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## S. 1 Absolute Energy Values

**Table S1: The absolute energies for the lowest energy Ins(1,3,4,5)P<sub>4</sub> isomers of each charge subset, for the QM geometry optimisation and MM energy minimisation calculations. Exact digits are given to facilitate the reproduction of the calculations.**

| Method                                                                    | Charge of isomer | Isomer | Absolute energy                 |
|---------------------------------------------------------------------------|------------------|--------|---------------------------------|
| QM geometry optimisation using DFT<br>level of theory in gas phase        | -4               | 1345H  | -2955.51054203 Hartree          |
|                                                                           | -5               | 5O134H | -2954.58116343 Hartree          |
|                                                                           | -6               | 13O45H | -2953.52631124 Hartree          |
|                                                                           | -7               | 134O5H | -2952.34906860 Hartree          |
|                                                                           | -8               | 1345O  | -2951.06867087 Hartree          |
| MM energy minimisation in gas phase,<br>with ff99SB atom types            | -4               | 1345H  | -11.0011 kcal mol <sup>-1</sup> |
|                                                                           | -5               | 5O134H | 2.38092 kcal mol <sup>-1</sup>  |
|                                                                           | -6               | 13O45H | 20.4906 kcal mol <sup>-1</sup>  |
|                                                                           | -7               | 134O5H | 43.8865 kcal mol <sup>-1</sup>  |
|                                                                           | -8               | 1345O  | 70.4274 kcal mol <sup>-1</sup>  |
| QM geometry optimisation using MP2<br>level of theory in gas phase        | -4               | 1345H  | -2944.74699756 Hartree          |
|                                                                           | -5               | 1O345H | -2943.81328454 Hartree          |
|                                                                           | -6               | 13O45H | -2942.76737024 Hartree          |
|                                                                           | -7               | 134O5H | -2941.60205502 Hartree          |
|                                                                           | -8               | 1345O  | -2940.35316876 Hartree          |
| MM energy minimisation in gas phase,<br>with GAFF atom types              | -4               | 1345H  | 3.4857 kcal mol <sup>-1</sup>   |
|                                                                           | -5               | 4O135H | 12.8553 kcal mol <sup>-1</sup>  |
|                                                                           | -6               | 45O13H | 22.0068 kcal mol <sup>-1</sup>  |
|                                                                           | -7               | 135O4H | 47.7466 kcal mol <sup>-1</sup>  |
|                                                                           | -8               | 1345O  | 74.9296 kcal mol <sup>-1</sup>  |
| QM geometry optimisation using DFT<br>level of theory in implicit solvent | -4               | 1345H  | -2956.29182024 Hartree          |
|                                                                           | -5               | 4O135H | -2955.78091556 Hartree          |
|                                                                           | -6               | 14O35H | -2955.28094982 Hartree          |
|                                                                           | -7               | 135O4H | -2954.75806732 Hartree          |
|                                                                           | -8               | 1345O  | -2954.21084339 Hartree          |
| MM energy minimisation in implicit<br>solvent                             | -4               | 1345H  | -705.72 kcal mol <sup>-1</sup>  |
|                                                                           | -5               | 5O134H | -803.51 kcal mol <sup>-1</sup>  |
|                                                                           | -6               | 14O35H | -904.07 kcal mol <sup>-1</sup>  |
|                                                                           | -7               | 135O4H | -992.43 kcal mol <sup>-1</sup>  |
|                                                                           | -8               | 1345O  | -1043.5 kcal mol <sup>-1</sup>  |



## S. 2 Free Energy Results

**Table S2: Computationally determined binding free energies (denoted  $\Delta G$ ) for the individual Ins(1,3,4,5)P<sub>4</sub>-PKB PH domain simulations.** Results are given for simulations in which the charge parameters for Ins(1,3,4,5)P<sub>4</sub> were taken from the geometry optimisation in gas phase and in implicit solvent. The MD simulations were carried out for 50 ns using the protocol outlined in section 5.6.2. The free energies of binding were calculated using the MM-PBSA method. Structural snapshots of the production MD simulations were saved every 10 ps, giving a total of 5000 snapshots for each 50 ns simulation (see section 5.6.3 for more details on the protocol). The statistical error was estimated from the deviation between block averages.

| Ligand                     | Charge | Isomer | $\Delta G$ in kcal mol <sup>-1</sup> for charges from optimisation in gas phase | $\Delta G$ in kcal mol <sup>-1</sup> for charges from optimisation in implicit solvent |
|----------------------------|--------|--------|---------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|
| Ins(1,3,4,5)P <sub>4</sub> | -4     | 1345H  | -71.86 ± 4.16                                                                   | -70.30 ± 5.95                                                                          |
|                            | -5     | 1O345H | -79.43 ± 3.06                                                                   | -61.09 ± 12.80                                                                         |
|                            |        | 3O145H | -60.33 ± 16.13                                                                  | -74.66 ± 4.67                                                                          |
|                            |        | 4O135H | -86.40 ± 5.40                                                                   | -88.03 ± 4.21                                                                          |
|                            |        | 5O134H | -69.46 ± 1.39                                                                   | -71.24 ± 8.03                                                                          |
|                            | -6     | 13O45H | -71.90 ± 9.09                                                                   | -72.10 ± 9.33                                                                          |
|                            |        | 14O35H | -65.58 ± 6.05                                                                   | -62.24 ± 13.13                                                                         |
|                            |        | 15O34H | -81.85 ± 5.48                                                                   | -62.97 ± 12.68                                                                         |
|                            |        | 34O15H | -60.81 ± 10.64                                                                  | -54.69 ± 2.67                                                                          |
|                            |        | 35O14H | -76.50 ± 6.99                                                                   | -76.40 ± 6.89                                                                          |
|                            |        | 45O13H | -96.31 ± 5.92                                                                   | -97.32 ± 1.37                                                                          |

**Table S3: Computationally determined binding free energies (denoted  $\Delta G$ ) for the PKB PH domain mutants to Ins(1,3,4,5)P<sub>4</sub> and Ins(1,3,4)P<sub>3</sub>.** Results are given for the 4O135H isomer of Ins(1,3,4,5)P<sub>4</sub> and 3O14H isomer of Ins(1,3,4)P<sub>3</sub>. The MD simulations were carried out for 150 ns using the protocol outlined in section 6.3.2. The free energies of binding were calculated for the final 50 ns using the MM-PBSA method. Structural snapshots were saved every 10 ps, giving a total of 5000 snapshots for each calculation (see section 6.3.3 for more details on the protocol). The statistical error was estimated from the deviation between block averages. The ability of these mutants to bind to PtdIns(3,4,5)P<sub>3</sub> and PtdIns(3,4)P<sub>2</sub> [the parent lipids of Ins(1,3,4,5)P<sub>4</sub> and Ins(1,3,4)P<sub>3</sub> respectively] were previously analysed using an *in vitro* protein lipid overlay assay, with results indicated in the final column.<sup>1</sup>

| Mutant | $\Delta G$ in kcal mol <sup>-1</sup><br>with Ins(1,3,4,5)P <sub>4</sub><br>ligand | $\Delta G$ in kcal mol <sup>-1</sup><br>with Ins(1,3,4)P <sub>3</sub><br>ligand | <i>In vitro</i> behavior with PtdIns(3,4,5)P <sub>3</sub> and<br>PtdIns(3,4)P <sub>2</sub> |
|--------|-----------------------------------------------------------------------------------|---------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Native | -86.40 ± 5.40                                                                     | -72.65 ± 9.63                                                                   | Binds to both phosphoinositides                                                            |
| K14A   | -26.81 ± 9.29                                                                     | -30.80 ± 7.87                                                                   | Complete loss of binding                                                                   |
| R23A   | -43.39 ± 6.11                                                                     | -41.67 ± 6.60                                                                   | Capable of interacting, with reduced affinity                                              |
| N53A   | -62.27 ± 8.07                                                                     | -54.55 ± 4.16                                                                   | Slight reduction in binding                                                                |
| R86A   | -42.47 ± 3.77                                                                     | -31.90 ± 5.89                                                                   | Complete loss of binding                                                                   |

**Table S4: Computationally determined binding free energies (denoted  $\Delta G$ ) for the individual inositol phosphate isomer-PKB PH domain simulations.** The free energies of binding were calculated using the MM-PBSA method. The statistical error was estimated from the deviation between block averages.

| Ligand                     | Charge | Isomer | $\Delta G$ in kcal/mol |
|----------------------------|--------|--------|------------------------|
| Ins(1,3,4,5)P <sub>4</sub> | -4     | 1345H  | -71.86 $\pm$ 4.16      |
|                            | -5     | 1O345H | -79.43 $\pm$ 3.06      |
|                            |        | 3O145H | -60.33 $\pm$ 16.13     |
|                            |        | 4O135H | -86.40 $\pm$ 5.40      |
|                            |        | 5O134H | -69.46 $\pm$ 1.39      |
|                            | -6     | 13O45H | -71.90 $\pm$ 9.09      |
|                            |        | 14O35H | -65.58 $\pm$ 6.05      |
|                            |        | 15O34H | -81.85 $\pm$ 5.48      |
|                            |        | 34O15H | -60.81 $\pm$ 10.64     |
|                            |        | 35O14H | -76.50 $\pm$ 6.99      |
|                            |        | 45O13H | -96.31 $\pm$ 5.92      |
|                            | -7     | 134O5H | -64.66 $\pm$ 15.77     |
|                            |        | 135O4H | -64.64 $\pm$ 9.46      |
|                            |        | 145O3H | -79.41 $\pm$ 2.49      |
|                            |        |        |                        |
| Ins(1,3,4)P <sub>3</sub>   | -3     | 134H   | -70.17 $\pm$ 8.55      |
|                            | -4     | 1O34H  | -57.97 $\pm$ 7.53      |
|                            |        | 3O14H  | -72.65 $\pm$ 9.63      |
|                            |        | 4O13H  | -62.66 $\pm$ 9.93      |
|                            | -5     | 13O4H  | -65.22 $\pm$ 9.55      |
|                            |        | 14O3H  | -63.67 $\pm$ 11.64     |
|                            |        | 34O1H  | -53.48 $\pm$ 4.58      |
|                            | -6     | 134O   | -61.46 $\pm$ 9.50      |
|                            |        |        |                        |
| Ins(1,4,5)P <sub>3</sub>   | -3     | 145H   | -30.01 $\pm$ 5.09      |
|                            | -4     | 1O45H  | -32.56 $\pm$ 11.82     |
|                            |        | 4O15H  | -42.79 $\pm$ 3.58      |
|                            |        | 5O14H  | -41.74 $\pm$ 5.68      |
|                            | -5     | 14O5H  | -47.08 $\pm$ 7.09      |
|                            |        | 15O4H  | -27.33 $\pm$ 8.17      |
|                            |        | 45O1H  | -42.52 $\pm$ 10.28     |
|                            | -6     | 145O   | -32.83 $\pm$ 12.40     |

**Table S5: Computationally determined binding free energies (denoted  $\Delta G$ ) for the individual flipped inositol phosphate isomer-PKB PH domain simulations.** The free energies of binding were calculated using the MM-PBSA method. The statistical error was estimated from the deviation between block averages.

| Ligand                          | Charge | Isomer             | $\Delta G$ in kcal/mol         |
|---------------------------------|--------|--------------------|--------------------------------|
| Ins(1,3,4,5)P <sub>4</sub> flip | -4     | 1345H              | -41.76 $\pm$ 6.04              |
|                                 | -5     | 1O345H             | -40.11 $\pm$ 8.88              |
|                                 |        | 3O145H             | -48.99 $\pm$ 6.94              |
|                                 |        | 4O135H             | -78.82 $\pm$ 6.53              |
|                                 |        | 5O134H             | -65.38 $\pm$ 6.88              |
|                                 |        |                    |                                |
|                                 | -6     | 13O45H             | -86.08 $\pm$ 3.99              |
|                                 |        | 14O35H             | -55.65 $\pm$ 3.99              |
|                                 |        | 15O34H             | -42.56 $\pm$ 10.54             |
|                                 |        | 34O15H             | -60.44 $\pm$ 9.80              |
|                                 |        | 35O14H             | -30.32 $\pm$ 10.53             |
|                                 |        | 45O13H             | -62.88 $\pm$ 8.00              |
|                                 | -7     | 134O5H             | -53.47 $\pm$ 8.14              |
|                                 |        | 135O4H             | -31.02 $\pm$ 7.09              |
| 145O3H                          |        | -50.02 $\pm$ 12.83 |                                |
|                                 |        |                    |                                |
| Ins(1,3,4)P <sub>3</sub> flip   | -3     | 134H               | -33.21 $\pm$ 1.74              |
|                                 | -4     | 1O34H              | -40.69 $\pm$ 12.6 <sup>f</sup> |
|                                 |        | 3O14H              | -38.35 $\pm$ 5.38              |
|                                 |        | 4O13H              | -52.34 $\pm$ 5.80              |
|                                 | -5     | 13O4H              | -36.49 $\pm$ 5.85              |
|                                 |        | 14O3H              | -47.87 $\pm$ 15.50             |
|                                 |        | 34O1H              | -43.65 $\pm$ 3.67              |
|                                 | -6     | 134O               | -30.15 $\pm$ 8.01              |
|                                 |        |                    |                                |
| Ins(1,4,5)P <sub>3</sub> flip   | -3     | 145H               | -48.84 $\pm$ 3.22              |
|                                 | -4     | 1O45H              | -45.90 $\pm$ 14.79             |
|                                 |        | 4O15H              | -77.72 $\pm$ 5.12              |
|                                 |        | 5O14H              | -60.81 $\pm$ 4.14              |
|                                 |        |                    |                                |
|                                 | -5     | 14O5H              | -59.74 $\pm$ 9.59              |
|                                 |        | 15O4H              | -32.31 $\pm$ 9.04              |
|                                 |        | 45O1H              | -65.51 $\pm$ 5.26              |
| -6                              | 145O   | -58.36 $\pm$ 3.47  |                                |

**Table S6: Computationally determined binding free energies (denoted  $\Delta G$ ) for the individual inositol phosphate isomer-E17K PKB PH domain simulations.** The free energies of binding were calculated using the MM-PBSA method. The statistical error was estimated from the deviation between block averages.

| Ligand                     | Charge | Isomer | $\Delta G$ in kcal/mol |
|----------------------------|--------|--------|------------------------|
| Ins(1,3,4,5)P <sub>4</sub> | -4     | 1345H  | -82.20 $\pm$ 4.73      |
|                            | -5     | 1O345H | -55.70 $\pm$ 1.39      |
|                            |        | 3O145H | -67.49 $\pm$ 6.70      |
|                            |        | 4O135H | -89.01 $\pm$ 6.38      |
|                            |        | 5O134H | -63.08 $\pm$ 6.00      |
|                            | -6     | 13O45H | -69.86 $\pm$ 16.28     |
|                            |        | 14O35H | -76.76 $\pm$ 6.16      |
|                            |        | 15O34H | -90.72 $\pm$ 2.26      |
|                            |        | 34O15H | -69.42 $\pm$ 8.68      |
|                            |        | 35O14H | -71.46 $\pm$ 3.68      |
|                            |        | 45O13H | -99.51 $\pm$ 4.54      |
|                            | -7     | 134O5H | -72.24 $\pm$ 10.89     |
|                            |        | 135O4H | -65.89 $\pm$ 8.79      |
|                            |        | 145O3H | -96.55 $\pm$ 4.15      |
|                            |        |        |                        |
| Ins(1,3,4)P <sub>3</sub>   | -3     | 134H   | -41.87 $\pm$ 5.75      |
|                            | -4     | 1O34H  | -65.96 $\pm$ 6.27      |
|                            |        | 3O14H  | -64.59 $\pm$ 5.52      |
|                            |        | 4O13H  | -47.12 $\pm$ 3.08      |
|                            | -5     | 13O4H  | -64.55 $\pm$ 5.14      |
|                            |        | 14O3H  | -77.29 $\pm$ 2.41      |
|                            |        | 34O1H  | -61.18 $\pm$ 6.09      |
|                            | -6     | 134O   | -65.88 $\pm$ 5.92      |
|                            |        |        |                        |
| Ins(1,4,5)P <sub>3</sub>   | -3     | 145H   | -38.67 $\pm$ 3.55      |
|                            | -4     | 1O45H  | -43.66 $\pm$ 5.89      |
|                            |        | 4O15H  | -41.70 $\pm$ 7.08      |
|                            |        | 5O14H  | -41.12 $\pm$ 3.16      |
|                            | -5     | 14O5H  | -64.77 $\pm$ 9.06      |
|                            |        | 15O4H  | -46.43 $\pm$ 5.69      |
|                            |        | 45O1H  | -63.86 $\pm$ 8.37      |
|                            | -6     | 145O   | -57.22 $\pm$ 6.86      |

**Table S7: Computationally determined binding free energies (denoted  $\Delta G$ ) for the individual inositol phosphate derivative-PKB PH domain simulations.** The free energies of binding were calculated using the MM-PBSA method. The statistical error was estimated from the deviation between block averages.

| Ligand | Charge | Isomer | $\Delta G$ in kcal/mol |
|--------|--------|--------|------------------------|
| 5A     | -3     | 134H   | $-88.49 \pm 5.81$      |
|        | -4     | 1O34H  | $-77.00 \pm 3.63$      |
|        |        | 3O14H  | $-81.33 \pm 4.10$      |
|        |        | 4O13H  | $-80.94 \pm 5.16$      |
|        | -5     | 13O4H  | $-73.25 \pm 9.64$      |
|        |        | 14O3H  | $-62.06 \pm 8.05$      |
|        |        | 34O1H  | $-59.12 \pm 10.93$     |
|        | -6     | 134O   | $-56.94 \pm 5.73$      |
|        |        |        |                        |
| 3M     | -3     | 145H   | $-69.73 \pm 1.36$      |
|        | -4     | 1O45H  | $-64.08 \pm 7.95$      |
|        |        | 4O15H  | $-67.58 \pm 5.22$      |
|        |        | 5O14H  | $-71.85 \pm 2.44$      |
|        | -5     | 14O5H  | $-68.08 \pm 1.18$      |
|        |        | 15O4H  | $-41.74 \pm 6.02$      |
|        |        | 45O1H  | $-81.29 \pm 2.97$      |
|        | -6     | 145O   | $-59.90 \pm 9.52$      |
|        |        |        |                        |
| 5S     | -3     | 134H   | $-71.96 \pm 4.85$      |
|        | -4     | 1O34H  | $-53.84 \pm 13.13$     |
|        |        | 3O14H  | $-79.53 \pm 8.38$      |
|        |        | 4O13H  | $-62.15 \pm 3.18$      |
|        | -5     | 13O4H  | $-48.93 \pm 11.69$     |
|        |        | 14O3H  | $-71.71 \pm 4.33$      |
|        |        | 34O1H  | $-67.71 \pm 3.69$      |
|        | -6     | 134O   | $-76.56 \pm 10.47$     |
|        |        |        |                        |
| 3S     | -3     | 145H   | $-32.40 \pm 5.07$      |
|        | -4     | 1O45H  | $-29.84 \pm 6.30$      |
|        |        | 4O15H  | $-61.23 \pm 1.58$      |
|        |        | 5O14H  | $-40.75 \pm 6.13$      |
|        | -5     | 14O5H  | $-60.52 \pm 5.52$      |
|        |        | 15O4H  | $-43.63 \pm 11.42$     |
|        |        | 45O1H  | $-61.24 \pm 5.47$      |
|        | -6     | 145O   | $-52.86 \pm 3.80$      |

### S. 3 Parameters for Ins(1,3,4,5)P<sub>4</sub>

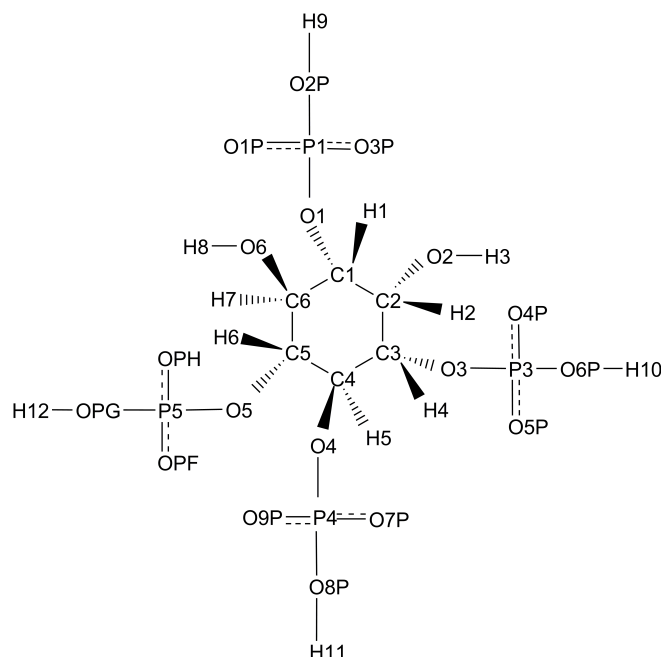


Figure S1: Atomic labelling scheme for the -4 isomer, 1345H, of Ins(1,3,4,5)P<sub>4</sub>.

Table S8: Atom names, atom types and charge parameters for the -4 1345H isomer of Ins(1,3,4,5)P<sub>4</sub>. Charge parameters for the isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.024812                                 | -0.004586                                       | P4   | P                   | 1.241543                                 | 1.183557                                        |
| O1   | OS                  | -0.467569                                | -0.355673                                       | O7P  | O2                  | -0.832113                                | -0.813621                                       |
| C2   | CT                  | 0.024704                                 | 0.026769                                        | O8P  | OH                  | -0.727447                                | -0.730850                                       |
| O2   | OH                  | -0.582613                                | -0.638301                                       | O9P  | O2                  | -0.804811                                | -0.808358                                       |
| C3   | CT                  | 0.042999                                 | 0.006967                                        | P5   | P                   | 1.208422                                 | 1.258253                                        |
| O3   | OS                  | -0.503174                                | -0.427697                                       | OPF  | O2                  | -0.829258                                | -0.843362                                       |
| C4   | CT                  | 0.020635                                 | 0.011566                                        | OPG  | OH                  | -0.702063                                | -0.744699                                       |
| O4   | OS                  | -0.473885                                | -0.409943                                       | OPH  | O2                  | -0.775938                                | -0.804044                                       |
| C5   | CT                  | 0.049358                                 | 0.010477                                        | H1   | HC                  | 0.122736                                 | 0.115305                                        |
| O5   | OS                  | -0.448672                                | -0.431320                                       | H2   | HC                  | 0.127450                                 | 0.121627                                        |
| C6   | CT                  | 0.077708                                 | 0.051829                                        | H3   | HO                  | 0.419241                                 | 0.420808                                        |
| O6   | OH                  | -0.585574                                | -0.648846                                       | H4   | HC                  | 0.155901                                 | 0.138762                                        |
| P1   | P                   | 1.263615                                 | 1.150816                                        | H5   | HC                  | 0.168002                                 | 0.185368                                        |
| O1P  | O2                  | -0.824174                                | -0.815060                                       | H6   | HC                  | 0.132010                                 | 0.141100                                        |
| O2P  | OH                  | -0.708093                                | -0.703597                                       | H7   | HC                  | 0.120269                                 | 0.158980                                        |
| O3P  | O2                  | -0.842697                                | -0.789944                                       | H8   | HO                  | 0.387273                                 | 0.461080                                        |
| P3   | P                   | 1.287731                                 | 1.186890                                        | H9   | HY                  | 0.381048                                 | 0.417880                                        |
| O4P  | O2                  | -0.830816                                | -0.816912                                       | H10  | HY                  | 0.484520                                 | 0.456781                                        |
| O5P  | O2                  | -0.853312                                | -0.852682                                       | H11  | HY                  | 0.444755                                 | 0.450091                                        |
| O6P  | OH                  | -0.769119                                | -0.733293                                       | H12  | HY                  | 0.376596                                 | 0.417885                                        |

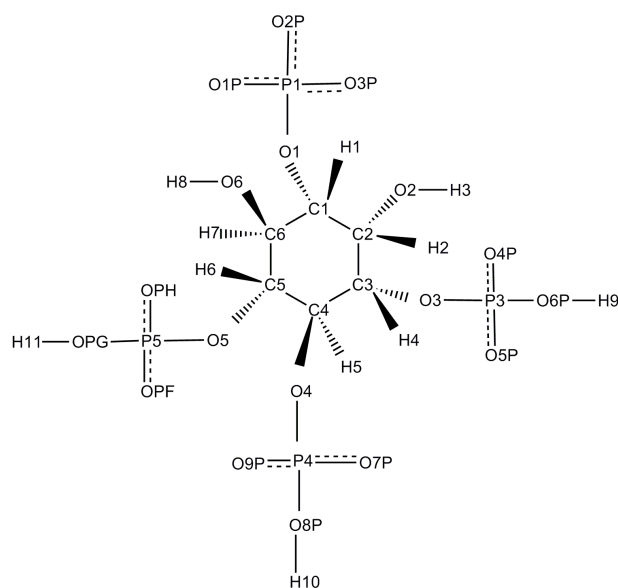


**Figure S2: Atomic labelling scheme for the -5 isomer, 1O345H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S9: Atom names, atom types and charge parameters for the -5 1O345H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.064457                                 | 0.054532                                        | P4   | P                   | 1.259818                                 | 1.144515                                        |
| O1   | OS                  | -0.440653                                | -0.442010                                       | O7P  | O2                  | -0.851880                                | -0.799032                                       |
| C2   | CT                  | 0.008829                                 | 0.075480                                        | O8P  | OH                  | -0.733737                                | -0.753892                                       |
| O2   | OH                  | -0.636875                                | -0.645566                                       | O9P  | O2                  | -0.823763                                | -0.816634                                       |
| C3   | CT                  | 0.029218                                 | -0.008141                                       | P5   | P                   | 1.206466                                 | 1.169697                                        |
| O3   | OS                  | -0.431196                                | -0.401554                                       | OPF  | O2                  | -0.847562                                | -0.834264                                       |
| C4   | CT                  | 0.024091                                 | -0.041055                                       | OPG  | OH                  | -0.759949                                | -0.728792                                       |
| O4   | OS                  | -0.430384                                | -0.390144                                       | OPH  | O2                  | -0.827282                                | -0.772197                                       |
| C5   | CT                  | 0.002732                                 | 0.142454                                        | H1   | HC                  | 0.100984                                 | 0.101834                                        |
| O5   | OS                  | -0.433905                                | -0.431229                                       | H2   | HC                  | 0.115432                                 | 0.172496                                        |
| C6   | CT                  | 0.051170                                 | 0.039379                                        | H3   | HO                  | 0.398446                                 | 0.379911                                        |
| O6   | OH                  | -0.646454                                | -0.615011                                       | H4   | HC                  | 0.133396                                 | 0.134667                                        |
| P1   | P                   | 1.221593                                 | 1.234204                                        | H5   | HC                  | 0.134542                                 | 0.170174                                        |
| O1P  | O2                  | -0.889876                                | -0.929479                                       | H6   | HC                  | 0.145124                                 | 0.154687                                        |
| O2P  | O2                  | -0.897616                                | -0.918606                                       | H7   | HC                  | 0.120302                                 | 0.077795                                        |
| O3P  | O2                  | -0.914072                                | -0.962883                                       | H8   | HO                  | 0.485539                                 | 0.378535                                        |
| P3   | P                   | 1.250309                                 | 1.173772                                        | H9   | HY                  | 0.449722                                 | 0.462144                                        |
| O4P  | O2                  | -0.842832                                | -0.817445                                       | H10  | HY                  | 0.427108                                 | 0.465369                                        |
| O5P  | O2                  | -0.878195                                | -0.854322                                       | H11  | HY                  | 0.415118                                 | 0.401025                                        |
| O6P  | OH                  | -0.758166                                | -0.770411                                       |      |                     |                                          |                                                 |



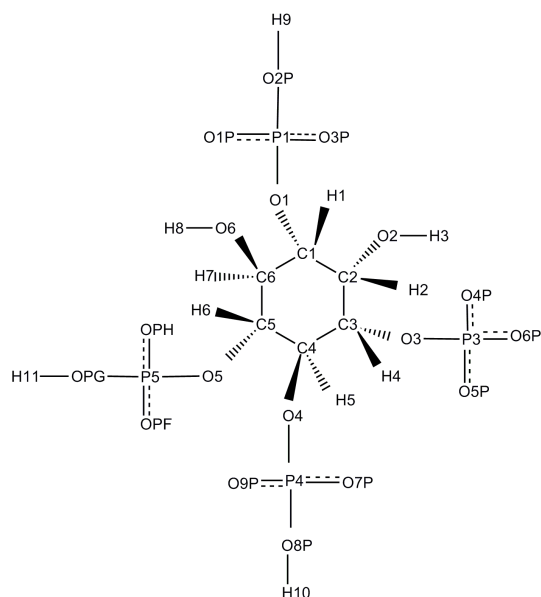


**Figure S3: Atomic labelling scheme for the -5 isomer, 3O145H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S10: Atom names, atom types and charge parameters for the -5 3O145H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 3O145H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.025348                                 | 0.040405                                        | P4   | P                   | 1.188686                                 | 1.153536                                        |
| O1   | OS                  | -0.439751                                | -0.454266                                       | O7P  | O2                  | -0.832640                                | -0.814351                                       |
| C2   | CT                  | 0.001280                                 | -0.045884                                       | O8P  | OH                  | -0.716692                                | -0.803411                                       |
| O2   | OH                  | -0.630477                                | -0.638411                                       | O9P  | O2                  | -0.827933                                | -0.833242                                       |
| C3   | CT                  | 0.024210                                 | -0.023493                                       | P5   | P                   | 1.171949                                 | 1.190142                                        |
| O3   | OS                  | -0.377692                                | -0.313868                                       | OPF  | O2                  | -0.816340                                | -0.853490                                       |
| C4   | CT                  | 0.007595                                 | -0.060309                                       | OPG  | OH                  | -0.732526                                | -0.744202                                       |
| O4   | OS                  | -0.420578                                | -0.394942                                       | OPH  | O2                  | -0.817281                                | -0.781105                                       |
| C5   | CT                  | 0.037849                                 | 0.025379                                        | H1   | HC                  | 0.077313                                 | 0.108082                                        |
| O5   | OS                  | -0.400404                                | -0.409433                                       | H2   | HC                  | 0.147599                                 | 0.195950                                        |
| C6   | CT                  | 0.021890                                 | 0.039179                                        | H3   | HO                  | 0.405027                                 | 0.447829                                        |
| O6   | OH                  | -0.540785                                | -0.594231                                       | H4   | HC                  | 0.099476                                 | 0.099343                                        |
| P1   | P                   | 1.182592                                 | 1.225168                                        | H5   | HC                  | 0.178396                                 | 0.209001                                        |
| O1P  | O2                  | -0.876489                                | -0.824608                                       | H6   | HC                  | 0.143069                                 | 0.179736                                        |
| O2P  | OH                  | -0.861566                                | -0.722824                                       | H7   | HC                  | 0.119300                                 | 0.127560                                        |
| O3P  | O2                  | -0.909832                                | -0.885626                                       | H8   | HO                  | 0.361842                                 | 0.358977                                        |
| P3   | P                   | 1.224346                                 | 1.161603                                        | H9   | HY                  | 0.454961                                 | 0.411932                                        |
| O4P  | O2                  | -0.841628                                | -0.891608                                       | H10  | HY                  | 0.396969                                 | 0.505050                                        |
| O5P  | O2                  | -0.745185                                | -0.890728                                       | H11  | HY                  | 0.372774                                 | 0.409618                                        |
| O6P  | O2                  | -0.854673                                | -0.908457                                       |      |                     |                                          |                                                 |

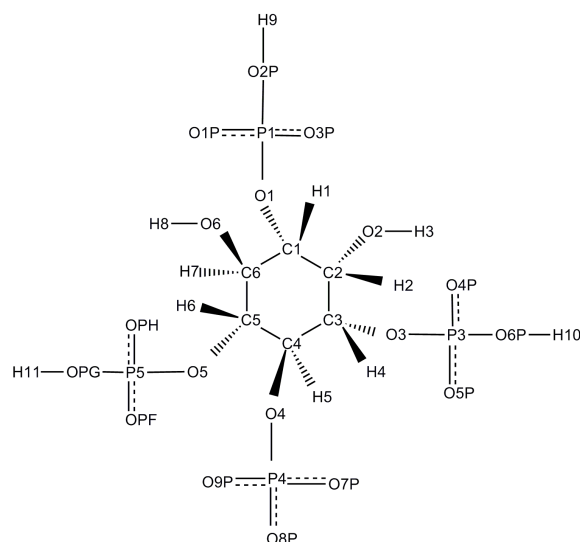


**Figure S4: Atomic labelling scheme for the -5 isomer, 4O135H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S11: Atom names, atom types and charge parameters for the -5 4O135H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 4O135H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.067152                                 | 0.051815                                        | P4   | P                   | 1.154384                                 | 1.150013                                        |
| O1   | OS                  | -0.454090                                | -0.410885                                       | O7P  | O2                  | -0.757781                                | -0.790807                                       |
| C2   | CT                  | 0.053995                                 | -0.003845                                       | O8P  | O2                  | -0.830031                                | -0.817402                                       |
| O2   | OH                  | -0.600429                                | -0.646364                                       | O9P  | O2                  | -0.818263                                | -0.840625                                       |
| C3   | CT                  | 0.029898                                 | -0.013041                                       | P5   | P                   | 1.178274                                 | 1.173690                                        |
| O3   | OS                  | -0.429845                                | -0.373467                                       | OPF  | O2                  | -0.823386                                | -0.818448                                       |
| C4   | CT                  | -0.015558                                | 0.001323                                        | OPG  | OH                  | -0.737023                                | -0.742525                                       |
| O4   | OS                  | -0.388140                                | -0.347744                                       | OPH  | O2                  | -0.859649                                | -0.860035                                       |
| C5   | CT                  | 0.075115                                 | 0.032396                                        | H1   | HC                  | 0.101603                                 | 0.146168                                        |
| O5   | OS                  | -0.450038                                | -0.451589                                       | H2   | HC                  | 0.102883                                 | 0.134737                                        |
| C6   | CT                  | 0.114987                                 | 0.057871                                        | H3   | HO                  | 0.389414                                 | 0.400567                                        |
| O6   | OH                  | -0.634800                                | -0.616467                                       | H4   | HC                  | 0.112576                                 | 0.120579                                        |
| P1   | P                   | 1.281418                                 | 1.196497                                        | H5   | HC                  | 0.150434                                 | 0.199870                                        |
| O1P  | O2                  | -0.853650                                | -0.824224                                       | H6   | HC                  | 0.126104                                 | 0.158223                                        |
| O2P  | OH                  | -0.745827                                | -0.721426                                       | H7   | HC                  | 0.078517                                 | 0.091487                                        |
| O3P  | O2                  | -0.881105                                | -0.840392                                       | H8   | HO                  | 0.383594                                 | 0.389899                                        |
| P3   | P                   | 1.226401                                 | 1.176660                                        | H9   | HY                  | 0.392764                                 | 0.400132                                        |
| O4P  | O2                  | -0.887978                                | -0.891130                                       | H10  | HY                  | 0.483249                                 | 0.499715                                        |
| O5P  | O2                  | -0.916960                                | -0.938514                                       | H11  | HY                  | 0.457309                                 | 0.440110                                        |
| O6P  | OH                  | -0.875517                                | -0.872821                                       |      |                     |                                          |                                                 |

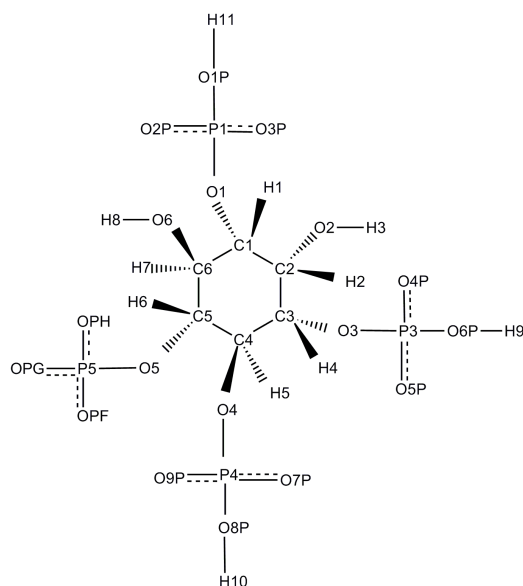


**Figure S5: Atomic labelling scheme for the -5 isomer, 5O134H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S12: Atom names, atom types and charge parameters for the -5 5O134H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 5O134H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atomtypes from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.123260                                 | 0.030379                                        | P4   | P                   | 1.289614                                 | 1.225117                                        |
| O1   | OS                  | -0.433811                                | -0.369027                                       | O7P  | O2                  | -0.860245                                | -0.859471                                       |
| C2   | CT                  | 0.017893                                 | -0.010909                                       | O8P  | OH                  | -0.762139                                | -0.813132                                       |
| O2   | OH                  | -0.647161                                | -0.670600                                       | O9P  | O2                  | -0.833095                                | -0.843760                                       |
| C3   | CT                  | 0.065885                                 | -0.000377                                       | P5   | P                   | 1.199519                                 | 1.253964                                        |
| O3   | OS                  | -0.432741                                | -0.433303                                       | OPF  | O2                  | -0.889507                                | -0.901468                                       |
| C4   | CT                  | 0.064609                                 | -0.036591                                       | OPG  | O2                  | -0.873313                                | -0.943645                                       |
| O4   | OS                  | -0.465430                                | -0.365711                                       | OPH  | O2                  | -0.867124                                | -0.891553                                       |
| C5   | CT                  | 0.041720                                 | 0.010190                                        | H1   | HC                  | 0.086896                                 | 0.127909                                        |
| O5   | OS                  | -0.457171                                | -0.474075                                       | H2   | HC                  | 0.099722                                 | 0.136338                                        |
| C6   | CT                  | 0.044590                                 | 0.164511                                        | H3   | HO                  | 0.403981                                 | 0.428157                                        |
| O6   | OH                  | -0.611761                                | -0.638011                                       | H4   | HC                  | 0.112986                                 | 0.145792                                        |
| P1   | P                   | 1.207331                                 | 1.144348                                        | H5   | HC                  | 0.104457                                 | 0.174036                                        |
| O1P  | OH                  | -0.751526                                | -0.728948                                       | H6   | HC                  | 0.111057                                 | 0.168703                                        |
| O2P  | O2                  | -0.849455                                | -0.816686                                       | H7   | HC                  | 0.109183                                 | 0.090943                                        |
| O3P  | O2                  | -0.868837                                | -0.825319                                       | H8   | HO                  | 0.434557                                 | 0.390874                                        |
| P3   | P                   | 1.240632                                 | 1.190137                                        | H9   | HY                  | 0.435962                                 | 0.440265                                        |
| O4P  | O2                  | -0.844004                                | -0.818523                                       | H10  | HY                  | 0.465059                                 | 0.524241                                        |
| O5P  | O2                  | -0.879797                                | -0.883693                                       | H11  | HY                  | 0.411683                                 | 0.419305                                        |
| O6P  | OH                  | -0.743478                                | -0.740407                                       |      |                     |                                          |                                                 |

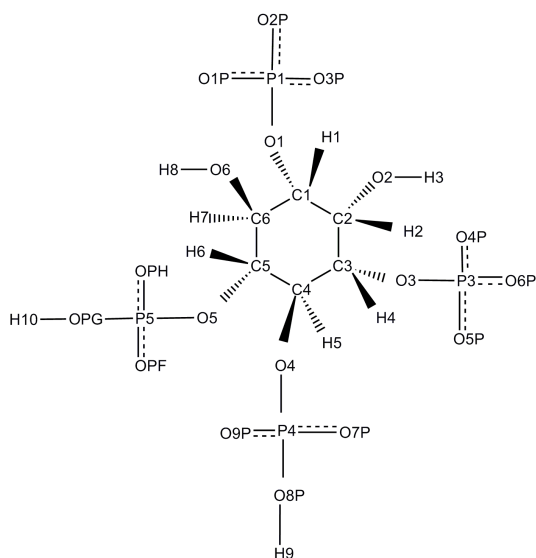


**Figure S6: Atomic labelling scheme for the -6 isomer, 13O45H.**

**Table S13: Atom names, atom types and charge parameters for the -6 13O45H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 13O45H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.093766                                 | 0.040495                                        | P4   | P                   | 1.196060                                 | 1.179730                                        |
| O1   | OS                  | -0.439348                                | -0.447475                                       | O7P  | O2                  | -0.886377                                | -0.839367                                       |
| C2   | CT                  | 0.007139                                 | -0.013715                                       | O8P  | OH                  | -0.796951                                | -0.818506                                       |
| O2   | OH                  | -0.714736                                | -0.659133                                       | O9P  | O2                  | -0.843762                                | -0.847359                                       |
| C3   | CT                  | 0.146969                                 | 0.016601                                        | P5   | P                   | 1.211750                                 | 1.229935                                        |
| O3   | OS                  | -0.477680                                | -0.354787                                       | OPF  | O2                  | -0.913455                                | -0.880024                                       |
| C4   | CT                  | 0.270887                                 | -0.010149                                       | OPG  | OH                  | -0.898445                                | -0.776595                                       |
| O4   | OS                  | -0.514047                                | -0.383884                                       | OPH  | O2                  | -0.892259                                | -0.837850                                       |
| C5   | CT                  | 0.096798                                 | -0.012868                                       | H1   | HC                  | 0.089053                                 | 0.119010                                        |
| O5   | OS                  | -0.505482                                | -0.417740                                       | H2   | HC                  | 0.113146                                 | 0.185572                                        |
| C6   | CT                  | 0.064200                                 | 0.151191                                        | H3   | HO                  | 0.478171                                 | 0.379343                                        |
| O6   | OH                  | -0.594670                                | -0.758614                                       | H4   | HC                  | 0.014214                                 | 0.107768                                        |
| P1   | P                   | 1.227467                                 | 1.212175                                        | H5   | HC                  | 0.067743                                 | 0.159592                                        |
| O1P  | O2                  | -0.753984                                | -0.930290                                       | H6   | HC                  | 0.063116                                 | 0.132246                                        |
| O2P  | O2                  | -0.869403                                | -0.909614                                       | H7   | HC                  | 0.115468                                 | 0.098671                                        |
| O3P  | O2                  | -0.896858                                | -0.945028                                       | H8   | HO                  | 0.373761                                 | 0.511653                                        |
| P3   | P                   | 1.207054                                 | 1.181518                                        | H9   | HY                  | 0.508429                                 | 0.489190                                        |
| O4P  | O2                  | -0.910409                                | -0.906625                                       | H10  | HY                  | 0.427991                                 | 0.455627                                        |
| O5P  | O2                  | -0.927561                                | -0.948150                                       |      |                     |                                          |                                                 |
| O6P  | O2                  | -0.937756                                | -0.952542                                       |      |                     |                                          |                                                 |

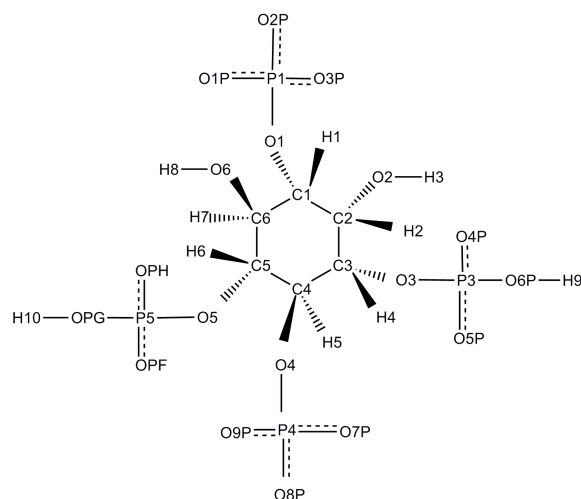


**Figure S7: Atomic labelling scheme for the -6 isomer, 14O35H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S14: Atom names, atom types and charge parameters for the -6 14O35H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 14O35H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.087105                                 | 0.075569                                        | P4   | P                   | 1.197861                                 | 1.167154                                        |
| O1   | OS                  | -0.488174                                | -0.440517                                       | O7P  | O2                  | -0.937085                                | -0.953144                                       |
| C2   | CT                  | -0.090218                                | 0.003380                                        | O8P  | O2                  | -0.934105                                | -0.883026                                       |
| O2   | OH                  | -0.563806                                | -0.660393                                       | O9P  | O2                  | -0.905005                                | -0.904629                                       |
| C3   | CT                  | 0.083548                                 | -0.025403                                       | P5   | P                   | 1.224824                                 | 1.276294                                        |
| O3   | OS                  | -0.491981                                | -0.394165                                       | OPF  | O2                  | -0.853650                                | -0.870950                                       |
| C4   | CT                  | 0.447407                                 | -0.009118                                       | OPG  | OH                  | -0.729417                                | -0.835885                                       |
| O4   | OS                  | -0.569679                                | -0.358995                                       | OPH  | O2                  | -0.834759                                | -0.859487                                       |
| C5   | CT                  | 0.027745                                 | -0.011861                                       | H1   | HC                  | 0.111064                                 | 0.117419                                        |
| O5   | OS                  | -0.505153                                | -0.404841                                       | H2   | HC                  | 0.162411                                 | 0.103312                                        |
| C6   | CT                  | 0.055585                                 | 0.054656                                        | H3   | HO                  | 0.378460                                 | 0.403045                                        |
| O6   | OH                  | -0.740504                                | -0.665474                                       | H4   | HC                  | 0.091560                                 | 0.140208                                        |
| P1   | P                   | 1.223743                                 | 1.224003                                        | H5   | HC                  | 0.013005                                 | 0.181653                                        |
| O1P  | O2                  | -0.918376                                | -0.929374                                       | H6   | HC                  | 0.189342                                 | 0.153761                                        |
| O2P  | O2                  | -0.921389                                | -0.919832                                       | H7   | HC                  | 0.130156                                 | 0.103834                                        |
| O3P  | O2                  | -0.946172                                | -0.951468                                       | H8   | HO                  | 0.498909                                 | 0.484436                                        |
| P3   | P                   | 1.281248                                 | 1.171237                                        | H9   | HY                  | 0.393041                                 | 0.552291                                        |
| O4P  | O2                  | -0.889496                                | -0.847431                                       | H10  | HY                  | 0.361793                                 | 0.433667                                        |
| O5P  | O2                  | -0.865293                                | -0.901082                                       |      |                     |                                          |                                                 |
| O6P  | OH                  | -0.774545                                | -0.818844                                       |      |                     |                                          |                                                 |

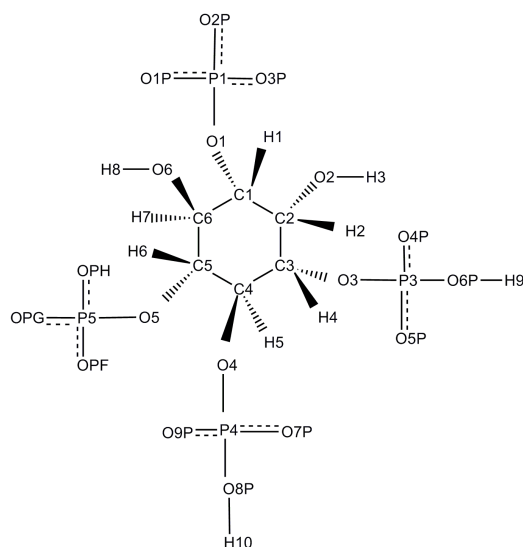


**Figure S8: Atomic labelling scheme for the -6 isomer, 15O34H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S15: Atom names, atom types and charge parameters for the -6 15O34H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 15O34H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.089395                                 | 0.039687                                        | P4   | P                   | 1.248110                                 | 1.163037                                        |
| O1   | OS                  | -0.454519                                | -0.442716                                       | O7P  | O2                  | -0.891912                                | -0.894236                                       |
| C2   | CT                  | 0.030986                                 | 0.075062                                        | O8P  | OH                  | -0.858599                                | -0.893942                                       |
| O2   | OH                  | -0.675099                                | -0.647495                                       | O9P  | O2                  | -0.808412                                | -0.885952                                       |
| C3   | CT                  | 0.016353                                 | 0.003448                                        | P5   | P                   | 1.264643                                 | 1.185748                                        |
| O3   | OS                  | -0.452271                                | -0.385701                                       | OPF  | O2                  | -0.895760                                | -0.893543                                       |
| C4   | CT                  | -0.010827                                | -0.055839                                       | OPG  | O2                  | -0.854938                                | -0.849694                                       |
| O4   | OS                  | -0.429786                                | -0.373607                                       | OPH  | O2                  | -0.820396                                | -0.809694                                       |
| C5   | CT                  | 0.044297                                 | 0.080212                                        | H1   | HC                  | 0.075113                                 | 0.110071                                        |
| O5   | OS                  | -0.479894                                | -0.414721                                       | H2   | HC                  | 0.110894                                 | 0.148078                                        |
| C6   | CT                  | 0.164636                                 | 0.095682                                        | H3   | HO                  | 0.408913                                 | 0.365325                                        |
| O6   | OH                  | -0.669131                                | -0.641789                                       | H4   | HC                  | 0.118709                                 | 0.122794                                        |
| P1   | P                   | 1.204602                                 | 1.208052                                        | H5   | HC                  | 0.156571                                 | 0.171731                                        |
| O1P  | O2                  | -0.915012                                | -0.928502                                       | H6   | HC                  | 0.139567                                 | 0.156188                                        |
| O2P  | O2                  | -0.921008                                | -0.923910                                       | H7   | HC                  | 0.072588                                 | 0.062780                                        |
| O3P  | O2                  | -0.950000                                | -0.971553                                       | H8   | HO                  | 0.432633                                 | 0.379792                                        |
| P3   | P                   | 1.242163                                 | 1.182467                                        | H9   | HY                  | 0.528178                                 | 0.498913                                        |
| O4P  | O2                  | -0.903789                                | -0.839136                                       | H10  | HY                  | 0.496733                                 | 0.501294                                        |
| O5P  | O2                  | -0.944388                                | -0.898412                                       |      |                     |                                          |                                                 |
| O6P  | OH                  | -0.909340                                | -0.799919                                       |      |                     |                                          |                                                 |

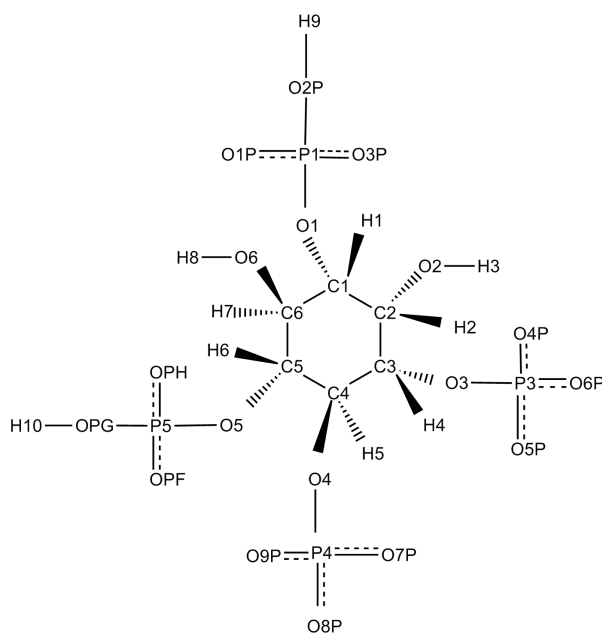


**Figure S9: Atomic labelling scheme for the -6 isomer, 34O15H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S16: Atom names, atom types and charge parameters for the -6 34O15H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 34O15H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.350123                                 | 0.099150                                        | P4   | P                   | 1.207097                                 | 1.110517                                        |
| O1   | OS                  | -0.541851                                | -0.446383                                       | O7P  | O2                  | -0.960478                                | -0.928569                                       |
| C2   | CT                  | -0.048199                                | -0.055548                                       | O8P  | O2                  | -0.930105                                | -0.931171                                       |
| O2   | OH                  | -0.699230                                | -0.650742                                       | O9P  | O2                  | -0.929292                                | -0.899224                                       |
| C3   | CT                  | 0.147357                                 | -0.058333                                       | P5   | P                   | 1.236009                                 | 1.195312                                        |
| O3   | OS                  | -0.517592                                | -0.228796                                       | OPF  | O2                  | -0.888834                                | -0.799040                                       |
| C4   | CT                  | 0.129352                                 | -0.075570                                       | OPG  | OH                  | -0.752439                                | -0.798958                                       |
| O4   | OS                  | -0.524221                                | -0.393788                                       | OPH  | O2                  | -0.873743                                | -0.871376                                       |
| C5   | CT                  | 0.144544                                 | 0.024916                                        | H1   | HC                  | 0.065585                                 | 0.091548                                        |
| O5   | OS                  | -0.512323                                | -0.330904                                       | H2   | HC                  | 0.178981                                 | 0.196624                                        |
| C6   | CT                  | 0.139986                                 | 0.076243                                        | H3   | HO                  | 0.481607                                 | 0.451336                                        |
| O6   | OH                  | -0.774836                                | -0.712871                                       | H4   | HC                  | 0.038017                                 | 0.068087                                        |
| P1   | P                   | 1.196935                                 | 1.210523                                        | H5   | HC                  | 0.091567                                 | 0.180668                                        |
| O1P  | O2                  | -0.866932                                | -0.841187                                       | H6   | HC                  | 0.166122                                 | 0.141642                                        |
| O2P  | OH                  | -0.742956                                | -0.730391                                       | H7   | HC                  | 0.086199                                 | 0.150563                                        |
| O3P  | O2                  | -0.891659                                | -0.900761                                       | H8   | HO                  | 0.445868                                 | 0.428784                                        |
| P3   | P                   | 1.211382                                 | 1.110367                                        | H9   | HY                  | 0.434454                                 | 0.405697                                        |
| O4P  | O2                  | -0.925456                                | -0.897580                                       | H10  | HY                  | 0.417632                                 | 0.423909                                        |
| O5P  | O2                  | -0.873079                                | -0.900964                                       |      |                     |                                          |                                                 |
| O6P  | O2                  | -0.915592                                | -0.913733                                       |      |                     |                                          |                                                 |

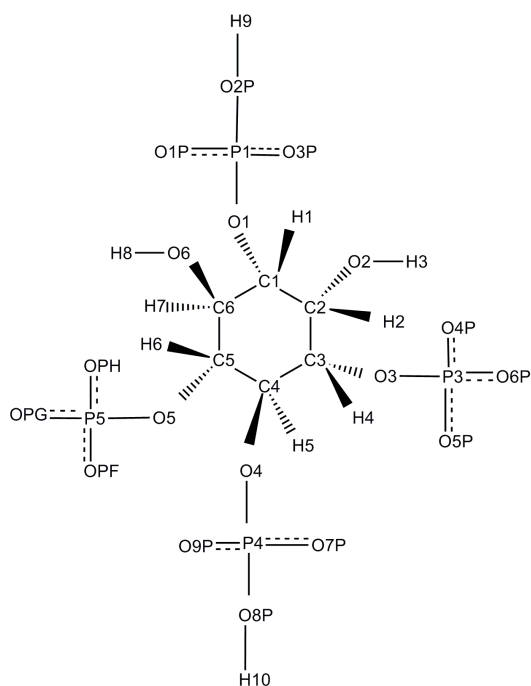


**Figure S10: Atomic labelling scheme for the -6 isomer, 35O14H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S17: Atom names, atom types and charge parameters for the -6 35O14H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 35O14H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.088364                                 | 0.049933                                        | P4   | P                   | 1.117351                                 | 1.160362                                        |
| O1   | OS                  | -0.572709                                | -0.453692                                       | O7P  | O2                  | -0.873062                                | -0.867087                                       |
| C2   | CT                  | 0.073581                                 | -0.031240                                       | O8P  | OH                  | -0.718967                                | -0.841467                                       |
| O2   | OH                  | -0.568190                                | -0.654825                                       | O9P  | O2                  | -0.864282                                | -0.854695                                       |
| C3   | CT                  | 0.079954                                 | -0.014676                                       | P5   | P                   | 1.139709                                 | 1.223066                                        |
| O3   | OS                  | -0.500754                                | -0.314370                                       | OPF  | O2                  | -0.910238                                | -0.952007                                       |
| C4   | CT                  | 0.374932                                 | -0.051223                                       | OPG  | O2                  | -0.906820                                | -0.915439                                       |
| O4   | OS                  | -0.498680                                | -0.390097                                       | OPH  | O2                  | -0.860828                                | -0.935988                                       |
| C5   | CT                  | 0.004386                                 | 0.025184                                        | H1   | HC                  | 0.090050                                 | 0.100207                                        |
| O5   | OS                  | -0.419084                                | -0.415170                                       | H2   | HC                  | 0.169918                                 | 0.186514                                        |
| C6   | CT                  | 0.128681                                 | 0.061959                                        | H3   | HO                  | 0.299892                                 | 0.455247                                        |
| O6   | OH                  | -0.743417                                | -0.603328                                       | H4   | HC                  | 0.035168                                 | 0.088403                                        |
| P1   | P                   | 1.299104                                 | 1.220359                                        | H5   | HC                  | 0.037156                                 | 0.189261                                        |
| O1P  | O2                  | -0.896096                                | -0.836482                                       | H6   | HC                  | 0.200170                                 | 0.168737                                        |
| O2P  | OH                  | -0.741868                                | -0.738611                                       | H7   | HC                  | 0.104527                                 | 0.108312                                        |
| O3P  | O2                  | -0.876369                                | -0.898820                                       | H8   | HO                  | 0.456439                                 | 0.346962                                        |
| P3   | P                   | 1.194056                                 | 1.153175                                        | H9   | HY                  | 0.407503                                 | 0.415917                                        |
| O4P  | O2                  | -0.916010                                | -0.902317                                       | H10  | HY                  | 0.437918                                 | 0.547294                                        |
| O5P  | O2                  | -0.930820                                | -0.907670                                       |      |                     |                                          |                                                 |
| O6P  | O2                  | -0.940664                                | -0.921685                                       |      |                     |                                          |                                                 |



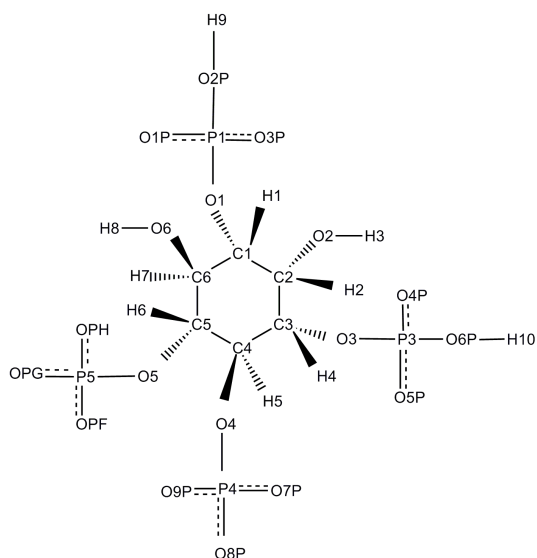


**Figure S11: Atomic labelling scheme for the -6 isomer, 45O13H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S18: Atom names, atom types and charge parameters for the -6 45O13H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the 45O13H isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.093976                                 | 0.040394                                        | P4   | P                   | 1.232417                                 | 1.235426                                        |
| O1   | OS                  | -0.469224                                | -0.369916                                       | O7P  | O2                  | -0.899018                                | -0.855161                                       |
| C2   | CT                  | 0.039703                                 | -0.001886                                       | O8P  | O2                  | -0.859343                                | -0.868003                                       |
| O2   | OH                  | -0.672906                                | -0.662217                                       | O9P  | O2                  | -0.791452                                | -0.872161                                       |
| C3   | CT                  | 0.030880                                 | -0.046226                                       | P5   | P                   | 1.183591                                 | 1.138666                                        |
| O3   | OS                  | -0.471469                                | -0.395765                                       | OPF  | O2                  | -0.924377                                | -0.894970                                       |
| C4   | CT                  | 0.234846                                 | -0.022232                                       | OPG  | O2                  | -0.887561                                | -0.974276                                       |
| O4   | OS                  | -0.552305                                | -0.383125                                       | OPH  | O2                  | -0.919193                                | -0.911625                                       |
| C5   | CT                  | 0.312545                                 | 0.072067                                        | H1   | HC                  | 0.123491                                 | 0.138234                                        |
| O5   | OS                  | -0.545313                                | -0.402341                                       | H2   | HC                  | 0.222211                                 | 0.153541                                        |
| C6   | CT                  | 0.052825                                 | 0.045002                                        | H3   | HO                  | 0.356090                                 | 0.409705                                        |
| O6   | OH                  | -0.718797                                | -0.563247                                       | H4   | HC                  | 0.072579                                 | 0.127197                                        |
| P1   | P                   | 1.210851                                 | 1.179642                                        | H5   | HC                  | 0.060597                                 | 0.167795                                        |
| O1P  | O2                  | -0.858163                                | -0.837686                                       | H6   | HC                  | 0.034403                                 | 0.145398                                        |
| O2P  | OH                  | -0.744083                                | -0.731502                                       | H7   | HC                  | 0.120220                                 | 0.085253                                        |
| O3P  | O2                  | -0.884459                                | -0.859626                                       | H8   | HO                  | 0.422779                                 | 0.331953                                        |
| P3   | P                   | 1.188794                                 | 1.193307                                        | H9   | HY                  | 0.422007                                 | 0.414980                                        |
| O4P  | O2                  | -0.888018                                | -0.920389                                       | H10  | HY                  | 0.505325                                 | 0.526224                                        |
| O5P  | O2                  | -0.928440                                | -0.936265                                       |      |                     |                                          |                                                 |
| O6P  | OH                  | -0.906012                                | -0.896165                                       |      |                     |                                          |                                                 |

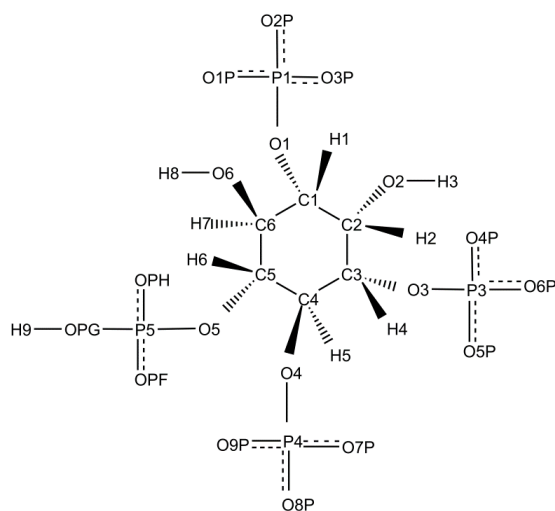


**Figure S12: Atomic labelling scheme for the -7 isomer, 134O5H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S19: Atom names, atom types and charge parameters for the -7 134O5H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB atom type | Charge from gas phase calculations | Charge from implicit solvent calculations | Atom | ff99SB atom type | Charge from gas phase calculations | Charge from implicit solvent calculations |
|------|------------------|------------------------------------|-------------------------------------------|------|------------------|------------------------------------|-------------------------------------------|
| C1   | CT               | 0.117757                           | 0.083131                                  | P4   | P                | 1.317919                           | 1.042426                                  |
| O1   | OS               | -0.448797                          | -0.458400                                 | O7P  | O2               | -0.978916                          | -0.910820                                 |
| C2   | CT               | -0.068199                          | -0.012904                                 | O8P  | O2               | -0.984588                          | -0.919529                                 |
| O2   | OH               | -0.747007                          | -0.660816                                 | O9P  | O2               | -0.946876                          | -0.917141                                 |
| C3   | CT               | 0.434004                           | -0.016586                                 | P5   | P                | 1.237755                           | 1.259566                                  |
| O3   | OS               | -0.605511                          | -0.285788                                 | OPF  | O2               | -0.903200                          | -0.879345                                 |
| C4   | CT               | -0.099412                          | 0.019680                                  | OPG  | OH               | -0.777543                          | -0.868494                                 |
| O4   | OS               | -0.569890                          | -0.332309                                 | OPH  | O2               | -0.876920                          | -0.863347                                 |
| C5   | CT               | 0.339144                           | 0.047618                                  | H1   | HC               | 0.063415                           | 0.122886                                  |
| O5   | OS               | -0.575180                          | -0.386574                                 | H2   | HC               | 0.063970                           | 0.176214                                  |
| C6   | CT               | 0.081703                           | 0.079410                                  | H3   | HO               | 0.525382                           | 0.350425                                  |
| O6   | OH               | -0.802417                          | -0.718849                                 | H4   | HC               | 0.028067                           | 0.077341                                  |
| P1   | P                | 1.235244                           | 1.198406                                  | H5   | HC               | 0.190370                           | 0.142376                                  |
| O1P  | O2               | -0.962850                          | -0.938261                                 | H6   | HC               | 0.125465                           | 0.115838                                  |
| O2P  | O2               | -0.934394                          | -0.919260                                 | H7   | HC               | 0.133349                           | 0.072052                                  |
| O3P  | O2               | -0.972889                          | -0.963166                                 | H8   | HO               | 0.561546                           | 0.495951                                  |
| P3   | P                | 1.265233                           | 1.171488                                  | H9   | HY               | 0.407729                           | 0.451478                                  |
| O4P  | O2               | -0.937750                          | -0.903043                                 |      |                  |                                    |                                           |
| O5P  | O2               | -0.969482                          | -0.981793                                 |      |                  |                                    |                                           |
| O6P  | O2               | -0.966231                          | -0.969865                                 |      |                  |                                    |                                           |

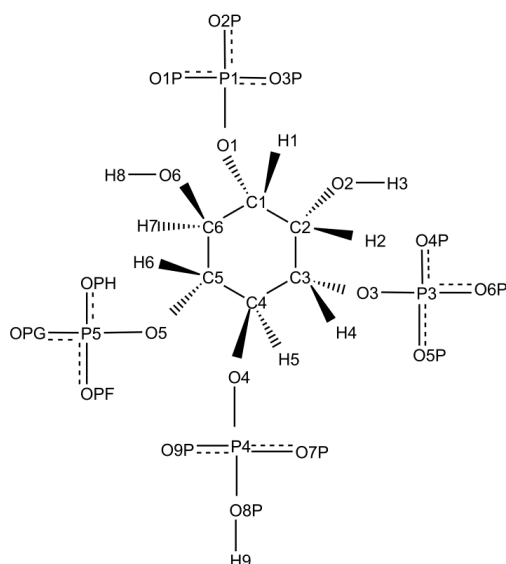


**Figure S13: Atomic labelling scheme for the -7 isomer, 135O4H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S20: Atom names, atom types and charge parameters for the -7 135O4H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.047183                                 | 0.043895                                        | P4   | P                   | 1.192988                                 | 1.150103                                        |
| O1   | OS                  | -0.434424                                | -0.455086                                       | O7P  | O2                  | -0.924064                                | -0.839812                                       |
| C2   | CT                  | -0.032919                                | -0.007198                                       | O8P  | OH                  | -0.817703                                | -0.885643                                       |
| O2   | OH                  | -0.703820                                | -0.665840                                       | O9P  | O2                  | -0.886364                                | -0.882308                                       |
| C3   | CT                  | 0.195195                                 | 0.011312                                        | P5   | P                   | 1.207011                                 | 1.192736                                        |
| O3   | OS                  | -0.475412                                | -0.324397                                       | OPF  | O2                  | -0.956737                                | -0.961483                                       |
| C4   | CT                  | 0.102599                                 | -0.039151                                       | OPG  | O2                  | -0.929827                                | -0.909896                                       |
| O4   | OS                  | -0.501788                                | -0.342089                                       | OPH  | O2                  | -0.915979                                | -0.952624                                       |
| C5   | CT                  | 0.071796                                 | 0.040604                                        | H1   | HC                  | 0.085212                                 | 0.135120                                        |
| O5   | OS                  | -0.493347                                | -0.423606                                       | H2   | HC                  | 0.108458                                 | 0.162649                                        |
| C6   | CT                  | 0.156312                                 | 0.121065                                        | H3   | HO                  | 0.478342                                 | 0.362217                                        |
| O6   | OH                  | -0.707886                                | -0.676917                                       | H4   | HC                  | 0.037208                                 | 0.094439                                        |
| P1   | P                   | 1.189999                                 | 1.210119                                        | H5   | HC                  | 0.127693                                 | 0.158138                                        |
| O1P  | O2                  | -0.929198                                | -0.940208                                       | H6   | HC                  | 0.154855                                 | 0.146772                                        |
| O2P  | O2                  | -0.932105                                | -0.930151                                       | H7   | HC                  | 0.095770                                 | 0.048266                                        |
| O3P  | O2                  | -0.971362                                | -0.976975                                       | H8   | HO                  | 0.432421                                 | 0.446136                                        |
| P3   | P                   | 1.180819                                 | 1.164135                                        | H9   | HY                  | 0.560674                                 | 0.564645                                        |
| O4P  | O2                  | -0.922530                                | -0.899231                                       |      |                     |                                          |                                                 |
| O5P  | O2                  | -0.935212                                | -0.970310                                       |      |                     |                                          |                                                 |
| O6P  | O2                  | -0.953857                                | -0.969427                                       |      |                     |                                          |                                                 |

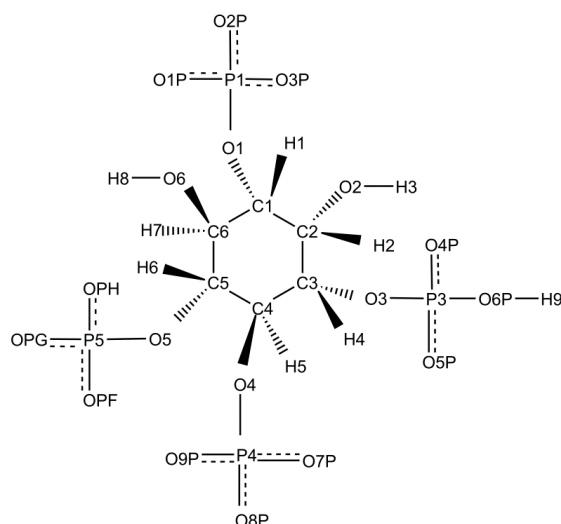


**Figure S14: Atomic labelling scheme for the -7 isomer, 145O3H, of Ins(1,3,4,5)P<sub>4</sub>.**

**Table S21: Atom names, atom types and charge parameters for the -7 145O3H isomer of Ins(1,3,4,5)P<sub>4</sub>.** Charge parameters for the isomer optimised using the DFT level of theory in both gas phase and in implicit solvent, plus assigned atom types from the ff99SB force field are provided.

| Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations | Atom | ff99SB<br>atom type | Charge from<br>gas phase<br>calculations | Charge from<br>implicit solvent<br>calculations |
|------|---------------------|------------------------------------------|-------------------------------------------------|------|---------------------|------------------------------------------|-------------------------------------------------|
| C1   | CT                  | 0.006741                                 | 0.058317                                        | P4   | P                   | 1.189919                                 | 1.258273                                        |
| O1   | OS                  | -0.503965                                | -0.429277                                       | O7P  | O2                  | -0.913490                                | -0.864350                                       |
| C2   | CT                  | 0.033204                                 | 0.028454                                        | O8P  | O2                  | -0.866078                                | -0.899365                                       |
| O2   | OH                  | -0.642457                                | -0.673358                                       | O9P  | O2                  | -0.815196                                | -0.884542                                       |
| C3   | CT                  | 0.003195                                 | -0.043292                                       | P5   | P                   | 1.211726                                 | 1.116421                                        |
| O3   | OS                  | -0.452007                                | -0.380157                                       | OPF  | O2                  | -0.963710                                | -0.912625                                       |
| C4   | CT                  | 0.059906                                 | -0.042721                                       | OPG  | O2                  | -0.945254                                | -0.982320                                       |
| O4   | OS                  | -0.460097                                | -0.361924                                       | OPH  | O2                  | -0.929396                                | -0.910459                                       |
| C5   | CT                  | 0.091729                                 | 0.025425                                        | H1   | HC                  | 0.126984                                 | 0.132016                                        |
| O5   | OS                  | -0.440696                                | -0.379266                                       | H2   | HC                  | 0.159233                                 | 0.136468                                        |
| C6   | CT                  | 0.176233                                 | 0.036592                                        | H3   | HO                  | 0.356530                                 | 0.384194                                        |
| O6   | OH                  | -0.816590                                | -0.612926                                       | H4   | HC                  | 0.106468                                 | 0.136079                                        |
| P1   | P                   | 1.228585                                 | 1.145399                                        | H5   | HC                  | 0.132802                                 | 0.164467                                        |
| O1P  | O2                  | -0.942964                                | -0.904048                                       | H6   | HC                  | 0.153732                                 | 0.151824                                        |
| O2P  | O2                  | -0.948476                                | -0.921876                                       | H7   | HC                  | 0.118083                                 | 0.071251                                        |
| O3P  | O2                  | -0.968999                                | -0.963695                                       | H8   | HO                  | 0.506506                                 | 0.413943                                        |
| P3   | P                   | 1.301262                                 | 1.166134                                        | H9   | HY                  | 0.545725                                 | 0.502921                                        |
| O4P  | O2                  | -0.958930                                | -0.916496                                       |      |                     |                                          |                                                 |
| O5P  | O2                  | -0.981268                                | -0.951767                                       |      |                     |                                          |                                                 |
| O6P  | OH                  | -0.958989                                | -0.893714                                       |      |                     |                                          |                                                 |

## S. 4 Parameters for Ins(1,3,4)P<sub>3</sub>

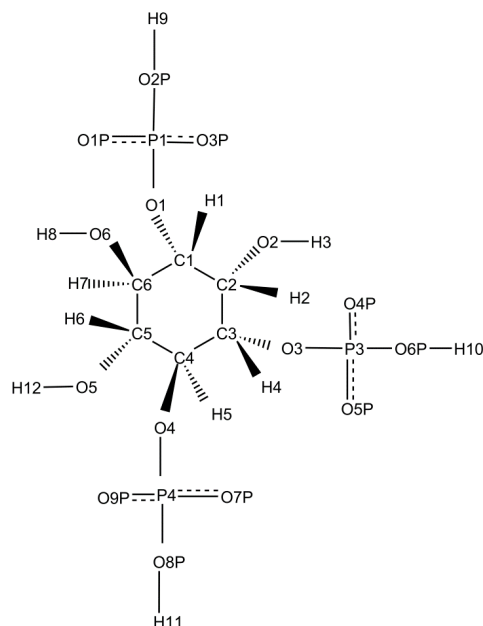


Figure S15: The atomic labelling scheme for the -3 isomer, 134H, of Ins(1,3,4)P<sub>3</sub>.

Table S22: Atom names, atom types and charge parameters for the -3 134H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.026167  | P4   | P                | 1.166716  |
| O1   | OS               | -0.489475 | O7P  | O2               | -0.764846 |
| C2   | CT               | 0.016310  | O8P  | OH               | -0.706027 |
| O2   | OH               | -0.572080 | O9P  | O2               | -0.788397 |
| C3   | CT               | 0.033117  | H1   | HC               | 0.115401  |
| O3   | OS               | -0.415327 | H2   | HC               | 0.147393  |
| C4   | CT               | 0.015759  | H3   | HO               | 0.389555  |
| O4   | OS               | -0.421136 | H4   | HC               | 0.122738  |
| C5   | CT               | 0.084103  | H5   | HC               | 0.158137  |
| O5   | OH               | -0.576136 | H6   | HC               | 0.101065  |
| C6   | CT               | 0.094965  | H7   | HC               | 0.112812  |
| O6   | OH               | -0.688429 | H8   | HO               | 0.434482  |
| P1   | P                | 1.279995  | H9   | HY               | 0.390760  |
| O1P  | O2               | -0.817592 | H10  | HY               | 0.399866  |
| O2P  | OH               | -0.710467 | H11  | HY               | 0.374215  |
| O3P  | O2               | -0.826135 | H12  | HO               | 0.404141  |
| P3   | P                | 1.194680  |      |                  |           |
| O4P  | O2               | -0.801728 |      |                  |           |
| O5P  | O2               | -0.806739 |      |                  |           |
| O6P  | OH               | -0.677859 |      |                  |           |

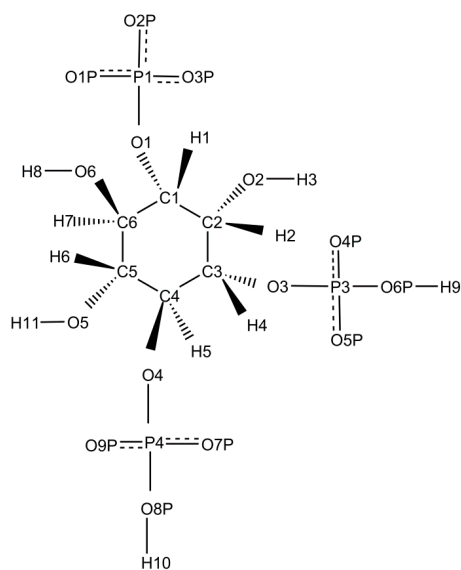


**Figure S16:** The atomic labelling scheme for the -4 isomer, 1O34H, of Ins(1,3,4)P<sub>3</sub>.

**Table S23:** Atom names, atom types and charge parameters for the -4 1O34H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.013873  | P4   | P                | 1.213326  |
| O1   | OS               | -0.481823 | O7P  | O2               | -0.821135 |
| C2   | CT               | 0.005823  | O8P  | OH               | -0.738796 |
| O2   | OH               | -0.655457 | O9P  | O2               | -0.770203 |
| C3   | CT               | 0.056183  | H1   | HC               | 0.134167  |
| O3   | OS               | -0.396201 | H2   | HC               | 0.152707  |
| C4   | CT               | 0.023906  | H3   | HO               | 0.408877  |
| O4   | OS               | -0.403256 | H4   | HC               | 0.102235  |
| C5   | CT               | 0.017627  | H5   | HC               | 0.175038  |
| O5   | OH               | -0.645426 | H6   | HC               | 0.081161  |
| C6   | CT               | 0.146188  | H7   | HC               | 0.087772  |
| O6   | OH               | -0.590467 | H8   | HO               | 0.344114  |
| P1   | P                | 1.239783  | H9   | HY               | 0.396609  |
| O1P  | O2               | -0.893159 | H10  | HY               | 0.392188  |
| O2P  | O2               | -0.914398 | H11  | HO               | 0.412141  |
| O3P  | O2               | -0.914600 |      |                  |           |
| P3   | P                | 1.164657  |      |                  |           |
| O4P  | O2               | -0.819055 |      |                  |           |
| O5P  | O2               | -0.821157 |      |                  |           |
| O6P  | OH               | -0.703241 |      |                  |           |

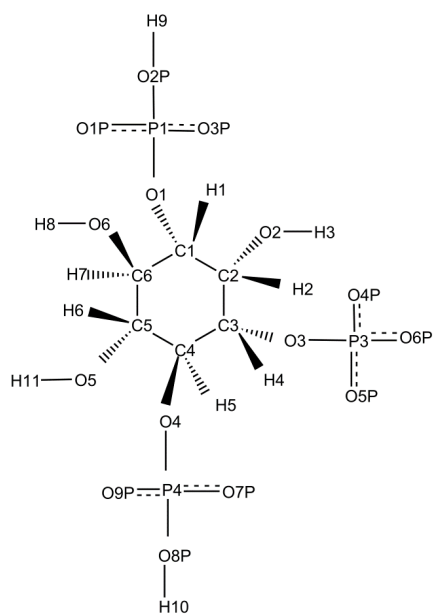


**Figure S17:** The atomic labelling scheme for the -4 isomer, 3O14H, of Ins(1,3,4)P<sub>3</sub>.

**Table S24:** Atom names, atom types and charge parameters for the -4 3O14H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.072263  | P4   | P                | 1.255551  |
| O1   | OS               | -0.461066 | O7P  | O2               | -0.836377 |
| C2   | CT               | -0.014129 | O8P  | OH               | -0.770734 |
| O2   | OH               | -0.668403 | O9P  | O2               | -0.782726 |
| C3   | CT               | 0.105859  | H1   | HC               | 0.090043  |
| O3   | OS               | -0.453311 | H2   | HC               | 0.122794  |
| C4   | CT               | 0.069741  | H3   | HO               | 0.467576  |
| O4   | OS               | -0.457824 | H4   | HC               | 0.055265  |
| C5   | CT               | 0.061335  | H5   | HC               | 0.139178  |
| O5   | OH               | -0.688663 | H6   | HC               | 0.059415  |
| C6   | CT               | 0.161356  | H7   | HC               | 0.117431  |
| O6   | OH               | -0.656745 | H8   | HO               | 0.373293  |
| P1   | P                | 1.277991  | H9   | HY               | 0.419020  |
| O1P  | O2               | -0.846400 | H10  | HY               | 0.391397  |
| O2P  | OH               | -0.731569 | H11  | HO               | 0.440484  |
| O3P  | O2               | -0.878450 |      |                  |           |
| P3   | P                | 1.198443  |      |                  |           |
| O4P  | O2               | -0.868236 |      |                  |           |
| O5P  | O2               | -0.871682 |      |                  |           |
| O6P  | O2               | -0.892117 |      |                  |           |

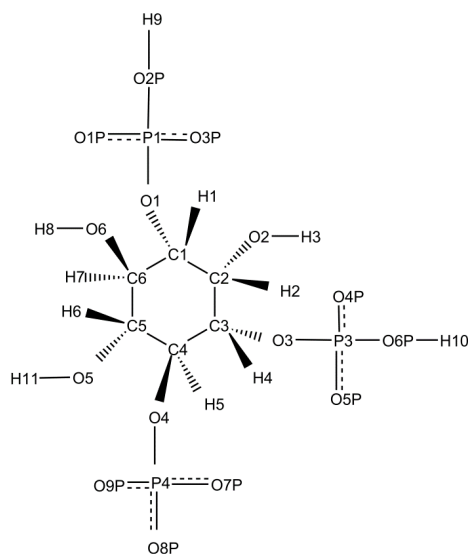


**Figure S18:** The atomic labelling scheme for the -4 isomer, 4O13H, of Ins(1,3,4)P<sub>3</sub>.

**Table S25:** Atom names, atom types and charge parameters for the -4 4O13H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.089514  | P4   | P                | 1.263174  |
| O1   | OS               | -0.477931 | O7P  | O2               | -0.866728 |
| C2   | CT               | 0.052506  | O8P  | O2               | -0.864020 |
| O2   | OH               | -0.692575 | O9P  | O2               | -0.778957 |
| C3   | CT               | 0.012065  | H1   | HC               | 0.043870  |
| O3   | OS               | -0.498877 | H2   | HC               | 0.079555  |
| C4   | CT               | 0.059773  | H3   | HO               | 0.493696  |
| O4   | OS               | -0.470764 | H4   | HC               | 0.060752  |
| C5   | CT               | 0.115809  | H5   | HC               | 0.139882  |
| O5   | OH               | -0.694383 | H6   | HC               | 0.039880  |
| C6   | CT               | 0.304750  | H7   | HC               | 0.068769  |
| O6   | OH               | -0.716496 | H8   | HO               | 0.399989  |
| P1   | P                | 1.228516  | H9   | HY               | 0.399106  |
| O1P  | O2               | -0.791703 | H10  | HY               | 0.505024  |
| O2P  | OH               | -0.733626 | H11  | HO               | 0.445125  |
| O3P  | O2               | -0.837263 |      |                  |           |
| P3   | P                | 1.268020  |      |                  |           |
| O4P  | O2               | -0.904410 |      |                  |           |
| O5P  | O2               | -0.884146 |      |                  |           |
| O6P  | OH               | -0.857895 |      |                  |           |



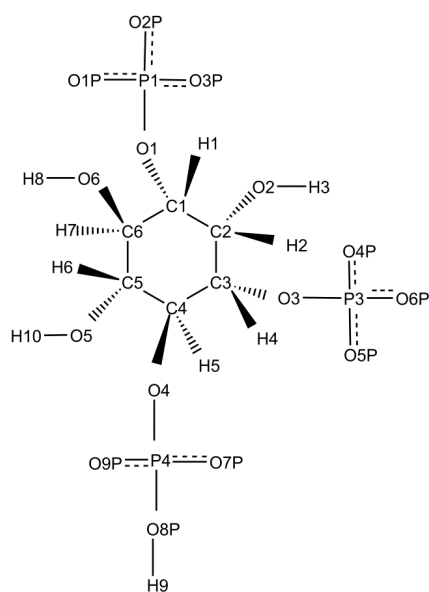


**Figure S19: The atomic labelling scheme for the -5 isomer, 13O4H, of Ins(1,3,4)P<sub>3</sub>.**

**Table S26: Atom names, atom types and charge parameters for the -5 13O4H isomer of Ins(1,3,4)P<sub>3</sub>.**

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | -0.003102 | P4   | P                | 1.208483  |
| O1   | OS               | -0.534171 | O7P  | O2               | -0.846325 |
| C2   | CT               | 0.149444  | O8P  | OH               | -0.778596 |
| O2   | OH               | -0.703444 | O9P  | O2               | -0.846236 |
| C3   | CT               | 0.062347  | H1   | HC               | 0.069463  |
| O3   | OS               | -0.430819 | H2   | HC               | 0.128716  |
| C4   | CT               | 0.067332  | H3   | HO               | 0.444990  |
| O4   | OS               | -0.418057 | H4   | HC               | 0.062523  |
| C5   | CT               | 0.045715  | H5   | HC               | 0.154233  |
| O5   | OH               | -0.605886 | H6   | HC               | 0.087999  |
| C6   | CT               | 0.143878  | H7   | HC               | 0.099654  |
| O6   | OH               | -0.745361 | H8   | HO               | 0.476636  |
| P1   | P                | 1.279962  | H9   | HY               | 0.392864  |
| O1P  | O2               | -0.925510 | H10  | HO               | 0.367580  |
| O2P  | O2               | -0.895923 |      |                  |           |
| O3P  | O2               | -0.926509 |      |                  |           |
| P3   | P                | 1.184179  |      |                  |           |
| O4P  | O2               | -0.914494 |      |                  |           |
| O5P  | O2               | -0.920363 |      |                  |           |
| O6P  | O2               | -0.931200 |      |                  |           |

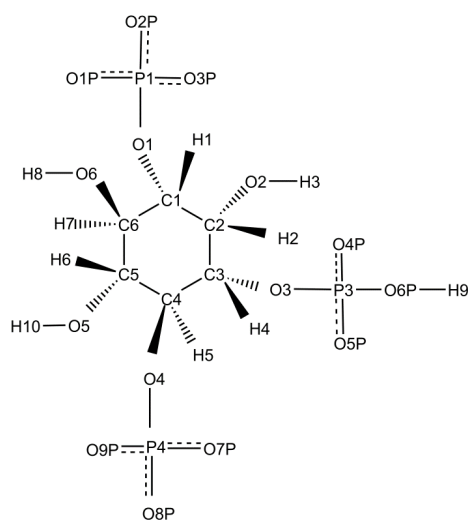


**Figure S20:** The atomic labelling scheme for the -5 isomer, 14O3H, of Ins(1,3,4)P<sub>3</sub>.

**Table S27:** Atom names, atom types and charge parameters for the -5 14O3H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.070152  | P4   | P                | 1.219236  |
| O1   | OS               | -0.442699 | O7P  | O2               | -0.930081 |
| C2   | CT               | -0.018542 | O8P  | O2               | -0.932143 |
| O2   | OH               | -0.618062 | O9P  | O2               | -0.908273 |
| C3   | CT               | 0.024692  | H1   | HC               | 0.086566  |
| O3   | OS               | -0.413644 | H2   | HC               | 0.136713  |
| C4   | CT               | 0.053059  | H3   | HO               | 0.367943  |
| O4   | OS               | -0.475342 | H4   | HC               | 0.106689  |
| C5   | CT               | 0.129298  | H5   | HC               | 0.141007  |
| O5   | OH               | -0.578109 | H6   | HC               | 0.040145  |
| C6   | CT               | 0.140422  | H7   | HC               | 0.050217  |
| O6   | OH               | -0.730523 | H8   | HO               | 0.470253  |
| P1   | P                | 1.211355  | H9   | HY               | 0.419862  |
| O1P  | O2               | -0.911127 | H10  | HO               | 0.339030  |
| O2P  | O2               | -0.902376 |      |                  |           |
| O3P  | O2               | -0.923113 |      |                  |           |
| P3   | P                | 1.261596  |      |                  |           |
| O4P  | O2               | -0.849748 |      |                  |           |
| O5P  | O2               | -0.843178 |      |                  |           |
| O6P  | OH               | -0.791275 |      |                  |           |

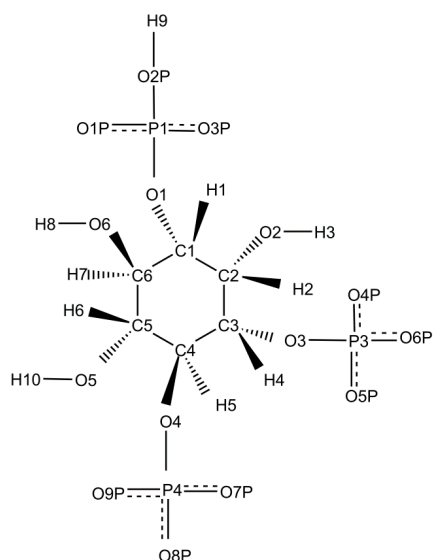


**Figure S21:** The atomic labelling scheme for the -5 isomer, 34O1H, of Ins(1,3,4)P<sub>3</sub>.

**Table S28:** Atom names, atom types and charge parameters for the -5 34O1H isomer of Ins(1,3,4)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.037401  | P4   | P                | 1.201063  |
| O1   | OS               | -0.467116 | O7P  | O2               | -0.917930 |
| C2   | CT               | 0.025270  | O8P  | O2               | -0.923224 |
| O2   | OH               | -0.693213 | O9P  | O2               | -0.892820 |
| C3   | CT               | 0.205926  | H1   | HC               | 0.066587  |
| O3   | OS               | -0.456932 | H2   | HC               | 0.102833  |
| C4   | CT               | 0.011744  | H3   | HO               | 0.467797  |
| O4   | OS               | -0.474859 | H4   | HC               | 0.017168  |
| C5   | CT               | 0.178663  | H5   | HC               | 0.100665  |
| O5   | OH               | -0.723483 | H6   | HC               | 0.028056  |
| C6   | CT               | 0.197837  | H7   | HC               | 0.073528  |
| O6   | OH               | -0.704797 | H8   | HO               | 0.380850  |
| P1   | P                | 1.239234  | H9   | HY               | 0.415835  |
| O1P  | O2               | -0.851133 | H10  | HO               | 0.462981  |
| O2P  | OH               | -0.724754 |      |                  |           |
| O3P  | O2               | -0.897006 |      |                  |           |
| P3   | P                | 1.191210  |      |                  |           |
| O4P  | O2               | -0.883131 |      |                  |           |
| O5P  | O2               | -0.889307 |      |                  |           |
| O6P  | O2               | -0.906946 |      |                  |           |

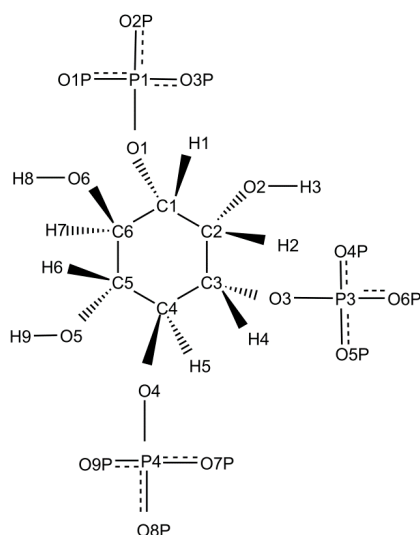


**Figure S22: The atomic labelling scheme for the -6 isomer, 134O, of Ins(1,3,4)P<sub>3</sub>.**

**Table S29: Atom names, atom types and charge parameters for the -6 134O isomer of Ins(1,3,4)P<sub>3</sub>.**

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.099410  | P4   | P                | 1.178651  |
| O1   | OS               | -0.460188 | O7P  | O2               | -0.953596 |
| C2   | CT               | -0.001150 | O8P  | O2               | -0.940626 |
| O2   | OH               | -0.700301 | O9P  | O2               | -0.910834 |
| C3   | CT               | 0.076315  | H1   | HC               | 0.062498  |
| O3   | OS               | -0.418785 | H2   | HC               | 0.116046  |
| C4   | CT               | 0.045328  | H3   | HO               | 0.452761  |
| O4   | OS               | -0.475477 | H4   | HC               | 0.039055  |
| C5   | CT               | 0.189355  | H5   | HC               | 0.120064  |
| O5   | OH               | -0.645536 | H6   | HC               | 0.062599  |
| C6   | CT               | 0.141750  | H7   | HC               | 0.067401  |
| O6   | OH               | -0.795789 | H8   | HO               | 0.495746  |
| P1   | P                | 1.214789  | H9   | HO               | 0.358485  |
| O1P  | O2               | -0.940650 |      |                  |           |
| O2P  | O2               | -0.921997 |      |                  |           |
| O3P  | O2               | -0.951626 |      |                  |           |
| P3   | P                | 1.175458  |      |                  |           |
| O4P  | O2               | -0.910339 |      |                  |           |
| O5P  | O2               | -0.924442 |      |                  |           |
| O6P  | O2               | -0.944377 |      |                  |           |

## S. 5 Parameters for Ins(1,4,5)P<sub>3</sub>

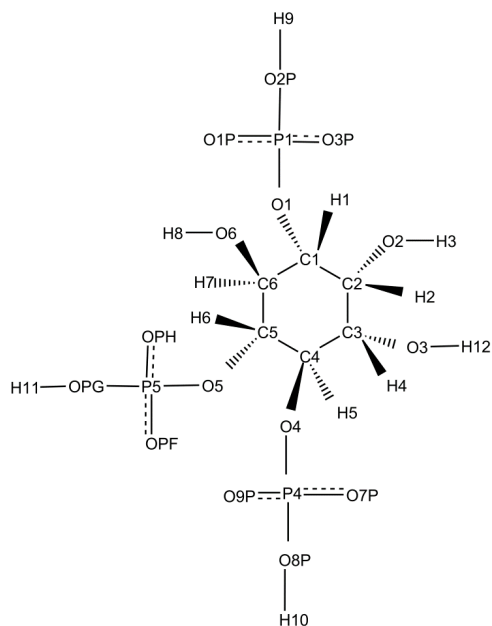


Figure S23: The atomic labelling scheme for the -3 isomer, 145H, of Ins(1,4,5)P<sub>3</sub>.

Table S30: Atom names, atom types and charge parameters for the -3 145H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | -0.003428 | P5   | P                | 1.226935  |
| O1   | OS               | -0.375440 | OPF  | O2               | -0.817259 |
| C2   | CT               | 0.056775  | OPG  | OH               | -0.706381 |
| O2   | OH               | -0.637025 | OPH  | O2               | -0.759779 |
| C3   | CT               | 0.200366  | H1   | HC               | 0.081431  |
| O3   | OH               | -0.717646 | H2   | HC               | 0.094212  |
| C4   | CT               | 0.143371  | H3   | HO               | 0.414492  |
| O4   | OS               | -0.526876 | H4   | HC               | 0.030619  |
| C5   | CT               | 0.094299  | H5   | HC               | 0.104241  |
| O5   | OS               | -0.493987 | H6   | HC               | 0.105801  |
| C6   | CT               | 0.094423  | H7   | HC               | 0.126715  |
| O6   | OH               | -0.638022 | H8   | HO               | 0.440763  |
| P1   | P                | 1.184252  | H9   | HY               | 0.410595  |
| O1P  | O2               | -0.814009 | H10  | HY               | 0.423189  |
| O2P  | OH               | -0.718754 | H11  | HY               | 0.395164  |
| O3P  | O2               | -0.775982 | H12  | HO               | 0.450229  |
| P4   | P                | 1.265521  |      |                  |           |
| O7P  | O2               | -0.822373 |      |                  |           |
| O8P  | OH               | -0.703148 |      |                  |           |
| O9P  | O2               | -0.833284 |      |                  |           |

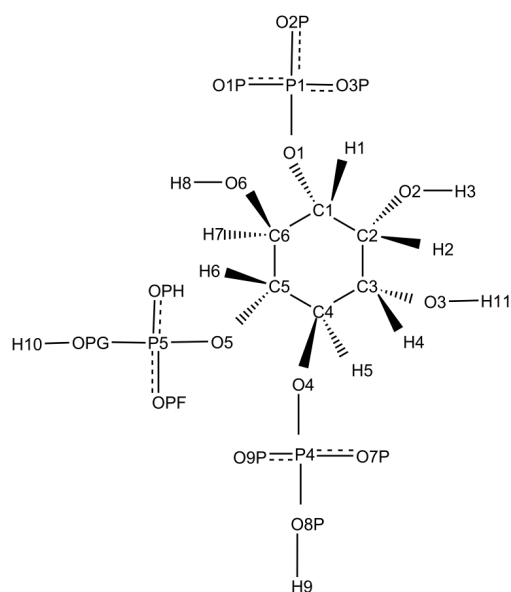


**Figure S24:** The atomic labelling scheme for the -4 isomer, 1O45H, of Ins(1,4,5)P<sub>3</sub>.

**Table S31:** Atom names, atom types and charge parameters for the -4 1O45H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | -0.039018 | P5   | P                | 1.252494  |
| O1   | OS               | -0.461582 | OPF  | O2               | -0.836610 |
| C2   | CT               | 0.161807  | OPG  | OH               | -0.755304 |
| O2   | OH               | -0.608807 | OPH  | O2               | -0.832421 |
| C3   | CT               | 0.004464  | H1   | HC               | 0.096019  |
| O3   | OH               | -0.678101 | H2   | HC               | 0.070252  |
| C4   | CT               | -0.002448 | H3   | HO               | 0.355665  |
| O4   | OS               | -0.469206 | H4   | HC               | 0.109754  |
| C5   | CT               | 0.006673  | H5   | HC               | 0.166066  |
| O5   | OS               | -0.475620 | H6   | HC               | 0.157070  |
| C6   | CT               | 0.120731  | H7   | HC               | 0.087597  |
| O6   | OH               | -0.608184 | H8   | HO               | 0.444720  |
| P1   | P                | 1.223028  | H9   | HY               | 0.431623  |
| O1P  | O2               | -0.875360 | H10  | HY               | 0.411765  |
| O2P  | O2               | -0.888313 | H11  | HO               | 0.467021  |
| O3P  | O2               | -0.899907 |      |                  |           |
| P4   | P                | 1.277407  |      |                  |           |
| O7P  | O2               | -0.842191 |      |                  |           |
| O8P  | OH               | -0.725433 |      |                  |           |
| O9P  | O2               | -0.845654 |      |                  |           |

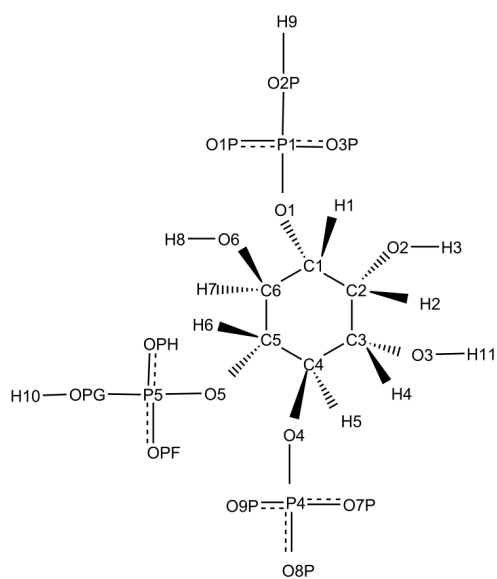


**Figure S25:** The atomic labelling scheme for the -4 isomer, 4O15H, of Ins(1,4,5)P<sub>3</sub>.

**Table S32:** Atom names, atom types and charge parameters for the -4 4O15H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.111359  | P5   | P                | 1.213028  |
| O1   | OS               | -0.445064 | OPF  | O2               | -0.830230 |
| C2   | CT               | -0.031348 | OPG  | OH               | -0.689157 |
| O2   | OH               | -0.594418 | OPH  | O2               | -0.842498 |
| C3   | CT               | 0.112454  | H1   | HC               | 0.101737  |
| O3   | OH               | -0.773570 | H2   | HC               | 0.099001  |
| C4   | CT               | 0.051656  | H3   | HO               | 0.381256  |
| O4   | OS               | -0.415319 | H4   | HC               | 0.016769  |
| C5   | CT               | 0.041130  | H5   | HC               | 0.135732  |
| O5   | OS               | -0.485044 | H6   | HC               | 0.115100  |
| C6   | CT               | 0.090340  | H7   | HC               | 0.085285  |
| O6   | OH               | -0.649986 | H8   | HO               | 0.412040  |
| P1   | P                | 1.266738  | H9   | HY               | 0.389808  |
| O1P  | O2               | -0.850465 | H10  | HY               | 0.395041  |
| O2P  | OH               | -0.743070 | H11  | HO               | 0.449366  |
| O3P  | O2               | -0.861430 |      |                  |           |
| P4   | P                | 1.228040  |      |                  |           |
| O7P  | O2               | -0.791778 |      |                  |           |
| O8P  | O2               | -0.848067 |      |                  |           |
| O9P  | O2               | -0.844437 |      |                  |           |

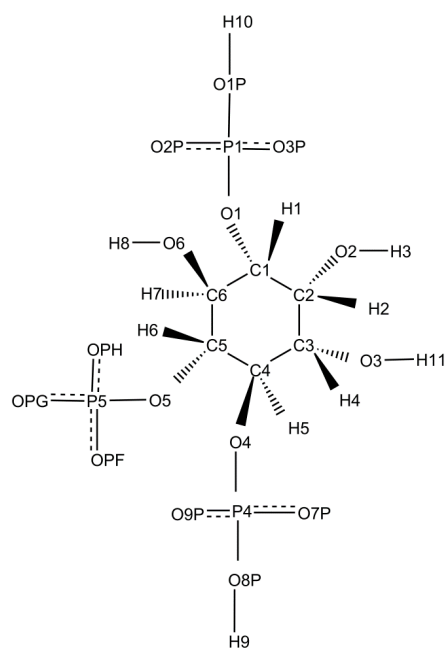


**Figure S26: The atomic labelling scheme for the -4 isomer, 5O14H, of Ins(1,4,5)P<sub>3</sub>.**

**Table S33: Atom names, atom types and charge parameters for the -4 5O14H isomer of Ins(1,4,5)P<sub>3</sub>.**

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | -0.037659 | P5   | P                | 1.244112  |
| O1   | OS               | -0.448720 | OPF  | O2               | -0.857172 |
| C2   | CT               | 0.159940  | OPG  | O2               | -0.767015 |
| O2   | OH               | -0.600046 | OPH  | O2               | -0.845105 |
| C3   | CT               | 0.001685  | H1   | HC               | 0.098839  |
| O3   | OH               | -0.675061 | H2   | HC               | 0.061157  |
| C4   | CT               | 0.010303  | H3   | HO               | 0.356062  |
| O4   | OS               | -0.480484 | H4   | HC               | 0.108611  |
| C5   | CT               | 0.034527  | H5   | HC               | 0.151342  |
| O5   | OS               | -0.465733 | H6   | HC               | 0.136592  |
| C6   | CT               | 0.117153  | H7   | HC               | 0.057280  |
| O6   | OH               | -0.690010 | H8   | HO               | 0.405840  |
| P1   | P                | 1.207573  | H9   | HY               | 0.427543  |
| O1P  | OH               | -0.756050 | H10  | HY               | 0.434525  |
| O2P  | O2               | -0.850812 | H11  | HO               | 0.463072  |
| O3P  | O2               | -0.863802 |      |                  |           |
| P4   | P                | 1.288862  |      |                  |           |
| O7P  | O2               | -0.850101 |      |                  |           |
| O8P  | OH               | -0.723337 |      |                  |           |
| O9P  | O2               | -0.853911 |      |                  |           |



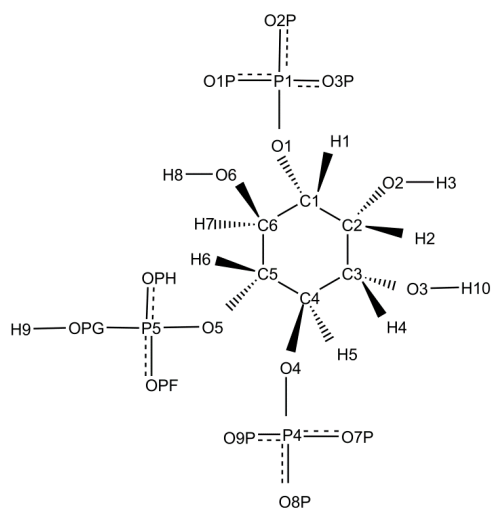


**Figure S27:** The atomic labelling scheme for the -5 isomer, 14O5H, of Ins(1,4,5)P<sub>3</sub>.

**Table S34:** Atom names, atom types and charge parameters for the -5 14O5H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.054765  | P5   | P                | 1.236822  |
| O1   | OS               | -0.440888 | OPF  | O2               | -0.867150 |
| C2   | CT               | 0.024615  | OPG  | OH               | -0.772361 |
| O2   | OH               | -0.662364 | OPH  | O2               | -0.846114 |
| C3   | CT               | 0.134880  | H1   | HC               | 0.099288  |
| O3   | OH               | -0.780696 | H2   | HC               | 0.086050  |
| C4   | CT               | 0.091978  | H3   | HO               | 0.399519  |
| O4   | OS               | -0.455165 | H4   | HC               | 0.043416  |
| C5   | CT               | -0.002006 | H5   | HC               | 0.115366  |
| O5   | OS               | -0.440875 | H6   | HC               | 0.128156  |
| C6   | CT               | 0.009215  | H7   | HC               | 0.124742  |
| O6   | OH               | -0.576623 | H8   | HO               | 0.425521  |
| P1   | P                | 1.219324  | H9   | HY               | 0.399494  |
| O1P  | O2               | -0.899464 | H10  | HO               | 0.509231  |
| O2P  | O2               | -0.917181 |      |                  |           |
| O3P  | O2               | -0.933231 |      |                  |           |
| P4   | P                | 1.238708  |      |                  |           |
| O7P  | O2               | -0.930884 |      |                  |           |
| O8P  | O2               | -0.895867 |      |                  |           |
| O9P  | O2               | -0.920221 |      |                  |           |

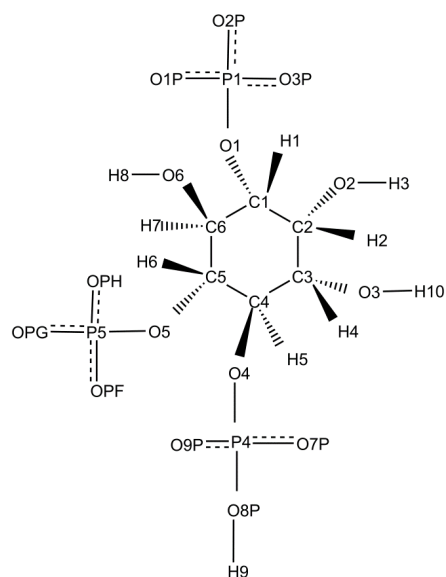


**Figure S28:** The atomic labelling scheme for the -5 isomer, 15O4H, of Ins(1,4,5)P<sub>3</sub>.

**Table S35:** Atom names, atom types and charge parameters for the -5 15O4H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.093358  | P5   | P                | 1.251949  |
| O1   | OS               | -0.457615 | OPF  | O2               | -0.886672 |
| C2   | CT               | 0.058093  | OPG  | O2               | -0.850299 |
| O2   | OH               | -0.660481 | OPH  | O2               | -0.794703 |
| C3   | CT               | 0.010834  | H1   | HC               | 0.063921  |
| O3   | OH               | -0.735515 | H2   | HC               | 0.082650  |
| C4   | CT               | -0.041722 | H3   | HO               | 0.401282  |
| O4   | OS               | -0.468270 | H4   | HC               | 0.106106  |
| C5   | CT               | 0.015168  | H5   | HC               | 0.172481  |
| O5   | OS               | -0.465439 | H6   | HC               | 0.151560  |
| C6   | CT               | 0.167962  | H7   | HC               | 0.063872  |
| O6   | OH               | -0.656771 | H8   | HO               | 0.419118  |
| P1   | P                | 1.209228  | H9   | HY               | 0.498680  |
| O1P  | O2               | -0.903891 | H10  | HO               | 0.494850  |
| O2P  | O2               | -0.921357 |      |                  |           |
| O3P  | O2               | -0.940705 |      |                  |           |
| P4   | P                | 1.285844  |      |                  |           |
| O7P  | O2               | -0.927680 |      |                  |           |
| O8P  | OH               | -0.904959 |      |                  |           |
| O9P  | O2               | -0.930875 |      |                  |           |

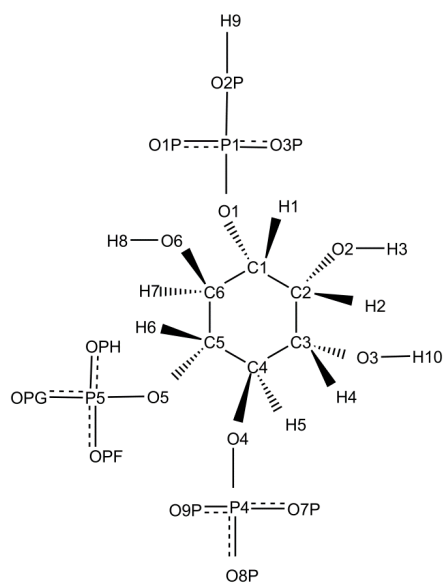


**Figure S29:** The atomic labelling scheme for the -5 isomer, 45O1H, of Ins(1,4,5)P<sub>3</sub>.

**Table S36:** Atom names, atom types and charge parameters for the -5 45O1H isomer of Ins(1,4,5)P<sub>3</sub>.

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.087423  | P5   | P                | 1.242584  |
| O1   | OS               | -0.448677 | OPF  | O2               | -0.924361 |
| C2   | CT               | 0.004243  | OPG  | O2               | -0.939798 |
| O2   | OH               | -0.613024 | OPH  | O2               | -0.906461 |
| C3   | CT               | 0.125078  | H1   | HC               | 0.092954  |
| O3   | OH               | -0.806299 | H2   | HC               | 0.072999  |
| C4   | CT               | 0.020970  | H3   | HO               | 0.382530  |
| O4   | OS               | -0.409337 | H4   | HC               | 0.010699  |
| C5   | CT               | 0.012637  | H5   | HC               | 0.133287  |
| O5   | OS               | -0.464182 | H6   | HC               | 0.108357  |
| C6   | CT               | 0.155764  | H7   | HC               | 0.051842  |
| O6   | OH               | -0.718157 | H8   | HO               | 0.476855  |
| P1   | P                | 1.269872  | H9   | HY               | 0.403111  |
| O1P  | O2               | -0.868173 | H10  | HO               | 0.454019  |
| O2P  | OH               | -0.774796 |      |                  |           |
| O3P  | O2               | -0.887605 |      |                  |           |
| P4   | P                | 1.239405  |      |                  |           |
| O7P  | O2               | -0.887221 |      |                  |           |
| O8P  | O2               | -0.869846 |      |                  |           |
| O9P  | O2               | -0.826693 |      |                  |           |

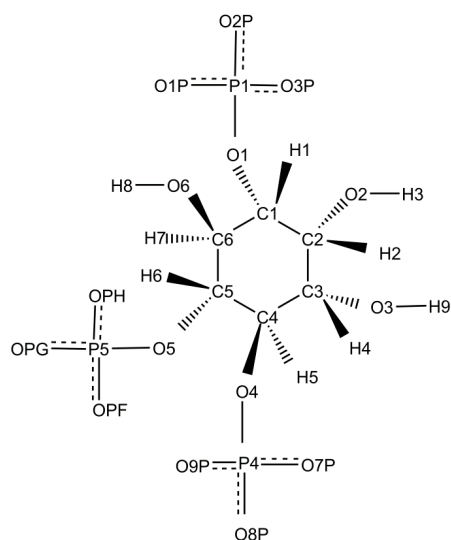


**Figure S30: The atomic labelling scheme for the -6 isomer, 145O, of Ins(1,4,5)P<sub>3</sub>.**

**Table S37: Atom names, atom types and charge parameters for the -6 145O isomer of Ins(1,4,5)P<sub>3</sub>.**

| Atom | ff99SB atom type | Charge    | Atom | ff99SB atom type | Charge    |
|------|------------------|-----------|------|------------------|-----------|
| C1   | CT               | 0.016906  | P5   | P                | 1.203981  |
| O1   | OS               | -0.527083 | OPF  | O2               | -0.952231 |
| C2   | CT               | 0.177777  | OPG  | O2               | -0.932364 |
| O2   | OH               | -0.706669 | OPH  | O2               | -0.914822 |
| C3   | CT               | 0.033974  | H1   | HC               | 0.076586  |
| O3   | OH               | -0.779108 | H2   | HC               | 0.074195  |
| C4   | CT               | 0.237039  | H3   | HO               | 0.400246  |
| O4   | OS               | -0.582251 | H4   | HC               | 0.052579  |
| C5   | CT               | 0.184988  | H5   | HC               | 0.074156  |
| O5   | OS               | -0.531031 | H6   | HC               | 0.081296  |
| C6   | CT               | 0.328378  | H7   | HC               | 0.051773  |
| O6   | OH               | -0.843179 | H8   | HO               | 0.483837  |
| P1   | P                | 1.229021  | H9   | HO               | 0.478490  |
| O1P  | O2               | -0.928954 |      |                  |           |
| O2P  | O2               | -0.948844 |      |                  |           |
| O3P  | O2               | -0.958965 |      |                  |           |
| P4   | P                | 1.225175  |      |                  |           |
| O7P  | O2               | -0.943621 |      |                  |           |
| O8P  | O2               | -0.933546 |      |                  |           |
| O9P  | O2               | -0.927729 |      |                  |           |

## S. 6 Parameters for PtdIns(4,5)P<sub>2</sub>

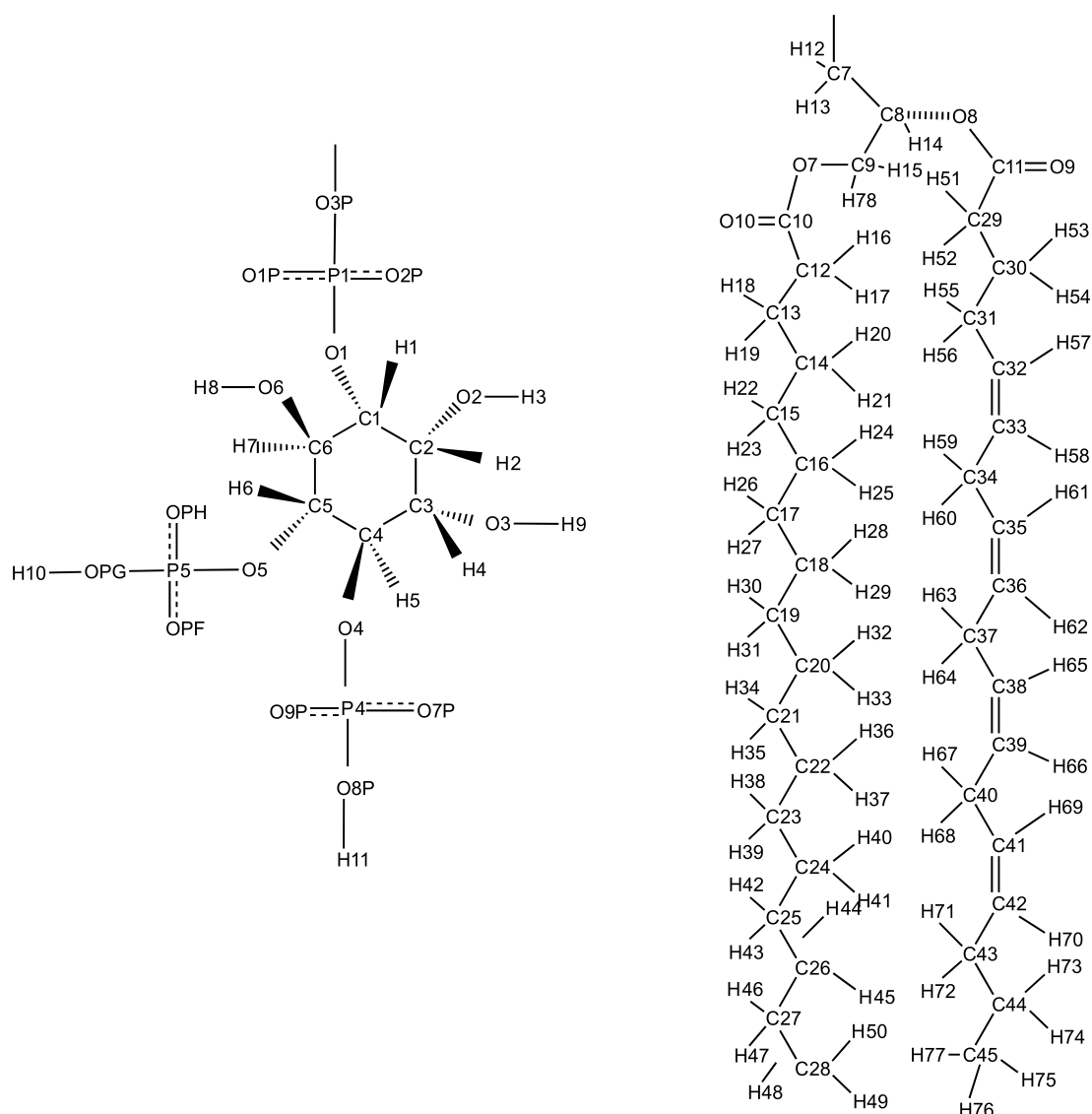


**Figure S31: The atomic labelling scheme for PtdIns(4,5)P<sub>2</sub>.** The fatty acid chains in this study are stearic acid at the 1-position and 5,8,11,14-octadecatetranoic acid at the 2-position. For ease of visualisation the inositol phosphate head-group and phosphatidate tail are drawn separately. These are bonded *via* atoms O3P and C7.

**Table S38: Atom names, atom types and charge parameters for PtdIns(4,5)P<sub>2</sub>.** Atom types for the inositol phosphate head-groups were taken from the ff99SB force field, whilst atom types for the phosphatidate tail were applied from the GAFF force field and assigned by analogy to DOPC and DMPC.<sup>2</sup> Table is shown on following page.

| Atom | ff99SB atom type | Charge    | Atom | GAFF atom type | Charge    |
|------|------------------|-----------|------|----------------|-----------|
| C1   | CT               | -0.007892 | H31  | hc             | 0.127449  |
| O1   | OS               | -0.329293 | C20  | c3             | -0.317377 |
| C2   | CT               | 0.010483  | H32  | hc             | 0.145037  |
| O2   | OH               | -0.626480 | H33  | hc             | 0.156847  |
| C3   | CT               | 0.201160  | C21  | c3             | -0.313223 |
| O3   | OS               | -0.711258 | H34  | hc             | 0.143451  |
| C4   | CT               | 0.093514  | H35  | hc             | 0.152481  |
| O4   | OS               | -0.511775 | C22  | c3             | -0.289072 |
| C5   | CT               | 0.072878  | H36  | hc             | 0.146392  |
| O5   | OS               | -0.475200 | H37  | hc             | 0.154311  |
| C6   | CT               | 0.060429  | C23  | c3             | -0.281396 |
| O6   | OH               | -0.583651 | H38  | hc             | 0.145484  |
| P1   | P                | 1.103976  | H39  | hc             | 0.151802  |
| O1P  | O2               | -0.759492 | C24  | c3             | -0.326471 |
| O2P  | O2               | -0.763350 | H40  | hc             | 0.147397  |
| O3P  | O2               | -0.436470 | H41  | hc             | 0.152962  |
| P4   | P                | 1.271394  | C25  | c3             | -0.314010 |
| O7P  | O2               | -0.823214 | H42  | hc             | 0.146688  |
| O8P  | OH               | -0.708211 | H43  | hc             | 0.151281  |
| O9P  | O2               | -0.830577 | C26  | c3             | -0.242019 |
| P5   | P                | 1.215553  | H44  | hc             | 0.147305  |
| OPF  | O2               | -0.813687 | H45  | hc             | 0.151378  |
| OPG  | OH               | -0.702181 | C27  | c3             | -0.385589 |
| OPH  | O2               | -0.753531 | H46  | hc             | 0.148809  |
| H1   | HC               | 0.118738  | H47  | hc             | 0.152328  |
| H2   | HC               | 0.092943  | C28  | c3             | -0.024803 |
| H3   | HO               | 0.422891  | H48  | hc             | 0.017039  |
| H4   | HC               | 0.046657  | H49  | hc             | 0.023122  |
| H5   | HC               | 0.125644  | H50  | hc             | 0.025196  |
| H6   | HC               | 0.135720  | C29  | c3             | -0.201885 |
| H7   | HC               | 0.108962  | H51  | hc             | 0.067182  |
| H8   | HO               | 0.409780  | H52  | hc             | 0.023592  |
| H9   | HO               | 0.453225  | C30  | c3             | 0.085756  |
| H10  | HY               | 0.385921  | H53  | hc             | 0.82607   |
| H11  | HY               | 0.430612  | H54  | hc             | 0.068043  |
|      |                  |           | C31  | c3             | -0.420171 |
|      |                  |           | H55  | hc             | 0.161456  |
|      |                  |           | H56  | hc             | 0.145907  |
|      |                  |           | C32  | c2             | -0.111977 |
|      |                  |           | H57  | hc             | 0.133058  |
|      |                  |           | C33  | c2             | -0.173807 |
|      |                  |           | H58  | hc             | 0.139805  |
|      |                  |           | C34  | c3             | -0.366602 |
|      |                  |           | H59  | hc             | 0.177039  |
|      |                  |           | H60  | hc             | 0.157694  |
|      |                  |           | C35  | c2             | -0.064823 |
|      |                  |           | H61  | hc             | 0.089994  |
|      |                  |           | C36  | c2             | -0.074487 |
|      |                  |           | H62  | hc             | 0.092892  |
|      |                  |           | C37  | c3             | -0.326674 |
|      |                  |           | H63  | hc             | 0.166166  |
|      |                  |           | H64  | hc             | 0.195626  |
|      |                  |           | C38  | c2             | -0.182059 |
|      |                  |           | H65  | hc             | 0.110292  |
|      |                  |           | C39  | c2             | -0.079491 |
|      |                  |           | H66  | hc             | 0.108238  |
|      |                  |           | C40  | c3             | -0.336421 |
|      |                  |           | H67  | hc             | 0.103550  |
|      |                  |           | H68  | hc             | 0.207144  |
|      |                  |           | C41  | c2             | -0.070816 |
|      |                  |           | H69  | hc             | 0.127505  |
|      |                  |           | C42  | c2             | -0.227918 |
|      |                  |           | H70  | hc             | 0.098200  |
|      |                  |           | C43  | c3             | -0.231989 |
|      |                  |           | H71  | hc             | 0.168862  |
|      |                  |           | H72  | hc             | 0.167289  |
|      |                  |           | C44  | c3             | -0.010990 |
|      |                  |           | H73  | hc             | 0.045032  |
|      |                  |           | H74  | hc             | 0.070065  |
|      |                  |           | C45  | c3             | -0.306709 |
|      |                  |           | H75  | hc             | 0.075239  |
|      |                  |           | H76  | hc             | 0.072774  |
|      |                  |           | H77  | hc             | 0.066776  |
|      |                  |           | H78  | hc             | 0.208214  |

| Atom | GAFF atom type | Charge    |
|------|----------------|-----------|
| C7   | c3             | 0.006650  |
| H12  | hc             | 0.076003  |
| H13  | hc             | 0.083821  |
| C8   | c3             | 0.018888  |
| H14  | hc             | 0.136849  |
| C9   | c3             | 0.019275  |
| H15  | hc             | 0.158297  |
| O7   | os             | -0.523019 |
| O8   | os             | -0.356749 |
| C10  | c              | 0.824405  |
| C11  | c              | 0.686414  |
| O9   | o              | -0.578146 |
| O10  | o              | -0.650149 |
| C12  | c3             | -0.096916 |
| H16  | hc             | 0.067229  |
| H17  | hc             | 0.025102  |
| C13  | c3             | -0.341768 |
| H18  | hc             | 0.170640  |
| H19  | hc             | 0.188647  |
| C14  | c3             | -0.236287 |
| H20  | hc             | 0.139592  |
| H21  | hc             | 0.116649  |
| C15  | c3             | -0.421411 |
| H22  | hc             | 0.145919  |
| H23  | hc             | 0.183324  |
| C16  | c3             | -0.224487 |
| H24  | hc             | 0.146202  |
| H25  | hc             | 0.140452  |
| C17  | c3             | -0.391526 |
| H26  | hc             | 0.135910  |
| H27  | hc             | 0.193092  |
| C18  | c3             | -0.315155 |
| H28  | hc             | 0.143265  |
| H29  | hc             | 0.166881  |
| C19  | c3             | -0.224105 |
| H30  | hc             | 0.140014  |

**Table S39: Parameters for PtdIns(4,5)P<sub>2</sub>.** Parameters for PtdIns(4,5)P<sub>2</sub> were largely taken from the ff99SB force field. Remaining parameters were taken from the GAFF force field.<sup>3</sup>

|            |              |         |               |     |                        |
|------------|--------------|---------|---------------|-----|------------------------|
| Bond       | $K_r$        |         | $r_{eq}$      |     |                        |
| c3-OS      | 301.5        |         | 1.439         |     | From c3-os in GAFF     |
|            |              |         |               |     |                        |
| Angle      | $K_\theta$   |         | $\theta_{eq}$ |     |                        |
| c3-OS-P    | 62.0         |         | 118.0         |     | From c3-os-p5 in GAFF  |
| hc-c3-OS   | 50.87        |         | 108.7         |     | From hc-c3-os in GAFF  |
| c3-c3-OS   | 67.78        |         | 108.42        |     | From c3-c3-os in GAFF  |
|            |              |         |               |     |                        |
| Dihedral   | No. of paths | $V_n/2$ | $\gamma$      | $n$ |                        |
| hc-c3-OS-P | 3            | 1.150   | 0.0           | 3   | From X-c3-os-X in GAFF |
| c3-c3-OS-P | 3            | 1.150   | 0.0           | 3   |                        |

## S. 7 Parameters for D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

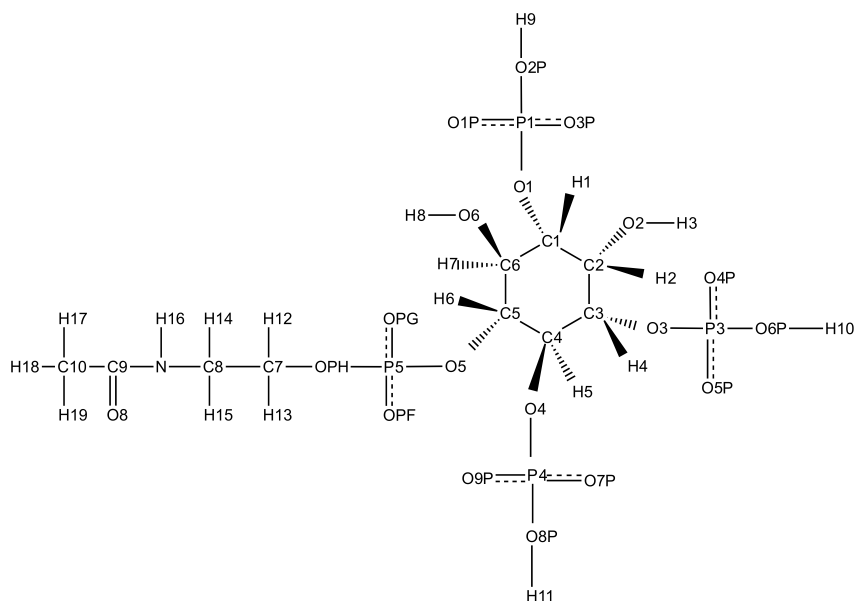


Figure S32: The atomic labelling scheme for the -4 isomer 134H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

Table S40: Atom names, atom types and charge parameters for the -4 isomer 134H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.040427  | H1   | HC                  | 0.101888  |
| O1   | OS                  | -0.470219 | H2   | HC                  | 0.117442  |
| C2   | CT                  | 0.046674  | H3   | HO                  | 0.408095  |
| O2   | OH                  | -0.589877 | H4   | HC                  | 0.114118  |
| C3   | CT                  | 0.113964  | H5   | HC                  | 0.133570  |
| O3   | OS                  | -0.493048 | H6   | HC                  | 0.150095  |
| C4   | CT                  | 0.020686  | H7   | HC                  | 0.101914  |
| O4   | OS                  | -0.437700 | H8   | HO                  | 0.392419  |
| C5   | CT                  | 0.033175  | H9   | HY                  | 0.387071  |
| O5   | OS                  | -0.323964 | H10  | HY                  | 0.488396  |
| C6   | CT                  | 0.080687  | H11  | HY                  | 0.378479  |
| O6   | OH                  | -0.604915 | C7   | CT                  | 0.049541  |
| P1   | P                   | 1.258975  | H12  | HC                  | 0.116898  |
| O1P  | O2                  | -0.820179 | H13  | HC                  | 0.045778  |
| O2P  | OH                  | -0.710965 | C8   | CT                  | 0.005834  |
| O3P  | O2                  | -0.839357 | H14  | H1                  | 0.033027  |
| P3   | P                   | 1.271703  | H15  | H1                  | 0.035549  |
| O4P  | O2                  | -0.828846 | N    | N                   | -0.255287 |
| O5P  | O2                  | -0.843923 | H16  | H                   | 0.199948  |
| O6P  | OH                  | -0.770804 | C9   | C                   | 0.622513  |
| P4   | P                   | 1.191717  | O8   | O                   | -0.726439 |
| O7P  | O2                  | -0.810702 | C10  | CT                  | -0.248065 |
| O8P  | OH                  | -0.686635 | H17  | HC                  | 0.075361  |
| O9P  | O2                  | -0.782943 | H18  | HC                  | 0.044940  |
| P5   | P                   | 0.940458  | H19  | HC                  | 0.046342  |
| OPF  | O2                  | -0.737835 |      |                     |           |
| OPG  | O2                  | -0.646022 |      |                     |           |
| OPH  | OS                  | -0.419956 |      |                     |           |



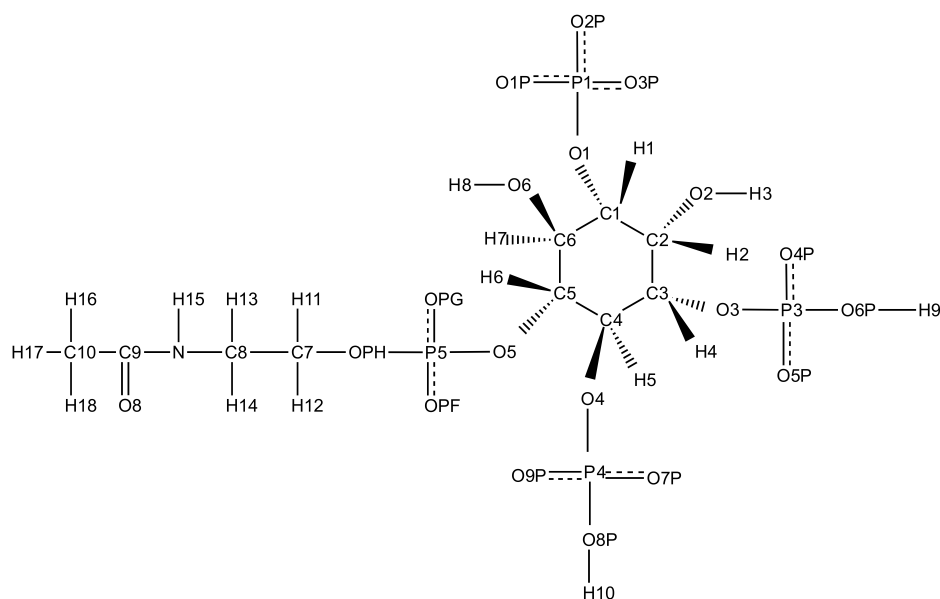


**Figure S33:** The atomic labelling scheme for the -5 isomer 1O34H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S41:** Atom names, atom types and charge parameters for the -5 isomer 1O34H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.030606  | H1   | HC                  | 0.128042  |
| O1   | OS                  | -0.494310 | H2   | HC                  | 0.179809  |
| C2   | CT                  | 0.032952  | H3   | HO                  | 0.330374  |
| O2   | OH                  | -0.600770 | H4   | HC                  | 0.137458  |
| C3   | CT                  | 0.003942  | H5   | HC                  | 0.152023  |
| O3   | OS                  | -0.456286 | H6   | HC                  | 0.137578  |
| C4   | CT                  | 0.110430  | H7   | HC                  | 0.060380  |
| O4   | OS                  | -0.494959 | H8   | HO                  | 0.414074  |
| C5   | CT                  | 0.059325  | H9   | HY                  | 0.462609  |
| O5   | OS                  | -0.342901 | H10  | HY                  | 0.435883  |
| C6   | CT                  | 0.313760  | C7   | CT                  | 0.110404  |
| O6   | OH                  | -0.642960 | H11  | HC                  | 0.008276  |
| P1   | P                   | 1.202461  | H12  | HC                  | 0.022757  |
| O1P  | O2                  | -0.725386 | C8   | CT                  | 0.116362  |
| O2P  | O2                  | -0.831307 | H13  | H1                  | 0.022443  |
| O3P  | O2                  | -0.837902 | H14  | H1                  | 0.012979  |
| P3   | P                   | 1.194692  | N    | N                   | -0.679615 |
| O4P  | O2                  | -0.829807 | H15  | H                   | 0.307923  |
| O5P  | O2                  | -0.846404 | C9   | C                   | 0.731143  |
| O6P  | OH                  | -0.750412 | O8   | O                   | -0.844533 |
| P4   | P                   | 1.222709  | C10  | CT                  | -0.300732 |
| O7P  | O2                  | -0.846699 | H16  | HC                  | 0.069424  |
| O8P  | OH                  | -0.731472 | H17  | HC                  | 0.022903  |
| O9P  | O2                  | -0.801690 | H18  | HC                  | 0.019805  |
| P5   | P                   | 1.005262  |      |                     |           |
| OPF  | O2                  | -0.775755 |      |                     |           |
| OPG  | O2                  | -0.717072 |      |                     |           |
| OPH  | OS                  | -0.507819 |      |                     |           |

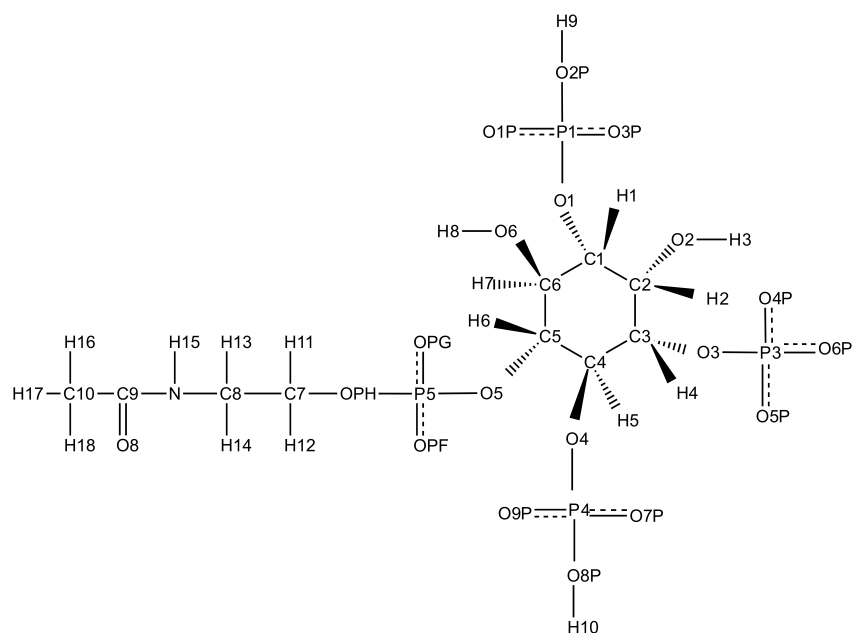


**Figure S34:** The atomic labelling scheme for the -5 isomer 3O14H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S42:** Atom names, atom types and charge parameters for the -5 isomer 3O14H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.212993  | H1   | HC                  | 0.066659  |
| O1   | OS                  | -0.516067 | H2   | HC                  | 0.034100  |
| C2   | CT                  | 0.104475  | H3   | HO                  | 0.431969  |
| O2   | OH                  | -0.668495 | H4   | HC                  | 0.147289  |
| C3   | CT                  | 0.040158  | H5   | HC                  | 0.170038  |
| O3   | OS                  | -0.459915 | H6   | HC                  | 0.195817  |
| C4   | CT                  | 0.014786  | H7   | HC                  | 0.139307  |
| O4   | OS                  | -0.460130 | H8   | HO                  | 0.393378  |
| C5   | CT                  | -0.044930 | H9   | HY                  | 0.479262  |
| O5   | OS                  | -0.300564 | H10  | HY                  | 0.382832  |
| C6   | CT                  | 0.021279  | C7   | CT                  | 0.033429  |
| O6   | OH                  | -0.639249 | H11  | HC                  | 0.180448  |
| P1   | P                   | 1.255377  | H12  | HC                  | 0.043755  |
| O1P  | O2                  | -0.904051 | C8   | CT                  | -0.032990 |
| O2P  | OH                  | -0.905062 | H13  | H1                  | 0.038181  |
| O3P  | O2                  | -0.916503 | H14  | H1                  | 0.025656  |
| P3   | P                   | 1.245712  | N    | N                   | -0.264640 |
| O4P  | O2                  | -0.857200 | H15  | H                   | 0.205979  |
| O5P  | O2                  | -0.755907 | C9   | C                   | 0.623907  |
| O6P  | O2                  | -0.855320 | O8   | O                   | -0.745265 |
| P4   | P                   | 1.205761  | C10  | CT                  | -0.240457 |
| O7P  | O2                  | -0.848478 | H16  | HC                  | 0.077040  |
| O8P  | OH                  | -0.707127 | H17  | HC                  | 0.036201  |
| O9P  | O2                  | -0.834651 | H18  | HC                  | 0.036776  |
| P5   | P                   | 0.891407  |      |                     |           |
| OPF  | O2                  | -0.750168 |      |                     |           |
| OPG  | O2                  | -0.622524 |      |                     |           |
| OPH  | OS                  | -0.404277 |      |                     |           |

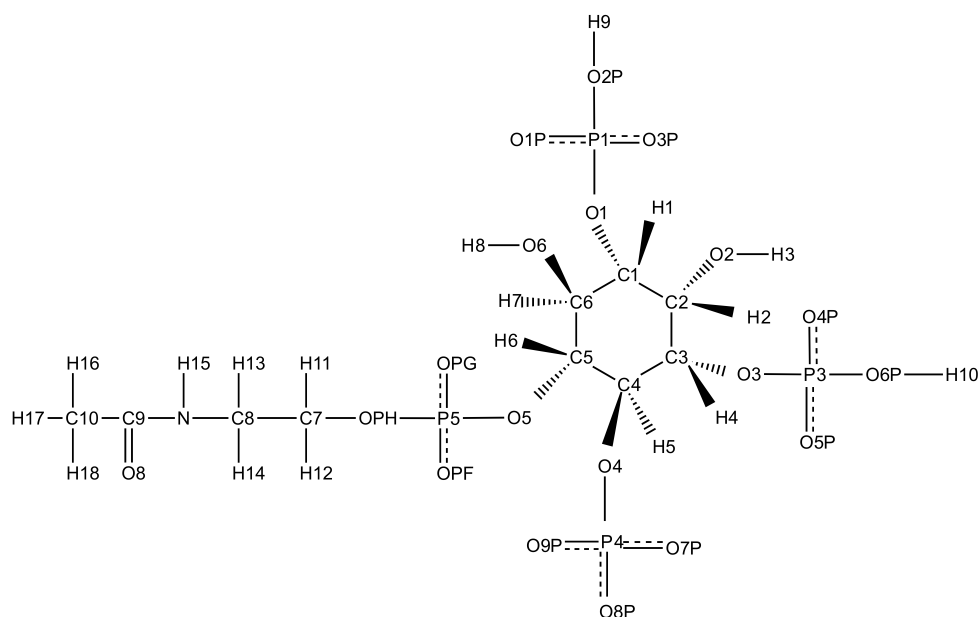


**Figure S35:** The atomic labelling scheme for the -5 isomer 4O13H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S43:** Atom names, atom types and charge parameters for the -5 isomer 4O13H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.041956  | H1   | HC                  | 0.099609  |
| O1   | OS                  | -0.426659 | H2   | HC                  | 0.076935  |
| C2   | CT                  | 0.148469  | H3   | HO                  | 0.446197  |
| O2   | OH                  | -0.693569 | H4   | HC                  | 0.116373  |
| C3   | CT                  | 0.019198  | H5   | HC                  | 0.155816  |
| O3   | OS                  | -0.530893 | H6   | HC                  | 0.102154  |
| C4   | CT                  | 0.136864  | H7   | HC                  | 0.143387  |
| O4   | OS                  | -0.511514 | H8   | HO                  | 0.410507  |
| C5   | CT                  | 0.191792  | H9   | HY                  | 0.398826  |
| O5   | OS                  | -0.469353 | H10  | HY                  | 0.488405  |
| C6   | CT                  | 0.102464  | C7   | CT                  | 0.074677  |
| O6   | OH                  | -0.655414 | H11  | HC                  | 0.094695  |
| P1   | P                   | 1.169206  | H12  | HC                  | 0.062498  |
| O1P  | O2                  | -0.838094 | C8   | CT                  | -0.046800 |
| O2P  | OH                  | -0.700901 | H13  | H1                  | 0.045203  |
| O3P  | O2                  | -0.813727 | H14  | H1                  | 0.016031  |
| P3   | P                   | 1.199318  | N    | N                   | -0.235712 |
| O4P  | O2                  | -0.887065 | H15  | H                   | 0.172762  |
| O5P  | O2                  | -0.894602 | C9   | C                   | 0.625360  |
| O6P  | OH                  | -0.864985 | O8   | O                   | -0.746931 |
| P4   | P                   | 1.175610  | C10  | CT                  | -0.285080 |
| O7P  | O2                  | -0.857709 | H16  | HC                  | 0.100215  |
| O8P  | O2                  | -0.832649 | H17  | HC                  | 0.048357  |
| O9P  | O2                  | -0.752714 | H18  | HC                  | 0.044340  |
| P5   | P                   | 1.102779  |      |                     |           |
| OPF  | O2                  | -0.775802 |      |                     |           |
| OPG  | O2                  | -0.688660 |      |                     |           |
| OPH  | OS                  | -0.501167 |      |                     |           |

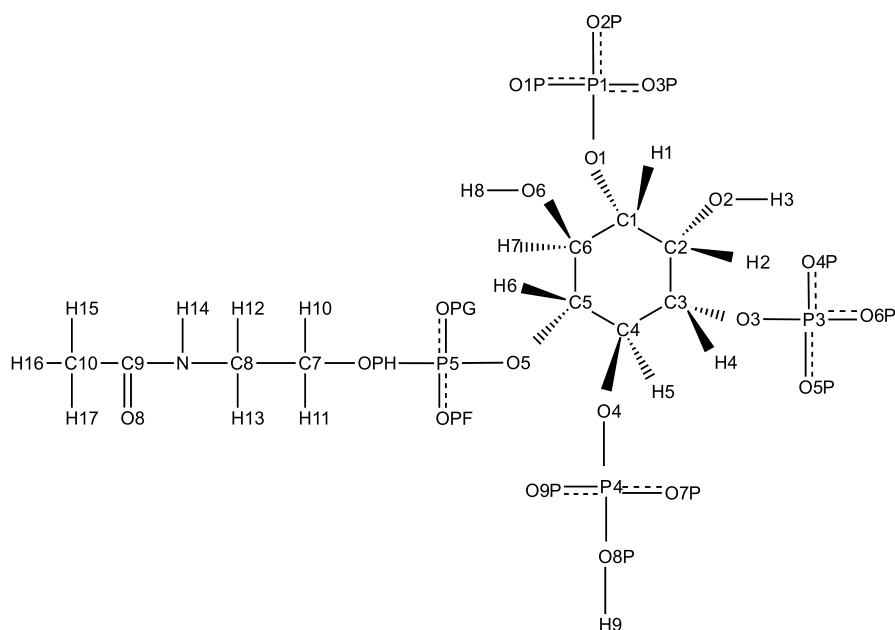


**Figure S36:** The atomic labelling scheme for the -6 isomer 13O4H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S44:** Atom names, atom types and charge parameters for the -6 isomer 13O4H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.094438  | H1   | HC                  | 0.070293  |
| O1   | OS                  | -0.467569 | H2   | HC                  | 0.127457  |
| C2   | CT                  | 0.015050  | H3   | HO                  | 0.488279  |
| O2   | OH                  | -0.729936 | H4   | HC                  | 0.046044  |
| C3   | CT                  | 0.072160  | H5   | HC                  | 0.104286  |
| O3   | OS                  | -0.446190 | H6   | HC                  | 0.128882  |
| C4   | CT                  | 0.118563  | H7   | HC                  | 0.082320  |
| O4   | OS                  | -0.436311 | H8   | HO                  | 0.459374  |
| C5   | CT                  | 0.023529  | H9   | HY                  | 0.340527  |
| O5   | OS                  | -0.255380 | C7   | CT                  | 0.059356  |
| C6   | CT                  | 0.233484  | H10  | HC                  | 0.179852  |
| O6   | OH                  | -0.715408 | H11  | HC                  | 0.032257  |
| P1   | P                   | 1.204054  | C8   | CT                  | -0.022674 |
| O1P  | O2                  | -0.915986 | H12  | H1                  | 0.021781  |
| O2P  | O2                  | -0.937539 | H13  | H1                  | 0.006687  |
| O3P  | O2                  | -0.914563 | N    | N                   | -0.254653 |
| P3   | P                   | 1.172499  | H14  | H                   | 0.222603  |
| O4P  | O2                  | -0.899190 | C9   | C                   | 0.595798  |
| O5P  | O2                  | -0.912917 | O8   | O                   | -0.775148 |
| O6P  | O2                  | -0.928830 | C10  | CT                  | -0.194139 |
| P4   | P                   | 1.152756  | H15  | HC                  | 0.055050  |
| O7P  | O2                  | -0.860207 | H16  | HC                  | 0.012499  |
| O8P  | OH                  | -0.675169 | H17  | HC                  | 0.016968  |
| O9P  | O2                  | -0.839987 |      |                     |           |
| P5   | P                   | 0.778044  |      |                     |           |
| OPF  | O2                  | -0.720186 |      |                     |           |
| OPG  | O2                  | -0.627470 |      |                     |           |
| OPH  | OS                  | -0.385438 |      |                     |           |

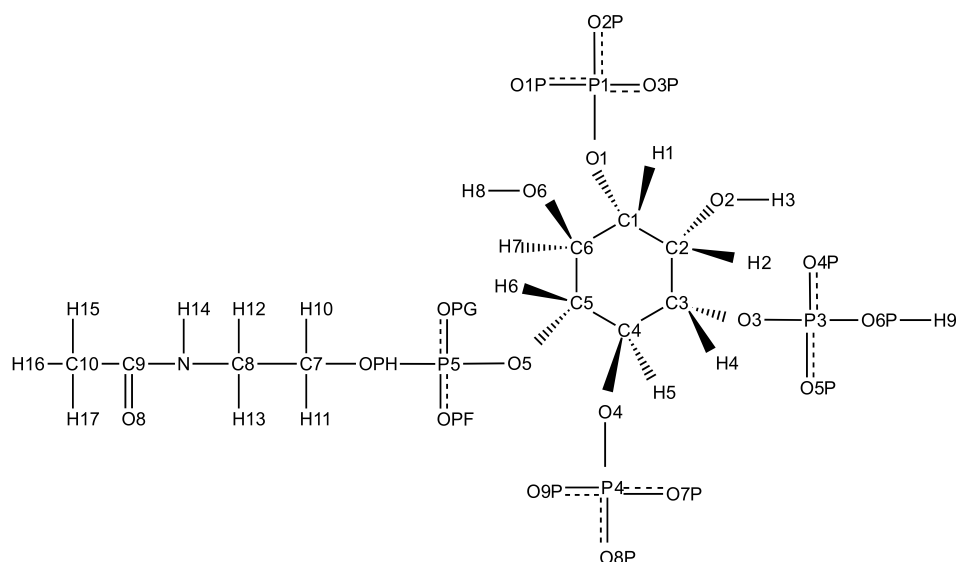


**Figure S37:** The atomic labelling scheme for the -6 isomer 14O3H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S45:** Atom names, atom types and charge parameters for the -6 isomer 14O3H of *D-myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.044513  | H1   | HC                  | 0.091341  |
| O1   | OS                  | -0.435882 | H2   | HC                  | 0.123628  |
| C2   | CT                  | 0.008998  | H3   | HO                  | 0.398426  |
| O2   | OH                  | -0.652623 | H4   | HC                  | 0.114284  |
| C3   | CT                  | 0.026510  | H5   | HC                  | 0.161784  |
| O3   | OS                  | -0.428096 | H6   | HC                  | 0.154657  |
| C4   | CT                  | 0.005260  | H7   | HC                  | 0.083036  |
| O4   | OS                  | -0.389959 | H8   | HO                  | 0.441542  |
| C5   | CT                  | -0.007253 | H9   | HY                  | 0.522444  |
| O5   | OS                  | -0.356207 | C7   | CT                  | 0.056072  |
| C6   | CT                  | 0.116161  | H10  | HC                  | 0.100734  |
| O6   | OH                  | -0.629171 | H11  | HC                  | 0.145166  |
| P1   | P                   | 1.222445  | C8   | CT                  | -0.052313 |
| O1P  | O2                  | -0.917903 | H12  | H1                  | 0.037208  |
| O2P  | O2                  | -0.947482 | H13  | H1                  | 0.013622  |
| O3P  | O2                  | -0.917493 | N    | N                   | -0.300694 |
| P3   | P                   | 1.265318  | H14  | H                   | 0.207876  |
| O4P  | O2                  | -0.910789 | C9   | C                   | 0.637203  |
| O5P  | O2                  | -0.937877 | O8   | O                   | -0.787761 |
| O6P  | OH                  | -0.935005 | C10  | CT                  | -0.232274 |
| P4   | P                   | 1.129413  | H15  | HC                  | 0.090656  |
| O7P  | O2                  | -0.857704 | H16  | HC                  | 0.014315  |
| O8P  | O2                  | -0.835549 | H17  | HC                  | 0.010621  |
| O9P  | O2                  | -0.773771 |      |                     |           |
| P5   | P                   | 0.994678  |      |                     |           |
| OPF  | O2                  | -0.737567 |      |                     |           |
| OPG  | O2                  | -0.722226 |      |                     |           |
| OPH  | OS                  | -0.452311 |      |                     |           |

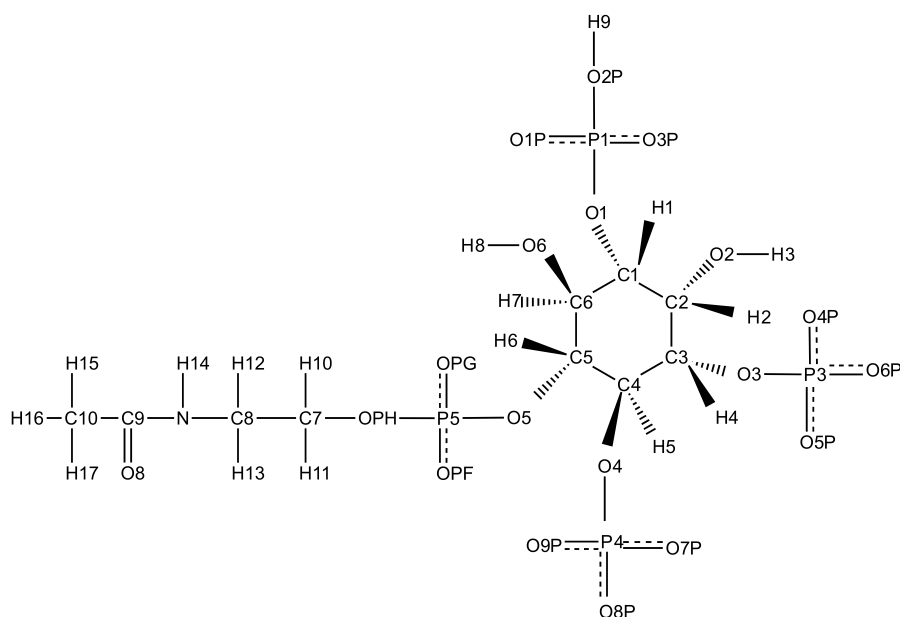


**Figure S38:** The atomic labelling scheme for the -6 isomer 34O1H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S46:** Atom names, atom types and charge parameters for the -6 isomer 34O1H of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.065532  | H1   | HC                  | 0.060126  |
| O1   | OS                  | -0.447718 | H2   | HC                  | 0.122240  |
| C2   | CT                  | -0.013316 | H3   | HO                  | 0.413220  |
| O2   | OH                  | -0.670278 | H4   | HC                  | 0.041439  |
| C3   | CT                  | 0.079300  | H5   | HC                  | 0.131360  |
| O3   | OS                  | -0.367872 | H6   | HC                  | 0.083820  |
| C4   | CT                  | 0.187370  | H7   | HC                  | 0.058159  |
| O4   | OS                  | -0.531830 | H8   | HO                  | 0.364149  |
| C5   | CT                  | 0.157472  | H9   | HY                  | 0.479449  |
| O5   | OS                  | -0.372970 | C7   | CT                  | 0.084215  |
| C6   | CT                  | 0.066182  | H10  | HC                  | 0.227024  |
| O6   | OH                  | -0.609024 | H11  | HC                  | 0.050521  |
| P1   | P                   | 1.204666  | C8   | CT                  | -0.032682 |
| O1P  | O2                  | -0.898545 | H12  | H1                  | 0.006666  |
| O2P  | OH                  | -0.894050 | H13  | H1                  | 0.034428  |
| O3P  | O2                  | -0.939501 | N    | N                   | -0.249163 |
| P3   | P                   | 1.205582  | H14  | H                   | 0.193325  |
| O4P  | O2                  | -0.852482 | C9   | C                   | 0.644522  |
| O5P  | O2                  | -0.757063 | O8   | O                   | -0.795145 |
| O6P  | O2                  | -0.864173 | C10  | CT                  | -0.230891 |
| P4   | P                   | 1.161790  | H15  | HC                  | 0.090220  |
| O7P  | O2                  | -0.911034 | H16  | HC                  | 0.009003  |
| O8P  | O2                  | -0.887420 | H17  | HC                  | 0.007004  |
| O9P  | O2                  | -0.896225 |      |                     |           |
| P5   | P                   | 1.048054  |      |                     |           |
| OPF  | O2                  | -0.775773 |      |                     |           |
| OPG  | O2                  | -0.755716 |      |                     |           |
| OPH  | OS                  | -0.523966 |      |                     |           |

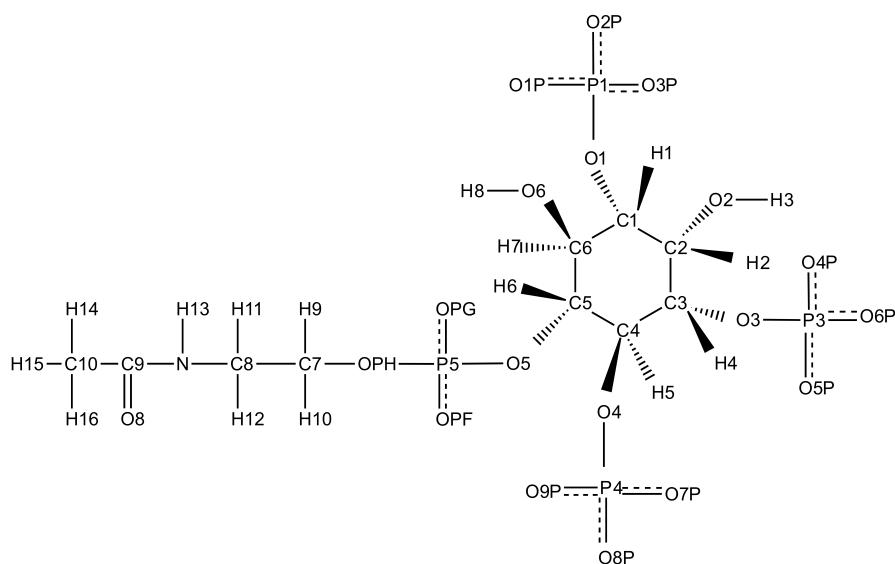


**Figure S39:** The atomic labelling scheme for the -7 isomer 134O of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

**Table S47:** Atom names, atom types and charge parameters for the -7 isomer 134O of D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.030231  | H1   | HC                  | 0.109232  |
| O1   | OS                  | -0.432715 | H2   | HC                  | 0.109309  |
| C2   | CT                  | -0.051885 | H3   | HO                  | 0.504629  |
| O2   | OH                  | -0.722223 | H4   | HC                  | 0.084038  |
| C3   | CT                  | 0.080283  | H5   | HC                  | 0.007547  |
| O3   | OS                  | -0.498246 | H6   | HC                  | 0.162547  |
| C4   | CT                  | 0.506590  | H7   | HC                  | 0.141111  |
| O4   | OS                  | -0.631836 | H8   | HO                  | 0.550524  |
| C5   | CT                  | 0.099001  | C7   | CT                  | 0.150367  |
| O5   | OS                  | -0.458174 | H9   | HC                  | 0.039127  |
| C6   | CT                  | 0.055292  | H10  | HC                  | 0.107466  |
| O6   | OH                  | -0.813058 | C8   | CT                  | 0.046183  |
| P1   | P                   | 1.234767  | H11  | H1                  | 0.063796  |
| O1P  | O2                  | -0.961956 | H12  | H1                  | 0.042443  |
| O2P  | O2                  | -0.929469 | N    | N                   | -0.586785 |
| O3P  | O2                  | -0.975276 | H13  | H                   | 0.316097  |
| P3   | P                   | 1.215912  | C9   | C                   | 0.778789  |
| O4P  | O2                  | -0.920708 | O8   | O                   | -0.721235 |
| O5P  | O2                  | -0.955618 | C10  | CT                  | -0.402040 |
| O6P  | O2                  | -0.961194 | H14  | HC                  | 0.120604  |
| P4   | P                   | 1.250337  | H15  | HC                  | 0.080098  |
| O7P  | O2                  | -0.973372 | H16  | HC                  | 0.065052  |
| O8P  | O2                  | -0.988033 |      |                     |           |
| O9P  | O2                  | -0.930272 |      |                     |           |
| P5   | P                   | 1.181432  |      |                     |           |
| OPF  | O2                  | -0.865692 |      |                     |           |
| OPG  | O2                  | -0.797259 |      |                     |           |
| OPH  | OS                  | -0.555759 |      |                     |           |

## S. 8 Parameters for D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

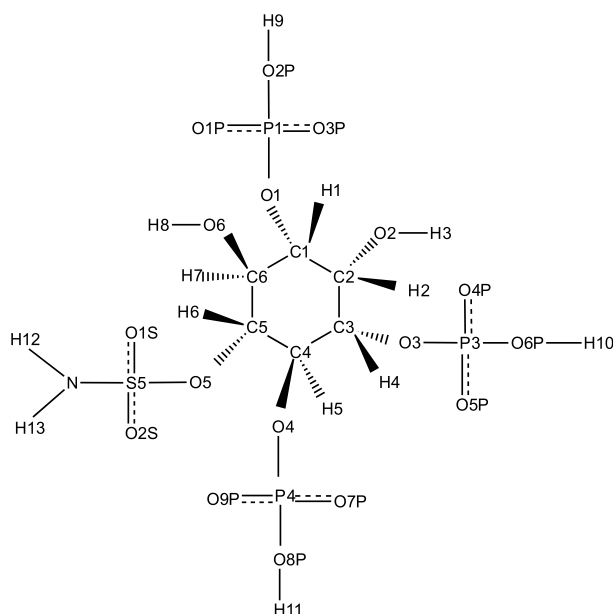


Figure S40: The atomic labelling scheme for the -3 isomer 134H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

Table S48: Atom names, atom types and charge parameters for the -3 isomer, 134H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.030628  | P4   | P                   | 1.176279  |
| O1   | OS                  | -0.360734 | O7P  | O2                  | -0.779530 |
| C2   | CT                  | 0.056471  | O8P  | OH                  | -0.744155 |
| O2   | OH                  | -0.655490 | O9P  | O2                  | -0.759856 |
| C3   | CT                  | -0.037089 | S5   | SO                  | 1.148687  |
| O3   | OS                  | -0.407865 | O1S  | O2                  | -0.579583 |
| C4   | CT                  | 0.030128  | O2S  | O2                  | -0.534360 |
| O4   | OS                  | -0.420120 | N    | NT                  | -0.942067 |
| C5   | CT                  | 0.003944  | H1   | HC                  | 0.150110  |
| O5   | OS                  | -0.343401 | H2   | HC                  | 0.150534  |
| C6   | CT                  | 0.039693  | H3   | HO                  | 0.444385  |
| O6   | OH                  | -0.581515 | H4   | HC                  | 0.135960  |
| P1   | P                   | 1.200650  | H5   | HC                  | 0.176739  |
| O1P  | O2                  | -0.831093 | H6   | HC                  | 0.184579  |
| O2P  | OH                  | -0.707733 | H7   | HC                  | 0.146811  |
| O3P  | O2                  | -0.820175 | H8   | HO                  | 0.398333  |
| P3   | P                   | 1.243437  | H9   | HY                  | 0.414323  |
| O4P  | O2                  | -0.828432 | H10  | HY                  | 0.458443  |
| O5P  | O2                  | -0.841890 | H11  | HY                  | 0.440085  |
| O6P  | OH                  | -0.745491 | H12  | H2                  | 0.428823  |
|      |                     |           | H13  | H2                  | 0.461537  |



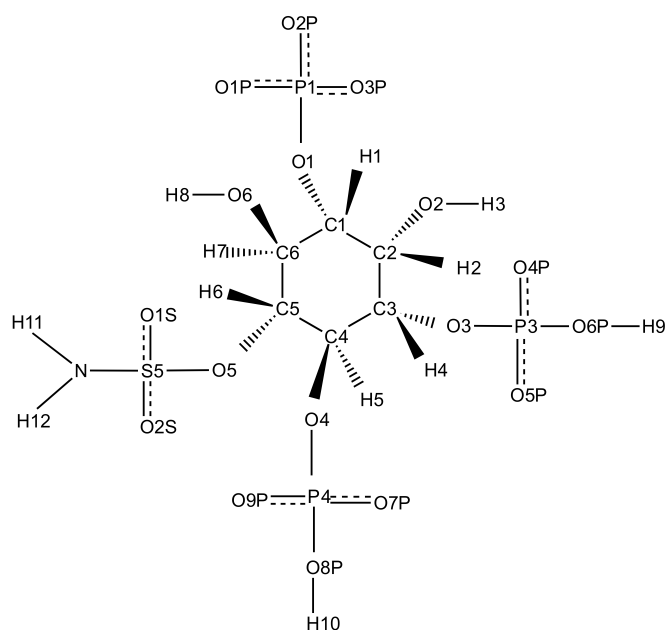


**Figure S41: The atomic labelling scheme for the -4 isomer 1O34H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>**

**Table S49: Atom names, atom types and charge parameters for the -4 isomer, 1O34H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.009136  | P4   | P                   | 1.150856  |
| O1   | OS                  | -0.479398 | O7P  | O2                  | -0.783800 |
| C2   | CT                  | 0.043868  | O8P  | OH                  | -0.765076 |
| O2   | OH                  | -0.676912 | O9P  | O2                  | -0.761929 |
| C3   | CT                  | -0.019781 | S5   | SO                  | 1.116883  |
| O3   | OS                  | -0.348615 | O1S  | O2                  | -0.582064 |
| C4   | CT                  | 0.008172  | O2S  | O2                  | -0.531009 |
| O4   | OS                  | -0.401720 | N    | NT                  | -0.953136 |
| C5   | CT                  | -0.027907 | H1   | HC                  | 0.149632  |
| O5   | OS                  | -0.336785 | H2   | HC                  | 0.190701  |
| C6   | CT                  | 0.126966  | H3   | HO                  | 0.442057  |
| O6   | OH                  | -0.581714 | H4   | HC                  | 0.127439  |
| P1   | P                   | 1.264874  | H5   | HC                  | 0.199269  |
| O1P  | O2                  | -0.925508 | H6   | HC                  | 0.185249  |
| O2P  | O2                  | -0.927797 | H7   | HC                  | 0.094918  |
| O3P  | O2                  | -0.955120 | H8   | HO                  | 0.380636  |
| P3   | P                   | 1.265178  | H9   | HY                  | 0.451563  |
| O4P  | O2                  | -0.840058 | H10  | HY                  | 0.443211  |
| O5P  | O2                  | -0.874913 | H11  | H2                  | 0.422098  |
| O6P  | OH                  | -0.769655 | H12  | H2                  | 0.470191  |

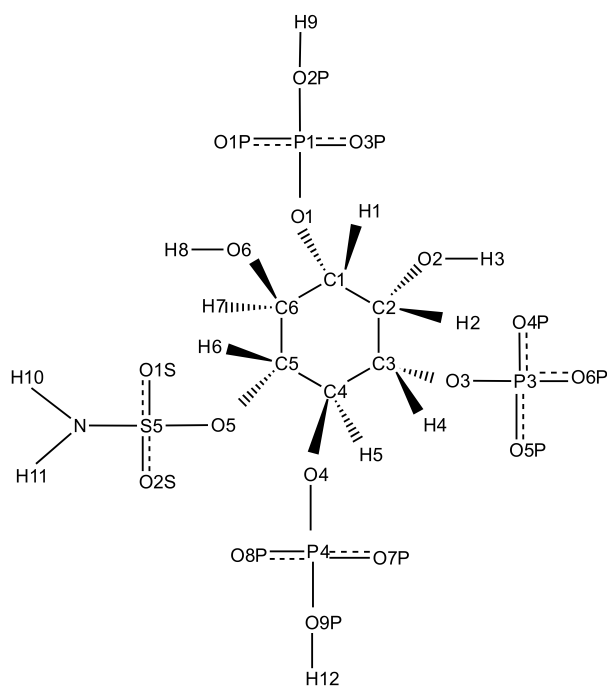


**Figure S42:** The atomic labelling scheme for the -4 isomer 3O14H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

**Table S50:** Atom names, atom types and charge parameters for the -4 isomer, 3O14H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.003120  | P4   | P                   | 1.223956  |
| O1   | OS                  | -0.377615 | O7P  | O2                  | -0.865942 |
| C2   | CT                  | 0.081531  | O8P  | O2                  | -0.827328 |
| O2   | OH                  | -0.651731 | O9P  | OH                  | -0.741212 |
| C3   | CT                  | -0.014075 | S5   | SO                  | 1.139562  |
| O3   | OS                  | -0.409759 | O1S  | O2                  | -0.581966 |
| C4   | CT                  | -0.005844 | O2S  | O2                  | -0.616313 |
| O4   | OS                  | -0.422015 | N    | NT                  | -0.986434 |
| C5   | CT                  | 0.027019  | H1   | HC                  | 0.129830  |
| O5   | OS                  | -0.249723 | H2   | HC                  | 0.132416  |
| C6   | CT                  | 0.023379  | H3   | HO                  | 0.424165  |
| O6   | OH                  | -0.640846 | H4   | HC                  | 0.132638  |
| P1   | P                   | 1.162464  | H5   | HC                  | 0.170945  |
| O1P  | O2                  | -0.836389 | H6   | HC                  | 0.197618  |
| O2P  | OH                  | -0.693723 | H7   | HC                  | 0.135937  |
| O3P  | O2                  | -0.820150 | H8   | HO                  | 0.433843  |
| P3   | P                   | 1.275051  | H9   | HY                  | 0.423720  |
| O4P  | O2                  | -0.893659 | H10  | H2                  | 0.480593  |
| O5P  | O2                  | -0.931917 | H11  | H2                  | 0.423324  |
| O6P  | O2                  | -0.932723 | H12  | HY                  | 0.478252  |

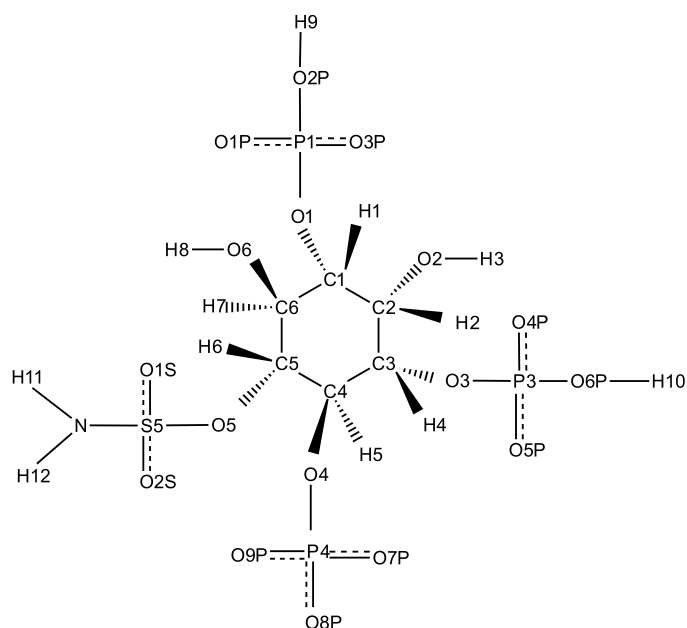


**Figure S43:** The atomic labelling scheme for the -4 isomer 4O13H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

**Table S51:** Atom names, atom types and charge parameters for the -4 isomer, 4O13H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.066132  | P4   | P                   | 1.265200  |
| O1   | OS                  | -0.377789 | O7P  | O2                  | -0.894771 |
| C2   | CT                  | 0.118334  | O8P  | O2                  | -0.902629 |
| O2   | OH                  | -0.704394 | O9P  | O2                  | -0.911491 |
| C3   | CT                  | -0.005080 | S5   | SO                  | 1.044092  |
| O3   | OS                  | -0.456884 | O1S  | O2                  | -0.604154 |
| C4   | CT                  | 0.035338  | O2S  | O2                  | -0.518751 |
| O4   | OS                  | -0.423826 | N    | NT                  | -0.904125 |
| C5   | CT                  | 0.018546  | H1   | HC                  | 0.127528  |
| O5   | OS                  | -0.316778 | H2   | HC                  | 0.096178  |
| C6   | CT                  | 0.079391  | H3   | HO                  | 0.491931  |
| O6   | OH                  | -0.612378 | H4   | HC                  | 0.073643  |
| P1   | P                   | 1.193343  | H5   | HC                  | 0.177372  |
| O1P  | O2                  | -0.843990 | H6   | HC                  | 0.156197  |
| O2P  | OH                  | -0.707755 | H7   | HC                  | 0.120149  |
| O3P  | O2                  | -0.831679 | H8   | HO                  | 0.394453  |
| P3   | P                   | 1.268175  | H9   | HY                  | 0.397997  |
| O4P  | O2                  | -0.873729 | H10  | HY                  | 0.501134  |
| O5P  | O2                  | -0.860880 | H11  | H2                  | 0.386470  |
| O6P  | OH                  | -0.750993 | H12  | H2                  | 0.490471  |

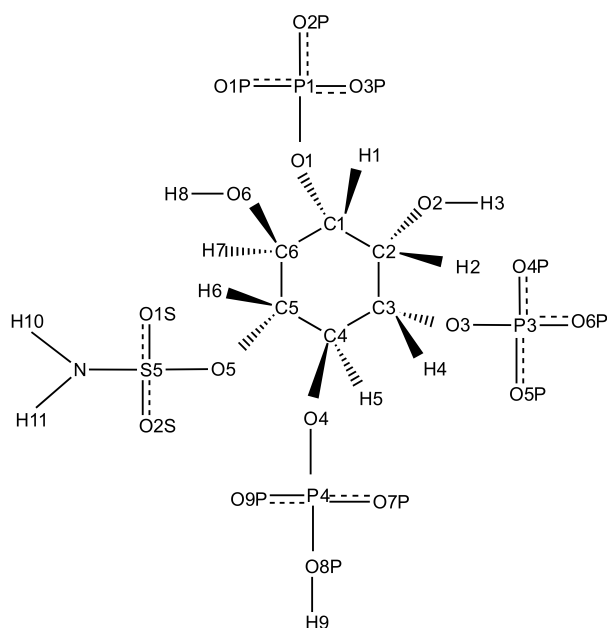


**Figure S44:** The atomic labelling scheme for the -5 isomer 13O4H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

**Table S52:** Atom names, atom types and charge parameters for the -5 isomer, 13O4H of D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.019967  | P4   | P                   | 1.237181  |
| O1   | OS                  | -0.449958 | O7P  | O2                  | -0.840342 |
| C2   | CT                  | 0.093228  | O8P  | OH                  | -0.836979 |
| O2   | OH                  | -0.678304 | O9P  | O2                  | -0.760091 |
| C3   | CT                  | -0.012378 | S5   | SO                  | 1.024973  |
| O3   | OS                  | -0.425911 | O1S  | O2                  | -0.578943 |
| C4   | CT                  | 0.053435  | O2S  | O2                  | -0.566557 |
| O4   | OS                  | -0.419530 | N    | NT                  | -0.928942 |
| C5   | CT                  | -0.006658 | H1   | HC                  | 0.127366  |
| O5   | OS                  | -0.265774 | H2   | HC                  | 0.183125  |
| C6   | CT                  | 0.229729  | H3   | HO                  | 0.428082  |
| O6   | OH                  | -0.637724 | H4   | HC                  | 0.036139  |
| P1   | P                   | 1.268915  | H5   | HC                  | 0.202844  |
| O1P  | O2                  | -0.968904 | H6   | HC                  | 0.161959  |
| O2P  | O2                  | -0.950496 | H7   | HC                  | 0.065487  |
| O3P  | O2                  | -0.971753 | H8   | HO                  | 0.387455  |
| P3   | P                   | 1.139573  | H9   | HY                  | 0.433252  |
| O4P  | O2                  | -0.931854 | H10  | H2                  | 0.469405  |
| O5P  | O2                  | -0.850537 | H11  | H2                  | 0.394941  |
| O6P  | O2                  | -0.875422 |      |                     |           |

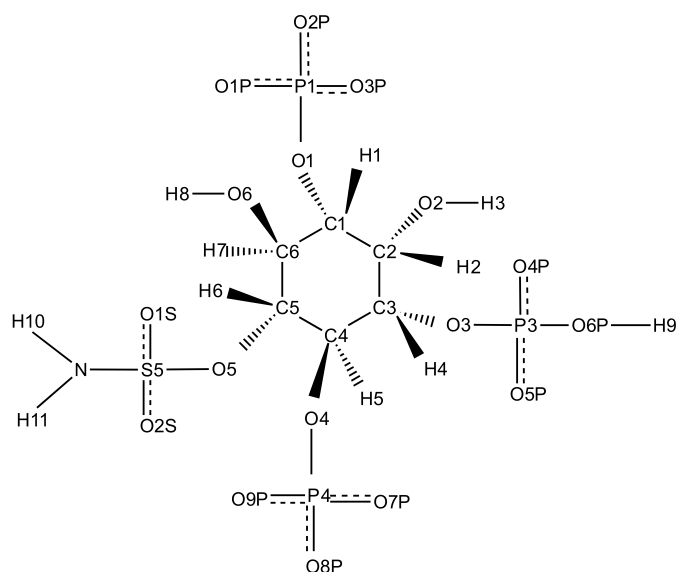


**Figure S45: The atomic labelling scheme for the -5 isomer 14O3H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>**

**Table S53: Atom names, atom types and charge parameters for the -5 isomer, 14O3H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.031643  | P4   | P                   | 1.331860  |
| O1   | OS                  | -0.437257 | O7P  | O2                  | -0.930513 |
| C2   | CT                  | 0.058414  | O8P  | O2                  | -0.986584 |
| O2   | OH                  | -0.704741 | O9P  | O2                  | -0.903894 |
| C3   | CT                  | 0.001268  | S5   | SO                  | 1.174135  |
| O3   | OS                  | -0.448014 | O1S  | O2                  | -0.627106 |
| C4   | CT                  | 0.035964  | O2S  | O2                  | -0.567733 |
| O4   | OS                  | -0.448239 | N    | NT                  | -1.041549 |
| C5   | CT                  | -0.001056 | H1   | HC                  | 0.109700  |
| O5   | OS                  | -0.330258 | H2   | HC                  | 0.119900  |
| C6   | CT                  | 0.110031  | H3   | HO                  | 0.486471  |
| O6   | OH                  | -0.693667 | H4   | HC                  | 0.086014  |
| P1   | P                   | 1.268664  | H5   | HC                  | 0.183533  |
| O1P  | O2                  | -0.935122 | H6   | HC                  | 0.171275  |
| O2P  | O2                  | -0.944319 | H7   | HC                  | 0.113257  |
| O3P  | O2                  | -0.955581 | H8   | HO                  | 0.466190  |
| P3   | P                   | 1.256415  | H9   | HY                  | 0.491692  |
| O4P  | O2                  | -0.886112 | H10  | H2                  | 0.392586  |
| O5P  | O2                  | -0.862065 | H11  | H2                  | 0.581551  |
| O6P  | OH                  | -0.766756 |      |                     |           |

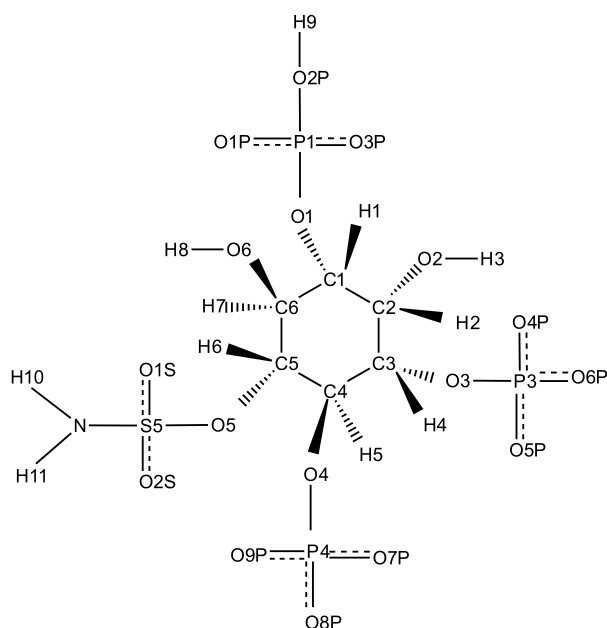


**Figure S46:** The atomic labelling scheme for the -5 isomer 3401H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

**Table S54:** Atom names, atom types and charge parameters for the -5 isomer, 3401H of D-5-O-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.023854  | P4   | P                   | 1.172321  |
| O1   | OS                  | -0.378478 | O7P  | O2                  | -0.849411 |
| C2   | CT                  | 0.021421  | O8P  | O2                  | -0.961462 |
| O2   | OH                  | -0.659660 | O9P  | O2                  | -0.911797 |
| C3   | CT                  | 0.014491  | S5   | SO                  | 1.120521  |
| O3   | OS                  | -0.334974 | O1S  | O2                  | -0.652201 |
| C4   | CT                  | -0.016511 | O2S  | O2                  | -0.602120 |
| O4   | OS                  | -0.370010 | N    | NT                  | -0.982203 |
| C5   | CT                  | -0.002629 | H1   | HC                  | 0.139889  |
| O5   | OS                  | -0.233936 | H2   | HC                  | 0.171145  |
| C6   | CT                  | 0.024935  | H3   | HO                  | 0.399930  |
| O6   | OH                  | -0.629254 | H4   | HC                  | 0.095618  |
| P1   | P                   | 1.187832  | H5   | HC                  | 0.180106  |
| O1P  | O2                  | -0.852053 | H6   | HC                  | 0.192653  |
| O2P  | OH                  | -0.719335 | H7   | HC                  | 0.121859  |
| O3P  | O2                  | -0.851298 | H8   | HO                  | 0.405082  |
| P3   | P                   | 1.244757  | H9   | HY                  | 0.433679  |
| O4P  | O2                  | -0.904205 | H10  | H2                  | 0.525313  |
| O5P  | O2                  | -0.989572 | H11  | H2                  | 0.390342  |
| O6P  | O2                  | -0.964639 |      |                     |           |

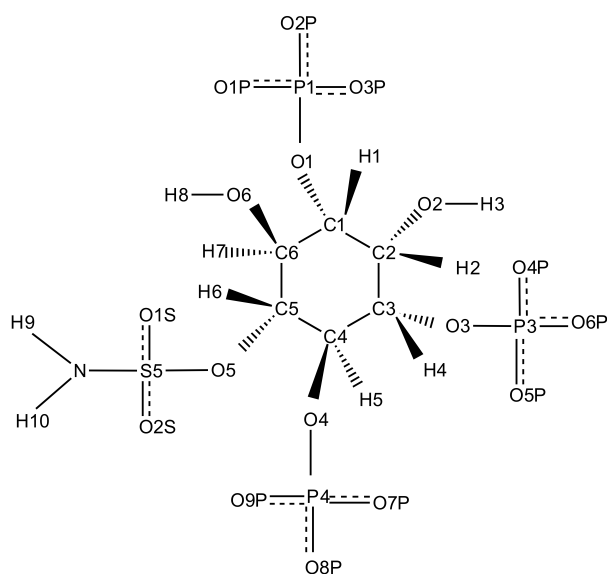


**Figure S47:** The atomic labelling scheme for the -6 isomer 134O of D-5-*O*-Sulfamoyl-*myo*-**Ins(1,3,4)P<sub>3</sub>**

**Table S55:** Atom names, atom types and charge parameters for the -6 isomer, 134O of D-5-*O*-Sulfamoyl-*myo*-**Ins(1,3,4)P<sub>3</sub>**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.043028  | P4   | P                   | 1.166169  |
| O1   | OS                  | -0.426200 | O7P  | O2                  | -0.863370 |
| C2   | CT                  | -0.010294 | O8P  | O2                  | -0.983225 |
| O2   | OH                  | -0.674921 | O9P  | O2                  | -0.918448 |
| C3   | CT                  | 0.011713  | S5   | SO                  | 1.107170  |
| O3   | OS                  | -0.317520 | O1S  | O2                  | -0.653794 |
| C4   | CT                  | -0.035613 | O2S  | O2                  | -0.607271 |
| O4   | OS                  | -0.354131 | N    | NT                  | -1.003685 |
| C5   | CT                  | -0.054078 | H1   | HC                  | 0.116438  |
| O5   | OS                  | -0.216032 | H2   | HC                  | 0.180377  |
| C6   | CT                  | 0.117239  | H3   | HO                  | 0.390298  |
| O6   | OH                  | -0.706932 | H4   | HC                  | 0.101583  |
| P1   | P                   | 1.266500  | H5   | HC                  | 0.177347  |
| O1P  | O2                  | -0.961141 | H6   | HC                  | 0.184117  |
| O2P  | O2                  | -0.940287 | H7   | HC                  | 0.094960  |
| O3P  | O2                  | -0.975262 | H8   | HO                  | 0.476106  |
| P3   | P                   | 1.252981  | H9   | H2                  | 0.551822  |
| O4P  | O2                  | -0.924965 | H10  | H2                  | 0.371112  |
| O5P  | O2                  | -0.993617 |      |                     |           |
| O6P  | O2                  | -0.988172 |      |                     |           |

## S. 9 Parameters for D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

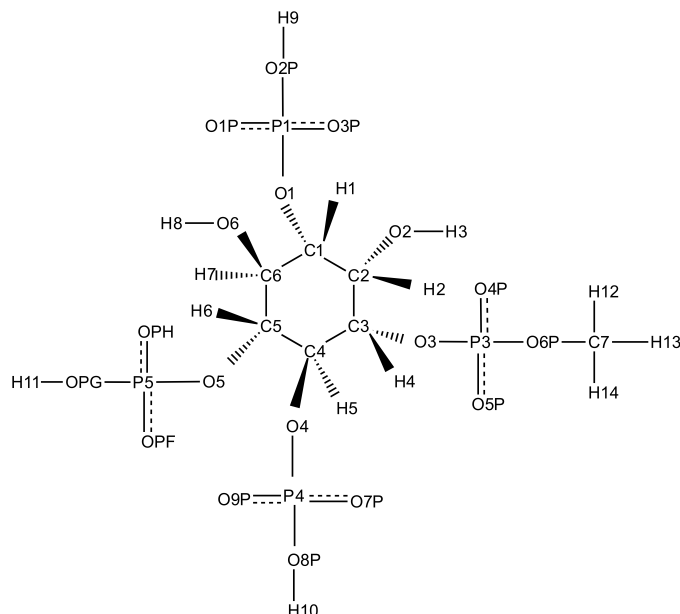


Figure S48: The atomic labelling scheme for the -4 isomer 145H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

Table S56: Atom names, atom types and charge parameters for the -4 isomer 145H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.053610  | P5   | P                   | 1.222911  |
| O1   | OS                  | -0.465343 | OPF  | O2                  | -0.831566 |
| C2   | CT                  | -0.006552 | OPG  | OH                  | -0.721597 |
| O2   | OH                  | -0.600292 | OPH  | O2                  | -0.785007 |
| C3   | CT                  | -0.008867 | H1   | HC                  | 0.105725  |
| O3   | OS                  | -0.234640 | H2   | HC                  | 0.159123  |
| C4   | CT                  | 0.027997  | H3   | HO                  | 0.427893  |
| O4   | OS                  | -0.476266 | H4   | HC                  | 0.096323  |
| C5   | CT                  | 0.056649  | H5   | HC                  | 0.173573  |
| O5   | OS                  | -0.442910 | H6   | HC                  | 0.141274  |
| C6   | CT                  | 0.045299  | H7   | HC                  | 0.129922  |
| O6   | OH                  | -0.589555 | H8   | HO                  | 0.392272  |
| P1   | P                   | 1.249676  | H9   | HY                  | 0.387092  |
| O1P  | O2                  | -0.821619 | H10  | HY                  | 0.447108  |
| O2P  | OH                  | -0.708570 | H11  | HY                  | 0.387382  |
| O3P  | O2                  | -0.842260 | C7   | CT                  | -0.215385 |
| P3   | P                   | 0.978418  | H12  | HC                  | 0.070480  |
| O4P  | O2                  | -0.763068 | H13  | HC                  | 0.181184  |
| O5P  | O2                  | -0.735992 | H14  | HC                  | 0.085762  |
| O6P  | OS                  | -0.410664 |      |                     |           |
| P4   | P                   | 1.223208  |      |                     |           |
| O7P  | O2                  | -0.838525 |      |                     |           |
| O8P  | OH                  | -0.735486 |      |                     |           |
| O9P  | O2                  | -0.808720 |      |                     |           |



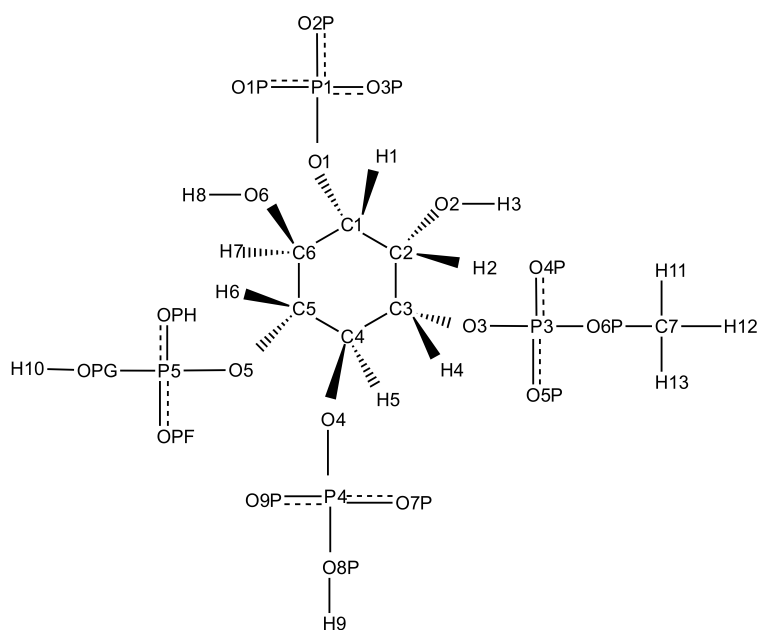


**Figure S49:** The atomic labelling scheme for the -5 isomer 1O45H of *D-myoinositol*(1,4,5)*P*<sub>3</sub>-3-*O*-methylphosphate ester

**Table S57:** Atom names, atom types and charge parameters for the -5 isomer 1O45H of *D-myoinositol*(1,4,5)*P*<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.026744  | P5   | P                   | 1.208953  |
| O1   | OS                  | -0.424438 | OPF  | O2                  | -0.893235 |
| C2   | CT                  | -0.015113 | OPG  | OH                  | -0.855657 |
| O2   | OH                  | -0.607994 | OPH  | O2                  | -0.869677 |
| C3   | CT                  | 0.158780  | H1   | HC                  | 0.112516  |
| O3   | OS                  | -0.395128 | H2   | HC                  | 0.144744  |
| C4   | CT                  | 0.025956  | H3   | HO                  | 0.379425  |
| O4   | OS                  | -0.462119 | H4   | HC                  | 0.091248  |
| C5   | CT                  | 0.007619  | H5   | HC                  | 0.142825  |
| O5   | OS                  | -0.464633 | H6   | HC                  | 0.125844  |
| C6   | CT                  | 0.076710  | H7   | HC                  | 0.092361  |
| O6   | OH                  | -0.494511 | H8   | HO                  | 0.363467  |
| P1   | P                   | 1.215246  | H9   | HY                  | 0.488749  |
| O1P  | O2                  | -0.735114 | H10  | HY                  | 0.352749  |
| O2P  | O2                  | -0.846183 | C7   | CT                  | -0.282264 |
| O3P  | O2                  | -0.871132 | H11  | HC                  | 0.061623  |
| P3   | P                   | 1.084024  | H12  | HC                  | 0.243594  |
| O4P  | O2                  | -0.810088 | H13  | HC                  | 0.090737  |
| O5P  | O2                  | -0.817067 |      |                     |           |
| O6P  | OS                  | -0.398934 |      |                     |           |
| P4   | P                   | 1.295029  |      |                     |           |
| O7P  | O2                  | -0.894465 |      |                     |           |
| O8P  | OH                  | -0.770211 |      |                     |           |
| O9P  | O2                  | -0.880978 |      |                     |           |

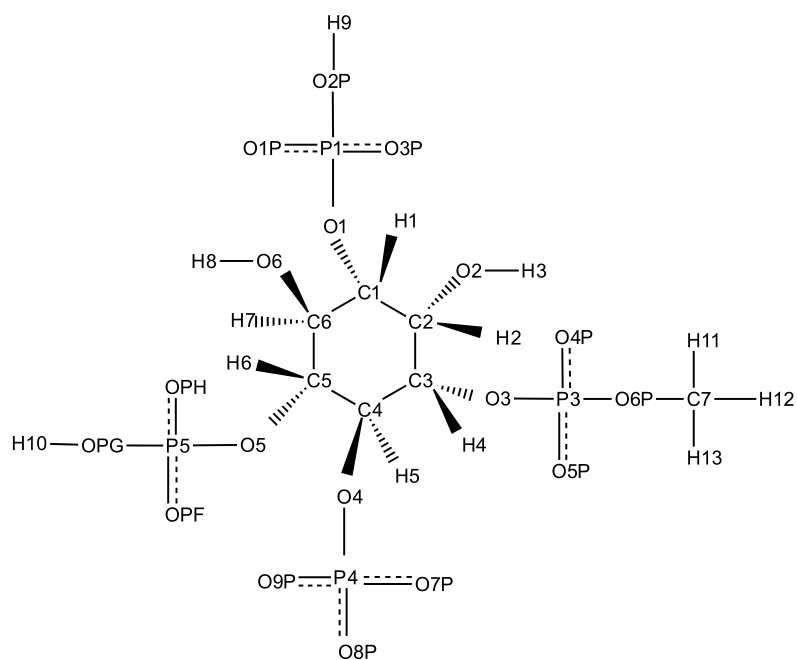


**Figure S50: The atomic labelling scheme for the -5 isomer 4O15H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester**

**Table S58: Atom names, atom types and charge parameters for the -5 isomer 4O15H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.043378  | P5   | P                   | 1.278541  |
| O1   | OS                  | -0.447020 | OPF  | O2                  | -0.873494 |
| C2   | CT                  | 0.035850  | OPG  | OH                  | -0.735630 |
| O2   | OH                  | -0.536055 | OPH  | O2                  | -0.830900 |
| C3   | CT                  | -0.009633 | H1   | HC                  | 0.153465  |
| O3   | OS                  | -0.374690 | H2   | HC                  | 0.106229  |
| C4   | CT                  | 0.017199  | H3   | HO                  | 0.447123  |
| O4   | OS                  | -0.490821 | H4   | HC                  | 0.192552  |
| C5   | CT                  | 0.098344  | H5   | HC                  | 0.149886  |
| O5   | OS                  | -0.497535 | H6   | HC                  | 0.171096  |
| C6   | CT                  | 0.081575  | H7   | HC                  | 0.122526  |
| O6   | OH                  | -0.667464 | H8   | HO                  | 0.388899  |
| P1   | P                   | 1.195884  | H9   | HY                  | 0.346181  |
| O1P  | O2                  | -0.825449 | H10  | HY                  | 0.382294  |
| O2P  | OH                  | -0.698524 | C7   | CT                  | -0.202540 |
| O3P  | O2                  | -0.865313 | H11  | HC                  | 0.044209  |
| P3   | P                   | 1.080124  | H12  | HC                  | 0.216485  |
| O4P  | O2                  | -0.822650 | H13  | HC                  | 0.082899  |
| O5P  | O2                  | -0.797557 |      |                     |           |
| O6P  | OS                  | -0.430859 |      |                     |           |
| P4   | P                   | 1.191367  |      |                     |           |
| O7P  | O2                  | -0.916535 |      |                     |           |
| O8P  | O2                  | -0.900556 |      |                     |           |
| O9P  | O2                  | -0.902881 |      |                     |           |

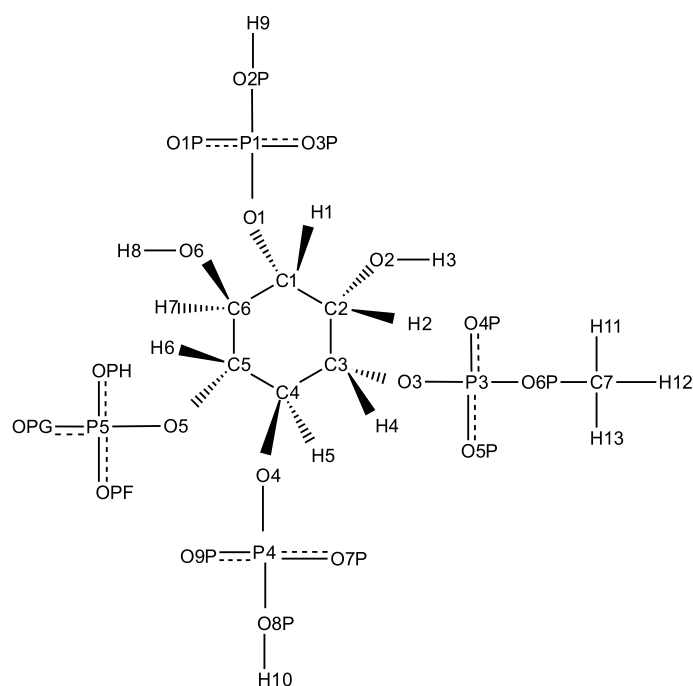


**Figure S51:** The atomic labelling scheme for the -4 isomer 5O14H of *D-myoinositol*(1,4,5)*P*<sub>3</sub>-3-*O*-methylphosphate ester

**Table S59:** Atom names, atom types and charge parameters for the -4 isomer 5O14H of *D-myoinositol*(1,4,5)*P*<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.054438  | P5   | P                   | 1.149559  |
| O1   | OS                  | -0.532735 | OPF  | O2                  | -0.887943 |
| C2   | CT                  | 0.117250  | OPG  | O2                  | -0.895276 |
| O2   | OH                  | -0.667819 | OPH  | O2                  | -0.841206 |
| C3   | CT                  | 0.071654  | H1   | HC                  | 0.070891  |
| O3   | OS                  | -0.418215 | H2   | HC                  | 0.164564  |
| C4   | CT                  | 0.097673  | H3   | HO                  | 0.379737  |
| O4   | OS                  | -0.500911 | H4   | HC                  | 0.088601  |
| C5   | CT                  | 0.093361  | H5   | HC                  | 0.119660  |
| O5   | OS                  | -0.463359 | H6   | HC                  | 0.169858  |
| C6   | CT                  | 0.324648  | H7   | HC                  | 0.054927  |
| O6   | OH                  | -0.796199 | H8   | HO                  | 0.460525  |
| P1   | P                   | 1.237766  | H9   | HY                  | 0.389321  |
| O1P  | O2                  | -0.836225 | H10  | HY                  | 0.447485  |
| O2P  | OH                  | -0.726721 | C7   | CT                  | -0.220143 |
| O3P  | O2                  | -0.828391 | H11  | HC                  | 0.051706  |
| P3   | P                   | 1.109865  | H12  | HC                  | 0.242764  |
| O4P  | O2                  | -0.825222 | H13  | HC                  | 0.088575  |
| O5P  | O2                  | -0.815897 |      |                     |           |
| O6P  | OS                  | -0.454439 |      |                     |           |
| P4   | P                   | 1.162932  |      |                     |           |
| O7P  | O2                  | -0.854155 |      |                     |           |
| O8P  | OH                  | -0.711519 |      |                     |           |
| O9P  | O2                  | -0.871381 |      |                     |           |

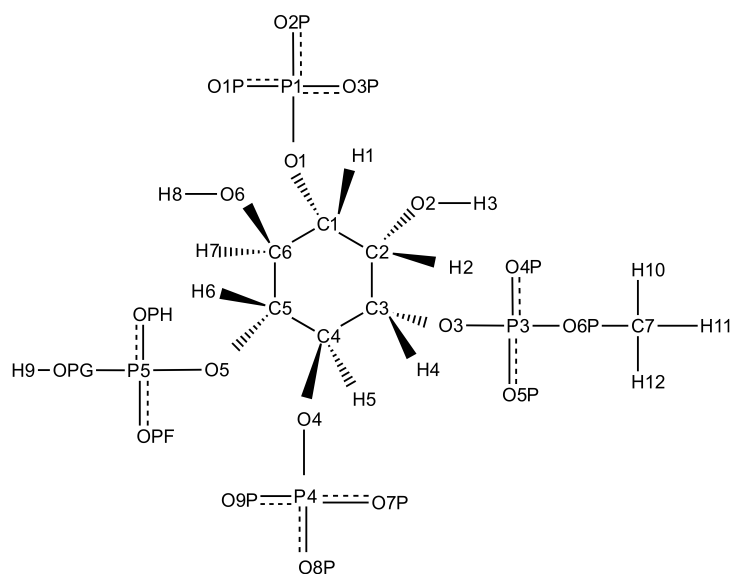


**Figure S52:** The atomic labelling scheme for the -6 isomer 14O5H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

**Table S60:** Atom names, atom types and charge parameters for the -6 isomer 14O5H of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.012460  | P5   | P                   | 1.219624  |
| O1   | OS                  | -0.434581 | OPF  | O2                  | -0.877050 |
| C2   | CT                  | 0.067916  | OPG  | OH                  | -0.766422 |
| O2   | OH                  | -0.663709 | OPH  | O2                  | -0.859577 |
| C3   | CT                  | -0.009834 | H1   | HC                  | 0.095116  |
| O3   | OS                  | -0.447037 | H2   | HC                  | 0.100010  |
| C4   | CT                  | 0.158049  | H3   | HO                  | 0.429071  |
| O4   | OS                  | -0.587715 | H4   | HC                  | 0.180519  |
| C5   | CT                  | 0.555923  | H5   | HC                  | 0.084397  |
| O5   | OS                  | -0.630261 | H6   | HC                  | 0.009489  |
| C6   | CT                  | 0.079892  | H7   | HC                  | 0.083893  |
| O6   | OH                  | -0.776989 | H8   | HO                  | 0.532757  |
| P1   | P                   | 1.219473  | H9   | HY                  | 0.420899  |
| O1P  | O2                  | -0.928534 | C7   | CT                  | -0.196514 |
| O2P  | O2                  | -0.914453 | H10  | HC                  | 0.016629  |
| O3P  | O2                  | -0.946908 | H11  | HC                  | 0.259357  |
| P3   | P                   | 1.062349  | H12  | HC                  | 0.060340  |
| O4P  | O2                  | -0.804104 |      |                     |           |
| O5P  | O2                  | -0.831536 |      |                     |           |
| O6P  | OS                  | -0.424402 |      |                     |           |
| P4   | P                   | 1.232546  |      |                     |           |
| O7P  | O2                  | -0.923773 |      |                     |           |
| O8P  | O2                  | -0.938116 |      |                     |           |
| O9P  | O2                  | -0.919195 |      |                     |           |

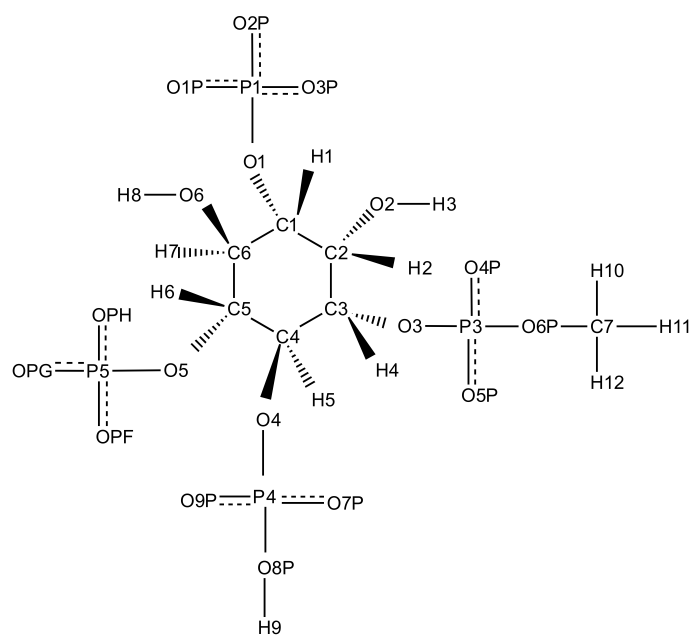


**Figure S53:** The atomic labelling scheme for the -6 isomer 15O4H of *D-my*o-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

**Table S61:** Atom names, atom types and charge parameters for the -6 isomer 15O4H of *D-my*o-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.052736  | P5   | P                   | 1.236467  |
| O1   | OS                  | -0.467875 | OPF  | O2                  | -0.906544 |
| C2   | CT                  | 0.095360  | OPG  | O2                  | -0.882075 |
| O2   | OH                  | -0.668556 | OPH  | O2                  | -0.797120 |
| C3   | CT                  | 0.019341  | H1   | HC                  | 0.083554  |
| O3   | OS                  | -0.429998 | H2   | HC                  | 0.098344  |
| C4   | CT                  | 0.081681  | H3   | HO                  | 0.412300  |
| O4   | OS                  | -0.546797 | H4   | HC                  | 0.121699  |
| C5   | CT                  | 0.249029  | H5   | HC                  | 0.133308  |
| O5   | OS                  | -0.555892 | H6   | HC                  | 0.109830  |
| C6   | CT                  | 0.225791  | H7   | HC                  | 0.059423  |
| O6   | OH                  | -0.769360 | H8   | HO                  | 0.467285  |
| P1   | P                   | 1.189412  | H9   | HY                  | 0.506209  |
| O1P  | O2                  | -0.909968 | C7   | CT                  | -0.198434 |
| O2P  | O2                  | -0.920415 | H10  | HC                  | 0.021078  |
| O3P  | O2                  | -0.944429 | H11  | HC                  | 0.085589  |
| P3   | P                   | 1.134438  | H12  | HC                  | 0.276840  |
| O4P  | O2                  | -0.807159 |      |                     |           |
| O5P  | O2                  | -0.851077 |      |                     |           |
| O6P  | OS                  | -0.492710 |      |                     |           |
| P4   | P                   | 1.253491  |      |                     |           |
| O7P  | O2                  | -0.934419 |      |                     |           |
| O8P  | OH                  | -0.879779 |      |                     |           |
| O9P  | O2                  | -0.950600 |      |                     |           |

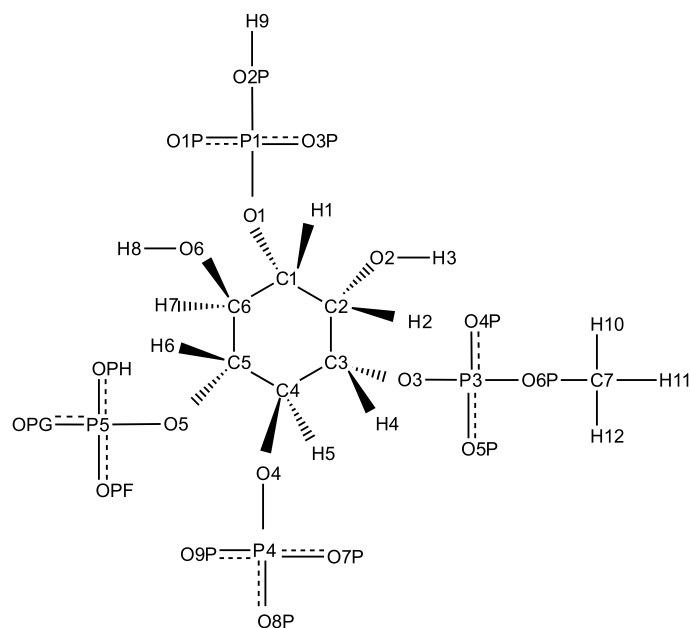


**Figure S54:** The atomic labelling scheme for the -6 isomer 45O1H of *D-my*o-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

**Table S62:** Atom names, atom types and charge parameters for the -6 isomer 45O1H of *D-my*o-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.103494  | P5   | P                   | 1.153759  |
| O1   | OS                  | -0.474352 | OPF  | O2                  | -0.911256 |
| C2   | CT                  | -0.132140 | OPG  | O2                  | -0.910628 |
| O2   | OH                  | -0.555462 | OPH  | O2                  | -0.872749 |
| C3   | CT                  | -0.036935 | H1   | HC                  | 0.140263  |
| O3   | OS                  | -0.358608 | H2   | HC                  | 0.216031  |
| C4   | CT                  | 0.305889  | H3   | HO                  | 0.369766  |
| O4   | OS                  | -0.556010 | H4   | HC                  | 0.138592  |
| C5   | CT                  | 0.045445  | H5   | HC                  | 0.057514  |
| O5   | OS                  | -0.494298 | H6   | HC                  | 0.133636  |
| C6   | CT                  | 0.131837  | H7   | HC                  | 0.107467  |
| O6   | OH                  | -0.688803 | H8   | HO                  | 0.398083  |
| P1   | P                   | 1.287206  | H9   | HY                  | 0.400007  |
| O1P  | O2                  | -0.858002 | C7   | CT                  | 0.052205  |
| O2P  | OH                  | -0.774931 | H10  | HC                  | -0.068746 |
| O3P  | O2                  | -0.888353 | H11  | HC                  | 0.195574  |
| P3   | P                   | 1.062402  | H12  | HC                  | 0.012079  |
| O4P  | O2                  | -0.812084 |      |                     |           |
| O5P  | O2                  | -0.830819 |      |                     |           |
| O6P  | OS                  | -0.505030 |      |                     |           |
| P4   | P                   | 1.203661  |      |                     |           |
| O7P  | O2                  | -0.938243 |      |                     |           |
| O8P  | O2                  | -0.910291 |      |                     |           |
| O9P  | O2                  | -0.937169 |      |                     |           |

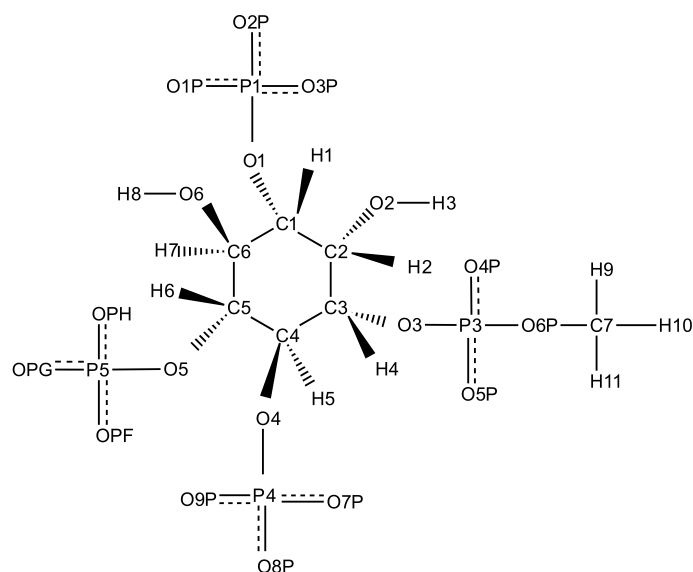


**Figure S55:** The atomic labelling scheme for the -7 isomer 145O of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

**Table S63:** Atom names, atom types and charge parameters for the -7 isomer 145O of D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | -0.030645 | P5   | P                   | 1.211952  |
| O1   | OS                  | -0.496342 | OPF  | O2                  | -0.963205 |
| C2   | CT                  | 0.065398  | OPG  | O2                  | -0.944278 |
| O2   | OH                  | -0.630199 | OPH  | O2                  | -0.931498 |
| C3   | CT                  | -0.073899 | H1   | HC                  | 0.139505  |
| O3   | OS                  | -0.387881 | H2   | HC                  | 0.157673  |
| C4   | CT                  | 0.047293  | H3   | HO                  | 0.368008  |
| O4   | OS                  | -0.455915 | H4   | HC                  | 0.152785  |
| C5   | CT                  | 0.191198  | H5   | HC                  | 0.125395  |
| O5   | OS                  | -0.465485 | H6   | HC                  | 0.146815  |
| C6   | CT                  | 0.082748  | H7   | HC                  | 0.149139  |
| O6   | OH                  | -0.807798 | H8   | HO                  | 0.517343  |
| P1   | P                   | 1.229923  | C7   | CT                  | 0.034226  |
| O1P  | O2                  | -0.941312 | H9   | HC                  | -0.079655 |
| O2P  | O2                  | -0.948550 | H10  | HC                  | 0.108468  |
| O3P  | O2                  | -0.969626 | H11  | HC                  | 0.132867  |
| P3   | P                   | 1.195872  |      |                     |           |
| O4P  | O2                  | -0.875160 |      |                     |           |
| O5P  | O2                  | -0.890116 |      |                     |           |
| O6P  | OS                  | -0.546569 |      |                     |           |
| P4   | P                   | 1.171121  |      |                     |           |
| O7P  | O2                  | -0.946417 |      |                     |           |
| O8P  | O2                  | -0.900047 |      |                     |           |
| O9P  | O2                  | -0.943131 |      |                     |           |

## S. 10 Parameters for D-3-O-Sulfamoyl-myo-Ins(1,4,5)P<sub>3</sub>

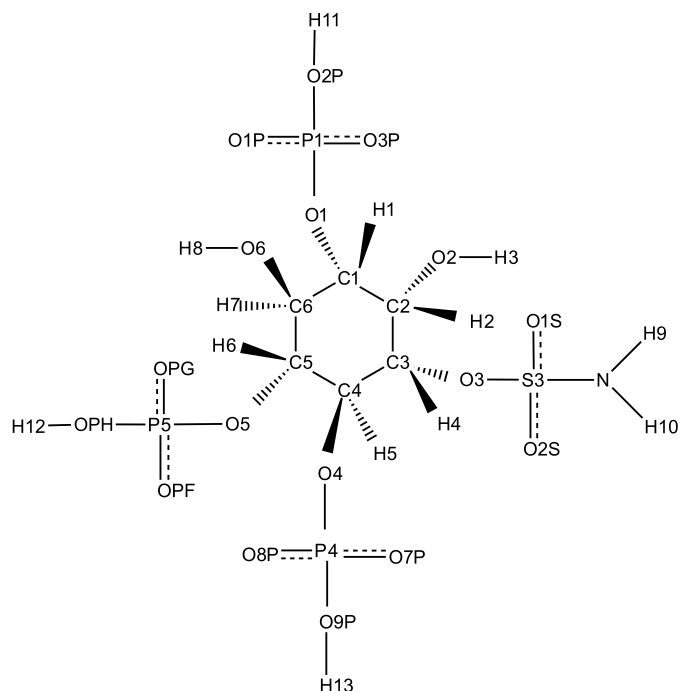


Figure S56: The atomic labelling scheme for the -3 isomer 145H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

Table S64: Atom names, atom types and charge parameters for the -3 isomer, 145H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | -0.001711 | P4   | P                   | 1.258278  |
| O1   | OS                  | -0.439683 | O7P  | O2                  | -0.877519 |
| C2   | CT                  | 0.005562  | O8P  | O2                  | -0.777476 |
| O2   | OH                  | -0.589960 | O9P  | OH                  | -0.686122 |
| C3   | CT                  | -0.069378 | P5   | P                   | 1.247232  |
| O3   | OS                  | -0.199394 | OPF  | O2                  | -0.845230 |
| C4   | CT                  | -0.029111 | OPG  | O2                  | -0.799284 |
| O4   | OS                  | -0.406944 | OPH  | OH                  | -0.744299 |
| C5   | CT                  | -0.011571 | H1   | HC                  | 0.158043  |
| O5   | OS                  | -0.402509 | H2   | HC                  | 0.137015  |
| C6   | CT                  | 0.078307  | H3   | HO                  | 0.408453  |
| O6   | OH                  | -0.585073 | H4   | HC                  | 0.166264  |
| P1   | P                   | 1.190621  | H5   | HC                  | 0.218267  |
| O1P  | O2                  | -0.817402 | H6   | HC                  | 0.191224  |
| O2P  | OH                  | -0.727418 | H7   | HC                  | 0.117781  |
| O3P  | O2                  | -0.760453 | H8   | HO                  | 0.407455  |
| S3   | SO                  | 1.147193  | H9   | H2                  | 0.495088  |
| O1S  | O2                  | -0.593401 | H10  | H2                  | 0.423566  |
| O2S  | O2                  | -0.591191 | H11  | HY                  | 0.430214  |
| N    | NT                  | -0.965247 | H12  | HY                  | 0.415389  |
|      |                     |           | H13  | HY                  | 0.424423  |



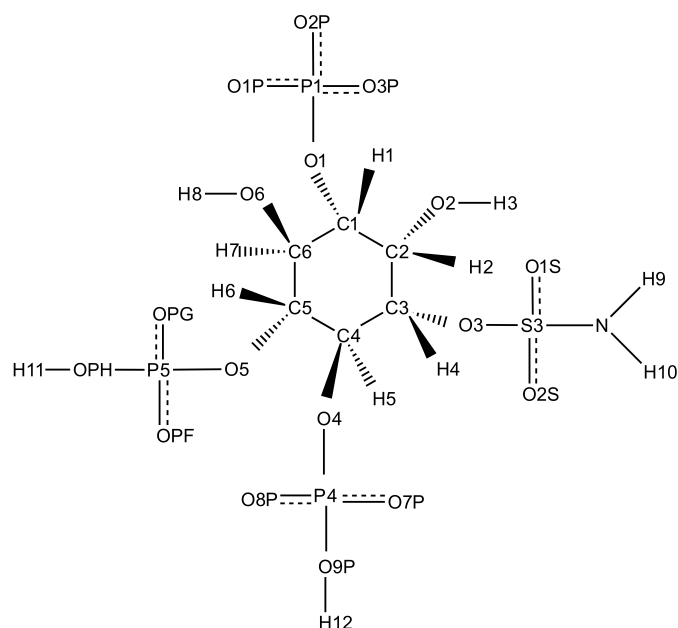


**Figure S57: The atomic labelling scheme for the -4 isomer 1O45H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>**

**Table S65: Atom names, atom types and charge parameters for the -4 isomer, 1O45H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.026261  | P4   | P                   | 1.300155  |
| O1   | OS                  | -0.485561 | O7P  | O2                  | -0.870275 |
| C2   | CT                  | 0.044707  | O8P  | O2                  | -0.826190 |
| O2   | OH                  | -0.649011 | O9P  | OH                  | -0.761770 |
| C3   | CT                  | -0.021741 | P5   | P                   | 1.273538  |
| O3   | OS                  | -0.230295 | OPF  | O2                  | -0.854904 |
| C4   | CT                  | 0.019722  | OPG  | O2                  | -0.823056 |
| O4   | OS                  | -0.468414 | OPH  | OH                  | -0.737232 |
| C5   | CT                  | 0.001556  | H1   | HC                  | 0.122493  |
| O5   | OS                  | -0.428355 | H2   | HC                  | 0.131619  |
| C6   | CT                  | 0.064145  | H3   | HO                  | 0.432909  |
| O6   | OH                  | -0.617400 | H4   | HC                  | 0.150911  |
| P1   | P                   | 1.275080  | H5   | HC                  | 0.207110  |
| O1P  | O2                  | -0.923935 | H6   | HC                  | 0.151930  |
| O2P  | O2                  | -0.901816 | H7   | HC                  | 0.114761  |
| O3P  | O2                  | -0.928312 | H8   | HO                  | 0.443438  |
| S3   | SO                  | 1.154519  | H9   | H2                  | 0.475165  |
| O1S  | O2                  | -0.619013 | H10  | H2                  | 0.407418  |
| O2S  | O2                  | -0.599170 | H11  | HY                  | 0.415547  |
| N    | NT                  | -0.934489 | H12  | HY                  | 0.467953  |

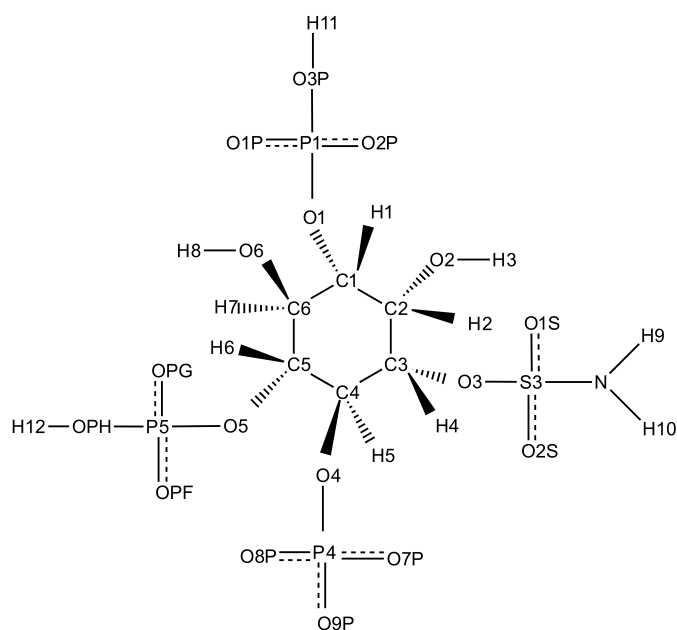


**Figure S58: The atomic labelling scheme for the -4 isomer 4O15H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>**

**Table S66: Atom names, atom types and charge parameters for the -4 isomer, 4O15H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>**

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.007158  | P4   | P                   | 1.241719  |
| O1   | OS                  | -0.419256 | O7P  | O2                  | -0.947068 |
| C2   | CT                  | -0.009987 | O8P  | O2                  | -0.877432 |
| O2   | OH                  | -0.590084 | O9P  | O2                  | -0.893701 |
| C3   | CT                  | -0.051155 | P5   | P                   | 1.264138  |
| O3   | OS                  | -0.187117 | OPF  | O2                  | -0.839174 |
| C4   | CT                  | 0.002390  | OPG  | O2                  | -0.812752 |
| O4   | OS                  | -0.403227 | OPH  | OH                  | -0.777057 |
| C5   | CT                  | 0.008812  | H1   | HC                  | 0.156981  |
| O5   | OS                  | -0.386665 | H2   | HC                  | 0.116185  |
| C6   | CT                  | 0.051879  | H3   | HO                  | 0.392895  |
| O6   | OH                  | -0.569721 | H4   | HC                  | 0.148115  |
| P1   | P                   | 1.163364  | H5   | HC                  | 0.195461  |
| O1P  | O2                  | -0.820807 | H6   | HC                  | 0.171654  |
| O2P  | O2                  | -0.763176 | H7   | HC                  | 0.111421  |
| O3P  | OH                  | -0.734099 | H8   | HO                  | 0.392479  |
| S3   | SO                  | 1.148988  | H9   | H2                  | 0.505518  |
| O1S  | O2                  | -0.627987 | H10  | H2                  | 0.398758  |
| O2S  | O2                  | -0.639412 | H11  | HY                  | 0.424527  |
| N    | NT                  | -0.951460 | H12  | HY                  | 0.398894  |

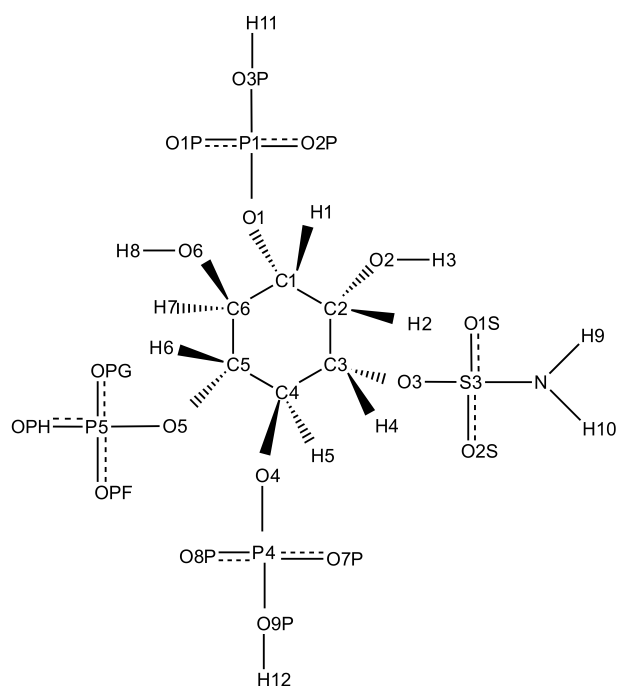


**Figure S59:** The atomic labelling scheme for the -4 isomer 5O14H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

**Table S67:** Atom names, atom types and charge parameters for the -4 isomer, 5O14H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.002866  | P4   | P                   | 1.260785  |
| O1   | OS                  | -0.442636 | O7P  | O2                  | -0.871801 |
| C2   | CT                  | 0.017912  | O8P  | O2                  | -0.841851 |
| O2   | OH                  | -0.604588 | O9P  | OH                  | -0.774576 |
| C3   | CT                  | -0.015625 | P5   | P                   | 1.260098  |
| O3   | OS                  | -0.216029 | OPF  | O2                  | -0.907629 |
| C4   | CT                  | -0.014516 | OPG  | O2                  | -0.911324 |
| O4   | OS                  | -0.420810 | OPH  | O2                  | -0.933577 |
| C5   | CT                  | 0.024944  | H1   | HC                  | 0.150225  |
| O5   | OS                  | -0.438037 | H2   | HC                  | 0.106350  |
| C6   | CT                  | 0.104690  | H3   | HO                  | 0.398632  |
| O6   | OH                  | -0.599975 | H4   | HC                  | 0.141004  |
| P1   | P                   | 1.209273  | H5   | HC                  | 0.200334  |
| O1P  | O2                  | -0.834896 | H6   | HC                  | 0.172571  |
| O2P  | O2                  | -0.774723 | H7   | HC                  | 0.098489  |
| O3P  | OH                  | -0.742476 | H8   | HO                  | 0.410692  |
| S3   | SO                  | 1.154310  | H9   | H2                  | 0.457307  |
| O1S  | O2                  | -0.623458 | H10  | H2                  | 0.397509  |
| O2S  | O2                  | -0.622839 | H11  | HY                  | 0.421802  |
| N    | NT                  | -0.900223 | H12  | HY                  | 0.501794  |

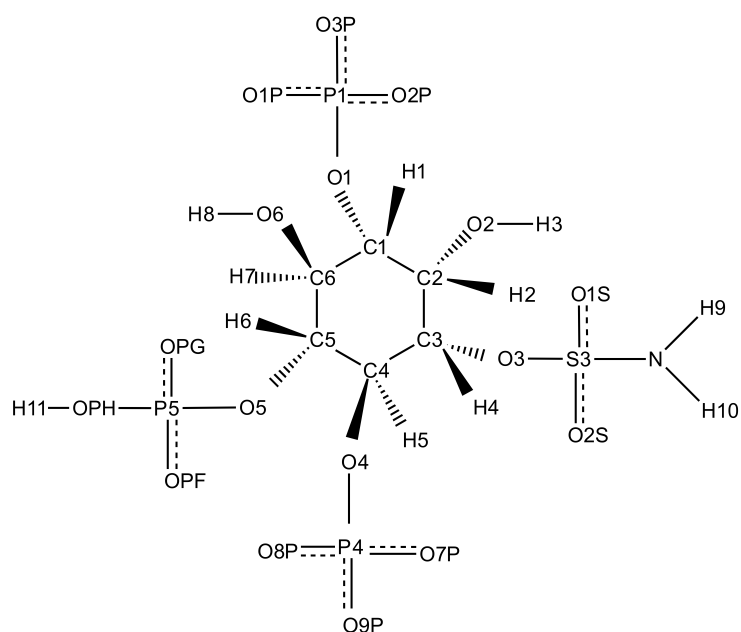


**Figure S60:** The atomic labelling scheme for the -5 isomer 1405H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

**Table S68:** Atom names, atom types and charge parameters for the -5 isomer, 1405H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.056006  | P4   | P                   | 1.238390  |
| O1   | OS                  | -0.484140 | O7P  | O2                  | -0.956338 |
| C2   | CT                  | 0.034374  | O8P  | O2                  | -0.897402 |
| O2   | OH                  | -0.655350 | O9P  | O2                  | -0.890002 |
| C3   | CT                  | -0.041563 | P5   | P                   | 1.266280  |
| O3   | OS                  | -0.185545 | OPF  | O2                  | -0.855936 |
| C4   | CT                  | 0.008086  | OPG  | O2                  | -0.812884 |
| O4   | OS                  | -0.413928 | OPH  | OH                  | -0.789861 |
| C5   | CT                  | 0.030329  | H1   | HC                  | 0.122423  |
| O5   | OS                  | -0.397085 | H2   | HC                  | 0.128487  |
| C6   | CT                  | 0.105674  | H3   | HO                  | 0.414289  |
| O6   | OH                  | -0.637636 | H4   | HC                  | 0.129394  |
| P1   | P                   | 1.255867  | H5   | HC                  | 0.185020  |
| O1P  | O2                  | -0.933392 | H6   | HC                  | 0.149522  |
| O2P  | O2                  | -0.912762 | H7   | HC                  | 0.063767  |
| O3P  | O2                  | -0.950980 | H8   | HO                  | 0.423889  |
| S3   | SO                  | 1.132186  | H9   | H2                  | 0.488726  |
| O1S  | O2                  | -0.637935 | H10  | H2                  | 0.375505  |
| O2S  | O2                  | -0.643532 | H11  | HY                  | 0.404255  |
| N    | NT                  | -0.916198 |      |                     |           |

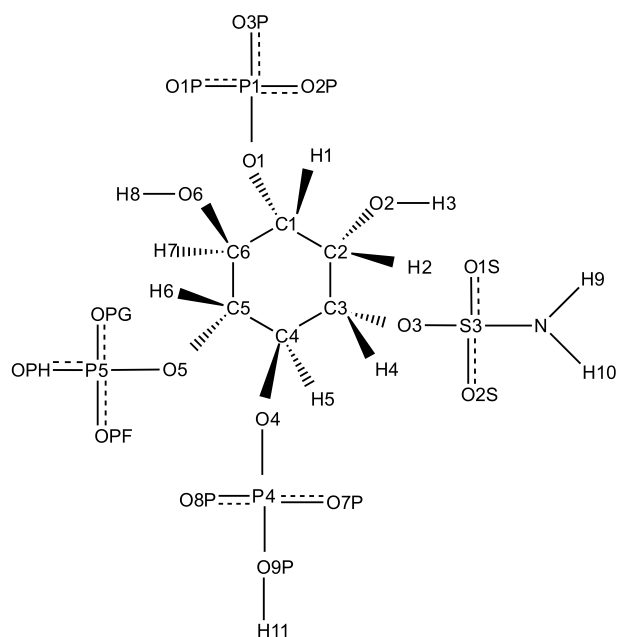


**Figure S61:** The atomic labelling scheme for the -5 isomer 15O4H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

**Table S69:** Atom names, atom types and charge parameters for the -5 isomer, 15O4H of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.022894  | P4   | P                   | 1.264327  |
| O1   | OS                  | -0.480166 | O7P  | O2                  | -0.889201 |
| C2   | CT                  | 0.050635  | O8P  | O2                  | -0.845931 |
| O2   | OH                  | -0.659931 | O9P  | OH                  | -0.798529 |
| C3   | CT                  | -0.016642 | P5   | P                   | 1.261633  |
| O3   | OS                  | -0.209854 | OPF  | O2                  | -0.935162 |
| C4   | CT                  | -0.022136 | OPG  | O2                  | -0.923059 |
| O4   | OS                  | -0.432118 | OPH  | O2                  | -0.944282 |
| C5   | CT                  | 0.025503  | H1   | HC                  | 0.126433  |
| O5   | OS                  | -0.423798 | H2   | HC                  | 0.117843  |
| C6   | CT                  | 0.112250  | H3   | HO                  | 0.419560  |
| O6   | OH                  | -0.619940 | H4   | HC                  | 0.134938  |
| P1   | P                   | 1.248132  | H5   | HC                  | 0.197023  |
| O1P  | O2                  | -0.937692 | H6   | HC                  | 0.165283  |
| O2P  | O2                  | -0.901707 | H7   | HC                  | 0.069031  |
| O3P  | O2                  | -0.950225 | H8   | HO                  | 0.424060  |
| S3   | SO                  | 1.148995  | H9   | H2                  | 0.464460  |
| O1S  | O2                  | -0.619591 | H10  | H2                  | 0.380497  |
| O2S  | O2                  | -0.644554 | H11  | HY                  | 0.518815  |
| N    | NT                  | -0.897797 |      |                     |           |

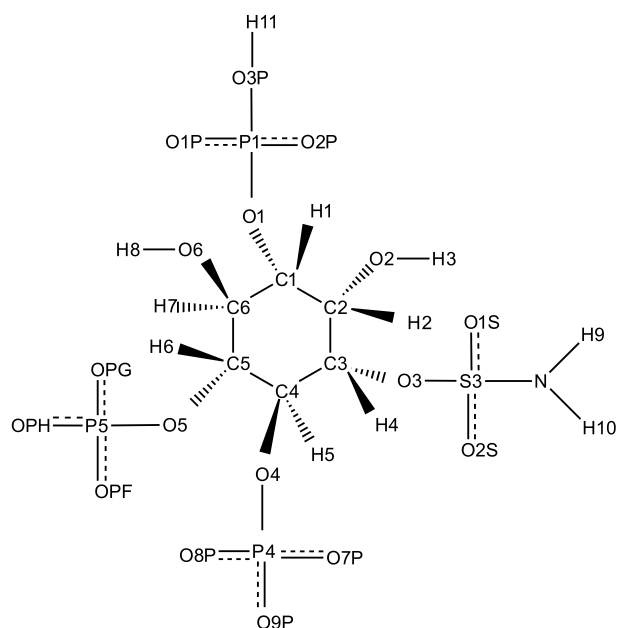


**Figure S62:** The atomic labelling scheme for the -5 isomer 45O1H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

**Table S70:** Atom names, atom types and charge parameters for the -5 isomer, 45O1H of D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | -0.010157 | P4   | P                   | 1.236479  |
| O1   | OS                  | -0.417337 | O7P  | O2                  | -0.969264 |
| C2   | CT                  | 0.030829  | O8P  | O2                  | -0.887547 |
| O2   | OH                  | -0.608578 | O9P  | O2                  | -0.889986 |
| C3   | CT                  | -0.043152 | P5   | P                   | 1.179407  |
| O3   | OS                  | -0.202236 | OPF  | O2                  | -0.889251 |
| C4   | CT                  | 0.007831  | OPG  | O2                  | -0.919162 |
| O4   | OS                  | -0.384966 | OPH  | O2                  | -0.985813 |
| C5   | CT                  | 0.037783  | H1   | HC                  | 0.150216  |
| O5   | OS                  | -0.396616 | H2   | HC                  | 0.094332  |
| C6   | CT                  | 0.103393  | H3   | HO                  | 0.384067  |
| O6   | OH                  | -0.587583 | H4   | HC                  | 0.135469  |
| P1   | P                   | 1.149402  | H5   | HC                  | 0.178192  |
| O1P  | O2                  | -0.829995 | H6   | HC                  | 0.149063  |
| O2P  | O2                  | -0.770527 | H7   | HC                  | 0.085434  |
| O3P  | OH                  | -0.742294 | H8   | HO                  | 0.402548  |
| S3   | SO                  | 1.183109  | H9   | H2                  | 0.502555  |
| O1S  | O2                  | -0.668746 | H10  | H2                  | 0.375414  |
| O2S  | O2                  | -0.660237 | H11  | HY                  | 0.414953  |
| N    | NT                  | -0.937031 |      |                     |           |

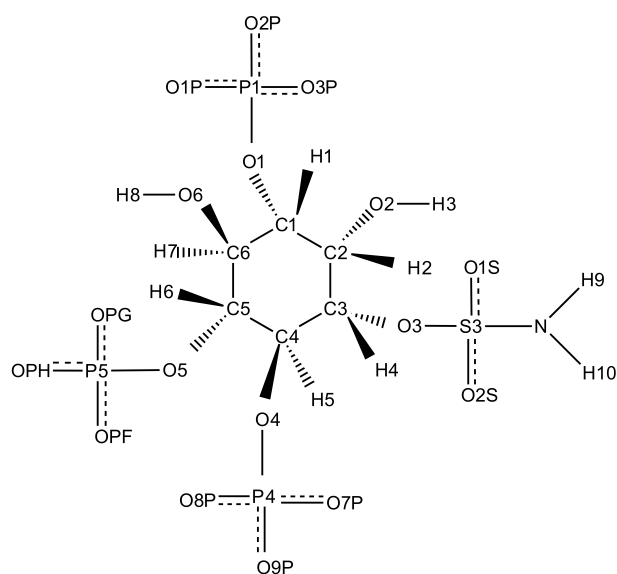


Figure S63: The atomic labelling scheme for the -6 isomer 145O of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

Table S71: Atom names, atom types and charge parameters for the -6 isomer, 145O of D-3-O-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub>

| Atom | ff99SB<br>atom type | Charge    | Atom | ff99SB<br>atom type | Charge    |
|------|---------------------|-----------|------|---------------------|-----------|
| C1   | CT                  | 0.065835  | P4   | P                   | 1.222515  |
| O1   | OS                  | -0.468949 | O7P  | O2                  | -0.984646 |
| C2   | CT                  | 0.027846  | O8P  | O2                  | -0.899895 |
| O2   | OH                  | -0.659359 | O9P  | O2                  | -0.896337 |
| C3   | CT                  | -0.055437 | P5   | P                   | 1.165109  |
| O3   | OS                  | -0.196035 | OPF  | O2                  | -0.913231 |
| C4   | CT                  | 0.017234  | OPG  | O2                  | -0.919943 |
| O4   | OS                  | -0.372103 | OPH  | O2                  | -0.991045 |
| C5   | CT                  | 0.031244  | H1   | HC                  | 0.127264  |
| O5   | OS                  | -0.373760 | H2   | HC                  | 0.115168  |
| C6   | CT                  | 0.060897  | H3   | HO                  | 0.405269  |
| O6   | OH                  | -0.583327 | H4   | HC                  | 0.131218  |
| P1   | P                   | 1.230905  | H5   | HC                  | 0.176727  |
| O1P  | O2                  | -0.945829 | H6   | HC                  | 0.130013  |
| O2P  | O2                  | -0.911143 | H7   | HC                  | 0.062402  |
| O3P  | O2                  | -0.967509 | H8   | HO                  | 0.401320  |
| S3   | SO                  | 1.181562  | H9   | H2                  | 0.502913  |
| O1S  | O2                  | -0.664015 | H10  | H2                  | 0.359542  |
| O2S  | O2                  | -0.679217 |      |                     |           |
| N    | NT                  | -0.933204 |      |                     |           |

## S. 11 Parameters for Sulfamate Group

**Table S72: Parameters for sulfamate groups.** Parameters for the sulfamate groups were largely taken from a study by Huige and Altona.<sup>4</sup> Remaining parameters were taken from the GAFF and ff99SB force fields.

| Mass          | Atomic mass  |         | Atomic polarisability |     |                                          |
|---------------|--------------|---------|-----------------------|-----|------------------------------------------|
| NT            | 14.01        |         | 0.530                 |     | From Morgantini and Kollman <sup>5</sup> |
| SO            | 32.06        |         | 2.900                 |     | From S in ff99SB <sup>6</sup>            |
|               |              |         |                       |     |                                          |
| Bond          | $K_r$        |         | $r_{eq}$              |     |                                          |
| SO-O2         | 525          |         | 1.44                  |     | From Huige and Altona <sup>4</sup>       |
| SO-OS         | 230          |         | 1.62                  |     | From Huige and Altona                    |
| NT-H2         | 410.2        |         | 1.009                 |     | From n-hn in GAFF <sup>3</sup>           |
| SO-NT         | 230          |         | 1.685                 |     | From Huige and Altona                    |
|               |              |         |                       |     |                                          |
| Angle         | $K_\theta$   |         | $\theta_{eq}$         |     |                                          |
| CT-OS-SO      | 100          |         | 120.5                 |     | From Huige and Altona                    |
| OS-SO-O2      | 100          |         | 108.23                |     | From Huige and Altona                    |
| OS-SO-NT      | 44.3         |         | 99.230                |     | From os-s6-n in GAFF                     |
| O2-SO-O2      | 140          |         | 119.9                 |     | From Huige and Altona                    |
| H2-NT-H2      | 39.730       |         | 117.850               |     | From hn-n-hn in GAFF                     |
| H2-NT-SO      | 45           |         | 109.5                 |     | From Huige and Altona                    |
| O2-SO-NT      | 100          |         | 109.6                 |     | From Huige and Altona                    |
|               |              |         |                       |     |                                          |
| Dihedral      | No. of paths | $V_n/2$ | $\gamma$              | $n$ |                                          |
| CT-CT-OS-SO   | 1            | -1.16   | 0.0                   | 1   | From Huige and Altona                    |
|               | 1            | 0.25    | 0.0                   | 2   |                                          |
|               | 1            | -0.15   | 0.0                   | 3   |                                          |
|               | 1            | -0.30   | 0.0                   | 4   |                                          |
| X-OS-SO-X     | 3            | 0.75    | 0.0                   | 3   | From Huige and Altona                    |
| X-NT-SO-X     | 6            | 0.75    | 0.0                   | 3   | From Huige and Altona                    |
|               |              |         |                       |     |                                          |
| Van der Waals | $R$          |         | $\epsilon$            |     |                                          |
| NT            | 1.875        |         | 0.1700                |     | From Morgantini and Kollman              |
| SO            | 2.000        |         | 0.2500                |     | From SH in ff99SB                        |



## S. 12 ELISA Data

**Table S73: Competitive ELISA binding assay for the Ins(1,3,4,5)P<sub>4</sub> derivatives.** Percent of control represents the amount of PKB PH domain bound to PtdIns(3,4,5)P<sub>3</sub> on the well plate for the given sample as a percentage of the amount of PKB PH domain bound to PtdIns(3,4,5)P<sub>3</sub> on the well plate for the control (i.e. with no competing ligand/derivative). Results are provided for the competing compounds D-3-*O*-Sulfamoyl-*myo*-Ins(1,4,5)P<sub>3</sub> (3S), D-*myo*-Ins(1,4,5)P<sub>3</sub>-3-*O*-methylphosphate ester (3M), D-5-*O*-Sulfamoyl-*myo*-Ins(1,3,4)P<sub>3</sub> (5S), D-*myo*-Ins(1,3,4)P<sub>3</sub>-5-*O*-acetamidoethylphosphate ester (5A) and D-*myo*-Ins(1,3,4,5)P<sub>4</sub> (IP4) at seven different concentrations. Data for the three independent experiments is provided. Each independent experiment is the mean of three repeats.

5A

| Concentration of derivative (μM) | 0   | 3.13 | 6.25 | 12.5 | 25   | 50   | 100  |
|----------------------------------|-----|------|------|------|------|------|------|
| Repeat 1 (% control)             | 100 | 38.3 | 40.3 | 30.5 | 52.7 | 31.9 | 39.0 |
| Repeat 2 (% control)             | 100 | 56.1 | 48.2 | 41.9 | 25.9 | 24.7 | 21.9 |
| Repeat 3 (% control)             | 100 | 47.9 | 62.6 | 44.1 | 36.4 | 30.6 | 32.5 |

5S

| Concentration of derivative (μM) | 0   | 3.13 | 6.25 | 12.5 | 25   | 50   | 100  |
|----------------------------------|-----|------|------|------|------|------|------|
| Repeat 1 (% control)             | 100 | 47.4 | 39.8 | 37.6 | 34.4 | 34.2 | 42.3 |
| Repeat 2 (% control)             | 100 | 55.7 | 55.6 | 55.5 | 52.7 | 61.2 | 50.9 |
| Repeat 3 (% control)             | 100 | 67.7 | 107  | 78.1 | 71.9 | 85.5 | 51.4 |

3M

| Concentration of derivative ( $\mu\text{M}$ ) | 0   | 3.13 | 6.25 | 12.5 | 25   | 50   | 100  |
|-----------------------------------------------|-----|------|------|------|------|------|------|
| Repeat 1<br>(% control)                       | 100 | 63.7 | 76.6 | 52.4 | 50.5 | 50.5 | 55.7 |
| Repeat 2<br>(% control)                       | 100 | 87.4 | 98.4 | 88.7 | 77.0 | 62.9 | 73.8 |
| Repeat 3<br>(% control)                       | 100 | 87.0 | 78.1 | 74.2 | 74.8 | 73.1 | 61.5 |

3S

| Concentration of derivative ( $\mu\text{M}$ ) | 0   | 3.13 | 6.25 | 12.5 | 25   | 50   | 100  |
|-----------------------------------------------|-----|------|------|------|------|------|------|
| Repeat 1<br>(% control)                       | 100 | 72.5 | 82.5 | 65.0 | 58.0 | 44.9 | 72.5 |
| Repeat 2<br>(% control)                       | 100 | 122  | 92.2 | 104  | 78.8 | 83.2 | 84.1 |
| Repeat 3<br>(% control)                       | 100 | 76.6 | 105  | 103  | 87.0 | 117  | 98.1 |

# IP4

| Concentration of derivative ( $\mu\text{M}$ ) | 0   | 3.13 | 6.25 | 12.5 | 25   | 50   | 100  |
|-----------------------------------------------|-----|------|------|------|------|------|------|
| Repeat 1<br>(% control)                       | 100 | 62.5 | 53.3 | 52.5 | 50.0 | 42.5 | 50.8 |
| Repeat 2<br>(% control)                       | 100 | 107  | 97.0 | 77.4 | 65.6 | 73.2 | 76.8 |
| Repeat 3<br>(% control)                       | 100 | 87.0 | 89.0 | 60.1 | 56.1 | 42.2 | 67.5 |

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