

# Supporting information

## Integrated Synthetic, Biophysical and Computational Investigations of Covalent Inhibitors of Prolyl Oligopeptidase and Fibroblast Activation Protein $\alpha$

Jessica Plescia,<sup>‡,1</sup> Stéphane De Cesco,<sup>‡,†,1</sup> Mihai Burai Patrascu,<sup>‡,1</sup> Jerry Kurian,<sup>1</sup> Justin Di Trani,<sup>1</sup> Caroline Dufresne,<sup>1</sup> Alexander S. Wahba,<sup>1</sup> Naëla Janmamode,<sup>1</sup> Anthony K. Mittermaier,<sup>1</sup> and Nicolas Moitessier\*

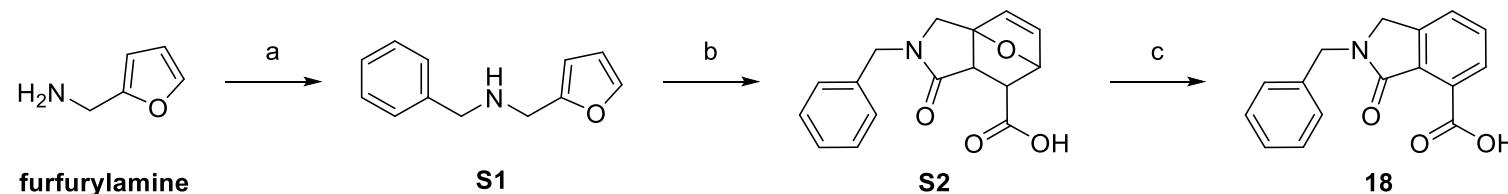
<sup>1</sup>Department of Chemistry, McGill University, Montréal, Quebec, Canada, H3A 0B8

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## I. Synthetic Chemistry – Experimental procedures to obtain scaffold **18**

**Scheme S1.**<sup>a</sup> Synthesis of intermediates for POP inhibitors



<sup>a</sup>Reagents: a) benzaldehyde, NaBH<sub>4</sub>, EtOH, 0°C→rt, 18h, 92%; b) maleic anhydride, toluene, rt, 18h, 94%; c) conc. HCl (aq.), reflux 3h, rt 18h, 86%

**N-benzyl-1-(furan-2-yl)methanamine (S1)** Furfurylamine (7.500 g, 77.22 mmol) was dissolved in EtOH (200 mL) under argon atmosphere, and benzaldehyde (8.195g, 77.22 mmol) was added. The solution stirred for 1h and was then cooled to 0°C. NaBH<sub>4</sub> was added, and the reaction stirred overnight at room temperature. The mixture was concentrated *in vacuo* to give a white solid, and water and DCM were added. The product was extracted with DCM, and the combined organic layers were washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated *in vacuo* to give a yellow oil which was taken to the next step without purification (13.282 g, 92%). <sup>1</sup>H NMR (300 MHz, Chloroform-*d*) δ 7.44 – 7.19 (m, 6H), 6.33 (dt, *J* = 3.0, 1.4 Hz, 1H), 6.19 (dt, *J* = 3.1, 0.8 Hz, 1H), 3.80 (s, 4H), 1.71 (s, 1H); <sup>13</sup>C NMR (75 MHz, Chloroform-*d*) δ 45.45, 52.88, 77.16, 107.13, 110.19, 127.11, 128.34 (2C), 128.50 (2C), 139.97, 141.91, 153.90. Spectral data previously published by our group.<sup>1</sup>

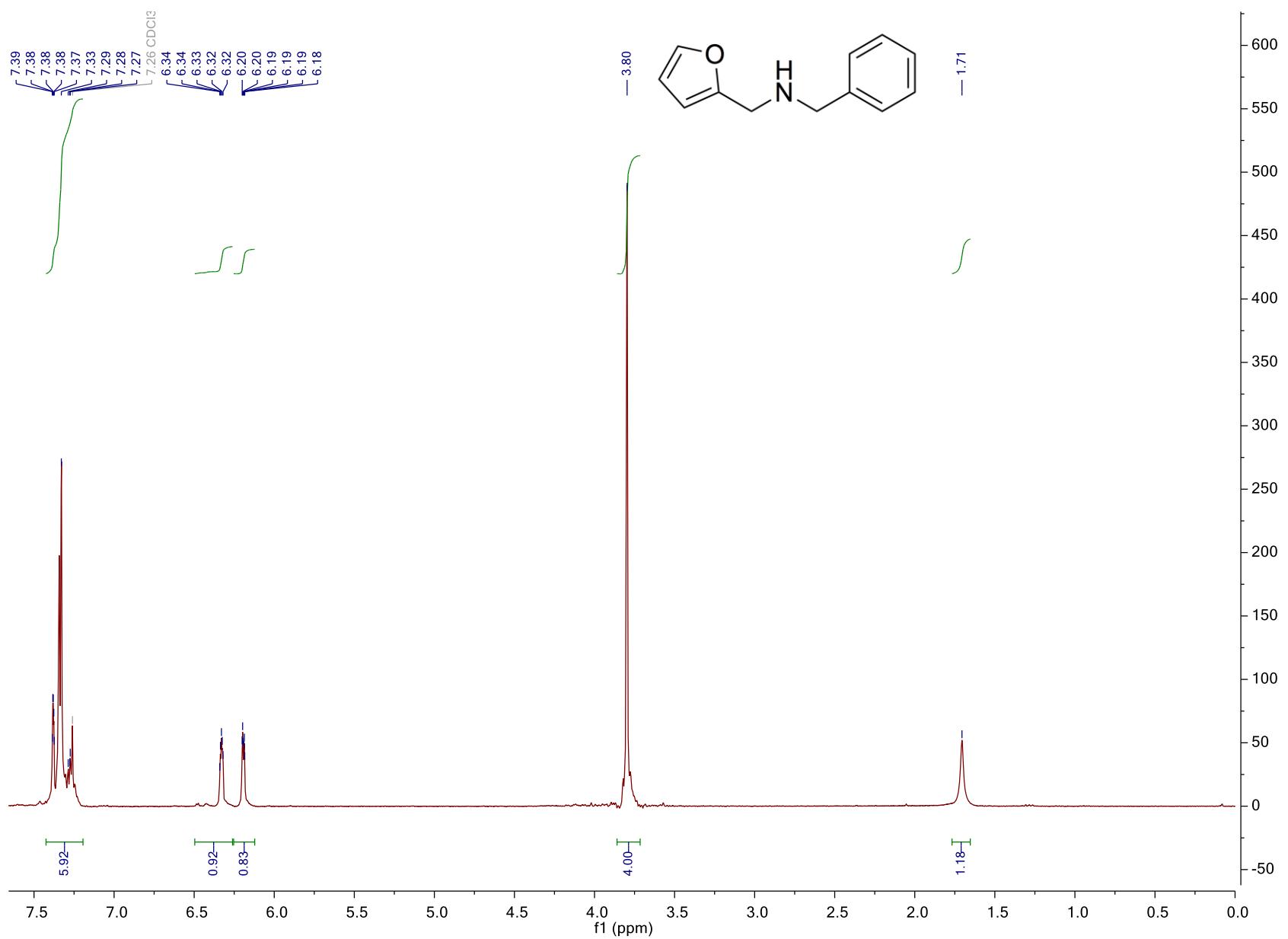
**2-benzyl-1-oxo-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole-7-carboxylic acid (S2).** Amine **S1** (13.282 g, 70.94 mmol) was dissolved in toluene (500 mL) under argon atmosphere, and maleic anhydride (7.652 g, 78.03 mmol) was added. The reaction stirred overnight at room temperature. The precipitate was then filtered under vacuum and rinsed with Et<sub>2</sub>O to give a white solid which was taken to the next step without purification (19.025 g, 94%). <sup>1</sup>H NMR (300 MHz, Chloroform-*d*) δ 10.74 (s, 1H), 7.35 – 7.11 (m, 5H), 6.44 – 6.31 (m, 2H), 5.21 (s, 1H), 4.61 (d, *J* = 15.0 Hz, 1H), 4.39 (d, *J* = 15.0 Hz, 1H), 3.81 (d, *J* = 11.9 Hz, 1H), 3.62 (d, *J* = 11.9 Hz, 1H), 2.95 (d, *J* = 9.1 Hz, 1H), 2.81 (d, *J* = 9.1 Hz, 1H); <sup>13</sup>C NMR (75 MHz, Chloroform-*d*) δ 45.60, 47.06, 48.61, 51.11, 77.16, 82.26, 88.78, 127.90, 128.02 (2C), 128.99 (2C), 135.09, 135.38, 137.17. Spectral data previously published by our group.<sup>1</sup>

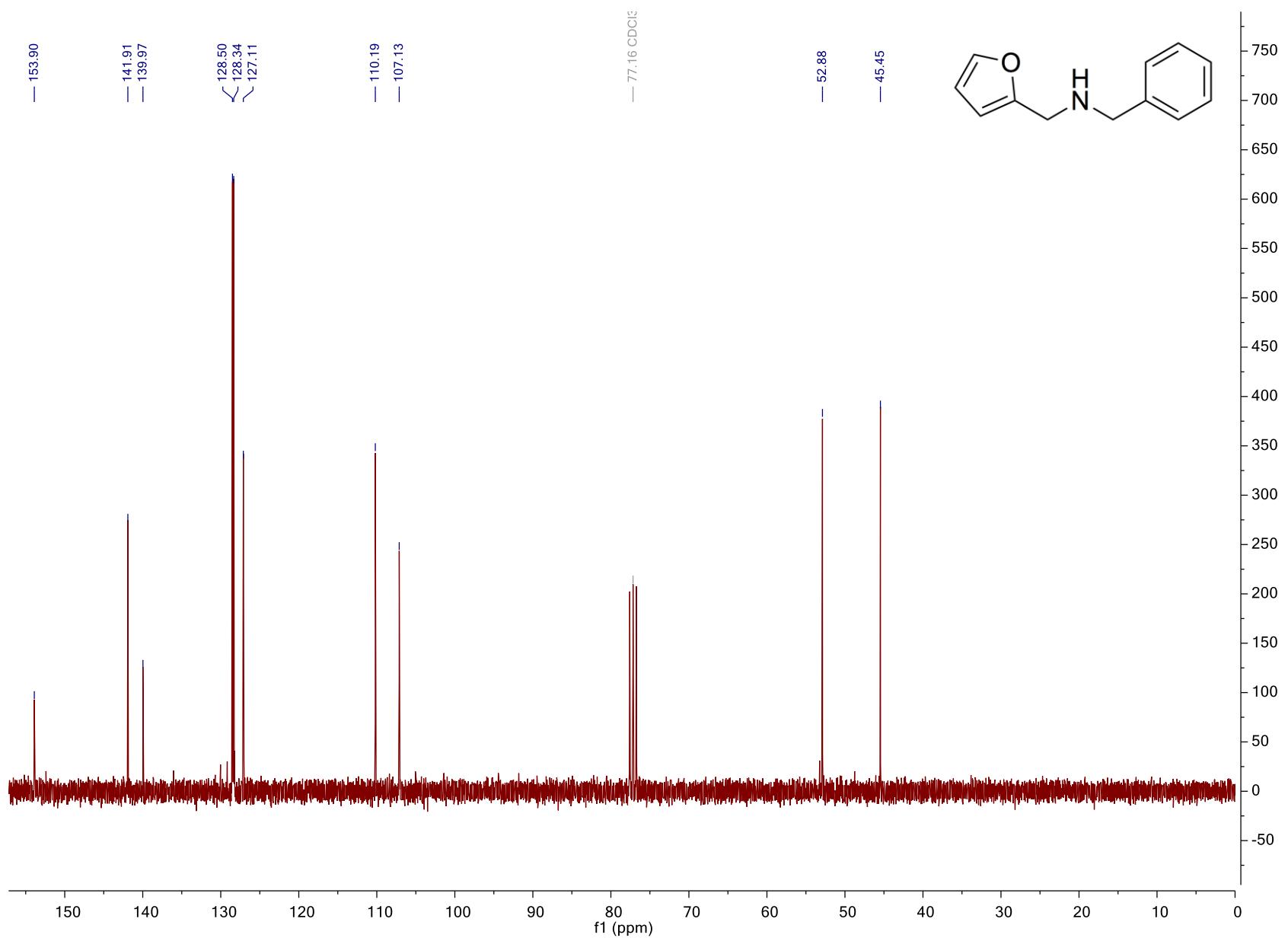
**2-benzyl-3-oxoisindoline-4-carboxylic acid (18).** Carboxylic acid **S2** (20.000 g, 70.10 mmol) was dissolved in concentrated HCl (150 mL), and the reaction was refluxed for 3h. The mixture was then cooled to room temperature and stirred overnight. The solvent was evaporated to give a dark brown solid, which was filtered and rinsed with copiously with MeOH to give a beige solid, which was taken to the next step without purification (8.700 g, 46%). <sup>1</sup>H NMR (500 MHz, Chloroform-*d*) δ 15.86 (s, 1H), 8.38 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.65 – 7.58 (m, 1H), 7.40 – 7.32 (m, 5H), 4.87 (s, 2H), 4.44 (s, 2H); <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 47.47,

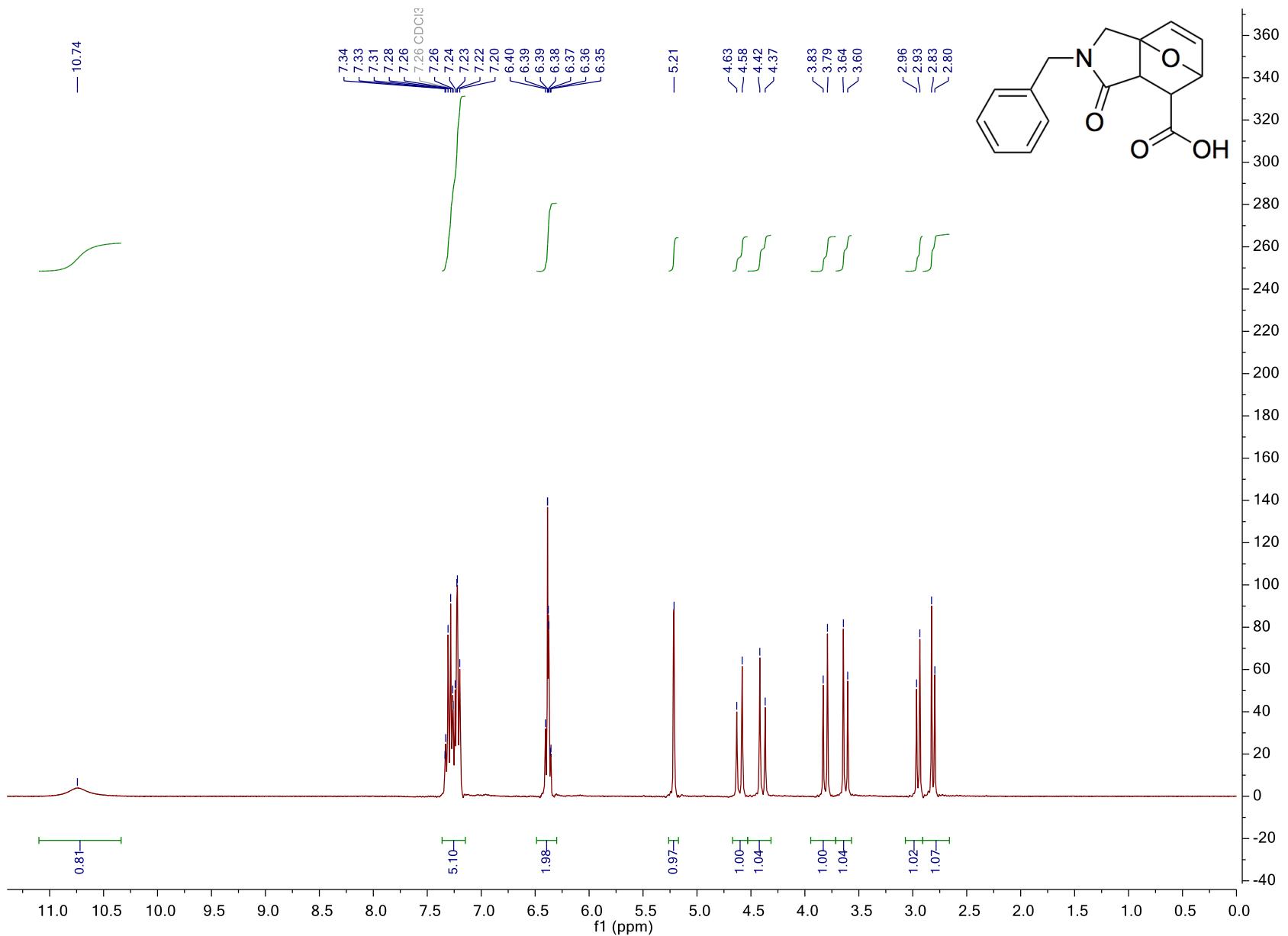
50.57, 77.16, 127.07, 128.52 (2C), 128.59, 129.30 (2C), 129.62, 129.63, 132.56, 133.66, 135.30, 142.01, 165.51, 169.79. Spectral data previously published by our group.<sup>1</sup>

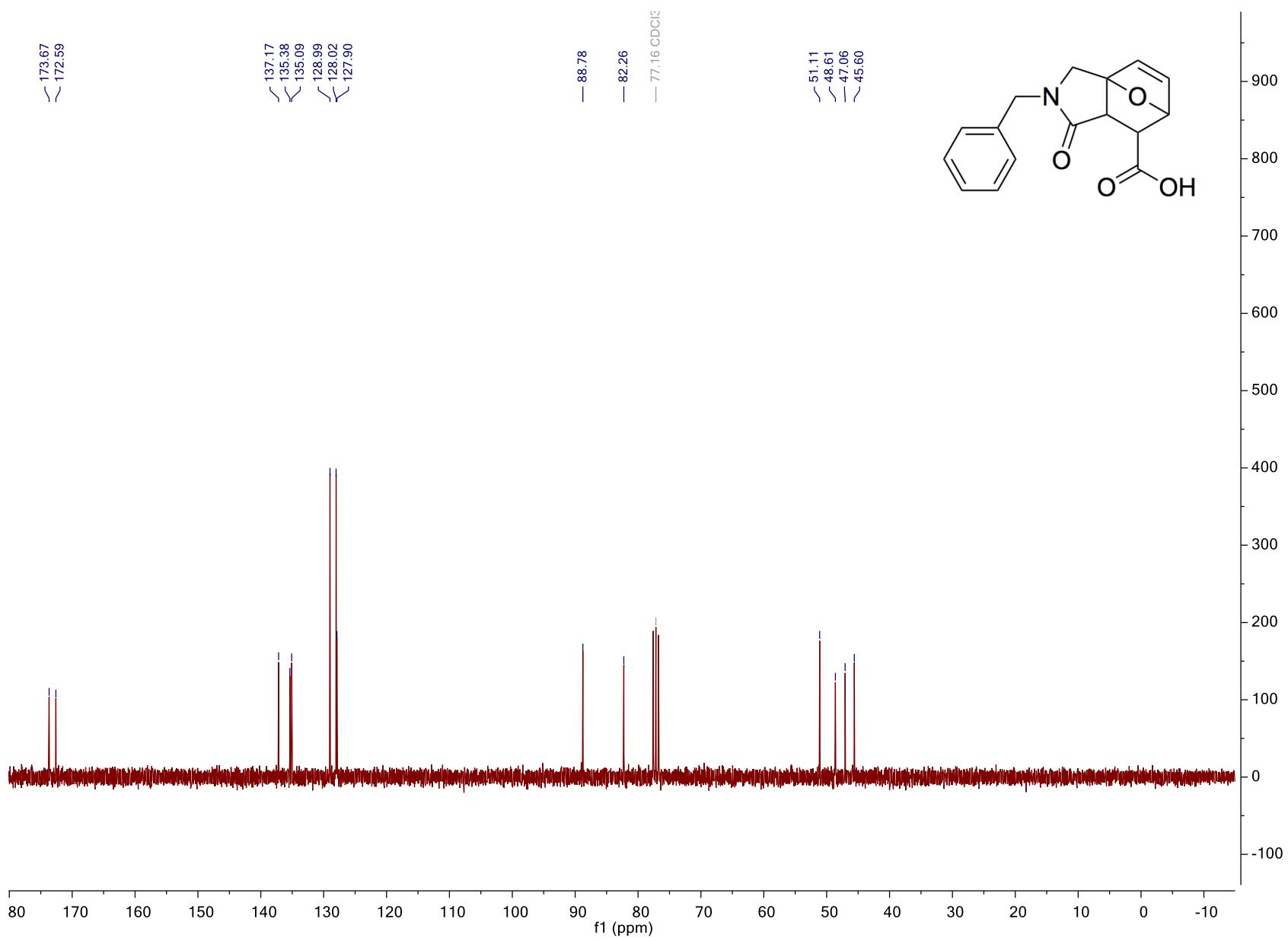
## II. Synthetic Chemistry – NMR spectra

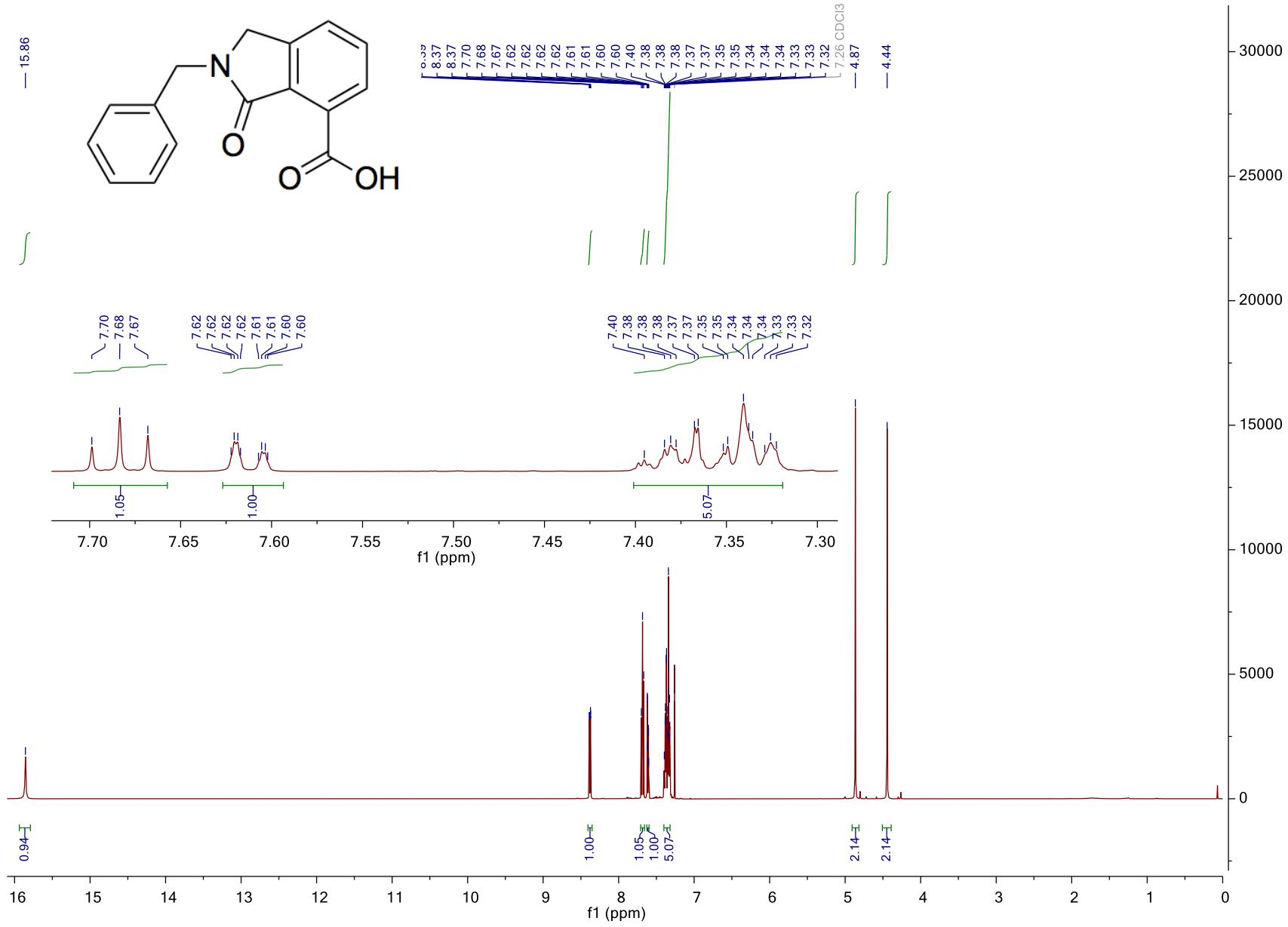
Spectra presented in the following order:  $^1\text{H}$ ,  $^{13}\text{C}$ , HSQC (if applicable),  $^{19}\text{F}/^{11}\text{B}$  (if applicable)

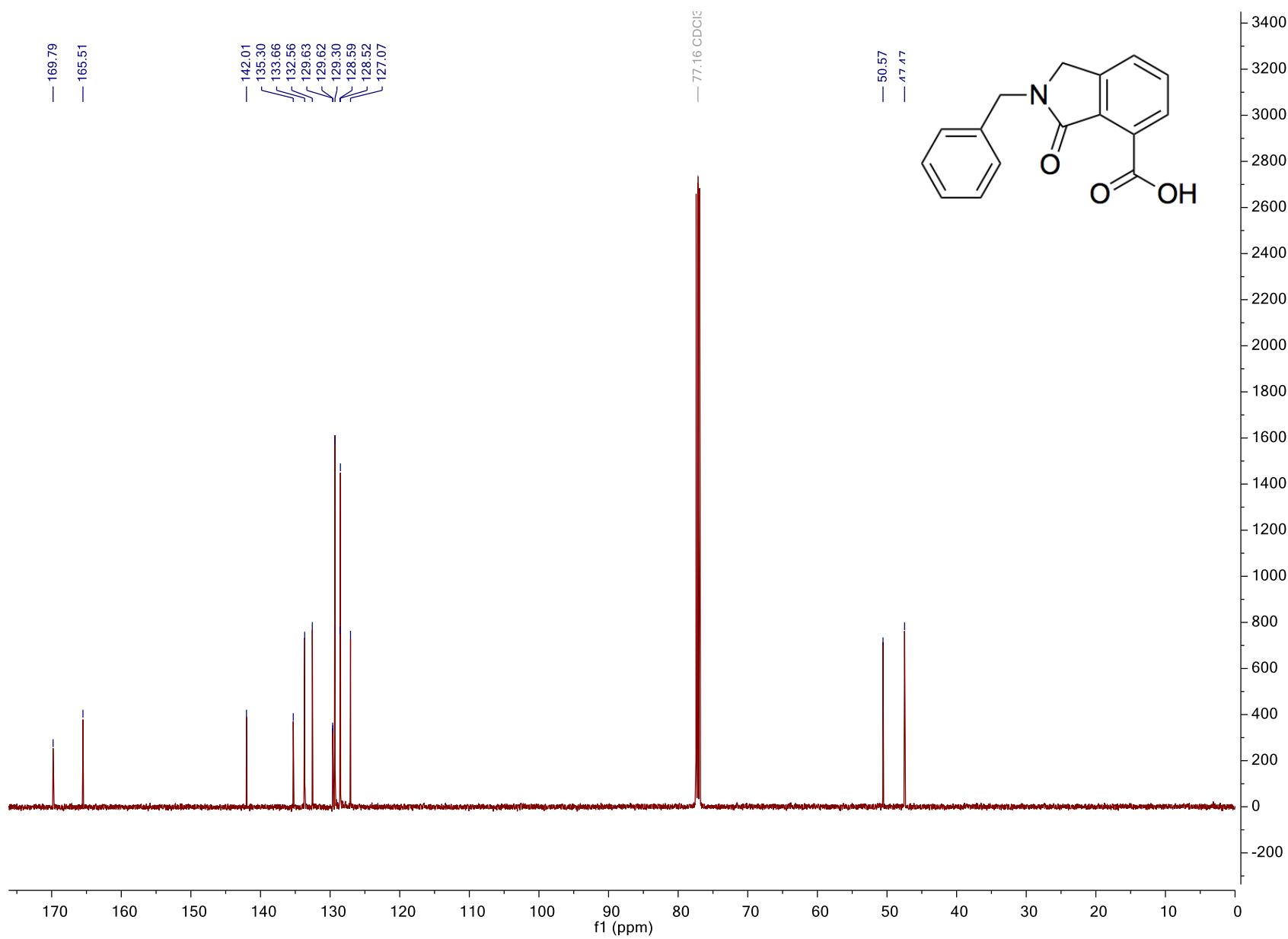


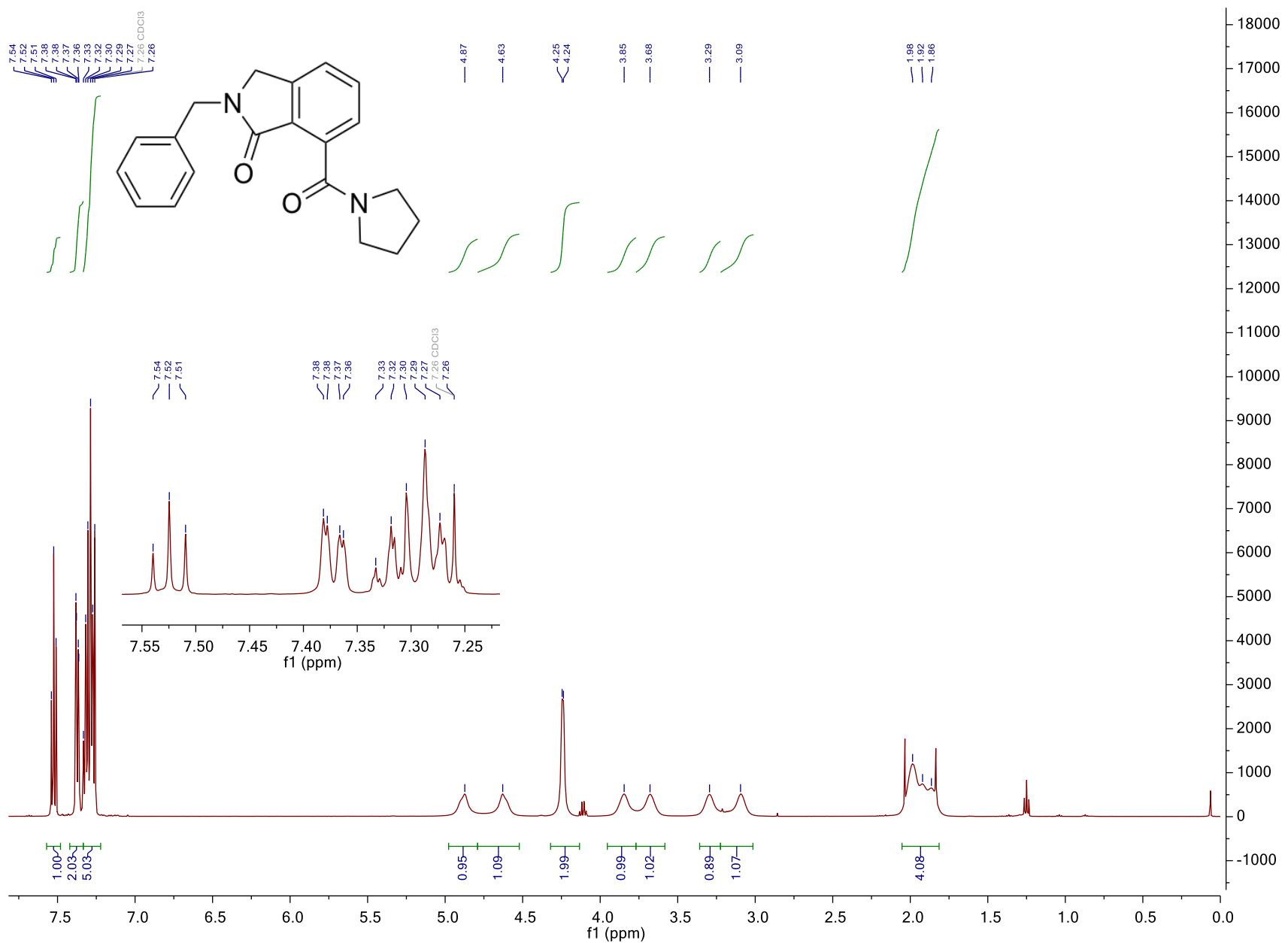


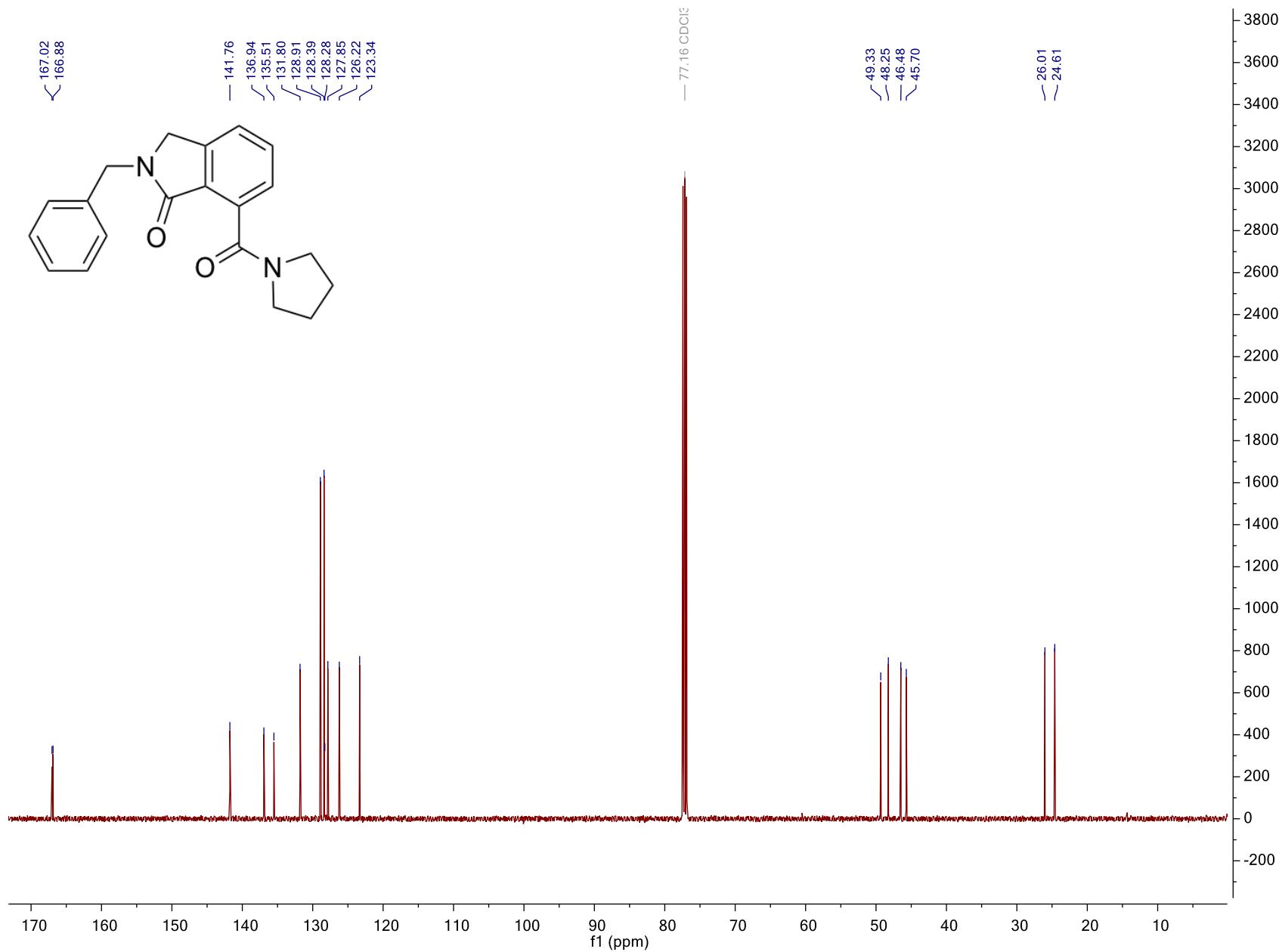


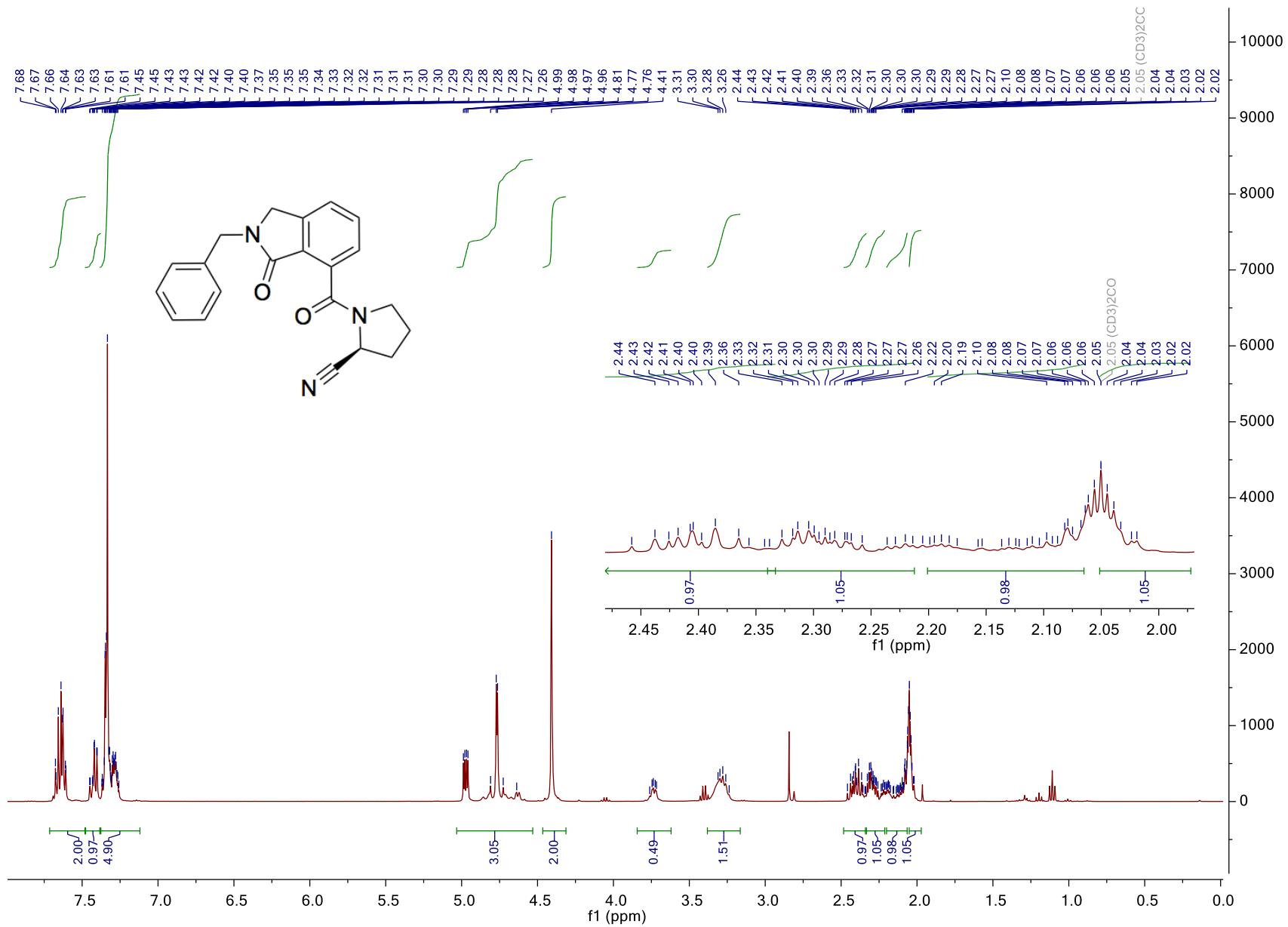


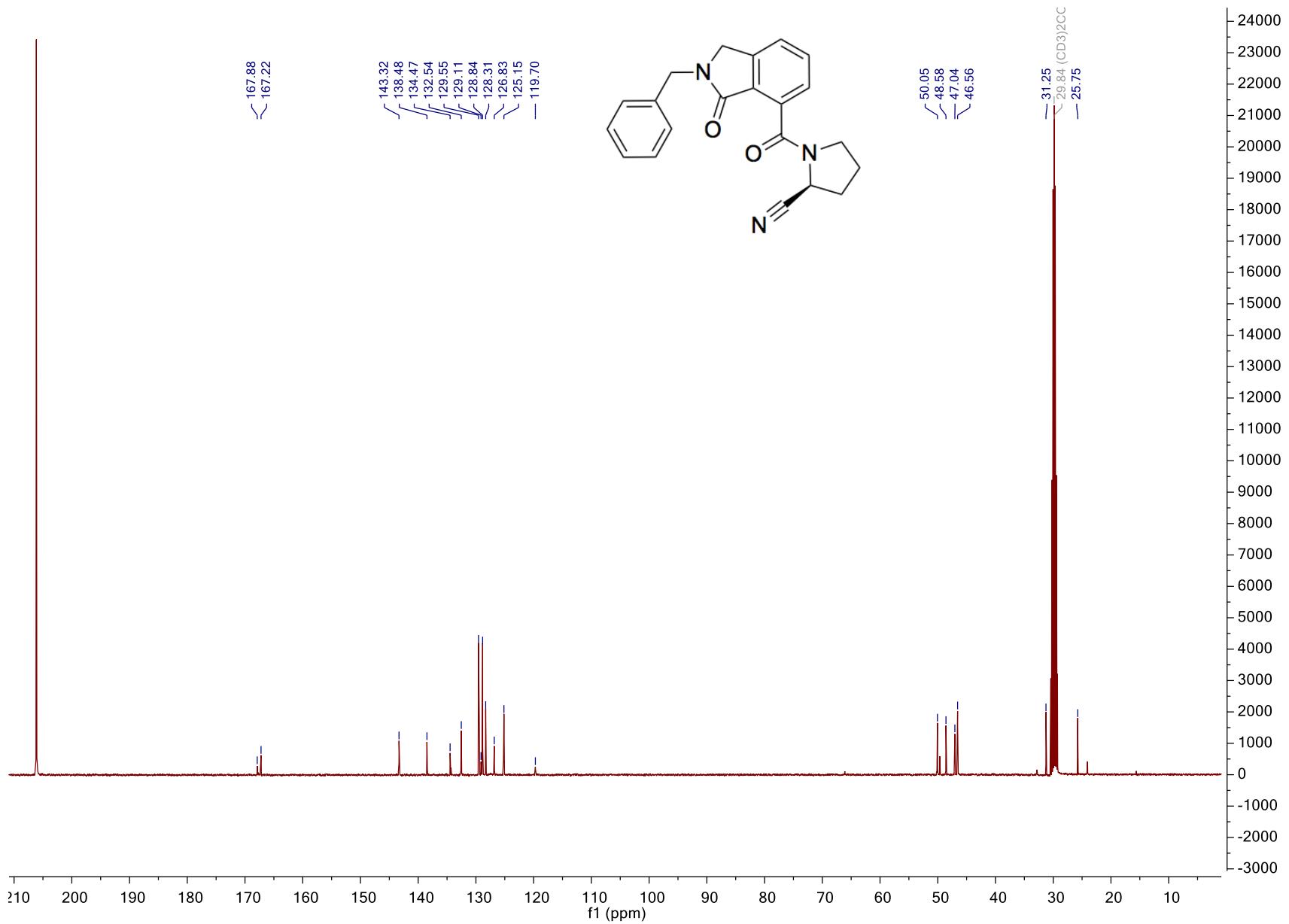


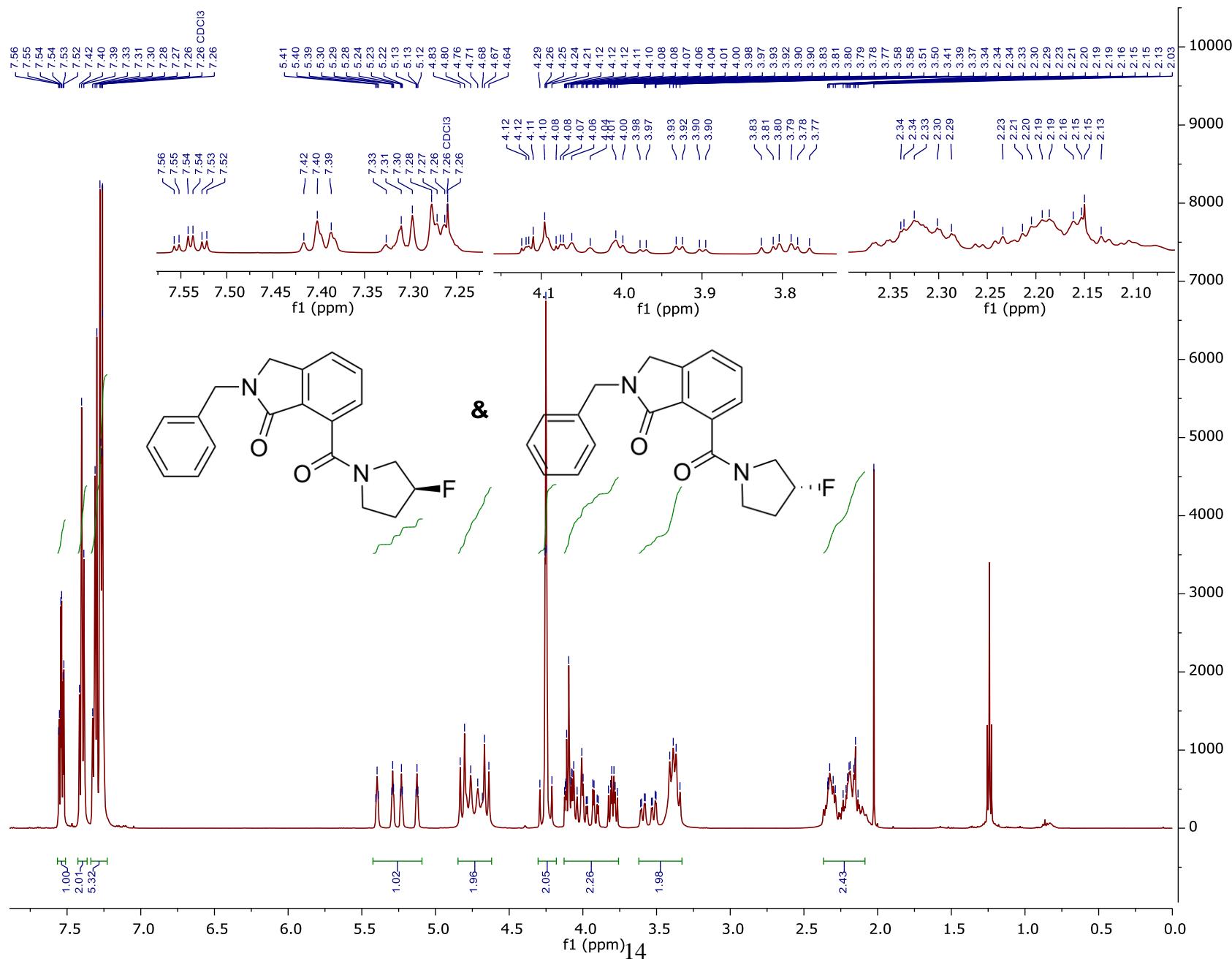


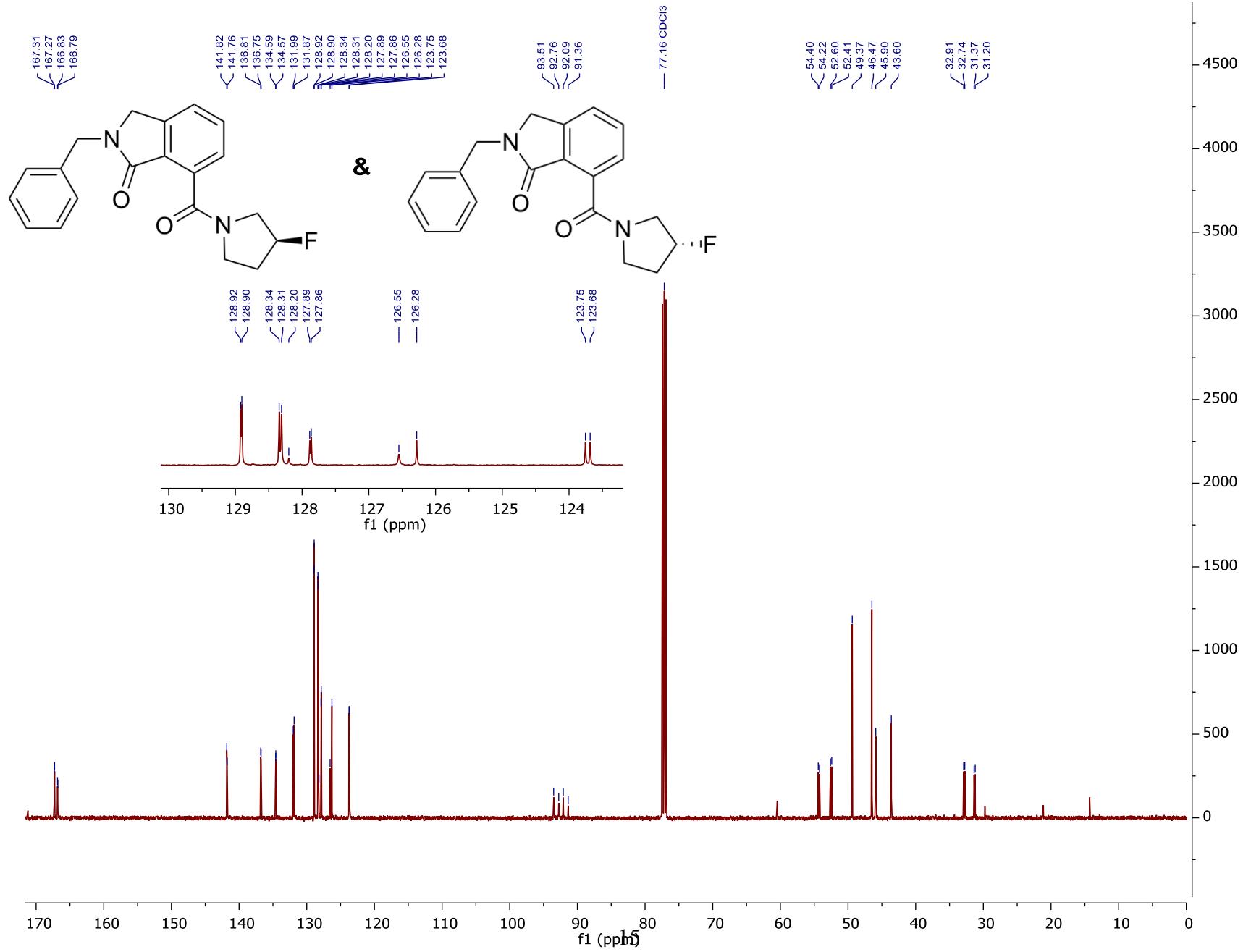


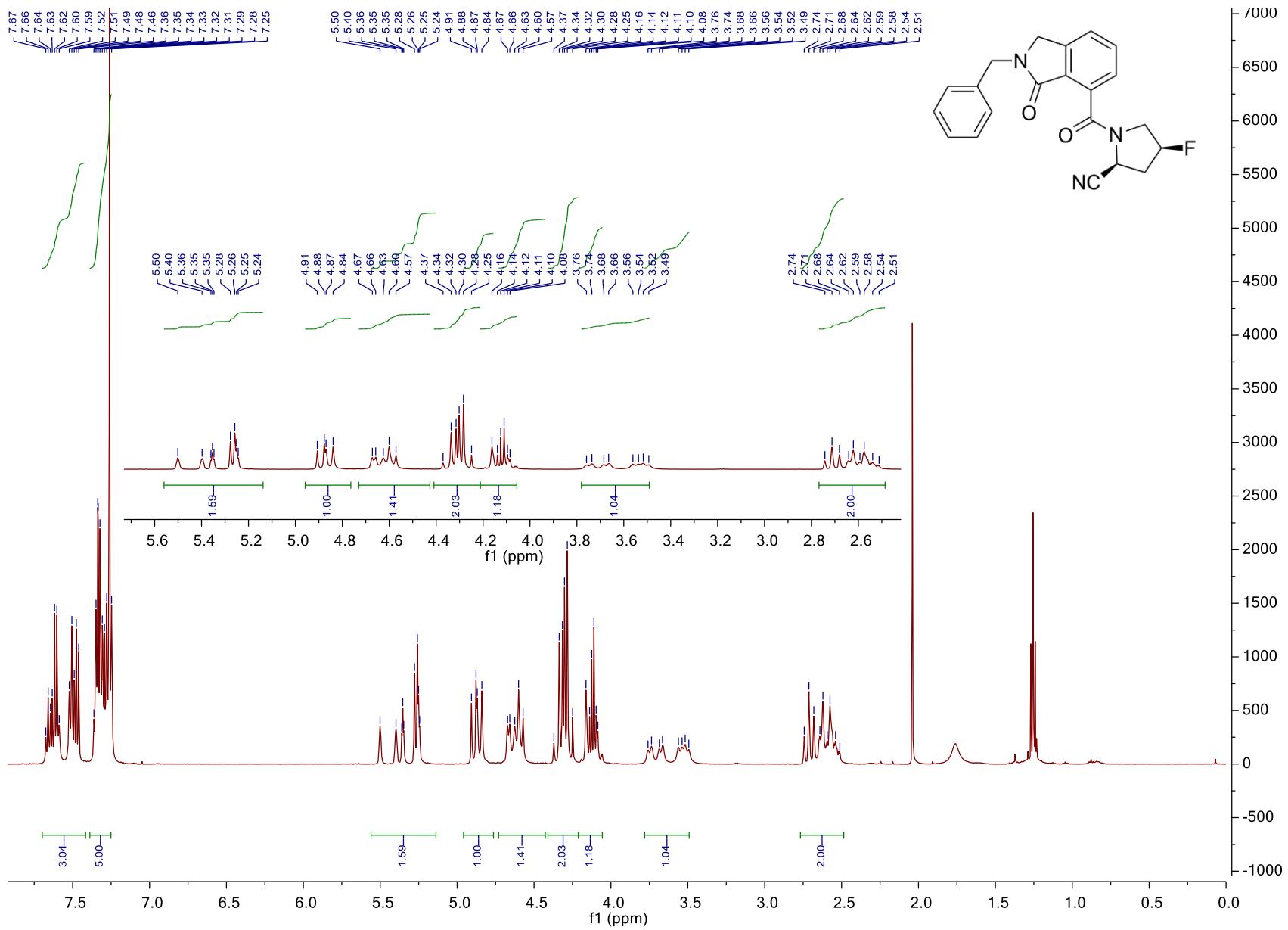


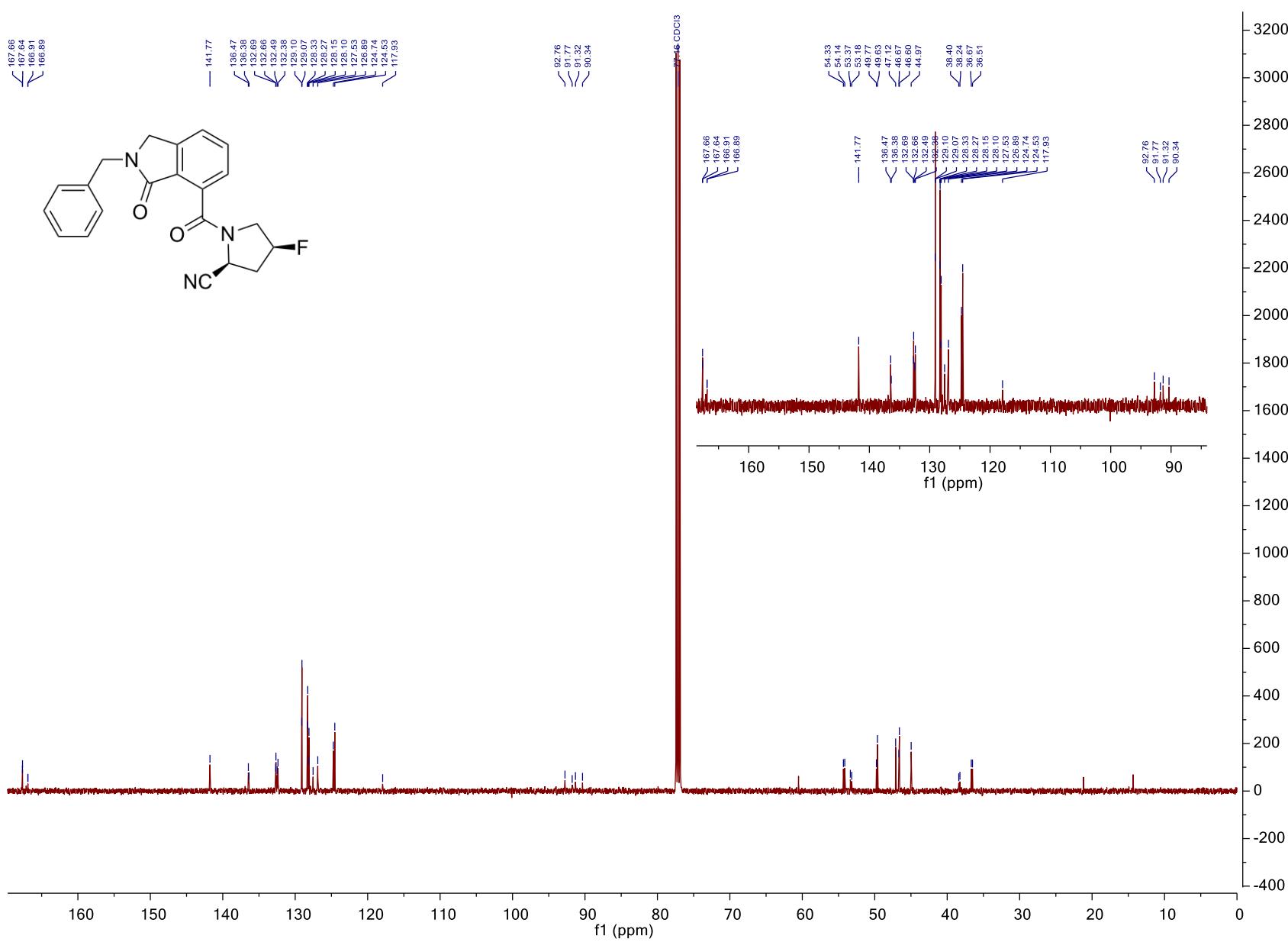


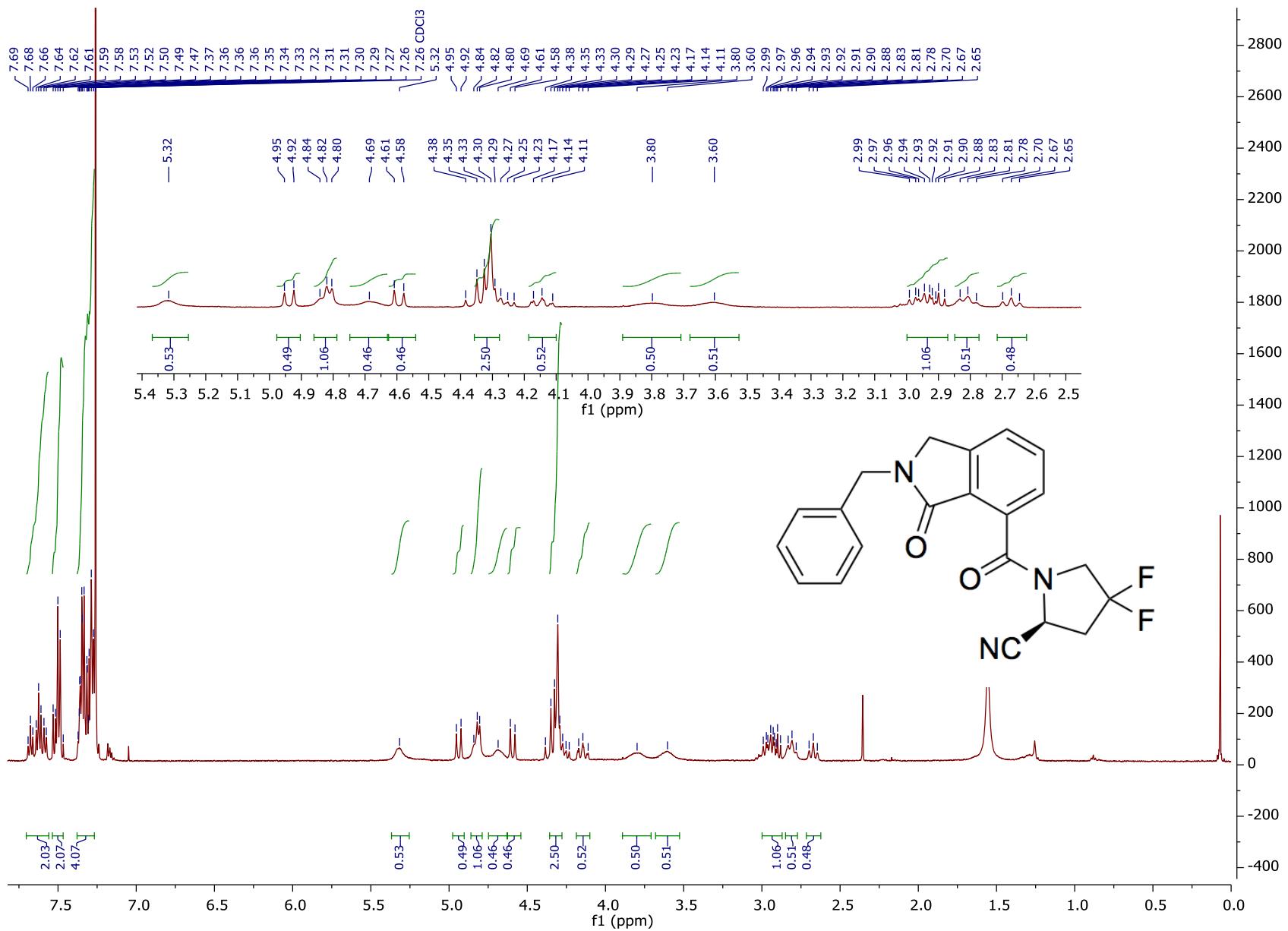


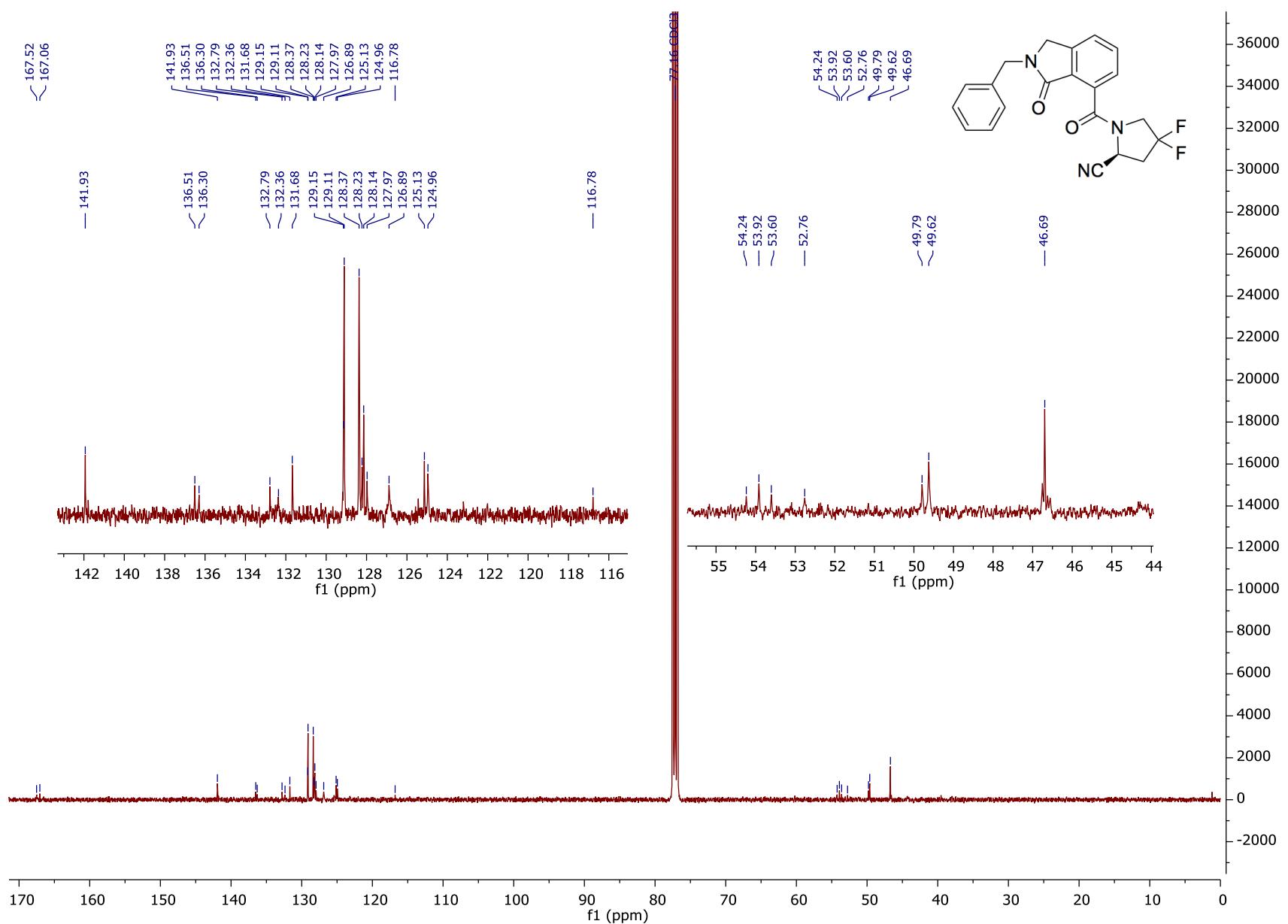


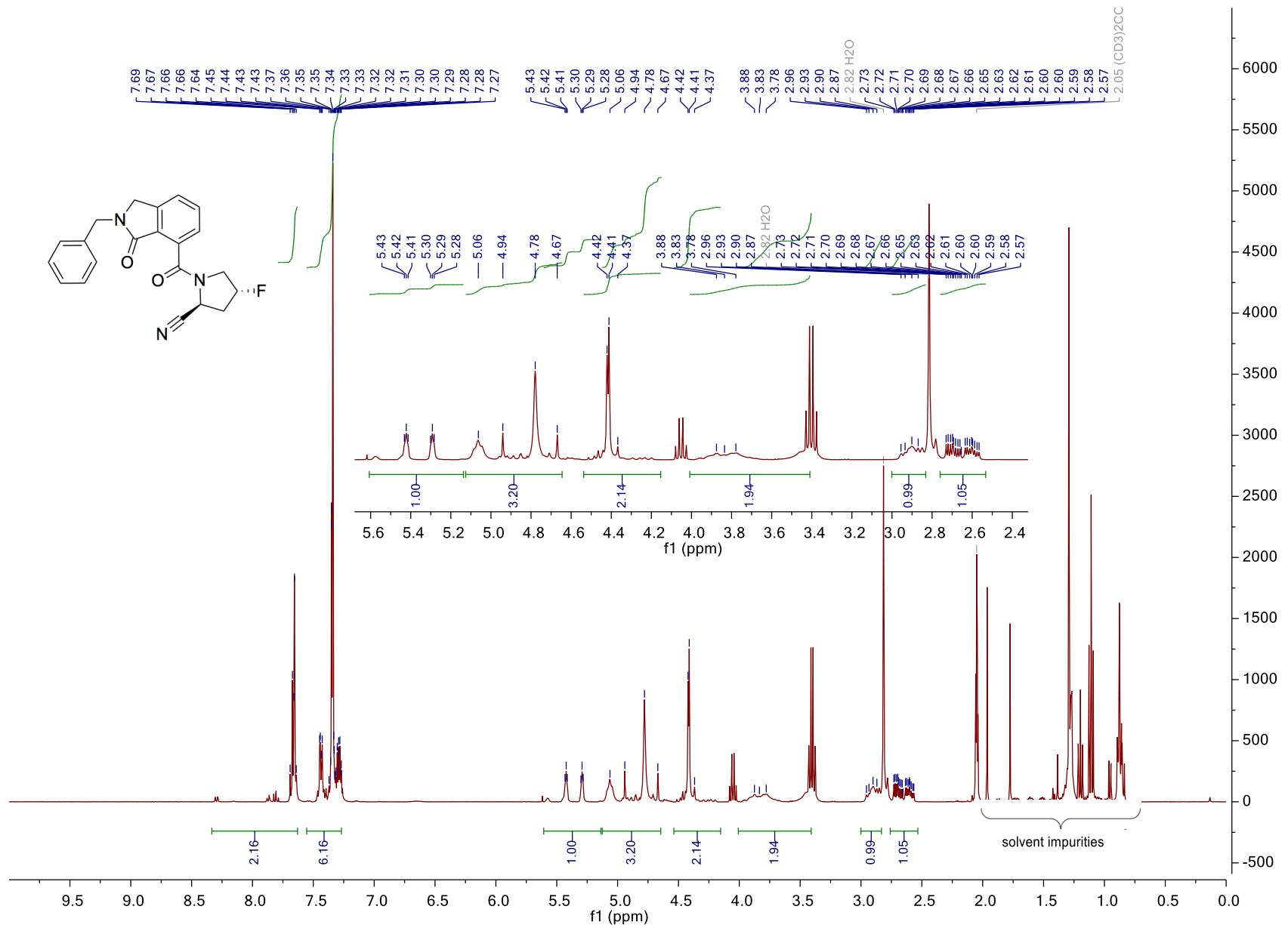


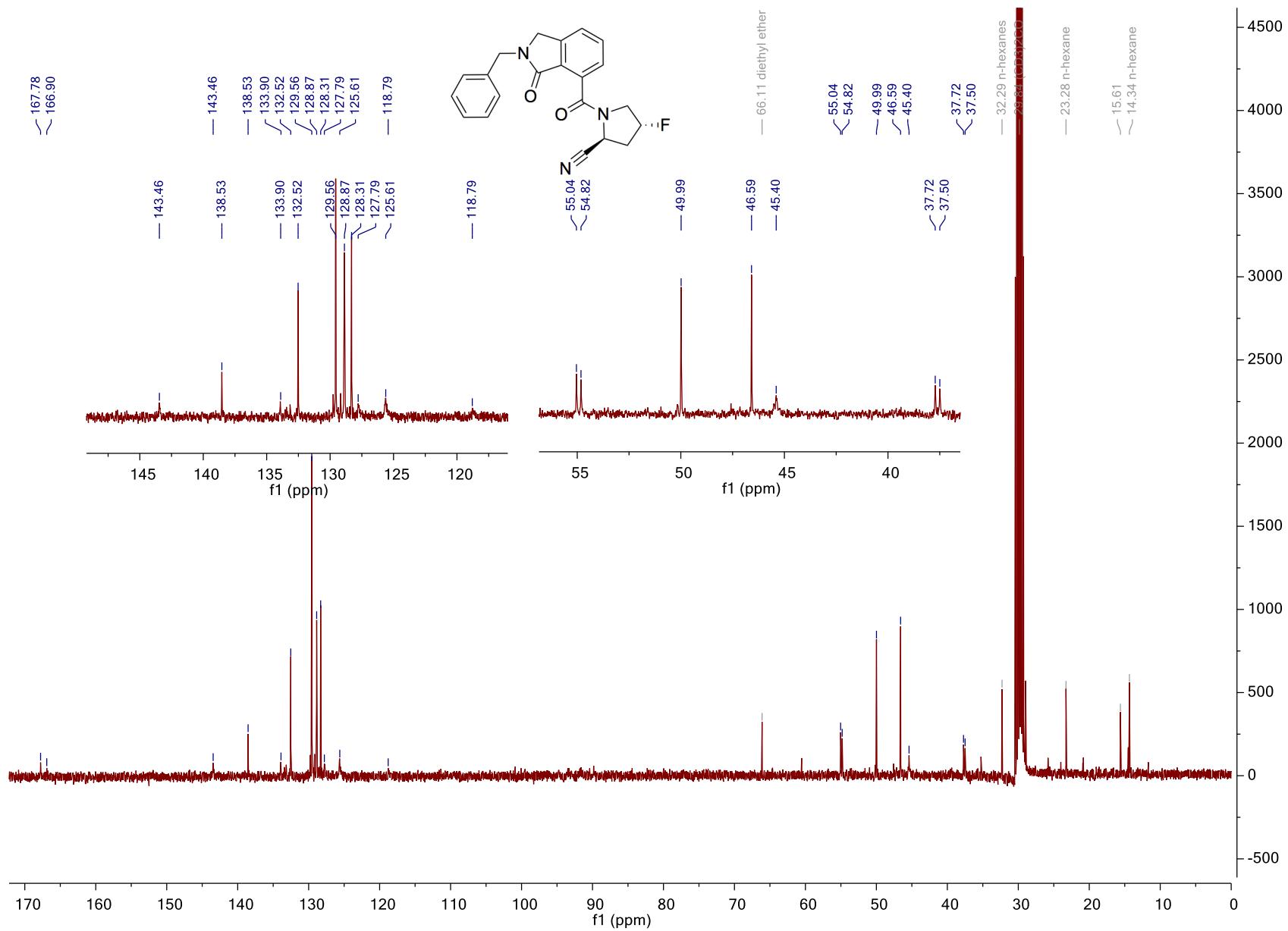


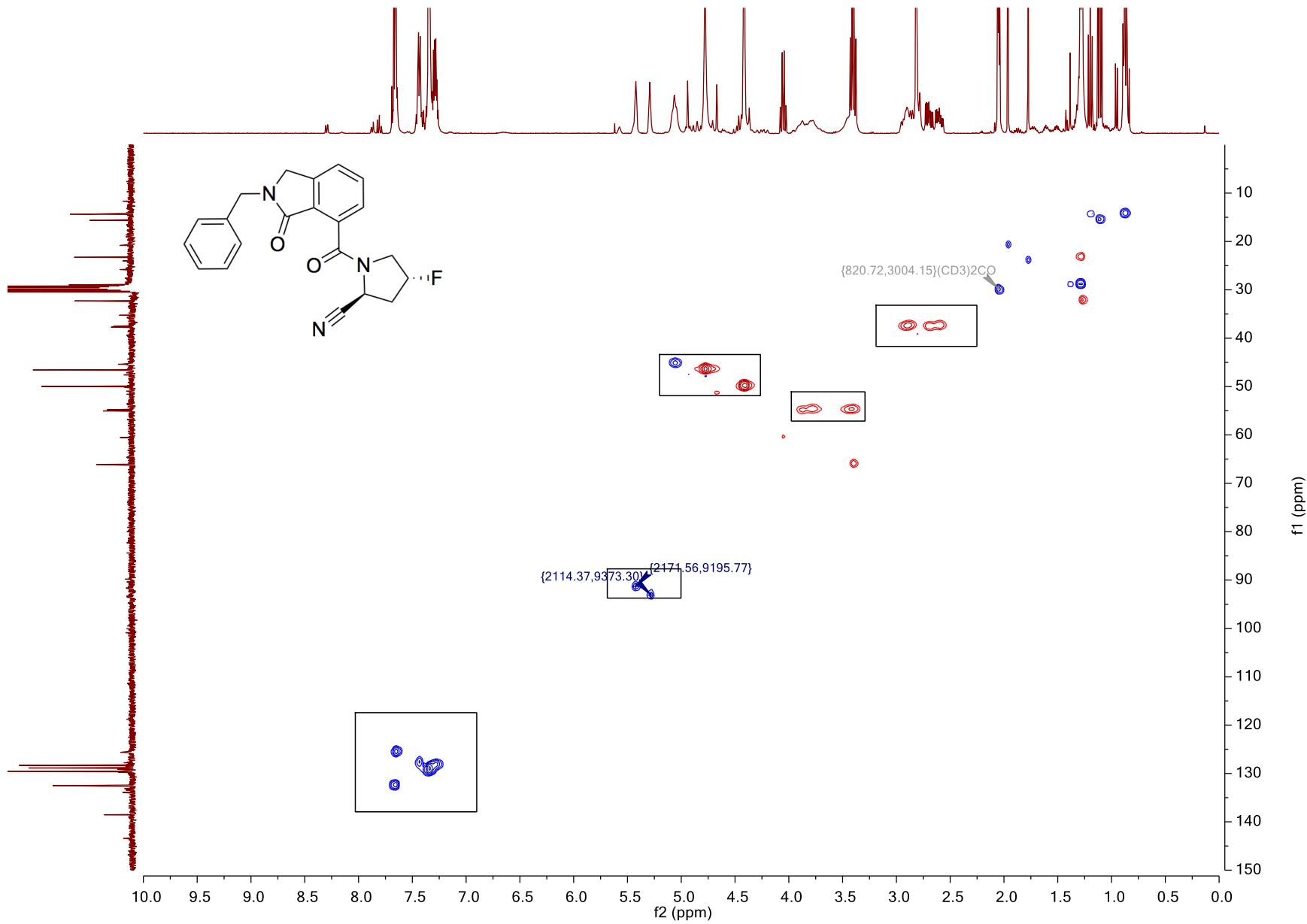


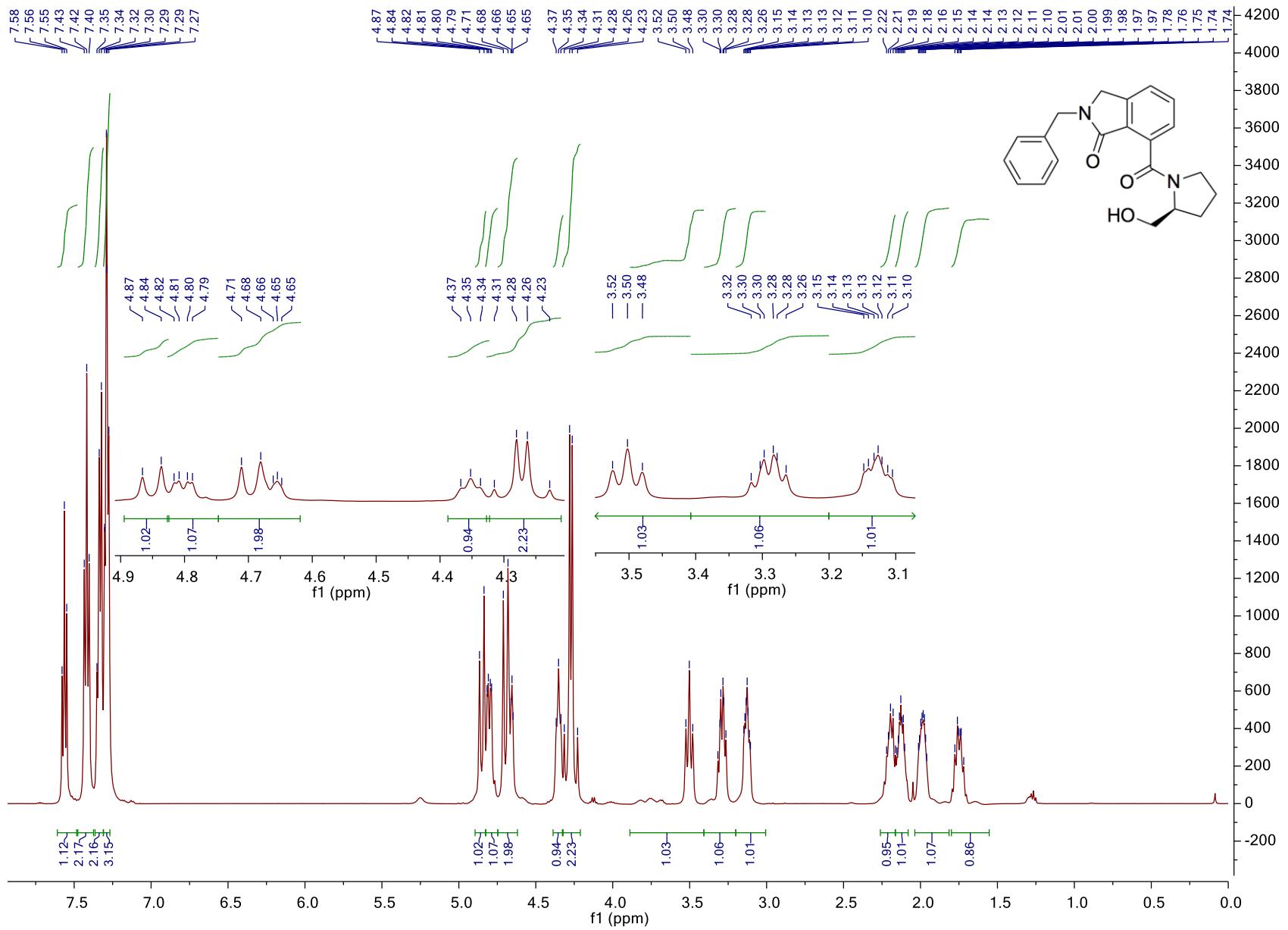


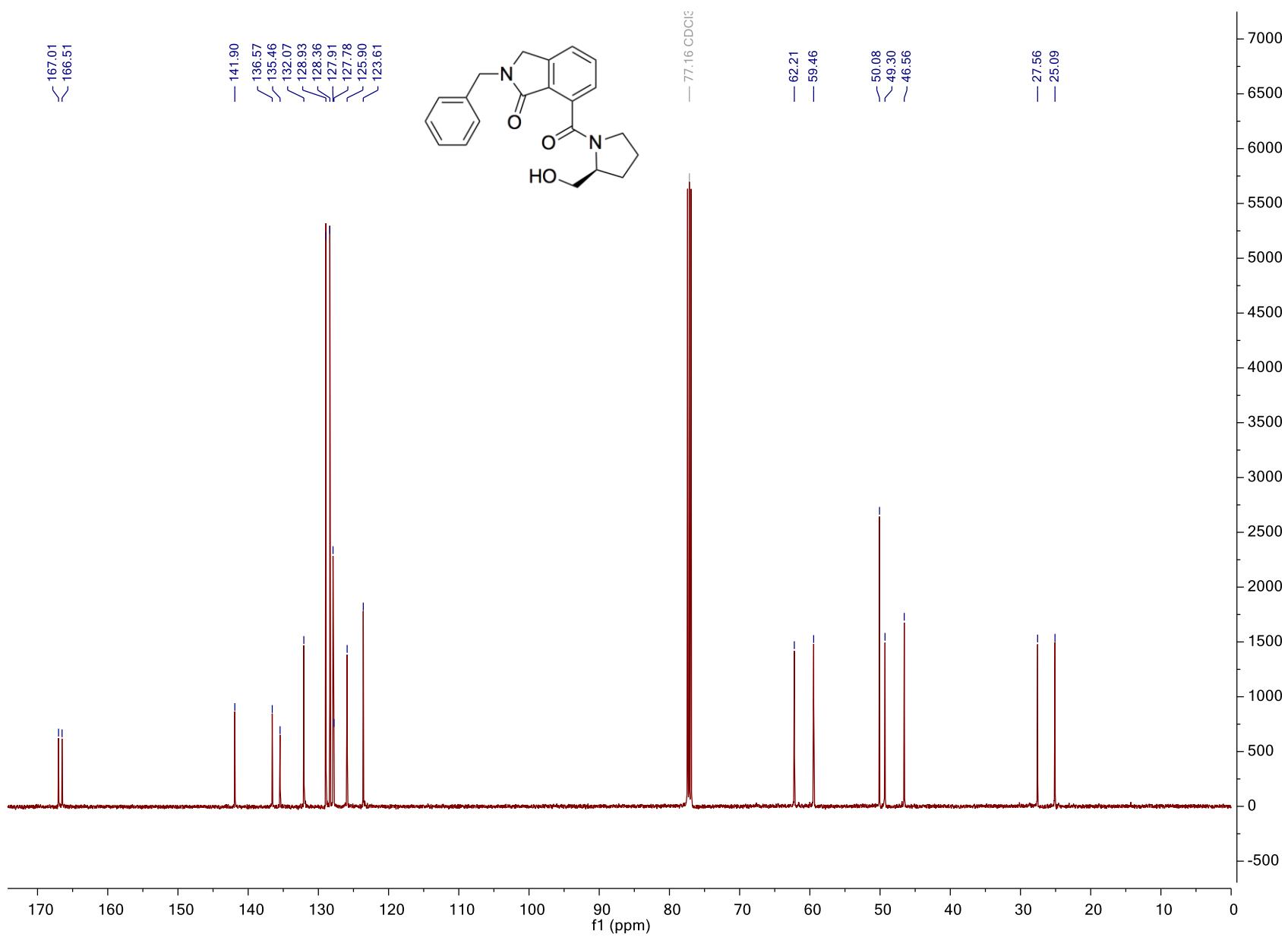


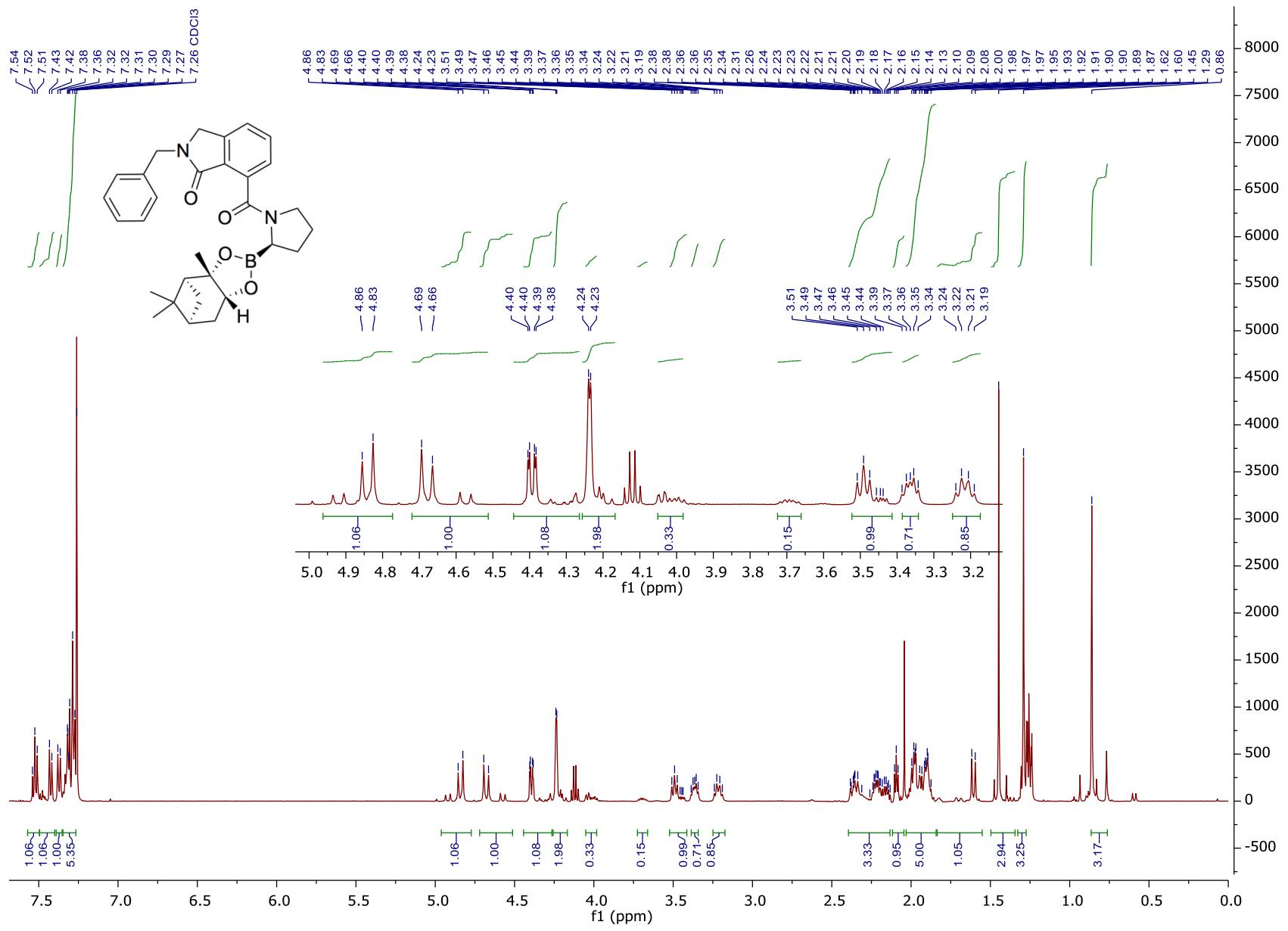


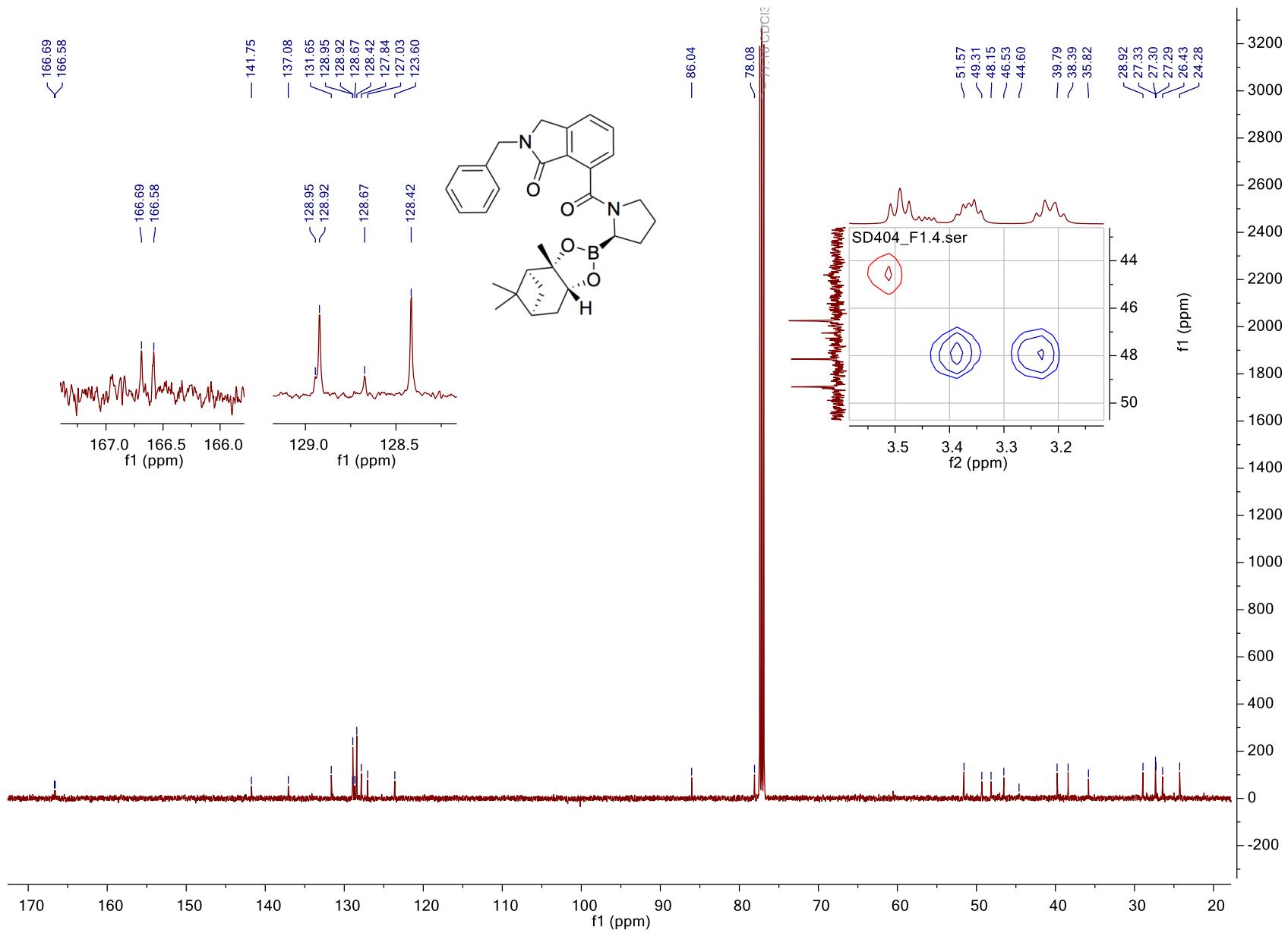


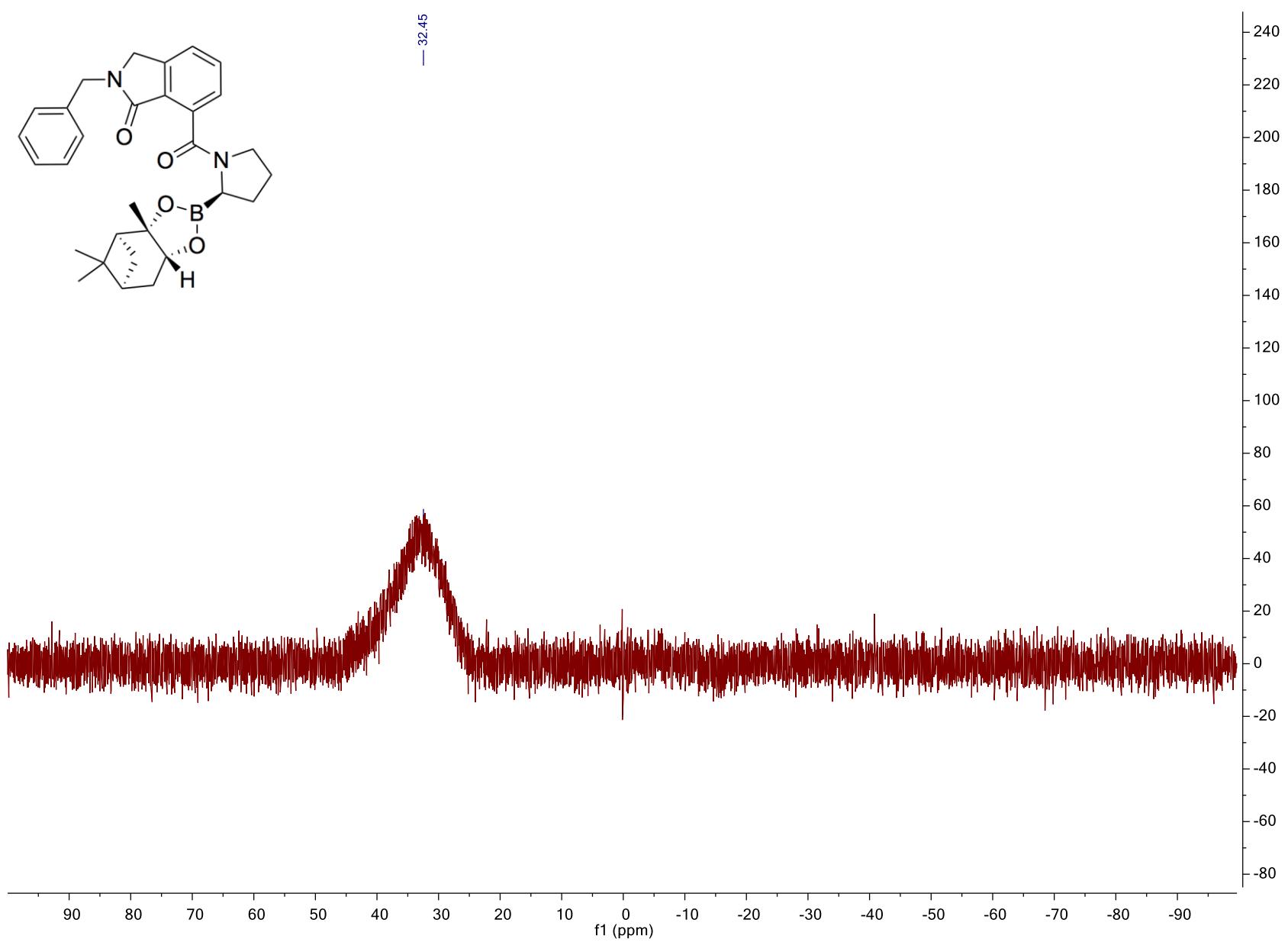


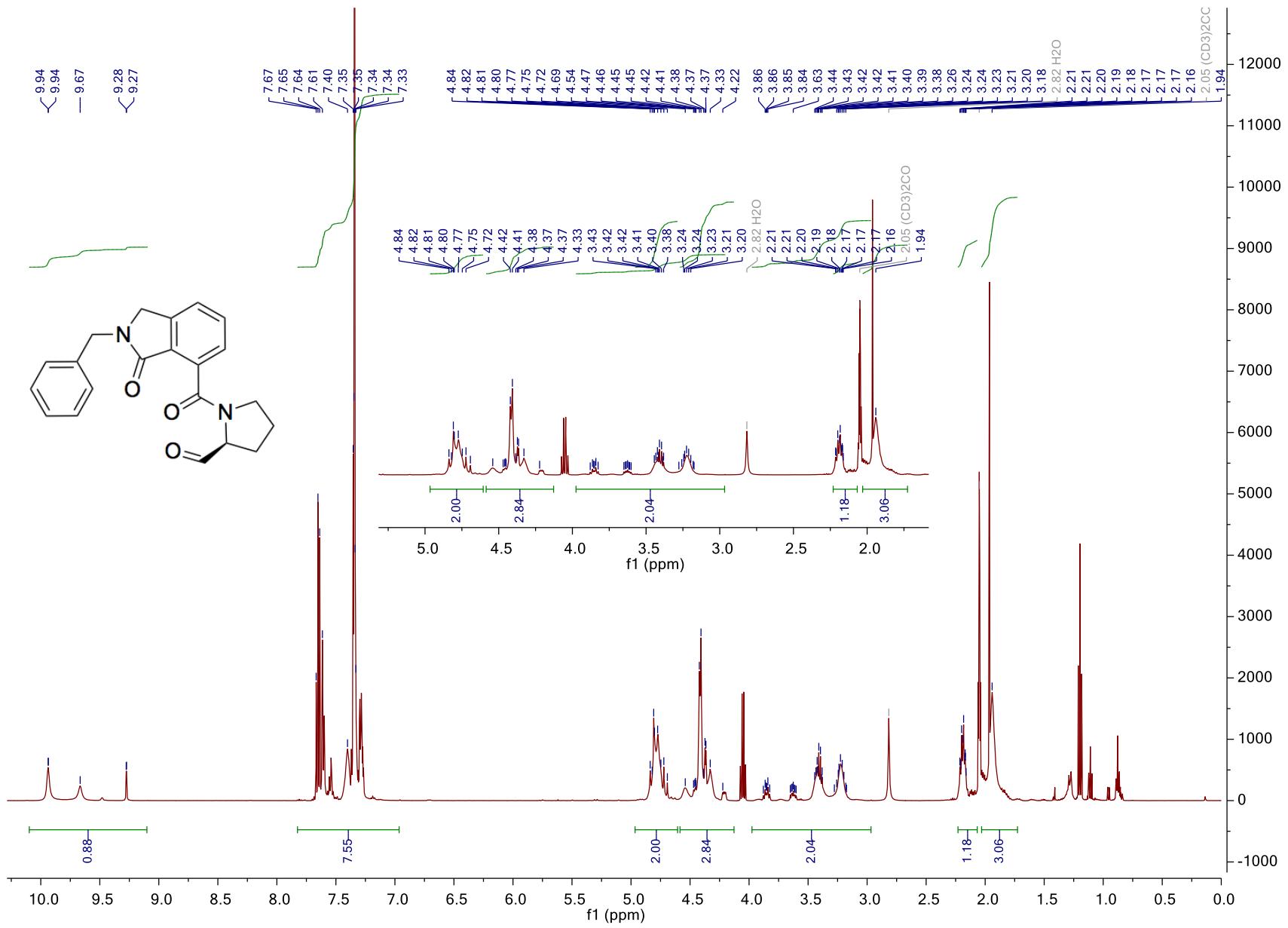


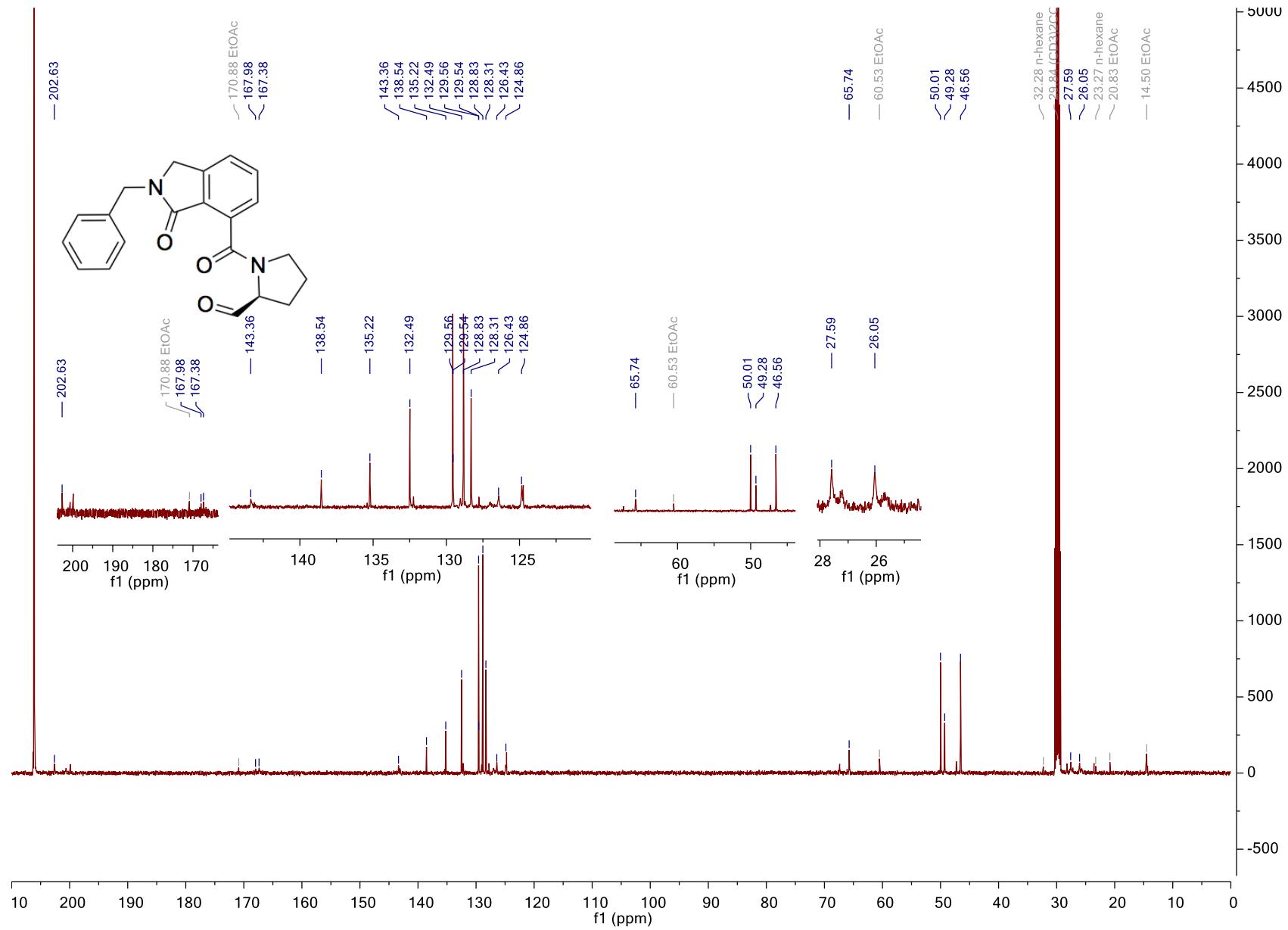












### III. Purity of Tested Compounds

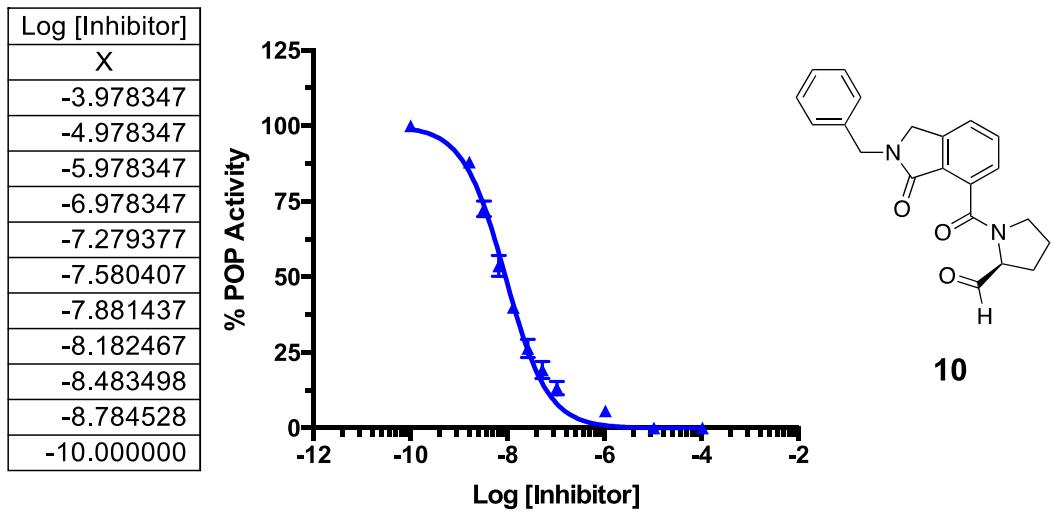
**Table S1.** Purity of Biologically Tested Compounds

Compound	Retention time (min.) <sup>a</sup>	purity (%) <sup>b</sup>
<b>4</b>	12.68	99.2
<b>5</b>	16.71	99.7
<b>10</b>	12.65	73.4
	13.26	23.4
		(96.8)
<b>12</b>	1.50	94.6
<b>13</b>	14.04	96.9
<b>14</b>	16.00	96.3
<b>15</b>	13.17	95.3
<b>16<sup>d</sup></b>	12.56	97.0
<b>17<sup>d</sup></b>	12.66	96.2
<b>20<sup>d</sup></b>	12.49	99.9

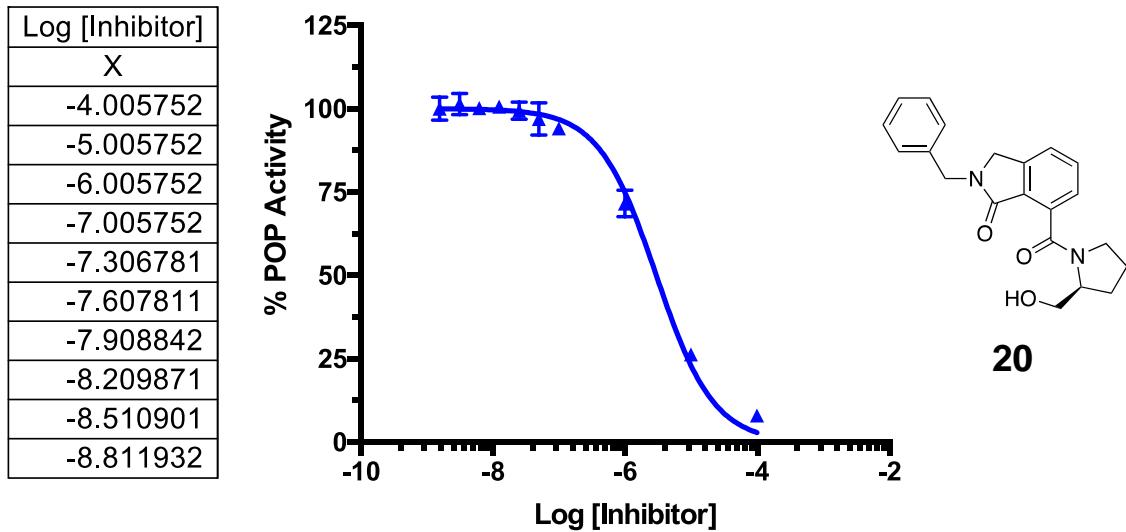
<sup>a</sup> Conditions: (gradient of 95% water, 5% MeOH or MeCN, 1 mL/min). <sup>b</sup> UV detection at 254 nm. <sup>c</sup> Hydrate and aldehyde form. <sup>d</sup> Slow rotation leads to “shoulders,” or rotamers partially separable over the time of this experiment.

## IV. Biological Assays

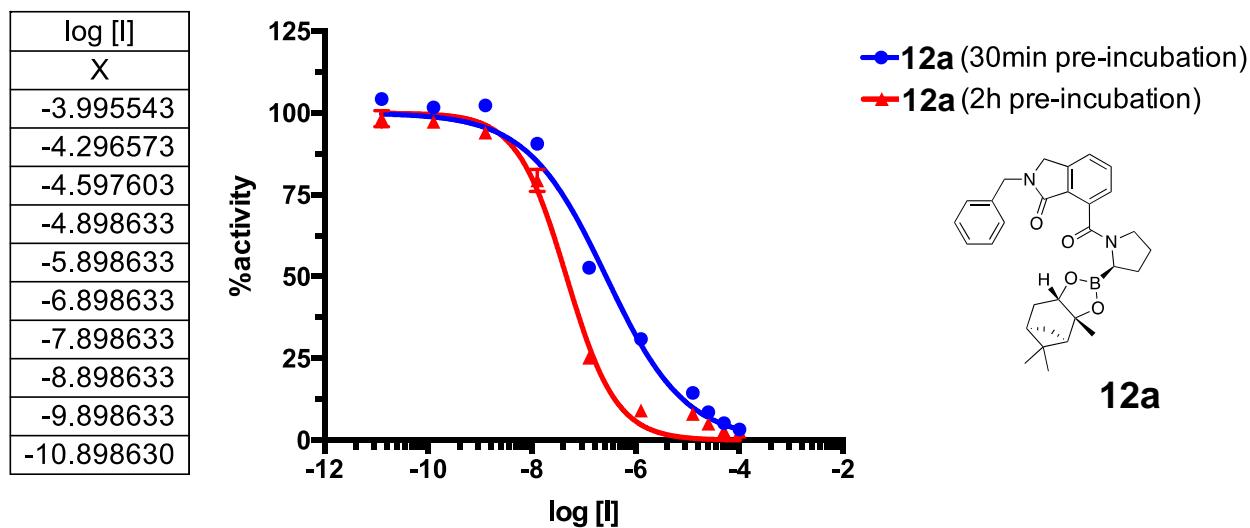
### Dose-Response Curves



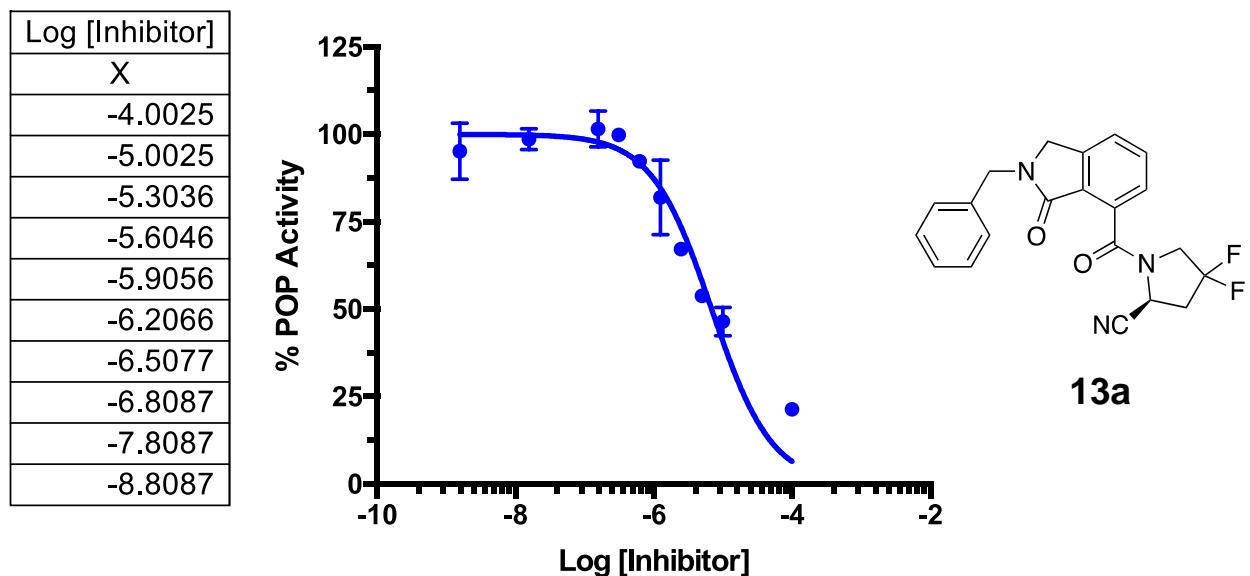
**Figure S2.** Inhibitory measurement for compound **10**.



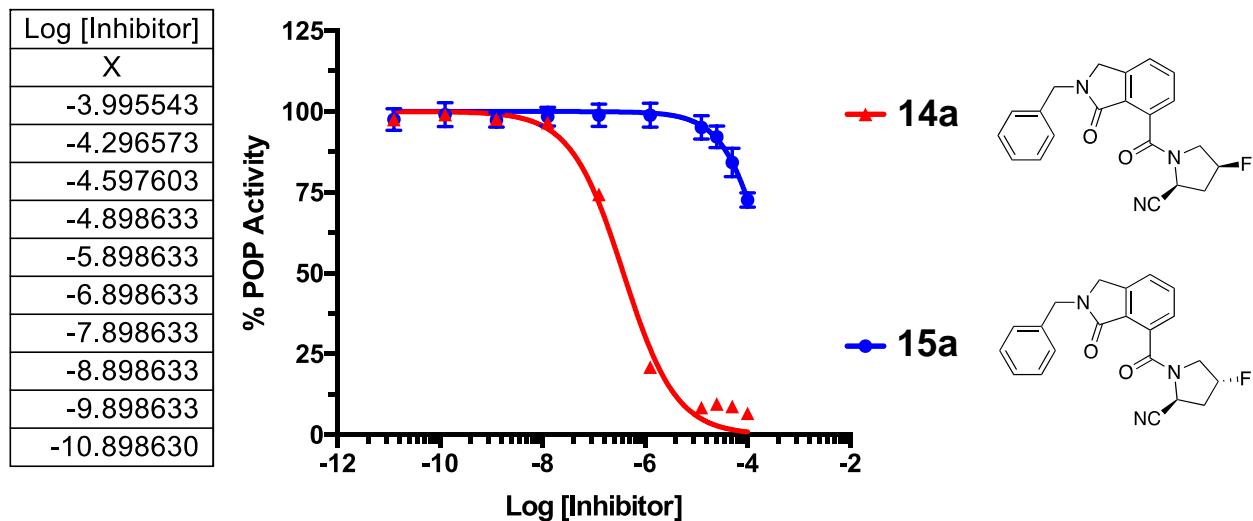
**Figure S3.** Inhibitory measurement for compound **22**



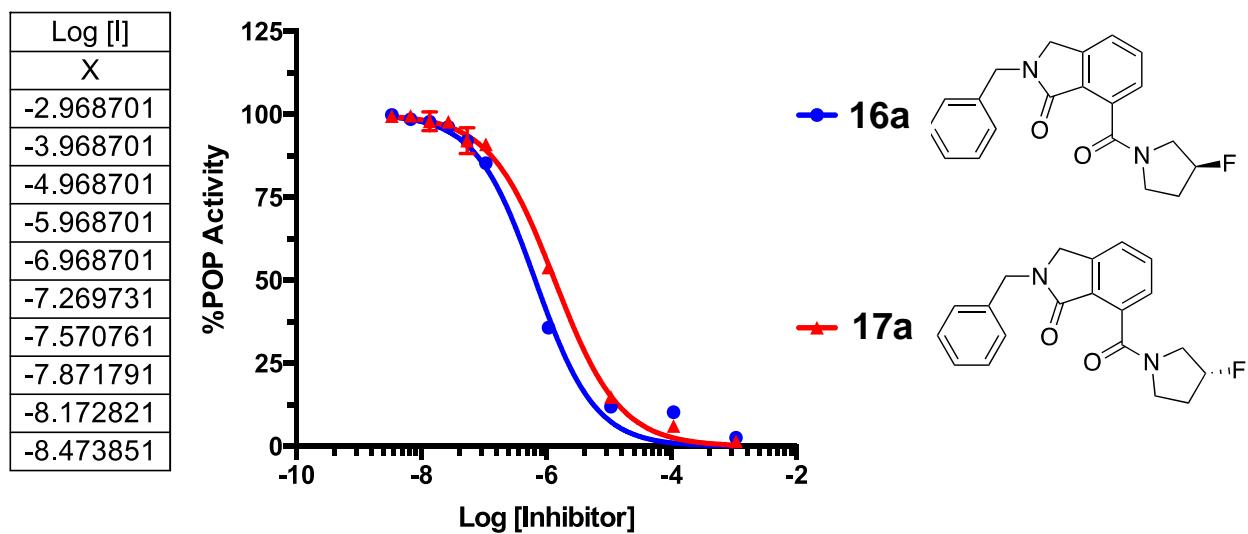
**Figure S4.** Inhibitory measurement for compound **12** at different pre-incubation time points.



**Figure S5.** Inhibitory measurement for compound **13**



**Figure S6.** Inhibitory measurement for compounds **14** and **15**



**Figure S7.** Inhibitory measurement for compound **16** and **17**

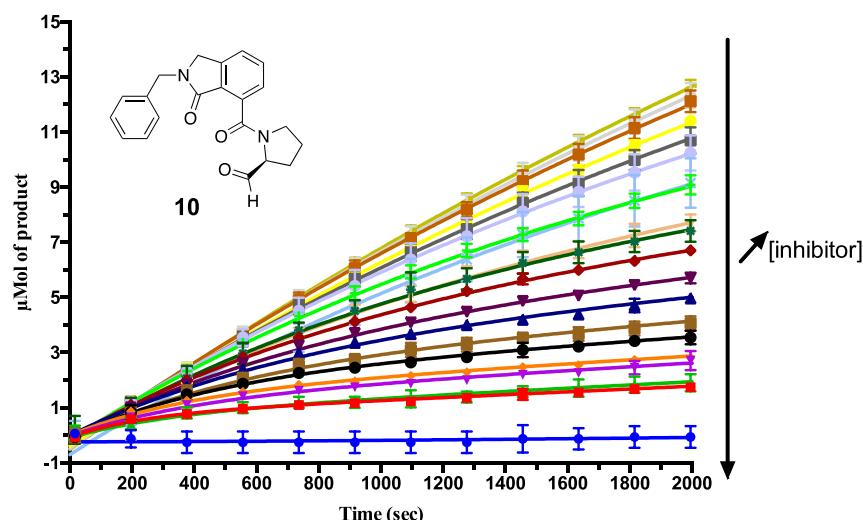
## Progress curves.

The reactions were performed in micro titer plates of 96 wells. For each reaction, 140  $\mu$ L of activity buffer was added, followed by 20  $\mu$ L of hPOP (10 nM in A.B.). After 15 min of equilibration at 30 °C, 20  $\mu$ L of inhibitor solution was added (different concentrations were prepared by serial dilution from an original 0.1M stock in DMSO that was kept at -80 °C). Directly afterwards, 20  $\mu$ L of a 800  $\mu$ M substrate solution (30 % MeCN in activity buffer). Once substrate was added, the absorbance at 405 nm was recorded every 30 sec. during a period of time ranging from 2h to 5h depending on the inhibitor. Data were then fitted to the equation S1 in order to extract  $k_{obs}$ . These values were further plotted against inhibitor concentration used and the data fitted to equation S2 in order to retrieve kinetic parameters.

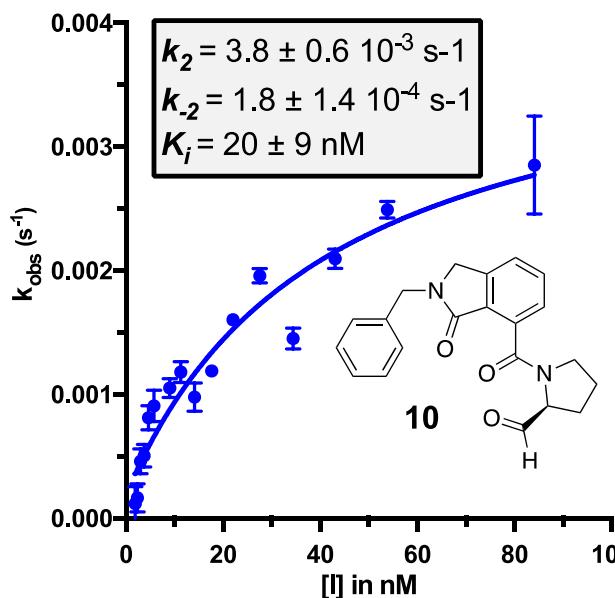
$$[P] = v_i t + \frac{v_0 - v_i}{k_{obs}} [1 - \exp(-k_{obs} t)] + y_{offset} \quad (\text{Eq. S1})$$

$$k_{obs} = k_{-2} + \left[ \frac{k_2[I]}{K_i^{\text{app}} + [I]} \right] \quad (\text{Eq. S2})$$

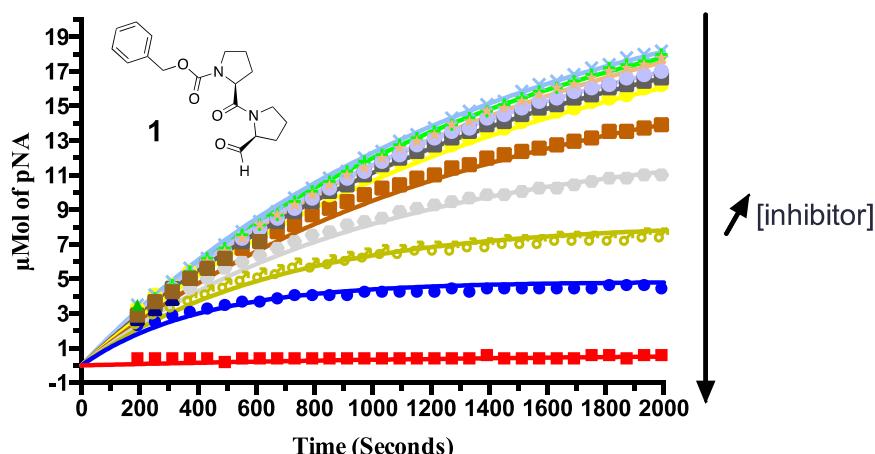
$$\text{with } K_i^{\text{app}} = K_i \left( 1 + \frac{[S]}{K_m} \right)$$



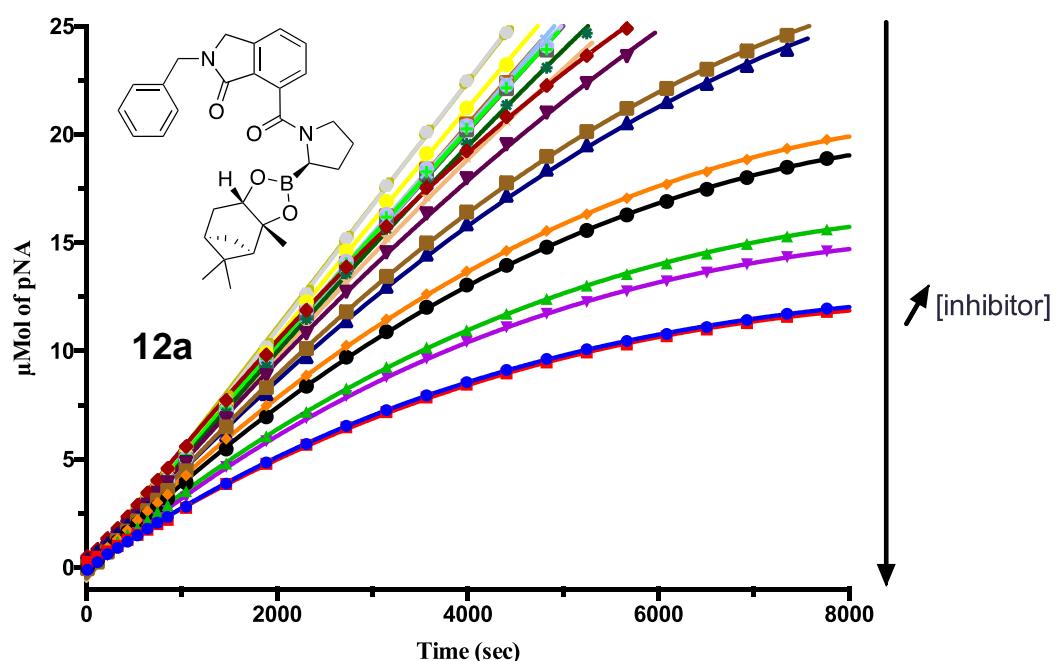
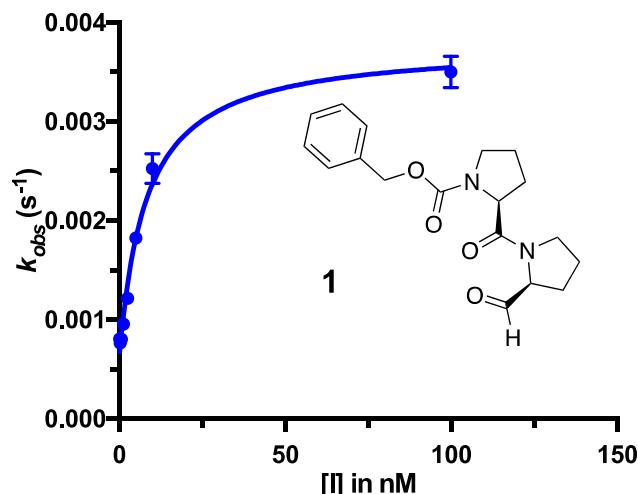
**Figure S8.** Progress curves at different inhibitor concentrations of **10**. Dots represent experimental data and the solid line represent the best fit to equation S1.

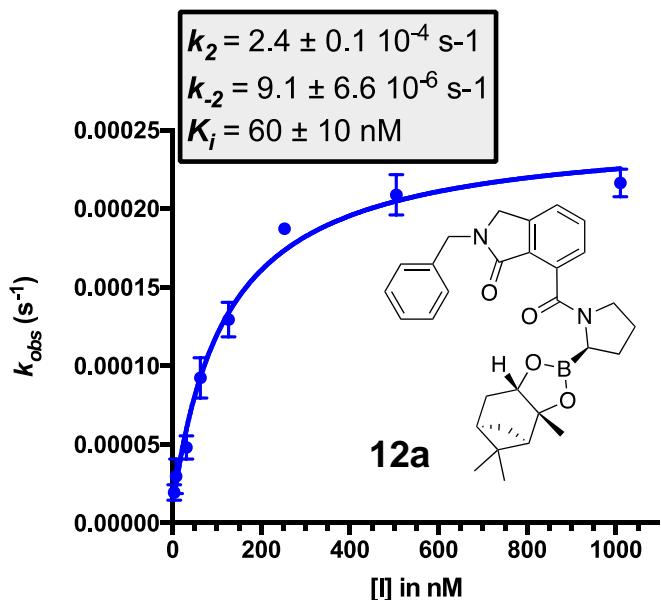


**Figure S9.** Relationship of  $k_{\text{obs}}$  obtained from fitting the progress curves to S1 and inhibitor concentration of **10**. Dots represents experimental data and the solid line represent the best fit to equation S2. to extract the corresponding kinetic parameters.



**Figure S10.** Progress curves at different inhibitor concentrations of **1**. Dots represents experimental data and the solid line represent the best fit to equation S1.

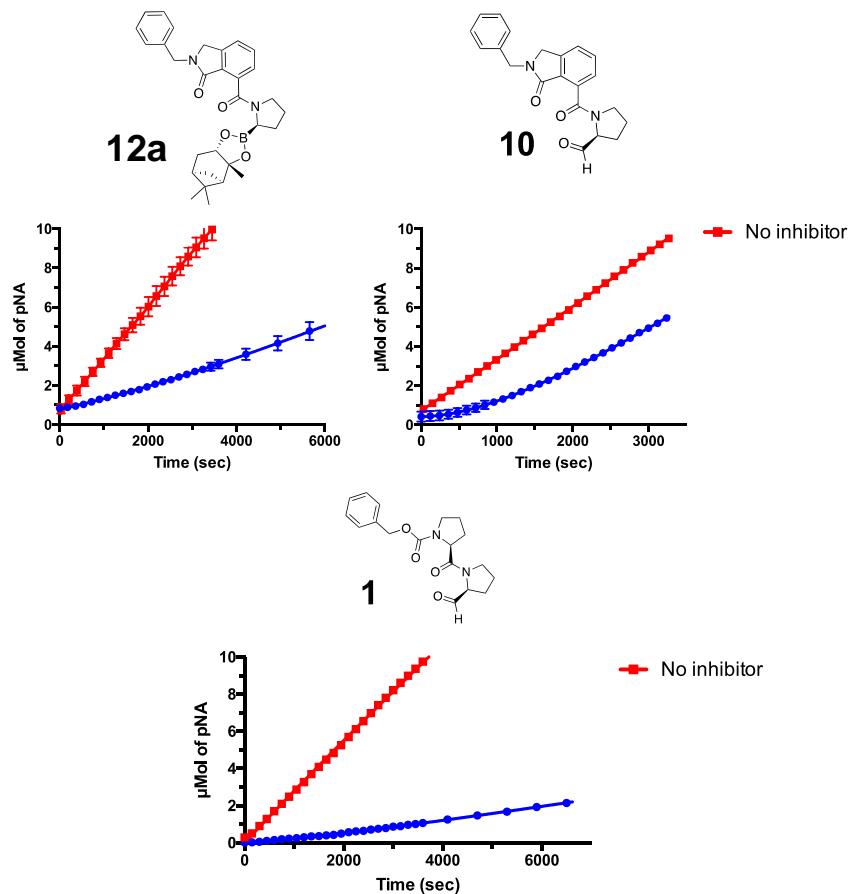




**Figure S3.** Relationship of  $k_{obs}$  obtained from fitting the progress curves to S1 and inhibitor concentration of **12**. Dots represents experimental data and the solid line represent the best fit to equation S2. to extract the corresponding kinetic parameters.

### Dilution experiment.

Inhibitor at a concentration of  $100 \times K_i$  was pre-incubated with 200 nM of hPOP in activity buffer for 2 h at 30 °C. Rapid serial dilutions (two times 40-fold dilution for a total of 1600-fold) were made with a substrate-containing buffer (Substrate concentration = 80 μM) pre-equilibrated at 30 °C. Final concentrations of inhibitor were  $0.06 \times K_i$  and the concentration of enzyme was 0.125 nM. The absorbance at 405 nm was immediately recorded every 30 sec for the first 60 minutes followed by every 2 minutes for the next 5 hours. Data were then fitted to above equation in order to extract  $k_{off}$ .



**Figure S4.** Curves from the rapid dilution experiments with the different inhibitors (blue) and in the absence of inhibitor (red).

## V. Definition of kinetic parameters.

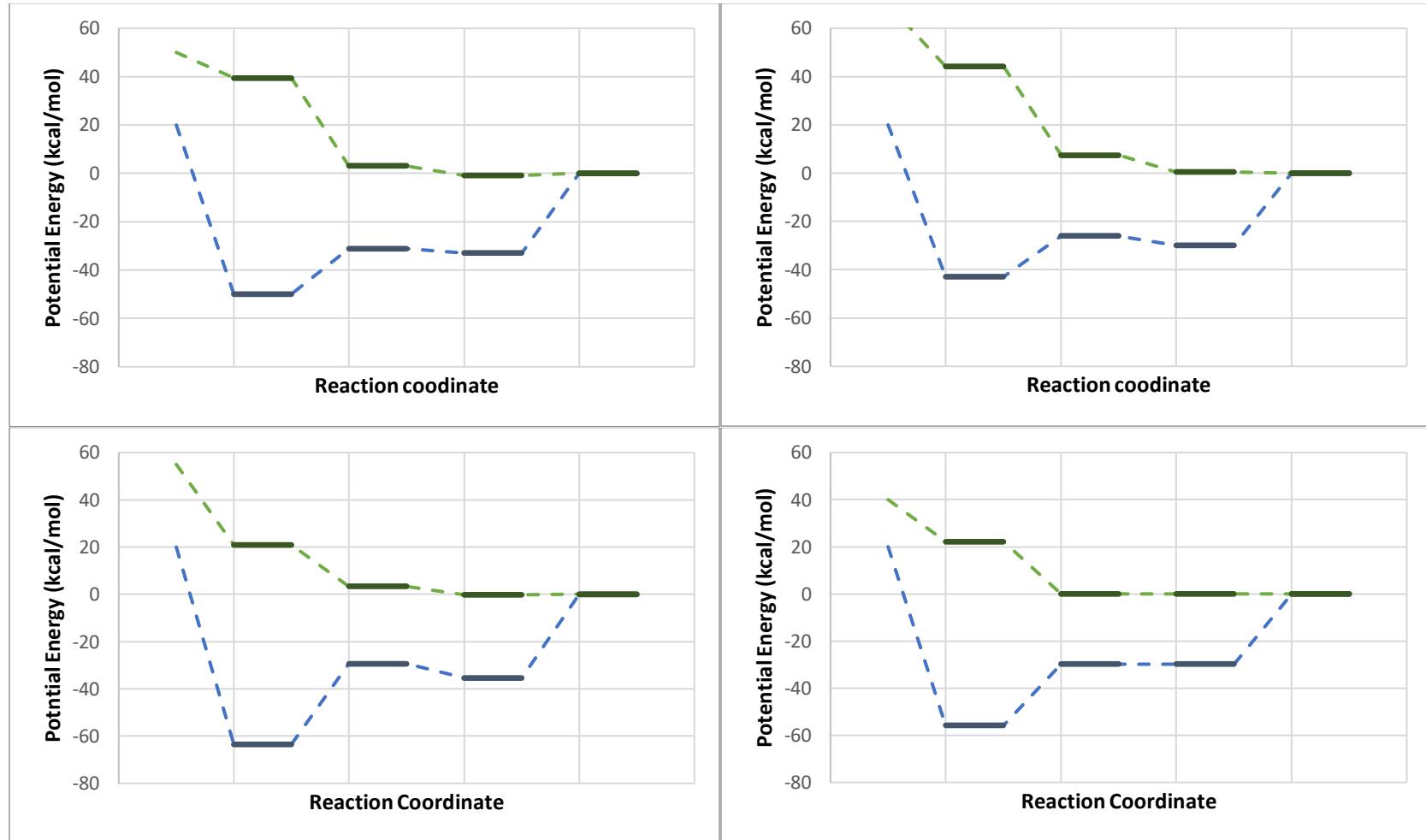
Kinetics parameters are defined as following:

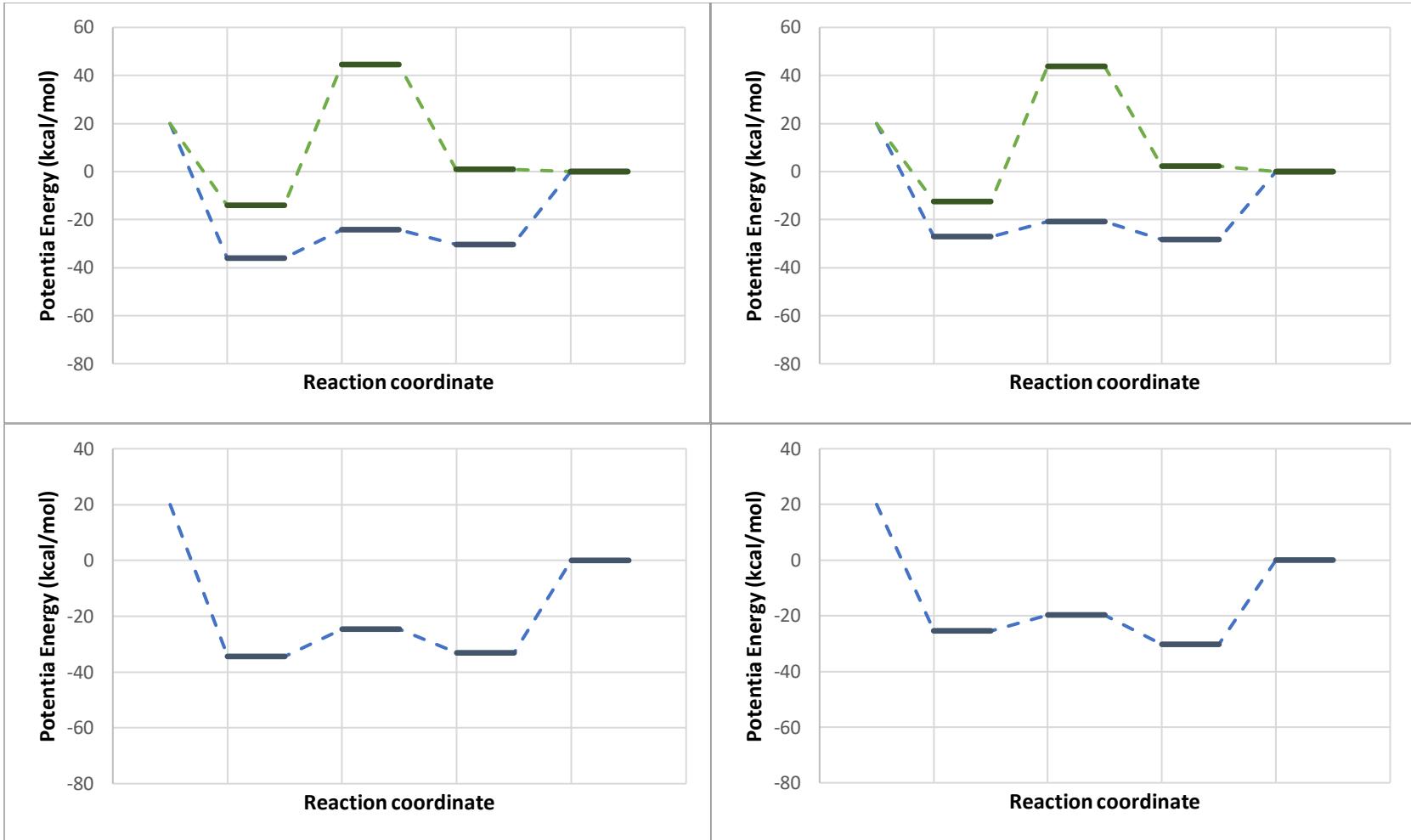
**Table S2.** Different relation of the kinetic parameters

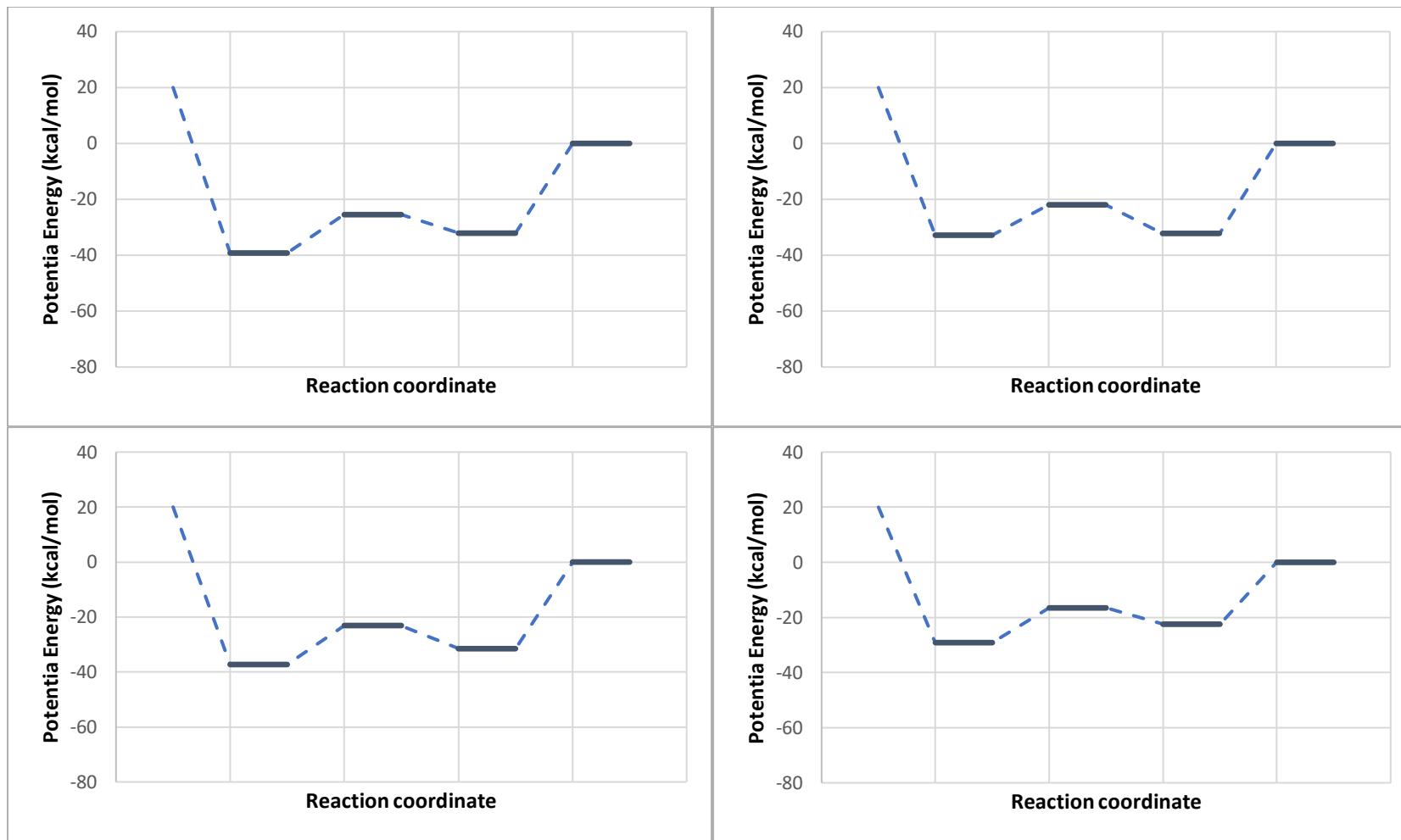
	One-step	Reversible covalent inhibition
$k_{on}$	$k_1$	$\frac{k_2}{K_i}$
$K_i$	$k_{-1}/k_1$	$k_{-1}/k_1$
$K_i^*$	-	$\frac{K_i}{\left(1 + \frac{k_2}{k_{-2}}\right)}$

<b>k<sub>off</sub></b>	$k_{-1}$	$\frac{k_{-1}k_{-2}}{(k_{-1} + k_2 + k_{-2})}$
<b>Residence-time</b>	$1/k_{-1}$	$1/k_{off}$

## VI. Computational Predictions







**Figure S15.** Computed binding energies for POP and FAP complexed with various inhibitors. Left: POP, right: FAP. From top to bottom: **10b**, **11b**, **5b**, **13b**, **14b** and **15b**. The uncatalyzed reactions were also computed for the first three inhibitors.

**Table S3.** Half-life of the covalent bond formation reaction computed using the Eyring eq. Energies are given in kcal/mol.

Cpd.	E <sub>on</sub> POP	k <sub>POP-theoretical</sub> (s <sup>-1</sup> )	E <sub>on</sub> FAP	k <sub>FAP-theoretical</sub> (s <sup>-1</sup> )	t <sub>1/2</sub> POP (s)	t <sub>1/2</sub> FAP (s)
5b	6.20	1.76E+08	7.50	1.96E+07	3.93E-09	3.53E-08
10b	1.80	2.97E+11	3.90	8.57E+09	2.33E-12	8.09E-11
11b	6.00	2.47E+08	0.50	2.67E+12	2.81E-09	2.60E-13
13b	8.40	4.29E+06	5.90	2.93E+08	1.61E-07	2.37E-09
14b	8.50	3.63E+06	10.60	1.05E+05	1.91E-07	6.63E-06
15b	6.60	8.97E+07	10.20	2.05E+05	7.73E-09	3.37E-06

**Table S4.** Half-life of the covalent bond breakage reaction computed using the Eyring eq. Energies are given in kcal/mol.

Cpd.	E <sub>off</sub> POP	k <sub>POP-theoretical</sub> (s <sup>-1</sup> )	E <sub>off</sub> FAP	k <sub>FAP-theoretical</sub> (s <sup>-1</sup> )	t <sub>1/2</sub> POP (s)	t <sub>1/2</sub> FAP (s)
5b	11.90	1.16E+04	6.20	1.76E+08	5.95E-05	3.93E-09
10b	18.80	1.01E-01	16.90	2.51E+00	6.84E+00	2.77E-01
11b	34.10	6.10E-13	26.00	5.31E-07	1.14E+12	1.30E+06
13b	14.20	2.39E+02	12.60	3.57E+03	2.89E-03	1.94E-04
14b	9.80	4.04E+05	5.70	4.10E+08	1.72E-06	1.69E-09
15b	13.70	5.57E+02	10.90	6.30E+04	1.24E-03	1.10E-05

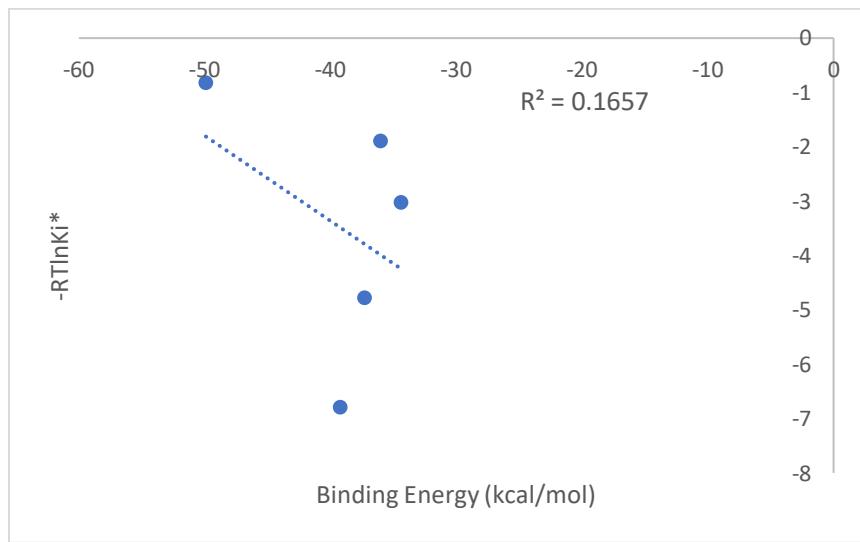
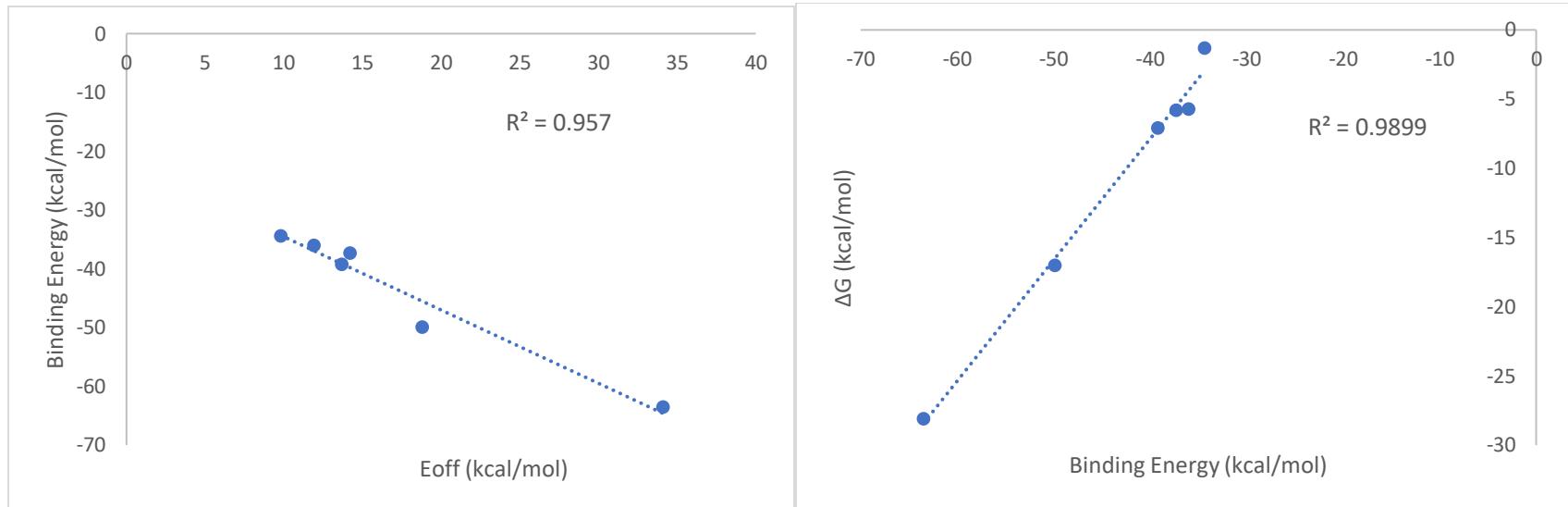
### Eyring equation:

$$k_{\text{theoretical}} = \kappa k_B T / h \times e^{-\Delta G / RT}$$

where:

$k$  = rate constant;  $\kappa$  = transmission coefficient (taken as unity);  $k_B$  = Boltzmann constant;  $T = 298$  K;  $h$  = Planck's constant;  $\Delta G = E_{\text{on}}$  or  $E_{\text{off}}$ ;  $R$  = ideal gas constant

$$t_{1/2} = 0.693 / k$$



**Figure S16.** Correlation for theoretical values obtained in POP for : top left : Binding energy vs. E<sub>off</sub>; top right: ΔG vs. binding energy; bottom left: -RTlnK<sub>i</sub>\* vs. binding energy.

**Table S5.** LUMO energies (in Hartrees) for compounds **5b**, **10b** and **11b**.

Cpd.	HF/def2-TZVP $E_{\text{LUMO}}$ (Eh)	Energy Difference (kcal/mol)
<b>5b</b>	0.1053	5.3203
<b>10b</b>	0.1086	7.4052
<b>11b</b>	0.0968	0.0000

**Table S6.** Intrinsic atomic orbital (IAO) atomic charges for the reactive atoms in compounds **5b**, **10b** and **11b**.

Cpd.	IAO Charge reactive atom
<b>5b</b> ( <chem>C#N</chem> )	0.1453
<b>10b</b> ( <chem>C=O</chem> )	0.3325
<b>11b</b> ( <chem>B</chem> )	0.7445

**Table S7.** Total atomic nucleophilic superdelocalizabilities (TANS) for the reactive atoms in compounds **5b**, **10b** and **11b**.

Cpd.	TANS reactive atom
<b>5b</b> ( <chem>C#N</chem> )	1.0600
<b>10b</b> ( <chem>C=O</chem> )	1.2400
<b>11b</b> ( <chem>B</chem> )	9.8400

## Potential Energy Surface Scan Coordinates

### FAP / 10b at 2.20 Å

C 0.96612 -1.54738 -1.68589  
N -0.48241 -0.06984 -2.90718  
C 0.21468 -0.23116 -1.62604  
C -0.91229 -0.23297 -0.60943  
C -2.07823 -0.86127 -1.37088  
C -1.91668 -0.31572 -2.78997  
H 1.91036 -1.50190 -2.26757  
C 0.17478 0.36428 -3.99757  
O 1.37882 0.65093 -3.95174  
C -0.63693 0.53322 -5.25450  
O 0.42066 -2.62730 -1.45390  
H 0.93798 0.58168 -1.49527  
H -1.13817 0.80940 -0.32645  
H -0.60945 -0.77342 0.29678  
H -3.06423 -0.61945 -0.95409  
H -1.95310 -1.95282 -1.36653  
H -2.46717 0.63161 -2.93221  
H -2.26984 -1.02728 -3.55227  
H 0.05099 0.69569 -6.09268  
H -1.29317 1.41233 -5.13460  
H -1.26842 -0.34348 -5.45823  
C 0.94400 9.25900 -7.06500  
H 1.82722 9.39228 -6.41950  
C 0.37300 7.84900 -6.94200  
H -0.54376 7.78058 -7.55379  
H 0.04855 7.64461 -5.90764  
C 1.34021 6.76634 -7.40556  
H 2.24994 6.78016 -6.77888  
H 1.66927 6.98688 -8.43765  
C 0.73644 5.36323 -7.37231  
H 1.35224 4.66585 -7.96353  
H -0.24447 5.38083 -7.87663  
N 0.53376 4.83942 -6.04588  
H -0.38917 5.07395 -5.54146  
C 1.29093 3.90698 -5.48034  
N 2.41533 3.45169 -6.09095  
H 2.97014 2.76085 -5.60439  
H 2.88101 4.01321 -6.78679  
N 0.94186 3.39490 -4.31092  
H 1.38634 2.51150 -4.04316  
H -0.08922 3.44964 -4.05859  
H 0.20467 10.01668 -6.76450  
H 1.25646 9.47876 -8.09911  
C -4.90900 5.91000 -5.26300  
H -4.11110 5.69521 -5.98992  
C -4.32100 5.98300 -3.85300  
H -5.12321 6.18831 -3.12358  
H -3.60623 6.81882 -3.78656  
C -3.60092 4.69782 -3.47587  
H -4.22199 3.81449 -3.70473  
H -3.41837 4.64112 -2.38909  
C -2.24351 4.47071 -4.13702  
O -1.68543 3.37210 -3.88357  
O -1.76305 5.37974 -4.85974  
H -5.39824 6.85207 -5.56019  
H -5.66419 5.11000 -5.34365  
C 4.24000 -9.06600 -1.92100  
H 4.48827 -8.30506 -1.16565

C 4.04500 -8.41900 -3.29700  
 H 3.84531 -9.20339 -4.04642  
 H 4.97557 -7.91744 -3.61073  
 C 2.91090 -7.42975 -3.27771  
 C 3.12819 -6.08865 -2.94583  
 H 4.15108 -5.73083 -2.78730  
 C 1.58562 -7.84032 -3.47037  
 H 1.38009 -8.88186 -3.73988  
 C 2.07479 -5.19404 -2.79057  
 H 2.26372 -4.15307 -2.51960  
 C 0.51967 -6.96101 -3.31804  
 H -0.51175 -7.29146 -3.46222  
 C 0.74846 -5.62627 -2.95256  
 O -0.29976 -4.81835 -2.77511  
 H -0.00069 -3.98674 -2.33683  
 H 5.05005 -9.81409 -1.92375  
 H 3.31810 -9.56800 -1.58857  
 C 3.66400 -2.43600 1.38200  
 H 3.31678 -1.74430 2.16929  
 C 3.22150 -3.84227 1.79163  
 O 3.89996 -4.53965 2.53025  
 C 3.12699 -1.93700 0.04100  
 H 2.81688 -2.82949 -0.54653  
 H 4.00901 -1.54415 -0.52413  
 O 2.11704 -1.00778 0.10971  
 H 4.76209 -2.45161 1.43513  
 N 2.03637 -4.26804 1.27040  
 H 1.52288 -3.64518 0.65491  
 C 1.55000 -5.61200 1.45100  
 H 2.35541 -6.19660 1.91641  
 H 1.27704 -6.06717 0.48509  
 H 0.66840 -5.65668 2.11480  
 C -5.52900 1.22600 5.75400  
 H -4.73973 1.99317 5.75270  
 C -5.05600 -0.04600 5.03800  
 H -5.83405 -0.82427 5.11198  
 H -4.16119 -0.45184 5.53707  
 C -4.75514 0.26358 3.59442  
 C -3.46705 0.60707 3.17445  
 H -2.63165 0.53740 3.87739  
 C -5.78936 0.35911 2.65313  
 H -6.80858 0.09425 2.95266  
 C -3.21510 1.04649 1.87654  
 H -2.19852 1.31834 1.58023  
 C -5.55509 0.78895 1.35247  
 H -6.36468 0.86679 0.62367  
 C -4.26292 1.15255 0.95790  
 O -4.09046 1.58175 -0.31310  
 H -3.16496 1.80523 -0.46580  
 H -5.81623 1.02786 6.80014  
 H -6.40279 1.65654 5.24019  
 C 4.04800 8.03900 3.82500  
 H 4.67058 8.25330 2.94291  
 C 4.36400 6.65100 4.38700  
 H 3.82310 6.48286 5.33523  
 H 5.43168 6.51537 4.61661  
 C 3.91654 5.56748 3.42544  
 O 4.56742 4.44163 3.55416  
 O 3.03284 5.77929 2.61715  
 H 4.23720 8.82840 4.56929  
 H 3.00028 8.08259 3.49793  
 H 4.31000 3.79726 2.73867  
 C 5.56700 5.31200 0.33900

H 5.69070 5.17632 1.42188  
 C 4.17900 4.89900 -0.11000  
 H 4.05940 5.02530 -1.19884  
 H 3.43949 5.55537 0.37660  
 C 3.82768 3.47559 0.25184  
 N 3.98848 2.99646 1.52916  
 C 3.28519 2.45396 -0.50850  
 H 2.98692 2.43113 -1.55498  
 C 3.55336 1.74637 1.52090  
 H 3.53254 1.08959 2.39024  
 N 3.12015 1.36618 0.31282  
 H 5.76315 6.37071 0.10320  
 H 6.34489 4.70797 -0.15623  
 H 2.66809 0.34865 0.13780

### FAP / 10b at 2.80 Å

C 0.63773 -1.69668 -2.30985  
 N -0.23610 0.12052 -3.58029  
 C 0.16858 -0.25498 -2.22328  
 C -1.11150 -0.08275 -1.41789  
 C -2.20617 -0.48002 -2.40692  
 C -1.69075 0.02708 -3.75621  
 H 1.66988 -1.83652 -2.70618  
 C 0.61163 0.73972 -4.43844  
 O 1.78848 0.95621 -4.15042  
 C 0.00739 1.16731 -5.75212  
 O -0.07691 -2.64735 -2.08422  
 H 1.01091 0.36761 -1.89185  
 H -1.19299 0.97957 -1.13386  
 H -1.10186 -0.68871 -0.50243  
 H -3.18571 -0.05266 -2.15372  
 H -2.30349 -1.57424 -2.40916  
 H -2.08487 1.03092 -3.98324  
 H -1.95090 -0.65506 -4.58109  
 H 0.80612 1.55196 -6.39678  
 H -0.73783 1.95824 -5.56102  
 H -0.50484 0.33373 -6.25575  
 C 0.94400 9.25900 -7.06500  
 H 1.70920 9.44520 -6.29447  
 C 0.37300 7.84900 -6.94200  
 H -0.40379 7.68574 -7.70873  
 H -0.13385 7.72607 -5.96999  
 C 1.46161 6.78265 -7.09320  
 H 2.25718 6.96418 -6.34962  
 H 1.93748 6.89331 -8.08444  
 C 0.99697 5.32996 -6.95858  
 H 1.77652 4.65681 -7.35527  
 H 0.11484 5.16671 -7.60117  
 N 0.64077 4.93745 -5.61860  
 H -0.36187 5.13869 -5.28678  
 C 1.34877 4.15367 -4.81318  
 N 2.60033 3.72785 -5.10822  
 H 2.80895 2.78230 -4.78358  
 H 3.02661 4.01575 -5.97618  
 N 0.81731 3.77262 -3.65458  
 H 1.38706 3.18060 -3.06213  
 H -0.22912 3.62175 -3.62509  
 H 0.16177 10.02308 -6.94019  
 H 1.42385 9.41701 -8.04492  
 C -4.90900 5.91000 -5.26300  
 H -4.12489 5.63085 -5.98273  
 C -4.32100 5.98300 -3.85300  
 H -5.11525 6.24501 -3.13288

H -3.56237 6.77854 -3.79798  
 C -3.67729 4.66786 -3.45449  
 H -4.33600 3.81155 -3.68109  
 H -3.49909 4.61084 -2.36709  
 C -2.33091 4.40399 -4.11100  
 O -1.77976 3.29980 -3.84541  
 O -1.83661 5.30239 -4.83295  
 H -5.34084 6.87156 -5.58560  
 H -5.71103 5.15523 -5.32477  
 C 4.24000 -9.06600 -1.92100  
 H 4.36875 -8.29960 -1.14112  
 C 4.04500 -8.41900 -3.29700  
 H 3.94257 -9.20063 -4.06723  
 H 4.94219 -7.83379 -3.56364  
 C 2.83010 -7.52958 -3.30849  
 C 2.84040 -6.30484 -2.63110  
 H 3.76128 -5.95449 -2.15371  
 C 1.62577 -7.92987 -3.89788  
 H 1.58512 -8.88304 -4.43460  
 C 1.69956 -5.51701 -2.53247  
 H 1.72277 -4.57430 -1.98009  
 C 0.47577 -7.15034 -3.81673  
 H -0.45852 -7.47245 -4.28205  
 C 0.49775 -5.93217 -3.12609  
 O -0.62894 -5.21019 -3.05321  
 H -0.43815 -4.34619 -2.64081  
 H 5.12410 -9.72384 -1.89352  
 H 3.36057 -9.66769 -1.64424  
 C 3.66400 -2.43600 1.38200  
 H 3.34998 -1.73242 2.17154  
 C 3.23340 -3.84578 1.78295  
 O 3.93535 -4.55851 2.47969  
 C 3.12699 -1.93700 0.04100  
 H 2.99650 -2.79546 -0.64442  
 H 3.89535 -1.28648 -0.41674  
 O 1.91947 -1.23306 0.13600  
 H 4.76332 -2.45397 1.40149  
 N 2.03652 -4.26373 1.27786  
 H 1.45932 -3.58453 0.79456  
 C 1.55000 -5.61200 1.45100  
 H 2.36867 -6.20095 1.88588  
 H 1.25325 -6.05319 0.48594  
 H 0.68869 -5.66454 2.13912  
 C -5.52900 1.22600 5.75400  
 H -4.75167 2.00472 5.72566  
 C -5.05600 -0.04600 5.03800  
 H -5.82038 -0.83409 5.14685  
 H -4.14363 -0.43192 5.52081  
 C -4.79253 0.22257 3.57782  
 C -3.50791 0.50377 3.10249  
 H -2.65324 0.43933 3.78220  
 C -5.85208 0.30838 2.66358  
 H -6.86924 0.08849 3.00368  
 C -3.28355 0.87337 1.77737  
 H -2.26834 1.09568 1.43486  
 C -5.64695 0.67418 1.33866  
 H -6.47783 0.75091 0.63418  
 C -4.35720 0.97649 0.88875  
 O -4.21064 1.35711 -0.40195  
 H -3.29638 1.61597 -0.56327  
 H -5.78394 1.03093 6.80854  
 H -6.42293 1.63971 5.26105  
 C 4.04800 8.03900 3.82500

H 4.63747 8.23303 2.91507  
 C 4.36400 6.65100 4.38700  
 H 3.87505 6.50305 5.36653  
 H 5.44021 6.48595 4.55054  
 C 3.83049 5.56403 3.43869  
 O 4.37215 4.41834 3.55535  
 O 2.94502 5.87806 2.63502  
 H 4.27294 8.84275 4.54707  
 H 2.99068 8.08372 3.53167  
 H 3.95380 3.63160 2.43436  
 C 5.56700 5.31200 0.33900  
 H 5.68561 5.16715 1.42342  
 C 4.17900 4.89900 -0.11000  
 H 4.05707 5.04121 -1.19750  
 H 3.45195 5.56127 0.39090  
 C 3.75484 3.48965 0.22353  
 N 3.68177 3.04381 1.51528  
 C 3.26985 2.44064 -0.54774  
 H 3.18035 2.37802 -1.63367  
 C 3.17169 1.80496 1.48533  
 H 2.99763 1.22353 2.39145  
 N 2.89788 1.38839 0.25585  
 H 5.74811 6.37509 0.11395  
 H 6.35039 4.72095 -0.16442  
 H 2.17138 -0.26197 0.17041

### FAP / 10b optimum structure

C 1.00206 -1.63364 -0.94201  
 N -0.94685 -0.61645 -2.00956  
 C -0.16121 -0.63729 -0.78043  
 C -1.15188 -1.07172 0.29035  
 C -2.15407 -1.93960 -0.46975  
 C -2.21126 -1.33866 -1.87610  
 H 1.53665 -1.35746 -1.88360  
 C -0.48257 0.01702 -3.10208  
 O 0.57598 0.66293 -3.06441  
 C -1.30900 -0.05704 -4.35947  
 O 0.66280 -2.91866 -0.88836  
 H 0.25176 0.36860 -0.60813  
 H -1.64314 -0.19612 0.74113  
 H -0.63513 -1.62568 1.08644  
 H -3.14625 -1.96358 0.00514  
 H -1.75242 -2.95947 -0.52712  
 H -3.05709 -0.63954 -1.98802  
 H -2.30330 -2.12429 -2.64295  
 H -0.63174 0.00935 -5.22050  
 H -1.98211 0.81652 -4.38950  
 H -1.90437 -0.97541 -4.43289  
 C 0.94400 9.25900 -7.06500  
 H 1.77326 9.41763 -6.35652  
 C 0.37300 7.84900 -6.94200  
 H -0.46398 7.72817 -7.65165  
 H -0.06060 7.68007 -5.94215  
 C 1.43356 6.78514 -7.24267  
 H 2.23222 6.83477 -6.48009  
 H 1.91711 7.04581 -8.20209  
 C 0.94706 5.33871 -7.36911  
 H 1.73169 4.73559 -7.85277  
 H 0.08578 5.31351 -8.06089  
 N 0.54973 4.68191 -6.14455  
 H -0.40299 4.90261 -5.72521  
 C 1.13042 3.58862 -5.63424  
 N 2.41857 3.28203 -5.97746

H 2.83378 2.49408 -5.49768  
 H 3.04879 4.05319 -6.15299  
 N 0.45332 2.79855 -4.83954  
 H 0.84696 2.02381 -4.28547  
 H -0.60266 2.95357 -4.68359  
 H 0.18218 10.02361 -6.84902  
 H 1.33936 9.44554 -8.07703  
 C -4.90900 5.91000 -5.26300  
 H -4.11001 5.70020 -5.98931  
 C -4.32100 5.98300 -3.85300  
 H -5.11057 6.20697 -3.11570  
 H -3.58197 6.79860 -3.79682  
 C -3.63236 4.67297 -3.49939  
 H -4.33159 3.82403 -3.57693  
 H -3.28050 4.67803 -2.45173  
 C -2.40692 4.31557 -4.34086  
 O -2.07166 3.10347 -4.32602  
 O -1.79755 5.22920 -4.94682  
 H -5.40274 6.84988 -5.56055  
 H -5.66099 5.10711 -5.34361  
 C 4.24000 -9.06600 -1.92100  
 H 4.65548 -8.34845 -1.19738  
 C 4.04500 -8.41900 -3.29700  
 H 3.70622 -9.18102 -4.01880  
 H 5.02381 -8.06262 -3.66970  
 C 3.05715 -7.27711 -3.27490  
 C 3.22291 -6.21177 -2.37864  
 H 4.09804 -6.18718 -1.72111  
 C 1.92162 -7.24125 -4.09441  
 H 1.74704 -8.05618 -4.80641  
 C 2.30075 -5.17972 -2.28298  
 H 2.42692 -4.38488 -1.54742  
 C 0.99115 -6.20397 -4.02255  
 H 0.10471 -6.20340 -4.66203  
 C 1.14996 -5.15071 -3.09997  
 O 0.24786 -4.18370 -3.01752  
 H 0.41413 -3.61521 -2.15611  
 H 4.93221 -9.92300 -1.96577  
 H 3.28187 -9.42402 -1.51277  
 C 3.66400 -2.43600 1.38200  
 H 3.49077 -1.68582 2.17093  
 C 3.10392 -3.77826 1.87202  
 O 3.65396 -4.35648 2.79987  
 C 3.12699 -1.93700 0.04100  
 H 3.04766 -2.78278 -0.65910  
 H 3.87830 -1.24989 -0.40310  
 O 1.90325 -1.26835 0.14743  
 H 4.75290 -2.58559 1.32469  
 N 2.04169 -4.28052 1.20032  
 H 1.53985 -3.72887 0.47821  
 C 1.55000 -5.61200 1.45100  
 H 2.34118 -6.19754 1.94017  
 H 1.26564 -6.08976 0.50143  
 H 0.66868 -5.62148 2.11826  
 C -5.52900 1.22600 5.75400  
 H -4.72367 1.97237 5.82622  
 C -5.05600 -0.04600 5.03800  
 H -5.85198 -0.80711 5.05584  
 H -4.19916 -0.48057 5.58237  
 C -4.67525 0.25713 3.60775  
 C -3.65443 1.17325 3.32051  
 H -3.07580 1.61291 4.13747  
 C -5.37357 -0.28373 2.52207

H -6.17243 -1.00842 2.70632  
 C -3.35216 1.55194 2.01634  
 H -2.55012 2.27212 1.82612  
 C -5.07988 0.07813 1.20947  
 H -5.62654 -0.35494 0.36929  
 C -4.07253 1.01131 0.94596  
 O -3.82986 1.34108 -0.33978  
 H -3.04439 1.89549 -0.40398  
 H -5.87701 1.00900 6.77755  
 H -6.36197 1.69420 5.20705  
 C 4.04800 8.03900 3.82500  
 H 4.67918 8.25961 2.95068  
 C 4.36400 6.65100 4.38700  
 H 3.81264 6.48116 5.32893  
 H 5.42902 6.52307 4.63208  
 C 3.93673 5.55937 3.43196  
 O 4.62134 4.44727 3.56617  
 O 3.04586 5.73225 2.62573  
 H 4.22708 8.82481 4.57471  
 H 3.00285 8.08174 3.48899  
 H 4.36935 3.80625 2.78456  
 C 5.56700 5.31200 0.33900  
 H 5.69057 5.19424 1.42369  
 C 4.17900 4.89900 -0.11000  
 H 4.06667 5.01392 -1.20091  
 H 3.44778 5.58069 0.35532  
 C 3.76676 3.50026 0.26564  
 N 3.98944 2.98132 1.51963  
 C 3.06112 2.56434 -0.46489  
 H 2.65778 2.57821 -1.47452  
 C 3.43835 1.78537 1.54339  
 H 3.43202 1.10496 2.39405  
 N 2.86392 1.48940 0.36544  
 H 5.76091 6.36609 0.08562  
 H 6.34703 4.70179 -0.14501  
 H 2.39533 0.58979 0.16046

### FAP / 11b at 3.40 Å

B 0.39399 -2.32317 -2.66968  
 N -1.49866 -0.74776 -3.19453  
 C -0.37795 -0.98991 -2.24803  
 C -1.07974 -1.00580 -0.89412  
 C -2.45231 -1.58424 -1.21463  
 C -2.80013 -0.92860 -2.54562  
 C -1.29937 -0.34214 -4.44952  
 C -2.49089 0.00842 -5.28715  
 O -0.14058 -0.24012 -4.91811  
 O 0.80549 -2.45740 -3.97603  
 O 0.58910 -3.33798 -1.79171  
 H 0.33393 -0.15039 -2.32980  
 H -1.18824 0.02509 -0.51654  
 H -0.49970 -1.56351 -0.14997  
 H -3.21074 -1.38509 -0.44463  
 H -2.37873 -2.67735 -1.33858  
 H -3.29136 0.04652 -2.38937  
 H -3.46636 -1.54842 -3.16460  
 H -2.21400 -0.10770 -6.34224  
 H -2.74496 1.06629 -5.09078  
 H -3.36522 -0.61395 -5.05979  
 H 0.61436 -1.61252 -4.46712  
 H 1.07211 -4.07907 -2.18647  
 C 0.94400 9.25900 -7.06500  
 H 1.84955 9.38391 -6.44927

C 0.37300 7.84900 -6.94200  
 H -0.55672 7.79726 -7.53600  
 H 0.06604 7.62956 -5.90560  
 C 1.32081 6.76818 -7.45571  
 H 2.16318 6.62726 -6.75611  
 H 1.76523 7.11682 -8.40639  
 C 0.65435 5.42207 -7.74071  
 H 1.29092 4.83341 -8.41782  
 H -0.27543 5.61191 -8.30861  
 N 0.32319 4.61283 -6.58744  
 H -0.51822 4.87776 -5.99553  
 C 0.76421 3.36520 -6.40173  
 N 1.84155 2.91332 -7.11156  
 H 2.21539 2.01510 -6.83511  
 H 2.54166 3.59175 -7.37856  
 N 0.14901 2.56306 -5.56627  
 H 0.44148 1.59664 -5.42092  
 H -0.80063 2.83549 -5.11368  
 H 0.21689 10.01356 -6.72915  
 H 1.21877 9.48956 -8.10731  
 C -4.90900 5.91000 -5.26300  
 H -4.10393 5.75456 -5.99584  
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 H -4.29700 3.83369 -3.51890  
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 O -1.80993 5.21704 -5.01914  
 H -5.44763 6.83165 -5.53781  
 H -5.62322 5.07455 -5.35789  
 C 4.24000 -9.06600 -1.92100  
 H 4.41563 -8.30583 -1.14428  
 C 4.04500 -8.41900 -3.29700  
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 C 2.89215 -7.47603 -3.48897  
 C 3.13070 -6.12998 -3.76885  
 H 4.16013 -5.75799 -3.76740  
 C 1.55964 -7.91467 -3.51426  
 H 1.33434 -8.96275 -3.29260  
 C 2.10117 -5.25166 -4.09378  
 H 2.31743 -4.21218 -4.34595  
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 H -0.51819 -7.40446 -3.86765  
 C 0.77723 -5.71320 -4.15193  
 O -0.24519 -4.92078 -4.51151  
 H 0.08113 -3.99701 -4.54713  
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 H 3.35661 -9.64961 -1.61564  
 C 3.66400 -2.43600 1.38200  
 H 3.35086 -1.73035 2.16945  
 C 3.21767 -3.83982 1.78798  
 O 3.88990 -4.54010 2.52754  
 C 3.12700 -1.93700 0.04100  
 H 2.97471 -2.78960 -0.64475  
 H 3.90737 -1.30349 -0.42341  
 O 1.93830 -1.21007 0.14744  
 H 4.76330 -2.46570 1.40766  
 N 2.04151 -4.27188 1.24744  
 H 1.50965 -3.63640 0.66156

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 H 2.35887 -6.19414 1.91333  
 H 1.26060 -6.07879 0.49503  
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 H -4.74207 1.99551 5.75035  
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 C -3.46853 0.57434 3.15588  
 H -2.63480 0.54228 3.86338  
 C -5.78591 0.28156 2.63712  
 H -6.80384 0.01804 2.94173  
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 C -5.55079 0.66088 1.32013  
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 H -3.18123 1.72059 -0.49579  
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 H 5.68477 5.17186 1.42387  
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 C 3.26350 1.78377 1.49482  
 H 3.15176 1.17964 2.39595  
 N 2.89579 1.40263 0.27977  
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 H 6.35005 4.71703 -0.16097  
 H 2.19704 -0.24231 0.16910

### FAP / 11b optimum structure

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 C 0.05597 -0.27906 -1.27306  
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 C -2.14329 -1.10991 -0.87872  
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 C -1.04865 0.15430 -4.90950  
 O 1.03340 0.46420 -3.76516  
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 H 0.64017 0.65642 -1.24582

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 H 2.22935 6.75660 -6.69669  
 H 1.73580 6.99826 -8.37732  
 C 0.74411 5.35750 -7.40796  
 H 1.38336 4.68949 -8.00689  
 H -0.21574 5.40025 -7.95155  
 N 0.49230 4.75846 -6.12028  
 H -0.42590 4.98373 -5.61780  
 C 1.15426 3.70988 -5.63132  
 N 2.29963 3.27587 -6.22867  
 H 2.82046 2.55561 -5.74640  
 H 2.84791 3.92810 -6.76953  
 N 0.69426 3.07219 -4.57721  
 H 1.09505 2.16398 -4.29914  
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 H -5.69256 5.13667 -5.33256  
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 H 4.73753 -8.37509 -1.22264  
 C 4.04500 -8.41900 -3.29700  
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 H 5.03719 -8.19902 -3.72758  
 C 3.21338 -7.16540 -3.33387  
 C 3.79676 -5.89998 -3.20007  
 H 4.87859 -5.82548 -3.04790  
 C 1.82769 -7.21436 -3.53410  
 H 1.33605 -8.18537 -3.65910  
 C 3.04558 -4.73005 -3.26438  
 H 3.51593 -3.75091 -3.14578  
 C 1.06063 -6.05678 -3.60147  
 H -0.01857 -6.09957 -3.76675  
 C 1.65778 -4.79344 -3.47208  
 O 0.88598 -3.70745 -3.55836  
 H 1.36536 -2.87473 -3.20525

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 H 3.27554 -9.34655 -1.46871  
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 H 3.51547 -1.69266 2.18374  
 C 3.09809 -3.77193 1.87906  
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 H 3.94690 -1.34420 -0.41973  
 O 1.96308 -1.17963 0.02684  
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 H -2.40715 1.79087 1.64400  
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 H 4.67401 8.25596 2.94609  
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 H 4.06280 5.02356 -1.19937  
 H 3.44475 5.56920 0.36664  
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 N 3.98201 2.97599 1.51134  
 C 3.15054 2.53246 -0.50929  
 H 2.79457 2.55047 -1.53689  
 C 3.47482 1.75850 1.50474  
 H 3.45800 1.07481 2.35256  
 N 2.96136 1.44412 0.30483  
 H 5.76039 6.36888 0.09569  
 H 6.34645 4.70658 -0.15200  
 H 2.50880 0.52350 0.09024

## FAP / 5b at 2.00 Å

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C 0.71833 1.09429 -3.80816  
C 0.04620 1.40739 -5.12235  
N -0.03986 0.46363 -2.88899  
C -1.46371 0.14382 -3.01306  
C -1.83502 -0.41239 -1.63461  
C -0.79742 0.20862 -0.70366  
C 0.46884 0.15547 -1.55753  
C 1.03342 -1.22190 -1.54013  
N 1.01356 -2.29583 -2.01987  
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H 0.80981 1.74791 -5.83105  
H -0.69504 2.20777 -4.96202  
H -2.02100 1.06525 -3.24889  
H -1.64571 -0.59427 -3.81051  
H -2.87168 -0.17723 -1.35911  
H -1.71929 -1.50682 -1.62408  
H -1.02843 1.26786 -0.49957  
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H 0.38064 -3.57664 -2.93909  
C 0.94398 9.25900 -7.06507  
H 1.62780 9.48283 -6.23080  
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H -0.20819 7.76291 -6.00787  
C 1.46536 6.77713 -6.95266  
H 2.24647 7.03929 -6.21750  
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H 1.77173 4.63497 -6.97824  
H 0.11351 5.11588 -7.28343  
N 0.62110 5.10756 -5.28639  
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 O 4.53178 4.43624 3.56672  
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## FAP / 5b at 2.60 Å

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 C -5.82506 0.35522 2.66233  
 H -6.83923 0.09178 2.97968  
 C -3.26580 1.04106 1.83469  
 H -2.25331 1.30816 1.51677  
 C -5.61602 0.79058 1.35911  
 H -6.44136 0.87789 0.64928  
 C -4.33280 1.15863 0.93964  
 O -4.19279 1.60207 -0.33257  
 H -3.30509 1.95138 -0.47761  
 H -5.80204 1.02963 6.80405  
 H -6.41161 1.64890 5.24908  
 C 4.04805 8.03905 3.82492  
 H 4.63806 8.23339 2.91544  
 C 4.36405 6.65105 4.38692  
 H 3.87182 6.50112 5.36442  
 H 5.43979 6.48589 4.55290  
 C 3.83212 5.56752 3.43338

O 4.37665 4.42119 3.54162  
 O 2.94515 5.88226 2.63236  
 H 4.27294 8.84236 4.54736  
 H 2.99083 8.08412 3.53154  
 H 3.95058 3.64012 2.43941  
 C 5.56703 5.31203 0.33892  
 H 5.68511 5.17071 1.42380  
 C 4.17902 4.89903 -0.11007  
 H 4.06139 5.03939 -1.19882  
 H 3.45482 5.56904 0.38508  
 C 3.73911 3.49890 0.22533  
 N 3.66345 3.05126 1.51527  
 C 3.22596 2.46648 -0.54986  
 H 3.13329 2.40493 -1.63587  
 C 3.12372 1.82534 1.48174  
 H 2.94230 1.24144 2.38484  
 N 2.83327 1.42075 0.25170  
 H 5.74773 6.37415 0.10994  
 H 6.35073 4.71938 -0.16200  
 H 2.18812 -0.24689 0.20562

### FAP / 5b optimum structure

O 1.49547 1.08765 -2.35622  
 C 0.79235 0.41779 -3.12205  
 C 0.77338 0.68727 -4.60515  
 N -0.01260 -0.56384 -2.68361  
 C -0.90967 -1.36077 -3.52580  
 C -1.82523 -2.09125 -2.53947  
 C -1.55706 -1.45076 -1.17456  
 C -0.12915 -0.90215 -1.26802  
 C 0.93831 -1.91125 -0.85901  
 N 1.08922 -3.08964 -1.24714  
 H 0.87016 -0.24136 -5.18444  
 H 1.59847 1.36573 -4.85098  
 H -0.17771 1.16986 -4.88303  
 H -1.46665 -0.69399 -4.20165  
 H -0.33902 -2.10485 -4.10731  
 H -2.88264 -1.99118 -2.82454  
 H -1.55628 -3.15755 -2.56269  
 H -2.25173 -0.61428 -1.00349  
 H -1.68030 -2.15498 -0.33990  
 H 0.01733 0.00887 -0.67054  
 H 0.53283 -3.48504 -2.06278  
 C 0.94398 9.25900 -7.06507  
 H 1.56845 9.51490 -6.19414  
 C 0.37298 7.84900 -6.94206  
 H -0.29548 7.63806 -7.79476  
 H -0.25914 7.76833 -6.04129  
 C 1.46857 6.78174 -6.88476  
 H 2.17083 7.02587 -6.06615  
 H 2.06643 6.83575 -7.81249  
 C 1.00473 5.32747 -6.72687  
 H 1.83636 4.65531 -7.00342  
 H 0.20759 5.12318 -7.46004  
 N 0.48914 4.94222 -5.43140  
 H -0.57625 4.88322 -5.28604  
 C 1.20671 4.34199 -4.48406  
 N 2.56374 4.29651 -4.58452  
 H 3.08745 3.89634 -3.81856  
 H 3.04409 4.98901 -5.13984  
 N 0.61049 3.76605 -3.45515  
 H 1.15685 3.18235 -2.82446  
 H -0.44039 3.52278 -3.48778

H 0.14519 10.01244 -7.13616  
 H 1.57930 9.35797 -7.96071  
 C -4.90901 5.91001 -5.26302  
 H -4.15255 5.52093 -5.95844  
 C -4.32100 5.98302 -3.85302  
 H -5.08278 6.37059 -3.15421  
 H -3.48081 6.69547 -3.83242  
 C -3.83068 4.62826 -3.36681  
 H -4.57896 3.83985 -3.56538  
 H -3.68061 4.60982 -2.27532  
 C -2.51134 4.18279 -3.98241  
 O -1.92815 3.21738 -3.42822  
 O -2.07482 4.82636 -4.97153  
 H -5.24485 6.89537 -5.62632  
 H -5.78158 5.23544 -5.29237  
 C 4.24000 -9.06598 -1.92100  
 H 4.58858 -8.32395 -1.18544  
 C 4.04499 -8.41899 -3.29700  
 H 3.79061 -9.21664 -4.01986  
 H 5.01010 -8.00785 -3.64056  
 C 3.00377 -7.33044 -3.36139  
 C 3.35532 -5.97920 -3.48648  
 H 4.41728 -5.71076 -3.55622  
 C 1.62970 -7.61726 -3.30903  
 H 1.30581 -8.66343 -3.22884  
 C 2.40264 -4.96874 -3.53354  
 H 2.71171 -3.92317 -3.63140  
 C 0.66362 -6.61968 -3.35009  
 H -0.40070 -6.87044 -3.29785  
 C 1.00293 -5.23547 -3.44057  
 O 0.11998 -4.29730 -3.40574  
 H 4.97938 -9.88420 -1.95149  
 H 3.29448 -9.48408 -1.53964  
 C 3.66402 -2.43596 1.38197  
 H 3.59282 -1.66740 2.16738  
 C 3.00919 -3.70476 1.94762  
 O 3.24108 -4.05643 3.09511  
 C 3.12702 -1.93696 0.04097  
 H 3.15507 -2.74558 -0.70331  
 H 3.81068 -1.14723 -0.32148  
 O 1.83052 -1.35614 0.03807  
 H 4.73512 -2.65861 1.24858  
 N 2.21424 -4.38580 1.09601  
 H 1.98506 -4.01284 0.16312  
 C 1.55002 -5.61196 1.45100  
 H 1.15829 -5.56577 2.47941  
 H 2.22970 -6.48045 1.38870  
 H 0.72292 -5.78177 0.74874  
 C -5.52894 1.22607 5.75401  
 H -4.74043 1.99430 5.75455  
 C -5.05595 -0.04594 5.03801  
 H -5.83412 -0.82328 5.12056  
 H -4.16396 -0.45032 5.54375  
 C -4.74717 0.22092 3.58342  
 C -3.44964 0.49390 3.13698  
 H -2.61392 0.43741 3.84088  
 C -5.77851 0.29489 2.63582  
 H -6.80581 0.08142 2.94833  
 C -3.18492 0.83763 1.81049  
 H -2.15885 1.04966 1.49394  
 C -5.53277 0.63242 1.31060  
 H -6.34155 0.69018 0.57905  
 C -4.22993 0.92056 0.88574

O -4.05657 1.25056 -0.41283  
 H -3.14981 1.52829 -0.58729  
 H -5.81493 1.02304 6.79923  
 H -6.40413 1.65751 5.24273  
 C 4.04805 8.03905 3.82492  
 H 4.64504 8.23909 2.92232  
 C 4.36405 6.65105 4.38692  
 H 3.84940 6.48853 5.35027  
 H 5.43614 6.50091 4.58456  
 C 3.87698 5.57754 3.43562  
 O 4.48304 4.42160 3.58054  
 O 3.01157 5.80644 2.61547  
 H 4.27234 8.82899 4.55825  
 H 2.99087 8.09832 3.53365  
 H 4.19567 3.79740 2.80346  
 C 5.56703 5.31203 0.33892  
 H 5.69120 5.16736 1.42120  
 C 4.17902 4.89903 -0.11007  
 H 4.06125 5.03562 -1.19900  
 H 3.44549 5.56665 0.37152  
 C 3.78044 3.49817 0.22920  
 N 3.82037 2.98259 1.50364  
 C 3.21803 2.55811 -0.59989  
 H 2.99358 2.53780 -1.65946  
 C 3.28384 1.78033 1.44163  
 H 3.14564 1.10052 2.28113  
 N 2.90177 1.48543 0.18621  
 H 5.75679 6.37297 0.11212  
 H 6.34773 4.71532 -0.16038  
 H 2.40647 0.64614 -0.12486

### FAP / 15b at 2.00 Å

O 1.62335 0.95170 -3.43745  
 C 0.49051 0.58094 -3.74445  
 C -0.06777 0.75574 -5.13410  
 N -0.34075 0.03302 -2.83005  
 C -1.70747 -0.39280 -3.07378  
 C -2.08971 -1.07039 -1.76356  
 C -1.25614 -0.35102 -0.71854  
 C 0.08205 -0.19855 -1.44687  
 C 0.84637 -1.47761 -1.37333  
 N 0.90976 -2.57463 -1.80082  
 H -0.51938 -0.17227 -5.51446  
 H 0.74938 1.06194 -5.79743  
 H -0.84281 1.54135 -5.11500  
 H -2.36942 0.47355 -3.25405  
 H -1.78997 -1.08391 -3.92644  
 F -3.45598 -0.97561 -1.54824  
 H -1.84527 -2.14324 -1.78571  
 H -1.68612 0.64523 -0.52698  
 H -1.15678 -0.89629 0.22867  
 H 0.68545 0.63479 -1.07341  
 H 0.24307 -3.73962 -2.80123  
 C 0.94400 9.25900 -7.06500  
 H 1.81604 9.39638 -6.40544  
 C 0.37300 7.84900 -6.94200  
 H -0.52914 7.76511 -7.57280  
 H 0.03300 7.64642 -5.91275  
 C 1.37694 6.78665 -7.37881  
 H 2.27884 6.84667 -6.74274  
 H 1.71183 6.99948 -8.41053  
 C 0.82993 5.36241 -7.32377  
 H 1.50769 4.66820 -7.84916

H -0.12106 5.31470 -7.87939  
 N 0.57144 4.88937 -5.98956  
 H -0.39779 5.08843 -5.55362  
 C 1.38350 4.10576 -5.29379  
 N 2.59938 3.75236 -5.78033  
 H 3.18798 3.15720 -5.21449  
 H 3.04011 4.28984 -6.51001  
 N 1.00098 3.64044 -4.11365  
 H 1.52311 2.84938 -3.73183  
 H -0.04739 3.60292 -3.94156  
 H 0.20107 10.02030 -6.78259  
 H 1.27432 9.47127 -8.09500  
 C -4.90900 5.91000 -5.26300  
 H -4.10697 5.72316 -5.99251  
 C -4.32100 5.98300 -3.85300  
 H -5.12476 6.16282 -3.11883  
 H -3.62649 6.83567 -3.78074  
 C -3.57106 4.71181 -3.49025  
 H -4.18596 3.81881 -3.69840  
 H -3.35438 4.66638 -2.40955  
 C -2.22929 4.49500 -4.18279  
 O -1.63678 3.41969 -3.90720  
 O -1.78728 5.38859 -4.94929  
 H -5.42295 6.84240 -5.54844  
 H -5.64464 5.09252 -5.35013  
 C 4.24000 -9.06600 -1.92100  
 H 4.53026 -8.31421 -1.17107  
 C 4.04500 -8.41900 -3.29700  
 H 3.83039 -9.21304 -4.03346  
 H 4.99248 -7.95628 -3.62005  
 C 2.95145 -7.39117 -3.34135  
 C 3.24235 -6.03085 -3.20762  
 H 4.28538 -5.71054 -3.11146  
 C 1.60618 -7.75554 -3.47898  
 H 1.34503 -8.81268 -3.59952  
 C 2.24136 -5.06851 -3.19405  
 H 2.48944 -4.01314 -3.07461  
 C 0.58962 -6.80642 -3.46287  
 H -0.45872 -7.09862 -3.56215  
 C 0.89169 -5.44584 -3.30292  
 O -0.10156 -4.55184 -3.26838  
 H 5.02370 -9.84074 -1.94070  
 H 3.30956 -9.53815 -1.56802  
 C 3.66400 -2.43600 1.38200  
 H 3.49533 -1.67449 2.16070  
 C 3.09258 -3.75622 1.90569  
 O 3.57980 -4.31053 2.87907  
 C 3.12700 -1.93699 0.04100  
 H 2.82865 -2.80018 -0.59575  
 H 3.99884 -1.50721 -0.50889  
 O 2.10156 -1.01932 0.11478  
 H 4.75131 -2.60634 1.34296  
 N 2.04839 -4.28290 1.20847  
 H 1.71124 -3.78744 0.38936  
 C 1.55000 -5.61200 1.45100  
 H 1.77094 -5.88576 2.49222  
 H 2.02712 -6.35993 0.79219  
 H 0.46356 -5.65687 1.28192  
 C -5.52900 1.22600 5.75400  
 H -5.01475 2.11269 5.35131  
 C -5.05600 -0.04600 5.03800  
 H -5.57123 -0.91370 5.48770  
 H -3.98266 -0.20505 5.23024

C -5.29587 -0.03955 3.55096  
 C -4.22997 -0.01495 2.64897  
 H -3.20328 -0.00001 3.02792  
 C -6.59096 -0.05164 3.01238  
 H -7.45289 -0.07306 3.68685  
 C -4.43905 -0.01765 1.27325  
 H -3.59014 -0.01018 0.59217  
 C -6.81739 -0.05073 1.63999  
 H -7.83063 -0.07089 1.23188  
 C -5.73568 -0.04122 0.75016  
 O -5.98856 -0.05302 -0.57454  
 H -5.15587 -0.17243 -1.05041  
 H -5.32178 1.17798 6.83491  
 H -6.61081 1.38551 5.62132  
 C 4.04800 8.03900 3.82500  
 H 4.67138 8.25394 2.94364  
 C 4.36400 6.65100 4.38700  
 H 3.82307 6.48310 5.33525  
 H 5.43152 6.51599 4.61762  
 C 3.91811 5.56674 3.42800  
 O 4.57155 4.44131 3.56085  
 O 3.03582 5.77284 2.61751  
 H 4.23655 8.82782 4.56989  
 H 3.00044 8.08278 3.49739  
 H 4.31378 3.80126 2.75199  
 C 5.56700 5.31200 0.33900  
 H 5.69085 5.17481 1.42164  
 C 4.17899 4.89900 -0.11000  
 H 4.05788 5.02804 -1.19855  
 H 3.44019 5.55561 0.37744  
 C 3.82686 3.47886 0.24940  
 N 3.98804 2.99932 1.52691  
 C 3.27981 2.46324 -0.51337  
 H 2.97726 2.42201 -1.55719  
 C 3.54702 1.75342 1.52210  
 H 3.52227 1.09359 2.38878  
 N 3.11140 1.38131 0.31202  
 H 5.76220 6.37114 0.10485  
 H 6.34528 4.70907 -0.15693  
 H 2.68064 0.39377 0.11951

## FAP / 15b at 2.60 Å

O 2.03188 0.97610 -4.27542  
 C 0.80769 0.90652 -4.34204  
 C 0.03387 1.22936 -5.59281  
 N 0.05697 0.53225 -3.27293  
 C -1.39756 0.57198 -3.18396  
 C -1.68725 0.37146 -1.69563  
 C -0.35645 0.54277 -0.97985  
 C 0.64489 0.06104 -2.02791  
 C 0.67257 -1.41287 -2.09588  
 N 0.49465 -2.52982 -2.34078  
 H -0.54021 0.35232 -5.92958  
 H 0.74160 1.51666 -6.37839  
 H -0.67767 2.04780 -5.39777  
 H -1.77434 1.56882 -3.47450  
 H -1.87016 -0.20963 -3.80030  
 F -2.61403 1.31991 -1.26617  
 H -2.13681 -0.61212 -1.48492  
 H -0.17653 1.61197 -0.79338  
 H -0.27425 -0.00711 -0.03518  
 H 1.65830 0.45082 -1.87398  
 H -0.10529 -3.99708 -3.27261

C 0.94400 9.25900 -7.06500  
 H 1.79413 9.40627 -6.37988  
 C 0.37300 7.84900 -6.94200  
 H -0.51260 7.75150 -7.59400  
 H 0.00508 7.66856 -5.91815  
 C 1.38884 6.77664 -7.32717  
 H 2.30147 6.89121 -6.71577  
 H 1.69900 6.92364 -8.37769  
 C 0.87799 5.34516 -7.16653  
 H 1.56060 4.63937 -7.66936  
 H -0.08816 5.23564 -7.68758  
 N 0.67951 4.96419 -5.79239  
 H -0.24829 5.25500 -5.33810  
 C 1.47194 4.18263 -5.07113  
 N 2.63674 3.68131 -5.54322  
 H 2.89192 2.76314 -5.17745  
 H 2.91618 3.88875 -6.48990  
 N 1.10850 3.88527 -3.82638  
 H 1.71841 3.28327 -3.28847  
 H 0.06596 3.83703 -3.65326  
 H 0.18927 10.01955 -6.81404  
 H 1.30640 9.46198 -8.08619  
 C -4.90900 5.91000 -5.26300  
 H -4.10500 5.75940 -6.00008  
 C -4.32100 5.98300 -3.85300  
 H -5.13376 6.13308 -3.12229  
 H -3.65375 6.85580 -3.76921  
 C -3.53550 4.73723 -3.49295  
 H -4.08059 3.82281 -3.78660  
 H -3.39302 4.64407 -2.40344  
 C -2.14421 4.63589 -4.09697  
 O -1.50542 3.57977 -3.82126  
 O -1.69631 5.57474 -4.79366  
 H -5.45083 6.83018 -5.53458  
 H -5.61820 5.07086 -5.36069  
 C 4.24000 -9.06600 -1.92100  
 H 4.42339 -8.30395 -1.14804  
 C 4.04500 -8.41900 -3.29700  
 H 3.92478 -9.22008 -4.04724  
 H 4.96570 -7.88151 -3.57875  
 C 2.88227 -7.47480 -3.39545  
 C 3.07435 -6.09333 -3.31392  
 H 4.08783 -5.69907 -3.18720  
 C 1.57207 -7.93905 -3.57097  
 H 1.38995 -9.01613 -3.64888  
 C 2.01064 -5.20281 -3.39988  
 H 2.18365 -4.12694 -3.34001  
 C 0.49554 -7.06356 -3.65209  
 H -0.52542 -7.42852 -3.78595  
 C 0.70213 -5.68041 -3.56489  
 O -0.35693 -4.86168 -3.65520  
 H 5.09456 -9.76134 -1.91786  
 H 3.34547 -9.63201 -1.61684  
 C 3.66400 -2.43600 1.38200  
 H 3.35810 -1.73082 2.17256  
 C 3.21517 -3.84220 1.78210  
 O 3.88793 -4.55274 2.50962  
 C 3.12700 -1.93699 0.04100  
 H 2.93314 -2.78762 -0.63657  
 H 3.91405 -1.32710 -0.44259  
 O 1.95498 -1.17385 0.15318  
 H 4.76295 -2.46853 1.40030  
 N 2.03185 -4.26404 1.25706

H 1.50268 -3.63184 0.66977  
 C 1.55000 -5.61200 1.45100  
 H 1.64568 -5.90295 2.50800  
 H 2.12289 -6.34239 0.85431  
 H 0.49611 -5.67089 1.14749  
 C -5.52900 1.22600 5.75400  
 H -4.90029 2.08568 5.47494  
 C -5.05600 -0.04600 5.03800  
 H -5.69405 -0.88811 5.35912  
 H -4.03725 -0.29775 5.37581  
 C -5.06487 0.04616 3.54056  
 C -3.87676 0.24122 2.83345  
 H -2.93157 0.31092 3.38034  
 C -6.25569 -0.03194 2.80670  
 H -7.20217 -0.18585 3.33479  
 C -3.86640 0.35186 1.44782  
 H -2.93002 0.53474 0.92029  
 C -6.26301 0.07182 1.42061  
 H -7.19144 0.00933 0.84885  
 C -5.06216 0.26221 0.72612  
 O -5.10508 0.34582 -0.61710  
 H -4.25074 0.66974 -0.93880  
 H -5.47592 1.11201 6.84830  
 H -6.56728 1.47591 5.48368  
 C 4.04800 8.03900 3.82500  
 H 4.64373 8.23631 2.91995  
 C 4.36400 6.65100 4.38700  
 H 3.86398 6.49770 5.35998  
 H 5.43883 6.48984 4.56251  
 C 3.84507 5.56780 3.42890  
 O 4.39849 4.42417 3.53853  
 O 2.96109 5.87619 2.62370  
 H 4.26613 8.84131 4.55043  
 H 2.99265 8.08246 3.52474  
 H 3.98905 3.64940 2.45483  
 C 5.56700 5.31200 0.33900  
 H 5.68456 5.17179 1.42388  
 C 4.17899 4.89900 -0.11000  
 H 4.05789 5.03620 -1.19822  
 H 3.45272 5.56568 0.38618  
 C 3.75605 3.49563 0.23261  
 N 3.70647 3.04813 1.52438  
 C 3.25586 2.45308 -0.53492  
 H 3.15254 2.39594 -1.62083  
 C 3.19522 1.81141 1.49905  
 H 3.03559 1.22432 2.40420  
 N 2.89945 1.39868 0.27176  
 H 5.75003 6.37364 0.10921  
 H 6.35009 4.71770 -0.16092  
 H 2.25111 -0.21347 0.21805

### FAP / 15b optimum structure

O 1.62668 0.30600 -3.35607  
 C 0.69773 -0.42316 -3.71392  
 C 0.51634 -0.85601 -5.14053  
 N -0.20628 -0.89949 -2.82826  
 C -1.40754 -1.66132 -3.15095  
 C -1.97466 -2.02100 -1.77676  
 C -1.38594 -0.99254 -0.83014  
 C 0.00793 -0.75550 -1.39791  
 C 0.99673 -1.81285 -0.91907  
 N 1.09616 -3.00016 -1.29137  
 H 0.63899 -1.95240 -5.18134

H 1.27448 -0.36659 -5.76218  
 H -0.48674 -0.61142 -5.52080  
 H -2.14064 -1.03692 -3.69079  
 H -1.15354 -2.56699 -3.72281  
 F -3.36243 -1.96188 -1.76727  
 H -1.69360 -3.04938 -1.50590  
 H -1.97700 -0.06631 -0.91556  
 H -1.37467 -1.31935 0.21898  
 H 0.39168 0.24737 -1.16734  
 H 0.59419 -3.37163 -2.16160  
 C 0.94400 9.25900 -7.06500  
 H 1.74782 9.43107 -6.33076  
 C 0.37300 7.84900 -6.94200  
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 H 1.37372 9.43566 -8.06494  
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 H -4.11442 5.67302 -5.98650  
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 C 4.04500 -8.41900 -3.29700  
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 C 3.43029 -5.95246 -3.46452  
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 H 1.29251 -8.57008 -3.28409  
 C 2.50984 -4.91135 -3.52943  
 H 2.85871 -3.87670 -3.60763  
 C 0.71911 -6.50544 -3.40643  
 H -0.35315 -6.72459 -3.38572  
 C 1.10144 -5.13317 -3.48605  
 O 0.24131 -4.16494 -3.48175  
 H 4.95055 -9.90854 -1.96187  
 H 3.28762 -9.45077 -1.52199

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 N 2.85759 1.49820 0.28022  
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 H 6.34803 4.71032 -0.15395  
 H 2.38347 0.62514 0.03374

## FAP / 14b at 2.00 Å

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 C -0.93134 -0.12106 -0.17657  
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 N 0.95896 -2.40853 -1.90740  
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 H -3.09861 -0.31790 -0.47486  
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 H 2.95186 4.18525 -6.69237  
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 H -4.11162 5.68159 -5.98541  
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 H 1.35459 -8.75033 -3.71646  
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 H 3.57642 1.08884 2.39718  
 N 3.15416 1.36238 0.32134  
 H 5.76511 6.37000 0.10129  
 H 6.34445 4.70603 -0.15442  
 H 2.71004 0.34567 0.14656

### FAP / 14b at 3.20 Å

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 C -2.18060 0.27063 -2.99779  
 C -2.38190 -0.03453 -1.51752  
 C -0.98704 -0.05295 -0.92294  
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 H -0.16313 0.63187 -6.43959  
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 H -3.04443 0.69164 -1.02664  
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 H -0.65385 0.96830 -0.69629  
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 H 1.79822 9.40654 -6.38474  
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 H 4.87571 -7.72047 -3.49436  
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 C 2.70488 -6.28890 -3.37163  
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 H 1.53433 -9.45940 -3.62566  
 C 1.50298 -5.59367 -3.42497  
 H 1.49229 -4.50417 -3.37727  
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 H -2.32593 0.14443 5.25545  
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 H -0.75035 1.19553 3.66889  
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 H -3.95569 1.76225 0.85953  
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 H 4.22206 8.83770 4.56582

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C 3.19582 1.83645 1.55781
H 3.12489 1.22915 2.46159
N 2.71080 1.48605 0.37194
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H 2.11280 -0.28524 0.23960

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### FAP / 14b optimum structure

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H 1.97466 6.98930 -8.08863
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H 1.00691 2.12627 -4.02660
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 N 2.09963 -4.31501 1.14729  
 H 1.74525 -3.84512 0.29895  
 C 1.55000 -5.61200 1.45100  
 H 1.67436 -5.81787 2.52390  
 H 2.06025 -6.41448 0.88860  
 H 0.48400 -5.63987 1.18131  
 C -5.52900 1.22600 5.75400  
 H -4.73397 1.98562 5.79475  
 C -5.05600 -0.04600 5.03800  
 H -5.83644 -0.82151 5.08779  
 H -4.17275 -0.45884 5.55586  
 C -4.73182 0.25798 3.59427  
 C -3.73146 1.18343 3.26638  
 H -3.12443 1.62891 4.05916  
 C -5.47384 -0.28248 2.53800  
 H -6.26274 -1.00931 2.75331  
 C -3.48435 1.56488 1.95076  
 H -2.69574 2.29088 1.72896  
 C -5.23644 0.08221 1.21494  
 H -5.81881 -0.35104 0.39909  
 C -4.23912 1.01423 0.90961  
 O -4.03093 1.31895 -0.38791  
 H -3.26461 1.89559 -0.48664  
 H -5.84480 1.01632 6.78938

H -6.38419 1.67442 5.22505  
 C 4.04800 8.03900 3.82500  
 H 4.67535 8.25693 2.94731  
 C 4.36400 6.65100 4.38700  
 H 3.81712 6.48085 5.33139  
 H 5.43011 6.51971 4.62569  
 C 3.92795 5.56310 3.42812  
 O 4.59906 4.44222 3.55947  
 O 3.04094 5.74905 2.62064  
 H 4.23262 8.82533 4.57293  
 H 3.00141 8.08350 3.49409  
 H 4.34226 3.80172 2.77949  
 C 5.56700 5.31200 0.33900  
 H 5.69121 5.18708 1.42296  
 C 4.17900 4.89900 -0.11000  
 H 4.06564 5.02365 -1.19988  
 H 3.44832 5.57721 0.36154  
 C 3.77224 3.49967 0.25014  
 N 3.97663 2.96742 1.50159  
 C 3.08722 2.57190 -0.50678  
 H 2.69825 2.60257 -1.52100  
 C 3.43502 1.76535 1.49395  
 H 3.42184 1.06843 2.33107  
 N 2.88354 1.48458 0.30139  
 H 5.76020 6.36790 0.09236  
 H 6.34705 4.70491 -0.14904  
 H 2.42750 0.58308 0.06750

### **POP / 10b at 2.20 Å**

C -0.54007 -0.94127 0.85475  
 N 1.62606 -1.92318 1.34241  
 C 0.81367 -1.30929 0.27275  
 C 0.74673 -2.40776 -0.77649  
 C 0.81287 -3.69729 0.03884  
 C 1.79977 -3.36058 1.15117  
 H -0.50610 -0.11557 1.59246  
 C 2.22436 -1.16960 2.28019  
 O 2.04986 0.05058 2.33402  
 C 3.11541 -1.88848 3.26640  
 O -1.50900 -1.70647 0.80596  
 H 1.30313 -0.38986 -0.07340  
 H 1.61566 -2.32932 -1.44394  
 H -0.16007 -2.31172 -1.38664  
 H 1.14798 -4.56511 -0.54772  
 H -0.17331 -3.92301 0.47219  
 H 2.83543 -3.58591 0.83602  
 H 1.59248 -3.91686 2.07867  
 H 3.65328 -1.14872 3.87217  
 H 3.83750 -2.54388 2.75680  
 H 2.51235 -2.52374 3.93526  
 C 8.86100 7.07200 3.43700  
 H 8.12080 7.64028 2.85432  
 C 8.88500 5.58700 2.98200  
 H 9.66517 5.03747 3.53805  
 H 9.15306 5.48804 1.91886  
 C 7.58735 4.82959 3.20780  
 O 6.78758 5.27081 4.06699  
 O 7.44397 3.78716 2.52259  
 H 9.84424 7.54745 3.29474  
 H 8.56470 7.14154 4.49322  
 C -8.79900 -3.70600 0.78800  
 H -8.37772 -3.13380 -0.05327  
 C -8.16000 -3.24700 2.12900

H -8.59810 -3.84383 2.94643  
 H -8.45769 -2.20236 2.32414  
 C -6.66431 -3.35770 2.17547  
 C -5.86455 -2.36772 1.59318  
 H -6.33910 -1.50747 1.11063  
 C -6.01739 -4.43916 2.78708  
 H -6.61576 -5.22568 3.25842  
 C -4.47823 -2.44139 1.61988  
 H -3.86545 -1.65078 1.18306  
 C -4.62882 -4.53444 2.81795  
 H -4.12664 -5.37757 3.29783  
 C -3.84089 -3.53478 2.23048  
 O -2.50880 -3.64481 2.28038  
 H -2.10782 -2.87920 1.80717  
 H -9.89014 -3.55394 0.78894  
 H -8.59131 -4.77085 0.59907  
 C -2.78800 0.52700 -2.29800  
 H -2.07903 0.98203 -3.00723  
 C -3.15534 -0.85900 -2.84531  
 O -3.55815 -0.99727 -3.98967  
 C -2.24700 0.60900 -0.89100  
 H -2.77262 -0.14392 -0.25808  
 H -2.60907 1.58162 -0.47034  
 O -0.88390 0.50911 -0.76333  
 H -3.72205 1.10597 -2.39458  
 N -3.09281 -1.89582 -1.96317  
 H -2.64868 -1.75239 -1.06019  
 C -3.62100 -3.20800 -2.24500  
 H -4.37941 -3.11477 -3.03489  
 H -4.07986 -3.63347 -1.34028  
 H -2.85010 -3.90888 -2.61349  
 C 4.91700 -7.80000 -0.78200  
 H 6.00685 -7.71830 -0.91709  
 C 4.17200 -6.80300 -1.69000  
 H 3.08218 -6.93910 -1.56602  
 H 4.38836 -7.04219 -2.74666  
 C 4.52818 -5.37174 -1.42518  
 C 5.33904 -4.88524 -0.42683  
 H 5.88752 -5.42806 0.34045  
 C 4.06956 -4.21749 -2.15836  
 N 5.40014 -3.51187 -0.48893  
 H 5.96787 -2.92274 0.10168  
 C 4.64016 -3.07203 -1.54244  
 C 3.22828 -4.03977 -3.27150  
 H 2.76382 -4.89933 -3.76193  
 C 4.39261 -1.77340 -2.00077  
 H 4.82579 -0.90240 -1.50253  
 C 2.98324 -2.75350 -3.73110  
 H 2.31690 -2.59934 -4.58300  
 C 3.55733 -1.63133 -3.10053  
 H 3.31975 -0.63102 -3.47092  
 H 4.62239 -8.83340 -1.02032  
 H 4.68331 -7.62310 0.27973  
 C 4.72800 7.90500 -3.55000  
 H 4.69508 8.08686 -2.46496  
 C 3.37000 7.45000 -4.07800  
 H 3.38351 7.36621 -5.17954  
 H 2.57427 8.17433 -3.84619  
 C 2.96684 6.10086 -3.51822  
 O 3.78674 5.30634 -3.09808  
 O 1.67299 5.91878 -3.51764  
 H 5.06229 8.83155 -4.04265  
 H 5.48066 7.12396 -3.72758

H 1.42152 5.21342 -2.74380  
 C 5.66500 3.07800 -1.29100  
 H 6.62130 2.77443 -0.83043  
 C 4.55800 3.22500 -0.25900  
 H 3.67478 3.62767 -0.77546  
 H 4.85046 3.98531 0.48551  
 C 4.14552 1.94846 0.46605  
 H 4.10984 1.10549 -0.24842  
 H 3.11370 2.06449 0.83005  
 C 5.02221 1.52178 1.64276  
 H 6.03532 1.26976 1.28992  
 H 4.59934 0.60177 2.08650  
 N 5.19939 2.52436 2.66750  
 H 6.13658 3.06587 2.65962  
 C 4.28967 2.90277 3.54908  
 N 3.06425 2.34300 3.58183  
 H 2.44885 2.58956 4.34207  
 H 2.81469 1.49286 3.05782  
 N 4.60584 3.85109 4.43981  
 H 3.85744 4.24316 4.99214  
 H 5.50222 4.43009 4.31209  
 H 5.81836 4.02598 -1.82518  
 H 5.39476 2.32616 -2.05135  
 C 1.42100 7.23500 -0.44800  
 H 1.33882 7.15237 -1.53944  
 C 2.11500 5.99500 0.13900  
 H 2.16782 6.05893 1.23683  
 H 3.14785 5.92456 -0.23801  
 C 1.36535 4.73011 -0.24497  
 N 1.07496 4.46368 -1.56209  
 C 0.85333 3.67956 0.50269  
 H 0.88443 3.48576 1.57252  
 C 0.43942 3.30813 -1.59544  
 H 0.08175 2.80543 -2.49315  
 N 0.27502 2.79293 -0.37394  
 H -0.22150 1.81084 -0.31119  
 H 1.98888 8.14927 -0.20972  
 H 0.40570 7.34842 -0.03708

### **POP / 10b at 2.30 Å**

C -0.36514 -0.36340 1.30609  
 N 1.46904 -1.98127 1.65504  
 C 0.66018 -1.27885 0.64364  
 C 0.07323 -2.41140 -0.21015  
 C 0.30250 -3.70310 0.57778  
 C 1.54460 -3.41807 1.41104  
 H -0.03806 0.67939 1.46490  
 C 2.23069 -1.28626 2.52136  
 O 2.16195 -0.05838 2.58577  
 C 3.15949 -2.07887 3.40991  
 O -1.40457 -0.76026 1.80947  
 H 1.31919 -0.62683 0.04954  
 H 0.61387 -2.43752 -1.16467  
 H -0.98335 -2.23498 -0.44590  
 H 0.44143 -4.56991 -0.08490  
 H -0.55025 -3.91461 1.23646  
 H 2.47105 -3.67083 0.86400  
 H 1.55589 -3.97894 2.35741  
 H 3.75266 -1.37897 4.01078  
 H 3.83128 -2.71815 2.81625  
 H 2.58768 -2.73711 4.08355  
 C 8.86100 7.07200 3.43700  
 H 8.01440 7.59770 2.97308

C 8.88500 5.58700 2.98200  
 H 9.73068 5.04870 3.44347  
 H 9.04476 5.49858 1.89472  
 C 7.62749 4.80236 3.31961  
 O 6.73476 5.38999 3.97718  
 O 7.59209 3.61698 2.90966  
 H 9.79059 7.59097 3.15366  
 H 8.72679 7.14409 4.52586  
 C -8.79900 -3.70600 0.78800  
 H -8.49693 -3.03458 -0.03024  
 C -8.16000 -3.24700 2.12900  
 H -8.48812 -3.93380 2.92818  
 H -8.55402 -2.25367 2.39958  
 C -6.65987 -3.19367 2.08305  
 C -5.96980 -1.97858 2.03688  
 H -6.53712 -1.04276 2.06828  
 C -5.90301 -4.37305 2.05630  
 H -6.41556 -5.33970 2.10077  
 C -4.57829 -1.92756 1.96869  
 H -4.04348 -0.97309 1.96831  
 C -4.51805 -4.34430 1.98422  
 H -3.92937 -5.26415 1.97113  
 C -3.83629 -3.11777 1.93946  
 O -2.50495 -3.13899 1.87470  
 H -2.11246 -2.22644 1.84808  
 H -9.89907 -3.69973 0.84336  
 H -8.47241 -4.72311 0.52174  
 C -2.78800 0.52700 -2.29800  
 H -2.14610 1.07600 -2.99950  
 C -2.91643 -0.90617 -2.83339  
 O -2.62835 -1.20926 -3.97585  
 C -2.24700 0.60900 -0.89100  
 H -2.75672 -0.10353 -0.21395  
 H -2.49811 1.60720 -0.48012  
 O -0.86980 0.41165 -0.79976  
 H -3.79226 0.98330 -2.33938  
 N -3.39571 -1.81996 -1.93412  
 H -3.67925 -1.49679 -1.01902  
 C -3.62100 -3.20800 -2.24500  
 H -2.99210 -3.47161 -3.10614  
 H -4.67148 -3.41883 -2.51539  
 H -3.34626 -3.83852 -1.38653  
 C 4.91700 -7.80000 -0.78200  
 H 6.00679 -7.64837 -0.83466  
 C 4.17200 -6.80300 -1.69000  
 H 3.09250 -7.03871 -1.67442  
 H 4.49268 -6.95994 -2.73613  
 C 4.36337 -5.36398 -1.32598  
 C 5.20461 -4.83943 -0.37390  
 H 5.88657 -5.35360 0.30110  
 C 3.69705 -4.23689 -1.93095  
 N 5.09755 -3.46667 -0.34911  
 H 5.65805 -2.84638 0.21627  
 C 4.18996 -3.06557 -1.29797  
 C 2.73277 -4.10392 -2.94681  
 H 2.32695 -4.98647 -3.44860  
 C 3.75455 -1.78449 -1.65496  
 H 4.14529 -0.89344 -1.15758  
 C 2.29748 -2.83512 -3.30313  
 H 1.54228 -2.71729 -4.08363  
 C 2.80434 -1.68567 -2.66261  
 H 2.43225 -0.70138 -2.95822  
 H 4.70755 -8.83456 -1.09342

H 4.60362 -7.69103 0.26822  
 C 4.72800 7.90500 -3.55000  
 H 4.68555 8.13026 -2.47269  
 C 3.37000 7.45000 -4.07800  
 H 3.40281 7.32774 -5.17600  
 H 2.58490 8.19890 -3.88768  
 C 2.91220 6.11773 -3.48373  
 O 3.74898 5.33469 -3.03161  
 O 1.64388 5.94715 -3.49699  
 H 5.09082 8.80572 -4.07237  
 H 5.46518 7.10033 -3.68343  
 H 1.32023 5.10961 -2.48529  
 C 5.66500 3.07800 -1.29100  
 H 6.64238 2.85757 -0.82638  
 C 4.55800 3.22500 -0.25900  
 H 3.66665 3.59240 -0.78919  
 H 4.82513 4.02144 0.45754  
 C 4.16476 1.97306 0.51885  
 H 4.12761 1.10923 -0.17036  
 H 3.13324 2.10150 0.88071  
 C 5.04630 1.56490 1.70144  
 H 6.06204 1.32298 1.35008  
 H 4.63081 0.63836 2.14164  
 N 5.21978 2.56295 2.73488  
 H 6.19688 3.00049 2.84334  
 C 4.28558 3.00109 3.56388  
 N 3.04475 2.47378 3.56347  
 H 2.38609 2.79697 4.25523  
 H 2.83099 1.57629 3.11989  
 N 4.59198 3.97571 4.42447  
 H 3.84550 4.36189 4.98317  
 H 5.48858 4.56206 4.27276  
 H 5.74539 4.00168 -1.88117  
 H 5.43427 2.26603 -2.00149  
 C 1.42100 7.23500 -0.44800  
 H 1.34689 7.15251 -1.54136  
 C 2.11500 5.99500 0.13900  
 H 2.16843 6.05102 1.23730  
 H 3.14475 5.92689 -0.24691  
 C 1.36084 4.74066 -0.25060  
 N 1.04162 4.48858 -1.55932  
 C 0.84290 3.66845 0.46290  
 H 0.89260 3.48074 1.53534  
 C 0.39282 3.32347 -1.59755  
 H 0.03873 2.87516 -2.52686  
 N 0.23895 2.78019 -0.39658  
 H -0.42679 1.31347 -0.58656  
 H 1.98734 8.14977 -0.20697  
 H 0.40425 7.34669 -0.03900

### **POP / 10b optimum structure**

C -0.56928 -0.80593 0.20795  
 N 1.45532 -2.13916 0.73301  
 C 0.84654 -1.23800 -0.24333  
 C 0.80123 -2.09032 -1.50514  
 C 0.58461 -3.51974 -0.99819  
 C 1.16802 -3.53835 0.42250  
 H -0.46164 -0.29129 1.20037  
 C 2.26247 -1.70948 1.71665  
 O 2.51108 -0.51173 1.90231  
 C 2.89312 -2.77228 2.58890  
 O -1.46965 -1.77205 0.21663  
 H 1.48162 -0.34582 -0.33517

H 1.75379 -2.01063 -2.04862  
 H 0.00088 -1.75443 -2.17740  
 H 1.07774 -4.26216 -1.64298  
 H -0.48784 -3.74430 -0.95498  
 H 2.09229 -4.13556 0.47812  
 H 0.44323 -3.95555 1.14063  
 H 3.51619 -2.27504 3.34251  
 H 3.51937 -3.44829 1.98441  
 H 2.13358 -3.39055 3.09011  
 C 8.86100 7.07200 3.43700  
 H 8.16298 7.65743 2.81932  
 C 8.88500 5.58700 2.98200  
 H 9.64881 5.04857 3.57203  
 H 9.20148 5.50225 1.93159  
 C 7.60694 4.77121 3.14073  
 O 6.88030 4.97542 4.14019  
 O 7.42939 3.89202 2.25918  
 H 9.85936 7.52587 3.34162  
 H 8.51950 7.14745 4.48018  
 C -8.79900 -3.70600 0.78800  
 H -8.45071 -3.07129 -0.04132  
 C -8.16000 -3.24700 2.12900  
 H -8.50634 -3.91169 2.93714  
 H -8.54209 -2.24050 2.37575  
 C -6.64861 -3.22808 2.11273  
 C -5.94129 -2.28530 1.35187  
 H -6.49570 -1.53843 0.77288  
 C -5.88348 -4.15559 2.83359  
 H -6.39621 -4.91256 3.43754  
 C -4.55076 -2.26436 1.30582  
 H -4.02412 -1.52668 0.69916  
 C -4.49023 -4.14777 2.80191  
 H -3.91132 -4.88280 3.36657  
 C -3.78572 -3.20122 2.03195  
 O -2.45873 -3.21983 2.02133  
 H -2.05840 -2.56131 1.34079  
 H -9.89859 -3.64153 0.82132  
 H -8.51349 -4.74271 0.55127  
 C -2.78800 0.52700 -2.29800  
 H -2.02912 0.87127 -3.02047  
 C -3.31699 -0.83568 -2.78560  
 O -3.94958 -0.89897 -3.83093  
 C -2.24700 0.60900 -0.89100  
 H -2.84801 -0.01568 -0.21250  
 H -2.35954 1.65354 -0.53610  
 O -0.88726 0.25275 -0.77132  
 H -3.64278 1.21156 -2.41373  
 N -3.08049 -1.89679 -1.98195  
 H -2.45224 -1.81413 -1.15352  
 C -3.62100 -3.20800 -2.24500  
 H -4.44587 -3.11507 -2.96535  
 H -3.99756 -3.65905 -1.31378  
 H -2.87010 -3.88845 -2.68510  
 C 4.91700 -7.80000 -0.78200  
 H 6.00622 -7.70883 -0.91278  
 C 4.17200 -6.80300 -1.69000  
 H 3.08135 -6.92847 -1.56398  
 H 4.39098 -7.03343 -2.74714  
 C 4.56176 -5.38263 -1.40309  
 C 5.26048 -4.92239 -0.31046  
 H 5.67022 -5.47535 0.53230  
 C 4.29406 -4.22258 -2.21386  
 N 5.43020 -3.55996 -0.39158

H 5.91662 -2.98789 0.28247  
 C 4.85383 -3.10026 -1.54669  
 C 3.63883 -4.02308 -3.44181  
 H 3.18325 -4.86396 -3.97149  
 C 4.78317 -1.80512 -2.07081  
 H 5.21654 -0.95315 -1.54105  
 C 3.56512 -2.74003 -3.96397  
 H 3.04531 -2.56799 -4.90944  
 C 4.13369 -1.64254 -3.28618  
 H 4.04657 -0.64320 -3.71941  
 H 4.62927 -8.83536 -1.02183  
 H 4.67615 -7.63005 0.27892  
 C 4.72800 7.90500 -3.55000  
 H 4.69654 8.08223 -2.46429  
 C 3.37000 7.45000 -4.07800  
 H 3.38186 7.36694 -5.17950  
 H 2.57293 8.17194 -3.84384  
 C 2.97366 6.10053 -3.51989  
 O 3.78586 5.30050 -3.10469  
 O 1.67263 5.91736 -3.51393  
 H 5.05739 8.83446 -4.03962  
 H 5.48324 7.12791 -3.73334  
 H 1.44108 5.20180 -2.79384  
 C 5.66500 3.07800 -1.29100  
 H 6.62584 2.79377 -0.83146  
 C 4.55800 3.22500 -0.25900  
 H 3.67346 3.63829 -0.76387  
 H 4.85955 3.96090 0.50586  
 C 4.17296 1.91175 0.41276  
 H 3.96717 1.14816 -0.35821  
 H 3.22897 2.02474 0.96778  
 C 5.23052 1.35068 1.35964  
 H 6.19343 1.25866 0.83301  
 H 4.93720 0.33758 1.68468  
 N 5.47891 2.18656 2.51038  
 H 6.26952 2.92188 2.43681  
 C 4.76305 2.15812 3.61996  
 N 3.77439 1.25340 3.79527  
 H 3.21416 1.30126 4.63249  
 H 3.42369 0.63558 3.05074  
 N 5.06812 3.02027 4.59856  
 H 4.47161 3.06662 5.41053  
 H 5.76825 3.80624 4.42286  
 H 5.81153 4.02002 -1.83785  
 H 5.39957 2.31418 -2.04151  
 C 1.42100 7.23500 -0.44800  
 H 1.33354 7.15432 -1.53912  
 C 2.11500 5.99500 0.13900  
 H 2.17543 6.07093 1.23551  
 H 3.14844 5.92970 -0.23817  
 C 1.39585 4.71847 -0.21612  
 N 1.10426 4.39929 -1.52270  
 C 0.95618 3.67858 0.58021  
 H 0.99993 3.52155 1.65479  
 C 0.53392 3.21529 -1.51537  
 H 0.18772 2.66208 -2.38679  
 N 0.42081 2.74100 -0.26578  
 H 0.01786 1.81160 -0.08338  
 H 1.99497 8.14499 -0.21102  
 H 0.40841 7.35472 -0.03224

## POP / 11b at 2.30 Å

B -0.41608 -0.62408 1.38982

N 1.59379 -2.23973 1.76541  
 C 0.64263 -1.66589 0.77582  
 C 0.05898 -2.91158 0.10568  
 C 0.19393 -4.01073 1.15364  
 C 1.53559 -3.69931 1.80250  
 C 2.46676 -1.49366 2.43624  
 C 3.46101 -2.19869 3.32599  
 O 2.49145 -0.25042 2.33232  
 O 0.02132 0.62199 1.80946  
 O -1.59789 -1.08493 1.98076  
 H 1.22543 -1.08109 0.04648  
 H 0.63977 -3.17127 -0.79426  
 H -0.97596 -2.73673 -0.20844  
 H 0.16164 -5.02312 0.72403  
 H -0.61048 -3.93628 1.90073  
 H 2.37244 -4.13069 1.22259  
 H 1.61461 -4.07235 2.83477  
 H 4.06886 -1.44941 3.84781  
 H 4.11887 -2.85162 2.72969  
 H 2.95541 -2.83597 4.06729  
 H 0.99631 0.56356 1.86112  
 H -2.06816 -0.33695 2.36783  
 C 8.86100 7.07200 3.43700  
 H 8.12676 7.64248 2.84881  
 C 8.88500 5.58700 2.98200  
 H 9.66372 5.03841 3.54110  
 H 9.15635 5.48849 1.91991  
 C 7.59073 4.82892 3.20456  
 O 6.79492 5.24384 4.07828  
 O 7.45108 3.80111 2.49380  
 H 9.84621 7.54536 3.30247  
 H 8.55673 7.14147 4.49107  
 C -8.79900 -3.70600 0.78800  
 H -8.36034 -3.15894 -0.06128  
 C -8.16000 -3.24700 2.12900  
 H -8.62794 -3.82159 2.94593  
 H -8.45579 -2.19699 2.30554  
 C -6.66810 -3.35119 2.26513  
 C -5.80912 -2.53484 1.51800  
 H -6.22060 -1.87105 0.75065  
 C -6.09185 -4.19560 3.22180  
 H -6.73981 -4.85099 3.81242  
 C -4.43690 -2.52275 1.74692  
 H -3.78335 -1.87421 1.15845  
 C -4.72325 -4.19283 3.47055  
 H -4.28163 -4.83052 4.24004  
 C -3.88351 -3.32993 2.75605  
 O -2.58112 -3.29781 3.07940  
 H -2.15089 -2.52708 2.63924  
 H -9.88388 -3.51853 0.78521  
 H -8.62445 -4.77935 0.61319  
 C -2.78800 0.52700 -2.29800  
 H -1.93383 0.60955 -2.99362  
 C -3.54821 -0.77064 -2.61599  
 O -4.54468 -0.78531 -3.32653  
 C -2.24700 0.60900 -0.89100  
 H -3.09095 0.36471 -0.18602  
 H -2.03213 1.69101 -0.68183  
 O -1.15312 -0.19797 -0.74681  
 H -3.49449 1.33782 -2.53868  
 N -3.03411 -1.89507 -2.04234  
 H -2.18957 -1.71633 -1.47739  
 C -3.62100 -3.20800 -2.24500

H -4.42659 -3.08733 -2.98206  
 H -4.05093 -3.62168 -1.31577  
 H -2.87840 -3.92368 -2.63582  
 C 4.91700 -7.80000 -0.78200  
 H 6.00451 -7.62653 -0.80829  
 C 4.17200 -6.80300 -1.69000  
 H 3.09666 -7.05595 -1.69826  
 H 4.51455 -6.93782 -2.73231  
 C 4.33540 -5.36884 -1.29758  
 C 5.17539 -4.84568 -0.34359  
 H 5.86904 -5.35856 0.32048  
 C 3.64703 -4.24481 -1.88163  
 N 5.04893 -3.47443 -0.30094  
 H 5.60635 -2.85301 0.26587  
 C 4.12964 -3.07490 -1.23979  
 C 2.66848 -4.11565 -2.88356  
 H 2.26579 -4.99917 -3.38608  
 C 3.68089 -1.79612 -1.58596  
 H 4.06998 -0.90469 -1.08833  
 C 2.21069 -2.84966 -3.21957  
 H 1.43806 -2.73477 -3.98314  
 C 2.71494 -1.70045 -2.57869  
 H 2.32306 -0.71939 -2.85758  
 H 4.73533 -8.83376 -1.11306  
 H 4.57847 -7.71283 0.26236  
 C 4.72800 7.90500 -3.55000  
 H 4.69600 8.07956 -2.46404  
 C 3.37000 7.45000 -4.07800  
 H 3.38032 7.35220 -5.17782  
 H 2.56844 8.16695 -3.84420  
 C 3.00112 6.09657 -3.48999  
 O 3.84032 5.32397 -3.07729  
 O 1.70573 5.87927 -3.45121  
 H 5.05748 8.83600 -4.03724  
 H 5.48223 7.12807 -3.73541  
 H 1.48911 5.14129 -2.75440  
 C 5.66500 3.07800 -1.29100  
 H 6.63804 2.85015 -0.82264  
 C 4.55800 3.22500 -0.25900  
 H 3.66172 3.58813 -0.78250  
 H 4.83026 4.01602 0.46121  
 C 4.17600 1.96433 0.50858  
 H 4.09103 1.11587 -0.19369  
 H 3.16540 2.09758 0.92458  
 C 5.10893 1.54052 1.64088  
 H 6.12329 1.36266 1.24903  
 H 4.75025 0.58359 2.05876  
 N 5.25889 2.51891 2.69371  
 H 6.17935 3.10382 2.66580  
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 N 3.22741 2.08784 3.74645  
 H 2.66949 2.20191 4.57922  
 H 3.05156 1.23931 3.19474  
 N 4.69654 3.68841 4.58237  
 H 3.95308 4.01350 5.18316  
 H 5.53217 4.33207 4.41238  
 H 5.76461 4.00401 -1.87387  
 H 5.43214 2.27165 -2.00690  
 C 1.42100 7.23500 -0.44800  
 H 1.29461 7.13861 -1.53399  
 C 2.11500 5.99500 0.13900  
 H 2.20427 6.09405 1.23198  
 H 3.14043 5.92301 -0.25945

C 1.39568 4.71247 -0.16309  
 N 1.10976 4.30846 -1.44894  
 C 0.95589 3.73399 0.70262  
 H 1.00692 3.64972 1.78494  
 C 0.53147 3.12590 -1.35366  
 H 0.17450 2.51152 -2.17826  
 N 0.41961 2.74184 -0.07259  
 H 0.03124 1.85135 0.26780  
 H 2.01657 8.13971 -0.24514  
 H 0.42477 7.37817 -0.00077

## POP / 11b at 2.40 Å

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 C 0.67067 -1.52150 0.64918  
 C 0.13660 -2.68039 -0.19256  
 C 0.22279 -3.89041 0.73141  
 C 1.52736 -3.65188 1.48453  
 C 2.46173 -1.51093 2.34612  
 C 3.42823 -2.30548 3.19046  
 O 2.48788 -0.26894 2.34853  
 O -0.07126 0.47508 2.11932  
 O -1.70364 -1.10411 1.64635  
 H 1.26664 -0.83655 0.02454  
 H 0.78721 -2.83534 -1.06548  
 H -0.87168 -2.47549 -0.57512  
 H 0.22517 -4.84652 0.18689  
 H -0.61985 -3.91446 1.43960  
 H 2.39110 -4.03305 0.91132  
 H 1.54344 -4.13224 2.47455  
 H 4.06166 -1.60858 3.75268  
 H 4.06027 -2.95062 2.55968  
 H 2.89312 -2.96030 3.89597  
 H 0.89474 0.59484 2.06343  
 H -2.15489 -0.45455 2.20257  
 C 8.86100 7.07200 3.43700  
 H 7.98848 7.58763 3.01093  
 C 8.88500 5.58700 2.98200  
 H 9.75467 5.06167 3.41309  
 H 9.01297 5.50345 1.89004  
 C 7.66010 4.76956 3.34979  
 O 6.75300 5.32706 4.01151  
 O 7.66622 3.57859 2.94942  
 H 9.77078 7.60172 3.11318  
 H 8.77585 7.14498 4.53105  
 C -8.79900 -3.70600 0.78800  
 H -8.36827 -3.14905 -0.05886  
 C -8.16000 -3.24700 2.12900  
 H -8.61849 -3.82765 2.94642  
 H -8.45178 -2.19788 2.31171  
 C -6.66920 -3.35977 2.22769  
 C -5.84498 -2.47534 1.52548  
 H -6.29392 -1.73526 0.85500  
 C -6.05423 -4.29725 3.06668  
 H -6.67747 -5.00708 3.61921  
 C -4.46554 -2.49591 1.68371  
 H -3.83384 -1.79038 1.14438  
 C -4.67433 -4.32703 3.24252  
 H -4.20031 -5.04253 3.91821  
 C -3.86445 -3.40500 2.56944  
 O -2.54359 -3.40845 2.81065  
 H -2.13701 -2.63358 2.36536  
 H -9.88606 -3.53196 0.78714

H -8.61227 -4.77621 0.60794  
 C -2.78800 0.52700 -2.29800  
 H -2.12323 1.04166 -3.00649  
 C -3.03211 -0.88119 -2.85718  
 O -3.05513 -1.10781 -4.05284  
 C -2.24700 0.60900 -0.89100  
 H -2.83649 -0.03980 -0.21417  
 H -2.44913 1.63313 -0.51881  
 O -0.89007 0.33296 -0.73797  
 H -3.75997 1.04714 -2.34673  
 N -3.28848 -1.84522 -1.92336  
 H -3.18681 -1.60085 -0.94860  
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 H -3.53512 -3.31970 -3.33471  
 H -4.64696 -3.46673 -1.93287  
 H -2.92808 -3.91354 -1.75954  
 C 4.91700 -7.80000 -0.78200  
 H 6.00595 -7.64020 -0.82539  
 C 4.17200 -6.80300 -1.69000  
 H 3.09308 -7.04111 -1.67945  
 H 4.49783 -6.95251 -2.73547  
 C 4.36265 -5.36689 -1.31353  
 C 5.19373 -4.85390 -0.34605  
 H 5.86452 -5.37618 0.33393  
 C 3.71149 -4.23177 -1.92012  
 N 5.09230 -3.48063 -0.31141  
 H 5.65894 -2.86625 0.25454  
 C 4.20224 -3.06785 -1.27237  
 C 2.76664 -4.08582 -2.95208  
 H 2.36239 -4.96204 -3.46597  
 C 3.78396 -1.78123 -1.62945  
 H 4.17083 -0.89535 -1.12004  
 C 2.34970 -2.81110 -3.30883  
 H 1.61037 -2.68272 -4.10262  
 C 2.85382 -1.66912 -2.65377  
 H 2.49547 -0.68006 -2.95003  
 H 4.71764 -8.83461 -1.09995  
 H 4.59406 -7.69891 0.26610  
 C 4.72800 7.90500 -3.55000  
 H 4.68684 8.12301 -2.47116  
 C 3.37000 7.45000 -4.07800  
 H 3.39962 7.33533 -5.17692  
 H 2.58288 8.19491 -3.88017  
 C 2.92050 6.11201 -3.48911  
 O 3.76598 5.33453 -3.04047  
 O 1.65562 5.93186 -3.50166  
 H 5.08883 8.80983 -4.06702  
 H 5.46600 7.10214 -3.68922  
 H 1.34912 5.07194 -2.47010  
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 H 6.65181 2.90065 -0.82821  
 C 4.55800 3.22500 -0.25900  
 H 3.65726 3.56840 -0.78955  
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 C 4.19528 1.97836 0.53793  
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 H 6.30052 2.96351 2.83513  
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 H 2.56315 2.43752 4.37843  
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 N 4.71103 3.76108 4.53116  
 H 3.97681 4.05905 5.15623  
 H 5.55010 4.41549 4.35680  
 H 5.71486 3.98573 -1.90909  
 H 5.45544 2.23810 -1.97562  
 C 1.42100 7.23500 -0.44800  
 H 1.34213 7.14928 -1.54115  
 C 2.11500 5.99500 0.13900  
 H 2.17179 6.05514 1.23702  
 H 3.14366 5.92584 -0.24953  
 C 1.36648 4.72962 -0.24332  
 N 1.08190 4.45482 -1.55548  
 C 0.83993 3.65722 0.46861  
 H 0.84333 3.48488 1.54485  
 C 0.44941 3.27910 -1.59575  
 H 0.12300 2.81930 -2.52963  
 N 0.27273 2.74742 -0.39405  
 H -0.41441 1.21390 -0.53522  
 H 1.99154 8.14841 -0.21183  
 H 0.40649 7.35052 -0.03450

### **POP / 11b optimum structure**

B -0.61941 -0.58349 0.59167  
 N 1.53582 -1.91850 1.40432  
 C 0.82573 -1.30674 0.25416  
 C 0.76802 -2.46968 -0.74072  
 C 0.72020 -3.71743 0.13458  
 C 1.66636 -3.36688 1.27265  
 C 2.10934 -1.20362 2.36450  
 C 2.93590 -1.94047 3.39143  
 O 1.99123 0.03958 2.42734  
 O -0.43846 0.65496 1.37300  
 O -1.52956 -1.46505 1.39346  
 H 1.47649 -0.50300 -0.13282  
 H 1.67075 -2.49439 -1.36938  
 H -0.09118 -2.37687 -1.41818  
 H 1.04298 -4.62848 -0.39225  
 H -0.29101 -3.89033 0.53540  
 H 2.70694 -3.63523 1.00670  
 H 1.40724 -3.87887 2.21227  
 H 3.48099 -1.21075 4.00304  
 H 3.64981 -2.63084 2.91770  
 H 2.28856 -2.54073 4.05115  
 H 0.39362 0.55312 1.87355  
 H -1.88530 -0.89576 2.08432  
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 H 8.12741 7.64244 2.84795  
 C 8.88500 5.58700 2.98200  
 H 9.65935 5.03655 3.54526  
 H 9.15949 5.48662 1.92080  
 C 7.58281 4.83676 3.20196  
 O 6.79754 5.26338 4.08138  
 O 7.42207 3.81411 2.49133  
 H 9.84640 7.54561 3.30372  
 H 8.55515 7.14068 4.49053  
 C -8.79900 -3.70600 0.78800  
 H -8.36749 -3.14224 -0.05354  
 C -8.16000 -3.24700 2.12900  
 H -8.59467 -3.83770 2.95213  
 H -8.44266 -2.19732 2.31987

C -6.66227 -3.38254 2.14448  
 C -5.86191 -2.47222 1.44272  
 H -6.33586 -1.64999 0.89621  
 C -6.01392 -4.42770 2.81490  
 H -6.61068 -5.16282 3.36516  
 C -4.47685 -2.58097 1.41923  
 H -3.86844 -1.86328 0.86632  
 C -4.62672 -4.55057 2.80695  
 H -4.12552 -5.36121 3.34116  
 C -3.83371 -3.62218 2.11422  
 O -2.50476 -3.75399 2.14583  
 H -2.06825 -2.92825 1.78534  
 H -9.88919 -3.54505 0.78017  
 H -8.59857 -4.77345 0.60642  
 C -2.78800 0.52700 -2.29800  
 H -1.95592 0.65025 -3.01377  
 C -3.52635 -0.77471 -2.65177  
 O -4.46447 -0.78278 -3.43415  
 C -2.24700 0.60900 -0.89100  
 H -3.06221 0.38605 -0.17008  
 H -1.93258 1.64885 -0.67892  
 O -1.18185 -0.28187 -0.73514  
 H -3.50642 1.33475 -2.50099  
 N -3.05390 -1.89504 -2.04189  
 H -2.25833 -1.75442 -1.41551  
 C -3.62100 -3.20800 -2.24500  
 H -4.45361 -3.10149 -2.95323  
 H -4.00410 -3.63448 -1.30293  
 H -2.88185 -3.90559 -2.67359  
 C 4.91700 -7.80000 -0.78200  
 H 6.00640 -7.72431 -0.92390  
 C 4.17200 -6.80300 -1.69000  
 H 3.08222 -6.92890 -1.55582  
 H 4.37851 -7.04944 -2.74701  
 C 4.54384 -5.37458 -1.43359  
 C 5.35380 -4.89020 -0.43332  
 H 5.89282 -5.43354 0.34024  
 C 4.09817 -4.22067 -2.17382  
 N 5.42713 -3.51831 -0.50213  
 H 5.98248 -2.92946 0.10021  
 C 4.67343 -3.07687 -1.55866  
 C 3.25935 -4.04169 -3.28838  
 H 2.79236 -4.90051 -3.77771  
 C 4.42855 -1.77779 -2.01710  
 H 4.86433 -0.90808 -1.51878  
 C 3.01565 -2.75479 -3.74658  
 H 2.34922 -2.59930 -4.59838  
 C 3.59078 -1.63414 -3.11464  
 H 3.35448 -0.63330 -3.48447  
 H 4.61558 -8.83314 -1.01314  
 H 4.69017 -7.61670 0.28010  
 C 4.72800 7.90500 -3.55000  
 H 4.69688 8.07492 -2.46333  
 C 3.37000 7.45000 -4.07800  
 H 3.37788 7.35492 -5.17798  
 H 2.56632 8.16250 -3.83809  
 C 3.01211 6.09062 -3.48926  
 O 3.85996 5.32142 -3.08919  
 O 1.71812 5.86403 -3.43491  
 H 5.05575 8.83851 -4.03370  
 H 5.48265 7.12958 -3.73943  
 H 1.50904 5.12053 -2.74401  
 C 5.66500 3.07800 -1.29100

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 H 3.67347 3.62213 -0.77647  
 H 4.84781 3.98975 0.48190  
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 H 6.11949 3.08776 2.64333  
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 N 4.64190 3.80464 4.49643  
 H 3.90437 4.17429 5.07815  
 H 5.52090 4.40254 4.34828  
 H 5.82088 4.02656 -1.82304  
 H 5.39569 2.32682 -2.05241  
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 H 1.28119 7.13245 -1.53186  
 C 2.11500 5.99500 0.13900  
 H 2.21498 6.10299 1.23029  
 H 3.13793 5.92074 -0.26617  
 C 1.39008 4.72522 -0.14464  
 N 1.11359 4.28561 -1.41777  
 C 0.92676 3.79040 0.75127  
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 H 0.16414 2.48048 -2.08906  
 N 0.37949 2.77929 0.01620  
 H -0.01848 1.89124 0.44126  
 H 2.02123 8.13973 -0.25811  
 H 0.43036 7.38447 0.00986

## POP / 5b at 2.20 Å

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 C 2.27567 -1.16233 2.18379  
 C 3.15395 -1.92134 3.15028  
 N 1.70979 -1.87446 1.19143  
 C 1.81953 -3.31588 0.97990  
 C 0.78705 -3.59612 -0.10919  
 C 0.73202 -2.28559 -0.88871  
 C 0.83376 -1.22728 0.21279  
 C -0.49896 -0.99657 0.81204  
 N -1.39123 -1.25510 1.52256  
 H 3.86045 -2.58395 2.62889  
 H 2.53295 -2.55192 3.80746  
 H 3.70646 -1.20581 3.77185  
 H 2.83712 -3.58094 0.64204  
 H 1.60834 -3.87310 1.90571  
 H 1.07007 -4.45569 -0.73302  
 H -0.18973 -3.81245 0.35374  
 H 1.60419 -2.19172 -1.55039  
 H -0.17371 -2.14452 -1.49162  
 H 1.25077 -0.27547 -0.13252  
 H -2.08873 -2.73182 2.01930  
 C 8.86100 7.07200 3.43700  
 H 8.11998 7.64001 2.85514  
 C 8.88500 5.58700 2.98200  
 H 9.66565 5.03730 3.53717

H 9.15274 5.48841 1.91869  
 C 7.58754 4.82825 3.20741  
 O 6.78199 5.27386 4.05866  
 O 7.45033 3.77994 2.52950  
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 H 8.56578 7.14180 4.49352  
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 H -8.38973 -3.12024 -0.04947  
 C -8.16000 -3.24700 2.12900  
 H -8.58372 -3.85868 2.94472  
 H -8.46163 -2.20805 2.34045  
 C -6.66078 -3.34030 2.14174  
 C -5.86634 -2.19098 2.09765  
 H -6.34885 -1.20849 2.07610  
 C -6.00515 -4.57904 2.16638  
 H -6.59857 -5.49884 2.20439  
 C -4.47703 -2.25995 2.08443  
 H -3.86721 -1.35448 2.05084  
 C -4.61843 -4.66995 2.14915  
 H -4.11215 -5.63782 2.17288  
 C -3.83307 -3.50732 2.10720  
 O -2.50134 -3.62947 2.10129  
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 H -2.08826 0.99784 -3.00461  
 C -3.10919 -0.86574 -2.85041  
 O -3.35163 -1.04339 -4.03248  
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 H -2.59087 1.59581 -0.48683  
 O -0.88864 0.48447 -0.76742  
 H -3.73612 1.08563 -2.38785  
 N -3.17302 -1.87511 -1.93362  
 H -2.95963 -1.65298 -0.96862  
 C -3.62100 -3.20800 -2.24500  
 H -3.94631 -3.21604 -3.29491  
 H -4.46491 -3.50347 -1.60053  
 H -2.81897 -3.95534 -2.11514  
 C 4.91700 -7.80000 -0.78200  
 H 6.00663 -7.72311 -0.92179  
 C 4.17200 -6.80300 -1.69000  
 H 3.08234 -6.93771 -1.56214  
 H 4.38323 -7.04882 -2.74627  
 C 4.52646 -5.36918 -1.44096  
 C 5.33661 -4.86698 -0.45023  
 H 5.88606 -5.39794 0.32470  
 C 4.06656 -4.22674 -2.19169  
 N 5.39583 -3.49439 -0.53326  
 H 5.96425 -2.89602 0.04749  
 C 4.63612 -3.07140 -1.59369  
 C 3.22669 -4.06682 -3.30870  
 H 2.76461 -4.93438 -3.78738  
 C 4.38870 -1.78010 -2.07264  
 H 4.82004 -0.90144 -1.58617  
 C 2.98363 -2.78832 -3.79077  
 H 2.32099 -2.64800 -4.64789  
 C 3.55640 -1.65597 -3.17696  
 H 3.32026 -0.66180 -3.56455  
 H 4.61666 -8.83245 -1.01669  
 H 4.68896 -7.61926 0.28039  
 C 4.72800 7.90500 -3.55000  
 H 4.69505 8.08580 -2.46477

C 3.37000 7.45000 -4.07800  
 H 3.38290 7.36664 -5.17956  
 H 2.57372 8.17333 -3.84492  
 C 2.96961 6.09939 -3.51720  
 O 3.79388 5.30719 -3.09965  
 O 1.67735 5.91405 -3.51209  
 H 5.06248 8.83207 -4.04170  
 H 5.48043 7.12390 -3.72815  
 H 1.42672 5.20415 -2.73391  
 C 5.66500 3.07800 -1.29100  
 H 6.62327 2.78175 -0.82974  
 C 4.55800 3.22500 -0.25900  
 H 3.67413 3.62583 -0.77574  
 H 4.84937 3.98681 0.48436  
 C 4.14748 1.94966 0.46836  
 H 4.10861 1.10543 -0.24501  
 H 3.11714 2.06819 0.83545  
 C 5.02909 1.52607 1.64219  
 H 6.04348 1.28275 1.28710  
 H 4.61494 0.60166 2.08492  
 N 5.20055 2.52759 2.66856  
 H 6.13873 3.06799 2.66489  
 C 4.28593 2.90513 3.54570  
 N 3.06258 2.34207 3.57426  
 H 2.43512 2.59495 4.32237  
 H 2.81582 1.49642 3.04364  
 N 4.59732 3.85536 4.43612  
 H 3.84771 4.24486 4.98851  
 H 5.49254 4.43471 4.30853  
 H 5.81234 4.02402 -1.83030  
 H 5.39812 2.32085 -2.04745  
 C 1.42100 7.23500 -0.44800  
 H 1.33744 7.15206 -1.53937  
 C 2.11500 5.99500 0.13900  
 H 2.16746 6.05823 1.23688  
 H 3.14740 5.92291 -0.23862  
 C 1.36525 4.72244 -0.24520  
 N 1.08394 4.45317 -1.56462  
 C 0.84976 3.66663 0.49627  
 H 0.86896 3.47040 1.56604  
 C 0.45267 3.29450 -1.60327  
 H 0.10205 2.79358 -2.50484  
 N 0.28054 2.77540 -0.38444  
 H -0.22247 1.78435 -0.32609  
 H 1.99066 8.14844 -0.21072  
 H 0.40651 7.34984 -0.03555

### **POP / 5b at 2.80 Å**

O 2.37420 -0.30240 2.74496  
 C 2.41448 -1.51604 2.58583  
 C 3.36716 -2.39993 3.35451  
 N 1.59166 -2.14044 1.70988  
 C 1.52944 -3.57561 1.43595  
 C 0.24654 -3.72280 0.62387  
 C 0.18095 -2.41064 -0.14979  
 C 0.66900 -1.37312 0.87234  
 C -0.44326 -0.87279 1.69696  
 N -1.31552 -0.62917 2.42006  
 H 3.97415 -3.01842 2.67552  
 H 2.81139 -3.08339 4.01686  
 H 4.02019 -1.76206 3.96215  
 H 2.41080 -3.89676 0.85326  
 H 1.51293 -4.15746 2.36970

H 0.26565 -4.60421 -0.03287  
 H -0.61907 -3.81762 1.30010  
 H 0.89172 -2.41071 -0.98807  
 H -0.80187 -2.14798 -0.55670  
 H 1.16807 -0.51413 0.40270  
 H -2.18716 -2.27637 2.79667  
 C 8.86100 7.07200 3.43700  
 H 8.02027 7.59993 2.96505  
 C 8.88500 5.58700 2.98200  
 H 9.72589 5.04640 3.44937  
 H 9.05213 5.49866 1.89581  
 C 7.62228 4.80415 3.30986  
 O 6.72192 5.39264 3.95570  
 O 7.59157 3.61707 2.90310  
 H 9.79474 7.58824 3.16251  
 H 8.71627 7.14439 4.52453  
 C -8.79900 -3.70600 0.78800  
 H -8.46048 -3.06701 -0.04200  
 C -8.16000 -3.24700 2.12900  
 H -8.54450 -3.90126 2.93088  
 H -8.53259 -2.23761 2.36950  
 C -6.65923 -3.22796 2.19298  
 C -5.95999 -2.01816 2.24832  
 H -6.51730 -1.07801 2.18952  
 C -5.91322 -4.41204 2.26812  
 H -6.43015 -5.37627 2.22668  
 C -4.57705 -1.97656 2.40790  
 H -4.04743 -1.02240 2.48091  
 C -4.53280 -4.39237 2.42728  
 H -3.95914 -5.31740 2.51763  
 C -3.85356 -3.17025 2.52288  
 O -2.52901 -3.18992 2.74890  
 H -9.89712 -3.64581 0.83598  
 H -8.51932 -4.74338 0.54573  
 C -2.78800 0.52700 -2.29800  
 H -2.12048 1.04735 -2.99864  
 C -2.99477 -0.88979 -2.84981  
 O -2.91192 -1.14702 -4.03654  
 C -2.24700 0.60900 -0.89100  
 H -2.82727 -0.03741 -0.19895  
 H -2.44029 1.63262 -0.51401  
 O -0.88707 0.32843 -0.79305  
 H -3.76937 1.02963 -2.35621  
 N -3.32758 -1.83754 -1.92069  
 H -3.38031 -1.55714 -0.95071  
 C -3.62100 -3.20800 -2.24500  
 H -3.43782 -3.33684 -3.32073  
 H -4.66940 -3.47033 -2.02172  
 H -2.97132 -3.90198 -1.68747  
 C 4.91700 -7.80000 -0.78200  
 H 6.00708 -7.65399 -0.84205  
 C 4.17200 -6.80300 -1.69000  
 H 3.09073 -7.02932 -1.66649  
 H 4.48562 -6.96330 -2.73757  
 C 4.38409 -5.36666 -1.32410  
 C 5.23497 -4.86094 -0.36993  
 H 5.90806 -5.38980 0.30253  
 C 3.74086 -4.22476 -1.92652  
 N 5.15386 -3.48661 -0.33953  
 H 5.73646 -2.87880 0.21739  
 C 4.25781 -3.06503 -1.29055  
 C 2.78178 -4.06882 -2.94402  
 H 2.35802 -4.94135 -3.44849

C 3.85366 -1.77399 -1.64859  
 H 4.26043 -0.89130 -1.14888  
 C 2.37913 -2.78975 -3.30235  
 H 1.63109 -2.65474 -4.08679  
 C 2.91085 -1.65223 -2.66105  
 H 2.56234 -0.65973 -2.95784  
 H 4.70113 -8.83519 -1.08705  
 H 4.60978 -7.68521 0.26944  
 C 4.72800 7.90500 -3.55000  
 H 4.68563 8.12797 -2.47219  
 C 3.37000 7.45000 -4.07800  
 H 3.40165 7.32802 -5.17607  
 H 2.58338 8.19684 -3.88533  
 C 2.91862 6.11331 -3.48006  
 O 3.76790 5.33817 -3.03232  
 O 1.65480 5.93181 -3.48551  
 H 5.09160 8.80685 -4.07043  
 H 5.46416 7.09968 -3.68442  
 H 1.33925 5.04883 -2.44713  
 C 5.66500 3.07800 -1.29100  
 H 6.64482 2.86841 -0.82634  
 C 4.55800 3.22500 -0.25900  
 H 3.66568 3.58848 -0.78999  
 H 4.82245 4.02402 0.45553  
 C 4.16840 1.97374 0.52176  
 H 4.12365 1.11031 -0.16751  
 H 3.14031 2.10701 0.89257  
 C 5.05915 1.56309 1.69628  
 H 6.07653 1.33824 1.33854  
 H 4.65811 0.62812 2.13090  
 N 5.22357 2.55531 2.73692  
 H 6.19861 3.00094 2.84540  
 C 4.28401 2.98522 3.56265  
 N 3.04652 2.44636 3.56261  
 H 2.37988 2.76584 4.24833  
 H 2.85130 1.54270 3.13235  
 N 4.57989 3.96666 4.41959  
 H 3.83166 4.34647 4.98026  
 H 5.46884 4.56029 4.26081  
 H 5.73640 3.99789 -1.88831  
 H 5.43933 2.25898 -1.99522  
 C 1.42100 7.23500 -0.44800  
 H 1.33869 7.14741 -1.54082  
 C 2.11500 5.99500 0.13900  
 H 2.17580 6.05889 1.23678  
 H 3.14382 5.92992 -0.25064  
 C 1.37640 4.72676 -0.23110  
 N 1.07642 4.43633 -1.53642  
 C 0.88170 3.65419 0.49921  
 H 0.92326 3.49252 1.57613  
 C 0.46228 3.24880 -1.55350  
 H 0.12628 2.77438 -2.47635  
 N 0.31489 2.72724 -0.34326  
 H -0.41722 1.18076 -0.52493  
 H 1.99470 8.14711 -0.21480  
 H 0.40809 7.35373 -0.03125

## **POP / 5b optimum structure**

O 1.98966 -0.24621 1.85587  
 C 1.75288 -1.44067 2.06980  
 C 2.29820 -2.13957 3.29448  
 N 1.03142 -2.20251 1.22754  
 C 0.71356 -3.62356 1.41447

C -0.00237 -4.01923 0.11963  
 C 0.38917 -2.94103 -0.88930  
 C 0.50884 -1.67734 -0.02697  
 C -0.84418 -1.00175 0.15156  
 N -1.79451 -1.28403 0.90369  
 H 3.01419 -2.92498 3.00438  
 H 1.50074 -2.63620 3.86720  
 H 2.81156 -1.40558 3.92755  
 H 1.64104 -4.19853 1.57790  
 H 0.03409 -3.77317 2.26949  
 H 0.28193 -5.02766 -0.21482  
 H -1.08330 -4.01298 0.33077  
 H 1.36886 -3.15679 -1.34420  
 H -0.34019 -2.81233 -1.70095  
 H 1.21320 -0.94793 -0.45001  
 H -1.86063 -2.15076 1.52905  
 C 8.86100 7.07200 3.43700  
 H 8.16058 7.65378 2.81905  
 C 8.88500 5.58700 2.98200  
 H 9.63584 5.03307 3.57298  
 H 9.19334 5.48679 1.93060  
 C 7.57108 4.83237 3.15657  
 O 6.79646 5.17535 4.07891  
 O 7.39372 3.87570 2.35840  
 H 9.85727 7.53143 3.34408  
 H 8.51484 7.14280 4.47820  
 C -8.79900 -3.70600 0.78800  
 H -8.40328 -3.10702 -0.04720  
 C -8.16000 -3.24700 2.12900  
 H -8.59111 -3.86416 2.93915  
 H -8.47601 -2.21165 2.34329  
 C -6.65358 -3.31443 2.16389  
 C -5.87138 -2.15200 2.20837  
 H -6.37707 -1.17822 2.23527  
 C -5.95242 -4.53250 2.14908  
 H -6.52054 -5.47152 2.12918  
 C -4.48211 -2.18740 2.23252  
 H -3.91295 -1.25657 2.27523  
 C -4.56324 -4.59015 2.15864  
 H -4.04782 -5.55570 2.14498  
 C -3.74693 -3.41534 2.19019  
 O -2.45856 -3.46584 2.17693  
 H -9.89647 -3.59453 0.79788  
 H -8.56069 -4.76086 0.57866  
 C -2.78800 0.52700 -2.29800  
 H -2.10736 0.98780 -3.02991  
 C -3.08185 -0.88433 -2.82689  
 O -3.13696 -1.09586 -4.02752  
 C -2.24700 0.60900 -0.89100  
 H -2.90774 0.12713 -0.15551  
 H -2.16737 1.66844 -0.58905  
 O -0.95095 0.03511 -0.76338  
 H -3.72989 1.09819 -2.34736  
 N -3.29322 -1.84687 -1.89354  
 H -3.19517 -1.63048 -0.90311  
 C -3.62100 -3.20800 -2.24500  
 H -3.43937 -3.33252 -3.32092  
 H -4.67534 -3.44383 -2.02310  
 H -2.99635 -3.91401 -1.67726  
 C 4.91700 -7.80000 -0.78200  
 H 5.96605 -7.49726 -0.64051  
 C 4.17200 -6.80300 -1.69000  
 H 3.12249 -7.12881 -1.80692

H 4.60856 -6.84928 -2.70215  
 C 4.21729 -5.38041 -1.22236  
 C 4.41733 -4.91096 0.05457  
 H 4.60081 -5.46351 0.97459  
 C 4.05630 -4.21239 -2.05027  
 N 4.37354 -3.53407 0.06748  
 H 4.56161 -2.94822 0.86755  
 C 4.16631 -3.07558 -1.20763  
 C 3.84032 -4.01692 -3.42509  
 H 3.74672 -4.87272 -4.09824  
 C 4.06990 -1.76904 -1.69928  
 H 4.15740 -0.90530 -1.03714  
 C 3.74698 -2.72295 -3.91663  
 H 3.57836 -2.55808 -4.98357  
 C 3.85896 -1.60946 -3.06119  
 H 3.77854 -0.60256 -3.47853  
 H 4.90108 -8.80920 -1.22072  
 H 4.44577 -7.86794 0.21125  
 C 4.72800 7.90500 -3.55000  
 H 4.69467 8.09204 -2.46611  
 C 3.37000 7.45000 -4.07800  
 H 3.38661 7.34597 -5.17739  
 H 2.57342 8.17673 -3.85761  
 C 2.97469 6.10737 -3.49475  
 O 3.78687 5.31290 -3.07269  
 O 1.67071 5.91926 -3.47533  
 H 5.06059 8.82898 -4.04734  
 H 5.48138 7.12455 -3.72562  
 H 1.44236 5.18797 -2.79157  
 C 5.66500 3.07800 -1.29100  
 H 6.62672 2.79552 -0.83051  
 C 4.55800 3.22500 -0.25900  
 H 3.67374 3.62480 -0.77547  
 H 4.84743 3.98156 0.49002  
 C 4.16068 1.93461 0.44695  
 H 4.05765 1.12364 -0.29487  
 H 3.15790 2.05125 0.88271  
 C 5.10800 1.45702 1.54392  
 H 6.10891 1.26020 1.12947  
 H 4.73974 0.49817 1.95426  
 N 5.28817 2.41342 2.61156  
 H 6.16779 3.06264 2.55401  
 C 4.42813 2.60962 3.59072  
 N 3.28158 1.89298 3.67500  
 H 2.69402 1.99037 4.48873  
 H 2.99385 1.19943 2.97904  
 N 4.71901 3.51489 4.53808  
 H 3.97328 3.82070 5.14661  
 H 5.53952 4.18112 4.38339  
 H 5.80707 4.02059 -1.83764  
 H 5.40432 2.31047 -2.03855  
 C 1.42100 7.23500 -0.44800  
 H 1.31263 7.14860 -1.53645  
 C 2.11500 5.99500 0.13900  
 H 2.19445 6.08832 1.23319  
 H 3.14489 5.93098 -0.24926  
 C 1.41709 4.70184 -0.17577  
 N 1.08292 4.33805 -1.46135  
 C 1.07577 3.66605 0.66783  
 H 1.20018 3.53413 1.73932  
 C 0.57827 3.12515 -1.39672  
 H 0.22115 2.53051 -2.23603  
 N 0.55307 2.67900 -0.12735

H 0.25447 1.74400 0.14433  
H 2.00940 8.13933 -0.22674  
H 0.41748 7.36980 -0.01498

### **POP / 13b at 2.20 Å**

O 2.15197 -0.04330 2.42090  
C 2.17187 -1.26905 2.38398  
C 2.93806 -2.10009 3.38402  
N 1.51000 -1.94988 1.42308  
C 1.38887 -3.39042 1.33161  
C 0.61959 -3.61600 0.02505  
C 0.65363 -2.29561 -0.71700  
C 0.72138 -1.25537 0.40047  
C -0.61380 -0.92413 0.94463  
N -1.50907 -1.03989 1.68696  
H 3.63805 -2.78232 2.87683  
H 2.25112 -2.71733 3.98503  
H 3.49451 -1.42906 4.04932  
H 2.36925 -3.88636 1.26508  
H 0.81513 -3.82520 2.16597  
F 1.16898 -4.63836 -0.67592  
F -0.65577 -3.99027 0.30135  
H 1.57533 -2.25433 -1.31354  
H -0.21055 -2.14824 -1.37480  
H 1.21825 -0.33125 0.08729  
H -2.16906 -2.33209 2.66206  
C 8.86100 7.07200 3.43700  
H 8.11856 7.63940 2.85643  
C 8.88500 5.58700 2.98200  
H 9.66516 5.03670 3.53716  
H 9.15300 5.48816 1.91875  
C 7.58697 4.83053 3.20673  
O 6.77899 5.28213 4.05262  
O 7.44993 3.77870 2.53406  
H 9.84351 7.54802 3.29179  
H 8.56782 7.14193 4.49403  
C -8.79900 -3.70600 0.78800  
H -8.43157 -3.09135 -0.04849  
C -8.16000 -3.24700 2.12900  
H -8.57925 -3.88033 2.93068  
H -8.51868 -2.22715 2.34851  
C -6.66250 -3.25083 2.24820  
C -5.94244 -2.05279 2.18083  
H -6.47855 -1.12234 1.96720  
C -5.94296 -4.42036 2.52785  
H -6.47392 -5.37601 2.59413  
C -4.57148 -2.00488 2.40848  
H -4.02517 -1.06012 2.36378  
C -4.57102 -4.39333 2.75638  
H -4.01679 -5.30519 2.98954  
C -3.86764 -3.17992 2.71784  
O -2.56095 -3.17395 3.00293  
H -9.89516 -3.60877 0.82455  
H -8.54904 -4.75490 0.56265  
C -2.78800 0.52700 -2.29800  
H -2.12351 1.04708 -3.00313  
C -3.01043 -0.88548 -2.86075  
O -3.01819 -1.11887 -4.05878  
C -2.24700 0.60900 -0.89100  
H -2.82493 -0.06656 -0.21063  
H -2.55338 1.61650 -0.50518  
O -0.89596 0.42878 -0.76710  
H -3.77134 1.02685 -2.36216

N -3.25986 -1.85049 -1.92797  
 H -3.20098 -1.58798 -0.95109  
 C -3.62100 -3.20800 -2.24500  
 H -2.97956 -3.91982 -1.70139  
 H -3.47925 -3.34571 -3.32618  
 H -4.67167 -3.42868 -1.98714  
 C 4.91700 -7.80000 -0.78200  
 H 6.00562 -7.74315 -0.93886  
 C 4.17200 -6.80300 -1.69000  
 H 3.08308 -6.90749 -1.53603  
 H 4.35946 -7.06144 -2.74775  
 C 4.56031 -5.37463 -1.44967  
 C 5.44288 -4.90019 -0.50776  
 H 6.03840 -5.45225 0.21677  
 C 4.06323 -4.21230 -2.14418  
 N 5.51211 -3.52672 -0.56626  
 H 6.12179 -2.94546 -0.01099  
 C 4.68150 -3.07506 -1.55950  
 C 3.14792 -4.01995 -3.19391  
 H 2.64316 -4.87271 -3.65445  
 C 4.40231 -1.77051 -1.98359  
 H 4.87281 -0.90558 -1.50881  
 C 2.87561 -2.72923 -3.62460  
 H 2.15489 -2.56633 -4.42946  
 C 3.49176 -1.61398 -3.02076  
 H 3.23309 -0.60921 -3.36466  
 H 4.59821 -8.83110 -0.99830  
 H 4.70681 -7.60127 0.28083  
 C 4.72800 7.90500 -3.55000  
 H 4.69500 8.08610 -2.46485  
 C 3.37000 7.45000 -4.07800  
 H 3.38316 7.36527 -5.17942  
 H 2.57411 8.17417 -3.84628  
 C 2.96830 6.10145 -3.51636  
 O 3.78800 5.30760 -3.09539  
 O 1.67392 5.91839 -3.51463  
 H 5.06181 8.83199 -4.04203  
 H 5.48095 7.12444 -3.72831  
 H 1.42520 5.21009 -2.74934  
 C 5.66500 3.07800 -1.29100  
 H 6.62516 2.79006 -0.82848  
 C 4.55800 3.22500 -0.25900  
 H 3.67285 3.62073 -0.77772  
 H 4.84647 3.99272 0.47958  
 C 4.14717 1.95449 0.47884  
 H 4.10351 1.10692 -0.22956  
 H 3.11856 2.08119 0.84979  
 C 5.02854 1.53425 1.65453  
 H 6.04388 1.29316 1.30043  
 H 4.61671 0.60925 2.09806  
 N 5.19751 2.53976 2.67829  
 H 6.13286 3.08719 2.66389  
 C 4.29140 2.91143 3.56563  
 N 3.06897 2.34237 3.60677  
 H 2.46319 2.57211 4.38007  
 H 2.85081 1.47030 3.11337  
 N 4.60375 3.86553 4.45066  
 H 3.85728 4.24969 5.01106  
 H 5.49670 4.44833 4.31433  
 H 5.80590 4.02225 -1.83499  
 H 5.40250 2.31487 -2.04294  
 C 1.42100 7.23500 -0.44800  
 H 1.33547 7.15184 -1.53912

C 2.11500 5.99500 0.13900  
 H 2.16964 6.05976 1.23665  
 H 3.14697 5.92271 -0.23978  
 C 1.36820 4.71970 -0.24180  
 N 1.08102 4.44876 -1.56002  
 C 0.86664 3.66080 0.50423  
 H 0.89471 3.46235 1.57337  
 C 0.45944 3.28622 -1.59681  
 H 0.10634 2.78118 -2.49496  
 N 0.29973 2.76666 -0.37539  
 H -0.18786 1.79302 -0.30012  
 H 1.99241 8.14748 -0.21182  
 H 0.40743 7.35160 -0.03385

### **POP / 13b at 2.60 Å**

O 2.32496 -0.32032 2.53768  
 C 2.39611 -1.53221 2.39838  
 C 3.32143 -2.39767 3.21737  
 N 1.62236 -2.17468 1.48578  
 C 1.57443 -3.60556 1.24835  
 C 0.35375 -3.75481 0.34921  
 C 0.26708 -2.45295 -0.41473  
 C 0.70093 -1.41900 0.62855  
 C -0.44257 -0.94458 1.42726  
 N -1.31293 -0.73753 2.16157  
 H 3.95280 -3.02844 2.57302  
 H 2.74119 -3.06597 3.87455  
 H 3.95217 -1.74720 3.83504  
 H 2.46553 -3.97544 0.71356  
 H 1.43587 -4.18551 2.17197  
 F 0.44236 -4.84562 -0.43874  
 F -0.75205 -3.92156 1.12400  
 H 0.99993 -2.47101 -1.23318  
 H -0.72580 -2.25181 -0.83317  
 H 1.20052 -0.54964 0.18040  
 H -2.26294 -2.05585 3.06844  
 C 8.86100 7.07200 3.43700  
 H 8.11552 7.63814 2.85930  
 C 8.88500 5.58700 2.98200  
 H 9.66963 5.03740 3.53163  
 H 9.14691 5.48984 1.91709  
 C 7.59014 4.82313 3.21126  
 O 6.77176 5.27669 4.04589  
 O 7.46726 3.76059 2.55208  
 H 9.84251 7.54870 3.28727  
 H 8.57256 7.14271 4.49541  
 C -8.79900 -3.70600 0.78800  
 H -8.44310 -3.08835 -0.05169  
 C -8.16000 -3.24700 2.12900  
 H -8.57480 -3.88837 2.92498  
 H -8.54116 -2.23527 2.35275  
 C -6.66553 -3.22424 2.28878  
 C -5.90644 -2.12157 1.87894  
 H -6.39169 -1.31189 1.32447  
 C -6.00311 -4.23025 3.00603  
 H -6.56935 -5.10088 3.35277  
 C -4.55939 -1.99707 2.21054  
 H -3.99334 -1.10655 1.92387  
 C -4.65812 -4.12657 3.34248  
 H -4.15572 -4.90111 3.92579  
 C -3.92707 -2.98732 2.97921  
 O -2.66481 -2.87982 3.40838  
 H -9.89461 -3.61173 0.83252

H -8.54469 -4.75306 0.55972  
 C -2.78800 0.52700 -2.29800  
 H -2.12160 1.04808 -2.99929  
 C -2.99995 -0.88845 -2.85137  
 O -2.94850 -1.13726 -4.04166  
 C -2.24700 0.60900 -0.89100  
 H -2.82355 -0.03841 -0.19758  
 H -2.43641 1.63192 -0.51176  
 O -0.88450 0.32784 -0.79662  
 H -3.76831 1.03163 -2.35550  
 N -3.29558 -1.84428 -1.91843  
 H -3.34142 -1.56747 -0.94699  
 C -3.62100 -3.20800 -2.24500  
 H -3.00897 -3.91285 -1.66006  
 H -3.41125 -3.35043 -3.31401  
 H -4.68308 -3.43851 -2.05291  
 C 4.91700 -7.80000 -0.78200  
 H 6.00826 -7.67925 -0.86958  
 C 4.17200 -6.80300 -1.69000  
 H 3.08572 -6.99494 -1.63045  
 H 4.45386 -6.98681 -2.74240  
 C 4.43265 -5.36671 -1.35063  
 C 5.29819 -4.87622 -0.40158  
 H 5.95545 -5.41800 0.27610  
 C 3.82734 -4.21104 -1.96782  
 N 5.25912 -3.49923 -0.38472  
 H 5.86697 -2.90339 0.15810  
 C 4.37932 -3.06090 -1.34302  
 C 2.87701 -4.03536 -2.99001  
 H 2.42330 -4.89900 -3.48260  
 C 4.01454 -1.76090 -1.71212  
 H 4.44635 -0.88696 -1.21788  
 C 2.51711 -2.74766 -3.36322  
 H 1.77819 -2.59791 -4.15366  
 C 3.07942 -1.62002 -2.72949  
 H 2.76357 -0.61980 -3.03742  
 H 4.67111 -8.83502 -1.06396  
 H 4.63518 -7.66214 0.27373  
 C 4.72800 7.90500 -3.55000  
 H 4.68592 8.12748 -2.47206  
 C 3.37000 7.45000 -4.07800  
 H 3.40133 7.33095 -5.17640  
 H 2.58306 8.19592 -3.88328  
 C 2.91942 6.11167 -3.48423  
 O 3.76779 5.33208 -3.04355  
 O 1.65455 5.93297 -3.48567  
 H 5.09107 8.80719 -4.07007  
 H 5.46443 7.10002 -3.68514  
 H 1.34233 5.05401 -2.45494  
 C 5.66500 3.07800 -1.29100  
 H 6.63951 2.84577 -0.82645  
 C 4.55800 3.22500 -0.25900  
 H 3.67433 3.61682 -0.78363  
 H 4.84032 3.99908 0.47502  
 C 4.14869 1.95843 0.48369  
 H 4.08874 1.11494 -0.22880  
 H 3.12412 2.09386 0.86393  
 C 5.04728 1.52828 1.64226  
 H 6.06114 1.30486 1.27302  
 H 4.65301 0.59286 2.08169  
 N 5.21685 2.52195 2.67746  
 H 6.15681 3.06624 2.67691  
 C 4.29654 2.89521 3.54762

N 3.07598 2.31741 3.57008  
 H 2.44436 2.54900 4.32129  
 H 2.88816 1.44343 3.07951  
 N 4.59040 3.85389 4.43348  
 H 3.83378 4.23925 4.97928  
 H 5.48060 4.44190 4.30095  
 H 5.75505 4.00646 -1.87213  
 H 5.42625 2.27658 -2.01102  
 C 1.42100 7.23500 -0.44800  
 H 1.34257 7.14946 -1.54125  
 C 2.11500 5.99500 0.13900  
 H 2.17020 6.05663 1.23723  
 H 3.14585 5.93194 -0.24550  
 C 1.37952 4.72400 -0.23577  
 N 1.08129 4.43639 -1.54225  
 C 0.89078 3.64536 0.49068  
 H 0.93174 3.47934 1.56706  
 C 0.47533 3.24535 -1.56444  
 H 0.14195 2.77281 -2.48926  
 N 0.33078 2.71707 -0.35625  
 H -0.41581 1.18499 -0.52765  
 H 1.99243 8.14749 -0.21097  
 H 0.40646 7.35130 -0.03465

### **POP / 13b optimum structure**

O 1.66943 -0.02779 2.26837  
 C 1.39146 -1.20907 2.49998  
 C 1.61487 -1.83301 3.85521  
 N 0.87355 -2.01191 1.54925  
 C 0.52098 -3.42218 1.66978  
 C 0.47680 -3.91182 0.21624  
 C 0.78384 -2.71521 -0.67237  
 C 0.55519 -1.50059 0.22728  
 C -0.88274 -1.00872 0.17087  
 N -1.89690 -1.42926 0.75543  
 H 2.28486 -2.70386 3.79160  
 H 0.65934 -2.18584 4.27423  
 H 2.05855 -1.08395 4.52092  
 H 1.28873 -3.98438 2.21871  
 H -0.47708 -3.58311 2.12509  
 F 1.38887 -4.90716 0.02139  
 F -0.72908 -4.44701 -0.07346  
 H 1.83712 -2.77424 -0.97566  
 H 0.15907 -2.71817 -1.57397  
 H 1.23304 -0.67464 -0.02270  
 H -1.95257 -2.21456 1.48657  
 C 8.86100 7.07200 3.43700  
 H 8.16553 7.65460 2.81421  
 C 8.88500 5.58700 2.98200  
 H 9.62483 5.02974 3.58343  
 H 9.20030 5.48346 1.93311  
 C 7.55852 4.85504 3.15039  
 O 6.81682 5.18710 4.10444  
 O 7.33031 3.93728 2.32200  
 H 9.85813 7.53103 3.35110  
 H 8.50797 7.14089 4.47581  
 C -8.79900 -3.70600 0.78800  
 H -8.41524 -3.09934 -0.04731  
 C -8.16000 -3.24700 2.12900  
 H -8.58961 -3.87081 2.93496  
 H -8.49337 -2.21736 2.34574  
 C -6.65318 -3.28658 2.19943  
 C -5.89912 -2.10570 2.26249

H -6.42715 -1.14371 2.24508  
 C -5.92670 -4.48898 2.24343  
 H -6.47246 -5.44063 2.20858  
 C -4.51301 -2.11137 2.36254  
 H -3.96369 -1.16829 2.42081  
 C -4.53854 -4.51542 2.33329  
 H -4.00134 -5.46833 2.36383  
 C -3.75296 -3.32244 2.39362  
 O -2.46479 -3.33108 2.46250  
 H -9.89690 -3.60454 0.80715  
 H -8.55187 -4.75770 0.57210  
 C -2.78800 0.52700 -2.29800  
 H -2.10401 0.98168 -3.03081  
 C -3.09571 -0.88188 -2.82932  
 O -3.14468 -1.08585 -4.03267  
 C -2.24700 0.60900 -0.89100  
 H -2.92391 0.13545 -0.16568  
 H -2.15785 1.67103 -0.60054  
 O -0.95724 0.03327 -0.73353  
 H -3.72379 1.10802 -2.34459  
 N -3.32654 -1.83768 -1.89792  
 H -3.18231 -1.63627 -0.90616  
 C -3.62100 -3.20800 -2.24500  
 H -2.94581 -3.89060 -1.70734  
 H -3.47941 -3.32250 -3.32814  
 H -4.65654 -3.47941 -1.98076  
 C 4.91700 -7.80000 -0.78200  
 H 6.00407 -7.76302 -0.95616  
 C 4.17200 -6.80300 -1.69000  
 H 3.08578 -6.89057 -1.50863  
 H 4.33157 -7.08491 -2.74666  
 C 4.57087 -5.37405 -1.49198  
 C 5.47304 -4.87212 -0.58562  
 H 6.08524 -5.40305 0.14082  
 C 4.04333 -4.23276 -2.19690  
 N 5.53005 -3.50025 -0.67815  
 H 6.11851 -2.89988 -0.12085  
 C 4.66257 -3.07626 -1.65037  
 C 3.09627 -4.07338 -3.22412  
 H 2.59610 -4.94276 -3.65868  
 C 4.34889 -1.78474 -2.08951  
 H 4.82409 -0.90506 -1.64725  
 C 2.78886 -2.79459 -3.66879  
 H 2.04441 -2.65840 -4.45718  
 C 3.40481 -1.66066 -3.10191  
 H 3.12512 -0.66608 -3.45905  
 H 4.57702 -8.82767 -0.98057  
 H 4.72583 -7.58353 0.28097  
 C 4.72800 7.90500 -3.55000  
 H 4.69274 8.09886 -2.46738  
 C 3.37000 7.45000 -4.07800  
 H 3.38814 7.33825 -5.17658  
 H 2.57478 8.18005 -3.86369  
 C 2.96920 6.11190 -3.48649  
 O 3.77763 5.31758 -3.05749  
 O 1.66404 5.92692 -3.46885  
 H 5.06282 8.82554 -4.05214  
 H 5.48059 7.12259 -3.72012  
 H 1.42984 5.19816 -2.78786  
 C 5.66500 3.07800 -1.29100  
 H 6.61898 2.76916 -0.83070  
 C 4.55800 3.22500 -0.25900  
 H 3.67624 3.63083 -0.77495

H 4.85068 3.97681 0.49307  
 C 4.14990 1.93266 0.44469  
 H 4.09685 1.10656 -0.28788  
 H 3.12570 2.04426 0.83181  
 C 5.04485 1.48055 1.59776  
 H 6.05368 1.24031 1.22576  
 H 4.63816 0.54775 2.03103  
 N 5.22132 2.47145 2.63389  
 H 6.09925 3.11094 2.55385  
 C 4.34904 2.74453 3.58704  
 N 3.16702 2.09336 3.67887  
 H 2.60025 2.23018 4.50207  
 H 2.86248 1.34235 3.05342  
 N 4.65917 3.67508 4.50010  
 H 3.91684 4.02737 5.08697  
 H 5.52870 4.28762 4.36202  
 H 5.82750 4.02801 -1.81875  
 H 5.39201 2.33098 -2.05494  
 C 1.42100 7.23500 -0.44800  
 H 1.29734 7.14238 -1.53413  
 C 2.11500 5.99500 0.13900  
 H 2.20449 6.09225 1.23199  
 H 3.14121 5.92554 -0.25795  
 C 1.40694 4.70730 -0.16591  
 N 1.04996 4.34622 -1.44632  
 C 1.06385 3.68003 0.68628  
 H 1.20856 3.54590 1.75508  
 C 0.52412 3.14310 -1.37006  
 H 0.14093 2.55286 -2.20105  
 N 0.51185 2.70096 -0.09823  
 H 0.18907 1.77972 0.18932  
 H 2.01731 8.13747 -0.24049  
 H 0.42418 7.37884 -0.00251

### **POP / 15b at 2.20 Å**

O 2.29247 -0.22490 2.34711  
 C 2.32140 -1.43620 2.14677  
 C 3.12337 -2.37526 3.01592  
 N 1.63088 -1.99731 1.13067  
 C 1.51518 -3.41771 0.83287  
 C 0.40561 -3.46427 -0.22228  
 C 0.53287 -2.12728 -0.92645  
 C 0.79996 -1.17875 0.23877  
 C -0.47901 -0.85261 0.90887  
 N -1.35038 -1.02593 1.66869  
 H 3.75247 -3.04651 2.41155  
 H 2.44988 -3.00513 3.61907  
 H 3.75071 -1.77964 3.69059  
 H 2.44000 -3.82483 0.38686  
 H 1.26509 -4.00762 1.72733  
 F 0.57285 -4.53079 -1.06977  
 H -0.58010 -3.57787 0.26169  
 H 1.41182 -2.15389 -1.58589  
 H -0.34576 -1.80545 -1.49578  
 H 1.31253 -0.25773 -0.05846  
 H -2.09945 -2.51437 2.10750  
 C 8.86100 7.07200 3.43700  
 H 8.12877 7.64288 2.84679  
 C 8.88500 5.58700 2.98200  
 H 9.65911 5.03580 3.54477  
 H 9.16200 5.48828 1.92125  
 C 7.58441 4.82908 3.19510  
 O 6.77678 5.25726 4.05247

O 7.44977 3.79244 2.49742  
 H 9.84717 7.54422 3.30502  
 H 8.55393 7.14228 4.49020  
 C -8.79900 -3.70600 0.78800  
 H -8.42349 -3.09145 -0.04455  
 C -8.16000 -3.24700 2.12900  
 H -8.55235 -3.88565 2.93952  
 H -8.49609 -2.22293 2.36027  
 C -6.65693 -3.28438 2.13102  
 C -5.90400 -2.10642 2.10270  
 H -6.42292 -1.14251 2.09188  
 C -5.95709 -4.49901 2.14289  
 H -6.51699 -5.43986 2.16872  
 C -4.51192 -2.12480 2.09670  
 H -3.93384 -1.19730 2.08249  
 C -4.56800 -4.53924 2.13352  
 H -4.02692 -5.48806 2.15141  
 C -3.82579 -3.34846 2.11446  
 O -2.48849 -3.42448 2.12480  
 H -9.89636 -3.61182 0.81222  
 H -8.54661 -4.75484 0.56726  
 C -2.78800 0.52700 -2.29800  
 H -2.11776 1.04407 -2.99965  
 C -3.02954 -0.88019 -2.86210  
 O -3.11287 -1.09317 -4.05991  
 C -2.24700 0.60900 -0.89100  
 H -2.78004 -0.10862 -0.21828  
 H -2.60407 1.59009 -0.48380  
 O -0.88734 0.50690 -0.77190  
 H -3.76661 1.03422 -2.36806  
 N -3.21664 -1.86198 -1.93079  
 H -3.10450 -1.61315 -0.95562  
 C -3.62100 -3.20800 -2.24500  
 H -3.89532 -3.23952 -3.30895  
 H -4.48707 -3.50913 -1.63452  
 H -2.81095 -3.93825 -2.07172  
 C 4.91700 -7.80000 -0.78200  
 H 6.00734 -7.71664 -0.91347  
 C 4.17200 -6.80300 -1.69000  
 H 3.08191 -6.93790 -1.56964  
 H 4.39267 -7.03866 -2.74656  
 C 4.51404 -5.36905 -1.42296  
 C 5.33166 -4.87270 -0.43555  
 H 5.89998 -5.40884 0.32217  
 C 4.02609 -4.22038 -2.14606  
 N 5.36840 -3.49709 -0.49368  
 H 5.94600 -2.90169 0.08096  
 C 4.58830 -3.06751 -1.53695  
 C 3.16446 -4.05554 -3.24464  
 H 2.69758 -4.92125 -3.72043  
 C 4.31506 -1.77243 -1.99211  
 H 4.74272 -0.89481 -1.50076  
 C 2.89964 -2.77443 -3.70589  
 H 2.22212 -2.63073 -4.55056  
 C 3.46690 -1.64353 -3.08399  
 H 3.21448 -0.64680 -3.45481  
 H 4.62475 -8.83330 -1.02355  
 H 4.68036 -7.62546 0.27957  
 C 4.72800 7.90500 -3.55000  
 H 4.69503 8.08682 -2.46494  
 C 3.37000 7.45000 -4.07800  
 H 3.38363 7.36578 -5.17952  
 H 2.57450 8.17479 -3.84674

C 2.96572 6.10130 -3.51759  
 O 3.78620 5.30701 -3.09705  
 O 1.67270 5.91918 -3.51799  
 H 5.06254 8.83152 -4.04263  
 H 5.48058 7.12383 -3.72741  
 H 1.41951 5.21403 -2.73805  
 C 5.66500 3.07800 -1.29100  
 H 6.62939 2.80611 -0.82791  
 C 4.55800 3.22500 -0.25900  
 H 3.66960 3.61544 -0.77635  
 H 4.84405 3.99271 0.48032  
 C 4.16226 1.94709 0.47290  
 H 4.10451 1.10925 -0.24603  
 H 3.14130 2.06361 0.86781  
 C 5.07407 1.51395 1.61936  
 H 6.08767 1.30529 1.24125  
 H 4.69185 0.56970 2.04795  
 N 5.23714 2.49867 2.66366  
 H 6.16104 3.07088 2.64777  
 C 4.33341 2.81596 3.57194  
 N 3.13348 2.19898 3.61669  
 H 2.53213 2.37907 4.40634  
 H 2.94044 1.33714 3.09720  
 N 4.62704 3.76140 4.47572  
 H 3.87329 4.12031 5.04329  
 H 5.49278 4.37521 4.33217  
 H 5.79498 4.01712 -1.84664  
 H 5.40890 2.30325 -2.03333  
 C 1.42100 7.23500 -0.44800  
 H 1.33906 7.15272 -1.53950  
 C 2.11500 5.99500 0.13900  
 H 2.16700 6.05788 1.23689  
 H 3.14754 5.92337 -0.23833  
 C 1.36389 4.72582 -0.24780  
 N 1.07602 4.46627 -1.56714  
 C 0.84910 3.66681 0.48961  
 H 0.87193 3.46231 1.55804  
 C 0.44066 3.31041 -1.61055  
 H 0.08563 2.81616 -2.51417  
 N 0.27201 2.78466 -0.39436  
 H -0.23495 1.79270 -0.34411  
 H 1.98933 8.14890 -0.20932  
 H 0.40577 7.34861 -0.03700

### POP / 15b at 2.60 Å

O 2.33519 -0.30230 2.59762  
 C 2.42897 -1.50853 2.41730  
 C 3.38510 -2.37440 3.19968  
 N 1.65896 -2.13840 1.49681  
 C 1.63101 -3.56353 1.21523  
 C 0.36067 -3.72317 0.38518  
 C 0.27135 -2.41558 -0.38225  
 C 0.74012 -1.37613 0.64319  
 C -0.38678 -0.87909 1.45153  
 N -1.25583 -0.68146 2.19274  
 H 4.00851 -2.98736 2.53111  
 H 2.83039 -3.05946 3.86159  
 H 4.02101 -1.72354 3.81183  
 H 2.49258 -3.88849 0.60465  
 H 1.61598 -4.16122 2.13793  
 F 0.45049 -4.81646 -0.43742  
 H -0.51892 -3.86377 1.03819  
 H 0.98533 -2.43709 -1.21832

H -0.71855 -2.17855 -0.78790  
 H 1.24309 -0.51755 0.17730  
 H -2.16021 -2.28212 2.52075  
 C 8.86100 7.07200 3.43700  
 H 8.11456 7.63776 2.86015  
 C 8.88500 5.58700 2.98200  
 H 9.67025 5.03756 3.53091  
 H 9.14536 5.48957 1.91674  
 C 7.58992 4.82437 3.21380  
 O 6.77382 5.27996 4.04964  
 O 7.46456 3.76184 2.55552  
 H 9.84207 7.54939 3.28625  
 H 8.57358 7.14242 4.49569  
 C -8.79900 -3.70600 0.78800  
 H -8.46682 -3.06019 -0.03918  
 C -8.16000 -3.24700 2.12900  
 H -8.52820 -3.90948 2.93155  
 H -8.53445 -2.24050 2.37787  
 C -6.65806 -3.22433 2.15336  
 C -5.95595 -2.01578 2.18541  
 H -6.51419 -1.07456 2.16660  
 C -5.91142 -4.41037 2.17732  
 H -6.43241 -5.37297 2.15392  
 C -4.56588 -1.97837 2.26622  
 H -4.03000 -1.02621 2.32011  
 C -4.52443 -4.39475 2.25521  
 H -3.94726 -5.32098 2.29759  
 C -3.83880 -3.17415 2.31848  
 O -2.50160 -3.19564 2.44977  
 H -9.89785 -3.65702 0.83601  
 H -8.50943 -4.73944 0.54134  
 C -2.78800 0.52700 -2.29800  
 H -2.11868 1.04470 -2.99905  
 C -3.00816 -0.88680 -2.85242  
 O -2.96801 -1.13190 -4.04396  
 C -2.24700 0.60900 -0.89100  
 H -2.82222 -0.04025 -0.19776  
 H -2.44425 1.63110 -0.51265  
 O -0.88373 0.33756 -0.79186  
 H -3.76567 1.03653 -2.35615  
 N -3.30071 -1.84337 -1.91928  
 H -3.33060 -1.56860 -0.94667  
 C -3.62100 -3.20800 -2.24500  
 H -3.47942 -3.32768 -3.32805  
 H -4.66340 -3.46044 -1.98648  
 H -2.95687 -3.91456 -1.72157  
 C 4.91700 -7.80000 -0.78200  
 H 6.00842 -7.69260 -0.88413  
 C 4.17200 -6.80300 -1.69000  
 H 3.08406 -6.97767 -1.61126  
 H 4.43606 -7.00082 -2.74450  
 C 4.45700 -5.36795 -1.36577  
 C 5.33824 -4.88153 -0.42932  
 H 5.99736 -5.42640 0.24400  
 C 3.85438 -4.20991 -1.98022  
 N 5.31118 -3.50438 -0.41751  
 H 5.92523 -2.91129 0.12103  
 C 4.42163 -3.06230 -1.36511  
 C 2.88976 -4.03078 -2.98776  
 H 2.42193 -4.89253 -3.47012  
 C 4.05608 -1.76087 -1.72799  
 H 4.49680 -0.88912 -1.23780  
 C 2.53010 -2.74202 -3.35575

H 1.77767 -2.58953 -4.13280  
 C 3.10577 -1.61658 -2.73052  
 H 2.78737 -0.61535 -3.03259  
 H 4.65590 -8.83504 -1.05036  
 H 4.64979 -7.64828 0.27566  
 C 4.72800 7.90500 -3.55000  
 H 4.68577 8.12836 -2.47223  
 C 3.37000 7.45000 -4.07800  
 H 3.40182 7.33017 -5.17632  
 H 2.58340 8.19656 -3.88426  
 C 2.91799 6.11239 -3.48400  
 O 3.76547 5.33243 -3.04242  
 O 1.65295 5.93497 -3.48652  
 H 5.09146 8.80666 -4.07075  
 H 5.46425 7.09970 -3.68432  
 H 1.33979 5.05639 -2.45454  
 C 5.66500 3.07800 -1.29100  
 H 6.63877 2.84349 -0.82599  
 C 4.55800 3.22500 -0.25900  
 H 3.67391 3.61610 -0.78343  
 H 4.84023 3.99897 0.47520  
 C 4.15088 1.95691 0.48321  
 H 4.10314 1.11168 -0.22812  
 H 3.12284 2.08599 0.85625  
 C 5.04283 1.53193 1.64900  
 H 6.05829 1.30573 1.28584  
 H 4.64467 0.59912 2.08995  
 N 5.20918 2.52940 2.68144  
 H 6.15143 3.06791 2.68385  
 C 4.28602 2.91262 3.54421  
 N 3.06017 2.34633 3.56152  
 H 2.43275 2.58107 4.31539  
 H 2.87240 1.46411 3.08479  
 N 4.58175 3.87272 4.42803  
 H 3.82419 4.26723 4.96585  
 H 5.47825 4.45166 4.30123  
 H 5.75715 4.00699 -1.87097  
 H 5.42523 2.27781 -2.01196  
 C 1.42100 7.23500 -0.44800  
 H 1.34274 7.14956 -1.54127  
 C 2.11500 5.99500 0.13900  
 H 2.17029 6.05648 1.23724  
 H 3.14585 5.93186 -0.24556  
 C 1.37891 4.72550 -0.23597  
 N 1.07755 4.43992 -1.54214  
 C 0.89024 3.64742 0.49067  
 H 0.93487 3.47982 1.56663  
 C 0.46967 3.24989 -1.56414  
 H 0.13405 2.77804 -2.48848  
 N 0.32686 2.72146 -0.35599  
 H -0.42202 1.19905 -0.52460  
 H 1.99202 8.14776 -0.21087  
 H 0.40627 7.35093 -0.03493

### **POP / 15b optimum structure**

O 1.44737 0.38425 2.07883  
 C 1.33909 -0.78635 2.47181  
 C 1.68462 -1.17834 3.88909  
 N 0.91491 -1.77644 1.66703  
 C 0.72255 -3.17381 2.04887  
 C 0.42202 -3.90709 0.73480  
 C 0.72658 -2.90089 -0.36833  
 C 0.54134 -1.52775 0.27672

C -0.89660 -1.03615 0.16207  
 N -1.92459 -1.49396 0.69705  
 H 2.43610 -1.98152 3.91904  
 H 0.79003 -1.55608 4.40856  
 H 2.07811 -0.30530 4.42315  
 H 1.63912 -3.60090 2.48666  
 H -0.12215 -3.28972 2.74812  
 F 1.23267 -5.01833 0.59474  
 H -0.62343 -4.25323 0.74847  
 H 1.78037 -3.03664 -0.65509  
 H 0.11042 -3.03498 -1.26615  
 H 1.21140 -0.77478 -0.15758  
 H -1.96421 -2.32432 1.37877  
 C 8.86100 7.07200 3.43700  
 H 8.15919 7.65274 2.81960  
 C 8.88500 5.58700 2.98200  
 H 9.62834 5.03122 3.58046  
 H 9.19446 5.48334 1.93140  
 C 7.55996 4.85784 3.15887  
 O 6.83403 5.18752 4.12693  
 O 7.31312 3.94990 2.32667  
 H 9.85630 7.53337 3.34283  
 H 8.51650 7.14012 4.47865  
 C -8.79900 -3.70600 0.78800  
 H -8.38760 -3.12252 -0.05054  
 C -8.16000 -3.24700 2.12900  
 H -8.60989 -3.84870 2.94075  
 H -8.45893 -2.20447 2.33248  
 C -6.65426 -3.34064 2.18481  
 C -5.85513 -2.19191 2.26778  
 H -6.34466 -1.21063 2.30887  
 C -5.97007 -4.56827 2.16009  
 H -6.55013 -5.49880 2.11428  
 C -4.46699 -2.25060 2.31066  
 H -3.88803 -1.32719 2.38179  
 C -4.58121 -4.64677 2.18614  
 H -4.07942 -5.61903 2.15524  
 C -3.74985 -3.48568 2.24232  
 O -2.45874 -3.54782 2.21801  
 H -9.89390 -3.57315 0.79243  
 H -8.58074 -4.76722 0.58914  
 C -2.78800 0.52700 -2.29800  
 H -2.10184 0.97923 -3.03005  
 C -3.10131 -0.88213 -2.82958  
 O -3.14996 -1.08738 -4.03280  
 C -2.24700 0.60900 -0.89100  
 H -2.93264 0.14831 -0.16551  
 H -2.14099 1.67121 -0.60861  
 O -0.95938 0.02395 -0.71701  
 H -3.72120 1.11216 -2.34359  
 N -3.33727 -1.83616 -1.89740  
 H -3.17946 -1.63732 -0.90506  
 C -3.62100 -3.20800 -2.24500  
 H -3.44114 -3.33334 -3.32151  
 H -4.66514 -3.47940 -2.01586  
 H -2.97011 -3.88992 -1.67716  
 C 4.91700 -7.80000 -0.78200  
 H 6.00549 -7.75261 -0.94514  
 C 4.17200 -6.80300 -1.69000  
 H 3.08520 -6.90535 -1.51936  
 H 4.34516 -7.07270 -2.74782  
 C 4.55082 -5.37220 -1.47054  
 C 5.46528 -4.87288 -0.57521

H 6.10293 -5.40738 0.12626  
 C 3.98480 -4.22681 -2.13789  
 N 5.49614 -3.49867 -0.64120  
 H 6.08412 -2.89916 -0.08256  
 C 4.59635 -3.07086 -1.58228  
 C 3.00666 -4.06360 -3.13468  
 H 2.51297 -4.93341 -3.57579  
 C 4.24583 -1.77711 -1.98380  
 H 4.71449 -0.89842 -1.53290  
 C 2.65997 -2.78190 -3.54009  
 H 1.89084 -2.64324 -4.30389  
 C 3.27023 -1.64907 -2.96544  
 H 2.96316 -0.65268 -3.29430  
 H 4.58878 -8.82939 -0.99147  
 H 4.71253 -7.59126 0.27995  
 C 4.72800 7.90500 -3.55000  
 H 4.69320 8.09405 -2.46656  
 C 3.37000 7.45000 -4.07800  
 H 3.38538 7.34045 -5.17669  
 H 2.57206 8.17529 -3.85780  
 C 2.98302 6.10677 -3.48387  
 O 3.80257 5.32012 -3.06233  
 O 1.67982 5.90867 -3.45260  
 H 5.06143 8.82823 -4.04829  
 H 5.48081 7.12391 -3.72413  
 H 1.45734 5.17058 -2.77968  
 C 5.66500 3.07800 -1.29100  
 H 6.60892 2.73567 -0.83337  
 C 4.55800 3.22500 -0.25900  
 H 3.67754 3.63573 -0.77220  
 H 4.85341 3.96809 0.50028  
 C 4.15581 1.91961 0.42670  
 H 4.17740 1.09369 -0.30719  
 H 3.10912 1.98496 0.75696  
 C 5.00861 1.49770 1.62350  
 H 6.02376 1.23027 1.28890  
 H 4.57552 0.58670 2.07758  
 N 5.17678 2.51834 2.63132  
 H 6.07176 3.12927 2.55855  
 C 4.28435 2.86731 3.54099  
 N 3.07320 2.26986 3.61686  
 H 2.43700 2.55282 4.34658  
 H 2.69367 1.61658 2.92390  
 N 4.60817 3.80612 4.43658  
 H 3.87123 4.19332 5.00738  
 H 5.52468 4.36302 4.33391  
 H 5.85397 4.03471 -1.79764  
 H 5.37739 2.35483 -2.07189  
 C 1.42100 7.23500 -0.44800  
 H 1.29089 7.13964 -1.53326  
 C 2.11500 5.99500 0.13900  
 H 2.21091 6.09904 1.23099  
 H 3.14032 5.92686 -0.26119  
 C 1.41655 4.70195 -0.15147  
 N 1.07245 4.30570 -1.42473  
 C 1.09645 3.68830 0.72288  
 H 1.24941 3.58730 1.79361  
 C 0.57839 3.08934 -1.31915  
 H 0.21519 2.46772 -2.13601  
 N 0.57200 2.67676 -0.03690  
 H 0.31614 1.74407 0.28394  
 H 2.02118 8.13634 -0.24653  
 H 0.42702 7.38330 0.00253

## **POP / 14b at 2.20 Å**

O 2.20947 -0.22717 2.46972  
C 2.22681 -1.43619 2.25504  
C 2.96757 -2.39418 3.15763  
N 1.57293 -1.97927 1.20380  
C 1.50674 -3.39478 0.85653  
C 0.54859 -3.45289 -0.32982  
C 0.58775 -2.05731 -0.91294  
C 0.76294 -1.15292 0.30637  
C -0.53800 -0.84857 0.93897  
N -1.41526 -0.97337 1.69861  
H 3.61570 -3.07887 2.58988  
H 2.25107 -3.01172 3.72237  
H 3.56985 -1.81151 3.86530  
H 2.49748 -3.78060 0.56235  
H 1.11285 -4.01156 1.67933  
H 0.83313 -4.23225 -1.05337  
F -0.72549 -3.75380 0.11859  
H 1.46547 -1.96075 -1.56587  
H -0.30725 -1.78760 -1.48417  
H 1.27055 -0.21284 0.06421  
H -2.15031 -2.28030 2.59902  
C 8.86100 7.07200 3.43700  
H 8.12792 7.64257 2.84758  
C 8.88500 5.58700 2.98200  
H 9.65855 5.03547 3.54522  
H 9.16173 5.48763 1.92122  
C 7.58278 4.83139 3.19618  
O 6.77892 5.26317 4.05569  
O 7.44142 3.79557 2.49914  
H 9.84685 7.54462 3.30397  
H 8.55506 7.14201 4.49049  
C -8.79900 -3.70600 0.78800  
H -8.42470 -3.09905 -0.05142  
C -8.16000 -3.24700 2.12900  
H -8.57654 -3.87940 2.93133  
H -8.52115 -2.22660 2.34696  
C -6.66106 -3.25686 2.24763  
C -5.89008 -2.19211 1.76426  
H -6.38023 -1.37743 1.22117  
C -5.98997 -4.27012 2.94592  
H -6.56347 -5.11220 3.34770  
C -4.51948 -2.11767 1.99082  
H -3.93785 -1.26126 1.64187  
C -4.61884 -4.21697 3.17767  
H -4.10667 -5.00302 3.73738  
C -3.86460 -3.12424 2.72290  
O -2.56566 -3.07269 3.02157  
H -9.89446 -3.59842 0.81851  
H -8.55389 -4.75745 0.56995  
C -2.78800 0.52700 -2.29800  
H -2.12214 1.04901 -3.00022  
C -3.01844 -0.88340 -2.86375  
O -3.04085 -1.11206 -4.06264  
C -2.24700 0.60900 -0.89100  
H -2.78985 -0.10119 -0.21864  
H -2.59752 1.59468 -0.48900  
O -0.89006 0.49634 -0.76610  
H -3.77033 1.02796 -2.36394  
N -3.26196 -1.84975 -1.93157  
H -3.16964 -1.59886 -0.95497  
C -3.62100 -3.20800 -2.24500

H -3.47212 -3.35194 -3.32456  
 H -4.67388 -3.42680 -1.99503  
 H -2.98318 -3.91356 -1.69045  
 C 4.91700 -7.80000 -0.78200  
 H 6.00775 -7.69030 -0.88686  
 C 4.17200 -6.80300 -1.69000  
 H 3.08369 -6.97722 -1.60651  
 H 4.42854 -7.01306 -2.74380  
 C 4.47032 -5.36597 -1.39275  
 C 5.23673 -4.86029 -0.36915  
 H 5.78087 -5.39027 0.41031  
 C 3.99831 -4.22230 -2.13337  
 N 5.25950 -3.48489 -0.42519  
 H 5.80112 -2.88337 0.17781  
 C 4.52179 -3.06296 -1.50160  
 C 3.18332 -4.06622 -3.26935  
 H 2.75531 -4.93770 -3.77205  
 C 4.26191 -1.77139 -1.97355  
 H 4.66222 -0.88998 -1.46650  
 C 2.92348 -2.78701 -3.74070  
 H 2.28151 -2.64915 -4.61367  
 C 3.45844 -1.65106 -3.09962  
 H 3.21540 -0.65748 -3.48460  
 H 4.65290 -8.83444 -1.04895  
 H 4.65255 -7.65078 0.27681  
 C 4.72800 7.90500 -3.55000  
 H 4.69556 8.08496 -2.46462  
 C 3.37000 7.45000 -4.07800  
 H 3.38274 7.36816 -5.17970  
 H 2.57393 8.17335 -3.84433  
 C 2.96813 6.09941 -3.51979  
 O 3.79053 5.30557 -3.10147  
 O 1.67567 5.91569 -3.51787  
 H 5.06175 8.83259 -4.04116  
 H 5.48093 7.12457 -3.72917  
 H 1.42453 5.20913 -2.73644  
 C 5.66500 3.07800 -1.29100  
 H 6.62657 2.79453 -0.82888  
 C 4.55800 3.22500 -0.25900  
 H 3.67232 3.62253 -0.77538  
 H 4.84781 3.98826 0.48336  
 C 4.15169 1.94767 0.46931  
 H 4.09915 1.11151 -0.25213  
 H 3.12719 2.06870 0.85431  
 C 5.04911 1.51155 1.62679  
 H 6.06195 1.28377 1.25735  
 H 4.65011 0.57682 2.06194  
 N 5.22005 2.50298 2.66319  
 H 6.14630 3.06833 2.64608  
 C 4.31314 2.84553 3.56089  
 N 3.10327 2.24865 3.60376  
 H 2.50015 2.44836 4.38750  
 H 2.90238 1.37674 3.10583  
 N 4.61288 3.79850 4.45266  
 H 3.86374 4.16489 5.02138  
 H 5.49195 4.39779 4.31657  
 H 5.80284 4.02084 -1.83828  
 H 5.40365 2.31215 -2.04070  
 C 1.42100 7.23500 -0.44800  
 H 1.33962 7.15292 -1.53962  
 C 2.11500 5.99500 0.13900  
 H 2.16572 6.05731 1.23699  
 H 3.14789 5.92358 -0.23731

C 1.36336 4.72376 -0.24864  
 N 1.08092 4.46186 -1.56876  
 C 0.84281 3.66572 0.48751  
 H 0.85794 3.46357 1.55656  
 C 0.44477 3.30626 -1.61370  
 H 0.09293 2.81198 -2.51860  
 N 0.26948 2.78144 -0.39792  
 H -0.24092 1.78712 -0.34950  
 H 1.98907 8.14891 -0.20880  
 H 0.40558 7.34828 -0.03749

## POP / 14b at 2.60 Å

O 2.42117 -0.52937 2.58922  
 C 2.46365 -1.71524 2.29037  
 C 3.34410 -2.69960 3.02113  
 N 1.70988 -2.21997 1.28021  
 C 1.62622 -3.61615 0.86205  
 C 0.58310 -3.61424 -0.25126  
 C 0.57171 -2.18937 -0.75720  
 C 0.82562 -1.35781 0.50122  
 C -0.41099 -1.11529 1.26565  
 N -1.33263 -1.08035 1.96513  
 H 3.96023 -3.28814 2.32478  
 H 2.72599 -3.40785 3.59586  
 H 3.98757 -2.14260 3.71284  
 H 2.59564 -3.97969 0.48388  
 H 1.29339 -4.27724 1.67773  
 H 0.80681 -4.35282 -1.03522  
 F -0.65844 -3.92883 0.27652  
 H 1.40544 -2.03253 -1.45495  
 H -0.35872 -1.90633 -1.25957  
 H 1.29847 -0.38898 0.29077  
 H -2.17250 -2.43684 2.86541  
 C 8.86100 7.07200 3.43700  
 H 8.12457 7.64131 2.85070  
 C 8.88500 5.58700 2.98200  
 H 9.66456 5.03714 3.53869  
 H 9.15432 5.48959 1.91917  
 C 7.58797 4.82266 3.20295  
 O 6.77962 5.24917 4.06038  
 O 7.45684 3.78092 2.51135  
 H 9.84578 7.54532 3.29885  
 H 8.56032 7.14263 4.49209  
 C -8.79900 -3.70600 0.78800  
 H -8.40062 -3.12225 -0.05679  
 C -8.16000 -3.24700 2.12900  
 H -8.61240 -3.84929 2.93497  
 H -8.48728 -2.21118 2.32505  
 C -6.66599 -3.30621 2.28073  
 C -5.85510 -2.24467 1.86242  
 H -6.30810 -1.39839 1.33602  
 C -6.04283 -4.36215 2.96042  
 H -6.64789 -5.20283 3.31551  
 C -4.49189 -2.21042 2.14133  
 H -3.88237 -1.35287 1.84691  
 C -4.68058 -4.34970 3.24236  
 H -4.20635 -5.16532 3.79265  
 C -3.89117 -3.25633 2.86056  
 O -2.60331 -3.24020 3.22240  
 H -9.89064 -3.56543 0.80943  
 H -8.58431 -4.76746 0.58694  
 C -2.78800 0.52700 -2.29800  
 H -2.11471 1.04238 -2.99686

C -3.02121 -0.88422 -2.85490  
 O -3.01298 -1.11976 -4.05018  
 C -2.24700 0.60900 -0.89100  
 H -2.79812 -0.06222 -0.20038  
 H -2.46337 1.62246 -0.50017  
 O -0.87771 0.36909 -0.81732  
 H -3.76314 1.04086 -2.36218  
 N -3.28921 -1.84503 -1.92255  
 H -3.26107 -1.58952 -0.94465  
 C -3.62100 -3.20800 -2.24500  
 H -3.44033 -3.34813 -3.31976  
 H -4.67699 -3.44124 -2.02472  
 H -2.98863 -3.90585 -1.67415  
 C 4.91700 -7.80000 -0.78200  
 H 6.00786 -7.69841 -0.89381  
 C 4.17200 -6.80300 -1.69000  
 H 3.08381 -6.97602 -1.60132  
 H 4.42243 -7.01926 -2.74417  
 C 4.46955 -5.36369 -1.40440  
 C 5.28287 -4.85080 -0.42138  
 H 5.87163 -5.37623 0.32840  
 C 3.95169 -4.22478 -2.12247  
 N 5.28934 -3.47487 -0.47819  
 H 5.86778 -2.86847 0.08499  
 C 4.49466 -3.06032 -1.51692  
 C 3.08315 -4.07586 -3.21960  
 H 2.64326 -4.95093 -3.70575  
 C 4.19872 -1.77087 -1.97357  
 H 4.61464 -0.88547 -1.48620  
 C 2.79101 -2.79885 -3.67844  
 H 2.11314 -2.66726 -4.52490  
 C 3.34237 -1.65745 -3.06080  
 H 3.07562 -0.66548 -3.43410  
 H 4.64515 -8.83367 -1.04358  
 H 4.66047 -7.64381 0.27785  
 C 4.72800 7.90500 -3.55000  
 H 4.68606 8.12631 -2.47184  
 C 3.37000 7.45000 -4.07800  
 H 3.40087 7.33058 -5.17636  
 H 2.58273 8.19543 -3.88286  
 C 2.92100 6.11105 -3.48272  
 O 3.77089 5.33311 -3.04171  
 O 1.65653 5.92981 -3.48299  
 H 5.09049 8.80793 -4.06922  
 H 5.46474 7.10052 -3.68622  
 H 1.34177 5.05150 -2.45081  
 C 5.66500 3.07800 -1.29100  
 H 6.64099 2.85113 -0.82723  
 C 4.55800 3.22500 -0.25900  
 H 3.67355 3.61699 -0.78219  
 H 4.84075 3.99630 0.47751  
 C 4.15427 1.95218 0.47635  
 H 4.07842 1.11930 -0.24761  
 H 3.13797 2.08800 0.87914  
 C 5.07403 1.50525 1.61156  
 H 6.08430 1.29989 1.22275  
 H 4.69817 0.55686 2.03924  
 N 5.24628 2.48247 2.66165  
 H 6.17243 3.05603 2.64846  
 C 4.34131 2.80071 3.56728  
 N 3.13998 2.18196 3.60918  
 H 2.53476 2.35456 4.39722  
 H 2.96274 1.32044 3.09438

N 4.63065 3.74556 4.47209  
 H 3.87261 4.11012 5.03052  
 H 5.49684 4.36108 4.33060  
 H 5.75190 4.00444 -1.87594  
 H 5.42802 2.27342 -2.00852  
 C 1.42100 7.23500 -0.44800  
 H 1.33971 7.14814 -1.54092  
 C 2.11500 5.99500 0.13900  
 H 2.17400 6.05898 1.23685  
 H 3.14448 5.92974 -0.24884  
 C 1.37511 4.72872 -0.23098  
 N 1.07600 4.43774 -1.53644  
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 H 0.91167 3.50240 1.57959  
 C 0.45693 3.25352 -1.55209  
 H 0.11864 2.77750 -2.47319  
 N 0.30567 2.73547 -0.34042  
 H -0.42231 1.22540 -0.52055  
 H 1.99370 8.14742 -0.21367  
 H 0.40767 7.35273 -0.03214

### **POP / 14b optimum structure**

O 1.58408 -0.14548 2.44165  
 C 1.26519 -1.33227 2.57707  
 C 1.34328 -2.04291 3.90430  
 N 0.81263 -2.07159 1.54297  
 C 0.46760 -3.49532 1.53776  
 C 0.37218 -3.86508 0.04959  
 C 0.80748 -2.62201 -0.71580  
 C 0.55111 -1.46919 0.25419  
 C -0.88406 -0.98095 0.19127  
 N -1.89848 -1.37906 0.79380  
 H 2.00983 -2.91775 3.85428  
 H 0.34295 -2.41068 4.18491  
 H 1.71721 -1.34434 4.66136  
 H 1.24815 -4.07958 2.04781  
 H -0.51721 -3.69787 2.00758  
 H 0.99669 -4.73863 -0.19836  
 F -0.92056 -4.20606 -0.27965  
 H 1.88053 -2.67901 -0.94771  
 H 0.26055 -2.52480 -1.66276  
 H 1.23410 -0.62603 0.08750  
 H -1.92656 -2.15101 1.52514  
 C 8.86100 7.07200 3.43700  
 H 8.16194 7.65354 2.81735  
 C 8.88500 5.58700 2.98200  
 H 9.62764 5.02979 3.58004  
 H 9.19747 5.48369 1.93217  
 C 7.56058 4.85180 3.15344  
 O 6.80533 5.19958 4.09087  
 O 7.34916 3.91433 2.34243  
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 H 8.51219 7.14126 4.47719  
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 C -8.16000 -3.24700 2.12900  
 H -8.58861 -3.87369 2.93348  
 H -8.49970 -2.21963 2.34729  
 C -6.65245 -3.27590 2.20878  
 C -5.90736 -2.08909 2.28380  
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 C -5.91582 -4.47170 2.26421  
 H -6.45211 -5.42846 2.21989

C -4.52322 -2.08328 2.40819  
 H -3.98288 -1.13551 2.47446  
 C -4.52907 -4.48663 2.37971  
 H -3.98673 -5.43629 2.42208  
 C -3.75160 -3.28767 2.45998  
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 H -9.89731 -3.60967 0.81014  
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 H -2.10448 0.98197 -3.03121  
 C -3.09579 -0.88195 -2.82880  
 O -3.14470 -1.08607 -4.03250  
 C -2.24700 0.60900 -0.89100  
 H -2.92337 0.13689 -0.16478  
 H -2.16258 1.67215 -0.60152  
 O -0.95870 0.03879 -0.73449  
 H -3.72393 1.10784 -2.34420  
 N -3.32671 -1.83722 -1.89763  
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 C -3.62100 -3.20800 -2.24500  
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 H 6.00408 -7.75817 -0.95377  
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 H 3.08401 -6.90760 -1.52577  
 H 4.34264 -7.08051 -2.74615  
 C 4.56512 -5.37318 -1.48712  
 C 5.47256 -4.87374 -0.58363  
 H 6.08398 -5.40610 0.14245  
 C 4.04616 -4.23100 -2.19866  
 N 5.54263 -3.50419 -0.68613  
 H 6.13672 -2.90553 -0.13264  
 C 4.67946 -3.07784 -1.66139  
 C 3.10439 -4.06896 -3.23163  
 H 2.59783 -4.93550 -3.66467  
 C 4.38441 -1.78656 -2.11382  
 H 4.87052 -0.90929 -1.67880  
 C 2.81542 -2.79008 -3.68779  
 H 2.07549 -2.65135 -4.47983  
 C 3.44543 -1.65966 -3.12980  
 H 3.17963 -0.66508 -3.49671  
 H 4.58158 -8.82828 -0.98458  
 H 4.72450 -7.58765 0.28166  
 C 4.72800 7.90500 -3.55000  
 H 4.69247 8.09861 -2.46737  
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 H 3.38780 7.33585 -5.17630  
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 O 3.77901 5.32528 -3.04328  
 O 1.66533 5.92333 -3.47104  
 H 5.06291 8.82564 -4.05196  
 H 5.48071 7.12270 -3.71990  
 H 1.43097 5.19682 -2.78664  
 C 5.66500 3.07800 -1.29100  
 H 6.61998 2.77227 -0.83068  
 C 4.55800 3.22500 -0.25900  
 H 3.67484 3.62758 -0.77510  
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 H 4.10850 1.10525 -0.29400

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H 6.11084 3.09806 2.56241
C 4.34910 2.73868 3.58051
N 3.16323 2.09240 3.66450
H 2.60931 2.20479 4.50042
H 2.88547 1.31052 3.06858
N 4.65441 3.67077 4.49367
H 3.90924 4.01982 5.07898
H 5.51886 4.28907 4.35502
H 5.82526 4.02686 -1.82154
H 5.39320 2.32856 -2.05305
C 1.42100 7.23500 -0.44800
H 1.29472 7.14115 -1.53380
C 2.11500 5.99500 0.13900
H 2.20459 6.09221 1.23199
H 3.14113 5.92596 -0.25833
C 1.40805 4.70649 -0.16615
N 1.05324 4.34609 -1.44756
C 1.06372 3.67830 0.68469
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C 0.52770 3.14277 -1.37331
H 0.14350 2.55391 -2.20478
N 0.51355 2.69956 -0.10193
H 0.18771 1.77833 0.18276
H 2.01891 8.13701 -0.24297
H 0.42530 7.38069 -0.00054

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## Initial systems (mol2 formats)

### FAP / 10b

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#FAP - 10b complex
#
```

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@<TRIPOS>MOLECULE
FAP-10b
 135   132      0 0 0
SMALL
USER_CHARGES
```

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@<TRIPOS>ATOM
    1 C          0.810326  -1.118251  -0.616207 C.2      1 MOL1      0.0438
    2 N         -1.653888  -0.967009  -1.303016 N.am     1 MOL1     -0.2650
    3 C         -0.680205  -0.632862  -0.251914 C.3      1 MOL1      0.0461
    4 C         -1.205592  -1.301120   1.036084 C.3      1 MOL1     -0.1143
    5 C         -1.997388  -2.509531   0.548314 C.3      1 MOL1     -0.1295
    6 C         -2.327991  -2.207285  -0.921789 C.3      1 MOL1     -0.0149
    7 H7        1.202168  -0.433880  -1.368630 H       1 MOL1     -0.3955
    8 C         -2.026115  -0.137215  -2.313941 C.2      1 MOL1      0.1952
    9 O         -1.596140   0.997260  -2.397703 O.2      1 MOL1     -0.3923
   10 C        -3.096537  -0.617276  -3.279712 C.3      1 MOL1     -0.1236
   11 O11       0.649029  -2.435860  -1.314595 O.2      1 MOL1      0.1445
   12 H1        -0.677291  0.448143  -0.086235 H       1 MOL1      0.1143
   13 H1        -1.866557  -0.617798  1.575770 H       1 MOL1      0.0830
   14 H1        -0.405180  -1.599864  1.715679 H       1 MOL1      0.0955
   15 H1        -2.909752  -2.641221  1.135569 H       1 MOL1      0.0754
   16 H1        -1.394359  -3.417219  0.625635 H       1 MOL1      0.0783
   17 H1        -3.410401  -2.108621  -1.032013 H      1 MOL1      0.1179
```

18	H1	-1.989897	-3.021838	-1.566022	H	1	MOL1	0.1131
19	H11	-3.139851	0.052400	-4.143110	H	1	MOL1	0.0896
20	H11	-4.077866	-0.610162	-2.798327	H	1	MOL1	0.1176
21	H11	-2.882516	-1.624751	-3.645890	H	1	MOL1	0.1207
22	CA	0.944000	9.259000	-7.065000	C.3	2	ARG123	-0.2637
23	HA	1.963134	9.273802	-6.678802	H	2	ARG123	0.1560
24	CB	0.373000	7.849000	-6.942000	C.3	2	ARG123	-0.0007
25	HB1	-0.646700	7.851900	-7.332700	H	2	ARG123	0.0327
26	HB2	0.354200	7.572800	-5.885700	H	2	ARG123	0.0327
27	CG	1.176000	6.809000	-7.698000	C.3	2	ARG123	0.0390
28	HG1	2.159100	6.725700	-7.229900	H	2	ARG123	0.0285
29	HG2	1.294600	7.148100	-8.729200	H	2	ARG123	0.0285
30	CD	0.543000	5.446000	-7.717000	C.3	2	ARG123	0.0486
31	HD1	1.058300	4.819900	-8.448400	H	2	ARG123	0.0687
32	HD2	-0.507600	5.540900	-7.999300	H	2	ARG123	0.0687
33	NE	0.633000	4.823000	-6.403000	N.pl3	2	ARG123	-0.5295
34	HE	-0.020700	5.141900	-5.675100	H	2	ARG123	0.3456
35	CZ	1.502000	3.871000	-6.081000	C.cat	2	ARG123	0.8076
36	NH1	2.364000	3.410000	-6.983000	N.pl3	2	ARG123	-0.8627
37	HH11	3.037000	2.672700	-6.733600	H	2	ARG123	0.4478
38	HH12	2.357800	3.801200	-7.934700	H	2	ARG123	0.4478
39	NH2	1.510000	3.367000	-4.855000	N.pl3	2	ARG123	-0.8627
40	HH21	2.183000	2.629700	-4.605600	H	2	ARG123	0.4478
41	HH22	0.843100	3.723600	-4.157200	H	2	ARG123	0.4478
42	H13	0.328562	9.952094	-6.491395	H	2	ARG123	0.0000
43	H14	0.948680	9.559529	-8.112772	H	2	ARG123	0.0000
44	CA	-4.909000	5.910000	-5.263000	C.3	3	GLU203	0.0397
45	HA	-4.100736	5.899014	-5.994156	H	3	GLU203	0.1105
46	CB	-4.321000	5.983000	-3.853000	C.3	3	GLU203	0.0560
47	HB1	-5.147700	5.992800	-3.139600	H	3	GLU203	-0.0173
48	HB2	-3.758500	6.915000	-3.766700	H	3	GLU203	-0.0173
49	CG	-3.391000	4.831000	-3.487000	C.3	3	GLU203	0.0136
50	HG1	-3.929200	3.893300	-3.640400	H	3	GLU203	-0.0425
51	HG2	-3.125100	4.926300	-2.432200	H	3	GLU203	-0.0425
52	CD	-2.106000	4.784000	-4.302000	C.2	3	GLU203	0.8054
53	OE1	-1.516000	3.687000	-4.356000	O.co2	3	GLU203	-0.8188
54	OE2	-1.674000	5.816000	-4.874000	O.co2	3	GLU203	-0.8188
55	H6	-5.544408	6.778288	-5.437637	H	3	GLU203	0.0000
56	H7	-5.501500	5.000599	-5.363494	H	3	GLU203	0.0000
57	CA	4.240000	-9.066000	-1.921000	C.3	4	TYR541	-0.0014
58	HA	4.706198	-8.349468	-1.244802	H	4	TYR541	0.0876
59	CB	4.045000	-8.419000	-3.297000	C.3	4	TYR541	-0.0152
60	HB1	3.577700	-9.149000	-3.961200	H	4	TYR541	0.0295
61	HB2	5.024600	-8.144700	-3.694000	H	4	TYR541	0.0295
62	CG	3.181000	-7.185000	-3.257000	C.ar	4	TYR541	-0.0011
63	CD1	3.557000	-6.075000	-2.504000	C.ar	4	TYR541	-0.1906
64	HD1	4.493500	-6.097600	-1.952600	H	4	TYR541	0.1699
65	CD2	1.975000	-7.130000	-3.954000	C.ar	4	TYR541	-0.1906
66	HD2	1.657300	-7.985700	-4.544200	H	4	TYR541	0.1699
67	CE1	2.758000	-4.939000	-2.444000	C.ar	4	TYR541	-0.2341
68	HE1	3.066900	-4.083400	-1.849000	H	4	TYR541	0.1656
69	CE2	1.168000	-5.988000	-3.904000	C.ar	4	TYR541	-0.2341
70	HE2	0.233300	-5.954600	-4.458000	H	4	TYR541	0.1656
71	CZ	1.565000	-4.905000	-3.148000	C.ar	4	TYR541	0.3226
72	OH	0.789000	-3.776000	-3.089000	O.3	4	TYR541	-0.5579
73	HH	1.080100	-3.215900	-3.808900	H	4	TYR541	0.3992
74	H9	4.880558	-9.942544	-2.018582	H	4	TYR541	0.0000
75	H10	3.272091	-9.366672	-1.519861	H	4	TYR541	0.0000
76	CA	3.664000	-2.436000	1.382000	C.3	5	SER624	-0.0249
77	HA	3.588100	-1.629342	2.111138	H	5	SER624	0.0843
78	C	2.883000	-3.658000	1.912000	C.2	5	SER624	0.5973
79	O	2.990000	-3.994000	3.088000	O.2	5	SER624	-0.5679
80	CB	3.127000	-1.937000	0.041000	C.3	5	SER624	0.2117

81	HB1	2.582200	-2.742600	-0.455600	H	5	SER624	0.0352
82	HB2	3.960400	-1.622000	-0.590400	H	5	SER624	0.0352
83	OG	2.260000	-0.845000	0.255000	O.3	5	SER624	-0.6546
84	H5	4.709867	-2.716580	1.257357	H	5	SER624	0.0000
85	N	2.100000	-4.317000	1.067000	N.am	6	TYR625	-0.4157
86	H	1.881900	-3.915900	0.144800	H	6	TYR625	0.2719
87	CA	1.550000	-5.612000	1.451000	C.3	6	TYR625	-0.0014
88	HA	1.889584	-5.868430	2.454458	H	6	TYR625	0.0876
89	H3	1.887636	-6.373596	0.748050	H	6	TYR625	0.0000
90	H4	0.461142	-5.563194	1.437890	H	6	TYR625	0.0000
91	CA	-5.529000	1.226000	5.754000	C.3	7	TYR656	-0.0014
92	HA	-4.687706	1.907731	5.878368	H	7	TYR656	0.0876
93	CB	-5.056000	-0.046000	5.038000	C.3	7	TYR656	-0.0152
94	HB1	-5.901000	-0.726700	4.915000	H	7	TYR656	0.0295
95	HB2	-4.284600	-0.532800	5.638300	H	7	TYR656	0.0295
96	CG	-4.490000	0.298000	3.681000	C.ar	7	TYR656	-0.0011
97	CD1	-3.659000	1.411000	3.537000	C.ar	7	TYR656	-0.1906
98	HD1	-3.412600	2.003300	4.414500	H	7	TYR656	0.1699
99	CD2	-4.810000	-0.439000	2.544000	C.ar	7	TYR656	-0.1906
100	HD2	-5.466400	-1.301800	2.623800	H	7	TYR656	0.1699
101	CE1	-3.146000	1.777000	2.322000	C.ar	7	TYR656	-0.2341
102	HE1	-2.489700	2.640000	2.244500	H	7	TYR656	0.1656
103	CE2	-4.288000	-0.071000	1.298000	C.ar	7	TYR656	-0.2341
104	HE2	-4.523300	-0.654500	0.411600	H	7	TYR656	0.1656
105	CZ	-3.463000	1.051000	1.203000	C.ar	7	TYR656	0.3226
106	OH	-2.925000	1.466000	0.010000	O.3	7	TYR656	-0.5579
107	HH	-3.108100	2.403700	-0.051800	H	7	TYR656	0.3992
108	H9	-5.931656	0.964346	6.732555	H	7	TYR656	0.0000
109	H10	-6.304118	1.710788	5.160419	H	7	TYR656	0.0000
110	CA	4.048000	8.039000	3.825000	C.3	8	ASP702	0.0381
111	HA	4.579375	8.180091	2.883865	H	8	ASP702	0.0880
112	CB	4.364000	6.651000	4.387000	C.3	8	ASP702	-0.0303
113	HB1	3.824800	6.525800	5.328300	H	8	ASP702	-0.0122
114	HB2	5.437900	6.588000	4.574900	H	8	ASP702	-0.0122
115	CG	3.972000	5.529000	3.455000	C.2	8	ASP702	0.7994
116	OD1	4.815000	4.639000	3.225000	O.3	8	ASP702	-0.8014
117	OD2	2.855000	5.433000	2.918000	O.2	8	ASP702	-0.8014
118	H4	4.364017	8.800732	4.537785	H	8	ASP702	0.0000
119	H5	2.975233	8.126113	3.652525	H	8	ASP702	0.0000
120	H6	4.425252	3.959308	2.525946	H	8	ASP702	0.0000
121	CA	5.567000	5.312000	0.339000	C.3	9	HIS734	0.0188
122	HA	5.688417	5.087594	1.398670	H	9	HIS734	0.0881
123	CB	4.179000	4.899000	-0.110000	C.3	9	HIS734	-0.0462
124	HB1	4.073100	5.129900	-1.172000	H	9	HIS734	0.0402
125	HB2	3.443700	5.471700	0.459100	H	9	HIS734	0.0402
126	CG	3.910000	3.449000	0.090000	C.2	9	HIS734	-0.0266
127	ND1	4.205000	2.800000	1.271000	N.2	9	HIS734	0.0000
128	CD2	3.409000	2.512000	-0.745000	C.2	9	HIS734	0.1292
129	HD2	3.076700	2.669200	-1.768000	H	9	HIS734	0.1147
130	CE1	3.882000	1.525000	1.157000	C.2	9	HIS734	0.2057
131	HE1	3.994200	0.769000	1.930000	H	9	HIS734	0.1392
132	NE2	3.399000	1.324000	-0.057000	N.pl3	9	HIS734	0.0000
133	H7	5.698357	6.381947	0.177369	H	9	HIS734	0.0000
134	H8	6.313491	4.763792	-0.235790	H	9	HIS734	0.0000
135	H9	3.055563	0.386392	-0.441503	H	9	HIS734	0.0000

@<TRIPOS>BOND

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4	4	3	1
5	5	4	1
6	6	5	1
7	7	1	1

8	8	2	1
9	9	8	2
10	10	8	1
11	11	1	2
12	12	3	1
13	13	4	1
14	14	4	1
15	15	5	1
16	16	5	1
17	17	6	1
18	18	6	1
19	19	10	1
20	20	10	1
21	21	10	1
22	22	23	1
23	22	24	1
24	24	25	1
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## FAP / 11b

```
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FAP-ligand_boronic_acid
 137   134      0 0 0
SMALL
USER_CHARGES

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 1 B          0.550355  -1.377554  -0.327136 B      1 MOL1    0.2803
 2 N         -1.815639  -0.805388  -0.886476 N.am   1 MOL1   -0.2432
 3 C         -0.792394  -0.751933   0.168695 C.3    1 MOL1    0.0234
 4 C         -1.346668  -1.541939   1.368595 C.3    1 MOL1   -0.1275
 5 C         -2.417935  -2.464996   0.790953 C.3    1 MOL1   -0.1269
 6 C         -2.670116  -1.968158  -0.642480 C.3    1 MOL1   -0.0110
 7 C         -1.969248  0.111348  -1.883186 C.2    1 MOL1    0.2099
 8 C         -2.986952  -0.188438  -2.962304 C.3    1 MOL1   -0.1167
 9 O         -1.333168  1.144239  -1.913729 O.2    1 MOL1   -0.3921
10 O          1.040705  -0.613615  -1.432743 O.3    1 MOL1   -0.5092
11 O          0.191658  -2.701329  -0.779660 O.3    1 MOL1   -0.4807
12 H1        -0.620167  0.284085   0.476154 H     1 MOL1    0.0944
13 H1        -1.798219  -0.860712  2.094346 H     1 MOL1    0.0769
14 H1        -0.562687  -2.110505  1.873781 H     1 MOL1    0.0700
15 H1        -3.333619  -2.406583  1.382470 H     1 MOL1    0.0731
16 H1        -2.077566  -3.501210  0.786781 H     1 MOL1    0.0738
17 H1        -3.720597  -1.688520  -0.748242 H    1 MOL1    0.1141
18 H1        -2.452394  -2.755794  -1.367156 H    1 MOL1    0.1190
19 H11       -2.778102  0.416950  -3.847229 H    1 MOL1    0.1147
20 H11       -3.992155  0.048436  -2.610175 H    1 MOL1    0.1507
21 H11       -2.947500  -1.237445  -3.260939 H    1 MOL1    0.0857
22 HO         1.540852  0.128669  -1.034342 H    1 MOL1    0.2562
23 HO         0.130227  -2.626138  -1.749673 H    1 MOL1    0.2650
24 CA         0.944000  9.259000  -7.065000 C.3    2 ARG123  -0.2637
25 HA         1.963134  9.273802  -6.678802 H    2 ARG123  0.1560
26 CB         0.373000  7.849000  -6.942000 C.3    2 ARG123  -0.0007
27 HB1       -0.646700  7.851900  -7.332700 H    2 ARG123  0.0327
28 HB2       0.354200  7.572800  -5.885700 H    2 ARG123  0.0327
29 CG         1.176000  6.809000  -7.698000 C.3    2 ARG123  0.0390
30 HG1       2.159100  6.725700  -7.229900 H    2 ARG123  0.0285
31 HG2       1.294600  7.148100  -8.729200 H    2 ARG123  0.0285
32 CD         0.543000  5.446000  -7.717000 C.3    2 ARG123  0.0486
33 HD1       1.058300  4.819900  -8.448400 H    2 ARG123  0.0687
34 HD2       -0.507600  5.540900  -7.999300 H    2 ARG123  0.0687
35 NE         0.633000  4.823000  -6.403000 N.pl3  2 ARG123  -0.5295
36 HE       -0.020700  5.141900  -5.675100 H    2 ARG123  0.3456
37 CZ         1.502000  3.871000  -6.081000 C.cat  2 ARG123  0.8076
38 NH1       2.364000  3.410000  -6.983000 N.pl3  2 ARG123  -0.8627
39 HH11      3.037000  2.672700  -6.733600 H    2 ARG123  0.4478
40 HH12      2.357800  3.801200  -7.934700 H    2 ARG123  0.4478
41 NH2         1.510000  3.367000  -4.855000 N.pl3  2 ARG123  -0.8627
42 HH21      2.183000  2.629700  -4.605600 H    2 ARG123  0.4478
43 HH22      0.843100  3.723600  -4.157200 H    2 ARG123  0.4478
44 H13        0.328562  9.952094  -6.491395 H    2 ARG123  0.0000
45 H14        0.948680  9.559529  -8.112772 H    2 ARG123  0.0000
46 CA        -4.909000  5.910000  -5.263000 C.3    3 GLU203  0.0397
47 HA        -4.100736  5.899014  -5.994156 H    3 GLU203  0.1105
48 CB        -4.321000  5.983000  -3.853000 C.3    3 GLU203  0.0560
49 HB1       -5.147700  5.992800  -3.139600 H    3 GLU203  -0.0173
50 HB2       -3.758500  6.915000  -3.766700 H    3 GLU203  -0.0173
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51	CG	-3.391000	4.831000	-3.487000 C.3	3	GLU203	0.0136
52	HG1	-3.929200	3.893300	-3.640400 H	3	GLU203	-0.0425
53	HG2	-3.125100	4.926300	-2.432200 H	3	GLU203	-0.0425
54	CD	-2.106000	4.784000	-4.302000 C.2	3	GLU203	0.8054
55	OE1	-1.516000	3.687000	-4.356000 O.co2	3	GLU203	-0.8188
56	OE2	-1.674000	5.816000	-4.874000 O.co2	3	GLU203	-0.8188
57	H6	-5.544408	6.778288	-5.437637 H	3	GLU203	0.0000
58	H7	-5.501500	5.000599	-5.363494 H	3	GLU203	0.0000
59	CA	4.240000	-9.066000	-1.921000 C.3	4	TYR541	-0.0014
60	HA	4.706198	-8.349468	-1.244802 H	4	TYR541	0.0876
61	CB	4.045000	-8.419000	-3.297000 C.3	4	TYR541	-0.0152
62	HB1	3.577700	-9.149000	-3.961200 H	4	TYR541	0.0295
63	HB2	5.024600	-8.144700	-3.694000 H	4	TYR541	0.0295
64	CG	3.181000	-7.185000	-3.257000 C.ar	4	TYR541	-0.0011
65	CD1	3.557000	-6.075000	-2.504000 C.ar	4	TYR541	-0.1906
66	HD1	4.493500	-6.097600	-1.952600 H	4	TYR541	0.1699
67	CD2	1.975000	-7.130000	-3.954000 C.ar	4	TYR541	-0.1906
68	HD2	1.657300	-7.985700	-4.544200 H	4	TYR541	0.1699
69	CE1	2.758000	-4.939000	-2.444000 C.ar	4	TYR541	-0.2341
70	HE1	3.066900	-4.083400	-1.849000 H	4	TYR541	0.1656
71	CE2	1.168000	-5.988000	-3.904000 C.ar	4	TYR541	-0.2341
72	HE2	0.233300	-5.954600	-4.458000 H	4	TYR541	0.1656
73	CZ	1.565000	-4.905000	-3.148000 C.ar	4	TYR541	0.3226
74	OH	0.789000	-3.776000	-3.089000 O.3	4	TYR541	-0.5579
75	HH	1.080100	-3.215900	-3.808900 H	4	TYR541	0.3992
76	H9	4.880558	-9.942544	-2.018582 H	4	TYR541	0.0000
77	H10	3.272091	-9.366672	-1.519861 H	4	TYR541	0.0000
78	CA	3.664000	-2.436000	1.382000 C.3	5	SER624	-0.0249
79	HA	3.588100	-1.629342	2.111138 H	5	SER624	0.0843
80	C	2.883000	-3.658000	1.912000 C.2	5	SER624	0.5973
81	O	2.990000	-3.994000	3.088000 O.2	5	SER624	-0.5679
82	CB	3.127000	-1.937000	0.041000 C.3	5	SER624	0.2117
83	HB1	2.582200	-2.742600	-0.455600 H	5	SER624	0.0352
84	HB2	3.960400	-1.622000	-0.590400 H	5	SER624	0.0352
85	OG	2.260000	-0.845000	0.255000 O.3	5	SER624	-0.6546
86	H5	4.709867	-2.716580	1.257357 H	5	SER624	0.0000
87	N	2.100000	-4.317000	1.067000 N.am	6	TYR625	-0.4157
88	H	1.881900	-3.915900	0.144800 H	6	TYR625	0.2719
89	CA	1.550000	-5.612000	1.451000 C.3	6	TYR625	-0.0014
90	HA	1.889584	-5.868430	2.454458 H	6	TYR625	0.0876
91	H3	1.887636	-6.373596	0.748050 H	6	TYR625	0.0000
92	H4	0.461142	-5.563194	1.437890 H	6	TYR625	0.0000
93	CA	-5.529000	1.226000	5.754000 C.3	7	TYR656	-0.0014
94	HA	-4.687706	1.907731	5.878368 H	7	TYR656	0.0876
95	CB	-5.056000	-0.046000	5.038000 C.3	7	TYR656	-0.0152
96	HB1	-5.901000	-0.726700	4.915000 H	7	TYR656	0.0295
97	HB2	-4.284600	-0.532800	5.638300 H	7	TYR656	0.0295
98	CG	-4.490000	0.298000	3.681000 C.ar	7	TYR656	-0.0011
99	CD1	-3.659000	1.411000	3.537000 C.ar	7	TYR656	-0.1906
100	HD1	-3.412600	2.003300	4.414500 H	7	TYR656	0.1699
101	CD2	-4.810000	-0.439000	2.544000 C.ar	7	TYR656	-0.1906
102	HD2	-5.466400	-1.301800	2.623800 H	7	TYR656	0.1699
103	CE1	-3.146000	1.777000	2.322000 C.ar	7	TYR656	-0.2341
104	HE1	-2.489700	2.640000	2.244500 H	7	TYR656	0.1656
105	CE2	-4.288000	-0.071000	1.298000 C.ar	7	TYR656	-0.2341
106	HE2	-4.523300	-0.654500	0.411600 H	7	TYR656	0.1656
107	CZ	-3.463000	1.051000	1.203000 C.ar	7	TYR656	0.3226
108	OH	-2.925000	1.466000	0.010000 O.3	7	TYR656	-0.5579
109	HH	-3.108100	2.403700	-0.051800 H	7	TYR656	0.3992
110	H9	-5.931656	0.964346	6.732555 H	7	TYR656	0.0000
111	H10	-6.304118	1.710788	5.160419 H	7	TYR656	0.0000
112	CA	4.048000	8.039000	3.825000 C.3	8	ASP702	0.0381
113	HA	4.579375	8.180091	2.883865 H	8	ASP702	0.0880

114	CB	4.364000	6.651000	4.387000	C.3	8	ASP702	-0.0303
115	HB1	3.824800	6.525800	5.328300	H	8	ASP702	-0.0122
116	HB2	5.437900	6.588000	4.574900	H	8	ASP702	-0.0122
117	CG	3.972000	5.529000	3.455000	C.2	8	ASP702	0.7994
118	OD1	4.815000	4.639000	3.225000	O.3	8	ASP702	-0.8014
119	OD2	2.855000	5.433000	2.918000	O.2	8	ASP702	-0.8014
120	H4	4.364017	8.800732	4.537785	H	8	ASP702	0.0000
121	H5	2.975233	8.126113	3.652525	H	8	ASP702	0.0000
122	H6	4.544754	4.116641	2.355133	H	8	ASP702	0.0000
123	CA	5.567000	5.312000	0.339000	C.3	9	HIS734	0.0188
124	HA	5.688417	5.087594	1.398670	H	9	HIS734	0.0881
125	CB	4.179000	4.899000	-0.110000	C.3	9	HIS734	-0.0462
126	HB1	4.073100	5.129900	-1.172000	H	9	HIS734	0.0402
127	HB2	3.443700	5.471700	0.459100	H	9	HIS734	0.0402
128	CG	3.910000	3.449000	0.090000	C.2	9	HIS734	-0.0266
129	ND1	4.205000	2.800000	1.271000	N.2	9	HIS734	0.0000
130	CD2	3.409000	2.512000	-0.745000	C.2	9	HIS734	0.1292
131	HD2	3.076700	2.669200	-1.768000	H	9	HIS734	0.1147
132	CE1	3.882000	1.525000	1.157000	C.2	9	HIS734	0.2057
133	HE1	3.994200	0.769000	1.930000	H	9	HIS734	0.1392
134	NE2	3.399000	1.324000	-0.057000	N.pl3	9	HIS734	0.0000
135	H7	5.698357	6.381947	0.177369	H	9	HIS734	0.0000
136	H8	6.313491	4.763792	-0.235790	H	9	HIS734	0.0000
137	H8	3.055563	0.386392	-0.441503	H	9	HIS734	0.0000

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## FAP / 5b

```
#FAP - 5b complex
#
```

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@<TRIPOS>MOLECULE
FAP-ligand_nitrile
 134   131      0 0 0
SMALL
USER_CHARGES
```

@<TRIPOS>ATOM

1	O9	-0.762910	0.888923	-2.268415	O.2	1	4I4791	-0.2702
2	C8	-1.544957	-0.057085	-2.036815	C.2	1	4I4791	0.2649
3	C10	-2.623985	-0.418996	-3.006770	C.3	1	4I4791	0.2514
4	N7	-1.515294	-0.788993	-0.898092	N.am	1	4I4791	-0.3285
5	C6	-2.411954	-1.901850	-0.505359	C.3	1	4I4791	0.1203
6	C5	-1.925479	-2.315671	0.876950	C.3	1	4I4791	0.0241
7	C4	-1.091223	-1.129682	1.361994	C.3	1	4I4791	0.0356
8	C3	-0.492011	-0.544653	0.097157	C.3	1	4I4791	0.1580
9	C1	0.793308	-1.285197	-0.229202	C.2	1	4I4791	0.1576
10	N2	0.798181	-2.357955	-0.880955	N.2	1	4I4791	-0.0909
11	H2	-3.191678	-1.265404	-2.620353	H	1	4I4791	0.0000
12	H3	-2.177439	-0.688311	-3.963971	H	1	4I4791	0.0000
13	H4	-3.290466	0.432554	-3.144000	H	1	4I4791	0.0000
14	H5	-3.447846	-1.565225	-0.464018	H	1	4I4791	0.0000
15	H6	-2.326593	-2.731076	-1.207640	H	1	4I4791	0.0000
16	H7	-2.768642	-2.491891	1.544873	H	1	4I4791	0.0000
17	H8	-1.314868	-3.216546	0.816308	H	1	4I4791	0.0000

18 H9	-1.720939	-0.395866	1.865055 H	1 4I4791	0.0000
19 H10	-0.306765	-1.462806	2.041520 H	1 4I4791	0.0000
20 H11	-0.307531	0.523497	0.211718 H	1 4I4791	0.0000
21 H11	-0.106853	-2.719931	-1.322301 H	1 4I4791	0.0000
22 CA	0.943981	9.259000	-7.065069 C.3	2 ARG123	-0.2637
23 HA	1.963117	9.273803	-6.678878 H	2 ARG123	0.1560
24 CB	0.372980	7.849001	-6.942059 C.3	2 ARG123	-0.0007
25 HB1	-0.646722	7.851900	-7.332752 H	2 ARG123	0.0327
26 HB2	0.354187	7.572806	-5.885757 H	2 ARG123	0.0327
27 CG	1.175974	6.808996	-7.698059 C.3	2 ARG123	0.0390
28 HG1	2.159077	6.725698	-7.229965 H	2 ARG123	0.0285
29 HG2	1.294568	7.148091	-8.729261 H	2 ARG123	0.0285
30 CD	0.542973	5.445997	-7.717048 C.3	2 ARG123	0.0486
31 HD1	1.058268	4.819893	-8.448449 H	2 ARG123	0.0687
32 HD2	-0.507629	5.540896	-7.999342 H	2 ARG123	0.0687
33 NE	0.632981	4.823003	-6.403046 N.pl3	2 ARG123	-0.5295
34 HE	-0.020714	5.141907	-5.675143 H	2 ARG123	0.3456
35 CZ	1.501982	3.871004	-6.081047 C.cat	2 ARG123	0.8076
36 NH1	2.363976	3.409999	-6.983050 N.pl3	2 ARG123	-0.8627
37 HH11	3.036977	2.672699	-6.733651 H	2 ARG123	0.4478
38 HH12	2.357770	3.801194	-7.934752 H	2 ARG123	0.4478
39 NH2	1.509990	3.367010	-4.855044 N.pl3	2 ARG123	-0.8627
40 HH21	2.182991	2.629710	-4.605645 H	2 ARG123	0.4478
41 HH22	0.843095	3.723614	-4.157242 H	2 ARG123	0.4478
42 H13	0.328547	9.952097	-6.491463 H	2 ARG123	0.0000
43 H14	0.948654	9.559524	-8.112843 H	2 ARG123	0.0000
44 CA	-4.909010	5.910013	-5.263015 C.3	3 GLU203	0.0397
45 HA	-4.100751	5.899023	-5.994176 H	3 GLU203	0.1105
46 CB	-4.321001	5.983020	-3.853019 C.3	3 GLU203	0.0560
47 HB1	-5.147696	5.992824	-3.139613 H	3 GLU203	-0.0173
48 HB2	-3.758500	6.915020	-3.766727 H	3 GLU203	-0.0173
49 CG	-3.391000	4.831021	-3.487019 C.3	3 GLU203	0.0136
50 HG1	-3.929202	3.893320	-3.640411 H	3 GLU203	-0.0425
51 HG2	-3.125093	4.926325	-2.432222 H	3 GLU203	-0.0425
52 CD	-2.106005	4.784016	-4.302028 C.2	3 GLU203	0.8054
53 OE1	-1.516006	3.687015	-4.356026 O.co2	3 GLU203	-0.8188
54 OE2	-1.674008	5.816012	-4.874035 O.co2	3 GLU203	-0.8188
55 H6	-5.544419	6.778301	-5.437652 H	3 GLU203	0.0000
56 H7	-5.501512	5.000612	-5.363500 H	3 GLU203	0.0000
57 CA	4.239999	-9.065978	-1.921002 C.3	4 TYR541	-0.0014
58 HA	4.706202	-8.349444	-1.244811 H	4 TYR541	0.0876
59 CB	4.044990	-8.418985	-3.297004 C.3	4 TYR541	-0.0152
60 HB1	3.577685	-9.148988	-3.961198 H	4 TYR541	0.0295
61 HB2	5.024588	-8.144688	-3.694012 H	4 TYR541	0.0295
62 CG	3.180992	-7.184984	-3.257005 C.ar	4 TYR541	-0.0011
63 CD1	3.556997	-6.074981	-2.504012 C.ar	4 TYR541	-0.1906
64 HD1	4.493501	-6.097579	-1.952618 H	4 TYR541	0.1699
65 CD2	1.974987	-7.129986	-3.953997 C.ar	4 TYR541	-0.1906
66 HD2	1.657282	-7.985689	-4.544191 H	4 TYR541	0.1699
67 CE1	2.757999	-4.938980	-2.444013 C.ar	4 TYR541	-0.2341
68 HE1	3.066903	-4.083377	-1.849019 H	4 TYR541	0.1656
69 CE2	1.167988	-5.987985	-3.903997 C.ar	4 TYR541	-0.2341
70 HE2	0.233285	-5.954587	-4.457991 H	4 TYR541	0.1656
71 CZ	1.564994	-4.904982	-3.148005 C.ar	4 TYR541	0.3226
72 OH	0.788996	-3.775981	-3.089005 O.3	4 TYR541	-0.5579
73 H9	4.880555	-9.942523	-2.018584 H	4 TYR541	0.0000
74 H10	3.272092	-9.366648	-1.519856 H	4 TYR541	0.0000
75 CA	3.664026	-2.435962	1.381969 C.3	5 SER624	-0.0249
76 HA	3.588132	-1.629300	2.111104 H	5 SER624	0.0843
77 C	2.883028	-3.657959	1.911980 C.2	5 SER624	0.5973
78 O	2.990036	-3.993953	3.087981 O.2	5 SER624	-0.5679
79 CB	3.127018	-1.936968	0.040971 C.3	5 SER624	0.2117
80 HB1	2.582214	-2.742570	-0.455622 H	5 SER624	0.0352

81	HB2	3.960414	-1.621972	-0.590436	H	5	SER624	0.0352
82	OG	2.260020	-0.844966	0.254971	O.3	5	SER624	-0.6546
83	H5	4.709892	-2.716543	1.257321	H	5	SER624	0.0000
84	N	2.100022	-4.316962	1.066989	N.am	6	TYR625	-0.4157
85	H	1.881917	-3.915866	0.144788	H	6	TYR625	0.2719
86	CA	1.550024	-5.611960	1.450999	C.3	6	TYR625	-0.0014
87	HA	1.889614	-5.868385	2.454456	H	6	TYR625	0.0876
88	H3	1.887655	-6.373560	0.748050	H	6	TYR625	0.0000
89	H4	0.461166	-5.563153	1.437896	H	6	TYR625	0.0000
90	CA	-5.528942	1.226067	5.754012	C.3	7	TYR656	-0.0014
91	HA	-4.687647	1.907798	5.878371	H	7	TYR656	0.0876
92	CB	-5.055948	-0.045937	5.038015	C.3	7	TYR656	-0.0152
93	HB1	-5.900949	-0.726637	4.915024	H	7	TYR656	0.0295
94	HB2	-4.284544	-0.532735	5.638312	H	7	TYR656	0.0295
95	CG	-4.489957	0.298056	3.681010	C.ar	7	TYR656	-0.0011
96	CD1	-3.658956	1.411055	3.536999	C.ar	7	TYR656	-0.1906
97	HD1	-3.412550	2.003359	4.414494	H	7	TYR656	0.1699
98	CD2	-4.809965	-0.438949	2.544015	C.ar	7	TYR656	-0.1906
99	HD2	-5.466365	-1.301748	2.623824	H	7	TYR656	0.1699
100	CE1	-3.145964	1.777048	2.321994	C.ar	7	TYR656	-0.2341
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102	CE2	-4.287972	-0.070956	1.298010	C.ar	7	TYR656	-0.2341
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104	CZ	-3.462972	1.051043	1.202999	C.ar	7	TYR656	0.3226
105	OH	-2.924980	1.466037	0.009994	O.3	7	TYR656	-0.5579
106	HH	-3.108079	2.403737	-0.051809	H	7	TYR656	0.3992
107	H9	-5.931592	0.964418	6.732571	H	7	TYR656	0.0000
108	H10	-6.304064	1.710853	5.160434	H	7	TYR656	0.0000
109	CA	4.048051	8.039049	3.824916	C.3	8	ASP702	0.0381
110	HA	4.579420	8.180135	2.883777	H	8	ASP702	0.0880
111	CB	4.364054	6.651052	4.386921	C.3	8	ASP702	-0.0303
112	HB1	3.824860	6.525857	5.328225	H	8	ASP702	-0.0122
113	HB2	5.437955	6.588052	4.574814	H	8	ASP702	-0.0122
114	CG	3.972046	5.529048	3.454929	C.2	8	ASP702	0.7994
115	OD1	4.815044	4.639046	3.224928	O.3	8	ASP702	-0.8014
116	OD2	2.855043	5.433046	2.917937	O.2	8	ASP702	-0.8014
117	H4	4.364073	8.800785	4.537696	H	8	ASP702	0.0000
118	H5	2.975283	8.126163	3.652448	H	8	ASP702	0.0000
119	H6	4.342493	3.816715	2.774341	H	8	ASP702	0.0000
120	CA	5.567026	5.312031	0.338919	C.3	9	HIS734	0.0188
121	HA	5.688450	5.087630	1.398590	H	9	HIS734	0.0881
122	CB	4.179023	4.899030	-0.110069	C.3	9	HIS734	-0.0462
123	HB1	4.073116	5.129925	-1.172070	H	9	HIS734	0.0402
124	HB2	3.443727	5.471734	0.459033	H	9	HIS734	0.0402
125	CG	3.910023	3.449032	0.089939	C.2	9	HIS734	-0.0266
126	ND1	4.205030	2.800037	1.270941	N.2	9	HIS734	0.0000
127	CD2	3.409016	2.512028	-0.745053	C.2	9	HIS734	0.1292
128	HD2	3.076710	2.669223	-1.768051	H	9	HIS734	0.1147
129	CE1	3.882028	1.525037	1.156949	C.2	9	HIS734	0.2057
130	HE1	3.994232	0.769040	1.929952	H	9	HIS734	0.1392
131	NE2	3.399020	1.324031	-0.057047	N.pl3	9	HIS734	0.0000
132	H7	5.698383	6.381977	0.177282	H	9	HIS734	0.0000
133	H8	6.313513	4.763820	-0.235873	H	9	HIS734	0.0000
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## FAP / 13b

#FAP - 13b complex

#

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SMALL  
USER\_CHARGES

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2 C8	-1.544945	-0.057108	-2.036786	C.2	1 4I4791	0.2649
3 C10	-2.624009	-0.419062	-3.006813	C.3	1 4I4791	0.2514
4 N7	-1.515275	-0.789038	-0.898137	N.am	1 4I4791	-0.3285
5 C6	-2.412016	-1.901895	-0.505351	C.3	1 4I4791	0.1203
6 C5	-1.925470	-2.315737	0.876938	C.3	1 4I4791	0.0241
7 C4	-1.091194	-1.129737	1.362032	C.3	1 4I4791	0.0356
8 C3	-0.492005	-0.544702	0.097181	C.3	1 4I4791	0.1580
9 C1	0.793262	-1.285260	-0.229172	C.2	1 4I4791	0.1576
10 N2	0.798161	-2.357927	-0.880974	N.2	1 4I4791	-0.0909
11 H2	-3.191711	-1.265466	-2.620325	H	1 4I4791	0.0000
12 H3	-2.177419	-0.688348	-3.963977	H	1 4I4791	0.0000
13 H4	-3.290479	0.432536	-3.144034	H	1 4I4791	0.0000
14 H5	-3.447878	-1.565237	-0.464051	H	1 4I4791	0.0000
15 H6	-2.326618	-2.731070	-1.207624	H	1 4I4791	0.0000
16 F7	-3.078102	-2.556662	1.790008	F	1 4I4791	0.0000
17 F17	-1.090835	-3.547243	0.794000	F	1 4I4791	0.0000
18 H9	-1.720983	-0.395955	1.865007	H	1 4I4791	0.0000
19 H10	-0.306776	-1.462817	2.041576	H	1 4I4791	0.0000
20 H11	-0.307544	0.523415	0.211698	H	1 4I4791	0.0000
21 H10	-0.088322	-2.681587	-1.385248	H	1 4I4791	0.0000
22 CA	0.944000	9.259000	-7.065000	C.3	2 ARG123	-0.2637
23 HA	1.963134	9.273802	-6.678802	H	2 ARG123	0.1560
24 CB	0.373000	7.849000	-6.942000	C.3	2 ARG123	-0.0007
25 HB1	-0.646700	7.851900	-7.332700	H	2 ARG123	0.0327
26 HB2	0.354200	7.572800	-5.885700	H	2 ARG123	0.0327
27 CG	1.176000	6.809000	-7.698000	C.3	2 ARG123	0.0390
28 HG1	2.159100	6.725700	-7.229900	H	2 ARG123	0.0285
29 HG2	1.294600	7.148100	-8.729200	H	2 ARG123	0.0285
30 CD	0.543000	5.446000	-7.717000	C.3	2 ARG123	0.0486
31 HD1	1.058300	4.819900	-8.448400	H	2 ARG123	0.0687
32 HD2	-0.507600	5.540900	-7.999300	H	2 ARG123	0.0687
33 NE	0.633000	4.823000	-6.403000	N.pl3	2 ARG123	-0.5295
34 HE	-0.020700	5.141900	-5.675100	H	2 ARG123	0.3456
35 CZ	1.502000	3.871000	-6.081000	C.cat	2 ARG123	0.8076
36 NH1	2.364000	3.410000	-6.983000	N.pl3	2 ARG123	-0.8627
37 HH11	3.037000	2.672700	-6.733600	H	2 ARG123	0.4478
38 HH12	2.357800	3.801200	-7.934700	H	2 ARG123	0.4478
39 NH2	1.510000	3.367000	-4.855000	N.pl3	2 ARG123	-0.8627
40 HH21	2.183000	2.629700	-4.605600	H	2 ARG123	0.4478
41 HH22	0.843100	3.723600	-4.157200	H	2 ARG123	0.4478
42 H13	0.328562	9.952094	-6.491395	H	2 ARG123	0.0000
43 H14	0.948680	9.559529	-8.112772	H	2 ARG123	0.0000
44 CA	-4.909000	5.910000	-5.263000	C.3	3 GLU203	0.0397
45 HA	-4.100736	5.899014	-5.994156	H	3 GLU203	0.1105
46 CB	-4.321000	5.983000	-3.853000	C.3	3 GLU203	0.0560
47 HB1	-5.147700	5.992800	-3.139600	H	3 GLU203	-0.0173
48 HB2	-3.758500	6.915000	-3.766700	H	3 GLU203	-0.0173
49 CG	-3.391000	4.831000	-3.487000	C.3	3 GLU203	0.0136
50 HG1	-3.929200	3.893300	-3.640400	H	3 GLU203	-0.0425
51 HG2	-3.125100	4.926300	-2.432200	H	3 GLU203	-0.0425
52 CD	-2.106000	4.784000	-4.302000	C.2	3 GLU203	0.8054

53	OE1	-1.516000	3.687000	-4.356000	O.co2	3	GLU203	-0.8188
54	OE2	-1.674000	5.816000	-4.874000	O.co2	3	GLU203	-0.8188
55	H6	-5.544408	6.778288	-5.437637	H	3	GLU203	0.0000
56	H7	-5.501500	5.000599	-5.363494	H	3	GLU203	0.0000
57	CA	4.240000	-9.066000	-1.921000	C.3	4	TYR541	-0.0014
58	HA	4.706198	-8.349468	-1.244802	H	4	TYR541	0.0876
59	CB	4.045000	-8.419000	-3.297000	C.3	4	TYR541	-0.0152
60	HB1	3.577700	-9.149000	-3.961200	H	4	TYR541	0.0295
61	HB2	5.024600	-8.144700	-3.694000	H	4	TYR541	0.0295
62	CG	3.181000	-7.185000	-3.257000	C.ar	4	TYR541	-0.0011
63	CD1	3.557000	-6.075000	-2.504000	C.ar	4	TYR541	-0.1906
64	HD1	4.493500	-6.097600	-1.952600	H	4	TYR541	0.1699
65	CD2	1.975000	-7.130000	-3.954000	C.ar	4	TYR541	-0.1906
66	HD2	1.657300	-7.985700	-4.544200	H	4	TYR541	0.1699
67	CE1	2.758000	-4.939000	-2.444000	C.ar	4	TYR541	-0.2341
68	HE1	3.066900	-4.083400	-1.849000	H	4	TYR541	0.1656
69	CE2	1.168000	-5.988000	-3.904000	C.ar	4	TYR541	-0.2341
70	HE2	0.233300	-5.954600	-4.458000	H	4	TYR541	0.1656
71	CZ	1.565000	-4.905000	-3.148000	C.ar	4	TYR541	0.3226
72	OH	0.789000	-3.776000	-3.089000	O.3	4	TYR541	-0.5579
73	H9	4.880558	-9.942544	-2.018582	H	4	TYR541	0.0000
74	H10	3.272091	-9.366672	-1.519861	H	4	TYR541	0.0000
75	CA	3.664000	-2.436000	1.382000	C.3	5	SER624	-0.0249
76	HA	3.588100	-1.629342	2.111138	H	5	SER624	0.0843
77	C	2.883000	-3.658000	1.912000	C.2	5	SER624	0.5973
78	O	2.990000	-3.994000	3.088000	O.2	5	SER624	-0.5679
79	CB	3.127000	-1.937000	0.041000	C.3	5	SER624	0.2117
80	HB1	2.582200	-2.742600	-0.455600	H	5	SER624	0.0352
81	HB2	3.960400	-1.622000	-0.590400	H	5	SER624	0.0352
82	OG	2.260000	-0.845000	0.255000	O.3	5	SER624	-0.6546
83	H5	4.709867	-2.716580	1.257357	H	5	SER624	0.0000
84	N	2.100000	-4.317000	1.067000	N.am	6	TYR625	-0.4157
85	H	1.881900	-3.915900	0.144800	H	6	TYR625	0.2719
86	CA	1.550000	-5.612000	1.451000	C.3	6	TYR625	-0.0014
87	HA	1.889584	-5.868430	2.454458	H	6	TYR625	0.0876
88	H3	1.887636	-6.373596	0.748050	H	6	TYR625	0.0000
89	H4	0.461142	-5.563194	1.437890	H	6	TYR625	0.0000
90	CA	-5.529000	1.226000	5.754000	C.3	7	TYR656	-0.0014
91	HA	-4.687706	1.907731	5.878368	H	7	TYR656	0.0876
92	CB	-5.056000	-0.046000	5.038000	C.3	7	TYR656	-0.0152
93	HB1	-5.901000	-0.726700	4.915000	H	7	TYR656	0.0295
94	HB2	-4.284600	-0.532800	5.638300	H	7	TYR656	0.0295
95	CG	-4.490000	0.298000	3.681000	C.ar	7	TYR656	-0.0011
96	CD1	-3.659000	1.411000	3.537000	C.ar	7	TYR656	-0.1906
97	HD1	-3.412600	2.003300	4.414500	H	7	TYR656	0.1699
98	CD2	-4.810000	-0.439000	2.544000	C.ar	7	TYR656	-0.1906
99	HD2	-5.466400	-1.301800	2.623800	H	7	TYR656	0.1699
100	CE1	-3.146000	1.777000	2.322000	C.ar	7	TYR656	-0.2341
101	HE1	-2.489700	2.640000	2.244500	H	7	TYR656	0.1656
102	CE2	-4.288000	-0.071000	1.298000	C.ar	7	TYR656	-0.2341
103	HE2	-4.523300	-0.654500	0.411600	H	7	TYR656	0.1656
104	CZ	-3.463000	1.051000	1.203000	C.ar	7	TYR656	0.3226
105	OH	-2.925000	1.466000	0.010000	O.3	7	TYR656	-0.5579
106	HH	-3.108100	2.403700	-0.051800	H	7	TYR656	0.3992
107	H9	-5.931656	0.964346	6.732555	H	7	TYR656	0.0000
108	H10	-6.304118	1.710788	5.160419	H	7	TYR656	0.0000
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110	HA	4.579375	8.180091	2.883865	H	8	ASP702	0.0880
111	CB	4.364000	6.651000	4.387000	C.3	8	ASP702	-0.0303
112	HB1	3.824800	6.525800	5.328300	H	8	ASP702	-0.0122
113	HB2	5.437900	6.588000	4.574900	H	8	ASP702	-0.0122
114	CG	3.972000	5.529000	3.455000	C.2	8	ASP702	0.7994
115	OD1	4.815000	4.639000	3.225000	O.3	8	ASP702	-0.8014

116	OD2	2.855000	5.433000	2.918000	O.2	8	ASP702	-0.8014
117	H4	4.364017	8.800732	4.537785	H	8	ASP702	0.0000
118	H5	2.975233	8.126113	3.652525	H	8	ASP702	0.0000
119	H6	4.568368	4.145026	2.331847	H	8	ASP702	0.0000
120	CA	5.567000	5.312000	0.339000	C.3	9	HIS734	0.0188
121	HA	5.688417	5.087594	1.398670	H	9	HIS734	0.0881
122	CB	4.179000	4.899000	-0.110000	C.3	9	HIS734	-0.0462
123	HB1	4.073100	5.129900	-1.172000	H	9	HIS734	0.0402
124	HB2	3.443700	5.471700	0.459100	H	9	HIS734	0.0402
125	CG	3.910000	3.449000	0.090000	C.2	9	HIS734	-0.0266
126	ND1	4.205000	2.800000	1.271000	N.2	9	HIS734	0.0000
127	CD2	3.409000	2.512000	-0.745000	C.2	9	HIS734	0.1292
128	HD2	3.076700	2.669200	-1.768000	H	9	HIS734	0.1147
129	CE1	3.882000	1.525000	1.157000	C.2	9	HIS734	0.2057
130	HE1	3.994200	0.769000	1.930000	H	9	HIS734	0.1392
131	NE2	3.399000	1.324000	-0.057000	N.pl3	9	HIS734	0.0000
132	H7	5.698357	6.381947	0.177369	H	9	HIS734	0.0000
133	H8	6.313491	4.763792	-0.235790	H	9	HIS734	0.0000
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## FAP / 15b

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#FAP - 15b complex
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SMALL
USER_CHARGES
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3	C10	-2.624009	-0.419062	-3.006813	C.3	1	4I4791	0.2514
4	N7	-1.515275	-0.789038	-0.898137	N.am	1	4I4791	-0.3285
5	C6	-2.412016	-1.901895	-0.505351	C.3	1	4I4791	0.1203
6	C5	-1.925470	-2.315737	0.876938	C.3	1	4I4791	0.0241
7	C4	-1.091194	-1.129737	1.362032	C.3	1	4I4791	0.0356
8	C3	-0.492005	-0.544702	0.097181	C.3	1	4I4791	0.1580
9	C1	0.793262	-1.285260	-0.229172	C.2	1	4I4791	0.1576
10	N2	0.798161	-2.357927	-0.880974	N.2	1	4I4791	-0.0909
11	H2	-3.191711	-1.265466	-2.620325	H	1	4I4791	0.0000
12	H3	-2.177419	-0.688348	-3.963977	H	1	4I4791	0.0000
13	H4	-3.290479	0.432536	-3.144034	H	1	4I4791	0.0000
14	H5	-3.447878	-1.565237	-0.464051	H	1	4I4791	0.0000
15	H6	-2.326618	-2.731070	-1.207624	H	1	4I4791	0.0000
16	F7	-3.078102	-2.556662	1.790008	F	1	4I4791	0.0000
17	H8	-1.314927	-3.216595	0.816268	H	1	4I4791	0.0000
18	H9	-1.720983	-0.395955	1.865007	H	1	4I4791	0.0000
19	H10	-0.306776	-1.462817	2.041576	H	1	4I4791	0.0000
20	H11	-0.307544	0.523415	0.211698	H	1	4I4791	0.0000
21	H10	-0.088322	-2.681587	-1.385248	H	1	4I4791	0.0000
22	CA	0.944000	9.259000	-7.065000	C.3	2	ARG123	-0.2637
23	HA	1.963134	9.273802	-6.678802	H	2	ARG123	0.1560
24	CB	0.373000	7.849000	-6.942000	C.3	2	ARG123	-0.0007
25	HB1	-0.646700	7.851900	-7.332700	H	2	ARG123	0.0327

26	HB2	0.354200	7.572800	-5.885700	H	2	ARG123	0.0327
27	CG	1.176000	6.809000	-7.698000	C.3	2	ARG123	0.0390
28	HG1	2.159100	6.725700	-7.229900	H	2	ARG123	0.0285
29	HG2	1.294600	7.148100	-8.729200	H	2	ARG123	0.0285
30	CD	0.543000	5.446000	-7.717000	C.3	2	ARG123	0.0486
31	HD1	1.058300	4.819900	-8.448400	H	2	ARG123	0.0687
32	HD2	-0.507600	5.540900	-7.999300	H	2	ARG123	0.0687
33	NE	0.633000	4.823000	-6.403000	N.pl3	2	ARG123	-0.5295
34	HE	-0.020700	5.141900	-5.675100	H	2	ARG123	0.3456
35	CZ	1.502000	3.871000	-6.081000	C.cat	2	ARG123	0.8076
36	NH1	2.364000	3.410000	-6.983000	N.pl3	2	ARG123	-0.8627
37	HH11	3.037000	2.672700	-6.733600	H	2	ARG123	0.4478
38	HH12	2.357800	3.801200	-7.934700	H	2	ARG123	0.4478
39	NH2	1.510000	3.367000	-4.855000	N.pl3	2	ARG123	-0.8627
40	HH21	2.183000	2.629700	-4.605600	H	2	ARG123	0.4478
41	HH22	0.843100	3.723600	-4.157200	H	2	ARG123	0.4478
42	H13	0.328562	9.952094	-6.491395	H	2	ARG123	0.0000
43	H14	0.948680	9.559529	-8.112772	H	2	ARG123	0.0000
44	CA	-4.909000	5.910000	-5.263000	C.3	3	GLU203	0.0397
45	HA	-4.100736	5.899014	-5.994156	H	3	GLU203	0.1105
46	CB	-4.321000	5.983000	-3.853000	C.3	3	GLU203	0.0560
47	HB1	-5.147700	5.992800	-3.139600	H	3	GLU203	-0.0173
48	HB2	-3.758500	6.915000	-3.766700	H	3	GLU203	-0.0173
49	CG	-3.391000	4.831000	-3.487000	C.3	3	GLU203	0.0136
50	HG1	-3.929200	3.893300	-3.640400	H	3	GLU203	-0.0425
51	HG2	-3.125100	4.926300	-2.432200	H	3	GLU203	-0.0425
52	CD	-2.106000	4.784000	-4.302000	C.2	3	GLU203	0.8054
53	OE1	-1.516000	3.687000	-4.356000	O.co2	3	GLU203	-0.8188
54	OE2	-1.674000	5.816000	-4.874000	O.co2	3	GLU203	-0.8188
55	H6	-5.544408	6.778288	-5.437637	H	3	GLU203	0.0000
56	H7	-5.501500	5.000599	-5.363494	H	3	GLU203	0.0000
57	CA	4.240000	-9.066000	-1.921000	C.3	4	TYR541	-0.0014
58	HA	4.706198	-8.349468	-1.244802	H	4	TYR541	0.0876
59	CB	4.045000	-8.419000	-3.297000	C.3	4	TYR541	-0.0152
60	HB1	3.577700	-9.149000	-3.961200	H	4	TYR541	0.0295
61	HB2	5.024600	-8.144700	-3.694000	H	4	TYR541	0.0295
62	CG	3.181000	-7.185000	-3.257000	C.ar	4	TYR541	-0.0011
63	CD1	3.557000	-6.075000	-2.504000	C.ar	4	TYR541	-0.1906
64	HD1	4.493500	-6.097600	-1.952600	H	4	TYR541	0.1699
65	CD2	1.975000	-7.130000	-3.954000	C.ar	4	TYR541	-0.1906
66	HD2	1.657300	-7.985700	-4.544200	H	4	TYR541	0.1699
67	CE1	2.758000	-4.939000	-2.444000	C.ar	4	TYR541	-0.2341
68	HE1	3.066900	-4.083400	-1.849000	H	4	TYR541	0.1656
69	CE2	1.168000	-5.988000	-3.904000	C.ar	4	TYR541	-0.2341
70	HE2	0.233300	-5.954600	-4.458000	H	4	TYR541	0.1656
71	CZ	1.565000	-4.905000	-3.148000	C.ar	4	TYR541	0.3226
72	OH	0.789000	-3.776000	-3.089000	O.3	4	TYR541	-0.5579
73	H9	4.880558	-9.942544	-2.018582	H	4	TYR541	0.0000
74	H10	3.272091	-9.366672	-1.519861	H	4	TYR541	0.0000
75	CA	3.664000	-2.436000	1.382000	C.3	5	SER624	-0.0249
76	HA	3.588100	-1.629342	2.111138	H	5	SER624	0.0843
77	C	2.883000	-3.658000	1.912000	C.2	5	SER624	0.5973
78	O	2.990000	-3.994000	3.088000	O.2	5	SER624	-0.5679
79	CB	3.127000	-1.937000	0.041000	C.3	5	SER624	0.2117
80	HB1	2.582200	-2.742600	-0.455600	H	5	SER624	0.0352
81	HB2	3.960400	-1.622000	-0.590400	H	5	SER624	0.0352
82	OG	2.260000	-0.845000	0.255000	O.3	5	SER624	-0.6546
83	H5	4.709867	-2.716580	1.257357	H	5	SER624	0.0000
84	N	2.100000	-4.317000	1.067000	N.am	6	TYR625	-0.4157
85	H	1.881900	-3.915900	0.144800	H	6	TYR625	0.2719
86	CA	1.550000	-5.612000	1.451000	C.3	6	TYR625	-0.0014
87	HA	1.889584	-5.868430	2.454458	H	6	TYR625	0.0876
88	H3	1.887636	-6.373596	0.748050	H	6	TYR625	0.0000

89	H4	0.461142	-5.563194	1.437890	H	6	TYR625	0.0000
90	CA	-5.529000	1.226000	5.754000	C.3	7	TYR656	-0.0014
91	HA	-4.687706	1.907731	5.878368	H	7	TYR656	0.0876
92	CB	-5.056000	-0.046000	5.038000	C.3	7	TYR656	-0.0152
93	HB1	-5.901000	-0.726700	4.915000	H	7	TYR656	0.0295
94	HB2	-4.284600	-0.532800	5.638300	H	7	TYR656	0.0295
95	CG	-4.490000	0.298000	3.681000	C.ar	7	TYR656	-0.0011
96	CD1	-3.659000	1.411000	3.537000	C.ar	7	TYR656	-0.1906
97	HD1	-3.412600	2.003300	4.414500	H	7	TYR656	0.1699
98	CD2	-4.810000	-0.439000	2.544000	C.ar	7	TYR656	-0.1906
99	HD2	-5.466400	-1.301800	2.623800	H	7	TYR656	0.1699
100	CE1	-3.146000	1.777000	2.322000	C.ar	7	TYR656	-0.2341
101	HE1	-2.489700	2.640000	2.244500	H	7	TYR656	0.1656
102	CE2	-4.288000	-0.071000	1.298000	C.ar	7	TYR656	-0.2341
103	HE2	-4.523300	-0.654500	0.411600	H	7	TYR656	0.1656
104	CZ	-3.463000	1.051000	1.203000	C.ar	7	TYR656	0.3226
105	OH	-2.925000	1.466000	0.010000	O.3	7	TYR656	-0.5579
106	HH	-3.108100	2.403700	-0.051800	H	7	TYR656	0.3992
107	H9	-5.931656	0.964346	6.732555	H	7	TYR656	0.0000
108	H10	-6.304118	1.710788	5.160419	H	7	TYR656	0.0000
109	CA	4.048000	8.039000	3.825000	C.3	8	ASP702	0.0381
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112	HB1	3.824800	6.525800	5.328300	H	8	ASP702	-0.0122
113	HB2	5.437900	6.588000	4.574900	H	8	ASP702	-0.0122
114	CG	3.972000	5.529000	3.455000	C.2	8	ASP702	0.7994
115	OD1	4.815000	4.639000	3.225000	O.3	8	ASP702	-0.8014
116	OD2	2.855000	5.433000	2.918000	O.2	8	ASP702	-0.8014
117	H4	4.364017	8.800732	4.537785	H	8	ASP702	0.0000
118	H5	2.975233	8.126113	3.652525	H	8	ASP702	0.0000
119	H6	4.568368	4.145026	2.331847	H	8	ASP702	0.0000
120	CA	5.567000	5.312000	0.339000	C.3	9	HIS734	0.0188
121	HA	5.688417	5.087594	1.398670	H	9	HIS734	0.0881
122	CB	4.179000	4.899000	-0.110000	C.3	9	HIS734	-0.0462
123	HB1	4.073100	5.129900	-1.172000	H	9	HIS734	0.0402
124	HB2	3.443700	5.471700	0.459100	H	9	HIS734	0.0402
125	CG	3.910000	3.449000	0.090000	C.2	9	HIS734	-0.0266
126	ND1	4.205000	2.800000	1.271000	N.2	9	HIS734	0.0000
127	CD2	3.409000	2.512000	-0.745000	C.2	9	HIS734	0.1292
128	HD2	3.076700	2.669200	-1.768000	H	9	HIS734	0.1147
129	CE1	3.882000	1.525000	1.157000	C.2	9	HIS734	0.2057
130	HE1	3.994200	0.769000	1.930000	H	9	HIS734	0.1392
131	NE2	3.399000	1.324000	-0.057000	N.p13	9	HIS734	0.0000
132	H7	5.698357	6.381947	0.177369	H	9	HIS734	0.0000
133	H8	6.313491	4.763792	-0.235790	H	9	HIS734	0.0000
134	H9	3.055563	0.386392	-0.441503	H	9	HIS734	0.0000

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126	129	131	1
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128	120	133	1
129	131	134	1
130	84	77	1
131	82	9	1

## FAP / 14b

```
#FAP - 14b complex
#
```

```
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FAP-ligand_nitrile_Fup
 134   131      0 0 0
SMALL
USER_CHARGES
```

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1 O9	-0.762954	0.888924	-2.268437	O.2	1 4I4791	-0.2702
2 C8	-1.544945	-0.057108	-2.036786	C.2	1 4I4791	0.2649
3 C10	-2.624009	-0.419062	-3.006813	C.3	1 4I4791	0.2514
4 N7	-1.515275	-0.789038	-0.898137	N.am	1 4I4791	-0.3285
5 C6	-2.412016	-1.901895	-0.505351	C.3	1 4I4791	0.1203
6 C5	-1.925470	-2.315737	0.876938	C.3	1 4I4791	0.0241
7 C4	-1.091194	-1.129737	1.362032	C.3	1 4I4791	0.0356
8 C3	-0.492005	-0.544702	0.097181	C.3	1 4I4791	0.1580
9 C1	0.793262	-1.285260	-0.229172	C.2	1 4I4791	0.1576
10 N2	0.798161	-2.357927	-0.880974	N.2	1 4I4791	-0.0909
11 H2	-3.191711	-1.265466	-2.620325	H	1 4I4791	0.0000
12 H3	-2.177419	-0.688348	-3.963977	H	1 4I4791	0.0000
13 H4	-3.290479	0.432536	-3.144034	H	1 4I4791	0.0000
14 H5	-3.447878	-1.565237	-0.464051	H	1 4I4791	0.0000
15 H6	-2.326618	-2.731070	-1.207624	H	1 4I4791	0.0000
16 H7	-2.768679	-2.491994	1.544901	H	1 4I4791	0.0000
17 F8	-1.090790	-3.547156	0.794051	F	1 4I4791	0.0000
18 H9	-1.720983	-0.395955	1.865007	H	1 4I4791	0.0000
19 H10	-0.306776	-1.462817	2.041576	H	1 4I4791	0.0000
20 H11	-0.307544	0.523415	0.211698	H	1 4I4791	0.0000
21 H10	-0.113357	-2.737756	-1.292998	H	1 4I4791	0.0000
22 CA	0.944000	9.259000	-7.065000	C.3	2 ARG123	-0.2637
23 HA	1.963134	9.273802	-6.678802	H	2 ARG123	0.1560
24 CB	0.373000	7.849000	-6.942000	C.3	2 ARG123	-0.0007
25 HB1	-0.646700	7.851900	-7.332700	H	2 ARG123	0.0327
26 HB2	0.354200	7.572800	-5.885700	H	2 ARG123	0.0327
27 CG	1.176000	6.809000	-7.698000	C.3	2 ARG123	0.0390
28 HG1	2.159100	6.725700	-7.229900	H	2 ARG123	0.0285
29 HG2	1.294600	7.148100	-8.729200	H	2 ARG123	0.0285
30 CD	0.543000	5.446000	-7.717000	C.3	2 ARG123	0.0486
31 HD1	1.058300	4.819900	-8.448400	H	2 ARG123	0.0687
32 HD2	-0.507600	5.540900	-7.999300	H	2 ARG123	0.0687
33 NE	0.633000	4.823000	-6.403000	N.pl3	2 ARG123	-0.5295
34 HE	-0.020700	5.141900	-5.675100	H	2 ARG123	0.3456
35 CZ	1.502000	3.871000	-6.081000	C.cat	2 ARG123	0.8076
36 NH1	2.364000	3.410000	-6.983000	N.pl3	2 ARG123	-0.8627
37 HH11	3.037000	2.672700	-6.733600	H	2 ARG123	0.4478
38 HH12	2.357800	3.801200	-7.934700	H	2 ARG123	0.4478
39 NH2	1.510000	3.367000	-4.855000	N.pl3	2 ARG123	-0.8627
40 HH21	2.183000	2.629700	-4.605600	H	2 ARG123	0.4478
41 HH22	0.843100	3.723600	-4.157200	H	2 ARG123	0.4478
42 H13	0.328562	9.952094	-6.491395	H	2 ARG123	0.0000
43 H14	0.948680	9.559529	-8.112772	H	2 ARG123	0.0000
44 CA	-4.909000	5.910000	-5.263000	C.3	3 GLU203	0.0397
45 HA	-4.100736	5.899014	-5.994156	H	3 GLU203	0.1105
46 CB	-4.321000	5.983000	-3.853000	C.3	3 GLU203	0.0560
47 HB1	-5.147700	5.992800	-3.139600	H	3 GLU203	-0.0173
48 HB2	-3.758500	6.915000	-3.766700	H	3 GLU203	-0.0173
49 CG	-3.391000	4.831000	-3.487000	C.3	3 GLU203	0.0136
50 HG1	-3.929200	3.893300	-3.640400	H	3 GLU203	-0.0425
51 HG2	-3.125100	4.926300	-2.432200	H	3 GLU203	-0.0425
52 CD	-2.106000	4.784000	-4.302000	C.2	3 GLU203	0.8054
53 OE1	-1.516000	3.687000	-4.356000	O.co2	3 GLU203	-0.8188
54 OE2	-1.674000	5.816000	-4.874000	O.co2	3 GLU203	-0.8188
55 H6	-5.544408	6.778288	-5.437637	H	3 GLU203	0.0000
56 H7	-5.501500	5.000599	-5.363494	H	3 GLU203	0.0000
57 CA	4.240000	-9.066000	-1.921000	C.3	4 TYR541	-0.0014
58 HA	4.706198	-8.349468	-1.244802	H	4 TYR541	0.0876
59 CB	4.045000	-8.419000	-3.297000	C.3	4 TYR541	-0.0152
60 HB1	3.577700	-9.149000	-3.961200	H	4 TYR541	0.0295

61	HB2	5.024600	-8.144700	-3.694000	H	4	TYR541	0.0295
62	CG	3.181000	-7.185000	-3.257000	C.ar	4	TYR541	-0.0011
63	CD1	3.557000	-6.075000	-2.504000	C.ar	4	TYR541	-0.1906
64	HD1	4.493500	-6.097600	-1.952600	H	4	TYR541	0.1699
65	CD2	1.975000	-7.130000	-3.954000	C.ar	4	TYR541	-0.1906
66	HD2	1.657300	-7.985700	-4.544200	H	4	TYR541	0.1699
67	CE1	2.758000	-4.939000	-2.444000	C.ar	4	TYR541	-0.2341
68	HE1	3.066900	-4.083400	-1.849000	H	4	TYR541	0.1656
69	CE2	1.168000	-5.988000	-3.904000	C.ar	4	TYR541	-0.2341
70	HE2	0.233300	-5.954600	-4.458000	H	4	TYR541	0.1656
71	CZ	1.565000	-4.905000	-3.148000	C.ar	4	TYR541	0.3226
72	OH	0.789000	-3.776000	-3.089000	O.3	4	TYR541	-0.5579
73	H9	4.880558	-9.942544	-2.018582	H	4	TYR541	0.0000
74	H10	3.272091	-9.366672	-1.519861	H	4	TYR541	0.0000
75	CA	3.664000	-2.436000	1.382000	C.3	5	SER624	-0.0249
76	HA	3.588100	-1.629342	2.111138	H	5	SER624	0.0843
77	C	2.883000	-3.658000	1.912000	C.2	5	SER624	0.5973
78	O	2.990000	-3.994000	3.088000	O.2	5	SER624	-0.5679
79	CB	3.127000	-1.937000	0.041000	C.3	5	SER624	0.2117
80	HB1	2.582200	-2.742600	-0.455600	H	5	SER624	0.0352
81	HB2	3.960400	-1.622000	-0.590400	H	5	SER624	0.0352
82	OG	2.260000	-0.845000	0.255000	O.3	5	SER624	-0.6546
83	H5	4.709867	-2.716580	1.257357	H	5	SER624	0.0000
84	N	2.100000	-4.317000	1.067000	N.am	6	TYR625	-0.4157
85	H	1.881900	-3.915900	0.144800	H	6	TYR625	0.2719
86	CA	1.550000	-5.612000	1.451000	C.3	6	TYR625	-0.0014
87	HA	1.889584	-5.868430	2.454458	H	6	TYR625	0.0876
88	H3	1.887636	-6.373596	0.748050	H	6	TYR625	0.0000
89	H4	0.461142	-5.563194	1.437890	H	6	TYR625	0.0000
90	CA	-5.529000	1.226000	5.754000	C.3	7	TYR656	-0.0014
91	HA	-4.687706	1.907731	5.878368	H	7	TYR656	0.0876
92	CB	-5.056000	-0.046000	5.038000	C.3	7	TYR656	-0.0152
93	HB1	-5.901000	-0.726700	4.915000	H	7	TYR656	0.0295
94	HB2	-4.284600	-0.532800	5.638300	H	7	TYR656	0.0295
95	CG	-4.490000	0.298000	3.681000	C.ar	7	TYR656	-0.0011
96	CD1	-3.659000	1.411000	3.537000	C.ar	7	TYR656	-0.1906
97	HD1	-3.412600	2.003300	4.414500	H	7	TYR656	0.1699
98	CD2	-4.810000	-0.439000	2.544000	C.ar	7	TYR656	-0.1906
99	HD2	-5.466400	-1.301800	2.623800	H	7	TYR656	0.1699
100	CE1	-3.146000	1.777000	2.322000	C.ar	7	TYR656	-0.2341
101	HE1	-2.489700	2.640000	2.244500	H	7	TYR656	0.1656
102	CE2	-4.288000	-0.071000	1.298000	C.ar	7	TYR656	-0.2341
103	HE2	-4.523300	-0.654500	0.411600	H	7	TYR656	0.1656
104	CZ	-3.463000	1.051000	1.203000	C.ar	7	TYR656	0.3226
105	OH	-2.925000	1.466000	0.010000	O.3	7	TYR656	-0.5579
106	HH	-3.108100	2.403700	-0.051800	H	7	TYR656	0.3992
107	H9	-5.931656	0.964346	6.732555	H	7	TYR656	0.0000
108	H10	-6.304118	1.710788	5.160419	H	7	TYR656	0.0000
109	CA	4.048000	8.039000	3.825000	C.3	8	ASP702	0.0381
110	HA	4.579375	8.180091	2.883865	H	8	ASP702	0.0880
111	CB	4.364000	6.651000	4.387000	C.3	8	ASP702	-0.0303
112	HB1	3.824800	6.525800	5.328300	H	8	ASP702	-0.0122
113	HB2	5.437900	6.588000	4.574900	H	8	ASP702	-0.0122
114	CG	3.972000	5.529000	3.455000	C.2	8	ASP702	0.7994
115	OD1	4.815000	4.639000	3.225000	O.3	8	ASP702	-0.8014
116	OD2	2.855000	5.433000	2.918000	O.2	8	ASP702	-0.8014
117	H4	4.364017	8.800732	4.537785	H	8	ASP702	0.0000
118	H5	2.975233	8.126113	3.652525	H	8	ASP702	0.0000
119	H6	4.413799	3.942375	2.549492	H	8	ASP702	0.0000
120	CA	5.567000	5.312000	0.339000	C.3	9	HIS734	0.0188
121	HA	5.688417	5.087594	1.398670	H	9	HIS734	0.0881
122	CB	4.179000	4.899000	-0.110000	C.3	9	HIS734	-0.0462
123	HB1	4.073100	5.129900	-1.172000	H	9	HIS734	0.0402

124	HB2	3.443700	5.471700	0.459100	H	9	HIS734	0.0402
125	CG	3.910000	3.449000	0.090000	C.2	9	HIS734	-0.0266
126	ND1	4.205000	2.800000	1.271000	N.2	9	HIS734	0.0000
127	CD2	3.409000	2.512000	-0.745000	C.2	9	HIS734	0.1292
128	HD2	3.076700	2.669200	-1.768000	H	9	HIS734	0.1147
129	CE1	3.882000	1.525000	1.157000	C.2	9	HIS734	0.2057
130	HE1	3.994200	0.769000	1.930000	H	9	HIS734	0.1392
131	NE2	3.399000	1.324000	-0.057000	N.p13	9	HIS734	0.0000
132	H7	5.698357	6.381947	0.177369	H	9	HIS734	0.0000
133	H8	6.313491	4.763792	-0.235790	H	9	HIS734	0.0000
134	H9	3.055563	0.386392	-0.441503	H	9	HIS734	0.0000

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51	52	53	am

52	52	54	am
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126	129	131	1
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128	120	133	1
129	131	134	1
130	84	77	1
131	82	9	1

## POP / 10b

```
#POP - 10b complex
#
```

```
@<TRIPOS>MOLECULE
POP-ligand_aldehyde
 135   133      0 0 0
SMALL
USER_CHARGES
```

### @<TRIPOS>ATOM

1	C	-0.281900	-0.749600	0.165200	C.3	1	MOL1	0.0438
2	N	1.413100	-2.485100	0.991000	N.am	1	MOL1	-0.2650
3	C	1.108200	-1.522800	-0.079300	C.3	1	MOL1	0.0461
4	C	1.090700	-2.340600	-1.387900	C.3	1	MOL1	-0.1143
5	C	0.683600	-3.746100	-0.959000	C.3	1	MOL1	-0.1295
6	C	0.986900	-3.811200	0.546200	C.3	1	MOL1	-0.0149
7	H7	-0.111900	-0.011600	0.949100	H	1	MOL1	-0.3955
8	C	2.176900	-2.219800	2.084300	C.2	1	MOL1	0.1952
9	O	2.717000	-1.141000	2.237300	O.2	1	MOL1	-0.3923
10	C	2.447200	-3.350400	3.062900	C.3	1	MOL1	-0.1236
11	O11	-1.211600	-1.764400	0.761600	O.3	1	MOL1	0.1445
12	H1	1.918600	-0.792500	-0.156400	H	1	MOL1	0.1143
13	H1	2.088200	-2.363400	-1.834600	H	1	MOL1	0.0830
14	H1	0.399900	-1.937300	-2.130800	H	1	MOL1	0.0955
15	H1	1.253400	-4.501500	-1.506100	H	1	MOL1	0.0754
16	H1	-0.381400	-3.907200	-1.141600	H	1	MOL1	0.0783
17	H1	1.773500	-4.548900	0.721000	H	1	MOL1	0.1179
18	H1	0.098800	-4.117400	1.103300	H	1	MOL1	0.1131
19	H11	2.887000	-2.946500	3.979000	H	1	MOL1	0.0896
20	H11	3.155300	-4.065400	2.636100	H	1	MOL1	0.1176
21	H11	1.526600	-3.873700	3.334100	H	1	MOL1	0.1207
22	CA	8.861000	7.072000	3.437000	C.3	2	ASP149	0.0381
23	HA	8.258100	7.655900	2.741600	H	2	ASP149	0.0880
24	CB	8.885000	5.587000	2.982000	C.3	2	ASP149	-0.0303
25	HB1	9.491800	5.015100	3.687100	H	2	ASP149	-0.0122
26	HB2	9.337300	5.532700	1.989500	H	2	ASP149	-0.0122
27	CG	7.490000	4.964000	2.919000	C.2	2	ASP149	0.7994
28	OD1	6.638000	5.270000	3.778000	O.co2	2	ASP149	-0.8014
29	OD2	7.310000	4.100000	2.019000	O.co2	2	ASP149	-0.8014
30	H4	9.877900	7.464100	3.453200	H	2	ASP149	0.0000
31	H5	8.430100	7.139500	4.436000	H	2	ASP149	0.0000
32	CA	-8.799000	-3.706000	0.788000	C.3	3	TYR473	-0.0014
33	HA	-8.519500	-3.012000	-0.004600	H	3	TYR473	0.0876

34	CB	-8.160000	-3.247000	2.129000 C.3	3	TYR473	-0.0152
35	HB1	-8.457500	-3.960000	2.900800 H	3	TYR473	0.0295
36	HB2	-8.565600	-2.262500	2.371200 H	3	TYR473	0.0295
37	CG	-6.665000	-3.144000	2.154000 C.2	3	TYR473	-0.0011
38	CD1	-6.020000	-2.031000	1.597000 C.2	3	TYR473	-0.1906
39	HD1	-6.601100	-1.248100	1.116300 H	3	TYR473	0.1699
40	CD2	-5.901000	-4.160000	2.733000 C.2	3	TYR473	-0.1906
41	HD2	-6.394500	-5.046800	3.122300 H	3	TYR473	0.1699
42	CE1	-4.641000	-1.932000	1.661000 C.2	3	TYR473	-0.2341
43	HE1	-4.135000	-1.072200	1.229400 H	3	TYR473	0.1656
44	CE2	-4.497000	-4.050000	2.819000 C.2	3	TYR473	-0.2341
45	HE2	-3.903500	-4.824400	3.298200 H	3	TYR473	0.1656
46	CZ	-3.904000	-2.939000	2.281000 C.2	3	TYR473	0.3226
47	OH	-2.513000	-2.831000	2.354000 O.3	3	TYR473	-0.5579
48	HH	-2.165100	-3.664600	2.036600 H	3	TYR473	0.3992
49	H9	-9.884200	-3.723200	0.889100 H	3	TYR473	0.0000
50	H10	-8.441900	-4.705100	0.538000 H	3	TYR473	0.0000
51	CA	-2.788000	0.527000	-2.298000 C.3	4	SER554	-0.0249
52	HA	-2.040000	0.943500	-2.972600 H	4	SER554	0.0843
53	C	-3.129000	-0.895000	-2.782000 C.2	4	SER554	0.5973
54	O	-3.466000	-1.066000	-3.962000 O.2	4	SER554	-0.5679
55	CB	-2.247000	0.609000	-0.891000 C.3	4	SER554	0.2117
56	HB1	-2.862200	0.009400	-0.216900 H	4	SER554	0.0352
57	HB2	-2.243600	1.646400	-0.550100 H	4	SER554	0.0352
58	OG	-0.912000	0.098000	-0.923000 O.3	4	SER554	-0.6546
59	H4	-3.696300	1.127600	-2.346500 H	4	SER554	0.0000
60	N	-3.079000	-1.892000	-1.903000 N.am	5	ASN555	-0.4157
61	H	-2.656900	-1.737300	-0.977400 H	5	ASN555	0.2719
62	CA	-3.621000	-3.208000	-2.245000 C.3	5	ASN555	0.0143
63	HA	-4.023500	-3.183800	-3.257600 H	5	ASN555	0.1048
64	H3	-4.415300	-3.467500	-1.545000 H	5	ASN555	0.0000
65	H4	-2.828400	-3.954100	-2.187400 H	5	ASN555	0.0000
66	CA	4.917000	-7.800000	-0.782000 C.3	6	TRP595	-0.0275
67	HA	5.987800	-7.600800	-0.824500 H	6	TRP595	0.1123
68	CB	4.172000	-6.803000	-1.690000 C.3	6	TRP595	-0.0050
69	HB1	3.102500	-7.016600	-1.635400 H	6	TRP595	0.0339
70	HB2	4.516600	-6.944600	-2.716500 H	6	TRP595	0.0339
71	CG	4.394000	-5.353000	-1.303000 C.2	6	TRP595	-0.1415
72	CD1	4.664000	-4.843000	-0.045000 C.2	6	TRP595	-0.1638
73	HD1	4.731300	-5.428600	0.868300 H	6	TRP595	0.2062
74	CD2	4.397000	-4.231000	-2.208000 C.2	6	TRP595	0.1243
75	NE1	4.836000	-3.465000	-0.130000 N.pl3	6	TRP595	-0.3418
76	HE1	5.033100	-2.838400	0.662100 H	6	TRP595	0.3412
77	CE2	4.701000	-3.075000	-1.438000 C.2	6	TRP595	0.1380
78	CE3	4.210000	-4.100000	-3.594000 C.2	6	TRP595	-0.2387
79	HE3	4.001400	-4.970700	-4.210300 H	6	TRP595	0.1700
80	CZ2	4.847000	-1.811000	-2.013000 C.2	6	TRP595	-0.2601
81	HZ2	5.112900	-0.944000	-1.413700 H	6	TRP595	0.1572
82	CZ3	4.298000	-2.823000	-4.166000 C.2	6	TRP595	-0.1972
83	HZ3	4.101700	-2.691200	-5.227000 H	6	TRP595	0.1447
84	CH2	4.640000	-1.708000	-3.372000 C.2	6	TRP595	-0.1134
85	HH2	4.743700	-0.736000	-3.847400 H	6	TRP595	0.1417
86	H10	4.723400	-8.817200	-1.122700 H	6	TRP595	0.0000
87	H11	4.567700	-7.688400	0.244500 H	6	TRP595	0.0000
88	CA	4.728000	7.905000	-3.550000 C.3	7	ASP641	0.0381
89	HA	4.652900	8.110600	-2.482200 H	7	ASP641	0.0880
90	CB	3.370000	7.450000	-4.078000 C.3	7	ASP641	-0.0303
91	HB1	3.454300	7.246400	-5.147500 H	7	ASP641	-0.0122
92	HB2	2.641100	8.247300	-3.918500 H	7	ASP641	-0.0122
93	CG	2.893000	6.198000	-3.374000 C.2	7	ASP641	0.7994
94	OD1	3.705000	5.595000	-2.630000 O.2	7	ASP641	-0.8014
95	OD2	1.749000	5.771000	-3.581000 O.3	7	ASP641	-0.8014
96	H4	5.037000	8.810100	-4.072900 H	7	ASP641	0.0000

97	H5	5.465200	7.119600	-3.717300	H	7	ASP641	0.0000
98	H6	1.525607	5.016082	-2.886194	H	7	ASP641	0.0000
99	CA	5.665000	3.078000	-1.291000	C.3	8	ARG643	-0.2637
100	HA	6.519900	2.575600	-0.838500	H	8	ARG643	0.1560
101	CB	4.558000	3.225000	-0.259000	C.3	8	ARG643	-0.0007
102	HB1	3.712000	3.729500	-0.730400	H	8	ARG643	0.0327
103	HB2	4.932200	3.839000	0.562900	H	8	ARG643	0.0327
104	CG	4.067000	1.893000	0.317000	C.3	8	ARG643	0.0390
105	HG1	3.914000	1.193700	-0.507600	H	8	ARG643	0.0285
106	HG2	3.116300	2.064500	0.826100	H	8	ARG643	0.0285
107	CD	5.040000	1.268000	1.307000	C.3	8	ARG643	0.0486
108	HD1	5.992900	1.081700	0.807200	H	8	ARG643	0.0687
109	HD2	4.630100	0.322000	1.667000	H	8	ARG643	0.0687
110	NE	5.257000	2.161000	2.440000	N.pl3	8	ARG643	-0.5295
111	HE	6.096800	2.755500	2.430500	H	8	ARG643	0.3456
112	CZ	4.448000	2.255000	3.473000	C.cat	8	ARG643	0.8076
113	NH1	3.401000	1.424000	3.588000	N.pl3	8	ARG643	-0.8627
114	HH11	2.768200	1.497500	4.396100	H	8	ARG643	0.4478
115	HH12	3.215100	0.715700	2.865100	H	8	ARG643	0.4478
116	NH2	4.689000	3.173000	4.410000	N.pl3	8	ARG643	-0.8627
117	HH21	4.056200	3.246500	5.218100	H	8	ARG643	0.4478
118	HH22	5.492000	3.810400	4.321800	H	8	ARG643	0.4478
119	H13	5.968100	4.064300	-1.642500	H	8	ARG643	0.0000
120	H14	5.301700	2.488600	-2.132900	H	8	ARG643	0.0000
121	CA	1.421000	7.235000	-0.448000	C.3	9	HIS680	0.0188
122	HA	1.293900	7.106200	-1.522800	H	9	HIS680	0.0881
123	CB	2.115000	5.995000	0.139000	C.3	9	HIS680	-0.0462
124	HB1	2.234700	6.139700	1.214700	H	9	HIS680	0.0402
125	HB2	3.099100	5.895200	-0.323700	H	9	HIS680	0.0402
126	CG	1.349000	4.728000	-0.090000	C.2	9	HIS680	-0.0266
127	ND1	1.020000	4.269000	-1.348000	N.2	9	HIS680	0.0000
128	CD2	0.895000	3.802000	0.789000	C.2	9	HIS680	0.1292
129	HD2	0.980900	3.840000	1.871900	H	9	HIS680	0.1147
130	CE1	0.372000	3.112000	-1.233000	C.2	9	HIS680	0.2057
131	HE1	-0.031100	2.523700	-2.053400	H	9	HIS680	0.1392
132	NE2	0.303000	2.802000	0.046000	N.pl3	9	HIS680	0.0000
133	H10777	-0.142100	1.914600	0.445100	H	9	HIS680	0.0000
134	H8	2.031600	8.117800	-0.258100	H	9	HIS680	0.0000
135	H9	0.444800	7.361400	0.020200	H	9	HIS680	0.0000

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## POP / 11b

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#POP - 11b complex
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SMALL
USER_CHARGES

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  1 B          -0.271300   -1.111800   -0.129900 B      1 MOL1      0.2803
  2 N          1.680300    -2.490000    0.598100 N.am    1 MOL1     -0.2432
  3 C          1.135800   -1.679300   -0.501700 C.3     1 MOL1      0.0234

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4 C	1.039500	-2.601600	-1.731000	C.3	1 MOL1	-0.1275
5 C	1.021100	-4.024100	-1.174700	C.3	1 MOL1	-0.1269
6 C	1.418800	-3.899900	0.305700	C.3	1 MOL1	-0.0110
7 C	2.363200	-2.004100	1.672800	C.2	1 MOL1	0.2099
8 C	2.720200	-2.976400	2.776100	C.3	1 MOL1	-0.1167
9 O	2.695600	-0.839900	1.753700	O.2	1 MOL1	-0.3921
10 O	-0.142400	-0.252900	1.006800	O.3	1 MOL1	-0.5092
11 O	-1.049900	-2.273200	0.231700	O.3	1 MOL1	-0.4807
12 H1	1.813300	-0.851500	-0.732500	H	1 MOL1	0.0944
13 H1	1.913100	-2.467700	-2.374100	H	1 MOL1	0.0769
14 H1	0.144200	-2.394300	-2.321400	H	1 MOL1	0.0700
15 H1	1.733600	-4.654300	-1.710400	H	1 MOL1	0.0731
16 H1	0.029400	-4.467400	-1.272800	H	1 MOL1	0.0738
17 H1	2.317800	-4.492400	0.489100	H	1 MOL1	0.1141
18 H1	0.623400	-4.278500	0.951400	H	1 MOL1	0.1190
19 H11	2.941800	-2.429100	3.695100	H	1 MOL1	0.1147
20 H11	3.601200	-3.556900	2.497900	H	1 MOL1	0.1507
21 H11	1.892300	-3.655900	2.985900	H	1 MOL1	0.0857
22 HO	0.818813	-0.088064	1.100365	H	1 MOL1	0.2562
23 HO	-1.046200	-2.283400	1.206500	H	1 MOL1	0.2650
24 CA	8.861000	7.072000	3.437000	C.3	2 ASP149	0.0381
25 HA	8.258100	7.655900	2.741600	H	2 ASP149	0.0880
26 CB	8.885000	5.587000	2.982000	C.3	2 ASP149	-0.0303
27 HB1	9.491800	5.015100	3.687100	H	2 ASP149	-0.0122
28 HB2	9.337300	5.532700	1.989500	H	2 ASP149	-0.0122
29 CG	7.490000	4.964000	2.919000	C.2	2 ASP149	0.7994
30 OD1	6.638000	5.270000	3.778000	O.co2	2 ASP149	-0.8014
31 OD2	7.310000	4.100000	2.019000	O.co2	2 ASP149	-0.8014
32 H4	9.877900	7.464100	3.453200	H	2 ASP149	0.0000
33 H5	8.430100	7.139500	4.436000	H	2 ASP149	0.0000
34 CA	-8.799000	-3.706000	0.788000	C.3	3 TYR473	-0.0014
35 HA	-8.519500	-3.012000	-0.004600	H	3 TYR473	0.0876
36 CB	-8.160000	-3.247000	2.129000	C.3	3 TYR473	-0.0152
37 HB1	-8.457500	-3.960000	2.900800	H	3 TYR473	0.0295
38 HB2	-8.565600	-2.262500	2.371200	H	3 TYR473	0.0295
39 CG	-6.665000	-3.144000	2.154000	C.2	3 TYR473	-0.0011
40 CD1	-6.020000	-2.031000	1.597000	C.2	3 TYR473	-0.1906
41 HD1	-6.601100	-1.248100	1.116300	H	3 TYR473	0.1699
42 CD2	-5.901000	-4.160000	2.733000	C.2	3 TYR473	-0.1906
43 HD2	-6.394500	-5.046800	3.122300	H	3 TYR473	0.1699
44 CE1	-4.641000	-1.932000	1.661000	C.2	3 TYR473	-0.2341
45 HE1	-4.135000	-1.072200	1.229400	H	3 TYR473	0.1656
46 CE2	-4.497000	-4.050000	2.819000	C.2	3 TYR473	-0.2341
47 HE2	-3.903500	-4.824400	3.298200	H	3 TYR473	0.1656
48 CZ	-3.904000	-2.939000	2.281000	C.2	3 TYR473	0.3226
49 OH	-2.513000	-2.831000	2.354000	O.3	3 TYR473	-0.5579
50 HH	-2.165100	-3.664600	2.036600	H	3 TYR473	0.3992
51 H9	-9.884200	-3.723200	0.889100	H	3 TYR473	0.0000
52 H10	-8.441900	-4.705100	0.538000	H	3 TYR473	0.0000
53 CA	-2.788000	0.527000	-2.298000	C.3	4 SER554	-0.0249
54 HA	-2.040000	0.943500	-2.972600	H	4 SER554	0.0843
55 C	-3.129000	-0.895000	-2.782000	C.2	4 SER554	0.5973
56 O	-3.466000	-1.066000	-3.962000	O.2	4 SER554	-0.5679
57 CB	-2.247000	0.609000	-0.891000	C.3	4 SER554	0.2117
58 HB1	-2.862200	0.009400	-0.216900	H	4 SER554	0.0352
59 HB2	-2.243600	1.646400	-0.550100	H	4 SER554	0.0352
60 OG	-0.912000	0.098000	-0.923000	O.3	4 SER554	-0.6546
61 H4	-3.696300	1.127600	-2.346500	H	4 SER554	0.0000
62 N	-3.079000	-1.892000	-1.903000	N.am	5 ASN555	-0.4157
63 H	-2.656900	-1.737300	-0.977400	H	5 ASN555	0.2719
64 CA	-3.621000	-3.208000	-2.245000	C.3	5 ASN555	0.0143
65 HA	-4.023500	-3.183800	-3.257600	H	5 ASN555	0.1048
66 H3	-4.415300	-3.467500	-1.545000	H	5 ASN555	0.0000

67	H4	-2.828400	-3.954100	-2.187400	H	5	ASN555	0.0000
68	CA	4.917000	-7.800000	-0.782000	C.3	6	TRP595	-0.0275
69	HA	5.987800	-7.600800	-0.824500	H	6	TRP595	0.1123
70	CB	4.172000	-6.803000	-1.690000	C.3	6	TRP595	-0.0050
71	HB1	3.102500	-7.016600	-1.635400	H	6	TRP595	0.0339
72	HB2	4.516600	-6.944600	-2.716500	H	6	TRP595	0.0339
73	CG	4.394000	-5.353000	-1.303000	C.2	6	TRP595	-0.1415
74	CD1	4.664000	-4.843000	-0.045000	C.2	6	TRP595	-0.1638
75	HD1	4.731300	-5.428600	0.868300	H	6	TRP595	0.2062
76	CD2	4.397000	-4.231000	-2.208000	C.2	6	TRP595	0.1243
77	NE1	4.836000	-3.465000	-0.130000	N.pl3	6	TRP595	-0.3418
78	HE1	5.033100	-2.838400	0.662100	H	6	TRP595	0.3412
79	CE2	4.701000	-3.075000	-1.438000	C.2	6	TRP595	0.1380
80	CE3	4.210000	-4.100000	-3.594000	C.2	6	TRP595	-0.2387
81	HE3	4.001400	-4.970700	-4.210300	H	6	TRP595	0.1700
82	CZ2	4.847000	-1.811000	-2.013000	C.2	6	TRP595	-0.2601
83	HZ2	5.112900	-0.944000	-1.413700	H	6	TRP595	0.1572
84	CZ3	4.298000	-2.823000	-4.166000	C.2	6	TRP595	-0.1972
85	HZ3	4.101700	-2.691200	-5.227000	H	6	TRP595	0.1447
86	CH2	4.640000	-1.708000	-3.372000	C.2	6	TRP595	-0.1134
87	HH2	4.743700	-0.736000	-3.847400	H	6	TRP595	0.1417
88	H10	4.723400	-8.817200	-1.122700	H	6	TRP595	0.0000
89	H11	4.567700	-7.688400	0.244500	H	6	TRP595	0.0000
90	CA	4.728000	7.905000	-3.550000	C.3	7	ASP641	0.0381
91	HA	4.652900	8.110600	-2.482200	H	7	ASP641	0.0880
92	CB	3.370000	7.450000	-4.078000	C.3	7	ASP641	-0.0303
93	HB1	3.454300	7.246400	-5.147500	H	7	ASP641	-0.0122
94	HB2	2.641100	8.247300	-3.918500	H	7	ASP641	-0.0122
95	CG	2.893000	6.198000	-3.374000	C.2	7	ASP641	0.7994
96	OD1	3.705000	5.595000	-2.630000	O.2	7	ASP641	-0.8014
97	OD2	1.749000	5.771000	-3.581000	O.3	7	ASP641	-0.8014
98	H4	5.037000	8.810100	-4.072900	H	7	ASP641	0.0000
99	H5	5.465200	7.119600	-3.717300	H	7	ASP641	0.0000
100	H6	1.378784	5.322456	-2.706753	H	7	ASP641	0.0000
101	CA	5.665000	3.078000	-1.291000	C.3	8	ARG643	-0.2637
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103	CB	4.558000	3.225000	-0.259000	C.3	8	ARG643	-0.0007
104	HB1	3.712000	3.729500	-0.730400	H	8	ARG643	0.0327
105	HB2	4.932200	3.839000	0.562900	H	8	ARG643	0.0327
106	CG	4.067000	1.893000	0.317000	C.3	8	ARG643	0.0390
107	HG1	3.914000	1.193700	-0.507600	H	8	ARG643	0.0285
108	HG2	3.116300	2.064500	0.826100	H	8	ARG643	0.0285
109	CD	5.040000	1.268000	1.307000	C.3	8	ARG643	0.0486
110	HD1	5.992900	1.081700	0.807200	H	8	ARG643	0.0687
111	HD2	4.630100	0.322000	1.667000	H	8	ARG643	0.0687
112	NE	5.257000	2.161000	2.440000	N.pl3	8	ARG643	-0.5295
113	HE	6.096800	2.755500	2.430500	H	8	ARG643	0.3456
114	CZ	4.448000	2.255000	3.473000	C.cat	8	ARG643	0.8076
115	NH1	3.401000	1.424000	3.588000	N.pl3	8	ARG643	-0.8627
116	HH11	2.768200	1.497500	4.396100	H	8	ARG643	0.4478
117	HH12	3.215100	0.715700	2.865100	H	8	ARG643	0.4478
118	NH2	4.689000	3.173000	4.410000	N.pl3	8	ARG643	-0.8627
119	HH21	4.056200	3.246500	5.218100	H	8	ARG643	0.4478
120	HH22	5.492000	3.810400	4.321800	H	8	ARG643	0.4478
121	H13	5.968100	4.064300	-1.642500	H	8	ARG643	0.0000
122	H14	5.301700	2.488600	-2.132900	H	8	ARG643	0.0000
123	CA	1.421000	7.235000	-0.448000	C.3	9	HIS680	0.0188
124	HA	1.293900	7.106200	-1.522800	H	9	HIS680	0.0881
125	CB	2.115000	5.995000	0.139000	C.3	9	HIS680	-0.0462
126	HB1	2.234700	6.139700	1.214700	H	9	HIS680	0.0402
127	HB2	3.099100	5.895200	-0.323700	H	9	HIS680	0.0402
128	CG	1.349000	4.728000	-0.090000	C.2	9	HIS680	-0.0266
129	ND1	1.020000	4.269000	-1.348000	N.2	9	HIS680	0.0000

130	CD2	0.895000	3.802000	0.789000	C.2	9	HIS680	0.1292
131	HD2	0.980900	3.840000	1.871900	H	9	HIS680	0.1147
132	CE1	0.372000	3.112000	-1.233000	C.2	9	HIS680	0.2057
133	HE1	-0.031100	2.523700	-2.053400	H	9	HIS680	0.1392
134	NE2	0.303000	2.802000	0.046000	N.pl3	9	HIS680	0.0000
135	H10777	-0.142100	1.914600	0.445100	H	9	HIS680	0.0000
136	H8	2.031600	8.117800	-0.258100	H	9	HIS680	0.0000
137	H9	0.444800	7.361400	0.020200	H	9	HIS680	0.0000

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## POP / 5b

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#POP - 5b complex
#
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SMALL
USER_CHARGES
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 2 C8          1.940407  -1.805116  1.789621 C.2       1 4I4791     0.2649
 3 C10         2.303119  -2.862851  2.782461 C.3       1 4I4791     0.2514
 4 N7          1.490236  -2.256613  0.595153 N.am     1 4I4791    -0.3285
 5 C6          1.307974  -3.661958  0.161014 C.3       1 4I4791     0.1203
 6 C5          0.809741  -3.557606  -1.274102 C.3      1 4I4791     0.0241
 7 C4          1.171644  -2.135733  -1.704365 C.3      1 4I4791     0.0356
 8 C3          1.080625  -1.318709  -0.429486 C.3      1 4I4791     0.1580
 9 C1          -0.356499 -0.868258  -0.232687 C.2      1 4I4791     0.1576
10 N2          -1.212546 -1.594832  0.328464 N.2      1 4I4791    -0.0909
11 H2          2.096402  -3.845652  2.358938 H        1 4I4791     0.0000
12 H3          1.714224  -2.727595  3.689695 H        1 4I4791     0.0000
13 H4          3.363491  -2.787392  3.023466 H        1 4I4791     0.0000
14 H5          2.253274  -4.203103  0.201876 H        1 4I4791     0.0000
15 H6          0.572660  -4.166213  0.788022 H        1 4I4791     0.0000
16 H7          1.308133  -4.290353  -1.908756 H       1 4I4791     0.0000
17 H8          -0.268515 -3.710666  -1.319235 H       1 4I4791     0.0000
18 H9          2.181929  -2.102060  -2.112150 H       1 4I4791     0.0000
19 H10         0.466184  -1.767338  -2.449155 H       1 4I4791     0.0000
20 H11         1.755143  -0.463274  -0.466335 H       1 4I4791     0.0000
21 H11         -0.922865 -2.534427  0.750536 H       1 4I4791     0.0000
22 CA           8.861000  7.072000  3.437000 C.3      2 ASP149     0.0381
23 HA           8.258100  7.655900  2.741600 H        2 ASP149     0.0880
24 CB           8.885000  5.587000  2.982000 C.3      2 ASP149    -0.0303
25 HB1          9.491800  5.015100  3.687100 H        2 ASP149    -0.0122
26 HB2          9.337300  5.532700  1.989500 H        2 ASP149    -0.0122
27 CG           7.490000  4.964000  2.919000 C.2      2 ASP149     0.7994
28 OD1          6.638000  5.270000  3.778000 O.co2    2 ASP149    -0.8014
29 OD2          7.310000  4.100000  2.019000 O.co2    2 ASP149    -0.8014
30 H4           9.877900  7.464100  3.453200 H        2 ASP149     0.0000
31 H5           8.430100  7.139500  4.436000 H        2 ASP149     0.0000
32 CA           -8.799000 -3.706000  0.788000 C.3      3 TYR473    -0.0014
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33	HA	-8.519500	-3.012000	-0.004600	H	3	TYR473	0.0876
34	CB	-8.160000	-3.247000	2.129000	C.3	3	TYR473	-0.0152
35	HB1	-8.457500	-3.960000	2.900800	H	3	TYR473	0.0295
36	HB2	-8.565600	-2.262500	2.371200	H	3	TYR473	0.0295
37	CG	-6.665000	-3.144000	2.154000	C.2	3	TYR473	-0.0011
38	CD1	-6.020000	-2.031000	1.597000	C.2	3	TYR473	-0.1906
39	HD1	-6.601100	-1.248100	1.116300	H	3	TYR473	0.1699
40	CD2	-5.901000	-4.160000	2.733000	C.2	3	TYR473	-0.1906
41	HD2	-6.394500	-5.046800	3.122300	H	3	TYR473	0.1699
42	CE1	-4.641000	-1.932000	1.661000	C.2	3	TYR473	-0.2341
43	HE1	-4.135000	-1.072200	1.229400	H	3	TYR473	0.1656
44	CE2	-4.497000	-4.050000	2.819000	C.2	3	TYR473	-0.2341
45	HE2	-3.903500	-4.824400	3.298200	H	3	TYR473	0.1656
46	CZ	-3.904000	-2.939000	2.281000	C.2	3	TYR473	0.3226
47	OH	-2.513000	-2.831000	2.354000	O.3	3	TYR473	-0.5579
48	H9	-9.884200	-3.723200	0.889100	H	3	TYR473	0.0000
49	H10	-8.441900	-4.705100	0.538000	H	3	TYR473	0.0000
50	CA	-2.788000	0.527000	-2.298000	C.3	4	SER554	-0.0249
51	HA	-2.040000	0.943500	-2.972600	H	4	SER554	0.0843
52	C	-3.129000	-0.895000	-2.782000	C.2	4	SER554	0.5973
53	O	-3.466000	-1.066000	-3.962000	O.2	4	SER554	-0.5679
54	CB	-2.247000	0.609000	-0.891000	C.3	4	SER554	0.2117
55	HB1	-2.862200	0.009400	-0.216900	H	4	SER554	0.0352
56	HB2	-2.243600	1.646400	-0.550100	H	4	SER554	0.0352
57	OG	-0.912000	0.098000	-0.923000	O.3	4	SER554	-0.6546
58	H4	-3.696300	1.127600	-2.346500	H	4	SER554	0.0000
59	N	-3.079000	-1.892000	-1.903000	N.am	5	ASN555	-0.4157
60	H	-2.656900	-1.737300	-0.977400	H	5	ASN555	0.2719
61	CA	-3.621000	-3.208000	-2.245000	C.3	5	ASN555	0.0143
62	HA	-4.023500	-3.183800	-3.257600	H	5	ASN555	0.1048
63	H3	-4.415300	-3.467500	-1.545000	H	5	ASN555	0.0000
64	H4	-2.828400	-3.954100	-2.187400	H	5	ASN555	0.0000
65	CA	4.917000	-7.800000	-0.782000	C.3	6	TRP595	-0.0275
66	HA	5.987800	-7.600800	-0.824500	H	6	TRP595	0.1123
67	CB	4.172000	-6.803000	-1.690000	C.3	6	TRP595	-0.0050
68	HB1	3.102500	-7.016600	-1.635400	H	6	TRP595	0.0339
69	HB2	4.516600	-6.944600	-2.716500	H	6	TRP595	0.0339
70	CG	4.394000	-5.353000	-1.303000	C.2	6	TRP595	-0.1415
71	CD1	4.664000	-4.843000	-0.045000	C.2	6	TRP595	-0.1638
72	HD1	4.731300	-5.428600	0.868300	H	6	TRP595	0.2062
73	CD2	4.397000	-4.231000	-2.208000	C.2	6	TRP595	0.1243
74	NE1	4.836000	-3.465000	-0.130000	N.pl3	6	TRP595	-0.3418
75	HE1	5.033100	-2.838400	0.662100	H	6	TRP595	0.3412
76	CE2	4.701000	-3.075000	-1.438000	C.2	6	TRP595	0.1380
77	CE3	4.210000	-4.100000	-3.594000	C.2	6	TRP595	-0.2387
78	HE3	4.001400	-4.970700	-4.210300	H	6	TRP595	0.1700
79	CZ2	4.847000	-1.811000	-2.013000	C.2	6	TRP595	-0.2601
80	HZ2	5.112900	-0.944000	-1.413700	H	6	TRP595	0.1572
81	CZ3	4.298000	-2.823000	-4.166000	C.2	6	TRP595	-0.1972
82	HZ3	4.101700	-2.691200	-5.227000	H	6	TRP595	0.1447
83	CH2	4.640000	-1.708000	-3.372000	C.2	6	TRP595	-0.1134
84	HH2	4.743700	-0.736000	-3.847400	H	6	TRP595	0.1417
85	H10	4.723400	-8.817200	-1.122700	H	6	TRP595	0.0000
86	H11	4.567700	-7.688400	0.244500	H	6	TRP595	0.0000
87	CA	4.728000	7.905000	-3.550000	C.3	7	ASP641	0.0381
88	HA	4.652900	8.110600	-2.482200	H	7	ASP641	0.0880
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91	HB2	2.641100	8.247300	-3.918500	H	7	ASP641	-0.0122
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93	OD1	3.705000	5.595000	-2.630000	O.2	7	ASP641	-0.8014
94	OD2	1.749000	5.771000	-3.581000	O.3	7	ASP641	-0.8014
95	H4	5.037000	8.810100	-4.072900	H	7	ASP641	0.0000

96	H5	5.465200	7.119600	-3.717300	H	7	ASP641	0.0000
97	H6	1.552947	4.966594	-2.935202	H	7	ASP641	0.0000
98	CA	5.665000	3.078000	-1.291000	C.3	8	ARG643	-0.2637
99	HA	6.519900	2.575600	-0.838500	H	8	ARG643	0.1560
100	CB	4.558000	3.225000	-0.259000	C.3	8	ARG643	-0.0007
101	HB1	3.712000	3.729500	-0.730400	H	8	ARG643	0.0327
102	HB2	4.932200	3.839000	0.562900	H	8	ARG643	0.0327
103	CG	4.067000	1.893000	0.317000	C.3	8	ARG643	0.0390
104	HG1	3.914000	1.193700	-0.507600	H	8	ARG643	0.0285
105	HG2	3.116300	2.064500	0.826100	H	8	ARG643	0.0285
106	CD	5.040000	1.268000	1.307000	C.3	8	ARG643	0.0486
107	HD1	5.992900	1.081700	0.807200	H	8	ARG643	0.0687
108	HD2	4.630100	0.322000	1.667000	H	8	ARG643	0.0687
109	NE	5.257000	2.161000	2.440000	N.pl3	8	ARG643	-0.5295
110	HE	6.096800	2.755500	2.430500	H	8	ARG643	0.3456
111	CZ	4.448000	2.255000	3.473000	C.cat	8	ARG643	0.8076
112	NH1	3.401000	1.424000	3.588000	N.pl3	8	ARG643	-0.8627
113	HH11	2.768200	1.497500	4.396100	H	8	ARG643	0.4478
114	HH12	3.215100	0.715700	2.865100	H	8	ARG643	0.4478
115	NH2	4.689000	3.173000	4.410000	N.pl3	8	ARG643	-0.8627
116	HH21	4.056200	3.246500	5.218100	H	8	ARG643	0.4478
117	HH22	5.492000	3.810400	4.321800	H	8	ARG643	0.4478
118	H13	5.968100	4.064300	-1.642500	H	8	ARG643	0.0000
119	H14	5.301700	2.488600	-2.132900	H	8	ARG643	0.0000
120	CA	1.421000	7.235000	-0.448000	C.3	9	HIS680	0.0188
121	HA	1.293900	7.106200	-1.522800	H	9	HIS680	0.0881
122	CB	2.115000	5.995000	0.139000	C.3	9	HIS680	-0.0462
123	HB1	2.234700	6.139700	1.214700	H	9	HIS680	0.0402
124	HB2	3.099100	5.895200	-0.323700	H	9	HIS680	0.0402
125	CG	1.349000	4.728000	-0.090000	C.2	9	HIS680	-0.0266
126	ND1	1.020000	4.269000	-1.348000	N.2	9	HIS680	0.0000
127	CD2	0.895000	3.802000	0.789000	C.2	9	HIS680	0.1292
128	HD2	0.980900	3.840000	1.871900	H	9	HIS680	0.1147
129	CE1	0.372000	3.112000	-1.233000	C.2	9	HIS680	0.2057
130	HE1	-0.031100	2.523700	-2.053400	H	9	HIS680	0.1392
131	NE2	0.303000	2.802000	0.046000	N.pl3	9	HIS680	0.0000
132	H10777	-0.142100	1.914600	0.445100	H	9	HIS680	0.0000
133	H8	2.031600	8.117800	-0.258100	H	9	HIS680	0.0000
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## POP / 13b

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SMALL
USER_CHARGES

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 2 C8          1.940400  -1.805100  1.789600 C.2      1 4I4791     0.2649
 3 C10         2.303100  -2.862900  2.782500 C.3      1 4I4791     0.2514
 4 N7          1.490200  -2.256600  0.595200 N.am     1 4I4791    -0.3285

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5	C6	1.308000	-3.662000	0.161000	C.3	1	4I4791	0.1203
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7	C4	1.171600	-2.135700	-1.704400	C.3	1	4I4791	0.0356
8	C3	1.080600	-1.318700	-0.429500	C.3	1	4I4791	0.1580
9	C1	-0.356500	-0.868300	-0.232700	C.2	1	4I4791	0.1576
10	N2	-1.212500	-1.594800	0.328500	N.2	1	4I4791	-0.0909
11	H2	2.096400	-3.845700	2.358900	H	1	4I4791	0.0000
12	H3	1.714200	-2.727600	3.689700	H	1	4I4791	0.0000
13	H4	3.363500	-2.787400	3.023500	H	1	4I4791	0.0000
14	H5	2.253300	-4.203100	0.201900	H	1	4I4791	0.0000
15	H6	0.572700	-4.166200	0.788000	H	1	4I4791	0.0000
16	F7	1.491000	-4.559300	-2.141700	F	1	4I4791	0.0000
17	F17	-0.664239	-3.766893	-1.335753	F	1	4I4791	0.0000
18	H9	2.181900	-2.102100	-2.112100	H	1	4I4791	0.0000
19	H10	0.466200	-1.767300	-2.449200	H	1	4I4791	0.0000
20	H11	1.755100	-0.463300	-0.466300	H	1	4I4791	0.0000
21	H9	-0.937954	-2.564089	0.689059	H	1	4I4791	0.0000
22	CA	8.861000	7.072000	3.437000	C.3	2	ASP149	0.0381
23	HA	8.258100	7.655900	2.741600	H	2	ASP149	0.0880
24	CB	8.885000	5.587000	2.982000	C.3	2	ASP149	-0.0303
25	HB1	9.491800	5.015100	3.687100	H	2	ASP149	-0.0122
26	HB2	9.337300	5.532700	1.989500	H	2	ASP149	-0.0122
27	CG	7.490000	4.964000	2.919000	C.2	2	ASP149	0.7994
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29	OD2	7.310000	4.100000	2.019000	O.co2	2	ASP149	-0.8014
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31	H5	8.430100	7.139500	4.436000	H	2	ASP149	0.0000
32	CA	-8.799000	-3.706000	0.788000	C.3	3	TYR473	-0.0014
33	HA	-8.519500	-3.012000	-0.004600	H	3	TYR473	0.0876
34	CB	-8.160000	-3.247000	2.129000	C.3	3	TYR473	-0.0152
35	HB1	-8.457500	-3.960000	2.900800	H	3	TYR473	0.0295
36	HB2	-8.565600	-2.262500	2.371200	H	3	TYR473	0.0295
37	CG	-6.665000	-3.144000	2.154000	C.2	3	TYR473	-0.0011
38	CD1	-6.020000	-2.031000	1.597000	C.2	3	TYR473	-0.1906
39	HD1	-6.601100	-1.248100	1.116300	H	3	TYR473	0.1699
40	CD2	-5.901000	-4.160000	2.733000	C.2	3	TYR473	-0.1906
41	HD2	-6.394500	-5.046800	3.122300	H	3	TYR473	0.1699
42	CE1	-4.641000	-1.932000	1.661000	C.2	3	TYR473	-0.2341
43	HE1	-4.135000	-1.072200	1.229400	H	3	TYR473	0.1656
44	CE2	-4.497000	-4.050000	2.819000	C.2	3	TYR473	-0.2341
45	HE2	-3.903500	-4.824400	3.298200	H	3	TYR473	0.1656
46	CZ	-3.904000	-2.939000	2.281000	C.2	3	TYR473	0.3226
47	OH	-2.513000	-2.831000	2.354000	O.3	3	TYR473	-0.5579
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54	CB	-2.247000	0.609000	-0.891000	C.3	4	SER554	0.2117
55	HB1	-2.862200	0.009400	-0.216900	H	4	SER554	0.0352
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58	H4	-3.696300	1.127600	-2.346500	H	4	SER554	0.0000
59	N	-3.079000	-1.892000	-1.903000	N.am	5	ASN555	-0.4157
60	H	-2.656900	-1.737300	-0.977400	H	5	ASN555	0.2719
61	CA	-3.621000	-3.208000	-2.245000	C.3	5	ASN555	0.0143
62	HA	-4.023500	-3.183800	-3.257600	H	5	ASN555	0.1048
63	H3	-4.415300	-3.467500	-1.545000	H	5	ASN555	0.0000
64	H4	-2.828400	-3.954100	-2.187400	H	5	ASN555	0.0000
65	CA	4.917000	-7.800000	-0.782000	C.3	6	TRP595	-0.0275
66	HA	5.987800	-7.600800	-0.824500	H	6	TRP595	0.1123
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68	HB1	3.102500	-7.016600	-1.635400	H	6	TRP595	0.0339
69	HB2	4.516600	-6.944600	-2.716500	H	6	TRP595	0.0339
70	CG	4.394000	-5.353000	-1.303000	C.2	6	TRP595	-0.1415
71	CD1	4.664000	-4.843000	-0.045000	C.2	6	TRP595	-0.1638
72	HD1	4.731300	-5.428600	0.868300	H	6	TRP595	0.2062
73	CD2	4.397000	-4.231000	-2.208000	C.2	6	TRP595	0.1243
74	NE1	4.836000	-3.465000	-0.130000	N.pl3	6	TRP595	-0.3418
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77	CE3	4.210000	-4.100000	-3.594000	C.2	6	TRP595	-0.2387
78	HE3	4.001400	-4.970700	-4.210300	H	6	TRP595	0.1700
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83	CH2	4.640000	-1.708000	-3.372000	C.2	6	TRP595	-0.1134
84	HH2	4.743700	-0.736000	-3.847400	H	6	TRP595	0.1417
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115	NH2	4.689000	3.173000	4.410000	N.pl3	8	ARG643	-0.8627
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124	125	127	2
125	127	128	1
126	127	131	1
127	129	126	2
128	129	130	1
129	129	131	1
130	131	132	1
131	59	52	1
132	57	9	1

## POP / 15b

```
#POP - 15b complex
#
```

```
@<TRIPOS>MOLECULE
POP-ligand_nitrile_Fdown
 134   132      0 0 0
SMALL
USER_CHARGES
```

```
@<TRIPOS>ATOM
 1 O9          2.091900  -0.594200  2.055900 O.2        1 4I4791  -0.2702
 2 C8          1.940400  -1.805100  1.789600 C.2        1 4I4791  0.2649
 3 C10         2.303100  -2.862900  2.782500 C.3        1 4I4791  0.2514
 4 N7          1.490200  -2.256600  0.595200 N.am       1 4I4791  -0.3285
 5 C6          1.308000  -3.662000  0.161000 C.3        1 4I4791  0.1203
 6 C5          0.809700  -3.557600  -1.274100 C.3       1 4I4791  0.0241
 7 C4          1.171600  -2.135700  -1.704400 C.3       1 4I4791  0.0356
 8 C3          1.080600  -1.318700  -0.429500 C.3       1 4I4791  0.1580
 9 C1          -0.356500  -0.868300  -0.232700 C.2       1 4I4791  0.1576
10 N2          -1.212500  -1.594800  0.328500 N.2       1 4I4791  -0.0909
11 H2          2.096400  -3.845700  2.358900 H          1 4I4791  0.0000
12 H3          1.714200  -2.727600  3.689700 H          1 4I4791  0.0000
13 H4          3.363500  -2.787400  3.023500 H          1 4I4791  0.0000
14 H5          2.253300  -4.203100  0.201900 H          1 4I4791  0.0000
15 H6          0.572700  -4.166200  0.788000 H          1 4I4791  0.0000
16 F7          1.491000  -4.559300  -2.141700 F         1 4I4791  0.0000
17 H8          -0.268500  -3.710700  -1.319200 H         1 4I4791  0.0000
18 H9          2.181900  -2.102100  -2.112100 H         1 4I4791  0.0000
19 H10         0.466200  -1.767300  -2.449200 H         1 4I4791  0.0000
20 H11         1.755100  -0.463300  -0.466300 H         1 4I4791  0.0000
21 H10         -0.916634  -2.518131  0.781073 H         1 4I4791  0.0000
22 CA          8.861000  7.072000  3.437000 C.3        2 ASP149  0.0381
23 HA          8.258100  7.655900  2.741600 H         2 ASP149  0.0880
24 CB          8.885000  5.587000  2.982000 C.3        2 ASP149  -0.0303
25 HB1         9.491800  5.015100  3.687100 H         2 ASP149  -0.0122
26 HB2         9.337300  5.532700  1.989500 H         2 ASP149  -0.0122
27 CG          7.490000  4.964000  2.919000 C.2       2 ASP149  0.7994
28 OD1         6.638000  5.270000  3.778000 O.co2      2 ASP149  -0.8014
29 OD2         7.310000  4.100000  2.019000 O.co2      2 ASP149  -0.8014
30 H4          9.877900  7.464100  3.453200 H         2 ASP149  0.0000
31 H5          8.430100  7.139500  4.436000 H         2 ASP149  0.0000
32 CA          -8.799000  -3.706000  0.788000 C.3       3 TYR473  -0.0014
33 HA          -8.519500  -3.012000  -0.004600 H        3 TYR473  0.0876
34 CB          -8.160000  -3.247000  2.129000 C.3       3 TYR473  -0.0152
35 HB1         -8.457500  -3.960000  2.900800 H        3 TYR473  0.0295
36 HB2         -8.565600  -2.262500  2.371200 H        3 TYR473  0.0295
37 CG          -6.665000  -3.144000  2.154000 C.2       3 TYR473  -0.0011
38 CD1         -6.020000  -2.031000  1.597000 C.2       3 TYR473  -0.1906
39 HD1         -6.601100  -1.248100  1.116300 H        3 TYR473  0.1699
```

40	CD2	-5.901000	-4.160000	2.733000 C.2	3	TYR473	-0.1906
41	HD2	-6.394500	-5.046800	3.122300 H	3	TYR473	0.1699
42	CE1	-4.641000	-1.932000	1.661000 C.2	3	TYR473	-0.2341
43	HE1	-4.135000	-1.072200	1.229400 H	3	TYR473	0.1656
44	CE2	-4.497000	-4.050000	2.819000 C.2	3	TYR473	-0.2341
45	HE2	-3.903500	-4.824400	3.298200 H	3	TYR473	0.1656
46	CZ	-3.904000	-2.939000	2.281000 C.2	3	TYR473	0.3226
47	OH	-2.513000	-2.831000	2.354000 O.3	3	TYR473	-0.5579
48	H9	-9.884200	-3.723200	0.889100 H	3	TYR473	0.0000
49	H10	-8.441900	-4.705100	0.538000 H	3	TYR473	0.0000
50	CA	-2.788000	0.527000	-2.298000 C.3	4	SER554	-0.0249
51	HA	-2.040000	0.943500	-2.972600 H	4	SER554	0.0843
52	C	-3.129000	-0.895000	-2.782000 C.2	4	SER554	0.5973
53	O	-3.466000	-1.066000	-3.962000 O.2	4	SER554	-0.5679
54	CB	-2.247000	0.609000	-0.891000 C.3	4	SER554	0.2117
55	HB1	-2.862200	0.009400	-0.216900 H	4	SER554	0.0352
56	HB2	-2.243600	1.646400	-0.550100 H	4	SER554	0.0352
57	OG	-0.912000	0.098000	-0.923000 O.3	4	SER554	-0.6546
58	H4	-3.696300	1.127600	-2.346500 H	4	SER554	0.0000
59	N	-3.079000	-1.892000	-1.903000 N.am	5	ASN555	-0.4157
60	H	-2.656900	-1.737300	-0.977400 H	5	ASN555	0.2719
61	CA	-3.621000	-3.208000	-2.245000 C.3	5	ASN555	0.0143
62	HA	-4.023500	-3.183800	-3.257600 H	5	ASN555	0.1048
63	H3	-4.415300	-3.467500	-1.545000 H	5	ASN555	0.0000
64	H4	-2.828400	-3.954100	-2.187400 H	5	ASN555	0.0000
65	CA	4.917000	-7.800000	-0.782000 C.3	6	TRP595	-0.0275
66	HA	5.987800	-7.600800	-0.824500 H	6	TRP595	0.1123
67	CB	4.172000	-6.803000	-1.690000 C.3	6	TRP595	-0.0050
68	HB1	3.102500	-7.016600	-1.635400 H	6	TRP595	0.0339
69	HB2	4.516600	-6.944600	-2.716500 H	6	TRP595	0.0339
70	CG	4.394000	-5.353000	-1.303000 C.2	6	TRP595	-0.1415
71	CD1	4.664000	-4.843000	-0.045000 C.2	6	TRP595	-0.1638
72	HD1	4.731300	-5.428600	0.868300 H	6	TRP595	0.2062
73	CD2	4.397000	-4.231000	-2.208000 C.2	6	TRP595	0.1243
74	NE1	4.836000	-3.465000	-0.130000 N.pl3	6	TRP595	-0.3418
75	HE1	5.033100	-2.838400	0.662100 H	6	TRP595	0.3412
76	CE2	4.701000	-3.075000	-1.438000 C.2	6	TRP595	0.1380
77	CE3	4.210000	-4.100000	-3.594000 C.2	6	TRP595	-0.2387
78	HE3	4.001400	-4.970700	-4.210300 H	6	TRP595	0.1700
79	CZ2	4.847000	-1.811000	-2.013000 C.2	6	TRP595	-0.2601
80	HZ2	5.112900	-0.944000	-1.413700 H	6	TRP595	0.1572
81	CZ3	4.298000	-2.823000	-4.166000 C.2	6	TRP595	-0.1972
82	HZ3	4.101700	-2.691200	-5.227000 H	6	TRP595	0.1447
83	CH2	4.640000	-1.708000	-3.372000 C.2	6	TRP595	-0.1134
84	HH2	4.743700	-0.736000	-3.847400 H	6	TRP595	0.1417
85	H10	4.723400	-8.817200	-1.122700 H	6	TRP595	0.0000
86	H11	4.567700	-7.688400	0.244500 H	6	TRP595	0.0000
87	CA	4.728000	7.905000	-3.550000 C.3	7	ASP641	0.0381
88	HA	4.652900	8.110600	-2.482200 H	7	ASP641	0.0880
89	CB	3.370000	7.450000	-4.078000 C.3	7	ASP641	-0.0303
90	HB1	3.454300	7.246400	-5.147500 H	7	ASP641	-0.0122
91	HB2	2.641100	8.247300	-3.918500 H	7	ASP641	-0.0122
92	CG	2.893000	6.198000	-3.374000 C.2	7	ASP641	0.7994
93	OD1	3.705000	5.595000	-2.630000 O.2	7	ASP641	-0.8014
94	OD2	1.749000	5.771000	-3.581000 O.3	7	ASP641	-0.8014
95	H4	5.037000	8.810100	-4.072900 H	7	ASP641	0.0000
96	H5	5.465200	7.119600	-3.717300 H	7	ASP641	0.0000
97	H6	1.575178	4.928327	-2.979129 H	7	ASP641	0.0000
98	CA	5.665000	3.078000	-1.291000 C.3	8	ARG643	-0.2637
99	HA	6.519900	2.575600	-0.838500 H	8	ARG643	0.1560
100	CB	4.558000	3.225000	-0.259000 C.3	8	ARG643	-0.0007
101	HB1	3.712000	3.729500	-0.730400 H	8	ARG643	0.0327
102	HB2	4.932200	3.839000	0.562900 H	8	ARG643	0.0327

103	CG	4.067000	1.893000	0.317000	C.3	8	ARG643	0.0390
104	HG1	3.914000	1.193700	-0.507600	H	8	ARG643	0.0285
105	HG2	3.116300	2.064500	0.826100	H	8	ARG643	0.0285
106	CD	5.040000	1.268000	1.307000	C.3	8	ARG643	0.0486
107	HD1	5.992900	1.081700	0.807200	H	8	ARG643	0.0687
108	HD2	4.630100	0.322000	1.667000	H	8	ARG643	0.0687
109	NE	5.257000	2.161000	2.440000	N.pl3	8	ARG643	-0.5295
110	HE	6.096800	2.755500	2.430500	H	8	ARG643	0.3456
111	CZ	4.448000	2.255000	3.473000	C.cat	8	ARG643	0.8076
112	NH1	3.401000	1.424000	3.588000	N.pl3	8	ARG643	-0.8627
113	HH11	2.768200	1.497500	4.396100	H	8	ARG643	0.4478
114	HH12	3.215100	0.715700	2.865100	H	8	ARG643	0.4478
115	NH2	4.689000	3.173000	4.410000	N.pl3	8	ARG643	-0.8627
116	HH21	4.056200	3.246500	5.218100	H	8	ARG643	0.4478
117	HH22	5.492000	3.810400	4.321800	H	8	ARG643	0.4478
118	H13	5.968100	4.064300	-1.642500	H	8	ARG643	0.0000
119	H14	5.301700	2.488600	-2.132900	H	8	ARG643	0.0000
120	CA	1.421000	7.235000	-0.448000	C.3	9	HIS680	0.0188
121	HA	1.293900	7.106200	-1.522800	H	9	HIS680	0.0881
122	CB	2.115000	5.995000	0.139000	C.3	9	HIS680	-0.0462
123	HB1	2.234700	6.139700	1.214700	H	9	HIS680	0.0402
124	HB2	3.099100	5.895200	-0.323700	H	9	HIS680	0.0402
125	CG	1.349000	4.728000	-0.090000	C.2	9	HIS680	-0.0266
126	ND1	1.020000	4.269000	-1.348000	N.2	9	HIS680	0.0000
127	CD2	0.895000	3.802000	0.789000	C.2	9	HIS680	0.1292
128	HD2	0.980900	3.840000	1.871900	H	9	HIS680	0.1147
129	CE1	0.372000	3.112000	-1.233000	C.2	9	HIS680	0.2057
130	HE1	-0.031100	2.523700	-2.053400	H	9	HIS680	0.1392
131	NE2	0.303000	2.802000	0.046000	N.pl3	9	HIS680	0.0000
132	H10777	-0.142100	1.914600	0.445100	H	9	HIS680	0.0000
133	H8	2.031600	8.117800	-0.258100	H	9	HIS680	0.0000
134	H9	0.444800	7.361400	0.020200	H	9	HIS680	0.0000

@<TRIPOS>BOND

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6	3	13	1
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8	4	8	1
9	5	6	1
10	5	14	1
11	5	15	1
12	6	7	1
13	6	16	1
14	6	17	1
15	7	8	1
16	7	18	1
17	7	19	1
18	8	9	1
19	8	20	1
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21	10	21	1
22	22	23	1
23	22	24	1
24	22	30	1
25	22	31	1
26	24	25	1
27	24	26	1
28	24	27	1
29	27	28	am
30	27	29	am

31	32	33	1
32	32	34	1
33	32	48	1
34	32	49	1
35	34	35	1
36	34	36	1
37	34	37	1
38	37	38	2
39	37	40	1
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41	40	41	1
42	42	38	1
43	42	43	1
44	42	46	2
45	44	40	2
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47	44	46	1
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50	50	52	1
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69	70	71	2
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81	79	83	2
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85	87	88	1
86	87	89	1
87	87	95	1
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90	89	91	1
91	89	92	1
92	92	93	2
93	92	94	1

```

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95    98    99  1
96    98   100  1
97    98   118  1
98    98   119  1
99   100   101  1
100   100   102  1
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105   106   107  1
106   106   108  1
107   106   109  1
108   109   110  1
109   111   109  am
110   111   112  am
111   111   115  am
112   112   113  1
113   112   114  1
114   115   116  1
115   115   117  1
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117   120   122  1
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119   120   134  1
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122   122   125  1
123   125   126  1
124   125   127  2
125   127   128  1
126   127   131  1
127   129   126  2
128   129   130  1
129   129   131  1
130   131   132  1
131    59    52  1
132     57     9  1

```

## POP / 14b

```
#POP - 14b complex
#
```

```
@<TRIPOS>MOLECULE
POP-ligand_nitrile_Fup
134    132      0 0 0
SMALL
USER_CHARGES
```

### @<TRIPOS>ATOM

1	O9	2.091900	-0.594200	2.055900	O.2	1	4I4791	-0.2702
2	C8	1.940400	-1.805100	1.789600	C.2	1	4I4791	0.2649
3	C10	2.303100	-2.862900	2.782500	C.3	1	4I4791	0.2514
4	N7	1.490200	-2.256600	0.595200	N.am	1	4I4791	-0.3285
5	C6	1.308000	-3.662000	0.161000	C.3	1	4I4791	0.1203
6	C5	0.809700	-3.557600	-1.274100	C.3	1	4I4791	0.0241
7	C4	1.171600	-2.135700	-1.704400	C.3	1	4I4791	0.0356
8	C3	1.080600	-1.318700	-0.429500	C.3	1	4I4791	0.1580
9	C1	-0.356500	-0.868300	-0.232700	C.2	1	4I4791	0.1576
10	N2	-1.212500	-1.594800	0.328500	N.2	1	4I4791	-0.0909
11	H2	2.096400	-3.845700	2.358900	H	1	4I4791	0.0000

12	H3	1.714200	-2.727600	3.689700	H	1	4I4791	0.0000
13	H4	3.363500	-2.787400	3.023500	H	1	4I4791	0.0000
14	H5	2.253300	-4.203100	0.201900	H	1	4I4791	0.0000
15	H6	0.572700	-4.166200	0.788000	H	1	4I4791	0.0000
16	H7	1.308100	-4.290400	-1.908800	H	1	4I4791	0.0000
17	F8	-0.664200	-3.766800	-1.335800	F	1	4I4791	0.0000
18	H9	2.181900	-2.102100	-2.112100	H	1	4I4791	0.0000
19	H10	0.466200	-1.767300	-2.449200	H	1	4I4791	0.0000
20	H11	1.755100	-0.463300	-0.466300	H	1	4I4791	0.0000
21	H10	-0.918588	-2.523639	0.770963	H	1	4I4791	0.0000
22	CA	8.861000	7.072000	3.437000	C.3	2	ASP149	0.0381
23	HA	8.258100	7.655900	2.741600	H	2	ASP149	0.0880
24	CB	8.885000	5.587000	2.982000	C.3	2	ASP149	-0.0303
25	HB1	9.491800	5.015100	3.687100	H	2	ASP149	-0.0122
26	HB2	9.337300	5.532700	1.989500	H	2	ASP149	-0.0122
27	CG	7.490000	4.964000	2.919000	C.2	2	ASP149	0.7994
28	OD1	6.638000	5.270000	3.778000	O.co2	2	ASP149	-0.8014
29	OD2	7.310000	4.100000	2.019000	O.co2	2	ASP149	-0.8014
30	H4	9.877900	7.464100	3.453200	H	2	ASP149	0.0000
31	H5	8.430100	7.139500	4.436000	H	2	ASP149	0.0000
32	CA	-8.799000	-3.706000	0.788000	C.3	3	TYR473	-0.0014
33	HA	-8.519500	-3.012000	-0.004600	H	3	TYR473	0.0876
34	CB	-8.160000	-3.247000	2.129000	C.3	3	TYR473	-0.0152
35	HB1	-8.457500	-3.960000	2.900800	H	3	TYR473	0.0295
36	HB2	-8.565600	-2.262500	2.371200	H	3	TYR473	0.0295
37	CG	-6.665000	-3.144000	2.154000	C.2	3	TYR473	-0.0011
38	CD1	-6.020000	-2.031000	1.597000	C.2	3	TYR473	-0.1906
39	HD1	-6.601100	-1.248100	1.116300	H	3	TYR473	0.1699
40	CD2	-5.901000	-4.160000	2.733000	C.2	3	TYR473	-0.1906
41	HD2	-6.394500	-5.046800	3.122300	H	3	TYR473	0.1699
42	CE1	-4.641000	-1.932000	1.661000	C.2	3	TYR473	-0.2341
43	HE1	-4.135000	-1.072200	1.229400	H	3	TYR473	0.1656
44	CE2	-4.497000	-4.050000	2.819000	C.2	3	TYR473	-0.2341
45	HE2	-3.903500	-4.824400	3.298200	H	3	TYR473	0.1656
46	CZ	-3.904000	-2.939000	2.281000	C.2	3	TYR473	0.3226
47	OH	-2.513000	-2.831000	2.354000	O.3	3	TYR473	-0.5579
48	H9	-9.884200	-3.723200	0.889100	H	3	TYR473	0.0000
49	H10	-8.441900	-4.705100	0.538000	H	3	TYR473	0.0000
50	CA	-2.788000	0.527000	-2.298000	C.3	4	SER554	-0.0249
51	HA	-2.040000	0.943500	-2.972600	H	4	SER554	0.0843
52	C	-3.129000	-0.895000	-2.782000	C.2	4	SER554	0.5973
53	O	-3.466000	-1.066000	-3.962000	O.2	4	SER554	-0.5679
54	CB	-2.247000	0.609000	-0.891000	C.3	4	SER554	0.2117
55	HB1	-2.862200	0.009400	-0.216900	H	4	SER554	0.0352
56	HB2	-2.243600	1.646400	-0.550100	H	4	SER554	0.0352
57	OG	-0.912000	0.098000	-0.923000	O.3	4	SER554	-0.6546
58	H4	-3.696300	1.127600	-2.346500	H	4	SER554	0.0000
59	N	-3.079000	-1.892000	-1.903000	N.am	5	ASN555	-0.4157
60	H	-2.656900	-1.737300	-0.977400	H	5	ASN555	0.2719
61	CA	-3.621000	-3.208000	-2.245000	C.3	5	ASN555	0.0143
62	HA	-4.023500	-3.183800	-3.257600	H	5	ASN555	0.1048
63	H3	-4.415300	-3.467500	-1.545000	H	5	ASN555	0.0000
64	H4	-2.828400	-3.954100	-2.187400	H	5	ASN555	0.0000
65	CA	4.917000	-7.800000	-0.782000	C.3	6	TRP595	-0.0275
66	HA	5.987800	-7.600800	-0.824500	H	6	TRP595	0.1123
67	CB	4.172000	-6.803000	-1.690000	C.3	6	TRP595	-0.0050
68	HB1	3.102500	-7.016600	-1.635400	H	6	TRP595	0.0339
69	HB2	4.516600	-6.944600	-2.716500	H	6	TRP595	0.0339
70	CG	4.394000	-5.353000	-1.303000	C.2	6	TRP595	-0.1415
71	CD1	4.664000	-4.843000	-0.045000	C.2	6	TRP595	-0.1638
72	HD1	4.731300	-5.428600	0.868300	H	6	TRP595	0.2062
73	CD2	4.397000	-4.231000	-2.208000	C.2	6	TRP595	0.1243
74	NE1	4.836000	-3.465000	-0.130000	N.pl3	6	TRP595	-0.3418

75 HE1	5.033100	-2.838400	0.662100 H	6 TRP595	0.3412
76 CE2	4.701000	-3.075000	-1.438000 C.2	6 TRP595	0.1380
77 CE3	4.210000	-4.100000	-3.594000 C.2	6 TRP595	-0.2387
78 HE3	4.001400	-4.970700	-4.210300 H	6 TRP595	0.1700
79 CZ2	4.847000	-1.811000	-2.013000 C.2	6 TRP595	-0.2601
80 HZ2	5.112900	-0.944000	-1.413700 H	6 TRP595	0.1572
81 CZ3	4.298000	-2.823000	-4.166000 C.2	6 TRP595	-0.1972
82 HZ3	4.101700	-2.691200	-5.227000 H	6 TRP595	0.1447
83 CH2	4.640000	-1.708000	-3.372000 C.2	6 TRP595	-0.1134
84 HH2	4.743700	-0.736000	-3.847400 H	6 TRP595	0.1417
85 H10	4.723400	-8.817200	-1.122700 H	6 TRP595	0.0000
86 H11	4.567700	-7.688400	0.244500 H	6 TRP595	0.0000
87 CA	4.728000	7.905000	-3.550000 C.3	7 ASP641	0.0381
88 HA	4.652900	8.110600	-2.482200 H	7 ASP641	0.0880
89 CB	3.370000	7.450000	-4.078000 C.3	7 ASP641	-0.0303
90 HB1	3.454300	7.246400	-5.147500 H	7 ASP641	-0.0122
91 HB2	2.641100	8.247300	-3.918500 H	7 ASP641	-0.0122
92 CG	2.893000	6.198000	-3.374000 C.2	7 ASP641	0.7994
93 OD1	3.705000	5.595000	-2.630000 O.2	7 ASP641	-0.8014
94 OD2	1.749000	5.771000	-3.581000 O.3	7 ASP641	-0.8014
95 H4	5.037000	8.810100	-4.072900 H	7 ASP641	0.0000
96 H5	5.465200	7.119600	-3.717300 H	7 ASP641	0.0000
97 H6	1.428492	5.211383	-2.752348 H	7 ASP641	0.0000
98 CA	5.665000	3.078000	-1.291000 C.3	8 ARG643	-0.2637
99 HA	6.519900	2.575600	-0.838500 H	8 ARG643	0.1560
100 CB	4.558000	3.225000	-0.259000 C.3	8 ARG643	-0.0007
101 HB1	3.712000	3.729500	-0.730400 H	8 ARG643	0.0327
102 HB2	4.932200	3.839000	0.562900 H	8 ARG643	0.0327
103 CG	4.067000	1.893000	0.317000 C.3	8 ARG643	0.0390
104 HG1	3.914000	1.193700	-0.507600 H	8 ARG643	0.0285
105 HG2	3.116300	2.064500	0.826100 H	8 ARG643	0.0285
106 CD	5.040000	1.268000	1.307000 C.3	8 ARG643	0.0486
107 HD1	5.992900	1.081700	0.807200 H	8 ARG643	0.0687
108 HD2	4.630100	0.322000	1.667000 H	8 ARG643	0.0687
109 NE	5.257000	2.161000	2.440000 N.pl3	8 ARG643	-0.5295
110 HE	6.096800	2.755500	2.430500 H	8 ARG643	0.3456
111 CZ	4.448000	2.255000	3.473000 C.cat	8 ARG643	0.8076
112 NH1	3.401000	1.424000	3.588000 N.pl3	8 ARG643	-0.8627
113 HH11	2.768200	1.497500	4.396100 H	8 ARG643	0.4478
114 HH12	3.215100	0.715700	2.865100 H	8 ARG643	0.4478
115 NH2	4.689000	3.173000	4.410000 N.pl3	8 ARG643	-0.8627
116 HH21	4.056200	3.246500	5.218100 H	8 ARG643	0.4478
117 HH22	5.492000	3.810400	4.321800 H	8 ARG643	0.4478
118 H13	5.968100	4.064300	-1.642500 H	8 ARG643	0.0000
119 H14	5.301700	2.488600	-2.132900 H	8 ARG643	0.0000
120 CA	1.421000	7.235000	-0.448000 C.3	9 HIS680	0.0188
121 HA	1.293900	7.106200	-1.522800 H	9 HIS680	0.0881
122 CB	2.115000	5.995000	0.139000 C.3	9 HIS680	-0.0462
123 HB1	2.234700	6.139700	1.214700 H	9 HIS680	0.0402
124 HB2	3.099100	5.895200	-0.323700 H	9 HIS680	0.0402
125 CG	1.349000	4.728000	-0.090000 C.2	9 HIS680	-0.0266
126 ND1	1.020000	4.269000	-1.348000 N.2	9 HIS680	0.0000
127 CD2	0.895000	3.802000	0.789000 C.2	9 HIS680	0.1292
128 HD2	0.980900	3.840000	1.871900 H	9 HIS680	0.1147
129 CE1	0.372000	3.112000	-1.233000 C.2	9 HIS680	0.2057
130 HE1	-0.031100	2.523700	-2.053400 H	9 HIS680	0.1392
131 NE2	0.303000	2.802000	0.046000 N.pl3	9 HIS680	0.0000
132 H10777	-0.142100	1.914600	0.445100 H	9 HIS680	0.0000
133 H8	2.031600	8.117800	-0.258100 H	9 HIS680	0.0000
134 H9	0.444800	7.361400	0.020200 H	9 HIS680	0.0000

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11	5	15	1
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13	6	16	1
14	6	17	1
15	7	8	1
16	7	18	1
17	7	19	1
18	8	9	1
19	8	20	1
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23	22	24	1
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25	22	31	1
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30	27	29	am
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126	127	131	1
127	129	126	2
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129	129	131	1
130	131	132	1
131	59	52	1
132	57	9	1

## Optimized standalone protein and ligand structures

### 10b

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 O 7.77557 8.29151 3.27484  
 C 7.72344 10.56469 4.04812  
 H 7.16582 11.33885 3.50084  
 C 7.14271 9.19401 3.79433  
 H 5.49850 7.86886 1.87849  
 H 7.68352 10.82494 5.11747  
 C 4.88071 7.34472 2.64957  
 H 5.98581 6.91642 4.39174  
 N 5.84847 9.00546 4.18703  
 O 4.01820 6.56407 2.35246  
 C 5.24922 7.68308 4.08943  
 H 4.91863 10.91098 4.32253  
 C 4.98938 9.95977 4.87321  
 H 5.37899 10.19289 5.88244  
 C 4.04474 7.75663 5.02331  
 H 3.06699 9.41979 4.03477  
 H 4.34862 7.48313 6.04580  
 C 3.64897 9.23208 4.95234  
 H 3.25148 7.06890 4.69948  
 H 3.03672 9.57011 5.79988

### 11b

H 10.67572 5.59200 5.25024  
 O 8.20790 6.00394 4.99953  
 C 10.49829 6.07063 4.28058  
 H 10.85479 5.40006 3.48350  
 C 9.01609 6.34000 4.15033  
 H 11.08896 6.99754 4.21722  
 H 7.70505 4.89634 2.35709  
 O 6.74362 4.88035 2.30186  
 N 8.60816 6.96250 3.00702  
 C 7.19846 7.35341 2.87056  
 H 10.22452 6.82624 1.63541  
 C 9.45232 7.53480 1.97152  
 H 9.97332 8.44440 2.33126  
 C 7.22002 8.31725 1.66802  
 C 8.45103 7.88204 0.87716  
 H 7.34291 9.35768 2.01245  
 H 8.22249 6.98234 0.28258  
 H 8.82622 8.64957 0.18529  
 H 6.87630 7.87065 3.79274  
 B 6.24177 6.09218 2.63447  
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 H 4.59307 7.08512 2.93708  
 H 6.29498 8.27692 1.07283

### 5b

O 7.39913 1.44464 0.63789  
 H 6.17793 -0.73305 0.19556  
 C 7.41188 0.50923 1.41306  
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 H 8.21381 2.66851 2.55077

H 5.95628 -1.00541 1.95187  
 H 7.40423 -1.63628 1.14204  
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 C 10.14172 1.88023 2.47409  
 C 8.75789 1.81424 2.98199  
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 C 8.71428 1.75651 4.51419  
 C 8.07749 -0.40647 3.67178  
 H 7.04066 -0.62755 3.98278  
 H 8.53452 -1.35845 3.35637  
 H 9.48808 2.37537 4.98676  
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 H 9.92755 -0.02133 4.74087  
 H 8.49674 -0.02593 5.79286

### **13b**

O 7.62462 1.56845 1.52135  
 H 6.35570 -0.49945 0.84652  
 C 7.63920 0.54759 2.17510  
 H 8.77978 2.50589 3.33633  
 C 6.86055 -0.68966 1.80051  
 N 11.68283 1.35471 2.90183  
 C 10.59092 1.45860 3.27042  
 H 7.52782 -1.55861 1.69704  
 H 6.10288 -0.93554 2.56011  
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 H 8.23418 2.06172 5.62841  
 C 9.11482 1.50315 5.28454  
 C 8.47509 -0.63746 4.25698  
 H 10.00252 1.87682 5.80911  
 H 7.51804 -1.16371 4.36485  
 H 9.25694 -1.36828 3.98618  
 C 8.87343 0.02561 5.58636  
 F 9.97143 -0.57831 6.09376  
 F 7.89816 -0.10459 6.51741

### **15b**

H 6.16757 -0.34449 -0.04254  
 O 7.26980 1.89447 0.30798  
 C 6.94171 -0.44805 0.72588  
 C 7.56113 0.90952 0.95451  
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 F 10.17198 0.09586 4.90120

### **14b**

O 6.00384 8.45494 6.11316  
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 H 6.60843 11.03263 3.11682  
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 C 5.22069 9.90620 1.84855  
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## FAP

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 H -0.21733 7.75112 -6.01606  
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 C 1.29317 5.50968 -6.25801  
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 C -3.69222 0.99768 3.16775  
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 H -6.09406 -1.37853 2.90186  
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 H 2.08517 -0.32661 0.13793

## POP

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 H -3.83060 -2.05193 0.74120  
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 H -4.16201 -5.16486 3.69099  
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 H 5.98839 -7.55396 -0.72260  
 C 4.17200 -6.80300 -1.69000  
 H 3.10866 -7.09921 -1.75081  
 H 4.56353 -6.90598 -2.71586  
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 C 4.31620 -4.83175 -0.02023

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 H 4.44470 -0.88615 -1.34667  
 C 4.34528 -2.85243 -4.15342  
 H 4.34034 -2.74303 -5.24069  
 C 4.39350 -1.69641 -3.34966  
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 H -0.39787 0.92250 -0.44230  
 H 2.01536 8.14084 -0.24472  
 H 0.42239 7.37576 -0.00417

## VII. References

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