

Electronic Supporting Information to:

**Derivatives of Cysteine Related to the Thiosulfate Metabolism of Sulfur Bacteria by the Multi-Enzyme Complex “Sox” – Studied by DFT-PCM and G3X(MP2) Calculations  
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Color code in all Figures of the online version: carbon gray, nitrogen green, oxygen blue, hydrogen red.

**Table S1a.** Negative absolute energies  $E$  enthalpies  $H$  and Gibbs energies  $G$  (all in Hartree) of various derivatives of cysteine as well as of some related molecules both in the gas phase (first line each) and in a polarizable continuum (PCM, second line). The dipole moments  $\mu$  calculated at the B3LYP/6-31G(2df,p) level are given in Debye. Global minimum data of isomeric species are shown in bold numbers. PCM calculations are with geometry optimization. The first dipole moment applies to the gas phase, the second to the polarizable continuum. In some cases, the energy difference (in  $\text{kJ mol}^{-1}$ ) to the global minimum structure is given in parentheses.

Species	$E_e$ B3LYP/6- 31G(2df,p)	$E_{298}$ (G3X/MP2)	$H_{298}$ (G3X/MP2)	$G_{298}^\circ$ (G3X/MP2)	$\mu$ B3LYP/6- 31G(2df,p)
SO <sub>2</sub>	548.62589 548.63254 PCM	548.05232	548.04829	548.07649	2.10 2.07
H <sub>2</sub> O	76.42608 76.43675 PCM	76.34357	76.33979	76.36122	1.85 2.18
SO <sub>2</sub> ·4H <sub>2</sub> O	854.39432		853.43729	853.49380	
[HSO <sub>3</sub> ] <sup>−</sup> (C <sub>3v</sub> )	<b>624.50447</b> <b>624.60975</b> PCM	<b>623.87680</b>	<b>623.87230</b>	<b>623.90324</b>	2.16 2.71
[SO <sub>3</sub> H] <sup>−</sup> (C <sub>1</sub> )	624.49972 624.60712 PCM	623.86938	623.8639 (+21.8)	623.89648 (+17.7)	1.24 2.33
[H–SO <sub>3</sub> ·H <sub>2</sub> O] <sup>−</sup>	700.95916 701.05381 PCM	<b>700.24148</b>	<b>700.23390</b>	<b>700.27278</b>	-
[HO–SO <sub>2</sub> ·H <sub>2</sub> O] <sup>−</sup>	<b>700.96355</b> <b>701.05703</b> PCM	700.23408	700.22674 (+18.8)	700.26398 (+23.1)	-

[HSO <sub>4</sub> ] <sup>-</sup>	699.75417 699.86384 PCM				
<b>Cysteine derivatives:</b>					
Cysteine <b>1a</b> <b>1a'</b>	<b>721.96642</b> <b>721.98616</b> PCM	<b>721.05883</b>	<b>721.04999</b>	<b>721.09148</b>	4.28 5.68
Cysteine <b>1a</b> <b>1b</b>	721.96386 721.97970 PCM (+17.0)	see <b>1c</b>			3.85 10.29
Cysteine <b>1c</b> <b>1c'</b>	721.96386 721.9858 PCM	721.05640	721.04742 (+6.7)	721.08928 (+5.8)	3.85 5.08
Cysteine <b>1d</b> <b>1d'</b>	721.96318 721.98380 PCM	721.05391	721.04503 (+13.0)	721.08654	4.92 6.59
Cys <sup>-</sup> <b>2a</b> <b>2a'</b>	<b>721.41214</b> 721.50583 PCM	<b>720.52937</b>	<b>720.52117</b>	<b>720.56135</b>	-
Cys <sup>-</sup> <b>2b</b> <b>2b'</b>	721.41002 721.50465 PCM	720.52708	720.51884 (+6.1)	720.55894	-
Cys <sup>-</sup> <b>2c</b> <b>2c'</b>	721.40109 <b>721.50716</b> PCM	720.51663	720.50852	720.54875	-
Cys <sup>-</sup> <b>2d</b> <b>2d'</b>	721.39661 721.49811 PCM	720.51956	720.51102 (+26.6)	720.55207	-
Cys <sup>-</sup> <b>2e</b> <b>2e'</b>	721.39460 721.50574 PCM (+3.7)	720.51189	720.50378 (+45.7)	720.54392	-
CysSH <b>3a</b> <b>3a'</b>	<b>1120.16268</b> <b>1120.18440</b> PCM	<b>1118.79002</b>	<b>1118.77957</b>	<b>1118.82552</b>	4.54 6.58
CysSH <b>3b</b> <b>3b'</b>	1120.16212 1120.18510 PCM	1118.78883	1118.77814 (+3.8)	1118.82522	4.21 6.08
CysS <sup>-</sup> <b>4</b>	<b>1119.61537</b> <b>1119.71760</b> PCM	1118.26579	1118.28520	1118.32940	-
CysSO <sub>3</sub> <sup>-</sup> <b>5a</b> <b>5a'</b>	1345.31191 1345.40460 PCM				-

CysSO <sub>3</sub> <sup>-</sup> <b>5b</b>	1345.30480 (+18.7)				-
<b>5b'</b>	1345.40264 PCM (+5.1)				
CysSSO <sub>3</sub> <sup>-</sup> <b>6</b>	1743.51917				-
<b>6'</b>	1743.61498 PCM				
CysSO <sub>2</sub> H <b>7a</b>	<b>1270.59867</b>	<b>1269.10895</b>	<b>1269.09694</b>	<b>1269.14711</b>	4.22
<b>7a'</b>	1270.63361 PCM				
<b>7a''</b>	1270.63353 PCM				
CysSO <sub>2</sub> H <b>7b</b>	1270.59362	1269.10469	1269.09210	1269.14355	4.71
<b>7b'</b>	1270.62105 PCM		(+12.7)		6.98
CysSO <sub>2</sub> H <b>7c</b>	1270.59278	1269.10258	1269.09047	1269.14083	2.77
<b>7c'</b>	<b>1270.63690</b> PCM		(+17.0)		
CysSO <sub>2</sub> <sup>-</sup> <b>8</b>	1270.07725	1268.61631	1268.60467	1268.65325	-
<b>8'</b>	1270.16837 PCM				
CysSSO <sub>2</sub> <sup>-</sup> <b>9a</b>	<b>1668.28941</b>	<b>1666.39254</b>	<b>1666.37908</b>	<b>1666.43254</b>	-
<b>9a'</b>	<b>1668.37648</b> PCM				
CysSSO <sub>2</sub> <sup>-</sup> <b>9b</b>	1668.28886	1666.39036	1666.37678	1666.43110	-
<b>9b'</b>	1668.37493 PCM (+4.1)		(+6.0)		
<b>RSH =</b> <b>C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>SH</b>					
RSH <b>10a</b>	815.43944	<b>814.39017</b>	<b>814.37853</b>	<b>814.42743</b>	5.29
<b>10a'</b>	815.47061 PCM				5.89
RSH <b>10b</b>	<b>815.43948</b>	814.38964	814.37820	814.42646	2.70
<b>10b'</b>	<b>815.47062</b> PCM		(+0.9)		5.11
RS <sup>-</sup> <b>11</b>	814.89495	813.86801	813.85767	813.90328	-
<b>11'</b>	814.99242 PCM				-
RSS <sup>-</sup> <b>12</b>	1213.10637				-
<b>12'</b>	1213.20151 PCM				-
RSSO <sub>2</sub> H <b>13a</b>	<b>1364.06740</b>	<b>1362.43928</b>	<b>1362.42414</b>	<b>1362.48154</b>	7.32
<b>13a'</b>	<b>1364.10500</b> PCM				10.60
RSSO <sub>2</sub> H <b>13b</b>	1364.06715	1362.43568	1362.42127	1362.47673	4.51

<b>13b'</b>	1364.09509 PCM		(+7.5)		6.07
RSSO <sub>2</sub> <sup>-</sup> <b>14</b>	1363.56653	1361.96380	1361.94944	1362.00530	-
<b>14'</b>	1363.65323 PCM				
RSSO <sub>2</sub> <sup>-</sup> ·2H <sub>2</sub> O <b>15</b>	1516.47143	1514.68239	1514.66319	1514.72993	-
<b>15'</b>	1516.55598 PCM				
RSSO <sub>3</sub> <sup>-</sup> <b>16</b>	1438.80231	1437.13622	1437.12152	1437.17804	-
<b>16'</b>	1438.89302 PCM				
RSSSO <sub>3</sub> <sup>-</sup> <b>17</b>	1837.00810				-
<b>17'</b>	1837.09645 PCM				
RSSO <sub>3</sub> <sup>-</sup> ·2H <sub>2</sub> O <b>18</b>	1591.70648	1589.85622	1589.83616	1589.90509	-
<b>18'</b>	1591.79532 PCM				

**Table S1b.** Negative absolute enthalpies  $H$  and Gibbs energies  $G$  (in Hartree) of molecules and ions related to the species in Table S1a, calculated by the polarizable continuum model (PCM) at the B3LYP/6-31G(2df,p) level of theory with geometry optimization at 298.15 K, 1.013 bar and  $\epsilon = 78.0$ . Global minimum data of isomeric species are shown in bold numbers (RSH = C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>SH).

Species	$H_{298}$	$G_{298}$
H <sub>2</sub> O	76.41254	76.43464
SO <sub>2</sub>	548.62164	548.65051
[HSO <sub>3</sub> ] <sup>-</sup>	<b>624.58321</b>	624.61419
[SO <sub>3</sub> H] <sup>-</sup>	624.58167	<b>624.61482</b>
[HSO <sub>3</sub> ] <sup>-</sup> ·H <sub>2</sub> O	701.00022	701.04121
[SO <sub>3</sub> H] <sup>-</sup> ·H <sub>2</sub> O	<b>701.00317</b>	<b>701.04147</b>
[SO <sub>4</sub> H] <sup>-</sup>	699.83192	699.86578
Cysteine <b>1a'</b>	<b>721.87109</b>	721.91303
Cysteine <b>1b'</b>	721.84406	721.90659
Cysteine <b>1c'</b>	721.87083	<b>721.91329</b>
Cysteine <b>1d'</b>	721.86854	721.91065
Cysteinate <b>2a'</b>	721.40038	721.44086
Cysteinate <b>2b'</b>	721.39935	721.43993
Cysteinate <b>2c'</b>	<b>721.40114</b>	<b>721.44167</b>
Cysteinate <b>2d'</b>	721.39564	721.43750

Cysteinate <b>2e'</b>	721.39891	721.43981
CysSH <b>3a'</b>	1120.06635	1120.11355
CysSH <b>3b'</b>	<b>1120.06706</b>	<b>1120.11408</b>
CysS <sup>-</sup> <b>4</b>	1119.60745	1119.65233
CysSO <sub>3</sub> <sup>-</sup> <b>5a'</b>	<b>1345.27851</b>	<b>1345.33011</b>
CysSO <sub>3</sub> <sup>-</sup> <b>5b'</b>	1345.27637	1345.32788
CysSSO <sub>3</sub> <sup>-</sup> <b>6</b>	1743.48772	1743.54365
CysSO <sub>2</sub> H <b>7a'</b>	1270.50377	1270.55541
CysSO <sub>2</sub> H <b>7a''</b>	1270.50383	1270.55552
CysSO <sub>2</sub> H <b>7b'</b>	1270.49127	1270.54274
CysSO <sub>2</sub> H <b>7c'</b>	<b>1270.50751</b>	<b>1270.55902</b>
CysSO <sub>2</sub> <sup>-</sup> <b>8'</b>	1270.04854	1270.09908
CysSSO <sub>2</sub> <sup>-</sup> <b>9a'</b>	1668.25309	<b>1668.30856</b>
CysSSO <sub>2</sub> <sup>-</sup> <b>9b'</b>	<b>1668.25351</b>	1668.30830
RSH <b>10a'</b>	815.33196	<b>815.38164</b>
RSH <b>10b'</b>	<b>815.33200</b>	815.38129
RS <sup>-</sup> <b>11</b>	814.86297	814.91059
RSS <sup>-</sup> <b>12</b>	1213.06829	1213.12050
RSSO <sub>2</sub> H <b>13a'</b>	<b>1363.95163</b>	<b>1364.00923</b>
RSSO <sub>2</sub> H <b>13b'</b>	1363.94082	1363.99745
RSSO <sub>2</sub> <sup>-</sup> <b>14'</b>	1363.51004	1363.56640
RSSO <sub>2</sub> <sup>-</sup> ·2H <sub>2</sub> O <b>15'</b>	1516.35740	1516.42564
RSSO <sub>3</sub> <sup>-</sup> <b>16'</b>	1438.74404	1438.80161
RSSSO <sub>3</sub> <sup>-</sup> <b>17'</b>	1836.94417	1837.00677
RSSO <sub>3</sub> <sup>-</sup> ·2H <sub>2</sub> O <b>18'</b>	1591.59088	1591.66069

**Table S2.** Harmonic vibrational frequencies of the most stable isomer of the cysteinate anion **2a** in the gas phase (region: 750–2900 cm<sup>-1</sup>,  $\nu$  stretching,  $\delta$  bending,  $\tau$  torsion vibration; wavenumbers in cm<sup>-1</sup> scaled by 0.9854; relative IR intensities in italics).

wavenumber/intensity	assignment
771 / 0.2	$\nu_{CC} + \delta_{OCO} + \tau$
832 / 0	$\nu_{CC} + \delta_{OCO}$

859 / 1.8	$\nu_{\text{CS}} + \delta_{\text{CCC}} + \nu_{\text{CO}}$
925 / 3.9	$\tau_{\text{HOCC}}$
950 / 3.8	$\nu_{\text{CC}} + \delta$
962 / 5.6	$\nu_{\text{CN}} + \delta$
1093 / 2.6	$\nu_{\text{CN}} + \nu_{\text{CC}}$
1129 / 0.2	$\delta_{\text{HCC}} + \delta_{\text{HNC}}$
1167 / 0.4	$\nu_{\text{CN}} + \delta_{\text{HCC}}$
1263 / 1	$\delta_{\text{H}_2\text{CCH}}$
1295 / 4.5	$\delta_{\text{HCC}}$
1318 / 0.4	$\delta_{\text{HCC}} + \delta_{\text{HCN}}$
1375 / 1	$\delta_{\text{HCN}}$
1445 / 0	$\delta_{\text{HCH}}$
1488 / 9.2	$\delta_{\text{COH}} + \nu_{\text{CO}}$
1607 / 2.6	$\delta_{\text{HNNH}}$
1761 / 32.9	$\nu_{\text{CO}} + \delta_{\text{COH}}$
2540 / 100	$\nu_{\text{OH}}$

**Table S3.** Torsion angles of the isomeric RSH molecules both in the gas phase (**10a,b**) and in the polarizable continuum (**10a',b'**), calculated by the B3LYP/6-31G(2df,p) method (RSH = C<sub>4</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>SH).

torsion axis	<b>10a</b>	<b>10b</b>	<b>10a'</b>	<b>10b'</b>
HSCC	80.6°	65.7°	76.9°	77.1°
SCCC	-69.7°	-75.5°	-66.6°	-66.8°
SCCN	171.7°	148.1°	174.4°	174.0°
CCCN	88.8°	-163.8°	119.9°	134.0°
CCNC	-92.8°/146.3°	-99.2°/135.2°	-110.5°/129.0°	-112.2°/126.7°
CNCO	-178.2°	170.5°	179.4°	179.3°
NCCN	-150.7°	-37.6°	-119.8°	-105.2°

**Table S4.** Torsion angles of the S-sulfinic and S-sulfonic species **13a,b**, **13a',b'**, **14**, **14'** and **15**, calculated at the B3LYP/6-31G(2df,p) level.

torsion	<b>13a</b>	<b>13a'</b>	<b>13b</b>	<b>13b'</b>	<b>14</b>	<b>14'</b>	<b>15</b>	<b>15'</b>
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axis								
SSCC	86.2°	86.5°	70.8°	70.4°	88.0°	88.2°	88.5°	93.4°
SCCC	-153.3°	-155.9°	-125.2°	-126.8°	-144.9°	-149.9°	-172.5°	-176.0°
SCCN	86.3°	81.5°	114.9°	112.4°	95.0°	87.5°	69.0°	64.2°
NCCN	-162.8°	-161.9°	-159.0°	-152.6°	-158.6°	-158.7°	-147.8°	-144.7°
NCCC	74.2°	74.5°	78.3°	85.0°	77.6°	77.3°	89.8°	92.8°

**Table S5.** Torsion angles of the S-sulfonic anions **16**, **16'**, **17**, **17'**, **18** and **18'**, calculated at the B3LYP/6-31G(2df,p) level.

torsion axis	<b>16</b>	<b>16'</b>	<b>17</b>	<b>17'</b>	<b>18</b>	<b>18'</b>
SSSC	–	–	-79.9°	-81.1°	–	–
SSSO(··H)	–	–	58.1°	59.5°	–	–
SSCC	82.3°	83.6°	99.3°	100.8°	82.7°	84.3°
SCCC	-137.9°	-144.9°	-151.6°	-155.0°	-173.2°	-178.3°
SCCN	102.2°	92.5°	88.8°	82.9°	68.3°	61.8°
NCCN	-159.9°	-159.3°	-157.4°	-154.4°	-152.0°	-148.4°
NCCC	76.6°	76.6°	80.0°	82.6°	86.0°	89.4°

**Atomic coordinates (Å) of all cysteine derivatives and related ions calculated in this work:**

**[HSO<sub>3</sub>]<sup>-</sup>H<sub>2</sub>O (PCM)**

S 0.7142036012 0.0023155707 0.2442614683  
O -0.2048064421 -1.1447524386 0.1158522108  
O 1.9431262817 -0.1551274579 -0.5343223272  
O 0.0508417296 1.2963507103 0.0671153508  
H 1.1112765159 -0.0219085096 1.5598372634  
H -2.5756841286 0.8634968494 -0.253067834  
O -2.8195144098 -0.07102465 -0.2045438142  
H -1.9488402046 -0.4979832839 -0.115406422

**[SO<sub>3</sub>H]<sup>-</sup>H<sub>2</sub>O (PCM)**

S -0.0319725596 -0.0688015873 0.9752434501  
O 1.4213225532 0.0993673348 0.1321830323  
H 1.1700020259 0.11067028 -0.8186322584  
O -0.7264702617 1.2314113104 0.7596975485  
O -0.7248754726 -1.1578909726 0.1872172642  
O -0.0153914327 -0.2520229102 -2.2797206825  
H -0.4894781319 0.5915681172 -2.3642500647

H -0.4596337207 -0.6852715724 -1.5143512895

**1a**

C 0.6722302876 -0.3135571994 0.4498374604  
H 0.9066215541 -1.3725198559 0.2716779548  
N 1.6254543713 0.1847968099 1.4451419136  
H 0.1996408371 -0.2171093744 2.6517219158  
H 2.5590595885 -0.1725003513 1.2769552467  
H 1.6673893469 1.2012333322 1.3899448824  
C -0.745945814 -0.3169818618 1.0650938811  
O -1.7499009605 -0.3462339073 0.401770405  
O -0.7456670315 -0.3141407195 2.3998871043  
C 0.6712921239 0.3927268682 -0.9131126559  
H -0.0911191079 -0.0466070533 -1.5561768431  
H 1.6450023253 0.2797864207 -1.3965455824  
S 0.3931942494 2.2040702715 -0.8117811893  
H -0.9094597701 2.1276296204 -0.4782634935

**1a'**

C 0.6671918179 -0.3095707607 0.447842186  
H 0.9065793153 -1.3661111304 0.2435575916  
N 1.6157431297 0.169644734 1.4512449127  
H 0.218409232 -0.1487256889 2.6385020189  
H 2.5367172096 -0.2454899122 1.3168054527  
H 1.719505078 1.1834865867 1.3964108833  
C -0.7407201961 -0.3482318052 1.0697655008  
O -1.7602233456 -0.4691779359 0.4276028012  
O -0.7374630764 -0.2742217477 2.3978387473  
C 0.6654554361 0.4100919781 -0.9081686682  
H -0.0850106659 -0.0314096255 -1.5653020797  
H 1.6460178256 0.3013987113 -1.3791086227  
S 0.3874030528 2.2243072541 -0.8221852556  
H -0.9418128131 2.1946023423 -0.5186544683

**1b**

C 0.1318666824 0.4082605309 -0.2221259969  
H -0.0818291383 1.4768308648 -0.110411337  
N 1.6234093317 0.2388319534 -0.1526609886  
H 2.1207273641 1.0943114711 0.1185547492  
H 1.9238500793 -0.5156517953 0.4766640319  
C -0.2686967908 -0.0298966626 -1.6804345498  
O -1.4793188612 -0.0446078589 -1.935451899  
O 0.7142407148 -0.3071041258 -2.420427285  
C -0.6089717056 -0.3931566537 0.8372891877  
H -0.3503494885 -1.4562959244 0.7717845346  
H -1.6768767326 -0.297683776 0.6412362904  
S -0.2371174374 0.0741009151 2.5738571218  
H -0.6922268749 1.3605094778 2.5089932146  
H 1.8267698568 -0.0247164164 -1.1606130738



**1c**

C -0.4101421029 0.5467379552 -0.0931450866  
H 0.1067861242 -0.3055531492 0.3652881145  
N -0.3372840287 0.5600610788 -1.5566011825  
H 0.1321906423 2.3818262406 -1.2867331658  
H 0.5191280824 0.1219260777 -1.8793977163  
H -1.1094679288 0.0270811974 -1.9485387255  
C 0.2532723279 1.8226261799 0.4744207219  
O 0.5337513581 1.9449135474 1.6364758383  
O 0.4391852272 2.7797277138 -0.4406756347  
C -1.8683560159 0.5474928643 0.3932963627  
H -2.4002144171 1.409420868 -0.0216002315  
H -1.8852412481 0.6311173464 1.4798184661  
S -2.857939871 -0.8989429287 -0.1450444506  
H -2.1501071495 -1.8346609914 0.51727969

**1c'**

C -0.4777702247 0.6265689009 -0.1256225424  
H 0.1521522401 -0.1844290068 0.2697914706  
N -0.3162124208 0.6506904804 -1.579590078  
H 0.8158331047 2.0603299494 -1.2506401479  
H -0.1669216004 -0.2856011497 -1.951118685  
H -1.1470364696 1.0308362654 -2.0372672421  
C 0.1343334438 1.9176517992 0.459880961  
O -0.0258822101 2.2871024927 1.6018245737  
O 0.8951086422 2.5809350225 -0.4060932744  
C -1.9069974065 0.4362814987 0.3989340897  
H -2.5741764818 1.1833360215 -0.0455553325  
H -1.9272316299 0.5719515258 1.4808483237  
S -2.6592357888 -1.178186392 -0.0343169622  
H -1.8304021982 -1.9636934077 0.713767846

**1d**

C 0.134686049 0.3171883697 -0.3631705031  
H -0.2482467062 1.3399581895 -0.4633576788  
N 1.5856889145 0.4201278974 -0.1271861538  
H 1.6627779817 0.2010131383 -2.0252134839  
H 1.7965615036 1.1632959778 0.5296600236  
H 1.9486756979 -0.4430223938 0.2689692907  
C -0.0849078372 -0.3489089942 -1.7407988827  
O -1.0990853851 -0.9129117389 -2.0623954435  
O 0.9592653146 -0.220726016 -2.5647497151  
C -0.6491885795 -0.3883343305 0.7555768834  
H -0.299357587 -0.0135072771 1.7214537693  
H -0.4683995057 -1.4667440532 0.7289799844  
S -2.4526775215 -0.0686409182 0.7609533479  
H -2.6650763392 -0.5725438508 -0.4692914385

**1d'**

C 0.1407971722 0.3238979421 -0.3763900494  
H -0.2390868724 1.3514830375 -0.4768062976

N 1.5848811418 0.415594003 -0.1329023129  
 H 1.7034818481 0.1761075002 -1.9896305739  
 H 1.7969126425 1.1779699806 0.5102703975  
 H 1.9423427973 -0.4463597336 0.2854024968  
 C -0.067127909 -0.3257206318 -1.7557409333  
 O -1.091926604 -0.8581856089 -2.1200044744  
 O 0.9950632821 -0.2287606539 -2.5533453096  
 C -0.6469687798 -0.3855525282 0.7379936491  
 H -0.2873105367 -0.0140216367 1.7016850597  
 H -0.477576571 -1.4655881851 0.7103053382  
 S -2.4513572194 -0.0545485825 0.7861798827  
 H -2.7814083919 -0.6600709028 -0.377586873

**2a**

C 0.8559099213 0.3716588043 -0.4990257186  
 H 1.5176927985 1.0549386556 -1.0484604518  
 N 1.5847092651 -0.8935251938 -0.2809426165  
 H 1.0505031418 -1.3950030811 0.4337797238  
 H 1.5492123737 -1.450254723 -1.1312938484  
 C -0.3540430457 0.1656828046 -1.4345687905  
 O -1.4698645871 -0.2989814383 -0.8873453674  
 O -0.2643866313 0.3623515306 -2.6331217968  
 C 0.5059901836 0.9929682874 0.8667667997  
 H 0.031397553 1.9667900968 0.6917093369  
 H 1.45298798 1.1820144438 1.3861374182  
 S -0.5772533113 -0.0685724296 1.9185248524  
 H -1.3519256415 -0.3430907572 0.1357524591

**2a'**

C 0.8473315769 0.355987419 -0.4778687478  
 H 1.5178433637 1.0287341636 -1.0289818778  
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 H 0.9721065761 -1.5304546961 0.2862564256  
 H 1.7304489647 -1.3691558294 -1.1574678135  
 C -0.360335232 0.1519720345 -1.4082460433  
 O -1.4749156647 -0.3321724171 -0.862664394  
 O -0.2977339232 0.3548686015 -2.607097073  
 C 0.5075035254 1.0200472339 0.8659416518  
 H 0.0666646647 2.0030328761 0.6694194339  
 H 1.4531646891 1.1820388038 1.3916492704  
 S -0.6305282768 0.0463618009 1.9604438624  
 H -1.3690676138 -0.3563367148 0.1473364757

**2b**

C 0.636682971 0.7114015281 -0.4567045758  
 H 1.1022890775 1.5377488259 -1.0070750635  
 N 1.6431428123 -0.3642716777 -0.3278651471  
 H 2.4545200361 0.0496337865 0.1310675403  
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 O -1.3527993584 -0.6381588245 -0.8420550146

O -0.5711605414 0.5580162598 -2.5451085612  
C 0.1080817558 1.2238815756 0.9066652372  
H -0.6535856328 1.9957149404 0.7270482392  
H 0.946181836 1.723327573 1.4137257185  
S -0.5643447657 -0.1146665804 1.9798089107  
H -1.2021767602 -0.6723517381 0.1709639646

**2b'**

C 0.6265359447 0.71623952 -0.4392677735  
H 1.0749595383 1.559020921 -0.9797060558  
N 1.6489482431 -0.3405212852 -0.3474860919  
H 2.4837609853 0.0675129816 0.0780128407  
H 1.3162763973 -1.0340689204 0.3259952311  
C -0.4777067188 0.1948692682 -1.3701376108  
O -1.3461859746 -0.6627055128 -0.8384101978  
O -0.5541697011 0.5075061167 -2.5420989955  
C 0.1017283244 1.2377776074 0.9168795369  
H -0.611481749 2.0514407647 0.7383337826  
H 0.9566757392 1.6702560124 1.4479620642  
S -0.680554964 -0.0538536693 1.9906066996  
H -1.2224310647 -0.6832498042 0.1701095701

**2c**

C 0.5947098507 0.7067557713 -0.3844671111  
H 0.8845388969 1.6893318452 -0.7864145447  
N 1.740624411 -0.217893193 -0.4945198993  
H 0.8145115243 -0.9631665958 -1.7696081696  
H 2.6132938843 0.2966133658 -0.4316458844  
H 1.6531238679 -0.7931693432 0.3723368059  
C -0.5108019007 0.2138508325 -1.3406816914  
O -1.5984761306 0.729434758 -1.4460038124  
O -0.1136533906 -0.810642093 -2.1072865171  
C 0.0853488845 0.8836274857 1.0747479277  
H -0.9433144068 1.2528249169 1.0089431367  
H 0.68322168 1.6830018145 1.5381278503  
S 0.1982758291 -0.6563065651 2.0592069094

**2c'**

C 0.5919048544 0.7062318784 -0.3731568537  
H 0.8405982086 1.6920782873 -0.7965534637  
N 1.7696494334 -0.163688455 -0.501753233  
H 0.862060696 -0.9502955595 -1.7904101904  
H 2.6309394242 0.3796831618 -0.5133708359  
H 1.7913084625 -0.78257678 0.3124522615  
C -0.5136824536 0.1503767483 -1.2884858483  
O -1.6445487902 0.5859754497 -1.3400039804  
O -0.0947071527 -0.8428306609 -2.0704596609  
C 0.0841252855 0.9073947942 1.0643021658  
H -0.8484160358 1.4760151286 1.0085057922  
H 0.8140654165 1.5256560196 1.5979087897  
S -0.1818943488 -0.6697570125 1.9837600571

**2d**

C -0.3349218211 0.3883698968 0.7536237936  
H -0.7558122604 0.4313162844 1.7723297298  
N -0.0980044128 1.7318783572 0.2179607022  
H -0.894772484 1.847661685 -0.4221768737  
H -0.1612055226 2.4371023141 0.9445112453  
C -1.4522396836 -0.3434733958 -0.1105216666  
O -1.5812920703 -1.5605822967 0.1133334649  
O -2.0968359682 0.4155363376 -0.8728758457  
C 0.9412624967 -0.4676993458 0.8831548426  
H 0.6151018694 -1.508648098 0.9219562786  
H 1.5061115774 -0.2228503152 1.7897754743  
S 2.0774140256 -0.2754989234 -0.55327108  
H 1.6375262552 0.9945862742 -0.7635447213

**2d'**

C -0.3901326737 0.3828711776 0.7618183448  
H -0.8473551577 0.3431493468 1.7677431676  
N -0.1515689437 1.7604592164 0.330497784  
H -0.9314874132 1.9954850847 -0.2826549648  
H -0.1712815003 2.3963853988 1.1246938984  
C -1.4140214108 -0.3434523178 -0.1714107877  
O -1.5543908877 -1.5736394056 0.0226571878  
O -2.02988941 0.3732394276 -0.9995584634  
C 0.9183833179 -0.4076924368 0.8907227572  
H 0.688812535 -1.4423921155 1.1495470641  
H 1.5594182643 0.0227545996 1.6651680247  
S 1.8879925729 -0.4886702638 -0.6704707135  
H 1.8378527083 0.8492010623 -0.9144979551

**2e**

C -0.390684264 0.661186878 0.1689744671  
H 0.1625097247 -0.1182807804 0.6955241399  
N -0.279586427 0.4437191739 -1.3078275233  
H -0.088649035 1.4627316928 -1.5840542651  
H 0.5038035471 -0.1472701963 -1.563479886  
H -1.2252420057 -0.0362825512 -1.5546234494  
C 0.2290286728 2.0837493567 0.4152521338  
O 0.4732645196 2.398895828 1.5812710648  
O 0.3767618391 2.7437698552 -0.6623496545  
C -1.8993910421 0.5808218436 0.5282358946  
H -2.3499106788 1.565664155 0.3563699276  
H -1.9704077398 0.3808581321 1.5999382751  
S -2.775826111 -0.6921283874 -0.4726671247

**2e'**

C -0.3993136304 0.6530816378 0.1462109832  
H 0.1351938027 -0.1567986513 0.6484089445  
N -0.2759555689 0.4491896593 -1.3318997496  
H -0.2004859511 1.4136767464 -1.7125100332

H 0.5679256147 -0.0706085162 -1.5934825073  
H -1.1218581721 -0.0749188866 -1.6458908164  
C 0.2248717555 2.0428591789 0.4719855362  
O 0.4753440684 2.2650101988 1.6696633815  
O 0.3624581253 2.8063708581 -0.5216361421  
C -1.8944166256 0.6243843261 0.516098883  
H -2.3516047714 1.5689779689 0.1977079811  
H -1.9524180367 0.589786974 1.6063766413  
S -2.8040696104 -0.7835764942 -0.2504691022

**3a**

C 0.1713876976 0.463632255 -0.9200968276  
H 0.133263563 1.5512137918 -0.7628491632  
N 1.5530028936 0.0442687483 -0.6540253141  
H 1.724453492 0.260705473 -2.5492368279  
H 1.9188033535 0.4753160289 0.1875770628  
H 1.59326568 -0.9652496139 -0.5308503272  
C -0.124626974 0.2671184355 -2.424171652  
O -1.2375540256 0.1874939934 -2.8756388926  
O 0.9740274032 0.2379701253 -3.1823841773  
C -0.9123067055 -0.1677634208 -0.0360738209  
H -1.9018624729 0.1860564454 -0.3255921059  
H -0.7339880358 0.0932427555 1.0115482342  
S -0.9284817196 -2.0103807303 -0.126371912  
S -2.6158893476 -2.4606434928 -1.2428338493  
H -2.1527948021 -2.124582794 -2.4668064272

**3a'**

C 0.1436164397 0.4793242289 -0.8968837702  
H 0.2565781781 1.5458751714 -0.6453620204  
N 1.4578453044 -0.1479469705 -0.7639950359  
H 1.4948074104 -0.0342219015 -2.6032920424  
H 2.0128110127 0.2981136065 -0.0354313203  
H 1.3756116254 -1.1382983966 -0.5331217903  
C -0.2632067612 0.4922722397 -2.3838203279  
O -1.3609591368 0.8120800127 -2.779352925  
O 0.731291984 0.1710827553 -3.2070044353  
C -0.9757960596 -0.0545496507 0.0123947551  
H -1.9392750976 0.368424515 -0.2774857076  
H -0.7669710811 0.229665554 1.0499810665  
S -1.1328263571 -1.8818534685 0.1207812744  
S -2.2797175493 -2.4604002941 -1.5098985176  
H -1.293109912 -2.6411694017 -2.4453152032

**3b**

C -0.4103514186 0.6687414702 -0.0411444362  
H 0.2144195673 -0.0985801444 0.4308925213  
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H 0.9269967017 2.1099981762 -1.1418039492  
H 0.0602014525 -0.3306399121 -1.7881370744  
H -0.9858192873 0.9012603875 -2.0110494007

C 0.1170276828 2.0172157392 0.5173254286  
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 O 0.9238124024 2.6626628664 -0.3274759067  
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 H -2.5355069337 1.1639954621 -0.0814243377  
 H -1.9144791336 0.6602377364 1.4895479842  
 S -2.5295956884 -1.2306862008 0.2208112743  
 S -3.2159733622 -1.3181139166 -1.7373240298  
 H -2.1304334161 -1.850206092 -2.3429027125

**3b'**

C -0.4248064801 0.6738277472 -0.0510900637  
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 H 0.9424163703 2.0788233426 -1.1331515576  
 H 0.0316268462 -0.2895339103 -1.8261835356  
 H -0.9632378642 1.0132811259 -2.0221739693  
 C 0.1286254219 1.9979445632 0.5242304671  
 O -0.1277939621 2.4142377485 1.6317518116  
 O 0.9544072091 2.6289068415 -0.3043174342  
 C -1.8745584274 0.4742979744 0.4037576079  
 H -2.5556212176 1.1535899136 -0.1181265083  
 H -1.9449166101 0.6833068808 1.476034276  
 S -2.5256564767 -1.2337933256 0.2492794396  
 S -3.2232714976 -1.3977513592 -1.6998383899  
 H -2.1030826009 -1.8896474832 -2.3190388309

**4**

C -0.4111624018 0.6372924869 0.1258080793  
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 H 0.0588009833 1.489086086 -1.5688661759  
 H 0.4717854011 -0.1772789203 -1.6026868794  
 H -1.1729585178 0.1297571733 -1.8161825152  
 C 0.1975681378 2.0613288456 0.4412556818  
 O 0.2685248955 2.3794367854 1.6282910832  
 O 0.5248041544 2.6941562026 -0.6088569472  
 C -1.8741604335 0.5214452158 0.5446667127  
 H -2.4632033368 1.3359223657 0.1109240291  
 H -1.9077967459 0.617247105 1.6333084977  
 S -2.6806038249 -1.064308817 0.0872123128  
 S -2.9638461501 -0.8373397361 -1.9972182878

**4'**

C -0.3998876021 0.6356130521 0.1089495493  
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 H -0.0243842979 1.4514487892 -1.6873295289  
 H 0.5650130082 -0.1181539255 -1.611251178  
 H -1.0939891357 0.0722488699 -1.829663225  
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O 0.2956579178 2.280434718 1.6913308282  
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H -2.4433334746 1.3752549266 0.0654200651  
H -1.9097051486 0.6751957447 1.6050618235  
S -2.724225788 -1.0185548232 0.1361706169  
S -3.0373680995 -0.9142755543 -1.9523736664

**5a**

C 0.0687874383 -0.4099919852 -1.1197607333  
H 0.3322335492 -1.4652919259 -1.0099862332  
N -1.3127443479 -0.2280502516 -0.5660100966  
H -1.8346895861 -0.1759441873 -1.5065831727  
H -1.5617812284 -0.9577019294 0.10743486  
H -1.3685944369 0.6343503273 -0.0005872654  
C -0.0925360998 -0.100546573 -2.6694132797  
O 0.9447072195 0.0039522305 -3.3215288943  
O -1.3084884148 -0.0285467837 -3.0183633907  
C 1.110488345 0.4564115785 -0.4319007866  
H 0.7740940849 1.4957737502 -0.3783143793  
H 2.005741859 0.4226293612 -1.0572124429  
S 1.6414225019 -0.0605322988 1.2483179097  
S -0.2413953308 0.148121568 2.3466584466  
O -0.9915918907 -1.0866804822 2.0739021236  
O -0.8700818685 1.3282472915 1.7226022701  
O 0.201928206 0.3121733099 3.7153340648

**5a'**

C 0.0425261274 -0.4167915679 -1.1291440548  
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N -1.3514649473 -0.2342963262 -0.5985140576  
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H -1.6637189129 -1.0233870253 -0.0251930591  
H -1.4307869437 0.6001518761 0.0003745485  
C -0.0433364945 -0.1127024161 -2.6744362135  
O 1.0367251839 -0.0663954806 -3.2803511957  
O -1.2152150084 0.0253906222 -3.1111569704  
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H 0.7191822315 1.5028993193 -0.374348998  
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S 1.6369388501 -0.0450561299 1.2327921181  
S -0.1857294012 0.157172531 2.3782250702  
O -0.9418608138 -1.0801263784 2.1635973963  
O -0.8529303307 1.3334615369 1.7951522281  
O 0.3113893677 0.3360799777 3.7353970126

**5b**

C 0.0678578598 0.0348207696 -1.4377063887  
H -0.8489725542 0.3651975682 -0.9452476017  
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H -0.1828464026 -1.569860744 -0.124557663

H -0.1758670127 -1.8229485279 -1.9673976692  
 H 1.2315137373 -1.6284845844 -0.970160737  
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 O -0.4495163813 -1.1832624559 -3.398648129  
 O -0.0666806274 1.0472998039 -3.6173166063  
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 H 2.0432805951 0.9010663436 -1.695529508  
 S 1.9752899093 0.4617635972 0.6356055976  
 S 0.1885164872 0.2474521997 1.924896982  
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 O -0.6524279691 1.3749818594 1.5532710003  
 O 0.791041832 0.2665859054 3.2434651942

**5b'**

C 0.0929574126 -0.0275492122 -1.428343265  
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 H -0.0124644703 -1.6822024979 -0.1586911499  
 H -0.1930637653 -1.967803658 -1.8701825386  
 H 1.3129269072 -1.7362454032 -1.1802175486  
 C -0.2172001773 0.0667183015 -2.9625593463  
 O -0.5296601787 -1.0296688907 -3.4927489086  
 O -0.1523510849 1.1997876656 -3.4644745818  
 C 1.2363567809 0.8724161874 -0.9742672227  
 H 0.893847285 1.9057348189 -1.0226346638  
 H 2.102965506 0.7712791034 -1.6371618224  
 S 1.9251582921 0.5250670907 0.6971423646  
 S 0.1478064906 0.3422181658 1.9162189457  
 O -0.461737678 -0.9443563043 1.5336976716  
 O -0.6869506352 1.4935837493 1.5878507764  
 O 0.7253376805 0.3399834853 3.2549351853

**6**

C 0.1657230136 -0.4557444092 -1.3800640635  
 H 0.6936640979 -1.3887596166 -1.6004205254  
 N -1.2071341796 -0.8223474147 -0.9162683488  
 H -1.7168115332 -0.6630589231 -1.8456281236  
 H -1.2771437879 -1.751966419 -0.5018290698  
 H -1.5792399366 -0.2000900844 -0.1639325607  
 C -0.0636654783 0.2805286874 -2.7723962168  
 O 0.9078022313 0.8677483021 -3.2462089561  
 O -1.2381860347 0.1131578649 -3.207333818  
 C 0.9671247415 0.3537848348 -0.3771203301  
 H 0.4013102716 1.2006375725 0.0176571932  
 H 1.8443560823 0.7348429759 -0.9034009937  
 S 1.5510342659 -0.6539522704 1.0661973123  
 S 0.4722597196 -0.0068068085 2.6940405746  
 S -1.5857349131 -0.754661552 2.3613395481  
 O -1.4462211146 -2.0771090505 1.7527734055  
 O -2.1192153234 -0.6932832803 3.7078433808



O -2.1572681223 0.2378775909 1.4269525919

**6'**

C 0.110486825 0.513344403 2.1612725788  
H 0.6346509948 1.4591775623 2.4747324124  
N -1.1538670817 0.8999172355 1.4486332979  
H -1.8837072455 0.5317331086 2.1082450605  
H -1.2548838727 1.9168330399 1.3528319966  
H -1.2589198738 0.4695350675 0.5065113902  
C -0.3275272916 -0.258820813 3.4593849191  
O 0.5908528113 -0.6977104888 4.1682650936  
O -1.5731228055 -0.3343461712 3.6284476216  
C 1.0258892994 -0.338797226 1.2949120225  
H 0.5013502061 -1.2018567802 0.8753319523  
H 1.8496754643 -0.6901425138 1.9183269667  
S 1.7273790117 0.6179890527 -0.1297134238  
S 1.3380967563 -0.556027165 -1.7731870067  
S -0.7302887665 -0.0632100352 -2.279695797  
O -0.7577462461 1.3353829189 -2.6849564693  
O -0.9658732012 -1.0369312992 -3.3403606459  
O -1.4951319842 -0.3321738962 -1.0465839694

**7a**

C -0.4634926284 0.6541675501 -0.0271405787  
H 0.1676170234 -0.099507592 0.4676138244  
N -0.4441035793 0.480645673 -1.4913245779  
H 0.3456165828 0.9669625877 -1.9007060062  
H -0.372377376 -0.5071013249 -1.7328427179  
C 0.1225638902 2.0003264208 0.3962234932  
O -0.1516131871 2.5719351895 1.4170981269  
O 1.0320994791 2.4671688606 -0.4893848703  
C -1.8914790463 0.5261968271 0.5277389443  
H -2.5396988953 1.2859102594 0.084275914  
H -1.8773779749 0.6885985608 1.6072304333  
S -2.6489806987 -1.1170437136 0.2875027614  
S -3.1793947832 -1.1263652876 -1.8988372672  
O -2.1067424431 -1.8830516489 -2.5549163712  
O -2.9906425348 0.432671567 -2.2191956197  
H 1.3694367544 3.3019706172 -0.1302697887  
H -1.9981805828 0.6512064537 -2.0880086995

**7a'**

C 1.3666495362 0.3645689223 0.5981680654  
H 1.6701800935 0.9904206308 1.5019777578  
N 0.5806885777 -0.7999959108 1.1252539569  
H 1.1912193765 -1.5261271967 1.5182294908  
H -0.0508336914 -0.4715085732 1.8662163681  
C 2.6539871381 -0.0818814744 -0.0770364417  
O 3.4083180415 0.6974776303 -0.6054485075  
O 2.8461905342 -1.4026144972 -0.0102757941  
C 0.5098546877 1.195990155 -0.3745650021

H 0.39625679 0.6460601678 -1.3142213734  
 H 1.0496173275 2.120893891 -0.5887061621  
 S -1.1519906369 1.5931943301 0.2596347281  
 S -2.3229165764 -0.3624691133 -0.5636803409  
 O -3.0592099136 -0.7863489798 0.6372543247  
 O -1.1431631887 -1.2462673195 -0.8650674462  
 H 3.7024031234 -1.6256827814 -0.449118618  
 H -0.0351319518 -1.2035116412 0.3601932531

**7a''**

C 1.3941453844 0.40258633 0.6019442116  
 H 1.7350316405 1.0594727797 1.4695117987  
 N 0.6183879621 -0.7345356685 1.1996168927  
 H 1.2374165911 -1.4412739852 1.6133090268  
 H 0.0051229451 -0.3688382525 1.9378768731  
 C 2.6487076914 -0.0842458213 -0.106728761  
 O 3.3736268284 0.6605910279 -0.7192951168  
 O 2.8460197131 -1.3992302579 0.0284515182  
 C 0.5088569681 1.2024116963 -0.3753498224  
 H 0.4004149414 0.63939876 -1.3076528149  
 H 1.0254772924 2.1362877855 -0.6065750462  
 S -1.1570959262 1.5697128157 0.2685938897  
 S -2.2929319217 -0.3804476651 -0.5908776207  
 O -3.1658258183 -0.7280258785 0.5406462006  
 O -1.1178737363 -1.3096201777 -0.7360896018  
 H 3.6772671458 -1.6503068116 -0.4417466976  
 H -0.0160034057 -1.1737959215 0.4680297142

**7b**

C -0.3571035882 0.5823246917 0.0475191185  
 H 0.2288891554 -0.0559420886 0.7176799126  
 N 0.0050139337 0.2817332977 -1.3411058523  
 H 0.8441330865 1.9417653521 -1.2650489708  
 H 0.4748059229 -0.6112182606 -1.4182813088  
 H -0.8176746797 0.2528705382 -1.9406057557  
 C 0.0616205263 2.0363333 0.4000371503  
 O -0.2427420719 2.5650396473 1.4372845942  
 O 0.7969210133 2.6171367473 -0.5464607069  
 C -1.8460281907 0.420325665 0.3902165596  
 H -2.4543051782 1.0256235146 -0.2876427708  
 H -2.0262581088 0.7702620318 1.4071033127  
 S -2.4539475502 -1.3056083677 0.2931865438  
 S -3.4953778757 -1.2446766706 -1.6305551163  
 O -3.0281588919 -2.7395492518 -2.0939287619  
 O -2.8154532528 -0.2153515554 -2.4278936558  
 H -2.07110525 -2.8492755909 -1.9653202925

**7b'**

C 1.4614664306 0.1166374955 0.563306178  
 H 1.6090121712 0.6561311197 1.508573221  
 N 1.0074121062 -1.2463276482 0.8469026587

H 2.6447188009 -1.7355852475 0.2978973832  
H 0.6758853243 -1.3362211686 1.8054191642  
H 0.2462596962 -1.5209795171 0.2287673664  
C 2.8630533 0.0481960189 -0.0880002571  
O 3.4513302232 1.0127539552 -0.5254533065  
O 3.371216218 -1.1781607329 -0.104389435  
C 0.5336911568 0.9451917825 -0.3404522341  
H 0.3489932573 0.4192723146 -1.2824104217  
H 1.0047651247 1.9016712347 -0.5748197289  
S -1.087801796 1.3276771372 0.4219151184  
S -2.3817054723 -0.1162405717 -0.6086743359  
O -3.3426319988 -0.4260690425 0.6519682244  
O -1.5271375465 -1.2754426155 -0.9190495625  
H -2.8408833162 -0.767784542 1.4426723988

**7c**

C -0.5068190718 0.6948764815 -0.0040011543  
H 0.0270388293 -0.0965943796 0.539443544  
N -0.4278282281 0.4824720486 -1.4567471601  
H 0.2530768862 1.1327825408 -1.8442329337  
H -0.1668062457 -0.4735590685 -1.682045788  
C 0.1979303591 2.0227105132 0.3237116389  
O 0.2409185798 2.3690355516 1.6244612502  
O 0.7001097599 2.7221913524 -0.5125822274  
C -1.9781267693 0.6962591884 0.4695526134  
H -2.5506465818 1.4330779802 -0.0999442112  
H -2.0584808134 0.9671839555 1.5274028891  
S -2.8025745049 -0.9320029811 0.3595871249  
S -3.1573799555 -1.1801290992 -1.8664766593  
O -2.0645423102 -2.0302430343 -2.3443400696  
O -2.8932160311 0.3239438471 -2.3228029087  
H -1.8968376879 0.5327237606 -2.1180515614  
H -0.1643972147 1.6911443427 2.1791156131

**7c'**

C 1.3808638614 0.2152927154 0.5820700818  
H 1.6289266649 0.7958927667 1.5359578848  
N 0.6458510274 -1.0313841279 0.9774351437  
H 1.3105427875 -1.818506203 0.9955254851  
H 0.2278794797 -0.9302635009 1.9090835119  
C 2.7027054535 -0.2214941718 -0.0359027424  
O 3.3899322659 0.8139969312 -0.5008249005  
O 3.0717916173 -1.3748841139 -0.0767870876  
C 0.5333072268 1.0827323342 -0.3636559209  
H 0.3780827543 0.5521392227 -1.3089293943  
H 1.0898716631 1.9975211553 -0.5778169027  
S -1.0934024726 1.5315555421 0.332798483  
S -2.4128150912 -0.2556411366 -0.5511734177  
O -3.2563284645 -0.5945725494 0.6059779602  
O -1.3228152537 -1.265269588 -0.8020859216  
H -0.1384708292 -1.2498647023 0.2868010224

H 4.2404118026 0.4863636839 -0.8811492575

### 8

C -0.459315569 0.6022919444 0.0744455605  
 H 0.1347333314 -0.1713326898 0.5694024154  
 N -0.2864871224 0.4234948594 -1.4055453085  
 H 0.4464147007 1.1921424775 -1.557713456  
 H -0.0669108534 -0.5353227515 -1.6906386195  
 H -1.1812313984 0.6134410823 -1.8962621934  
 C 0.2212483344 2.0017219248 0.3759138927  
 O 0.0240170006 2.4860461235 1.4900464288  
 O 0.9209121519 2.4165734382 -0.5971014376  
 C -1.9133938871 0.4826779314 0.5045109706  
 H -2.5450069065 1.1225200046 -0.1215980951  
 H -1.9800361283 0.8449206623 1.5320515228  
 S -2.596045773 -1.2182313251 0.4548865127  
 S -2.7730103349 -1.44148098 -1.9113434726  
 O -1.4593584305 -2.0279970451 -2.2964489447  
 O -2.8662291154 0.0006933429 -2.3160127764

### 8'

C -0.3296424067 0.6574474299 0.1362863915  
 H 0.3007216889 -0.015156523 0.7255762958  
 N -0.0340107886 0.4149356159 -1.3169773151  
 H 0.3858902438 1.3340656812 -1.5995139987  
 H 0.6406423881 -0.3415711449 -1.4638497261  
 H -0.8982455505 0.2135163825 -1.8720251961  
 C 0.1028227961 2.1375985238 0.4324860711  
 O -0.0801774883 2.5359940686 1.5935437124  
 O 0.5924335649 2.7533684494 -0.5522567284  
 C -1.8023775394 0.4236898585 0.4658142177  
 H -2.4304834655 1.0637037959 -0.1626351318  
 H -1.9557982451 0.7235498547 1.5038461083  
 S -2.3726488669 -1.3075385298 0.2669003639  
 S -3.2447214857 -1.2270958307 -1.9574018768  
 O -2.7736990022 -2.5194213446 -2.4932622898  
 O -2.4804058429 -0.0549272872 -2.4979378981

### 9a

C -0.3271478739 -0.3993891787 -1.4102731018  
 H -0.4506814408 -1.4581361237 -1.1801263609  
 N -1.2189464543 0.3775636717 -0.4956243213  
 H -1.7976622241 0.8772752417 -1.2557389262  
 H -1.7628192147 -0.2535504562 0.1219452672  
 H -0.7133285204 0.9811068278 0.1608083563  
 C -0.8661531297 -0.079512805 -2.8683501298  
 O -0.3023661717 -0.6510590103 -3.7999148228  
 O -1.8146048869 0.7606811603 -2.8570031484  
 C 1.1422375278 -0.0235824075 -1.2929799954  
 H 1.3112361124 1.0032997323 -1.6415148822  
 H 1.7002814696 -0.6931334513 -1.9485189582

S 1.8697665778 -0.0117642741 0.4070860744  
 S -0.8219142621 -0.8605167147 2.4863563449  
 O -1.9205554913 -1.3330172591 1.5917296277  
 O -0.5898858654 0.5970510082 2.3652033554  
 S 1.2228698479 -1.7210069615 1.3327706211

**9a'**

C -1.4392964533 -0.0581033459 -0.0566715767  
 H -0.9216127438 -0.2028894018 -1.0101365417  
 N -0.9543658769 -1.1393862472 0.8607774266  
 H -1.8096707187 -1.7376428042 0.9571584642  
 H -0.1540405154 -1.6406681917 0.4255197559  
 H -0.6580154143 -0.792732795 1.7801747833  
 C -2.9728217818 -0.3141201842 -0.2858889813  
 O -3.5688691635 0.5243592484 -0.9786429998  
 O -3.4131167077 -1.3614917065 0.2570687794  
 C -1.1635032934 1.3427376647 0.4604835929  
 H -1.6456329876 1.5120226701 1.4324213676  
 H -1.5830372459 2.0491785292 -0.2568016937  
 S 0.6052274525 1.7532094828 0.788562409  
 S 2.3738766352 -1.0342210113 -0.3238081389  
 O 1.2061308863 -1.8794470984 -0.7207827971  
 O 2.4675513546 -0.8915685076 1.1422161001  
 S 1.6215371594 1.2648333061 -0.9291220074

**9b**

C 1.6156147267 -0.0107502272 0.3439264623  
 H 1.3867150074 -0.0179129246 1.4122603999  
 N 0.8407958577 -1.1312535814 -0.2788935349  
 H 1.6731870771 -1.7924549438 -0.4541534425  
 H 0.0762123301 -1.4672026448 0.3481624617  
 H 0.3822611322 -0.8331024253 -1.1410183219  
 C 3.137548 -0.416688417 0.1434158371  
 O 3.9757477895 0.4295312319 0.4525579308  
 O 3.2655466326 -1.5918391748 -0.3092659207  
 C 1.2961556729 1.3501288984 -0.2435185068  
 H 1.4245003501 1.3453349576 -1.3314601238  
 H 2.0252842141 2.0514039477 0.1722253306  
 S -0.3565984104 2.060757083 0.1397870369  
 S -1.6984041203 0.8897654728 -0.9180757111  
 S -2.5600125772 -0.8806001629 0.6230661945  
 O -1.3244907938 -1.3457523038 1.3201481915  
 O -3.0437872173 -1.810103942 -0.408776546

**9b'**

C -1.6971829446 -0.1497124288 -0.2235723036  
 H -1.502514919 -0.2959061469 -1.3273340362  
 N -0.8842996117 -1.1845398492 0.4892966376  
 H -1.5281452239 -1.9998541373 0.5348486515  
 H 0.0197002224 -1.3953049035 -0.0012326743  
 H -0.6811836343 -0.9074472675 1.45747046

C -3.2074014375 -0.5185460373 0.0077967697  
O -4.0399620666 0.3655345613 -0.2573707171  
O -3.4012687622 -1.6983023627 0.3985231998  
C -1.3544399923 1.2687743136 0.1911494344  
H -1.3774936719 1.3846999113 1.2813814595  
H -2.1284975295 1.9182809692 -0.2297965958  
S 0.2231581362 1.9825025044 -0.4304721764  
S 1.7223114287 1.1708856982 0.7347891064  
S 2.6402380115 -0.7148975086 -0.482480643  
O 1.4106864801 -1.4459560419 -0.9224964553  
O 3.3361859537 -1.3612578342 0.6463682489

**10a**

C -0.0842742185 0.2334226333 0.4417241005  
H -0.3075406555 1.3048926751 0.4061657173  
N -0.283030246 -0.2607775444 1.7849502089  
H 0.3363269678 -1.0084180588 2.0749293301  
C 1.3930518704 -0.0159503129 0.082768362  
O 2.0022606926 -0.9521581097 0.5659911284  
C -1.0270655522 -0.4977082628 -0.5480156494  
H -2.0510896712 -0.3944874164 -0.1819284817  
H -0.7922859214 -1.5637790143 -0.57482575  
S -1.072483421 0.1716486312 -2.2557111244  
N 1.9387069101 0.8623442616 -0.7946968345  
H 2.8744765483 0.6846586591 -1.1247493735  
H 1.3756676223 1.5469020853 -1.2716191747  
C -1.1320712524 0.2825344186 2.6999910225  
H -1.6917782038 1.1468963931 2.2825289749  
O -1.2769692328 -0.1102236287 3.8346765696  
H 0.0507817634 -0.4174194091 -2.7048660262

**10a'**

C -0.1429859171 -0.0676461134 -0.2090154333  
H -0.1716304694 -0.2480232362 -1.2899577872  
N -1.5063069284 -0.1416739127 0.2938764595  
H -1.6707126394 0.1408997116 1.2644092295  
C 0.3984782041 1.3395531762 0.099631523  
O 0.4576733021 1.7304714743 1.2617035416  
C 0.7278724345 -1.1397792465 0.4695535713  
H 0.2796214034 -2.1219496019 0.2987997795  
H 0.768923085 -0.9601229686 1.5461648914  
S 2.4354211308 -1.2663761307 -0.1873294329  
N 0.7692523783 2.0737786444 -0.9614183302  
H 1.1433112578 3.0073750662 -0.8161630094  
H 0.7285280386 1.7113794641 -1.9072765241  
C -2.5671182082 -0.5596752896 -0.4289406836  
H -2.2913802598 -0.8336032671 -1.4674521973  
O -3.7124619608 -0.6344247009 -0.0083206096  
H 2.9577881134 -0.1667298297 0.4277163932

**10b**

C 0.0141459687 0.0609103692 0.1742758715  
 H -0.176096755 1.1395220026 0.1128620606  
 N -0.0223550386 -0.2897088979 1.5872156331  
 H 0.1631153191 -1.2493686078 1.8514406344  
 C 1.4233540533 -0.1766221598 -0.4194430675  
 O 1.5882481426 -0.5810003423 -1.5555948258  
 C -1.0698309221 -0.6661713645 -0.6425174403  
 H -2.0006951939 -0.6573349467 -0.071173123  
 H -0.7871877328 -1.7059329825 -0.8202413652  
 S -1.4849314399 0.1314943666 -2.2369339142  
 N 2.4479268764 0.1307536455 0.4148376839  
 H 3.3896106469 -0.0059501773 0.0861122199  
 H 2.2865379981 0.3601198223 1.3799428186  
 C -0.6108608174 0.477703517 2.5591564756  
 H -0.8823240809 1.483416434 2.1785769748  
 O -0.7896968877 0.123748159 3.699769512  
 H -0.2797701371 -0.0813068374 -2.7962931484

**10b'**

C -0.1348584195 -0.0821383504 -0.1936400416  
 H -0.1918131599 -0.2368456469 -1.2777205911  
 N -1.4819746364 -0.2136104917 0.3449493892  
 H -1.6249087581 0.0013038995 1.3369427204  
 C 0.3600259212 1.3426186335 0.12444342  
 O 0.6714021366 1.6485045807 1.2714330058  
 C 0.793944167 -1.1331850184 0.4290941342  
 H 0.37745795 -2.1288108868 0.2566834222  
 H 0.876982331 -0.9700722213 1.5053540718  
 S 2.4755858996 -1.1736040989 -0.3029429126  
 N 0.3805386638 2.1955457331 -0.9127918063  
 H 0.6590847839 3.1607251164 -0.7612273069  
 H 0.1267113146 1.9080276462 -1.851186145  
 C -2.5551598648 -0.6194416742 -0.3678778535  
 H -2.3048498444 -0.8296713667 -1.4274691407  
 O -3.6846675406 -0.7437594377 0.0817905309  
 H 2.9760631883 -0.0699923608 0.3215236634

**11**

C -0.0102625821 0.3209408788 0.5148294527  
 H -0.2074512593 1.3994964632 0.4864707377  
 N -0.2265621133 -0.2004142519 1.8589397752  
 H 0.5611677597 -0.7172933018 2.2358726647  
 C 1.4815180872 0.0869234295 0.2089751048  
 O 2.2182370557 -0.501093155 1.0003819271  
 C -0.9318860395 -0.3357706711 -0.5551825884  
 H -1.9406147524 -0.3363548348 -0.124757658  
 H -0.6390005812 -1.3911284989 -0.6527117525  
 S -0.9485276422 0.5214254872 -2.1747372591  
 N 1.8780029805 0.5820533266 -0.9822295014  
 H 2.7816823105 0.2592641441 -1.2986224177  
 H 1.106615569 0.7382915021 -1.6780949305

C -1.2798566169 0.0719548302 2.648137461  
 H -2.0218278834 0.723547209 2.1398119671  
 O -1.4418622924 -0.3268975572 3.7920030171

**11'**

C -0.032272676 0.2591342917 0.4992367269  
 H -0.2691274763 1.3313601737 0.4978971642  
 N -0.2837852261 -0.2713410578 1.8293021013  
 H 0.3385375507 -1.0084405827 2.1624874529  
 C 1.4727814861 0.0941892132 0.2116538699  
 O 2.2240009996 -0.4639711011 1.0095236523  
 C -0.9261645655 -0.4260796663 -0.5723796268  
 H -1.9239485023 -0.5049712142 -0.1304775782  
 H -0.5679841222 -1.4507655893 -0.7297882357  
 S -1.0538082778 0.4701201938 -2.1796098369  
 N 1.8787727803 0.6174897976 -0.959542929  
 H 2.8260396032 0.4144469899 -1.2654002148  
 H 1.1601180102 0.8390784718 -1.6559379151  
 C -1.2227541667 0.1948594675 2.6689943298  
 H -1.7942995545 1.0440944095 2.2412078364  
 O -1.4467338624 -0.2442587974 3.7919192029

**12**

C -0.0334623292 0.044493085 0.3648820498  
 H -0.2484739587 1.0555841762 0.0030435943  
 N -0.2929580548 -0.0491875658 1.7891746048  
 H 0.448793279 -0.4896728188 2.3228700488  
 C 1.4722690982 -0.2163416442 0.170090228  
 O 2.1763935317 -0.6531913189 1.0773753431  
 C -0.8821862822 -0.9440541158 -0.5001832224  
 H -1.5440993438 -1.511420309 0.1619240213  
 H -0.233851162 -1.6546935015 -1.0217748972  
 S -1.9637054123 -0.1210171532 -1.7274296921  
 N 1.9032289743 0.0606709924 -1.0711411597  
 H 1.2339826129 0.3729346544 -1.799671383  
 H 2.8575836338 -0.1621589799 -1.3007935689  
 C -1.3181000392 0.537709304 2.4410288566  
 H -2.001033721 1.0672981121 1.745831973  
 O -1.5036340518 0.5001391424 3.6465338151  
 S -0.612835775 0.9402819405 -2.9395506114

**12'**

C -0.0516989311 -0.0581300683 0.348762533  
 H -0.2959733331 0.9503158535 -0.0043839057  
 N -0.4412261956 -0.1494112441 1.7365362007  
 H -0.0810666814 -0.9377926138 2.2793716164  
 C 1.4730519445 -0.2342020484 0.2119500484  
 O 2.1611015567 -0.7073089062 1.1099608141  
 C -0.7969208875 -1.0846331787 -0.5534066108  
 H -1.2864763843 -1.836097389 0.0746878322  
 H -0.1023184561 -1.5975773074 -1.2230549519



S -2.1162197952 -0.340179793 -1.5815006722  
N 1.9490947002 0.1665319932 -0.9814890051  
H 1.3179055967 0.5121818402 -1.6990461233  
H 2.9289659667 0.0274926793 -1.2051908762  
C -1.180109516 0.7717494265 2.3848536686  
H -1.4763944639 1.6143790444 1.7277420269  
O -1.5052693203 0.7085572802 3.5633286652  
S -1.0385348002 0.9714984315 -2.8269112605

**13a**

C -1.2846377906 0.313838191 0.0357514932  
H -0.7957404382 0.0662226847 -0.9089011574  
N -2.5385595613 -0.3866662476 0.1294583697  
H -3.2837730835 0.1228619588 0.5917040338  
C -1.5649370442 1.8351273545 0.0627485703  
O -2.6182776324 2.2794316978 0.4782311757  
C -0.3146331999 -0.0309592756 1.1975697816  
H -0.8810063577 -0.2398781206 2.1076460418  
H 0.3773411093 0.7875896717 1.4077296603  
S 0.7084786113 -1.524072418 0.8867949705  
N -0.533058048 2.5903340911 -0.3818654516  
H 0.3254052889 2.1704577322 -0.7103446644  
H -0.6249095288 3.5927965334 -0.3564700419  
C -2.8842598131 -1.4676133725 -0.628692755  
H -2.030210111 -1.839265956 -1.2318868764  
O -3.9783522207 -1.9824705853 -0.6414615422  
S 2.2974294495 -0.5113509627 -0.1833756803  
O 2.9442443196 0.3781924151 1.0538987234  
O 1.7002801384 0.5409924411 -1.0132482949  
H 3.3028709126 -0.2289758329 1.7196486438

**13a'**

C 1.0266197687 0.3109647863 -0.0222447948  
H 0.6275422328 0.0905311776 0.9716541484  
N 2.223781713 -0.4710151496 -0.2075554634  
H 2.8398028143 -0.216796692 -0.9845528742  
C 1.3555243467 1.8197840872 -0.0835089453  
O 2.3864344985 2.2360732062 -0.5954617691  
C -0.05370694 -0.0139293657 -1.0832073799  
H 0.4133275413 -0.1944711323 -2.0557887097  
H -0.7598873444 0.8110313518 -1.2027415641  
S -1.0334330792 -1.5135241676 -0.7004293835  
N 0.4004373932 2.6034507891 0.4523548511  
H -0.4396069177 2.2078964655 0.8534514615  
H 0.4979310487 3.6130990186 0.408652433  
C 2.648070115 -1.4294767532 0.6430667354  
H 1.9488959151 -1.583939878 1.489524672  
O 3.679939266 -2.0719373967 0.5135669819  
S -2.5254226299 -0.5161994896 0.5499798729  
O -3.2880327052 0.3913527366 -0.5671532456  
O -1.8080082602 0.5088888778 1.3286183152

H -3.9053240153 -0.1925951014 -1.0866148574

**13b**

C 0.9987009674 0.182359231 -0.0333897614  
H 0.6429238582 -0.1889143293 0.930620538  
N 2.4020773781 -0.1147804318 -0.161969506  
H 2.948855314 0.5333039037 -0.7163625476  
C 0.8234442867 1.7124207277 -0.1000163731  
O 1.6212860947 2.4214144511 -0.6713972045  
C 0.1348210198 -0.4696117262 -1.168559905  
H 0.8019025411 -0.9996315686 -1.8524015377  
H -0.4077600075 0.2726878242 -1.7594182158  
S -1.0622521994 -1.7474269556 -0.6360391499  
N -0.3531354142 2.1852844811 0.4467797415  
H -0.4004060086 3.1932976484 0.5221727193  
H -0.7738942206 1.6527933724 1.2050097206  
C 3.0748522159 -1.0293060122 0.5977434464  
H 2.3920406418 -1.5948491861 1.2650876243  
O 4.2672544527 -1.219032473 0.5521086541  
S -2.5452155489 -0.5347519467 0.4074278419  
O -2.7270601963 0.6942525744 -0.6466661634  
O -1.9070274899 0.0264947422 1.6155575227  
H -2.013269444 1.3521599217 -0.4918167525

**13b'**

C 0.9985526618 0.1872932483 -0.0501262203  
H 0.6415506367 -0.1881871331 0.9138154108  
N 2.3972935315 -0.1505465819 -0.1619906054  
H 2.9376759615 0.2932057515 -0.9100221391  
C 0.8288975668 1.717140922 -0.1085386813  
O 1.5666389446 2.415178074 -0.7796066336  
C 0.1446477441 -0.4326351397 -1.2056901651  
H 0.8099336154 -0.933281823 -1.9156557081  
H -0.4063941801 0.3295302715 -1.7642189306  
S -1.0425472928 -1.7356297211 -0.7201662668  
N -0.2751828493 2.1914651983 0.5467603988  
H -0.3622516682 3.2067067325 0.5970675059  
H -0.6195003476 1.677709274 1.3531227312  
C 3.0516781315 -0.9658544466 0.6941880123  
H 2.3910869705 -1.3600867792 1.4930125699  
O 4.2367388642 -1.2510426432 0.6154172517  
S -2.5411291473 -0.5725027309 0.3788704838  
O -2.6788920312 0.7282476295 -0.5855232485  
O -1.9145484905 -0.1199933919 1.6363759483  
H -1.9746520531 1.3839838682 -0.3753763243

**14**

C -1.2450095238 0.2543565813 -0.0255160153  
H -0.7764232532 -0.0193788643 -0.9727130516  
N -2.5737743217 -0.3201040602 0.0531355079  
H -3.2702813686 0.2778322609 0.4826687168

C -1.4068239009 1.7844113567 0.0182942517  
 O -2.4058149326 2.3177515183 0.4884353519  
 C -0.2967859242 -0.2148496464 1.119868844  
 H -0.8991447155 -0.4710384808 1.995330677  
 H 0.386356612 0.5927525841 1.4108664973  
 S 0.7547883214 -1.6349975515 0.6679881008  
 N -0.352322054 2.453980973 -0.4920308633  
 H 0.4926130654 1.9488283477 -0.7797575603  
 H -0.3283257718 3.451736653 -0.3591049338  
 C -2.9710101174 -1.4810543488 -0.5114932257  
 H -2.1334024798 -2.0031713275 -1.0139071071  
 O -4.1064464111 -1.9261414057 -0.4782004444  
 S 2.451377999 -0.1081530249 -0.2136436883  
 O 2.6814674971 0.761987018 0.9578189417  
 O 1.6945462795 0.6115924171 -1.2848069993

**14'**

C 0.9694076681 0.2980690108 -0.0391934914  
 H 0.5827513285 0.033846291 0.9482714132  
 N 2.281554799 -0.2915930261 -0.1797817943  
 H 2.8669491655 0.0415281825 -0.9493223118  
 C 1.0723089487 1.834068793 -0.1235244681  
 O 2.0186085959 2.3939386665 -0.6684460628  
 C -0.0291713213 -0.2177477044 -1.1096165818  
 H 0.5015078927 -0.3921306207 -2.0498108697  
 H -0.8031254193 0.5324608449 -1.30489343  
 S -0.9014469017 -1.7492834582 -0.6270740335  
 N 0.0271304961 2.4741140572 0.4334352097  
 H -0.7527794949 1.9480035129 0.8197210995  
 H -0.0405438748 3.4828541693 0.3457378973  
 C 2.8127211874 -1.1901486577 0.670188036  
 H 2.1233068504 -1.4459383483 1.4995834901  
 O 3.9274217732 -1.6863820475 0.5631042541  
 S -2.6576947186 -0.4577736132 0.4645064379  
 O -3.1546378566 0.3504524164 -0.6715967226  
 O -1.8718913893 0.378157915 1.4180994827

**15**

C 1.1026656581 0.5501448503 -0.1167683743  
 H 0.5712252206 0.3129597927 0.8067896439  
 N 2.5258640701 0.3807766173 0.0891414143  
 H 3.1187483256 0.9470683411 -0.5042913889  
 C 0.881975487 2.0213174523 -0.5132928052  
 O 1.7069733135 2.6165828431 -1.1951559163  
 C 0.5367589408 -0.3602047295 -1.2376815369  
 H 1.1195928119 -0.2142513099 -2.151716505  
 H -0.5013064332 -0.0793956728 -1.4533089696  
 S 0.5283990321 -2.1298315401 -0.8154600241  
 N -0.290728801 2.5654487901 -0.1092645486  
 H -0.8905860598 2.139352581 0.6160932409  
 H -0.4116641028 3.5452958045 -0.3175533748

C 3.1113568774 -0.3803069249 1.0433047714  
 H 2.3661632584 -0.9130333851 1.6631022244  
 O 4.3136602599 -0.4750087475 1.2166156044  
 S -1.6231137126 -2.0708727089 0.1969355111  
 O -2.4052808295 -1.3118126325 -0.8248425131  
 O -1.4044988491 -1.2656777623 1.4337251789  
 O -2.1633871563 1.4103613835 1.6627770443  
 H -1.9092382397 0.4655579194 1.7092536853  
 H -2.7907541627 1.4154844907 0.9135280155  
 O -3.2792825245 1.2882091517 -0.910079563  
 H -3.0355611111 0.3356255762 -0.9247164301  
 H -2.4647311841 1.7202869558 -1.1932498383

**15'**

C 1.2774175679 0.4745184342 -0.1179083097  
 H 0.7563669796 0.3341502566 0.8313981845  
 N 2.6233215712 -0.0394653591 0.0208929055  
 H 3.2976614685 0.2296877006 -0.6992353388  
 C 1.3636727518 1.9728461137 -0.4715050564  
 O 2.2525068713 2.3813224023 -1.2182765788  
 C 0.4783590411 -0.2385381868 -1.2335743826  
 H 1.009445299 -0.138773683 -2.1849439258  
 H -0.5031085222 0.2378658158 -1.3459598981  
 S 0.1751186306 -2.0097250524 -0.9242918901  
 N 0.3995265451 2.7399947973 0.0542570337  
 H -0.3299621699 2.3670926104 0.674820816  
 H 0.3761833982 3.7224348481 -0.2021760868  
 C 3.0542435689 -0.8095394009 1.0367381781  
 H 2.2612893407 -1.0119832712 1.7832512553  
 O 4.1929002899 -1.2465488844 1.1525332606  
 S -1.9413541127 -1.7262369623 0.0926767307  
 O -2.5746946951 -0.7465680732 -0.8427165817  
 O -1.6221035105 -1.0966605735 1.4070679825  
 O -1.681690264 1.7061367541 1.7166795948  
 H -1.6110357908 0.7325150862 1.711318787  
 H -2.4368139903 1.8560697142 1.1089043197  
 O -3.6793627686 1.7193032393 -0.2036997387  
 H -3.3136008487 0.8590612232 -0.4942840417  
 H -4.5115853365 1.4812804776 0.2378013275

**16**

C -1.2431964462 0.2539937893 -0.0175418468  
 H -0.7703005423 -0.0290538333 -0.9600896336  
 N -2.5724871585 -0.3161978193 0.063496708  
 H -3.2693111932 0.2916417883 0.4793297558  
 C -1.4010974264 1.7871380611 0.0105079154  
 O -2.4103805898 2.3206413748 0.4571018201  
 C -0.3044889652 -0.2033727023 1.1429442246  
 H -0.9157840687 -0.602078407 1.9561274175  
 H 0.2820424873 0.6308934823 1.535140515  
 S 0.9000411324 -1.4966327829 0.6720393805

N -0.333037044 2.4470699126 -0.4755981108  
 H 0.5009983576 1.934153442 -0.7827790285  
 H -0.3162350587 3.4487819624 -0.3789278496  
 C -2.9747724924 -1.4689233541 -0.517208016  
 H -2.1378833073 -1.9898145581 -1.0243002056  
 O -4.1107351915 -1.9087394715 -0.4936456858  
 S 2.37998899 -0.1362752553 -0.2137185983  
 O 2.7662881825 0.7429109462 0.8821960344  
 O 1.6250593455 0.5688763944 -1.2713343503  
 O 3.3827900325 -1.0629769899 -0.7021798557

**16'**

C -1.2640958416 0.2699490537 0.0344040616  
 H -0.7799231326 0.0031750839 -0.9089783591  
 N -2.479898787 -0.5001278312 0.1507892501  
 H -3.1730193657 -0.1878748481 0.8357395521  
 C -1.5957168698 1.7759050521 -0.0107125877  
 O -2.6505194911 2.2204057086 0.428128859  
 C -0.2730978389 -0.010715585 1.1975964103  
 H -0.825924813 -0.3338115546 2.0840357208  
 H 0.2967142823 0.8813289075 1.4673532982  
 S 0.9407528314 -1.3316360177 0.8309287071  
 N -0.6148750411 2.5241248073 -0.5470018406  
 H 0.2413885319 2.0943198136 -0.8817507276  
 H -0.7078357432 3.534695623 -0.5601152854  
 C -2.7907653403 -1.559927573 -0.6223520222  
 H -2.0028353709 -1.7853436447 -1.3690328616  
 O -3.8206936384 -2.2142808342 -0.532620686  
 S 2.3793013475 -0.1181904502 -0.2362347573  
 O 2.9672782282 0.770283927 0.7626331109  
 O 1.6013034085 0.6002651197 -1.2592527683  
 O 3.2803232166 -1.132749333 -0.7719028422

**17**

C -1.5723370445 0.3027507661 0.1170549018  
 H -0.8432691504 0.1796207758 -0.6861726558  
 N -2.7938570785 -0.4050973529 -0.2021044022  
 H -3.6419761348 0.0346944362 0.1364710883  
 C -1.9138480969 1.7999348276 0.250434971  
 O -3.043319949 2.1767200985 0.5376999886  
 C -0.9271486455 -0.1829252331 1.4430089165  
 H -1.7153958448 -0.5090816301 2.1281668065  
 H -0.3570127166 0.616104368 1.9185597239  
 S 0.2463139922 -1.588595248 1.2398967199  
 N -0.8548831214 2.6128088342 0.0669018643  
 H 0.0442858487 2.2424814557 -0.2480050953  
 H -0.9982534341 3.604242276 0.163688296  
 C -2.9122735478 -1.4148085171 -1.0986075924  
 H -1.9292505194 -1.7310176494 -1.4994493298  
 O -3.9623043436 -1.9353114864 -1.426745672  
 S 2.0886802674 -0.6575887664 1.2526246608

S 2.4122331569 0.1875859783 -0.7782274462  
 O 1.2699464556 1.0956775141 -0.9864739832  
 O 3.6765047486 0.8550108955 -0.5088875279  
 O 2.4353068748 -0.9313326038 -1.6994287131

**17'**

C -1.5993362845 0.2893664255 0.1327563351  
 H -0.8730753935 0.1681760154 -0.6731471381  
 N -2.7260844163 -0.5749111992 -0.1309607046  
 H -3.5539175885 -0.463667889 0.4604501987  
 C -2.0497671694 1.7660623456 0.1650890678  
 O -3.1903983374 2.0845914916 0.4796674484  
 C -0.9165997966 -0.0494687099 1.4790598541  
 H -1.6719477586 -0.3398704466 2.2162190007  
 H -0.3620686447 0.8048386592 1.8710417249  
 S 0.2821470977 -1.4444162779 1.36964299  
 N -1.0690892454 2.6355713639 -0.1391518699  
 H -0.149918422 2.3117008722 -0.4180923466  
 H -1.2534645377 3.6323006932 -0.0875498075  
 C -2.8080026481 -1.4401957317 -1.16298892  
 H -1.8892474801 -1.450748008 -1.7831856066  
 O -3.7750642418 -2.1471562983 -1.4069830354  
 S 2.1102117257 -0.4935905677 1.2983991143  
 S 2.410230681 0.1514415619 -0.7739794215  
 O 1.2891342053 1.048985039 -1.0848250772  
 O 3.6945298948 0.8269465464 -0.603039127  
 O 2.4395359198 -1.0491002327 -1.5988962834

**18**

C 1.4287161777 0.3581061911 -0.0852430009  
 H 0.8543446083 0.2431954017 0.8359031881  
 N 2.6373800514 -0.432507994 -0.0099676261  
 H 3.425783615 -0.0623381051 -0.5266643046  
 C 1.8536158651 1.8260956228 -0.2849835424  
 O 2.8853044894 2.1005931847 -0.8874264236  
 C 0.5187473885 -0.0509250738 -1.2702953634  
 H 1.110024377 -0.0643012379 -2.1906206712  
 H -0.2901990427 0.6729406077 -1.3972704487  
 S -0.2439624005 -1.7021486867 -1.1062945472  
 N 0.9893787031 2.7443189008 0.1932142819  
 H 0.1960604423 2.5149792134 0.8150998279  
 H 1.2609082585 3.7091179874 0.0836569662  
 C 2.842950054 -1.4936766713 0.8087156077  
 H 1.9346272364 -1.7557816822 1.3831929523  
 O 3.8948279115 -2.0981157033 0.9084869496  
 S -1.9292709073 -1.1581852411 0.1490259983  
 O -2.6828487484 -0.1759617353 -0.646749369  
 O -1.3317860846 -0.5702798534 1.3587702793  
 O -1.2628672235 2.1989490668 1.7934887067  
 H -1.3351397363 1.2244041553 1.8022603373  
 H -1.9206609401 2.4478619764 1.1138835182

O -2.7876850832 2.5402354995 -0.5280024565  
H -2.8426032738 1.5590788146 -0.585325221  
H -2.0280189757 2.7495946685 -1.0807545426  
O -2.5863757772 -2.4339768886 0.3352082946

**18'**

C 1.4883728715 0.3659042493 -0.0992271047  
H 0.9265404578 0.3268579657 0.8352445768  
N 2.5963903086 -0.5573066472 -0.0062295871  
H 3.3551214435 -0.4447054016 -0.682671082  
C 2.0428984586 1.7874173204 -0.3337886823  
O 3.0651969375 1.9494683851 -0.9972563624  
C 0.538319929 0.0268738417 -1.2710875366  
H 1.1024319449 0.007789705 -2.2091516622  
H -0.2454862576 0.7826238997 -1.3652524597  
S -0.2630679764 -1.6128889167 -1.147205504  
N 1.3073073402 2.7756074297 0.1915473017  
H 0.4626005205 2.6001217513 0.7506146521  
H 1.5944484406 3.7335330981 0.0135778044  
C 2.7278579864 -1.5043728152 0.9437560165  
H 1.8783462837 -1.5157250022 1.6541182862  
O 3.6725909773 -2.2769294421 1.034803019  
S -1.9346865288 -1.1320830199 0.1098611307  
O -2.7413968854 -0.1646307575 -0.6478962616  
O -1.3775527166 -0.5709233601 1.3492949209  
O -1.087120277 2.2516903619 1.6550110577  
H -1.1886413691 1.2851565734 1.6998985731  
H -1.7770535357 2.5069352513 1.0050405109  
O -2.9905629963 2.5919117585 -0.3217807615  
H -2.9639457384 1.6311002656 -0.4953138698  
H -3.8539136157 2.7324841003 0.1021261594  
O -2.5608726525 -2.4376496462 0.2673219071