

Supporting information:

Photocurable acylhydrazone covalent adaptable networks with fast dynamic exchange and tunable viscoelastic properties

Yunsheng Xu^a, Chonglin Liu^a, Yanying Zhao^b, Xianming Zhang^{a,*} and Minna Hakkarainen^{c,*}

^a School of Materials Science and Engineering, Zhejiang Sci-Tech University, Hangzhou 310018, China

^b School of Chemistry and Chemical Engineering, Zhejiang Sci-Tech University, Hangzhou 310018, China

^c Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Teknikringen 58, 100 44 Stockholm, Sweden

Correspondence: Xianming Zhang, Email: zhangxm@zstu.edu.cn

Minna Hakkarainen, Email: minna@kth.se

This supporting information contains 26 figures and 4 tables on 47 pages.

1. Synthesis small molecules for model reactions:

Compound b: vanillin (1.50 g, 10 mmol) and acetyl hydrazine (0.74 g, 10 mmol) were dissolved in 20 ml ethanol, and 4-5 drops of acetic acid were added. The mixture was stirred for 3 h at room temperature. After the reaction, the powder was filtered under reduced pressure and washed with ethanol to obtain a white solid powder. The crude product was recrystallized with ethanol:water =1:1 (v/v) and characterized by ^1H nuclear magnetic resonance (^1H NMR) spectroscopy. All samples were dissolved in DMSO-d_6 for ^1H NMR characterization. Compounds a, c and d were obtained and characterized by following the same protocol

2. ^1H NMR characterization

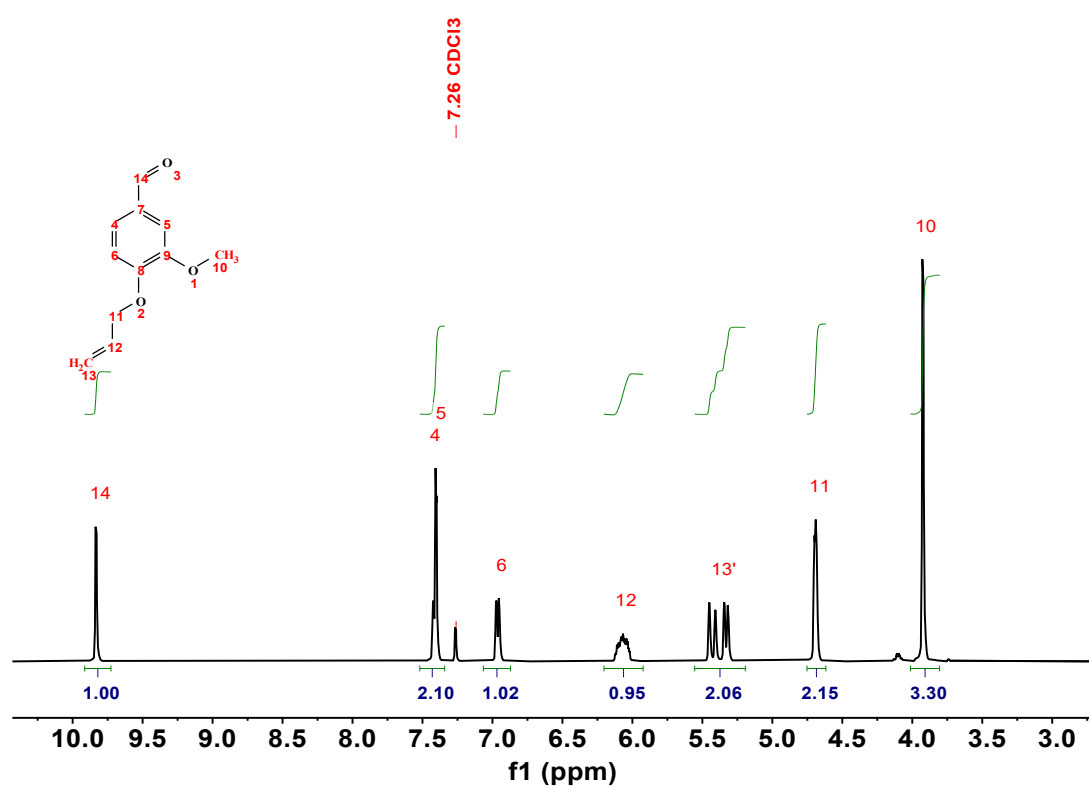


Figure S1. ^1H NMR spectrum of AVL.

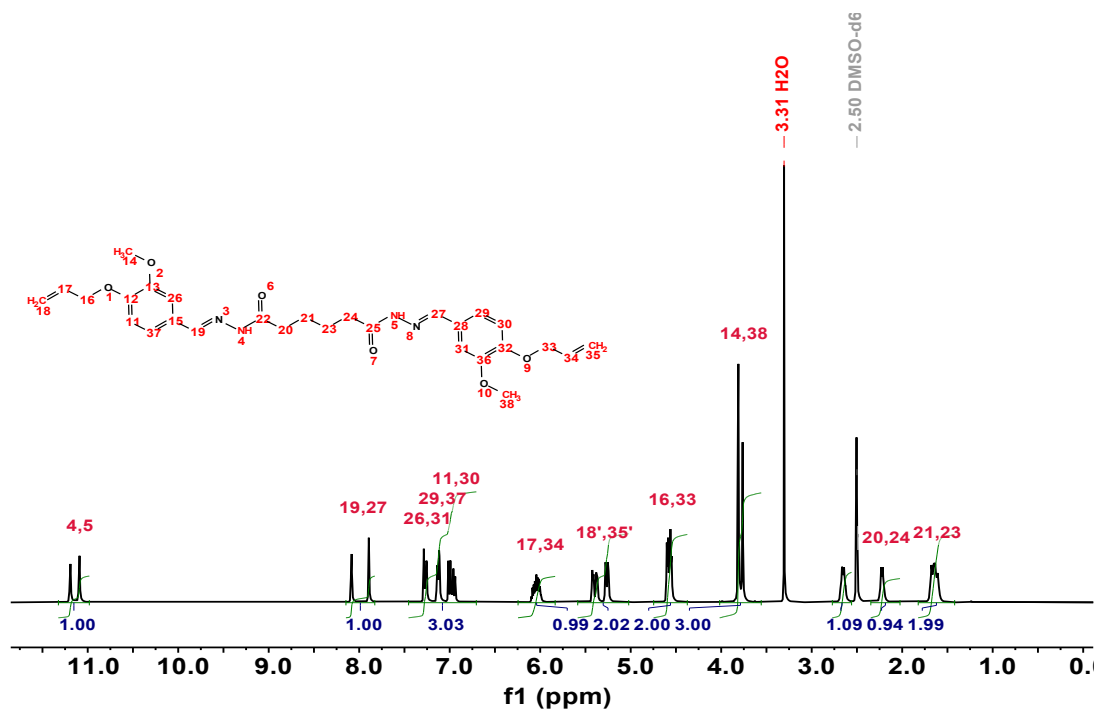


Figure S2. ¹H NMR spectrum of AVH.

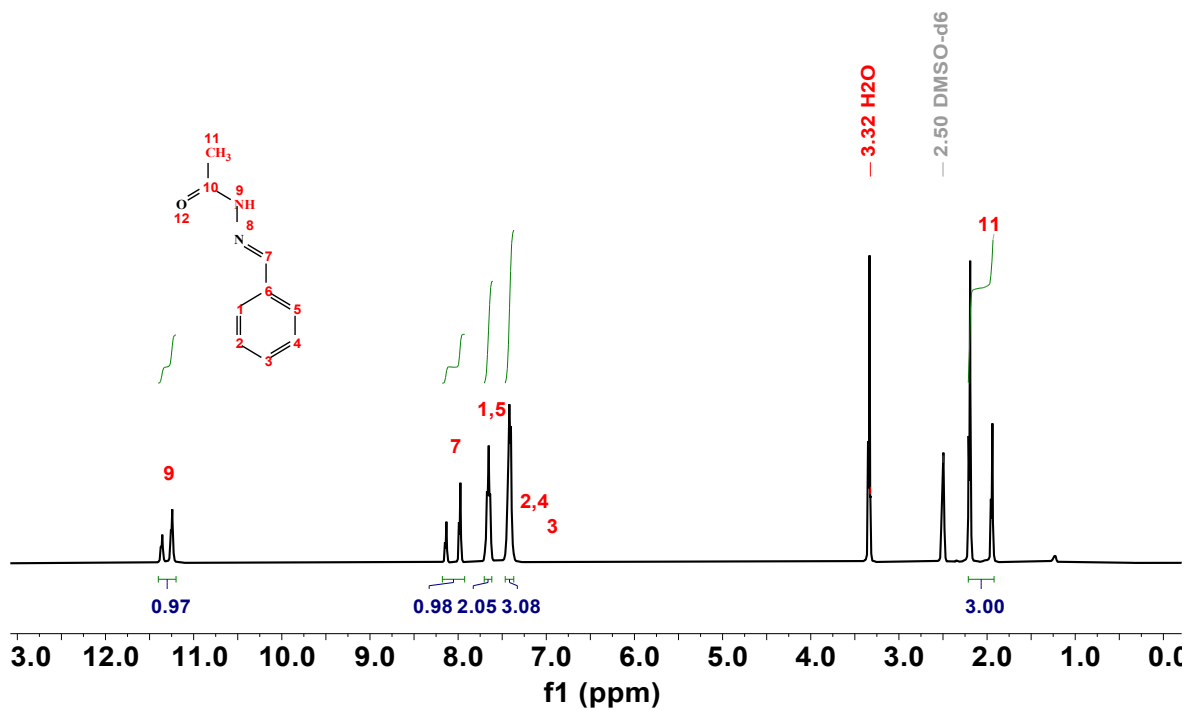


Figure S3. ¹H NMR spectrum of compound a.

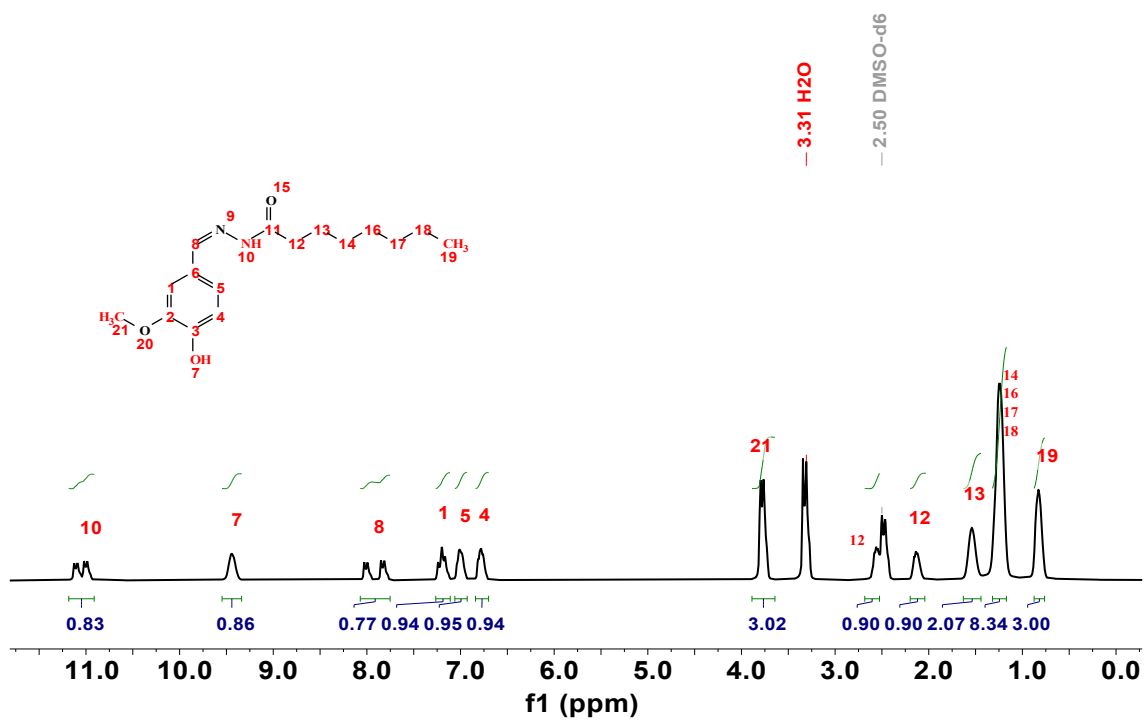


Figure S4. ¹H NMR spectrum of compound b.

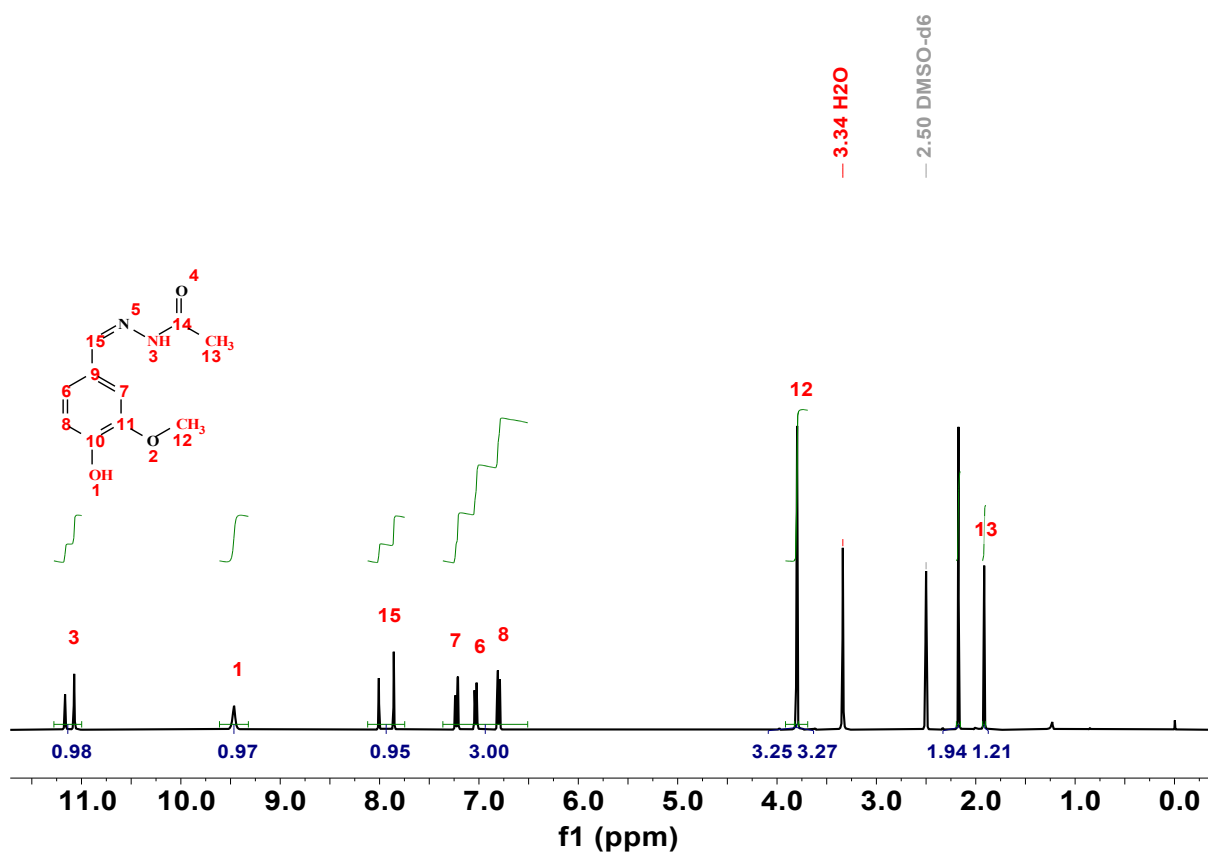


Figure S5. ¹H NMR spectrum of compound c.

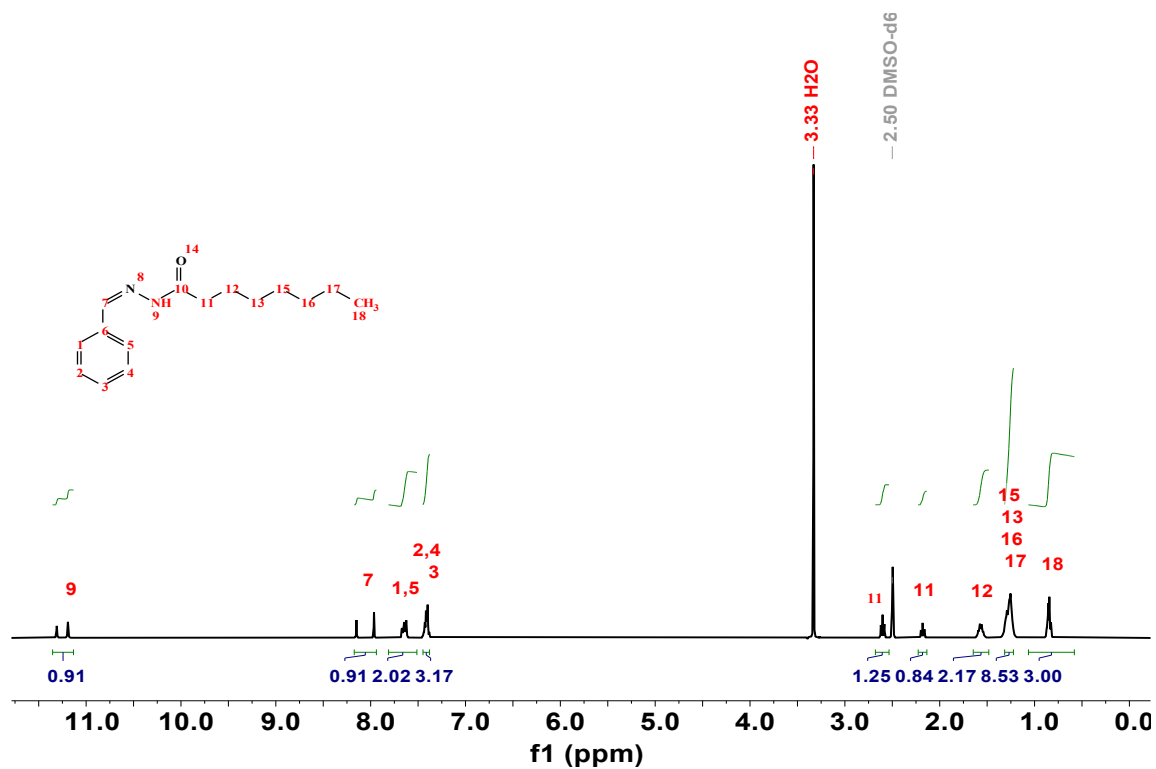


Figure S6. ¹H NMR spectrum of compound d.

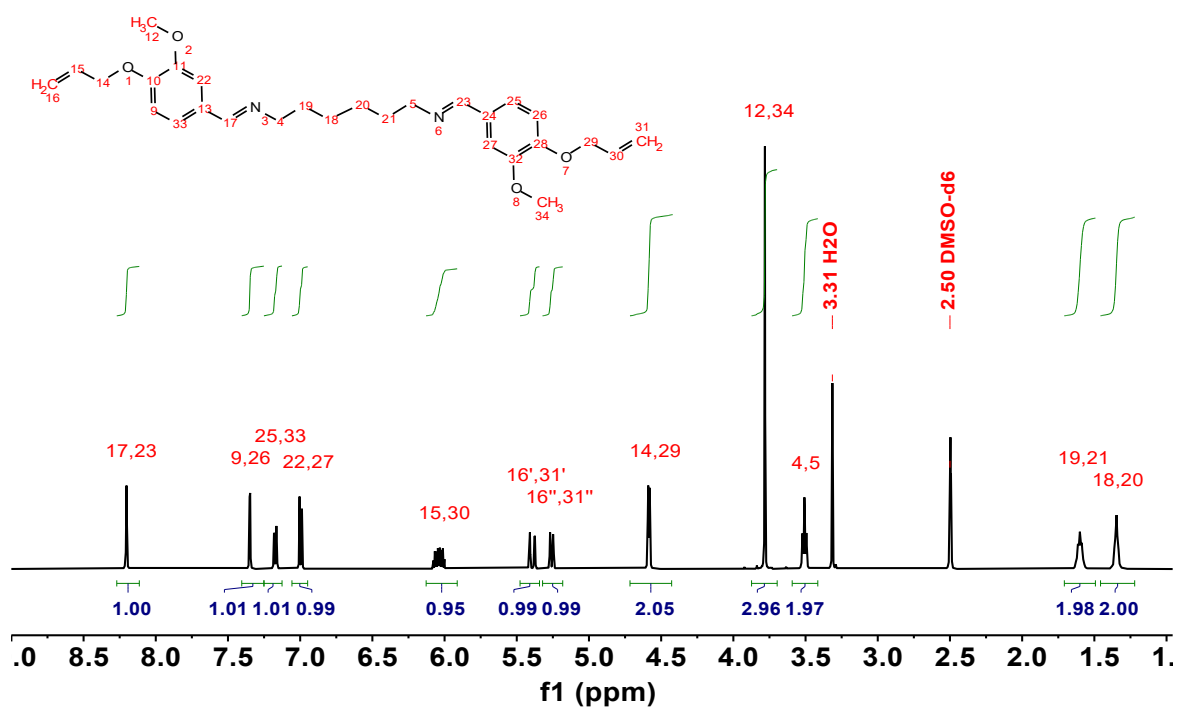


Figure S7. ¹H NMR spectrum of SVH.

2. The presence of AD influence on the thiol-ene model reaction

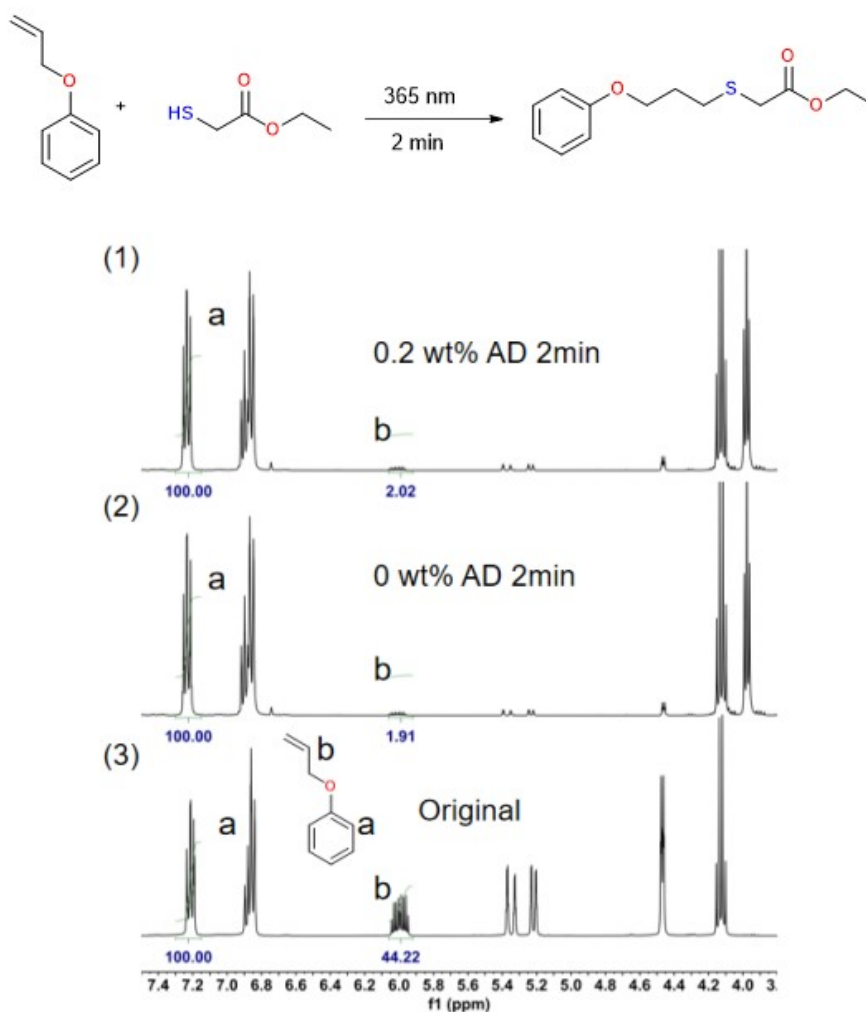


Figure S8. Comparison of ¹H NMR spectra of components with and without catalyst before and after photocuring (in the figure, a and b are proton peaks on the double bond of allyl phenyl ether and benzene ring respectively, and the peaks on benzene ring are used as reference).

3. GC-MS test

Figure S9. Mass spectra of model compounds a-d.

Figure S10. Mass spectrum of catalyst AD.

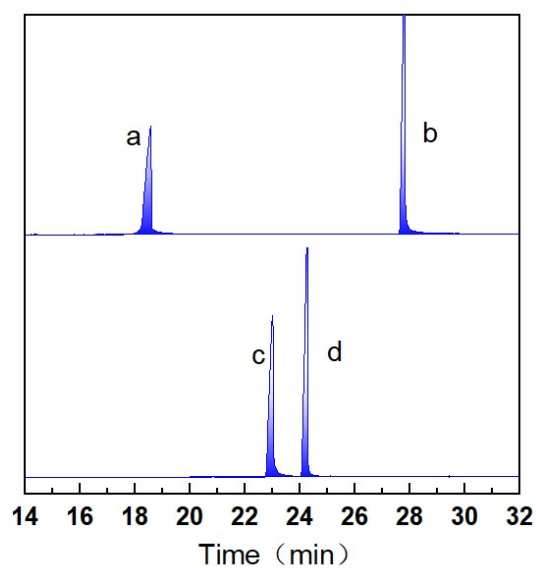


Figure S11. Gas chromatography of model compound reference material

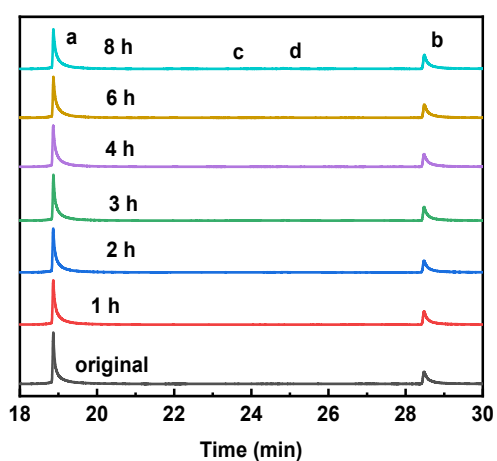


Figure S12. Gas chromatogram of acylhydrazone fractions a and b after exchange at different time at 160 °C.

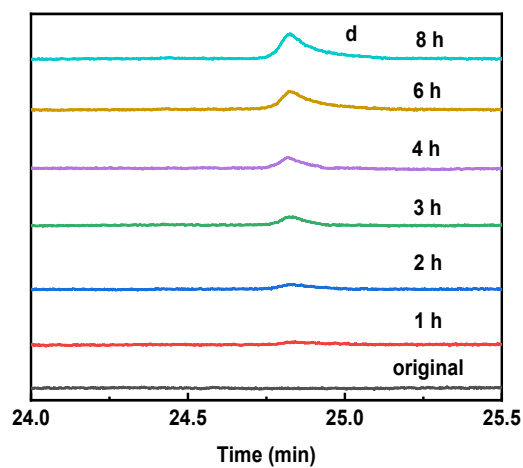


Figure S13. Magnified figure of peak position of c and d gas chromatographic products.

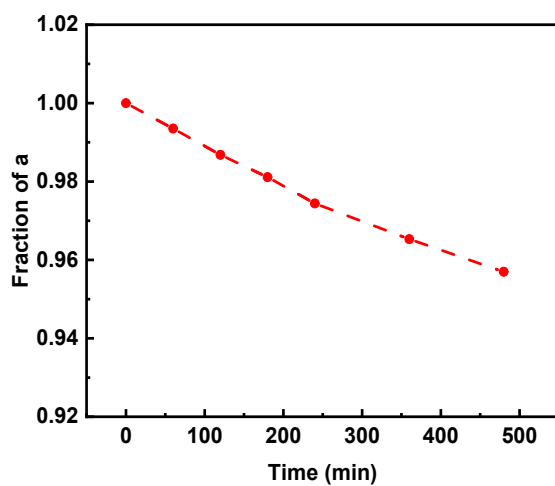


Figure S14. Reaction fraction of compound a

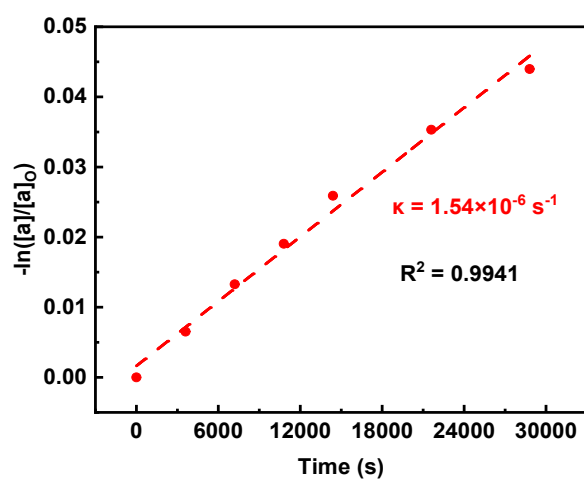


Figure S15. Pseudo-first order kinetics of acylhydrazone exchange.

4. Infrared spectra

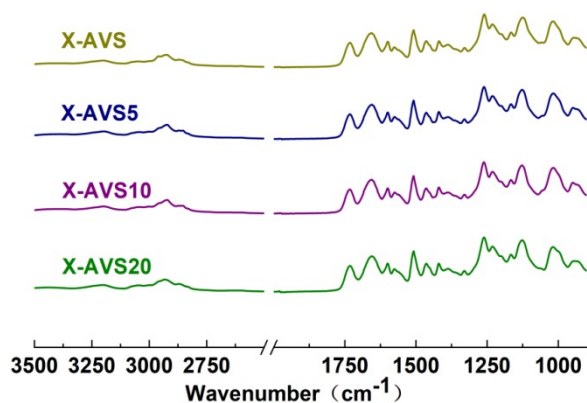


Figure S16. ATR-FTIR spectra of different loadings of AD acylhydrazone resins after UV curing

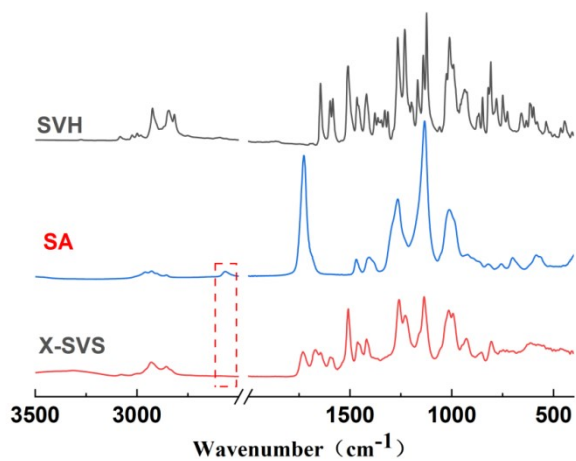


Figure S17. ATR-FTIR spectra of schiff base resins before and after UV curing

5. Reprocessability of acylhydrazone CANs

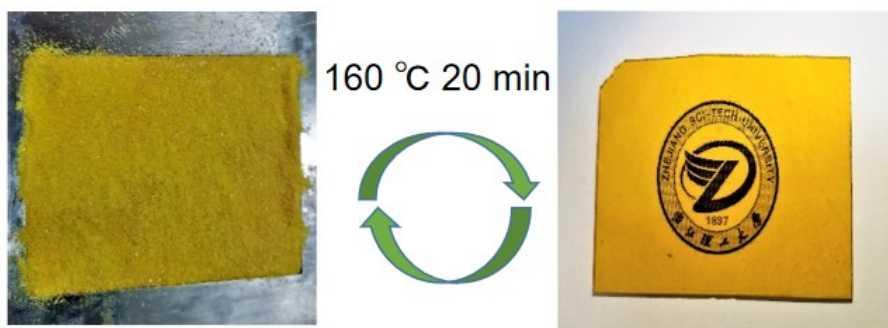


Figure S18. Illustration of the thermal reprocessing of X-AVS

6. Tensile properties

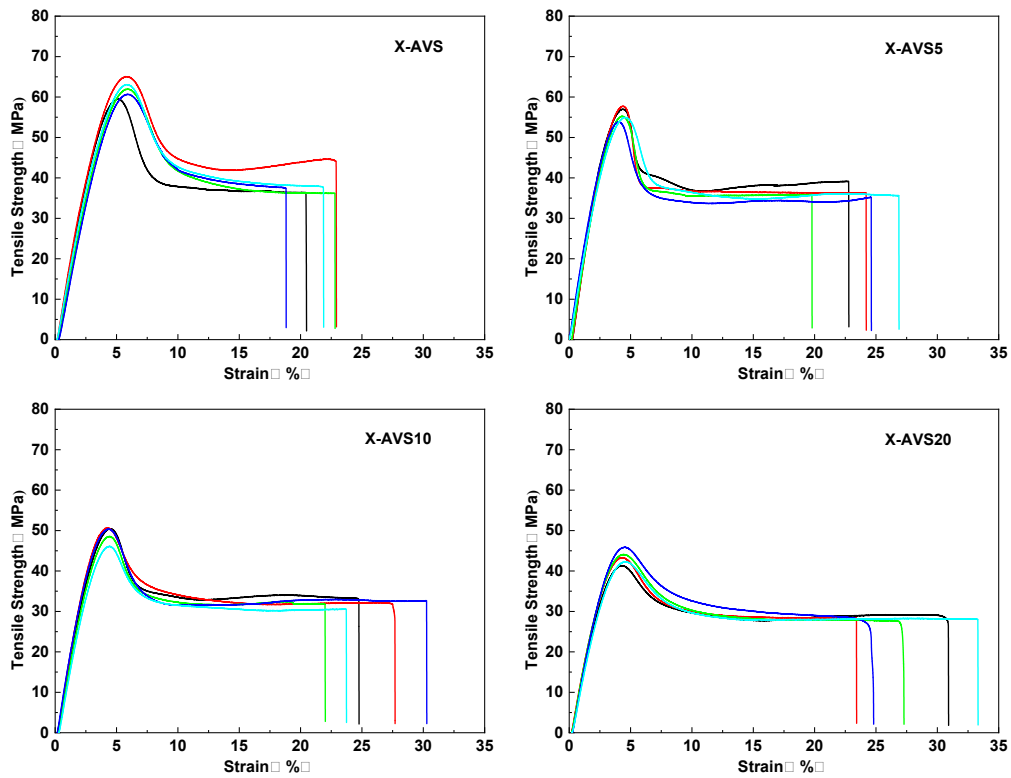


Figure S19. The tensile testing curves of the different CANs including five replicates for each material.

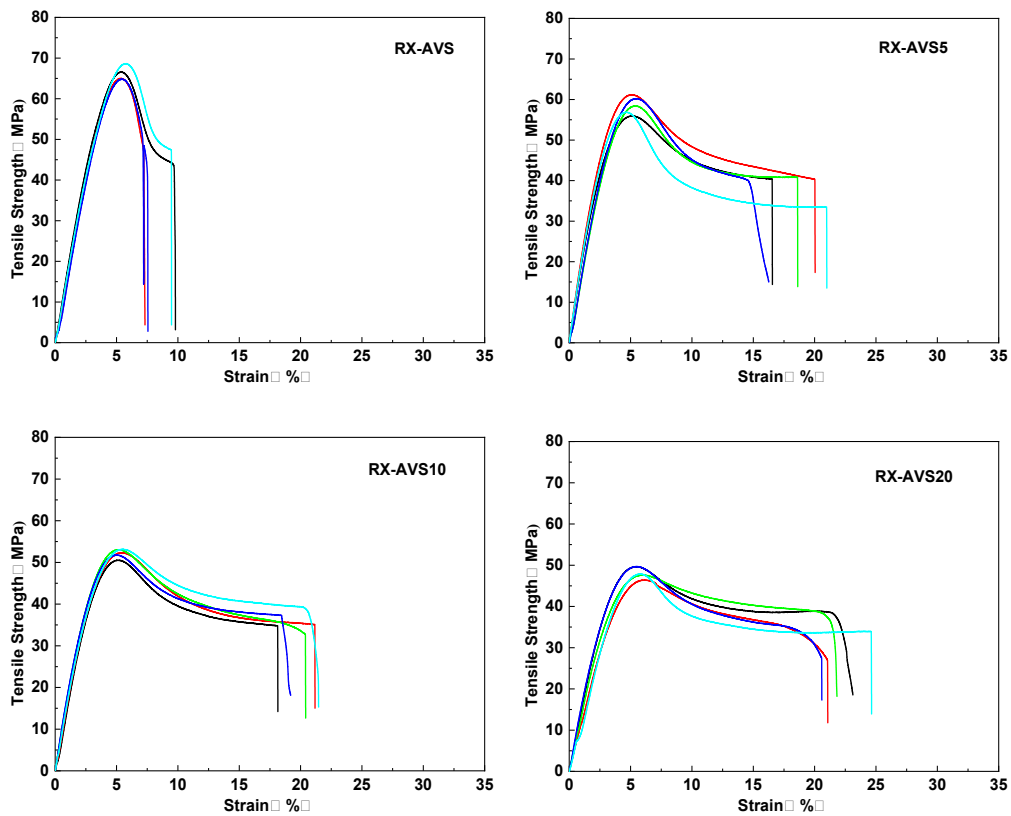


Figure S20. The tensile testing curves of the different CANs after reprocessing including five replicates for each material.

7. Stoichiometric comparison

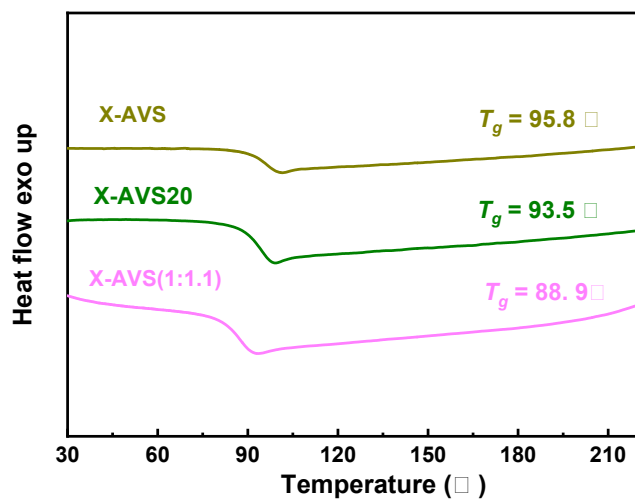


Figure S21. DSC test of hydrazone materials with different stoichiometric ratios

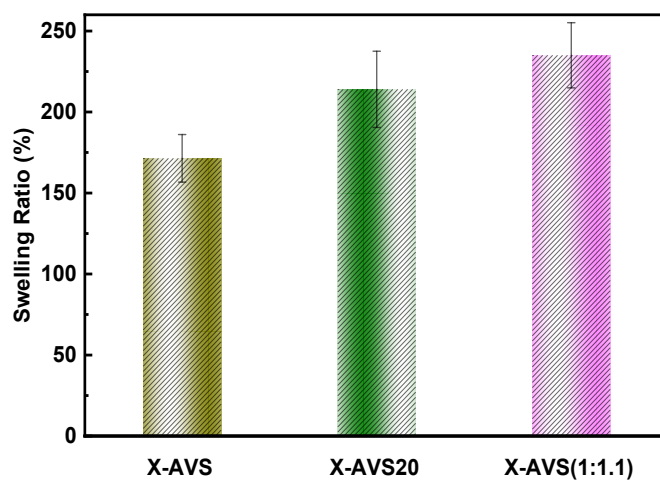


Figure S22. Swelling ratios of different catalyst loads and different stoichiometric ratios

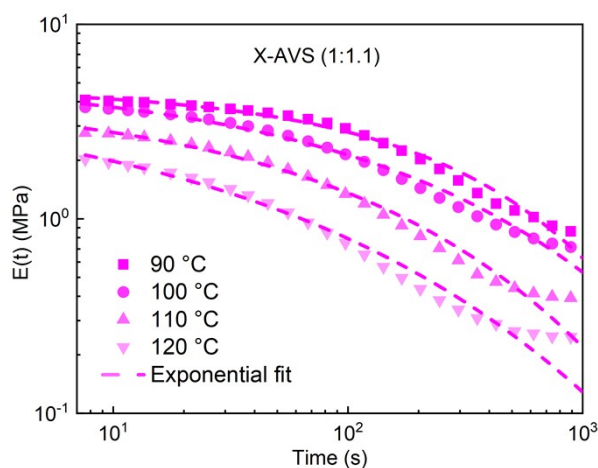


Figure S23. The stretched exponential to the stress relaxation data of acylhydrazone CANs with different stoichiometric ratios.

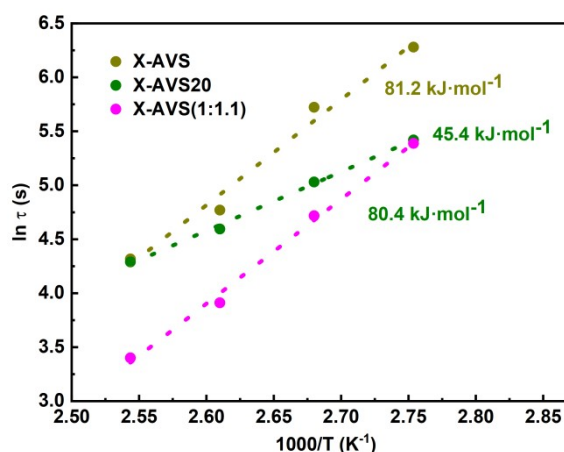


Figure S24. The relaxation time (τ) of acylhydrazone CANs as a function of $1000/T$.

8. Calculation details of activation energy

Double Maxwell model:
$$G(t) = G_0 \cdot e^{-\left(\frac{t}{\tau}\right)^\beta} \quad (S1)$$

X-AVS: $y=9.77x-20.6$, $E_a = 81.2 \text{ kJ}\cdot\text{mol}^{-1}$, $R^2=0.983$

X-AVS5: $y=6.86x-12.6$, $E_a = 57.0 \text{ kJ}\cdot\text{mol}^{-1}$, $R^2=0.997$

X-AVS10: $y=5.73x-10.0$, $E_a = 47.6 \text{ kJ}\cdot\text{mol}^{-1}$, $R^2=0.998$

X-AVS20: $y=5.47x-9.6$, $E_a = 45.4 \text{ kJ}\cdot\text{mol}^{-1}$, $R^2=0.997$

X-AVS(1:1.1): $y=9.67x-21.2$, $E_a = 80.4 \text{ kJ}\cdot\text{mol}^{-1}$, $R^2=0.995$

9. Creep test

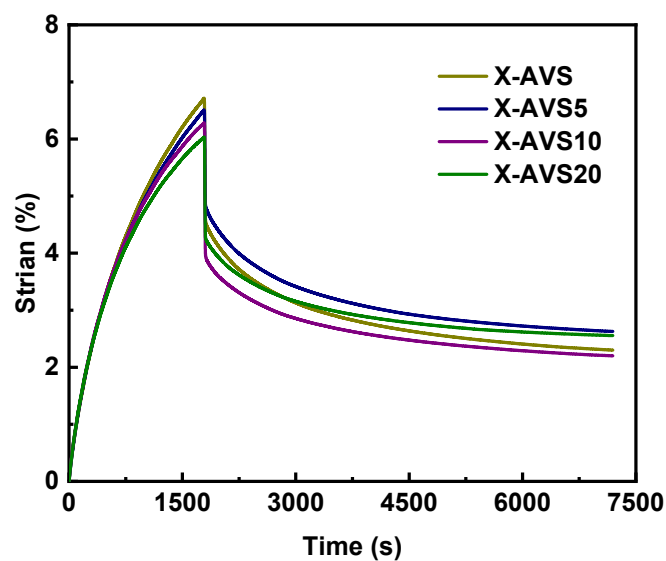


Figure S25. The creep curves of acylhydrazone CANs under different catalyst loadings at 100 °C.

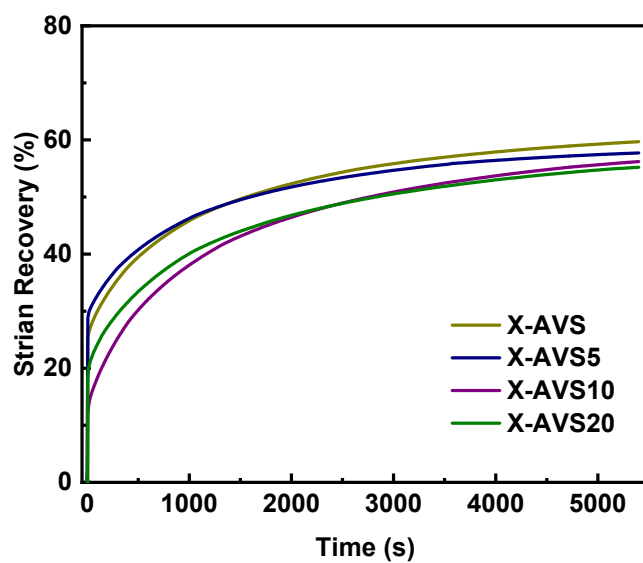


Figure S26. The strain recovery curves of acylhydrazone CANs under different catalyst loadings at 70 °C

10. GC-MS analysis date

Table S1 GC-MS retention times, peak height and peak areas.

Group	Peak #	Retention time min	Peak height %	Corrected area %
0.2 wt% AD	---	-----	-----	-----
	1	18.543	1896053	216109773
	2	22.785	499259	28026965
	3	24.147	1655989	69490773
	4	27.783	4842435	299246160
0 wt% AD	---	-----	-----	-----
	1	18.561	2041390	256102246
	2	22.78	100189	10182719
	3	24.125	902246	33366878
	4	27.801	5350630	365414547

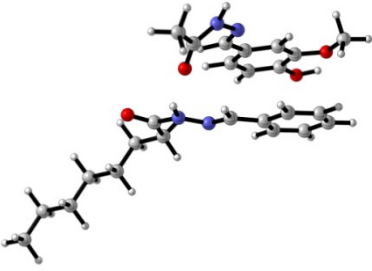
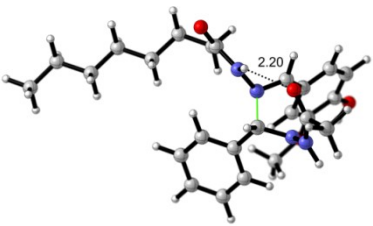
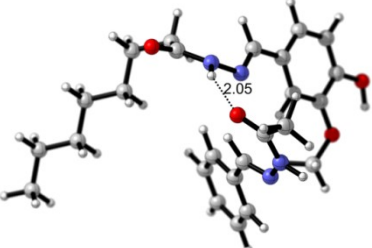
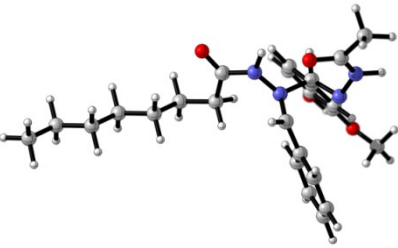
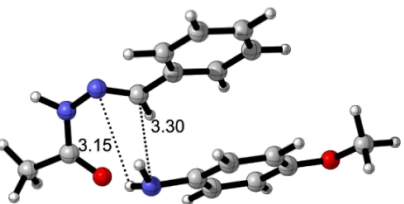
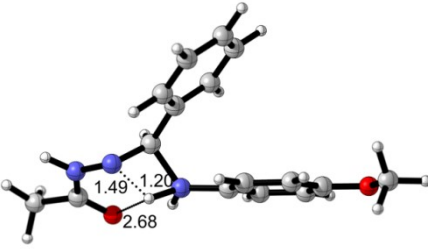
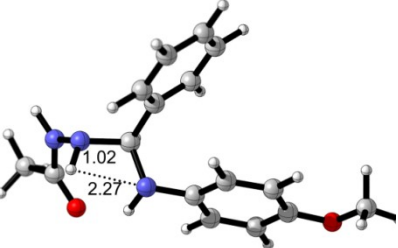
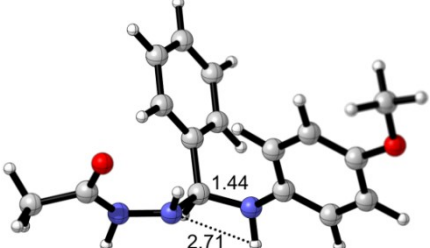
11. Mechanical properties after reprocessing

Table S2 Comparison of tensile properties before and after reprocessing.

sample	Young's modulus (MPa)	Tensile strength (MPa)	Elongation at break (%)
X-AVS	1620±27	62.1±2.1	21.4±1.7
RX-AVS	1630±32	66.2±1.7	8.6±1.1
X-AVS5	1850±89	55.8±1.6	23.7±2.6
RX-AVS5	1610±21	58.5±2.2	18.5±2.1
X-AVS10	1620±41	49.2±1.9	25.7±2.3
RX-AVS10	1620±25	52.2±1.1	20.1±1.4
X-AVS20	1560±39	43.4±1.7	27.9±4.0
RX-AVS20	1520±40	48.3±1.4	22.3±1.6

12. Transition state geometry

Table S3 Transition state geometry.

	
1-1	ts1-2
	
1-3	ts1-4
	
2-1	2-2
	
2-3	2-4

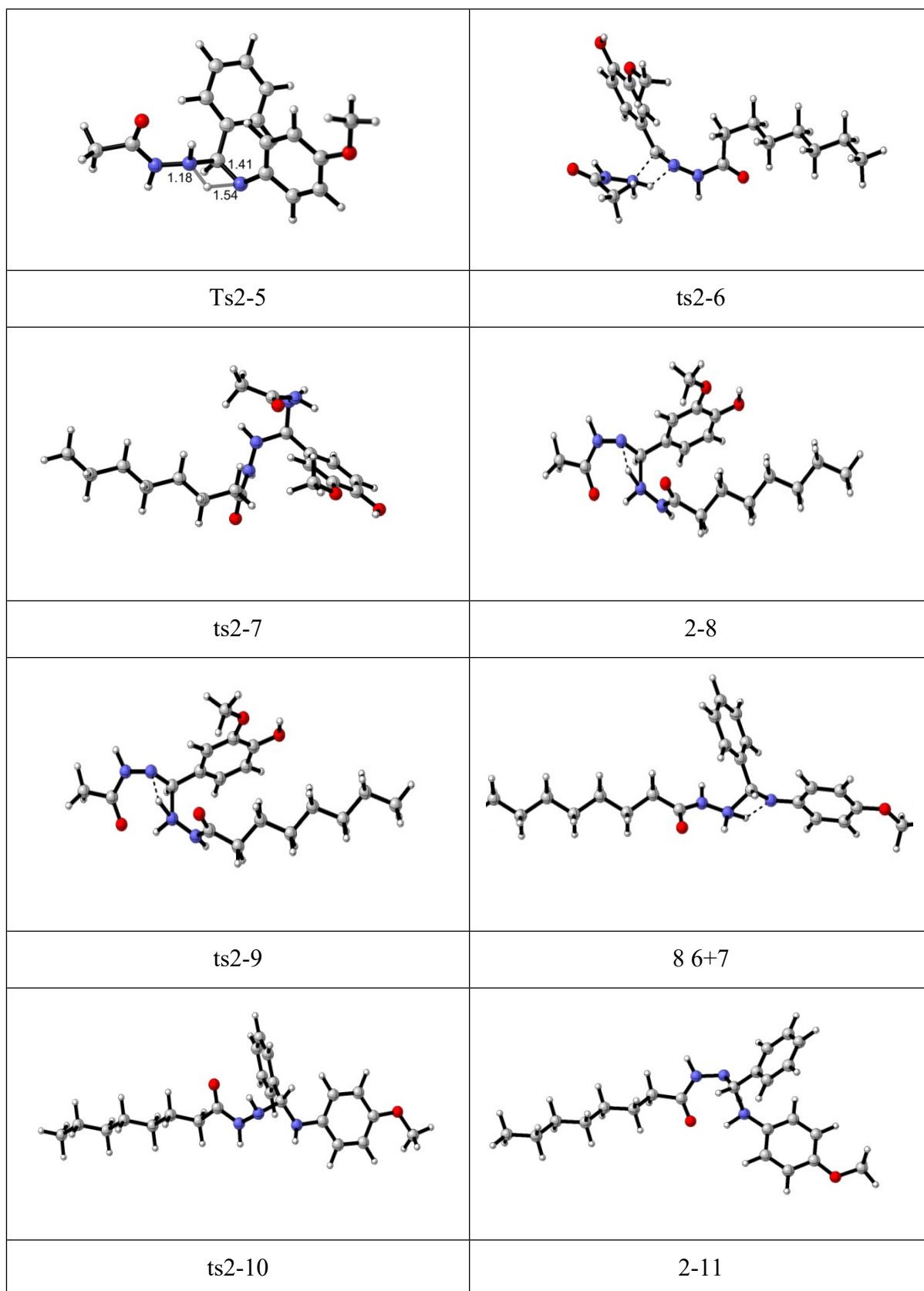


Table S4. Cartesian Coordinates of all Calculated Structures

Structure		Cartesian coordinates		
		x	y	z
1+2	C	-4.029541	0.009290	0.000043
	C	-3.374488	-1.212527	0.000000
	C	-1.987192	-1.253265	-0.000030
	C	-1.243678	-0.075764	-0.000016
	C	-1.910405	1.150814	0.000015
	C	-3.292781	1.190239	0.000048
	H	-5.111254	0.045343	0.000068
	H	-3.941790	-2.134064	-0.000008
	H	-1.471267	-2.206295	-0.000063
	H	-1.328130	2.062512	0.000020
	H	-3.803853	2.144411	0.000077
	C	0.223200	-0.172757	-0.000053
	H	0.662485	-1.163392	-0.000082
	N	0.920927	0.894262	-0.000055
	N	2.282336	0.854115	-0.000084
	C	3.138675	-0.214690	-0.000006
	H	2.682050	1.776032	-0.000088
	O	2.777437	-1.370980	0.000030
	C	4.602321	0.165144	0.000076
	H	4.777940	1.239264	-0.000341
H	5.067264	-0.276387	0.880268	
H	5.067551	-0.277136	-0.879584	
1-1	C	-8.974652	-1.459856	-0.041945
	C	-7.804083	-1.643762	-0.999257
	H	-9.901139	-1.858236	-0.456595
	H	-8.785464	-1.968806	0.905365
	H	-9.133496	-0.402289	0.177777
	C	-6.497109	-1.092442	-0.442712
	H	-7.677710	-2.706295	-1.227606
	H	-8.024690	-1.150340	-1.950288

C	-5.316575	-1.268120	-1.389190
H	-6.621846	-0.028293	-0.215489
H	-6.274763	-1.584279	0.510841
H	-5.189566	-2.332713	-1.615866
H	-5.540333	-0.775901	-2.341321
C	-4.014495	-0.707482	-0.832534
C	-2.835510	-0.894382	-1.780932
H	-3.789042	-1.192603	0.124226
H	-4.138800	0.358942	-0.626666
C	-1.541799	-0.314102	-1.230435
H	-2.691741	-1.961217	-1.973752
H	-3.062332	-0.420067	-2.737935
H	-0.673963	-0.629776	-1.818011
H	-1.352025	-0.659136	-0.210845
C	-1.548125	1.202449	-1.243869
O	-2.382176	1.868663	-1.815446
N	-0.521006	1.816130	-0.575189
H	-0.507419	2.831920	-0.567882
C	2.612166	0.515868	-1.042570
C	2.326908	-0.851553	-0.979510
C	3.602919	0.972327	-1.892804
C	3.036227	-1.736683	-1.762131
H	1.534155	-1.184799	-0.322739
C	4.327520	0.079541	-2.678808
H	3.814264	2.033212	-1.951569
C	4.049489	-1.269990	-2.617613
H	5.103736	0.417559	-3.351906
O	4.740710	-2.145142	-3.383555
H	4.392904	-3.030278	-3.215655
O	2.846867	-3.086316	-1.804974
C	1.816486	-3.619306	-1.000036
H	1.807527	-4.690418	-1.181027
H	2.010034	-3.426768	0.058309
H	0.848385	-3.191216	-1.272667

N	0.447132	1.120507	0.103495
C	1.858991	1.457797	-0.162905
H	1.979792	2.495502	-0.487735
C	-1.269088	-1.436148	4.090090
C	-1.853764	-0.196998	3.873451
C	-1.212740	0.741435	3.075218
C	0.007167	0.442264	2.479692
C	0.589699	-0.802971	2.699362
C	-0.043963	-1.735930	3.505330
H	-1.763512	-2.166551	4.717310
H	-2.805915	0.041745	4.329015
H	-1.665067	1.712245	2.907062
H	1.545632	-1.021833	2.239401
H	0.416554	-2.699850	3.681169
C	0.631295	1.428468	1.541444
H	0.322298	2.452793	1.770114
N	2.083907	1.312340	1.303634
N	2.930879	2.202227	1.932703
C	2.814179	3.559968	1.863492
H	3.689262	1.784554	2.444673
O	1.927272	4.108902	1.241118
C	3.867904	4.330650	2.619860
H	4.389190	4.976727	1.915120
H	3.367565	4.966984	3.348121
H	4.588390	3.693466	3.129107

ts1-2

C	-8.361150	-0.724440	0.872660
C	-7.519660	-0.736250	-0.396980
H	-9.407310	-0.951010	0.664890
H	-7.993870	-1.462460	1.588800
H	-8.319250	0.253600	1.356140
C	-6.053400	-0.418480	-0.131340
H	-7.593920	-1.715080	-0.880340
H	-7.919320	-0.010820	-1.111550

C	-5.194700	-0.426240	-1.389470
H	-5.977850	0.562150	0.351110
H	-5.652200	-1.143540	0.586280
H	-5.259870	-1.409760	-1.867790
H	-5.597490	0.293640	-2.109210
C	-3.735290	-0.092060	-1.112070
C	-2.861000	-0.121690	-2.360140
H	-3.334590	-0.800570	-0.377200
H	-3.676600	0.903240	-0.657510
C	-1.418610	0.258270	-2.052330
H	-2.881200	-1.123130	-2.796950
H	-3.259890	0.569630	-3.104620
H	-0.773370	0.080180	-2.919240
H	-1.016470	-0.350100	-1.240170
C	-1.296700	1.736000	-1.724640
O	-2.042790	2.574540	-2.173960
N	-0.268890	2.112420	-0.893180
H	-0.060260	3.098180	-0.752100
C	2.504430	-0.229240	-1.196200
C	2.293260	-1.331050	-0.345530
C	3.449110	-0.319940	-2.219690
C	3.017410	-2.477840	-0.534350
H	1.569130	-1.260220	0.451740
C	4.197650	-1.472570	-2.395590
H	3.600860	0.524480	-2.880220
C	3.985450	-2.553400	-1.561540
H	4.939130	-1.557290	-3.177900
O	4.690370	-3.684450	-1.724500
H	4.409570	-4.316040	-1.048030
O	2.908960	-3.615810	0.199590
C	2.070500	-3.566250	1.340980
H	2.138450	-4.542730	1.812300
H	2.411350	-2.790670	2.029940
H	1.033950	-3.362250	1.060690

N	0.650260	1.237460	-0.373320
C	1.732340	0.974360	-1.124930
H	1.823530	1.637390	-1.983810
C	-1.169560	-1.717740	3.336850
C	-1.830150	-0.984580	2.357740
C	-1.146730	-0.019270	1.634730
C	0.206820	0.220090	1.868860
C	0.857490	-0.504800	2.858300
C	0.171560	-1.469890	3.588250
H	-1.702100	-2.469170	3.905560
H	-2.881000	-1.159140	2.161530
H	-1.674680	0.561670	0.887080
H	1.907350	-0.303880	3.029480
H	0.689120	-2.027440	4.359680
C	0.938090	1.302700	1.081900
H	0.516840	2.268690	1.390800
N	2.376940	1.251870	1.187190
N	2.867390	2.495110	1.544180
C	2.701980	3.622830	0.832260
H	3.548090	2.501920	2.289060
O	1.982870	3.676520	-0.167570
C	3.438330	4.841680	1.331360
H	4.069330	5.214350	0.525090
H	2.713500	5.619260	1.570210
H	4.051230	4.641230	2.209090

1-3

C	-8.459880	-0.732850	0.883970
C	-7.618350	-0.744850	-0.385760
H	-9.506080	-0.959340	0.676240
H	-8.092670	-1.470810	1.600220
H	-8.417900	0.245260	1.367350
C	-6.151950	-0.427100	-0.120220
H	-7.692810	-1.723710	-0.869010
H	-8.018030	-0.019420	-1.100320

C	-5.292180	-0.434440	-1.377830
H	-6.076560	0.553540	0.362240
H	-5.750940	-1.152110	0.597590
H	-5.356180	-1.418040	-1.856190
H	-5.694840	0.285230	-2.097830
C	-3.833180	-0.098500	-1.098770
C	-2.957190	-0.125240	-2.345730
H	-3.432310	-0.807260	-0.364180
H	-3.775940	0.896550	-0.643580
C	-1.517120	0.260680	-2.038110
H	-2.972430	-1.127450	-2.781340
H	-3.358570	0.563370	-3.091290
H	-0.870690	0.068310	-2.900890
H	-1.119890	-0.341760	-1.218590
C	-1.396470	1.747350	-1.722370
O	-2.161560	2.573880	-2.162320
N	-0.366330	2.123850	-0.903630
H	-0.115920	3.099980	-0.769160
C	2.393550	-0.236160	-1.225090
C	2.200120	-1.313780	-0.339760
C	3.353680	-0.333910	-2.227990
C	2.930710	-2.466680	-0.512720
H	1.446550	-1.250030	0.430730
C	4.115730	-1.477940	-2.377840
H	3.483460	0.489760	-2.918600
C	3.893190	-2.552940	-1.539010
H	4.859370	-1.571260	-3.157000
O	4.584930	-3.691550	-1.710590
H	4.302460	-4.321870	-1.033870
O	2.809440	-3.610520	0.214070
C	1.969170	-3.568510	1.353530
H	2.038230	-4.547210	1.820430
H	2.307530	-2.796120	2.047210
H	0.932300	-3.365360	1.073580

N	0.583000	1.207330	-0.495650
C	1.476830	0.875850	-1.341260
H	1.505920	1.428500	-2.279750
C	-1.288420	-1.728810	3.343760
C	-1.925960	-0.985520	2.356670
C	-1.222400	-0.030140	1.633780
C	0.131650	0.181000	1.893800
C	0.755780	-0.559170	2.887630
C	0.055040	-1.510610	3.608130
H	-1.843620	-2.462520	3.913930
H	-2.979850	-1.138800	2.159360
H	-1.733120	0.568630	0.888460
H	1.797470	-0.352610	3.090810
H	0.555010	-2.070300	4.389270
C	0.938870	1.291630	1.297400
H	0.426670	2.256840	1.357270
N	2.234110	1.248370	1.480570
N	2.819220	2.515560	1.553850
C	2.608260	3.617250	0.821610
H	3.479920	2.581190	2.309020
O	1.876840	3.676580	-0.165600
C	3.342110	4.842730	1.318980
H	3.958690	5.233530	0.510790
H	2.601220	5.602340	1.567050
H	3.964530	4.652370	2.191720

ts1-4

C	9.441400	0.138030	0.964090
C	8.299300	0.901690	0.306660
H	10.397670	0.643020	0.824070
H	9.271730	0.033250	2.037690
H	9.528970	-0.866160	0.544490
C	6.951410	0.214650	0.488610
H	8.244770	1.913120	0.720620
H	8.500460	1.018790	-0.762310

C	5.800070	0.967430	-0.165040
H	7.003080	-0.798100	0.074620
H	6.748520	0.097110	1.559010
H	5.752900	1.982970	0.244010
H	6.000580	1.076790	-1.236030
C	4.452270	0.283060	0.022130
C	3.308250	1.056520	-0.623280
H	4.251650	0.168080	1.093670
H	4.492350	-0.722240	-0.405060
C	1.955620	0.381760	-0.450990
H	3.256530	2.057410	-0.186920
H	3.510010	1.179410	-1.689540
H	1.133930	1.061500	-0.698230
H	1.797360	0.092560	0.592730
C	1.809930	-0.843660	-1.333640
O	2.636450	-1.200410	-2.138210
N	0.645820	-1.565990	-1.186810
H	0.460250	-2.382240	-1.763090
C	-1.987790	0.620850	-1.175620
C	-2.977350	1.250770	-0.424170
C	-1.233800	1.362650	-2.072760
C	-3.178140	2.611980	-0.554580
H	-3.562310	0.641430	0.250530
C	-1.435340	2.732390	-2.206800
H	-0.481190	0.873180	-2.681940
C	-2.401850	3.362820	-1.447540
H	-0.856550	3.324010	-2.903630
O	-2.608110	4.695930	-1.573600
H	-3.329520	4.942580	-0.981110
O	-4.107010	3.340910	0.130870
C	-4.938230	2.639180	1.031880
H	-5.601860	3.376670	1.475420
H	-5.526410	1.881740	0.508210
H	-4.346350	2.155150	1.813220

N	-0.394640	-1.161920	-0.393040
C	-1.728080	-0.866100	-1.016140
H	-1.626910	-1.301690	-2.018000
C	-2.125330	0.146990	4.266930
C	-1.715530	0.935000	3.200250
C	-1.200090	0.348100	2.055660
C	-1.093930	-1.041970	1.975540
C	-1.457110	-1.828520	3.073210
C	-1.988660	-1.236960	4.202190
H	-2.529200	0.608460	5.158660
H	-1.785860	2.013770	3.261350
H	-0.857610	0.959700	1.231520
H	-1.347070	-2.904720	3.016510
H	-2.288230	-1.850410	5.041730
C	-0.485060	-1.674900	0.822790
H	0.193900	-2.505790	1.009920
N	-2.689460	-1.546650	-0.180750
N	-3.165300	-2.671640	-0.822890
C	-2.412520	-3.709950	-1.226300
H	-4.168900	-2.778020	-0.840970
O	-1.182870	-3.705770	-1.144980
C	-3.154800	-4.889680	-1.803900
H	-2.833940	-5.038510	-2.834410
H	-2.876610	-5.779220	-1.239620
H	-4.236730	-4.767990	-1.780490

3+4

C	9.755670	0.163300	0.818640
C	8.576520	1.047460	0.414420
H	10.709850	0.713220	0.780170
H	9.634580	-0.221070	1.845620
H	9.847990	-0.710020	0.151070
C	7.228370	0.324540	0.451380
H	8.532730	1.931260	1.077210
H	8.745040	1.445990	-0.602740

C	6.049940	1.207940	0.045030
H	7.268440	-0.558360	-0.213720
H	7.055450	-0.075290	1.468570
H	6.004160	2.087600	0.714930
H	6.232420	1.613200	-0.967460
C	4.702780	0.491080	0.055420
C	3.547490	1.398700	-0.368820
H	4.503510	0.091660	1.068340
H	4.743070	-0.377520	-0.622840
C	2.207050	0.687570	-0.377360
H	3.486630	2.259390	0.320130
H	3.755130	1.808640	-1.371390
H	1.361800	1.395030	-0.411760
H	2.070230	0.144140	0.570150
C	2.035550	-0.300910	-1.528620
O	2.848220	-0.486450	-2.414100
N	0.858900	-1.020180	-1.457090
H	0.771530	-1.912120	-1.951620
C	-2.206120	0.945590	-0.992610
C	-3.250380	1.352560	-0.143160
C	-1.384420	1.914590	-1.585770
C	-3.526200	2.693980	0.031720
H	-3.869920	0.576010	0.299830
C	-1.644070	3.276250	-1.386820
H	-0.562960	1.606850	-2.236420
C	-2.733800	3.677620	-0.611160
H	-1.033930	4.046500	-1.862840
O	-3.059570	4.981730	-0.483610
H	-3.847090	5.026810	0.082540
O	-4.575650	3.182550	0.757080
C	-5.440260	2.250810	1.374600
H	-6.215170	2.831780	1.891750
H	-5.918500	1.588350	0.631840
H	-4.903040	1.626750	2.110200

N	0.115500	-0.837780	-0.305150
C	-2.138780	-0.471410	-1.352000
H	-1.484860	-0.748830	-2.186220
C	-1.771190	-1.587820	4.354350
C	-1.802600	-0.459100	3.523330
C	-1.255630	-0.510610	2.242180
C	-0.664610	-1.705640	1.781030
C	-0.656900	-2.834380	2.614150
C	-1.203540	-2.778910	3.894320
H	-2.189860	-1.536540	5.362820
H	-2.247860	0.471110	3.886400
H	-1.260100	0.366280	1.594360
H	-0.198990	-3.759530	2.253350
H	-1.179480	-3.661900	4.537750
C	0.021070	-1.824050	0.496880
H	0.481700	-2.798120	0.264820
N	-2.936210	-1.305340	-0.784850
N	-3.039580	-2.584830	-1.280640
C	-2.147830	-3.404640	-1.923380
H	-3.968430	-2.958970	-1.127760
O	-0.938830	-3.227510	-1.983280
C	-2.815300	-4.583070	-2.613290
H	-2.624650	-4.479210	-3.693180
H	-2.343900	-5.523200	-2.290980
H	-3.901740	-4.640310	-2.454820

2-1

C	-1.198842	3.574424	0.455830
C	-1.083665	2.639110	1.476165
C	-0.145132	1.618587	1.380538
C	0.687939	1.524144	0.265548
C	0.575930	2.474658	-0.741128
C	-0.364049	3.489791	-0.650590
H	-1.927261	4.372032	0.529205
H	-1.722605	2.703971	2.347681

H	-0.061839	0.887571	2.177837
H	1.254608	2.405191	-1.581231
H	-0.438991	4.225044	-1.442005
C	1.740816	0.454965	0.146671
H	2.131214	0.159012	1.123993
N	2.603975	0.542568	-0.881038
N	3.875296	0.067422	-0.564227
C	4.208877	-1.109798	-0.031817
H	4.617679	0.697895	-0.817792
O	3.389927	-1.975662	0.295551
C	5.690026	-1.324805	0.178266
H	5.991063	-2.217742	-0.368650
H	6.296659	-0.480428	-0.145543
H	5.868224	-1.509098	1.237072
C	-1.355848	-0.465607	-1.067343
C	-2.734016	-0.578421	-0.980825
C	-3.292418	-1.354811	0.030605
C	-2.472287	-2.002388	0.952555
C	-1.104000	-1.880950	0.863317
C	-0.549943	-1.125577	-0.155618
H	-0.905713	0.135632	-1.848012
H	-3.353682	-0.064413	-1.700294
H	-2.936522	-2.600366	1.724838
H	-0.457515	-2.388789	1.569030
O	-4.622603	-1.542373	0.199025
C	-5.494971	-0.900291	-0.701600
H	-5.322999	-1.237986	-1.727528
H	-6.501473	-1.172914	-0.396208
H	-5.381875	0.186411	-0.654412
N	0.853397	-1.005268	-0.263126
H	1.163506	-0.970778	-1.232844
H	1.425221	-1.731752	0.178010

ts2-2

C	-1.199670	3.572256	0.455819
---	-----------	----------	----------

C	-1.093148	2.642134	1.482805
C	-0.156747	1.624470	1.396761
C	0.681362	1.524195	0.289109
C	0.579759	2.462650	-0.729342
C	-0.360605	3.482237	-0.645829
H	-1.929208	4.369579	0.520513
H	-1.739409	2.710608	2.348521
H	-0.079171	0.891916	2.193212
H	1.253489	2.377987	-1.572104
H	-0.434942	4.212314	-1.442111
C	1.653316	0.378251	0.193244
H	2.126117	0.186263	1.157976
N	2.553546	0.408166	-0.927397
N	3.855671	0.058874	-0.572995
C	4.215140	-1.113391	-0.030071
H	4.575074	0.719969	-0.818223
O	3.401898	-1.978083	0.297517
C	5.694242	-1.322825	0.183705
H	5.994720	-2.212810	-0.368302
H	6.299182	-0.476414	-0.137733
H	5.871603	-1.513289	1.241344
C	-1.349760	-0.461502	-1.069807
C	-2.729644	-0.585255	-0.980554
C	-3.287956	-1.361673	0.030837
C	-2.457428	-2.009482	0.944667
C	-1.087151	-1.874717	0.849764
C	-0.525840	-1.098645	-0.159202
H	-0.910745	0.145142	-1.851796
H	-3.350921	-0.074145	-1.700878
H	-2.911800	-2.611393	1.720086
H	-0.442657	-2.372844	1.564829
O	-4.618665	-1.548084	0.202630
C	-5.493788	-0.906607	-0.697955
H	-5.322504	-1.245100	-1.723543

H	-6.499594	-1.179894	-0.390904
H	-5.381039	0.180010	-0.651466
N	0.892895	-0.928737	-0.238547
H	1.582007	-0.688615	-1.190012
H	1.426660	-1.690651	0.188287

2-3

C	-0.540061	3.993154	0.492873
C	-0.641389	2.988151	1.443029
C	0.024836	1.784160	1.251798
C	0.793215	1.576045	0.114970
C	0.896750	2.589560	-0.831582
C	0.232876	3.791899	-0.645314
H	-1.057078	4.932903	0.638438
H	-1.240624	3.138133	2.331794
H	-0.068758	0.989869	1.983982
H	1.502719	2.428403	-1.714170
H	0.317995	4.576030	-1.386833
C	1.454274	0.237324	-0.118628
H	1.574506	-0.262619	0.851908
N	2.799082	0.388463	-0.704257
N	3.809957	-0.215920	0.027853
C	3.883081	-1.562038	0.188697
H	4.506923	0.395775	0.416724
O	3.051580	-2.310417	-0.290208
C	5.055899	-2.062361	0.992433
H	5.639467	-2.734609	0.365225
H	5.696000	-1.262557	1.360413
H	4.674311	-2.638641	1.833746
C	-1.689624	0.040951	-0.951568
C	-3.003506	-0.220282	-0.581365
C	-3.315793	-1.410792	0.067025
C	-2.304605	-2.327024	0.345914
C	-0.998860	-2.045250	-0.007911
C	-0.672724	-0.858395	-0.665840

H	-1.448668	0.960150	-1.470114
H	-3.768991	0.504862	-0.816166
H	-2.566038	-3.250295	0.845675
H	-0.210654	-2.754354	0.221329
O	-4.569066	-1.765248	0.459460
C	-5.616962	-0.867004	0.183430
H	-5.724809	-0.700989	-0.892226
H	-6.523031	-1.326534	0.569659
H	-5.457715	0.094268	0.680429
N	0.674073	-0.587012	-1.049570
H	2.785900	-0.006037	-1.640083
H	1.182196	-1.465752	-1.119685

2-4

C	-1.967374	3.413631	1.173421
C	-1.485802	3.591990	-0.117716
C	-1.214696	2.492061	-0.914760
C	-1.417931	1.199496	-0.436811
C	-1.898951	1.025782	0.853677
C	-2.169321	2.130055	1.654757
H	-2.177465	4.270800	1.799903
H	-1.316372	4.589842	-0.501521
H	-0.822546	2.626597	-1.915526
H	-2.039855	0.032896	1.260507
H	-2.536028	1.978766	2.661950
C	-1.130692	0.041106	-1.390224
H	-1.828875	0.159986	-2.224178
N	-1.366593	-1.328821	-0.905783
N	-2.724522	-1.602973	-0.683875
C	-3.128768	-2.127042	0.505756
H	-3.215660	-1.907138	-1.511054
O	-2.399001	-2.153905	1.478398
C	-4.539700	-2.655366	0.531632
H	-5.090027	-2.446285	-0.384045
H	-4.504744	-3.731615	0.698651

H	-5.056476	-2.203334	1.376127
C	1.410998	-0.059542	0.163175
C	2.621417	-0.229716	0.835961
C	3.797722	-0.410290	0.128056
C	3.752474	-0.415192	-1.266221
C	2.556857	-0.238510	-1.924623
C	1.356925	-0.059183	-1.223874
H	0.518449	0.084775	0.754082
H	2.614754	-0.222207	1.916259
H	4.674970	-0.556158	-1.813832
H	2.540198	-0.231702	-3.008531
O	5.025266	-0.589512	0.690277
C	5.096395	-0.591495	2.095496
H	4.496363	-1.400590	2.522273
H	6.141916	-0.745550	2.349466
H	4.758775	0.362315	2.511550
N	0.183498	0.147860	-1.975094
H	-0.879482	-1.533753	-0.036380
H	0.227985	-0.339474	-2.858051

ts2-5

C	-0.887743	3.841470	0.477893
C	-0.099168	3.500020	-0.614023
C	-0.184584	2.232849	-1.166815
C	-1.064150	1.293789	-0.634611
C	-1.855970	1.638598	0.454378
C	-1.763752	2.908644	1.011238
H	-0.813245	4.829141	0.914224
H	0.594115	4.220341	-1.028866
H	0.442213	1.948484	-2.002741
H	-2.537168	0.918243	0.893610
H	-2.376115	3.164188	1.866435
C	-1.147815	-0.047858	-1.315136
H	-1.899318	0.010524	-2.113113
N	-1.739388	-1.206930	-0.419630

N	-3.105349	-1.491785	-0.431121
C	-3.782074	-1.585747	0.755733
H	-3.463134	-1.874205	-1.290845
O	-3.237501	-1.305668	1.800002
C	-5.210329	-2.041677	0.650014
H	-5.568638	-2.082670	-0.376872
H	-5.288639	-3.030857	1.100972
H	-5.830476	-1.360055	1.228595
C	1.358618	-0.302060	0.262939
C	2.607958	-0.334444	0.885699
C	3.721953	-0.769605	0.189097
C	3.572459	-1.167238	-1.140228
C	2.338731	-1.119919	-1.748394
C	1.183681	-0.685639	-1.070467
H	0.522558	0.049474	0.855295
H	2.681462	-0.017551	1.916552
H	4.449218	-1.502785	-1.679772
H	2.225723	-1.420011	-2.782577
O	4.985624	-0.843628	0.704726
C	5.154793	-0.455770	2.043989
H	4.556909	-1.077778	2.717666
H	6.209574	-0.589131	2.272845
H	4.881833	0.593780	2.193678
N	-0.018874	-0.747662	-1.787925
H	-1.459114	-1.128544	0.564433
H	-0.923103	-1.764043	-1.064440

5+6

C	-4.131797	1.789200	1.064583
C	-3.160561	2.330511	0.230398
C	-2.391929	1.504431	-0.572691
C	-2.597842	0.125257	-0.556435
C	-3.591552	-0.408126	0.260676
C	-4.346111	0.418314	1.080107
H	-4.725801	2.437707	1.695432

H	-3.002534	3.400784	0.206542
H	-1.632774	1.926368	-1.218328
H	-3.754060	-1.479532	0.262010
H	-5.105719	-0.005996	1.723507
C	-1.838657	-0.802390	-1.428309
H	-2.430023	-1.624668	-1.833619
N	-0.783342	-3.007513	0.763417
N	0.371912	-2.977622	-0.035370
C	1.560434	-2.629216	0.539668
H	0.197181	-2.640133	-0.974129
O	1.697932	-2.575022	1.746439
C	2.667199	-2.308068	-0.430002
H	2.391950	-2.515673	-1.462851
H	2.906673	-1.247640	-0.331749
H	3.549001	-2.885407	-0.157901
C	0.457245	0.261245	0.168288
C	1.478707	1.031118	0.709055
C	2.369394	1.685918	-0.136042
C	2.237321	1.543712	-1.518378
C	1.237405	0.751083	-2.044332
C	0.319633	0.115113	-1.206608
H	-0.228845	-0.254869	0.828869
H	1.574377	1.093026	1.783023
H	2.948315	2.048727	-2.158585
H	1.153441	0.609239	-3.114207
O	3.398447	2.461025	0.288196
C	3.589221	2.588602	1.679481
H	3.778967	1.616627	2.142779
H	4.457799	3.228276	1.809830
H	2.721475	3.052341	2.156533
N	-0.619179	-0.775090	-1.774380
H	-0.962171	-3.973196	1.020589
H	-0.542688	-2.532648	1.632751

2+5

C	0.603455	-0.153848	0.000074
O	1.547187	-0.913091	-0.000150
N	-0.672395	-0.647963	0.000293
H	-0.757121	-1.655313	-0.000117
C	0.740276	1.346535	0.000074
H	0.254834	1.774790	-0.875927
H	0.253182	1.775073	0.874997
H	1.799567	1.583646	0.000890
N	-1.795406	0.169475	-0.000100
H	-2.357450	0.010136	-0.826918
H	-2.358288	0.009692	0.826044

ts2-6

C	9.045419	0.507066	1.524562
C	8.031563	0.875695	0.440365
H	10.039093	0.934871	1.314774
H	8.726833	0.876230	2.514184
H	9.164916	-0.586531	1.606013
C	6.632701	0.301611	0.685602
H	7.962973	1.976089	0.358361
H	8.399277	0.526321	-0.541794
C	5.611080	0.665836	-0.395455
H	6.699522	-0.799447	0.765861
H	6.264339	0.649967	1.669260
H	5.543157	1.767581	-0.476117
H	5.981137	0.316680	-1.377235
C	4.216074	0.084184	-0.150701
C	3.199258	0.452572	-1.236393
H	3.843489	0.432839	0.831823
H	4.283565	-1.014391	-0.087998
C	1.797492	-0.112176	-0.999795
H	3.128231	1.552596	-1.310031
H	3.567434	0.092777	-2.211487
H	1.062869	0.372116	-1.666220
H	1.437762	0.104271	0.020291

C	1.707175	-1.617240	-1.224915
O	2.637929	-2.290336	-1.646449
N	0.496367	-2.203900	-0.952946
H	0.540314	-3.224142	-0.993397
C	-2.439142	-0.087456	-0.975328
C	-2.066877	0.882863	-0.024500
C	-3.502724	0.178546	-1.848505
C	-2.759612	2.086691	0.046875
H	-1.215258	0.664472	0.619419
C	-4.199519	1.389307	-1.780287
H	-3.784109	-0.558430	-2.607004
C	-3.839476	2.348286	-0.833878
H	-5.023432	1.613525	-2.460480
O	-4.495285	3.523242	-0.756496
H	-4.085784	4.034679	-0.039219
O	-2.501343	3.112438	0.908592
C	-1.450510	2.978884	1.844588
H	-1.427439	3.909094	2.427217
H	-1.625001	2.128573	2.526677
H	-0.477372	2.841361	1.342047
N	-0.553198	-1.585311	-0.265333
C	-1.706222	-1.387178	-1.045049
H	-1.682756	-1.808603	-2.065468
C	-3.947555	-1.840682	1.830171
O	-4.976024	-1.330500	2.216521
N	-3.849482	-2.254074	0.501304
H	-4.586608	-1.890146	-0.102869
C	-2.757126	-2.125469	2.722902
H	-2.488702	-3.193702	2.699614
H	-1.869881	-1.556307	2.403588
H	-3.028970	-1.838874	3.745577
N	-2.639234	-2.538338	-0.129190
H	-1.583714	-2.430371	0.397543
H	-2.701276	-3.428527	-0.638673

C	4.456350	-0.987215	1.810220
O	4.659744	-0.503353	2.900720
N	3.413723	-1.870170	1.647730
H	2.784156	-1.922648	2.442129
C	5.298788	-0.678622	0.602287
H	5.332704	-1.506246	-0.100816
H	4.860639	0.181734	0.091268
H	6.291934	-0.409057	0.951200
N	2.969880	-2.311542	0.409539
H	2.819166	-3.313941	0.456624
C	1.748879	-1.623275	-0.022274
H	1.017349	-1.582759	0.799447
C	2.083153	-0.219495	-0.460001
C	1.857423	0.850811	0.392070
C	2.687289	0.008737	-1.690146
C	2.235628	2.143727	0.050811
H	1.390002	0.705287	1.359016
C	3.067980	1.291645	-2.044417
H	2.876994	-0.825207	-2.353301
C	2.865157	2.360882	-1.178874
H	3.554163	1.473942	-2.997078
N	1.215719	-2.404810	-1.142111
H	1.100304	-3.369835	-0.839908
N	-0.057758	-1.957505	-1.485395
C	-1.153616	-2.362412	-0.788274
H	-0.130564	-1.425976	-2.335742
O	-1.050128	-3.099772	0.173075
C	-2.479938	-1.840396	-1.286887
C	-3.253705	-1.158044	-0.160930
H	-3.047154	-2.699899	-1.653336
H	-2.338931	-1.155343	-2.126213
C	-4.631731	-0.686412	-0.604803
H	-3.343826	-1.860467	0.669965

H	-2.674649	-0.306394	0.209497
C	-5.411579	-0.004592	0.512371
H	-4.529891	0.004566	-1.448700
H	-5.204656	-1.542608	-0.976601
H	-5.514600	-0.696618	1.354599
H	-4.836401	0.848848	0.886740
C	-6.791837	0.469853	0.076410
C	-7.574349	1.149348	1.193544
H	-7.366959	-0.383163	-0.299852
H	-6.688592	1.163286	-0.765421
H	-7.678033	0.454880	2.032297
H	-6.997922	1.999641	1.569608
C	-8.950986	1.620459	0.743092
H	-9.552051	0.781014	0.388205
H	-9.496314	2.102783	1.554597
H	-8.867699	2.336792	-0.076589
O	3.271041	3.626276	-1.477475
H	3.713930	3.626381	-2.331559
O	2.021181	3.129910	0.958762
C	1.411232	4.331103	0.502956
H	0.904913	4.758876	1.365649
H	2.152412	5.030591	0.121860
H	0.679082	4.118631	-0.279521

ts2-8

C	-0.953004	-2.044688	-1.025177
C	-0.358733	-1.431307	-2.125973
C	0.905193	-0.839347	-1.998066
C	1.588572	-0.867624	-0.777533
C	1.005194	-1.516144	0.325046
C	-0.255697	-2.089659	0.206735
H	-0.902091	-1.418897	-3.073124
H	1.360244	-0.356314	-2.868290
H	1.570924	-1.540306	1.255590
O	-2.193356	-2.583107	-1.112270

H	-2.400337	-2.955284	-0.239119
O	-0.946618	-2.714848	1.206210
C	-0.403138	-2.708204	2.513292
H	-1.143004	-3.193537	3.163695
H	0.543608	-3.274086	2.558861
H	-0.220768	-1.678476	2.865496
C	2.908574	-0.158611	-0.611835
H	3.453298	-0.107602	-1.567956
N	3.692541	-0.516662	0.533768
N	5.064153	-0.551780	0.284489
C	5.813444	0.484234	-0.154659
H	5.541954	-1.396927	0.582818
O	5.334368	1.569155	-0.513273
C	7.309134	0.238450	-0.219867
H	7.608848	-0.758090	0.136845
H	7.651064	0.367370	-1.258349
H	7.816522	1.006155	0.384339
C	-8.234012	0.426286	-0.502866
C	-6.833498	0.030099	-0.033258
H	-8.955651	-0.394980	-0.365847
H	-8.612719	1.298453	0.056383
H	-8.236896	0.696011	-1.572489
C	-5.792317	1.140877	-0.203797
H	-6.872270	-0.270050	1.029947
H	-6.498728	-0.867028	-0.585187
C	-4.387071	0.750693	0.262024
H	-5.753619	1.441754	-1.267663
H	-6.124968	2.039803	0.348704
H	-4.426353	0.445111	1.324324
H	-4.048259	-0.143860	-0.292962
C	-3.346448	1.864596	0.101441
C	-1.940513	1.423422	0.510580
H	-3.651103	2.745872	0.696322
H	-3.334040	2.201744	-0.952015

C	-0.865884	2.510156	0.354339
H	-1.937049	1.088177	1.560935
H	-1.648364	0.546015	-0.090617
H	-0.860287	2.905701	-0.675451
H	-1.085432	3.357872	1.025424
C	0.498742	1.962362	0.742939
O	0.743511	1.499301	1.838017
N	1.447803	2.024712	-0.262858
H	1.166216	2.263622	-1.208935
N	2.648660	1.337335	-0.121101
H	3.493280	1.866274	-0.415929
H	3.079402	0.812713	0.874510

6+7

C	-7.180374	-0.474866	-0.264783
C	-6.379315	-1.573562	0.005754
C	-5.004755	-1.416590	0.116351
C	-4.419419	-0.162928	-0.042045
C	-5.232700	0.938784	-0.314062
C	-6.602229	0.781251	-0.424201
H	-8.252705	-0.592966	-0.351707
H	-6.822792	-2.552716	0.131001
H	-4.374998	-2.272856	0.327828
H	-4.773124	1.910481	-0.435938
H	-7.227377	1.639362	-0.635218
C	-2.959081	-0.049589	0.084078
H	-2.400701	-0.953257	0.298203
N	-2.404562	1.089176	-0.060443
N	-1.055886	1.242726	0.048712
C	-0.080966	0.338362	0.378854
H	-0.775898	2.197544	-0.094724
O	-0.294649	-0.836651	0.585046
C	1.305126	0.946975	0.492575
C	2.388947	-0.018361	0.030952
H	1.455779	1.192877	1.548822

H	1.363478	1.886379	-0.062797
C	3.790628	0.536432	0.246742
H	2.267202	-0.960012	0.568983
H	2.240959	-0.247441	-1.028321
C	4.883020	-0.419499	-0.215792
H	3.896537	1.489304	-0.283412
H	3.932168	0.760168	1.309681
H	4.774998	-1.372866	0.311791
H	4.743335	-0.641361	-1.279084
C	6.288574	0.124156	0.005652
C	7.382414	-0.830319	-0.457501
H	6.428911	0.344829	1.069448
H	6.396113	1.078969	-0.520647
C	8.781934	-0.274348	-0.228829
H	7.273246	-1.783198	0.068543
H	7.241260	-1.049251	-1.519974
H	9.551000	-0.969528	-0.566309
H	8.919696	0.665052	-0.767817
H	8.952415	-0.074995	0.830935

ts2-9

C	3.998789	-0.516166	-0.313333
C	4.893459	-1.270153	-1.109907
C	6.247391	-1.394997	-0.794362
C	6.772553	-0.764539	0.344827
C	5.910180	-0.003057	1.143386
C	4.559659	0.127604	0.822269
H	4.496755	-1.770435	-1.997299
H	6.884801	-1.993420	-1.447410
H	6.325758	0.500082	2.020103
H	3.933454	0.763826	1.452903
O	8.084401	-0.826548	0.741365
C	8.989685	-1.558323	-0.039912
H	9.972593	-1.472735	0.445543
H	8.719852	-2.630367	-0.102604

H	9.069515	-1.162857	-1.071026
C	1.179244	1.453993	0.105129
C	1.461826	2.207672	-1.042924
C	0.412903	2.028898	1.131229
C	0.974727	3.512338	-1.168169
H	2.087215	1.749740	-1.813730
C	-0.072606	3.333730	1.007939
H	0.203857	1.452203	2.038135
C	0.205248	4.076654	-0.145110
H	1.206883	4.096783	-2.062508
H	-0.661181	3.776166	1.816041
H	-0.167718	5.099852	-0.239783
C	1.691339	0.027481	0.220517
H	1.838446	-0.219650	1.295057
N	2.672777	-0.437869	-0.676310
C	-10.737295	-0.370424	0.014980
C	-9.429402	-1.128105	0.247379
H	-11.613693	-0.987613	0.269322
H	-10.785588	0.544451	0.629287
H	-10.841521	-0.063736	-1.039440
C	-8.179071	-0.311087	-0.093034
H	-9.373474	-1.453260	1.302294
H	-9.429476	-2.057121	-0.351569
C	-6.865017	-1.062380	0.138468
H	-8.232974	0.014172	-1.149044
H	-8.178293	0.619131	0.505689
H	-6.810016	-1.387620	1.193784
H	-6.864887	-1.991862	-0.460622
C	-5.615966	-0.243690	-0.200567
C	-4.307058	-0.998919	0.042849
H	-5.616429	0.687517	0.396336
H	-5.666645	0.078892	-1.257411
C	-3.064831	-0.172060	-0.296993
H	-4.238431	-1.314197	1.096543

H	-4.297167	-1.929875	-0.550934
H	-3.050556	0.107770	-1.364232
H	-3.078632	0.778753	0.268296
C	-1.769142	-0.865841	0.071889
O	-1.638788	-1.645823	0.997863
N	-0.689259	-0.564433	-0.737533
H	-0.691266	0.225149	-1.374873
N	0.575293	-0.990519	-0.327455
H	0.398896	-1.737159	0.362195
H	1.443651	-1.245622	-1.053076

2-10

C	-1.195668	-2.139319	-0.505989
C	-0.474795	-2.130473	-1.700942
C	0.821445	-1.601454	-1.708225
C	1.396291	-1.093064	-0.536809
C	0.682724	-1.122077	0.675449
C	-0.607065	-1.639076	0.688013
H	-0.929043	-2.531504	-2.605738
H	1.382170	-1.600038	-2.642677
H	1.158427	-0.752167	1.589154
O	-2.475488	-2.628086	-0.538196
H	-2.886198	-2.599233	0.374050
O	-1.436829	-1.750712	1.792061
C	-1.191254	-0.809352	2.868504
H	-2.019170	-1.024418	3.554089
H	-0.224963	-1.017640	3.338698
H	-1.241869	0.220448	2.480780
C	2.779297	-0.499478	-0.599060
H	3.361464	-0.885110	-1.468285
N	3.467129	-0.439475	0.694390
N	4.834814	-0.713772	0.640472
C	5.741751	0.012601	-0.129068
H	5.134406	-1.308647	1.414388
O	5.353242	0.796045	-0.996395

C	7.193638	-0.281751	0.116335
H	7.434968	-1.346165	0.001767
H	7.813725	0.270128	-0.610119
H	7.515521	0.035129	1.117105
C	-7.794185	0.107521	-0.480996
C	-6.333425	-0.237840	-0.200941
H	-8.434961	-0.776404	-0.385600
H	-8.172332	0.863379	0.216533
H	-7.928989	0.500945	-1.495041
C	-5.424243	0.992434	-0.331995
H	-6.240154	-0.669446	0.814603
H	-5.996697	-1.030069	-0.898798
C	-3.958403	0.637574	-0.052546
H	-5.522752	1.422348	-1.347491
H	-5.762681	1.784340	0.363324
H	-3.861088	0.210518	0.964384
H	-3.625672	-0.163092	-0.745030
C	-3.047577	1.865694	-0.193245
C	-1.583861	1.485086	0.053754
H	-3.363600	2.654279	0.516668
H	-3.162064	2.305843	-1.202802
C	-0.644260	2.688312	-0.084690
H	-1.477173	1.045802	1.074608
H	-1.285109	0.682956	-0.652069
H	-0.741094	3.156201	-1.084487
H	-0.927923	3.484768	0.638638
C	0.778353	2.263258	0.205386
O	1.339037	2.399499	1.272198
N	1.477868	1.746982	-0.931768
H	0.924923	1.320487	-1.688288
N	2.704846	1.078208	-0.647773
H	3.464807	1.480736	-1.258211
H	3.148241	1.036485	0.603650

ts2-11

C	-0.953004	-2.044688	-1.025177
C	-0.358733	-1.431307	-2.125973
C	0.905193	-0.839347	-1.998066
C	1.588572	-0.867624	-0.777533
C	1.005194	-1.516144	0.325046
C	-0.255697	-2.089659	0.206735
H	-0.902091	-1.418897	-3.073124
H	1.360244	-0.356314	-2.868290
H	1.570924	-1.540306	1.255590
O	-2.193356	-2.583107	-1.112270
H	-2.400337	-2.955284	-0.239119
O	-0.946618	-2.714848	1.206210
C	-0.403138	-2.708204	2.513292
H	-1.143004	-3.193537	3.163695
H	0.543608	-3.274086	2.558861
H	-0.220768	-1.678476	2.865496
C	2.908574	-0.158611	-0.611835
H	3.453298	-0.107602	-1.567956
N	3.692541	-0.516662	0.533768
N	5.064153	-0.551780	0.284489
C	5.813444	0.484234	-0.154659
H	5.541954	-1.396927	0.582818
O	5.334368	1.569155	-0.513273
C	7.309134	0.238450	-0.219867
H	7.608848	-0.758090	0.136845
H	7.651064	0.367370	-1.258349
H	7.816522	1.006155	0.384339
C	-8.234012	0.426286	-0.502866
C	-6.833498	0.030099	-0.033258
H	-8.955651	-0.394980	-0.365847
H	-8.612719	1.298453	0.056383
H	-8.236896	0.696011	-1.572489
C	-5.792317	1.140877	-0.203797
H	-6.872270	-0.270050	1.029947

H	-6.498728	-0.867028	-0.585187
C	-4.387071	0.750693	0.262024
H	-5.753619	1.441754	-1.267663
H	-6.124968	2.039803	0.348704
H	-4.426353	0.445111	1.324324
H	-4.048259	-0.143860	-0.292962
C	-3.346448	1.864596	0.101441
C	-1.940513	1.423422	0.510580
H	-3.651103	2.745872	0.696322
H	-3.334040	2.201744	-0.952015
C	-0.865884	2.510156	0.354339
H	-1.937049	1.088177	1.560935
H	-1.648364	0.546015	-0.090617
H	-0.860287	2.905701	-0.675451
H	-1.085432	3.357872	1.025424
C	0.498742	1.962362	0.742939
O	0.743511	1.499301	1.838017
N	1.447803	2.024712	-0.262858
H	1.166216	2.263622	-1.208935
N	2.648660	1.337335	-0.121101
H	3.493280	1.866274	-0.415929
H	3.079402	0.812713	0.874510
