



## Organic & Biomolecular Chemistry

### SUPPORTING INFORMATION

#### **Exploring the origins of selectivity in soluble Epoxide Hydrolase from *Bacillus megaterium***

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### SUPPORTING INFORMATION

### Computational methods

Full geometry optimizations were performed with the hybrid DFT B3LYP functional<sup>1, 2</sup> and the 6-31G(d) basis set<sup>3, 4</sup> using Gaussian 09,<sup>5</sup> a widely accepted level of theory for studying mechanisms of organic reactions.<sup>6, 7</sup> The effects of the active site environment of the protein were implicitly included in all calculations using the Conductor-like Polarizable Continuum Model (CPCM)<sup>8, 9</sup> with diethyl ether as the solvent ( $\epsilon=4$ ). The transition states (TS) were located by using a Bofill update TS search on a reduced potential energy surface.<sup>10</sup> Analytical frequency calculations were performed at the same level of theory as the geometry optimizations to obtain the zero point energies (ZPE). The nature of the stationary points was determined in each case according to the Hessian matrix eigenvalues. We have also checked that imaginary frequencies exhibit the expected motion, while transition states have also been verified by intrinsic reaction coordinate (IRC) calculations. More accurate energies were obtained by single-point calculations including the DFT hybrid B3LYP-D3BJ dispersion correction with the larger 6-311+G(2d,2p) basis set. All energies are ZPE-corrected.

**Active site model.** The quantum chemical model used has been devised based on the most populated cluster from a 1000-ns MD simulation on the alkyl-enzyme intermediate (**Int1**, see full details of MD simulation below). The starting structure was obtained from the X-ray crystal structure of wild-type BmEH from the PDB structure: 4NZZ. The cluster model consists of: Asp239-His267-Asp97 catalytic triad, the two active Tyr144 and Tyr203, the nucleophilic water molecule and two hydrogen bonded amide bonds (Gly29-Phe30 and Phe30-Pro31 from the oxyanion motif HGFP). In addition, Trp98, Leu168, Met145, Thr241, Pro240 residues were also included to appropriately describe the shape of the active site cavity of BmEH<sub>4NZZ</sub> enzyme. All amino acids were truncated at the  $\alpha$ - or  $\beta$ -carbon, except for the tyrosines, which are modelled as phenols and for the Pro240, in which only the  $\alpha$ - and its side-chain carbon attached are included to properly simulate the conformational rigidity of proline. Atoms in black in Figure 2 are those maintained fixed to their initial Cartesian coordinates during the optimizations. Hydrogen atoms were included manually based either on literature and BmEH<sub>4NZZ</sub> active site rearrangement, resulting the two aspartate Asp97 and Asp239 active site residues modelled as in the negatively charged state, whereas His267 was modelled in the neutral form, obtaining a quantum model with an overall charge of -2 (see Figure 2).

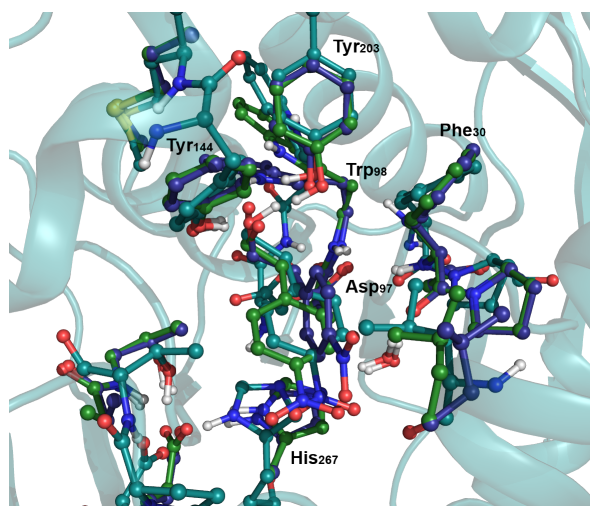
The epoxide substrates used to model the mechanisms were the racemic styrene oxide (*rac*-SO) and its racemic *para* nitro substituted derivative (*rac-p*-NSO, cluster models of 195 and 197 atoms, respectively). To explore the origins of the enantio- and regioselectivity of BmEH and the effect of the presence of the NO<sub>2</sub> group, all plausible reaction mechanism should be considered. Thus, a total of 16 reaction pathways need to be computed to take into account that EHs hydrolysis of *rac*-epoxides can take place via attack on either carbon atom of each enantiomer, but also two possible binding orientations of the substrate on the basis of the proposed BmEH active site tunnel.<sup>11</sup> The two possible binding poses arise from the orientation of the phenyl moiety of the substrate towards either region 1 (**r1**) placing the phenyl moiety close to His267, or region 3 (**r3**) when it is pointing towards Trp98 (see Figure 1 and 2).

**Molecular Dynamics of the alkyl intermediate.** 1000 ns MD simulation in explicit water was performed using AMBER 16 package<sup>12</sup> in our in-house GPU cluster *Galatea*.

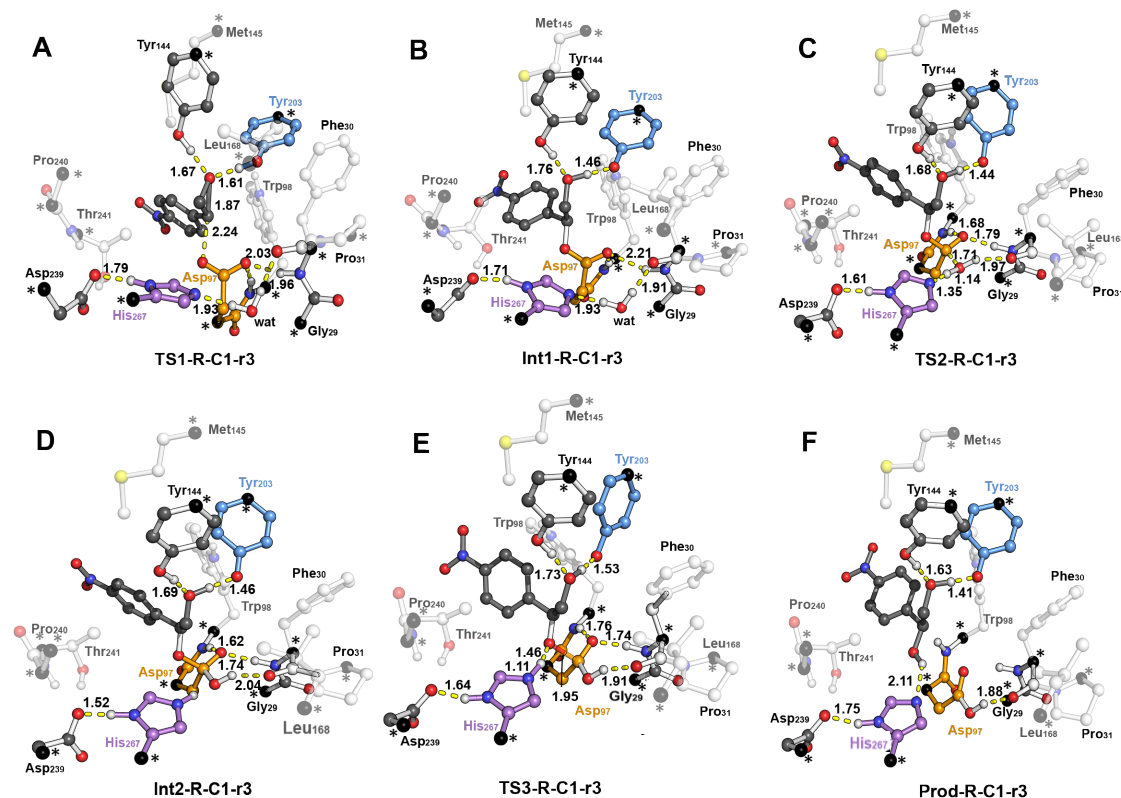
Parameters for the non-standard alkyl-intermediate were generated within the *antechamber* module of AMBER 16 using the general AMBER force field (GAFF),<sup>13</sup> with partial charges set to fit the electrostatic potential generated at the HF/6-31G(d) level by the restrained electrostatic potential (RESP) model.<sup>14</sup> The charges were calculated according to the Merz-Singh-Kollman scheme<sup>15, 16</sup> using Gaussian 09.<sup>5</sup> Amino acid protonation states were predicted using the H++ server (<http://biophysics.cs.vt.edu/H++>).<sup>17</sup> Then, the covalently modified enzyme (PD: 4NZZ) was solvated in a pre-equilibrated truncated cuboid box with a 10-Å buffer of TIP3P<sup>18</sup> water molecules using the AMBER16 *leap* module, resulting in the addition of ~9,000 solvent molecules. The systems were neutralized by addition of explicit counterions (Na<sup>+</sup>). All subsequent calculations were done using the widely tested Stony Brook modification of the Amber 99 force field (ff99SB).<sup>19</sup>

A two-stage geometry optimization approach was performed. The first stage minimizes the positions of solvent molecules and ions imposing positional restraints on solute by a harmonic potential with a force constant of 500 kcal·mol<sup>-1</sup>·Å<sup>-2</sup>, and the second stage is an unrestrained minimization of all the atoms in the simulation cell. The systems are gently heated using six 50-ps steps, incrementing the temperature 50 K each step (0–300 K) under constant volume and periodic boundary conditions. Water molecules were treated with the SHAKE algorithm such that the angle between the hydrogen atoms is kept fixed. Long-range electrostatic effects were modeled using the particle-mesh-Ewald method.<sup>20</sup>

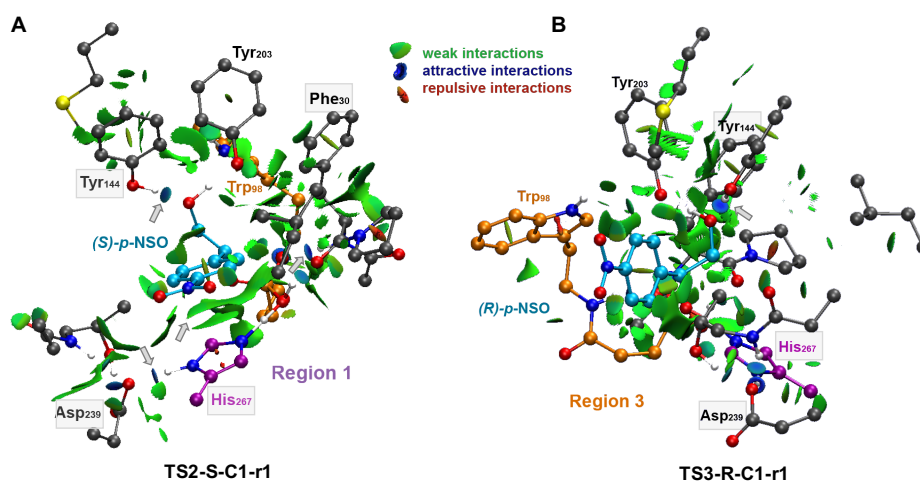
An 8-Å cutoff was applied to Lennard-Jones and electrostatic interactions. Harmonic restraints of 10 kcal·mol<sup>-1</sup> were applied to the solute, and the Langevin equilibration scheme was used to control and equalize the temperature. The time step was kept at 1 fs during the heating stages, allowing potential inhomogeneities to self-adjust. Each system was then equilibrated without restraints for 2 ns with a 2-fs time-step at a constant pressure of 1 atm and temperature of 300 K. After the systems were equilibrated in the NPT ensemble, 1 μs MD simulation was performed under the NVT ensemble and periodic-boundary conditions.



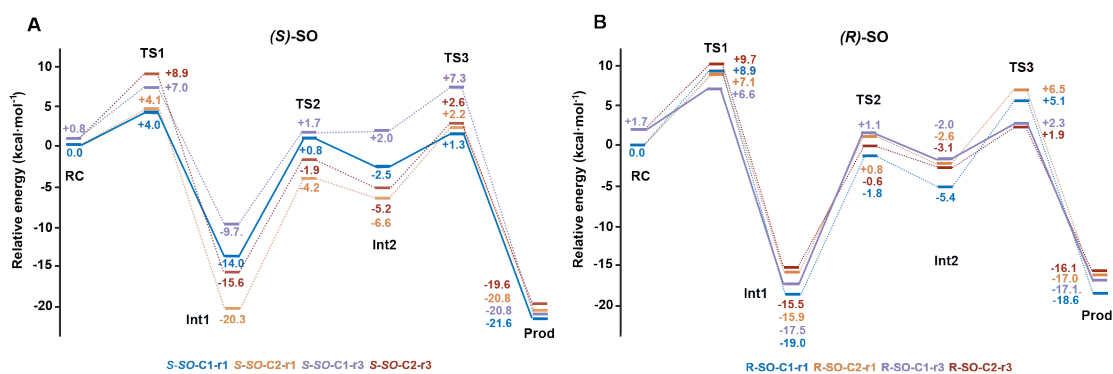
**Figure S1.** Representation of the overlay of the most populated 1 μs MD BmEH simulation (in teal), the cluster model structures **TS1-S-C1-r1** (in green) and **Int1-S-C1-r1** (in purple).



**Figure S2.** B3LYP-D3BJ/6-311+g(2d,2p)//6-31g(d) level corresponding to the different steps of the BmEH mechanism of action for (*R*)-*p*-NSO substrate oriented towards region 3 for the attack at the benzylic position (C1): **A**) epoxide ring opening (**TS1-R-C1-r3**), **B**) alkyl-enzyme intermediate (**Int1-R-C1-r3**), **C**) hydrolysis of alkyl-enzyme intermediate (**TS2-R-C1-r3**), **D**) tetrahedral intermediate (**Int2-R-C1-r3**), **E**) dissociation of tetrahedral (**TS3-R-C1-r3**) and **F**) product complex (**Prod-R-C1-r3**). All distances are in Å. Active site pocket residues are shown as transparent sticks and spheres and non-polar hydrogen atoms are omitted for clarity. Atoms in black spheres and asterisks are those maintained fixed.

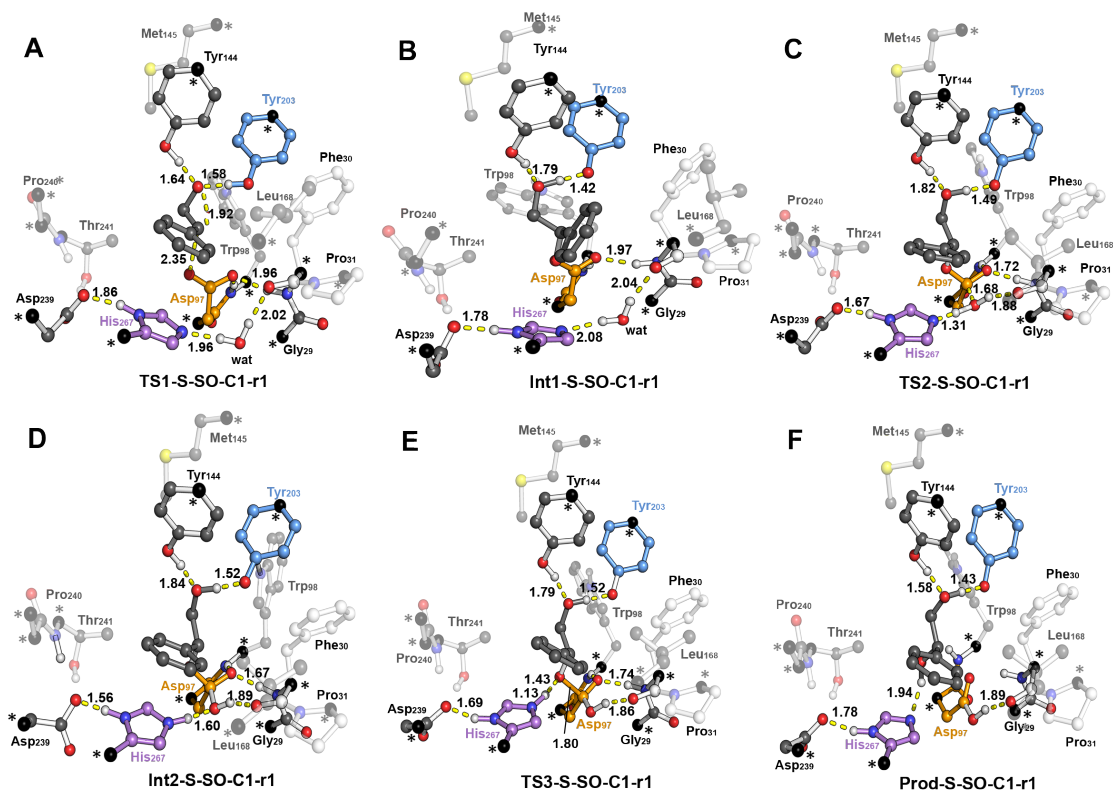


**Figure S3.** Non-covalent interactions representation of transition states **A) TS2-S-C1-r1** and **B) TS3-R-C1-r1** for the most favoured attack of (*S*)-*p*-NSO hydrolysis using the NCIplot computational tool.<sup>21, 22</sup> NCI surface show intermolecular interactions between the epoxide substrate and the active site residues included in the CM model. All residues are represented as balls and sticks and the two possible orientations of each substrate is indicated for each case (region 1, His267 and region 3, Trp98). Only the most important catalytically residues are labelled regarding BmEH (PDB: 4NZZ) numbering and non-polar hydrogen are not shown for clarity. Grey arrows are used to highlight the most important noncovalent interactions. The most important residues are framed.



**Figure S4.** Energy profiles at B3LYP-D3BJ/6-311+g(2d,2p)//B3LYP/6-31g(d,p) level of theory for all possible BmEH-mediated epoxide *rac*-SO hydrolysis outcomes. All energies are in kcal·mol<sup>-1</sup> and referenced to the lowest energy RC for each enantiomer, RC-S-SO-r1 and RC-R-SO-r1, respectively.





**Figure S5.** B3LYP-D3BJ/6-311+g(2d,2p)//6-31g(d) level corresponding to the different steps of the BmEH mechanism of action for (*S*)-SO substrate oriented towards region 1 for the attack at the benzylic position (C1): **A**) epoxide ring opening (**TS1-S-SO-C1-r1**), **B**) alkyl-enzyme intermediate (**Int1-S-SO-C1-r1**), **C**) hydrolysis of alkyl-enzyme intermediate (**TS2-S-SO-C1-r1**), **D**) tetrahedral intermediate (**Int2-S-SO-C1-r1**), **E**) dissociation of tetrahedral (**TS3-S-SO-C1-r1**) and **F**) product complex (**Prod-S-SO-C1-r1**). All distances are in Å. Active site pocket residues are shown as transparent sticks and spheres and non-polar hydrogen atoms are omitted for clarity. Atoms in black spheres and asterisks are those maintained fixed.

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## Cartesian coordinates of all analyzed structures

## RC-S-r1

C	3.121825	0.913373	-6.063232	C	-2.483863	7.302576	1.587327
C	2.372582	-0.417722	-6.004175	O	-2.820906	6.067724	1.576492
O	2.344332	-1.174090	-6.982210	O	-1.323102	7.735666	1.787114
N	1.735075	-0.702694	-4.831440	C	-4.495848	5.226966	4.777165
C	1.026467	-1.966736	-4.654905	C	-3.039671	5.310866	5.273471
C	-0.493547	-1.735401	-4.577687	O	-2.772654	5.192605	6.476862
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**TS1-S-C1-r1**

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**TS2-S-C1-r1**

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**Int2-S-C1-r1**

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H	-4.654811	4.891860	-2.568465				
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				<b>TS3-S-C1-r1</b>			
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				C	1.773110	-1.877565	-5.901177
				O	1.298682	-2.441535	-6.894168
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				C	0.277985	-3.083193	-4.361081
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				O	-1.229304	-1.206458	-4.147647
				C	0.397126	-3.642416	-2.922209

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C	5.739255	-3.053774	1.422247	H	-1.640916	-5.102368	-5.114597
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**Prod-S-C1-r1**

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**TS1-S-C2-r1**

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**Int1-S-C2-r1**

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**Int2-S-C2-r1**

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C	-5.348323	-5.046320	-1.459643	O	-0.761582	-1.257458	3.880358
H	-4.336231	-4.791821	-1.126870	C	0.674500	-6.469600	7.438900
H	-5.843801	-5.575778	-0.636233	C	1.163021	-5.142427	8.031692
H	-5.261725	-5.744702	-2.299738	C	1.360427	-4.070424	6.956666
C	-6.201124	-2.802745	-0.678900	C	-8.347800	-2.949500	-2.995400
H	-6.683997	-1.859389	-0.950530	C	-7.709080	-4.327445	-2.792587
H	-6.759654	-3.235542	0.160869	C	-6.175727	-4.316184	-2.631769
H	-5.195828	-2.561271	-0.317621	C	3.447700	-6.135700	2.790200
H	2.412444	-5.523381	8.312125	C	3.271290	-4.845741	3.304299
S	2.394636	-2.726341	7.414321	C	2.701336	-6.500276	1.659444
C	2.530001	-1.726941	5.887311	C	2.389297	-3.937117	2.708675
H	1.552153	-1.569708	5.426067	C	1.816313	-5.613136	1.058140
H	2.950368	-0.761361	6.176762	C	1.620521	-4.284006	1.552625
H	3.200625	-2.205906	5.170138	O	0.786660	-3.465747	0.975557
N	-5.102751	1.300924	0.705534	C	-4.746100	7.723200	1.403300
O	-5.428812	1.945232	1.707921	C	-3.539653	8.542929	1.868045
O	-5.887201	1.032320	-0.211646	C	-2.230505	8.010465	1.263691
<b>TS3-S-C2-r1</b>							
C	3.309000	-0.272400	-5.874600	O	-2.072752	6.729271	1.375924
C	2.428579	-1.518981	-5.759712	O	-1.433252	8.791345	0.725910
O	2.158525	-2.204069	-6.752225	C	-4.523500	5.194100	4.270400
N	1.975692	-1.819557	-4.510877	C	-3.077344	5.176562	4.795679
C	1.104200	-2.963700	-4.273100	O	-2.824635	4.944113	5.981331
C	-0.373440	-2.572739	-4.439337	C	-5.503000	4.497400	5.220300
O	-0.800194	-1.521564	-3.922281	N	-2.111671	5.431838	3.867307
C	1.357391	-3.552305	-2.860258	C	-0.698400	5.608600	4.215800
C	0.680630	-4.887901	-2.636228	C	0.123821	4.316416	4.032005
C	1.304927	-6.078851	-3.036157	C	-0.152223	3.249217	5.089925
C	-0.585561	-4.965995	-2.040068	C	-4.293200	4.766100	-1.841400
				C	-2.922619	4.296286	-1.456534
				C	-2.158939	3.249004	-1.916514

N	-2.163614	4.898139	-0.467963	H	-0.252523	4.463463	0.387695
C	-1.008124	4.231077	-0.347738	H	-0.067685	2.444957	-1.210065
N	-0.972139	3.222928	-1.212211	H	-5.675681	8.067656	1.870783
O	0.464179	1.011973	-3.393192	H	-9.428973	-3.036293	-3.147382
O	0.662425	-0.965621	1.415044	H	4.182753	-0.521419	-6.481571
H	3.629122	0.114474	-4.906759	H	6.736268	0.405676	-3.213381
H	2.748681	0.504834	-6.403849	H	3.849861	3.946365	-3.216250
H	2.440875	-3.661372	-2.749414	H	4.136680	-6.833331	3.256556
H	1.025349	-2.836012	-2.103285	H	0.531817	-7.220641	8.222749
H	2.294475	-6.037294	-3.485128	H	-0.304894	6.373404	3.541752
H	-1.068767	-4.056986	-1.695015	H	-3.283257	-5.445482	5.842093
H	1.180473	-8.224607	-3.169163	H	-2.343805	5.725489	0.161454
H	-2.194307	-6.238939	-1.387920	H	0.180512	0.073315	-3.375573
H	-1.078479	-8.335540	-2.129246	H	-0.280220	-6.339020	6.918087
H	1.369541	-3.710813	-5.023888	H	-2.368135	5.825542	2.951341
H	-2.209953	-5.919839	-7.011875	H	2.131957	-1.157501	-3.739205
H	-2.634913	-5.829825	-5.295604	H	3.983896	0.488641	-2.238034
H	-2.924068	-3.591387	-7.369760	H	4.052293	-3.485967	1.253970
H	-4.184812	-4.199976	-6.286644	C	0.310983	-0.318827	0.189201
H	-2.699386	-1.980284	-5.578957	C	1.215774	0.938777	0.044104
H	-3.147224	-3.165922	-4.348241	H	1.075170	1.566866	0.936620
H	-0.300203	-5.337111	-5.136765	H	0.538020	-0.976328	-0.657530
H	2.487010	2.194488	-4.323133	C	-1.178439	-0.016107	0.161835
H	1.578333	3.213811	-3.234583	C	-1.793098	0.639454	1.243329
H	3.473466	3.279892	-1.633543	C	-1.970519	-0.417404	-0.924202
H	6.577002	-1.891675	-3.132040	C	-3.159907	0.887939	1.246145
H	4.865461	-1.531272	-3.169055	H	-1.194419	0.949238	2.093089
H	3.443624	-2.131654	-0.767937	C	-3.342235	-0.181172	-0.938094
H	8.545358	-2.484934	-1.583458	H	-1.515342	-0.921695	-1.771106
H	9.896617	-3.739339	0.070228	C	-3.921645	0.468042	0.151510
H	6.375603	-4.611531	2.415645	H	-3.642681	1.388995	2.075479
H	8.834576	-4.789041	2.046190	H	-3.959891	-0.492934	-1.770437
H	6.688399	0.211737	-1.469200	H	2.247996	0.568585	0.058091
H	-2.185730	-5.597785	3.606553	H	-4.279183	5.802453	-2.195833
H	-3.161269	-3.288738	7.102689	H	-4.609425	6.668001	1.644566
H	-0.981497	-3.651460	2.645853	H	-4.550907	4.739227	3.274047
H	-1.969793	-1.340960	6.130049	H	-7.928756	-2.447050	-3.875128
H	-0.383656	-1.344401	2.975413	H	-0.274068	-4.489271	-6.699047
H	0.439894	-4.782902	8.774373	H	1.184690	4.591762	4.067476
H	2.100408	-4.397167	6.218415	O	-0.079780	3.785868	2.713757
H	0.420833	-3.873794	6.431037	H	-1.039938	3.687614	2.616798
H	1.394749	-6.869800	6.716971	H	-5.266884	3.433719	5.319379
H	-7.964597	-4.965431	-3.649573	H	-8.152500	-4.812730	-1.910931
H	-5.756217	-3.784464	-3.500274	C	-5.622139	-5.748760	-2.648735
H	-8.188886	-2.293015	-2.134382	H	-5.908230	-6.278090	-3.564771
H	2.816606	-7.498117	1.239100	H	-4.528394	-5.753688	-2.585199
H	3.834636	-4.533721	4.182395	H	-6.005612	-6.325918	-1.797963
H	1.246463	-5.912139	0.183155	C	-5.723180	-3.578605	-1.362602
H	2.262035	-2.941861	3.128590	H	-6.036237	-2.530360	-1.353569
H	0.772713	-1.976373	1.240474	H	-6.137720	-4.059739	-0.467576
H	-3.652297	9.600116	1.608284	H	-4.631797	-3.593958	-1.268966
H	-3.456275	8.482574	2.962226	N	-5.359422	0.714706	0.147804
H	-4.876869	7.801265	0.317392	O	-5.853274	1.325021	1.101173
H	-5.453147	4.941127	6.217220	O	-6.024480	0.305583	-0.811765
H	-6.527571	4.586046	4.847070	H	2.107439	-5.301179	8.566856
H	-4.813462	6.244005	4.134025	C	2.169786	-1.469961	6.216554
H	0.446051	2.356910	4.883623	H	1.237045	-1.368250	5.656970
H	0.098295	3.616603	6.090275	H	2.492555	-0.483001	6.555166
H	-1.209243	2.968473	5.096612	H	2.943534	-1.892433	5.570811
H	-0.615407	5.960485	5.248603	S	1.943580	-2.496547	7.714217
H	-4.689661	4.137662	-2.641668				
H	-4.984752	4.714222	-0.993681				
H	-2.375098	2.523502	-2.684551				
				<b>Prod-S-C2-r1</b>			
				C	-3.093510	-0.349000	5.973608



C	-2.167066	-1.562358	5.866325	C	2.424958	5.098859	-5.088334
O	-1.779790	-2.168163	6.868189	O	2.161659	4.650861	-6.210033
N	-1.773453	-1.930083	4.605348	C	4.881814	4.604763	-5.557264
C	-0.682132	-2.890886	4.426624	N	1.470019	5.416037	-4.172642
C	0.643689	-2.211491	4.832203	C	0.041698	5.391900	-4.498912
O	0.830427	-1.005760	4.561793	C	-0.877268	4.825388	-3.410208
C	-0.665420	-3.418529	2.970680	C	-0.478980	3.415041	-2.984109
C	0.203377	-4.643692	2.775193	C	3.867380	5.193894	1.471557
C	-0.290676	-5.917742	3.093466	C	2.537190	4.570131	1.196165
C	1.513812	-4.535957	2.292495	C	1.949941	3.416540	1.664303
C	0.507389	-7.053839	2.946798	N	1.602859	5.121546	0.341013
C	2.314648	-5.670126	2.142938	C	0.525259	4.300987	0.321181
C	1.815913	-6.932192	2.472664	N	0.693486	3.251347	1.112391
N	1.583599	-2.935705	5.469359	O	-0.676421	1.416760	4.205304
C	1.490878	-4.337629	5.964994	O	-0.217091	-1.595553	-1.683716
C	2.926035	-4.643449	6.408136	H	-3.726340	-0.196067	5.100516
C	3.450017	-3.282495	6.891371	H	-2.475402	0.543428	6.115401
C	2.847845	-2.292730	5.886979	H	-1.701989	-3.660555	2.714200
C	-3.833698	2.731691	2.650198	H	-0.343787	-2.622384	2.294045
C	-4.823284	1.657248	3.119249	H	-1.310964	-6.019359	3.455302
O	-5.290243	1.702793	4.262855	H	1.903589	-3.560144	2.018646
C	-2.536204	2.714934	3.481985	H	0.105621	-8.031973	3.195567
C	-1.787250	1.394344	3.459880	H	3.324147	-5.568417	1.755063
O	-1.185554	1.470690	0.030741	H	2.437841	-7.814371	2.351823
O	-2.170254	0.393857	2.869286	H	-0.883126	-3.721612	5.106188
N	-5.156672	0.691039	2.218737	H	2.957995	-5.419638	7.176806
C	-6.002499	-0.451094	2.565902	H	3.510720	-4.990906	5.549625
C	-5.288003	-1.817888	2.569293	H	3.074485	-3.070503	7.898543
C	-5.139438	-2.455368	1.218674	H	4.540944	-3.226677	6.919770
C	-3.982368	-2.647765	0.500114	H	2.639620	-1.307416	6.309282
C	-6.200646	-3.033478	0.428115	H	3.495685	-2.150223	5.013765
C	-5.603086	-3.557335	-0.755164	H	1.138905	-5.009352	5.183833
C	-7.589046	-3.180252	0.607494	H	-2.757483	2.940377	4.531053
N	-4.254349	-3.297111	-0.685091	H	-1.848422	3.493035	3.134503
C	-6.351119	-4.211516	-1.742077	H	-3.586963	2.613645	1.590901
C	-8.334678	-3.827211	-0.371637	H	-5.883101	-2.482431	3.210902
C	-7.720702	-4.337386	-1.535564	H	-4.311990	-1.715860	3.052970
C	3.053787	-4.608230	-5.307039	H	-2.966609	-2.374893	0.748417
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C	2.913684	-3.482520	-6.124760	H	-9.406818	-3.945029	-0.240935
C	1.742114	-3.505266	-3.585915	H	-5.873175	-4.612810	-2.630374
C	2.191702	-2.373967	-5.686624	H	-8.328251	-4.840303	-2.282677
C	1.596156	-2.378804	-4.414355	H	-6.855954	-0.486447	1.878810
O	0.898625	-1.276087	-4.041553	H	2.567124	-5.474570	-3.393975
C	-0.236460	-6.904593	-7.120618	H	3.369013	-3.466111	-7.111576
C	-0.890124	-5.686735	-7.785000	H	1.285121	-3.524494	-2.602014
C	-1.077687	-4.529634	-6.800431	H	2.076000	-1.494653	-6.313092
C	8.684642	-2.031586	2.845988	H	0.476479	-1.399707	-3.140365
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C	-2.899591	-6.612845	-2.405047	H	-0.112440	-4.199294	-6.404292
C	-2.680946	-5.383332	-3.032018	H	-0.850863	-7.281708	-6.295815
C	-2.190898	-6.900511	-1.231432	H	8.031876	-3.154765	4.568348
C	-1.786803	-4.449806	-2.500461	H	6.110633	-3.124897	3.027499
C	-1.294027	-5.987207	-0.691364	H	9.017410	-2.194721	1.815825
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C	3.940408	8.019613	-1.917782	H	-0.749310	-6.217073	0.219347
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O	1.346680	6.890015	-1.753763	H	2.738746	9.835449	-2.050033
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**React-S-C2-r3**

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**TS2-S-C1-r3**

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**Int2-S-C1-r3**

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N	4.749893	0.356780	-2.397278	H	-2.960194	-5.985240	-6.562294
C	5.850299	-0.571596	-2.154801	H	-3.330867	-5.847741	-4.836379
C	5.571759	-2.021798	-2.611862	H	-3.533611	-3.618465	-6.930462
C	5.039258	-2.951197	-1.551394	H	-4.803875	-4.136658	-5.811777
C	3.967378	-2.751117	-0.709744	H	-3.169014	-2.007585	-5.161687
C	5.593315	-4.234733	-1.194973	H	-3.655825	-3.154078	-3.908854
C	4.804233	-4.752177	-0.125344	H	-0.966541	-5.502808	-4.750232
C	6.676484	-5.001501	-1.665110	H	2.325411	1.579527	-4.059617
N	3.822120	-3.827336	0.142455	H	1.619860	2.837040	-3.073599
C	5.071402	-5.990532	0.472151	H	3.684252	3.098420	-1.758210
C	6.945227	-6.231184	-1.074984	H	6.518880	-2.437424	-2.973123
C	6.149734	-6.720735	-0.016133	H	4.910673	-1.993974	-3.487264
C	-3.595500	-3.708199	5.733099	H	3.284322	-1.913927	-0.668423
C	-2.875832	-4.013095	4.571585	H	7.296892	-4.639116	-2.480969
C	-3.734940	-2.363899	6.096113	H	7.780000	-6.827983	-1.432819
C	-2.298535	-3.011703	3.782923	H	4.454950	-6.358509	1.287489
C	-3.166029	-1.352308	5.322638	H	6.384227	-7.685518	0.425366
C	-2.439298	-1.665895	4.160251	H	6.116602	-0.577405	-1.088731
O	-1.908695	-0.625770	3.463750	H	-2.754744	-5.049460	4.266293
C	-0.412499	-5.776300	7.965000	H	-4.291779	-2.096024	6.990524
C	0.683321	-4.733749	7.710991	H	-1.739277	-3.268552	2.884660
C	0.102060	-3.332206	7.506782	H	-3.273539	-0.308416	5.602002
C	-8.821603	-2.128903	-2.927600	H	-1.411898	-0.895275	2.653591
C	-8.100488	-3.463061	-2.705889	H	1.382117	-4.722522	8.556932
C	-6.759947	-3.362542	-1.951229	H	-0.517255	-3.302290	6.604921
C	2.467600	-6.070800	3.379100	H	-0.525672	-3.048967	8.359371
C	2.570371	-4.677408	3.459256	H	-1.124795	-5.808640	7.133711
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C	1.705185	-3.843282	2.745817	H	-6.123019	-2.653265	-2.502103
C	0.592250	-5.799354	1.849064	H	-9.120575	-1.662810	-1.983598
C	0.671964	-4.372842	1.911372	H	1.362579	-7.695451	2.482802
O	-0.165433	-3.623441	1.249215	H	3.336480	-4.227260	4.087798
C	-4.213725	8.413900	0.793183	H	-0.178899	-6.233411	1.218330
C	-2.716651	8.677853	0.655916	H	1.789049	-2.763109	2.835615
C	-1.876070	7.402153	0.722408	H	-0.122149	-2.137784	1.309587
O	-2.538263	6.302737	0.718341	H	-2.491507	9.170058	-0.299837
O	-0.628167	7.494749	0.787439	H	-2.355375	9.362976	1.431794
C	-4.309341	6.093202	3.838019	H	-4.560891	7.721707	0.023454
C	-2.887954	6.188015	4.418641	H	-5.135428	5.240218	5.657737
O	-2.707501	6.465229	5.610542	H	-6.177427	5.034001	4.234655
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N	-1.880125	5.936229	3.546702	H	0.829417	2.940273	3.141166
C	-0.461451	6.108970	3.854816	H	0.463446	3.597142	4.746373
C	0.411766	5.059967	3.143436	H	-0.844183	3.346580	3.568879
C	0.200568	3.650245	3.684887	H	-0.336112	6.041022	4.938007
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C	-2.860059	4.273521	-1.984781	H	-4.656644	5.253397	-1.339317
C	-2.416352	3.183905	-2.686244	H	-2.805236	2.715760	-3.576122
N	-1.983914	4.432552	-0.926114	H	-0.219040	3.382521	-0.304921
C	-1.047573	3.486509	-0.986679	H	-0.691951	1.890711	-2.345003
N	-1.289791	2.712458	-2.046223	H	-4.783362	9.346278	0.698255

H	-9.728487	-2.267979	-3.525736	C	-0.058043	-3.647795	-3.670544
H	3.978559	-1.307939	-6.174187	C	-1.319428	-2.816851	-3.958897
H	6.715705	-0.171697	-2.691249	O	-1.382853	-1.631480	-3.585799
H	3.940697	3.352265	-3.472502	C	-0.026108	-4.088973	-2.183648
H	3.141626	-6.712991	3.938291	C	-1.095214	-5.106718	-1.845268
H	0.017083	-6.776749	8.079065	C	-0.874380	-6.472763	-2.079426
H	-0.139555	7.111075	3.540575	C	-2.333095	-4.711507	-1.320185
H	-4.038439	-4.495898	6.334505	C	-1.868563	-7.416153	-1.813536
H	-2.080188	5.186572	-0.161973	C	-3.331601	-5.651844	-1.056747
H	0.019945	-0.163895	-2.890625	C	-3.104480	-7.007307	-1.306433
H	-0.974724	-5.546243	8.877033	N	-2.355529	-3.406825	-4.599121
H	-2.112155	5.809539	2.562747	C	-2.469131	-4.807837	-5.092332
H	1.809786	-1.470580	-3.496109	C	-3.957155	-4.934663	-5.443478
H	3.770420	0.021045	-2.261985	C	-4.351103	-3.511039	-5.866435
H	3.132313	-3.898483	0.885008	C	-3.573662	-2.626692	-4.885277
C	0.263864	-0.592488	0.090031	C	4.359404	1.281033	-2.723202
C	1.028922	0.744753	0.314176	C	5.312519	0.079660	-2.579548
H	0.309209	1.388801	0.840385	O	6.524435	0.255463	-2.767272
H	0.927369	-1.314480	-0.387473	C	2.881535	1.120699	-3.178355
C	4.356360	0.402631	3.045818	C	1.822335	0.233618	-2.463046
C	3.057860	0.183866	3.510446	O	1.519714	1.221558	-0.976824
C	4.606513	0.724770	1.712616	O	2.090352	-0.964345	-2.123444
C	1.997630	0.293807	2.618019	N	4.787062	-1.103487	-2.173306
H	2.893009	-0.062181	4.551676	C	5.635903	-2.245607	-1.843398
C	3.532944	0.824730	0.832715	C	5.066571	-3.612415	-2.251808
H	5.622666	0.896788	1.381282	C	4.109761	-4.255704	-1.283639
C	2.217688	0.603697	1.260828	C	3.479965	-3.701987	-0.192469
H	0.987298	0.124074	2.966959	C	3.717274	-5.643986	-1.306048
H	3.716983	1.074373	-0.201117	C	2.851896	-5.857729	-0.193556
H	-0.557190	-0.379457	-0.609284	C	4.020777	-6.730201	-2.147866
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H	-4.451349	7.974447	1.762883	C	2.295974	-7.111548	0.090804
H	-4.277089	5.882863	2.766078	C	3.470486	-7.976596	-1.869617
H	-8.179611	-1.417106	-3.459668	C	2.616669	-8.164062	-0.760755
H	-0.931487	-4.671914	-6.320628	C	-4.473892	-2.358493	5.841586
H	1.458413	5.355524	3.335213	C	-3.792308	-2.905588	4.746953
H	-4.729941	4.031882	4.427582	C	-4.375375	-0.979572	6.062850
O	0.164128	5.021407	1.740342	C	-3.027014	-2.110904	3.886919
H	0.010910	5.933625	1.391784	C	-3.615867	-0.171366	5.215948
H	-8.762657	-4.152058	-2.161401	C	-2.931616	-0.728813	4.120518
C	-6.045154	-4.721761	-1.939288	O	-2.213367	0.121769	3.341536
H	-5.881448	-5.096883	-2.955953	C	-1.952297	-4.961096	8.343097
H	-5.069913	-4.654400	-1.445128	C	-1.135394	-3.758053	8.827142
H	-6.638828	-5.470882	-1.400434	C	-0.835588	-2.777993	7.691013
C	-6.927794	-2.829395	-0.520548	C	-8.944305	-0.229351	-3.119073
H	-7.364940	-1.826489	-0.502974	C	-8.607925	-1.423383	-2.219080
H	-7.579618	-3.489099	0.066244	C	-7.148034	-1.480764	-1.727210
H	-5.961897	-2.776148	-0.007425	C	0.872904	-6.305303	3.913300
N	5.474506	0.304909	3.978412	C	1.385602	-5.003286	3.896727
O	5.231691	0.036422	5.159603	C	-0.253200	-6.579355	3.121212
O	6.616443	0.496724	3.547049	C	0.802994	-3.999366	3.115654
H	1.265410	-5.014971	6.825289	C	-0.846425	-5.593990	2.340047
S	1.445227	-2.085560	7.334930	C	-0.346668	-4.252923	2.300819
C	0.448028	-0.586779	7.016017	O	-0.924432	-3.344108	1.571543
H	-0.218998	-0.374911	7.855670	C	-1.967950	9.126087	0.048818
H	1.146967	0.244398	6.901162	C	-0.537148	9.509652	0.438829
H	-0.136931	-0.692273	6.099561	C	0.455331	8.448807	-0.054142
<b>TS3-S-C1-r3</b>				O	0.154947	7.239404	0.311811
C	2.981155	-2.144503	-5.452644	O	1.424626	8.768849	-0.753091
C	1.710505	-2.969930	-5.239569	C	-2.704266	7.142504	3.240952
O	1.245786	-3.666581	-6.149501	C	-1.353259	6.759167	3.862729
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				C	-3.858286	6.412056	3.947038

N	-0.341678	6.510776	2.987429	H	0.920970	2.901569	4.553091
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C	1.332007	4.708946	3.444840	H	-0.418973	4.069034	4.566082
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C	-2.493189	5.730870	-2.721554	H	-3.091302	5.173483	-3.445203
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N	0.008977	3.213370	-1.619823	H	-2.702192	9.837641	0.443005
O	0.626379	0.447240	-3.135077	H	-9.974993	-0.291618	-3.484342
O	-0.473198	-0.847557	1.407876	H	3.748407	-2.797164	-5.877321
H	3.356450	-1.687352	-4.536913	H	6.584913	-2.076912	-2.357729
H	2.772137	-1.361531	-6.188377	H	4.848678	1.952850	-3.432827
H	0.964687	-4.513268	-1.996160	H	1.332291	-7.078920	4.521157
H	-0.131154	-3.206895	-1.545998	H	-2.163734	-5.649861	9.167586
H	0.088920	-6.799235	-2.462426	H	1.693022	6.698415	2.694738
H	-2.506502	-3.663175	-1.098366	H	-5.067650	-2.987140	6.497817
H	-1.675381	-8.469568	-1.996524	H	-0.362936	6.227396	-0.719189
H	-4.283604	-5.325248	-0.647517	H	0.071500	-0.357613	-3.059245
H	-3.879329	-7.739444	-1.097178	H	-2.909231	-4.641515	7.916848
H	-0.047136	-4.534003	-4.307949	H	-0.428265	6.787094	2.000425
H	-4.131056	-5.683568	-6.220317	H	1.515153	-2.234150	-3.309851
H	-4.520853	-5.232704	-4.552734	H	3.761763	-1.162869	-2.049932
H	-4.017484	-3.316600	-6.891925	H	2.158561	-4.490735	1.290132
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H	-3.304324	-1.648144	-5.289106	C	1.053388	0.709621	0.265504
H	-4.134952	-2.458826	-3.956920	H	0.434052	1.502865	0.719286
H	-2.158688	-5.518972	-4.326553	H	0.669752	-1.373616	-0.238420
H	2.878418	0.725812	-4.201960	C	4.215942	0.020403	3.123831
H	2.460957	2.127761	-3.251882	C	2.905800	0.197405	3.576290
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H	5.920804	-4.291372	-2.380114	C	1.896785	0.414989	2.645739
H	4.613938	-3.526039	-3.248934	H	2.697996	0.171124	4.638270
H	3.503281	-2.686906	0.177029	C	3.501358	0.274833	0.849396
H	4.674953	-6.597530	-3.005697	H	5.550913	-0.083490	1.441822
H	3.698736	-8.821403	-2.513815	C	2.176463	0.455336	1.266074
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H	2.202063	-9.149730	-0.568061	H	3.724308	0.304758	-0.205996
H	5.860077	-2.254142	-0.767173	H	-0.665464	-0.266635	-0.591611
H	-3.849558	-3.973687	4.552751	H	-2.076459	6.609789	-3.224205
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H	-3.541189	0.898771	5.385333	H	-8.284401	-0.195480	-3.994033
H	-1.716427	-0.320470	2.610886	H	-1.831478	-4.940244	-5.974928
H	-1.683438	-3.236237	9.621592	H	2.419630	4.592461	3.518245
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H	-1.766174	-2.418246	7.240848	O	0.977532	4.113404	2.188681
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H	2.256116	-4.759055	4.503342	C	-6.886198	-2.792376	-0.972431
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**Prod-S-C1-r3**

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**TS1-S-C2-r3**

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**TS2-S-C2-r3**

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H	0.417311	5.275671	2.274251	C	-1.373051	6.955022	2.119947
<b>Int2-S-C2-r3</b>				O	-2.132591	5.924407	2.027672
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**TS3-S-C2-r3**

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C	-3.774386	-4.212018	-6.437998	H	2.952276	-0.001307	-5.203118
C	-4.401762	-2.813339	-6.543604	H	2.048113	0.667587	-6.581233
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C	3.607700	2.641100	-2.764100	H	0.174213	-2.619027	-2.465634
C	4.750278	1.638388	-3.032030	H	0.432125	-5.975993	-4.051835
O	5.837447	2.050436	-3.459437	H	-2.078527	-3.301757	-1.821206
C	2.152924	2.404204	-3.245744	H	-1.158494	-7.825548	-3.636098
C	1.332516	1.145232	-2.893560	H	-3.673001	-5.148088	-1.397673
O	0.846211	1.405146	-1.143225	H	-3.226462	-7.418842	-2.311460
O	1.881333	-0.003082	-2.911682	H	0.108203	-3.434525	-5.425601
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C	5.569200	-0.670900	-2.918100	H	-4.223570	-4.765069	-5.605795
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C	3.894877	-2.823441	-0.455245	H	-3.593025	-0.957424	-5.648206
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C	5.603032	-3.057311	0.984719	H	-1.833455	-4.713917	-5.542095
C	7.525903	-2.462618	-0.389534	H	2.149461	2.398917	-4.342930
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C	6.418867	-3.303456	2.095679	H	3.594349	2.803070	-1.677635
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C	-3.383700	-4.614700	5.179600	H	2.854034	-2.856035	-0.747201
C	-2.685072	-4.691274	3.969345	H	7.964759	-2.146752	-1.332206
C	-3.479208	-3.374642	5.821621	H	9.414335	-2.579246	0.625689
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C	-2.889124	-2.238427	5.268942	H	8.448383	-3.301043	2.789226
C	-2.186469	-2.319671	4.053136	H	6.453857	-0.441623	-2.313014
O	-1.637127	-1.179189	3.572889	H	-2.598950	-5.643447	3.452440
C	-0.171700	-7.192500	6.737700	H	-4.020706	-3.287805	6.759973
C	-0.284948	-6.343922	8.009115	H	-1.544718	-3.636055	2.465155
C	-0.119134	-4.851960	7.712892	H	-2.966470	-1.272454	5.758960
C	-9.187300	-1.320100	-2.584300	H	-1.191324	-1.294525	2.688372
C	-8.799603	-2.795541	-2.730235	H	-1.261415	-6.514068	8.479307
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C	2.296600	-6.850200	1.920700	H	-0.872615	-4.520568	6.991401
C	2.052723	-5.740018	2.738017	H	0.805172	-7.063561	6.258771
C	1.965276	-6.746469	0.562071	H	-9.161838	-3.162611	-3.700092
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C	1.419804	-5.580877	0.036738	H	-8.936753	-0.926675	-1.594306
C	1.159751	-4.426997	0.843545	H	2.140655	-7.592793	-0.100699
O	0.668090	-3.340447	0.318151	H	2.294885	-5.789162	3.798827
C	-3.604300	8.186400	2.384000	H	1.166977	-5.522222	-1.017878
C	-2.217319	8.756671	2.693931	H	1.308722	-3.717718	2.888251
C	-1.094377	8.042197	1.931270	H	0.162348	-2.024937	0.932674
O	-1.167752	6.737603	1.972394	H	-2.167633	9.826699	2.471388
O	-0.210993	8.686376	1.360718	H	-2.006959	8.638207	3.766038
C	-3.602600	5.389600	5.000200	H	-3.870310	8.352392	1.333501
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O	-1.870435	4.567224	6.474237	H	-5.603343	4.619630	5.392706
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C	0.927871	4.430399	3.542936	H	-0.765398	3.224517	2.902756

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H	-2.583521	2.984170	-2.349233	C	2.141592	0.298605	-6.406995
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H	3.946066	3.578718	-3.210552	C	-0.235723	-2.910903	-3.579768
H	2.726435	-7.760810	2.327162	C	-1.341348	-3.899312	-3.275346
H	-0.295375	-8.256547	6.963769	C	-1.241918	-5.236776	-3.688574
H	0.724744	6.177414	4.778937	C	-2.488472	-3.500631	-2.576208
H	-3.846849	-5.498124	5.607676	C	-2.264546	-6.148431	-3.419156
H	-1.586072	5.860001	0.648660	C	-3.512469	-4.409828	-2.302538
H	-0.326790	0.402729	-3.589446	C	-3.405303	-5.736255	-2.726369
H	-0.937996	-6.911121	6.007784	N	-2.655381	-1.999070	-5.803169
H	-1.478414	5.886438	3.593562	C	-2.737846	-3.322372	-6.477938
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H	3.564257	0.054414	-2.578262	C	-4.693865	-2.016416	-7.010347
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H	0.961688	-0.644291	-1.070958	C	2.062072	2.934632	-3.421102
C	4.223215	0.079727	2.870406	C	1.234489	1.661027	-3.479372
C	3.112689	-0.456378	3.526280	O	1.060663	1.418750	-0.034960
C	4.128648	0.601966	1.581722	O	1.615033	0.567226	-3.082781
C	1.891141	-0.470440	2.866299	N	4.648167	0.618228	-2.782090
H	3.218311	-0.847871	4.529899	C	5.346999	-0.517696	-3.383000
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H	5.009567	1.003262	1.097377	C	4.720390	-2.580115	-1.981704
C	1.761419	0.041571	1.561802	C	3.705324	-2.904461	-1.111513
H	1.018356	-0.877918	3.363593	C	5.929991	-3.128109	-1.410807
H	2.799378	0.988556	-0.062320	C	5.563930	-3.764098	-0.187712
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H	-3.647435	6.542931	-1.453421	N	4.207087	-3.604009	-0.033692
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H	-3.704275	5.447802	3.912819	C	8.209401	-3.817572	-1.009201
H	-8.670534	-0.701150	-3.327118	C	7.823782	-4.432323	0.200540
H	-1.716188	-3.778025	-7.048127	C	-3.223299	-5.191599	4.740000
H	1.947567	4.237218	3.904644	C	-2.718595	-4.905716	3.467984
H	-4.384705	3.358314	5.141508	C	-2.789801	-4.428411	5.828602
O	1.087989	5.204098	2.351311	C	-1.790818	-3.881269	3.274602
H	0.316227	5.805095	2.222815	C	-1.863918	-3.401770	5.652475
H	-9.322688	-3.389888	-1.966920	C	-1.350615	-3.121844	4.373906
C	-6.998635	-4.555094	-2.969027	O	-0.440313	-2.127705	4.261125
H	-5.923694	-4.764918	-2.945227	C	0.023100	-7.955999	5.839200
H	-7.482402	-5.222922	-2.245139	C	0.537844	-7.026503	6.944135
H	-7.371997	-4.819285	-3.964953	C	1.140706	-5.742063	6.371618
C	-6.706802	-2.720442	-1.259524	C	-9.378883	-1.029636	-2.302788
H	-6.837739	-1.660191	-1.023098	C	-8.259526	-1.819235	-2.997437
H	-7.191910	-3.302503	-0.465798	C	-8.627737	-3.313337	-3.089346
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**Int1-R-C1-r1**

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C	-2.491316	-3.866057	6.146716	H	6.004648	-6.475147	-4.149592
C	-1.489800	-3.825516	3.541314	H	4.323500	-6.315552	-0.171739
C	-1.503844	-2.944332	5.801613	H	5.058956	-7.618482	-2.166470
C	-0.978528	-2.928501	4.497722	H	6.432880	0.060042	-1.132851
O	0.005750	-2.051785	4.206944	H	-2.850386	-5.438388	3.155388
C	0.402900	-6.746200	7.237600	H	-2.883002	-3.872101	7.160773
C	1.092938	-5.592085	7.973957	H	-1.093157	-3.788856	2.533028
C	1.696190	-4.578173	7.000104	H	-1.116717	-2.237714	6.529730
C	-8.326600	-2.803900	-3.294300	H	0.423281	-2.289414	3.311654
C	-9.550811	-2.646040	-2.386597	H	0.366834	-5.084372	8.620596
C	-9.317224	-3.011317	-0.906937	H	2.471792	-5.045870	6.384232
C	3.301900	-6.242300	2.681900	H	0.921639	-4.188067	6.333954
C	3.771851	-5.006271	3.139789	H	1.104387	-7.274993	6.582785
C	2.113748	-6.268165	1.938664	H	-10.363210	-3.274757	-2.776229
C	3.064733	-3.826159	2.888268	H	-8.906748	-4.032661	-0.879511
C	1.401799	-5.100889	1.679386	H	-7.507722	-2.142513	-2.994744
C	1.834450	-3.836639	2.170604	H	1.736479	-7.215148	1.557805
O	1.114559	-2.750757	1.977291	H	4.700686	-4.956482	3.704546
C	-4.827000	7.682500	1.606500	H	0.485770	-5.135079	1.096418
C	-3.333680	7.970837	1.835431	H	3.428703	-2.872102	3.262099
C	-2.495069	7.126130	0.868868	H	1.774661	-1.206928	1.974803
O	-2.137798	5.954594	1.299860	H	-3.129787	9.029868	1.647442
O	-2.284299	7.552717	-0.277562	H	-3.062723	7.743851	2.871269
C	-4.686700	5.044700	4.379400	H	-5.111653	7.938221	0.580797
C	-3.268805	5.126307	4.977503	H	-5.613126	4.673405	6.304187
O	-3.082912	5.065567	6.197993	H	-6.652384	4.277041	4.916774
C	-5.626400	4.252900	5.296600	H	-5.054151	6.072085	4.262257
N	-2.265611	5.282697	4.078060	H	0.455294	2.248347	3.935686
C	-0.860800	5.450400	4.444300	H	0.094661	2.993778	5.505363
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C	-0.168384	2.990945	4.442325	H	-0.791022	5.424999	5.533501
C	-4.291300	4.850500	-1.735800	H	-4.892624	4.629637	-2.621029
C	-2.983242	4.160082	-1.813016	H	-4.865815	4.538710	-0.855010
C	-2.500466	3.214248	-2.680472	H	-2.988997	2.752875	-3.525874
N	-1.964369	4.407562	-0.918246	H	0.013884	3.607042	-0.720035
C	-0.922679	3.630755	-1.249759	H	-0.433390	1.941182	-2.803155
N	-1.212818	2.891116	-2.315837	H	-5.456550	8.264659	2.287898
O	0.339262	1.182414	-3.207128	H	-8.575707	-2.569586	-4.334809
O	2.115078	-0.274833	1.921028	H	4.284399	-0.252066	-6.373363
H	3.724502	0.280066	-4.763311	H	6.897977	0.696266	-2.695851
H	2.839603	0.752716	-6.231205	H	3.896205	4.027537	-2.977964
H	2.567195	-3.581442	-2.911197	H	3.850869	-7.156305	2.887662
H	1.223717	-2.742126	-2.148241	H	-0.006426	-7.474145	7.946030



C	-2.512438	3.068195	-2.693085	H	-2.801210	2.631539	-3.635457
N	-2.350774	4.155324	-0.784213	H	-0.378250	3.472759	-0.285805
C	-1.217649	3.477047	-0.959060	H	-0.568733	2.140630	-2.489930
N	-1.291903	2.810348	-2.111947	H	-6.114849	8.168663	1.540749
O	0.513468	1.188831	-3.130744	H	-8.199341	-3.117667	-4.604134
O	2.207719	-0.198503	1.913777	H	4.599693	-0.055755	-6.095700
H	3.852664	0.508153	-4.572399	H	6.948373	1.145538	-2.381877
H	3.090564	0.857813	-6.142565	H	3.758563	4.278707	-2.810939
H	2.889381	-3.399286	-2.658683	H	4.203968	-6.797475	3.242730
H	1.416930	-2.688276	-2.012782	H	0.219427	-7.330453	8.121722
H	2.929290	-5.754495	-3.445997	H	-1.317673	6.526275	4.080258
H	-0.599282	-4.081318	-1.658009	H	-3.562211	-5.647285	5.507589
H	1.975135	-8.024874	-3.208495	H	-2.634359	4.738903	0.079221
H	-1.558419	-6.345975	-1.419157	H	0.335707	0.232339	-3.226987
H	-0.278725	-8.333848	-2.198885	H	-0.316912	-6.341071	6.754417
H	1.894242	-3.449203	-4.944073	H	-2.919965	4.869590	2.966281
H	-1.375438	-5.840110	-7.222028	H	2.364632	-0.855735	-3.565054
H	-1.888648	-5.880834	-5.527901	H	4.014774	0.774603	-2.058530
H	-2.273159	-3.565071	-7.499130	H	4.416431	-3.363543	1.046508
H	-3.527223	-4.337717	-6.517506	C	1.110417	1.067564	0.158584
H	-2.278933	-2.041801	-5.619335	C	2.305148	0.168981	0.549366
H	-2.680497	-3.327526	-4.476715	H	3.214671	0.763449	0.395924
H	0.382639	-5.199676	-5.222143	H	1.053657	1.811702	0.961905
H	2.664566	2.317636	-4.005168	C	-0.223486	0.326332	0.160270
H	1.582667	3.367696	-3.115916	C	-0.501891	-0.681803	-0.773284
H	3.245912	3.596041	-1.275780	C	-1.217406	0.666812	1.091417
H	7.203750	-1.101898	-2.776141	C	-1.745246	-1.298171	-0.820806
H	5.600347	-0.859967	-3.420081	H	0.254253	-0.962697	-1.492250
H	4.894447	-1.034813	0.270047	C	-2.463781	0.046019	1.080124
H	6.653235	-3.598552	-3.867144	H	-1.021850	1.443822	1.823064
H	6.574605	-6.075308	-3.812260	C	-2.716124	-0.924287	0.109987
H	4.802445	-6.016665	0.128737	H	-1.970987	-2.034895	-1.579719
H	5.663346	-7.273853	-1.845484	H	-3.234343	0.311510	1.792457
H	6.465353	0.500362	-0.828405	H	2.370019	-0.702976	-0.102638
H	-2.496089	-5.772177	3.258715	H	-4.455230	5.627923	-2.084648
H	-3.046171	-3.717380	6.996923	H	-5.674145	6.475884	1.835580
H	-0.911311	-4.001484	2.526003	H	-5.064623	4.312129	3.141984
H	-1.447724	-1.961285	6.259386	H	-7.581695	-4.421704	-3.581137
H	0.337898	-2.204449	3.177329	H	0.409833	-4.267943	-6.734921
H	0.265706	-4.896268	8.728229	H	0.630193	5.184570	3.834867
H	2.370715	-4.637709	6.505578	O	-0.535709	4.639966	2.198819
H	0.721661	-3.992294	6.422071	H	-0.828390	5.532411	1.889327
H	1.314129	-7.027143	6.764388	H	-5.781934	2.975817	5.168672
H	-10.004850	-3.886270	-3.097494	H	-9.564900	-2.236920	-2.688490
H	-8.568123	-4.719030	-1.215534	C	-10.324858	-3.746820	-0.460671
H	-7.148294	-2.744156	-3.235039	H	-10.194308	-4.088356	0.572011
H	2.224392	-7.085762	1.746723	H	-10.786075	-2.751881	-0.423439
H	4.784788	-4.508052	4.048022	H	-11.033394	-4.423277	-0.952176
H	0.838813	-5.140081	1.109638	C	-7.989424	-2.791019	-0.465128
H	3.380561	-2.559457	3.421913	H	-6.986974	-2.804418	-0.900960
H	1.833453	-1.117688	1.946778	H	-8.340872	-1.751155	-0.467154
H	-3.683469	8.710003	1.065794	H	-7.887657	-3.099304	0.581273
H	-3.883865	8.077597	2.681855	N	-4.035268	-1.548685	0.048741
H	-5.504193	7.157136	0.223319	O	-4.887160	-1.205076	0.873189
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H	-5.642876	5.781363	3.912418	S	2.071144	-2.731222	7.976166
H	0.546046	2.684650	3.528580	C	2.491699	-1.678777	6.539163
H	0.062801	3.197840	5.154770	H	2.731258	-0.686672	6.927781
H	-1.172680	2.711994	3.977906	H	3.361416	-2.074311	6.009461
H	-1.312335	5.364399	5.417526	H	1.646222	-1.605336	5.850533
H	-5.051485	4.145445	-2.847741				
H	-5.133282	4.343003	-1.087275				

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C	3.647996	0.062967	-5.617978	C	-5.099932	4.754770	4.160903
C	2.869916	-1.260083	-5.612361	C	-3.682925	4.779221	4.763597
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C	0.076196	-2.402055	-4.645792	C	-1.309038	5.386036	4.360015
O	-0.396962	-1.313446	-4.268711	C	-0.370791	4.213851	4.012765
C	1.542827	-3.239741	-2.749325	C	-0.650232	2.942508	4.812156
C	0.673973	-4.436932	-2.427357	C	-4.469071	4.534016	-1.934007
C	1.172505	-5.743073	-2.549226	C	-3.044639	4.236429	-1.592024
C	-0.653469	-4.267026	-2.008097	C	-2.164249	3.331955	-2.132298
C	0.364073	-6.847367	-2.270896	N	-2.356384	4.867461	-0.569829
C	-1.464748	-5.368211	-1.728005	C	-1.125174	4.354141	-0.500861
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C	-0.263002	-4.578002	-5.929968	O	2.055463	-0.002126	1.799676
C	-1.591046	-5.167894	-6.422288	C	0.834300	1.148175	0.008890
C	-2.397461	-3.930185	-6.845020	C	2.081121	0.309863	0.418457
C	-2.035297	-2.892746	-5.776120	C	-0.436760	0.301900	0.038859
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C	4.953266	2.537971	-2.259643	C	-1.143320	-0.021872	-1.128970
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C	2.433920	2.649755	-3.129761	C	-2.276945	-0.825734	-1.089832
C	1.745435	1.339202	-2.685581	C	-2.719600	-1.307450	0.142382
O	1.019257	1.900665	-1.188527	O	-0.408647	3.945796	2.603167
O	2.423236	0.284937	-2.438133	N	-3.891136	-2.172017	0.184241
N	4.951391	1.214211	-1.963246	O	-4.340128	-2.508346	1.283256
C	6.198011	0.446983	-1.951992	O	-4.384598	-2.537935	-0.892365
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C	5.907973	-1.491406	-0.272343	C	-5.534992	-5.316105	-3.580689
C	4.843548	-2.083322	0.365057	C	2.157520	-1.602855	7.184857
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C	6.470446	-2.009175	1.906990	H	3.970437	0.366068	-4.622232
C	8.306477	-0.984180	0.675197	H	2.999841	0.842063	-6.031954
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C	7.252002	-2.122568	3.063173	H	1.240961	-2.381064	-2.141552
C	9.086035	-1.098321	1.821101	H	2.204384	-5.894272	-2.857251
C	8.562344	-1.659429	3.005103	H	-1.051110	-3.263119	-1.893752
C	-2.844034	-4.946040	5.150024	H	0.770085	-7.850459	-2.366691
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C	-1.692005	-2.880104	5.697376	H	-1.443552	-5.888541	-7.230516
C	-0.981726	-2.933806	4.483209	H	-2.094432	-5.682153	-5.596389
O	-0.078815	-1.967181	4.219376	H	-2.068312	-3.583803	-7.831047
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**Prod-R-C1-r1**

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C	-3.309476	5.606778	4.726609	H	-2.991596	8.542297	1.003425
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**Int1-R-C2-r1**

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C	7.815634	-2.873129	2.177837	H	4.344851	-2.209209	-3.043108
C	-3.286128	-4.845138	4.984255	H	3.017504	-2.830098	-0.761362
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C	-3.202561	-3.852659	5.966900	H	9.482786	-2.292512	0.931137
C	-1.752271	-3.559770	3.593009	H	5.986641	-3.420012	3.197028
C	-2.407109	-2.724874	5.773970	H	8.439053	-3.024940	3.054427
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C	0.385596	-6.473773	7.304077	H	-1.185788	-3.446955	2.672400
C	0.855815	-5.247246	6.517925	H	-2.338998	-1.950680	6.532097
C	-8.997710	-0.947209	-2.565519	H	-0.434756	-1.401347	3.596485
C	-8.778424	-2.313252	-3.225111	H	-0.405218	-6.175130	8.002979
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C	2.354242	-6.992517	1.599492	H	0.030090	-4.818275	5.941692
C	2.377042	-5.992665	2.577073	H	0.644671	-7.918508	5.687628
C	1.773836	-6.690969	0.359893	H	-8.125261	-2.181278	-4.098269
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C	1.243023	-5.432994	0.098991	H	-9.709417	-1.002008	-1.735315
C	1.261477	-4.391192	1.073218	H	1.737948	-7.451220	-0.418448
O	0.784918	-3.203745	0.795063	H	2.818177	-6.200719	3.550388
C	-3.227797	8.107805	2.997196	H	0.796726	-5.214135	-0.866302
C	-1.794924	8.189757	2.467767	H	1.845938	-3.967422	3.116357
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C	-3.292405	5.153064	5.432716	H	-3.818866	7.410607	2.400590
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C	-3.531306	5.673388	-0.671500	H	-4.215792	5.716125	-1.522743
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H	0.637326	-3.356535	-5.329101	H	-1.512144	5.700854	3.453764
H	-3.272621	-4.938283	-7.277363	H	1.742794	-1.017970	-3.890125
H	-3.558340	-5.005324	-5.530366	H	3.914346	0.133462	-2.337354
H	-3.757553	-2.525792	-7.320981	H	3.906316	-3.274589	1.923140
H	-4.996083	-3.130595	-6.211049	C	0.257973	0.030463	0.960869
H	-3.223903	-1.162903	-5.403782	C	1.454166	0.107587	-0.019298
H	-3.736136	-2.408845	-4.264787	H	2.358040	0.131727	0.600160
H	-1.176394	-4.769255	-5.532931	H	0.221160	0.959489	1.538607
H	2.379905	2.124654	-3.956207	C	-1.105965	-0.167229	0.309290
H	1.803305	3.166725	-2.674091	C	-2.060194	0.859937	0.327415
H	3.934220	3.085910	-1.492124	C	-1.453185	-1.405980	-0.257989
H	6.194598	-2.632345	-2.692716	C	-3.321254	0.685829	-0.234653
H	4.511663	-2.145049	-2.707844	H	-1.816685	1.810838	0.788541
H	3.218402	-2.673114	-0.375772	C	-2.706761	-1.597718	-0.823635
H	8.325063	-1.887951	-0.857986	H	-0.742923	-2.228165	-0.225489
H	9.736869	-2.245859	1.142435	C	-3.624477	-0.545859	-0.814196
H	6.277923	-3.268351	3.513108	H	-4.056892	1.479201	-0.229858
H	8.733377	-2.925529	3.302661	H	-2.989890	-2.543728	-1.265289
H	6.797225	-0.243779	-1.952461	H	1.487883	-0.795984	-0.626456
H	-2.666200	-5.389081	3.304009	H	-3.346446	6.517097	-1.137936
H	-3.632580	-3.456403	7.023792	H	-3.908175	7.159676	2.466308
H	-1.253808	-3.458469	2.660167	H	-3.729160	5.491161	3.806737
H	-2.222415	-1.521034	6.368275	H	-7.762753	-1.296704	-2.548718
H	-0.458169	-1.298497	3.304721	H	-1.184254	-3.728244	-6.973128
H	-0.379047	-5.522254	8.421331	H	2.000301	4.503399	4.056183
H	1.634861	-4.978602	6.168461	H	-9.970489	-2.333924	-4.440982
H	-0.017469	-4.339540	6.240804	H	-4.151990	3.298511	4.969163
H	0.739939	-7.421013	6.266073	H	1.269325	-6.134504	8.377494
H	-8.546753	-1.447741	-4.958937	S	1.426601	-3.254526	7.852856
H	-7.087553	-3.272807	-4.083677	C	1.891838	-2.088730	6.521188
H	-9.246235	-2.111645	-2.034754	H	2.267865	-1.185625	7.006825
H	2.288691	-7.504069	0.226587	H	2.684935	-2.511176	5.898783
H	2.764154	-5.622531	4.061465	H	1.031485	-1.828643	5.900004
H	1.309710	-5.425947	-0.672887	C	-8.167613	-3.952695	-5.810432
H	1.750507	-3.545910	3.174458	H	-7.584023	-4.870535	-5.943149
H	0.747928	-1.907647	1.412018	H	-9.195891	-4.165438	-6.129684
H	-1.841004	9.388840	1.957842	H	-7.761263	-3.194346	-6.489330
H	-1.694733	8.150965	3.225260	C	-8.657303	-4.573040	-3.413839
H	-4.054448	8.454776	1.272923	H	-8.573122	-4.288345	-2.360917
H	-4.404641	4.155989	6.496920	H	-9.713636	-4.789653	-3.619024
H	-5.559326	4.357076	5.160517	H	-8.095646	-5.503998	-3.549433
H	-4.073573	6.364772	5.303487	O	1.177407	5.431386	2.474730
H	1.123515	2.768339	2.537002	H	0.296775	5.669641	2.113311
H	0.407262	2.582807	4.151506	N	-4.934160	-0.745537	-1.422373
H	-0.543621	3.300338	2.840593	O	-5.749814	0.180250	-1.379370
H	0.245933	4.773964	5.661115	O	-5.172122	-1.836225	-1.956806
H	-4.354999	5.408211	-2.095740				
H	-4.269018	5.241499	-0.335877				
H	-2.809524	3.277748	-3.184635	<b>Int2-R-C2-r1</b>			
H	0.343486	3.403698	-0.415119	C	3.153723	-0.283886	-5.877048
H	-0.369502	1.995584	-2.561612	C	2.140875	-1.433945	-5.817021
H	-4.096919	8.836496	3.000787	O	1.821727	-2.057069	-6.838101
H	-9.335087	-0.530990	-2.809523	N	1.641717	-1.712586	-4.584540
H	3.869970	-0.506670	-6.564269	C	0.692381	-2.799038	-4.365988
H	6.292262	-0.509588	-3.609204	C	-0.753376	-2.282711	-4.433154
H	4.138177	3.614369	-3.152686	O	-1.075281	-1.252430	-3.815084
H	3.037428	-7.629418	2.607803	C	0.967918	-3.495600	-3.007654
H	-0.346021	-7.880559	7.586708	C	0.307357	-4.852896	-2.889083
H	0.600956	6.318968	4.881560	C	0.966390	-6.003289	-3.348840
H	-3.869557	-5.414960	5.488649	C	-0.977747	-4.997235	-2.347825
H	-1.358850	5.210879	0.313487	C	0.358674	-7.257649	-3.275811
				C	-1.591851	-6.249534	-2.274589

C	-0.925329	-7.384814	-2.740108	N	-1.065886	2.968561	-2.103359
N	-1.663032	-2.977637	-5.153494	O	0.457360	1.032775	-3.021284
C	-1.469684	-4.226472	-5.937272	O	0.538441	-0.873409	1.962574
C	-2.906199	-4.685255	-6.215044	H	3.438395	0.078317	-4.889496
C	-3.690502	-3.367915	-6.318712	H	2.718730	0.538217	-6.454324
C	-3.052764	-2.485961	-5.237808	H	2.052666	-3.608870	-2.921566
C	3.870811	2.794574	-2.546486	H	0.648460	-2.837868	-2.194561
C	5.104412	1.871124	-2.624629	H	1.968115	-5.913114	-3.761613
O	6.221683	2.368899	-2.836287	H	-1.497669	-4.121018	-1.974256
C	2.456096	2.280296	-2.943604	H	0.890034	-8.135832	-3.631729
C	1.753157	1.018832	-2.317092	H	-2.586276	-6.337380	-1.846413
O	1.437394	1.317352	-0.893242	H	-1.398674	-8.360498	-2.679235
O	2.348993	-0.138806	-2.474984	H	0.862952	-3.514897	-5.173016
N	4.911771	0.555246	-2.385612	H	-2.972194	-5.302540	-7.114608
C	6.005962	-0.409318	-2.422408	H	-3.271598	-5.277513	-5.368942
C	5.531903	-1.839948	-2.776486	H	-3.542177	-2.918621	-7.307100
C	5.344423	-2.754818	-1.598234	H	-4.765320	-3.494303	-6.165567
C	4.226237	-2.899774	-0.808946	H	-3.057004	-1.421112	-5.483812
C	6.339548	-3.642585	-1.047925	H	-3.549706	-2.598425	-4.266767
C	5.745613	-4.298156	0.070713	H	-0.898871	-4.962254	-5.370089
C	7.667758	-3.959567	-1.389080	H	2.456680	2.065998	-4.016829
N	4.461700	-3.823291	0.188617	H	1.776427	3.129903	-2.812181
C	6.435778	-5.248442	0.833694	H	3.842963	3.165323	-1.512510
C	8.357647	-4.899143	-0.631137	H	6.277783	-2.286543	-3.444153
C	7.746650	-5.537930	0.469950	H	4.607834	-1.773395	-3.359757
C	-3.218012	-4.463608	5.308102	H	3.269189	-2.403197	-0.879851
C	-2.511447	-4.456620	4.099427	H	8.150363	-3.475355	-2.234340
C	-3.153198	-3.329991	6.126210	H	9.383744	-5.148438	-0.887633
C	-1.750787	-3.351068	3.704963	H	5.955682	-5.742455	1.673289
C	-2.401192	-2.218783	5.747411	H	8.309948	-6.269918	1.042177
C	-1.692372	-2.217579	4.532843	H	6.536672	-0.427870	-1.460407
O	-0.974859	-1.104711	4.235700	H	-2.545370	-5.326001	3.447859
C	0.019401	-6.789896	7.178205	H	-3.693171	-3.307409	7.069317
C	0.682220	-5.574728	7.838116	H	-1.199657	-3.359833	2.767482
C	0.938883	-4.443961	6.838153	H	-2.349770	-1.337015	6.378929
C	-8.689674	-1.843794	-2.938891	H	-0.508237	-1.146206	3.360335
C	-8.453821	-3.202689	-3.607792	H	0.044825	-5.203827	8.650440
C	-7.882066	-4.293928	-2.680843	H	1.595421	-4.785630	6.030655
C	2.761399	-6.532185	2.506189	H	-0.000175	-4.104009	6.390279
C	2.907906	-5.269174	3.092199	H	0.650391	-7.200601	6.382464
C	1.904454	-6.651191	1.402335	H	-7.758958	-3.065138	-4.447398
C	2.231533	-4.152169	2.591169	H	-6.968454	-3.888933	-2.223101
C	1.221515	-5.552091	0.893944	H	-9.430993	-1.907028	-2.135191
C	1.357674	-4.248176	1.464365	H	1.770414	-7.621782	0.927862
O	0.723274	-3.222140	0.967915	H	3.566251	-5.145153	3.950344
C	-3.923050	8.166979	1.887179	H	0.563831	-5.660997	0.036567
C	-2.402508	8.381582	1.849564	H	2.358730	-3.177527	3.056568
C	-1.791519	7.395553	0.857509	H	0.686237	-1.801197	1.542880
O	-1.593091	6.192664	1.328005	H	-2.172984	9.402082	1.529386
O	-1.602369	7.726837	-0.319543	H	-1.977308	8.222515	2.845656
C	-3.939925	5.495573	4.631602	H	-4.362532	8.366143	0.904121
C	-2.485778	5.454982	5.125633	H	-4.655106	4.380479	6.349656
O	-2.238977	5.326044	6.330653	H	-5.800237	4.410186	4.990159
C	-4.742287	4.344090	5.261595	H	-4.367077	6.459143	4.933594
N	-1.514146	5.541307	4.180644	H	1.076396	3.036876	2.357323
C	-0.093562	5.504766	4.534783	H	0.347474	2.787714	3.957338
C	0.804307	4.865043	3.466210	H	-0.628231	3.451256	2.637572
C	0.371237	3.448524	3.084210	H	-0.013975	4.948240	5.472273
C	-3.823483	5.335411	-1.496559	H	-4.472813	5.188301	-2.362157
C	-2.625237	4.455672	-1.594173	H	-4.404837	5.116972	-0.593975
C	-2.292931	3.466228	-2.482653	H	-2.827025	3.084290	-3.337562
N	-1.579667	4.534219	-0.692075	H	0.263588	3.422816	-0.497166
C	-0.657801	3.627443	-1.018662	H	-0.523545	2.156790	-2.520321



H	-4.402810	8.834311	2.610717	N	1.634525	-1.824878	-4.692734
H	-9.061534	-1.112509	-3.665289	C	0.660600	-2.884100	-4.463400
H	4.038903	-0.631357	-6.416570	C	-0.770492	-2.326200	-4.533859
H	6.730569	-0.052603	-3.162985	O	-1.055851	-1.265535	-3.950057
H	4.105177	3.657770	-3.174484	C	0.933068	-3.596677	-3.113402
H	3.291928	-7.394268	2.898934	C	0.288603	-4.964955	-3.027427
H	-0.158869	-7.584735	7.909827	C	0.926632	-6.080467	-3.593204
H	0.280040	6.520396	4.726277	C	-0.956771	-5.155300	-2.414681
H	-3.806758	-5.327474	5.600378	C	0.334348	-7.343444	-3.555874
H	-1.525963	5.226783	0.132839	C	-1.555208	-6.416607	-2.375832
H	0.105171	0.119474	-3.077083	C	-0.912498	-7.515164	-2.949119
H	-0.943607	-6.518869	6.732174	N	-1.704002	-3.018966	-5.227022
H	-1.755374	5.755008	3.209697	C	-1.540100	-4.271700	-6.016700
H	1.904365	-1.106451	-3.781154	C	-2.986386	-4.682450	-6.316737
H	3.935189	0.200053	-2.321817	C	-3.727040	-3.340396	-6.421481
H	3.794557	-4.079913	0.909359	C	-3.079566	-2.489192	-5.322403
C	0.261022	0.134558	0.985995	C	3.960900	2.649600	-2.677400
C	1.453798	0.196241	-0.004102	C	5.142358	1.674679	-2.853095
H	2.357096	0.237399	0.620241	O	6.234288	2.099243	-3.256306
H	0.217036	1.081941	1.532677	C	2.527211	2.311634	-3.174102
C	-1.100440	-0.092175	0.340067	C	1.728927	1.061057	-2.739746
C	-2.080878	0.910610	0.372455	O	1.204837	1.499575	-0.957859
C	-1.419165	-1.330045	-0.245300	O	2.277796	-0.076024	-2.643392
C	-3.336177	0.717227	-0.196560	N	4.962498	0.393465	-2.452033
H	-1.862542	1.856455	0.857023	C	6.033700	-0.595500	-2.562500
C	-2.664715	-1.539956	-0.822093	C	5.580115	-2.005071	-2.154766
H	-0.702156	-2.145140	-0.205887	C	5.441308	-2.244437	-0.678468
C	-3.606436	-0.509854	-0.802076	C	4.285667	-2.523863	0.011415
H	-4.092995	1.490436	-0.176855	C	6.510802	-2.290759	0.291500
H	-2.924311	-2.485930	-1.277837	C	5.919554	-2.604255	1.551476
H	1.493595	-0.732175	-0.576548	C	7.906402	-2.121865	0.225201
H	-3.520009	6.385629	-1.450182	N	4.564128	-2.723534	1.348890
H	-4.167851	7.138665	2.161969	C	6.680318	-2.746912	2.717894
H	-3.981234	5.444079	3.539732	C	8.664925	-2.263810	1.382492
H	-7.761944	-1.449268	-2.512766	C	8.057173	-2.572416	2.617576
H	-0.929157	-4.002660	-6.865310	C	-3.212200	-4.454600	5.241400
H	1.803242	4.809074	3.918728	C	-2.540062	-4.471456	4.013361
H	-4.365151	3.373803	4.923232	C	-3.068329	-3.333218	6.066275
O	0.966664	5.696362	2.321837	C	-1.736277	-3.400968	3.607869
H	-9.392893	-3.568958	-4.049268	C	-2.272312	-2.257408	5.675833
C	-7.493696	-5.539492	-3.490744	C	-1.597088	-2.279298	4.442108
H	-7.049782	-6.310296	-2.850978	O	-0.830796	-1.203278	4.136294
H	-8.373102	-5.979502	-3.978312	C	-0.007600	-6.840500	7.092800
H	-6.767221	-5.295456	-4.274075	C	0.454212	-5.607506	7.879219
C	-8.852159	-4.669840	-1.550499	C	0.868719	-4.460862	6.954069
H	-9.095864	-3.812866	-0.915266	C	-8.690500	-1.742900	-2.971400
H	-9.792797	-5.061841	-1.958566	C	-9.699110	-1.804322	-1.818352
H	-8.422195	-5.444837	-0.906272	C	-9.515865	-2.993464	-0.854629
H	1.631176	-5.876133	8.298738	C	2.705400	-6.644800	2.400900
C	2.020973	-1.903284	6.248224	C	2.508821	-5.491902	3.169366
H	1.083073	-1.633492	5.757164	C	2.313621	-6.609417	1.055303
H	2.492070	-0.998963	6.639719	C	1.944847	-4.335075	2.622382
H	2.695904	-2.368657	5.525780	C	1.757022	-5.465996	0.492708
S	1.738799	-3.012134	7.675708	C	1.550151	-4.271464	1.249496
N	-4.907208	-0.731433	-1.421436	O	1.051728	-3.197157	0.696584
O	-5.759775	0.157966	-1.336177	C	-3.694600	8.181300	1.801400
O	-5.100407	-1.803161	-2.008771	C	-2.383854	8.852835	2.216644
H	0.086655	5.853234	1.920121	C	-1.131814	8.184505	1.630588
<b>TS3-R-C2-r1</b>							
C	3.159900	-0.420100	-5.996900	O	-1.159395	6.878848	1.634670
C	2.153962	-1.573132	-5.924247	O	-0.187092	8.872954	1.235513
O	1.847784	-2.219557	-6.933170	C	-3.744000	5.515700	4.550600
				C	-2.296631	5.262482	5.015793
				O	-2.060724	4.852732	6.157627

C	-4.728900	4.588700	5.273300	H	-3.982923	6.564812	4.768020
N	-1.324053	5.524640	4.103208	H	1.136695	2.805789	2.401032
C	0.101300	5.449200	4.426900	H	0.467885	2.699091	4.040110
C	0.960246	4.716896	3.389510	H	-0.543138	3.298343	2.713936
C	0.473023	3.293462	3.119986	H	0.177041	4.938768	5.389520
C	-3.674500	5.342300	-1.577500	H	-4.240876	4.776014	-2.319459
C	-2.377335	4.645748	-1.282385	H	-4.287014	5.434104	-0.674680
C	-1.821935	3.488544	-1.774672	H	-2.194774	2.800911	-2.516239
N	-1.467552	5.122729	-0.351193	H	0.414719	4.417731	0.384888
C	-0.424704	4.285045	-0.285609	H	0.086151	2.409142	-1.135208
N	-0.611376	3.282213	-1.138134	H	-4.554481	8.646220	2.295815
O	0.494561	1.134017	-3.346382	H	-8.942119	-0.929495	-3.661338
O	0.566036	-0.916391	1.814971	H	4.008569	-0.739088	-6.606455
H	3.506159	-0.099917	-5.013612	H	6.399483	-0.618354	-3.598335
H	2.687643	0.428083	-6.503039	H	4.269249	3.569845	-3.177524
H	2.019224	-3.703891	-3.030353	H	3.145682	-7.537630	2.834592
H	0.611842	-2.960851	-2.284003	H	-0.303790	-7.648725	7.769425
H	1.898951	-5.955626	-4.063514	H	0.507682	6.462246	4.555122
H	-1.456568	-4.309604	-1.954375	H	-3.834839	-5.290961	5.543038
H	0.848552	-8.193538	-3.995352	H	-1.528888	5.943799	0.292678
H	-2.519265	-6.539925	-1.890822	H	0.095779	0.237199	-3.360452
H	-1.373977	-8.497802	-2.915761	H	-0.866590	-6.600784	6.456928
H	0.810218	-3.600574	-5.273922	H	-1.561932	5.980672	3.217809
H	-3.058998	-5.291237	-7.221573	H	1.872711	-1.204007	-3.907610
H	-3.382473	-5.268561	-5.480235	H	3.993675	0.075724	-2.323342
H	-3.547660	-2.887475	-7.403083	H	3.888126	-3.084297	2.011650
H	-4.807538	-3.433963	-6.287203	C	0.175378	0.120889	0.909705
H	-3.050935	-1.421855	-5.554437	C	1.349607	0.412892	-0.077830
H	-3.592004	-2.602611	-4.359402	H	2.227781	0.553597	0.576232
H	-1.000174	-5.028257	-5.446916	H	0.028652	1.012358	1.528182
H	2.554798	2.217973	-4.267728	C	-1.158399	-0.194998	0.251909
H	1.902068	3.185359	-2.968861	C	-2.187857	0.758265	0.257887
H	3.906967	2.873638	-1.603505	C	-1.405914	-1.454587	-0.322318
H	6.322567	-2.703930	-2.563856	C	-3.423064	0.496532	-0.323132
H	4.635571	-2.238073	-2.660812	H	-2.022108	1.719024	0.732902
H	3.263052	-2.606250	-0.331084	C	-2.633939	-1.733846	-0.908592
H	8.390072	-1.887948	-0.719383	H	-0.641837	-2.226500	-0.274392
H	9.742888	-2.134933	1.337705	C	-3.626587	-0.751841	-0.910688
H	6.210619	-2.987249	3.667361	H	-4.218045	1.230740	-0.321006
H	8.674151	-2.676570	3.505742	H	-2.842864	-2.696387	-1.355840
H	6.882773	-0.275754	-1.947248	H	1.535277	-0.506295	-0.652918
H	-2.635980	-5.331505	3.355730	H	-3.505553	6.350200	-1.970854
H	-3.580305	-3.292620	7.024212	H	-3.685285	7.120484	2.053739
H	-1.210848	-3.428546	2.657133	H	-3.814182	5.394430	3.465168
H	-2.159098	-1.385733	6.313113	H	-8.699225	-2.676097	-3.548264
H	-0.404644	-1.244797	3.239108	H	-0.980579	-4.058732	-6.935909
H	-0.353596	-5.268023	8.539260	H	1.964489	4.653091	3.833216
H	1.685696	-4.777831	6.296930	O	1.120845	5.454359	2.175646
H	0.028180	-4.148444	6.326577	H	0.337067	6.030799	2.003127
H	0.790495	-7.219836	6.445361	H	-4.545853	3.541688	5.012742
H	-10.715330	-1.850821	-2.233728	H	-9.651674	-0.870212	-1.239618
H	-9.531375	-3.913346	-1.459941	C	-10.684810	-3.067756	0.138989
H	-7.670327	-1.572386	-2.621085	H	-11.647250	-3.147563	-0.379255
H	2.450370	-7.491189	0.431148	H	-10.588872	-3.932581	0.804937
H	2.801788	-5.489176	4.218080	H	-10.719400	-2.169064	0.767540
H	1.462652	-5.459763	-0.552346	C	-8.174954	-2.944005	-0.107294
H	1.776190	-3.459802	3.247228	H	-7.320608	-2.953764	-0.789668
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**Prod-R-C2-r1**

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**TS1-R-C1-r3**

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H	2.164770	3.963512	4.165537	C	-3.180941	-3.084830	6.107538
O	0.732244	4.095611	2.663576	C	-2.099655	-3.387165	3.546840
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<b>TS2-R-C1-r3</b>				O	-1.518790	6.327998	1.363125
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**Int2-R-C1-r3**

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C	-1.968538	-7.191680	-2.596616	N	-1.358354	2.796292	-1.753200
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C	3.613105	2.561296	-2.870496	H	0.288769	-2.933887	-2.285953
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C	2.159163	2.074776	-3.142558	H	-0.405825	-8.199974	-3.691005
C	1.493842	0.867697	-2.386951	H	-3.331522	-5.917822	-1.514741
O	1.444666	1.254362	-0.953262	H	-2.572995	-8.085459	-2.470892
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C	5.609698	-0.732494	-2.799803	H	-4.014308	-5.241601	-5.309194
C	5.076793	-2.169425	-2.641910	H	-4.234388	-2.809763	-7.162351
C	4.983138	-2.673077	-1.229518	H	-5.450812	-3.371912	-6.005873
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C	7.493308	-2.886637	-0.482770	H	2.065215	1.816956	-4.202394
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C	6.354022	-3.870237	1.935175	H	3.671656	2.974565	-1.855215
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C	-3.408093	-4.278294	5.409095	H	2.808270	-2.939106	-0.815915
C	-2.819618	-4.427440	4.147397	H	7.943226	-2.517270	-1.400548
C	-3.271650	-3.052392	6.070078	H	9.378302	-3.218077	0.490377
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C	-0.190982	-6.722519	7.159769	H	-3.721316	-2.908622	7.049208
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C	-9.142564	-1.520511	-2.611312	H	-0.876597	-1.271657	2.824967
C	-8.438380	-2.847103	-2.305602	H	-0.118331	-5.193275	8.689304
C	-7.063899	-2.712886	-1.620469	H	1.200087	-4.608181	5.975360
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C	1.131851	-5.773415	0.434415	H	-9.390203	-0.968756	-1.699153
C	0.943266	-4.496525	1.048623	H	1.922835	-7.759560	0.561783
O	0.317033	-3.536036	0.423776	H	2.574416	-5.247888	3.989025
C	-3.721052	8.327994	1.843212	H	0.730809	-5.915092	-0.564284
C	-2.217748	8.586700	1.662659	H	1.360542	-3.402135	2.873261
C	-1.628460	7.498944	0.769641	H	0.212544	-2.193583	0.988731
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C	-3.725342	5.694137	4.623315	H	-4.237182	8.363729	0.877481
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H	-0.030980	3.325067	-0.151761	O	0.585157	-1.967011	-7.292634
H	-0.827339	1.979510	-2.169338	N	0.705305	-1.868132	-5.014751
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H	3.429221	-0.913060	-6.723876	O	-1.778217	-0.792354	-4.087127
H	6.089731	-0.627292	-3.782082	C	-0.226339	-3.398640	-3.368052
H	3.831203	3.386932	-3.552650	C	-1.372097	-4.261884	-2.885108
H	2.866579	-7.452629	2.856924	C	-1.597061	-5.535172	-3.430922
H	-0.285962	-7.549043	7.871218	C	-2.227594	-3.811391	-1.869976
H	0.708026	6.442683	4.228627	C	-2.659693	-6.327151	-2.992399
H	-3.963133	-5.094587	5.860720	C	-3.289802	-4.602564	-1.425899
H	-1.669739	5.273113	0.252615	C	-3.513870	-5.860092	-1.990358
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H	-0.502772	-0.424141	-0.407318	C	2.425393	1.965705	-3.368210
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C	4.665381	1.528332	1.683835	N	4.539359	-0.366364	-2.814933
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H	2.858752	0.902672	4.504501	C	4.952836	-2.796003	-2.369135
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H	1.226673	0.129901	2.809554	C	6.477001	-2.865730	1.080811
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C	-2.261670	-2.447980	5.700470	H	7.798195	-6.235299	0.595233
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C	-0.040100	-7.178700	6.645600	H	-3.478507	-3.570877	7.064534
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C	0.814520	-4.825075	7.057048	H	-2.082457	-1.629703	6.391133
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C	1.599223	-4.469996	2.097939	H	-6.507806	-1.729634	-2.002583
C	0.718479	-5.815901	0.280496	H	-9.503788	-0.711523	-1.531732
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**Int1-R-C2-r3**

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C	2.075262	2.297617	-3.080310	H	-0.121745	-8.048283	-3.847887
C	1.465309	1.092884	-2.305299	H	-3.160896	-5.897620	-1.692701
O	1.228194	1.467067	-0.968383	H	-2.311306	-8.024820	-2.663286
O	1.885921	-0.098345	-2.501952	H	0.341751	-3.408065	-5.363210
N	4.523862	0.574275	-2.691563	H	-3.579159	-5.118855	-7.188842
C	5.625300	-0.376599	-2.805599	H	-3.826344	-5.161945	-5.435581
C	5.162873	-1.846952	-2.878015	H	-4.118256	-2.716060	-7.260403
C	5.052962	-2.552794	-1.556127	H	-5.321439	-3.332063	-6.117544
C	3.912116	-3.007898	-0.937821	H	-3.598725	-1.314335	-5.355580
C	6.149791	-2.931977	-0.696948	H	-4.019527	-2.586535	-4.204417
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N	4.225394	-3.642468	0.245669	H	1.387822	3.138899	-2.957175
C	6.378135	-4.118609	1.462881	H	3.525854	3.229683	-1.744840
C	8.335393	-3.289421	0.262962	H	5.894790	-2.379154	-3.499755
C	7.755210	-3.948581	1.367934	H	4.211546	-1.905550	-3.418340
C	-3.223504	-4.541399	5.295799	H	2.882494	-2.933174	-1.255147
C	-2.667381	-4.612947	4.012336	H	8.009393	-2.279730	-1.610649
C	-2.990385	-3.391488	6.058737	H	9.415086	-3.176485	0.218539
C	-1.892267	-3.570966	3.490341	H	5.927299	-4.631939	2.306939
C	-2.220642	-2.343398	5.554135	H	8.395651	-4.331830	2.157370
C	-1.662300	-2.423829	4.266415	H	6.320886	-0.246660	-1.967032
O	-0.920929	-1.361441	3.850533	H	-2.834742	-5.494825	3.399365
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C	1.106460	-5.809040	0.411235	H	-9.386907	-1.281040	-1.691295
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**Int2-R-C2-r3**

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O	0.115854	1.092608	-3.068676	H	-9.878013	-2.017765	-3.399398
O	0.404978	-1.181996	1.411401	H	3.589019	-0.495052	-6.665920
H	3.115262	0.147624	-5.067542	H	6.414685	0.111402	-3.404289
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H	1.725322	-3.663962	-3.104539	H	3.331380	-7.266880	2.720756
H	0.459612	-2.727465	-2.313527	H	-0.072883	-7.651580	7.752029
H	1.298279	-5.969168	-3.896070	H	0.206869	6.458828	4.522561
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H	-0.024091	-8.043305	-3.618854	H	-1.882943	5.214616	0.226123
H	-3.091872	-5.804571	-1.597910	H	-0.182096	0.169736	-3.209264
H	-2.235522	-7.968562	-2.477182	H	-0.881580	-6.529083	6.645365
H	0.532019	-3.455309	-5.292652	H	-1.995979	5.824718	3.283651
H	-3.319167	-5.234313	-7.202920	H	1.599922	-1.059407	-3.894647
H	-3.621749	-5.241226	-5.458136	H	3.611739	0.278221	-2.521241
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H	-5.108216	-3.439088	-6.225690	C	0.495999	0.566667	-0.224369
H	-3.423043	-1.388683	-5.463653	C	1.325403	-0.418874	0.649030
H	-3.871821	-2.634051	-4.293834	H	-0.169224	-0.042742	-0.844783
H	-1.254134	-4.927163	-5.430001	H	-0.132529	1.148469	0.460961
H	2.160461	2.054944	-4.181613	C	4.223237	1.598064	3.115009
H	1.425231	3.164588	-3.051504	C	3.086381	1.054337	3.713364
H	3.469907	3.242696	-1.669449	C	4.445024	1.496691	1.739456
H	6.055251	-2.133454	-3.714995	C	2.154686	0.399006	2.913478
H	4.368214	-1.670966	-3.671214	H	2.946802	1.146072	4.782903
H	2.940304	-2.458195	-1.355197	C	3.502915	0.841821	0.955933
H	7.968341	-3.170849	-2.330629	H	5.342477	1.919783	1.306458
H	9.214713	-4.761966	-0.898638	C	2.343085	0.288189	1.527720
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H	8.082219	-5.972984	0.941170	H	3.669889	0.751286	-0.110828
H	6.234682	-0.310157	-1.711752	H	1.877303	-1.071502	-0.036023
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H	0.679416	-7.233640	6.204824	H	-0.244097	5.610437	1.908166
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**TS1-S-SO-C1-r1**

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H	-4.246320	-4.047537	-5.877186	H	3.752335	0.059790	-2.665611
H	-4.022796	-1.563034	-7.659159	H	3.305467	-2.135108	1.905541
H	-5.376916	-1.984701	-6.600151	C	0.695817	-0.065148	0.073183
H	-3.387755	-0.291426	-5.698520	C	1.275908	-0.212752	1.498914
H	-4.085159	-1.486589	-4.600494	H	0.848591	0.552668	2.152865
H	-1.858100	-4.145652	-5.781241	H	1.015120	-0.925907	-0.511575
H	2.005306	2.204737	-3.399605	C	-0.813518	0.040621	0.042040
H	1.848321	3.117725	-1.924926	C	-1.563556	-1.144114	0.108082
H	4.182835	3.088692	-1.436420	C	-1.479860	1.270709	0.015730
H	6.127000	-2.714485	-2.487889	C	-2.957750	-1.092454	0.154916
H	4.423993	-2.378843	-2.728160	H	-1.046016	-2.099512	0.124091
H	2.952812	-2.479054	-0.513518	C	-2.875741	1.316358	0.050224
H	8.000931	-1.278076	-0.640950	H	-0.910695	2.190306	-0.050905
H	9.133695	-0.850243	1.516655	C	-3.619131	0.137606	0.124390
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H	7.887321	-0.968172	3.653597	H	-3.377459	2.278607	0.013694
H	6.655028	-0.276717	-2.459349	H	2.357218	-0.027355	1.427160
H	-2.794714	-5.684131	2.886845	H	-3.421790	6.765437	-0.297317
H	-3.616700	-4.079396	6.792634	H	-2.746478	7.853623	4.339216
H	-1.194610	-3.844807	2.459942	H	-3.267658	5.358383	4.633616
H	-2.014929	-2.235910	6.356247	H	-8.177546	-0.316749	-2.013783
H	-0.165165	-1.852066	3.364085	H	-1.663529	-3.140269	-7.233145
H	-0.492930	-6.443982	7.769522	H	-9.472304	-2.410126	-3.870799
H	1.735757	-5.892378	5.731437	C	-8.542757	-3.769186	-1.614504
H	0.146039	-5.107299	5.743211	H	-7.926206	-4.540132	-1.139756
H	0.595939	-8.220899	5.498160	H	-8.882541	-3.089274	-0.827480
H	-7.997951	-1.529459	-4.233835	H	-9.427726	-4.263958	-2.034820
H	-6.893751	-2.544822	-2.238585	C	-7.215121	-4.039461	-3.743057
H	-9.714003	-1.135784	-1.706755	H	-6.619870	-3.536829	-4.513581
H	1.869324	-7.597929	-0.704748	H	-6.579164	-4.795120	-3.269013
H	2.520693	-6.355049	3.358789	H	-8.036132	-4.564950	-4.246940
H	1.069480	-5.326497	-1.268094	H	1.088206	-7.214982	7.770932
H	1.710381	-4.089621	2.800492	S	1.537536	-4.318448	7.559475
H	0.999316	-2.269536	1.345131	C	2.135960	-3.045838	6.388820
H	-2.348351	8.711362	1.408276	H	1.319859	-2.658506	5.774026
H	-1.658714	9.547934	2.783861	H	2.549275	-2.232077	6.988682
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H	-3.820610	3.230161	6.794049	H	2.345073	3.904429	4.262723
H	-5.022400	3.786503	5.608433	O	1.605660	5.373818	3.107824
H	-3.572520	5.701283	6.342093	H	0.746801	5.750094	2.794893
H	1.215539	2.858220	2.326635	H	-3.592942	2.889009	5.071171
H	0.528679	2.247043	3.849393	H	-4.704476	0.176396	0.154092
H	-0.358813	3.441247	2.888208				
H	0.685024	3.845372	5.985413	<b>TS2-S-SO-C1-r1</b>			
H	-4.227264	5.461244	-1.179643	C	2.903200	-0.242907	-6.026199
H	-3.773424	5.239675	0.516226	C	1.889879	-1.391414	-5.956045
H	-2.398980	4.206423	-2.879868	O	1.520243	-1.982512	-6.977995
H	1.011032	4.574368	-0.469259	N	1.442081	-1.707071	-4.711366
H	-0.221982	2.751753	-3.526850	C	0.451078	-2.753887	-4.490800
H	-3.957335	8.649241	3.324128	C	-0.971457	-2.169364	-4.555939
H	-9.565481	-0.024186	-3.069028	O	-1.241679	-1.106548	-3.963555
H	3.251416	0.207990	-7.003220	C	0.700884	-3.465059	-3.137244
H	5.946268	-0.847899	-3.961506	C	-0.149339	-4.704023	-2.947148
H	3.989101	3.514574	-3.120124	C	0.253943	-5.934406	-3.489018
H	2.607190	-8.138564	1.618473	C	-1.362258	-4.651717	-2.246475
H	-0.609994	-8.706838	6.699521	C	-0.535846	-7.077049	-3.346279
H	1.185055	5.516306	5.697576	C	-2.156035	-5.791542	-2.102649
H	-4.024300	-5.830584	5.053600	C	-1.747773	-7.007588	-2.655196
H	-0.910798	5.650345	0.805724	N	-1.923589	-2.830203	-5.247020
H	-0.558528	1.338871	-4.090336	C	-1.796903	-4.094403	-6.015800
H	-0.996527	-7.449522	5.513785	C	-3.252506	-4.458759	-6.336417
H	-1.034850	5.485844	4.217475	C	-3.951187	-3.094375	-6.440173
H	1.404256	-0.752291	-4.064724	C	-3.287981	-2.274411	-5.328110

C	3.808092	2.725294	-2.641799	H	0.537185	-2.770184	-2.310372
C	4.995598	1.760196	-2.828002	H	1.199435	-5.996700	-4.022719
O	6.096973	2.211922	-3.172449	H	-1.675789	-3.715816	-1.793585
C	2.350691	2.283572	-2.948881	H	-0.201814	-8.020591	-3.768717
C	1.664502	1.030670	-2.317776	H	-3.087114	-5.732020	-1.545916
O	1.270376	1.258111	-0.967794	H	-2.362187	-7.895562	-2.537757
O	2.144836	-0.129273	-2.570820	H	0.581406	-3.473713	-5.301739
N	4.807972	0.454658	-2.522591	H	-3.332186	-5.058608	-7.246467
C	5.882299	-0.520699	-2.689599	H	-3.678102	-5.038328	-5.510045
C	5.429833	-1.962776	-2.411693	H	-3.746902	-2.638300	-7.415306
C	5.348409	-2.350448	-0.963044	H	-5.035418	-3.155389	-6.317382
C	4.221939	-2.696270	-0.254741	H	-3.242141	-1.203087	-5.534623
C	6.458502	-2.497930	-0.050882	H	-3.798710	-2.404962	-4.365405
C	5.920480	-2.935246	1.195975	H	-1.294202	-4.863590	-5.429570
C	7.851157	-2.326665	-0.161527	H	2.272584	2.095778	-4.022292
N	4.557866	-3.033406	1.041473	H	1.715090	3.150961	-2.748059
C	6.730446	-3.195439	2.308015	H	3.871862	3.077969	-1.603075
C	8.658163	-2.585121	0.941415	H	6.151739	-2.619686	-2.915899
C	8.102518	-3.014374	2.165205	H	4.466163	-2.140543	-2.903365
C	-3.117801	-4.619001	5.277900	H	3.185232	-2.739161	-0.560349
C	-2.515986	-4.650291	4.013247	H	8.294549	-2.000110	-1.098429
C	-2.878570	-3.509863	6.097909	H	9.734008	-2.454726	0.862622
C	-1.689941	-3.611085	3.568136	H	6.300645	-3.529158	3.248080
C	-2.058714	-2.466403	5.669383	H	8.756963	-3.207808	3.010589
C	-1.451715	-2.505136	4.400537	H	6.720284	-0.253518	-2.035191
O	-0.654942	-1.456662	4.069729	H	-2.685949	-5.498036	3.354530
C	0.141800	-7.058100	6.955700	H	-3.333285	-3.452876	7.083522
C	0.604371	-5.835137	7.757043	H	-1.225885	-3.653619	2.586196
C	1.067346	-4.696606	6.845150	H	-1.872792	-1.606789	6.305930
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C	-8.407608	-3.111119	-2.916652	H	-0.216021	-5.480078	8.392840
C	-6.922357	-3.399672	-2.618625	H	1.900090	-5.027446	6.215004
C	2.707600	-6.719198	2.189701	H	0.252027	-4.372512	6.190995
C	2.505468	-5.544143	2.919611	H	0.949853	-7.450706	6.328802
C	2.282897	-6.754426	0.855117	H	-8.607940	-3.371845	-3.964638
C	1.903217	-4.425427	2.340257	H	-6.323047	-2.695336	-3.216498
C	1.685105	-5.650641	0.259746	H	-8.761343	-1.379003	-1.621362
C	1.470691	-4.433346	0.975843	H	2.427364	-7.660503	0.268488
O	0.926124	-3.396349	0.401027	H	2.824762	-5.494349	3.959356
C	-3.701901	8.114900	2.238399	H	1.361307	-5.690900	-0.775855
C	-2.483783	8.371502	1.351235	H	1.739163	-3.522329	2.923609
C	-1.412472	7.288030	1.512275	H	0.890469	-2.127972	1.189332
O	-1.834873	6.076320	1.574160	H	-2.791366	8.381056	0.296149
O	-0.213550	7.638747	1.575976	H	-2.031434	9.345448	1.560497
C	-3.666899	5.367300	4.906000	H	-4.133276	7.136364	2.019069
C	-2.190102	5.226925	5.319331	H	-4.429913	4.682406	6.816367
O	-1.887819	5.048440	6.506440	H	-5.643089	4.689571	5.516311
C	-4.594300	4.487900	5.754300	H	-3.934759	6.422852	5.044758
N	-1.258050	5.333765	4.334891	H	1.417730	3.367188	2.028124
C	0.172700	5.306699	4.660701	H	0.411319	2.836433	3.393928
C	1.143850	4.882243	3.541750	H	-0.255809	3.941159	2.175816
C	0.645369	3.681435	2.736561	H	0.279008	4.616556	5.503009
C	-3.788302	5.379402	-1.223799	H	-4.595150	5.106718	-1.908270
C	-2.602878	4.511956	-1.452045	H	-4.156227	5.281708	-0.198124
C	-2.312210	3.572181	-2.408061	H	-2.907298	3.247015	-3.248130
N	-1.509005	4.542074	-0.611018	H	0.316734	3.405495	-0.565518
C	-0.615715	3.640828	-1.050530	H	-0.456347	2.023516	-2.695459
N	-1.069135	3.035825	-2.143397	H	-4.473203	8.878621	2.088247
O	0.225700	1.178927	-3.168913	H	-9.892224	-1.516358	-2.968955
O	0.844138	-1.250456	1.735337	H	3.739569	-0.556340	-6.655913
H	3.267954	0.056555	-5.043213	H	6.267833	-0.453728	-3.716323
H	2.427830	0.615948	-6.510618	H	4.029413	3.589279	-3.272518
H	1.760751	-3.738652	-3.116929	H	3.179044	-7.583985	2.647746

H	-0.186917	-7.862253	7.622124	C	0.089975	-7.267504	-2.797889
H	0.501097	6.292010	5.020754	C	-1.694306	-6.016972	-1.759548
H	-3.757254	-5.431068	5.608711	C	-1.167444	-7.236889	-2.190092
H	-1.462193	5.119344	0.259936	N	-1.468187	-3.234271	-5.072191
H	-0.193128	0.298077	-3.289235	C	-1.234000	-4.540000	-5.740000
H	-0.695669	-6.801509	6.298083	C	-2.649427	-5.005702	-6.105446
H	-1.544523	5.545309	3.375224	C	-3.409180	-3.692213	-6.346490
H	1.709059	-1.107373	-3.914586	C	-2.852614	-2.761484	-5.263190
H	3.844559	0.110724	-2.411070	C	3.804000	2.805000	-2.580000
H	3.900794	-3.432028	1.703633	C	5.064057	1.915452	-2.605590
C	0.642945	0.114542	-0.296465	O	6.166887	2.434988	-2.840951
C	1.428174	-0.192743	0.994078	C	2.414733	2.238363	-2.982725
H	1.465028	0.697500	1.632736	C	1.712961	0.975826	-2.352825
H	0.755337	-0.745335	-0.958118	O	1.286272	1.296717	-0.971473
C	-0.841670	0.332785	-0.031871	O	2.362133	-0.165855	-2.420469
C	-1.298174	1.106798	1.043659	N	4.914919	0.608031	-2.297451
C	-1.795672	-0.297449	-0.840980	C	6.051000	-0.311000	-2.298000
C	-2.662071	1.263007	1.292386	C	5.627711	-1.785026	-2.488195
H	-0.585497	1.584251	1.704901	C	5.450520	-2.561384	-1.214548
C	-3.162988	-0.147574	-0.595959	C	4.290394	-2.771750	-0.505009
H	-1.473387	-0.904153	-1.680481	C	6.495936	-3.229586	-0.478732
C	-3.602647	0.635849	0.471401	C	5.887906	-3.828219	0.663984
H	-2.988657	1.868635	2.133259	C	7.880483	-3.393848	-0.671613
H	-3.882031	-0.646671	-1.240331	N	4.547620	-3.529976	0.618298
H	2.463520	-0.427615	0.708270	C	6.620679	-4.575356	1.594921
H	-3.554784	6.438294	-1.384343	C	8.611616	-4.131530	0.252880
H	-3.424316	8.127269	3.297583	C	7.986939	-4.716745	1.375780
H	-3.783033	5.157426	3.837762	C	-3.123000	-4.380000	5.484000
H	-8.237529	-0.962932	-3.257358	C	-2.475296	-4.453143	4.243515
H	-1.215971	-3.913283	-6.928479	C	-2.971753	-3.212953	6.242204
H	-9.027757	-3.789010	-2.312051	C	-1.689758	-3.399505	3.760572
C	-6.550014	-4.822778	-3.059118	C	-2.193134	-2.153451	5.776695
H	-6.760464	-4.980576	-4.122969	C	-1.541841	-2.235389	4.532458
H	-5.486199	-5.025291	-2.892931	O	-0.794236	-1.162916	4.160906
H	-7.121659	-5.568845	-2.493008	C	0.170000	-6.507000	7.487000
C	-6.566194	-3.182483	-1.140408	C	0.783100	-5.241921	8.099445
H	-6.752922	-2.153977	-0.817386	C	1.080517	-4.178213	7.039747
H	-7.155947	-3.847330	-0.496565	C	-8.575000	-2.302000	-2.929000
H	-5.507854	-3.396269	-0.956738	C	-7.980351	-3.711882	-2.842616
H	-4.404027	3.424703	5.575310	C	-6.459388	-3.762780	-2.597063
H	2.052231	4.571974	4.077328	C	2.964000	-6.341000	2.842000
O	1.573149	5.947075	2.712970	C	2.896304	-5.040747	3.354479
H	0.815070	6.400513	2.270304	C	2.226953	-6.635254	1.685597
H	1.422032	-6.120571	8.430511	C	2.127453	-4.053808	2.731653
S	1.627892	-3.248894	7.833222	C	1.454608	-5.668190	1.053580
C	2.114796	-2.110934	6.485270	C	1.373409	-4.326247	1.544530
H	1.267989	-1.882386	5.833806	O	0.658168	-3.422866	0.937754
H	2.462494	-1.189376	6.957041	C	-4.237900	8.066100	1.533900
H	2.931360	-2.536486	5.896376	C	-2.740933	8.387121	1.417525
H	-4.664978	0.751879	0.667824	C	-2.108844	7.396178	0.443773
<b>Int2-S-SO-C1-r1</b>							
C	3.243000	-0.432000	-5.788000	O	-1.774539	6.248073	0.966047
C	2.266377	-1.611050	-5.688692	O	-2.023337	7.673015	-0.760411
O	1.941731	-2.258587	-6.692910	C	-4.195000	5.509900	4.386100
N	1.803812	-1.889249	-4.441499	C	-2.736098	5.454112	4.872670
C	0.854000	-2.971000	-4.204000	O	-2.476635	5.322367	6.073889
C	-0.590573	-2.475408	-4.382963	C	-5.141000	4.729000	5.304900
O	-0.944493	-1.392157	-3.879120	N	-1.759459	5.573004	3.931305
C	1.059196	-3.569758	-2.788624	C	-0.350000	5.656000	4.335100
C	0.284825	-4.850418	-2.560916	C	0.659755	5.393692	3.211088
C	0.807283	-6.083370	-2.979762	C	0.505268	4.013816	2.570609
C	-0.972446	-4.835480	-1.941521	C	-3.990100	5.103000	-1.727900
				C	-2.740961	4.306158	-1.845913
				C	-2.382820	3.298243	-2.700504

N	-1.675554	4.482511	-0.981649	H	-4.487285	6.567647	4.362200
C	-0.720291	3.606513	-1.291603	H	1.287117	3.859836	1.821065
N	-1.121597	2.880919	-2.335181	H	0.585080	3.220072	3.321135
O	0.476529	0.930279	-3.158590	H	-0.467099	3.918204	2.079752
O	0.815661	-1.058039	1.863958	H	-0.197826	4.933534	5.142585
C	0.654201	0.184572	-0.276227	H	-4.657729	4.888471	-2.565392
C	1.430812	-0.088524	1.029901	H	-4.522771	4.865133	-0.800177
C	-0.833482	0.409845	-0.021519	H	-2.921933	2.847623	-3.517824
C	-1.292219	1.171749	1.062224	H	0.213148	3.454309	-0.776044
C	-1.788066	-0.191488	-0.853333	H	-0.565154	2.068635	-2.718423
C	-2.656632	1.347425	1.297240	H	-4.736654	8.730398	2.247590
C	-3.155590	-0.023223	-0.620872	H	-9.643089	-2.340791	-3.168061
C	-3.596712	0.749856	0.454018	H	4.127153	-0.760091	-6.341150
H	3.535100	-0.045831	-4.811515	H	6.723664	-0.002791	-3.106826
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H	0.785079	-2.830180	-2.031810	H	-0.040360	-7.254413	8.259072
H	1.789143	-6.114969	-3.446209	H	-0.138725	6.649687	4.754186
H	-1.376028	-3.894736	-1.579576	H	-3.730632	-5.204600	5.842875
H	0.515486	-8.212294	-3.124522	H	-1.644536	5.212855	-0.193534
H	-2.662060	-5.985899	-1.266768	H	0.170009	0.004628	-3.259345
H	-1.726425	-8.156555	-2.042821	H	-0.769844	-6.279104	6.972626
H	1.066227	-3.740276	-4.950054	H	-1.992913	5.792375	2.961492
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H	-3.089473	-5.546012	-5.260222	H	3.949561	0.222098	-2.227528
H	-3.171481	-3.295763	-7.339922	H	3.849933	-3.807241	1.303204
H	-4.494339	-3.802916	-6.278451	H	1.518831	0.842980	1.602644
H	-2.850622	-1.706010	-5.543835	H	0.760848	-0.699455	-0.909332
H	-3.409298	-2.853264	-4.321758	H	-0.579198	1.618650	1.744963
H	-0.724413	-5.236453	-5.073765	H	-1.463159	-0.793325	-1.696348
H	2.450703	1.985299	-4.046512	H	-2.983932	1.941507	2.146313
H	1.710872	3.074380	-2.905922	H	-3.875795	-0.501016	-1.280039
H	3.751738	3.215129	-1.561613	H	2.451702	-0.387557	0.751860
H	6.401255	-2.277752	-3.089680	H	-3.760699	6.172544	-1.714893
H	4.711213	-1.820327	-3.086272	H	-4.391469	7.036367	1.865454
H	3.287524	-2.428558	-0.715246	H	-4.259425	5.146468	3.354490
H	8.374203	-2.949094	-1.531958	H	-8.081622	-1.712810	-3.710934
H	9.681206	-4.261853	0.111948	H	-0.614508	-4.390933	-6.632939
H	6.131649	-5.031494	2.450495	H	-8.486375	-4.275921	-2.045593
H	8.583744	-5.289744	2.080113	C	-6.060993	-3.150191	-1.246075
H	6.627654	-0.210585	-1.368293	H	-4.976588	-3.194048	-1.098894
H	-2.576452	-5.347454	3.633876	H	-6.360446	-2.100844	-1.164233
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H	-1.187450	-3.473110	2.798154	C	-5.943359	-5.204886	-2.708290
H	-2.074935	-1.248440	6.364841	H	-6.191417	-5.644416	-3.681116
H	-0.339686	-1.250958	3.288686	H	-4.855654	-5.249717	-2.586296
H	0.098298	-4.826756	8.849419	H	-6.389888	-5.840156	-1.933089
H	1.781298	-4.565720	6.292584	O	0.670056	6.432729	2.240695
H	0.162533	-3.883090	6.522209	H	-0.160144	6.364649	1.721880
H	0.847791	-6.960758	6.755765	H	1.643965	5.440940	3.696217
H	-8.198999	-4.246300	-3.777039	H	-4.912683	3.658781	5.288160
H	-5.977074	-3.171301	-3.390982	H	1.708740	-5.498474	8.629547
H	-8.470280	-1.754786	-1.987037	S	1.819248	-2.679338	7.812854
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H	3.458856	-4.784610	4.251125	H	2.567435	-0.720532	6.672126
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H	2.084099	-3.047426	3.139884	H	1.226419	-1.464959	5.768577
H	0.803325	-1.991551	1.432281	H	-4.659628	0.878418	0.639734
H	-2.600423	9.404641	1.040854				
H	-2.259427	8.305447	2.397267				
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H	-5.039370	5.074678	6.335775	C	2.857900	-0.802300	-6.037800
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				O	1.306446	-2.448946	-6.893687



N	1.381011	-2.166103	-4.630204	C	-4.312900	5.163800	5.602400
C	0.278000	-3.083200	-4.361100	N	-0.880333	5.631196	4.102696
C	-1.068511	-2.366689	-4.573692	C	0.546700	5.438000	4.363000
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C	-0.625777	-4.700433	-2.585202	C	-3.453800	5.440500	-1.495100
C	-0.416350	-6.037950	-2.955063	C	-2.142174	4.748065	-1.284701
C	-1.807349	-4.376323	-1.905009	C	-1.633862	3.587509	-1.812102
C	-1.363410	-7.022402	-2.664448	N	-1.166094	5.218462	-0.419323
C	-2.756375	-5.357414	-1.610618	C	-0.131102	4.367278	-0.423750
C	-2.540190	-6.683542	-1.992969	N	-0.385202	3.369419	-1.264162
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C	3.963000	2.277500	-2.816500	H	0.326270	-2.817594	-2.202656
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C	2.493118	2.026773	-3.247636	H	-1.178004	-8.052719	-2.955029
C	1.614814	0.829214	-2.787180	H	-3.658657	-5.088129	-1.068873
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O	2.118070	-0.340837	-2.685483	H	0.364929	-3.905570	-5.075113
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C	5.228199	-2.685895	-0.795380	H	-5.174559	-3.159284	-6.332656
C	4.078764	-2.921956	-0.080081	H	-3.197770	-1.311212	-5.755678
C	6.316470	-2.761415	0.151346	H	-3.909921	-2.274934	-4.457453
C	5.741922	-3.045644	1.426478	H	-1.645089	-5.101735	-5.111314
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C	1.330543	-4.567061	1.055713	H	2.252552	-7.852840	0.606859
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**Prod-S-SO-C1-r1**

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C 2.426999 -7.154000 1.714992  
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C 1.769890 -5.916668 -0.271276  
C 1.417934 -4.767498 0.495921  
O 0.975793 -3.681236 -0.085358

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C	-1.798265	8.644038	3.078190	H	1.325494	-4.025011	2.530858
C	-0.582182	7.959937	2.432631	H	0.425890	-2.665170	0.756908
O	-0.674592	6.666180	2.340623	H	-1.788582	9.703404	2.802910
O	0.390944	8.638359	2.083507	H	-1.644638	8.603077	4.166423
C	-3.185497	5.099899	5.241902	H	-3.338768	8.070839	1.651696
C	-1.740371	4.681238	5.578042	H	-3.981962	4.929641	7.260857
O	-1.492600	3.966112	6.555632	H	-5.214710	4.887161	5.984699
C	-4.203800	4.565800	6.254099	H	-3.228301	6.194230	5.196533
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C	0.637195	4.841400	4.886499	H	0.355660	2.265006	3.873713
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C	0.485893	3.031674	3.100137	H	0.714437	4.150943	5.729706
C	-3.458904	5.450704	-0.873001	H	-4.054559	5.008137	-1.675245
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N	-1.097178	5.230919	0.016438	H	0.903378	4.570052	0.338039
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O	0.001197	-1.899649	1.347719	H	3.387677	-0.395364	-7.048736
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H	1.298199	-3.730765	-3.128620	H	2.808965	-8.059678	2.177448
H	0.196934	-2.511313	-2.522795	H	-0.577834	-8.321548	7.155430
H	0.301752	-5.913565	-4.093105	H	1.196182	5.751192	5.142778
H	-1.981338	-3.137027	-1.742739	H	-3.963000	-5.602866	5.387946
H	-1.369932	-7.679352	-3.642267	H	-1.145501	5.877882	0.819441
H	-3.653176	-4.901083	-1.283303	H	0.101438	0.594299	-4.071235
H	-3.365165	-7.179270	-2.238628	H	-0.744312	-7.183184	5.810261
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H	2.739118	2.867121	-4.413512	C	-1.347490	0.357063	-0.002594
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H	-0.134231	-2.167372	2.898245	H	-1.479467	-3.834011	-7.098091
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**TS1-S-SO-C2-r1**

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**Int1-S-SO-C2-r1**

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C	2.138467	-4.400193	2.199005	H	-5.974292	-1.788634	-2.397763
C	1.985812	-5.723389	0.174482	H	-9.118443	-2.213500	-2.183856
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**TS2-S-SO-C2-r1**

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C	1.651380	-4.271114	6.729910	H	-1.652327	-1.585654	6.201466
C	-8.344736	-3.014124	-2.973649	H	-0.222059	-1.519606	2.969287
C	-7.173383	-3.798974	-2.372205	H	0.825522	-4.862358	8.633908
C	-6.159118	-2.949433	-1.581533	H	2.300571	-4.672637	5.944334
C	3.545906	-6.077509	2.682005	H	0.691838	-4.005709	6.275406
C	3.503758	-4.700176	2.922553	H	1.424071	-7.068141	6.566921
C	2.590267	-6.628573	1.814036	H	-6.639407	-4.313011	-3.182809
C	2.543404	-3.886774	2.315267	H	-5.819553	-2.139016	-2.245219
C	1.624895	-5.836419	1.205337	H	-8.965399	-2.547443	-2.202052
C	1.555929	-4.425636	1.430440	H	2.603462	-7.698258	1.611154
O	0.637929	-3.693956	0.863456	H	4.236159	-4.246797	3.588365
C	-4.963101	7.623602	1.677201	H	0.892222	-6.275134	0.533360
C	-3.495865	8.026922	1.786040	H	2.519487	-2.818926	2.517553
C	-2.521959	6.877429	1.516340	H	0.713520	-2.230212	1.141680
O	-3.048043	5.721962	1.347499	H	-3.252396	8.843801	1.095560
O	-1.291014	7.123022	1.513771	H	-3.269423	8.414144	2.788024
C	-4.670500	5.029201	4.478902	H	-5.199102	7.269171	0.669633
C	-3.248331	5.204493	5.046144	H	-5.544183	4.531109	6.399325
O	-3.066558	5.424484	6.248928	H	-6.595959	4.165655	5.014415
C	-5.562099	4.157999	5.372299	H	-5.095218	6.039237	4.423631
N	-2.239116	5.134276	4.138789	H	0.942803	2.709491	3.410521
C	-0.855901	5.531001	4.419000	H	0.590865	3.189820	5.082162
C	0.157413	4.713344	3.597527	H	-0.737761	2.778035	3.977317
C	0.242543	3.258609	4.046644	H	-0.674652	5.403227	5.488834
C	-4.458996	4.759595	-1.642599	H	-5.015996	4.484739	-2.540944
C	-3.149316	4.052826	-1.614789	H	-5.065023	4.501291	-0.768564
C	-2.574189	3.181566	-2.499244	H	-2.931703	2.801142	-3.442386
N	-2.258738	4.182335	-0.564111	H	-0.340476	3.300509	-0.152181
C	-1.195320	3.413612	-0.797135	H	-0.703772	2.076882	-2.368309
N	-1.360775	2.799765	-1.969079	H	-5.619702	8.473990	1.896583
O	0.353581	1.049092	-3.015521	H	-8.994377	-3.668823	-3.564448
O	0.717623	-1.224473	1.393184	H	4.148699	-0.259394	-6.375832
H	3.489788	0.409711	-4.856463	H	6.784591	0.840700	-2.946838
H	2.704222	0.752931	-6.418368	H	3.653017	4.097607	-3.183481
H	2.559063	-3.467798	-2.879398	H	4.293032	-6.704294	3.160005
H	1.106874	-2.836165	-2.111669	H	0.659798	-7.308528	8.145744
H	2.584123	-5.766604	-3.850814	H	-0.729184	6.595245	4.179904
H	-0.825836	-4.298835	-1.695871	H	-3.240252	-5.580207	5.780724
H	1.681449	-8.067185	-3.724486	H	-2.436193	4.786662	0.303760
H	-1.754835	-6.590775	-1.598214	H	0.131319	0.096878	-3.043018
H	-0.505038	-8.489660	-2.610950	H	-0.176705	-6.386521	6.885118
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**TS3-S-SO-C2-r1**

C 3.308974 -0.272393 -5.874559  
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H	2.453210	-3.670441	-2.763625	H	4.140092	-6.824179	3.265086
H	1.041557	-2.850995	-2.100860	H	0.511160	-7.217966	8.221228
H	2.307828	-6.042575	-3.503787	H	-0.307114	6.373254	3.540216
H	-1.054251	-4.073549	-1.700406	H	-3.303790	-5.434952	5.837329
H	1.194179	-8.232144	-3.200903	H	-2.335122	5.724971	0.149688
H	-2.181408	-6.257281	-1.408862	H	0.167615	0.074474	-3.346324
H	-1.065337	-8.349510	-2.162928	H	-0.271949	-6.324509	6.906983
H	1.367902	-3.704856	-5.030702	H	-2.366487	5.812228	2.947760
H	-2.210266	-5.915770	-7.015986	H	2.121615	-1.150200	-3.740222
H	-2.628813	-5.840497	-5.297482	H	3.981133	0.486722	-2.242159
H	-2.935059	-3.587433	-7.353209	H	4.031465	-3.475555	1.250019
H	-4.189084	-4.209370	-6.269886	C	0.260463	-0.304101	0.209934
H	-2.710790	-1.989160	-5.550252	C	1.207965	0.916118	0.042527
H	-3.146485	-3.186760	-4.327184	H	1.117083	1.553348	0.934331
H	-0.296476	-5.339208	-5.142168	H	0.423108	-0.957672	-0.655346
H	2.475216	2.191603	-4.313548	C	-1.218686	0.044645	0.267864
H	1.575193	3.216058	-3.222584	C	-1.747225	0.728564	1.374109
H	3.480222	3.286954	-1.634161	C	-2.090866	-0.347244	-0.755075
H	6.583199	-1.892577	-3.125546	C	-3.111007	1.009494	1.455032
H	4.871635	-1.532876	-3.174159	H	-1.086686	1.030765	2.180937
H	3.436867	-2.117214	-0.774239	C	-3.458584	-0.066193	-0.676651
H	8.539307	-2.498058	-1.572561	H	-1.700538	-0.876662	-1.620890
H	9.878797	-3.757281	0.087017	C	-3.973772	0.610876	0.429060
H	6.345373	-4.609199	2.421466	H	-3.503623	1.533687	2.322493
H	8.804877	-4.799467	2.060647	H	-4.120459	-0.382545	-1.478729
H	6.685928	0.213466	-1.467879	H	2.227124	0.513730	0.022717
H	-2.267202	-5.577680	3.571875	H	-4.286663	5.804007	-2.191748
H	-3.070844	-3.310830	7.138586	H	-4.608895	6.665643	1.634067
H	-1.013406	-3.657580	2.622730	H	-4.550657	4.740227	3.273560
H	-1.833724	-1.387538	6.176021	H	-7.895663	-2.361820	-3.803135
H	-0.341926	-1.363072	2.975337	H	-0.277606	-4.482801	-6.699648
H	0.450087	-4.778283	8.769993	H	1.191428	4.605983	4.098807
H	2.148034	-4.421325	6.234691	O	-0.034980	3.797616	2.714949
H	0.473150	-3.874576	6.424639	H	-0.986580	3.646576	2.605950
H	1.396835	-6.881392	6.725454	H	-5.267960	3.433301	5.318481
H	-7.948625	-4.898445	-3.822236	H	-8.177938	-4.904155	-2.081897
H	-5.743322	-3.762477	-3.529953	C	-5.635552	-5.780473	-2.810001
H	-8.226298	-2.383310	-2.066910	H	-5.902656	-6.244935	-3.766023
H	2.843720	-7.510714	1.239408	H	-4.543654	-5.795467	-2.721889
H	3.805657	-4.524397	4.179252	H	-6.040870	-6.411511	-2.009152
H	1.265994	-5.945897	0.163686	C	-5.757098	-3.700793	-1.384096
H	2.223235	-2.953918	3.107442	H	-6.073634	-2.655756	-1.313971
H	0.762242	-1.985815	1.211520	H	-6.189403	-4.238832	-0.530980
H	-3.651860	9.597497	1.627682	H	-4.668026	-3.720094	-1.270018
H	-3.458211	8.466776	2.971320	H	2.111904	-5.322604	8.583422
H	-4.875437	7.812217	0.318046	C	2.249512	-1.493886	6.226125
H	-5.451133	4.940000	6.217580	H	1.324246	-1.387194	5.655069
H	-6.528150	4.587916	4.848802	H	2.575536	-0.508446	6.566074
H	-4.813615	6.244072	4.134769	H	3.027950	-1.923897	5.591072
H	0.455847	2.362900	4.891370	S	1.997022	-2.514766	7.723677
H	0.067310	3.614441	6.094362	H	-5.037100	0.824786	0.495050
H	-1.209751	2.957032	5.067745				
H	-0.619124	5.964480	5.247657				
H	-4.692313	4.139400	-2.641827				
H	-4.978854	4.708000	-0.989151				
H	-2.375993	2.523318	-2.692700				
H	-0.241614	4.463648	0.368670				
H	-0.056360	2.426389	-1.214724				
H	-5.676433	8.062654	1.873124				
H	-9.421571	-3.020119	-3.198263				
H	4.186624	-0.522039	-6.475622				
H	6.737626	0.405867	-3.212274				
H	3.848648	3.943126	-3.222524				

**Prod-S-SO-C2-r1**

C	-3.093500	-0.349000	5.973600
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N	-1.777671	-1.935099	4.606557
C	-0.682100	-2.890900	4.426600
C	0.639094	-2.207992	4.843270
O	0.825171	-1.001946	4.578601
C	-0.651399	-3.398204	2.964083
C	0.256836	-4.591357	2.751994
C	-0.195638	-5.885916	3.047944

C	1.564452	-4.431976	2.275648	C	1.922931	3.449688	1.683417
C	0.640468	-6.992479	2.886742	N	1.591063	5.156776	0.359014
C	2.402464	-5.536574	2.110557	C	0.501363	4.350890	0.349685
C	1.945541	-6.819791	2.418948	N	0.660209	3.300785	1.141655
N	1.577505	-2.931088	5.485587	O	-0.670962	1.402145	4.180694
C	1.490900	-4.337600	5.965000	O	-0.202131	-1.623346	-1.631282
C	2.920076	-4.634458	6.434182	H	-3.732308	-0.201004	5.104094
C	3.425670	-3.271085	6.929981	H	-2.474325	0.544262	6.105285
C	2.834390	-2.285239	5.915746	H	-1.679978	-3.667910	2.703143
C	-3.833700	2.731700	2.650200	H	-0.353310	-2.581161	2.301491
C	-4.824136	1.657931	3.119605	H	-1.213412	-6.027488	3.403664
O	-5.292184	1.704049	4.262760	H	1.921817	-3.439150	2.018210
C	-2.529023	2.708193	3.470667	H	0.270749	-7.987312	3.118602
C	-1.790345	1.381759	3.448993	H	3.408321	-5.395195	1.725544
O	-1.193713	1.467699	0.028454	H	2.596601	-7.678913	2.285506
O	-2.190189	0.379478	2.872960	H	-0.881556	-3.730641	5.095462
N	-5.159251	0.692869	2.217948	H	2.943305	-5.412316	7.201478
C	-6.002500	-0.451100	2.565900	H	3.523168	-4.975964	5.586093
C	-5.280843	-1.814255	2.594391	H	3.029606	-3.063175	7.930122
C	-5.125517	-2.473454	1.255169	H	4.515591	-3.207478	6.979311
C	-3.968300	-2.659421	0.534961	H	2.620671	-1.297956	6.330363
C	-6.180401	-3.081199	0.478884	H	3.492655	-2.148210	5.049185
C	-5.579154	-3.615904	-0.697727	H	1.161669	-5.005383	5.170512
C	-7.565789	-3.245434	0.666163	H	-2.738723	2.940317	4.520749
N	-4.234439	-3.333772	-0.637391	H	-1.838080	3.478474	3.112316
C	-6.321058	-4.297785	-1.670501	H	-3.595069	2.617889	1.588561
C	-8.305339	-3.919569	-0.299162	H	-5.874213	-2.471444	3.245080
C	-7.687925	-4.440210	-1.456671	H	-4.306953	-1.698933	3.078859
C	3.053800	-4.608200	-5.307000	H	-2.956479	-2.363891	0.773123
C	2.488854	-4.613154	-4.030172	H	-8.053433	-2.855277	1.555732
C	2.872521	-3.490392	-6.127400	H	-9.375203	-4.050861	-0.162502
C	1.747680	-3.526336	-3.567053	H	-5.840044	-4.707380	-2.553245
C	2.132625	-2.396740	-5.681504	H	-8.290634	-4.964581	-2.192918
C	1.559586	-2.408099	-4.398612	H	-6.845927	-0.498826	1.867384
O	0.838931	-1.323098	-4.021677	H	2.622051	-5.474557	-3.380677
C	-0.236500	-6.904600	-7.120600	H	3.309345	-3.468424	-7.122516
C	-0.907405	-5.690104	-7.774040	H	1.306807	-3.551285	-2.575660
C	-1.116619	-4.547911	-6.776618	H	1.985010	-1.523901	-6.310391
C	8.684600	-2.031600	2.846000	H	0.454109	-1.441125	-3.101622
C	8.143882	-3.283005	3.545997	H	-0.293769	-5.335255	-8.611375
C	6.947640	-3.955860	2.845093	H	-1.736004	-4.882668	-5.937880
C	-2.899600	-6.612800	-2.405000	H	-0.157679	-4.205829	-6.375188
C	-2.676752	-5.370783	-3.005906	H	-0.847489	-7.299980	-6.301860
C	-2.178497	-6.933597	-1.247362	H	7.840317	-3.014053	4.566672
C	-1.769228	-4.456808	-2.463702	H	6.162236	-3.193969	2.725656
C	-1.267146	-6.041000	-0.697533	H	9.092163	-2.258848	1.855950
C	-1.028262	-4.759834	-1.279150	H	-2.334664	-7.897847	-0.766592
O	-0.172930	-3.931337	-0.743650	H	-3.223042	-5.102376	-3.908715
C	3.940400	8.019600	-1.917800	H	-0.712714	-6.297725	0.200211
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C	1.377869	8.208104	-1.821960	H	-0.186638	-2.619274	-1.264704
O	1.343332	6.910343	-1.756587	H	2.753846	9.844755	-2.057991
O	0.445600	8.967578	-1.532258	H	2.625394	8.782187	-3.452656
C	3.886000	5.344300	-4.657500	H	4.068264	8.063571	-0.829959
C	2.425184	5.099937	-5.088397	H	4.734565	4.883264	-6.602994
O	2.162171	4.639679	-6.205313	H	5.910407	4.844925	-5.270829
C	4.881800	4.604800	-5.557300	H	4.068542	6.425867	-4.697476
N	1.470554	5.431961	-4.178504	H	-1.115587	3.077653	-2.163966
C	0.041700	5.391900	-4.498900	H	-0.470103	2.726537	-3.782838
C	-0.866160	4.829165	-3.397615	H	0.574963	3.441749	-2.542988
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C	2.524084	4.592944	1.208226	H	4.453260	5.303361	0.551272

H	2.331864	2.722414	2.370457	O	1.082936	-1.134004	-7.166917
H	-0.360663	4.568158	-0.265216	N	0.780540	-0.666233	-4.953102
H	-0.421538	1.922388	0.435806	C	-0.170199	-1.758084	-4.757097
H	4.848055	8.432788	-2.372407	C	-1.611268	-1.210487	-4.720519
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H	-4.314260	3.703846	2.790164	C	-0.140308	-5.015061	-3.873292
H	-3.611007	-7.314863	-2.829908	C	-1.906540	-3.852575	-2.719760
H	-0.087350	-7.709373	-7.847916	C	-0.872499	-6.202986	-3.805758
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H	-3.527939	-3.663366	-1.289717	C	4.455318	2.707120	-2.997934
C	-0.149672	-0.719236	-0.538431	O	5.597522	3.161640	-3.141489
C	-0.796247	0.597110	-1.010743	C	1.842128	3.097586	-3.093560
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H	-0.774153	-1.102016	0.281957	O	1.209254	2.410307	-0.886979
C	1.266597	-0.530195	-0.009576	O	1.409127	0.807146	-2.454751
C	1.506976	-0.426765	1.364882	N	4.220502	1.371900	-2.920921
C	2.358198	-0.442214	-0.887084	C	5.307006	0.401487	-3.007495
C	2.803086	-0.255204	1.860249	C	4.798613	-1.044743	-2.886639
H	0.678143	-0.485168	2.061936	C	4.498908	-1.487508	-1.481772
C	3.652488	-0.264125	-0.397760	C	3.349021	-1.257673	-0.763090
H	2.190823	-0.522248	-1.956333	C	5.392830	-2.202606	-0.603978
C	3.881952	-0.174376	0.978655	C	4.712309	-2.378275	0.636443
H	2.954058	-0.195139	2.933958	C	6.695606	-2.717191	-0.737626
H	4.485734	-0.201315	-1.092707	N	3.475543	-1.789568	0.505219
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H	3.790070	6.187957	1.928347	C	7.278828	-3.378243	0.337660
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H	7.896528	-1.280787	2.715199	C	-2.772730	-3.896670	3.899084
H	0.776731	-4.395486	6.795845	C	-4.560550	-2.798510	5.086133
H	-1.860299	4.746393	-3.861724	C	-2.929125	-3.012696	2.830536
H	4.750336	3.521412	-5.482297	C	-4.722590	-1.904170	4.029481
H	8.951751	-4.021415	3.655302	C	-3.900615	-2.002602	2.897604
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H	5.494609	-5.537775	3.259755	C	-0.455238	-5.535068	7.930281
H	7.122119	-5.877936	3.865247	C	-0.422437	-4.017234	7.735185
C	7.305192	-4.484459	1.448085	C	-9.428395	-0.642100	-2.756195
H	7.644736	-3.687015	0.780392	C	-8.650443	-1.937436	-2.496558
H	8.104478	-5.234272	1.508369	C	-7.307326	-1.760683	-1.758866
H	6.438853	-4.960582	0.976277	C	2.174304	-5.872709	1.801704
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H	-1.874627	-5.986305	-8.198786	C	0.911949	-3.803433	1.988749
S	-1.950585	-3.118441	-7.583718	C	0.808572	-5.112526	-0.051581
C	-2.150957	-2.002400	-6.147655	C	0.426665	-3.981001	0.684768
H	-1.188062	-1.755401	-5.694485	O	-0.426611	-3.112520	0.078670
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<b>RC-S-SO-C1-r3</b>				O	-2.423002	6.808879	1.572439
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				C	-2.590624	6.112521	5.292119

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C	-1.251936	4.342196	-1.306581	H	-1.133454	2.959009	-4.033097
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O	-1.561616	-0.726718	0.833477	H	2.917093	0.627030	-7.153080
H	2.875043	0.905158	-5.384780	H	5.823231	0.531466	-3.967963
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H	-0.459628	-7.116277	-4.225133	H	-2.002327	5.712870	0.185266
H	-3.616147	-5.037819	-2.169356	H	-1.208298	1.540578	-4.589168
H	-2.701008	-7.138214	-3.141747	H	-1.130263	-6.051131	5.919228
H	-0.038086	-2.421367	-5.612963	H	-1.985712	6.392605	3.340860
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H	6.050573	0.606619	-2.227824	H	-2.016068	1.020522	-0.330795
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H	-3.295389	-1.086652	1.315206	H	-1.933376	-2.818317	-7.206262
H	-1.397640	-5.819296	8.414349	H	1.505595	5.093629	3.927012
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**Int1-S-SO-C1-r3**

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C 2.147111 0.704758 1.284342

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**Int2-S-SO-C1-r3**

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C 0.765799 -6.307843 -2.799016  
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C 0.127582 -7.539807 -2.646230  
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C 5.542613 -4.267713 -1.259986  
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C	6.823957	-6.313053	-1.200692	H	6.549735	-2.432646	-2.956096
C	6.022459	-6.798807	-0.144667	H	4.955291	-1.994862	-3.516334
C	-3.595500	-3.708200	5.733100	H	3.324884	-1.878613	-0.650383
C	-2.883545	-4.014714	4.567335	H	7.216934	-4.702000	-2.574113
C	-3.715209	-2.364515	6.105469	H	7.633112	-6.930573	-1.581606
C	-2.294572	-3.016082	3.783518	H	4.355189	-6.407368	1.185918
C	-3.134632	-1.355647	5.337166	H	6.226952	-7.781367	0.271934
C	-2.415680	-1.670894	4.170296	H	6.095888	-0.579041	-1.083683
O	-1.872429	-0.633187	3.480458	H	-2.777583	-5.050551	4.254540
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C	0.123126	-3.344593	7.461141	H	-3.226662	-0.312350	5.624179
C	-8.821600	-2.128900	-2.927600	H	-1.387507	-0.900074	2.661843
C	-8.103279	-3.464352	-2.704510	H	1.296859	-4.673033	8.698915
C	-6.763634	-3.366194	-1.947941	H	-0.374221	-3.351885	6.486215
C	2.467600	-6.078000	3.379100	H	-0.613634	-3.045830	8.215250
C	2.576490	-4.676505	3.433580	H	-1.034089	-5.852641	7.066543
C	1.449911	-6.623985	2.585852	H	-7.916406	-3.932787	-3.680223
C	1.705055	-3.850718	2.718358	H	-6.124519	-2.658352	-2.498081
C	0.570725	-5.818023	1.872524	H	-9.121037	-1.662035	-1.984124
C	0.656806	-4.390304	1.907853	H	1.343069	-7.706206	2.527489
O	-0.185641	-3.648869	1.246115	H	3.353024	-4.218686	4.043780
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O	-0.628839	7.496845	0.786095	H	-2.350513	9.373963	1.401401
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C	-4.009500	5.195300	-2.219600	H	-4.602249	4.850443	-3.069431
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H	1.943164	-3.899801	-2.431573	H	3.147266	-6.706082	3.939491
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H	-2.655224	-6.489966	-0.998053	H	0.014783	-0.155965	-2.897443
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H	-3.328408	-5.851646	-4.835561	H	3.768747	0.018968	-2.273195
H	-3.537750	-3.619724	-6.926127	H	3.117914	-3.892359	0.855721
H	-4.805446	-4.141295	-5.806115	C	0.276617	-0.602852	0.073777
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H	-4.521021	-5.230831	-4.552087	H	3.760806	-1.164460	-2.058970
H	-4.016559	-3.319389	-6.894839	H	2.155176	-4.477324	1.296184
H	-5.427217	-3.330440	-5.825245	C	0.074180	-0.519044	0.116837
H	-3.301729	-1.648620	-5.295383	C	1.026917	0.704506	0.248387
H	-4.133830	-2.455213	-3.961756	H	0.408002	1.500370	0.696770
H	-2.158914	-5.518320	-4.325857	H	0.638173	-1.373558	-0.263618
H	2.885210	0.737037	-4.212976	C	4.206845	-0.034135	3.128489
H	2.466941	2.136631	-3.259354	C	2.892549	0.177373	3.554424
H	4.374287	1.786344	-1.748747	C	4.491585	-0.005558	1.763196
H	5.927406	-4.295044	-2.363823	C	1.877851	0.414652	2.625249
H	4.622066	-3.538313	-3.242655	H	2.657358	0.166139	4.615302
H	3.506619	-2.679226	0.182071	C	3.472201	0.231961	0.835689
H	4.675997	-6.602531	-2.987695	H	5.509055	-0.161939	1.413834
H	3.695592	-8.823381	-2.489958	C	2.152703	0.441754	1.247310
H	1.633404	-7.236289	0.960233	H	0.859985	0.569469	2.965689
H	2.195593	-9.142882	-0.545202	H	3.698063	0.253056	-0.219995
H	5.853755	-2.243768	-0.765759	H	-0.689197	-0.262159	-0.634169
H	-3.836620	-3.978006	4.564467	H	-2.077770	6.607225	-3.229958
H	-4.911170	-0.518965	6.886772	H	-2.208046	8.129102	0.419311
H	-2.509152	-2.558535	3.036992	H	-2.708022	6.929242	2.168748
H	-3.582007	0.905077	5.349846	H	-8.284547	-0.195068	-3.994151
H	-1.752286	-0.316046	2.579414	H	-1.831613	-4.941744	-5.974859
H	-1.628954	-3.232216	9.603742	H	2.420992	4.593477	3.506338
H	-0.271729	-3.291324	6.847862	H	-3.794757	5.331174	3.785816
H	-1.771231	-2.425469	7.222704	O	0.985350	4.129550	2.165689
H	-1.442716	-5.528429	7.556640	H	0.040094	4.308637	2.045768
H	-8.824984	-2.351153	-2.765487	H	-9.274408	-1.423430	-1.345069
H	-6.497800	-1.468288	-2.617116	C	-6.884504	-2.791597	-0.973067
H	-8.841957	0.723643	-2.590686	H	-7.106183	-3.664008	-1.598088
H	-0.673063	-7.592151	3.126616	H	-5.839616	-2.863041	-0.652627
H	2.250221	-4.750681	4.495283	H	-7.511259	-2.857254	-0.074979
H	-1.726054	-5.840688	1.737763	C	-6.771867	-0.272593	-0.855865
H	1.183288	-2.986363	3.127415	H	-6.873837	0.673564	-1.396129
H	-0.580133	-1.856795	1.464124	H	-7.412866	-0.221160	0.033352
H	-0.268814	10.496419	0.045987	H	-5.734697	-0.345663	-0.512342
H	-0.474231	9.577345	1.544463	H	-0.159403	-4.117580	9.216897
H	-2.075672	9.110550	-1.042400	S	0.144338	-1.349450	8.236310
H	-3.816115	6.595382	5.022843	C	0.245533	-0.387666	6.684551
H	-4.825990	6.754946	3.568600	H	-0.751392	-0.119108	6.327514
H	-2.823640	8.227182	3.356061	H	0.805486	0.523526	6.905191
H	0.921523	2.888695	4.513132	H	0.770690	-0.952887	5.910866
H	1.001811	4.335439	5.545239	H	4.996871	-0.213385	3.852667
H	-0.420807	4.053517	4.536420				
H	1.194498	6.646349	4.410855	<b>Prod-S-SO-C1-r3</b>			
H	-3.094734	5.170881	-3.440448	C	2.707803	-2.402712	-5.533602
H	-3.153776	6.088172	-1.924942	C	1.394829	-3.146943	-5.285842
H	-1.516981	2.817900	-3.077239	O	0.778029	-3.682596	-6.209831
H	1.117000	4.357368	-0.171394	N	0.934597	-3.176215	-4.000789
H	0.585387	2.259656	-1.461050	C	-0.408667	-3.670672	-3.703629
H	-2.709678	9.830679	0.441722	C	-1.444674	-2.703382	-4.312038
H	-9.975038	-0.292103	-3.484202	O	-1.254388	-1.471239	-4.250535
H	3.748965	-2.793928	-5.881258	C	-0.600517	-3.802385	-2.173486
H	6.587248	-2.078974	-2.354099	C	-1.848900	-4.571402	-1.793934
H	4.854130	1.959034	-3.423118	C	-1.834220	-5.973840	-1.771618
H	1.338338	-7.075374	4.521149	C	-3.043948	-3.910500	-1.482776
H	-2.146863	-5.643677	9.176838	C	-2.987749	-6.697133	-1.461131
H	1.694693	6.706271	2.701572	C	-4.199151	-4.629828	-1.171359
H	-5.057129	-2.987927	6.506512	C	-4.176523	-6.026667	-1.163874
H	-0.361490	6.230326	-0.730481	N	-2.559392	-3.205842	-4.877850
H	0.071475	-0.351547	-3.084476	C	-2.927105	-4.633002	-5.086680
H	-2.917791	-4.633635	7.942951	C	-4.387250	-4.551072	-5.546889

C	-4.450998	-3.216544	-6.305491	H	2.476279	-1.470631	-6.057502
C	-3.554803	-2.291786	-5.473262	H	0.282423	-4.315511	-1.780865
C	4.395927	0.893862	-2.819442	H	-0.620238	-2.800499	-1.733691
C	5.251531	-0.386257	-2.772581	H	-0.909314	-6.502806	-1.985689
O	6.415286	-0.374839	-3.184771	H	-3.065683	-2.824460	-1.468835
C	3.165939	0.917382	-3.755869	H	-2.954920	-7.783003	-1.444891
C	1.986079	0.021013	-3.413070	H	-5.112812	-4.098809	-0.921243
O	1.519586	1.078588	-0.092546	H	-5.074175	-6.586740	-0.917665
O	1.969465	-0.819465	-2.518791	H	-0.504779	-4.653622	-4.169990
N	4.673770	-1.483920	-2.207781	H	-4.671338	-5.412117	-6.157054
C	5.407239	-2.725046	-1.970747	H	-5.046589	-4.522365	-4.672606
C	4.679619	-4.011357	-2.378304	H	-4.035392	-3.335113	-7.312330
C	3.651218	-4.539758	-1.415341	H	-5.466720	-2.825723	-6.404816
C	3.151157	-3.968581	-0.266278	H	-3.048641	-1.521892	-6.059853
C	3.035372	-5.840303	-1.513944	H	-4.115739	-1.787122	-4.677306
C	2.176699	-5.988935	-0.387450	H	-2.807362	-5.208297	-4.169864
C	3.137764	-6.898204	-2.436442	H	3.455515	0.671825	-4.784863
N	2.267044	-4.832006	0.352072	H	2.777005	1.940602	-3.799593
C	1.431706	-7.154332	-0.164907	H	4.059626	1.131157	-1.803379
C	2.400606	-8.056770	-2.219899	H	5.451374	-4.783513	-2.506305
C	1.556683	-8.182117	-1.094690	H	4.241122	-3.875950	-3.375646
C	-4.549441	-2.076174	5.886005	H	3.358681	-3.006801	0.182532
C	-3.961038	-2.672291	4.767158	H	3.783059	-6.811222	-3.306603
C	-4.322977	-0.716693	6.125551	H	2.471972	-8.880038	-2.925368
C	-3.154831	-1.937914	3.896699	H	0.781955	-7.243353	0.700250
C	-3.517785	0.031620	5.267998	H	0.994247	-9.100522	-0.950601
C	-2.922095	-0.572842	4.146103	H	5.694451	-2.792195	-0.912211
O	-2.151165	0.199681	3.348173	H	-4.129117	-3.726665	4.562274
C	-2.197576	-4.877714	8.337493	H	-4.776663	-0.232650	6.986840
C	-0.908236	-4.067781	8.157093	H	-2.711868	-2.419500	3.028906
C	-1.171712	-2.561918	8.226819	H	-3.338293	1.088055	5.445257
C	-8.990402	0.430906	-2.991406	H	-1.698391	-0.342563	2.634314
C	-9.103941	-0.988705	-2.426260	H	-0.182544	-4.351147	8.929794
C	-7.941156	-1.929710	-2.797612	H	-1.848434	-2.256200	7.422581
C	0.438523	-6.421860	3.856715	H	-1.638938	-2.298280	9.182644
C	0.924146	-5.111973	3.791018	H	-2.932190	-4.621872	7.566588
C	-0.695348	-6.750144	3.099917	H	-10.041263	-1.438125	-2.781345
C	0.306065	-4.148943	2.989615	H	-7.865017	-1.942663	-3.896084
C	-1.323796	-5.805067	2.296030	H	-8.123582	0.964612	-2.589638
C	-0.848512	-4.460930	2.206634	H	-1.095204	-7.762211	3.141725
O	-1.455029	-3.586566	1.452756	H	1.797845	-4.828950	4.375523
C	-1.250104	9.199300	0.080002	H	-2.201494	-6.069356	1.711881
C	0.203332	9.477334	0.472374	H	0.672774	-3.125687	2.976923
C	1.171585	8.373288	0.019065	H	-1.023308	-2.224000	1.499005
O	0.763199	7.164747	0.276544	H	0.547737	10.434808	0.069696
O	2.244337	8.669505	-0.519158	H	0.277579	9.541694	1.567120
C	-2.085500	7.267311	3.279411	H	-1.369605	9.203214	-1.009790
C	-0.758502	6.749249	3.863513	H	-3.162115	6.898815	5.125612
O	-0.637436	6.568340	5.081731	H	-4.218779	7.123327	3.712385
C	-3.276003	6.689692	4.060091	H	-2.079284	8.361993	3.357640
N	0.237658	6.509252	2.974656	H	1.685532	2.946800	1.816714
C	1.564805	6.054798	3.389688	H	0.998552	3.309827	3.414650
C	2.152254	4.927571	2.528687	H	0.269054	4.002778	1.954992
C	1.217500	3.723527	2.423654	H	1.469689	5.717225	4.424276
C	-2.086198	5.866310	-2.689500	H	-2.872729	5.390581	-3.280713
C	-1.122568	4.832476	-2.191742	H	-2.564917	6.405588	-1.863852
C	-1.044926	3.468007	-2.372883	H	-1.708770	2.838346	-2.949994
N	-0.042868	5.142791	-1.389186	H	1.494645	3.972617	-0.488241
C	0.618145	3.991322	-1.120009	H	0.859696	1.503678	-0.684367
N	0.044985	2.945875	-1.698499	H	-1.928587	9.956330	0.488560
O	0.960116	0.204617	-4.239445	H	-9.879527	1.022182	-2.747811
O	-0.812477	-1.195827	1.587061	H	3.332703	-3.008934	-6.193021
H	3.257614	-2.174775	-4.620184	H	6.331331	-2.632472	-2.544627

H	5.073947	1.685617	-3.140861	C	0.256288	-5.511377	-3.764636
H	0.925681	-7.165375	4.480778	C	-1.443241	-4.287807	-2.572217
H	-1.998402	-5.951880	8.267996	C	-0.475986	-6.690022	-3.606464
H	2.270975	6.897100	3.379935	C	-2.179697	-5.463437	-2.414287
H	-5.178493	-2.656493	6.554562	C	-1.699110	-6.668681	-2.931730
H	0.196990	6.042894	-0.940517	N	-2.163630	-2.445188	-5.464192
H	0.227335	-0.448727	-4.062337	C	-1.979200	-3.635492	-6.320495
H	-2.655556	-4.683962	9.314106	C	-3.417038	-4.099479	-6.593224
H	0.137690	6.785970	1.992664	C	-4.223886	-2.791750	-6.572141
H	1.368350	-2.571437	-3.309045	C	-3.567932	-1.994417	-5.439235
H	3.697486	-1.405132	-1.939525	C	3.274524	3.269387	-2.573903
H	1.743246	-4.634314	1.200607	C	4.532016	2.418512	-2.803389
C	-0.048550	-0.689936	0.517120	O	5.626576	2.972678	-2.957878
C	0.862609	0.459434	1.002401	C	1.881462	2.623974	-2.740646
H	0.210293	1.178113	1.522658	C	1.585652	1.417266	-1.827940
H	0.578005	-1.475523	0.072824	O	1.313732	1.666058	-0.607373
C	3.810943	-1.009298	3.820290	O	1.663886	0.254547	-2.323299
C	2.507427	-0.732470	4.240104	N	4.403718	1.065715	-2.787078
C	4.163270	-0.790903	2.486814	C	5.558985	0.190618	-2.951901
C	1.565930	-0.241500	3.333206	C	5.166119	-1.240327	-3.385827
H	2.220230	-0.896992	5.275250	C	5.068706	-2.235205	-2.263903
C	3.217867	-0.306307	1.578752	C	3.978308	-2.507663	-1.471614
H	5.177369	-0.992678	2.151598	C	6.137544	-3.074988	-1.781119
C	1.907163	-0.029091	1.989723	C	5.616005	-3.835777	-0.694665
H	0.554491	-0.027831	3.663455	C	7.479429	-3.267662	-2.158972
H	3.494043	-0.128386	0.545707	N	4.300475	-3.468224	-0.534058
H	-0.690216	-0.287928	-0.286576	C	6.391169	-4.769300	0.004339
H	-1.592268	6.611747	-3.323936	C	8.253343	-4.190624	-1.464765
H	-1.566937	8.220311	0.442036	C	7.713861	-4.934127	-0.392884
H	-2.156025	7.022155	2.215840	C	-2.848101	-5.148715	4.928007
H	-8.892959	0.414426	-4.083427	C	-2.272156	-4.928224	3.673560
H	-2.284770	-5.064985	-5.864090	C	-2.786722	-4.130809	5.885985
H	-3.335399	5.603909	3.935440	C	-1.639077	-3.720520	3.371274
H	3.064298	4.605974	3.052263	C	-2.157344	-2.920447	5.599929
O	2.595344	5.373869	1.248824	C	-1.571409	-2.704319	4.339819
H	1.953212	6.018732	0.865245	O	-0.964508	-1.512881	4.126826
H	-9.185698	-0.942476	-1.330716	C	0.627200	-7.479697	6.298301
C	-8.237634	-3.362311	-2.330586	C	0.861805	-6.427751	7.388499
H	-7.435697	-4.050432	-2.619805	C	1.093335	-5.034550	6.798586
H	-8.331251	-3.404303	-1.238244	C	-9.050906	-1.976800	-2.573998
H	-9.173849	-3.738114	-2.758760	C	-8.613505	-2.911459	-1.440786
C	-6.594950	-1.446828	-2.237968	C	-7.805050	-2.236443	-0.315208
H	-6.326372	-0.453153	-2.608775	C	2.988490	-6.583589	1.498899
H	-6.623648	-1.396752	-1.142201	C	2.970415	-5.422174	2.274086
H	-5.786835	-2.131759	-2.516294	C	2.133318	-6.677077	0.395345
H	-0.451189	-4.312298	7.190928	C	2.122180	-4.358485	1.951042
S	0.393724	-1.608500	8.062471	C	1.281441	-5.627946	0.061401
C	-0.278461	0.091510	8.044600	C	1.274161	-4.452208	0.832863
H	0.564504	0.770487	7.901580	O	0.444623	-3.453242	0.456810
H	-0.983616	0.218217	7.219734	C	-4.397300	7.714700	2.962000
H	-0.771124	0.329122	8.990992	C	-3.217424	8.035336	2.043616
H	4.545512	-1.386051	4.526832	C	-2.129889	6.952580	2.075046
<b>TS1-S-SO-C2-r3</b>							
C	2.447793	0.524001	-6.160499	O	-2.531040	5.736413	2.101640
C	1.616222	-0.756824	-6.134124	O	-0.932377	7.323769	2.077965
O	1.404651	-1.410793	-7.160559	C	-4.080300	4.772600	5.393000
N	1.114987	-1.115633	-4.916877	C	-2.592614	4.791198	5.778814
C	0.228517	-2.266115	-4.760912	O	-2.252391	4.569186	6.949344
C	-1.240281	-1.793210	-4.726150	C	-4.656600	3.354700	5.574600
O	-1.561653	-0.835376	-4.004280	N	-1.702209	5.019745	4.780564
C	0.571333	-3.016594	-3.448984	C	-0.256800	5.000400	5.024699
C	-0.216909	-4.293682	-3.252746	C	0.624514	4.579399	3.829697
				C	0.049611	3.397557	3.042681
				C	-4.426102	5.264302	-0.708499



C	-3.227864	4.472010	-1.101397	H	-4.826837	4.938111	0.256634
C	-2.908415	3.767802	-2.238277	H	-3.505840	3.637536	-3.130686
N	-2.138239	4.326941	-0.269385	H	-0.276224	3.265083	-0.487283
C	-1.224515	3.558932	-0.916233	H	-0.979760	2.352589	-3.724973
N	-1.656648	3.198950	-2.117358	H	-5.165772	8.494281	2.908740
O	-0.790214	1.912165	-4.581447	H	-9.560083	-2.534175	-3.367518
O	0.336909	-1.228544	1.830031	H	3.060450	0.525963	-7.062384
H	3.079519	0.631663	-5.275929	H	6.207103	0.652095	-3.703840
H	1.764574	1.380077	-6.187459	H	3.362916	4.125776	-3.248334
H	1.642893	-3.237821	-3.474015	H	3.651795	-7.404449	1.753111
H	0.398847	-2.331388	-2.613355	H	0.463243	-8.469363	6.736786
H	1.210880	-5.535001	-4.284709	H	0.091161	5.987993	5.357724
H	-1.816542	-3.355203	-2.158912	H	-3.341091	-6.089703	5.151951
H	-0.089320	-7.623612	-4.005475	H	-2.072397	4.764625	0.664346
H	-3.124886	-5.438830	-1.879440	H	-0.946373	0.973563	-4.382997
H	-2.268952	-7.584499	-2.803729	H	-0.250902	-7.228613	5.693704
H	0.407343	-2.910988	-5.622128	H	-2.042017	5.219604	3.835053
H	-3.499607	-4.648023	-7.534873	H	1.245595	-0.503409	-4.107146
H	-3.749279	-4.759980	-5.784859	H	3.487413	0.636623	-2.667837
H	-4.105665	-2.260315	-7.523001	H	3.674191	-3.817174	0.179297
H	-5.292449	-2.947099	-6.403709	C	0.613092	-0.014119	0.473076
H	-3.615100	-0.911450	-5.573301	C	1.160729	-0.065603	1.829084
H	-4.014248	-2.226569	-4.464168	H	0.756982	0.705200	2.494516
H	-1.386083	-4.398425	-5.813810	H	1.026458	-0.642303	-0.299697
H	1.716098	2.311222	-3.772394	C	5.330948	-0.659880	2.761156
H	1.137371	3.394049	-2.522215	C	4.330311	-1.126930	3.619146
H	3.368782	3.671536	-1.556935	C	4.978254	0.002447	1.585019
H	5.919753	-1.593280	-4.098639	C	2.988209	-0.934602	3.294801
H	4.224139	-1.200553	-3.944432	H	4.597857	-1.636512	4.540763
H	2.990303	-2.070248	-1.500632	C	3.632174	0.192779	1.257596
H	7.907618	-2.700833	-2.981663	H	5.750468	0.373214	0.917023
H	9.290721	-4.344371	-1.748850	C	2.627688	-0.282168	2.106624
H	5.968789	-5.344075	0.823039	H	2.206106	-1.288861	3.961531
H	8.342652	-5.649119	0.130281	H	3.357297	0.721999	0.352282
H	6.144766	0.148353	-2.024261	H	-0.373336	0.400106	0.338044
H	-2.313124	-5.704116	2.913517	H	-4.198102	6.332486	-0.615569
H	-3.233086	-4.277813	6.865983	H	-4.074643	7.637244	4.005381
H	-1.198689	-3.564078	2.391409	H	-4.220302	5.111949	4.363396
H	-2.111136	-2.125453	6.338022	H	-8.188101	-1.472640	-3.024525
H	-0.573245	-1.442913	3.210041	H	-1.465250	-3.355346	-7.248784
H	-0.003061	-6.397277	8.062453	H	1.570090	4.252323	4.285200
H	1.971793	-5.037077	6.143676	H	-4.177572	2.648147	4.889297
H	0.227512	-4.717363	6.208884	H	-9.498038	-3.395397	-1.001038
H	1.487171	-7.549883	5.623226	C	-7.270814	-3.286218	0.670050
H	-8.005559	-3.721626	-1.865121	H	-6.658002	-2.823594	1.451055
H	-6.939121	-1.741814	-0.780917	H	-8.096137	-3.813639	1.164884
H	-9.740823	-1.202307	-2.224229	H	-6.654587	-4.035564	0.161093
H	2.133915	-7.575030	-0.216645	C	-8.614919	-1.164146	0.428851
H	3.623204	-5.332913	3.138271	H	-8.950540	-0.363552	-0.237300
H	0.623155	-5.689608	-0.798125	H	-9.504221	-1.604410	0.897940
H	2.117585	-3.454053	2.549388	H	-8.016049	-0.703210	1.221601
H	0.553500	-2.632347	1.021556	S	1.363202	-3.797657	8.134901
H	-3.570840	8.121868	1.006588	H	1.725780	-6.714064	8.000990
H	-2.758878	8.994621	2.302128	C	1.613769	-2.291372	7.129195
H	-4.851722	6.762457	2.681257	H	0.747514	-2.095603	6.493009
H	-4.486317	3.006404	6.596895	H	1.742504	-1.458710	7.823736
H	-5.733025	3.341140	5.377274	H	2.512235	-2.381030	6.513370
H	-4.596825	5.473972	6.056987	O	0.991315	5.655479	2.985330
H	0.763884	3.089944	2.273919	H	0.196130	6.116204	2.617226
H	-0.153346	2.543510	3.699324	H	6.377411	-0.808179	3.011816
H	-0.885016	3.677046	2.550188				
H	-0.095425	4.309724	5.857910				
H	-5.212057	5.155042	-1.460648				
				<b>Int1-S-SO-C2-r3</b>			
				C	2.284501	0.322797	-6.302402

C	1.351970	-0.888188	-6.278719	C	-1.877689	4.983505	5.935051
O	1.113164	-1.550519	-7.291919	O	-1.545859	4.951895	7.127346
N	0.802375	-1.172931	-5.061765	C	-4.088800	3.738002	5.752103
C	-0.190199	-2.224606	-4.868714	N	-1.000751	4.924926	4.903808
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O	-1.778254	-0.615707	-4.031485	C	1.057399	3.793637	4.124521
C	0.117938	-3.027069	-3.580043	C	0.658107	2.392251	4.577386
C	-0.828629	-4.186030	-3.347768	C	-3.835805	5.708499	-0.559411
C	-0.581640	-5.440177	-3.927235	C	-2.792214	4.685171	-0.861867
C	-1.978066	-4.029537	-2.560289	C	-2.481554	3.988866	-2.007171
C	-1.460276	-6.507519	-3.729258	N	-1.874656	4.261578	0.075624
C	-2.857765	-5.094993	-2.358487	C	-1.063049	3.356514	-0.521867
C	-2.603313	-6.337051	-2.944569	N	-1.398725	3.159871	-1.790510
N	-2.609095	-2.124258	-5.489232	O	-0.655660	2.033624	-4.336810
C	-2.586200	-3.309801	-6.372896	O	0.616854	-1.479964	1.919070
C	-4.074488	-3.607557	-6.601285	H	2.986494	0.312132	-5.464671
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C	-3.952701	-1.519679	-5.410459	H	1.145669	-3.393985	-3.667806
C	3.528111	2.894569	-2.707522	H	0.086150	-2.338717	-2.730127
C	4.629112	1.890282	-3.073190	H	0.312080	-5.582410	-4.530187
O	5.742286	2.327822	-3.381954	H	-2.175181	-3.068968	-2.093078
C	2.032069	2.495773	-2.479696	H	-1.248121	-7.472217	-4.181541
C	1.667549	1.149052	-1.868910	H	-3.734377	-4.957522	-1.731951
O	1.413448	1.132007	-0.559962	H	-3.283887	-7.167823	-2.782515
O	1.581583	0.128271	-2.551888	H	-0.115026	-2.875701	-5.740666
N	4.384669	0.561918	-2.964465	H	-4.247961	-4.124462	-7.548455
C	5.437678	-0.414124	-3.203983	H	-4.450381	-4.244633	-5.793244
C	4.912789	-1.861390	-3.304926	H	-4.590532	-1.686509	-7.476680
C	4.870508	-2.625484	-2.012111	H	-5.803796	-2.261417	-6.323540
C	3.762134	-3.079781	-1.337730	H	-3.882684	-0.436136	-5.529359
C	6.013697	-3.082182	-1.256943	H	-4.389139	-1.716464	-4.423207
C	5.513299	-3.803721	-0.134242	H	-2.064295	-4.143156	-5.900027
C	7.407018	-2.969961	-1.421367	H	1.500858	2.483579	-3.434672
N	4.140933	-3.787398	-0.215412	H	1.578495	3.280660	-1.871174
C	6.359629	-4.394633	0.812225	H	3.905203	3.369664	-1.794574
C	8.250405	-3.556219	-0.484124	H	5.574255	-2.390374	-4.003021
C	7.731136	-4.259556	0.623617	H	3.923316	-1.861136	-3.777241
C	-3.265899	-4.913191	4.876107	H	2.714313	-2.959576	-1.572816
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C	-2.885609	-4.021288	5.886400	H	9.326997	-3.472566	-0.603322
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C	2.260813	-6.934031	1.235208	H	0.220443	-4.885016	5.764593
C	2.299396	-5.875929	2.148126	H	0.557906	-7.974583	5.237279
C	1.539270	-6.767220	0.047930	H	-9.318150	-2.762669	-3.508589
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**TS2-S-SO-C2-r3**

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C	-2.173019	8.277572	2.177276	H	1.721404	-3.699797	2.815516
C	-1.440703	6.936633	2.057632	H	0.329620	-1.955032	1.213002
O	-2.180364	5.893302	2.013991	H	-2.143944	8.751874	1.186087
O	-0.185785	6.939963	2.007475	H	-1.589163	8.929664	2.836223
C	-3.545700	5.263700	5.189400	H	-4.179058	7.468795	2.003223
C	-2.066926	5.206302	5.610954	H	-4.215944	4.161315	6.938544
O	-1.744822	5.294051	6.802939	H	-5.419202	4.231664	5.634316
C	-4.351600	4.133200	5.854000	H	-3.929843	6.232201	5.530456
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H	1.907491	0.890208	-6.733747	H	3.722848	3.666823	-3.411462
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H	0.143950	-2.558233	-2.600742	H	-0.218608	-8.283523	7.009142
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H	-3.046136	-7.514506	-2.676987	H	-0.939724	-7.045600	5.967115
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H	6.312060	-0.399232	-2.387628	H	-0.310118	-0.127583	-0.659225
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H	-0.317969	-6.091975	8.217944	H	1.351396	-6.590005	7.976615
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**Int2-S-SO-C2-r3**

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**TS3-S-SO-C2-r3**

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C	-0.171717	-7.192520	6.737709	H	-4.002193	-3.308974	6.784939
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C	2.296610	-6.850183	1.920693	H	-0.618446	-4.446236	6.609996
C	2.189586	-5.693008	2.702484	H	0.471987	-7.301878	5.858109
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C	1.576501	-4.532692	2.216124	H	-6.652340	-2.347144	-3.082252
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C	-3.602598	5.389593	5.000191	H	-3.864243	8.352800	1.332049
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H	-3.644860	-5.139137	-1.329850	H	-0.326363	0.402364	-3.598559
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**Prod-S-SO-C2-r3**

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**RC-R-SO-r1**

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C	5.312921	-1.647147	-1.537704	H	-4.766171	-1.572444	-6.604849
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**TS1-R-SO-C1-r1**

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H	4.798912	-1.440523	-3.554019	H	-0.469370	-0.666700	-1.548748
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H	-2.876411	-5.233014	3.067542	H	-3.951530	6.274876	-1.047703
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H	-4.812476	5.051126	-1.990691	<b>Int1-R-SO-C1-r1</b>			
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C	-1.551964	-4.615907	-1.888817	C	-0.681111	4.690154	-1.774451
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C	2.047341	2.254502	-1.758193	H	-2.578423	-4.476779	-1.561329
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C	-8.194092	-1.937192	-3.344495	H	0.679702	-1.384352	3.569681
C	-9.463164	-1.885886	-2.486787	H	0.479404	-4.226312	8.580312
C	-9.239066	-2.107873	-0.977848	H	2.711820	-4.259471	6.471774
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C	3.981754	-4.199693	3.155648	H	1.254803	-6.432572	6.573257
C	2.233250	-5.292809	1.914896	H	-10.166537	-2.648167	-2.848351
C	3.333978	-2.970840	2.998216	H	-8.716729	-3.069664	-0.859431
C	1.580179	-4.075711	1.748588	H	-7.495938	-1.133046	-3.092570
C	2.088563	-2.873546	2.316429	H	1.800229	-6.191577	1.480645
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**TS3-R-SO-C1-r1**

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**Prod-R-SO-C1-r1**

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**TS1-R-SO-C2-r1**

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C	7.538953	-3.940087	-1.777300	H	2.297313	2.130281	-3.501133
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C	6.213422	-5.350719	0.313348	H	4.042152	3.399244	-1.301997
C	8.185747	-4.945325	-1.067753	H	6.255944	-2.077278	-3.739133
C	7.528315	-5.643945	-0.032116	H	4.589821	-1.556016	-3.676481
C	-3.137900	-4.881800	4.978100	H	3.169449	-2.302228	-1.289202
C	-2.574229	-4.672722	3.716735	H	8.056570	-3.409083	-2.572025
C	-2.766308	-4.038696	6.031003	H	9.213581	-5.199687	-1.311232
C	-1.651151	-3.647937	3.499723	H	5.701325	-5.890187	1.104281
C	-1.843909	-3.012253	5.830794	H	8.058570	-6.425780	0.504424
C	-1.273668	-2.811172	4.562521	H	6.472402	-0.375167	-1.617858
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C	0.966382	-6.505609	7.281608	H	-1.226352	-3.495731	2.513518
C	1.363354	-5.286864	6.445961	H	-1.551492	-2.355354	6.644270
C	-8.774500	-1.266100	-2.765800	H	0.014347	-1.753914	3.517237
C	-8.303349	-2.416784	-3.661554	H	0.431806	-6.172205	8.179604
C	-7.464354	-3.495869	-2.948428	H	1.931798	-5.596886	5.562390
C	2.690900	-6.800900	1.780100	H	0.471467	-4.752077	6.105020
C	2.748718	-5.584268	2.465029	H	0.604154	-7.845423	5.596856
C	1.816759	-6.921305	0.693321	H	-7.705953	-2.002361	-4.484536
C	1.954207	-4.499056	2.076843	H	-6.613441	-2.989236	-2.468022
C	1.018074	-5.852657	0.294594	H	-9.456077	-1.608921	-1.980850
C	1.077798	-4.625605	0.981491	H	1.758638	-7.858473	0.146179
O	0.283528	-3.620601	0.553258	H	3.422755	-5.467416	3.309490
C	-3.570700	8.052600	2.918000	H	0.343837	-5.941320	-0.550689
C	-2.036571	8.110046	2.898362	H	2.005361	-3.555798	2.611776
C	-1.499106	7.205267	1.782151	H	0.424092	-2.772160	1.080044
O	-1.359203	5.951952	2.098369	H	-1.705818	9.136732	2.712509
O	-1.299448	7.685425	0.656596	H	-1.638754	7.788677	3.866406
C	-3.584400	5.109400	5.367600	H	-3.979352	8.430048	1.974523
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H	-3.540635	-1.938091	-7.674510	H	3.597406	-4.134356	0.387940
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**Int1-R-SO-C2-r1**

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H	-3.788765	-4.305363	-7.460974	H	1.348376	-0.700224	-4.083017
H	-4.055686	-4.350775	-5.710416	H	3.771183	0.076528	-2.604565
H	-4.093536	-1.861315	-7.498735	H	3.652944	-3.688006	1.379311
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H	-3.431688	-0.545356	-5.580512	C	1.614266	-0.142684	0.351835
H	-4.007687	-1.765950	-4.441948	H	2.597199	-0.384524	0.763010
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H	1.956166	2.219069	-3.397784	C	-0.841653	0.142562	1.086123
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H	8.111097	-2.145290	-1.261488	H	-1.024144	-1.789546	0.139804
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H	-1.184079	-3.479205	2.652341	H	-3.339626	5.388909	4.366601
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H	-0.234006	-1.536572	3.650463	H	-1.611443	-3.265669	-7.188631
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H	-7.054711	-2.711594	-1.639371	C	-7.402624	-4.531328	-2.720355
H	-9.764975	-1.013209	-1.788043	H	-6.704715	-4.305640	-3.534648
H	1.608185	-7.540645	-0.350786	H	-6.882069	-5.173172	-2.001292
H	2.936543	-6.118682	3.482396	H	-8.231021	-5.112833	-3.144456
H	0.569981	-5.347164	-0.806016	C	-8.859667	-3.594513	-0.884747
H	1.869637	-3.928086	3.042914	H	-9.186406	-2.702191	-0.342466
H	0.737009	-2.086877	1.688417	H	-9.756428	-4.112845	-1.247651
H	-1.812554	8.552189	1.417796	H	-8.363585	-4.254231	-0.164688
H	-1.160962	8.814668	3.022701	S	1.974486	-4.144809	7.484440
H	-3.844794	7.409951	2.427730	H	1.595701	-7.057776	7.574566
H	-4.024222	3.612883	6.791856	C	2.287039	-2.816102	6.265224
H	-5.143524	3.996331	5.470519	H	1.352290	-2.407509	5.873487
H	-3.722573	5.991706	5.990312	H	2.832349	-2.026806	6.787216
H	1.683892	1.835809	3.895628	H	2.903182	-3.185269	5.441282
H	1.496268	2.324950	5.586715	H	-4.595899	0.613203	0.155266
H	0.067949	2.190912	4.538908				
H	0.741636	4.676918	6.139428	<b>TS2-R-SO-C2-r1</b>			
H	-4.219410	5.737701	-1.518691	C	3.019700	-0.190000	-5.955500
H	-4.086803	5.291695	0.191329	C	1.998638	-1.333334	-5.919105
H	-2.531869	4.124887	-3.119546	O	1.676718	-1.939602	-6.948301
H	0.351730	3.262809	-0.199539	N	1.488884	-1.620503	-4.692224
H	-0.348576	2.402334	-3.538867	C	0.511700	-2.680700	-4.480500
H	-3.692634	9.099592	2.955063	C	-0.918783	-2.113430	-4.505694
H	-9.401258	-0.326009	-3.371931	O	-1.202075	-1.100163	-3.841784
H	3.293133	0.122971	-7.012211	C	0.782725	-3.414807	-3.144021
H	6.181010	-0.495012	-3.851577	C	-0.042996	-4.674378	-2.984301
H	3.965634	3.518594	-3.244264	C	0.433193	-5.904887	-3.462204
H	2.815649	-7.955073	1.798405	C	-1.308719	-4.639380	-2.381768
H	-0.371558	-8.485056	6.956053	C	-0.333167	-7.066185	-3.345117
H	0.878627	5.931801	4.895819	C	-2.079162	-5.797735	-2.264392
H	-3.964992	-5.681781	5.117169	C	-1.594253	-7.015369	-2.746631
H	-1.395562	4.818277	0.880148	N	-1.859634	-2.745321	-5.243333

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C	-3.233725	-2.210579	-5.283869	H	1.847886	-3.665893	-3.126497
C	3.900300	2.745000	-2.535800	H	0.597855	-2.731046	-2.311032
C	5.087052	1.774026	-2.707156	H	1.416820	-5.952331	-3.923134
O	6.195031	2.219657	-3.037705	H	-1.688450	-3.696067	-2.000377
C	2.437976	2.309387	-2.858857	H	0.057121	-8.009905	-3.715655
C	1.781122	1.037991	-2.237303	H	-3.054300	-5.749826	-1.788083
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C	5.899533	-3.001152	1.286715	H	-1.202733	-4.763129	-5.497297
C	7.849114	-2.415217	-0.053525	H	2.355207	2.147513	-3.936370
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C	8.075317	-3.148920	2.261722	H	4.480833	-2.106992	-2.804369
C	-3.251800	-4.566700	5.211100	H	3.178481	-2.703677	-0.475856
C	-2.569854	-4.546231	3.988331	H	8.303521	-2.083038	-0.983132
C	-3.104585	-3.475712	6.075293	H	9.724496	-2.605741	0.974548
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C	0.467881	-5.859260	7.735409	H	-1.223013	-3.468706	2.676913
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**Int2-R-SO-C2-r1**

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H	-3.465538	-2.883519	-7.384843	H	3.695045	-4.063317	0.815158
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H	-2.244758	-1.382100	6.418955	H	-7.774309	-1.502697	-2.441501
H	-0.427219	-1.188294	3.384409	H	-0.888331	-4.045746	-6.849783
H	0.107273	-5.206278	8.650669	H	1.839650	4.961870	3.888935
H	1.625023	-4.826120	6.005767	H	-4.372041	3.374116	4.915002
H	0.054253	-4.103544	6.393636	O	0.968544	5.932261	2.359602
H	0.628673	-7.216728	6.374079	H	-9.384668	-3.476354	-4.178941
H	-7.740699	-2.961953	-4.516424	C	-7.535065	-5.510592	-3.731024
H	-6.981491	-3.959183	-2.356853	H	-7.109047	-6.328404	-3.139659
H	-9.463210	-1.950136	-2.171694	H	-8.420983	-5.901136	-4.247377
H	1.720045	-7.664446	0.991143	H	-6.800936	-5.231570	-4.495106
H	3.608618	-5.104440	3.885107	C	-8.883203	-4.740660	-1.740920
H	0.453616	-5.738658	0.110319	H	-9.104750	-3.924471	-1.046741
H	2.342609	-3.170469	3.001395	H	-9.833228	-5.077873	-2.174861
H	0.673306	-1.835388	1.550625	H	-8.473660	-5.570000	-1.154079
H	-2.200795	9.422233	1.469583	H	1.670617	-5.918263	8.274594
H	-1.954505	8.263261	2.795784	C	2.113683	-1.950484	6.217010
H	-4.389407	8.345137	0.912492	H	1.169941	-1.665983	5.745801
H	-4.646715	4.374214	6.349196	H	2.607037	-1.054424	6.600000
H	-5.802005	4.416562	4.998706	H	2.765713	-2.425470	5.480019
H	-4.361116	6.459468	4.940753	S	1.842555	-3.057507	7.648194
H	1.208521	3.287054	2.169467	H	0.096010	6.016891	1.920532
H	0.506119	2.870277	3.746499	H	-4.819054	-0.282728	-0.612887
H	-0.513266	3.585551	2.489851				

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C	3.159894	-0.420114	-5.996893	O	-0.202733	8.837822	1.166725
C	2.154366	-1.574674	-5.925583	C	-3.743997	5.515692	4.550594
O	1.832259	-2.207723	-6.938282	C	-2.296997	5.267551	5.019377
N	1.655485	-1.843925	-4.689595	O	-2.062015	4.864604	6.163952
C	0.660613	-2.884097	-4.463432	C	-4.728901	4.588706	5.273304
C	-0.759035	-2.302351	-4.576029	N	-1.324585	5.527772	4.106678
O	-1.038883	-1.224892	-4.022193	C	0.101300	5.449199	4.426906
C	0.888608	-3.564098	-3.089991	C	0.951856	4.698811	3.395002
C	0.148320	-4.877827	-2.949402	C	0.454607	3.275519	3.144546
C	0.723061	-6.071603	-3.412865	C	-3.674525	5.342322	-1.577508
C	-1.131191	-4.934223	-2.380664	C	-2.386688	4.625384	-1.290233
C	0.037677	-7.283889	-3.315335	C	-1.849936	3.461314	-1.787352
C	-1.821863	-6.143848	-2.282967	N	-1.465603	5.087548	-0.363096
C	-1.239956	-7.323388	-2.751568	C	-0.434256	4.233967	-0.306640
N	-1.691884	-2.992202	-5.272806	N	-0.638706	3.235960	-1.160203
C	-1.540100	-4.271696	-6.016688	O	0.507622	1.133290	-3.403260
C	-2.988246	-4.661122	-6.338124	O	0.511408	-0.914793	1.788589
C	-3.698927	-3.307469	-6.491572	H	3.507066	-0.102674	-5.013260
C	-3.055860	-2.443917	-5.400010	H	2.684468	0.428462	-6.499334
C	3.960895	2.649588	-2.677400	H	1.965175	-3.740789	-3.001553
C	5.142427	1.674602	-2.854080	H	0.609825	-2.878738	-2.284770
O	6.234702	2.099994	-3.256129	H	1.719331	-6.049510	-3.847908
C	2.526092	2.319235	-3.176528	H	-1.584963	-4.021382	-2.008660
C	1.726107	1.060955	-2.763208	H	0.503556	-8.197289	-3.674366
O	1.160815	1.459467	-1.007584	H	-2.810330	-6.164795	-1.832853
O	2.286207	-0.073823	-2.675356	H	-1.773046	-8.266271	-2.670738
N	4.962597	0.393777	-2.452450	H	0.813687	-3.622956	-5.253132
C	6.033703	-0.595500	-2.562500	H	-3.054054	-5.290547	-7.229234
C	5.568772	-2.011081	-2.187974	H	-3.414203	-5.218609	-5.496737
C	5.418607	-2.281111	-0.717931	H	-3.488539	-2.881924	-7.479146
C	4.257773	-2.564475	-0.037678	H	-4.783924	-3.375431	-6.379184
C	6.483810	-2.359177	0.254600	H	-3.009181	-1.381277	-5.648976
C	5.884925	-2.694393	1.505317	H	-3.582494	-2.534819	-4.441852
C	7.881235	-2.202441	0.196703	H	-1.031099	-5.021688	-5.410648
N	4.529485	-2.796445	1.295731	H	2.553905	2.240831	-4.271157
C	6.640181	-2.870178	2.670913	H	1.901832	3.190870	-2.959263
C	8.634187	-2.377080	1.353160	H	3.907856	2.869504	-1.602431
C	8.018954	-2.706829	2.579147	H	6.310351	-2.705783	-2.605672
C	-3.212208	-4.454609	5.241405	H	4.626907	-2.227981	-2.705938
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C	-3.066639	-3.331474	6.063563	H	8.370433	-1.952512	-0.740945
C	-1.756613	-3.395491	3.592727	H	9.713516	-2.257658	1.314922
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O	-0.856782	-1.193503	4.111513	H	6.873779	-0.290421	-1.927440
C	-0.007600	-6.840500	7.092801	H	-2.648419	-5.330842	3.351689
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C	0.860483	-4.458625	6.933445	H	-1.239964	-3.421581	2.637215
C	-8.690471	-1.742893	-2.971388	H	-2.165162	-1.379115	6.299517
C	-9.784361	-1.889484	-1.908133	H	-0.439996	-1.229657	3.207277
C	-9.587843	-3.064170	-0.929434	H	-0.345505	-5.261027	8.533482
C	2.705398	-6.644796	2.400899	H	1.672015	-4.776653	6.270163
C	2.510348	-5.484616	3.159305	H	0.013551	-4.150868	6.312295
C	2.282450	-6.629335	1.063905	H	0.785749	-7.220924	6.440186
C	1.920956	-4.340627	2.611345	H	-10.752425	-2.015911	-2.411498
C	1.699556	-5.499912	0.500145	H	-9.479094	-3.980361	-1.530245
C	1.495462	-4.295214	1.244996	H	-7.714946	-1.518345	-2.528790
O	0.974662	-3.235450	0.691128	H	2.415378	-7.517125	0.447134
C	-3.694602	8.181300	1.801400	H	2.825641	-5.465494	4.201546
C	-2.372139	8.835393	2.208638	H	1.381161	-5.511158	-0.537892
C	-1.136628	8.157002	1.599327	H	1.755034	-3.460326	3.229857
O	-1.168050	6.851860	1.622353	H	0.728560	-1.796777	1.329888
				H	-2.353258	9.896237	1.941296

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**Prod-R-SO-C2-r1**

C 2.747597 -0.068799 -6.188799  
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C	1.497277	-4.834360	1.991031	H	-6.845706	-2.137816	-2.913224
C	0.804554	-5.790207	-0.124066	H	-9.412896	-0.781654	-1.576331
C	0.841690	-4.648073	0.732811	H	1.326362	-7.842108	-0.449762
O	0.310295	-3.514646	0.361542	H	2.570805	-6.155051	3.302363
C	-2.589612	8.254801	2.977110	H	0.305111	-5.682957	-1.082345
C	-1.306808	8.868644	2.407945	H	1.528969	-3.998681	2.686129
C	-0.057010	8.015260	2.679138	H	0.436754	-2.359841	1.235520
O	-0.206014	6.743961	2.457588	H	-1.406163	8.974822	1.318383
O	0.983906	8.555266	3.073932	H	-1.134129	9.870785	2.812328
C	-2.801201	5.303701	5.408400	H	-2.759134	7.260812	2.556727
C	-1.367931	4.859253	5.743202	H	-3.673638	3.925853	6.836970
O	-1.128413	4.263263	6.800863	H	-4.835942	4.552639	5.645824
C	-3.807499	4.207496	5.790392	H	-3.005698	6.213855	5.986655
N	-0.415942	5.156264	4.824151	H	1.385493	2.474446	2.460581
C	0.996000	4.824108	5.011685	H	0.810420	2.172077	4.119294
C	1.658710	4.149503	3.801947	H	-0.131179	3.193714	3.019209
C	0.884606	2.921360	3.321927	H	1.046090	4.163002	5.879845
C	-3.096116	5.853153	-0.690729	H	-3.766517	5.485442	-1.471791
C	-1.858847	5.009957	-0.638607	H	-3.644325	5.831566	0.258705
C	-1.452561	3.907904	-1.360015	H	-1.985236	3.406056	-2.156594
N	-0.830203	5.246382	0.251503	H	1.023940	4.267701	0.638070
C	0.123274	4.304798	0.041188	H	0.907595	1.806924	-0.339882
N	-0.212789	3.468223	-0.930240	H	-3.463157	8.876617	2.751013
O	0.707818	1.760421	-4.083047	H	-9.660016	0.363937	-2.895444
O	0.524190	-1.564395	1.917171	H	3.324448	-0.200744	-7.105646
H	3.415916	-0.092977	-5.328859	H	6.000292	-0.751717	-4.047185
H	2.269757	0.915272	-6.229656	H	4.697546	3.383368	-2.682499
H	1.040700	-3.523002	-3.230916	H	2.481466	-8.104954	1.750549
H	-0.064976	-2.305873	-2.602762	H	-0.698198	-8.492416	6.871367
H	0.164701	-5.691632	-4.123923	H	1.563025	5.734785	5.248762
H	-2.432824	-2.836215	-2.237509	H	-4.163365	-5.443198	5.130614
H	-1.589487	-7.425517	-3.924673	H	-0.772592	5.950949	1.007352
H	-4.193052	-4.563125	-2.045168	H	0.139131	0.948814	-4.119475
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H	-4.022346	-4.039651	-7.568704	H	1.571449	-1.056691	-4.100967
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H	9.211218	-4.422269	-0.367616	C	-3.604907	-0.041511	-0.508436
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H	6.719665	-1.118364	-2.478631	H	1.552149	-0.519853	-0.464528
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H	-3.535278	-3.831974	6.927935	H	-2.528670	8.152775	4.065683
H	-1.380098	-3.510423	2.460187	H	-2.888479	5.568415	4.351028
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H	-0.174417	-1.727717	3.353282	H	-1.717859	-3.377295	-7.193227
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**RC-R-SO-C1-r3**

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**TS1-R-SO-C1-r3**

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H	-4.188858	-2.116261	-4.297483	H	-0.773556	-0.213595	0.318036
H	-1.699106	-4.444851	-5.659319	H	-0.384255	0.512857	1.918485
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**Int1-R-SO-C1-r3**

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C	1.550549	0.887009	-2.307180	H	-3.331885	-5.755784	-1.347137
O	1.444731	1.245275	-0.943176	H	-2.693880	-7.958503	-2.313617
O	1.935237	-0.304421	-2.568553	H	0.187486	-3.613769	-5.287958
N	4.560622	0.289614	-2.700745	H	-3.791734	-5.212129	-7.066993
C	5.600100	-0.724200	-2.821200	H	-4.029289	-5.240604	-5.312507
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C	5.020597	-2.511349	-1.054917	H	-5.470650	-3.368840	-5.989306
C	3.895171	-2.868881	-0.349663	H	-3.683359	-1.399806	-5.252431
C	6.126886	-2.635125	-0.134262	H	-4.128318	-2.654799	-4.091652
C	5.586371	-3.065573	1.114244	H	-1.651988	-5.017865	-5.365498
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N	4.227567	-3.191364	0.949908	H	1.491682	2.950015	-2.930014
C	6.391562	-3.299923	2.235428	H	3.688580	2.996408	-1.875972
C	8.320899	-2.683747	0.874265	H	5.801859	-2.832591	-3.008549
C	7.762035	-3.102698	2.100148	H	4.131403	-2.305203	-2.991781
C	-3.392900	-4.279500	5.410800	H	2.861878	-2.930775	-0.662845
C	-2.843107	-4.421024	4.131409	H	7.965373	-2.131988	-1.175605
C	-3.188645	-3.078436	6.098873	H	9.395683	-2.542062	0.800595
C	-2.100270	-3.393599	3.542430	H	5.959045	-3.627083	3.176520
C	-2.451191	-2.044356	5.524862	H	8.412756	-3.275954	2.952759
C	-1.896431	-2.190724	4.240431	H	6.439026	-0.465155	-2.164824
O	-1.183949	-1.151792	3.745846	H	-2.989891	-5.344957	3.577966
C	-0.169900	-6.724200	7.150200	H	-3.607078	-2.942276	7.092754
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C	0.653777	-4.331377	6.920067	H	-2.292585	-1.110177	6.054934
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C	-8.775993	-2.990850	-2.780382	H	-0.638818	-5.079910	8.476795
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C	2.343700	-6.641200	2.345200	H	-0.155859	-4.079204	6.228090
C	2.095126	-5.424450	2.989717	H	0.671473	-7.115072	6.567638
C	1.951727	-6.769872	1.005881	H	-8.969460	-3.274391	-3.823708
C	1.482181	-4.358313	2.324406	H	-6.669165	-2.681402	-3.051271
C	1.342429	-5.721191	0.327251	H	-9.068856	-1.204786	-1.545102
C	1.081624	-4.464441	0.955336	H	2.130385	-7.707047	0.480801
O	0.526512	-3.485175	0.293419	H	2.385126	-5.297965	4.031584
C	-3.719900	8.329700	1.856500	H	1.043389	-5.836907	-0.709829
C	-2.215806	8.586975	1.684590	H	1.285181	-3.425031	2.847130
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O	-1.523326	6.329708	1.358912	H	-2.043781	9.565571	1.227008
O	-1.326979	7.740122	-0.386996	H	-1.725001	8.570482	2.664372
C	-3.715300	5.693500	4.634300	H	-4.231275	8.369757	0.888292
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C	-0.225131	3.238601	3.284336	H	0.222873	5.164102	5.370969
C	-3.912400	5.457700	-1.489000	H	-4.536274	5.321834	-2.375591
C	-2.833932	4.425882	-1.451947	H	-4.561253	5.399389	-0.607194
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O	0.024512	-1.284305	1.385444	H	3.399075	-0.871513	-6.768839
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H	2.127001	0.344943	-6.632967	H	3.800707	3.384497	-3.583024
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H	0.344690	-2.911228	-2.300524	H	-0.478259	-7.501236	7.857227
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H	-1.880653	-3.779044	-1.695090	H	-3.969665	-5.083810	5.856673

H	-1.667721	5.209029	0.208298	N	-2.288154	-3.002557	-5.109985
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H	-1.001019	-6.548251	6.458939	C	-3.648266	-4.644157	-6.146705
H	-1.590115	6.052335	3.188050	C	-4.379202	-3.293219	-6.178781
H	1.380916	-1.246898	-3.973244	C	-3.668199	-2.484838	-5.088140
H	3.592230	-0.038054	-2.579258	C	3.613100	2.561300	-2.870500
H	3.563657	-3.553800	1.625872	C	4.797329	1.579632	-3.001450
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C	1.500158	0.180839	0.050611	C	2.159750	2.073602	-3.142492
H	-0.511658	-0.390764	-0.421280	C	1.495564	0.869056	-2.380074
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C	4.291314	1.476950	3.124371	O	1.986481	-0.330293	-2.589170
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C	2.130529	0.554564	2.520190	C	5.057540	-2.173517	-2.776110
H	2.773749	0.903545	4.542919	C	4.957289	-2.799608	-1.414025
C	3.711964	1.130259	0.801144	C	3.820766	-3.082378	-0.692352
H	5.596514	1.923638	1.464154	C	6.064679	-3.262912	-0.612086
C	2.445659	0.637966	1.156933	C	5.515741	-3.814309	0.583413
H	1.181267	0.139124	2.831893	C	7.461122	-3.284182	-0.786305
H	3.987231	1.172832	-0.246285	N	4.150283	-3.686420	0.503219
H	1.932496	-0.695017	-0.440057	C	6.319086	-4.372057	1.585687
H	-3.478638	6.462759	-1.513598	C	8.261661	-3.836935	0.207662
H	-3.901099	7.345476	2.290199	C	7.695432	-4.374716	1.383370
H	-3.781999	5.604810	3.546396	C	-3.408100	-4.278300	5.409100
H	-8.498781	-0.864585	-3.183137	C	-2.841377	-4.421530	4.136620
H	-1.676868	-4.041852	-6.850076	C	-3.221887	-3.070803	6.091343
H	1.651098	4.200284	3.699984	C	-2.100610	-3.391586	3.548195
O	0.868044	5.045350	2.048726	C	-2.487132	-2.033851	5.518607
H	0.052129	5.506191	1.761005	C	-1.916841	-2.182208	4.240908
H	-4.235319	3.608258	5.017018	O	-1.210957	-1.136874	3.749151
H	-9.438017	-3.620065	-2.167606	C	-0.191000	-6.722500	7.159800
C	-6.998399	-4.790297	-2.835486	C	0.332794	-5.448036	7.832139
H	-7.197048	-4.970798	-3.898027	C	0.657179	-4.352119	6.813893
H	-5.948268	-5.036523	-2.643148	C	-9.142600	-1.520500	-2.611300
H	-7.614171	-5.491585	-2.258416	C	-8.421857	-2.853196	-2.380311
C	-6.972566	-3.093566	-0.967004	C	-7.091384	-2.749711	-1.608465
H	-7.113233	-2.047655	-0.678615	C	2.336600	-6.644200	2.362100
H	-7.606478	-3.708642	-0.315655	C	2.219645	-5.380911	2.953761
H	-5.929789	-3.353778	-0.756482	C	1.726971	-6.844641	1.115552
H	1.023863	-5.641543	8.596881	C	1.527082	-4.341189	2.324712
C	1.574889	-1.714912	6.444642	C	1.033090	-5.824259	0.475428
H	0.726121	-1.558431	5.774931	C	0.902127	-4.520495	1.049249
H	1.871114	-0.756209	6.875906	O	0.256879	-3.571918	0.428587
H	2.417780	-2.126270	5.883805	C	-3.721100	8.328000	1.843200
S	1.125241	-2.808820	7.840112	C	-2.218014	8.589183	1.665875
H	4.999415	1.801703	3.881678	C	-1.629993	7.504506	0.767557
<b>Int2-R-SO-C1-r3</b>				O	-1.533801	6.332000	1.336212
C	2.606200	-0.523100	-6.119500	O	-1.369848	7.732590	-0.419504
C	1.542974	-1.618112	-5.986286	C	-3.725300	5.694100	4.623300
O	1.142074	-2.237177	-6.980578	C	-2.257500	5.594262	5.086690
N	1.088992	-1.857280	-4.727116	O	-1.986064	5.302105	6.257167
C	0.111100	-2.908100	-4.459300	C	-4.559300	4.609200	5.326500
C	-1.317600	-2.345638	-4.430055	N	-1.311172	5.831841	4.143195
O	-1.570296	-1.321910	-3.770824	C	0.109100	5.531500	4.347900
C	0.433628	-3.629505	-3.124613	C	0.629894	4.464771	3.364871
C	-0.385538	-4.887116	-2.925252	C	-0.255474	3.217647	3.335063
C	0.050055	-6.112462	-3.451607	C	-3.904800	5.453300	-1.500400
C	-1.607702	-4.853869	-2.239250	C	-2.800168	4.450116	-1.448131
C	-0.715995	-7.271236	-3.306121	C	-2.524046	3.359727	-2.231270
C	-2.379608	-6.008172	-2.096702	N	-1.787725	4.512495	-0.508071
C	-1.937990	-7.220875	-2.631474	C	-0.933867	3.509141	-0.716410
				N	-1.362286	2.790497	-1.754388

O	0.098172	0.926331	-2.867806	H	-10.042436	-1.661473	-3.219551
O	0.076276	-1.264732	1.420732	H	3.428897	-0.913843	-6.723805
H	2.983633	-0.181274	-5.155310	H	6.164850	-0.565002	-3.731871
H	2.174237	0.325248	-6.659843	H	3.832030	3.387404	-3.552145
H	1.498400	-3.882959	-3.148860	H	2.880869	-7.443728	2.855734
H	0.282338	-2.946230	-2.284952	H	-0.419075	-7.492815	7.903731
H	1.002215	-6.158302	-3.975003	H	0.710958	6.441071	4.231429
H	-1.942801	-3.919962	-1.799319	H	-3.982786	-5.085165	5.853021
H	-0.356827	-8.211310	-3.715725	H	-1.667912	5.270286	0.246572
H	-3.321604	-5.962370	-1.557284	H	-0.230639	0.013950	-2.994194
H	-2.535431	-8.120507	-2.513930	H	-1.105880	-6.519433	6.592820
H	0.206070	-3.621017	-5.280784	H	-1.598275	6.051495	3.185184
H	-3.772496	-5.228363	-7.062057	H	1.424707	-1.270840	-3.939728
H	-4.010041	-5.247896	-5.307266	H	3.577481	-0.040958	-2.586994
H	-4.240966	-2.811771	-7.153464	H	3.471995	-3.997841	1.191974
H	-5.453209	-3.380124	-5.995552	C	0.103926	-0.191125	0.490682
H	-3.666267	-1.407202	-5.266841	C	1.525372	0.200488	0.027895
H	-4.114946	-2.655274	-4.099882	H	-0.477644	-0.431512	-0.410128
H	-1.633694	-5.024845	-5.361863	H	-0.376878	0.675540	0.962390
H	2.065823	1.812565	-4.201572	C	4.330009	1.525347	3.084716
H	1.510120	2.942618	-2.988595	C	3.083605	1.028658	3.463379
H	3.670335	2.973168	-1.854675	C	4.656567	1.578266	1.726814
H	5.730292	-2.785205	-3.391539	C	2.166345	0.596308	2.498952
H	4.084153	-2.197103	-3.277074	H	2.816688	0.971499	4.515392
H	2.782807	-2.904750	-0.935274	C	3.739821	1.151084	0.767938
H	7.911063	-2.874787	-1.687102	H	5.628158	1.951046	1.413261
H	9.340652	-3.856033	0.080428	C	2.474684	0.661461	1.132787
H	5.878500	-4.791596	2.485384	H	1.218811	0.183633	2.819792
H	8.345484	-4.799848	2.143126	H	4.006036	1.184217	-0.281957
H	6.338756	-0.601213	-1.989402	H	1.966857	-0.672457	-0.464353
H	-2.972388	-5.350581	3.587676	H	-3.492787	6.466907	-1.526594
H	-3.652147	-2.931769	7.079852	H	-3.898531	7.342765	2.275971
H	-1.659369	-3.514992	2.562245	H	-3.788745	5.595571	3.536002
H	-2.341907	-1.095347	6.045017	H	-8.495791	-0.808074	-3.136622
H	-0.821217	-1.295036	2.842029	H	-1.658383	-4.052861	-6.849039
H	-0.414006	-5.073365	8.543171	H	1.629533	4.176253	3.714847
H	1.416536	-4.700484	6.105472	O	0.835892	4.992145	2.052355
H	-0.236372	-4.075286	6.245661	H	0.039127	5.491238	1.780348
H	0.546964	-7.135667	6.463538	H	-4.233057	3.609099	5.024741
H	-8.222052	-3.320755	-3.353849	H	-9.089556	-3.543466	-1.844249
H	-6.448908	-2.038865	-2.150584	C	-6.373429	-4.107108	-1.587455
H	-9.452956	-1.054156	-1.671048	H	-5.408389	-4.037822	-1.073949
H	1.800837	-7.817392	0.631558	H	-6.975159	-4.859631	-1.062450
H	2.683226	-5.194080	3.921332	H	-6.188662	-4.477897	-2.601920
H	0.571749	-5.996359	-0.492045	C	-7.279426	-2.217899	-0.179737
H	1.447052	-3.367770	2.802616	H	-7.719722	-1.216268	-0.167053
H	0.200060	-2.199508	0.981494	H	-7.936800	-2.879907	0.398232
H	-2.048550	9.568435	1.209308	H	-6.320355	-2.162170	0.345863
H	-1.721268	8.568175	2.642217	H	1.231672	-5.680591	8.416584
H	-4.236064	8.369609	0.877089	C	1.668741	-1.791411	6.215200
H	-4.440352	4.689034	6.408598	H	2.058775	-0.848473	6.604668
H	-5.620393	4.709427	5.077776	H	2.429651	-2.253477	5.581394
H	-4.103183	6.689775	4.886144	H	0.770132	-1.590774	5.627446
H	0.196521	2.460859	2.692161	S	1.298637	-2.848941	7.661102
H	-0.374466	2.791341	4.337421	H	5.041221	1.859047	3.835416
H	-1.251116	3.455531	2.948527				
H	0.212182	5.181671	5.377358	<b>TS3-R-SO-C1-r3</b>			
H	-4.516467	5.295064	-2.391030	C	2.333000	-0.600000	-6.312700
H	-4.555370	5.379851	-0.621945	C	1.129208	-1.548194	-6.260217
H	-3.052406	2.953086	-3.078451	O	0.599585	-1.986326	-7.287754
H	-0.031940	3.317501	-0.156331	N	0.700735	-1.859425	-5.010293
H	-0.828199	1.972630	-2.171952	C	-0.454500	-2.703200	-4.738800
H	-4.181452	9.075828	2.497672	C	-1.746404	-1.870264	-4.709516

O	-1.785812	-0.802711	-4.070397	C	1.489604	3.990392	3.503238
C	-0.222518	-3.409786	-3.374421	C	0.439934	2.907624	3.245039
C	-1.367696	-4.276724	-2.896439	C	-3.042200	5.905900	-0.999700
C	-1.597039	-5.543770	-3.454836	C	-1.926075	4.911818	-0.848291
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C	-2.659963	-6.338326	-3.021501	N	-0.871657	5.118115	0.025956
C	-3.281201	-4.629265	-1.434697	C	-0.031474	4.077949	-0.047100
C	-3.510193	-5.880070	-2.012104	N	-0.488429	3.198126	-0.931028
N	-2.833779	-2.331839	-5.368708	O	0.213844	1.156201	-3.466733
C	-2.969300	-3.566200	-6.192200	O	-0.460593	-1.567852	0.805862
C	-4.476288	-3.639715	-6.470350	H	2.824277	-0.488778	-5.346019
C	-4.913864	-2.167047	-6.485449	H	1.991545	0.382435	-6.654645
C	-4.079587	-1.541695	-5.362480	H	0.684877	-4.013477	-3.482560
C	3.895700	2.022900	-2.883100	H	-0.002873	-2.648031	-2.622288
C	4.883295	0.886663	-3.224080	H	-0.927629	-5.916392	-4.226896
O	5.985538	1.154062	-3.721022	H	-2.026088	-2.879799	-1.394141
C	2.415200	1.966721	-3.340478	H	-2.817001	-7.318200	-3.463731
C	1.443347	0.833029	-2.954904	H	-3.923038	-4.273500	-0.633661
O	1.093664	1.234213	-1.100487	H	-4.333277	-6.499419	-1.667530
O	1.796258	-0.380150	-2.936002	H	-0.510915	-3.444560	-5.538527
N	4.522904	-0.368911	-2.857390	H	-4.692999	-4.167655	-7.402462
C	5.359000	-1.531400	-3.140800	H	-4.977057	-4.173464	-5.655152
C	4.970296	-2.768453	-2.315925	H	-4.654733	-1.706612	-7.445347
C	5.268307	-2.672721	-0.848216	H	-5.987101	-2.035113	-6.326622
C	4.342754	-2.656214	0.167255	H	-3.850261	-0.485094	-5.516169
C	6.566989	-2.586190	-0.222595	H	-4.574538	-1.635257	-4.387239
C	6.346676	-2.508384	1.184879	H	-2.604574	-4.439940	-5.650601
C	7.891887	-2.578640	-0.696868	H	2.393066	1.955080	-4.438279
N	4.986590	-2.570978	1.386892	H	1.945613	2.909245	-3.045995
C	7.398722	-2.406344	2.101698	H	3.926286	2.140679	-1.793839
C	8.940695	-2.481383	0.212159	H	5.508660	-3.619356	-2.756550
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C	-3.867200	-4.313100	5.130700	H	3.260387	-2.733429	0.117295
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C	-3.208598	-3.338273	5.888970	H	9.965539	-2.472814	-0.148847
C	-2.726478	-3.485284	3.140999	H	7.208256	-2.343589	3.169395
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O	-1.154792	-1.643959	3.404278	H	-4.120740	-5.115140	3.143696
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C	1.354300	-7.272700	1.687100	H	-0.455340	-4.719737	5.843845
C	0.636885	-6.254766	2.330400	H	-0.425798	-7.875236	5.805463
C	1.989956	-6.954066	0.478252	H	-9.535387	-2.121845	-3.066280
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C	1.913509	-5.674507	-0.067970	H	-8.906141	0.515071	-1.603981
C	1.189573	-4.617726	0.566936	H	2.557678	-7.719291	-0.049710
O	1.138009	-3.419901	0.043745	H	0.124618	-6.466860	3.267736
C	-2.322300	8.440000	2.541200	H	2.413921	-5.449455	-1.007207
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C -6.718090 -1.315012 -1.171539  
H -6.772145 -0.222132 -1.169942  
H -7.096264 -1.669820 -0.204459  
H -5.660325 -1.591708 -1.235075  
H 0.652066 -6.794005 7.820679  
S 1.352075 -3.983996 7.265237  
C 1.821789 -2.884330 5.881304  
H 2.394264 -2.059137 6.310085  
H 2.445431 -3.415426 5.157843  
H 0.938060 -2.484121 5.378688  
H 4.609703 0.981740 3.870655

**Prod-R-SO-C1-r3**

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C 1.346082 -1.542017 -6.075941  
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N 1.004796 -1.923879 -4.805443  
C -0.120500 -2.832800 -4.575900  
C -1.434953 -2.076645 -4.862651  
O -1.554187 -0.888009 -4.505890  
C -0.071181 -3.344845 -3.116118  
C -1.052271 -4.459271 -2.821121  
C -0.733315 -5.787863 -3.141833  
C -2.295161 -4.194512 -2.231554  
C -1.635792 -6.822780 -2.890344  
C -3.199052 -5.227923 -1.974244  
C -2.874260 -6.544586 -2.306714  
N -2.444005 -2.724674 -5.479020  
C -2.459100 -4.111600 -6.017100  
C -3.935937 -4.331897 -6.366005  
C -4.422415 -2.930396 -6.766043  
C -3.701495 -2.009197 -5.774885  
C 3.444500 2.552900 -2.847500  
C 4.329426 1.430937 -3.404987  
O 4.701923 1.464525 -4.583663  
C 2.079660 2.602646 -3.564567  
C 1.265406 1.320627 -3.490132  
O 1.113066 1.511309 0.049402  
O 1.623866 0.301480 -2.913463  
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C 5.430400 -0.745500 -2.978000  
C 4.614045 -2.057261 -3.104919  
C 4.612387 -2.929071 -1.881870  
C 3.551826 -3.235695 -1.060645  
C 5.745086 -3.655686 -1.357109  
C 5.289952 -4.374379 -0.213126  
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C 7.464406 -5.297447 0.133434  
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C -3.049041 -3.669436 6.286073  
C -1.863667 -3.515014 3.756768  
C -2.146929 -2.644799 6.004055  
C -1.541241 -2.559098 4.737378  
O -0.662763 -1.552484 4.527139  
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C 0.788273 -6.127861 7.567413  
C 1.114339 -4.940956 6.658001  
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C -8.939036 -2.940377 -2.021563  
C -7.652598 -3.475957 -2.679916  
C 2.282000 -6.871100 2.009100  
C 2.410989 -5.660712 2.698145  
C 1.405228 -6.923815 0.916960  
C 1.694649 -4.525931 2.309133  
C 0.682838 -5.805348 0.517027  
C 0.799624 -4.553387 1.193778  
O 0.123925 -3.507815 0.796263  
C -3.733600 8.123800 2.320100  
C -2.332501 8.714327 2.506839  
C -1.248416 7.944848 1.735027

O	-1.317742	6.651985	1.862408	H	-2.300359	9.765071	2.202530
O	-0.400312	8.558022	1.076419	H	-2.062382	8.677768	3.571701
C	-3.669400	5.369900	4.980700	H	-4.054252	8.198926	1.274474
C	-2.201575	5.071864	5.347209	H	-4.478499	4.711892	6.886833
O	-1.913807	4.486486	6.397762	H	-5.680935	4.804980	5.581548
C	-4.646300	4.540500	5.821300	H	-3.847628	6.441802	5.134268
N	-1.271996	5.509314	4.459165	H	0.307249	2.601348	2.290902
C	0.155200	5.210500	4.590500	H	-0.222619	2.509741	3.988545
C	0.725483	4.385162	3.424429	H	-1.145250	3.463023	2.814269
C	-0.136477	3.163044	3.112628	H	0.272440	4.661568	5.527750
C	-4.021500	5.399600	-1.140100	H	-4.757978	4.912393	-1.784276
C	-2.799836	4.540889	-1.014429	H	-4.492280	5.579980	-0.166623
C	-2.441393	3.335553	-1.580575	H	-3.015452	2.736319	-2.275123
N	-1.725671	4.888773	-0.220440	H	0.131731	3.939390	0.221078
C	-0.796128	3.907702	-0.330326	H	0.264709	1.500919	-0.432147
N	-1.186993	2.940571	-1.147456	H	-4.475118	8.651081	2.930721
O	0.124777	1.397992	-4.181502	H	-10.271064	-1.217107	-1.962215
O	0.493926	-1.462609	2.169133	H	2.887939	-0.501264	-7.132875
H	3.034719	-0.305619	-5.367497	H	5.845012	-0.475407	-3.950772
H	1.766033	0.550068	-6.258991	H	3.962941	3.499502	-3.021904
H	0.949861	-3.697238	-2.937715	H	2.844845	-7.748048	2.314953
H	-0.245155	-2.500072	-2.441536	H	-0.337926	-7.994280	7.533137
H	0.233890	-6.012183	-3.585003	H	0.727587	6.143654	4.667823
H	-2.550074	-3.174251	-1.958539	H	-4.070323	-5.424780	5.538661
H	-1.368204	-7.845160	-3.141594	H	-1.645755	5.676789	0.445293
H	-4.152047	-5.004310	-1.504515	H	-0.365541	0.536190	-4.147543
H	-3.574970	-7.348757	-2.102076	H	-1.058371	-6.702210	6.558284
H	-0.009379	-3.669023	-5.268438	H	-1.560770	5.951232	3.580239
H	-4.062160	-5.078000	-7.154501	H	1.253525	-1.301128	-4.038111
H	-4.475729	-4.680640	-5.478915	H	4.222585	0.404741	-1.644644
H	-4.107029	-2.700212	-7.789768	H	3.347495	-4.441655	0.678724
H	-5.508540	-2.820893	-6.715665	C	0.244619	-0.250219	1.489355
H	-3.479608	-1.017003	-6.173868	C	1.425551	0.240894	0.609354
H	-4.276269	-1.874648	-4.850484	H	-0.642422	-0.330671	0.839529
H	-2.090716	-4.824080	-5.279312	H	0.033436	0.520529	2.236014
H	2.220619	2.828744	-4.627127	C	5.127768	0.603164	2.842716
H	1.462907	3.409659	-3.155166	C	4.403745	1.745249	2.497519
H	3.283181	2.440006	-1.771764	C	4.653412	-0.651843	2.453137
H	5.048938	-2.624336	-3.939464	C	3.213132	1.636066	1.773883
H	3.589346	-1.816081	-3.400155	H	4.765517	2.728133	2.787797
H	2.522593	-2.907718	-1.102194	C	3.465449	-0.760480	1.729211
H	7.469318	-3.258423	-2.617009	H	5.211572	-1.549390	2.705353
H	8.978523	-4.704650	-1.290928	C	2.725374	0.380347	1.384513
H	5.765950	-5.739536	1.402966	H	2.660545	2.527408	1.501780
H	8.147832	-5.926966	0.696362	H	3.106236	-1.738465	1.431863
H	6.267336	-0.897952	-2.288292	H	1.578994	-0.499261	-0.191357
H	-3.003790	-5.269775	3.290711	H	-3.788704	6.378376	-1.576289
H	-3.506128	-3.718558	7.271179	H	-3.748962	7.068646	2.594087
H	-1.403694	-3.455548	2.773686	H	-3.818064	5.183334	3.911531
H	-1.895373	-1.898379	6.751579	H	-9.410324	-1.402649	-3.495826
H	-0.258836	-1.583823	3.606536	H	-1.823520	-4.165855	-6.909712
H	0.293182	-5.764021	8.476353	H	1.716047	4.038159	3.749530
H	1.638739	-5.279200	5.757915	H	-4.514799	3.470825	5.634429
H	0.195992	-4.434943	6.344339	O	0.975240	5.177015	2.264424
H	0.373436	-7.558183	5.971687	H	0.177984	5.722285	2.060756
H	-9.769209	-3.608387	-2.288144	H	-8.832908	-3.009830	-0.929333
H	-7.774386	-3.380100	-3.770082	C	-7.463517	-4.965750	-2.358520
H	-8.565271	-0.781661	-2.072460	H	-6.574521	-5.371013	-2.854017
H	1.287299	-7.855603	0.366411	H	-7.339682	-5.118785	-1.279130
H	3.086383	-5.592984	3.549331	H	-8.327564	-5.557852	-2.680687
H	0.008912	-5.858965	-0.332944	C	-6.407954	-2.673504	-2.272521
H	1.806803	-3.594589	2.856768	H	-6.482322	-1.620624	-2.560870
H	0.352652	-2.306070	1.554094	H	-6.258556	-2.711086	-1.186096



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H 2.992119 -2.899915 5.382914  
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**TS1-R-SO-C2-r3**

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C -0.152349 -5.732708 -3.627215  
C -1.796368 -4.414607 -2.458709  
C -0.944257 -6.871409 -3.465814  
C -2.593049 -5.550118 -2.298139  
C -2.170341 -6.782554 -2.802049  
N -2.421678 -2.503134 -5.317589  
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C -3.830758 -4.072061 -6.383960  
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C -3.779805 -1.928314 -5.291857  
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C 4.747092 1.821752 -2.954757  
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C 2.134464 2.278518 -2.889943  
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O 1.669011 -0.025558 -2.325330  
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H 0.235077 -0.429720 -0.367844  
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C 3.077939 0.646628 4.563620  
C 4.440683 1.434344 2.732721  
C 2.247874 -0.024459 3.660089  
H 2.862754 0.599685 5.627474  
C 3.618034 0.761121 1.831188  
H 5.289676 2.004040 2.365903  
C 2.511462 0.030390 2.288750  
H 1.392000 -0.584544 4.019018  
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H -7.061175 -4.524852 -0.857660  
C -7.337181 -1.862721 -0.025233  
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H 2.386749 -2.302572 6.431521  
H 4.816785 1.899774 4.807209

**Int1-R-SO-C2-r3**

C 2.367500 -0.003101 -6.236300  
C 1.408968 -1.189428 -6.155960  
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C	-9.280900	-0.863900	-2.375200	H	-0.399677	-1.584196	3.165681
C	-8.533655	-2.183899	-2.155930	H	0.111147	-6.042656	8.105394
C	-7.197205	-2.058304	-1.397736	H	1.504268	-5.481222	5.426413
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C	1.519140	-4.612970	1.986013	H	-6.573558	-1.334082	-1.943961
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C	0.694756	-4.578481	0.819644	H	1.230089	-7.829878	-0.158100
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C	-3.261400	8.245300	2.822499	H	-0.004072	-5.792884	-0.820547
C	-2.019360	8.456306	1.956713	H	1.593834	-3.710773	2.586885
C	-1.075296	7.248709	1.987615	H	0.342562	-2.306993	1.117568
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**TS2-R-SO-C2-r3**

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**Int2-R-SO-C2-r3**

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O 5.877185 2.500949 -2.970637  
C 2.128858 2.329109 -3.119333  
C 1.444244 1.101918 -2.415715  
O 1.220207 1.499679 -1.024216  
O 2.011719 -0.081416 -2.532095  
N 4.582485 0.651934 -2.631243  
C 5.702400 -0.284900 -2.672400  
C 5.291364 -1.708177 -3.120132

C	5.061128	-2.682443	-1.998676	H	-5.110152	-3.445493	-6.217736
C	3.905996	-2.864550	-1.274352	H	-3.427058	-1.392893	-5.456544
C	6.030271	-3.593078	-1.440921	H	-3.871364	-2.640401	-4.287413
C	5.383110	-4.298665	-0.383288	H	-1.251374	-4.927091	-5.432553
C	7.374916	-3.892924	-1.729530	H	2.156282	2.055891	-4.178467
N	4.090824	-3.834413	-0.310591	H	1.424712	3.164973	-3.045307
C	6.039223	-5.278922	0.371880	H	3.472233	3.241442	-1.668937
C	8.030253	-4.862869	-0.979468	H	6.086991	-2.101350	-3.763522
C	7.367882	-5.549113	0.061700	H	4.400107	-1.638352	-3.752435
C	-3.232100	-4.544800	5.284200	H	2.957734	-2.358113	-1.379662
C	-2.644533	-4.598716	4.014010	H	7.896653	-3.371393	-2.528070
C	-3.036839	-3.396063	6.059592	H	9.068844	-5.098867	-1.195126
C	-1.876897	-3.540135	3.515357	H	5.519644	-5.808073	1.165166
C	-2.275029	-2.331026	5.579018	H	7.905334	-6.303293	0.630030
C	-1.688671	-2.393058	4.302881	H	6.195213	-0.339547	-1.692037
O	-0.961382	-1.313084	3.907570	H	-2.779986	-5.480775	3.393328
C	0.092900	-6.836200	7.040300	H	-3.481454	-3.324044	7.048826
C	0.870879	-5.663210	7.647155	H	-1.420498	-3.598029	2.528667
C	1.099617	-4.543422	6.629723	H	-2.124362	-1.437572	6.177338
C	-8.978600	-1.941700	-2.779100	H	-0.565138	-1.393462	3.009634
C	-8.455914	-3.329166	-2.390538	H	0.323355	-5.264573	8.510252
C	-7.137867	-3.329170	-1.590918	H	1.665903	-4.914631	5.768672
C	2.694800	-6.497600	2.293900	H	0.143561	-4.155052	6.263946
C	2.769516	-5.173186	2.741075	H	0.636209	-7.277237	6.197463
C	1.762072	-6.804822	1.291821	H	-8.306950	-3.920473	-3.303975
C	1.945362	-4.178715	2.207335	H	-6.391204	-2.778371	-2.183475
C	0.931066	-5.829584	0.752570	H	-9.237324	-1.341147	-1.901480
C	0.983558	-4.467683	1.188442	H	1.685436	-7.827298	0.925270
O	0.193358	-3.564199	0.679338	H	3.487254	-4.904879	3.514611
C	-4.227500	8.101200	1.995200	H	0.213566	-6.081752	-0.023326
C	-2.723328	8.392360	1.885993	H	2.010083	-3.156071	2.569247
C	-2.093603	7.393990	0.917537	H	0.370946	-2.141397	1.096193
O	-1.908833	6.198659	1.410693	H	-2.557805	9.407486	1.513794
O	-1.879632	7.707769	-0.260026	H	-2.254602	8.300283	2.871535
C	-4.124700	5.407600	4.715200	H	-4.715139	8.224665	1.022143
C	-2.662016	5.395970	5.194404	H	-4.793043	4.310841	6.463313
O	-2.391177	5.164860	6.378849	H	-5.956683	4.289635	5.118366
C	-4.894200	4.251900	5.377900	H	-4.569771	6.368197	5.001782
N	-1.716444	5.633847	4.251205	H	0.280682	2.624766	2.568956
C	-0.282900	5.476600	4.508400	H	-0.409505	2.709209	4.197518
C	0.413466	4.589512	3.458472	H	-1.295926	3.399544	2.828644
C	-0.297691	3.250529	3.251527	H	-0.188628	5.036334	5.503719
C	-4.182300	5.299600	-1.414700	H	-4.824711	5.139170	-2.283113
C	-2.992598	4.406504	-1.480335	H	-4.775342	5.110952	-0.512889
C	-2.662562	3.395361	-2.343499	H	-3.196289	2.993049	-3.189299
N	-1.945475	4.506978	-0.583152	H	-0.079822	3.440955	-0.387382
C	-1.019724	3.598755	-0.891940	H	-0.871969	2.133959	-2.415226
N	-1.433283	2.908181	-1.955874	H	-4.715334	8.780847	2.701856
O	0.113211	1.094080	-3.065567	H	-9.878283	-2.020756	-3.398658
O	0.401738	-1.164841	1.436025	H	3.594067	-0.497945	-6.657682
H	3.107572	0.154319	-5.067014	H	6.442338	0.131956	-3.363941
H	2.272527	0.666429	-6.554983	H	3.737410	3.761893	-3.323914
H	1.730067	-3.659865	-3.106177	H	3.338032	-7.265250	2.713851
H	0.461864	-2.728986	-2.314137	H	-0.072063	-7.624251	7.782456
H	1.310675	-5.966424	-3.900573	H	0.216080	6.454201	4.521420
H	-1.746558	-3.750052	-1.859528	H	-3.827721	-5.372785	5.655510
H	-0.005331	-8.045214	-3.627932	H	-1.883924	5.212923	0.227210
H	-3.080877	-5.819898	-1.603953	H	-0.184971	0.170965	-3.201708
H	-2.217742	-7.979464	-2.487516	H	-0.885390	-6.510316	6.670553
H	0.531955	-3.454128	-5.293689	H	-1.995935	5.835952	3.287820
H	-3.319619	-5.235946	-7.201231	H	1.596284	-1.055179	-3.895379
H	-3.618383	-5.245708	-5.455765	H	3.611593	0.280537	-2.531155
H	-3.881871	-2.842579	-7.340605	H	3.403381	-4.099817	0.388177

C	0.502014	0.559710	-0.217614	O	6.037293	2.089748	-3.070935
C	1.333522	-0.402970	0.674335	C	2.322586	2.266263	-3.230070
H	-0.153905	-0.058314	-0.839779	C	1.477924	1.067050	-2.723218
H	-0.137711	1.144715	0.454975	O	0.967802	1.621574	-1.106384
C	4.225071	1.672286	3.161379	O	2.004031	-0.086338	-2.566559
C	3.059936	1.153684	3.727786	N	4.699301	0.354132	-2.465172
C	4.451715	1.507626	1.792117	C	5.789200	-0.620400	-2.539300
C	2.127189	0.479488	2.933247	C	5.320093	-2.069994	-2.330621
H	2.874093	1.269270	4.792499	C	5.136334	-2.498214	-0.902388
C	3.519856	0.836198	1.000146	C	3.969730	-2.900050	-0.294690
H	5.359622	1.897552	1.339429	C	6.173961	-2.640185	0.092357
C	2.340723	0.317510	1.558814	C	5.551385	-3.127549	1.279991
H	1.231254	0.067296	3.382007	C	7.565560	-2.427272	0.099994
H	3.708088	0.709352	-0.060569	N	4.211242	-3.269795	1.011453
H	1.889776	-1.068382	0.005750	C	6.276024	-3.391977	2.448705
H	-3.867887	6.347556	-1.391950	C	8.287770	-2.689907	1.259077
H	-4.404749	7.078096	2.331729	C	7.648273	-3.166022	2.423392
H	-4.172952	5.335358	3.624959	C	-3.474400	-4.403600	5.280700
H	-8.229068	-1.384005	-3.352747	C	-2.734864	-4.614074	4.109249
H	-1.265110	-3.969188	-6.929196	C	-3.606439	-3.092747	5.754482
H	1.423212	4.393192	3.841881	C	-2.135757	-3.553515	3.419477
H	-4.499884	3.283674	5.053881	C	-3.015036	-2.024759	5.079361
O	0.616212	5.274345	2.222709	C	-2.271200	-2.243042	3.905315
H	-0.246230	5.611482	1.904592	O	-1.734183	-1.148007	3.307291
H	-9.223080	-3.860095	-1.808122	C	-0.278600	-6.787900	7.149200
C	-6.621325	-4.763188	-1.403653	C	0.148488	-5.579241	7.990022
H	-5.664582	-4.773700	-0.870240	C	0.222058	-4.300448	7.152551
H	-7.331912	-5.361844	-0.819983	C	-8.938200	-1.725500	-2.952900
H	-6.475450	-5.265323	-2.366540	C	-8.428813	-3.115478	-2.555675
C	-7.272918	-2.624696	-0.232714	C	-7.112563	-3.123014	-1.753105
H	-7.564390	-1.575365	-0.338703	C	2.438600	-6.629100	2.458300
H	-8.028994	-3.121167	0.388845	C	2.163190	-5.406502	3.081293
H	-6.325282	-2.648596	0.315574	C	2.007775	-6.809237	1.136777
H	1.837804	-6.016625	8.026322	C	1.486230	-4.383557	2.409851
C	2.166993	-2.036560	5.945942	C	1.332897	-5.805224	0.453720
H	2.675461	-1.131660	6.284626	C	1.040307	-4.541939	1.058658
H	2.757616	-2.497694	5.151027	O	0.411907	-3.612245	0.399262
H	1.179450	-1.771574	5.561422	C	-3.915700	8.212500	1.763100
S	2.034995	-3.151974	7.389378	C	-2.631391	8.950381	2.143347
H	4.951816	2.192754	3.779256	C	-1.355873	8.289514	1.600189
<b>TS3-R-SO-C2-r3</b>							
C	2.918600	-0.457400	-5.977100	O	-1.376371	6.985610	1.608441
C	1.904114	-1.601066	-5.888049	O	-0.404129	8.986093	1.234893
O	1.564228	-2.231046	-6.896639	C	-3.975400	5.563900	4.528500
N	1.414606	-1.869020	-4.646616	C	-2.531509	5.291542	4.992196
C	0.410600	-2.904300	-4.430500	O	-2.304313	4.733363	6.071766
C	-1.007318	-2.319366	-4.544176	C	-4.976500	4.641500	5.234300
O	-1.287201	-1.243976	-3.983447	N	-1.552075	5.716467	4.153815
C	0.616925	-3.590950	-3.056530	C	-0.130200	5.485000	4.408200
C	-0.207525	-4.850940	-2.895889	C	0.591925	4.732933	3.277563
C	0.258395	-6.075700	-3.397904	C	-0.160055	3.471007	2.850974
C	-1.460736	-4.821970	-2.269197	C	-3.901700	5.352700	-1.598400
C	-0.508718	-7.237563	-3.286733	C	-2.550282	4.743999	-1.353527
C	-2.233106	-5.979670	-2.160178	C	-1.927147	3.635924	-1.878592
C	-1.761301	-7.191462	-2.670454	N	-1.643544	5.277134	-0.451010
N	-1.940442	-3.007286	-5.241889	C	-0.540244	4.514185	-0.438575
C	-1.793200	-4.294600	-5.976900	N	-0.676958	3.509898	-1.297185
C	-3.241735	-4.674017	-6.310051	O	0.269882	1.119078	-3.406421
C	-3.944261	-3.316398	-6.464712	O	0.016428	-1.211806	1.096992
C	-3.306098	-2.462859	-5.363125	H	3.298660	-0.152478	-5.001470
C	3.726300	2.630200	-2.675800	H	2.438276	0.401235	-6.457221
C	4.913844	1.654366	-2.780298	H	1.681464	-3.836865	-2.983911
				H	0.391378	-2.891842	-2.247526
				H	1.234600	-6.118984	-3.875362

H	-1.821577	-3.888568	-1.848521	H	-3.937277	-5.235274	5.802122
H	-0.126287	-8.176780	-3.676706	H	-1.747385	6.068579	0.217964
H	-3.200082	-5.937088	-1.666618	H	-0.110868	0.215748	-3.452045
H	-2.359568	-8.093541	-2.579124	H	-1.262835	-6.624624	6.697399
H	0.563254	-3.640378	-5.222470	H	-1.786092	6.175392	3.269759
H	-3.304422	-5.300625	-7.203388	H	1.649894	-1.243462	-3.861606
H	-3.677434	-5.231413	-5.473695	H	3.720131	0.040274	-2.373375
H	-3.722241	-2.887021	-7.448110	H	3.503543	-3.648913	1.633584
H	-5.030549	-3.379083	-6.362226	C	0.208962	0.632924	-0.407748
H	-3.263325	-1.397069	-5.598247	C	0.991413	-0.365534	0.488907
H	-3.834994	-2.569852	-4.407342	H	-0.371823	0.024778	-1.115249
H	-1.296467	-5.044280	-5.361308	H	-0.512680	1.155689	0.236148
H	2.411916	2.072972	-4.305857	C	3.647473	1.475750	3.391834
H	1.700878	3.162863	-3.144869	C	2.465262	0.864865	3.812875
H	3.628949	2.887663	-1.612543	C	3.963987	1.486218	2.030511
H	6.077729	-2.713305	-2.798869	C	1.603000	0.276312	2.883101
H	4.394846	-2.236700	-2.894763	H	2.211752	0.841634	4.869749
H	2.964728	-2.961584	-0.687700	C	3.103982	0.895706	1.104100
H	8.074201	-2.065006	-0.789380	H	4.888487	1.944952	1.689816
H	9.361952	-2.526744	1.271321	C	1.905858	0.290290	1.515869
H	5.781428	-3.764136	3.341166	H	0.689693	-0.201646	3.218055
H	8.237686	-3.361020	3.314993	H	3.369654	0.887153	0.052781
H	6.559606	-0.361825	-1.803624	H	1.619863	-0.963908	-0.179377
H	-2.617198	-5.621163	3.717813	H	-3.816090	6.372051	-1.989790
H	-4.176652	-2.895068	6.658433	H	-3.873133	7.169120	2.074677
H	-1.565680	-3.733578	2.511473	H	-4.037940	5.448739	3.441578
H	-3.121210	-1.007221	5.443211	H	-8.182492	-1.177724	-3.527997
H	-1.175658	-1.333552	2.515707	H	-1.198289	-4.133697	-6.884301
H	-0.560731	-5.433365	8.814128	H	-4.795798	3.594330	4.974109
H	0.944536	-4.417343	6.337389	H	1.566187	4.431111	3.684929
H	-0.753719	-4.075752	6.710245	O	0.898859	5.581970	2.169693
H	0.431720	-6.975587	6.336712	H	0.116037	6.147116	1.954997
H	-8.283179	-3.713000	-3.465613	H	-9.201996	-3.636379	-1.972150
H	-6.359665	-2.582096	-2.346894	C	-6.609332	-4.560630	-1.557056
H	-9.193294	-1.117850	-2.079115	H	-6.465959	-5.069234	-2.516948
H	2.208793	-7.752055	0.630004	H	-5.653828	-4.576737	-1.021585
H	2.484421	-5.240613	4.108739	H	-7.326530	-5.149661	-0.971718
H	1.006147	-5.958265	-0.570303	C	-7.244186	-2.410172	-0.398948
H	1.272296	-3.442158	2.910870	H	-7.525863	-1.358820	-0.511190
H	0.224318	-2.190552	0.861987	H	-8.006110	-2.896444	0.223540
H	-2.653185	9.992257	1.809140	H	-6.298031	-2.439754	0.151581
H	-2.533417	8.973772	3.238322	H	1.125730	-5.773865	8.449013
H	-4.070289	8.226754	0.677845	C	0.669524	-1.535631	6.938522
H	-4.882045	4.734001	6.318192	H	-0.331559	-1.457386	6.508189
H	-6.002226	4.892428	4.946896	H	0.914062	-0.602345	7.449900
H	-4.207841	6.614664	4.744895	H	1.399074	-1.708360	6.143530
H	0.420110	2.914951	2.111884	S	0.732977	-2.868155	8.189374
H	-0.331150	2.812163	3.708548	H	4.320000	1.928862	4.115130
H	-1.133299	3.722539	2.419159				
H	-0.071094	4.908000	5.333810				
H	-4.453737	4.753374	-2.325318	<b>Prod-R-SO-C2-r3</b>			
H	-4.488984	5.397880	-0.675278	C	2.685000	-0.270400	-6.146000
H	-2.276366	2.932483	-2.618041	C	1.679193	-1.420560	-6.071222
H	0.301890	4.692200	0.217143	O	1.215945	-1.942566	-7.087924
H	0.109508	2.610176	-1.310211	N	1.303236	-1.826680	-4.818332
H	-4.794078	8.675926	2.226055	C	0.157600	-2.721200	-4.637400
H	-9.837298	-1.799860	-3.573904	C	-1.136665	-1.950159	-4.970137
H	3.744703	-0.776321	-6.616848	O	-1.261438	-0.764762	-4.603513
H	6.268756	-0.532456	-3.522955	C	0.136899	-3.237799	-3.177990
H	4.057243	3.536917	-3.186938	C	-0.915633	-4.295139	-2.922053
H	2.969633	-7.415789	2.986155	C	-0.659378	-5.641424	-3.223710
H	-0.334416	-7.693198	7.762415	C	-2.169753	-3.955575	-2.398174
H	0.384369	6.440850	4.571951	C	-1.633302	-6.620536	-3.017427
				C	-3.146761	-4.931441	-2.190816



C	-2.882712	-6.266904	-2.502221	N	-0.674058	3.450114	-1.221604
N	-2.125495	-2.582771	-5.632629	O	0.407155	1.483209	-4.153868
C	-2.136600	-3.968600	-6.174200	O	0.254973	-1.517087	2.020965
C	-3.605714	-4.177145	-6.561820	H	3.342411	-0.201500	-5.280124
C	-4.072068	-2.770852	-6.968731	H	2.126623	0.667346	-6.233005
C	-3.371938	-1.859496	-5.954130	H	1.131115	-3.644333	-2.966202
C	3.693300	2.621400	-2.724800	H	-0.015184	-2.386271	-2.506857
C	4.608762	1.512863	-3.260876	H	0.313833	-5.924119	-3.617745
O	5.065067	1.585422	-4.407396	H	-2.378060	-2.920369	-2.142139
C	2.348788	2.675769	-3.479221	H	-1.413662	-7.658155	-3.252236
C	1.542224	1.387704	-3.455008	H	-4.110425	-4.648748	-1.776823
O	0.979264	1.429327	-0.004587	H	-3.640131	-7.027250	-2.335496
O	1.901334	0.353875	-2.907117	H	0.282999	-3.557640	-5.327333
N	4.889534	0.484043	-2.413005	H	-3.716940	-4.919465	-7.356128
C	5.661700	-0.688600	-2.821900	H	-4.169676	-4.525146	-5.689683
C	4.891397	-2.024615	-2.793871	H	-3.727365	-2.538310	-7.982423
C	4.791184	-2.672465	-1.442702	H	-5.158373	-2.653971	-6.947213
C	3.653328	-2.905199	-0.704376	H	-3.136713	-0.865305	-6.340224
C	5.882523	-3.235389	-0.681795	H	-3.968069	-1.729947	-5.042516
C	5.322186	-3.785756	0.508193	H	-1.794363	-4.685692	-5.428792
C	7.269866	-3.352450	-0.891170	H	2.518173	2.926135	-4.532366
N	3.966819	-3.562275	0.466452	H	1.713108	3.467295	-3.068406
C	6.104856	-4.430405	1.474244	H	3.506295	2.499370	-1.654021
C	8.049641	-3.991824	0.066202	H	5.422522	-2.704509	-3.474833
C	7.472216	-4.524106	1.238883	H	3.894730	-1.878031	-3.221361
C	-3.446700	-4.602200	5.115400	H	2.622779	-2.666562	-0.926526
C	-2.697932	-4.616872	3.935005	H	7.729183	-2.954424	-1.792078
C	-3.594932	-3.395902	5.807952	H	9.120912	-4.085892	-0.088750
C	-2.095620	-3.456258	3.447475	H	5.654488	-4.847532	2.369932
C	-2.996899	-2.228209	5.336502	H	8.106430	-5.018770	1.969155
C	-2.235039	-2.247976	4.154552	H	6.554486	-0.768539	-2.190628
O	-1.676193	-1.086765	3.744436	H	-2.577889	-5.543799	3.380072
C	-0.263300	-7.167200	6.751200	H	-4.179619	-3.361998	6.723754
C	0.180590	-6.110774	7.768965	H	-1.526072	-3.481687	2.522571
C	0.213106	-4.708324	7.157685	H	-3.106480	-1.287340	5.867787
C	-9.097700	-1.356500	-2.780600	H	-1.005531	-1.240240	3.014742
C	-8.634190	-2.089185	-1.516647	H	-0.501622	-6.116946	8.628193
C	-7.113723	-2.057480	-1.264543	H	0.922176	-4.669079	6.323643
C	2.300700	-6.846900	1.982900	H	-0.774834	-4.433654	6.774701
C	2.212384	-5.692366	2.766773	H	0.417863	-7.203226	5.893914
C	1.618485	-6.876754	0.759696	H	-8.953800	-3.138188	-1.579187
C	1.476166	-4.583448	2.341670	H	-6.621144	-2.457129	-2.164656
C	0.878038	-5.785143	0.322252	H	-8.891654	-0.282665	-2.731599
C	0.785048	-4.587844	1.091106	H	1.669926	-7.768042	0.136581
O	0.102636	-3.561127	0.650629	H	2.726664	-5.649297	3.725491
C	-3.627500	8.183700	2.248300	H	0.352670	-5.816599	-0.627638
C	-2.308873	8.862399	2.621000	H	1.411153	-3.692062	2.958915
C	-1.074582	8.195395	1.992355	H	0.198065	-2.397327	1.424477
O	-1.130704	6.897499	1.936756	H	-2.311250	9.921645	2.345192
O	-0.122001	8.890608	1.619925	H	-2.171853	8.821358	3.711297
C	-3.674700	5.400800	4.878700	H	-3.819053	8.262817	1.171799
C	-2.220251	5.091932	5.282843	H	-4.516537	4.518933	6.674465
O	-1.968305	4.520545	6.350926	H	-5.690570	4.731324	5.355966
C	-4.656200	4.463300	5.593100	H	-3.886007	6.445286	5.141928
N	-1.261487	5.490511	4.410593	H	0.633254	2.861515	2.096506
C	0.160400	5.219900	4.621800	H	-0.052900	2.602793	3.710729
C	0.857290	4.555606	3.422458	H	-0.901363	3.629639	2.542559
C	0.086716	3.338444	2.911558	H	0.224725	4.568197	5.496164
C	-3.810200	5.499300	-1.250000	H	-4.437424	4.947988	-1.954963
C	-2.485882	4.816007	-1.101756	H	-4.346400	5.556588	-0.295570
C	-1.952737	3.691657	-1.693090	H	-2.414970	3.047757	-2.429074
N	-1.494734	5.271088	-0.253262	H	0.450034	4.554666	0.242321
C	-0.440846	4.426672	-0.356659	H	0.379447	2.007489	-0.526777

H	-4.475781	8.643189	2.768252	H	1.718892	-1.040913	0.650996
H	-10.176091	-1.476090	-2.930262	H	-3.701295	6.523592	-1.625798
H	3.280681	-0.392789	-7.051976	H	-3.602921	7.123334	2.498730
H	5.995956	-0.473576	-3.838821	H	-3.779707	5.324533	3.791791
H	4.211673	3.572325	-2.873033	H	-8.594043	-1.749864	-3.671573
H	2.880351	-7.702180	2.317807	H	-1.478019	-4.025209	-7.049811
H	-0.285889	-8.163790	7.204053	H	1.833079	4.213816	3.794431
H	0.692631	6.151474	4.857657	H	-4.495561	3.424118	5.290931
H	-3.914730	-5.510448	5.483351	O	1.162454	5.481340	2.380868
H	-1.527747	6.028274	0.448461	H	0.361622	6.022920	2.173554
H	-0.077690	0.617002	-4.163230	H	-9.146901	-1.668352	-0.639496
H	-1.265395	-6.947495	6.367682	C	-6.743786	-2.967837	-0.084396
H	-1.507581	5.990300	3.551405	H	-5.661451	-2.983455	0.083088
H	1.542375	-1.222725	-4.032669	H	-7.215136	-2.617178	0.842185
H	4.342225	0.414023	-1.566573	H	-7.073757	-3.998807	-0.255020
H	3.284260	-3.897255	1.140460	C	-6.585865	-0.633924	-1.032090
C	0.195763	0.459615	0.666504	H	-6.772165	0.020341	-1.889237
C	1.090692	-0.551454	1.409904	H	-7.064406	-0.180723	-0.154770
H	-0.420039	-0.121236	-0.037943	H	-5.505721	-0.641850	-0.851992
H	-0.485724	0.918410	1.399634	H	1.174681	-6.364412	8.157476
C	3.768841	1.275903	4.298011	C	0.624432	-1.940517	7.403146
C	2.606845	0.631813	4.727493	H	0.851391	-1.100628	8.063066
C	4.060252	1.323840	2.932182	H	1.355959	-1.964879	6.591843
C	1.743023	0.040690	3.801604	H	-0.378369	-1.810901	6.989444
H	2.370655	0.586849	5.787418	S	0.714916	-3.460993	8.414765
C	3.195772	0.732420	2.010415	H	4.442621	1.731137	5.018663
H	4.964378	1.816621	2.584746				
C	2.023372	0.088686	2.430092				
H	0.843072	-0.460543	4.139615				
H	3.424556	0.775540	0.950476				