

## Supplementary material

### Heteroditopic chemosensor for detecting $\gamma$ -hydroxybutiric acid (GHB) in soft drinks and alcoholic beverages

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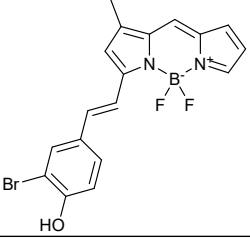
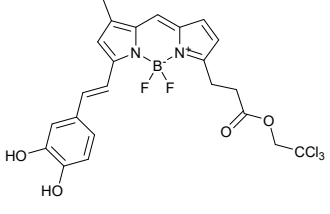
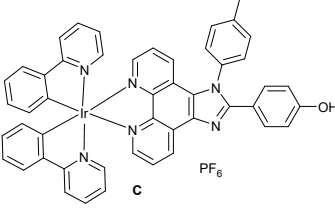
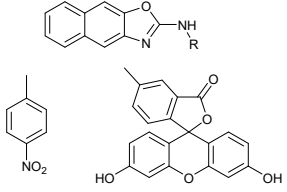
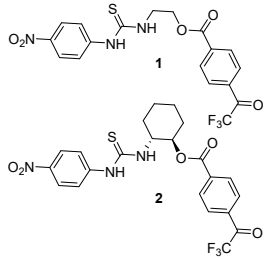
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## Reported data and comparison

**Table S1.** Comparison with other sensors published

SENSOR	DETECTION	RECOGNITION	LoDs (mg/mL)	INTERFERENTS	REFERENCE
	FLUORESCENCE On-Off	Acid moiety by hydrogen bond	5	Some Acids	<i>Chem. Commun.</i> , <b>2014</b> , 50, 2904
	FLUORESCENCE Off-On Pre-treatment is required	No data available	10	No data available	<i>Chem. Commun.</i> , <b>2013</b> , 49, 6170-6172
	FLUORESCENCE On-Off	No data available	0.15	No data available	<i>J. Mater. Chem. B</i> , <b>2017</b> , 5, 2739--2742
	COLOUR Yellow to red FLUORESCENCE Off-On	Deprotonation of acid moiety	0.04	Some Acids and sugars	<i>Chem. Commun.</i> , <b>2020</b> , 56, 12600-12603
	COLOUR Yellow to orange	Double recognition: Acid-base and hemiacetal formation	0.17	Some Acids and sugars	<i>This work</i>

## NMR Spectra

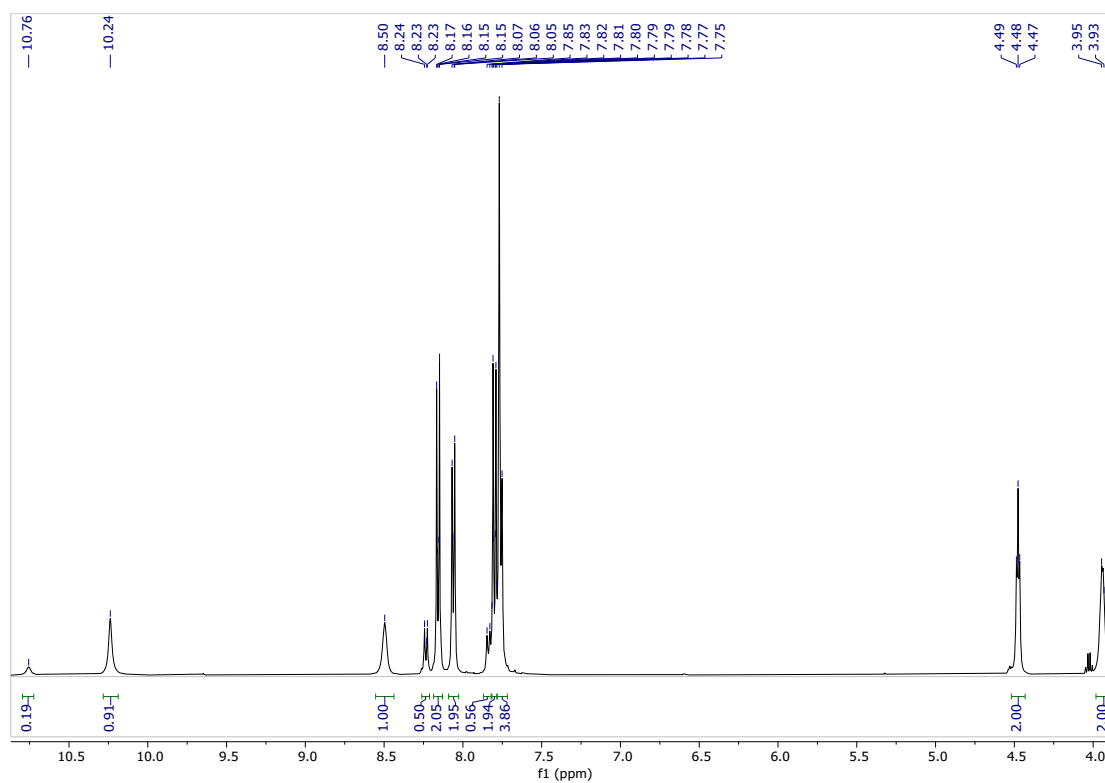


Figure S1.  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{DMSO-}d_6$ .

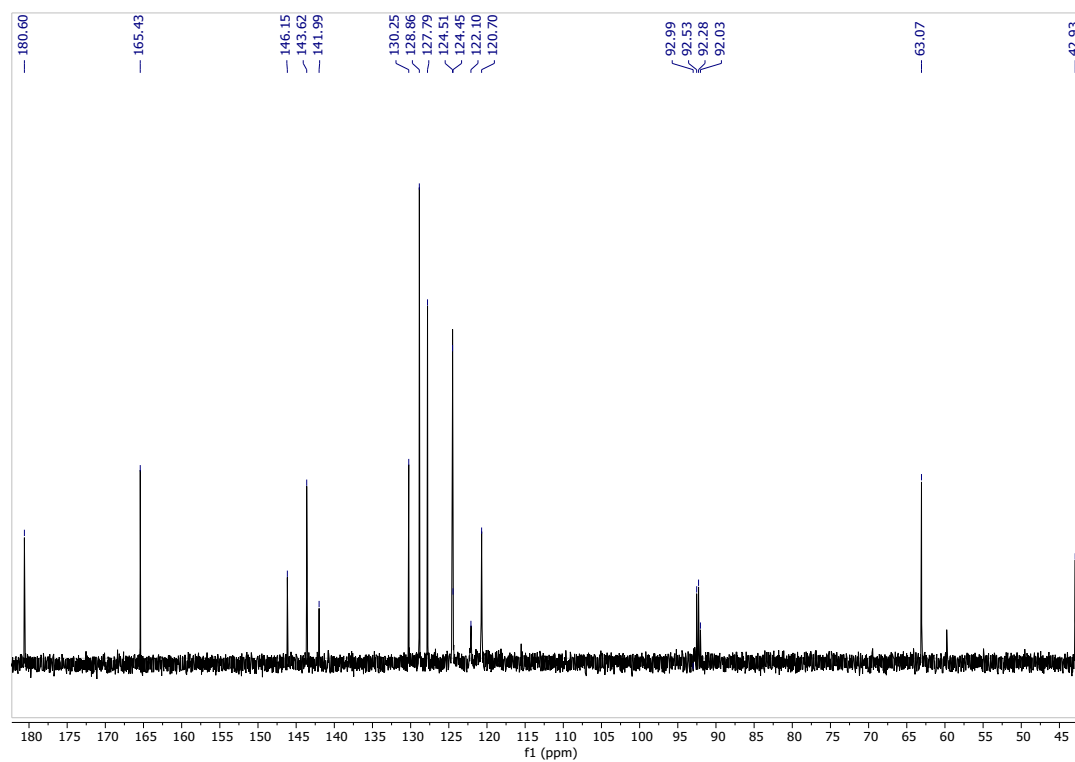


Figure S2.  $^{13}\text{C}$  NMR spectrum of compound 1 in  $\text{DMSO-}d_6$ .

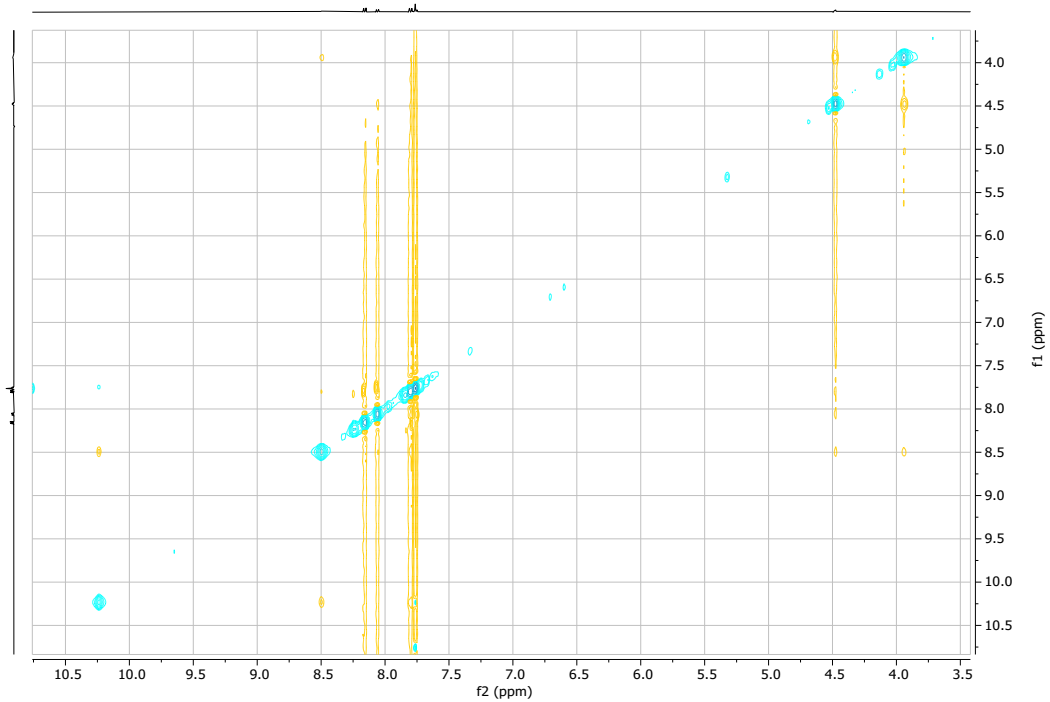


Figure S3. NOESY spectrum of compound **1** in DMSO- $d_6$ .

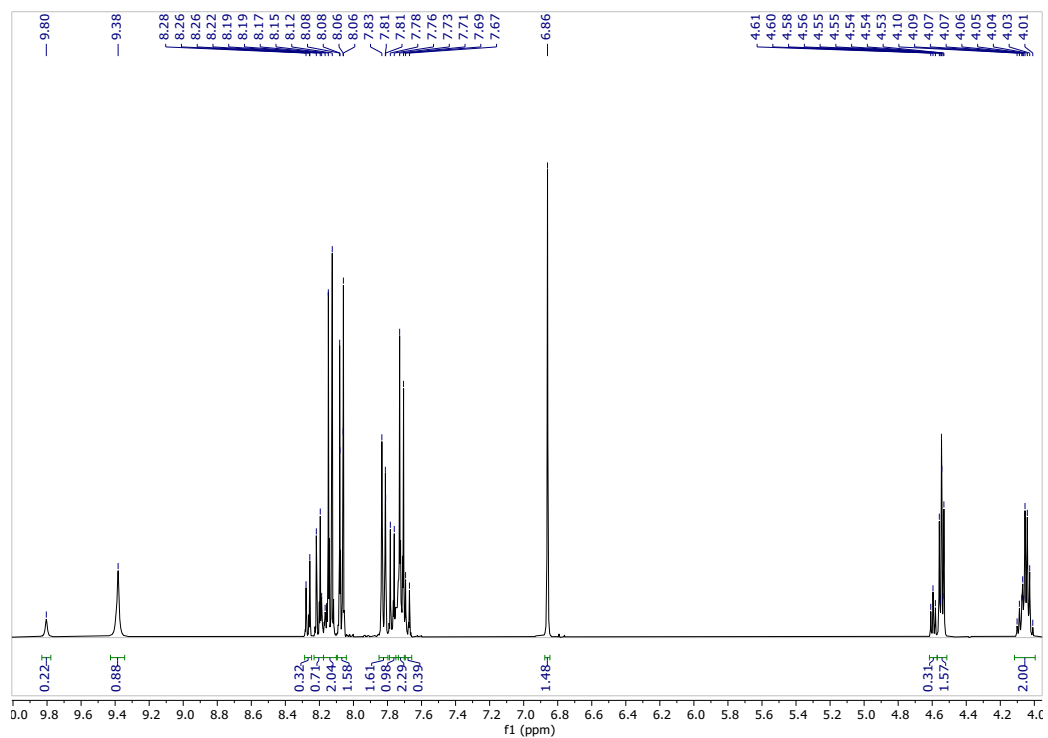


Figure S4.  $^1\text{H}$  NMR spectrum of compound **1** in THF- $d_8$ .



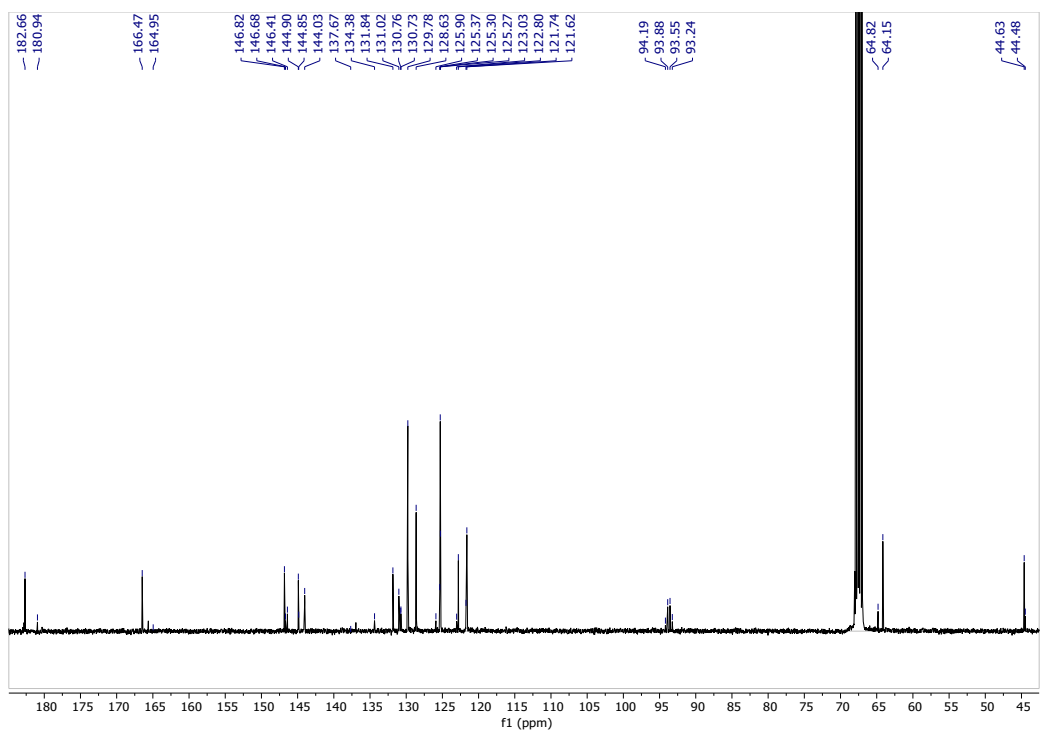


Figure S5.  $^{13}\text{C}$  NMR spectrum of compound **1** in  $\text{THF-}d_8$ .

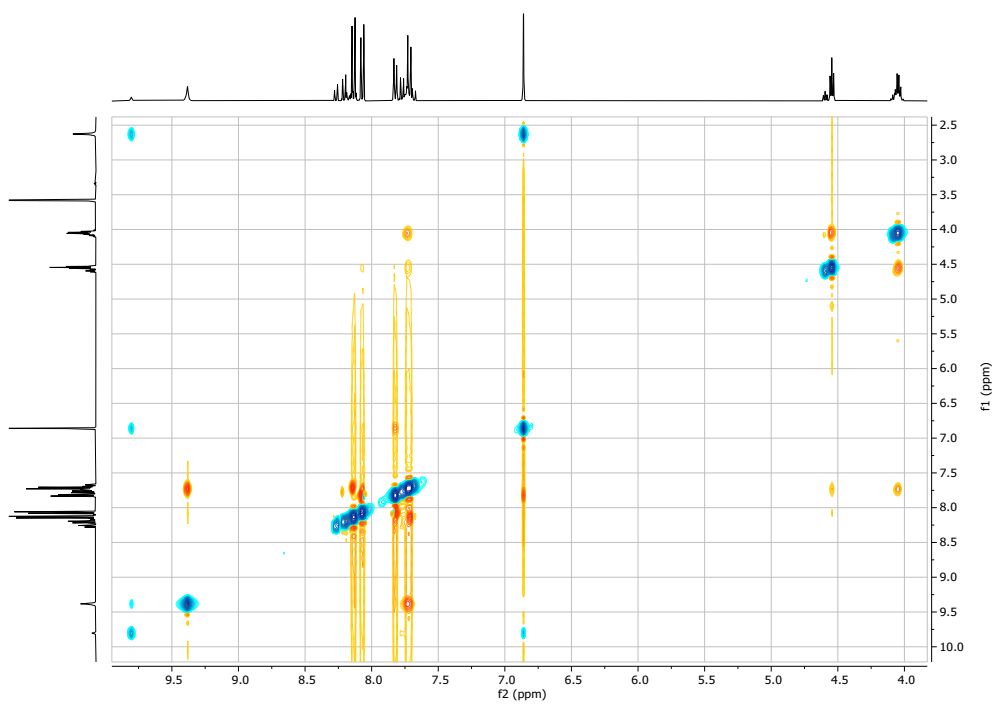


Figure S6. NOESY spectrum of compound **1** in  $\text{THF-}d_8$ .

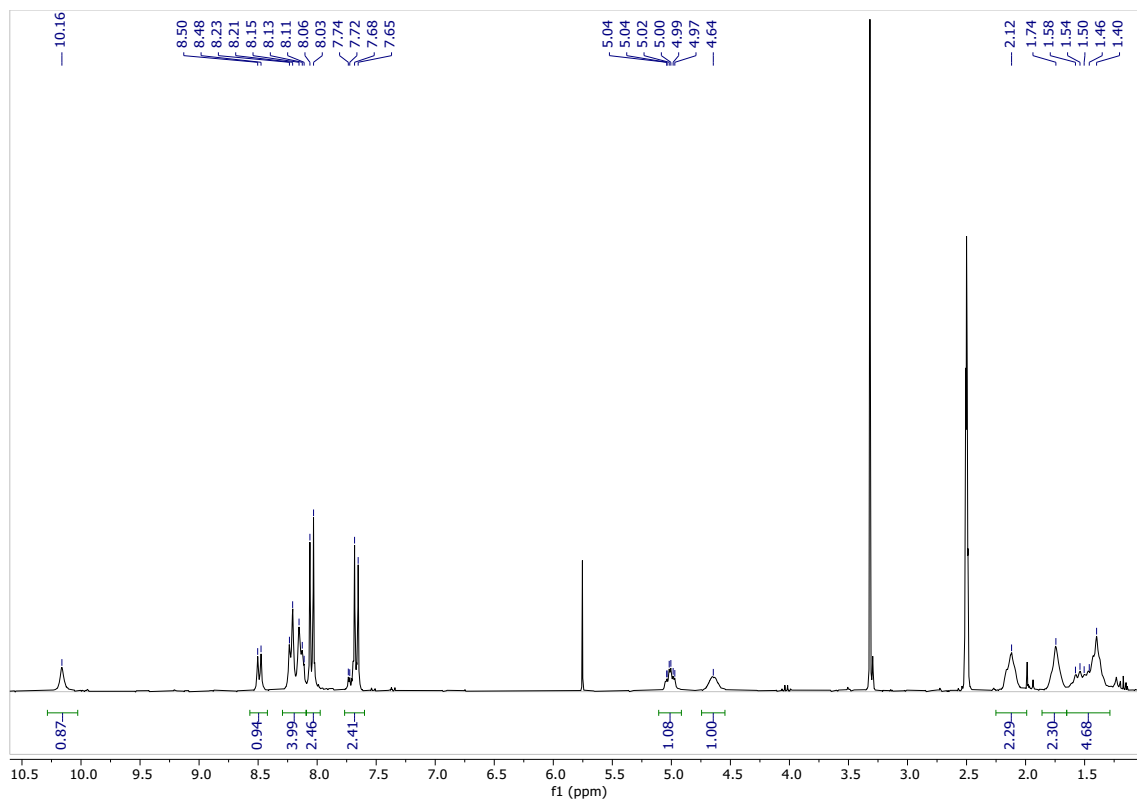


Figure S7.  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{DMSO-}d_6$ .

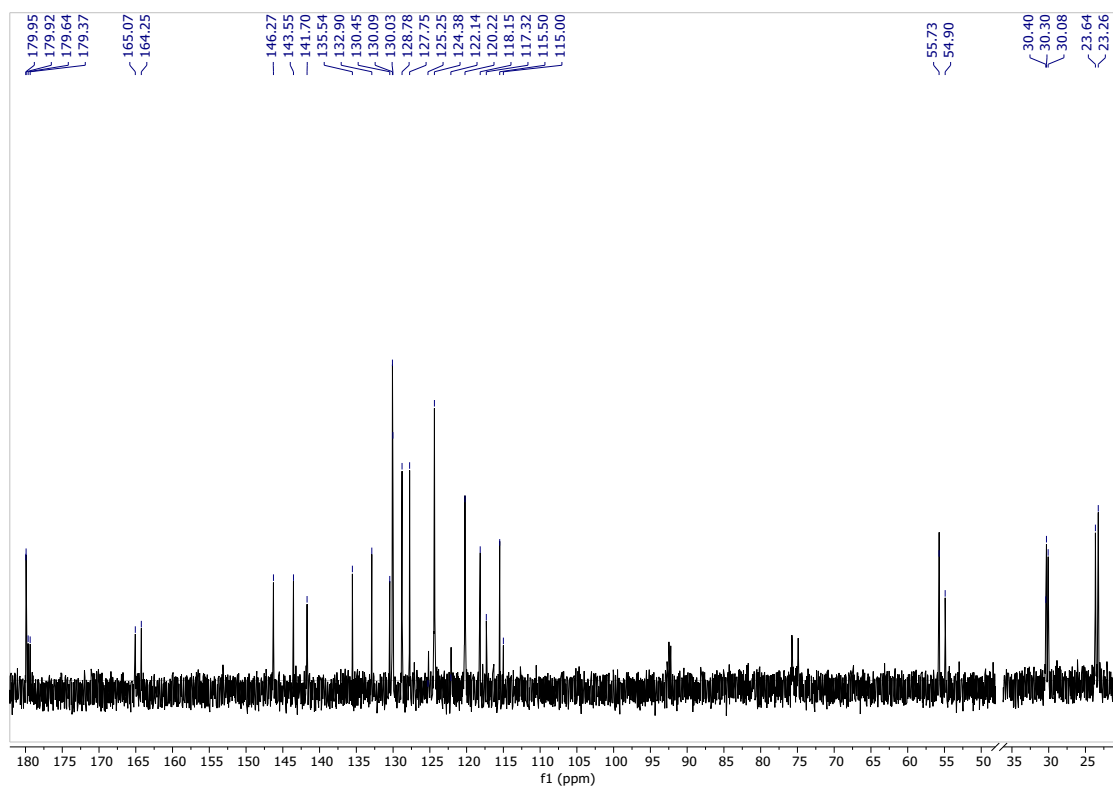


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{DMSO-}d_6$ .

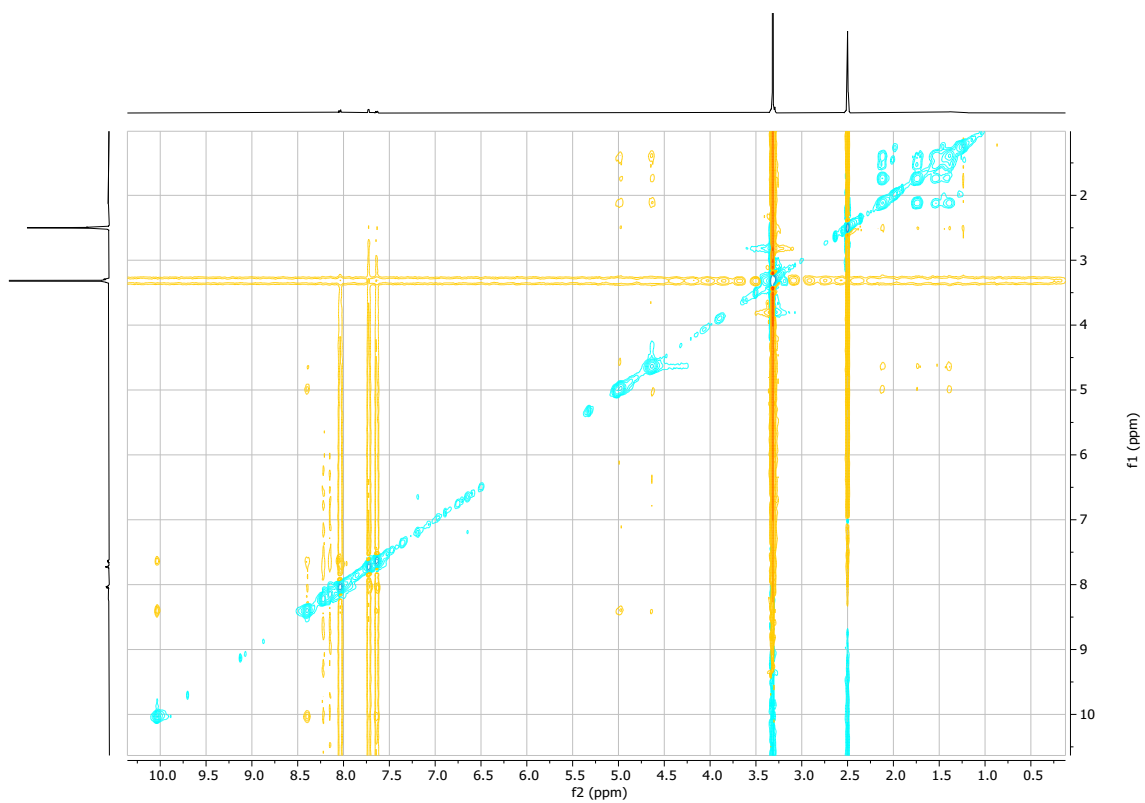


Figure S9. NOESY spectrum of compound **2** in DMSO- $d_6$ .

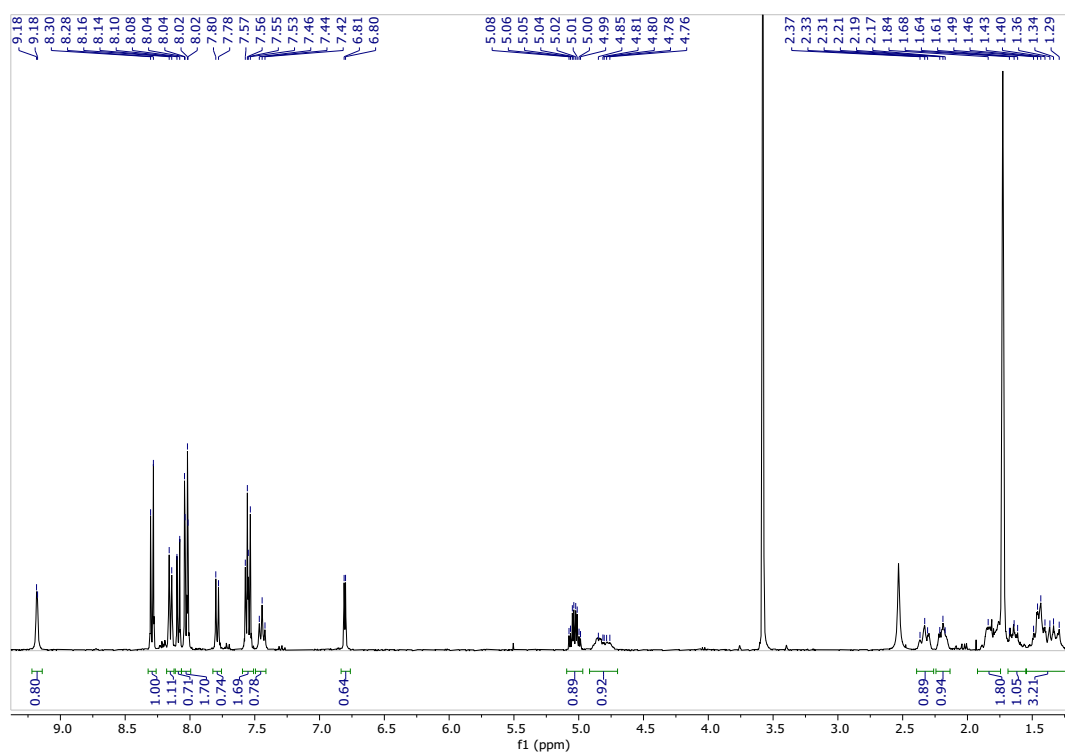


Figure S10.  $^1\text{H}$  NMR spectrum of compound **2** in THF- $d_8$ .

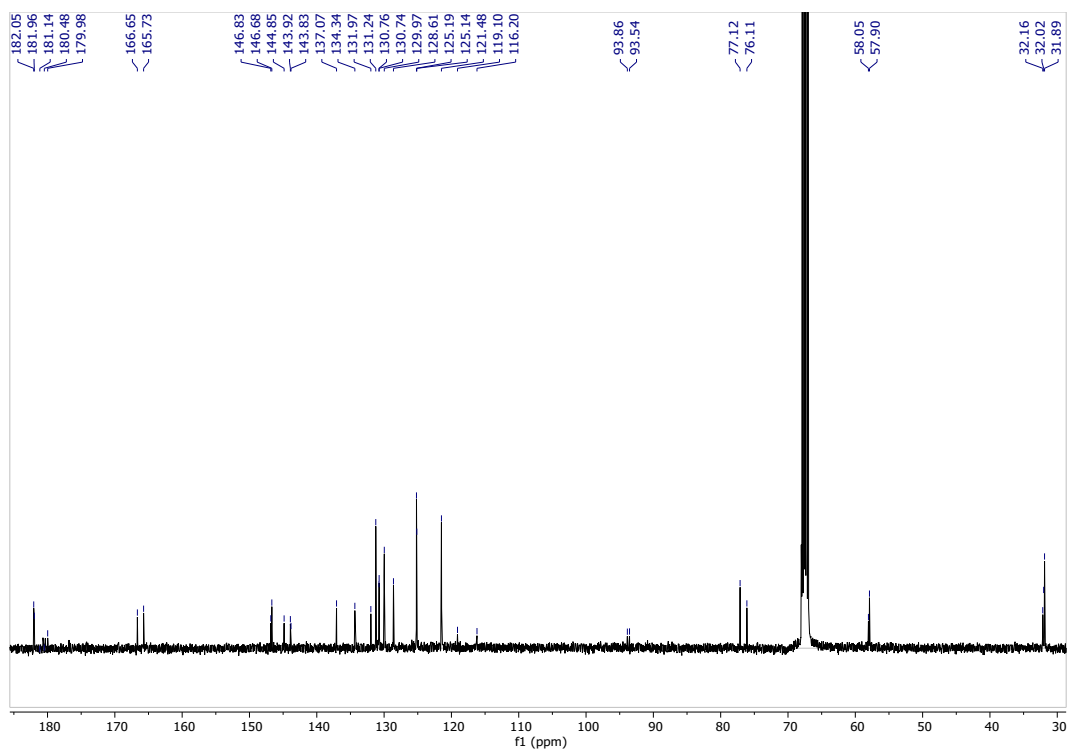


Figure S11.  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{THF-}d_8$ .

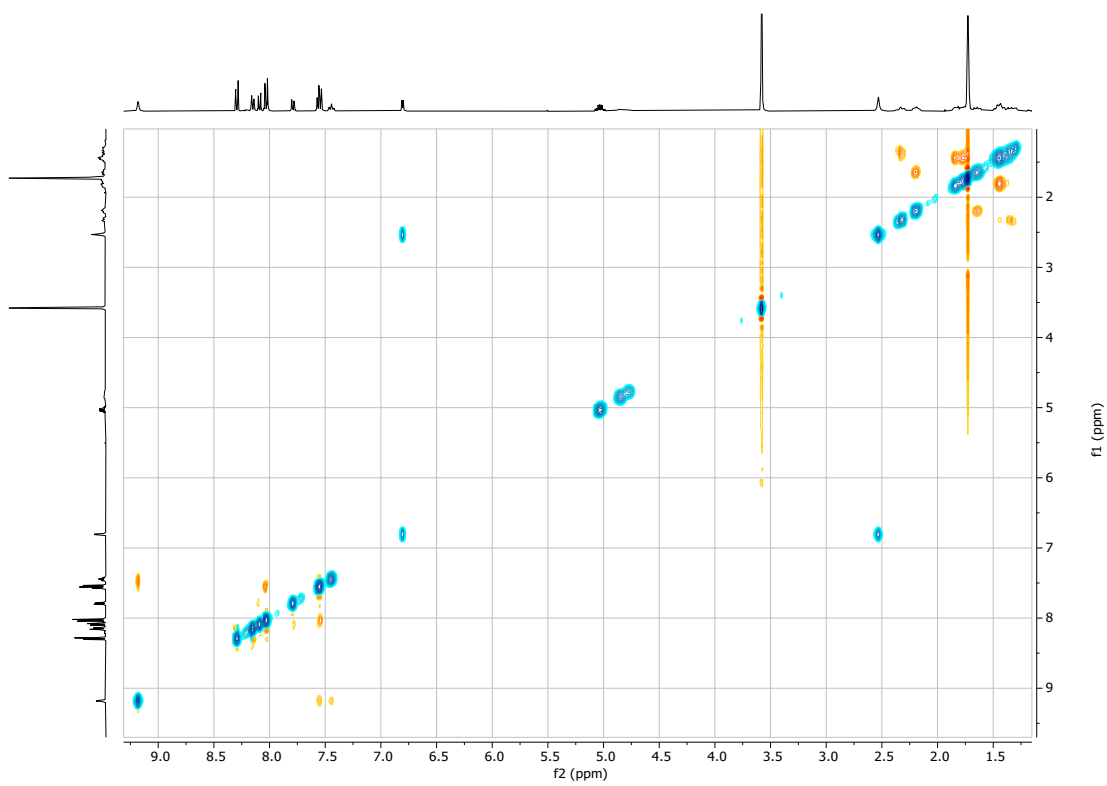


Figure S12. NOESY spectrum of compound **2** in  $\text{THF-}d_8$ .

## Mass Spectrometry Spectra

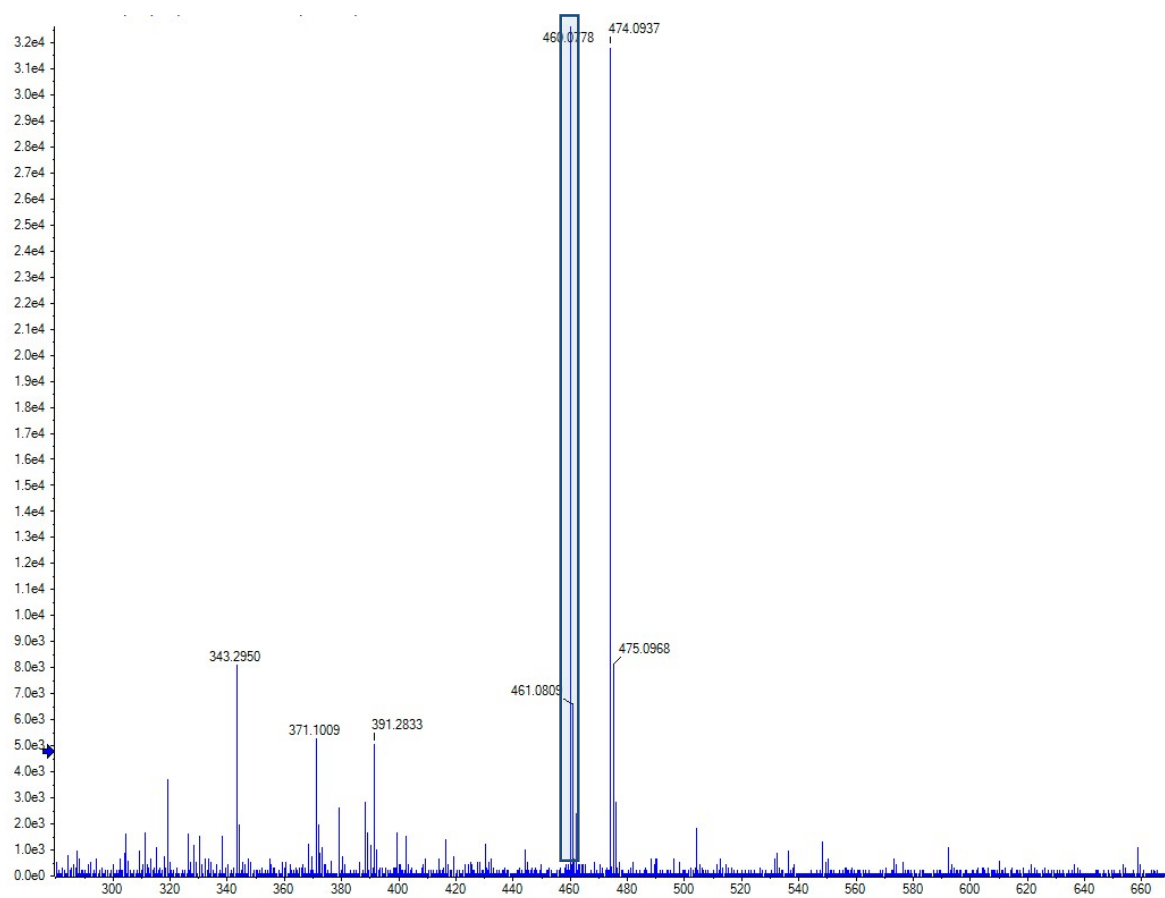
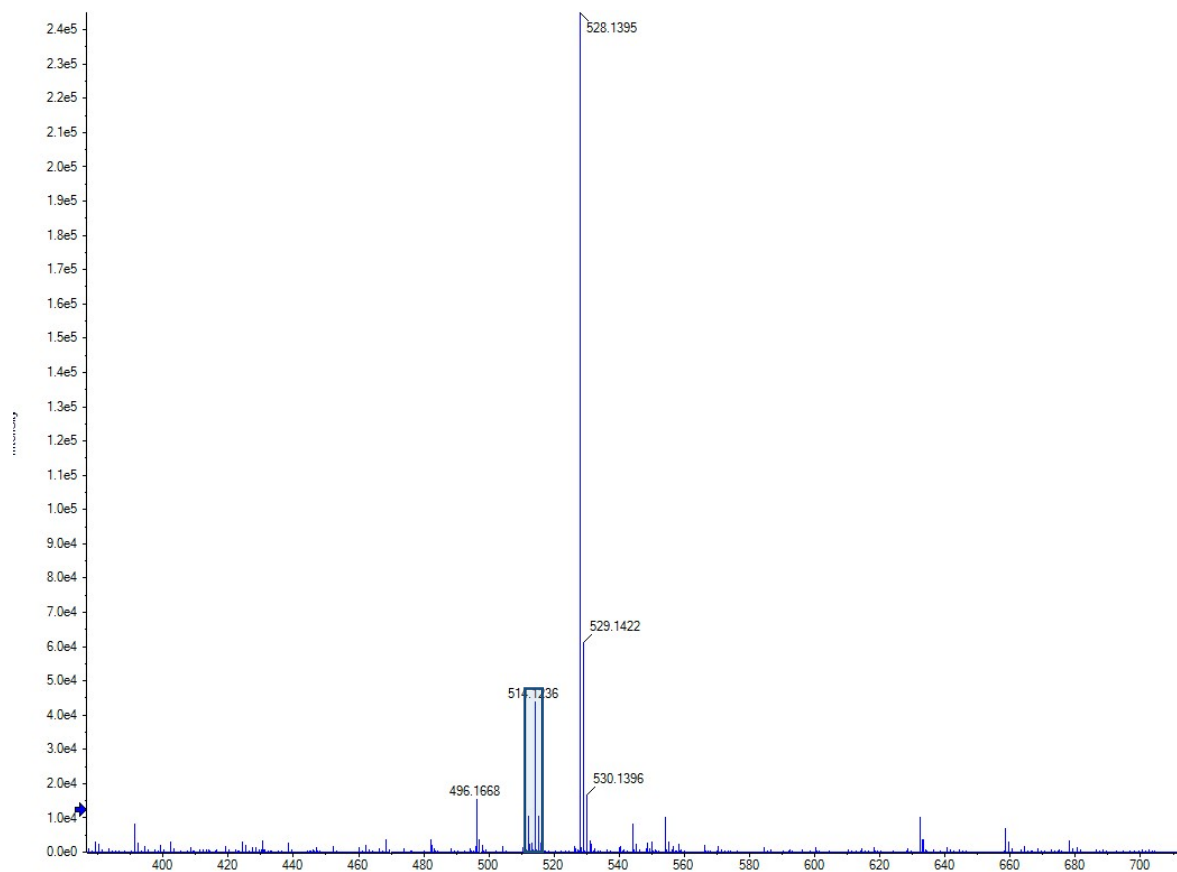
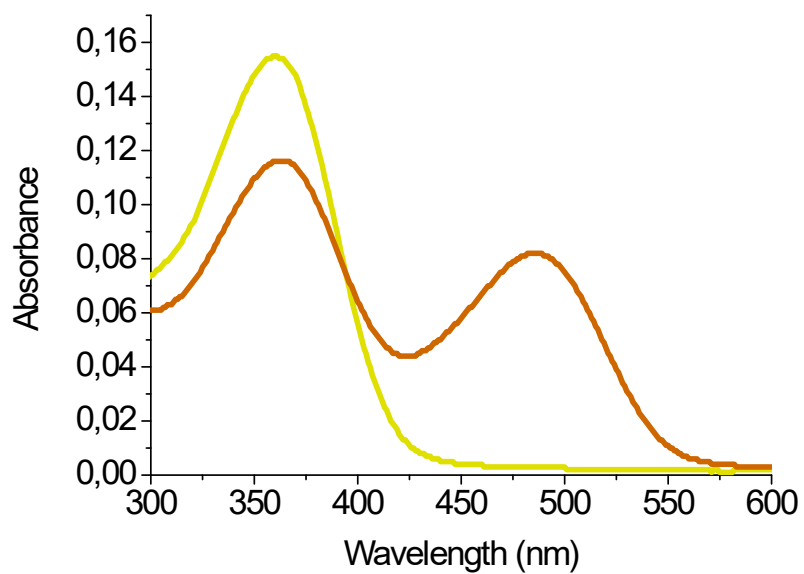


Figure S13. Mass Spectrum of compound 1.



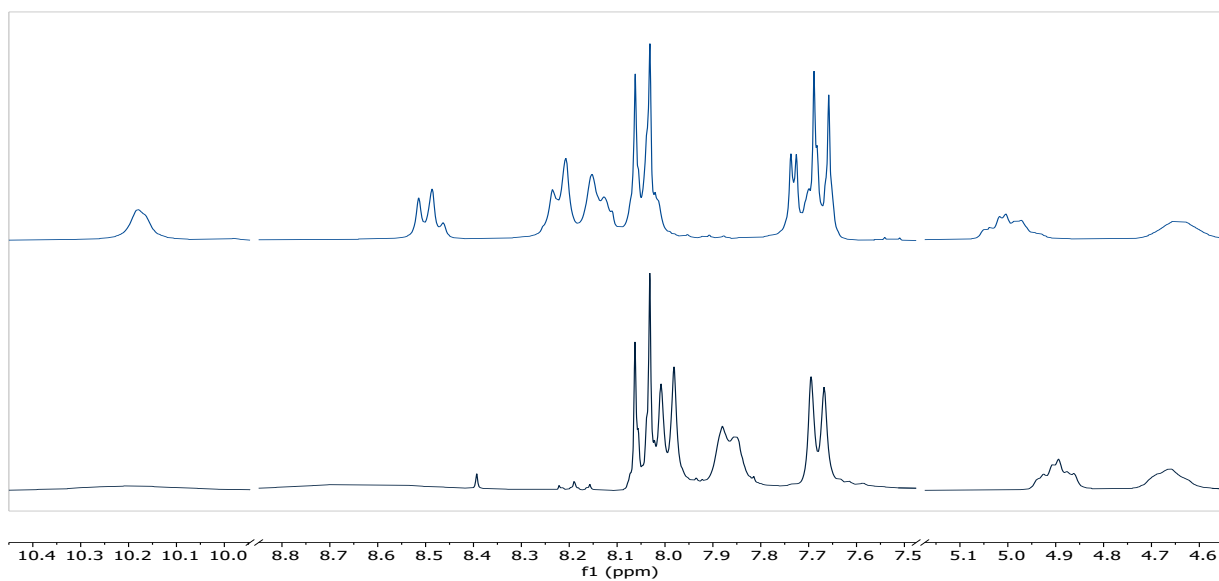
**Figure S14.** Mass Spectrum of compound 2.

## UV-Vis analysis

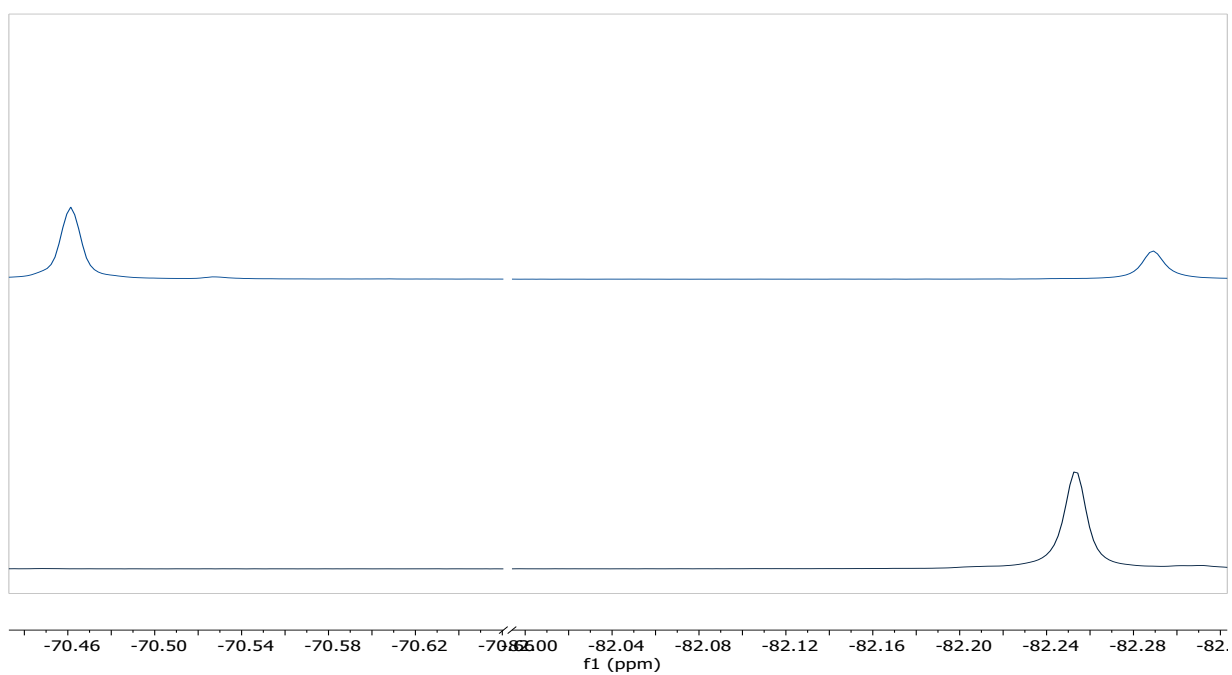


**Figure S15.** Changes observed in UV spectrum of compound **2** in presence of an excess of NaGHB.

## NMR Analysis



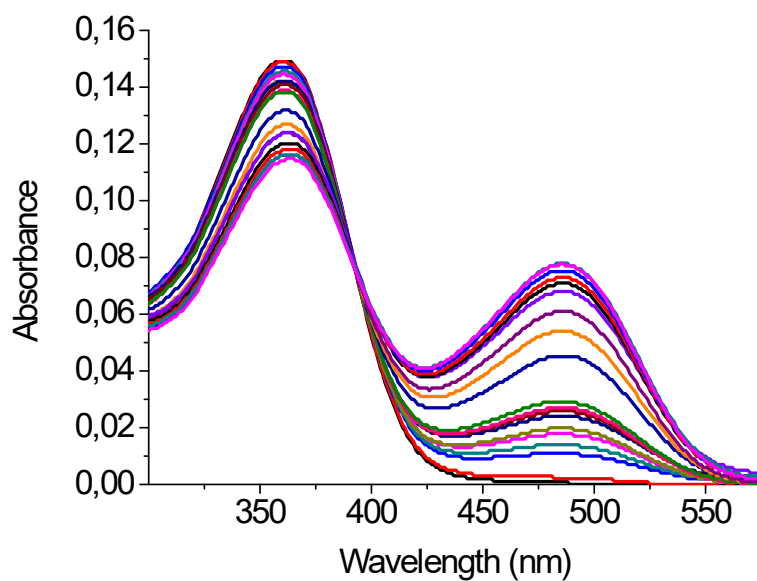
**Figure S16.** Changes observed in  $^1\text{H}$  NMR spectrum of **2** in presence of an excess of GHB in  $\text{DMSO-}d_6$ .



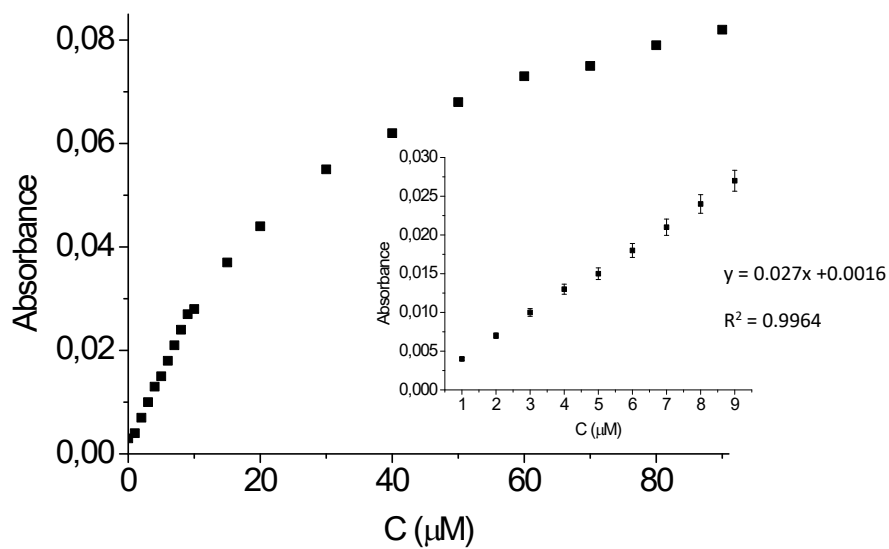
**Figure S17.** Changes observed in  $^{19}\text{F}$  NMR spectrum of **2** in presence of an excess of GHB in  $\text{DMSO-}d_6$ .



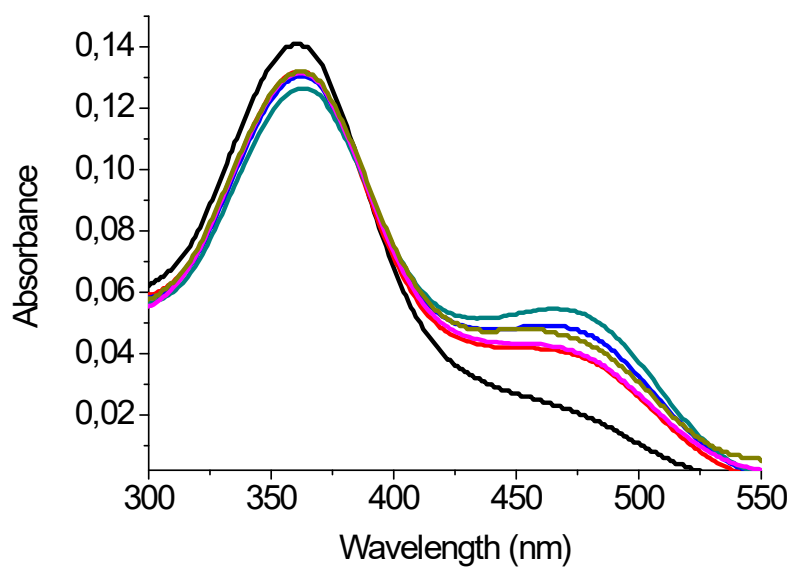
## UV-Vis titrations spectra



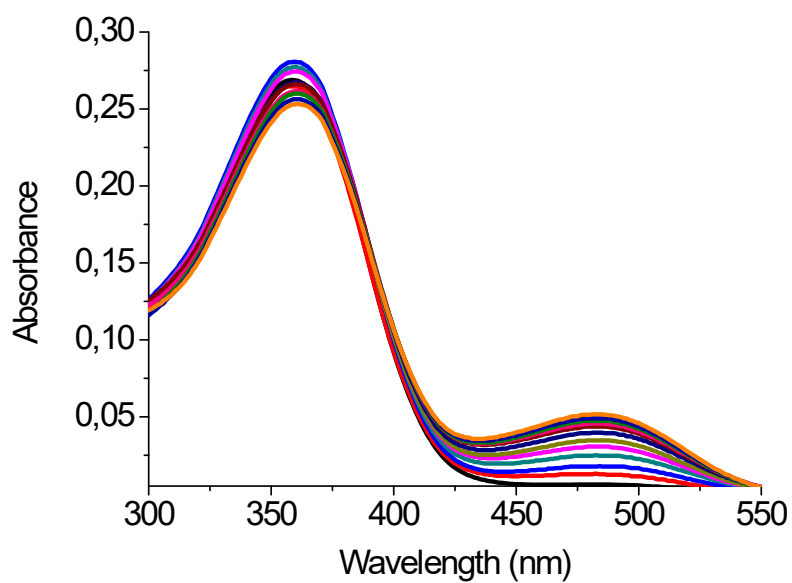
**Figure S18.** UV-visible spectra of probe **2** with increasing amounts of GHB (0–10 eq.) in DMSO (10  $\mu$ M of **2**)



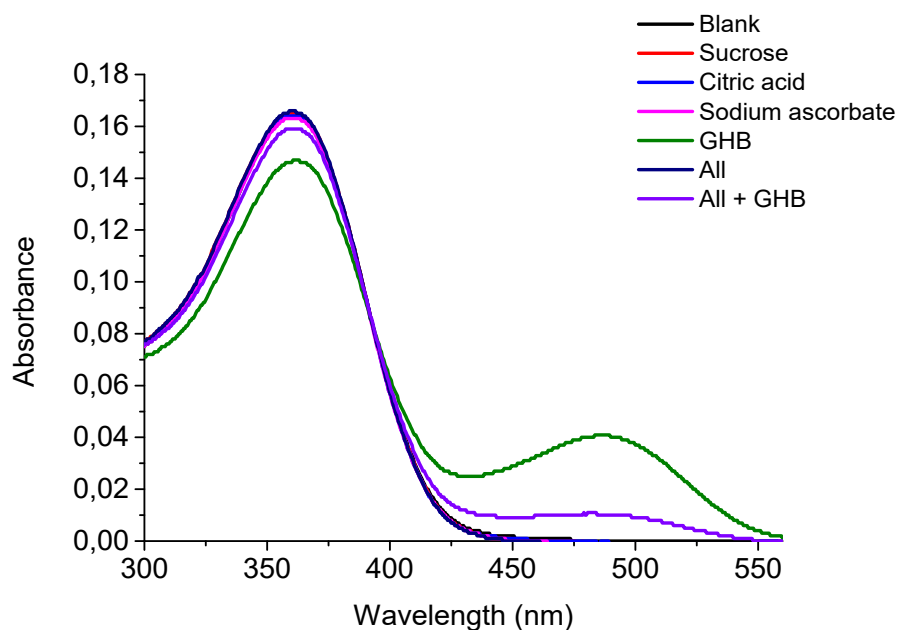
**Figure S19.** Changes in the absorbance at 485 nm of DMSO solutions of probe **2** upon the addition of increasing amounts of GHB



**Figure S20.** UV-visible changes of probe **1** with increasing amounts of GHB (0–21 eq.) in DMSO:H<sub>2</sub>O 95:5 media (10  $\mu$ M of **1**).



**Figure S21.** UV-visible changes of probe **2** with increasing amounts of GHB (0–42 eq.) in DMSO:H<sub>2</sub>O 95:5 media (10  $\mu$ M of **2**).



**Figure S22.** Absorbance spectra of **2** (10  $\mu\text{M}$  in DMSO) in the presence of citric acid, sodium ascorbate, sucrose (in real concentration present in beverages) and NaGHB (1 eq).

**Table S2.** Recovery and accuracy determination of the method to probe **1**. Recovery and accuracy of the method were calculated according to reference K. A. Rawat, R.K. Singhal, S. K. Kailasa, *RSC Advances*, 2016, **6**, 32025.

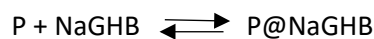
KNOWN CONCENTRATION ( $\mu\text{M}$ )	FOUND CONCENTRATION ( $\mu\text{M}$ )	RECOVERY % <sup>a</sup>	ACCURACY % <sup>b</sup>
5	4.48	89.50	-10,50

<sup>a</sup> % recovery (found concentration/known concentration) x 100

<sup>b</sup> % accuracy (found concentration – known concentration/known concentration) x 100

### Constant determination

The binding process can be described by the reaction



P= Probe, P@NaGHB = complex

The equilibrium constant was defined as  $K = \frac{[P@NaGHB]}{[P][NaGHB]}$

The analysis of the titration curves were done according to the following equation:[1]

$$\left[ \frac{C_P C_{NaGHB}}{\Delta A} \right] + \left( \frac{\Delta A}{\Delta \epsilon^2} \right) = \left( \frac{1}{K \Delta \epsilon} \right) + \left[ \frac{C_P + C_{NaGHB}}{\Delta \epsilon} \right]$$

where:

$C_P$  and  $C_{NaGHB}$  are the total probe and drug concentrations

$$\Delta A = A - \epsilon_p C_p$$

$$\epsilon_p = \Delta A^0 / C_p, A^0 \text{ initial absorbance of NaGHB}$$

$$\Delta\varepsilon = \varepsilon_{p@NaGHB} - \varepsilon_p$$

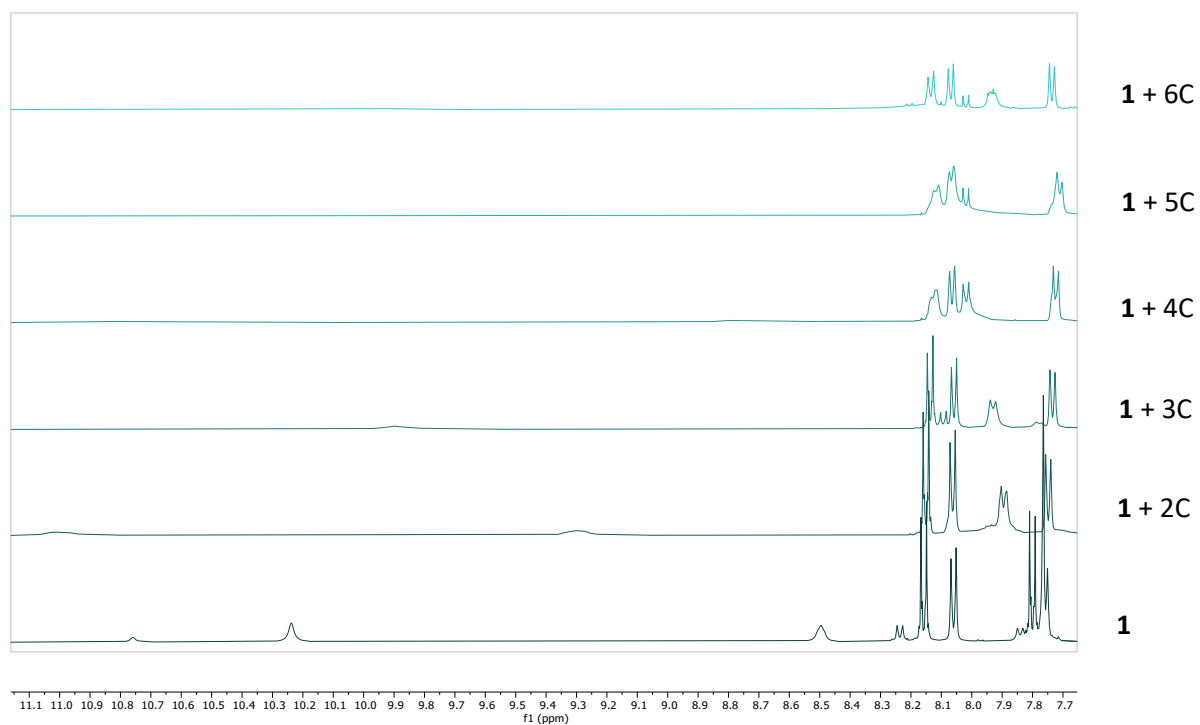
Iterations were carried out using Origin 2000.

[1] Borja Díaz de Greñu, José García-Calvo, José Cuevas, Gabriel García-Herbosa,<sup>a</sup> Begoña Garía, Natalia Busto, Saturnino Ibeas, Tomás Torroba, Blanca Torroba, Antonio Herrera and Sebastian Pons, *Chem. Sci.*, 2015, 6, 3757

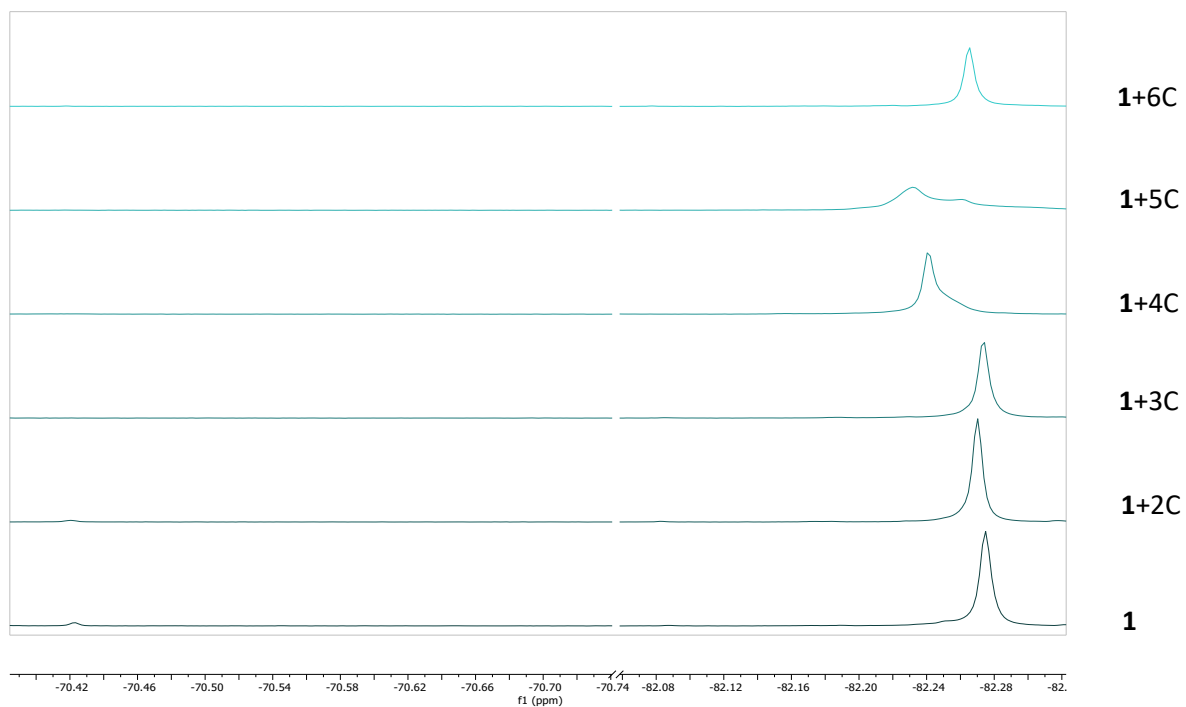
## $\omega$ -hydroxyacids analysis

### NMR essays

A solution 100 mM of **1** and 100 mM of each  $\omega$ -hydroxyacid were prepared in DMSO- $d_6$ . 50  $\mu$ L of solution of **1** and 50  $\mu$ L of solution of each  $\omega$ -hydroxyacid were mixed and then diluted until 500  $\mu$ L with DMSO- $d_6$ .



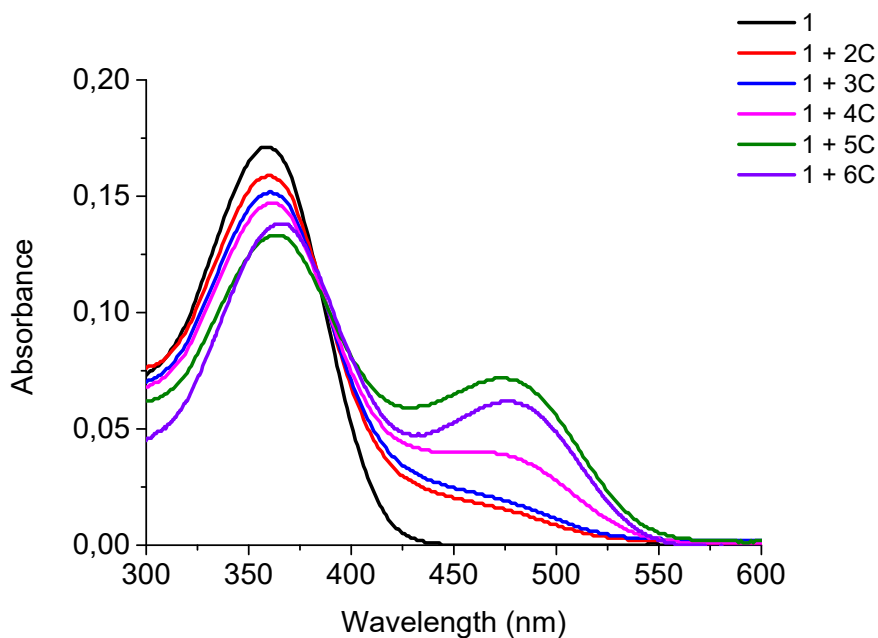
**Figure S23.** Changes observed in  $^1\text{H}$  NMR spectrum of **1** in presence of 1 eq. of  $\omega$ -hydroxyacids of  $n$  carbon atoms in DMSO- $d_6$ .



**Figure S24.** Changes observed in  $^{19}\text{F}$  NMR spectrum of **1** in presence of 1 eq of  $\omega$ -hydroxyacid in  $\text{DMSO-}d_6$ .

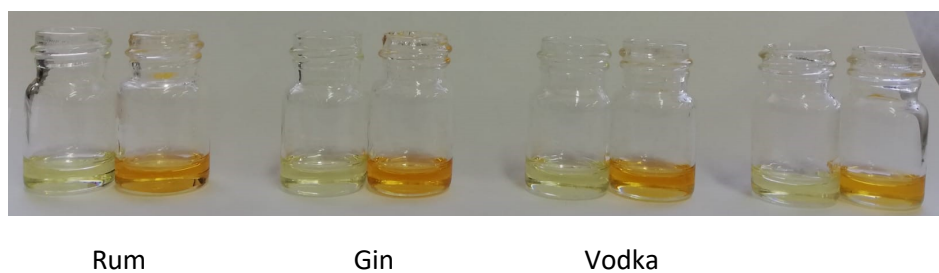
#### UV-Vis essays

In a cuvette of 3 mL, 3  $\mu\text{L}$  of solution of **1** (100 mM in DMSO) and 9.9  $\mu\text{L}$  of solution of each  $\omega$ -hydroxyacid (100 mM in DMSO) were mixed and diluted until 3000  $\mu\text{L}$  with DMSO.

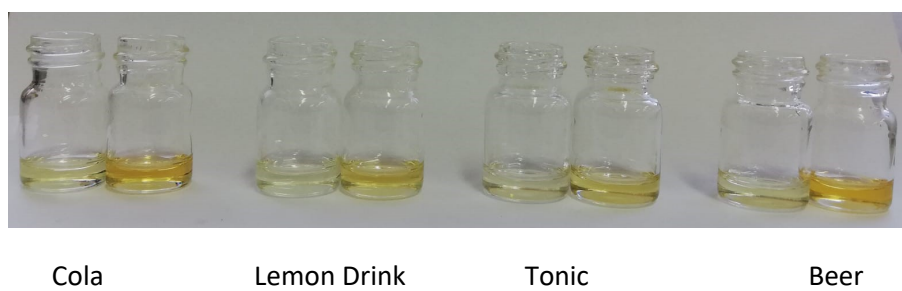


**Figure S25.** Changes observed in UV-Vis spectrum of **1** in presence of 3.3 eq. of  $\omega$ -hydroxyacids in DMSO.

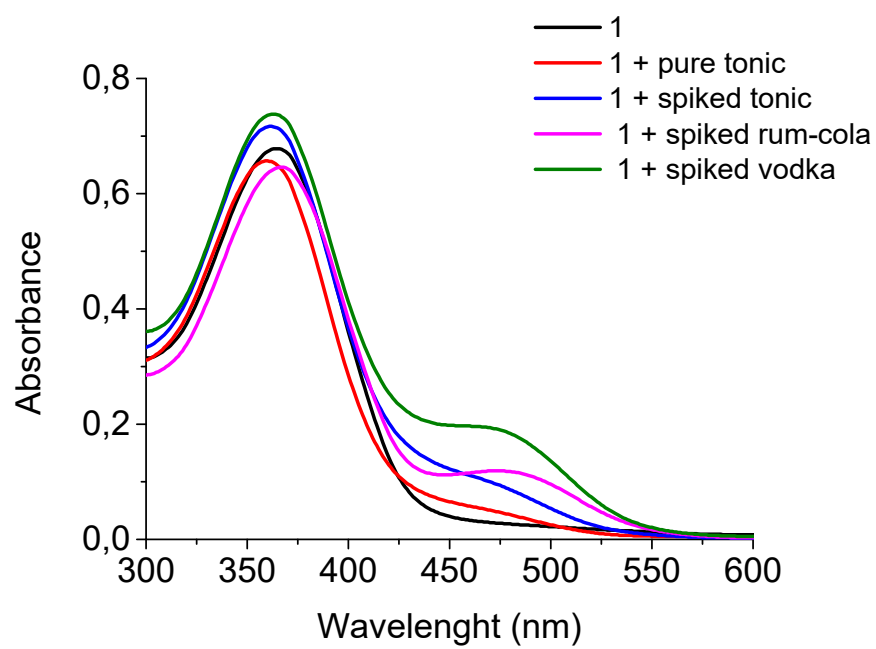
## Real Samples Analysis



**Figure S26.** Colour changes observed in real samples with compound **2** (alcoholic drinks).



**Figure S27.** Colour changes observed in real samples with compound **2** (soft drinks and beverages).



**Figure S28.** Changes observed in UV-Vis spectrum of **1** pure and in presence of spiked rum-cola, spiked vodka, spiked tonic and pure tonic. Sensor 60  $\mu$ M in DMSO in presence of GHB 0.75 mM in the spiked samples. (percent of water < 5%)



## Theoretical calculations

Complete reference for Gaussian09, Rev. D.01:

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

The following Supporting Information section, which contains the details of computational calculations performed in this work, has been structured in the following subsections (which, in turn, has its own bibliographic references included at the end):

- **Part 1** - Computational methods. In this section, computational details about the geometrical optimizations and the vertical excitation analysis are given.
- **Part 2** - Figure of X3LYP/6-31G(d)/PCM(DMSO) energy barrier profiles along restricted singlet potential energy hypersurface (PES) of the dihedral angle of both NH-C bonds at the reduced 1-methyl-3-(4-nitrophenyl)thiourea going from *Z* to *E* rotamer (relaxed PES scan, 12 points, 15° each one at the corresponding dihedral angle).
- **Part 3** -Figure of X3LYP/6-31G(d)/PCM(DMSO) energy barrier profiles along restricted singlet PES of the dihedral angle of both NH-C bonds of compound **1** (starting from one of its selected minimum-energy optimized conformations) going from *Z* to *E* rotamer (relaxed PES scan, 12 points, 15° each one at the corresponding dihedral angle).
- **Part 4** -Figure of X3LYP/6-31G(d)/PCM(DMSO) energy barrier profiles along restricted singlet PES of the dihedral angle of both NH-C bonds of compound **2** (starting from one of its selected minimum-energy optimized conformations) going from *Z* to *E* rotamer (relaxed PES scan, 12 points, 15° each one at the corresponding dihedral angle).
- **Part 5** -X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures for the different 32 starting rotamers found along the full-search of the PES for chemosensor **1**. Starting structures were the six different eclipsed and staggered conformers along the C-C ethylenic bond as well as the *E,E*-, *E,Z*-, *Z,E*- and *Z,Z*- thiourea conformers and rotamers around –CH<sub>2</sub>-O-C(=O)-Ar dihedral angle. Distances between C=O of trifluoromethyl acetate group and C=S thiourea carbon atoms are also depicted.
- **Part 6** -X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures for the different 28 starting rotamers found along the full-search of the PES for chemosensor **2**. Starting structures were the different ester and thiourea diaxial 1,2-*anti*- or diequatorial 1,2-*anti*- diastereoisomers over the cyclohexane ring together with the rotamers around –CH<sub>2</sub>-O-C(=O)-Ar dihedral angle. Distances between C=O of trifluoromethyl acetate group and C=S thiourea carbon atoms are also depicted.

- **Part 7** - Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **1** at the same theory level (30 states, singlets only).
- **Part 8** - Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **2** at the same theory level (30 states, singlets only).
- **Part 9** - X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures of **1-GHB** derivatives with hydrogen bonds between the thiourea and carboxylate moieties and between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group.
- **Part 10** - X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures of **2-GHB** derivatives with hydrogen bonds between the thiourea and carboxylate moieties and between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group.
- **Part 11** - Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of X3LYP/6-31+G(d,p)/PCM(DMSO) **1-GHB** optimized geometries at the same theory level (15 states, singlets only).
- **Part 12** - Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of X3LYP/6-31+G(d,p)/PCM(DMSO) **2-GHB** optimized geometries at the same theory level (15 states, singlets only).
- **Part 13** - X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures for chemosensor **2-GHB** with and without hydrogen bond between the hydroxyacid carboxylate and thiourea moiety with increasing hydroxyacid chain (3 to 7 carbon atoms).
- **Part 14** – X3LYP/6-31+G(d,p)/PCM(DMSO) energies of butyric acid and 1-methyl-3-(4-nitrophenyl)thiourea in different hydrogen-bonded complexes in different protonation states.
- **Annex I**: XYZ cartesian coordinates of the optimized energies of 32 starting rotamers of chemosensor **1**.
- **Annex II**: XYZ cartesian coordinates of the optimized energies of 28 starting rotamers of chemosensor **1**.
- **Annex III**: XYZ cartesian coordinates of the optimized energies of several **1-GHB** geometries bearing different hydrogen bonding modes between the thiourea and carboxylate moieties.
- **Annex IV**: XYZ cartesian coordinates of the optimized energies of several **2-GHB** geometries bearing different hydrogen bonding modes between the thiourea and carboxylate moieties.
- **Annex V**: XYZ cartesian coordinates of the optimized energies of the two **2-GHB** series (with and without hydrogen bond) with increasing hydroxyacid chain.

#### Part 1 - Computational methods.

In order to gain insight in the behavior of chemosensors **1** and **2** with and without the presence of GHB, DFT calculations have been carried out using Gaussian09 rev. D01 program package[a] and GaussView 5 [b] was employed to visualize the results. The geometrical optimization was performed using the X3LYP hybrid DFT functional of Xu and Goddard[c] which accounts for the accurate description of nonbonding interactions as those we are dealing here with **1-GHB** and **2-GHB** structures. The double- $\zeta$  6-31+G(d,p) basis set[d] was used in the optimization of the real systems although for the sake of simplicity, 6-31G(d) basis set was used to perform the relaxed PES scan along the dihedral angle of both NH-C thiourea bonds at the reduced and complete

models. To take into account the effect of the solvent, DMSO, PCM solvation model was used[e]. Frequency calculations were performed over optimized structures to properly characterize minima structures (no imaginary frequencies).

On the other hand, to explore the electronic transitions responsible for the UV-Vis spectra, vertical excitation energies were computed over X3LYP/6-31+G(d,p)/PCM(DMSO) geometries through single-point TD-DFT[f] calculations (15 states, singlets only) in solution using non-equilibrium formalism at the same theory level. Geometry details of all optimized geometries as well as excitation energies, oscillator strengths, spin and spatial symmetry,  $S^2$  and largest coefficients in the CI expansion for all TD-DFT vertical excitation energies computed for **1**, **2**, **1-GHB** and **2-GHB** geometries can be found in the different Annex sections.

[a] Gaussian 09, Revision D.01. See complete reference at the beginning of the theoretical calculations at the Supporting Information.

[b] GaussView, Version 5, Roy Dennington, Todd Keith, and John Millam, Semichem Inc., Shawnee Mission, KS, 2009.

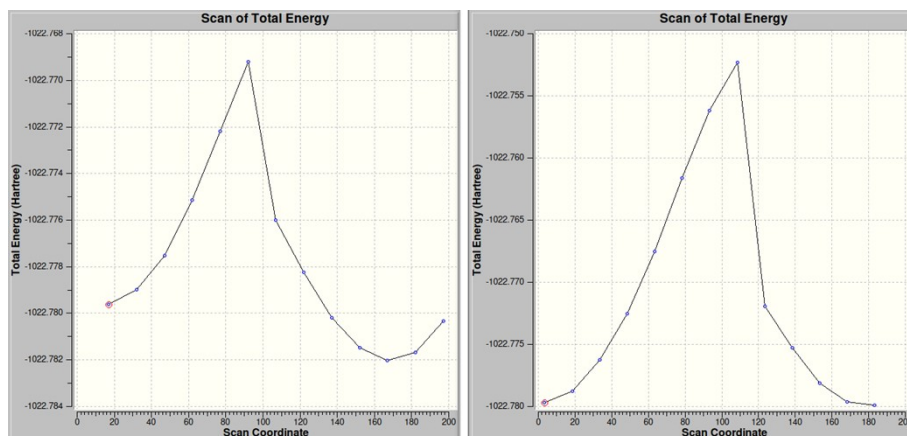
[c] X. Xu, W. A. Goddard III, Proc. Natl. Acad. Sci. USA, 101 (2004) 2673-77.

[d] a) G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Al-Laham, W. A. Shirley, and J. Mantzaris, "A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row atoms," J. Chem. Phys., 89 (1988) 2193-218. b) G. A. Petersson and M. A. Al-Laham, "A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms," J. Chem. Phys., 94 (1991) 6081-90. c) A. D. McLean and G. S. Chandler, "Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18," J. Chem. Phys., 72 (1980) 5639-48. d) K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, "Self-Consistent Molecular Orbital Methods. 20. Basis set for correlated wave-functions," J. Chem. Phys., 72 (1980) 650-54. e) J.-P. Blaudeau, M. P. McGrath, L. A. Curtiss, and L. Radom, "Extension of Gaussian-2 (G2) theory to molecules containing third-row atoms K and Ca," J. Chem. Phys., 107 (1997) 5016- 21. f) A. J. H. Wachters, "Gaussian basis set for molecular wavefunctions containing third-row atoms," J. Chem. Phys., 52 (1970) 1033. g) P. J. Hay, "Gaussian basis sets for molecular calculations – representation of 3D orbitals in transition-metal atoms," J. Chem. Phys., 66 (1977) 4377-84. h) K. Raghavachari and G. W. Trucks, "Highly correlated systems: Excitation energies of first row transition metals Sc-Cu," J. Chem. Phys., 91 (1989) 1062-65. i) R. C. Binning Jr. and L. A. Curtiss, 16 "Compact contracted basis-sets for 3rd-row atoms – GA-KR," J. Comp. Chem., 11 (1990) 1206-16. j) M. P. McGrath and L. Radom, "Extension of Gaussian-1 (G1) theory to bromine-containing molecules," J. Chem. Phys., 94 (1991) 511-16. k) L. A. Curtiss, M. P. McGrath, J.-P. Blaudeau, N. E. Davis, R. C. Binning Jr., and L. Radom, "Extension of Gaussian-2 theory to molecules containing third-row atoms Ga-Kr," J. Chem. Phys., 103 (1995) 6104-13.

[e] G. Scalmani and M. J. Frisch, "Continuous surface charge polarizable continuum models of solvation. I. General formalism," J. Chem. Phys., 132 (2010) 114110.

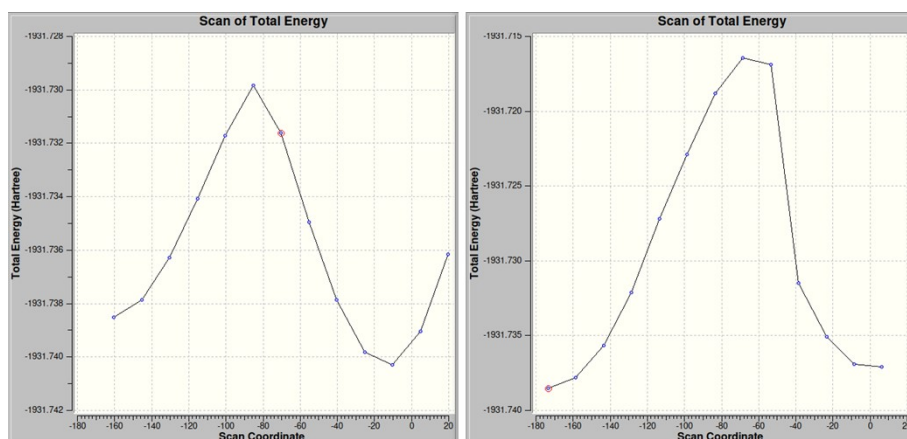
[f] a) C. Adamo and D. Jacquemin, "The calculations of excited-state properties with Time-Dependent Density Functional Theory," Chem. Soc. Rev., 2013, 42, 845. b) A. D. Laurent, C. Adamo, D. Jacquemin, "Dye chemistry with time-dependent density functional theory," Phys. Chem. Chem. Phys., 2014, 16, 14334-56.

**Part 2** –X3LYP/6-31G(d)/PCM(DMSO) energy profile of the dihedral bond rotation from Z to E rotamer for both NH-C thiourea bonds (N3H-C, left and N1H-C, right) at the reduced 1-methyl-3-(4-nitrophenyl)thiourea model. The energy difference between the first and the most energetic rotamer in the profile is 6.5 (N<sub>3</sub>H-C) and 17.2 kcal/mol (N<sub>1</sub>H-C), respectively.



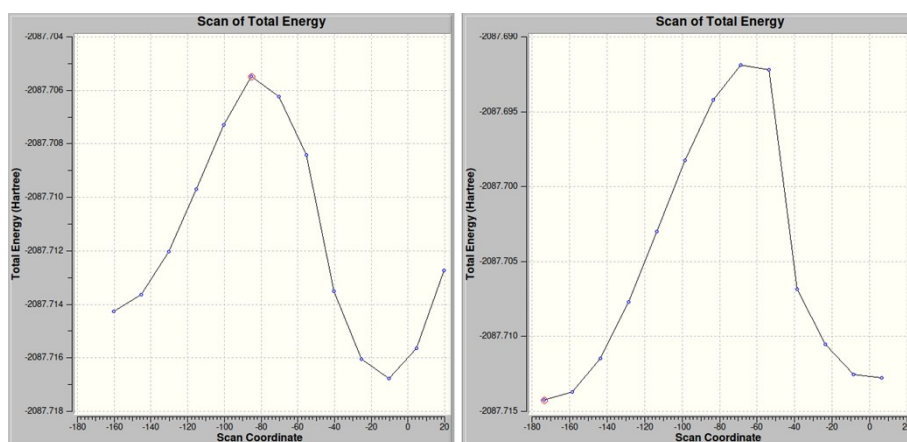
**Figure S29.** N<sub>3</sub>H-C (left) and N<sub>1</sub>H-C (right) energy profile of the dihedral bond-rotation from Z to E rotamer at 1-methyl-3-(4-nitrophenyl)thiourea.

**Part 3** –X3LYP/6-31G(d)/PCM(DMSO) energy profile of the dihedral bond rotation from Z to E rotamer for both NH-C thiourea bonds (N3H-C, left and N1H-C, right) at chemosensor **1**. The energy difference between the first and the most energetic rotamer in the profile is 5.5 (N<sub>3</sub>H-C) and 13.9 kcal/mol (N<sub>1</sub>H-C), respectively.



**Figure S30.** N<sub>3</sub>H-C (left) and N<sub>1</sub>H-C (right) energy profile of the dihedral bond-rotation from Z to E rotamer at chemosensor **1**.

**Part 4** –X3LYP/6-31G(d)/PCM(DMSO) energy profile of the dihedral bond rotation from Z to E rotamer for both NH-C thiourea bonds (N3H-C, left and N1H-C, right) at chemosensor **2**. The energy difference between the first and the most energetic rotamer in the profile is 5.5 (N<sub>3</sub>H-C) and 13.9 kcal/mol (N<sub>1</sub>H-C), respectively.



**Figure S31.**  $N_3H-C$  (left) and  $N_1H-C$  (right) energy profile of the dihedral bond-rotation from Z to E rotamer at chemosensor **2**.

**Part 5** -X3LYP/6-31+G(d,p)/PCM(DMSO) energy and (C=O)-(C=S) distance of the optimized structures of the rotamers found along the full-search of the PES for chemosensor 1.

**Table S3.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy (E, in hartrees), energy difference ( $\Delta E$ , in kcal/mol) with respect to the most stable structure and distance between C=O of trifluoromethyl acetate group and C=S thiourea carbon atoms ( $d_{(C=O)-(C=S)}$ , in angstroms) for the optimized structures of chemosensor **1** rotamers.

Structure	E (hartrees)	$\Delta E$ (kcal/mol)	$d_{(C=O)-(C=S)}$ ( $\text{\AA}$ )
<b>1-conf1</b>	-1931,820057	10,6	8,14
<b>1-conf2</b>	-1931,833730	2,0	10,83
<b>1-conf3</b>	-1931,821545	9,6	8,08
<b>1-conf4</b>	-1931,835218	1,1	10,82
<b>1-conf5</b>	-1931,818129	11,8	7,93
<b>1-conf6</b>	-1931,831972	3,1	10,87
<b>1-conf7</b>	-1931,815870	13,2	8,67
<b>1-conf8</b>	-1931,829810	4,5	10,98
<b>1-conf9</b>	-1931,820038	10,6	9,40
<b>1-conf10</b>	-1931,834990	1,2	9,43
<b>1-conf11</b>	-1931,823127	8,7	9,39
<b>1-conf12</b>	-1931,836035	0,6	8,15
<b>1-conf13</b>	-1931,823717	8,3	9,11
<b>1-conf14</b>	-1931,833079	2,4	8,07
<b>1-conf15</b>	-1931,817851	12,0	9,22
<b>1-conf16</b>	-1931,831860	3,2	8,40
<b>1-conf17</b>	-1931,820042	10,6	9,22
<b>1-conf18</b>	-1931,834246	1,7	8,16
<b>1-conf19</b>	-1931,821940	9,4	9,40
<b>1-conf20</b>	-1931,836066	0,5	8,23
<b>1-conf21</b>	-1931,823759	8,3	9,13
<b>1-conf22</b>	-1931,834246	1,7	8,05
<b>1-conf23</b>	-1931,817851	12,0	9,22
<b>1-conf24</b>	-1931,831879	3,2	8,39
<b>1-conf25</b>	-1931,821427	9,7	9,42
<b>1-conf26</b>	-1931,835008	1,2	9,44

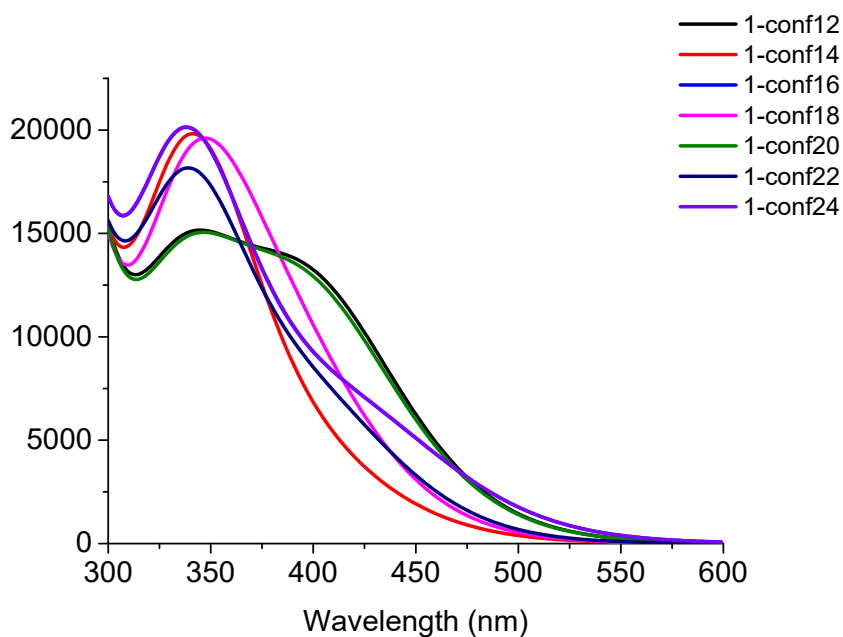
<b>1-conf27</b>	-1931,823127	8,7	9,39
<b>1-conf28</b>	-1931,836917	0,0	9,39
<b>1-conf29</b>	-1931,819072	11,2	9,36
<b>1-conf30</b>	-1931,833163	2,4	9,26
<b>1-conf31</b>	-1931,818218	11,7	9,83
<b>1-conf32</b>	-1931,832086	3,0	9,49

**Part 6** -X3LYP/6-31+G(d,p)/PCM(DMSO) energy and (C=O)-(C=S) distance of the optimized structures of the rotamers found along the full-search of the PES for chemosensor **2**.

**Table S4.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy (*E*, in hartrees), energy difference ( $\Delta E$ , in kcal/mol) with respect to the most stable structure and distance between C=O of trifluoromethyl acetate group and C=S thiourea carbon atoms ( $d_{(C=O)-(C=S)}$ , in angstroms) for the optimized structures of chemosensor **2** rotamers.

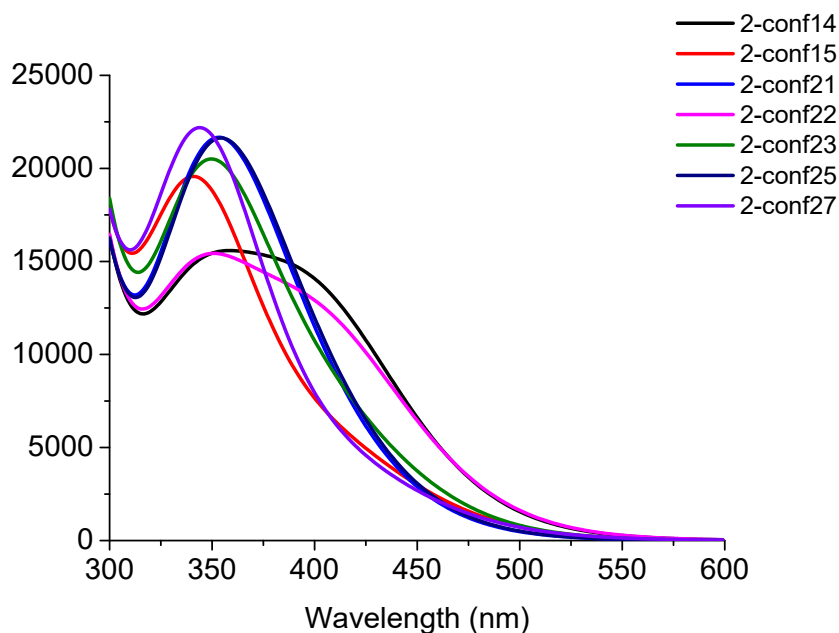
<b>Structure</b>	<b><i>E</i> (hartrees)</b>	<b><math>\Delta E</math> (kcal/mol)</b>	<b><math>d_{(C=O)-(C=S)}</math> (Å)</b>
<b>2-conf1</b>	-2087,804293	12,1	7,20
<b>2-conf2</b>	-2087,805636	11,3	7,29
<b>2-conf3</b>	-2087,803340	12,7	7,03
<b>2-conf4</b>	-2087,800198	14,7	7,06
<b>2-conf5</b>	-2087,804254	12,1	7,24
<b>2-conf6</b>	-2087,805538	11,3	7,35
<b>2-conf7</b>	-2087,803070	12,9	7,05
<b>2-conf8</b>	-2087,800157	14,7	7,04
<b>2-conf9</b>	-2087,817794	3,6	10,52
<b>2-conf10</b>	-2087,819088	2,8	10,48
<b>2-conf11</b>	-2087,816545	4,4	10,57
<b>2-conf12</b>	-2087,813976	6,0	10,51
<b>2-conf13</b>	-2087,815185	5,3	8,49
<b>2-conf14</b>	-2087,817538	3,8	8,61
<b>2-conf15</b>	-2087,815219	5,2	8,38
<b>2-conf16</b>	-2087,807389	10,2	7,84
<b>2-conf17</b>	-2087,810663	8,1	8,32
<b>2-conf18</b>	-2087,812682	6,8	8,54
<b>2-conf19</b>	-2087,810178	8,4	8,32
<b>2-conf20</b>	-2087,803182	12,8	9,09
<b>2-conf21</b>	-2087,815893	4,8	8,43
<b>2-conf22</b>	-2087,817592	3,8	8,45
<b>2-conf23</b>	-2087,818135	3,4	8,56
<b>2-conf24</b>	-2087,811224	7,8	9,07
<b>2-conf25</b>	-2087,821879	1,1	8,63
<b>2-conf26</b>	-2087,823581	0,0	8,77
<b>2-conf27</b>	-2087,820226	2,1	8,84
<b>2-conf28</b>	-2087,817651	3,7	9,03

**Part 7** -Simulated UV-Vis spectra of selected optimized geometries of rotamers of **1**.



**Figure S32.** Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **1** at the same theory level (15 states, singlets only). Please, note that the main band is centered around 340-350 nm and that whenever  $N_3H-C$  thiourea bond adopts an *E* conformation (see **1-conf12** and **1-conf20**), a shoulder at 390 nm appears, which is not seen at the experimental UV-Vis spectra, fact that agrees with the appearance of *Z,Z*-rotamers (the ones that enables chemosensors to establish readily an effective hydrogen-bond interaction with the carboxylate of GHB) as the main ones.

**Part 8** -Simulated UV-Vis spectra of selected optimized geometries of rotamers of **2**.



**Figure S33.** Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **2** at the same theory level (15 states, singlets only). Please, note that the main band is centered around 340-350 nm and that whenever N<sub>3</sub>H-C thiourea bond adopts an *E* conformation (see **1-conf14** and **1-conf22**), a shoulder at 390 nm appears, which is not seen at the experimental UV-Vis spectra, fact that agrees with the appearance of *Z,Z*- rotamers (the ones that enables chemosensors to establish readily an effective hydrogen-bond interaction with the carboxylate of GHB) as the main ones.

**Part 9** - X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures of 1-GHB derivatives with hydrogen bonds between the thiourea and carboxylate moieties and between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group.

**Table S5.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy (*E*, in hartrees), relative energy ( $\Delta E$ , in kcal/mol) and hydrogen-bond type, of the optimized structures of **1-GHB** derivatives with single/double hydrogen bonds between the thiourea and carboxylate or between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group.

Structure	<i>E</i> (hartrees)	$\Delta E$ (kcal/mol)	Hydrogen-bond type
<b>1-GHB-a</b>	-2314,199679	0,00	double HB (carboxylate-thiourea)
<b>1-GHB-b</b>	-2314,191321	5,24	double HB (carboxylate-thiourea)
<b>1-GHB-c</b>	-2314,195948	2,34	double HB (carboxylate-thiourea)
<b>1-GHB-d</b>	-2314,184309	9,64	single HB (carboxylate-thiourea)
<b>1-GHB-e</b>	-2314,181783	11,23	double HB (carboxylic acid-N <sub>3</sub> -deprotonated thiourea)
<b>1-GHB-f</b>	-2314,190573	5,71	double HB (carboxylic acid-N <sub>3</sub> -deprotonated thiourea)
<b>1-GHB-g</b>	-2314,186472	8,29	double HB (carboxylic acid-N <sub>3</sub> -deprotonated thiourea)

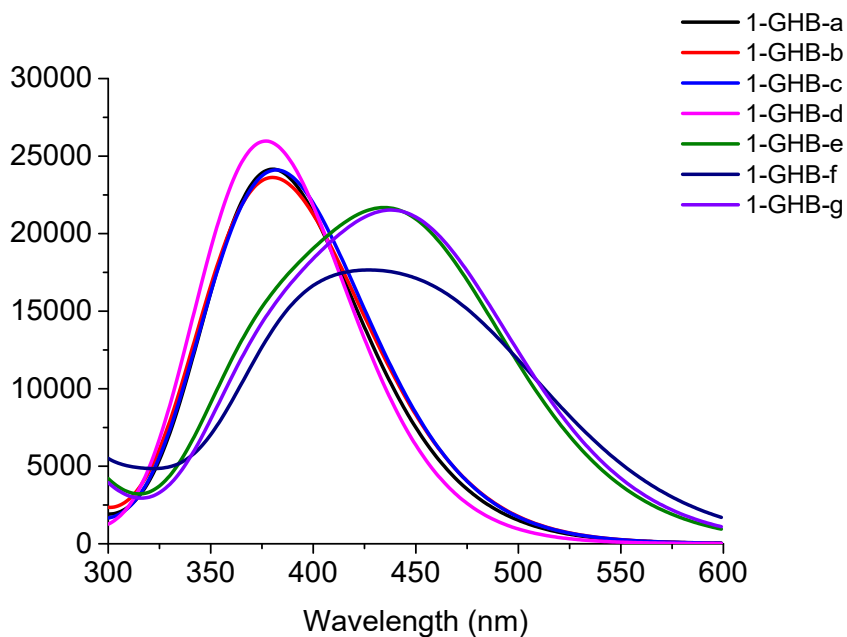


**Part 10** - X3LYP/6-31+G(d,p)/PCM(DMSO) energies of the optimized structures of 2-GHB derivatives with hydrogen bonds between the thiourea and carboxylate moieties and between the N3-deprotonated thiourea and the carboxylic acid group.

**Table S6.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy (*E*, in hartrees), relative energy ( $\Delta E$ , in kcal/mol) and hydrogen-bond type, of the optimized structures of **2-GHB** derivatives with single/double hydrogen bonds between the thiourea and carboxylate or between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group.

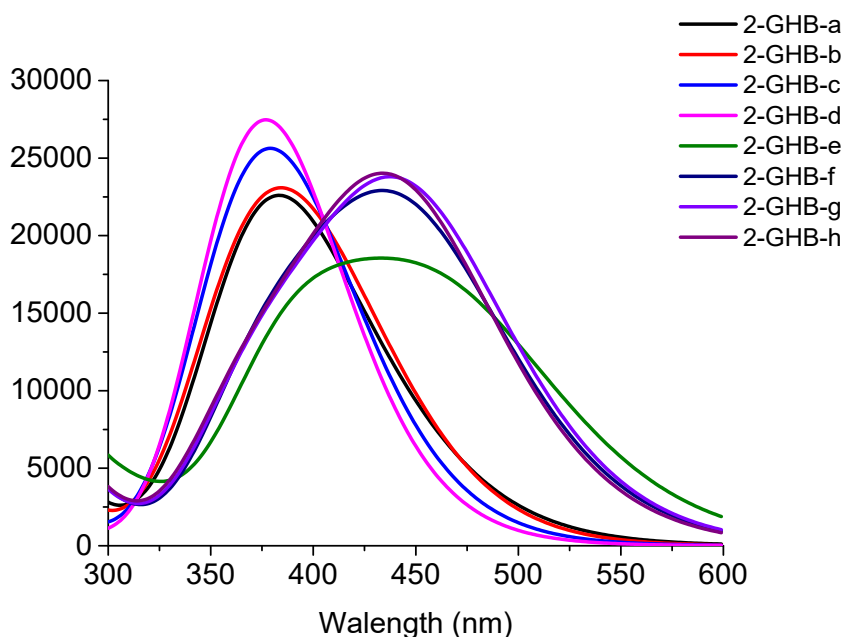
Structure	<i>E</i> (hartrees)	$\Delta E$ (kcal/mol)	Hydrogen-bond type
<b>2-GHB-a</b>	-2470,1733572	0,18	double HB (carboxylate-thiourea)
<b>2-GHB-b</b>	-2470,1736486	0,00	double HB (carboxylate-thiourea)
<b>2-GHB-c</b>	-2470,1715432	1,32	single HB (carboxylate-thiourea)
<b>2-GHB-d</b>	-2470,1664388	4,52	single HB (carboxylate-thiourea)
<b>2-GHB-e</b>	-2470,1646541	5,64	double HB (carboxylic acid-N3-deprotonated thiourea)
<b>2-GHB-f</b>	-2470,1651804	5,31	double HB (carboxylic acid-N3-deprotonated thiourea)
<b>2-GHB-g</b>	-2470,1660697	4,76	single HB (carboxylic acid-N3-deprotonated thiourea)
<b>2-GHB-h</b>	-2470,1586224	9,43	single HB (carboxylic acid-N3-deprotonated thiourea)

**Part 11** - Simulated UV-Vis spectra of selected optimized geometries of rotamers of **1-GHB** derivatives.



**Figure S34.** Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **1-GHB** derivatives at the same theory level (15 states, singlets only). Please, note that the main band is centered around 380 nm for species where the hydrogen bond takes place between the thiourea moiety and the carboxylate (**1-GHB-a to 1-GHB-d**) regardless of the number of hydrogen bonds formed and the main band is centered around 430-440 nm for species where the hydrogen bond takes place between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group (**1-GHB-e to 1-GHB-g**).

**Part 12** - Simulated UV-Vis spectra of selected optimized geometries of rotamers of **2-GHB** derivatives.



**Figure S35.** Simulated UV-Vis spectra from the TD-DFT vertical excitation energies analysis of selected X3LYP/6-31+G(d,p)/PCM(DMSO) optimized geometries of rotamers of **2-GHB** derivatives at the same theory level (15 states, singlets only). Please, note that the main band is centered around 380 nm for species where the hydrogen bond takes place between the thiourea moiety and the carboxylate (**2-GHB-a to 2-GHB-d**) regardless of the number of hydrogen bonds formed and the main band is centered around 430-440 nm for species where the hydrogen bond takes place between the N<sub>3</sub>-deprotonated thiourea and the carboxylic acid group (**2-GHB-e to 2-GHB-h**).

**Part 13** - X3LYP/6-31+G(d,p)/PCM(DMSO) absolute ( $E$ , in hartrees) and relative ( $\Delta E$ , in kcal/mol) of chemosensor 2-GHB-a (double hydrogen bond between thiourea and carboxylate) and 2-GHB-a' (no hydrogen bond, equivalent 1,2-trans cyclohexane ring substituents, Z,Z- thiourea and ester conformations) of increasing hydroxyacid chain.

**Table S7.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy ( $E$ , in hartrees), relative energy ( $\Delta E$ , in kcal/mol) and hydrogen-bond type, of the optimized structures of 2-GHB derivatives with (2-GHB-a) and without (2-GHB-a') double hydrogen bonds between the thiourea and carboxylate of increasing hydroxyacid chain (3 to 7 carbon atoms, noted as XC) with equivalent conformations of cyclohexane ring substituents, thiourea moiety and ester group. Please, note that the lowest stabilization due to the hydrogen bond formation takes place at the 3-hydroxypropionate, is maximum at GHB and, from there, decreases.

Structure	$E$ (hartrees)	$\Delta E$ (2-GHB-a vs 2-GHB-a') (kcal/mol)
2-GHB-a(3C)	-2430,872711	4,02
2-GHB-a	-2470,173357	0,09
2-GHB-a(5C)	-2509,467970	0,56
2-GHB-a(6C)	-2548,762117	1,50
2-GHB-a(7C)	-2588,057222	1,82

<b>2-GHB-a'(3C)</b>	-2430,879116
<b>2-GHB-a'</b>	-2470,173500
<b>2-GHB-a'(5C)</b>	-2509,468869
<b>2-GHB-a'(6C)</b>	-2548,764502
<b>2-GHB-a'(7C)</b>	-2588,060122

**Part 14** –Stabilization of butyric acid and 1-methyl-3-(4-nitrophenyl)thiourea in different hydrogen-bonded complexes and protonation states.

**Table S8.** X3LYP/6-31+G(d,p)/PCM(DMSO) energy (E, in hartrees), relative energy ( $\Delta E$ , in kcal/mol) of butyric acid/butyrate, 1-methyl-3-(4-nitrophenyl)thiourea and N<sub>3</sub>-deprotonated 1-methyl-3-(4-nitrophenyl)thiourea in different hydrogen-bonded complexes.

Structure	E (hartrees)	$\Delta E$ (kcal/mol)	Hydrogen bond
<b>butyrate</b>	-307,14534413		
<b>butyric acid</b>	-307,61249807		
<b>1-methyl-3-(4-nitrophenyl)thiourea</b>	-1022,82522452		
<b>N<sub>3</sub>-deprotonated thiourea</b>	-1022,35725196		
<b>acid + thiourea<sub>conformation 1</sub></b>	-1330,44706964	-5,87	single hydrogen bond
<b>acid + thiourea<sub>conformation 2</sub></b>	-1330,44612229	-5,27	single hydrogen bond
<b>carboxylate + thiourea<sub>conformation 1</sub></b>	-1329,99267431	-13,87	single hydrogen bond
<b>carboxylate + thiourea<sub>conformation 2</sub></b>	-1329,99140705	-13,08	single hydrogen bond
<b>carboxylate + thiourea<sub>conformation 3</sub></b>	-1329,99773512	-17,05	double hydrogen bond
<b>carboxylate + thiourea<sub>conformation 4</sub></b>	-1329,99773511	-17,05	double hydrogen bond
<b>acid + N<sub>3</sub>-deprotonated thiourea</b>	-1329,98884260	-11,98	double hydrogen bond

**Annex I: XYZ cartesian coordinates of the optimized energies of 32 starting rotamers of chemosensor 1 (1-conf1 to 1-conf32).**

**1-conf1**

C	-0.84887900	2.91940100	0.61635600
C	0.44303800	3.64159000	0.22984900
H	0.50358900	3.73840300	-0.85548300
N	1.61221500	2.92354400	0.71417100
H	-0.88405600	1.92857900	0.16159400
O	-1.93278200	3.74540400	0.12192000
H	1.98879000	3.23071900	1.60282500
C	-3.09008000	3.24423000	-0.34520000
O	-3.82661700	3.97019000	-0.98688100
C	-3.46363900	1.82256700	-0.04119200
C	-3.91025000	1.01476100	-1.09410100
C	-4.33120500	-0.28855000	-0.84728900
C	-4.33465700	-0.78908300	0.46645200
C	-3.90614600	0.03469100	1.52268100
C	-3.46514000	1.32738800	1.27214200
C	2.23385100	1.91044800	0.06643700
N	3.24904700	1.35178800	0.81378200
S	1.75991000	1.38087200	-1.46700300
C	4.24751500	0.43101300	0.47691300
C	4.80710400	-0.30781900	1.53956800
C	5.83398000	-1.20924900	1.31326600
C	6.30954700	-1.37840700	0.00932300
C	5.77840400	-0.64701700	-1.05616600
C	4.75293600	0.25972000	-0.82503200
F	-6.34209200	-2.57968600	-0.96505700
C	-5.27280300	-3.10569800	-0.32386200
F	-5.63461000	-4.29785800	0.16380900
F	-4.30265000	-3.31296800	-1.24416200
N	7.37995800	-2.32581800	-0.23982800
O	7.76999800	-2.48349400	-1.40326100
O	7.86089800	-2.93843300	0.72161700
H	-3.92342600	1.40604900	-2.10503200
H	-4.65741600	-0.89633400	-1.68148700
H	-3.92317900	-0.35146900	2.53519100
H	-3.14519300	1.95173000	2.09894400
H	3.23195800	1.57973400	1.80161400
H	4.42498300	-0.17631500	2.54689600
H	6.25775100	-1.78168900	2.12798900
H	6.17623900	-0.77860200	-2.05415800
H	4.34983100	0.83470300	-1.64495400
C	-4.77744200	-2.15957700	0.81444100
O	-4.78316900	-2.60702600	1.94490200
H	0.45916300	4.63902500	0.67411800
H	-0.93539500	2.83395700	1.70192800

**1-conf2**

C	-0.06916200	-0.94576700	-0.57962500
C	-0.84667800	-0.02449300	-1.51699600
H	-0.76869900	1.00958100	-1.17780400
N	-2.25191100	-0.39911000	-1.57420900
H	-0.45083000	-0.88578700	0.44225400
O	1.29971300	-0.48177800	-0.60598800

H	-2.51001300	-1.05124300	-2.30503000
C	2.19088600	-1.17999200	0.11381500
O	1.90047500	-2.16556000	0.77048100
C	3.57339700	-0.61814500	0.01966200
C	4.60037800	-1.27834300	0.70502300
C	5.90453200	-0.79712400	0.64819100
C	6.19367300	0.35882100	-0.09869800
C	5.15776100	1.01952100	-0.78404100
C	3.85739500	0.53591300	-0.72741800
C	-3.22149300	0.05544400	-0.74772300
N	-4.43420500	-0.56547900	-0.96436500
S	-2.93991300	1.22060500	0.44449100
C	-5.71353800	-0.27145800	-0.47787000
C	-6.62332800	-1.34435200	-0.39245700
C	-7.92559000	-1.13691300	0.03266700
C	-8.32534700	0.15732100	0.37838500
C	-7.44355400	1.23773800	0.28730400
C	-6.14140800	1.02670400	-0.14443800
F	8.53277100	0.17701200	1.85439600
C	8.73893900	0.22592000	0.51792200
F	9.89125200	0.87220400	0.30605000
F	8.89151500	-1.04478000	0.07834900
N	-9.68454100	0.38357300	0.83395700
O	-10.01543300	1.53100900	1.15707000
O	-10.45902500	-0.58017700	0.88082500
H	4.36949500	-2.16790200	1.27923300
H	6.67982100	-1.32713700	1.18644800
H	5.38760700	1.91014800	-1.35726200
H	3.06355500	1.04767200	-1.25713700
H	-4.38940500	-1.43551400	-1.48336700
H	-6.29942700	-2.34681900	-0.65313700
H	-8.62185700	-1.96198400	0.10721500
H	-7.78153900	2.23468100	0.53919800
H	-5.46191100	1.86162900	-0.22873000
C	7.55444500	0.93567400	-0.21022000
O	7.81875700	1.94024000	-0.84193300
H	-0.44348600	-0.09329000	-2.52983900
H	-0.10367000	-1.98520200	-0.91528500

### 1-conf3

C	0.02285200	2.09523100	-0.86711400
C	-1.15239500	2.85044400	-0.24441200
H	-0.79465200	3.48975000	0.56482700
N	-2.15337800	1.92631200	0.27386900
H	0.52015100	1.47848600	-0.11753000
O	0.92480200	3.10877000	-1.37628200
H	-2.96939100	1.77826400	-0.30609600
C	2.26460900	3.00696400	-1.31588600
O	2.93719900	4.00298900	-1.50685300
C	2.89927400	1.67295100	-1.05073800
C	3.90009900	1.59594800	-0.07460200
C	4.56117600	0.39336200	0.15698200
C	4.24506500	-0.74150400	-0.61027100
C	3.25476600	-0.65162000	-1.60483200
C	2.57872000	0.54242600	-1.81820500
C	-2.13873900	1.39208200	1.50880300

N	-3.16429800	0.53987900	1.84450000
S	-0.95566400	1.73924900	2.67547700
C	-4.16182200	-0.06184500	1.06053600
C	-5.40451500	-0.31572700	1.67268700
C	-6.41759300	-0.95103000	0.97246300
C	-6.18991900	-1.32990200	-0.35400500
C	-4.96114500	-1.10247500	-0.97617000
C	-3.94392000	-0.47679800	-0.26682200
F	7.03822400	-1.36386000	0.45199400
C	6.00158900	-2.20581500	0.67082100
F	6.48705200	-3.45222200	0.70043800
F	5.49850500	-1.92917200	1.89602900
N	-7.25257100	-1.98678800	-1.09827400
O	-7.04199700	-2.29379600	-2.27690300
O	-8.32208700	-2.21069200	-0.52061000
H	4.15582200	2.47535200	0.50563300
H	5.32024300	0.35735900	0.92787900
H	3.02331800	-1.52613300	-2.20170800
H	1.82083200	0.59656500	-2.59192100
H	-3.21315100	0.36135000	2.83986400
H	-5.57119900	-0.00318600	2.69804000
H	-7.37668200	-1.14138900	1.43629100
H	-4.79860400	-1.43186500	-1.99420000
H	-2.97485100	-0.35648500	-0.73508400
C	4.91004900	-2.05383300	-0.43453000
O	4.66012500	-3.03892100	-1.10184100
H	-1.63637200	3.47363900	-0.99861400
H	-0.31038300	1.47180700	-1.70014800

#### 1-conf4

C	-0.54896700	0.36194100	0.35045600
C	-1.28481100	1.02681500	-0.81036400
H	-0.91029800	2.04028900	-0.96375600
N	-2.71898800	1.07999300	-0.55369900
H	-0.67714000	0.92618500	1.27716400
O	0.84940300	0.35357400	-0.01431500
H	-3.27466500	0.34193800	-0.96674500
C	1.69795500	-0.22125200	0.85171100
O	1.34487700	-0.72398800	1.90495600
C	3.11708000	-0.17602400	0.38314600
C	4.09864600	-0.74785800	1.20154600
C	5.43418300	-0.73149300	0.81211800
C	5.80133700	-0.13809100	-0.40881900
C	4.81108300	0.43476800	-1.22771900
C	3.47885600	0.41706700	-0.83670500
C	-3.35610500	2.08600400	0.07133000
N	-4.71497900	1.96164900	0.24639700
S	-2.59351900	3.50249000	0.61328000
C	-5.56965800	0.85899000	0.08775200
C	-6.89904200	1.11589000	-0.30052400
C	-7.80859900	0.07823800	-0.42807500
C	-7.38537700	-1.22953400	-0.17219900
C	-6.07722200	-1.50625800	0.22901700
C	-5.17171300	-0.46229600	0.36748000
F	8.39543500	-0.10264700	1.19365200
C	8.33359900	-0.69838300	-0.01963600

F	9.52788600	-0.55534000	-0.60581700
F	8.12806800	-2.02068800	0.18136500
N	-8.33143900	-2.32430600	-0.31540500
O	-7.93334900	-3.47631300	-0.10953700
O	-9.49458500	-2.05695500	-0.63714500
H	3.80774700	-1.20316400	2.14087400
H	6.17278900	-1.18086600	1.46346500
H	5.10125600	0.89056300	-2.16721300
H	2.72047100	0.85992400	-1.47029600
H	-5.15714500	2.83549200	0.50299600
H	-7.21028000	2.13376800	-0.50963700
H	-8.82883300	0.27048800	-0.73376800
H	-5.78049000	-2.52320500	0.45059000
H	-4.17559500	-0.67723000	0.73385700
C	7.19999200	-0.07832300	-0.89580500
O	7.53335300	0.42915200	-1.94909400
H	-1.13398800	0.45321400	-1.72725700
H	-0.88720100	-0.66549000	0.50621800

### 1-conf5

C	0.28259700	-3.53398100	-0.08935400
C	1.72067800	-3.92216400	0.27167900
H	1.96911900	-3.56211800	1.27523600
N	2.67290700	-3.43959700	-0.72328000
H	0.16679000	-2.45035200	-0.13691100
O	-0.56023700	-4.09357600	0.94458200
H	2.95969200	-4.08915900	-1.44306900
C	-1.60659200	-3.44195000	1.48861600
O	-2.07116900	-3.85513500	2.53394300
C	-2.19274500	-2.25493800	0.78258500
C	-2.45880900	-1.10245100	1.53209300
C	-3.05949900	-0.00005200	0.93147400
C	-3.42839000	-0.05248100	-0.42409600
C	-3.18019200	-1.22147900	-1.16536300
C	-2.55723300	-2.31131100	-0.57164000
C	3.14783900	-2.18359700	-0.89697200
N	2.83128700	-1.30168500	0.10513200
S	4.10543900	-1.82130600	-2.24793600
C	3.01029900	0.08848000	0.18545200
C	3.17002800	0.63730300	1.47189300
C	3.29479200	2.00730100	1.64459300
C	3.25932900	2.83498400	0.51936700
C	3.08767900	2.31089400	-0.76451800
C	2.95847100	0.93897900	-0.93246900
F	-5.15727100	2.20013200	0.70103200
C	-4.34420300	2.40299800	-0.36144000
F	-4.92435500	3.31287600	-1.15211700
F	-3.18827500	2.93350700	0.10055600
N	3.39481400	4.27174300	0.68950200
O	3.38177900	4.98819700	-0.31819600
O	3.51684300	4.71994800	1.83558100
H	-2.19079000	-1.06843400	2.58199300
H	-3.24032900	0.88372100	1.52979700
H	-3.47722200	-1.26104500	-2.20687600
H	-2.37437500	-3.20628200	-1.15601400
H	2.52844800	-1.71713100	0.97772300



H	3.20421500	-0.01633900	2.33767600
H	3.42618700	2.43191400	2.63123100
H	3.04191100	2.97399400	-1.61869200
H	2.81246500	0.52950000	-1.92119400
C	-4.08252200	1.07224600	-1.13384900
O	-4.43190700	1.03170900	-2.29747100
H	1.81277500	-5.00891600	0.30427800
H	-0.00150800	-3.97215100	-1.04872000

### 1-conf6

C	-0.50430400	-2.07759600	0.42794600
C	-1.18127600	-2.55848600	-0.85610700
H	-1.21299600	-1.75482400	-1.59931000
N	-2.51358400	-3.09373600	-0.59309800
H	-1.06012300	-1.26882500	0.90880700
O	0.79743900	-1.59412200	0.03438100
H	-2.59392000	-4.09433900	-0.47307300
C	1.59109100	-1.12828600	1.01322400
O	1.25938400	-1.09635700	2.18554200
C	2.91573300	-0.65877100	0.50487900
C	3.83647100	-0.15761900	1.43300700
C	5.08458600	0.28970800	1.01143800
C	5.42372200	0.23974000	-0.35237700
C	4.49447000	-0.26370400	-1.28093100
C	3.24977000	-0.71045300	-0.85763500
C	-3.67103600	-2.42330900	-0.38735600
N	-3.60615600	-1.07112400	-0.60206300
S	-5.07269000	-3.27441300	0.04738400
C	-4.56726800	-0.06938600	-0.38528700
C	-4.53517900	1.04258200	-1.24717300
C	-5.41236300	2.10132200	-1.06666700
C	-6.32905400	2.04490900	-0.01388700
C	-6.36730400	0.95635200	0.86134600
C	-5.48392800	-0.09915800	0.67954300
F	7.33742900	2.33428700	0.77294000
C	7.79971500	1.24745200	0.11249200
F	8.91714900	1.60522800	-0.53064500
F	8.13470400	0.31663100	1.03565000
N	-7.25629600	3.14743600	0.18029600
O	-8.07391100	3.07370100	1.10479400
O	-7.18935000	4.11479700	-0.58702800
H	3.56794300	-0.12218700	2.48228100
H	5.77800900	0.67197200	1.74948200
H	4.76255100	-0.29947100	-2.33044100
H	2.53846300	-1.09822700	-1.57620700
H	-2.79553800	-0.74363100	-1.11305900
H	-3.82598700	1.06954300	-2.06822500
H	-5.39701300	2.95372300	-1.73316200
H	-7.07169400	0.94624600	1.68301100
H	-5.49856100	-0.93691700	1.36120500
C	6.73111600	0.69524300	-0.88235800
O	7.03582500	0.66728100	-2.05889300
H	-0.59568300	-3.36391300	-1.30274800
H	-0.38856400	-2.89753000	1.14088000

### 1-conf7

C	0.15906200	0.07119100	1.39108600
C	1.64100700	-0.26122800	1.20999300
H	1.97815900	0.11088600	0.24399400
N	1.82746000	-1.71049400	1.27078500
H	-0.43178800	-0.32254200	0.56203200
O	0.08617400	1.51596200	1.42980600
H	1.36181200	-2.19322600	2.03028200
C	-0.97821500	2.21101700	0.98341500
O	-0.85600300	3.40549100	0.79110200
C	-2.28590600	1.50833500	0.76558100
C	-2.95450100	1.71042700	-0.44803200
C	-4.20048800	1.12987300	-0.66573300
C	-4.80371500	0.36085000	0.34474000
C	-4.13711900	0.18077500	1.56981700
C	-2.88365200	0.74123500	1.77756400
C	2.24553000	-2.53199900	0.28616200
N	3.02749000	-1.99977700	-0.71813600
S	1.81920900	-4.17005000	0.24601100
C	4.08486500	-1.07856300	-0.62712200
C	4.58290100	-0.54136700	-1.82977800
C	5.65527400	0.33576800	-1.81588000
C	6.23199900	0.68350500	-0.59007800
C	5.75773700	0.15488800	0.61281400
C	4.68741000	-0.72854000	0.59485800
F	-7.16169300	1.19718400	-1.39819500
C	-6.90968000	-0.10794800	-1.14496600
F	-8.08236800	-0.75076000	-1.10783200
F	-6.20143200	-0.59991900	-2.18782100
N	7.35124400	1.60841200	-0.56756100
O	7.84001900	1.91573200	0.52613100
O	7.77061400	2.05118500	-1.64347400
H	-2.49714500	2.31744500	-1.22111900
H	-4.68899500	1.28957700	-1.61841400
H	-4.61248900	-0.40179800	2.35033600
H	-2.38725800	0.59973200	2.73115500
H	3.03244300	-2.57304700	-1.55313500
H	4.11857600	-0.81078500	-2.77249300
H	6.03851400	0.75602700	-2.73662800
H	6.23245200	0.42281000	1.54781600
H	4.33866100	-1.15918200	1.52496900
C	-6.13110200	-0.28137600	0.19677300
O	-6.66589100	-0.94610000	1.06277700
H	2.22855000	0.23042700	1.99167200
H	-0.22050400	-0.33026400	2.33436900

### 1-conf8

C	-1.02403200	-2.54372700	-0.36223700
C	-2.20882700	-1.59773400	-0.54106200
H	-2.29939200	-0.95662700	0.33476700
N	-3.43443200	-2.38087800	-0.69874700
H	-1.10627500	-3.11946400	0.56283100
O	0.14602500	-1.70163600	-0.30434900
H	-3.38171200	-3.18056700	-1.31873800
C	1.32980400	-2.32232600	-0.16650400

O	1.44539800	-3.53312100	-0.09018200
C	2.47777800	-1.36666800	-0.11893800
C	3.76649300	-1.89408500	0.02721800
C	4.86941000	-1.04744800	0.07567300
C	4.69051300	0.34384500	-0.02291800
C	3.39348100	0.86855700	-0.16957000
C	2.29416400	0.02161800	-0.21723900
C	-4.52106400	-2.38914000	0.09835900
N	-4.77016200	-1.27576700	0.87516000
S	-5.55701200	-3.72614900	0.18551600
C	-4.66654300	0.08406900	0.53949500
C	-4.80179800	1.02238400	1.58140200
C	-4.75529900	2.38064300	1.31325300
C	-4.56835100	2.80685000	-0.00581200
C	-4.44324700	1.89222600	-1.05423500
C	-4.49615600	0.53208900	-0.78317600
F	7.40675400	0.08149000	1.33657400
C	7.26881900	0.77621700	0.18363700
F	8.15212800	1.78096900	0.20414400
F	7.60443100	-0.04788300	-0.83586700
N	-4.51123200	4.22882400	-0.29240300
O	-4.33065900	4.58778700	-1.46219700
O	-4.64540100	5.02427300	0.64519500
H	3.89616400	-2.96730300	0.10208300
H	5.85481400	-1.48073400	0.18917400
H	3.26315800	1.94181100	-0.24496100
H	1.29786800	0.43054700	-0.33033300
H	-5.38469000	-1.47697200	1.65458300
H	-4.93697400	0.67913700	2.60170800
H	-4.85286900	3.10563600	2.11081200
H	-4.32082200	2.24484000	-2.07016000
H	-4.42871600	-0.17487500	-1.60027700
C	5.81206300	1.31237700	0.01848100
O	5.67505000	2.51711200	-0.06917600
H	-2.04813700	-0.96134400	-1.41725300
H	-0.92580900	-3.23594500	-1.20349200

### 1-conf9

C	0.89069400	2.42773800	-0.61480100
C	-0.46042500	2.74835600	-1.23646500
H	-0.95698000	3.54351500	-0.68064100
N	-1.35070600	1.59826100	-1.26724800
H	1.36597800	1.57384900	-1.10289400
O	0.67218600	2.13913400	0.78998900
H	-1.05588500	0.82556800	-1.85365100
C	1.43400900	1.28679300	1.49685100
O	1.03055100	0.89671100	2.57702700
C	2.76987300	0.85911500	0.96180200
C	3.07778500	-0.50688200	0.95896600
C	4.32925600	-0.94197500	0.53314300
C	5.29893700	-0.00680400	0.13079900
C	4.99163600	1.36527700	0.15862000
C	3.73432200	1.79651400	0.56075500
C	-2.55031800	1.49558000	-0.65153700
N	-3.07820100	0.22354200	-0.75260600
S	-3.28904700	2.76470800	0.18604000

C	-4.36329400	-0.26077400	-0.48495400
C	-4.47182100	-1.62700800	-0.15626300
C	-5.71038500	-2.20447200	0.07240300
C	-6.85564500	-1.40874600	-0.02572200
C	-6.77139300	-0.05467100	-0.36247500
C	-5.52950900	0.51876400	-0.59589800
F	6.95019800	-2.47344600	0.83694700
C	7.03876400	-1.89876500	-0.38488400
F	8.29224600	-2.06206600	-0.82304800
F	6.21768000	-2.57770900	-1.21938200
N	-8.15675800	-2.00215400	0.21844100
O	-9.15775600	-1.27792900	0.15252300
O	-8.21457700	-3.20980500	0.48211400
H	2.33653600	-1.22711000	1.28630100
H	4.53589900	-2.00455100	0.52715800
H	5.74704300	2.08288500	-0.13967200
H	3.51528400	2.85824600	0.58239800
H	-2.40927100	-0.50423700	-0.97770200
H	-3.57558200	-2.23361700	-0.07309900
H	-5.79365500	-3.25157500	0.33270900
H	-7.67306700	0.53708600	-0.45382800
H	-5.46245600	1.56146100	-0.86889200
C	6.65618900	-0.38652800	-0.32651400
O	7.50765800	0.41104500	-0.66855600
H	-0.28724700	3.10057000	-2.25931300
H	1.54015100	3.30173200	-0.70402100

### 1-conf10

C	0.02205900	3.41379400	-0.06799900
C	1.01811500	3.34631300	1.07744900
H	1.76328800	4.13105500	0.93707300
N	1.70095200	2.06284700	1.17620300
H	-0.42123800	4.41125000	-0.12813100
O	-1.02158700	2.44720800	0.20822900
H	1.24763300	1.36294800	1.75059300
C	-2.00907800	2.34406000	-0.69286600
O	-2.06779800	3.01783100	-1.70785200
C	-3.02721100	1.31538500	-0.31543100
C	-4.11620800	1.12015300	-1.17337100
C	-5.09044100	0.17507000	-0.86750800
C	-4.98224000	-0.58853800	0.30841500
C	-3.88641900	-0.38793800	1.16766200
C	-2.91579600	0.55606800	0.86003500
C	2.84592600	1.72991000	0.54077000
N	3.18436100	0.40395400	0.71904300
S	3.72380400	2.82589700	-0.40284500
C	4.35145300	-0.29877100	0.39802800
C	4.21925200	-1.68689100	0.19059600
C	5.32742600	-2.47099900	-0.08584600
C	6.58452900	-1.86339000	-0.15775200
C	6.74011200	-0.49161600	0.05889300
C	5.62824300	0.28990200	0.34107900
F	-7.95219100	-0.75562400	-0.36303900
C	-7.20601500	-1.87502200	-0.21721000
F	-7.99558000	-2.82888900	0.28980500
F	-6.81658300	-2.27366700	-1.45030800

N	7.75026500	-2.67450500	-0.45540500
O	8.85198400	-2.11743500	-0.53644100
O	7.59672000	-3.89172300	-0.61601400
H	-4.19263700	1.71234300	-2.07765500
H	-5.92213000	0.04473400	-1.54795100
H	-3.80945800	-0.97958900	2.07244400
H	-2.07463200	0.70709900	1.52508800
H	2.43707600	-0.19121100	1.05897000
H	3.23789400	-2.14798700	0.23797200
H	5.22470400	-3.53505400	-0.25404100
H	7.72581100	-0.04613700	0.02015300
H	5.74739400	1.34764000	0.52163900
C	-5.97450900	-1.61542900	0.70589600
O	-5.89504000	-2.28300800	1.71889300
H	0.50735300	3.52000100	2.02764000
H	0.48881500	3.17074400	-1.02483600

### 1-conf11

C	-0.18558100	1.14714700	0.88466300
C	0.91269500	1.78896200	1.71849200
H	0.67457300	2.84603900	1.85334400
N	2.23149500	1.66904400	1.10791600
H	-1.15076700	1.28524100	1.37622200
O	0.12799400	-0.26823400	0.77806500
H	2.79911200	0.89248400	1.42095300
C	-0.80892400	-1.22036500	0.63243100
O	-0.49350400	-2.38456200	0.79645700
C	-2.20987100	-0.83556100	0.25334500
C	-3.26650100	-1.33282600	1.02594900
C	-4.58355000	-1.05278900	0.67414200
C	-4.85730100	-0.29194500	-0.47591600
C	-3.79204000	0.18404300	-1.26116700
C	-2.47761500	-0.07614200	-0.89622200
C	2.75532000	2.52805600	0.21812200
N	3.98693100	2.21701000	-0.31069000
S	2.01153900	3.98063200	-0.25271900
C	4.72593000	1.02365800	-0.28262300
C	6.13027900	1.12598800	-0.31747800
C	6.91911800	-0.01303600	-0.34285800
C	6.30026300	-1.26671200	-0.32604200
C	4.90997500	-1.39233000	-0.30528100
C	4.12221800	-0.24855200	-0.29147700
F	-7.46213800	-1.81012600	-0.00532900
C	-7.44244900	-0.45901100	-0.07810500
F	-8.60143100	-0.06192700	-0.61570200
F	-7.38831900	0.01994800	1.18636100
N	7.12220000	-2.46580100	-0.34157400
O	6.55860400	-3.56560600	-0.31216900
O	8.35074100	-2.33545000	-0.38371000
H	-3.05674700	-1.93413500	1.90336400
H	-5.38082800	-1.43711600	1.29733100
H	-4.00863600	0.75869600	-2.15418200
H	-1.66829500	0.29196500	-1.51709500
H	4.42397400	3.00268800	-0.77614500
H	6.59731400	2.10512100	-0.31590000
H	7.99862200	0.06118500	-0.36226200

H	4.45264200	-2.37311200	-0.32128300
H	3.04480100	-0.35348000	-0.32953600
C	-6.22961900	0.04185200	-0.92347200
O	-6.48250700	0.69072500	-1.92006600
H	0.96191400	1.31326300	2.70010400
H	-0.21439600	1.58062400	-0.11659000

### 1-conf12

C	0.99868900	-3.00171700	-1.88979900
C	1.93795700	-3.53530900	-0.82067700
H	1.39582100	-4.15589800	-0.10737800
N	2.60445900	-2.47027000	-0.07988000
H	1.49962500	-2.31134100	-2.57381000
O	-0.07258200	-2.30322300	-1.21602500
H	3.33051200	-1.97167300	-0.58023100
C	-0.99460300	-1.70479100	-1.98275600
O	-0.97408500	-1.72352900	-3.20227700
C	-2.04720400	-1.01571300	-1.17405000
C	-3.07071100	-0.34627900	-1.85534900
C	-4.07386500	0.30795500	-1.14719500
C	-4.06138200	0.29624900	0.25908000
C	-3.03030100	-0.37801100	0.93859600
C	-2.02946800	-1.02943500	0.22992700
C	2.42428100	-2.17778700	1.21898200
N	3.10518600	-1.08750700	1.71385100
S	1.46330300	-3.07785500	2.29278100
C	3.76731000	-0.03764000	1.05896100
C	4.85151400	0.56547900	1.72621700
C	5.51830400	1.63955100	1.15889500
C	5.10375500	2.11264500	-0.08986900
C	4.02225200	1.54053500	-0.76254900
C	3.34914100	0.47176900	-0.18551900
F	-5.76678300	2.73375500	-0.40090700
C	-6.24934300	1.73664000	0.37636000
F	-7.08401200	2.28212100	1.26866800
F	-6.97348200	0.91187700	-0.41514700
N	5.80724600	3.23082100	-0.69592700
O	5.44144900	3.62196000	-1.81022300
O	6.74252400	3.74434800	-0.07159600
H	-3.07409000	-0.34292100	-2.93902200
H	-4.85353800	0.81808400	-1.69820700
H	-3.02685000	-0.38269000	2.02240000
H	-1.23743700	-1.54721300	0.75788700
H	3.13385700	-1.06969700	2.72547800
H	5.17245300	0.17952900	2.68793200
H	6.35680200	2.10043200	1.66462600
H	3.70041000	1.94210700	-1.71469300
H	2.47879600	0.06698300	-0.68634900
C	-5.09259900	0.96574600	1.08676200
O	-5.10126000	0.95820800	2.30253100
H	2.69838900	-4.15288600	-1.30858600
H	0.58194300	-3.82967300	-2.46976400

### 1-conf13

C	-0.39710300	2.00250800	-1.49226600
C	0.77964500	2.95260500	-1.31598300
H	1.57166700	2.70346700	-2.02845200
N	1.33176200	3.00068800	0.03785400
H	-1.15106300	2.15396000	-0.71846500
O	0.12829300	0.64577400	-1.41803700
H	1.02295200	3.75781700	0.63247400
C	-0.54746900	-0.40486400	-0.89799800
O	0.08591900	-1.39517900	-0.58945000
C	-2.03509100	-0.32822900	-0.74794300
C	-2.59927400	-0.77235500	0.45448600
C	-3.98117600	-0.77755600	0.61854100
C	-4.81503600	-0.36219600	-0.43415200
C	-4.24303200	0.05999000	-1.64724400
C	-2.86331700	0.08661600	-1.80228400
C	2.37651000	2.30212900	0.54113000
N	2.74090500	1.20151900	-0.19097300
S	3.08829300	2.77635100	2.00772000
C	3.86734700	0.37729900	-0.05501600
C	3.70226600	-0.98930400	-0.34976000
C	4.78377500	-1.85591400	-0.29393800
C	6.03773000	-1.35029700	0.06000900
C	6.22326600	0.00615600	0.34464000
C	5.13969900	0.87069800	0.28288800
F	-6.65752000	-2.10998600	1.25266400
C	-6.97655100	-0.82429600	0.97733900
F	-8.30882500	-0.74335400	0.88798500
F	-6.58616500	-0.06917000	2.03011000
N	7.17385500	-2.25233100	0.12742900
O	8.27286800	-1.79319700	0.46150400
O	6.99810500	-3.44438000	-0.15267500
H	-1.95595600	-1.10710900	1.26020100
H	-4.39125200	-1.11074400	1.56324800
H	-4.89113600	0.36521100	-2.46043300
H	-2.43893600	0.40503700	-2.74755800
H	2.00543000	0.81223700	-0.77792600
H	2.71702200	-1.36662000	-0.60598200
H	4.66163200	-2.90952900	-0.50893900
H	7.20846400	0.37677100	0.59652600
H	5.27800300	1.92288800	0.48744800
C	-6.29501800	-0.34667400	-0.34332900
O	-7.02730300	0.01699000	-1.24252200
H	0.42991300	3.95939800	-1.55789200
H	-0.83855000	2.15109800	-2.48004400

#### 1-conf14

C	1.89573500	4.10467800	-0.80964500
C	3.27575200	3.47198600	-0.90067400
H	3.32986800	2.78384800	-1.74863700
N	3.71427500	2.82123200	0.33200800
H	1.83386100	4.80744100	0.02498900
O	0.92728200	3.04966500	-0.60450000
H	4.14817000	3.41538200	1.02621200
C	-0.36418700	3.42336000	-0.57060500
O	-0.72996300	4.57496800	-0.72995900
C	-1.29483300	2.28107500	-0.32107300

C	-2.67116600	2.52836700	-0.39307900
C	-3.58164600	1.50088100	-0.16758200
C	-3.11918400	0.20835400	0.13736100
C	-1.73568100	-0.03350900	0.21425200
C	-0.82933400	0.99342800	-0.01339100
C	3.65869200	1.52107700	0.70399100
N	3.08811600	0.67118600	-0.20564100
S	4.31419800	1.06879100	2.20549200
C	2.87904000	-0.71689600	-0.20415700
C	2.65889600	-1.30669800	-1.46660100
C	2.40287500	-2.66252500	-1.58272400
C	2.36475700	-3.44351200	-0.42374600
C	2.56801900	-2.87884900	0.83664700
C	2.82071900	-1.51732600	0.95054800
F	-5.96096300	0.19929700	1.24300600
C	-5.56557900	-0.71704300	0.32926800
F	-6.22658200	-1.85342000	0.57787600
F	-5.94980100	-0.27435800	-0.89038700
N	2.10269500	-4.86805500	-0.53398900
O	2.08721500	-5.54647000	0.49975900
O	1.90502000	-5.34483900	-1.65795200
H	-3.02006100	3.52704200	-0.62778700
H	-4.63999200	1.71847200	-0.23281800
H	-1.38572200	-1.03068800	0.45448500
H	0.23381400	0.80272300	0.05340500
H	2.82315700	1.09913900	-1.08377800
H	2.69824500	-0.69442000	-2.36191200
H	2.24193100	-3.11458700	-2.55264800
H	2.51774000	-3.49930600	1.72218000
H	2.97190800	-1.07557200	1.92352000
C	-4.02190000	-0.94060000	0.38844000
O	-3.63729500	-2.06524200	0.64331000
H	3.99136400	4.26977600	-1.11707600
H	1.66513700	4.63372500	-1.73773500

### 1-conf15

C	0.18407000	-0.53759100	0.56217100
C	1.57139700	-0.32467800	-0.02413400
H	2.29359700	-0.21746500	0.78468700
N	1.61536800	0.86776600	-0.87228800
H	-0.58316000	-0.54476900	-0.21538600
O	-0.06109900	0.53175200	1.50783400
H	0.81674000	1.01698900	-1.47752800
C	-1.26627600	1.09875300	1.70378000
O	-1.32317700	2.15043000	2.31267900
C	-2.50522600	0.41751300	1.20092400
C	-3.44008000	1.18560600	0.49588900
C	-4.63524700	0.61556200	0.06798900
C	-4.91884400	-0.72872600	0.36629200
C	-3.98586400	-1.48867300	1.09402900
C	-2.78374400	-0.92492700	1.50129900
C	2.38521200	1.96215000	-0.71913300
N	3.57259600	1.83181200	-0.02703100
S	1.92490200	3.47501300	-1.32624800
C	4.53096600	0.80784100	-0.09323200
C	5.57123500	0.83032500	0.85640900



C	6.57589300	-0.12260700	0.82012600
C	6.54003000	-1.11046900	-0.16966800
C	5.52276500	-1.14361400	-1.12649300
C	4.52127900	-0.18341000	-1.09170800
F	-7.67497100	0.46976000	-0.13889500
C	-7.24012800	-0.59959200	-0.84473400
F	-8.30307100	-1.35967400	-1.13147700
F	-6.73193000	-0.14239900	-2.01271400
N	7.58417800	-2.11798300	-0.20728800
O	7.52265500	-2.99906000	-1.07329300
O	8.49381600	-2.05494200	0.62844700
H	-3.22859800	2.22689700	0.28086200
H	-5.33392500	1.22813700	-0.48726100
H	-4.21512400	-2.52067200	1.33273900
H	-2.07925200	-1.52289600	2.06874600
H	3.91927900	2.71781900	0.32017600
H	5.58183300	1.59610600	1.62497000
H	7.37417200	-0.11296500	1.55085700
H	5.52667500	-1.90438100	-1.89634000
H	3.75088500	-0.19226900	-1.85233500
C	-6.17127500	-1.40691000	-0.04335900
O	-6.42938500	-2.56850000	0.20558300
H	1.83798100	-1.21587500	-0.60246000
H	0.16576400	-1.49195600	1.09359200

### 1-conf16

C	0.99846900	2.52666700	-0.58602500
C	2.20645400	1.75814200	-0.08162700
H	2.26034200	0.79047400	-0.58101200
N	2.13698600	1.54696800	1.36690600
H	0.85253800	3.46837600	-0.04868300
O	-0.16416400	1.68932700	-0.39867100
H	1.74899000	2.30700800	1.91277600
C	-1.34053500	2.18502700	-0.81474600
O	-1.46074000	3.28300500	-1.33099400
C	-2.47681800	1.24302000	-0.57842800
C	-3.75255900	1.63074300	-1.00542700
C	-4.84348600	0.78970700	-0.81017100
C	-4.66539300	-0.45537400	-0.18122500
C	-3.38159100	-0.83945900	0.24714000
C	-2.29431000	0.00160800	0.05108500
C	2.19097300	0.37923100	2.03404300
N	2.81685700	-0.69034800	1.42696200
S	1.49049600	0.18787300	3.56580300
C	4.00800800	-0.71505500	0.68246600
C	4.31280200	-1.89824800	-0.01791100
C	5.49534500	-2.00681000	-0.73134600
C	6.37883500	-0.92254300	-0.75039000
C	6.09890300	0.25601100	-0.05468600
C	4.91638300	0.35883100	0.66480500
F	-7.62719500	0.11678300	0.23533100
C	-7.21910400	-1.01765600	-0.37891700
F	-8.09367300	-1.98363300	-0.07509400
F	-7.28271400	-0.80812000	-1.71435700
N	7.61560500	-1.02650700	-1.50386600
O	8.37760100	-0.05250700	-1.52395000

O	7.85726100	-2.08561400	-2.09509300
H	-3.88168300	2.59138500	-1.48993500
H	-5.81870700	1.11293800	-1.15097300
H	-3.25180700	-1.79972000	0.73254900
H	-1.30840500	-0.29804200	0.38407400
H	2.54476900	-1.57997400	1.82784400
H	3.61291300	-2.72706400	-0.00344200
H	5.73221100	-2.91154900	-1.27594100
H	6.80733700	1.07416800	-0.06608700
H	4.71449100	1.26018200	1.22980500
C	-5.77363600	-1.40954700	0.06141400
O	-5.63396000	-2.49561100	0.58949300
H	3.10544700	2.32616300	-0.34432700
H	1.11929400	2.74907300	-1.64903500

### 1-conf17

C	0.91217800	2.67821600	-0.60800100
C	-0.44681500	2.92404100	-1.24762700
H	-0.98625900	3.70599100	-0.71349500
N	-1.27869100	1.73069900	-1.25858300
H	1.42800000	1.83783600	-1.07674100
O	0.69971400	2.41190500	0.80173800
H	-0.93536400	0.95599900	-1.81507300
C	1.40494200	1.50719800	1.50228000
O	0.98418100	1.14683300	2.58619600
C	2.70424100	0.98785000	0.95833700
C	2.92187800	-0.39533000	0.96606100
C	4.13876700	-0.91518400	0.53492000
C	5.16386300	-0.04906200	0.11570700
C	4.94696700	1.34038700	0.13176200
C	3.72411600	1.85653000	0.54008000
C	-2.47784400	1.58205000	-0.65198800
N	-2.92911700	0.27772700	-0.70629200
S	-3.30126200	2.83670000	0.12565000
C	-4.19520900	-0.26161400	-0.45347000
C	-4.24523300	-1.60910600	-0.04468800
C	-5.46053600	-2.23831400	0.17301700
C	-6.64071000	-1.51370200	-0.01756800
C	-6.61376900	-0.17945900	-0.43393500
C	-5.39494000	0.44558500	-0.65517200
F	6.66554000	-2.59407600	0.86062900
C	6.77940400	-2.05434800	-0.37492700
F	8.01725800	-2.30350000	-0.81707500
F	5.91218400	-2.70121300	-1.18803800
N	-7.91784600	-2.16224600	0.21280000
O	-8.95219900	-1.50062400	0.06036100
O	-7.92262200	-3.35235700	0.55169600
H	2.13756500	-1.06225100	1.30580600
H	4.27526700	-1.98906000	0.53666200
H	5.74490100	2.00412800	-0.18020700
H	3.57375000	2.93039400	0.55183700
H	-2.21338300	-0.42076200	-0.87318600
H	-3.32278600	-2.16001400	0.10921600
H	-5.49966600	-3.27083700	0.49474500
H	-7.54062500	0.35555700	-0.59594200
H	-5.37122700	1.47223000	-0.98997900

C	6.48970800	-0.52086500	-0.34833900
O	7.38407300	0.21553600	-0.71687700
H	-0.28148200	3.26223200	-2.27653900
H	1.52503300	3.57761500	-0.70622400

### 1-conf18

C	0.25632100	4.39567800	-0.27432700
C	-1.11659600	4.32167200	0.37377500
H	-1.02906200	4.06598500	1.42964400
N	-1.98591600	3.33792400	-0.25659700
H	0.19580800	4.57733100	-1.35099100
O	0.91647200	3.12915500	-0.04980200
H	-2.28938500	3.55734200	-1.19874800
C	2.15462500	2.98887300	-0.54323000
O	2.74181300	3.86799600	-1.15194100
C	2.73170800	1.63770500	-0.26371200
C	4.03344500	1.37255600	-0.70538200
C	4.61373800	0.12934600	-0.47434700
C	3.88956300	-0.86725500	0.20402800
C	2.58231300	-0.59490400	0.64715000
C	2.00592000	0.64750400	0.41759400
C	-2.43181700	2.18823300	0.29655200
N	-3.10028900	1.39549800	-0.61581000
S	-2.15818800	1.75353300	1.90803600
C	-3.90270800	0.26365700	-0.43556800
C	-3.99480100	-0.62768700	-1.52349800
C	-4.80532500	-1.74912400	-1.45498300
C	-5.53308700	-1.98623200	-0.28504000
C	-5.46698800	-1.10802100	0.80038200
C	-4.65717600	0.01652200	0.72625400
F	6.00413400	-2.43849600	-1.32500800
C	5.88102200	-2.56240500	0.01682700
F	6.20676100	-3.81898600	0.34181700
F	6.78823900	-1.73886500	0.59128900
N	-6.37839500	-3.16203700	-0.19952000
O	-7.00287200	-3.36545900	0.84905700
O	-6.44232400	-3.91542800	-1.17914400
H	4.58438100	2.14489200	-1.22914100
H	5.62193500	-0.04896300	-0.82575200
H	2.03041700	-1.36712200	1.17042300
H	0.99935500	0.85232000	0.76225000
H	-2.91496400	1.60781700	-1.58974100
H	-3.41836000	-0.43855900	-2.42341700
H	-4.86923300	-2.43793300	-2.28720900
H	-6.05611300	-1.29995600	1.68788500
H	-4.61402700	0.70273400	1.55889900
C	4.43253100	-2.21741600	0.48518100
O	3.81877900	-3.09155400	1.06598800
H	-1.58407400	5.30866200	0.29527400
H	0.84327500	5.19645800	0.18345200

### 1-conf19

C	0.36081700	-2.84292600	-0.97864900
C	1.78346700	-2.99222600	-1.49488500

H	2.21418500	-3.93514900	-1.15893900
N	2.65538500	-1.91388600	-1.04740100
H	-0.05488600	-1.86168000	-1.21796700
O	0.39152000	-3.03266400	0.45932500
H	2.43617900	-0.99154600	-1.40474400
C	-0.46014500	-2.42478600	1.30347000
O	-0.21029800	-2.43164400	2.49461300
C	-1.70485400	-1.77698100	0.76935800
C	-1.99304400	-0.46525900	1.16573500
C	-3.16581100	0.15275200	0.74199800
C	-4.07972300	-0.55021600	-0.06237800
C	-3.79673500	-1.87628400	-0.43572200
C	-2.61461600	-2.48351000	-0.03251300
C	3.80572200	-2.06254500	-0.36768700
N	4.47936000	-0.91335000	-0.01878400
S	4.50000000	-3.55589100	0.04799600
C	4.08394500	0.43302600	-0.03135400
C	5.08822000	1.40199900	-0.22486100
C	4.77938600	2.75239500	-0.19958300
C	3.45317700	3.14076700	0.01372200
C	2.44393800	2.19904900	0.22234900
C	2.75945900	0.84669000	0.20866400
F	-5.78385400	1.65552600	1.17704600
C	-5.70435100	1.50440600	-0.16526600
F	-6.88028800	1.87024400	-0.68795600
F	-4.76428400	2.36466200	-0.62082600
N	3.11983600	4.55540500	0.02963200
O	1.93798800	4.87965700	0.19244200
O	4.03244800	5.37567700	-0.12033500
H	-1.29725400	0.07135400	1.80084100
H	-3.35636600	1.17282400	1.04998500
H	-4.51095400	-2.41856000	-1.04439400
H	-2.41424900	-3.50867200	-0.32384700
H	5.43370200	-1.09245700	0.26717400
H	6.11063300	1.08688400	-0.40375400
H	5.54725000	3.49900900	-0.35516700
H	1.42959300	2.52377500	0.41471900
H	1.98265700	0.12504000	0.42640500
C	-5.35312700	0.03218600	-0.54699900
O	-6.15746800	-0.56595900	-1.23496600
H	1.74914800	-3.00082800	-2.58986500
H	-0.26373200	-3.61857200	-1.42792400

### 1-conf20

C	-1.06322200	-2.98499000	1.95408500
C	-2.01988000	-3.52727000	0.90564200
H	-1.49538500	-4.17042900	0.19924500
N	-2.67347800	-2.46584100	0.14893700
H	-1.54781100	-2.27623300	2.63104300
O	0.00975600	-2.31155200	1.25697200
H	-3.33666900	-1.89937800	0.66449100
C	0.93948600	-1.70267500	2.00662900
O	0.92485000	-1.69756500	3.22630700
C	1.99183400	-1.03374100	1.18096300
C	3.02426000	-0.36234400	1.84681400
C	4.02751500	0.27528400	1.12394700

C	4.00609300	0.24517500	-0.28188500
C	2.96635500	-0.43101900	-0.94604200
C	1.96573900	-1.06611100	-0.22246700
C	-2.56778400	-2.25768200	-1.17406500
N	-3.22227300	-1.15938000	-1.68608500
S	-1.73058100	-3.26932500	-2.25199500
C	-3.76612500	-0.03385500	-1.04730500
C	-4.87331400	0.59130300	-1.65302100
C	-5.42622000	1.73501900	-1.09887800
C	-4.87292300	2.25572000	0.07486900
C	-3.76578200	1.66162700	0.68393100
C	-3.20721900	0.52273600	0.11907200
F	5.73286900	2.68123900	0.33332900
C	6.20333800	1.66835000	-0.43079200
F	7.03844700	2.19283700	-1.33511500
F	6.92406100	0.84958300	0.37003400
N	-5.45571800	3.44774400	0.66844200
O	-4.97069300	3.87773000	1.72114900
O	-6.41221300	3.98181000	0.09566300
H	3.03422100	-0.34472400	2.93029700
H	4.81429200	0.78703600	1.66324800
H	2.95599900	-0.44974400	-2.02964500
H	1.16731400	-1.58516500	-0.73883000
H	-3.32522400	-1.19618900	-2.69231100
H	-5.30269400	0.16846400	-2.55497300
H	-6.28225400	2.21368000	-1.55649800
H	-3.33599900	2.09939200	1.57556900
H	-2.31736300	0.09608200	0.56482700
C	5.03640800	0.89742100	-1.12441400
O	5.03651100	0.87581900	-2.34000200
H	-2.78370800	-4.12483700	1.41381400
H	-0.65056500	-3.80698100	2.54515600

### 1-conf21

C	-0.41868000	1.89504000	-1.52250900
C	0.74786900	2.86572700	-1.40011900
H	1.53585900	2.59555900	-2.10926100
N	1.31317000	2.97908700	-0.05548700
H	-1.16596800	2.07059100	-0.74731300
O	0.12395000	0.54877800	-1.39404800
H	0.99909900	3.75564100	0.51075900
C	-0.54982900	-0.48853400	-0.84565700
O	0.08488700	-1.46352000	-0.49514900
C	-2.03961200	-0.41210900	-0.71755600
C	-2.61810200	-0.76622200	0.50741900
C	-4.00203800	-0.75804900	0.65451900
C	-4.82256000	-0.42369000	-0.43671400
C	-4.23556600	-0.09655000	-1.67192000
C	-2.85405100	-0.07937700	-1.81102000
C	2.37062500	2.31431000	0.46651500
N	2.74155700	1.18880400	-0.22377100
S	3.08957300	2.85581200	1.90571100
C	3.87801400	0.38285900	-0.06616000
C	3.72591700	-0.99503700	-0.31181700
C	4.81677700	-1.84789300	-0.23353800
C	6.06763700	-1.31716800	0.09373500

C	6.24024900	0.05022100	0.33000700
C	5.14719800	0.90087800	0.24607200
F	-6.70951300	-1.97200600	1.40961500
C	-6.99892600	-0.71646200	0.99602400
F	-8.32874900	-0.61661500	0.89171000
F	-6.59461500	0.13921000	1.96297600
N	7.21395400	-2.20402900	0.18368700
O	8.31016200	-1.72203200	0.49405600
O	7.04932600	-3.40677600	-0.05434200
H	-1.98513700	-1.03925500	1.34411500
H	-4.42402800	-1.01908500	1.61653300
H	-4.87364900	0.14587000	-2.51370400
H	-2.41667900	0.16786800	-2.77182400
H	2.00420400	0.76689900	-0.78513900
H	2.74329000	-1.39153800	-0.54825200
H	4.70437000	-2.90951400	-0.41120100
H	7.22302400	0.43963400	0.56215100
H	5.27590300	1.96086500	0.41306500
C	-6.30327600	-0.39805000	-0.36426600
O	-7.02566700	-0.13777200	-1.30637400
H	0.38355000	3.85678400	-1.68196500
H	-0.87300900	1.99555900	-2.51029100

### 1-conf22

C	-1.41250100	-4.20392100	-0.86647500
C	-2.84449700	-3.69520300	-0.83369700
H	-3.00649200	-2.94703800	-1.61360400
N	-3.25964900	-3.14986700	0.45761400
H	-1.24161000	-4.97893800	-0.11475700
O	-0.53000800	-3.08942900	-0.57171100
H	-3.63496600	-3.79940000	1.13626900
C	0.77495700	-3.25416900	-0.87141300
O	1.20854700	-4.23160500	-1.45284800
C	1.62458100	-2.11458300	-0.41371200
C	2.88144700	-1.95051600	-1.00903600
C	3.71817500	-0.91527300	-0.60472800
C	3.30798900	-0.03902000	0.41584400
C	2.05096100	-0.21760400	1.02082700
C	1.21262900	-1.24499800	0.60790000
C	-3.35311100	-1.85354100	0.82421000
N	-2.73475700	-0.96691200	-0.02728300
S	-4.13294900	-1.42949400	2.26983500
C	-2.87227100	0.42144300	-0.14255200
C	-1.79291900	1.12811000	-0.70896700
C	-1.86948100	2.49731300	-0.90827000
C	-3.03730400	3.17026100	-0.53829300
C	-4.12498800	2.48626000	0.01230300
C	-4.04556600	1.11476500	0.20687700
F	6.34269900	0.22530500	0.45233300
C	5.55276300	1.31000600	0.27874500
F	6.16774800	2.35744300	0.83940700
F	5.46414000	1.54593700	-1.05078100
N	-3.12486500	4.60474600	-0.73833300
O	-4.15750900	5.18786400	-0.38584500
O	-2.16356200	5.18810300	-1.25448500
H	3.19493100	-2.63316500	-1.79018700

H	4.68008900	-0.80378700	-1.08838400
H	1.74495600	0.45467400	1.81389600
H	0.25118300	-1.38472100	1.08711600
H	-1.98165700	-1.35955100	-0.58265600
H	-0.88755500	0.59908800	-0.98789100
H	-1.03777000	3.04167000	-1.33611600
H	-5.02731500	3.02451100	0.27228100
H	-4.88878400	0.58222300	0.62180600
C	4.14139700	1.08517700	0.90623400
O	3.79637000	1.85742500	1.77912000
H	-3.50034000	-4.54008900	-1.06154900
H	-1.17812900	-4.60341800	-1.85481800

### 1-conf23

C	0.18438700	-0.53709800	0.56342800
C	1.57165100	-0.32384600	-0.02289400
H	2.29382400	-0.21612500	0.78588700
N	1.61517500	0.86838000	-0.87138300
H	-0.58278700	-0.54466800	-0.21418200
O	-0.06122200	0.53225700	1.50895100
H	0.81624000	1.01746100	-1.47624700
C	-1.26645900	1.09937100	1.70422100
O	-1.32359100	2.15124700	2.31274800
C	-2.50520200	0.41793300	1.20112300
C	-3.44002600	1.18579400	0.49578700
C	-4.63503900	0.61552200	0.06777400
C	-4.91851100	-0.72875800	0.36625100
C	-3.98555700	-1.48847500	1.09425200
C	-2.78358500	-0.92449800	1.50164800
C	2.38537000	1.96265700	-0.71923000
N	3.57306200	1.83244000	-0.02764800
S	1.92507700	3.47530100	-1.32689900
C	4.53109800	0.80809600	-0.09369300
C	5.57142100	0.83040000	0.85586600
C	6.57573300	-0.12292300	0.81971000
C	6.53940800	-1.11097500	-0.16986000
C	5.52207200	-1.14394000	-1.12662100
C	4.52096900	-0.18333200	-1.09197800
F	-7.67478100	0.46929700	-0.13939300
C	-7.23966000	-0.60007000	-0.84506500
F	-8.30245100	-1.36033300	-1.13189200
F	-6.73133500	-0.14290400	-2.01298500
N	7.58315900	-2.11893300	-0.20731500
O	7.52120500	-3.00019200	-1.07309600
O	8.49288000	-2.05604500	0.62833300
H	-3.22865000	2.22708400	0.28064700
H	-5.33371800	1.22790600	-0.48769000
H	-4.21472300	-2.52046300	1.33310000
H	-2.07909500	-1.52227700	2.06930000
H	3.92023000	2.71858700	0.31871700
H	5.58234500	1.59630900	1.62429400
H	7.37405000	-0.11343300	1.55040100
H	5.52565200	-1.90486900	-1.89630900
H	3.75051600	-0.19202800	-1.85255000
C	-6.17080300	-1.40715300	-0.04346400
O	-6.42880500	-2.56873900	0.20560300

H	1.83852100	-1.21512900	-0.60096900
H	0.16636800	-1.49137700	1.09500700

### 1-conf24

C	0.99532900	2.53932500	-0.56941700
C	2.20448800	1.76844400	-0.07140400
H	2.26058800	0.80620200	-0.58095900
N	2.13412800	1.54168900	1.37471200
H	0.84780900	3.47668900	-0.02490400
O	-0.16584800	1.69863800	-0.38806800
H	1.74842800	2.29661800	1.92935100
C	-1.34254400	2.19385100	-0.80379300
O	-1.46396000	3.29364200	-1.31584500
C	-2.47752700	1.24902300	-0.57242000
C	-3.75354000	1.63636200	-0.99900200
C	-4.84333700	0.79305200	-0.80726500
C	-4.66386500	-0.45388400	-0.18241200
C	-3.37978900	-0.83769200	0.24532700
C	-2.29367600	0.00562900	0.05280900
C	2.18594500	0.36662800	2.02878500
N	2.80861400	-0.69757200	1.40863700
S	1.48833300	0.15917800	3.55964300
C	4.00287000	-0.71721200	0.66908200
C	4.30793000	-1.89473400	-0.04074000
C	5.49421700	-2.00075700	-0.74823100
C	6.38112900	-0.91914400	-0.75232700
C	6.10045400	0.25420300	-0.04815900
C	4.91394000	0.35449200	0.66532200
F	-7.62623300	0.11388300	0.23287100
C	-7.21693500	-1.01940200	-0.38264300
F	-8.08999800	-1.98675000	-0.07909400
F	-7.28182100	-0.80848700	-1.71780800
N	7.62233300	-1.02079700	-1.49868900
O	8.38776800	-0.04931200	-1.50560600
O	7.86386900	-2.07538400	-2.09799100
H	-3.88382700	2.59853400	-1.48018100
H	-5.81894100	1.11569900	-1.14753000
H	-3.24888500	-1.79938100	0.72762400
H	-1.30753700	-0.29361100	0.38545500
H	2.53462700	-1.59086000	1.79995900
H	3.60544300	-2.72147500	-0.03704100
H	5.73154300	-2.90147900	-1.29925100
H	6.81126100	1.07041800	-0.04865200
H	4.71192600	1.25182800	1.23668000
C	-5.77081500	-1.41046400	0.05650200
O	-5.62966300	-2.49815000	0.58083100
H	3.10258400	2.34102700	-0.32711800
H	1.11564100	2.77008700	-1.63071700

### 1-conf25

C	0.63545600	1.04114100	0.95744700
C	-0.48479700	1.56530300	1.84353500
H	-0.59367400	0.89447600	2.69752800
N	-1.76443600	1.66074300	1.15549300



H	1.55656000	0.95654400	1.53808800
O	0.80955400	1.99648200	-0.12457100
H	-1.94819500	2.53545200	0.67907800
C	1.98109500	2.19720400	-0.75086200
O	2.10825800	3.18116300	-1.45650100
C	3.09329500	1.20154400	-0.59074200
C	4.36782200	1.67784500	-0.25954200
C	5.44205600	0.79801600	-0.16628500
C	5.25530800	-0.56999200	-0.43175500
C	3.97751700	-1.03852800	-0.78593800
C	2.90180100	-0.16313600	-0.85632000
C	-2.68553700	0.67590600	1.06781400
N	-3.72489900	0.99733800	0.21854800
S	-2.53511300	-0.80088300	1.87875200
C	-4.96800700	0.38559100	0.02144500
C	-5.57866600	0.57382100	-1.23474200
C	-6.83157700	0.04492700	-1.49950500
C	-7.48356200	-0.68231200	-0.49924300
C	-6.90223900	-0.86864000	0.75811200
C	-5.64946600	-0.33260000	1.02122400
F	8.24625400	-0.18105500	-0.87437800
C	7.78531900	-1.09330800	0.01234700
F	8.64414000	-2.11906400	0.02616800
F	7.80515200	-0.52133700	1.23853500
N	-8.79271200	-1.24667700	-0.76949700
O	-9.34714000	-1.90423800	0.11980900
O	-9.30354600	-1.04735700	-1.87868000
H	4.51605500	2.73525500	-0.07170800
H	6.41326700	1.19087100	0.10636800
H	3.84131600	-2.09162300	-1.00286100
H	1.92509100	-0.53961300	-1.13885300
H	-3.53531200	1.75058600	-0.43323800
H	-5.06000300	1.13252900	-2.00711700
H	-7.29750300	0.18210500	-2.46655900
H	-7.43490200	-1.41635700	1.52483700
H	-5.20384500	-0.46341300	1.99610600
C	6.34738200	-1.56913300	-0.36512000
O	6.20006800	-2.75519500	-0.58812700
H	-0.23210600	2.56227100	2.21153900
H	0.37272900	0.06957000	0.53537600

### 1-conf26

C	0.02511000	3.41072700	-0.03290700
C	1.01747300	3.34604900	1.11587700
H	1.75383200	4.14065700	0.98261500
N	1.71355100	2.06929500	1.21285300
H	-0.42117300	4.40693300	-0.09271700
O	-1.01726900	2.44082000	0.23647900
H	1.28673300	1.37677300	1.81557000
C	-1.99507300	2.33345800	-0.67470700
O	-2.04302900	3.00307800	-1.69303900
C	-3.01791500	1.30689200	-0.30460400
C	-4.09295600	1.10465800	-1.17836100
C	-5.07299000	0.16340000	-0.87969200
C	-4.98489700	-0.58887300	0.30511300
C	-3.90282700	-0.38162100	1.18010800

C	-2.92600600	0.55837000	0.87941600
C	2.84379900	1.73841100	0.54996700
N	3.20686500	0.42197900	0.74946800
S	3.67177000	2.82844200	-0.44356300
C	4.36693000	-0.28377800	0.41379700
C	4.24728100	-1.68714000	0.33449600
C	5.34726500	-2.47848700	0.04948900
C	6.58606400	-1.86456900	-0.16036200
C	6.73034400	-0.47765100	-0.07221500
C	5.62662700	0.31266400	0.21836300
F	-7.94245600	-0.75376700	-0.41372400
C	-7.20319000	-1.87450700	-0.24451900
F	-8.00464500	-2.82035600	0.25901700
F	-6.79533900	-2.28688700	-1.46709200
N	7.74285600	-2.68379000	-0.46780200
O	8.82716600	-2.12295300	-0.66945800
O	7.60014300	-3.91206200	-0.51579400
H	-4.15411800	1.68881300	-2.08899700
H	-5.89377300	0.02697000	-1.57194000
H	-3.84147000	-0.96476300	2.09160300
H	-2.09540200	0.71540900	1.55629700
H	2.48386300	-0.16711000	1.14748500
H	3.28050900	-2.15500100	0.49102000
H	5.25213100	-3.55427300	-0.01910400
H	7.70251700	-0.02461100	-0.21804500
H	5.73873300	1.38333300	0.29627900
C	-5.98563200	-1.61013400	0.69595000
O	-5.92410100	-2.26881200	1.71596100
H	0.50178800	3.50894100	2.06515800
H	0.49682700	3.17177800	-0.98809900

### 1-conf27

C	-0.18552300	1.14722700	0.88402700
C	0.91263900	1.78890600	1.71803300
H	0.67447600	2.84597600	1.85293000
N	2.23150300	1.66904900	1.10756900
H	-1.15074800	1.28519900	1.37554100
O	0.12810400	-0.26814800	0.77712600
H	2.79890100	0.89221100	1.42029600
C	-0.80892400	-1.22032700	0.63200600
O	-0.49345600	-2.38446600	0.79624400
C	-2.20989000	-0.83556400	0.25300100
C	-3.26642100	-1.33284300	1.02573600
C	-4.58352200	-1.05282900	0.67408100
C	-4.85741000	-0.29202800	-0.47596600
C	-3.79225000	0.18396200	-1.26135700
C	-2.47778100	-0.07618000	-0.89655700
C	2.75552300	2.52825400	0.21803300
N	3.98697000	2.21695600	-0.31106700
S	2.01216300	3.98117200	-0.25225500
C	4.72593900	1.02359800	-0.28278800
C	6.13028900	1.12583300	-0.31701200
C	6.91908400	-0.01325200	-0.34222700
C	6.30016300	-1.26688200	-0.32581800
C	4.90983300	-1.39240700	-0.30559700
C	4.12214700	-0.24860000	-0.29201300

F	-7.46229200	-1.81003700	-0.00479200
C	-7.44248800	-0.45892700	-0.07770300
F	-8.60154500	-0.06177600	-0.61510000
F	-7.38799500	0.02014600	1.18670600
N	7.12200900	-2.46601600	-0.34123800
O	6.55835900	-3.56579400	-0.31159000
O	8.35055900	-2.33576000	-0.38352700
H	-3.05654300	-1.93415100	1.90312100
H	-5.38071900	-1.43716600	1.29736800
H	-4.00897300	0.75857100	-2.15436900
H	-1.66853000	0.29192800	-1.51752000
H	4.42435000	3.00274700	-0.77601400
H	6.59742200	2.10491800	-0.31502700
H	7.99859800	0.06094800	-0.36113700
H	4.45247700	-2.37317400	-0.32184800
H	3.04473800	-0.35346800	-0.33049200
C	-6.22979300	0.04170900	-0.92338200
O	-6.48282800	0.69040400	-1.92005300
H	0.96174600	1.31316200	2.69963400
H	-0.21426500	1.58083600	-0.11717600

### 1-conf28

C	-2.04576800	-3.48964300	0.48854800
C	-3.12763400	-2.83952000	1.33385900
H	-4.00971600	-3.48224700	1.33002600
N	-3.50307500	-1.51475000	0.85105800
H	-1.82090300	-4.49254400	0.86137000
O	-0.85960400	-2.66527800	0.60012800
H	-3.01385000	-0.73335700	1.26731900
C	0.19700900	-3.01121300	-0.15070400
O	0.20245500	-3.97011800	-0.90396900
C	1.36177800	-2.09239800	0.03901100
C	2.51129700	-2.31758800	-0.72782000
C	3.62191500	-1.49129300	-0.58709100
C	3.59338000	-0.42833000	0.33306600
C	2.43675500	-0.20773200	1.10303300
C	1.32827800	-1.03102500	0.95720400
C	-4.46905700	-1.25891600	-0.04620300
N	-4.62832700	0.04897600	-0.44564700
S	-5.52202600	-2.43348300	-0.67493400
C	-3.79205200	1.16607800	-0.29911000
C	-4.40413800	2.43373300	-0.24454200
C	-3.63666600	3.58364200	-0.15149200
C	-2.24394100	3.46762100	-0.10553400
C	-1.61508300	2.22287900	-0.17242100
C	-2.38692000	1.07324000	-0.27723900
F	6.57823000	-0.90358400	-0.11731000
C	6.02381700	0.31509700	-0.31419600
F	6.94276800	1.23613100	-0.00204800
F	5.75049300	0.43470500	-1.63384200
N	-1.43289700	4.66866300	0.00364600
O	-0.20429400	4.54542200	0.06550200
O	-2.00551700	5.76396800	0.02992800
H	2.52736500	-3.14078500	-1.43237900
H	4.49719800	-1.68637300	-1.19340300
H	2.42119600	0.61329300	1.81037500

H	0.44019500	-0.85661900	1.55174800
H	-5.50976400	0.21077100	-0.91651600
H	-5.48611000	2.50799900	-0.26684200
H	-4.10391600	4.55855000	-0.10128100
H	-0.53467500	2.15876900	-0.16439800
H	-1.89012300	0.11684300	-0.38317000
C	4.73395600	0.49415200	0.54656100
O	4.73477600	1.39921900	1.35825800
H	-2.78361400	-2.72752900	2.36452900
H	-2.33827100	-3.55493700	-0.56138800

### 1-conf29

C	0.20665600	1.88467600	0.75567200
C	-0.83087700	2.60153000	1.61266200
H	-1.13174100	1.94178000	2.43339900
N	-1.99001800	3.07791500	0.86234900
H	1.01514400	1.52013800	1.39274200
O	0.71136000	2.85304900	-0.19806200
H	-1.96424300	4.03535900	0.53929400
C	1.95831800	2.80277300	-0.70120100
O	2.39173100	3.77463800	-1.29047000
C	2.77301600	1.55134700	-0.54476400
C	4.06800500	1.66266700	-0.02399100
C	4.88008100	0.53702900	0.07923000
C	4.41119800	-0.71134600	-0.36553700
C	3.11839800	-0.81184600	-0.90989000
C	2.30015800	0.30727300	-0.99081000
C	-3.05272900	2.37702200	0.40594300
N	-3.13313100	1.08221300	0.85190900
S	-4.19305600	3.13270200	-0.59781600
C	-4.03059800	0.05676900	0.50966800
C	-4.32781900	-0.88969900	1.50803300
C	-5.16025800	-1.96497200	1.23685900
C	-5.69969500	-2.09302500	-0.04551000
C	-5.40505100	-1.17263600	-1.05471500
C	-4.56711900	-0.10028100	-0.77985600
F	7.44379800	-1.04782700	-0.40665600
C	6.65567100	-1.89125200	0.29938300
F	7.23460400	-3.09720300	0.28797600
F	6.63208500	-1.45612800	1.58063100
N	-6.58028600	-3.21195300	-0.33720500
O	-7.06709900	-3.29841600	-1.47040800
O	-6.80649000	-4.03256400	0.55973500
H	4.43708800	2.62805300	0.30343800
H	5.87187900	0.64809000	0.49847600
H	2.76661000	-1.77373500	-1.26445000
H	1.30874700	0.21344800	-1.42021900
H	-2.54965000	0.85082600	1.64641000
H	-3.91240700	-0.77372200	2.50379000
H	-5.39851500	-2.68885100	2.00516000
H	-5.81754700	-1.30548400	-2.04650800
H	-4.32516000	0.60728000	-1.55926000
C	5.21611200	-1.95364500	-0.30081000
O	4.82663200	-3.03830000	-0.68784000
H	-0.37611000	3.47724900	2.07915800
H	-0.23541000	1.04797400	0.21087600

### 1-conf30

C	-0.62643500	-2.00782200	-1.53619200
C	-1.28982000	-2.99945900	-0.59023500
H	-2.19637800	-3.39120900	-1.06385400
N	-1.57747000	-2.45270400	0.73470000
H	-0.48463600	-2.46411300	-2.51951600
O	0.66314800	-1.67701600	-0.97339400
H	-0.90307700	-2.63719000	1.46453900
C	1.39361000	-0.76404400	-1.63322000
O	1.02084300	-0.22096500	-2.65924400
C	2.70745900	-0.49170400	-0.97442100
C	3.56122500	0.44273200	-1.57290600
C	4.79712400	0.73019600	-1.00259200
C	5.19179300	0.08017500	0.18032000
C	4.32971100	-0.85702300	0.77837100
C	3.09669000	-1.14237100	0.20698800
C	-2.56152100	-1.60234400	1.10360300
N	-3.51569500	-1.36807500	0.14589500
S	-2.57817700	-0.95970500	2.67419200
C	-4.59055200	-0.46508900	0.12894400
C	-5.71501900	-0.82886300	-0.63631500
C	-6.79890300	0.02782300	-0.75094100
C	-6.75683600	1.26052800	-0.09428000
C	-5.64375800	1.64704500	0.65674700
C	-4.55872900	0.78788600	0.76539900
F	7.83360900	0.97992300	-1.03970000
C	7.48513100	1.35108300	0.21407700
F	8.60637800	1.44642300	0.93793600
F	6.93525400	2.58527500	0.14003300
N	-7.89105600	2.16216400	-0.20225400
O	-7.84564100	3.24113900	0.40011300
O	-8.85626300	1.81421200	-0.89277200
H	3.24991600	0.93901900	-2.48450700
H	5.43814100	1.45644200	-1.48560600
H	4.64031600	-1.35394100	1.69005100
H	2.43712600	-1.86534900	0.67063700
H	-3.53546400	-2.02458500	-0.62472200
H	-5.74051800	-1.79237500	-1.13528100
H	-7.66836800	-0.25308500	-1.33073100
H	-5.62511000	2.61626900	1.13808500
H	-3.69074600	1.08686400	1.33414300
C	6.49116100	0.32854500	0.84915500
O	6.84440500	-0.21847700	1.87577100
H	-0.63461100	-3.85930700	-0.43851600
H	-1.20929100	-1.09134700	-1.65341100

### 1-conf31

C	0.11545900	-1.05673400	0.02625500
C	1.60910500	-0.80412500	0.15999300
H	1.93764900	-0.24181300	-0.71484300
N	2.34068100	-2.07026100	0.23098800
H	-0.41644900	-0.10401600	-0.00172800
O	-0.28405700	-1.82925400	1.18904700

H	1.89874600	-2.80289900	0.77391100
C	-1.50785600	-1.75416400	1.74786800
O	-1.67338000	-2.22641600	2.85586100
C	-2.63237300	-1.11597200	0.98681700
C	-3.41156100	-0.15252300	1.63919200
C	-4.50520000	0.41733400	0.99406300
C	-4.84638700	0.00636600	-0.30637200
C	-4.07288200	-0.97757700	-0.94745600
C	-2.96855400	-1.52945000	-0.31153400
C	3.33554700	-2.49684400	-0.56855300
N	4.08254500	-1.55001300	-1.24045800
S	3.66504600	-4.14424100	-0.79163900
C	4.57792900	-0.31981000	-0.77796800
C	5.12330900	0.56201400	-1.73120900
C	5.66942500	1.77234400	-1.33643000
C	5.66716200	2.10772700	0.02157700
C	5.14186000	1.24168900	0.98351700
C	4.60177800	0.02662200	0.58523700
F	-7.45137800	1.16843700	0.76173800
C	-6.89812300	1.63673300	-0.38070000
F	-7.89286300	2.01382800	-1.19193400
F	-6.17919700	2.73972100	-0.06770900
N	6.22894700	3.37918000	0.44077000
O	6.20250500	3.66784800	1.64313600
O	6.71110200	4.12272400	-0.42199500
H	-3.15869800	0.15249000	2.64837300
H	-5.08182400	1.17043500	1.51576600
H	-4.34831700	-1.30079600	-1.94456500
H	-2.38886200	-2.29397400	-0.81677500
H	4.56720900	-1.93246100	-2.04333200
H	5.10848700	0.29374300	-2.78217800
H	6.08409200	2.45641800	-2.06534100
H	5.17144700	1.51220600	2.03105500
H	4.22436500	-0.65818400	1.33420000
C	-6.00077600	0.55384200	-1.05750000
O	-6.30356500	0.21197300	-2.18411200
H	1.80401400	-0.19945900	1.05149600
H	-0.10488100	-1.63387700	-0.87404000

### 1-conf32

C	-0.87819700	0.89822000	-1.90195800
C	-2.02801200	0.59027400	-0.95961700
H	-2.95819100	0.86736400	-1.45693900
N	-1.89594400	1.35177800	0.28489700
H	-0.98365000	0.32436400	-2.82562600
O	0.34014800	0.50216900	-1.22697400
H	-0.95217900	1.45966000	0.63725400
C	1.49209500	0.69263700	-1.89422500
O	1.54237200	1.16035200	-3.01815500
C	2.69053900	0.26763300	-1.10944800
C	3.95031600	0.42069900	-1.70103400
C	5.09898500	0.04170300	-1.01373200
C	4.99567200	-0.49769200	0.28079800
C	3.72755100	-0.64977800	0.87044800
C	2.58246500	-0.27096400	0.18239900
C	-2.79142100	2.18659600	0.84276900

N	-4.12339100	2.02499500	0.51775600
S	-2.32478700	3.43463800	1.89096300
C	-4.86533400	0.84015500	0.38163700
C	-6.15344000	0.93904200	-0.17912800
C	-6.95469100	-0.18462800	-0.29980200
C	-6.46430400	-1.41874100	0.13969100
C	-5.19432500	-1.53538000	0.70964700
C	-4.39677000	-0.40633400	0.83490200
F	7.70984800	-1.49947000	-0.67782700
C	7.59626100	-0.78147700	0.46347600
F	8.53413300	-1.21490600	1.31356900
F	7.87273400	0.50947500	0.16669600
N	-7.29512100	-2.60208600	0.00724200
O	-6.84071300	-3.68729900	0.38875200
O	-8.42413700	-2.47693100	-0.48194500
H	4.02171400	0.83745100	-2.69874300
H	6.06044400	0.17135900	-1.49378300
H	3.65532400	-1.06646100	1.86828600
H	1.60909000	-0.39163500	0.64131800
H	-4.67318500	2.85635600	0.69762800
H	-6.51695500	1.90061900	-0.52559000
H	-7.94276700	-0.11562000	-0.73590900
H	-4.84451200	-2.49661000	1.06330700
H	-3.42544900	-0.49105700	1.30571500
C	6.16929700	-0.92463700	1.07990100
O	6.09722100	-1.38721700	2.20176500
H	-2.06003400	-0.48367900	-0.74904300
H	-0.82154400	1.96242900	-2.14235700

**Annex II:** XYZ cartesian coordinates of the optimized energies of 28 starting rotamers of chemosensor **2** (**2-conf1** to **2-conf28**).

### **2-conf1**

C	-1.57220300	5.05566500	1.51664000
C	-1.51293500	3.52813800	1.66910400
C	-1.46874400	2.80235300	0.32585900
C	-0.35667000	3.33896900	-0.61084800
C	-0.39172100	4.87178100	-0.71905000
C	-0.41785900	5.57492200	0.64800900
H	-0.49911800	2.89111900	-1.59681300
N	0.95208800	2.89868600	-0.12246700
H	-1.32833900	1.72927000	0.45812300
O	-2.73228900	3.04118100	-0.37129500
H	1.48412200	3.57866200	0.40788900
C	-3.51132700	2.07573200	-0.88525500
O	-4.33376100	2.37286400	-1.73372200
C	-3.40408500	0.66528000	-0.37877200
C	-3.32729200	-0.37135600	-1.31685200
C	-3.30156400	-1.69770900	-0.89674400
C	-3.38032200	-2.00242000	0.47368500
C	-3.48049600	-0.95798300	1.41016200
C	-3.48320500	0.36559800	0.99013700
C	1.53454200	1.70643000	-0.38256800
N	2.72322400	1.54000900	0.30052300
S	0.83810100	0.54105100	-1.38934500
C	3.73052000	0.57804300	0.17016700

C	4.53176800	0.34044500	1.30557400
C	5.58356200	-0.55956000	1.25498600
C	5.84014900	-1.23299200	0.05682200
C	5.06724400	-1.00185100	-1.08444200
C	4.01706800	-0.09602400	-1.03141700
F	-4.26534600	-4.58930400	-0.87928900
C	-3.24001800	-4.57695100	0.00386000
F	-3.24296000	-5.74965000	0.64833700
F	-2.08880900	-4.49689100	-0.70253500
N	6.93408600	-2.18396300	-0.00391400
O	7.13468100	-2.78630800	-1.06590400
O	7.62413700	-2.35492500	1.00895000
H	-1.54212300	5.52096700	2.50746900
H	-2.52832500	5.34113500	1.06118200
H	-0.60930700	3.24477100	2.22367200
H	-2.36328900	3.16086400	2.25254800
H	-1.29743600	5.13655200	-1.27462200
H	0.45955300	5.20624800	-1.32186800
H	-0.51169000	6.65534300	0.49552900
H	0.53385500	5.42855100	1.17939000
H	-3.28206100	-0.13788100	-2.37454400
H	-3.22633700	-2.47810800	-1.64335500
H	-3.55288800	-1.19785800	2.46460400
H	-3.56614800	1.15926900	1.72426800
H	2.85583400	2.15823000	1.09308600
H	4.31868900	0.86177100	2.23351100
H	6.19331900	-0.74841100	2.12883300
H	5.29756700	-1.51824800	-2.00741500
H	3.42625800	0.09294500	-1.91518600
C	-3.36973200	-3.38559000	1.00362300
O	-3.45321300	-3.66381500	2.18441000

## 2-conf2

C	1.54249100	3.66884000	1.59242400
C	0.68102200	2.39717700	1.60535400
C	-0.02124100	2.14409300	0.27308400
C	0.94636800	2.18270000	-0.93652000
C	1.83789000	3.43382400	-0.91437100
C	2.54722900	3.65071000	0.43208000
H	0.34547400	2.16772300	-1.84889200
N	1.77587600	0.97053500	-0.94671800
H	-0.54588200	1.18806600	0.27513100
O	-0.98220100	3.22269600	0.04561500
H	2.73936400	1.08438800	-0.65570300
C	-2.28055600	3.04036000	-0.24571900
O	-2.90090000	3.95366600	-0.76100600
C	-2.96456700	1.75187700	0.11242100
C	-3.77134200	1.13959900	-0.85440800
C	-4.48401600	-0.01464200	-0.54468200
C	-4.41722300	-0.55580000	0.75134600
C	-3.62400500	0.07662700	1.72526000
C	-2.89605900	1.21582000	1.40768100
C	1.43519700	-0.19039500	-1.53577300
N	2.36424900	-1.20577800	-1.53104200
S	-0.05138200	-0.46198500	-2.30985600
C	3.59398900	-1.33054800	-0.86475100
C	4.61975300	-2.04672600	-1.51176500



C	5.84131100	-2.24446000	-0.88770000
C	6.04318700	-1.71603100	0.39099800
C	5.03567100	-1.01755400	1.05825100
C	3.80854500	-0.83319900	0.43412200
F	-7.01649000	-1.71361200	-0.35586400
C	-6.03265500	-2.51735800	0.11033200
F	-6.60883400	-3.60127200	0.64278800
F	-5.29440600	-2.92087100	-0.94948900
N	7.32753500	-1.90899700	1.04552900
O	7.49585900	-1.41668800	2.16667700
O	8.19695900	-2.55705400	0.45255200
H	2.06735200	3.76105700	2.54901500
H	0.89426100	4.54887800	1.50062300
H	1.31079500	1.52359900	1.81428600
H	-0.06395500	2.43928800	2.40628200
H	1.19224100	4.29354800	-1.12179300
H	2.55812300	3.37385400	-1.73772400
H	3.10581300	4.59203700	0.39685500
H	3.29490400	2.86400100	0.60826200
H	-3.83582000	1.56518400	-1.84936500
H	-5.08764500	-0.47577200	-1.31589200
H	-3.58501700	-0.33660900	2.72644500
H	-2.29420200	1.69531100	2.17145000
H	2.12668000	-1.95202800	-2.17277500
H	4.45473400	-2.43765700	-2.51001100
H	6.63531600	-2.78701800	-1.38414100
H	5.20418400	-0.64452100	2.06014200
H	3.01073600	-0.34409800	0.97831400
C	-5.15131100	-1.77473800	1.16291800
O	-5.11464900	-2.24725200	2.28271200

## 2-conf3

C	5.71369500	-0.96403100	-1.05155200
C	4.22002200	-0.91295600	-1.40551500
C	3.33216400	-0.66686200	-0.18682000
C	3.77807900	0.57011300	0.63858200
C	5.28535500	0.53646800	0.94586500
C	6.15083800	0.30199700	-0.30222100
H	3.24362300	0.56061200	1.59541500
N	3.44731000	1.80214200	-0.08922400
H	2.29078300	-0.54672000	-0.48787700
O	3.44585800	-1.81519900	0.70726400
H	4.19678200	2.26789300	-0.58405200
C	2.40102500	-2.48374400	1.22686800
O	2.58348300	-3.19155400	2.20043800
C	1.04802300	-2.38936500	0.58143400
C	-0.05755800	-2.11279100	1.39459400
C	-1.33823200	-2.08534300	0.85015400
C	-1.52811200	-2.36091600	-0.51513500
C	-0.41628100	-2.66308200	-1.32176300
C	0.86304300	-2.66956900	-0.78151600
C	2.24279500	2.39231000	-0.26161600
N	1.21714200	1.85605600	0.47522000
S	2.09400600	3.73420700	-1.28928500
C	-0.16185500	2.12101300	0.41888100
C	-0.88254500	2.04768700	1.62420300
C	-2.25759600	2.23079400	1.63561800

C	-2.91262200	2.49031400	0.42962100
C	-2.21547200	2.55797300	-0.77982400
C	-0.84035400	2.36910500	-0.78634100
F	-4.27678400	-2.92306500	0.68887900
C	-4.12042600	-2.02573100	-0.31182600
F	-5.22962500	-2.04971100	-1.05920400
F	-4.02628500	-0.79738100	0.24872000
N	-4.35389600	2.68214500	0.43114400
O	-4.91635700	2.92763900	-0.64205500
O	-4.95885800	2.58986200	1.50555300
H	6.29950200	-1.08458800	-1.96860000
H	5.91314000	-1.84466100	-0.42902600
H	4.03292400	-0.09861200	-2.11640500
H	3.90250100	-1.83726300	-1.89847000
H	5.45231000	-0.27892700	1.65701400
H	5.56313600	1.46513200	1.45515500
H	7.19972300	0.22253700	0.00185900
H	6.09839600	1.16530900	-0.98026000
H	0.08538800	-1.91656000	2.45126300
H	-2.17376800	-1.85426200	1.49851200
H	-0.56878200	-2.88831200	-2.37089800
H	1.71063300	-2.90994500	-1.41387900
H	1.48906900	1.28981500	1.26992500
H	-0.35946300	1.85577900	2.55531600
H	-2.81582700	2.18284500	2.56147900
H	-2.74928500	2.73939400	-1.70370600
H	-0.29637400	2.40318000	-1.71940300
C	-2.85791100	-2.35511700	-1.16875500
O	-3.03845000	-2.59331600	-2.34719700

## 2-conf4

C	-2.19721600	-4.61037500	-0.97502100
C	-0.96150500	-3.94988800	-0.34496000
C	-0.95417700	-2.43176100	-0.51220100
C	-2.27677000	-1.76564000	-0.04754900
C	-3.50863300	-2.46473400	-0.64538100
C	-3.49615900	-3.98876000	-0.44312400
H	-2.26230400	-0.72719400	-0.37693200
N	-2.34848200	-1.79192000	1.42561200
H	-0.11781700	-1.98344000	0.02668200
O	-0.83047000	-2.12382000	-1.93451500
H	-2.67368800	-2.66031300	1.83293800
C	0.07676200	-1.27713500	-2.45288400
O	-0.11920000	-0.81265900	-3.56107500
C	1.33291700	-0.96072100	-1.69261900
C	1.70989600	0.38111400	-1.55964300
C	2.90501100	0.71367300	-0.92858700
C	3.75191900	-0.29993800	-0.44708700
C	3.37862100	-1.64672500	-0.60376400
C	2.17507500	-1.97614400	-1.21319700
C	-1.62632500	-1.05237400	2.29690300
N	-1.20963800	0.20526600	1.90455100
S	-1.20466700	-1.63364600	3.82780700
C	-1.91034600	1.20655700	1.21311900
C	-1.18363400	2.34747700	0.81991000
C	-1.81726000	3.39553500	0.17270600
C	-3.18822000	3.30272700	-0.08862100

C	-3.92847600	2.18440800	0.30207500
C	-3.29185500	1.13866900	0.95611200
F	5.62196500	2.08809200	-0.76132700
C	5.49640100	1.45058100	0.42560900
F	6.67787900	1.51337500	1.04978900
F	4.59902600	2.13870400	1.16918400
N	-3.85659500	4.39315300	-0.77587100
O	-5.06544600	4.28646800	-1.01461400
O	-3.18969100	5.38470900	-1.09474200
H	-2.17753300	-5.68553600	-0.76927200
H	-2.15702500	-4.49489700	-2.06491300
H	-0.93039900	-4.16406300	0.73099500
H	-0.03995900	-4.36209700	-0.76791800
H	-3.51706300	-2.24628700	-1.71836300
H	-4.41343800	-2.01722300	-0.22119400
H	-4.36219300	-4.42337400	-0.95306100
H	-3.61807700	-4.24187700	0.61976300
H	1.06635100	1.16323000	-1.94644100
H	3.16567200	1.75941500	-0.82681200
H	4.04009300	-2.42501400	-0.24133800
H	1.90252300	-3.01907500	-1.33140700
H	-0.44070900	0.54651300	2.46884200
H	-0.11914100	2.40306100	1.02198600
H	-1.26226900	4.27180900	-0.13621600
H	-4.99197600	2.14198800	0.10578600
H	-3.87077700	0.28275700	1.27979100
C	5.04433400	-0.02993200	0.22526000
O	5.79048300	-0.89554400	0.64006800

## 2-conf5

C	1.71121100	4.63971100	-1.96380200
C	1.65454000	3.11032600	-1.82895300
C	1.45100600	2.65190100	-0.38624000
C	0.24485000	3.34276400	0.29891700
C	0.27957700	4.86865100	0.11616700
C	0.47163300	5.30226400	-1.34634600
H	0.27084100	3.09327700	1.36200400
N	-1.00333400	2.79448500	-0.23634800
H	1.31667200	1.57134000	-0.32798500
O	2.62881700	3.03410000	0.39245600
H	-1.46262300	3.33883500	-0.95689500
C	3.33852500	2.19239000	1.16120700
O	4.05615000	2.65331200	2.03136100
C	3.28914400	0.71213700	0.90991400
C	3.10512200	-0.14438900	2.00633900
C	3.13048700	-1.51976200	1.82440600
C	3.36633400	-2.06371300	0.54815200
C	3.57372300	-1.20302500	-0.54296300
C	3.52654500	0.17699500	-0.36207600
C	-1.63003300	1.68142100	0.20692200
N	-2.73990400	1.36093400	-0.54930000
S	-1.06672400	0.76429600	1.51085500
C	-3.77039400	0.44342600	-0.31357500
C	-4.42466800	-0.08645900	-1.44352900
C	-5.49097100	-0.95976200	-1.29951600
C	-5.90798500	-1.31068100	-0.01217800
C	-5.28093500	-0.78707700	1.12190200

C	-4.21721900	0.09175400	0.97340100
F	2.69645200	-3.80293300	-1.85946000
C	3.63922800	-4.18460800	-0.96679600
F	3.61507600	-5.52031900	-0.89350900
F	4.84474000	-3.81987200	-1.46215300
N	-7.01880400	-2.23047700	0.14969600
O	-7.35968900	-2.54841500	1.29565800
O	-7.58180500	-2.65977100	-0.86497100
H	1.79885800	4.90779300	-3.02192600
H	2.61262100	5.01700800	-1.46570000
H	0.81756100	2.71520300	-2.41864500
H	2.56248300	2.65023700	-2.23202500
H	1.11636700	5.24612300	0.71326500
H	-0.63332800	5.29959000	0.54143800
H	0.56230300	6.39288400	-1.38888600
H	-0.41538700	5.05228500	-1.94616300
H	2.93861300	0.27284000	2.99315400
H	2.97436300	-2.18781200	2.66350600
H	3.77083300	-1.58994300	-1.53443200
H	3.69436200	0.82935400	-1.21145900
H	-2.77942400	1.79056000	-1.46689600
H	-4.08561200	0.18346600	-2.43857600
H	-5.98866600	-1.37382500	-2.16669600
H	-5.63547100	-1.05566900	2.10867900
H	-3.74100000	0.51026500	1.84758800
C	3.38481100	-3.54011700	0.43213200
O	3.21076500	-4.29971600	1.36547200

## 2-conf6

C	-1.17490800	3.14640000	-2.38381300
C	-0.36022700	1.92362400	-1.93610200
C	0.17830100	2.06063000	-0.51341500
C	-0.91629700	2.44378800	0.51437700
C	-1.75928400	3.63518500	0.03357100
C	-2.30519800	3.45817400	-1.39265200
H	-0.41985500	2.69301100	1.45518300
N	-1.78040000	1.28508900	0.77519900
H	0.66768000	1.14404000	-0.18210600
O	1.14236500	3.16022100	-0.48900500
H	-2.70462700	1.31390300	0.36175900
C	2.39684700	3.06715500	-0.01862900
O	2.98397900	4.08784800	0.29442300
C	3.08142100	1.73269200	0.06225900
C	3.77223200	1.40969500	1.24038800
C	4.48644700	0.22294700	1.32273900
C	4.54488700	-0.64984400	0.22033600
C	3.86882400	-0.31344200	-0.96455500
C	3.13525800	0.86814600	-1.03778200
C	-1.54300300	0.34203300	1.70541600
N	-2.49497600	-0.63691900	1.87934200
S	-0.16378700	0.30774700	2.69451800
C	-3.63568400	-0.96568000	1.13081600
C	-4.73595600	-1.50770000	1.82393500
C	-5.87561600	-1.89920700	1.13994200
C	-5.92097900	-1.74206300	-0.24878500
C	-4.83724800	-1.22217100	-0.95839800
C	-3.69181000	-0.84310100	-0.27035200

F	4.21513200	-3.33746000	-1.18417200
C	5.43730300	-2.88333700	-0.82117100
F	6.19068500	-3.94381800	-0.50818700
F	5.99206800	-2.28788200	-1.90237200
N	-7.11814800	-2.14058800	-0.97114500
O	-7.15080600	-1.96929200	-2.19490500
O	-8.05322300	-2.63423200	-0.33103600
H	-1.58399500	2.96388400	-3.38299100
H	-0.51253100	4.01663800	-2.46618300
H	-0.98925200	1.02519100	-1.96548300
H	0.47216200	1.73911100	-2.62249200
H	-1.11366400	4.51907400	0.06218600
H	-2.56865400	3.81217800	0.75027500
H	-2.83316600	4.36994300	-1.69141100
H	-3.05305900	2.65312500	-1.42572900
H	3.74136600	2.08854800	2.08521300
H	5.01140100	-0.03988100	2.23382600
H	3.90305800	-0.95703600	-1.83423000
H	2.62567300	1.11886200	-1.96101000
H	-2.35364100	-1.16738800	2.73004200
H	-4.69330200	-1.61116000	2.90286300
H	-6.72596400	-2.30870000	1.66958400
H	-4.88328700	-1.13807700	-2.03640800
H	-2.83317000	-0.49810400	-0.83211700
C	5.33576200	-1.89194900	0.38025400
O	5.92202100	-2.19999600	1.39995400

## 2-conf7

C	5.42197500	-1.28379800	-1.11631300
C	3.89855300	-1.22893200	-1.30399800
C	3.17051200	-0.67937100	-0.07830300
C	3.74777000	0.68082400	0.39712300
C	5.27873500	0.63196800	0.53825000
C	5.98362300	0.08701300	-0.71422900
H	3.32961300	0.90939900	1.38336100
N	3.36954000	1.73768800	-0.55055800
H	2.10439100	-0.56895400	-0.27960200
O	3.35645500	-1.61047900	1.03026700
H	4.05824600	2.01148600	-1.23908000
C	2.36033600	-2.12908700	1.77033600
O	2.63047600	-2.62854300	2.84734600
C	0.94972700	-2.12399500	1.25362100
C	-0.06481800	-1.66308300	2.10655900
C	-1.38875900	-1.69642700	1.69192000
C	-1.72496100	-2.21631000	0.42859000
C	-0.70930800	-2.70357600	-0.41127400
C	0.62099000	-2.64939300	-0.00231700
C	2.16745000	2.33205500	-0.72817400
N	1.23510700	2.06321500	0.24292100
S	1.92013500	3.37169300	-2.04509800
C	-0.13875400	2.34982900	0.28196300
C	-0.71302300	2.56995200	1.54765100
C	-2.07610400	2.79165600	1.67497800
C	-2.86934700	2.79375200	0.52498600
C	-2.31947900	2.56786300	-0.73988800
C	-0.95548800	2.34139100	-0.86192700

F	-2.98099400	-2.08459100	-2.33988200
C	-3.57829700	-2.77355700	-1.33995600
F	-4.90130100	-2.68449700	-1.51644800
F	-3.23014000	-4.07468700	-1.47180000
N	-4.29827100	3.03010600	0.64776300
O	-4.98271300	3.04833200	-0.38178100
O	-4.77177400	3.20203600	1.77707900
H	5.88875900	-1.62852500	-2.04474000
H	5.66985100	-2.02152600	-0.34355900
H	3.65075300	-0.57695800	-2.15066800
H	3.49859800	-2.21905300	-1.54428600
H	5.50375800	-0.02009700	1.38827900
H	5.64266800	1.63181300	0.79674400
H	7.05783000	0.01507400	-0.51459700
H	5.88120100	0.78712000	-1.55526400
H	0.19025000	-1.27589000	3.08677200
H	-2.17602200	-1.32731600	2.33899700
H	-0.93593100	-3.12406700	-1.38267200
H	1.39299000	-3.03355600	-0.65956400
H	1.60152900	1.71849500	1.12203100
H	-0.08501000	2.57511700	2.43284500
H	-2.52070500	2.96895600	2.64553400
H	-2.95807000	2.55488700	-1.61364700
H	-0.52632500	2.15049300	-1.83491200
C	-3.15942300	-2.21827600	0.05719700
O	-4.04928400	-1.80885200	0.77723000

## 2-conf8

C	1.23272800	-4.73245600	1.13330100
C	0.17660700	-3.81454800	0.49836200
C	0.53390300	-2.33474200	0.61823300
C	1.96564600	-2.01722200	0.10942100
C	3.00932800	-2.96936600	0.71540100
C	2.63263600	-4.45277100	0.56806100
H	2.20789400	-0.99506300	0.40067000
N	1.99836500	-2.11234600	-1.36269300
H	-0.18407600	-1.71250700	0.08159400
O	0.52174000	-1.97401400	2.03315300
H	2.15269200	-3.03976300	-1.73925500
C	-0.12392100	-0.91234800	2.54682500
O	0.20774700	-0.49874600	3.64298100
C	-1.26688300	-0.28644200	1.80001900
C	-1.28937500	1.11090300	1.67167600
C	-2.36565400	1.73385600	1.05592000
C	-3.45209100	0.97433600	0.58413300
C	-3.43700200	-0.42242500	0.73557300
C	-2.34478900	-1.04821900	1.33156100
C	1.41039400	-1.28432200	-2.25476500
N	1.24304800	0.04273400	-1.90720600
S	0.85863400	-1.83345500	-3.75579600
C	2.14037100	0.91924800	-1.27554600
C	1.65556600	2.19175900	-0.91558700
C	2.49703100	3.12510100	-0.33261000
C	3.83351800	2.78375700	-0.10116300
C	4.33556400	1.53008200	-0.45812000
C	3.49138100	0.59961400	-1.04819100
F	-5.45527400	0.01014000	-1.50617500

C	-5.80923900	0.91288600	-0.56211800
F	-6.72043900	1.73113000	-1.10074900
F	-6.40534200	0.23872000	0.44837200
N	4.71886900	3.75446900	0.51689200
O	5.89294900	3.42943900	0.73017400
O	4.26266100	4.86736200	0.80487400
H	0.95473800	-5.77732500	0.96082500
H	1.24140100	-4.58167100	2.21951800
H	0.07339800	-4.04362400	-0.56971500
H	-0.80742800	-3.98372600	0.94722600
H	3.09231000	-2.72468200	1.77926400
H	3.98509900	-2.76294700	0.26348900
H	3.38007400	-5.06353600	1.08499100
H	2.67284200	-4.76185900	-0.48609800
H	-0.46232000	1.70012300	2.05172700
H	-2.38374700	2.81142200	0.94080800
H	-4.26234800	-1.03438900	0.39509900
H	-2.35036400	-2.12644000	1.44549800
H	0.54036900	0.50035400	-2.47563300
H	0.61447200	2.44074600	-1.09157200
H	2.12785100	4.10258900	-0.05054000
H	5.37776900	1.29394600	-0.28653000
H	3.88669900	-0.36305200	-1.34722500
C	-4.56901800	1.71163300	-0.05160700
O	-4.58861700	2.91756900	-0.20443800

## 2-conf9

C	-0.35887200	3.93902700	0.63240500
C	0.09856000	2.70060500	1.41702200
C	0.07772500	1.42539900	0.57263200
C	0.82124000	1.57434600	-0.77325300
C	0.39339000	2.84368500	-1.52780800
C	0.45097500	4.11231400	-0.66097600
H	0.60734100	0.68952200	-1.37676800
N	2.26658600	1.59455500	-0.53514300
H	0.48861400	0.58144300	1.12818600
O	-1.29618600	1.09111900	0.20690500
H	2.70734000	2.50667400	-0.52337200
C	-2.00596400	0.32409000	1.04647800
O	-1.57733900	-0.11622400	2.10033800
C	-3.39339800	0.06451000	0.54727800
C	-4.24585000	-0.70981800	1.34353100
C	-5.54532600	-0.97916500	0.92582400
C	-6.00664500	-0.47230700	-0.30217900
C	-5.14617700	0.30509400	-1.09889200
C	-3.85022800	0.57319000	-0.67871900
C	3.06379800	0.51123100	-0.40452900
N	4.36172100	0.85071000	-0.07318300
S	2.50413900	-1.07478500	-0.57385400
C	5.53436500	0.08845400	-0.06157500
C	6.56391400	0.51639100	0.80123200
C	7.77704100	-0.15137700	0.84249500
C	7.96684900	-1.26116800	0.01351000
C	6.96483700	-1.69341700	-0.85979900
C	5.75255700	-1.01927900	-0.90178500
F	-7.88869300	-2.81182800	0.24123100
C	-8.36719400	-1.56319500	0.03483800

F	-9.55250200	-1.67612000	-0.57579900
F	-8.57924000	-0.99864200	1.24630700
N	9.23021000	-1.97280000	0.05587600
O	9.37365100	-2.96498600	-0.66937800
O	10.11540900	-1.55956300	0.81548500
H	-0.26158400	4.82832200	1.26419200
H	-1.42326600	3.84281800	0.38397900
H	1.12810100	2.84246600	1.77058400
H	-0.51634000	2.54758400	2.30933300
H	-0.63691300	2.68852400	-1.86578400
H	1.00883200	2.94968900	-2.42784100
H	0.07003400	4.96102100	-1.23901700
H	1.49156000	4.36375300	-0.40961000
H	-3.88327000	-1.09669800	2.28859400
H	-6.18362200	-1.57967200	1.56120200
H	-5.50778100	0.69252200	-2.04432100
H	-3.19198700	1.17304000	-1.29473900
H	4.47780000	1.78009300	0.31534100
H	6.40436100	1.37343500	1.44781100
H	8.56412100	0.17142900	1.51141600
H	7.14143400	-2.54180500	-1.50834600
H	4.98178600	-1.34355600	-1.58495600
C	-7.37494400	-0.71176600	-0.81820800
O	-7.78833300	-0.28322700	-1.87833300

## 2-conf10

C	-0.80150800	-2.65250900	0.13965700
C	-0.85318200	-1.46190000	1.10794800
C	-0.41060100	-0.15096600	0.45611100
C	-1.13314100	0.14497700	-0.87615000
C	-1.13106200	-1.07183200	-1.81504800
C	-1.60458900	-2.36836500	-1.13702700
H	-0.62303500	0.98481800	-1.35404500
N	-2.51253100	0.57326800	-0.60527700
H	-0.53896400	0.68909200	1.13991600
O	1.00402600	-0.22240500	0.10097200
H	-3.24138300	-0.09495000	-0.82439300
C	1.90771700	0.12168700	1.02961800
O	1.62406300	0.49210200	2.15671700
C	3.31369700	0.00029200	0.52961800
C	4.35628300	0.29851100	1.41525000
C	5.68055700	0.20028100	0.99989500
C	5.97514800	-0.19891700	-0.31596900
C	4.92398000	-0.49743500	-1.20213900
C	3.60345800	-0.40018900	-0.78415300
C	-2.88590700	1.83588700	-0.33154000
N	-4.23072900	2.08370100	-0.16996100
S	-1.80832600	3.14276900	-0.20872800
C	-5.32826400	1.21551100	-0.06625700
C	-6.56533900	1.66776200	-0.56633200
C	-7.70030500	0.88088300	-0.45553900
C	-7.59891800	-0.37338600	0.15441000
C	-6.38788000	-0.83504800	0.67289900
C	-5.25511900	-0.03764600	0.57116700
F	8.50026200	1.27310700	0.55240900
C	8.55522500	-0.00455400	0.11021400
F	9.72429200	-0.16836000	-0.51986000



F	8.55314300	-0.81535400	1.19378400
N	-8.78334500	-1.20939000	0.26277900
O	-8.67068800	-2.32400700	0.78525000
O	-9.85372500	-0.77057000	-0.17271200
H	-1.18622800	-3.54766200	0.63973600
H	0.24189500	-2.86312200	-0.12680300
H	-1.88000900	-1.31721000	1.46793400
H	-0.23893000	-1.64505200	1.99493600
H	-0.10129100	-1.20705600	-2.16317400
H	-1.73387300	-0.84287300	-2.70094100
H	-1.50538000	-3.19930400	-1.84369000
H	-2.67433600	-2.30965100	-0.89072000
H	4.12128500	0.60572400	2.42751000
H	6.46749400	0.43491100	1.70518800
H	5.15782600	-0.80410000	-2.21502800
H	2.79771200	-0.63135600	-1.46957500
H	-4.44671200	3.07274100	-0.18883100
H	-6.62653500	2.63680400	-1.04998700
H	-8.65052200	1.22161500	-0.84580300
H	-6.34017600	-1.79586000	1.16877600
H	-4.33405300	-0.37448700	1.02988200
C	7.35654600	-0.32632800	-0.83697400
O	7.62815000	-0.66952300	-1.97134600

## 2-conf11

C	-0.07625700	4.58373600	0.99476400
C	0.59088600	3.33327400	1.58514500
C	0.68166000	2.18099500	0.58310900
C	1.31418600	2.60234500	-0.76514000
C	0.67056500	3.88352700	-1.32372900
C	0.61990700	5.02807100	-0.29917600
H	1.14572900	1.80053600	-1.49346300
N	2.75885200	2.80999900	-0.59898200
H	1.22940900	1.34234400	1.01644500
O	-0.65363100	1.70706000	0.23886400
H	3.08918700	3.76419500	-0.53915200
C	-1.18656700	0.72313700	0.98115200
O	-0.61987200	0.19643200	1.92366900
C	-2.55799200	0.34048000	0.52144200
C	-3.22001200	-0.68389600	1.20901800
C	-4.49696100	-1.07803800	0.82211700
C	-5.12797700	-0.44406900	-0.26300400
C	-4.45926200	0.58583500	-0.94956600
C	-3.18427600	0.97623000	-0.56213400
C	3.74147500	1.89154200	-0.46317600
N	3.34868900	0.58801000	-0.63210900
S	5.33451800	2.39501900	-0.16161300
C	4.05832100	-0.60771300	-0.43598700
C	3.70523000	-1.70020500	-1.24998100
C	4.31724400	-2.93298500	-1.08201300
C	5.29227600	-3.07211700	-0.09092800
C	5.64705100	-2.00339600	0.73665500
C	5.02767400	-0.77250600	0.56839900
F	-6.58125200	-3.11696400	-0.07899200
C	-7.26110000	-1.94881000	-0.01346200
F	-8.46206000	-2.14361900	-0.57023800
F	-7.45449000	-1.65842700	1.29398100

N	5.94421900	-4.35835400	0.08844600
O	6.82301200	-4.45807100	0.95264800
O	5.59328700	-5.30173800	-0.63007000
H	-0.05550900	5.39100300	1.73434600
H	-1.13253500	4.37280500	0.78613000
H	1.61416400	3.57061200	1.90269700
H	0.06136700	2.98441600	2.47714400
H	-0.34996700	3.62819000	-1.62755200
H	1.20637400	4.18368900	-2.23041100
H	0.09512100	5.88065500	-0.74279400
H	1.63280500	5.38548600	-0.06597800
H	-2.72760500	-1.16657200	2.04497400
H	-4.98587300	-1.87311900	1.37032200
H	-4.95160800	1.07030800	-1.78474700
H	-2.67363300	1.76946900	-1.09374800
H	2.45543500	0.45376400	-1.09048500
H	2.95420700	-1.57615300	-2.02345600
H	4.05450200	-3.77266800	-1.71200700
H	6.38939200	-2.14191600	1.51198700
H	5.28708500	0.05348100	1.21427700
C	-6.48530400	-0.80372500	-0.73743100
O	-7.04742500	-0.26088300	-1.66878800

## 2-conf12

C	1.40499500	-4.02103000	1.72052500
C	1.58644000	-3.72869700	0.22354900
C	1.53441700	-2.23446800	-0.09866300
C	2.47586500	-1.38535300	0.78734900
C	2.31868200	-1.72123600	2.27929400
C	2.40689000	-3.22815800	2.57206700
H	2.22260500	-0.33666700	0.63389500
N	3.87541700	-1.60444100	0.37227200
H	1.75307200	-2.05942000	-1.15379900
O	0.19989200	-1.70922800	0.16829100
H	4.33664500	-2.40394900	0.78931400
C	-0.69994800	-1.73311300	-0.82742900
O	-0.47453700	-2.17711800	-1.94067100
C	-2.01681900	-1.15019000	-0.42074700
C	-3.05926200	-1.16524200	-1.35532500
C	-4.30329800	-0.63516300	-1.02822500
C	-4.51560500	-0.07863100	0.24564900
C	-3.46452100	-0.06437600	1.18064800
C	-2.22469900	-0.59661700	0.85236900
C	4.45876200	-1.21728300	-0.78329500
N	3.98989900	-0.07628600	-1.40568300
S	5.71588800	-2.10005300	-1.49144700
C	3.63296900	1.16257800	-0.85028400
C	3.03508600	2.10687000	-1.70736000
C	2.70065500	3.36737200	-1.24007900
C	2.96132200	3.68721800	0.09648400
C	3.56158600	2.76773000	0.96013700
C	3.90087200	1.50792100	0.48713000
F	-6.71369800	1.18383200	-1.45369400
C	-7.00906400	0.49504500	-0.32682700
F	-8.09593300	1.05267400	0.21935200
F	-7.33115900	-0.76814200	-0.68932300
N	2.60660300	5.00361000	0.59511500

O	2.82517300	5.26200400	1.78479800
O	2.10031100	5.81395100	-0.19020300
H	1.52209600	-5.09526900	1.89777800
H	0.38338800	-3.76052900	2.02436700
H	2.56116400	-4.10354900	-0.11504000
H	0.83237200	-4.24765800	-0.37619200
H	1.33590600	-1.35315500	2.59271700
H	3.06556700	-1.16238900	2.85289800
H	2.21905000	-3.39678400	3.63758200
H	3.42395900	-3.60105800	2.38565600
H	-2.88730400	-1.59443100	-2.33534700
H	-5.09231500	-0.66063700	-1.76886500
H	-3.63487000	0.36650100	2.16041500
H	-1.41892200	-0.58344900	1.57567700
H	4.24796900	-0.03909900	-2.38456800
H	2.83153400	1.84279800	-2.73976600
H	2.23646500	4.09458700	-1.89346500
H	3.77066300	3.04326000	1.98571100
H	4.38736000	0.80318900	1.14978300
C	-5.80923700	0.50593500	0.67174500
O	-6.00627200	1.00119600	1.76443200

## 2-conf13

C	-0.90857800	5.94888200	0.45246200
C	0.22349200	4.92032800	0.30861900
C	-0.33102100	3.49912800	0.19428000
C	-1.32898800	3.38589200	-0.96579300
C	-2.46364000	4.42032300	-0.83529000
C	-1.89932600	5.84274600	-0.71372500
N	-1.80996500	2.01236800	-1.19636000
O	0.75508300	2.57402500	-0.10872000
H	-1.59063900	1.65380500	-2.11742100
C	1.39256100	1.97921300	0.90855300
O	1.13855900	2.17194800	2.08626100
C	2.45935600	1.03847700	0.43904600
C	3.17887900	0.32327000	1.40388800
C	4.17395500	-0.56993200	1.01923800
C	4.46383400	-0.75264800	-0.34473700
C	3.74176300	-0.02772700	-1.31042200
C	2.74575900	0.85900600	-0.92349500
C	-2.47477400	1.17266300	-0.37490800
N	-2.57528500	-0.10104800	-0.91441000
S	-3.06688400	1.58082800	1.15427900
C	-3.39300900	-1.17746900	-0.55912800
C	-2.92690700	-2.46818700	-0.88149800
C	-3.69813200	-3.58763300	-0.61397200
C	-4.95032600	-3.41934600	-0.01512000
C	-5.43779800	-2.14733100	0.30029400
C	-4.66472800	-1.02856400	0.02607900
F	6.97276400	-1.78449700	1.07082400
C	6.28960700	-2.55601500	0.19376900
F	7.17129900	-3.35260400	-0.42145000
F	5.44912600	-3.34232500	0.90535100
N	-5.76161000	-4.58527100	0.27608300
O	-6.85820400	-4.42010600	0.82538200
O	-5.32615600	-5.70087900	-0.03650300
H	-0.48000800	6.95557000	0.50212900

H	-1.43775800	5.78352600	1.40041300
H	0.81138300	5.14001400	-0.59220800
H	0.90547600	4.96842800	1.16334200
H	-3.07135000	4.18263600	0.04223000
H	-3.11100200	4.33344900	-1.71447900
H	-2.72414900	6.55099300	-0.57940700
H	-1.39285300	6.12129000	-1.64824400
H	2.95085700	0.47062100	2.45297000
H	4.71359900	-1.11127500	1.78575400
H	3.97022000	-0.17272700	-2.35994400
H	2.18988600	1.41206500	-1.67026800
H	-1.88556100	-0.32973100	-1.62148300
H	-1.94953500	-2.58903900	-1.33765800
H	-3.33660700	-4.57910200	-0.85362500
H	-6.41976800	-2.03883900	0.74252800
H	-5.04519900	-0.04419700	0.25576300
C	5.50623300	-1.68369900	-0.83705400
O	5.79520500	-1.82478800	-2.00965900
H	-0.79008600	3.18460500	1.13122400
H	-0.77260500	3.61728900	-1.88040900

## 2-conf14

C	2.35273200	-5.24833800	-1.33363400
C	1.07729000	-4.39302500	-1.33897200
C	1.22392900	-3.18081900	-0.41765200
C	2.45141300	-2.34047300	-0.79577000
C	3.73468000	-3.19052700	-0.80690500
C	3.57725000	-4.41159200	-1.72524100
N	2.57564300	-1.10163900	-0.00503100
O	0.06749700	-2.30507700	-0.56970500
H	2.33813800	-0.26399000	-0.52062500
C	-0.99169000	-2.50429500	0.22660900
O	-1.06370900	-3.38785700	1.06491800
C	-2.08735200	-1.51416500	-0.02238500
C	-3.24616900	-1.60523800	0.75796200
C	-4.29226000	-0.70743200	0.57040300
C	-4.18818100	0.29649700	-0.40898800
C	-3.02243600	0.38309300	-1.19193100
C	-1.97955000	-0.51382800	-1.00138100
C	2.82015700	-0.94027400	1.30582100
N	2.94510100	0.36141400	1.75160300
S	2.94150900	-2.17768300	2.46177100
C	3.13146000	1.56635700	1.06035500
C	2.65232700	2.74405100	1.66905000
C	2.84285500	3.97710600	1.06734700
C	3.51302200	4.03759500	-0.15869500
C	4.01054400	2.88639400	-0.77261000
C	3.82721700	1.65307800	-0.16160000
F	-7.19296400	0.04447000	0.03208100
C	-6.56467200	1.23392000	0.17911000
F	-7.41993900	2.19489600	-0.18891800
F	-6.29981900	1.39915700	1.49578400
N	3.70576800	5.32587000	-0.80131800
O	4.27882300	5.35761000	-1.89664300
O	3.28865300	6.33808900	-0.22654100
H	2.22811800	-6.09075900	-2.02231000
H	2.50435400	-5.67691900	-0.33403000

H	0.87368300	-4.03666500	-2.35736900
H	0.21153400	-4.98154700	-1.01983600
H	3.96415400	-3.51921800	0.21055200
H	4.56387900	-2.55801800	-1.14115100
H	4.48682200	-5.02013300	-1.67805600
H	3.47282700	-4.07962700	-2.76741100
H	-3.31927300	-2.38178300	1.51022500
H	-5.17594200	-0.80033900	1.18866100
H	-2.94838700	1.15897300	-1.94510400
H	-1.08455000	-0.44316900	-1.60690400
H	2.87146700	0.43449500	2.75855400
H	2.12250000	2.68201300	2.61371200
H	2.46918000	4.88192400	1.52883000
H	4.55243300	2.96036500	-1.70656800
H	4.26095700	0.77217300	-0.61767400
C	-5.25624500	1.28979500	-0.67047200
O	-5.18485900	2.16175700	-1.51491300
H	1.27886400	-3.48784500	0.62678100
H	2.28484700	-1.97667400	-1.81537800

## 2-conf15

C	2.32623400	4.48061300	-1.97400400
C	0.97084700	3.79627600	-1.74343300
C	1.07705900	2.68863900	-0.69235400
C	1.65803700	3.23232800	0.62387500
C	3.01903100	3.92315700	0.39657200
C	2.89885900	5.03001100	-0.66116300
N	1.65027300	2.24552600	1.72348600
O	-0.25015100	2.18311000	-0.37939600
H	1.05431200	2.47761600	2.50635600
C	-0.71561600	1.13758800	-1.08108700
O	-0.09243600	0.57853100	-1.96812400
C	-2.08903100	0.72830900	-0.65119300
C	-2.69094800	-0.34865500	-1.31308900
C	-3.96541800	-0.77254700	-0.95037600
C	-4.65428500	-0.11679800	0.08558000
C	-4.04586000	0.96598300	0.74631400
C	-2.77364600	1.38680500	0.38231900
C	2.13205500	0.98575200	1.80318100
N	3.02251500	0.62351700	0.82156700
S	1.67482300	-0.01432100	3.09701800
C	3.54205200	-0.63996500	0.50092200
C	4.84373900	-0.68642600	-0.03158400
C	5.40256800	-1.89283500	-0.42585900
C	4.65176600	-3.06257900	-0.28470300
C	3.35180500	-3.03579500	0.22868100
C	2.79517900	-1.82549700	0.61706400
F	-6.88755500	-1.48260300	-1.48464500
C	-6.72107900	-1.71125900	-0.16124300
F	-7.92920100	-1.93082000	0.37008300
F	-5.99913100	-2.84781100	-0.02761800
N	5.23179700	-4.33180200	-0.68824900
O	4.56221400	-5.36050400	-0.53702900
O	6.37208300	-4.33264200	-1.16730800
H	2.20547600	5.28651900	-2.70525800
H	3.03288000	3.76229200	-2.41092500
H	0.23588100	4.53326200	-1.39569300

H	0.58796700	3.36661900	-2.67413400
H	3.78491900	3.21139000	0.06146100
H	3.36514700	4.32709100	1.35270200
H	3.88244000	5.48036400	-0.83008900
H	2.24581400	5.82629800	-0.28003500
H	-2.15358700	-0.84900500	-2.11006400
H	-4.40654400	-1.60802800	-1.47886200
H	-4.58224600	1.46689100	1.54382500
H	-2.30995400	2.22037000	0.89495500
H	3.49256700	1.38955900	0.35693300
H	5.42209100	0.22684700	-0.12587300
H	6.40707400	-1.93318600	-0.82640900
H	2.78139100	-3.95221300	0.30732800
H	1.78530600	-1.79619000	1.00022900
C	-6.01201100	-0.50684200	0.53392000
O	-6.62379100	0.05463700	1.42199900
H	1.66526400	1.85557300	-1.08201100
H	0.96615900	4.00485500	0.97409400

## 2-conf16

C	2.86171000	3.02940500	-2.12884900
C	1.40127900	2.62667600	-1.87833600
C	1.27903200	1.65971100	-0.69506000
C	1.89671800	2.27616700	0.56318600
C	3.36732500	2.66293700	0.32025200
C	3.49138800	3.62936800	-0.86576100
N	1.69308300	1.49994500	1.81873900
O	-0.12712000	1.42450600	-0.40273800
H	1.45026600	2.09544400	2.60093200
C	-0.76225800	0.45361700	-1.07840400
O	-0.22800600	-0.26094900	-1.90980400
C	-2.20476400	0.34364900	-0.69625600
C	-2.97411000	-0.65258000	-1.30947000
C	-4.32109200	-0.79482400	-0.99162600
C	-4.91492500	0.06711400	-0.05241300
C	-4.13789700	1.06729800	0.56001500
C	-2.79329400	1.20562300	0.24245100
C	1.30979600	0.22638300	2.04235200
N	1.69263200	-0.75400000	1.14030500
S	0.36325200	-0.19286700	3.38228300
C	2.99768200	-1.03784600	0.69396600
C	3.14073100	-1.93923000	-0.37732800
C	4.40175700	-2.30547400	-0.82219000
C	5.52658500	-1.76187900	-0.19430200
C	5.40490100	-0.87233500	0.87649600
C	4.14060100	-0.51326700	1.32215300
F	-7.29688400	-0.98560700	-1.64684500
C	-7.23929700	-1.12122000	-0.30162900
F	-8.49037400	-1.05845200	0.16884200
F	-6.75895300	-2.35742400	-0.03309400
N	6.85084400	-2.13599400	-0.65977600
O	7.83446700	-1.63119100	-0.10565700
O	6.94094400	-2.94402500	-1.59162400
H	2.90281100	3.74444100	-2.95718500
H	3.43760100	2.14874400	-2.44312800
H	0.80032600	3.51871000	-1.66116700
H	0.97222400	2.15059300	-2.76482600

H	3.96039200	1.76571800	0.12115500
H	3.76378000	3.11627900	1.23473900
H	4.54768800	3.86194300	-1.03740700
H	2.99330800	4.57758400	-0.62212800
H	-2.50996200	-1.31134000	-2.03391700
H	-4.89281700	-1.57361300	-1.47980600
H	-4.60175500	1.72802600	1.28309600
H	-2.19906800	1.97644000	0.71697100
H	1.08453800	-1.56422300	1.17429000
H	2.25805400	-2.34427700	-0.86051300
H	4.51904100	-2.99345800	-1.64933700
H	6.29060100	-0.48117400	1.36025500
H	4.04273200	0.15952100	2.16499700
C	-6.34215700	-0.01561600	0.33852400
O	-6.87371400	0.73004100	1.13827400
H	1.73543800	0.70243900	-0.94734400
H	1.34189900	3.20263400	0.75457200

## 2-conf17

C	-0.80504900	5.98170500	0.70747400
C	0.30687900	4.92079500	0.63884900
C	-0.31089500	3.52460200	0.53316800
C	-1.21594200	3.41166800	-0.70706800
C	-2.34160200	4.46247800	-0.62419300
C	-1.75206300	5.87518100	-0.49576800
N	-1.69503300	2.04770100	-0.98399700
O	0.69087600	2.46322100	0.61305900
H	-1.47906400	1.72778500	-1.92030000
C	1.60278300	2.26961100	-0.34620900
O	1.69239300	2.92738800	-1.37069700
C	2.51746900	1.12550800	-0.02523500
C	3.48078500	0.76517300	-0.97528900
C	4.34861800	-0.29438400	-0.72984300
C	4.26353700	-1.00469000	0.48107000
C	3.29755400	-0.63544100	1.43497700
C	2.42959900	0.41908700	1.18473900
C	-2.40324900	1.19401500	-0.21409200
N	-2.51654800	-0.05514300	-0.80527100
S	-3.02720600	1.56069600	1.31247700
C	-3.36216400	-1.12968900	-0.51695100
C	-2.92010700	-2.41078100	-0.90621700
C	-3.71766400	-3.52619000	-0.70977300
C	-4.97271500	-3.36451800	-0.11482200
C	-5.43581800	-2.10189400	0.26746300
C	-4.63636700	-0.98637600	0.06437800
F	5.61004100	-2.99533100	-1.38200600
C	6.20396100	-2.62023500	-0.22552700
F	6.89923900	-3.66699200	0.23413300
F	7.08519100	-1.63501800	-0.51593800
N	-5.81214700	-4.52669500	0.10104400
O	-6.90840100	-4.36971300	0.65350400
O	-5.40027300	-5.63110700	-0.27659400
H	-0.35341400	6.97851600	0.75146800
H	-1.37708500	5.85228400	1.63601200
H	0.94943200	5.11046700	-0.22695800
H	0.93494100	4.96056400	1.53513200
H	-2.98510400	4.24293900	0.23300400

H	-2.95742400	4.38131500	-1.52627500
H	-2.56537700	6.60325500	-0.40377300
H	-1.20397700	6.12816100	-1.41372500
H	3.54169500	1.31884100	-1.90488800
H	5.08210100	-0.55312000	-1.48285800
H	3.23743400	-1.18665800	2.36625400
H	1.68531600	0.69751500	1.92031900
H	-1.81825900	-0.26620000	-1.50942400
H	-1.94065000	-2.52761400	-1.35913800
H	-3.37463600	-4.51020100	-1.00171500
H	-6.41985600	-1.99685700	0.70596400
H	-4.99765300	-0.00869800	0.34700500
C	5.14836100	-2.14382200	0.82068200
O	5.10648400	-2.74875700	1.87464100
H	-0.90721800	3.32447400	1.42338400
H	-0.60413400	3.64806200	-1.57944800

## 2-conf18

C	3.93763300	-4.50784100	-1.00403500
C	2.46929000	-4.06833500	-0.88772300
C	2.36625900	-2.77445800	-0.07627200
C	3.20920000	-1.64803400	-0.69990400
C	4.68118500	-2.09122100	-0.82329700
C	4.79808700	-3.39758400	-1.62190400
N	3.04791100	-0.34187800	-0.03145800
O	0.97728300	-2.38291100	0.16303800
H	2.85183300	0.41578800	-0.67356200
C	0.15597300	-2.02920000	-0.83226900
O	0.47544300	-1.94574700	-2.00754200
C	-1.22771100	-1.72898900	-0.33860800
C	-2.17780800	-1.29347900	-1.27045400
C	-3.47623900	-0.99986800	-0.86602500
C	-3.83931900	-1.14307300	0.48514600
C	-2.88216600	-1.58389200	1.41733300
C	-1.58645700	-1.87432700	1.01082200
C	3.29612800	0.00879900	1.24116700
N	3.07730700	1.33074400	1.57622500
S	3.88219600	-1.01552600	2.46336600
C	2.44548000	2.37535300	0.88629000
C	2.91010900	3.68468500	1.12239900
C	2.30383700	4.76942500	0.51010300
C	1.22498500	4.54647300	-0.35146400
C	0.73545700	3.26038900	-0.58634900
C	1.33911800	2.17675500	0.03803300
F	-5.92145200	0.80099600	-0.59860800
C	-6.29195700	-0.35490600	-0.00057100
F	-7.45324400	-0.13559400	0.62711800
F	-6.51484600	-1.26836000	-0.97379700
N	0.59264200	5.67850500	-1.00758600
O	-0.34914400	5.46102600	-1.77846400
O	1.02307900	6.81237200	-0.76764100
H	3.99600900	-5.41925100	-1.60856000
H	4.32678600	-4.76238000	-0.00910000
H	2.04923600	-3.91649600	-1.88683100
H	1.87232300	-4.83994400	-0.39005300
H	5.10629900	-2.22359000	0.17615400
H	5.24138100	-1.28743900	-1.31308700



H	5.84827600	-3.70674200	-1.66161900
H	4.47994200	-3.22517800	-2.65931100
H	-1.89097800	-1.18650100	-2.30999000
H	-4.18979500	-0.66344400	-1.60734600
H	-3.16855500	-1.69318000	2.45693000
H	-0.85319700	-2.21302000	1.73206500
H	3.50085800	1.57765600	2.46201400
H	3.75649000	3.84182700	1.78242900
H	2.66451800	5.77527900	0.68177000
H	-0.12038700	3.11423800	-1.23252200
H	0.91867800	1.18951600	-0.10334600
C	-5.19864600	-0.85042600	0.99733100
O	-5.52928900	-0.97037500	2.16124500
H	2.71747500	-2.95500200	0.93988400
H	2.82495700	-1.47109100	-1.70605200

## 2-conf19

C	-2.12866600	-4.50476100	-1.99221300
C	-0.83586400	-3.68731300	-1.83589800
C	-1.03711100	-2.56097000	-0.81866400
C	-1.48817800	-3.12019600	0.54737500
C	-2.79915500	-3.91809300	0.38292300
C	-2.61562400	-5.04809800	-0.64185700
N	-1.50509000	-2.11352300	1.62676700
O	0.12585800	-1.68520900	-0.72830400
H	-0.87003500	-2.29440400	2.39262000
C	1.29803800	-2.11145000	-0.23704100
O	1.49640000	-3.22340700	0.22398200
C	2.35591100	-1.05351700	-0.31302800
C	3.61381700	-1.34361700	0.22902800
C	4.63503200	-0.40018500	0.17894500
C	4.40620500	0.84971500	-0.42365800
C	3.14065200	1.13653500	-0.96711400
C	2.12193100	0.19457100	-0.91151400
C	-2.07048200	-0.88849400	1.70603900
N	-3.03414800	-0.61646800	0.76489100
S	-1.62150100	0.17273300	2.95220700
C	-3.66280800	0.59612600	0.44385300
C	-4.98558700	0.52828100	-0.03183700
C	-5.65543700	1.67763900	-0.42300400
C	-4.99498300	2.90582100	-0.33660300
C	-3.67645400	2.99287900	0.11943200
C	-3.00887100	1.83924600	0.50553400
F	6.76606800	1.40093800	1.41933000
C	6.85191400	1.64208400	0.09075100
F	7.65755900	2.69648900	-0.08166700
F	7.44595500	0.57070900	-0.48431400
N	-5.69035000	4.11593600	-0.73931900
O	-5.10011300	5.19757800	-0.63443700
O	-6.84490400	4.01589600	-1.17147700
H	-1.95276900	-5.32811300	-2.69218500
H	-2.91093900	-3.87518800	-2.43725600
H	-0.02169000	-4.33898500	-1.50401100
H	-0.54031800	-3.24585000	-2.79319500
H	-3.62628700	-3.27849100	0.04688800
H	-3.08682000	-4.31667000	1.36054700
H	-3.56167400	-5.58522100	-0.76573700

H	-1.88783000	-5.77248600	-0.25281900
H	3.78354000	-2.31047200	0.68796200
H	5.59757600	-0.65020200	0.60649600
H	2.97083200	2.10194400	-1.42952200
H	1.14914400	0.42001900	-1.33037400
H	-3.47338400	-1.42660100	0.34646300
H	-5.49134600	-0.43027800	-0.08483300
H	-6.67569400	1.63001300	-0.78054500
H	-3.17817800	3.95300400	0.15612200
H	-1.98546900	1.89893400	0.84628200
C	5.44224100	1.90449700	-0.52620200
O	5.26819400	2.98068900	-1.06446200
H	-1.79058800	-1.87014000	-1.20380300
H	-0.72577600	-3.82796400	0.87518700

## 2-conf20

C	-3.19685400	-1.90920500	-3.16480800
C	-1.73552200	-1.58777500	-2.80978100
C	-1.63937200	-1.15447300	-1.34504700
C	-2.17246600	-2.25887400	-0.41211300
C	-3.64983900	-2.52916900	-0.74185400
C	-3.78853800	-2.95787800	-2.21242600
N	-1.87440600	-2.04487900	1.03093200
O	-0.30311000	-0.68079800	-0.99702100
H	-1.09579800	-2.60855200	1.34949500
C	0.75230500	-1.50372100	-0.95083000
O	0.70072200	-2.71057400	-1.12576400
C	2.02336700	-0.77226100	-0.64473700
C	3.20515200	-1.51778800	-0.55627400
C	4.41356200	-0.88772400	-0.27639200
C	4.45023000	0.50430500	-0.08048900
C	3.26016600	1.24924900	-0.17039400
C	2.05567400	0.61779800	-0.45079000
C	-2.69324000	-1.73540700	2.06271200
N	-3.72610100	-0.84191600	1.85356200
S	-2.48702500	-2.42628700	3.59452400
C	-3.67652600	0.41584600	1.22938600
C	-2.46620300	1.07841800	0.95763100
C	-2.48060000	2.34789500	0.39742100
C	-3.70499800	2.95939100	0.11466600
C	-4.91854400	2.32194000	0.39090900
C	-4.89984600	1.05195700	0.94595100
F	6.98864400	-0.46976300	1.30432000
C	7.04061600	0.46370900	0.32611600
F	8.05826500	1.28743000	0.60209400
F	7.32666500	-0.17172200	-0.83392300
N	-3.71725400	4.28814400	-0.47123700
O	-4.80980300	4.82291600	-0.69442700
O	-2.63514600	4.83132200	-0.72308100
H	-3.25059600	-2.26162400	-4.20012900
H	-3.79505000	-0.98963100	-3.11270600
H	-1.10621500	-2.46811900	-2.97592000
H	-1.35277300	-0.78038900	-3.44253200
H	-4.25866100	-1.63688900	-0.56654100
H	-4.02529300	-3.31335600	-0.07648000
H	-4.84674500	-3.12271800	-2.44140100
H	-3.27884300	-3.91881400	-2.36216300

H	3.16879800	-2.59013100	-0.70791100
H	5.31246900	-1.48737400	-0.21424700
H	3.29536400	2.32185500	-0.01890800
H	1.14223400	1.19515500	-0.52041200
H	-4.46935700	-0.94060100	2.53492400
H	-1.51858400	0.60896600	1.18976300
H	-1.55384700	2.86826400	0.19245400
H	-5.85582900	2.81384700	0.16552500
H	-5.83279100	0.54157900	1.16038600
C	5.69533400	1.24913500	0.22197900
O	5.74484200	2.45122700	0.39707400
H	-2.23050100	-0.24854100	-1.20738200
H	-1.61661600	-3.17022800	-0.64268800

## 2-conf21

C	-0.35084700	6.29479300	0.29634000
C	0.65472800	5.13611900	0.20366200
C	0.03160600	3.84747400	0.74526200
C	-1.26461200	3.47421700	0.00841700
C	-2.26281900	4.64641000	0.10251100
C	-1.65666300	5.95098100	-0.43229200
N	-1.82437400	2.24783900	0.57643100
O	0.98807700	2.74373400	0.80186100
H	-1.77510700	2.16430600	1.58620700
C	1.52556300	2.21669500	-0.30728000
O	1.28688500	2.58889100	-1.44366100
C	2.46774500	1.09367300	0.00664500
C	3.09070400	0.44172500	-1.06441300
C	3.97049300	-0.61051200	-0.83141800
C	4.23834500	-1.02221300	0.48631800
C	3.61178400	-0.36275000	1.55960900
C	2.73358800	0.68678200	1.32368600
C	-2.49005800	1.28998800	-0.10319000
N	-3.03820400	0.33404500	0.73026600
S	-2.66785600	1.30005100	-1.78671000
C	-3.64135800	-0.89699800	0.45180900
C	-4.55126300	-1.38654700	1.41143000
C	-5.16406000	-2.61758800	1.24507400
C	-4.86734900	-3.37208900	0.10582300
C	-3.95681100	-2.91317500	-0.84991400
C	-3.34028100	-1.68168000	-0.67712000
F	4.97650300	-3.46659300	-1.17708800
C	5.87487000	-2.89539200	-0.34175600
F	6.66487500	-3.86552600	0.13285900
F	6.64438000	-2.05848300	-1.07573500
N	-5.51086400	-4.65825200	-0.08271100
O	-5.25546700	-5.30202600	-1.10810300
O	-6.29007800	-5.06178700	0.78994100
H	0.09928300	7.19896800	-0.12694300
H	-0.56648500	6.51315800	1.35114800
H	0.95483500	4.98802900	-0.83755400
H	1.55738900	5.35825400	0.78254900
H	-2.55995200	4.77795400	1.15174400
H	-3.16443100	4.37551200	-0.45590700
H	-2.38166500	6.76450800	-0.32037300
H	-1.45965800	5.84868800	-1.50796700
H	2.87916800	0.76460100	-2.07693300

H	4.43716400	-1.09763600	-1.67791900
H	3.82277300	-0.68467200	2.57279900
H	2.25373500	1.19121200	2.15308700
H	-3.09682300	0.59538800	1.70812400
H	-4.78203700	-0.78940200	2.28794500
H	-5.86907900	-2.98840800	1.97759200
H	-3.72496400	-3.52387400	-1.71301400
H	-2.62722800	-1.33096400	-1.40797700
C	5.16094100	-2.13315800	0.81877600
O	5.40601300	-2.50013400	1.95180800
H	-0.19466200	3.98736900	1.80810100
H	-1.04319400	3.26619800	-1.03820100

## 2-conf22

C	-2.28050700	-4.80637800	-2.03822100
C	-0.95600100	-4.05253900	-1.83593100
C	-1.22249600	-2.65011200	-1.28303600
C	-2.01193200	-2.68928900	0.03427600
C	-3.33675100	-3.44749700	-0.18314500
C	-3.09270700	-4.85735800	-0.73771300
N	-2.25114900	-1.32494900	0.51469400
O	-0.00923700	-1.84081900	-1.19205100
H	-2.38980500	-0.61445200	-0.19411700
C	0.99333400	-2.15796700	-0.35940900
O	0.99991800	-3.11943200	0.39008000
C	2.12412600	-1.17823300	-0.44804300
C	3.21052100	-1.34955200	0.41842400
C	4.28610900	-0.46790100	0.38014300
C	4.28645700	0.59874700	-0.53637600
C	3.19374800	0.76540700	-1.40678100
C	2.11978400	-0.11366900	-1.36316500
C	-2.28686200	-0.94406600	1.80020600
N	-2.60557300	0.37138700	2.06291700
S	-1.92881700	-1.95828100	3.11641300
C	-3.15181800	1.37104400	1.24527500
C	-2.80379700	2.70662300	1.52853600
C	-3.34529700	3.74742400	0.79157100
C	-4.23766700	3.45305000	-0.24413100
C	-4.61039100	2.13859100	-0.53183700
C	-4.07552500	1.09902100	0.21748900
F	6.23957300	1.54300500	1.60797700
C	6.61898500	1.44316900	0.31293400
F	7.52280000	2.40141400	0.07705000
F	7.23466000	0.24856100	0.15530200
N	-4.79948800	4.53898500	-1.02940100
O	-5.56226200	4.25798800	-1.96098500
O	-4.49115000	5.69908300	-0.73349400
H	-2.06827100	-5.81826500	-2.39911100
H	-2.87171300	-4.30980800	-2.81946400
H	-0.31666500	-4.60506100	-1.14142900
H	-0.41539200	-3.95716700	-2.78336600
H	-3.96551600	-2.87757800	-0.88017100
H	-3.86983300	-3.48961400	0.77189700
H	-4.05315100	-5.35583300	-0.90728400
H	-2.55253700	-5.45537400	0.00848300
H	3.20401000	-2.17482700	1.12066800
H	5.11167800	-0.62203400	1.06313100

H	3.20037600	1.58904500	-2.11123300
H	1.28045100	0.01912200	-2.03434600
H	-2.36945600	0.64840500	3.00750100
H	-2.09940100	2.91942800	2.32553900
H	-3.07404000	4.77402300	1.00100900
H	-5.32720200	1.93684300	-1.31722800
H	-4.41483500	0.08808000	0.02901000
C	5.39312600	1.57841000	-0.64405300
O	5.41375600	2.49877200	-1.43835300
H	-1.79901200	-2.08567400	-2.02409100
H	-1.42329100	-3.19785000	0.79788100

## 2-conf23

C	1.90150000	-5.43408500	-1.67995700
C	0.76511200	-4.40970000	-1.52709000
C	0.87176700	-3.70340000	-0.17448500
C	2.22526000	-2.98331800	-0.01996300
C	3.35091800	-4.03268200	-0.13684400
C	3.27573500	-4.78279400	-1.47490000
N	2.32120300	-2.26522600	1.25410400
O	-0.30991400	-2.87850900	0.08100700
H	2.37874500	-2.83562600	2.08970100
C	-0.55103600	-1.73648800	-0.56060200
O	0.24664300	-1.17343300	-1.30331700
C	-1.90854100	-1.18760200	-0.25893500
C	-2.27150200	0.03278800	-0.84177100
C	-3.52385600	0.58472200	-0.59102400
C	-4.42971200	-0.08546300	0.24987900
C	-4.06071600	-1.31198600	0.83176100
C	-2.81053000	-1.86077200	0.58035000
C	2.61563300	-0.96400000	1.47707700
N	2.46275600	-0.13529200	0.39189000
S	3.05753100	-0.45303100	3.03579600
C	2.89066700	1.18055700	0.19034200
C	2.16787400	1.94418100	-0.74909200
C	2.55163200	3.24001200	-1.05353000
C	3.67183700	3.78168300	-0.41556500
C	4.41218200	3.03582300	0.50666200
C	4.02610400	1.73755800	0.80752600
F	-5.40642400	2.80032600	0.34308600
C	-6.23059200	1.79910900	-0.04291300
F	-7.47029100	2.11660300	0.34746900
F	-6.22150800	1.75671400	-1.39535100
N	4.07867300	5.13879600	-0.72410000
O	5.06127000	5.60919800	-0.13686700
O	3.42781300	5.77423800	-1.56351200
H	1.84199300	-5.89703300	-2.67036200
H	1.76456800	-6.23917600	-0.94585500
H	0.81640800	-3.66785200	-2.33217500
H	-0.20984600	-4.90297800	-1.59153000
H	3.27146400	-4.74348500	0.69696000
H	4.31186900	-3.51913700	-0.03250800
H	4.06490400	-5.54114400	-1.51263600
H	3.47404300	-4.07950100	-2.29467200
H	-1.56908100	0.54290500	-1.49007100
H	-3.77957800	1.52909000	-1.05400100
H	-4.76428300	-1.82297500	1.47858100

H	-2.53012700	-2.80490700	1.03024600
H	1.82147200	-0.47055300	-0.32607700
H	1.29877800	1.51261400	-1.23478500
H	1.99222400	3.82973000	-1.76799100
H	5.28846400	3.46800400	0.97243200
H	4.60234800	1.15572900	1.51184400
C	-5.78197500	0.43422000	0.56722600
O	-6.57947000	-0.13821900	1.28390600
H	0.78471100	-4.44317700	0.62684700
H	2.34870400	-2.26912100	-0.83144400

## 2-conf24

C	2.88407600	-2.99720300	-3.08975700
C	1.51008000	-2.39406000	-2.75657300
C	1.23895700	-2.50635100	-1.25560600
C	2.31953900	-1.80079100	-0.41966800
C	3.68492600	-2.44045000	-0.74825400
C	3.99162700	-2.34754800	-2.25019300
N	1.95867000	-1.93344300	1.00866700
O	-0.11964400	-2.10631400	-0.89598200
H	1.24757600	-2.62517800	1.21461900
C	-0.55569000	-0.84794200	-1.06512000
O	0.12816100	0.07292400	-1.47756900
C	-1.99422700	-0.69634600	-0.67702900
C	-2.57460500	0.57264400	-0.79313100
C	-3.90796400	0.76940400	-0.44820800
C	-4.67783600	-0.31024200	0.02014700
C	-4.09018800	-1.58328900	0.13517700
C	-2.75935400	-1.77691800	-0.21060100
C	2.69212400	-1.62340300	2.09707800
N	3.64994800	-0.63676100	2.01056700
S	2.48771500	-2.44875300	3.56720600
C	3.63653900	0.58640000	1.32182900
C	4.86145900	1.26791500	1.18425000
C	4.90949400	2.50678700	0.56574500
C	3.72488000	3.06677200	0.07625900
C	2.49927200	2.41072800	0.21107300
C	2.45446700	1.17332500	0.83833300
F	-6.18916200	2.13410100	1.04993100
C	-6.80213800	1.20506100	0.28034800
F	-8.08220800	1.13741400	0.66401600
F	-6.77732600	1.64807600	-0.99802400
N	3.76935400	4.36150300	-0.58073200
O	2.71544500	4.83577200	-1.02074700
O	4.86002700	4.93706100	-0.67354100
H	3.08688700	-2.86858400	-4.15803900
H	2.86677200	-4.07848500	-2.89847800
H	1.47891000	-1.34366000	-3.05975900
H	0.71483000	-2.92057100	-3.29414300
H	3.66776000	-3.49133100	-0.43170200
H	4.46872600	-1.94407200	-0.16981800
H	4.95485700	-2.82752500	-2.45311800
H	4.09819300	-1.29256900	-2.53594800
H	-1.97477300	1.39954200	-1.15470100
H	-4.33153600	1.76061100	-0.54721000
H	-4.68936100	-2.41107800	0.49627300
H	-2.31163700	-2.75883100	-0.12174700

H	4.33045900	-0.69552900	2.75848500
H	5.77341300	0.81700700	1.56100100
H	5.84834500	3.03284600	0.45154100
H	1.59262300	2.87080000	-0.15965500
H	1.50132100	0.67733500	0.96798600
C	-6.10271800	-0.18472900	0.40869700
O	-6.77849300	-1.10500600	0.82640300
H	1.22741100	-3.56564500	-0.97716000
H	2.33797600	-0.74454000	-0.69382300

## 2-conf25

C	0.54654100	6.30148100	-0.10326100
C	-0.46988900	5.18043400	0.16208800
C	0.01009700	3.85444300	-0.42279000
C	1.38499400	3.46368000	0.13413100
C	2.40422800	4.58386400	-0.15298000
C	1.93744600	5.92605500	0.42470000
N	1.81189400	2.18392700	-0.43289400
O	-0.98240800	2.84668100	-0.06123500
H	1.44853700	1.96502100	-1.35622000
C	-1.27077600	1.87651600	-0.93884800
O	-0.69857100	1.73086500	-2.00999300
C	-2.37084600	0.98153000	-0.46641500
C	-2.77833600	-0.06147300	-1.30718400
C	-3.79942700	-0.92086400	-0.91435500
C	-4.42167900	-0.74611000	0.33446200
C	-4.00587100	0.30093700	1.17710900
C	-2.99016300	1.16066100	0.78054800
C	2.59171200	1.27194400	0.18145300
N	2.93026700	0.22233800	-0.65253800
S	3.13356800	1.43548100	1.77718100
C	3.54263900	-1.00528300	-0.38323600
C	4.23277900	-1.61918200	-1.44865800
C	4.83282200	-2.85697600	-1.28534800
C	4.74484900	-3.49291000	-0.04310700
C	4.05206200	-2.90974100	1.02165300
C	3.44814700	-1.67173400	0.85287700
F	-6.50534200	-2.26752300	-1.26925300
C	-6.04455100	-2.76056400	-0.09653800
F	-7.04678100	-3.42638600	0.48839100
F	-5.06689000	-3.65212800	-0.38085400
N	5.37824400	-4.78438200	0.14079400
O	5.30832600	-5.32386800	1.25230600
O	5.96392000	-5.29717700	-0.82135900
H	0.19423100	7.22728100	0.36349600
H	0.60467900	6.49440000	-1.18294000
H	-0.61726000	5.05709500	1.24238100
H	-1.44357700	5.42537000	-0.27394900
H	2.53954500	4.66925000	-1.23924300
H	3.36901500	4.28969000	0.27101500
H	2.66362400	6.70695200	0.17456900
H	1.90783500	5.86049000	1.52076000
H	-2.29178000	-0.19186500	-2.26657900
H	-4.09660400	-1.71779700	-1.58385800
H	-4.48979000	0.42981500	2.13826300
H	-2.67538200	1.96726400	1.43080800
H	2.80153800	0.40248000	-1.64194900

H	4.30391400	-1.11339000	-2.40630700
H	5.37106700	-3.32301500	-2.10033900
H	3.97737300	-3.42974400	1.96805600
H	2.90232300	-1.22464300	1.67008500
C	-5.51485600	-1.61834100	0.82637400
O	-6.04048600	-1.50202900	1.91629200
H	0.04605100	3.90932300	-1.51497500
H	1.29807000	3.32348900	1.21579400

## 2-conf26

C	-2.77891900	-4.71114500	-2.03259800
C	-1.39380900	-4.17471000	-1.64205800
C	-1.48304500	-2.74511800	-1.11314700
C	-2.44525900	-2.64633600	0.07654600
C	-3.83695600	-3.17380700	-0.32587700
C	-3.76183000	-4.60995400	-0.85940900
N	-2.51509000	-1.25978100	0.55143400
O	-0.13140100	-2.36718800	-0.70659700
H	-2.23850500	-0.54797200	-0.11882500
C	0.28128100	-1.10928600	-0.90819600
O	-0.44432300	-0.20863300	-1.30727500
C	1.72796000	-0.91890300	-0.58654900
C	2.26323800	0.37057700	-0.69290400
C	3.60665700	0.59724700	-0.41109000
C	4.43060100	-0.47191800	-0.01682700
C	3.88703900	-1.76501300	0.09073500
C	2.54626700	-1.98907900	-0.19200700
C	-2.74632000	-0.88937700	1.81840500
N	-2.81372500	0.46270800	2.08234200
S	-2.92220300	-1.96858200	3.12059800
C	-2.94073300	1.56962900	1.23180700
C	-2.42682100	2.79989800	1.68912600
C	-2.55826300	3.94768100	0.92484300
C	-3.20424000	3.86822600	-0.31312100
C	-3.73624400	2.66389400	-0.77880400
C	-3.61187900	1.51767800	-0.00555000
F	6.40141200	1.56995000	-1.10499500
C	6.52621100	1.09556700	0.15598200
F	7.83106300	1.05169900	0.44837400
F	5.94544200	1.98848000	0.99059500
N	-3.33497900	5.06462700	-1.12563100
O	-3.89086600	4.97146900	-2.22642900
O	-2.88449000	6.12814500	-0.68357800
H	-2.68334500	-5.74939600	-2.36718800
H	-3.16673800	-4.13875600	-2.88594500
H	-0.95252500	-4.81043900	-0.86427600
H	-0.71338700	-4.18947200	-2.49933200
H	-4.25805200	-2.51084800	-1.09295700
H	-4.49328800	-3.11440300	0.54752300
H	-4.75986200	-4.93929800	-1.16779200
H	-3.44144000	-5.28374000	-0.05325000
H	1.62183800	1.18911100	-0.99754500
H	3.99587500	1.60324400	-0.50096900
H	4.52820600	-2.58429100	0.39448200
H	2.13165500	-2.98613800	-0.11101900
H	-2.74903300	0.66851700	3.07151200
H	-1.91623500	2.84518900	2.64523900



H	-2.15708400	4.89165700	1.27029100
H	-4.25810500	2.63188600	-1.72645600
H	-4.07052300	0.60001400	-0.35099900
C	5.87123000	-0.31447600	0.29680500
O	6.59222000	-1.22323000	0.65999500
H	-1.79365300	-2.06075300	-1.90849300
H	-2.05136800	-3.25300200	0.89805800

## 2-conf27

C	-1.02012300	5.35582100	-1.04954700
C	0.10827900	4.32526400	-1.20226700
C	0.04622600	3.26910500	-0.10099300
C	-1.31658000	2.56307300	-0.07417800
C	-2.44205100	3.60491900	0.09510200
C	-2.39286500	4.67284900	-1.00552100
N	-1.32919500	1.56149600	1.00062800
O	1.10202300	2.30328000	-0.37830200
H	-0.67633000	1.69989400	1.76457500
C	1.79961700	1.79234800	0.64809800
O	1.54784600	2.01873900	1.82227400
C	2.91725500	0.90775800	0.20066600
C	3.71450700	0.30780700	1.18309100
C	4.76683800	-0.52620000	0.81919400
C	5.02925600	-0.77147500	-0.54035500
C	4.22492900	-0.16641100	-1.52329200
C	3.17742200	0.66853200	-1.15785000
C	-2.16187300	0.51374200	1.16694200
N	-3.00244200	0.25979700	0.11122100
S	-2.07745300	-0.41903000	2.58554900
C	-4.07721700	-0.63349000	-0.00959200
C	-4.37108600	-1.10393800	-1.30412300
C	-5.45113900	-1.94467800	-1.52313000
C	-6.24629700	-2.31891900	-0.43647000
C	-5.98056100	-1.85165600	0.85342900
C	-4.90051600	-1.00648400	1.06762300
F	7.69915200	-1.38942000	0.79195400
C	7.06403200	-2.32002600	0.04264000
F	7.99718300	-3.07188900	-0.55238500
F	6.36496400	-3.11792200	0.88256000
N	-7.37645800	-3.20449800	-0.65437800
O	-8.05763800	-3.54224900	0.32113600
O	-7.61322900	-3.58509700	-1.80725100
H	-0.97225800	6.06972700	-1.87825800
H	-0.86802400	5.93146100	-0.12692500
H	0.02999300	3.82482000	-2.17560100
H	1.08829000	4.81109100	-1.16468100
H	-2.32861400	4.07475100	1.08029400
H	-3.40953800	3.09332300	0.09764400
H	-3.18179000	5.41212900	-0.83161400
H	-2.60443200	4.20800800	-1.97795800
H	3.50367300	0.49890500	2.22864500
H	5.36788800	-0.97706600	1.59839600
H	4.43379000	-0.35917900	-2.56914800
H	2.56188700	1.13403500	-1.91745900
H	-2.75877300	0.71279000	-0.76104400
H	-3.74141700	-0.81473900	-2.13940300
H	-5.67267300	-2.31459700	-2.51568000

H	-6.62328700	-2.13775300	1.67598300
H	-4.69796600	-0.63282400	2.06042100
C	6.12727400	-1.64987300	-1.01066200
O	6.35543800	-1.88686800	-2.18088600
H	0.24813600	3.71772000	0.87587600
H	-1.42181000	2.05665900	-1.04290400

## 2-conf28

C	3.45877600	-2.70513200	-3.15459000
C	2.08915400	-2.06748600	-2.87682200
C	1.69665900	-2.22853400	-1.41009600
C	2.75662200	-1.62941500	-0.47790800
C	4.12393300	-2.29048100	-0.74754600
C	4.53427700	-2.13892400	-2.21867800
N	2.32952600	-1.81293700	0.92381200
O	0.42476200	-1.53973200	-1.22805200
H	1.78811400	-2.65311100	1.10133300
C	-0.51085500	-2.10290400	-0.44713000
O	-0.33573400	-3.12376900	0.20022400
C	-1.79479700	-1.33770900	-0.45033700
C	-2.82820600	-1.78318700	0.38285500
C	-4.04376900	-1.10721800	0.41554900
C	-4.23683200	0.02778300	-0.39185200
C	-3.19569600	0.47058800	-1.22797800
C	-1.98298100	-0.20501300	-1.25807600
C	2.92950900	-1.32633900	2.02797700
N	3.62645500	-0.13609700	1.93494600
S	2.88200400	-2.14653700	3.51003400
C	3.29138000	1.05189900	1.26851900
C	4.28098600	2.05151200	1.19096200
C	4.00400900	3.26971100	0.59252900
C	2.72859900	3.49176400	0.06242300
C	1.73071200	2.51677100	0.13735400
C	2.01016200	1.29961900	0.74249000
F	-7.07837300	-0.90971000	0.19334100
C	-6.68372100	0.34894600	0.49523200
F	-7.74165500	1.15486500	0.34876300
F	-6.32856700	0.36694800	1.80076000
N	2.43359600	4.76332000	-0.57193400
O	1.30493400	4.93778800	-1.04717900
O	3.32319600	5.62193600	-0.61179500
H	3.73194200	-2.53535800	-4.20118700
H	3.39040400	-3.79264900	-3.01796200
H	2.11691300	-0.99788500	-3.11999100
H	1.31297000	-2.52332100	-3.49947600
H	4.06128100	-3.35393800	-0.48290300
H	4.87184700	-1.83838300	-0.08866800
H	5.49046500	-2.64644500	-2.38445000
H	4.69649900	-1.07657700	-2.44523600
H	-2.67166000	-2.65848400	1.00211000
H	-4.82578300	-1.47199500	1.06907300
H	-3.35204800	1.34514300	-1.84867500
H	-1.18477000	0.13854400	-1.90416600
H	4.29090800	-0.02043500	2.69063300
H	5.26825000	1.86266200	1.59927300
H	4.76266600	4.03864000	0.52582700
H	0.74521900	2.71701100	-0.26285400

H	1.23095500	0.55248200	0.82151800
C	-5.50081700	0.80251200	-0.41664400
O	-5.68407200	1.78402500	-1.10999100
H	1.54279900	-3.28401500	-1.16790700
H	2.82396500	-0.56077900	-0.69545900

**Annex III:** XYZ cartesian coordinates of the optimized energies of several **1-GHB** geometries bearing different hydrogen bonding modes between the thiourea and carboxylate moieties.

**1-GHB-a**

C	0.48976600	4.21120700	-0.55083100
C	1.11882300	3.73960200	0.76160400
N	1.61319800	2.37104200	0.72743800
O	-0.56928100	3.31199700	-0.95504000
H	0.98517200	1.64987800	1.13560800
C	-1.77316500	3.44426300	-0.37061600
O	-2.09023300	4.39564200	0.32553100
C	-2.62703600	2.24609000	-0.60477500
C	-3.67344100	1.99353300	0.29100200
C	-4.33620100	0.77071400	0.26574900
C	-3.98806400	-0.20642100	-0.67954000
C	-3.00768900	0.09091400	-1.63416300
C	-2.31930300	1.30121700	-1.58970900
C	2.80878100	1.99931100	0.23599300
N	2.99572300	0.63355900	0.26833000
S	3.92456900	3.12298000	-0.40384700
C	4.13049000	-0.13603100	0.03978100
C	3.90997500	-1.50606200	-0.24576100
C	4.96920700	-2.37026500	-0.45525900
C	6.27877600	-1.87839400	-0.37729500
C	6.52275500	-0.53408900	-0.07597800
C	5.45976300	0.33129600	0.13428500
F	-6.58816300	-1.10113700	0.62068800
C	-6.06678400	-1.73411300	-0.45073100
F	-6.47974600	-3.01414500	-0.39048400
F	-6.62271900	-1.18230300	-1.55733900
N	7.38988700	-2.77162100	-0.60133500
O	8.54201900	-2.31592800	-0.54428400
O	7.15445900	-3.96522200	-0.84274500
H	-3.91611900	2.73031600	1.04855200
H	-5.08545100	0.56561400	1.01944900
H	-2.71931600	-0.64566100	-2.37458900
H	-1.51584800	1.48939400	-2.29151000
H	2.14373300	0.05897600	0.46429600
H	2.89196800	-1.87517400	-0.29386500
H	4.79384800	-3.41388000	-0.68287200
H	7.54130800	-0.17586500	0.00337400
H	5.65086200	1.36626600	0.37309200
C	-4.51182600	-1.64525700	-0.54022700
O	-4.06588700	-2.23469800	0.64167600
H	1.20950900	4.17574700	-1.36724500
H	0.37670600	3.78873900	1.56218900
O	-4.12463100	-2.47027500	-1.61905000
C	-2.62794400	-2.30477600	0.84859500
H	-2.35127700	-3.36250100	0.79895100

H	-2.10817100	-1.78356600	0.04225900
C	-2.27664500	-1.70994100	2.20739700
H	-2.79959100	-2.27945600	2.98425000
H	-2.64026000	-0.67897500	2.26069900
C	-0.76133700	-1.73892500	2.48732900
H	-0.35655400	-2.73489100	2.28116000
H	-0.60644600	-1.53345300	3.55235900
C	0.04895600	-0.69276900	1.70425500
O	-0.16105800	0.52935300	1.96335200
O	0.90038900	-1.10828200	0.85742500
H	-4.38992800	-2.07661200	-2.46406000
H	0.09793900	5.22416700	-0.43840900
H	1.93543500	4.42332900	1.00950000

### 1-GHB-b

C	-0.70378900	3.29997500	1.27740000
C	0.26983600	3.11698300	0.11239100
H	-0.28661200	2.88669900	-0.80710200
N	1.18020700	2.02949800	0.43297400
H	-1.11583100	2.34428400	1.59621300
O	-1.75437000	4.22977500	0.91086700
H	0.81333800	1.28704900	1.06561400
C	-2.81917100	3.89064700	0.15123700
O	-3.47831100	4.78634100	-0.34581600
C	-3.16698700	2.44630900	-0.04574500
C	-3.37696500	1.98349500	-1.35014300
C	-3.69069600	0.64332100	-1.57823700
C	-3.79345600	-0.25000800	-0.50624100
C	-3.64428400	0.23061600	0.80087900
C	-3.33615700	1.56720000	1.03289500
C	2.36207200	1.82207400	-0.17305600
N	2.88265800	0.57635700	0.11801400
S	3.06831400	2.94700100	-1.24158400
C	4.16823900	0.08193400	-0.03448600
C	4.30601700	-1.32755100	-0.05088300
C	5.55133000	-1.91970000	-0.15665000
C	6.68951700	-1.10694800	-0.24403300
C	6.57984200	0.28842000	-0.21062100
C	5.33114500	0.88037200	-0.10460900
F	-5.82815800	-1.88560800	0.90768000
C	-5.53898900	-2.10311100	-0.39195400
F	-5.80660300	-3.39787500	-0.65240300
F	-6.39289800	-1.35843100	-1.12678200
N	7.99153800	-1.71597900	-0.36223600
O	8.98718300	-0.98173000	-0.45425700
O	8.07179500	-2.95393200	-0.36723600
H	-3.28150400	2.66698100	-2.18696600
H	-3.85178500	0.30672800	-2.59641400
H	-3.74758200	-0.44677000	1.63938400
H	-3.22937500	1.91790500	2.05373200
H	2.17649400	-0.14016800	0.41346900
H	3.41621400	-1.94355700	0.01979300
H	5.65098300	-2.99731800	-0.17875200
H	7.47204000	0.89982000	-0.25696800
H	5.24942000	1.95670900	-0.07184900
O	-3.91962700	-2.14335100	-2.05853200

H	-3.11043100	-1.76986700	-2.43623300
C	-4.06041500	-1.74553400	-0.72125900
O	-3.30952300	-2.53104100	0.17549700
C	-1.91848400	-2.72134600	-0.17926500
H	-1.86774000	-3.45379000	-0.99125900
H	-1.49275500	-1.77479500	-0.53507700
C	-1.15326600	-3.22269100	1.03820600
H	-0.21462900	-3.65398700	0.67664200
H	-1.72542400	-4.03663100	1.49879100
C	-0.83668900	-2.14597900	2.08225700
H	-0.37686400	-2.62269000	2.95835300
H	-1.74761700	-1.65938500	2.44112500
C	0.14362400	-1.06202400	1.60971100
O	0.02504400	0.09712800	2.10967300
O	1.03398500	-1.38484200	0.76432200
H	-0.21255500	3.76995000	2.13011200
H	0.83424500	4.03340800	-0.06789700

### 1-GHB-c

C	0.68168600	2.67032600	0.50722500
C	-0.75529300	3.03041000	0.15466500
H	-1.15093200	3.76722600	0.86089900
N	-1.54959600	1.81065500	0.19530100
H	0.75355700	2.29606200	1.53088600
O	1.46545200	3.88553900	0.39734300
H	-1.04417200	0.91894100	0.38061500
C	2.76869800	3.86204100	0.04277600
O	3.32427300	4.91493900	-0.21073100
C	3.44963500	2.53025200	-0.03460800
C	3.52249300	1.68771200	1.08256100
C	4.04800400	0.40689500	0.95257600
C	4.49351500	-0.05175600	-0.29396600
C	4.48948400	0.81535100	-1.39002700
C	3.97585700	2.10687100	-1.25964000
C	-2.86833200	1.77527000	-0.05853400
N	-3.36465600	0.48859200	-0.11013700
S	-3.76980900	3.19131900	-0.35699400
C	-4.66985700	0.02005300	-0.08386700
C	-4.86621500	-1.31488700	-0.51718000
C	-6.12188200	-1.89342200	-0.49630700
C	-7.21285500	-1.14477900	-0.03440000
C	-7.04082800	0.16920300	0.41622300
C	-5.78164100	0.74846300	0.39476100
F	7.21745800	-1.01377900	-0.20012200
C	6.24435700	-1.82629100	0.26238600
F	6.63509400	-3.09921300	0.01288300
F	6.19355300	-1.67735100	1.60064400
N	-8.52690800	-1.73819100	-0.01521400
O	-9.48450800	-1.05477600	0.37870600
O	-8.65550700	-2.91306600	-0.39265500
H	3.14444900	2.01474800	2.04551600
H	4.06032500	-0.25388300	1.81131600
H	4.84900700	0.47219400	-2.35211400
H	3.94112300	2.76562400	-2.12106400
H	-2.64817000	-0.26627100	-0.23699400
H	-4.01181800	-1.88454800	-0.86541000

H	-6.26692800	-2.91057500	-0.83701800
H	-7.89087200	0.72585500	0.78994200
H	-5.65158100	1.76039400	0.74764000
C	4.88526600	-1.52189900	-0.43833500
O	5.03422200	-1.81062700	-1.80324000
H	5.22910800	-2.75561300	-1.90248800
O	3.97769700	-2.37587700	0.20515300
C	2.61656600	-2.36057400	-0.29966400
H	2.34939400	-1.34677500	-0.60987300
H	2.56052800	-3.01969600	-1.17307400
C	1.69355800	-2.84094800	0.80952000
H	1.78700200	-2.17003200	1.66885600
H	2.01861200	-3.83741000	1.13117400
C	0.22821200	-2.90897400	0.36441800
H	-0.34738600	-3.46492400	1.11562700
H	0.12580400	-3.48052200	-0.56527800
C	-0.50635800	-1.57084400	0.18287000
O	-1.60008200	-1.61431600	-0.46439100
O	-0.02815100	-0.52288200	0.70488700
H	-0.79297800	3.48032400	-0.84427500
H	1.06445400	1.91114800	-0.17457300

#### 1-GHB-d

C	-0.58455500	2.85295000	0.36990400
C	0.74155000	3.13795500	-0.32911900
H	0.56109100	3.37530900	-1.38583100
N	1.57247600	1.95458400	-0.19243300
H	-1.03632400	1.94241400	-0.02671100
O	-1.45770500	3.98273700	0.13701600
H	1.10112500	1.04300400	-0.20913900
C	-2.78182100	3.84818300	-0.09218100
O	-3.40272400	4.81782800	-0.48756200
C	-3.42686500	2.51648600	0.14170800
C	-4.17268600	1.94319600	-0.89241700
C	-4.74190500	0.67845800	-0.73221200
C	-4.59272100	-0.01512000	0.47392200
C	-3.89831200	0.59279200	1.52988100
C	-3.31326600	1.84349500	1.36642000
C	2.92377000	1.93417200	-0.17071000
N	3.40359600	0.64812200	-0.06370400
S	3.85641200	3.35166100	-0.29054600
C	4.68425400	0.11486500	0.01131400
C	4.75663200	-1.29718600	-0.09991100
C	5.97090600	-1.95257200	-0.01938900
C	7.14160600	-1.20605800	0.17506600
C	7.09212800	0.18623600	0.29218200
C	5.87403300	0.84669100	0.21370400
F	-7.23875100	-1.09597000	-0.26823500
C	-6.18027400	-1.93421600	-0.27349100
F	-6.62930400	-3.15106600	0.10711000
F	-5.76550700	-2.05419300	-1.55640900
N	8.41362600	-1.88337600	0.25859900
O	9.43993700	-1.20687800	0.42339500
O	8.43620900	-3.11964400	0.16304700
H	-4.28549700	2.46943500	-1.83412700
H	-5.28477500	0.24906500	-1.56500800

H	-3.80185700	0.07298000	2.47541400
H	-2.76600300	2.28704700	2.19143700
H	2.64918600	-0.06960700	-0.05331800
H	3.84220000	-1.86601500	-0.25823800
H	6.02297700	-3.03013700	-0.10958900
H	8.00493900	0.74639800	0.45075000
H	5.83478500	1.92115300	0.30686800
C	-5.05061200	-1.45631000	0.69520700
O	-5.57491100	-1.54564200	1.98865200
H	-5.62282000	-2.48430200	2.23098400
O	-3.98954500	-2.38742900	0.63171600
C	-3.03741400	-2.36174700	-0.46481000
H	-3.14917300	-3.30946700	-1.00127400
H	-3.27500200	-1.55153800	-1.15763500
C	-1.62375000	-2.19479900	0.07794200
H	-1.54624500	-1.23285700	0.59383700
H	-1.42745700	-2.98104300	0.81717500
C	-0.58263700	-2.26180200	-1.05164600
H	-0.83957600	-1.52231400	-1.82218800
H	-0.59435600	-3.24925900	-1.52249100
C	0.84615500	-1.95395300	-0.57910300
O	1.03680200	-0.80149700	-0.05305800
O	1.73803200	-2.82241400	-0.73532700
H	-0.43758000	2.74122200	1.44696000
H	1.24788800	3.99091300	0.12481600

### 1-GHB-e

C	-0.60392100	3.35320500	1.27459200
C	0.22873800	3.02622200	0.03443800
H	-0.42847300	2.71205100	-0.78903800
N	1.16043500	1.96801400	0.38133200
H	-0.99696700	2.44754100	1.73458700
O	-1.67635600	4.27596800	0.95971000
H	0.83106600	1.26686500	1.05150500
C	-2.79904000	3.93387400	0.29176300
O	-3.51079000	4.83100200	-0.12399700
C	-3.14494500	2.49097200	0.07524000
C	-3.48878500	2.08826000	-1.22128100
C	-3.81826500	0.75853300	-1.48177600
C	-3.80200500	-0.18802800	-0.45121000
C	-3.51414700	0.22940300	0.85427500
C	-3.19355000	1.55752900	1.11982800
C	2.28770200	1.63985500	-0.29976700
N	2.77006300	0.41715200	0.04085200
S	2.90253600	2.67101300	-1.53802600
C	4.07509700	0.02311500	-0.06792800
C	4.34309100	-1.37039300	-0.19450400
C	5.63368600	-1.85837500	-0.24273800
C	6.71559600	-0.96578100	-0.15321000
C	6.48737900	0.41392800	-0.00546300
C	5.19483200	0.89812600	0.03430900
F	-5.67332600	-1.89911700	1.09495200
C	-5.53100200	-2.04824600	-0.23819100
F	-5.82980100	-3.32829300	-0.53433500
F	-6.45754100	-1.26811900	-0.83445800
N	8.05325500	-1.46371600	-0.20480700

O	9.00160900	-0.65765700	-0.14042800
O	8.23771200	-2.69169600	-0.31247500
H	-3.48867800	2.81342800	-2.02774100
H	-4.08948400	0.47416700	-2.49249200
H	-3.52605000	-0.48813000	1.66543700
H	-2.99381300	1.85719800	2.14249100
H	1.76429500	-0.65338300	0.40073800
H	3.50808700	-2.05869700	-0.26471200
H	5.81984100	-2.91910000	-0.35479300
H	7.32991500	1.08815500	0.08669900
H	5.02696500	1.95944900	0.15803300
O	-4.10371200	-2.00255700	-2.07274400
H	-3.36202200	-1.58003500	-2.52887400
C	-4.09642100	-1.67103300	-0.71111800
O	-3.25650900	-2.50311400	0.05715800
C	-1.90857900	-2.65527700	-0.44045600
H	-1.93512400	-3.27256600	-1.34382800
H	-1.49578100	-1.67240200	-0.70223100
C	-1.06076300	-3.33163500	0.62794000
H	-0.14416400	-3.68490600	0.14641000
H	-1.59422400	-4.21786300	0.98838100
C	-0.69798200	-2.44083200	1.82397900
H	-0.15654400	-3.04298500	2.56528100
H	-1.58984800	-2.05715200	2.32459400
C	0.19729500	-1.25626100	1.50316400
O	0.08915900	-0.17726400	2.09651100
O	1.09918900	-1.48112000	0.57208800
H	-0.00587300	3.88474400	2.01548500
H	0.77956600	3.90556700	-0.30250200

### 1-GHB-f

C	0.48068600	4.18619200	-0.48268200
C	1.16419500	3.67142200	0.78604400
N	1.63279000	2.29948700	0.70416300
O	-0.62459000	3.32531400	-0.85352100
H	0.98510700	1.57130300	1.00721200
C	-1.78464200	3.45817700	-0.18860900
O	-2.02873200	4.37421200	0.58089700
C	-2.69079500	2.30187100	-0.43998800
C	-3.64605800	1.98605600	0.53408600
C	-4.34546700	0.78529400	0.46502300
C	-4.13171900	-0.10055000	-0.60220500
C	-3.24665300	0.26705000	-1.62335300
C	-2.51657200	1.45065400	-1.53642800
C	2.81758200	1.87871900	0.18474900
N	2.94968500	0.53774000	0.14411000
S	3.94866800	3.04078500	-0.43419000
C	4.13871900	-0.12704700	-0.03595700
C	4.10382700	-1.36568000	-0.73359800
C	5.23630200	-2.14164400	-0.89459800
C	6.45209800	-1.70680000	-0.34309400
C	6.51929400	-0.49928700	0.37298200
C	5.38472600	0.27585200	0.52089600
F	-6.60986200	-1.05930800	0.88064400
C	-6.22749700	-1.59214500	-0.29821500
F	-6.67651500	-2.86101800	-0.32042200



F	-6.87603500	-0.91686400	-1.27865400
N	7.63040500	-2.50377400	-0.50465100
O	8.70481400	-2.09563800	-0.02580100
O	7.54877400	-3.58383600	-1.11884000
H	-3.78664700	2.65151600	1.37858900
H	-5.01773700	0.52407000	1.27208700
H	-3.06416500	-0.39868000	-2.45854200
H	-1.78440800	1.68905800	-2.29859300
H	1.82148900	-0.53908000	0.57895800
H	3.16205000	-1.69420900	-1.15958700
H	5.19683700	-3.07323700	-1.44497500
H	7.45879200	-0.19044600	0.81433100
H	5.43801000	1.19823200	1.08297100
C	-4.68894500	-1.53272100	-0.54767500
O	-4.13915400	-2.24545500	0.51897800
H	1.15735200	4.14558500	-1.33520100
H	0.46467600	3.72777100	1.62442700
O	-4.44653200	-2.25680200	-1.73445400
C	-2.69820300	-2.41308500	0.52116200
H	-2.48403100	-3.43918000	0.20594100
H	-2.24240200	-1.73402500	-0.20301200
C	-2.16464400	-2.14515600	1.92357700
H	-2.60817000	-2.86475300	2.61931700
H	-2.47016900	-1.14512100	2.24497500
C	-0.63467000	-2.26059000	1.98672000
H	-0.27650500	-3.16402200	1.48437500
H	-0.32243600	-2.34784200	3.03518400
C	0.11785300	-1.05811900	1.43964000
O	-0.27873300	0.10071100	1.56454300
O	1.26327100	-1.37357100	0.86130000
H	-4.79233000	-1.77964900	-2.50387100
H	0.12153000	5.20698100	-0.33447200
H	2.00658100	4.33344300	1.00179400

### 1-GHB-g

C	-0.63865200	2.71793800	-0.59714500
C	0.77713800	3.05028000	-0.14341200
H	1.21290200	3.82724200	-0.78039200
N	1.55642600	1.82470400	-0.21653700
H	-0.65141200	2.39387600	-1.64115100
O	-1.43699900	3.92134900	-0.48259100
H	1.07190000	0.96924400	-0.50152600
C	-2.74142600	3.88933200	-0.13298300
O	-3.30467900	4.94030900	0.11193300
C	-3.41780200	2.55557500	-0.04397600
C	-3.46614500	1.68604800	-1.14187100
C	-3.99516300	0.40842100	-0.99338200
C	-4.47067200	-0.01980400	0.25315400
C	-4.48976000	0.87328700	1.32799100
C	-3.97189000	2.16090900	1.17839000
C	2.83726400	1.67765800	0.19868200
N	3.25123500	0.38583300	0.22172900
S	3.72737700	3.05412400	0.74102400
C	4.55542800	-0.02106300	0.14481600
C	4.89606100	-1.28016600	0.71847500
C	6.17231400	-1.79873700	0.62569700

C	7.16442600	-1.07823600	-0.06119600
C	6.85843500	0.15813100	-0.65777100
C	5.58279500	0.67630100	-0.55472500
F	-7.18736900	-0.98826900	0.07377700
C	-6.19666300	-1.81522700	-0.31979000
F	-6.59715200	-3.07920500	-0.04224400
F	-6.08992200	-1.71302200	-1.65888000
N	8.48660500	-1.60784200	-0.16096600
O	9.36046900	-0.94549200	-0.75382700
O	8.73333500	-2.71956100	0.34629800
H	-3.06590800	1.98962600	-2.10349600
H	-3.98797700	-0.27215000	-1.83667300
H	-4.87188100	0.55390900	2.28947200
H	-3.95683100	2.84026500	2.02416300
H	2.22837100	-0.76691700	0.37256200
H	4.13114300	-1.83471600	1.25037400
H	6.41723200	-2.74950200	1.08227500
H	7.62550100	0.69127900	-1.20579000
H	5.35299100	1.62231800	-1.02577900
C	-4.86830700	-1.48523200	0.42682800
O	-5.07238600	-1.73246200	1.79174600
H	-5.27862000	-2.67261800	1.91202300
O	-3.93341600	-2.35945500	-0.15170300
C	-2.59727400	-2.32023800	0.40552300
H	-2.30401500	-1.28178800	0.58472800
H	-2.59410500	-2.85404800	1.36202700
C	-1.65579100	-2.98009200	-0.59136100
H	-1.71944600	-2.45569400	-1.54966000
H	-1.98043200	-4.01246600	-0.75890000
C	-0.20360800	-2.99196900	-0.10280700
H	0.38848500	-3.67583800	-0.72369500
H	-0.12343100	-3.38030000	0.91865200
C	0.51402900	-1.65411600	-0.15990400
O	1.64727300	-1.64648000	0.51351800
O	0.09470400	-0.68464700	-0.79700400
H	0.75875200	3.43791700	0.88164100
H	-1.05593200	1.92746800	0.02695100

**Annex IV:** XYZ cartesian coordinates of the optimized energies of several **2-GHB** geometries bearing different hydrogen bonding modes between the thiourea and carboxylate moieties.

#### **2-GHB-a**

C	2.14939500	6.07075800	-0.56496500
C	0.86711500	5.32244200	-0.95876400
C	1.07524000	3.80968300	-0.84480100
C	1.58089000	3.36633700	0.54467200
C	2.81482900	4.18419300	0.98322100
C	2.57396900	5.69462000	0.86060800
N	1.78359600	1.91065800	0.65668500
O	-0.10544900	3.02592800	-1.22054100
H	1.15933800	1.44754200	1.34323000
C	-1.24852000	3.09936000	-0.52156700
O	-1.52193800	3.98340500	0.27660900
C	-2.13967900	1.92540300	-0.76039900

C	-3.35941700	1.87530400	-0.07207300
C	-4.10857600	0.70530500	-0.05510500
C	-3.65584000	-0.43790600	-0.73328300
C	-2.48551800	-0.35423300	-1.49557500
C	-1.72839300	0.81731400	-1.50848300
C	2.63239900	1.11747700	-0.02350800
N	2.46596000	-0.21878600	0.28891300
S	3.73988100	1.65815300	-1.20668800
C	3.30944700	-1.29629100	0.05286900
C	2.70993400	-2.57798600	0.00654700
C	3.47520800	-3.71646500	-0.17550300
C	4.86407800	-3.59298500	-0.30951500
C	5.48304300	-2.33855800	-0.24269000
C	4.71437000	-1.20013600	-0.06086300
F	-6.55287800	-0.94419100	-0.00313800
C	-5.84858000	-1.81028800	-0.76080900
F	-6.37853000	-3.03144300	-0.55843400
F	-6.06984200	-1.48485400	-2.05864400
N	5.66798600	-4.77391600	-0.50777100
O	6.89471600	-4.64492200	-0.64128900
O	5.10576400	-5.87947000	-0.53757400
H	1.97706700	7.14984800	-0.64342800
H	2.95974800	5.82742500	-1.26569100
H	0.04965600	5.63724900	-0.30675600
H	0.57788900	5.55712800	-1.98950600
H	3.67170900	3.89972500	0.36725900
H	3.05119800	3.91108300	2.01769500
H	3.48716600	6.23064800	1.14296700
H	1.79217200	6.00898100	1.56615100
H	-3.68149100	2.73809300	0.49968300
H	-5.01209600	0.66917300	0.53998500
H	-2.11012500	-1.22145700	-2.02558900
H	-0.79103600	0.84725500	-2.05040400
H	1.54729700	-0.49421100	0.71811900
H	1.63515300	-2.65912000	0.12003200
H	3.01032700	-4.69290100	-0.22238800
H	6.56029700	-2.26444600	-0.32003500
H	5.19552500	-0.23544400	0.00170700
C	-4.31643800	-1.80130100	-0.46860600
O	-4.21934900	-2.16520100	0.87326900
H	1.79917600	3.49034700	-1.59446500
H	0.78110700	3.57347300	1.26157500
O	-3.75495500	-2.83750900	-1.24789600
C	-2.88234600	-2.20644200	1.45210800
H	-2.72655400	-3.23494600	1.79187300
H	-2.13442200	-1.98753300	0.69057700
C	-2.79022200	-1.22676700	2.61884700
H	-3.50669100	-1.53140600	3.39071500
H	-3.09373300	-0.23146900	2.27976200
C	-1.38258500	-1.14706400	3.25038000
H	-1.03260300	-2.15677600	3.49573400
H	-1.45276300	-0.57823800	4.18128100
C	-0.34390700	-0.47626100	2.34038600
O	-0.05043700	0.73838700	2.54708800
O	0.16057700	-1.18664900	1.41358900
H	-3.79374700	-2.61657800	-2.19074100

## 2-GHB-b

C	0.02253200	0.00304900	-0.00835500
C	0.01770700	0.01154100	1.52527200
C	1.41675700	-0.00177400	2.14252000
C	2.39665300	1.02365300	1.52469800
C	2.31646900	1.05291300	-0.01485100
C	0.88281600	1.15167900	-0.54821200
H	3.41284900	0.73629400	1.81388400
N	2.12399000	2.32668900	2.14978800
H	1.35054900	0.19214200	3.21086800
O	2.00123400	-1.32757500	1.93203300
H	1.24939200	2.42122200	2.69934900
C	2.51079300	-2.08961800	2.91940400
O	3.21882800	-3.03560400	2.61704700
C	2.18763200	-1.76654500	4.34771700
C	3.23499500	-1.69919400	5.27253300
C	2.97882200	-1.35195200	6.60046800
C	1.67501400	-1.06306600	7.01602000
C	0.62056700	-1.20149200	6.10350800
C	0.87173100	-1.55212000	4.78223700
C	3.03654300	3.30648000	2.28199900
N	2.62125000	4.30761000	3.14213000
S	4.57493000	3.26113700	1.55060400
C	3.05947400	5.61681200	3.24620700
C	2.79820400	6.28485300	4.46761900
C	3.15498700	7.60945100	4.64412600
C	3.78011700	8.29665200	3.59484400
C	4.03110100	7.66257100	2.37103300
C	3.67361500	6.33601200	2.19594200
F	-0.49343500	-2.06361700	8.78568200
C	0.70101700	-1.68897400	9.28872900
F	0.49408600	-1.28867500	10.55863400
F	1.48381600	-2.78850600	9.33404200
N	4.16128300	9.67453600	3.77377900
O	4.73215900	10.26208900	2.84143800
O	3.90542600	10.22875700	4.85442200
H	-1.00729000	0.08497800	-0.37337400
H	0.41468400	-0.95339100	-0.37794000
H	-0.48229900	0.91609200	1.88872700
H	-0.54942000	-0.83821200	1.92123000
H	2.77424200	0.12500100	-0.38158600
H	2.93545100	1.87593000	-0.37955500
H	0.89908200	1.13707500	-1.64386200
H	0.43969700	2.11274800	-0.25282500
H	4.25192400	-1.89587400	4.95060300
H	3.80624200	-1.30210500	7.29962300
H	-0.39654400	-1.00621400	6.42001100
H	0.04131600	-1.64116800	4.09058400
H	1.96541500	4.00738100	3.90695500
H	2.31095900	5.74121300	5.26942100
H	2.96253100	8.11286000	5.58291000
H	4.49359600	8.21536900	1.56323800
H	3.86130400	5.85259300	1.24826200
O	2.51011000	-0.23679600	9.16937700
H	3.10689400	0.30535800	8.63392300
C	1.36261000	-0.56897800	8.43446900

O	0.40060900	0.45995800	8.40838600
C	0.89662800	1.76213500	8.00826700
H	1.43357900	2.19835800	8.85684300
H	1.59451800	1.65282000	7.16998100
C	-0.27753300	2.64705800	7.60803800
H	0.05841500	3.68603700	7.67930200
H	-1.07543300	2.51779400	8.34901200
C	-0.82557400	2.39605600	6.19955100
H	-1.75208400	2.96952700	6.06395400
H	-1.10458300	1.34673200	6.06211700
C	0.10505000	2.79859800	5.04327800
O	-0.16438000	2.33678400	3.89492100
O	1.07275600	3.58268000	5.28940400

## 2-GHB-c

C	-0.55231400	4.14767500	2.23738600
C	-1.01563200	2.80369100	1.65863600
C	-0.73814200	2.67016700	0.15812100
C	0.71452600	3.01511700	-0.22950600
C	1.17653100	4.34401000	0.40180200
C	0.92570300	4.40338700	1.91370100
H	0.76289000	3.10110700	-1.31877800
N	1.56107700	1.88258200	0.15792100
H	-0.96535000	1.66079800	-0.18518400
O	-1.55854100	3.62236900	-0.59434000
H	1.19437000	1.19427500	0.82068100
C	-2.85882100	3.41275400	-0.88333900
O	-3.52589600	4.35181700	-1.27968400
C	-3.42762200	2.03620600	-0.70947400
C	-2.94793400	0.94979300	-1.45346700
C	-3.43623400	-0.33013700	-1.20800300
C	-4.39436000	-0.54340000	-0.20795800
C	-4.92326000	0.55066600	0.48195400
C	-4.44948900	1.83802000	0.22475800
C	2.72944900	1.54736000	-0.43414400
N	3.22441600	0.36302300	0.06432700
S	3.42983100	2.46726400	-1.67993400
C	4.44579100	-0.27306000	-0.09156000
C	4.49466500	-1.62822600	0.31883700
C	5.66861100	-2.35433700	0.24902100
C	6.82711800	-1.73282900	-0.23578400
C	6.80760500	-0.39219100	-0.63562600
C	5.62916500	0.33524600	-0.56450100
F	-6.68803600	-2.00011000	-1.22505000
C	-5.57266700	-2.69745800	-0.92322100
F	-5.96850700	-3.92304700	-0.50368000
F	-4.88101700	-2.86993600	-2.06688900
N	8.05674700	-2.48371600	-0.31673400
O	9.06781800	-1.92466600	-0.76738200
O	8.05989700	-3.66258700	0.06856200
H	-0.71706300	4.15078500	3.32025400
H	-1.16379100	4.95830000	1.82120800
H	-0.48974200	1.98417200	2.16644500
H	-2.08157100	2.63720700	1.84502700
H	0.62705900	5.15414800	-0.09334700

H	2.23493300	4.48842000	0.16938000
H	1.23609100	5.38092700	2.29904800
H	1.54725500	3.65374500	2.42201800
H	-2.17800700	1.09396100	-2.20466000
H	-3.02537800	-1.16934900	-1.75714800
H	-5.67665000	0.39634900	1.24412000
H	-4.84668800	2.68041800	0.78157100
H	2.52732300	-0.15989000	0.64052500
H	3.59223800	-2.10098700	0.69126400
H	5.69630700	-3.39127200	0.55804800
H	7.71621500	0.07678600	-0.99149200
H	5.61681300	1.37019600	-0.87092400
C	-4.75065900	-1.97630300	0.18764000
O	-5.54743900	-1.93302800	1.34297100
H	-5.69948600	-2.84162200	1.64628700
O	-3.61706500	-2.78939800	0.34745200
C	-2.60944600	-2.30787900	1.27209700
H	-2.26837000	-1.32242100	0.94313900
H	-3.05214300	-2.20903300	2.26914000
C	-1.44349200	-3.28527200	1.27640900
H	-1.21405200	-3.56675100	0.24479700
H	-1.72072200	-4.19506600	1.82033300
C	-0.19716500	-2.64683900	1.90355900
H	0.55071500	-3.42595800	2.10104300
H	-0.42502200	-2.19541600	2.87573600
C	0.49780100	-1.59552200	1.01507100
O	1.20234700	-0.71180700	1.62527700
O	0.37994500	-1.68011000	-0.22936300

## 2-GHB-d

C	-0.64443100	4.92280600	1.71963000
C	-1.13952800	3.47298500	1.61079400
C	-1.08016700	2.93050800	0.18210600
C	0.28454100	3.15229400	-0.50821000
C	0.78397500	4.60105300	-0.34559600
C	0.75813600	5.07506700	1.11391900
H	0.16622200	2.93204100	-1.57162800
N	1.23059800	2.16985100	0.02238700
H	-1.31682500	1.86592700	0.16386000
O	-2.06301100	3.64762200	-0.63093000
H	1.11981600	1.84435300	0.98752700
C	-3.06111000	3.03535900	-1.29535100
O	-3.66526700	3.65822700	-2.15012900
C	-3.40871700	1.61820000	-0.94249100
C	-3.23399700	0.61035400	-1.89418000
C	-3.51969100	-0.71820200	-1.57148400
C	-4.01087100	-1.04804700	-0.30384900
C	-4.24355900	-0.02320600	0.62468400
C	-3.93552000	1.29766800	0.31640700
C	2.22156200	1.58304800	-0.68749500
N	2.88448400	0.63714300	0.06431600
S	2.54502200	1.97765100	-2.30936700
C	4.01294600	-0.13744700	-0.16227400
C	4.33065200	-1.05981100	0.86728200
C	5.43356500	-1.88623400	0.77386900
C	6.25224400	-1.80454900	-0.36083800

C	5.96593600	-0.89749700	-1.38539900
C	4.85681000	-0.06896000	-1.29214100
F	-5.18943100	-3.25868300	-1.88937400
C	-4.27715800	-3.55478000	-0.93836500
F	-4.61801500	-4.75484500	-0.41812300
F	-3.08479300	-3.71904400	-1.55799900
N	7.40507500	-2.66611600	-0.47158600
O	8.11749200	-2.58080100	-1.48283800
O	7.64258500	-3.46177700	0.44935900
H	-0.64322600	5.22585800	2.77217900
H	-1.34291900	5.58960200	1.19857400
H	-0.51681400	2.82368900	2.24034000
H	-2.16266700	3.37489500	1.98800000
H	0.13697900	5.24734000	-0.95154200
H	1.79090500	4.66995400	-0.76797700
H	1.08234300	6.12025000	1.16657500
H	1.47861200	4.49440800	1.70605500
H	-2.84762200	0.85222200	-2.87864100
H	-3.33784000	-1.47879600	-2.32025300
H	-4.64769600	-0.26732400	1.60010600
H	-4.10042300	2.07248300	1.05796600
H	2.43958100	0.47492600	0.99178800
H	3.69467100	-1.11265100	1.74477600
H	5.66634900	-2.58849700	1.56391600
H	6.61272500	-0.84263800	-2.25188800
H	4.63398900	0.62696300	-2.08602800
C	-4.22888000	-2.47734100	0.19130800
O	-5.46760600	-2.52052200	0.84154100
H	-5.49900700	-3.32770600	1.37998600
O	-3.26345700	-2.89493300	1.13563300
C	-1.85626700	-2.58904800	0.94120900
H	-1.32856300	-3.54788200	0.92689800
H	-1.70611600	-2.10908600	-0.02819000
C	-1.35653500	-1.69224500	2.06717200
H	-1.99426000	-0.80330500	2.11439200
H	-1.45822300	-2.20916700	3.02616000
C	0.09844700	-1.26561100	1.84325500
H	0.21735400	-0.83823400	0.84153000
H	0.76080000	-2.14207500	1.88483100
C	0.62497200	-0.25065300	2.87423900
O	1.49400500	0.59494600	2.44924800
O	0.20606500	-0.30991700	4.05124100

## 2-GHB-e

C	2.25822000	6.07208600	-0.53998000
C	0.92954500	5.36609600	-0.85097500
C	1.11485000	3.84777800	-0.79939800
C	1.68345200	3.35786100	0.54947400
C	2.98522400	4.11392300	0.89261100
C	2.79499900	5.63575600	0.82998300
N	1.81189500	1.89675700	0.64903500
O	-0.09533600	3.09969500	-1.14882300
H	1.23938400	1.46432600	1.37550000
C	-1.19248700	3.13946700	-0.38095700
O	-1.41051200	3.97679500	0.48252100
C	-2.10830000	1.98815300	-0.64045100

C	-3.28871500	1.90086100	0.10953200
C	-4.05399800	0.74119800	0.08175200
C	-3.65703000	-0.35334800	-0.70325300
C	-2.52503700	-0.22961200	-1.51633900
C	-1.75231700	0.93126000	-1.48522300
C	2.53521300	1.01747400	-0.09324800
N	2.29223300	-0.27872200	0.22190200
S	3.56684600	1.52541800	-1.38775900
C	3.16465400	-1.30964700	-0.01286800
C	2.62596000	-2.60072500	-0.27512600
C	3.43798200	-3.70653600	-0.43902700
C	4.83122900	-3.56330600	-0.33255300
C	5.39763000	-2.30594500	-0.05464300
C	4.58115400	-1.20310600	0.09758100
F	-6.53983100	-0.84300700	0.05695100
C	-5.87526800	-1.67996100	-0.76606300
F	-6.42733300	-2.89904000	-0.61950400
F	-6.11906100	-1.27639000	-2.03729900
N	5.67701400	-4.70287000	-0.49897600
O	6.91187000	-4.55596500	-0.41780900
O	5.15840200	-5.81439400	-0.71992400
H	2.10845400	7.15714500	-0.56674600
H	2.99890700	5.83532600	-1.31607100
H	0.17274500	5.67568700	-0.12599200
H	0.56585100	5.64147000	-1.84756900
H	3.76887500	3.80880600	0.19350900
H	3.30303200	3.80443600	1.89468600
H	3.74919400	6.13145200	1.04228300
H	2.09222600	5.95628500	1.61203500
H	-3.56772700	2.72405400	0.75730600
H	-4.92662400	0.67181000	0.71868500
H	-2.19171700	-1.05947300	-2.12810100
H	-0.84499500	0.99071000	-2.07369000
H	1.55063000	-2.70921000	-0.36037700
H	3.01218100	-4.67809400	-0.65613600
H	6.47169900	-2.21452800	0.04976700
H	5.02148600	-0.24100900	0.32328500
C	-4.33676300	-1.71941000	-0.51289000
O	-4.21520300	-2.17116900	0.80127100
H	1.79810000	3.53962700	-1.59083300
H	0.94930100	3.61010700	1.32042900
O	-3.81313300	-2.71378700	-1.36738400
C	-2.86827800	-2.27903500	1.33727400
H	-2.70596400	-3.33608500	1.56867700
H	-2.13916200	-1.98533300	0.58155200
C	-2.75145200	-1.42089400	2.59433600
H	-3.45820000	-1.79462000	3.34290900
H	-3.04567400	-0.39283700	2.36343100
C	-1.33834000	-1.42645100	3.22154000
H	-0.98258300	-2.45607400	3.33348600
H	-1.39488300	-0.97352400	4.21363400
C	-0.31512100	-0.63740100	2.42306600
O	-0.02682200	0.53418700	2.68153600
O	0.22794000	-1.31192600	1.42798400
H	-3.87675800	-2.43901600	-2.29457600
H	1.01101900	-0.78508400	0.94809000



## 2-GHB-f

C	-0.11463900	-4.88874200	-2.09646600
C	-0.77073300	-3.51380300	-1.91493400
C	-0.74474500	-3.01840300	-0.46802000
C	0.64023000	-3.12697400	0.20934800
C	1.30938900	-4.49099200	-0.04760400
C	1.31101400	-4.89058400	-1.52855800
H	0.50217200	-3.00257600	1.28735200
N	1.44308200	-1.98916900	-0.25109600
H	-1.06366100	-1.97928100	-0.42056400
O	-1.67434100	-3.83869900	0.31025700
H	1.14587000	-1.50827900	-1.10208700
C	-2.66258300	-3.34094800	1.07832600
O	-3.19848800	-4.08088700	1.88642000
C	-3.08164100	-1.91000500	0.91719200
C	-3.21280700	-1.11983300	2.06402800
C	-3.55176200	0.23015500	1.95315400
C	-3.75547200	0.80608100	0.69510700
C	-3.69310800	-0.00570300	-0.44586100
C	-3.36414900	-1.35176200	-0.33784700
C	2.36451200	-1.32018200	0.48646900
N	2.70874800	-0.11790700	-0.04999800
S	2.90068400	-1.92937800	2.00741500
C	3.91672100	0.49718100	0.11602700
C	3.97559300	1.91399000	-0.03367700
C	5.16812200	2.60299900	0.05479300
C	6.36248300	1.89803200	0.28571900
C	6.34423900	0.49702300	0.41517600
C	5.14864800	-0.18731500	0.33475900
F	-5.84871700	2.03144500	-1.02277200
C	-5.50620400	2.58382000	0.15937400
F	-5.75816600	3.90463200	0.07374000
F	-6.33121200	2.07409000	1.09867900
N	7.59735800	2.60483500	0.38193900
O	8.64544000	1.96596000	0.60286300
O	7.59882800	3.84429300	0.24246500
H	-0.10675000	-5.14781300	-3.16097400
H	-0.71198600	-5.65650100	-1.58812700
H	-0.24426100	-2.77048500	-2.52494500
H	-1.80778400	-3.52394700	-2.26797000
H	0.75775500	-5.24429800	0.52969700
H	2.32431100	-4.45928900	0.35817700
H	1.76587300	-5.88109600	-1.64190500
H	1.93505700	-4.19071800	-2.10121500
H	-3.02952900	-1.55353100	3.04109000
H	-3.64631000	0.82219300	2.85684700
H	-3.87747700	0.42129600	-1.42389800
H	-3.31584400	-1.95901600	-1.23498800
H	3.05535900	2.45940900	-0.21036500
H	5.19175300	3.68098300	-0.04461700
H	7.27388100	-0.03706800	0.56855600
H	5.14524400	-1.26515700	0.42641900
O	-3.82501300	3.04656200	1.69335500
H	-3.00966500	2.77236700	2.13671200
C	-4.01736900	2.30699300	0.51862900

O	-3.29687200	2.81574400	-0.58225600
C	-1.88536300	3.03374500	-0.34912800
H	-1.76977500	3.93586800	0.25987300
H	-1.46181800	2.18477400	0.20047300
C	-1.18129600	3.21261400	-1.68797600
H	-0.22028600	3.69791500	-1.49318000
H	-1.76914500	3.90815600	-2.29717900
C	-0.94867700	1.92346100	-2.48397800
H	-0.58228300	2.17692200	-3.48702200
H	-1.88138300	1.37373600	-2.64066000
C	0.06325200	0.94009700	-1.91466400
O	0.13780700	-0.21843300	-2.33696100
O	0.85150400	1.41942000	-0.97739400
H	1.59542700	0.72232300	-0.64319400

## 2-GHB-g

C	-0.13465500	4.54976500	2.10409700
C	-0.73829500	3.17343600	1.78771300
C	-0.62606800	2.80124500	0.30654700
C	0.79835200	2.96773200	-0.26073100
C	1.39816700	4.34249500	0.09759000
C	1.31234900	4.65168500	1.59917300
H	0.74823400	2.86647800	-1.34629500
N	1.62178500	1.85840400	0.21397500
H	-0.95649400	1.77609400	0.14047700
O	-1.46308600	3.71066500	-0.48241800
H	1.57282200	1.60748800	1.19395800
C	-2.77650600	3.50330100	-0.69450000
O	-3.46515300	4.43791400	-1.06514500
C	-3.33714800	2.12641300	-0.49725500
C	-2.89067700	1.04944700	-1.27513600
C	-3.40957600	-0.22424900	-1.06216100
C	-4.35930000	-0.44288300	-0.05560200
C	-4.83544000	0.63985600	0.68902100
C	-4.33538900	1.92280800	0.46082300
C	2.55708200	1.17044100	-0.49706000
N	3.07200400	0.12066700	0.18773500
S	2.89175700	1.57547900	-2.13903900
C	4.32675900	-0.38484700	0.01224100
C	4.56832800	-1.73810200	0.39379100
C	5.82465200	-2.30259700	0.31255900
C	6.90702300	-1.52861300	-0.14289200
C	6.71070000	-0.18276800	-0.50483800
C	5.45080900	0.37473700	-0.43176200
F	-6.83614000	-1.59713500	-0.99680700
C	-5.77123800	-2.41237800	-0.84868400
F	-6.24773400	-3.63362600	-0.50747000
F	-5.18136900	-2.53307700	-2.05385900
N	8.20701000	-2.10574600	-0.22875000
O	9.15434200	-1.40793600	-0.64386600
O	8.36703900	-3.29477600	0.11402400
H	-0.17782600	4.72484200	3.18447600
H	-0.74152400	5.33217000	1.63170400
H	-0.21876900	2.39852900	2.36762700
H	-1.78873200	3.12114900	2.09473800
H	0.84762300	5.10802000	-0.46275600

H	2.43457600	4.37092000	-0.25339900
H	1.71036200	5.65401200	1.79209000
H	1.94789900	3.95368300	2.16180200
H	-2.13041400	1.19862200	-2.03510800
H	-3.03954100	-1.05593600	-1.65087800
H	-5.57810000	0.48017800	1.46071100
H	-4.70186400	2.75754500	1.04930500
H	3.73761900	-2.33625400	0.75045200
H	5.98434200	-3.33633700	0.59256000
H	7.55585300	0.41093000	-0.83089400
H	5.31220300	1.41251500	-0.70395700
C	-4.80489100	-1.87239100	0.24974700
O	-5.49957900	-1.87007100	1.46887300
H	-5.73606900	-2.78376400	1.69287600
O	-3.74408900	-2.79216800	0.23538000
C	-2.64668900	-2.51959800	1.13694200
H	-2.23807500	-1.52950000	0.91424600
H	-3.01342800	-2.51992600	2.16879400
C	-1.58486400	-3.59024300	0.92657700
H	-1.43926000	-3.74032300	-0.14713200
H	-1.92348100	-4.53992200	1.35226100
C	-0.25119100	-3.18450500	1.56311400
H	0.41869600	-4.05227500	1.61141600
H	-0.37687700	-2.84583400	2.59702900
C	0.49788300	-2.11611200	0.78103300
O	1.40228200	-1.47556000	1.51505400
O	0.31204600	-1.89388600	-0.40964400
H	1.99221900	-0.83739600	0.95087500

## 2-GHB-h

C	-0.88566500	5.14083800	1.46612400
C	-1.23286300	3.64497100	1.42476100
C	-1.09454900	3.04067600	0.02818500
C	0.27160400	3.34770100	-0.63443000
C	0.62900800	4.84171800	-0.54095800
C	0.51052200	5.40357900	0.88423600
H	0.21112200	3.04591700	-1.68114000
N	1.30696500	2.51502000	-0.03068200
H	-1.23292900	1.95961500	0.05564000
O	-2.11751400	3.62855500	-0.84252300
H	1.69416600	2.80870400	0.85829700
C	-3.03057400	2.90224100	-1.51233100
O	-3.62371500	3.41797200	-2.44409400
C	-3.31011200	1.49527100	-1.07259900
C	-3.12991500	0.44760800	-1.97930600
C	-3.35060800	-0.87298600	-1.58216300
C	-3.78416400	-1.15590700	-0.28271500
C	-4.02768700	-0.09525100	0.60201200
C	-3.78252000	1.21852200	0.21808400
C	1.85826800	1.38054400	-0.54412800
N	2.69093200	0.76154400	0.33099500
S	1.39209100	0.78716600	-2.09255400
C	3.76980900	0.00078000	-0.01672000
C	4.26120700	-0.94048900	0.93500200
C	5.38497400	-1.70260800	0.68951000
C	6.08018900	-1.54382200	-0.52217100

C	5.63990100	-0.60530200	-1.47290800
C	4.51008600	0.14845300	-1.22688900
F	-4.80733900	-3.54038100	-1.73535400
C	-3.88720400	-3.71011000	-0.76152800
F	-4.15024000	-4.89479100	-0.16599100
F	-2.67921600	-3.82859600	-1.35964000
N	7.24192300	-2.32963700	-0.78292700
O	7.84080100	-2.18435100	-1.86695400
O	7.62961200	-3.14197800	0.08008700
H	-0.94284600	5.49816800	2.49988700
H	-1.63147000	5.70638800	0.89366300
H	-0.55699100	3.09084700	2.08898800
H	-2.24627400	3.46811200	1.79894900
H	-0.05962700	5.38728300	-1.19644800
H	1.63738700	4.98946500	-0.94197600
H	0.72078200	6.47864100	0.87089700
H	1.27138600	4.95460700	1.53853500
H	-2.78578900	0.65532000	-2.98675400
H	-3.16223400	-1.66299800	-2.29809800
H	-4.38951300	-0.30507400	1.60184100
H	-3.95608100	2.02300600	0.92481300
H	3.73412300	-1.05944500	1.87500300
H	5.73451200	-2.42204200	1.41928900
H	6.19800600	-0.47362300	-2.39169600
H	4.18493500	0.87379800	-1.96037800
C	-3.92521200	-2.56258500	0.29584400
O	-5.16697700	-2.64096800	0.93560700
H	-5.16355500	-3.42178100	1.51259400
O	-2.94794700	-2.85451100	1.27619400
C	-1.56133200	-2.48548400	1.06597800
H	-0.98425600	-3.41326100	0.99855600
H	-1.45266200	-1.95040200	0.12003100
C	-1.09242700	-1.61857100	2.22857400
H	-1.77582300	-0.76975700	2.33204800
H	-1.14359000	-2.18812200	3.16106800
C	0.33049800	-1.10234200	1.99737500
H	0.40156800	-0.57546000	1.04046400
H	1.04058800	-1.93860100	1.93279000
C	0.82665100	-0.18914200	3.10919500
O	1.83216700	0.62982200	2.81459900
O	0.35661400	-0.20607700	4.23995700
H	2.14239000	0.63393200	1.82196700

**Annex V:** XYZ cartesian coordinates of the optimized energies of the two **2-GHB** series (with and without hydrogen bond) with increasing hydroxyacid chain (XYZ cartesian coordinates of 2-GHB-a is present already on previous Annex IV).

#### **2-GHB-a(3C)**

C	2.33343900	5.61463400	-0.55956600
C	1.00453000	5.01377600	-1.03982000
C	0.99338500	3.49537100	-0.83712100
C	1.34642800	3.05403200	0.60022800
C	2.61424400	3.75839100	1.13103100
C	2.56657000	5.27673800	0.91833300
N	1.40156600	1.58749500	0.75819900
O	-0.26541000	2.86173700	-1.24764500

H	0.66664300	1.19632400	1.37242300
C	-1.42745600	3.14486800	-0.63727700
O	-1.62244500	4.11760400	0.07608500
C	-2.45496100	2.08215300	-0.84625300
C	-3.69445500	2.23025600	-0.20875800
C	-4.57566900	1.15861800	-0.12516100
C	-4.23569300	-0.08331400	-0.68546900
C	-3.04825200	-0.19096200	-1.41996900
C	-2.15977400	0.88060700	-1.49767800
C	2.25015500	0.70614200	0.19431600
N	1.95422300	-0.60178100	0.53113200
S	3.50455900	1.11475300	-0.89022000
C	2.73851300	-1.74232500	0.41541000
C	2.05847300	-2.98061500	0.32732800
C	2.75721200	-4.17350200	0.26126000
C	4.15734200	-4.14850600	0.28729300
C	4.85227800	-2.93755200	0.39721700
C	4.15040700	-1.74483600	0.46357600
F	-7.02286700	-0.34257600	0.59197500
C	-6.55253900	-1.20551700	-0.33404500
F	-7.16400600	-2.38473100	-0.11385800
F	-6.95991500	-0.76044500	-1.54759000
N	4.89313600	-5.38676200	0.20996400
O	6.13301000	-5.34453100	0.21303400
O	4.26133900	-6.45239600	0.14376200
H	2.31345300	6.69979400	-0.70895600
H	3.16674700	5.22680900	-1.16123100
H	0.18323300	5.47046200	-0.48451600
H	0.84097000	5.22191000	-2.10338400
H	3.49058600	3.35015900	0.62218500
H	2.71213900	3.51675700	2.19531200
H	3.50511800	5.71932400	1.27081600
H	1.76207300	5.71914700	1.52235600
H	-3.93062000	3.16855200	0.28002300
H	-5.49307300	1.28177600	0.43553200
H	-2.76814900	-1.13457500	-1.87300000
H	-1.21182200	0.75852300	-2.00721800
H	0.97491400	-0.80145200	0.85150800
H	0.97471200	-2.98499900	0.31314400
H	2.23291300	-5.11716200	0.18142000
H	5.93388000	-2.93912400	0.44337100
H	4.68866600	-0.81357800	0.56049500
C	-5.00074800	-1.36456200	-0.31730200
O	-4.72145100	-1.77956300	0.98811800
H	1.70623100	3.03814900	-1.52327600
H	0.51452300	3.35543900	1.24326700
O	-4.70177100	-2.43276500	-1.19200500
C	-3.32262300	-2.00130000	1.33332600
H	-3.32074500	-2.94388500	1.88383100
H	-2.73614500	-2.14823500	0.42757700
C	-2.74924800	-0.85148700	2.17583200
H	-2.83483300	-1.07860300	3.24520200
H	-3.33361400	0.05632000	2.01493600
C	-1.27500000	-0.51664800	1.89223600
H	-4.76783700	-2.14318000	-2.11451100
O	-0.83821100	0.59310900	2.31449300
O	-0.58165400	-1.37002100	1.25875200

## 2-GHB-a(5C)

C	2.06864100	6.11806900	-0.55660500
C	0.77891200	5.34711400	-0.87976900
C	1.03399600	3.84035300	-0.79977800
C	1.59187200	3.40875300	0.57267500
C	2.86166300	4.21478400	0.91742400
C	2.60641300	5.72609700	0.82663900
N	1.75501400	1.95338000	0.71465100
O	-0.12748900	3.02733400	-1.16296300
H	1.15339200	1.53221400	1.45122500
C	-1.23454600	3.01094700	-0.40515700
O	-1.49946100	3.83763100	0.45487200
C	-2.08877500	1.81663300	-0.67570900
C	-3.20840100	1.61286000	0.14183500
C	-3.91556200	0.41853600	0.07842100
C	-3.52660200	-0.59183200	-0.81478000
C	-2.45375500	-0.35568100	-1.68089100
C	-1.73447200	0.83764600	-1.61050900
C	2.51269800	1.10648600	-0.00351200
N	2.27301300	-0.21531400	0.32959000
S	3.59044000	1.56882100	-1.24497700
C	3.03787900	-1.34609800	0.08190700
C	2.36013200	-2.58922700	0.09189300
C	3.04583900	-3.77618000	-0.09541300
C	4.43239900	-3.74157300	-0.29307200
C	5.12829200	-2.52611800	-0.28549500
C	4.43930400	-1.33879000	-0.09789800
F	-6.36162600	-1.22187400	0.02504400
C	-5.71089300	-1.96391400	-0.89471000
F	-6.23076200	-3.20487400	-0.83948600
F	-6.01537300	-1.45432700	-2.11461100
N	5.15369300	-4.97357300	-0.49502500
O	6.37884700	-4.92336500	-0.68500500
O	4.52516200	-6.04319700	-0.47124200
H	1.86900900	7.19442100	-0.59983100
H	2.83089200	5.90670700	-1.31900600
H	-0.00542600	5.63064900	-0.17346000
H	0.42230800	5.59007200	-1.88711300
H	3.66619000	3.93277900	0.23273900
H	3.17960900	3.93582700	1.92815100
H	3.53575500	6.26561800	1.04151500
H	1.88143100	6.02745000	1.59565500
H	-3.48339900	2.37399400	0.86303800
H	-4.73927200	0.25773200	0.76207600
H	-2.12468700	-1.12173000	-2.37318000
H	-0.87106300	0.98489500	-2.24778800
H	1.35522100	-0.42219700	0.79499600
H	1.28847000	-2.60104900	0.25373800
H	2.52086300	-4.72281600	-0.09754300
H	6.20336300	-2.52020800	-0.41294100
H	4.98013100	-0.40422200	-0.08115000
C	-4.16229200	-1.98756800	-0.70378100
O	-3.97775500	-2.52569900	0.56761100
H	1.75000700	3.55560400	-1.57110300
H	0.83570900	3.65644200	1.32296300

O	-3.65585200	-2.89800400	-1.65655600
C	-1.30465600	-0.83879000	3.63914200
C	-0.38405200	-0.25187400	2.56160400
O	0.04390800	0.93068300	2.73056200
O	-0.06249300	-0.98827700	1.57746800
H	-3.77025300	-2.55241000	-2.55432100
C	-2.60317600	-2.82118000	0.95245300
H	-2.33729200	-3.79201400	0.52291900
H	-1.92912200	-2.05921600	0.55849500
C	-2.52915400	-2.86107600	2.47163000
H	-3.32904700	-3.52193800	2.82788700
H	-1.58537900	-3.35204800	2.73696900
C	-2.62798800	-1.49252400	3.18346600
H	-3.18771100	-0.78978300	2.55573300
H	-3.23056800	-1.62214100	4.08986500
H	-1.53392700	-0.03732000	4.34727900
H	-0.71352300	-1.58581100	4.18814000

## 2-GHB-a(6C)

C	2.00070500	6.09820800	-0.59573100
C	0.74875300	5.27470800	-0.93244800
C	1.04302200	3.77686200	-0.80720400
C	1.62979600	3.37965100	0.56379800
C	2.82759400	4.27500000	0.94898500
C	2.49578300	5.76720700	0.81808300
N	1.93131800	1.94104800	0.67228400
O	-0.11075200	2.93107000	-1.12952600
H	1.37947800	1.44263100	1.39558100
C	-1.23427900	2.96988900	-0.39686800
O	-1.48861300	3.82383100	0.44036200
C	-2.13502900	1.80983700	-0.66198900
C	-3.38224700	1.78682200	-0.02121300
C	-4.16875000	0.64290800	-0.05873100
C	-3.71623800	-0.50382600	-0.72877400
C	-2.51033200	-0.45510400	-1.43201500
C	-1.72229200	0.69678900	-1.40292100
C	2.79691900	1.20051800	-0.04486200
N	2.71595900	-0.14373200	0.26906800
S	3.82364100	1.80316600	-1.27004400
C	3.61772200	-1.16818800	0.02505700
C	3.09940700	-2.48643600	0.02191700
C	3.92865900	-3.57792400	-0.16395800
C	5.30237800	-3.37109300	-0.34706000
C	5.84218400	-2.07876800	-0.32510700
C	5.00989800	-0.98708600	-0.13869100
F	-6.63333800	-0.84515400	-0.94078200
C	-5.82522600	-1.86684600	-1.28327300
F	-6.50093000	-3.01057200	-1.04052800
F	-5.62888400	-1.79739700	-2.62640500
N	6.17167300	-4.50240100	-0.55059900
O	7.38211300	-4.29969900	-0.73486500
O	5.68110000	-5.64223700	-0.53439700
H	1.76595400	7.16487200	-0.68205800
H	2.79793000	5.88917600	-1.32211600
H	-0.06057200	5.55481600	-0.25493500
H	0.41048300	5.47757500	-1.95499500

H	3.67754300	4.03256000	0.30603700
H	3.11549000	4.02948400	1.97732400
H	3.38600500	6.35837100	1.06112200
H	1.72241900	6.04634700	1.54732000
H	-3.70273800	2.65329700	0.54593800
H	-5.10386600	0.62002100	0.48698900
H	-2.13944200	-1.33056600	-1.95177100
H	-0.76346600	0.70751400	-1.90700400
H	1.81013900	-0.46705400	0.69914800
H	2.03568600	-2.63137600	0.17224600
H	3.52527200	-4.58235300	-0.17661600
H	6.90944000	-1.93902500	-0.44142800
H	5.43094300	0.00698900	-0.11270100
C	-4.45852500	-1.83360600	-0.52645800
O	-4.68879300	-1.90509900	0.84727100
H	1.75177600	3.48698600	-1.58285600
H	0.84729400	3.54061500	1.31050400
O	-3.71582600	-2.94799100	-0.95141400
C	-0.90259600	-1.35910200	3.32563300
C	0.02125300	-0.56193200	2.39869800
O	0.31374700	0.63670400	2.68665300
O	0.44990200	-1.17075700	1.36570800
H	-3.68945000	-2.99809000	-1.91829300
C	-4.82433700	-3.16810400	1.54505100
H	-5.84215700	-3.54804100	1.40524600
H	-4.11790700	-3.89422500	1.13625600
C	-4.55076700	-2.88598400	3.02000100
H	-5.12717700	-1.99796200	3.30991700
H	-4.96982100	-3.72447800	3.59046800
C	-3.07441500	-2.71483100	3.42482200
H	-3.04789800	-2.53073000	4.50767100
H	-2.54921600	-3.66777100	3.26728300
C	-2.29443100	-1.60199100	2.70707200
H	-2.17284900	-1.86391100	1.65253200
H	-2.86985900	-0.66853200	2.72952200
H	-0.42104800	-2.32760800	3.51130900
H	-1.00036000	-0.84188700	4.28553500

## 2-GHB-a(7C)

C	1.88729700	6.03126100	-0.53960700
C	0.62941300	5.20161300	-0.84291000
C	0.95412300	3.70781000	-0.76659400
C	1.55055400	3.30456800	0.59772600
C	2.78903100	4.16667100	0.92076100
C	2.46511600	5.66495400	0.83434200
N	1.78190600	1.85934700	0.74292400
O	-0.17609700	2.84787900	-1.12063300
H	1.21473700	1.42592600	1.49831000
C	-1.27878600	2.79550800	-0.35926700
O	-1.53328400	3.57657300	0.54586200
C	-2.15406200	1.63505000	-0.69935100
C	-3.29840100	1.43173600	0.08394100
C	-4.06492400	0.28533800	-0.07939500
C	-3.70653300	-0.67507000	-1.03706800
C	-2.59749200	-0.44773600	-1.85539800
C	-1.82086700	0.70020000	-1.68657900



C	2.56878300	1.04523600	0.01703200
N	2.42560300	-0.28015200	0.38276900
S	3.57533200	1.55362900	-1.26647600
C	3.21971400	-1.37980500	0.08694600
C	2.59964100	-2.65040300	0.16782300
C	3.31677800	-3.81009800	-0.06643600
C	4.67873800	-3.72018400	-0.38231500
C	5.32026700	-2.47701900	-0.44393500
C	4.59971000	-1.31676700	-0.20945700
F	-6.64602000	-1.09197900	-0.60350900
C	-5.94681700	-1.83314200	-1.48534400
F	-6.59218700	-3.01262500	-1.61144000
F	-6.02268100	-1.21434700	-2.69156200
N	5.43180500	-4.92334000	-0.63657700
O	6.63280700	-4.82426000	-0.93204800
O	4.85353000	-6.01779300	-0.55101600
H	1.63772000	7.09730900	-0.57916000
H	2.64598400	5.85489700	-1.31435300
H	-0.15636100	5.45029500	-0.12498700
H	0.24746900	5.42712800	-1.84500600
H	3.59424800	3.92042400	0.22299200
H	3.13559800	3.90314800	1.92621700
H	3.37269700	6.24599700	1.03358800
H	1.74037200	5.93387600	1.61550300
H	-3.55264600	2.15738500	0.84798600
H	-4.91494100	0.11797200	0.57008100
H	-2.30027200	-1.18494900	-2.59193800
H	-0.93770900	0.84873600	-2.29612500
H	1.56146200	-0.52406500	0.92775100
H	1.54719100	-2.70529500	0.42106400
H	2.83423600	-4.77770600	-0.01507600
H	6.37948200	-2.42771000	-0.66228600
H	5.09938600	-0.36048100	-0.24858500
C	-4.44716300	-2.01932400	-1.06666400
O	-4.32267300	-2.50505000	0.22590900
H	1.67226400	3.45615700	-1.54701200
H	0.79557200	3.52014200	1.35847600
O	-3.88274700	-2.95146500	-1.96243500
C	-0.74103000	-1.03818800	4.03905600
C	-0.05869800	-0.38880200	2.82867400
O	0.15357100	0.86199500	2.85464100
O	0.28607400	-1.14624200	1.86729800
H	-4.07015600	-2.71194800	-2.88255400
C	-4.88862600	-3.78002700	0.61947900
H	-5.92649400	-3.61017900	0.93027300
H	-4.87798800	-4.47257900	-0.22502300
C	-2.39525600	-2.65147900	2.82530600
H	-1.63956400	-3.42800300	3.01081800
C	-2.19851000	-1.50511900	3.82612800
H	-2.81831900	-0.64848700	3.52717200
H	-2.57703000	-1.82395500	4.80734100
H	-0.71867000	-0.32201800	4.86592800
H	-0.13787500	-1.90672700	4.33283700
C	-3.78864200	-3.29865800	2.91163300
H	-3.88245700	-3.79767300	3.88437000
H	-4.56105200	-2.51800900	2.89522000
C	-4.06057400	-4.31969700	1.78153200

H	-4.60748100	-5.18734700	2.17009700
H	-3.10700200	-4.70182600	1.39645800
H	-2.22015100	-2.29112300	1.80806700

## 2-GHB-a'(3C)

C	-2.21730900	6.34231100	-0.17495700
C	-1.12758300	5.26049300	-0.21251400
C	-1.62555500	3.95140900	0.39580100
C	-2.89070500	3.45254100	-0.31536600
C	-3.98633700	4.53533200	-0.25353500
C	-3.50252400	5.85891500	-0.85951400
N	-3.33743500	2.19472000	0.28550300
O	-0.54341500	2.98377400	0.25383200
H	-3.03970500	2.03612800	1.24505600
C	-0.34568100	2.08028500	1.22732300
O	-1.09735800	1.94405100	2.18547400
C	0.87798000	1.25978200	1.01424500
C	1.13331800	0.20385500	1.89882100
C	2.26801800	-0.58685300	1.73725000
C	3.16802400	-0.32484300	0.69683000
C	2.91235800	0.72990700	-0.18870100
C	1.77413800	1.51735800	-0.03325700
C	-3.99382800	1.20650800	-0.35262600
N	-4.36589100	0.18632600	0.50481700
S	-4.36647300	1.24874400	-2.00388700
C	-4.85232600	-1.09910400	0.25460300
C	-5.58826300	-1.71138400	1.29071300
C	-6.07221800	-3.00138700	1.15120700
C	-5.82133500	-3.69348700	-0.03801400
C	-5.08129600	-3.11170300	-1.07128000
C	-4.59342500	-1.82079700	-0.92617100
F	2.99061500	-3.08230500	0.01489700
C	4.08428200	-2.40926600	-0.40761500
F	5.09265500	-3.30468400	-0.47483500
F	3.83744000	-1.98668900	-1.66561000
N	-6.33140800	-5.04078800	-0.19820200
O	-6.12298300	-5.62872800	-1.26720300
O	-6.95562700	-5.55164000	0.74075800
H	-1.84215100	7.25116500	-0.65707000
H	-2.43546200	6.60579300	0.86879600
H	-0.82326900	5.07284400	-1.24986300
H	-0.23669400	5.58530300	0.33431900
H	-4.27387600	4.68650200	0.79535400
H	-4.86983300	4.16342400	-0.78069200
H	-4.29038100	6.61450200	-0.76894100
H	-3.31704000	5.72285400	-1.93362100
H	0.43806300	0.00704700	2.70695500
H	2.45353100	-1.40809700	2.41980100
H	3.60837500	0.93848400	-0.99162400
H	1.58325900	2.33401000	-0.71888700
H	-4.35682100	0.43083600	1.48867800
H	-5.78543400	-1.16344100	2.20669700
H	-6.64394500	-3.46666400	1.94355400
H	-4.87937200	-3.67356300	-1.97416700
H	-4.01124300	-1.37469500	-1.71834400
C	4.41631700	-1.19832700	0.52713900

O	4.81212500	-1.81532500	1.72588900
H	-1.82153000	4.07650600	1.46515200
H	-2.64727400	3.24340800	-1.36196500
H	4.96575800	-1.12747600	2.39141400
O	5.40380400	-0.38396700	-0.03052700
C	6.74198100	-0.91931200	-0.23484600
H	6.75329700	-1.52118500	-1.14722300
H	7.01193600	-1.55613200	0.60920600
C	7.67871400	0.26923300	-0.35462400
H	7.34718600	0.92402800	-1.16942000
H	7.63356300	0.87097300	0.56068100
C	9.15532600	-0.10690900	-0.61287400
O	9.96306000	0.86278800	-0.69763800
O	9.44376400	-1.33326500	-0.71868300

## 2-GHB-a'

C	2.26312100	6.39593300	0.15170300
C	1.20117600	5.28569900	0.16194600
C	1.74758200	3.99297400	-0.43941100
C	3.00923400	3.52629100	0.29964000
C	4.07795700	4.63637100	0.26422400
C	3.54632000	5.94486900	0.86227200
N	3.50351100	2.28022700	-0.28775200
O	0.69320600	2.99230600	-0.32381700
H	3.26001400	2.12495200	-1.26261200
C	0.54915300	2.08475500	-1.30310400
O	1.31185800	1.99345100	-2.25752800
C	-0.62885200	1.19688400	-1.10061100
C	-0.83942600	0.15622000	-2.01467100
C	-1.92546500	-0.70152300	-1.86281100
C	-2.82033600	-0.52443800	-0.80001300
C	-2.60947000	0.51460400	0.11517000
C	-1.52074300	1.37091300	-0.03265100
C	4.16123500	1.30718100	0.37229100
N	4.59850900	0.30181900	-0.47120300
S	4.46325300	1.35052700	2.03808500
C	5.12630700	-0.96276200	-0.19567700
C	5.95931400	-1.53288500	-1.18028000
C	6.49129300	-2.80072100	-1.01215400
C	6.19035200	-3.51141400	0.15403300
C	5.35394800	-2.97185500	1.13550500
C	4.81868800	-1.70350900	0.96121600
F	-2.48145500	-3.31804800	-0.30445700
C	-3.57898200	-2.71836100	0.20721400
F	-4.54570200	-3.65937900	0.27216300
F	-3.28787600	-2.35319700	1.47345300
N	6.75024200	-4.83521700	0.34460600
O	6.49233700	-5.44077400	1.39263800
O	7.46434800	-5.30861800	-0.54869700
H	1.85363300	7.29287000	0.62820900
H	2.49636200	6.66889400	-0.88634800
H	0.87859200	5.08630300	1.19156700
H	0.31450600	5.58941400	-0.40363400
H	4.38562900	4.79797800	-0.77736300
H	4.95857200	4.28584900	0.81070300

H	4.31507900	6.72180500	0.79007100
H	3.34187300	5.80079300	1.93188400
H	-0.14714200	0.02371700	-2.83822800
H	-2.07605300	-1.50955200	-2.56935000
H	-3.30106000	0.65661000	0.93614400
H	-1.36465200	2.17443300	0.67686100
H	4.62981500	0.54947700	-1.45393500
H	6.19518500	-0.96898700	-2.07719300
H	7.13804800	-3.23387100	-1.76397100
H	5.11593100	-3.54887400	2.01983400
H	4.16293700	-1.28940800	1.71243100
C	-4.01094400	-1.47551800	-0.64014300
O	-4.42085000	-2.03970500	-1.85901100
H	1.96378900	4.12759100	-1.50357400
H	2.74742400	3.30998700	1.34009600
H	-4.61303300	-1.32352200	-2.48350600
O	-5.02035800	-0.75560500	0.00529100
C	-6.31875700	-1.36950000	0.20836000
H	-6.28318800	-1.99031000	1.11061800
H	-6.56042800	-2.00469600	-0.64793400
C	-7.33577700	-0.24941900	0.36224400
H	-7.02416000	0.40624500	1.18430300
H	-7.34226900	0.35334000	-0.55319100
C	-8.74783400	-0.79422700	0.63824700
H	-8.74012200	-1.38194500	1.56263200
H	-9.05113200	-1.45117700	-0.18507800
C	-9.77137100	0.35324400	0.77001500
O	-10.01653600	0.77831200	1.93751100
O	-10.26938600	0.80221100	-0.30439800

## 2-GHB-a'(5C)

C	-2.78638000	6.37357700	-0.18181100
C	-1.70181200	5.28566900	-0.18226800
C	-2.22560500	3.98238200	0.41641400
C	-3.47134600	3.48822600	-0.33180100
C	-4.56300100	4.57613100	-0.30701500
C	-4.05390600	5.89499800	-0.90231400
N	-3.94315200	2.23324300	0.25529600
O	-1.14811100	3.00527400	0.31084800
H	-3.69632700	2.08342100	1.23030700
C	-0.99079800	2.10290700	1.29273600
O	-1.76398100	1.98893100	2.23630200
C	0.21641500	1.25133000	1.10777700
C	0.43120500	0.20052100	2.00901500
C	1.54501900	-0.62358200	1.87256400
C	2.46438700	-0.40098600	0.83975200
C	2.25003500	0.64916800	-0.06197800
C	1.13275800	1.47059700	0.06916200
C	-4.57012300	1.24166900	-0.40728900
N	-4.98002600	0.22436000	0.43572500
S	-4.86774100	1.27733600	-2.07395900
C	-5.46367100	-1.05865800	0.16654000
C	-6.25115400	-1.66260900	1.16892000
C	-6.73802700	-2.94933400	1.01007600
C	-6.43793300	-3.64621600	-0.16479100
C	-5.64641100	-3.07291100	-1.16404500

C	-5.15587800	-1.78531100	-0.99935500
F	2.21608200	-3.17887400	0.23939500
C	3.32074100	-2.54060300	-0.20572600
F	4.31035500	-3.45835400	-0.25552200
F	3.07660400	-2.14376400	-1.47230800
N	-6.95067700	-4.99010600	-0.34540700
O	-6.69613900	-5.58299100	-1.40155500
O	-7.62301800	-5.49295200	0.56414200
H	-2.39181100	7.27828000	-0.65620600
H	-3.03374300	6.64283000	0.85392000
H	-1.36727900	5.09185300	-1.20911700
H	-0.82607500	5.60838400	0.38977200
H	-4.88279000	4.73244300	0.73169500
H	-5.43153000	4.20678200	-0.86035800
H	-4.83952800	6.65550900	-0.83739900
H	-3.83750500	5.75414700	-1.97000700
H	-0.27984300	0.03312400	2.80992500
H	1.69810700	-1.44079600	2.56790600
H	2.96090300	0.82732100	-0.85918200
H	0.97358000	2.28291600	-0.62957900
H	-5.01214200	0.47040400	1.41875000
H	-6.48628800	-1.11082600	2.07355000
H	-7.34919800	-3.40835600	1.77617300
H	-5.40755800	-3.63855900	-2.05548000
H	-4.53491100	-1.34522700	-1.76499700
C	3.68578000	-1.31501900	0.69654300
O	4.06453500	-1.90771600	1.91161900
H	-2.45316600	4.11358600	1.47871300
H	-3.19683900	3.27537600	-1.36975400
H	4.21573200	-1.20765500	2.56495000
O	4.69883700	-0.54697200	0.11420000
C	6.02025000	-1.12011100	-0.05397500
H	6.02796400	-1.74727300	-0.95234100
H	6.25973300	-1.74307400	0.81210300
C	7.00611900	0.02976600	-0.19023100
H	6.70788500	0.66013800	-1.03755300
H	6.95080700	0.65408800	0.71030100
C	8.44314000	-0.46774100	-0.39175400
H	8.48959300	-1.10233100	-1.28648600
H	8.73244500	-1.09859600	0.45907300
C	9.45648100	0.68108900	-0.53505300
H	9.40798100	1.31704100	0.35619600
H	9.18907500	1.29036900	-1.40606100
C	10.89455700	0.15239800	-0.70405700
O	11.28573400	-0.09237100	-1.88436700
O	11.57228400	-0.02624500	0.35193000

## 2-GHB-a'(6C)

C	-2.73245500	6.41633600	-0.07711200
C	-1.70479900	5.27446100	-0.05673500
C	-2.31665600	3.98970900	0.49713400
C	-3.55872100	3.57293000	-0.30159700
C	-4.59277300	4.71622800	-0.29868900
C	-3.99353600	6.01483700	-0.85310900
N	-4.11611200	2.33748000	0.25121900
O	-1.28845300	2.95943600	0.40711500

H	-3.91124700	2.16309700	1.23155600
C	-1.20659300	2.03476900	1.37734000
O	-2.00695700	1.95153500	2.30113500
C	-0.04554900	1.11830500	1.20611900
C	0.11506100	0.07221500	2.12412300
C	1.18552700	-0.80968900	2.00238500
C	2.11384800	-0.65295200	0.96529700
C	1.95157700	0.39018200	0.04490400
C	0.87955800	1.27169200	0.16355800
C	-4.78531700	1.39660200	-0.44318400
N	-5.28498600	0.39648700	0.37165300
S	-5.02777900	1.47294000	-2.11747900
C	-5.85682000	-0.84141700	0.06568100
C	-6.72117400	-1.39631500	1.03226900
C	-7.30021500	-2.63913600	0.83681100
C	-7.01532100	-3.34081000	-0.33895600
C	-6.14935400	-2.81671900	-1.30288400
C	-5.56715600	-1.57316400	-1.10158400
F	1.73372600	-3.44457500	0.47827700
C	2.85400500	-2.86824600	-0.01015200
F	3.80454800	-3.82719700	-0.04613300
F	2.60038800	-2.50560300	-1.28514000
N	-7.62328000	-4.63867400	-0.55769900
O	-7.37786100	-5.23604900	-1.61342900
O	-8.36409500	-5.09934300	0.32044500
H	-2.27475500	7.30739500	-0.51958900
H	-3.00578400	6.68073600	0.95331000
H	-1.34059500	5.08093300	-1.07356800
H	-0.83651900	5.54223100	0.55384900
H	-4.94213800	4.87412100	0.73028400
H	-5.45817000	4.40065200	-0.88901600
H	-4.74072000	6.81443500	-0.80591000
H	-3.74363000	5.87798400	-1.91400100
H	-0.60277700	-0.04497900	2.92792300
H	1.29764000	-1.62026800	2.71322000
H	2.66832100	0.51645300	-0.75680000
H	0.76273800	2.07879400	-0.54938200
H	-5.33104300	0.62926300	1.35752200
H	-6.94336500	-0.83987500	1.93741300
H	-7.97047000	-3.05980300	1.57501400
H	-5.92535500	-3.38669000	-2.19540900
H	-4.88937000	-1.17150700	-1.83978000
C	3.28861600	-1.62852400	0.84019600
O	3.65729900	-2.19228000	2.07229200
H	-2.57351900	4.11275700	1.55368700
H	-3.25863800	3.35966800	-1.33227100
H	3.84004700	-1.47594700	2.69941600
O	4.32735300	-0.93227300	0.21524500
C	5.61926000	-1.56997500	0.05076100
H	5.59103800	-2.21301200	-0.83595300
H	5.83548800	-2.18727500	0.92678900
C	6.65499600	-0.46905500	-0.11387900
H	6.36668700	0.16897600	-0.95890400
H	6.64689000	0.16318700	0.78282700
C	8.06426200	-1.02982300	-0.34421600
H	8.06417300	-1.66583200	-1.24036500
H	8.34209000	-1.67971100	0.49733400

C	9.12255000	0.06834100	-0.50314500
H	9.12370100	0.70117100	0.39419700
H	8.84627000	0.71694700	-1.34537800
C	10.54011500	-0.48398300	-0.73294500
H	10.54652000	-1.09566900	-1.64237300
H	10.81705100	-1.12463500	0.11254600
C	11.57638200	0.64814900	-0.87044400
O	12.08378100	1.09863200	0.20031700
O	11.82526600	1.06896900	-2.04005200

## 2-GHB-a'(7C)

C	-3.35852700	6.41936700	-0.17179700
C	-2.28601400	5.32076500	-0.11594500
C	-2.85543100	4.02246300	0.45082600
C	-4.06334400	3.54266400	-0.36564700
C	-5.14430500	4.64065100	-0.39898500
C	-4.58984900	5.95565100	-0.96158000
N	-4.57876500	2.29096100	0.19030900
O	-1.78773600	3.03119600	0.40073200
H	-4.41384800	2.14983200	1.18336300
C	-1.69412100	2.12726000	1.38959800
O	-2.50470200	2.03868300	2.30369800
C	-0.50687900	1.23919400	1.25096500
C	-0.33540000	0.21112200	2.18713500
C	0.75532700	-0.64895900	2.09272500
C	1.69366900	-0.48760100	1.06551200
C	1.52221200	0.53925700	0.12853100
C	0.42944800	1.39837600	0.21934800
C	-5.16415400	1.30068500	-0.51173000
N	-5.63942800	0.28867100	0.30210900
S	-5.34110500	1.33284400	-2.19578300
C	-6.13121800	-0.98448900	0.00144300
C	-6.99443000	-1.56962400	0.95122100
C	-7.49768600	-2.84583000	0.76171700
C	-7.13734000	-3.55093600	-0.39107100
C	-6.27092100	-2.99654400	-1.33739600
C	-5.76449400	-1.71929500	-1.14196900
F	1.36530200	-3.28280300	0.58582500
C	2.48708500	-2.69441600	0.11568700
F	3.45074200	-3.64068800	0.10473800
F	2.25384400	-2.34335800	-1.16644500
N	-7.66660400	-4.88384200	-0.60394000
O	-7.35608400	-5.48455100	-1.64043300
O	-8.40850100	-5.36954600	0.25965600
H	-2.92982300	7.32125900	-0.62133600
H	-3.65940700	6.68864700	0.84963300
H	-1.89776300	5.12513100	-1.12342700
H	-1.43958200	5.63423500	0.50348200
H	-5.52082600	4.79787300	0.62042600
H	-5.98388400	4.28066500	-1.00124300
H	-5.36979200	6.72433500	-0.93736100
H	-4.31701900	5.81488500	-2.01629500
H	-1.06192700	0.08954200	2.98243100
H	0.87449600	-1.44711100	2.81637100
H	2.24702000	0.66956800	-0.66530400
H	0.30439900	2.19176000	-0.50750400

H	-5.73198300	0.53457000	1.28125300
H	-7.27569700	-1.01094400	1.83842100
H	-8.16692000	-3.29031500	1.48675000
H	-5.98754200	-3.56857900	-2.21154500
H	-5.08686300	-1.29328500	-1.86646100
C	2.88718000	-1.44315400	0.96639400
O	3.24457700	-1.99426000	2.20743800
H	-3.13899200	4.15491800	1.49937300
H	-3.73402500	3.32877600	-1.38700000
H	3.40801700	-1.27170600	2.83274400
O	3.92457100	-0.73224400	0.35555400
C	5.22736300	-1.35247000	0.21206400
H	5.21734800	-2.00870800	-0.66527200
H	5.44445100	-1.95378600	1.09902100
C	6.24919400	-0.23971300	0.04044200
H	5.96259000	0.37933100	-0.81919000
H	6.22206300	0.40798700	0.92566700
C	7.66786300	-0.78646300	-0.16337200
H	7.68348100	-1.44475400	-1.04316000
H	7.94504400	-1.41243400	0.69634400
C	8.71636500	0.31823300	-0.34153800
H	8.69823400	0.97963600	0.53628800
H	8.44165200	0.94240300	-1.20376200
C	10.13761400	-0.22094000	-0.54050500
H	10.15644500	-0.87952300	-1.41871500
H	10.41185700	-0.84201900	0.32366100
C	11.18898500	0.88799900	-0.72087500
H	10.92248000	1.49290700	-1.59623500
H	11.18319300	1.54137300	0.15875300
C	12.60356400	0.31106200	-0.92156300
O	12.89390100	-0.10644600	-2.08288900
O	13.36708000	0.26882500	0.08976500