Electronic Supplementary Material (ESI) for Dalton Transactions
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Supporting Information for:

Selective $NaNO_2$ recognition by a simple heteroditopic salt receptor based on L-ornithine molecular scaffold

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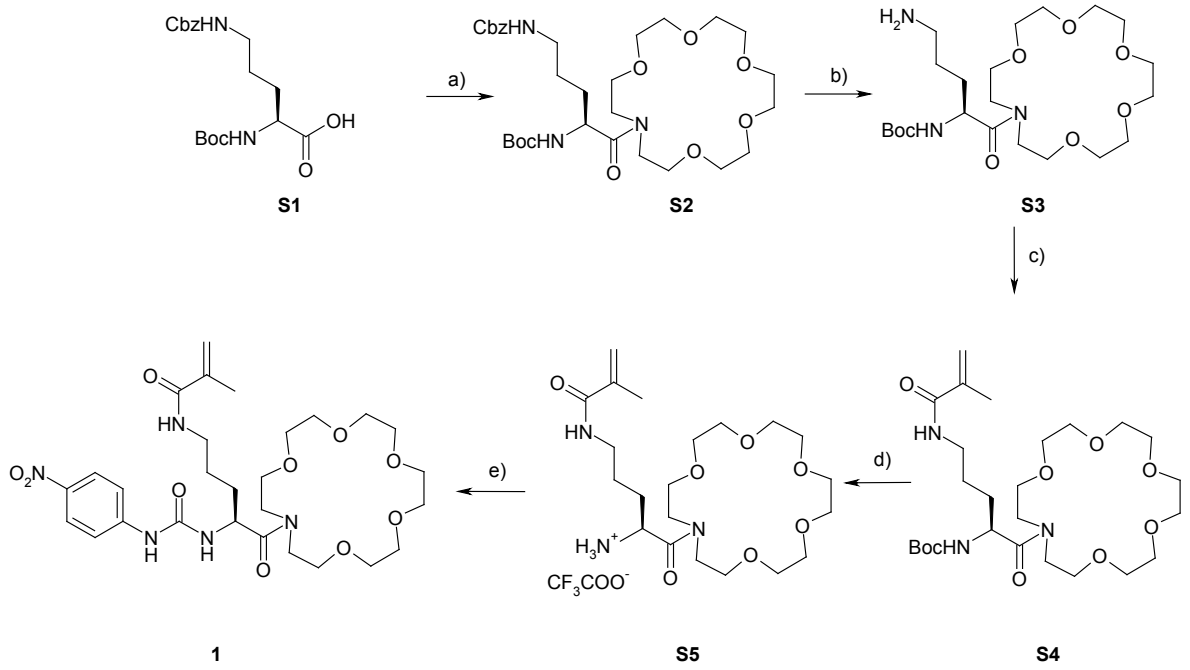
GENERAL INFORMATIONS

Unless specifically indicated, all other chemicals and reagents used in this study were purchased from commercial sources and used as received. 18-Aza-crown-6 was prepared according to literature procedure.[1] Compounds S2-S5 were prepared according to literature procedure.[2] Purification of products was performed using column chromatography on silica gel (Merck Kieselgel 60, 230-400 mesh) with mixtures of chloroform/methanol. Thin-layer chromatography (TLC) was performed on silica gel plates (Merck Kieselgel 60 F254).
^{1}H and ^{13}C NMR spectra used in the characterization of products were recorded on Varian Unity 200 spectrometer using a TMS (δ=0.00) or residual protonated solvent as internal standard. The following abbreviations are used to indicate the multiplicity: s - singlet; d - doublet; t - triplet; q - quartet; m - multiplet, b – broad signal.
High resolution mass spectra (HRMS) were measured on a Quattro LC Micromass unit using ESI technique.
UV-vis analyses were performed using Thermo Spectronic Unicam UV500 Spectrophotometer.

SYNTHESIS

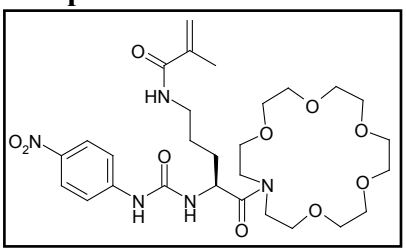


Scheme S1. Synthesis of receptor **1**. *Reagents and conditions*: a) DCC, 1-aza-18-crown-6, CH_2Cl_2, 0˚C to r.t., 92%; b) H_2, Pd/C, MeOH-THF, r.t., quantitative; c) methacryloyl chloride, Et_3N, CH_2Cl_2, 0˚C to r.t., 50%; d) TFA- CH_2Cl_2 (1:1), r.t., quantitative; e) 4-nitrophenyl isocyanate, Et_3N, THF, 75%.

[1] Maeda, H. Furuyoshi, S. Nakatsuji, Y. Okahara, M. *Bull. Chem. Soc. Jpn.*, **1983**, *56*, 212-218.

[2] Romański, J. Piątek, P. *Chem. Commun.* **2012**, *48*, 11346-11348.

Receptor 1:

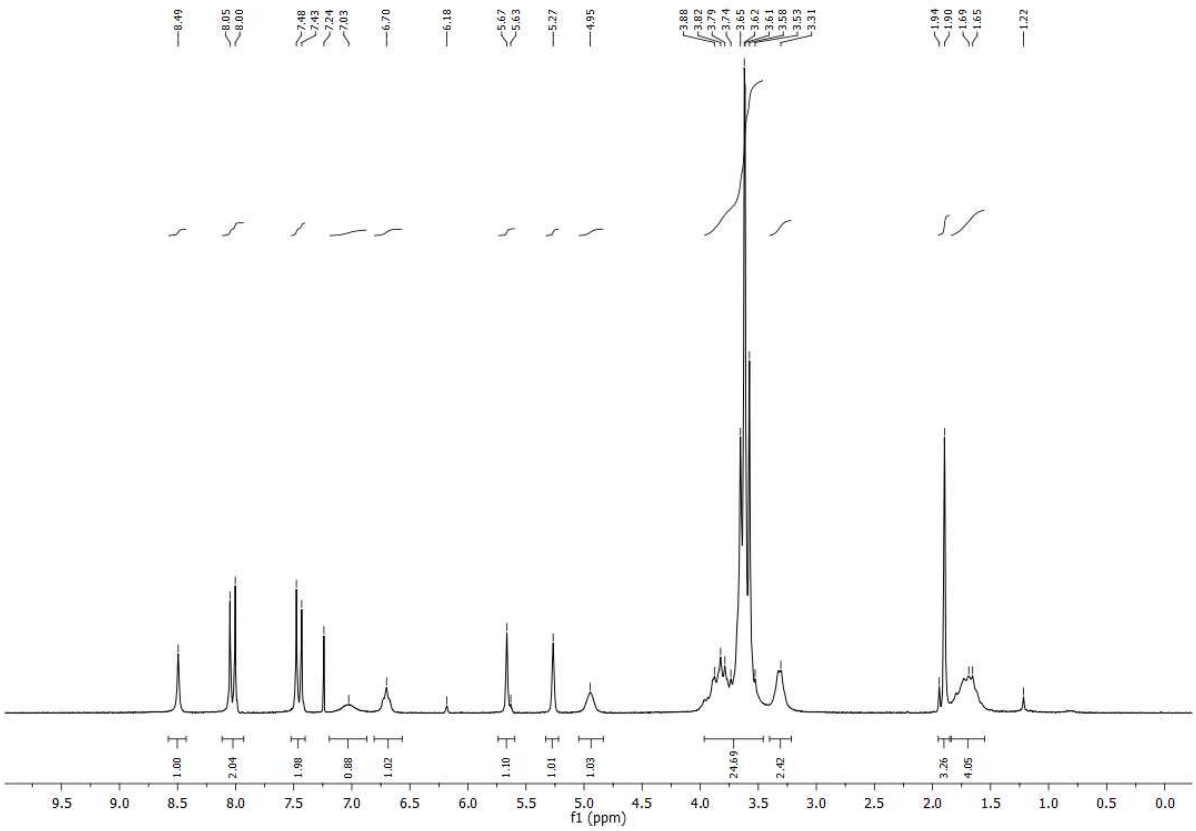


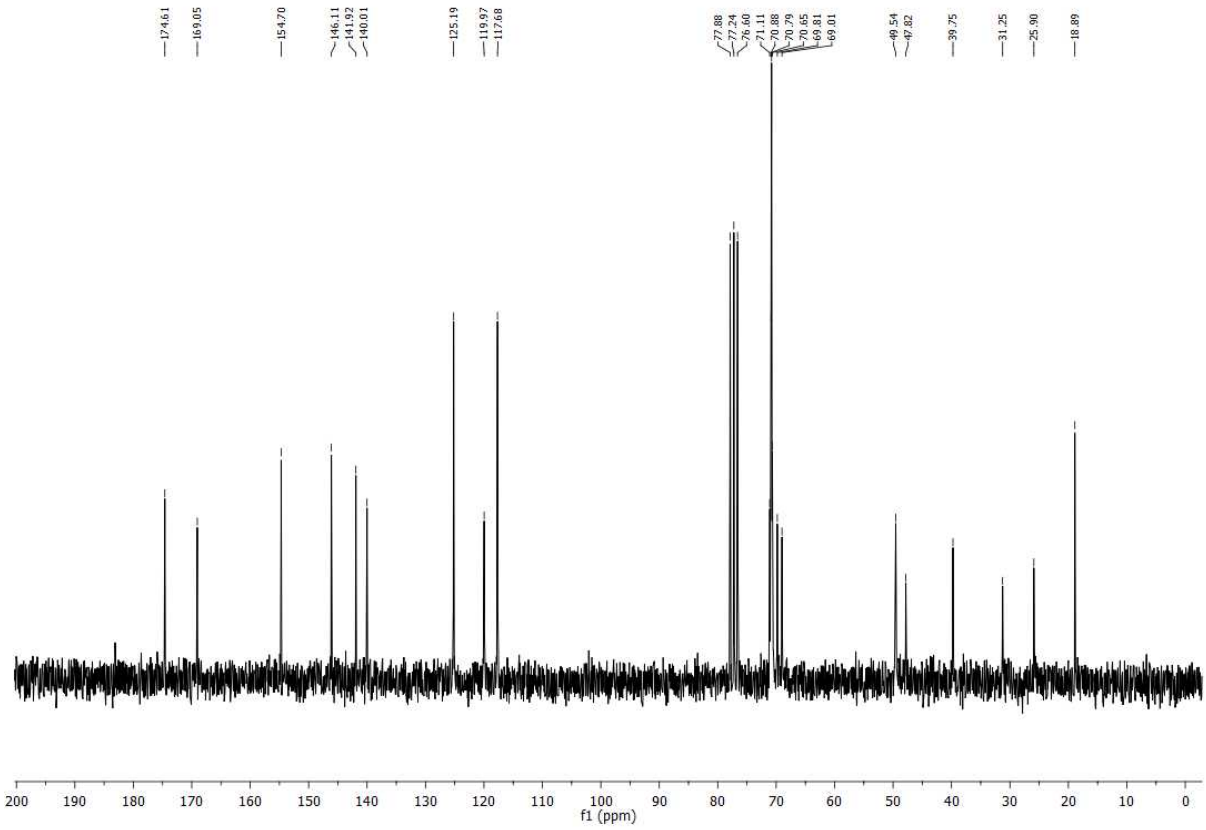
To the solution of **S7** (2 g, 3.58 mmol) and triethylamine (0.725 g, 7.16 mmol) in 40 ml of dry THF the 4-nitrophenyl isocyanate (0.587 g, 3.58 mmol) was added. After stirring overnight at room temperature, the reaction mixture was concentrated and residue was partitioned between dichloromethane and water. The organic layer was dried over anhydrous $MgSO_4$. After filtration the solvent was evaporated, and the crude material was purified by silica gel column chromatography (2,5% methanol in chloroform) to give receptor **1** as pale-yellow solid (1.64 g, 75% yield).

HRMS (ESI): calcd for $C_{28}H_{43}N_5O_{10}Na$ $[M+Na]^+$: 632.2902, found: 632.2872.

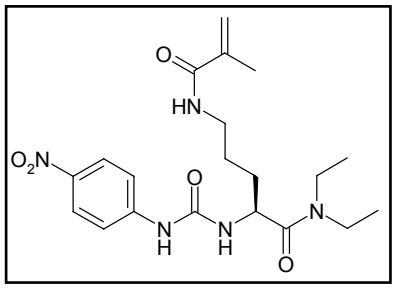
^{1}HNMR (200 MHz, $CDCl_3$) δ: 1.50- 1.85 (m, 4H, C<u>H</u>$_2$-C<u>H</u>$_2$), 1.90 (s, 3H, methacryl C<u>H</u>$_3$), 3.20-3.40 (m, 2H, δ-C<u>H</u>$_2$), 3.45- 4.10 (m, 24H, crown ether C<u>H</u>$_2$), 4.95 (bs, 1H, α-C<u>H</u>), 5.27 (s, 1H, C=C<u>H</u>$_2$), 5.67 (s, 1H, C=C<u>H</u>$_2$), 6.70 (bt, 1H, CH$_2$-N<u>H</u>-methacryl), 7.02 (bs, 1H, N<u>H</u>CONHAr), 7.45 (d, J=9.4, 2H, ArH), 8.02 (d, J=9.4, 2H, ArH), 8.49 (s, 1H, NHCON<u>H</u>Ar).

^{13}CNMR (50 MHz, $CDCl_3$) δ: 18.9 (methacryl CH_3), 25.9 (γ-CH_2), 31.2 (β-CH_2), 39.7 (δ-CH_2), 47.8, 49.5 (crown ether <u>C</u>H$_2$-N rotamers), 69.0 (α-CH), 69.8, 70.6, 70.8, 70.9, 71.1 (all crown ether rotamers), 117.7 (C=<u>C</u>H$_2$), 120.0 (ArH), 125.2 (ArH), 140.0 (<u>C</u>=CH$_2$), 141.9 (ArNO$_2$), 146.1 (ArNH), 154.7 (<u>C</u>O-C=CH$_2$), 169.0 (CO-crown), 174.6 (C=O).





Receptor 3:

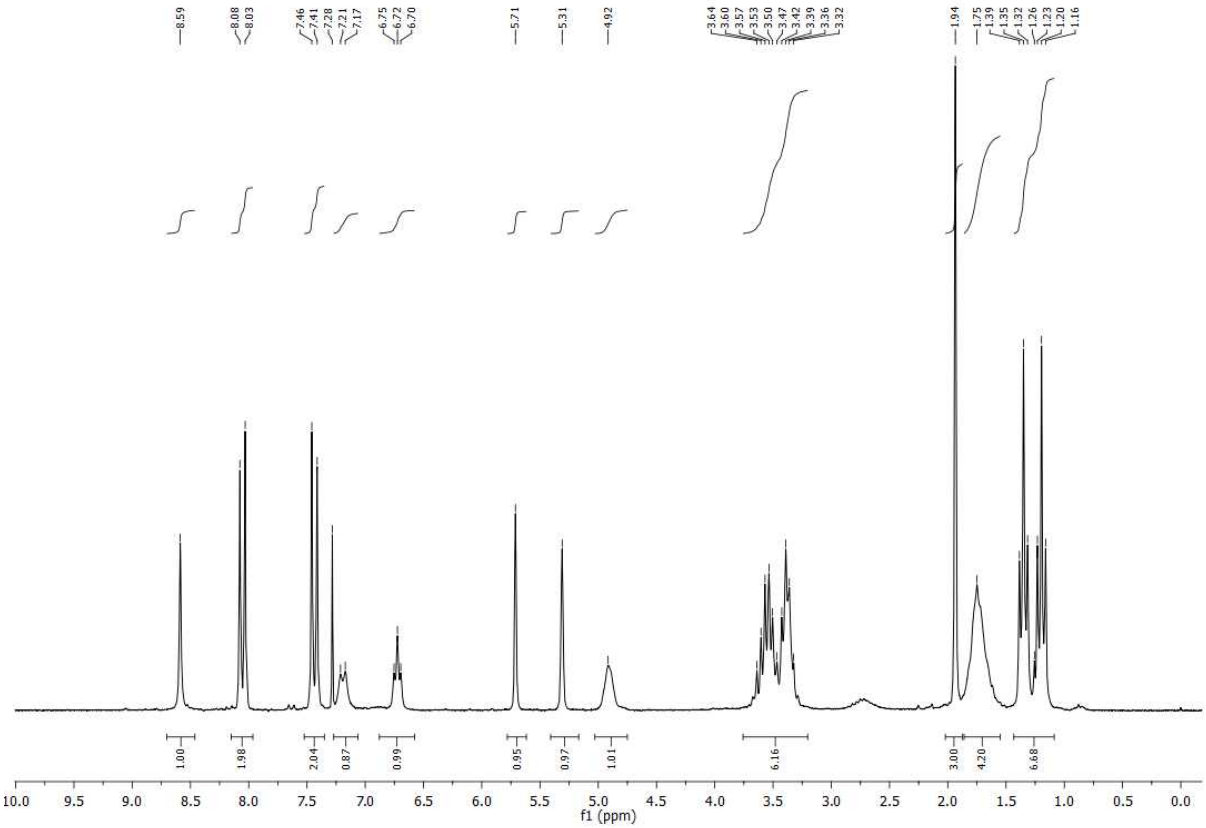


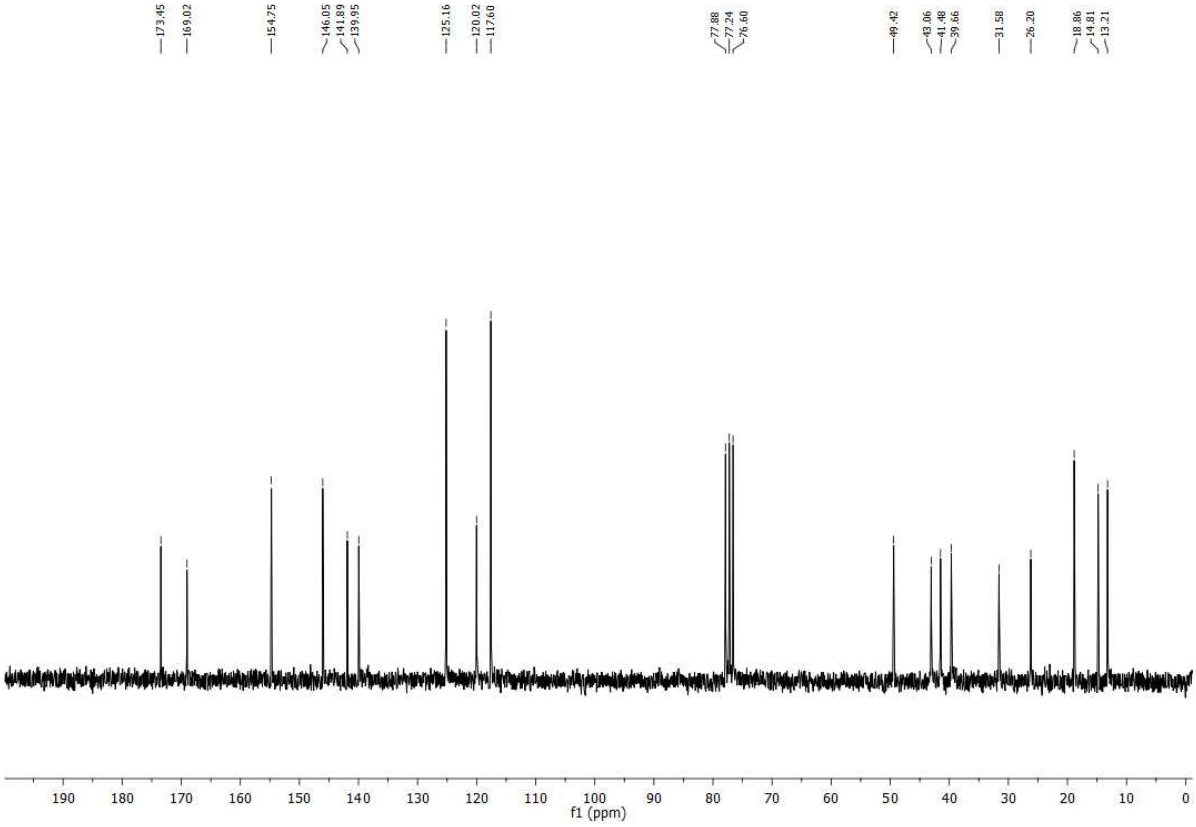
Reference compound was synthesized in analogues manner as receptor **1**. Instead of 1-aza-18-crown-6 at first step the diethylamine was used.

HRMS (ESI): calcd for $C_{20}H_{29}N_5O_5Na$ $[M+Na]^+$: 442.2066, found: 442.2092.

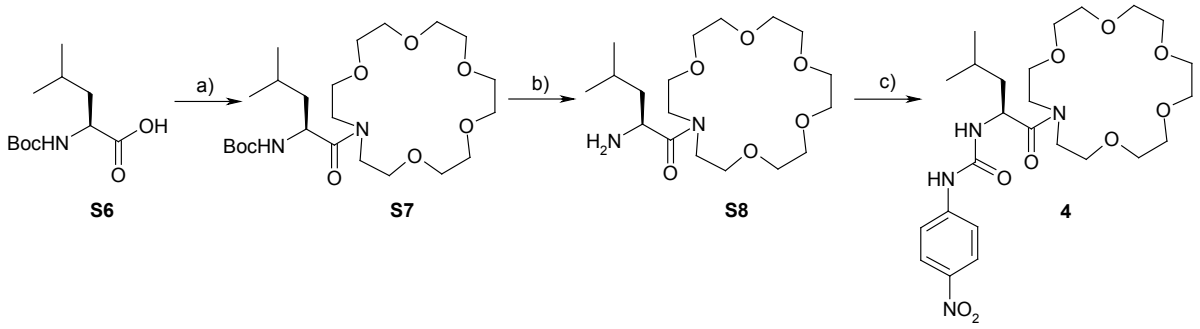
^{1}**HNMR** (200 MHz, $CDCl_3$) δ: 1.15 (t, J=7.1, 3H, $CH_2C\underline{H}_3$ rotamer), 1.30 (t, J=7.0, 3H, $CH_2C\underline{H}_3$ rotamer), 1.50-1.80 (m, 4H, $C\underline{H}_2$-$C\underline{H}_2$), 1.94 (s, 3H, methacryl CH_3), 3.20-3.65 (m, 6H, δ-CH_2+$C\underline{H}_2CH_3$), 4.87 (bs, 1H, α-C$\underline{H}$), 5.26 (s, 1H, C=$C\underline{H}_2$), 5.67 (s, 1H, C=$C\underline{H}_2$), 6.68 (t, J=5.7, 1H, CH_2-N$\underline{H}$-methacryl), 7.15 (bd, J=7.8, 1H, N$\underline{H}$CONHAr), 7.39 (d, J=9.2, ArH), 8.01 (d, J=9.2, ArH), 8.54 (s, 1H, NHCON$\underline{H}$Ar).

^{13}**CNMR** (50 MHz, $CDCl_3$) δ: 13.2, 14.8 ($CH_2\underline{C}H_3$ rotamers), 18.8 (methacryl CH_3), 26.2 (γ-CH_2), 31.6 (β-CH_2), 39.6 (δ-CH_2), 41.5, 43.0 ($\underline{C}H_2CH_3$ rotamers), 49.4.5 (α-CH), 117.6 (C=$\underline{C}H_2$), 120.0 (ArH), 125.2 (ArH), 140.0 ($\underline{C}$=CH_2), 141.9 ($ArNO_2$), 146.1 (ArNH), 154.8 ($\underline{C}$O-C=CH_2), 169.0 ($\underline{C}$O-NEt_2), 173.5.0 (C=O).

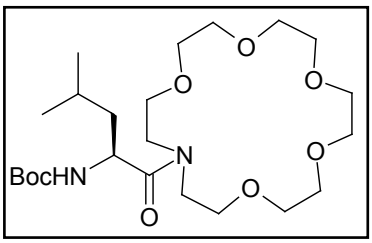

8.59
8.08
8.03
7.46
7.41
7.28
7.21
7.17
6.75
6.72
6.70
5.71
5.31
4.92
3.64
3.60
3.57
3.53
3.50
3.47
3.42
3.39
3.36
3.32
1.94
1.75
1.39
1.35
1.32
1.26
1.23
1.20
1.16
1.00
1.98
2.04
0.87
0.99
0.95
0.97
1.01
6.16
3.00
4.20
6.68
f1 (ppm)


173.45
169.02
154.75
146.05
141.89
139.95
125.16
120.02
117.60
77.88
77.24
76.60
49.42
43.06
41.48
39.66
31.58
26.20
18.86
14.81
13.21
f1 (ppm)

Leucine based salt receptor 4:



Scheme S2. Synthesis of receptor **4**. *Reagents and conditions*: a) DCC, 1-aza-18-crown-6, CH_2Cl_2, 0˚C to r.t., 81%; b) TFA- CH_2Cl_2 (1:1), r.t., quantitative; c) 4-nitrophenyl isocyanate, THF, reflux, 75%.

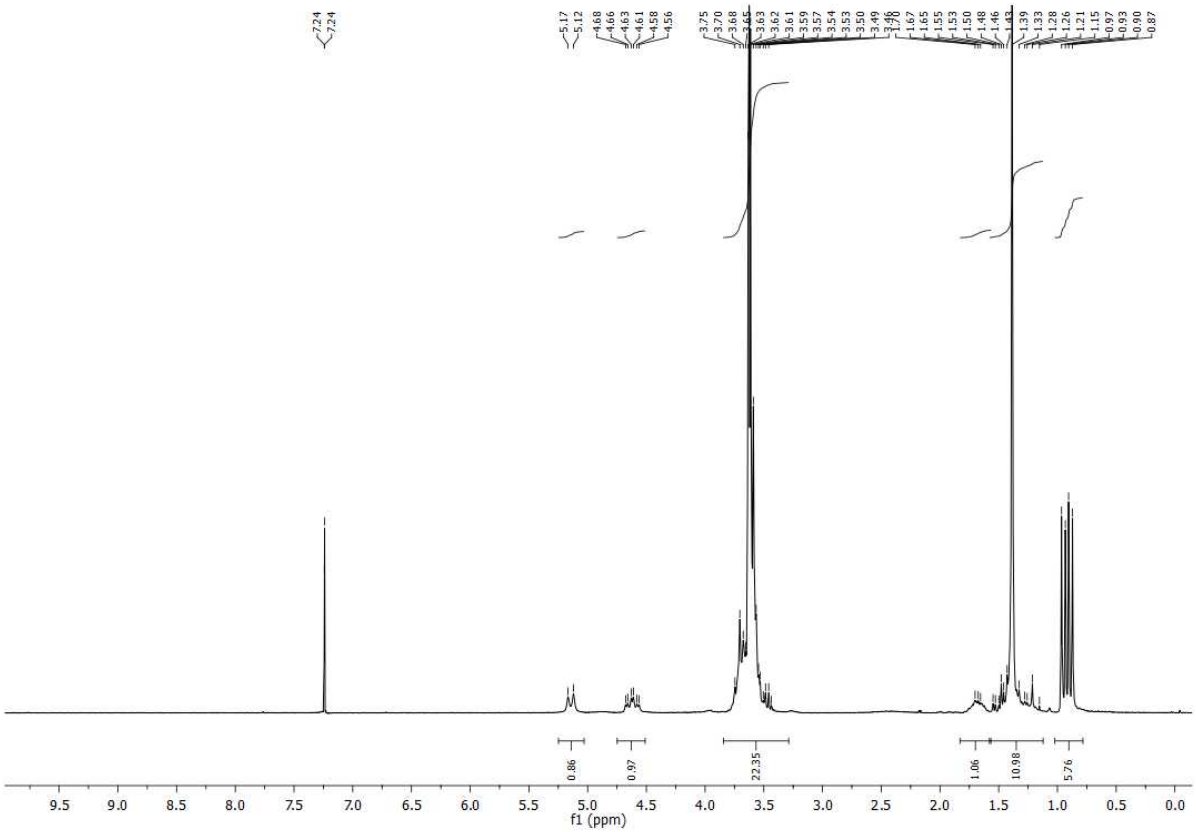


To a solution of N_α-Boc-L-leucine (**S6**) (0.693 g, 3 mmol) and 1,3-dicyclohexylocarbodiimide (DCC) (0.680 g, 3.3 mmol) in 20 ml of dry dichloromethane 0.789 g, 3 mmol of 1-aza-18-crown-6 in 10 ml of dry dichloromethane at 0 °C (ice bath) was added. The reaction mixture was stirred for 30 min and then left at room temperature overnight. The precipitate was filtered off, washed with dichloromethane and solvent was evaporated. The residue was purified by silica gel column chromatography (5% methanol in chloroform) to give the **S7** as a white oil (1.04 g, 81% yield)

HRMS (ESI): calcd for $C_{23}H_{44}N_2O_8Na$ $[M+Na]^+$: 449.2993, found: 499.2995.

^{1}**HNMR** (200 MHz, $CDCl_3$) δ: 0.80-1.00 (m, 6H, $CH(C\underline{H}_3)_2$), 1.30-1.60 (m, 2H, $CH\text{-}C\underline{H}_2\text{-}CH$), 1.45 (s, 9H, $C(C\underline{H}_3)_3$); 1.60-1.80 (m, 1H, $CH_2\text{-}C\underline{H}(CH_3)_2$); 3,50- 3,80 (m, 24H, crown ether $C\underline{H}_2$); 4,62 (dt, J_1=4, J_2=10, 1H, α-$C\underline{H}$); 5.14 (bd, J=10 Hz , 1H, $N\underline{H}$-Boc).

^{13}**CNMR** (50 MHz, $CDCl_3$) δ: 22.0 and 23.7 ($CH_2\text{-}CH(\underline{C}H_3)_2$), 24.8 (γ-CH), 28.5 ($COC(\underline{C}H_3)_3$), 43.2 (β-CH2), 47.2 (α-CH), 48.8, 69.8, 70.6, 70.8, 70.9, 71.0, (all crown ether), 79.5($CO\underline{C}(CH_3)_3$), 155.6 ($\underline{C}OC(CH_3)_3$), 173.6 (CO-crown).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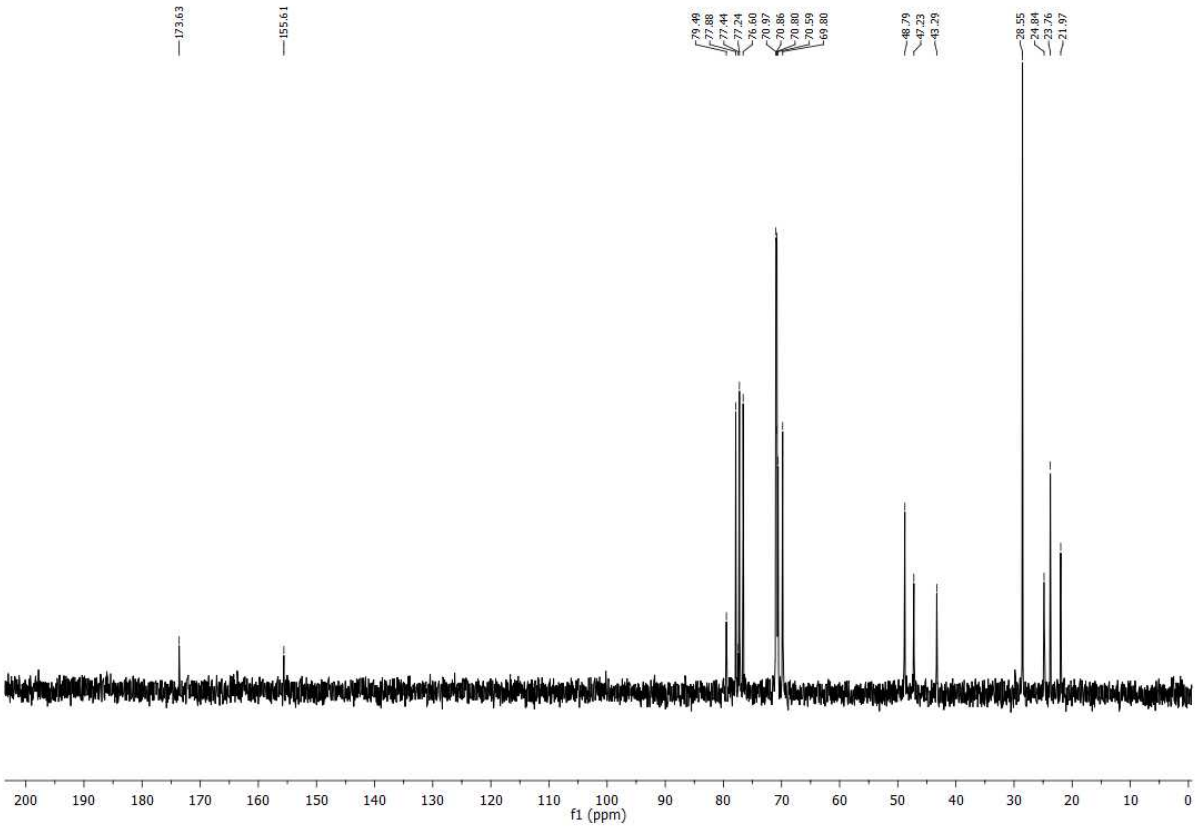
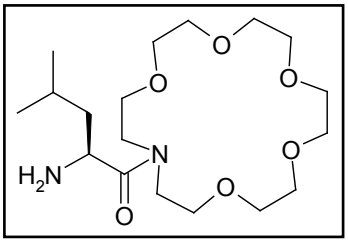
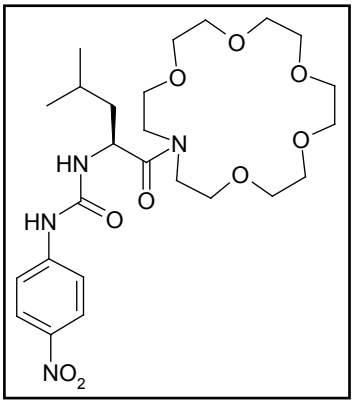
7.24
5.17
5.12
4.68
4.66
4.63
4.61
4.58
4.56
3.75
3.70
3.68
3.65
3.63
3.62
3.61
3.59
3.57
3.54
3.53
3.50
3.49
1.67
1.65
1.55
1.53
1.50
1.48
1.46
1.39
1.33
1.28
1.26
1.21
1.15
0.97
0.93
0.90
0.87
0.86
0.97
22.35
1.06
10.98
5.76
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


173.63
155.61
79.49
77.88
77.44
77.24
76.60
70.97
70.86
70.80
70.59
69.80
48.79
47.23
43.29
28.55
24.84
23.76
21.97
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



The compound **S7** (1g, 2.1 mmol) was dissolved in 20 ml of dichloromethane and 5 ml of trifluoroacetic acid was added. The reaction mixture was stirred at room temperature until starting material was consumed (TLC monitoring). The mixture was evaporated and neutralized with 20 ml of saturated solution and solid sodium bicarbonate. After phase separation the aqueous layer was extracted twice with dichloromethane. The combined organic phase was dried over $MgSO_4$ and the organic solvent was removed under reduced pressure to yield the 0.750 g (95 % yield) of amine **S8**. The amine was used in next step without further purification.

LRMS (ESI): 399.3 $[M+Na]^+$

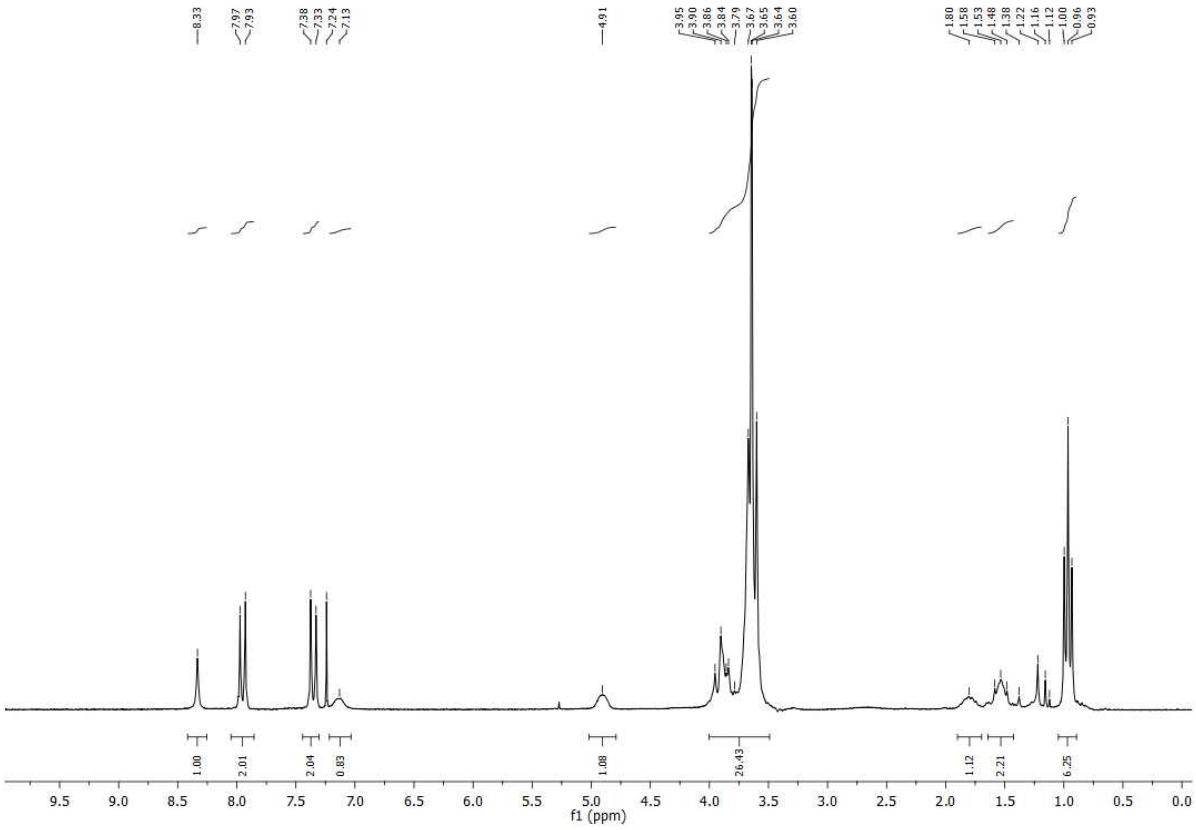


To the solution of **S8** (0.564 g, 1.5 mmol) in 20 ml of dry THF the 4-nitrophenyl isocyanate (0.246 g, 1.5 mmol) was added. After stirring overnight at room temperature, the reaction mixture was concentrated and residue was purified by silica gel column chromatography (2,5% methanol in chloroform) to give L-leucine based receptor **4** as pale-yellow oil (0.599 g, 74 % yield).

HRMS (ESI): calcd for $C_{25}H_{40}N_4O_9Na$ $[M+Na]^+$: 563.2688, found: 563.2668.

^{1}**HNMR** (200 MHz, $CDCl_3$) δ: 0.96 (t, J= 6.5, 6H, $CH(C\underline{H}_3)_2$), 1.45- 1.68 (m, 2H, , $CH-C\underline{H}_2-CH$); 1.70-1.80 (m, 1H, $CH_2-C\underline{H}(CH_3)_2$); 3.50- 4.00 (m, 24H, crown ether $C\underline{H}_2$); 4.90 (bs, 1H, α-C<u>H</u>); 7.13 (bs, 1H, N<u>H</u>CONHAr); 7.35 (d, J=9.4, 2H, ArH), 7.95 (d, J=9.2, 2H, ArH), 8.33 (s, 1H, NHCON<u>H</u>Ar).

^{13}**CNMR** (50 MHz, $CDCl_3$) δ: 21.7 and 23.8 ($CH_2-CH(\underline{C}H_3)_2$), 25.0 (γ-CH), 42.2 (β-CH2), 47.0 and 48.5 (crown ether), 49.4 (α-CH), 70.1, 70.9, 70.8, 69.8, 69.1 (all ether), 69.0 (α-CH), 69.8, 70.6, 70.8, 70.9, 71.1 (all crown ether), 117.6, 125.0, 141.8, 146.0 (all $ArNO_2$), 154.9 (NH-CONH), 175.9 (CO-crown ether).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7.97
7.93
7.38
7.33
7.24
7.13
4.91
3.95
3.90
3.86
3.84
3.79
3.67
3.65
3.64
3.60
1.80
1.58
1.53
1.48
1.38
1.22
1.16
1.12
1.00
0.96
0.93
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2.01
2.04
0.83
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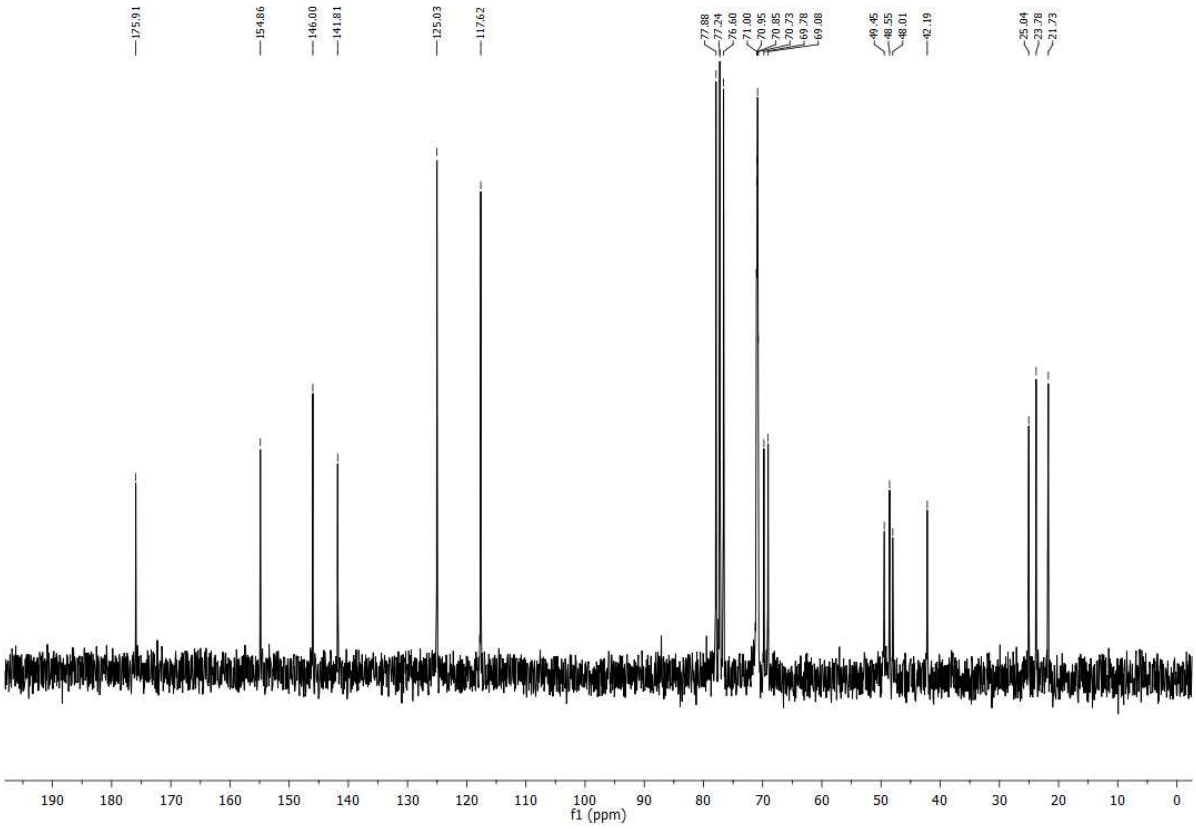
2.21
6.25
f1 (ppm)


175.91
154.86
146.00
141.81
125.03
117.62
77.88
77.24
76.60
71.00
70.95
70.85
70.73
69.78
69.08
49.45
48.55
48.01
42.19
25.04
23.78
21.73
f1 (ppm)

BINDING STUDIES

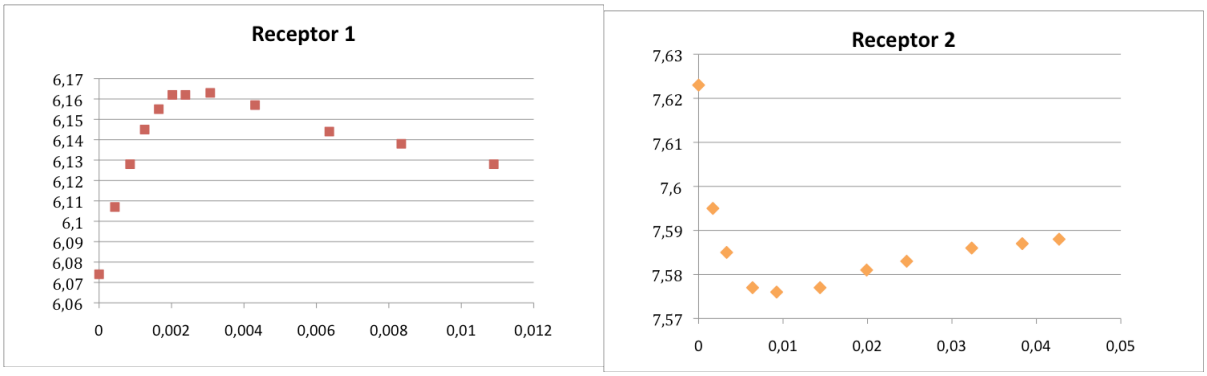


Figure S1. The comparison of urea NH proton shift of receptors **1** and **2** upon addition of $NaPF_6$.

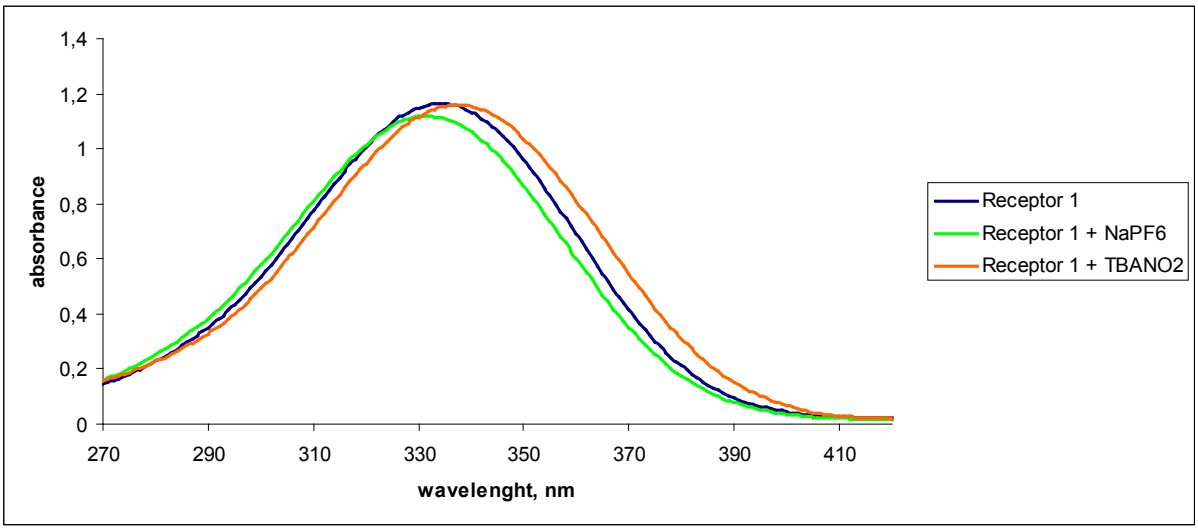
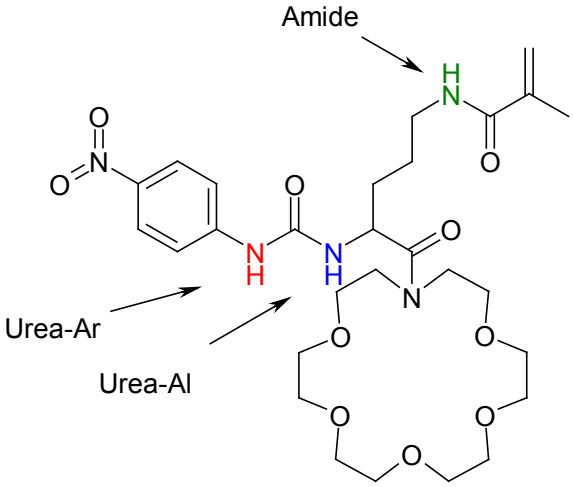
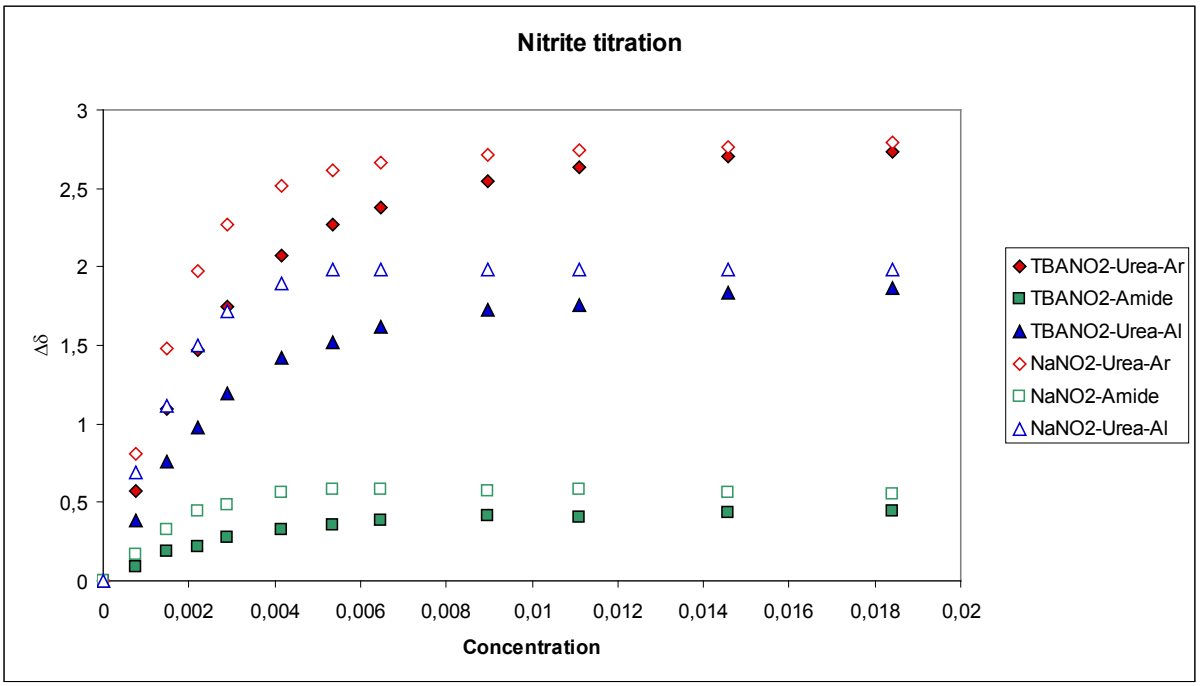


Figure S2. UV/vis spectra changes of receptor **1** CH_3CN solution in the presence of excess of $NaPF_6$ and $TBANO_2$.

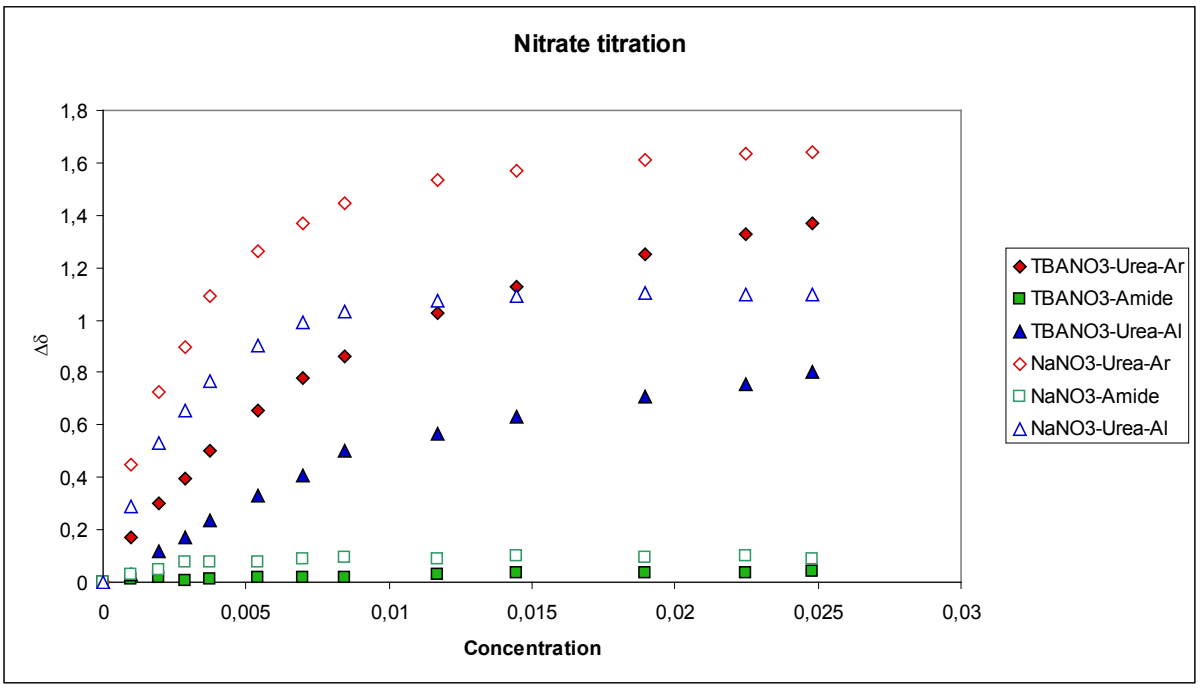
NMR titrations

The ^1H NMR titrations were performed on a Varian UnityPlus 200MHz spectrometer, at 298K in CD_3CN. In each case, a 500 µL of freshly prepared 2.7 mM solution of receptor **1** was added to a 5mm NMR tube. Where applicable the solution also contained 1 molar equivalent of sodium hexafluorophosphate. Small aliquots of 10-20 mM solution of tetrabutylammonium anion salts, containing **1** at 2.7 mM concentration, were added and a spectrum was acquired after each addition. Titration isotherms for NH protons were fitted to a 1:1 binding model using the HypNMR 2000 program. The 1:1 binding stoichiometries were verified by a Job plot analysis.

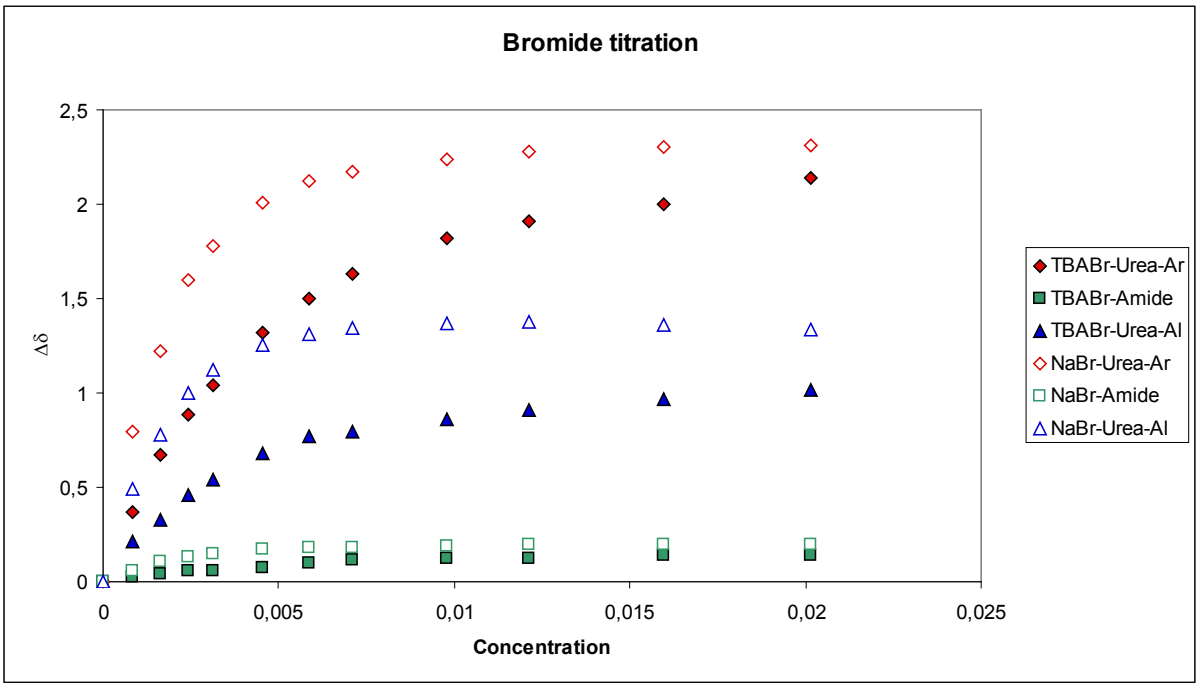




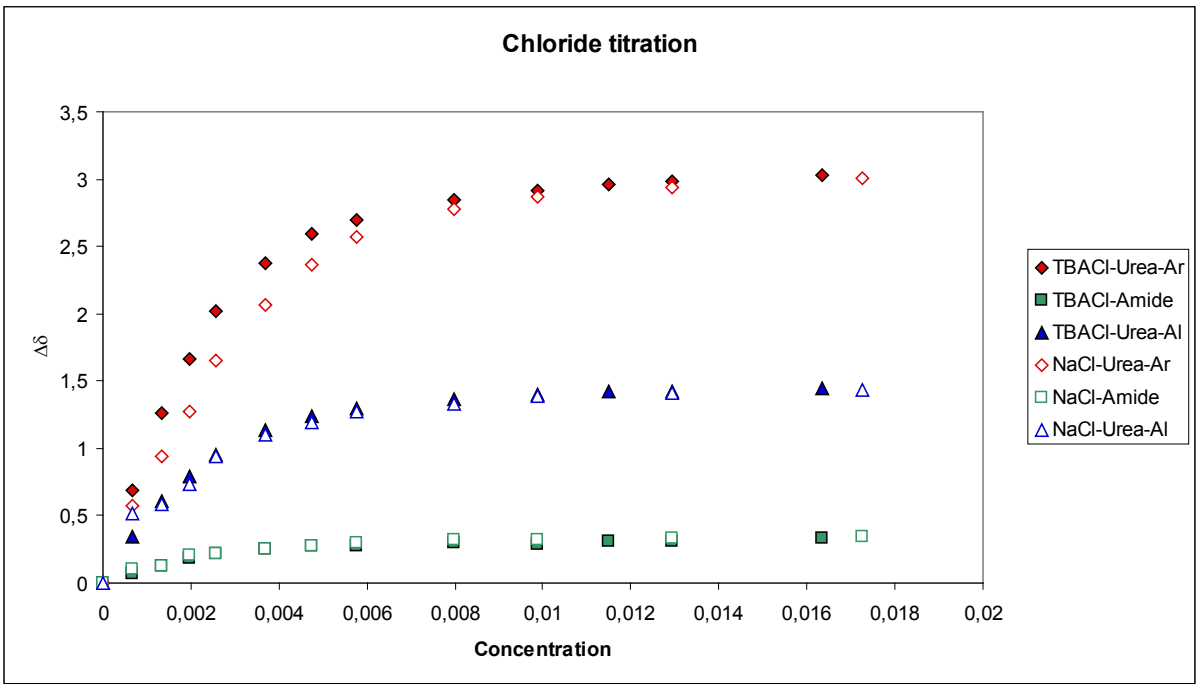
	K_{TBA}	K_{Na}	K_{Na}/K_{TBA}
NO_2^-	1 180	7 590	6,43



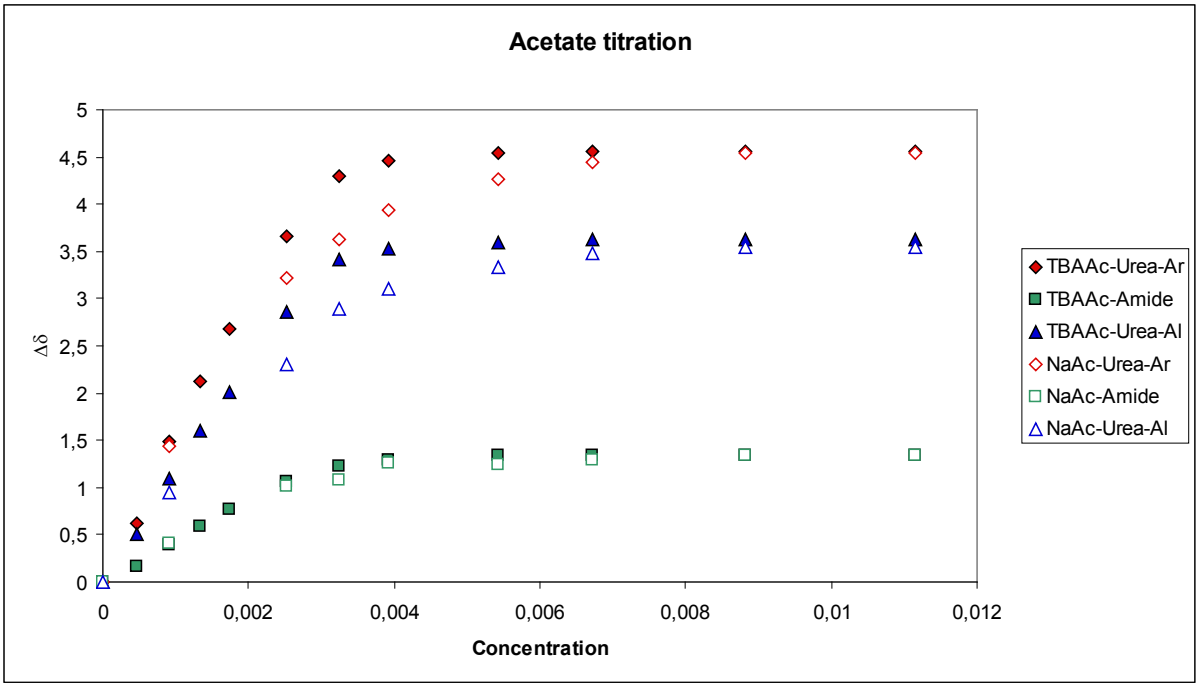
	K_{TBA}	K_{Na}	K_{Na}/K_{TBA}
NO_3^-	110	850	7,73



	K_{TBA}	K_{Na}	K_{Na}/K_{TBA}
Br^-	320	3 310	10,34



	K_{TBA}	K_{Na}	K_{Na}/K_{TBA}
Cl^-	2 040	930	0,46



	K_{TBA}	K_{Na}	K_{Na}/K_{TBA}
Cl^-	10 710	2 340	0,22

Figure S3. Selected binding isotherms.

MOLECULAR MODELING

The structure of **1** was prepared manually in Maestro (Maestro, version 9.3, Schrödinger, LLC, New York, NY, 2012) using the crystal structure of the corresponding crown ether. This structure was subject to a conformational search using MacroModel (MacroModel, version 9.9, Schrödinger, LLC, New York, NY, 2012). We have used systematic torsional sampling method on all rotatable bonds of this molecule and requested 10,000 hits. In this step we obtained a total of 514 conformations of **1**. We have selected the best 20 conformations by OPLS energy; the range of the energies of these 20 conformers was 9.7 kJ/mol. The coordinates of all selected conformers of **1** are presented below.

For each of the 20 conformers of **1** we have additionally built complexes with Na^+, NO_2^- as well as complexes with both ions, to obtain 80 different systems. For these complexes, the ions were placed manually with the Na^+ cation always close to the crown ether group and the NO_2^- anion close to the urea group.

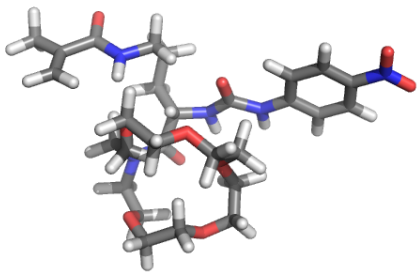
Geometry optimization calculations for the conformer of **1** and its complexes with ions were performed using a two-step approach and utilizing the M06-2X functional[3], as implemented in Gaussian09 software[4]. In the first step we optimized the structures of all 20 conformers using a small 3-21+G* basis set and no solvent model. In the second step for each system we chose either five lowest-energy conformers or all conformers within 10 kcal/mol of the best one and for these conformers we performed DFT calculations using the same M06-2X functional, but the 6-31+G* basis set and in the proper solvent (acetonitrile, modeled using the polarizable continuum method[5]).

[3] Zhao, Y. and Truhlar, D. G. (2008) The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06 Functionals and Twelve Other Functionals, Theor. Chem. Acc. 120, 215.

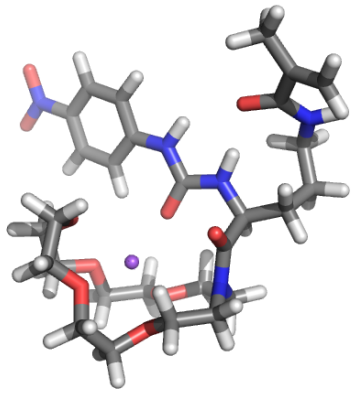
[4] Gaussian 09, Revision C.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[5] Miertuš, S.; Scrocco, E.; Tomasi, J. "Electrostatic Interaction of a Solute with a Continuum. A Direct Utilization of ab initio Molecular Potentials for the Prevision of Solvent Effects," Chem. Phys., 55 (1981) 117-29.

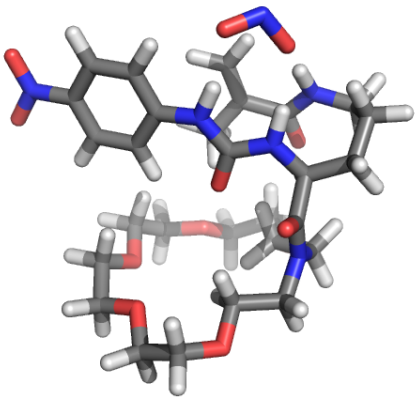
Optimized structure of 1



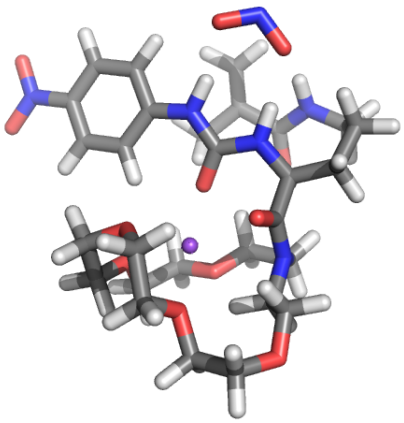
Optimized structure of 1•Na$^+$



Optimized structure of 1•NO$_2^-$



Optimized structure of 1•NaNO$_2$



Cartesian coordinates for the optimized structure of 1.

C	2.738407	3.698879	-1.436563
O	2.948439	3.683724	-0.032971
C	2.221505	4.663033	0.688548
C	0.773933	4.280934	0.935212
O	0.015349	4.486170	-0.245478
C	-1.316752	4.005080	-0.186436
C	-1.430287	2.549208	-0.616303
O	-0.892217	1.638333	0.328776
C	-1.764540	1.313055	1.404943
C	-1.012645	1.393590	2.715547
O	0.038969	0.448971	2.686727
C	1.165098	0.809412	3.450481
C	2.291631	-0.155762	3.129010
O	2.543011	-0.291184	1.738515
C	2.685034	0.932102	1.028478
C	3.399796	0.611007	-0.294720
N	2.811888	1.230219	-1.480659
C	3.403695	2.461704	-2.007588
H	3.188620	4.602474	-1.875258
H	1.669122	3.687253	-1.667487
H	2.274037	5.634713	0.175638
H	2.723702	4.756419	1.656212
H	0.726988	3.229979	1.240256
H	0.364244	4.901910	1.748167
H	-1.899996	4.619244	-0.880906
H	-1.730715	4.150980	0.824071
H	-2.485945	2.310411	-0.820940
H	-0.854441	2.409283	-1.539950
H	-2.144949	0.294405	1.254497
H	-2.618024	2.003238	1.442768
H	-0.606866	2.407193	2.844119
H	-1.692958	1.187412	3.554710
H	0.954769	0.765672	4.530357
H	1.462238	1.842422	3.211759
H	3.202231	0.181715	3.645488
H	2.040663	-1.161650	3.476396
H	3.265015	1.648140	1.623596
H	1.693618	1.360508	0.832982
H	4.444381	0.926178	-0.252677
H	3.410730	-0.474193	-0.421137
H	3.301176	2.462782	-3.094998
H	4.467495	2.453983	-1.756970
C	1.652345	0.809246	-2.032758
O	1.112621	1.412092	-2.967661
C	1.027804	-0.500254	-1.525128
H	1.048481	-0.539404	-0.429822
H	-0.547788	0.185321	-2.690845
N	-0.363153	-0.483246	-1.947686
C	1.775800	-1.702371	-2.136870
H	2.854519	-1.598562	-1.973529
H	1.620196	-1.664473	-3.221975
C	1.306960	-3.055491	-1.602061
H	1.847734	-3.841353	-2.138622
H	0.239761	-3.190761	-1.817146
C	1.503509	-3.249414	-0.092175
H	1.302676	-4.296425	0.160839
H	0.793735	-2.627761	0.457848
H	2.918105	-2.044398	0.933785
N	2.833606	-2.895052	0.383767
C	3.919119	-3.644309	0.106093
O	3.847911	-4.673515	-0.574655
C	5.252514	-3.185754	0.644908
C	5.365926	-2.281480	1.623611
C	6.442130	-3.858057	0.018282
H	6.403792	-4.939397	0.182398
H	6.452780	-3.701009	-1.064894
H	7.370573	-3.468545	0.441108
H	6.345513	-1.988306	1.992120
H	4.513284	-1.805969	2.100126
C	-1.363850	-0.870652	-1.113585
O	-1.187068	-1.550014	-0.107920
H	-2.661010	0.134224	-2.356674
N	-2.624349	-0.452206	-1.530974
C	-6.401424	-1.206585	0.052008
C	-5.305807	-1.831702	0.640045
C	-4.032101	-1.603871	0.140016
C	-3.856806	-0.739689	-0.958016
C	-4.983922	-0.119056	-1.534621
C	-6.253168	-0.350133	-1.038571
H	-5.449970	-2.497237	1.484088
H	-3.178246	-2.088063	0.591042
H	-4.855209	0.549924	-2.381843
H	-7.118233	0.126290	-1.485031
O	-8.684500	-0.918568	0.034268
N	-7.731044	-1.452850	0.585651
O	-7.838498	-2.182089	1.563514

Cartesian coordinates for the optimized structure of 1•Na$^+$.

Na	-1.654341	-1.385653	0.178523
C	-0.792210	-4.185207	1.372725
O	-1.895155	-3.843576	0.548558
C	-3.162392	-4.083527	1.132740
C	-3.379927	-3.262501	2.391341
O	-2.966198	-1.940131	2.100200
C	-3.435943	-0.973266	3.021297
C	-2.693422	0.317199	2.729162
O	-2.687141	0.626332	1.345426
C	-3.943336	0.978114	0.780641
C	-4.460057	-0.121581	-0.129993
O	-3.411577	-0.426196	-1.036301
C	-3.772607	-1.324807	-2.070241
C	-2.519639	-1.635829	-2.853508
O	-1.638605	-2.382728	-2.027322
C	-0.374636	-2.553707	-2.641027
C	0.464791	-3.584824	-1.895778
N	0.715202	-3.353305	-0.463220
C	0.399325	-4.446598	0.470842
H	-1.007345	-5.101974	1.940287
H	-0.579836	-3.375710	2.082997
H	-3.287262	-5.151943	1.357359
H	-3.892193	-3.796305	0.370523
H	-4.444767	-3.287013	2.660897
H	-2.800676	-3.648180	3.242167
H	-3.232823	-1.287563	4.054377
H	-4.523785	-0.856410	2.905444
H	-3.124920	1.141062	3.313543
H	-1.640072	0.205636	3.003236
H	-3.782876	1.886739	0.192483
H	-4.681286	1.200806	1.561343
H	-4.734004	-1.024355	0.434976
H	-5.345139	0.237146	-0.673835
H	-4.521871	-0.865615	-2.728959
H	-4.195717	-2.246299	-1.644137
H	-2.771228	-2.214717	-3.752554
H	-2.036584	-0.696302	-3.159800
H	0.116070	-1.577418	-2.713357
H	-0.508077	-2.945289	-3.660669
H	-0.059268	-4.539594	-1.958127
H	1.410822	-3.707468	-2.438913
H	1.276168	-4.635624	1.097839
H	0.203995	-5.339655	-0.125882
C	1.507738	-2.364623	0.033863
O	1.670362	-2.220388	1.245091
C	2.303113	-1.474255	-0.930671
H	1.953377	-1.586770	-1.958286
H	2.995676	0.409890	-0.173078
N	2.184895	-0.085873	-0.546980
C	3.772639	-1.919267	-0.858961
H	3.787604	-3.012138	-0.937163
H	4.165172	-1.679653	0.138259
C	4.678203	-1.356645	-1.960143
H	4.202121	-1.501215	-2.937558
H	5.598894	-1.951383	-1.972226
C	5.076384	0.120092	-1.843540
H	4.210906	0.785121	-1.871689
H	5.714656	0.382233	-2.692490
H	6.789032	0.109628	-0.584303
N	5.821439	0.407383	-0.622154
C	5.348738	1.116347	0.416690
O	4.206769	1.611474	0.431650
C	6.263083	1.295145	1.593521
C	7.056141	0.297386	1.995329
C	6.140083	2.612359	2.306031
H	6.821166	2.652929	3.158949
H	6.369229	3.444238	1.630802
H	5.115640	2.756928	2.662539
H	7.688799	0.408177	2.871857
H	7.081750	-0.665278	1.491211
C	0.982882	0.521225	-0.505782
O	-0.065137	-0.056550	-0.817851
H	1.956968	2.168644	0.206988
N	1.040860	1.840029	-0.090307
C	-1.789960	4.874614	-0.397280
C	-2.091373	3.633997	-0.951533
C	-1.184244	2.590488	-0.842233
C	0.046417	2.807089	-0.197063
C	0.329893	4.071943	0.353314
C	-0.584085	5.105844	0.261995
H	-3.034085	3.487262	-1.467190
H	-1.429107	1.615507	-1.242417
H	1.277181	4.238481	0.858066
H	-0.370746	6.077801	0.691975
O	-2.495670	7.023269	0.030502
N	-2.760227	5.953379	-0.500480
O	-3.800468	5.741660	-1.110914

Cartesian coordinates for the optimized structure of 1•NO$_2^-$.

C	-3.793849	-0.535826	-0.015012
C	-4.661945	-1.589202	-0.290142
C	-4.212964	-2.755473	-0.911572
C	-2.879344	-2.860640	-1.257363
C	-1.976813	-1.806326	-0.991676
C	-2.457673	-0.637858	-0.364974
N	-6.058423	-1.468794	0.076167
O	-6.810750	-2.400162	-0.184855
N	-0.659909	-1.996684	-1.367393
C	0.407967	-1.172801	-1.045261
O	0.284115	-0.042474	-0.571323
N	1.628617	-1.701712	-1.322506
C	2.791695	-0.955190	-0.881485
C	4.095865	-1.706509	-1.168472
C	4.229118	-3.097400	-0.531778
C	3.891465	-3.167296	0.961250
N	2.452120	-3.225106	1.184402
C	1.780388	-2.335311	1.943545
C	0.272721	-2.408373	1.949445
C	-0.412049	-1.195805	2.519380
C	2.816010	0.384958	-1.637746
O	2.565808	0.408080	-2.843456
N	3.143373	1.512094	-0.956287
C	3.016691	2.777913	-1.677942
C	1.554358	3.158429	-1.890491
O	1.536783	4.353472	-2.655026
C	0.336669	4.588185	-3.364704
C	-0.803239	5.097970	-2.507064
O	-1.270698	4.063045	-1.665490
C	-2.454778	4.419956	-0.981515
C	-2.822571	3.317016	-0.016578
O	-1.939996	3.357672	1.088880
C	-2.273003	2.399371	2.073762
C	-1.390524	2.590548	3.284085
O	-0.086967	2.149727	2.978006
C	0.823476	2.349494	4.040190
C	2.083987	1.552606	3.774684
O	2.844987	2.025792	2.675614
C	2.315768	1.708995	1.396270
C	3.509623	1.552047	0.458644
O	2.355919	-1.461055	2.604644
C	-0.398570	-3.471120	1.492920
O	-6.431786	-0.434514	0.617101
O	-0.417465	-4.755439	-2.289919
N	0.500745	-5.365043	-1.716017
O	1.388610	-4.638257	-1.206006
H	1.042220	2.354386	-2.433492
H	1.043021	3.301095	-0.931418
H	0.022610	3.670747	-3.884643
H	0.570951	5.350123	-4.114120
H	-0.470093	5.955195	-1.902266
H	-1.615284	5.438219	-3.169512
H	-3.273956	4.569562	-1.701662
H	-2.307196	5.358621	-0.425314
H	-3.863102	3.456534	0.323623
H	-2.751588	2.343186	-0.529939
H	-2.130242	1.378617	1.681988
H	-3.328735	2.513026	2.370444
H	-1.382587	3.652395	3.575840
H	-1.793815	2.003984	4.124751
H	0.381661	1.994018	4.985318
H	1.050533	3.421785	4.147224
H	2.736624	1.634728	4.650229
H	1.831726	0.496515	3.617341
H	1.651381	2.510117	1.047357
H	1.730502	0.782891	1.437566
H	4.182886	2.403803	0.596938
H	4.082111	0.659585	0.727680
H	3.506008	2.687479	-2.652017
H	3.529428	3.553605	-1.103103
H	2.705285	-0.771508	0.194098
H	1.695436	-2.705930	-1.493802
H	4.914944	-1.071354	-0.806434
H	4.219250	-1.789888	-2.254844
H	5.268233	-3.420018	-0.662688
H	3.614503	-3.830829	-1.067773
H	4.272895	-2.292516	1.496453
H	4.358816	-4.055401	1.401813
H	1.926888	-3.835039	0.562912
H	-0.129027	-1.040326	3.567103
H	-0.122835	-0.289589	1.976629
H	-1.498988	-1.309136	2.455868
H	-1.486487	-3.483234	1.509922
H	0.082192	-4.357129	1.085968
H	-0.435045	-2.940683	-1.713012
H	-4.904737	-3.565316	-1.113349
H	-2.509258	-3.765313	-1.730869
H	-1.772393	0.169902	-0.154380
H	-4.169745	0.358565	0.471245

Cartesian coordinates for the optimized structure of 1•NaNO$_2$.

C	-2.733998	3.131129	0.260139
C	-4.087157	3.214098	-0.056424
C	-4.743130	2.181847	-0.725919
C	-4.027931	1.049210	-1.070406
C	-2.659239	0.935081	-0.751322
C	-2.014179	1.997547	-0.086881
N	-4.833002	4.403821	0.318391
O	-6.024536	4.452595	0.041857
N	-2.028708	-0.243222	-1.137676
C	-0.853001	-0.732203	-0.622805
O	-0.150701	-0.091722	0.175102
N	-0.496859	-1.973444	-1.040507
C	0.566480	-2.645868	-0.311169
C	0.877239	-4.036499	-0.879225
C	-0.279182	-5.044003	-0.845879
C	-1.028202	-5.127047	0.490580
N	-2.047579	-4.091403	0.596452
C	-2.080580	-3.143092	1.553813
C	-3.156124	-2.091717	1.433467
C	-2.881147	-0.817946	2.184408
C	1.849414	-1.810954	-0.391946
O	2.107290	-1.162695	-1.411317
N	2.705550	-1.848878	0.662648
C	3.968651	-1.095899	0.596548
C	4.811369	-1.231816	-0.672996
O	6.075541	-0.637860	-0.402054
C	6.246618	0.681727	-0.889297
C	5.355612	1.732805	-0.234643
O	4.040392	1.774072	-0.796653
C	3.939327	2.712097	-1.861467
C	2.581217	2.570618	-2.517865
O	1.504874	2.631719	-1.591873
C	1.296842	3.878764	-0.935863
C	1.836186	3.852362	0.484563
O	1.273005	2.713660	1.118267
C	1.657219	2.557712	2.476254
C	1.143654	1.220451	2.955797
O	1.892147	0.187528	2.330222
C	1.361559	-1.098078	2.633046
C	2.264122	-2.173119	2.029451
O	-1.261872	-3.091772	2.481524

C	-4.277750	-2.291870	0.733140
O	-4.239269	5.305354	0.895749
Na	1.856636	0.879150	-0.121443
O	-3.940762	-1.731625	-2.719197
N	-3.903819	-2.971161	-2.630675
O	-2.854519	-3.440757	-2.125565
H	4.982182	-2.291013	-0.895150
H	4.347320	-0.755643	-1.537011
H	6.098213	0.701937	-1.979524
H	7.291113	0.929849	-0.681850
H	5.251563	1.528011	0.835382
H	5.820067	2.721133	-0.342639
H	4.713928	2.529690	-2.618295
H	4.088242	3.726727	-1.464157
H	2.467157	3.344307	-3.287937
H	2.495916	1.588487	-2.992223
H	0.213887	4.035897	-0.909196
H	1.754143	4.699679	-1.501336
H	2.932308	3.774271	0.505042
H	1.537833	4.770316	1.009775
H	1.226041	3.365246	3.082219
H	2.753238	2.595679	2.561296
H	1.250711	1.150385	4.046588
H	0.080185	1.116407	2.693782
H	0.342424	-1.168841	2.237101
H	1.322093	-1.242432	3.722260
H	3.169353	-2.282886	2.628870
H	1.747000	-3.136146	2.059765
H	4.589260	-1.463866	1.417009
H	3.786115	-0.038565	0.812885
H	0.263456	-2.749030	0.734472
H	-1.199286	-2.536219	-1.528966
H	1.708987	-4.436154	-0.285213
H	1.243021	-3.927518	-1.907270
H	0.141125	-6.030375	-1.070027
H	-1.001997	-4.833505	-1.642664
H	-0.348747	-5.015834	1.341085
H	-1.511434	-6.106103	0.578799
H	-2.641024	-3.966225	-0.220538
H	-2.792579	-1.016224	3.257709
H	-1.935307	-0.367400	1.861412
H	-3.685695	-0.095421	2.020659
H	-5.031954	-1.511584	0.664782
H	-4.499849	-3.223706	0.220906
H	-2.608254	-0.888668	-1.695669
H	-5.796940	2.267043	-0.963920
H	-4.521434	0.230543	-1.585828
H	-0.965046	1.935644	0.167644
H	-2.245440	3.951479	0.774303

Cartesian coordinates for the 20 starting conformers of 1.

C	4.07850	5.16220	-7.21340
O	4.41520	6.19460	-8.12860
C	4.67100	5.74330	-9.45510
C	3.38120	5.53400	-10.26250
O	2.78240	4.28790	-9.93440
C	1.63130	4.02620	-10.72620
C	1.01900	2.67970	-10.32690
O	0.34730	2.80720	-9.08060
C	-0.27190	1.59240	-8.67830
C	-1.09960	1.83220	-7.41040
O	-0.24300	1.92450	-6.27940
C	-0.96600	2.19100	-5.08450
C	-0.03340	2.14440	-3.86420
O	0.70950	3.34850	-3.70200
C	1.88330	3.42300	-4.49910
C	2.66480	4.67640	-4.07240
N	3.97850	4.76320	-4.73420
C	4.07980	5.77370	-5.80170
H	4.80530	4.35590	-7.29290
H	3.09890	4.74080	-7.44150
H	5.30670	4.85750	-9.47380
H	5.24520	6.53340	-9.93990
H	2.68780	6.35960	-10.09390
H	3.63250	5.53670	-11.32460
H	1.92140	3.98650	-11.77750
H	0.89310	4.82330	-10.62330
H	0.30300	2.37700	-11.09290
H	1.78740	1.90850	-10.28210
H	0.47000	0.80890	-8.51480
H	-0.93890	1.24690	-9.47010
H	-1.70710	2.73220	-7.52050
H	-1.78550	0.99510	-7.26980
H	-1.73710	1.42880	-4.95870
H	-1.47440	3.15490	-5.14110
H	-0.65380	2.04780	-2.97270
H	0.60790	1.26150	-3.87980
H	1.63170	3.48100	-5.55850
H	2.48730	2.52620	-4.35280
H	2.05400	5.55840	-4.26450
H	2.80430	4.66880	-2.98960
H	4.97220	6.38070	-5.64590
H	3.26580	6.49600	-5.74230
C	5.01650	4.00720	-4.28620
O	4.89420	3.24410	-3.32180
C	6.39800	4.04510	-4.98700
H	6.49400	4.88360	-5.67350
H	7.95020	3.29430	-3.75740
N	7.46350	4.14700	-3.98730
C	6.59050	2.72690	-5.77060
H	5.67060	2.49420	-6.30850
H	6.73920	1.89130	-5.08440
C	7.75400	2.79300	-6.78010
H	8.68760	2.99660	-6.25400
H	7.60230	3.63950	-7.45160
C	7.92590	1.51070	-7.61700
H	8.22190	0.68470	-6.96920
H	8.73470	1.63720	-8.33910
H	6.16350	0.36520	-7.91980
N	6.69610	1.13230	-8.30700
C	6.18970	1.71450	-9.40230
O	6.78580	2.61410	-9.99650
C	4.90220	1.16090	-9.82080
C	4.05320	0.61260	-8.92490
C	4.55710	1.22710	-11.29770
H	4.44260	2.26550	-11.61120
H	5.35030	0.77530	-11.89460
H	3.62810	0.70120	-11.51880
H	3.10890	0.19700	-9.24330
H	4.26150	0.56480	-7.86550
C	7.74910	5.25700	-3.30210
O	7.16380	6.32360	-3.49810
H	9.17900	4.16400	-2.43450
N	8.73460	5.07020	-2.41330
C	10.52530	7.72140	0.41520
C	11.19660	6.57080	-0.05830
C	10.58530	5.71330	-0.99420
C	9.29320	5.99200	-1.48600
C	8.61000	7.13460	-1.00530
C	9.22410	7.98970	-0.06850
H	12.18970	6.33930	0.29860
H	11.12530	4.84050	-1.33450
H	7.60820	7.37290	-1.33130
H	8.68540	8.85760	0.28330
O	10.54520	9.60930	1.78500
N	11.16760	8.62080	1.39780
O	12.30030	8.34740	1.79150
C	3.37080	6.38440	-5.24930
O	2.86700	7.16490	-6.32220
C	3.84760	7.51430	-7.29350
C	3.14860	7.69060	-8.64530
O	2.84790	6.39840	-9.15410
C	2.04360	6.43450	-10.32390
C	1.89020	5.00670	-10.86180
O	1.13160	4.22970	-9.94320
C	0.97500	2.88490	-10.37660
C	0.22510	2.07770	-9.30910
O	1.07590	1.84740	-8.19310
C	0.43610	1.08970	-7.17400
C	1.38910	0.89600	-5.98780
O	1.62440	2.15310	-5.37060
C	2.35640	2.05110	-4.15850
C	2.73220	3.46910	-3.69910
N	3.79840	4.03570	-4.54010
C	3.32360	4.89360	-5.63400
H	2.72640	6.54960	-4.38510
H	4.36870	6.71310	-4.95520
H	4.63690	6.76600	-7.38490
H	4.32530	8.44490	-6.98470
H	2.24890	8.29820	-8.53270
H	3.80940	8.20700	-9.34320
H	2.52070	7.05770	-11.08220
H	1.06700	6.87060	-10.10800
H	1.38150	5.03360	-11.82690
H	2.87360	4.56240	-11.02460
H	1.94180	2.42630	-10.58610
H	0.40450	2.87320	-11.30670
H	-0.68360	2.60140	-9.00760
H	-0.07820	1.11900	-9.73320
H	0.15090	0.11380	-7.57050
H	-0.47760	1.58500	-6.84100
H	0.93420	0.21060	-5.27060
H	2.32820	0.44960	-6.31480
H	3.24810	1.43410	-4.28610
H	1.73450	1.56780	-3.40340
H	1.84990	4.11070	-3.69980
H	3.05310	3.43930	-2.65620
H	2.29690	4.63100	-5.89230
H	3.88280	4.70030	-6.54880
C	5.10120	3.74520	-4.29820
O	5.44180	3.06370	-3.32480
C	6.20930	4.23420	-5.26820
H	5.91540	5.16730	-5.74690
H	8.20490	3.84530	-4.67720
N	7.45990	4.51310	-4.55520
C	6.48330	3.18100	-6.37330
H	7.18980	3.60070	-7.09070
H	5.56310	3.02240	-6.93740
C	7.01690	1.81270	-5.88590
H	6.30730	1.35270	-5.19790
H	7.93270	1.95530	-5.31190
C	7.31670	0.81860	-7.02320
H	7.71240	-0.11140	-6.61080
H	8.09810	1.22010	-7.66960
H	6.12410	0.91420	-8.77800
N	6.14400	0.52920	-7.84360
C	5.11120	-0.25290	-7.49970
O	5.05560	-0.81310	-6.40370
C	4.10460	-0.40350	-8.55070
C	3.92870	0.54320	-9.49630
C	3.26470	-1.66860	-8.54210
H	3.90490	-2.54860	-8.61330
H	2.69090	-1.73900	-7.61750
H	2.56300	-1.69180	-9.37630
H	3.18810	0.40970	-10.27050
H	4.49480	1.46320	-9.52890
C	7.63130	5.51220	-3.68430
O	6.75870	6.35360	-3.46250
H	9.48560	4.79790	-3.47270
N	8.84670	5.49510	-3.11960
C	10.63070	8.02540	-0.17830
C	9.22220	7.95100	-0.27510
C	8.60570	7.12770	-1.23850
C	9.39140	6.36480	-2.13550
C	10.79660	6.42510	-2.03130
C	11.40960	7.24970	-1.06740
H	8.60360	8.52680	0.39790
H	7.52650	7.09170	-1.26110
H	11.42130	5.84300	-2.69480
H	12.48800	7.28350	-1.01200
O	12.50360	8.92370	0.88290
N	11.27440	8.89100	0.83340
O	10.55720	9.54630	1.58770
C	1.53180	1.68590	-4.05290

O	1.22080	3.07190	-4.08060
C	1.16930	3.63090	-2.77290
C	0.92260	5.14250	-2.85010
O	2.08480	5.77510	-3.36590
C	2.03380	7.19240	-3.27720
C	3.23420	7.77900	-4.03000
O	2.97600	7.69700	-5.42350
C	4.10550	8.02560	-6.22020
C	3.68970	7.93410	-7.69240
O	3.41110	6.57490	-7.99710
C	2.74660	6.40730	-9.23940
C	2.39820	4.92510	-9.44010
O	1.34220	4.52890	-8.56510
C	1.76850	3.94250	-7.33880
C	2.05130	2.44250	-7.54710
N	2.59870	1.80480	-6.33820
C	1.60210	1.12640	-5.48720
H	0.75930	1.15000	-3.49890
H	2.46640	1.51830	-3.51680
H	2.09540	3.43680	-2.22870
H	0.36050	3.15960	-2.21210
H	0.05300	5.36380	-3.47080
H	0.71310	5.51910	-1.84740
H	2.07830	7.48450	-2.22680
H	1.10110	7.58480	-3.68620
H	3.37310	8.82560	-3.75480
H	4.14700	7.24640	-3.75940
H	4.93790	7.35010	-6.01510
H	4.43860	9.03920	-5.99180
H	2.81770	8.56750	-7.86510
H	4.49050	8.29630	-8.33860
H	3.39970	6.74600	-10.04530
H	1.83730	7.00920	-9.28210
H	2.03320	4.79500	-10.45930
H	3.28390	4.29480	-9.35230
H	0.95870	4.05310	-6.61710
H	2.62240	4.46940	-6.91340
H	1.13120	1.94890	-7.86080
H	2.72210	2.28640	-8.39080
H	1.83940	0.06180	-5.44820
H	0.60360	1.18410	-5.92070
C	3.92710	1.72620	-6.06530
O	4.36130	1.04830	-5.12750
C	4.95750	2.46220	-6.95990
H	4.50740	3.32120	-7.45390
H	6.95720	2.48840	-6.24860
N	6.06550	2.96080	-6.14710
C	5.51870	1.47810	-8.01600
H	4.68280	0.93410	-8.45920
H	6.12800	0.70750	-7.54140
C	6.28320	2.14040	-9.18490
H	5.68580	2.95830	-9.59010
H	6.35890	1.41360	-9.99500
C	7.70350	2.65590	-8.87600
H	7.67310	3.49400	-8.17900
H	8.13820	3.06230	-9.79010
H	8.88870	0.90690	-9.08770
N	8.58490	1.58910	-8.40610
C	9.08310	1.44690	-7.17020
O	8.81810	2.23890	-6.26370
C	9.97460	0.29920	-7.02310
C	9.78330	-0.82590	-7.74320
C	11.11890	0.42350	-6.03400
H	11.74880	1.27680	-6.28820
H	10.73380	0.57380	-5.02460
H	11.74460	-0.46940	-6.02800
H	10.44950	-1.66950	-7.63570
H	8.96880	-0.94370	-8.44430
C	5.99550	3.96080	-5.26880
O	4.96330	4.59670	-5.06460
H	7.94910	3.63600	-5.03170
N	7.17540	4.18890	-4.67820
C	8.33330	7.02970	-1.71220
C	9.27280	6.44740	-2.59400
C	8.86590	5.51260	-3.56650
C	7.50940	5.14760	-3.68510
C	6.56610	5.71330	-2.79460
C	6.97620	6.64850	-1.82380
H	10.31690	6.71680	-2.52640
H	9.60800	5.08330	-4.22570
H	5.52220	5.43720	-2.82980
H	6.23940	7.07060	-1.15600
O	7.90960	8.49480	0.05250
N	8.76150	8.01130	-0.69230
O	9.95330	8.30820	-0.62670
C	2.32470	1.69430	-3.33790
O	1.92880	3.00280	-3.72520
C	1.61100	3.81650	-2.60180
C	1.27100	5.24080	-3.05730
O	2.45310	5.87110	-3.52910
C	2.28290	7.26060	-3.77390
C	3.54070	7.80170	-4.46490
O	3.51570	7.40000	-5.82650
C	4.72390	7.69140	-6.51520
C	4.56690	7.23170	-7.96880
O	4.47240	5.81470	-7.98320
C	4.07350	5.29450	-9.24140
C	3.88970	3.77460	-9.12880
O	2.71830	3.46030	-8.37520
C	2.94260	3.21730	-6.98920
C	3.41030	1.76410	-6.78630
N	3.77790	1.47680	-5.38900
C	2.70590	0.86540	-4.58000
H	1.50100	1.20230	-2.81790
H	3.15080	1.74280	-2.62790
H	2.44130	3.84530	-1.89390
H	0.75450	3.38870	-2.07810
H	0.50320	5.22830	-3.83240
H	0.87010	5.79810	-2.20880
H	2.13570	7.77320	-2.82200
H	1.40130	7.45290	-4.38800
H	3.55350	8.89150	-4.41570
H	4.43640	7.44130	-3.95670
H	5.57180	7.18940	-6.04600
H	4.91800	8.76480	-6.48510
H	3.67940	7.69320	-8.40530
H	5.42610	7.54670	-8.56280
H	4.84080	5.52010	-9.98380
H	3.14450	5.75540	-9.58130
H	3.74400	3.37040	-10.13110
H	4.78990	3.29970	-8.73780
H	1.99680	3.36140	-6.46610
H	3.63480	3.94110	-6.55980
H	2.62410	1.08850	-7.12440
H	4.24050	1.53330	-7.44970
H	3.02330	-0.13090	-4.26750
H	1.80280	0.71000	-5.17050
C	5.03250	1.63330	-4.89080
O	5.34710	1.21500	-3.77120
C	6.13170	2.32500	-5.73700
H	5.68670	3.04090	-6.42640
H	7.93850	2.60210	-4.66110
N	7.06240	3.05490	-4.87090
C	6.92390	1.26300	-6.53090
H	6.21970	0.59670	-7.02790
H	7.49310	0.61840	-5.85900
C	7.86470	1.89090	-7.58090
H	8.75780	2.27280	-7.08450
H	7.38780	2.76300	-8.03040
C	8.28020	0.92390	-8.70590
H	8.80190	0.06330	-8.28550
H	8.98700	1.41250	-9.37920
H	6.79940	-0.48980	-9.27860
N	7.12490	0.44930	-9.46400
C	6.42760	1.15730	-10.36320
O	6.77100	2.28590	-10.71790
C	5.25020	0.45890	-10.87270
C	4.54540	-0.37670	-10.08100
C	4.85080	0.71160	-12.31480
H	4.59700	1.76240	-12.45960
H	5.67460	0.46450	-12.98540
H	3.98730	0.11200	-12.60390
H	3.67720	-0.89520	-10.46090
H	4.80160	-0.56270	-9.04750
C	6.76060	4.20120	-4.25490
O	5.69250	4.78390	-4.43290
H	8.60850	4.11340	-3.49040
N	7.74560	4.63640	-3.45720
C	7.94660	8.05000	-0.90050
C	9.11030	7.44750	-1.43160
C	9.01950	6.32290	-2.27550
C	7.76250	5.78220	-2.61580
C	6.59430	6.37000	-2.07360
C	6.68870	7.49500	-1.23050
H	10.08430	7.84830	-1.19080
H	9.92850	5.88490	-2.66430
H	5.61300	5.96880	-2.28240
H	5.78420	7.92970	-0.83040
O	7.00460	9.72430	0.42220
N	8.04350	9.23050	-0.01510
O	9.15890	9.67520	0.25100
C	4.26970	5.63230	-6.96990
O	4.48970	6.84860	-7.66970
C	4.70180	6.69430	-9.07000
C	3.40600	6.40570	-9.84420
O	3.06140	5.03100	-9.73480
C	1.96570	4.68450	-10.57110
C	1.59990	3.21180	-10.35810
O	0.86900	3.07250	-9.14790
C	0.46200	1.73040	-8.91570
C	-0.44130	1.68360	-7.67860
O	0.35120	1.79400	-6.50470
C	-0.43940	1.89340	-5.32830
C	0.45140	1.82620	-4.07810
O	1.11780	3.05700	-3.81120
C	2.28310	3.27560	-4.59550
C	3.03410	4.47790	-3.99830
N	4.34010	4.70320	-4.64470
C	4.42490	5.91970	-5.47040
H	4.99210	4.88540	-7.28870
H	3.27460	5.23950	-7.18180
H	5.46950	5.94870	-9.28370
H	5.10150	7.64510	-9.42390
H	2.59440	7.04320	-9.49000
H	3.57100	6.64930	-10.89530
H	2.25310	4.83420	-11.61320
H	1.10130	5.32230	-10.37830
H	0.98330	2.87470	-11.19310
H	2.49670	2.59330	-10.34610
H	1.32480	1.07450	-8.79070
H	-0.10150	1.36680	-9.77670
H	-1.18980	2.47650	-7.72970
H	-0.97710	0.73320	-7.65640
H	-1.14250	1.05900	-5.29840
H	-1.02910	2.81140	-5.33090
H	-0.19120	1.63390	-3.21840
H	1.14640	0.98620	-4.12560
H	2.01940	3.47730	-5.63400
H	2.91160	2.38400	-4.58420
H	2.39190	5.35620	-4.06140
H	3.18600	4.31970	-2.92880
H	5.36360	6.43930	-5.28250
H	3.66830	6.64660	-5.17480
C	5.38770	3.88380	-4.35950
O	5.27850	2.96220	-3.54350
C	6.77320	4.06300	-5.03540
H	6.81660	4.90490	-5.72420
H	8.31570	3.43810	-3.73190
N	7.77780	4.25260	-3.98620
C	7.16540	2.77090	-5.80010
H	7.08150	1.90430	-5.14140
H	8.22020	2.82700	-6.07430
C	6.36290	2.50470	-7.08550
H	6.54410	3.31380	-7.79390
H	5.29420	2.50650	-6.86730
C	6.73810	1.16690	-7.74440

H	6.53130	0.33480	-7.06840
H	7.80920	1.13880	-7.94910
H	6.53740	1.17160	-9.85830
N	6.03060	0.97660	-9.00530
C	4.77400	0.53350	-9.14730
O	4.07950	0.21700	-8.18050
C	4.34390	0.42980	-10.54070
C	4.80800	1.28470	-11.47670
C	3.36050	-0.67120	-10.89420
H	3.76920	-1.64520	-10.62280
H	2.42330	-0.53340	-10.35440
H	3.13690	-0.68350	-11.96120
H	4.49270	1.19950	-12.50630
H	5.49770	2.08600	-11.25080
C	7.95400	5.37450	-3.28350
O	7.30710	6.39970	-3.49930
H	9.41470	4.37490	-2.35630
N	8.90790	5.24790	-2.35070
C	10.37940	7.99000	0.57360
C	11.14820	6.89070	0.12740
C	10.64110	6.00190	-0.84110
C	9.35810	6.19760	-1.39300
C	8.57760	7.28810	-0.94010
C	9.08770	8.17480	0.02920
H	12.13650	6.72310	0.53050
H	11.25420	5.16990	-1.15920
H	7.57870	7.46170	-1.31260
H	8.47580	9.00190	0.35900
O	10.20820	9.86510	1.95040
N	10.91250	8.92240	1.59020
O	12.04030	8.72110	2.03790
C	1.69130	2.11130	-4.67990
O	0.43780	1.69480	-4.15420
C	-0.11670	2.57720	-3.18260
C	-0.78770	3.80890	-3.81040
O	0.19080	4.76730	-4.18970
C	-0.39310	5.98880	-4.62210
C	0.69950	6.92530	-5.15000
O	1.10300	6.48960	-6.44150
C	2.04270	7.36960	-7.04390
C	2.32920	6.89850	-8.47410
O	3.19630	5.77330	-8.44370
C	3.40960	5.22340	-9.73680
C	4.51640	4.15940	-9.68480
O	4.06340	2.90220	-9.19270
C	3.83240	2.86100	-7.79140
C	3.79990	1.37950	-7.38160
N	3.66280	1.19680	-5.92730
C	2.29460	0.92520	-5.45180
H	2.35210	2.41920	-3.86850
H	1.56570	2.96750	-5.34340
H	0.61540	2.86220	-2.42520
H	-0.88420	2.00840	-2.65680
H	-1.40200	3.51830	-4.66410
H	-1.45530	4.25420	-3.07050
H	-0.89700	6.46020	-3.77670
H	-1.14610	5.81810	-5.39360
H	0.29370	7.93600	-5.21870
H	1.54680	6.96060	-4.46320
H	2.96320	7.42360	-6.46030
H	1.62270	8.37620	-7.08320
H	1.39510	6.66590	-8.98880
H	2.81270	7.70410	-9.02920
H	3.72720	6.01730	-10.41520
H	2.48720	4.80380	-10.14150
H	4.86570	3.98210	-10.70230
H	5.38290	4.51800	-9.13000
H	2.88550	3.34550	-7.55030
H	4.61590	3.39770	-7.25590
H	2.98810	0.88340	-7.91390
H	4.69610	0.87600	-7.74410
H	2.30890	0.04190	-4.81040
H	1.62690	0.66480	-6.27300
C	4.70590	1.17970	-5.05680
O	4.54230	0.94700	-3.85370

C	6.15330	1.42620	-5.55150
H	6.15980	2.02550	-6.45850
H	7.55270	1.59560	-3.96670
N	6.91410	2.14220	-4.52330
C	6.83150	0.06160	-5.82130
H	6.25620	-0.47660	-6.57620
H	6.77670	-0.55990	-4.92550
C	8.30420	0.11290	-6.28990
H	8.61490	-0.91370	-6.49000
H	8.95190	0.44860	-5.47900
C	8.57030	0.94200	-7.56150
H	7.77980	0.77450	-8.29570
H	9.49910	0.60820	-8.02640
H	9.14330	2.58980	-6.35260
N	8.72560	2.35740	-7.24210
C	8.35450	3.39280	-8.00550
O	7.83430	3.23800	-9.11070
C	8.58370	4.69000	-7.37090
C	9.63420	4.88240	-6.54550
C	7.59420	5.80390	-7.66110
H	7.52780	5.98880	-8.73380
H	6.60310	5.53080	-7.29720
H	7.88550	6.73580	-7.17610
H	9.79220	5.83850	-6.06800
H	10.35980	4.11150	-6.32730
C	6.77630	3.44680	-4.27160
O	5.95690	4.15140	-4.86200
H	8.13510	3.16320	-2.82980
N	7.61530	3.87650	-3.31970
C	8.55070	7.82100	-1.97970
C	8.80810	6.68200	-1.18250
C	8.48520	5.39050	-1.64410
C	7.88780	5.20970	-2.90850
C	7.63900	6.34500	-3.71670
C	7.96490	7.63480	-3.25300
H	9.25990	6.79560	-0.20770
H	8.69850	4.54000	-1.01150
H	7.21000	6.25140	-4.70350
H	7.76560	8.48710	-3.88630
O	8.65100	10.13860	-2.22230
N	8.89150	9.17580	-1.49480
O	9.40280	9.28990	-0.38190
C	1.72640	2.48720	-5.43630
O	0.65790	1.71140	-4.91040
C	0.19830	2.13290	-3.62990
C	-0.78810	3.30750	-3.71690
O	-0.08960	4.53220	-3.89690
C	-0.95970	5.65530	-3.84820
C	-0.16640	6.93860	-4.11810
O	0.12720	7.02850	-5.50610
C	0.77210	8.24940	-5.84330
C	0.97460	8.31720	-7.36110
O	2.05070	7.46940	-7.73980
C	2.26430	7.46920	-9.14500
C	3.53080	6.67100	-9.49140
O	3.30410	5.26560	-9.53620
C	3.20140	4.64180	-8.26390
C	3.30860	3.12400	-8.48720
N	3.47720	2.38370	-7.22660
C	2.25450	1.76410	-6.68690
H	2.51360	2.58900	-4.68800
H	1.38780	3.49080	-5.69570
H	1.02120	2.34720	-2.94600
H	-0.33210	1.28160	-3.20190
H	-1.50760	3.14490	-4.52100
H	-1.35360	3.35430	-2.78450
H	-1.41070	5.71460	-2.85610
H	-1.77390	5.55650	-4.56830
H	-0.77260	7.79560	-3.81950
H	0.74640	6.96250	-3.52040
H	1.72560	8.34840	-5.32170
H	0.14450	9.08720	-5.53430
H	0.05430	8.04290	-7.87980
H	1.21170	9.34430	-7.64370
H	2.40100	8.49770	-9.48400

H	1.39860	7.06850	-9.67480
H	3.84700	6.95950	-10.49430
H	4.36030	6.92780	-8.83040
H	2.25150	4.88870	-7.78820
H	3.99360	4.99640	-7.60410
H	2.42820	2.78290	-9.03220
H	4.13580	2.90260	-9.16220
H	2.46290	0.72050	-6.44310
H	1.46090	1.72370	-7.43300
C	4.67440	2.18650	-6.61500
O	4.77200	1.51260	-5.58320
C	5.97590	2.77350	-7.21940
H	5.77840	3.65570	-7.82540
H	7.69680	2.57300	-5.99730
N	6.88870	3.16720	-6.14820
C	6.66290	1.68760	-8.08400
H	5.91090	1.25110	-8.74400
H	7.00320	0.85660	-7.46420
C	7.80460	2.19620	-8.99380
H	7.46530	3.07630	-9.54190
H	7.99110	1.43910	-9.75690
C	9.14780	2.51470	-8.30560
H	9.05510	3.37780	-7.64580
H	9.87090	2.81480	-9.06510
H	10.07330	0.60780	-8.17800
N	9.69790	1.35400	-7.60840
C	9.80990	1.19480	-6.28250
O	9.42520	2.05380	-5.48650
C	10.44740	-0.05990	-5.89180
C	10.29700	-1.17640	-6.63470
C	11.28180	-0.05640	-4.62410
H	11.74490	-1.02700	-4.44430
H	12.07460	0.68940	-4.69410
H	10.66060	0.18740	-3.76130
H	10.77620	-2.10020	-6.34530
H	9.69780	-1.20750	-7.53420
C	6.73350	4.20900	-5.33180
O	5.78420	4.98870	-5.41970
H	8.47100	3.60540	-4.57170
N	7.73630	4.29430	-4.44820
C	8.55460	7.02930	-1.27460
C	7.25520	6.97380	-1.82920
C	6.95390	6.08400	-2.87970
C	7.95550	5.23220	-3.40370
C	9.24940	5.27660	-2.84480
C	9.54720	6.16760	-1.79500
H	6.47650	7.61660	-1.44490
H	5.94250	6.07080	-3.25770
H	10.02990	4.62850	-3.21970
H	10.54750	6.18590	-1.38720
O	10.01030	7.97600	0.28280
N	8.86700	7.96460	-0.17250
O	7.97250	8.69650	0.24820
C	1.67790	6.00120	-6.27300
O	1.58540	7.21440	-7.01340
C	2.77510	7.59570	-7.70500
C	2.81640	7.00020	-9.12090
O	3.14210	5.61980	-9.05500
C	3.10850	4.98390	-10.32500
C	3.18450	3.46810	-10.11570
O	2.00150	3.05790	-9.44440
C	1.92050	1.65230	-9.26420
C	0.66410	1.33850	-8.44310
O	0.88600	1.69210	-7.08380
C	-0.29490	1.59410	-6.29800
C	0.05610	1.79500	-4.81930
O	0.44950	3.14270	-4.59560
C	0.81980	3.37880	-3.24350
C	1.44850	4.78130	-3.12140
N	2.50700	5.02480	-4.12040
C	2.33750	6.25730	-4.90610
H	2.19180	5.22820	-6.83790
H	0.66510	5.63000	-6.11170
H	3.68450	7.36170	-7.15090
H	2.74820	8.68190	-7.79610

H	1.85670	7.15690	-9.61610
H	3.57470	7.51510	-9.71290
H	3.94930	5.32740	-10.92950
H	2.19360	5.23040	-10.86670
H	3.25820	2.96780	-11.08270
H	4.07170	3.20250	-9.53900
H	2.81040	1.26170	-8.76940
H	1.85170	1.16940	-10.24010
H	-0.19500	1.87010	-8.85630
H	0.44450	0.27130	-8.50170
H	-0.74050	0.60590	-6.42470
H	-1.03460	2.32860	-6.62050
H	-0.81410	1.56450	-4.20260
H	0.85100	1.10480	-4.53160
H	1.51470	2.61320	-2.89660
H	-0.05940	3.30850	-2.60120
H	0.64500	5.51190	-3.21700
H	1.85740	4.91820	-2.11900
H	3.29690	6.76330	-5.00780
H	1.73380	6.97980	-4.35620
C	3.61130	4.23630	-4.17940
O	3.87350	3.42490	-3.28500
C	4.58110	4.30510	-5.38960
H	4.46760	5.23680	-5.93910
H	6.51330	3.45180	-5.21010
N	5.97790	4.27280	-4.95620
C	4.33230	3.15210	-6.40480
H	5.04530	3.23750	-7.22530
H	3.36220	3.32610	-6.87040
C	4.31040	1.68980	-5.88900
H	3.94720	1.05560	-6.69790
H	3.56310	1.57560	-5.10370
C	5.65160	1.10880	-5.40550
H	5.50120	0.07250	-5.10040
H	5.99430	1.62590	-4.50830
H	6.46630	0.55200	-7.28570
N	6.65350	1.11700	-6.46860
C	7.82620	1.76320	-6.45840
O	8.18510	2.44450	-5.49660
C	8.62030	1.56350	-7.66760
C	8.02600	1.38640	-8.86630
C	10.13080	1.56390	-7.52170
H	10.47610	2.52880	-7.14850
H	10.44370	0.79430	-6.81500
H	10.62710	1.37170	-8.47330
H	8.61690	1.23280	-9.75740
H	6.95290	1.39560	-8.99750
C	6.58220	5.18790	-4.19560
O	6.02490	6.22350	-3.82850
H	8.16770	3.99420	-4.37220
N	7.84710	4.84580	-3.91940
C	10.90980	6.75360	-1.64000
C	9.56210	7.14100	-1.45900
C	8.52840	6.53260	-2.19900
C	8.82660	5.52360	-3.14570
C	10.16810	5.12570	-3.31960
C	11.19890	5.73650	-2.57860
H	9.31320	7.91040	-0.74260
H	7.51430	6.85320	-2.01260
H	10.42050	4.34850	-4.02830
H	12.21950	5.41770	-2.73370
O	13.15030	7.02520	-1.05090
N	11.99180	7.39470	-0.86190
O	11.69350	8.27360	-0.05480
C	2.41430	5.82710	-6.05950
O	2.49270	6.94770	-6.93460
C	3.76480	7.13090	-7.55430
C	3.76360	6.51320	-8.95950
O	3.73020	5.09890	-8.85090
C	3.55820	4.45040	-10.10280
C	3.27870	2.96900	-9.83710
O	2.03430	2.86470	-9.16030
C	1.67020	1.52360	-8.87070
C	0.37750	1.53850	-8.04630
O	0.67300	1.92800	-6.71040

C	-0.50030	2.12500	-5.93160
C	-0.11700	2.31240	-4.45870
O	0.53840	3.56170	-4.27830
C	0.91120	3.77850	-2.92400
C	1.72090	5.08470	-2.80840
N	2.89280	5.11630	-3.70460
C	2.91320	6.23440	-4.66140
H	2.95130	4.96520	-6.45580
H	1.36780	5.52840	-5.99170
H	4.59110	6.75000	-6.95240
H	3.92590	8.20500	-7.64990
H	2.90530	6.88550	-9.52160
H	4.66240	6.81250	-9.50070
H	4.46080	4.56610	-10.70470
H	2.72920	4.88430	-10.66460
H	3.24230	2.42040	-10.77970
H	4.07940	2.54150	-9.23620
H	2.46030	1.00130	-8.32940
H	1.50580	0.98730	-9.80650
H	-0.35210	2.20920	-8.50380
H	-0.06150	0.53960	-8.03640
H	-1.14880	1.25110	-6.01670
H	-1.06470	2.98480	-6.29570
H	-1.01950	2.28600	-3.84570
H	0.52030	1.48870	-4.13250
H	1.48240	2.92970	-2.54640
H	0.01680	3.84890	-2.30290
H	1.04450	5.91620	-3.00650
H	2.05350	5.21920	-1.77770
H	3.91250	6.66670	-4.70650
H	2.30100	7.06090	-4.30010
C	3.91500	4.23660	-3.54570
O	3.96590	3.46720	-2.58000
C	5.05430	4.13740	-4.59080
H	5.04220	4.94630	-5.31780
H	6.76700	3.23480	-3.73350
N	6.34600	4.13570	-3.90070
C	4.90010	2.79400	-5.34010
H	3.87260	2.69400	-5.69740
H	5.05460	1.96010	-4.65250
C	5.84050	2.65270	-6.54900
H	6.87270	2.83150	-6.24520
H	5.59580	3.42490	-7.28050
C	5.73830	1.26580	-7.20080
H	4.69360	1.04300	-7.42230
H	6.07920	0.49540	-6.50770
H	7.41760	1.72380	-8.42340
N	6.55130	1.20310	-8.41010
C	6.24330	0.53080	-9.52730
O	5.20540	-0.12440	-9.63450
C	7.21910	0.70750	-10.59940
C	8.53520	0.82090	-10.32460
C	6.69580	0.76390	-12.02300
H	6.20710	-0.17500	-12.28580
H	5.96640	1.56820	-12.12680
H	7.49830	0.94000	-12.73980
H	9.25540	0.95990	-11.11770
H	8.92950	0.77280	-9.31900
C	6.92760	5.22420	-3.39130
O	6.44250	6.35020	-3.51240
H	8.39110	3.98550	-2.82920
N	8.07830	4.94310	-2.76440
C	10.83520	7.43970	-0.66610
C	11.21930	6.18930	-1.20230
C	10.29130	5.38550	-1.89360
C	8.96100	5.81790	-2.07360
C	8.56640	7.06260	-1.52690
C	9.49700	7.86360	-0.83530
H	12.23430	5.83880	-1.08310
H	10.61700	4.43350	-2.28960
H	7.55180	7.42240	-1.61460
H	9.17490	8.81100	-0.42810
O	11.43130	9.36290	0.51170
N	11.80980	8.28260	0.05970
O	12.96260	7.87250	0.18470

C	4.53640	6.62270	-7.88200
O	3.47770	5.78100	-8.31230
C	3.69510	5.28890	-9.62820
C	2.57480	4.32070	-10.02140
O	2.67690	3.14650	-9.22880
C	1.84900	2.09360	-9.70310
C	1.86380	0.94910	-8.68350
O	1.03490	1.31600	-7.59200
C	1.06250	0.37770	-6.52580
C	0.12200	0.88960	-5.43000
O	0.66150	2.10020	-4.91970
C	-0.25010	2.82400	-4.10840
C	0.37450	4.17200	-3.71740
O	0.42270	5.05050	-4.84160
C	1.65740	5.03610	-5.55250
C	2.65700	6.00110	-4.88760
N	3.99300	5.93420	-5.50820
C	4.31640	7.05030	-6.41900
H	4.58010	7.51080	-8.51460
H	5.49280	6.11810	-8.00730
H	4.65850	4.78160	-9.69410
H	3.71930	6.12420	-10.32980
H	1.59590	4.78570	-9.89590
H	2.68370	4.06710	-11.07740
H	2.23550	1.74150	-10.66060
H	0.82630	2.43550	-9.87200
H	1.47320	0.03890	-9.14120
H	2.88420	0.74180	-8.35720
H	2.07520	0.26040	-6.13650
H	0.72730	-0.59910	-6.87820
H	-0.87500	1.04320	-5.84690
H	0.03310	0.15770	-4.62590
H	-0.47300	2.24330	-3.21200
H	-1.19350	2.99260	-4.63060
H	-0.26540	4.64260	-2.97050
H	1.34790	4.03550	-3.24380
H	1.46190	5.37130	-6.57140
H	2.06130	4.02700	-5.63680
H	2.24880	7.01130	-4.91350
H	2.74590	5.78050	-3.82280
H	5.18950	7.58850	-6.04710
H	3.51850	7.79260	-6.41810
C	4.85000	4.94510	-5.14190
O	4.50850	4.04800	-4.36260
C	6.30430	4.90520	-5.67050
H	6.60340	5.84660	-6.12730
H	7.52340	3.68580	-4.44080
N	7.21480	4.63910	-4.55300
C	6.43810	3.74860	-6.69030
H	5.63260	3.80640	-7.42450
H	6.29960	2.79050	-6.18580
C	7.78740	3.75370	-7.43600
H	8.60140	3.84530	-6.71590
H	7.85390	4.63900	-8.06980
C	8.04820	2.48910	-8.27310
H	8.04200	1.60500	-7.63250
H	9.05300	2.54030	-8.69430
H	7.31800	2.85090	-10.23320
N	7.11100	2.34320	-9.38390
C	6.07020	1.50000	-9.43890
O	5.75070	0.79260	-8.48220
C	5.41500	1.45930	-10.74640
C	5.40050	2.53820	-11.55740
C	4.76530	0.15210	-11.16530
H	5.51620	-0.63560	-11.23380
H	4.01670	-0.15810	-10.43640
H	4.27560	0.23860	-12.13560
H	4.92150	2.49310	-12.52450
H	5.85120	3.48310	-11.29070
C	7.55990	5.54080	-3.63020
O	7.17710	6.71140	-3.67470
H	8.66230	4.07450	-2.83910
N	8.36430	5.02730	-2.68930
C	10.12320	6.77840	0.78570
C	10.66500	5.62370	0.17590
C	10.06750	5.06680	-0.97210

C	8.92080	5.65730	-1.54260
C	8.36480	6.80500	-0.92830
C	8.96470	7.35900	0.22030
H	11.54680	5.15680	0.59020
H	10.50610	4.18220	-1.41290
H	7.47130	7.27480	-1.31220
H	8.52520	8.23670	0.67160
O	10.24480	8.36690	2.48940
N	10.75120	7.36240	1.99050
O	11.75680	6.82260	2.44900
C	4.01010	5.04570	-7.89750
O	4.47380	5.83470	-8.98310
C	4.37840	5.20830	-10.25700
C	2.96920	5.33770	-10.85460
O	2.14040	4.27870	-10.39850
C	0.80400	4.40130	-10.86750
C	0.02950	3.12090	-10.53920
O	-0.18140	3.03180	-9.13620
C	-0.79540	1.80420	-8.76770
C	-1.11380	1.81010	-7.26890
O	0.08710	1.71140	-6.51320
C	-0.17460	1.58040	-5.12250
C	1.13670	1.53390	-4.32630
O	1.66170	2.84380	-4.14300
C	2.67090	3.19500	-5.07750
C	3.11320	4.63830	-4.77780
N	4.39260	4.97940	-5.42470
C	4.26380	5.84490	-6.60870
H	4.53020	4.08870	-7.88150
H	2.94670	4.82480	-7.99620
H	4.72100	4.17290	-10.23630
H	5.07070	5.74210	-10.90880
H	2.54180	6.31230	-10.61230
H	3.03920	5.27860	-11.94210
H	0.80280	4.54270	-11.94980
H	0.31790	5.27240	-10.42540
H	-0.93620	3.14190	-11.04670
H	0.57040	2.25160	-10.91560
H	-0.15370	0.95750	-9.01700
H	-1.72520	1.68080	-9.32580
H	-1.66740	2.71140	-7.00050
H	-1.75710	0.95730	-7.04490
H	-0.72310	0.65220	-4.95370
H	-0.80440	2.39540	-4.76120
H	0.91500	1.14740	-3.33110
H	1.85660	0.84170	-4.76730
H	2.29860	3.12000	-6.09950
H	3.50590	2.49900	-4.98180
H	2.31710	5.32250	-5.07240
H	3.21110	4.77500	-3.69900
H	5.13720	6.47740	-6.74040
H	3.45720	6.56560	-6.47040
C	5.56330	4.55780	-4.87190
O	5.56740	3.84500	-3.86120
C	6.94380	4.93820	-5.48260
H	6.92630	5.94880	-5.88520
H	8.62460	4.15290	-4.46220
N	7.99430	4.93920	-4.45790
C	7.36490	3.95790	-6.60560
H	8.30410	4.30060	-7.04190
H	6.64710	4.03500	-7.41770
C	7.52590	2.47680	-6.18850
H	6.66230	2.13840	-5.61670
H	8.37780	2.37840	-5.51500
C	7.72460	1.51850	-7.37720
H	7.88920	0.50220	-7.01420
H	8.62280	1.79350	-7.93150
H	6.71270	1.99600	-9.18350
N	6.58790	1.53080	-8.29480
C	5.39210	0.96540	-8.07740
O	5.12850	0.37640	-7.02810
C	4.44340	1.15970	-9.17190
C	4.86410	1.24530	-10.45140
C	2.97220	1.27040	-8.81700
H	2.65180	0.42030	-8.21360
H	2.78380	2.18170	-8.25030
H	2.35180	1.29740	-9.71150
H	4.15760	1.40060	-11.25360
H	5.90320	1.15930	-10.73650
C	8.09070	5.83030	-3.46640
O	7.34000	6.80370	-3.37450
H	9.68380	4.77280	-2.88560
N	9.09600	5.55090	-2.62490
C	10.42820	7.50450	0.93100
C	9.09940	7.69210	0.48590
C	8.63350	7.06340	-0.68610
C	9.49600	6.23690	-1.44550
C	10.81740	6.03520	-0.99580
C	11.28010	6.66590	0.17610
H	8.42510	8.32090	1.04910
H	7.60520	7.22360	-0.97530
H	11.49390	5.39840	-1.54890
H	12.29870	6.50080	0.49610
O	12.07780	7.97330	2.51210
N	10.91420	8.16630	2.16090
O	10.13740	8.88540	2.78730
C	0.98000	5.90120	-7.19460
O	-0.20180	5.63230	-7.94020
C	-0.02270	4.75270	-9.05080
C	-0.02000	3.26910	-8.63500
O	1.26060	2.89490	-8.14550
C	1.35210	1.51870	-7.80610
C	2.74710	1.23980	-7.23120
O	2.81770	1.73630	-5.90060
C	4.11630	1.60810	-5.33830
C	4.11980	2.06880	-3.87310
O	4.05430	3.48820	-3.77710
C	2.72510	3.98460	-3.66930
C	2.76930	5.51230	-3.59540
O	3.25530	5.99340	-4.83860
C	3.11330	7.39820	-4.98600
C	3.64620	7.83860	-6.36050
N	3.23740	6.91740	-7.43700
C	1.82310	7.02750	-7.83320
H	1.56470	4.99640	-7.03930
H	0.67390	6.21490	-6.19680
H	0.85980	5.00050	-9.64170
H	-0.87800	4.91510	-9.70730
H	-0.79610	3.07820	-7.89220
H	-0.25310	2.65800	-9.50860
H	1.20160	0.91800	-8.70450
H	0.57990	1.23430	-7.08940
H	2.92820	0.16390	-7.21950
H	3.51260	1.69070	-7.86490
H	4.84160	2.18800	-5.90740
H	4.42880	0.56340	-5.38330
H	3.34070	1.57240	-3.29190
H	5.06710	1.76820	-3.42520
H	2.25630	3.59040	-2.76630
H	2.11180	3.67680	-4.51620
H	1.76260	5.89000	-3.40850
H	3.40690	5.84820	-2.77630
H	3.64690	7.92300	-4.19180
H	2.06110	7.67270	-4.89770
H	3.29250	8.84620	-6.58280
H	4.72650	7.94610	-6.29610
H	1.74910	7.00070	-8.92120
H	1.40620	7.99570	-7.55370
C	4.05140	6.02960	-8.07170
O	3.62950	5.33170	-8.99710
C	5.52520	5.84400	-7.64280
H	5.95710	6.84530	-7.66850
H	4.78930	4.87070	-5.92330
N	5.61650	5.33680	-6.27340
C	6.42780	5.00680	-8.58840
H	7.45980	5.11940	-8.25620
H	6.41380	5.44740	-9.58650
C	6.07020	3.50660	-8.70490
H	5.40300	3.36360	-9.55600
H	5.49940	3.18090	-7.83770
C	7.29580	2.59060	-8.86200
H	7.90190	2.91500	-9.70880
H	6.97540	1.57240	-9.09070
H	8.82570	3.32400	-7.58230
N	8.11860	2.60590	-7.65490
C	7.98000	1.79450	-6.59750
O	7.14410	0.88980	-6.57940
C	8.86140	2.11810	-5.47500
C	10.02340	2.78120	-5.65660
C	8.41480	1.68370	-4.09030
H	7.43250	2.09780	-3.86380
H	8.34700	0.59680	-4.03550
H	9.10730	2.02030	-3.31840
H	10.65550	3.01900	-4.81360
H	10.38170	3.09840	-6.62530
C	6.61060	5.57000	-5.41670
O	7.59780	6.24410	-5.71300
H	5.48530	4.56490	-4.09680
N	6.39040	5.00960	-4.22010
C	8.82820	4.66660	-0.73280
C	7.43170	4.45100	-0.69340
C	6.64940	4.58010	-1.85770
C	7.24350	4.93550	-3.08600
C	8.64270	5.14450	-3.13380
C	9.42260	5.01290	-1.96790
H	6.95230	4.18050	0.23630
H	5.58490	4.40200	-1.79520
H	9.14820	5.38790	-4.05630
H	10.48910	5.17420	-2.02810
O	10.86180	4.72160	0.40800
N	9.64940	4.52800	0.48920
O	9.08970	4.22440	1.54140
C	1.56160	2.76660	-4.23710
O	0.40940	2.25580	-3.57950
C	0.01520	2.99040	-2.42430
C	-0.76740	4.26640	-2.77110
O	0.12170	5.30150	-3.16890
C	-0.54780	6.54210	-3.35020
C	0.43620	7.58800	-3.88600
O	0.67670	7.34190	-5.26520
C	1.49710	8.33930	-5.85880
C	1.62240	8.06550	-7.36180
O	2.52710	6.99140	-7.57990
C	2.63730	6.65180	-8.95590
C	3.75930	5.62180	-9.16140
O	3.35560	4.28920	-8.86060
C	3.22980	4.00850	-7.47360
C	3.20580	2.47950	-7.31090
N	3.29990	2.06670	-5.90150
C	2.02220	1.71290	-5.25870
H	2.34820	2.96660	-3.50840
H	1.33440	3.70640	-4.74120
H	0.85960	3.20350	-1.76680
H	-0.64660	2.33470	-1.85770
H	-1.50590	4.06450	-3.54850
H	-1.31490	4.58850	-1.88350
H	-0.94270	6.87700	-2.38960
H	-1.39520	6.43970	-4.03060
H	-0.00470	8.57910	-3.76580
H	1.36620	7.57450	-3.31530
H	2.48070	8.37240	-5.38730
H	1.03580	9.31830	-5.71720
H	0.64210	7.85060	-7.79090
H	2.00410	8.95940	-7.85790
H	2.88460	7.54920	-9.52580
H	1.69000	6.27480	-9.34470
H	4.03270	5.62620	-10.21700
H	4.66270	5.90180	-8.61700
H	2.31390	4.44760	-7.07600
H	4.06160	4.44530	-6.92100
H	2.30220	2.08740	-7.77800
H	4.01480	2.02930	-7.88690
H	2.12970	0.74660	-4.76200
H	1.23040	1.56390	-5.99290
C	4.47010	1.92830	-5.22490

O	4.49960	1.53030	-4.05500
C	5.82440	2.23450	-5.91450
H	5.71240	2.94360	-6.73310
H	7.44120	2.17820	-4.54630
N	6.76060	2.80770	-4.94270
C	6.41810	0.91370	-6.45420
H	5.66890	0.40330	-7.06240
H	6.63970	0.23420	-5.62890
C	7.67700	1.11920	-7.31510
H	8.45440	1.60690	-6.72570
H	7.44260	1.79840	-8.13620
C	8.22210	-0.20250	-7.88130
H	7.46140	-0.70530	-8.48180
H	8.46830	-0.88360	-7.06570
H	10.31890	-0.08710	-8.20570
N	9.42790	0.01450	-8.67300
C	9.46960	0.33440	-9.97370
O	8.44570	0.50420	-10.63800
C	10.82590	0.49910	-10.49370
C	11.84800	-0.24050	-10.01450
C	11.03990	1.53130	-11.58610
H	10.46430	1.26940	-12.47470
H	10.71360	2.51520	-11.24670
H	12.08960	1.60310	-11.87210
H	12.85010	-0.11020	-10.39650
H	11.72080	-0.99000	-9.24580
C	6.68740	4.05620	-4.47330
O	5.85050	4.86540	-4.87590
H	8.29690	3.57680	-3.39040
N	7.62320	4.31170	-3.54850
C	8.42230	7.81070	-1.23410
C	9.41000	6.82560	-1.46340
C	9.12200	5.68130	-2.23340
C	7.84330	5.50060	-2.80000
C	6.84560	6.47640	-2.56220
C	7.13690	7.61940	-1.79100
H	10.39910	6.94430	-1.04520
H	9.89960	4.94600	-2.38820
H	5.84400	6.36760	-2.95140
H	6.36120	8.35260	-1.62400
O	7.83500	9.84240	-0.25020
N	8.72550	9.01150	-0.42580
O	9.85680	9.13510	0.04080
C	1.65400	2.33620	-5.07360
O	0.77390	1.48860	-4.34750
C	-0.16250	2.17750	-3.52490
C	-1.39500	2.65110	-4.31010
O	-1.10470	3.84890	-5.01800
C	-2.25700	4.38490	-5.65500
C	-1.87580	5.64070	-6.44650
O	-1.19950	5.26120	-7.63790
C	-0.90610	6.37600	-8.46960
C	-0.26470	5.88640	-9.77270
O	1.08590	5.51380	-9.53280
C	1.72390	5.02820	-10.70650
C	3.21640	4.77960	-10.43890
O	3.46200	3.52960	-9.80200
C	3.17020	3.50650	-8.41190
C	3.79370	2.22520	-7.83320
N	3.80160	2.22360	-6.36170
C	2.72720	1.44520	-5.72160
H	2.11030	3.06130	-4.39840
H	1.11420	2.89400	-5.83940
H	0.29920	2.99400	-2.96730
H	-0.49820	1.45740	-2.77790
H	-1.74120	1.86910	-4.98790
H	-2.20340	2.84360	-3.60240
H	-2.99410	4.65090	-4.89530
H	-2.72240	3.64970	-6.31390
H	-2.78700	6.18340	-6.70430
H	-1.26080	6.30810	-5.84050
H	-0.25210	7.08580	-7.96030
H	-1.83190	6.90200	-8.70930
H	-0.83600	5.05430	-10.18810
H	-0.28850	6.69370	-10.50670

H	1.63450	5.77750	-11.49510
H	1.24100	4.11970	-11.07020
H	3.72800	4.73570	-11.40090
H	3.67090	5.60960	-9.89550
H	2.09290	3.51320	-8.24220
H	3.57830	4.39330	-7.92590
H	3.25910	1.36110	-8.22820
H	4.80900	2.09980	-8.21040
H	3.16490	0.79310	-4.96320
H	2.24570	0.76860	-6.42760
C	4.76530	2.81370	-5.60770
O	4.75190	2.75230	-4.37290
C	5.94530	3.55850	-6.28080
H	5.67890	3.95260	-7.26010
H	7.18530	4.52150	-4.86060
N	6.37210	4.67300	-5.43710
C	7.14290	2.59100	-6.40440
H	6.82450	1.65100	-6.85850
H	7.49350	2.32620	-5.40550
C	8.29790	3.16940	-7.24870
H	8.48170	4.21090	-6.98280
H	7.99670	3.18720	-8.29700
C	9.61690	2.38680	-7.11320
H	10.36300	2.78830	-7.80150
H	9.46570	1.34550	-7.40060
H	10.00460	1.60520	-5.17390
N	10.13400	2.42770	-5.74730
C	10.76920	3.46130	-5.17670
O	11.03420	4.48990	-5.80080
C	11.13240	3.23080	-3.77980
C	10.36840	2.45560	-2.98170
C	12.39630	3.89400	-3.26320
H	13.25830	3.57410	-3.84970
H	12.31580	4.97890	-3.34090
H	12.58490	3.64270	-2.21910
H	10.64510	2.28480	-1.95150
H	9.45710	1.98210	-3.31880
C	5.73920	5.83930	-5.28890
O	4.72890	6.13650	-5.92480
H	5.93060	7.62060	-4.41300
N	6.30270	6.68060	-4.40900
C	9.53760	6.01150	-1.71330
C	8.46800	5.08910	-1.78260
C	7.39290	5.29640	-2.66820
C	7.37450	6.43250	-3.50950
C	8.41980	7.37350	-3.42370
C	9.49680	7.15840	-2.54050
H	8.47050	4.21080	-1.15340
H	6.58490	4.57730	-2.68780
H	8.41370	8.25790	-4.04570
H	10.29770	7.88240	-2.50070
O	11.58630	6.60530	-0.77180
N	10.67220	5.78250	-0.79310
O	10.66020	4.77740	-0.08520
C	1.65400	2.33620	-5.07360
O	0.77390	1.48860	-4.34750
C	-0.16250	2.17750	-3.52490
C	-1.39500	2.65110	-4.31010
O	-1.10470	3.84890	-5.01800
C	-2.25700	4.38490	-5.65500
C	-1.87580	5.64070	-6.44650
O	-1.19950	5.26120	-7.63790
C	-0.90610	6.37600	-8.46960
C	-0.26470	5.88640	-9.77270
O	1.08590	5.51380	-9.53280
C	1.72390	5.02820	-10.70650
C	3.21640	4.77960	-10.43890
O	3.46200	3.52960	-9.80200
C	3.17020	3.50650	-8.41190
C	3.79370	2.22520	-7.83320
N	3.80160	2.22360	-6.36170
C	2.72720	1.44520	-5.72160
H	2.11030	3.06130	-4.39840
H	1.11420	2.89400	-5.83940
H	0.29920	2.99400	-2.96730

H	-0.49820	1.45740	-2.77790
H	-1.74120	1.86910	-4.98790
H	-2.20340	2.84360	-3.60240
H	-2.99410	4.65090	-4.89530
H	-2.72240	3.64970	-6.31390
H	-2.78700	6.18340	-6.70430
H	-1.26080	6.30810	-5.84050
H	-0.25210	7.08580	-7.96030
H	-1.83190	6.90200	-8.70930
H	-0.83600	5.05430	-10.18810
H	-0.28850	6.69370	-10.50670
H	1.63450	5.77750	-11.49510
H	1.24100	4.11970	-11.07020
H	3.72800	4.73570	-11.40090
H	3.67090	5.60960	-9.89550
H	2.09290	3.51320	-8.24220
H	3.57830	4.39330	-7.92590
H	3.25910	1.36110	-8.22820
H	4.80900	2.09980	-8.21040
H	3.16490	0.79310	-4.96320
H	2.24570	0.76860	-6.42760
C	4.76530	2.81370	-5.60770
O	4.75190	2.75230	-4.37290
C	5.94530	3.55850	-6.28080
H	5.67890	3.95260	-7.26010
H	7.18530	4.52150	-4.86060
N	6.37210	4.67300	-5.43710
C	7.14290	2.59100	-6.40440
H	6.82450	1.65100	-6.85850
H	7.49350	2.32620	-5.40550
C	8.29790	3.16940	-7.24870
H	8.48170	4.21090	-6.98280
H	7.99670	3.18720	-8.29700
C	9.61690	2.38680	-7.11320
H	10.36300	2.78830	-7.80150
H	9.46570	1.34550	-7.40060
H	10.00460	1.60520	-5.17390
N	10.13400	2.42770	-5.74730
C	10.76920	3.46130	-5.17670
O	11.03420	4.48990	-5.80080
C	11.13240	3.23080	-3.77980
C	10.36840	2.45560	-2.98170
C	12.39630	3.89400	-3.26320
H	13.25830	3.57410	-3.84970
H	12.31580	4.97890	-3.34090
H	12.58490	3.64270	-2.21910
H	10.64510	2.28480	-1.95150
H	9.45710	1.98210	-3.31880
C	5.73920	5.83930	-5.28890
O	4.72890	6.13650	-5.92480
H	5.93060	7.62060	-4.41300
N	6.30270	6.68060	-4.40900
C	9.53760	6.01150	-1.71330
C	8.46800	5.08910	-1.78260
C	7.39290	5.29640	-2.66820
C	7.37450	6.43250	-3.50950
C	8.41980	7.37350	-3.42370
C	9.49680	7.15840	-2.54050
H	8.47050	4.21080	-1.15340
H	6.58490	4.57730	-2.68780
H	8.41370	8.25790	-4.04570
H	10.29770	7.88240	-2.50070
O	11.58630	6.60530	-0.77180
N	10.67220	5.78250	-0.79310
O	10.66020	4.77740	-0.08520
C	2.41460	5.22090	-6.95770
O	2.69370	6.04280	-8.08620
C	3.96410	5.80630	-8.68850
C	3.82580	4.81930	-9.85760
O	3.52800	3.52960	-9.34860
C	3.31810	2.55840	-10.36150
C	2.85660	1.26240	-9.68630
O	1.59630	1.50740	-9.07880
C	1.06440	0.37010	-8.41680
C	-0.24550	0.78010	-7.73400

O	0.05150	1.53640	-6.56700
C	-1.10580	2.13360	-5.99710
C	-0.75640	2.71150	-4.62100
O	0.11690	3.82500	-4.76490
C	0.48150	4.37900	-3.50830
C	1.51920	5.50120	-3.70800
N	2.70410	5.07890	-4.48230
C	2.96760	5.88450	-5.68570
H	2.79550	4.20820	-7.08430
H	1.33130	5.13060	-6.87120
H	4.71270	5.47400	-7.96810
H	4.32000	6.75900	-9.08160
H	3.04510	5.15730	-10.54100
H	4.75890	4.78070	-10.42160
H	4.24580	2.38960	-10.91040
H	2.56630	2.89500	-11.07730
H	2.76550	0.46870	-10.42950
H	3.58770	0.93770	-8.94420
H	1.76800	-0.03120	-7.68530
H	0.86890	-0.41400	-9.15000
H	-0.86860	1.34650	-8.42880
H	-0.80650	-0.11050	-7.44660
H	-1.88790	1.38210	-5.87510
H	-1.50050	2.91060	-6.65370
H	-1.67180	3.03070	-4.11980
H	-0.30020	1.93820	-4.00060
H	0.86520	3.60230	-2.84630
H	-0.40330	4.78780	-3.01770
H	1.01060	6.33930	-4.18460
H	1.84460	5.87370	-2.73530
H	4.03120	6.10170	-5.77730
H	2.52310	6.87520	-5.58850
C	3.53100	4.10490	-4.01990
O	3.37120	3.59820	-2.90400
C	4.71750	3.57680	-4.86870
H	4.93220	4.19550	-5.73670
H	6.12720	2.62780	-3.60060
N	5.90620	3.52090	-4.01340
C	4.37530	2.14490	-5.35460
H	3.51520	2.20100	-6.02430
H	4.03910	1.53650	-4.51270
C	5.50080	1.36800	-6.07830
H	5.07720	0.41500	-6.39890
H	6.29210	1.10030	-5.37710
C	6.10260	2.05270	-7.31950
H	5.31550	2.51590	-7.91310
H	6.57650	1.30560	-7.95790
H	7.54890	2.92970	-6.03730
N	7.11920	3.02730	-6.94540
C	7.52480	4.06600	-7.68470
O	7.07220	4.29360	-8.80680
C	8.50110	4.90660	-6.99920
C	9.46230	4.35470	-6.23000
C	8.38490	6.40880	-7.17660
H	8.48370	6.67790	-8.22880
H	7.41180	6.75430	-6.82490
H	9.15510	6.93980	-6.61670
H	10.18030	4.97370	-5.71230
H	9.56380	3.28620	-6.10010
C	6.63710	4.59180	-3.69160
O	6.36200	5.72340	-4.09260
H	7.69840	3.34190	-2.54350
N	7.66980	4.28800	-2.89440
C	10.93150	6.66860	-1.50750
C	10.22600	7.05670	-2.66970
C	9.14110	6.29370	-3.14490
C	8.73380	5.12420	-2.45920
C	9.44520	4.72560	-1.30870
C	10.52820	5.49220	-0.83480
H	10.51930	7.94610	-3.20810
H	8.64490	6.61970	-4.04730
H	9.16430	3.82920	-0.77330
H	11.05340	5.16970	0.05260
O	12.65600	7.09570	0.00380
N	12.06900	7.47210	-1.01010
O	12.38580	8.48710	-1.62820
C	2.44970	1.64430	-3.65250
O	2.00270	2.98810	-3.76910
C	1.79460	3.59050	-2.49650
C	1.35670	5.05080	-2.66320
O	2.45310	5.81570	-3.14320
C	2.20010	7.21430	-3.13210
C	3.34560	7.93470	-3.85370
O	3.18300	7.75430	-5.25250
C	4.29210	8.22450	-6.00590
C	3.99430	7.99040	-7.49090
O	3.96750	6.59030	-7.72820
C	3.45970	6.25150	-9.00890
C	3.37000	4.72370	-9.13570
O	2.30850	4.21250	-8.33010
C	2.70240	3.76100	-7.03780
C	3.21980	2.31330	-7.12870
N	3.71200	1.81410	-5.83400
C	2.72390	1.04970	-5.04820
H	1.68350	1.04780	-3.15450
H	3.33620	1.59270	-3.01990
H	2.70160	3.54390	-1.89100
H	1.01950	3.04070	-1.96010
H	0.50590	5.12560	-3.34200
H	1.03610	5.43700	-1.69400
H	2.14320	7.55630	-2.09760
H	1.24630	7.45140	-3.60700
H	3.31700	9.00150	-3.62660
H	4.30830	7.55380	-3.51020
H	5.20880	7.70850	-5.71520
H	4.44030	9.28970	-5.82140
H	3.04200	8.45560	-7.75180
H	4.76490	8.45130	-8.11060
H	4.12590	6.64800	-9.77670
H	2.47560	6.69450	-9.17070
H	3.13120	4.47950	-10.17120
H	4.33060	4.25140	-8.92560
H	1.82240	3.78340	-6.39430
H	3.42820	4.43150	-6.57780
H	2.42160	1.67410	-7.50720
H	3.99490	2.22660	-7.88850
H	3.07760	0.02290	-4.94100
H	1.77180	0.97530	-5.57410
C	5.00240	1.92630	-5.42510
O	5.41900	1.35030	-4.41410
C	6.01730	2.76490	-6.24370
H	5.51420	3.54260	-6.81670
H	7.86780	2.96540	-5.22720
N	6.97230	3.41480	-5.34050
C	6.79350	1.83150	-7.19870
H	6.08180	1.21390	-7.74740
H	7.40750	1.13060	-6.63010
C	7.67110	2.59480	-8.21080
H	8.41090	3.19140	-7.67570
H	7.05750	3.30800	-8.76320
C	8.40920	1.68070	-9.20450
H	9.07780	1.00420	-8.66880
H	9.04850	2.28580	-9.84870
H	6.98010	1.47770	-10.76290
N	7.47380	0.95010	-10.05580
C	7.20140	-0.36090	-10.00110
O	7.77850	-1.12260	-9.22340
C	6.18730	-0.78100	-10.96490
C	5.14990	0.02680	-11.26920
C	6.34500	-2.14830	-11.60440
H	7.30590	-2.21920	-12.11530
H	6.30460	-2.93000	-10.84490
H	5.55850	-2.34420	-12.33370
H	4.40270	-0.27980	-11.98650
H	5.01200	0.99870	-10.81580
C	6.66980	4.45960	-4.56510
O	5.58060	5.02800	-4.61940
H	8.55600	4.34000	-3.90150
N	7.67690	4.81440	-3.75560
C	7.84830	7.78750	-0.69690
C	6.60570	7.20880	-1.04380
C	6.52230	6.22750	-2.05140
C	7.68490	5.81330	-2.74450
C	8.92850	6.37500	-2.38910
C	9.00840	7.35560	-1.38040
H	5.70540	7.51340	-0.53020
H	5.55490	5.79850	-2.27020
H	9.83420	6.06500	-2.89200
H	9.97140	7.77700	-1.13090
O	9.03670	9.28610	0.63830
N	7.93330	8.81700	0.36130
O	6.89750	9.16630	0.92500
C	2.33900	2.39970	-4.25130
O	1.20240	1.82650	-3.62170
C	0.45040	2.73960	-2.82960
C	-0.54750	3.55190	-3.67090
O	0.09220	4.67180	-4.27040
C	-0.82250	5.47960	-5.00140
C	-0.10770	6.71900	-5.55340
O	0.68520	6.36440	-6.67940
C	1.30200	7.49910	-7.27600
C	2.10550	7.06720	-8.50810
O	3.27530	6.38000	-8.08770
C	4.10360	5.99590	-9.17690
C	5.32830	5.22960	-8.65100
O	5.05980	3.84800	-8.43020
C	4.19640	3.58370	-7.33180
C	4.24790	2.07130	-7.05050
N	4.32410	1.76690	-5.61330
C	3.07500	1.28210	-5.00600
H	2.99090	2.85000	-3.50090
H	2.04380	3.18590	-4.94690
H	1.08750	3.38370	-2.22110
H	-0.12080	2.13170	-2.12720
H	-1.01800	2.91710	-4.42360
H	-1.34140	3.91080	-3.01350
H	-1.62370	5.80660	-4.33630
H	-1.28650	4.91300	-5.81050
H	-0.85930	7.44880	-5.85960
H	0.49980	7.18790	-4.77760
H	1.94770	8.01320	-6.56210
H	0.53280	8.20860	-7.58620
H	1.49650	6.44060	-9.16180
H	2.39020	7.95300	-9.07850
H	4.44040	6.89490	-9.69580
H	3.55720	5.38930	-9.90120
H	6.11150	5.27170	-9.40850
H	5.74390	5.70230	-7.75950
H	3.17200	3.88350	-7.55550
H	4.51110	4.16190	-6.46120
H	3.38890	1.59520	-7.52370
H	5.09980	1.61840	-7.55360
H	3.29030	0.45830	-4.32290
H	2.40910	0.85330	-5.75500
C	5.45950	1.87360	-4.87400
O	5.48660	1.55950	-3.67880
C	6.77230	2.38570	-5.52300
H	6.55490	3.09780	-6.31450
H	8.36160	2.53370	-4.13000
N	7.60390	3.06750	-4.52710
C	7.56810	1.19020	-6.09530
H	6.92140	0.57260	-6.71930
H	7.87900	0.53180	-5.28220
C	8.81090	1.58850	-6.92280
H	9.28670	0.67520	-7.28270
H	9.55060	2.05830	-6.27340
C	8.54780	2.51990	-8.12840
H	9.45080	2.60680	-8.73530
H	8.32960	3.52910	-7.77730
H	6.57180	2.61960	-8.90910
N	7.43250	2.08390	-8.96450
C	7.43820	1.04190	-9.80620
O	8.42670	0.32250	-9.95800
C	6.15430	0.82790	-10.46580
C	5.43020	1.87460	-10.91120
C	5.67190	-0.60180	-10.62410

H	6.36800	-1.17220	-11.24020
H	5.60220	-1.08700	-9.64980
H	4.68930	-0.64430	-11.09470
H	4.47540	1.72430	-11.39300
H	5.76750	2.89710	-10.81380
C	7.34630	4.28360	-4.03840
O	6.40930	4.97410	-4.44240
H	8.99190	4.01480	-2.93720
N	8.22440	4.65130	-3.09490
C	8.50030	8.18860	-0.71870
C	7.26040	7.82800	-1.29450
C	7.14050	6.66860	-2.08650
C	8.26780	5.84700	-2.32690
C	9.50260	6.19560	-1.74120
C	9.61900	7.35590	-0.95050
H	6.38780	8.44230	-1.12580
H	6.16830	6.42630	-2.49000
H	10.37720	5.57920	-1.89720
H	10.57740	7.60480	-0.51830
O	9.72100	9.68080	0.59440
N	8.62290	9.40650	0.11130
O	7.62270	10.10020	0.28770
C	2.64500	6.96090	-6.34390
O	2.30120	7.15410	-7.70770
C	3.42230	7.28130	-8.57710
C	3.03590	6.73400	-9.95540
O	3.02590	5.31420	-9.88440
C	2.54470	4.70520	-11.07440
C	2.67260	3.18160	-10.94940
O	1.77280	2.70630	-9.95630
C	1.80850	1.29080	-9.82670
C	0.93690	0.85890	-8.64210
O	1.58120	1.22060	-7.42780
C	0.83270	0.83740	-6.28220
C	1.55720	1.30280	-5.01360
O	1.52720	2.72210	-4.96210
C	2.00230	3.24530	-3.73140
C	2.08220	4.77570	-3.85330
N	3.22410	5.19120	-4.68320
C	2.89370	5.46250	-6.08840
H	1.80150	7.29080	-5.73640
H	3.49240	7.58580	-6.05770
H	4.30630	6.75670	-8.21070
H	3.68700	8.33710	-8.64570
H	2.06500	7.12670	-10.26240
H	3.76860	7.05160	-10.69890
H	3.13380	5.04740	-11.92690
H	1.50710	4.98720	-11.26020
H	2.43640	2.71960	-11.90940
H	3.69990	2.90920	-10.70130
H	2.82740	0.93110	-9.68630
H	1.43000	0.83770	-10.74430
H	-0.05260	1.31360	-8.71270
H	0.80150	-0.22360	-8.67050
H	0.72660	-0.24850	-6.26300
H	-0.17200	1.26230	-6.31550
H	1.05020	0.88910	-4.14010
H	2.58500	0.93820	-4.99860
H	2.97390	2.82090	-3.47140
H	1.30790	2.97400	-2.93470
H	1.14560	5.17050	-4.24930
H	2.16860	5.21350	-2.85700
H	2.00010	4.90470	-6.37170
H	3.66740	5.07310	-6.74810
C	4.46940	5.27730	-4.15310
O	4.67830	5.05160	-2.95540
C	5.68480	5.63630	-5.04830
H	5.38340	6.30340	-5.85480
H	7.52430	5.81990	-4.00430
N	6.70780	6.34450	-4.27720
C	6.32850	4.36940	-5.66670
H	7.16920	4.67460	-6.29130
H	5.61380	3.91550	-6.35360
C	6.81010	3.29190	-4.66570
H	5.95670	2.87940	-4.12640

H	7.44980	3.74180	-3.90610
C	7.58460	2.13330	-5.32220
H	7.81240	1.36460	-4.58150
H	8.54540	2.49690	-5.68880
H	7.22280	1.73380	-7.37430
N	6.86770	1.54150	-6.44780
C	5.79130	0.74650	-6.37980
O	5.30710	0.40120	-5.30070
C	5.29070	0.31330	-7.68600
C	5.55700	1.01200	-8.81120
C	4.46200	-0.95840	-7.73100
H	5.02820	-1.79530	-7.32070
H	3.55350	-0.83860	-7.13950
H	4.16970	-1.21410	-8.74970
H	5.19200	0.67060	-9.76840
H	6.12880	1.92880	-8.82210
C	6.58440	7.57850	-3.77630
O	5.63550	8.31440	-4.04630
H	7.57740	8.96100	-2.74770
N	7.57960	7.97460	-2.96960
C	10.70210	5.76970	-1.07650
C	9.40420	5.21580	-1.17230
C	8.36020	5.92700	-1.79600
C	8.60300	7.20450	-2.35330
C	9.88770	7.77240	-2.23980
C	10.92880	7.05810	-1.61440
H	9.20140	4.23930	-0.75670
H	7.37440	5.48270	-1.82530
H	10.08910	8.75660	-2.64000
H	11.90910	7.50730	-1.54700
O	12.90810	5.54410	-0.35300
N	11.79610	5.02150	-0.42050
O	11.55380	3.90410	0.03290
C	2.21010	1.72900	-4.51540
O	1.73430	3.03830	-4.23590
C	1.65540	3.28570	-2.83650
C	1.21180	4.72990	-2.57390
O	2.26130	5.61250	-2.94330
C	2.02920	6.95400	-2.53610
C	3.09850	7.85550	-3.16500
O	2.77770	8.04590	-4.53470
C	3.80320	8.70970	-5.26000
C	3.33120	8.87200	-6.70890
O	3.24960	7.58340	-7.30110
C	2.57200	7.58450	-8.54770
C	2.45080	6.14420	-9.06720
O	1.50090	5.40690	-8.29850
C	2.05740	4.64370	-7.23220
C	2.54680	3.28310	-7.76330
N	3.20340	2.48260	-6.71660
C	2.32340	1.51090	-6.03740
H	1.51670	0.99470	-4.10180
H	3.16560	1.55930	-4.01880
H	2.61700	3.10310	-2.35360
H	0.93430	2.59900	-2.38990
H	0.29860	4.96250	-3.12390
H	0.99140	4.84510	-1.51110
H	2.09140	7.01030	-1.44830
H	1.03230	7.29240	-2.82420
H	3.11170	8.82470	-2.66400
H	4.08740	7.41120	-3.04320
H	4.73620	8.14450	-5.22330
H	3.99330	9.69010	-4.82010
H	2.36460	9.37870	-6.72450
H	4.03340	9.48870	-7.27180
H	3.13370	8.18870	-9.26190
H	1.57970	8.02890	-8.45420
H	2.07440	6.18010	-10.08990
H	3.42580	5.65780	-9.11890
H	1.26930	4.47500	-6.49770
H	2.84300	5.18930	-6.70990
H	1.70020	2.74240	-8.18720
H	3.21280	3.41630	-8.61380
H	2.69870	0.50440	-6.23020
H	1.31640	1.52830	-6.45460

C	4.53430	2.53450	-6.44830
O	5.06600	1.76100	-5.64450
C	5.44890	3.56260	-7.16920
H	4.87310	4.43880	-7.46370
H	7.43520	3.70800	-6.44370
N	6.50320	4.05210	-6.27420
C	6.10530	2.96300	-8.44000
H	6.65340	3.75530	-8.95200
H	5.32320	2.66210	-9.13800
C	7.05030	1.76230	-8.22270
H	6.50250	0.93660	-7.76750
H	7.84150	2.03010	-7.52190
C	7.68360	1.27600	-9.53700
H	8.25490	2.08340	-9.99700
H	6.90980	0.99950	-10.25610
H	9.57160	0.35580	-9.21530
N	8.58540	0.15240	-9.30940
C	8.23430	-1.13930	-9.24510
O	7.06790	-1.50780	-9.39430
C	9.36260	-2.04300	-9.02830
C	10.42420	-1.66210	-8.28710
C	9.29610	-3.41810	-9.66790
H	8.44820	-3.97980	-9.27410
H	9.17290	-3.32820	-10.74780
H	10.20160	-3.99490	-9.47750
H	11.25950	-2.33000	-8.13520
H	10.49070	-0.69360	-7.81130
C	6.28040	4.80080	-5.18940
O	5.16600	5.23690	-4.90620
H	8.25870	4.71040	-4.89050
N	7.39410	5.03270	-4.48100
C	7.95180	7.11020	-0.79290
C	6.69540	6.53330	-1.08930
C	6.48470	5.84410	-2.30000
C	7.52870	5.72920	-3.24900
C	8.78810	6.28820	-2.94920
C	8.99570	6.97580	-1.73710
H	5.88350	6.61270	-0.38090
H	5.51370	5.40350	-2.47520
H	9.60730	6.20210	-3.64970
H	9.96730	7.40200	-1.53320
O	9.28250	8.31150	0.69930
N	8.17050	7.83290	0.47870
O	7.23240	7.92900	1.26820