

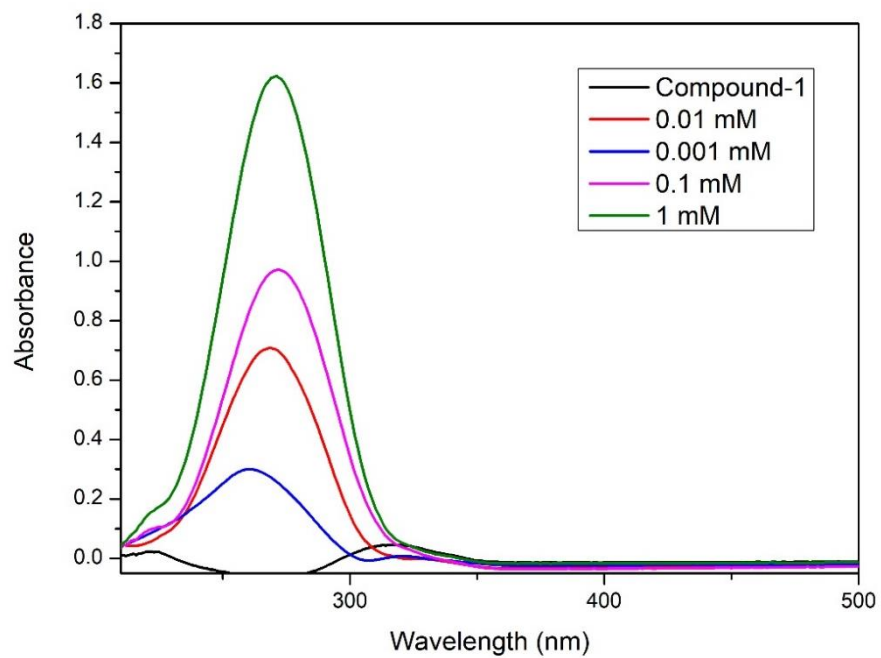
Photophysical studies of diazines: Effect of solvent and complexation with Cu^{2+} , Ni^{2+} , Co^{2+} and Pb^{2+} ions

Packirisamy Kuzhalmozhi Madarasi^a and Chinnappan Sivasankar*^a

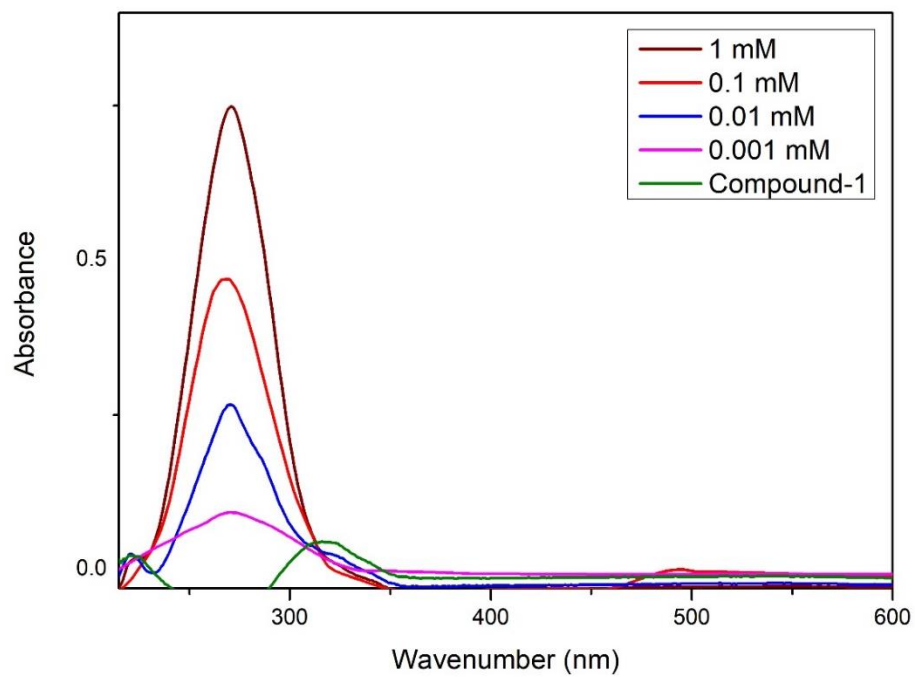
^a Catalysis and Energy Laboratory, Department of Chemistry, Pondicherry University (A Central University),
Puducherry 605014, India.

Table of Contents

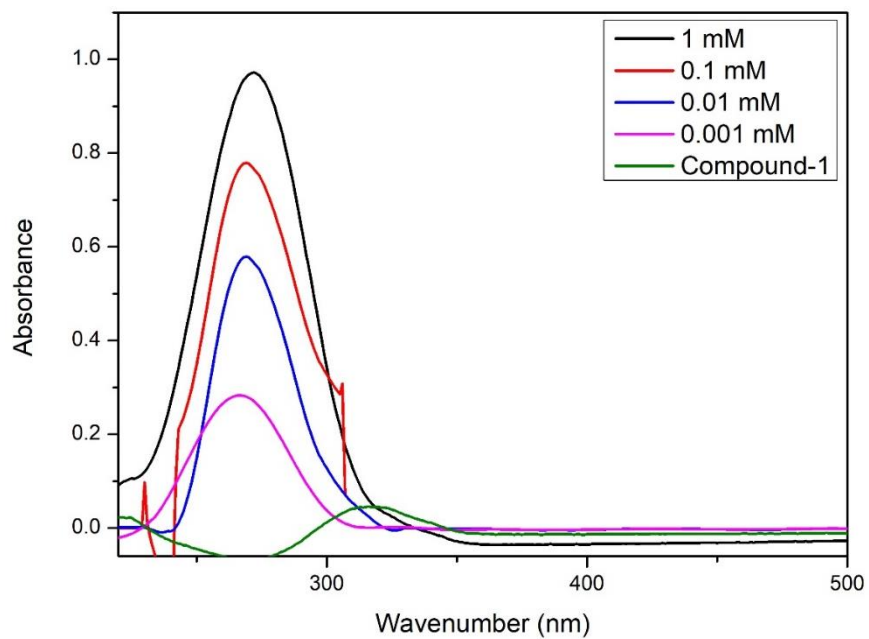
1. Figure S1. Absorption spectra of 1 after the addition of metal ion at different concentrations.....	S2 – S3
2. Figure S2. Optimized geometries of diazines 1 – 4 using CAM-B3LYP theory in gas phase...S4	
3. Figure S3. Optimized geometries of diazines 1 – 4 using CAM-B3LYP theory in hexane.....S4	
4. Figure S4. Simulated UV-Vis spectrum of 1 – 4 using different solvent systems.....S5 – S6	
5. Figure S5. Simulated UV-Vis spectrum of 1 – 4 using CAM-B3LYP theory and hexane as solvent.....S7	
6. Table S1. NBO analysis of all the system only C_α , C_β , N_α and N_β	S7 – S8
7. Fig. S6. Possible transitions from TD-DFT calculation for the compounds in different solvent system.....	S9 – S14
8. Table S2. Cartesian coordinates of all the systems.....	S14 – S59



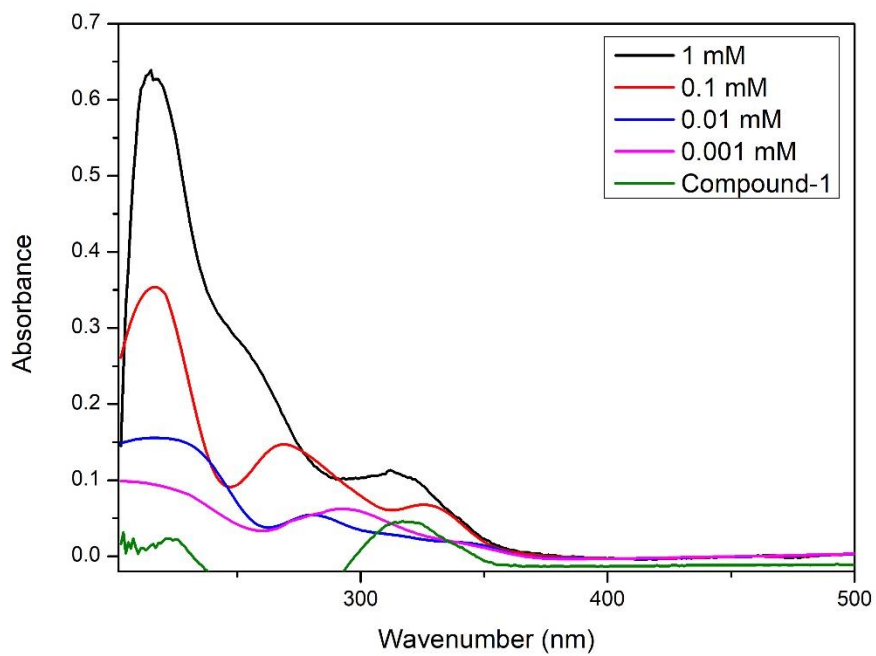
1-Lead



1-Nickel



1-Cobalt



1-Copper

Fig. S1. Absorption spectra of 1 after the addition of metal ion at different concentrations.

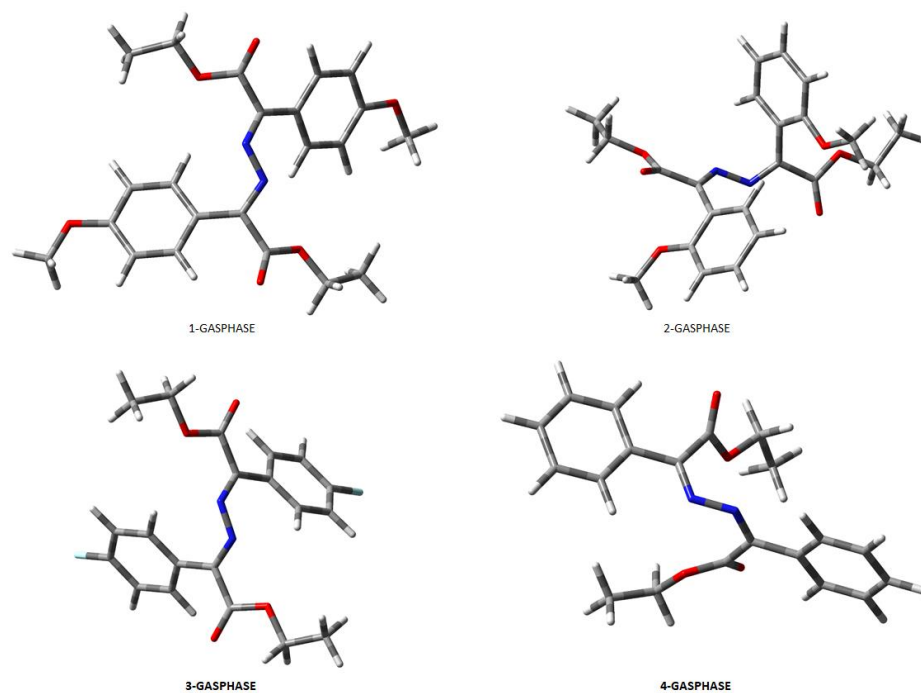


Fig. S2. Optimized geometries of diazines **1** – **4** using CAM-B3LYP theory in gas phase.

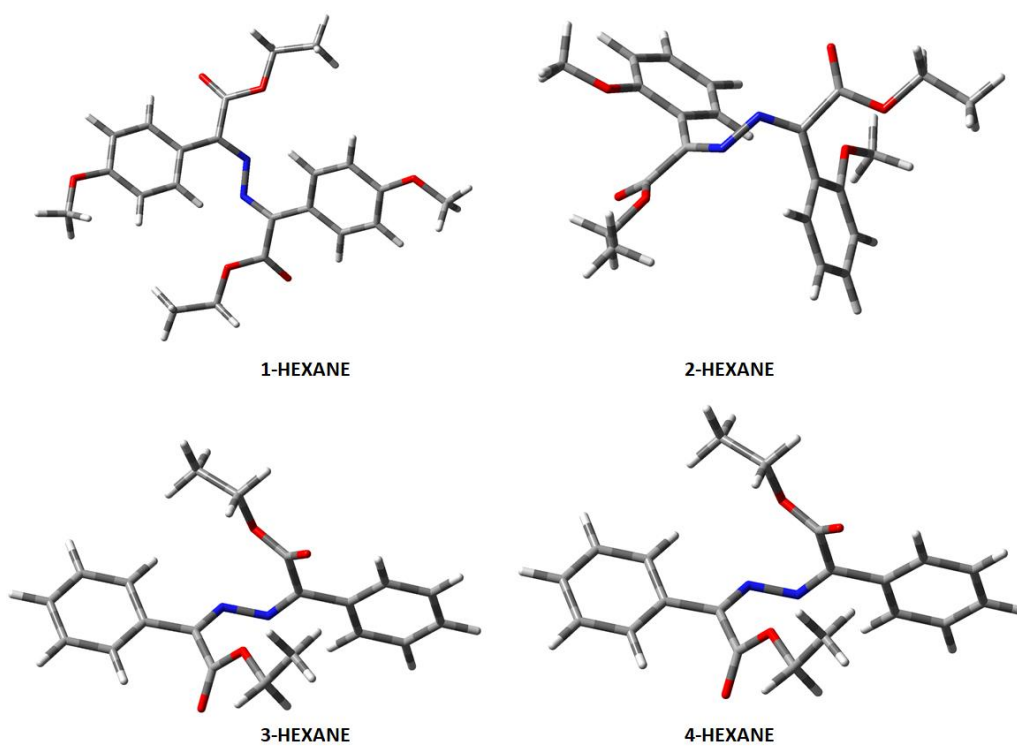
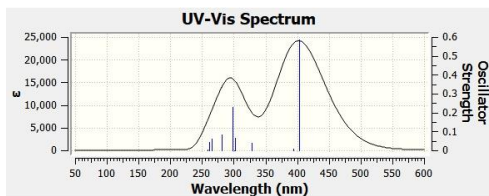
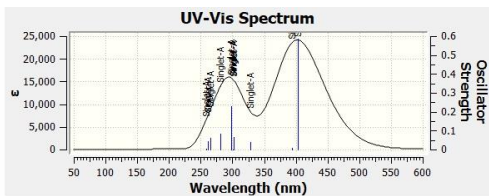


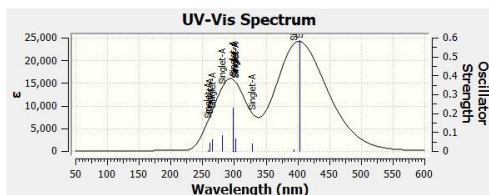
Fig. S3. Optimized geometries of diazines **1** – **4** using CAM-B3LYP theory in hexane.



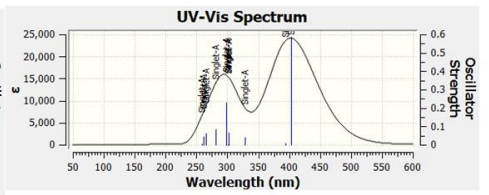
1-THF



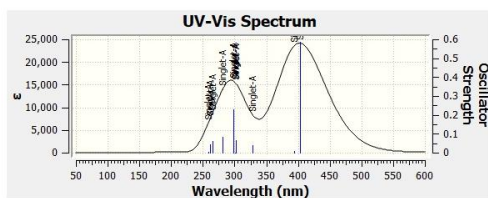
1-HEXANE



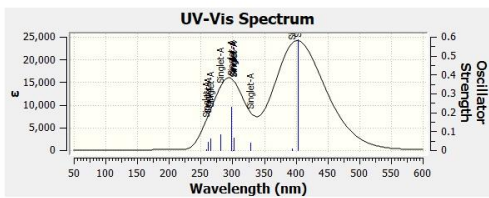
1-DMSO



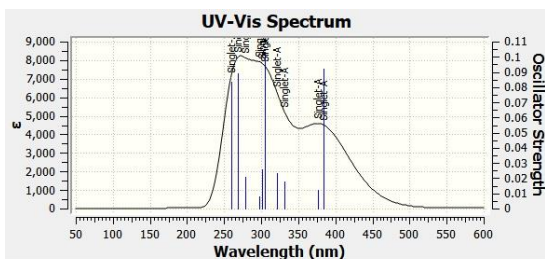
1-DCM



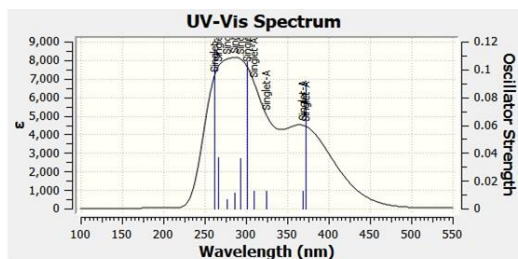
1-CH₃OH



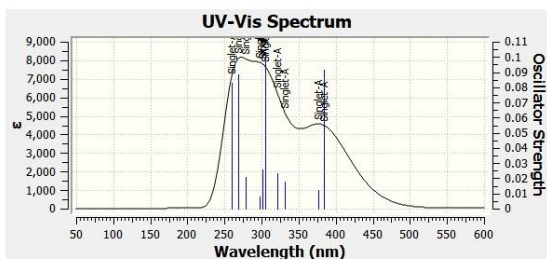
1-CH₃CN



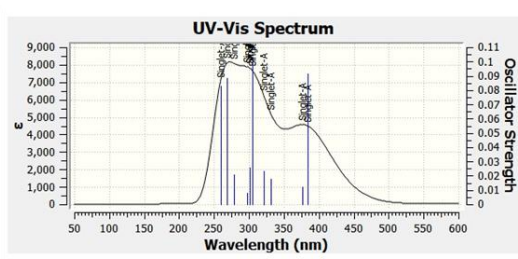
2-THF



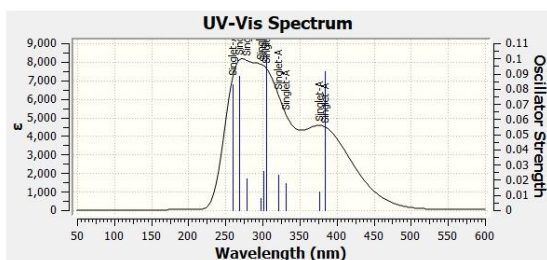
2-HEXANE



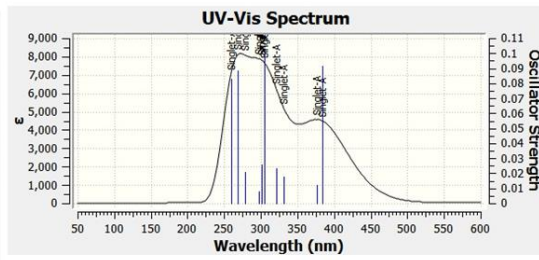
2-DMSO



2-DCM



2-MeOH



2-CH₃CN

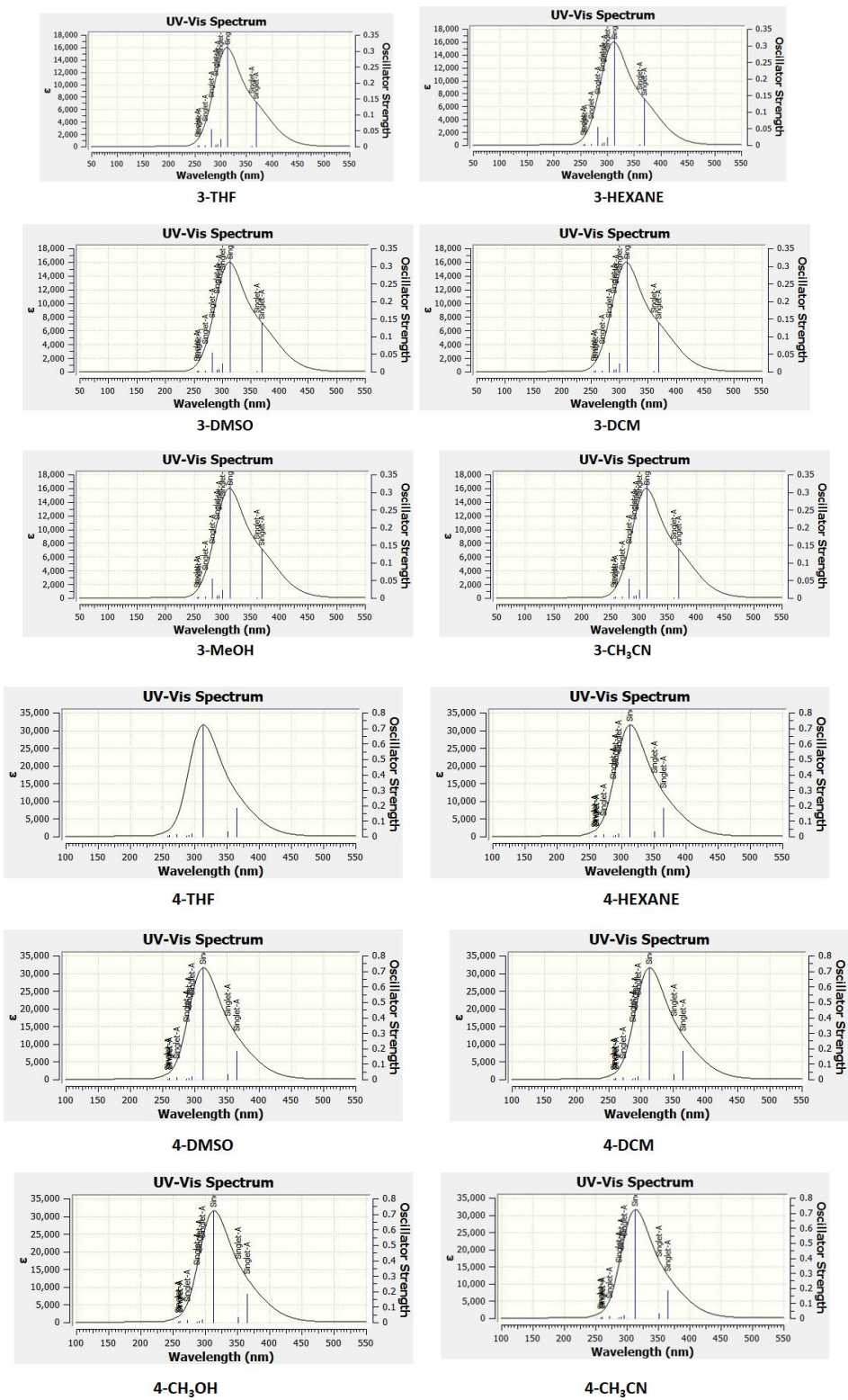


Fig. S4. Simulated UV-Vis spectrum of 1 – 4 using different solvent systems.

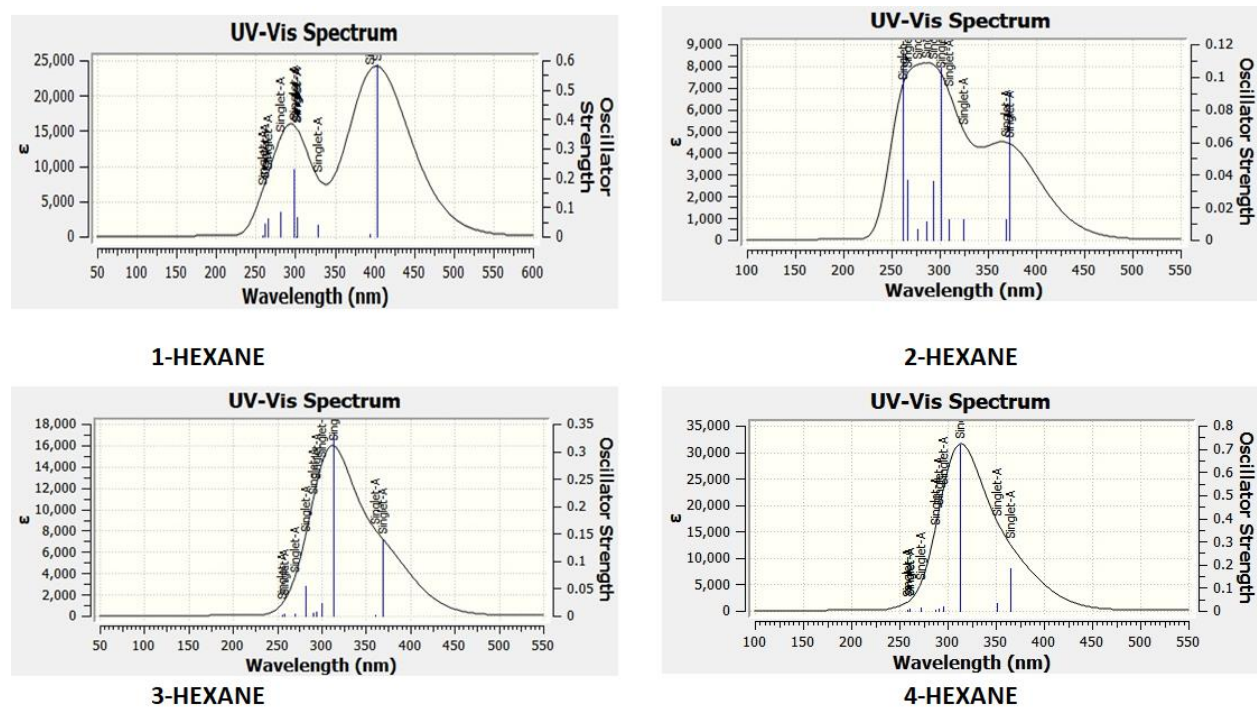
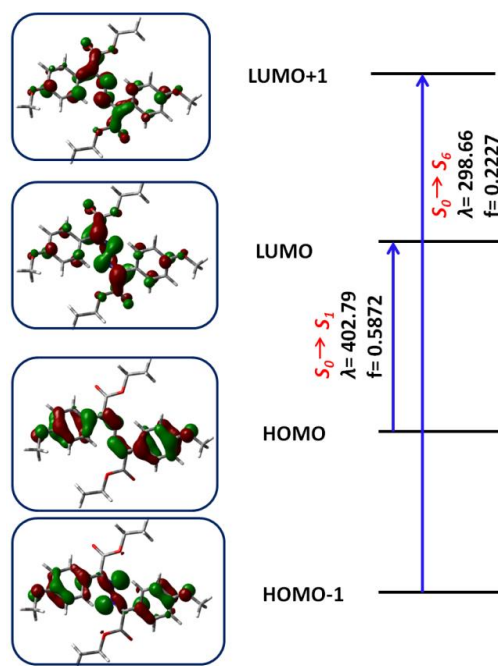
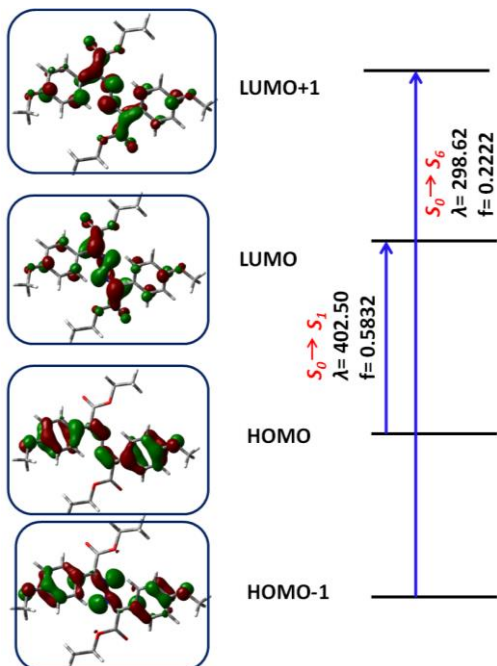


Fig. S5. Simulated UV-Vis spectrum of 1 – 4 using CAM-B3LYP theory and hexane as solvent.

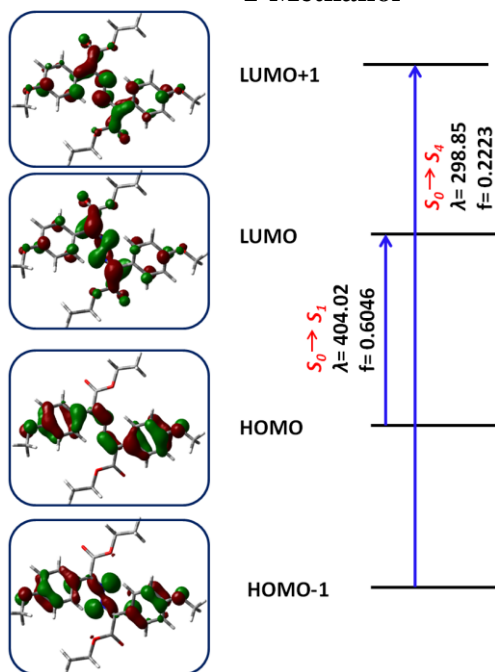
Table S1. NBO analysis of all the system only C_α , C_β , N_α and N_β .

Systems	Bond	Population		Contribution %				Hybrid	
		C-N	C_α - N_α	C_β - N_β	C_α	N_α	C_β	N_β	C/N
1-MeOH	1	1.989	1.989	40.67	59.33	40.52	59.48	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.715	1.715	43.11	56.89	42.87	57.13	$sp^{99.99}d^{0.61}/sp^{99.99}d^{3.88}$	$sp^{99.99}d^{0.30}/sp^{99.99}d^{0.40}$
1-CH ₃ CN	1	1.980	1.982	40.67	59.33	40.52	59.48	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.928	1.924	43.11	56.89	42.87	57.13	$sp^{99.99}d^{0.61}/sp^{99.99}d^{3.88}$	$sp^{99.99}d^{0.30}/sp^{99.99}d^{0.40}$
1-DMSO	1	1.980	1.982	40.67	59.33	40.52	59.48	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.928	1.922	43.10	56.90	42.86	57.14	$sp^{99.99}d^{0.61}/sp^{99.99}d^{3.88}$	$sp^{99.99}d^{0.30}/sp^{99.99}d^{0.40}$
1-DCM	1	1.980	1.981	40.67	59.33	40.52	59.48	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.928	1.922	43.18	56.82	42.94	57.06	$sp^{99.99}d^{0.61}/sp^{99.99}d^{3.86}$	$sp^{99.99}d^{0.29}/sp^{99.99}d^{0.40}$
1-THF	1	1.980	1.981	40.68	59.32	40.52	59.48	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.927	1.922	43.19	56.81	42.96	57.04	$sp^{99.99}d^{0.60}/sp^{99.99}d^{3.85}$	$sp^{99.99}d^{0.29}/sp^{99.99}d^{0.40}$
1-Hexane	1	1.980	1.981	40.69	59.31	40.55	59.45	$sp^{2.09}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.926	1.921	43.35	56.65	43.18	56.82	$sp^{99.99}d^{0.61}/sp^{99.99}d^{3.90}$	$sp^{99.99}d^{0.28}/sp^{99.99}d^{0.41}$
2-MeOH	1	1.981	1.982	40.95	59.05	40.95	59.05	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$
	2	1.885	1.886	42.26	57.74	42.30	57.70	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.92}$	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.87}$
2-CH ₃ CN	1	1.982	1.982	40.95	59.05	40.95	59.05	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$
	2	1.880	1.886	42.26	57.74	42.29	57.71	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.92}$	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.87}$
2-DMSO	1	1.997	1.968	50.00	50.00	50.21	49.79	$sp^{1.40}d^{0.00}/sp^{1.40}d^{0.00}$	$sp^{99.99}d^{0.51}/sp^{83.36}d^{0.34}$

	2	1.884	1.884	42.26	57.74	42.29	57.71	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.92}$	$sp^{1.00}d^{0.00}/sp^{99.99}d^{1.87}$
2-DCM	1	1.982	1.982	40.96	59.04	40.96	59.04	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$
	2	1.885	1.885	42.35	57.65	42.41	57.59	$sp^{99.99}d^{11.81}/sp^{99.99}d^{1.95}$	$sp^{99.99}d^{13.90}/sp^{99.99}d^{1.90}$
2-THF	1	1.982	1.982	40.96	59.04	40.96	59.04	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$	$sp^{2.07}d^{0.00}/sp^{1.48}d^{0.00}$
	2	1.885	1.885	42.37	57.63	42.43	57.57	$sp^{99.99}d^{11.65}/sp^{99.99}d^{1.95}$	$sp^{99.99}d^{13.69}/sp^{99.99}d^{1.91}$
2-Hexane	1	1.981	1.982	40.98	59.02	41.00	59.00	$sp^{2.07}d^{0.00}/sp^{1.49}d^{0.00}$	$sp^{2.07}d^{0.00}/sp^{1.49}d^{0.00}$
	2	1.884	1.884	42.58	57.42	42.72	57.28	$sp^{99.99}d^{10.75}/sp^{99.99}d^{1.94}$	$sp^{99.99}d^{11.38}/sp^{99.99}d^{2.01}$
3-MeOH	1	1.982	1.981	40.55	59.45	40.40	59.60	$sp^{2.07}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.919	1.920	43.86	56.14	43.56	56.44	$sp^{99.99}d^{0.87}/sp^{99.99}d^{1.35}$	$sp^{99.99}d^{0.42}/sp^{99.99}d^{0.56}$
3-CH ₃ CN	1	1.982	1.981	40.55	59.45	40.40	59.60	$sp^{2.07}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.919	1.920	43.85	56.15	43.56	56.44	$sp^{99.99}d^{0.87}/sp^{99.99}d^{1.35}$	$sp^{99.99}d^{0.42}/sp^{99.99}d^{0.56}$
3-DMSO	1	1.982	1.981	40.55	59.45	40.40	59.60	$sp^{2.07}d^{0.00}/sp^{1.42}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.919	1.920	43.84	56.16	43.54	56.46	$sp^{99.99}d^{0.87}/sp^{99.99}d^{1.35}$	$sp^{99.99}d^{0.42}/sp^{99.99}d^{0.56}$
3-DCM	1	1.981	1.981	40.57	59.43	40.42	59.58	$sp^{2.07}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.918	1.919	43.99	56.01	43.68	56.32	$sp^{99.99}d^{0.85}/sp^{99.99}d^{1.34}$	$sp^{99.99}d^{0.43}/sp^{99.99}d^{0.58}$
3-THF	1	1.981	1.981	40.57	59.43	40.42	59.58	$sp^{2.07}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.11}d^{0.00}/sp^{1.42}d^{0.00}$
	2	1.918	1.920	44.02	55.98	43.71	56.29	$sp^{99.99}d^{0.84}/sp^{99.99}d^{1.33}$	$sp^{99.99}d^{0.43}/sp^{99.99}d^{0.58}$
3-Hexane	1	1.982	1.981	40.61	59.39	40.47	59.53	$sp^{2.07}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.10}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.918	1.918	44.38	55.62	44.06	55.94	$sp^{99.99}d^{0.77}/sp^{99.99}d^{1.30}$	$sp^{99.99}d^{0.44}/sp^{99.99}d^{0.63}$
4-MeOH	1	1.980	1.980	40.44	59.56	40.44	59.56	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.10}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.908	1.908	43.77	56.23	43.77	56.23	$sp^{31.99}d^{2.12}/sp^{41.13}d^{0.00}$	$sp^{99.99}d^{1.22}/sp^{99.99}d^{0.76}$
4-CH ₃ CN	1	1.980	1.980	40.44	59.56	40.44	59.56	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.908	1.908	43.76	56.24	43.76	56.24	$sp^{99.99}d^{1.12}/sp^{99.99}d^{0.76}$	$sp^{99.99}d^{1.22}/sp^{99.99}d^{0.76}$
4-DMSO	1	1.980	1.980	40.44	59.56	40.44	59.56	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.908	1.908	43.76	56.24	43.76	56.24	$sp^{99.99}d^{1.22}/sp^{99.99}d^{0.76}$	$sp^{99.99}d^{1.22}/sp^{99.99}d^{0.76}$
4-DCM	1	1.980	1.980	40.44	59.56	40.44	59.56	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.907	1.907	43.82	56.18	43.82	56.18	$sp^{99.99}d^{1.21}/sp^{99.99}d^{0.76}$	$sp^{99.99}d^{1.21}/sp^{99.99}d^{0.76}$
4-THF	1	1.980	1.980	40.44	59.56	40.44	59.56	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.12}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.907	1.907	43.84	56.16	43.84	56.16	$sp^{99.99}d^{1.20}/sp^{99.99}d^{0.76}$	$sp^{99.99}d^{1.20}/sp^{99.99}d^{0.76}$
4-Hexane	1	1.980	1.980	40.46	59.54	40.46	59.54	$sp^{2.13}d^{0.00}/sp^{1.43}d^{0.00}$	$sp^{2.13}d^{0.00}/sp^{1.43}d^{0.00}$
	2	1.907	1.907	44.00	56.00	44.00	56.00	$sp^{99.99}d^{1.16}/sp^{99.99}d^{0.77}$	$sp^{99.99}d^{1.16}/sp^{99.99}d^{0.77}$

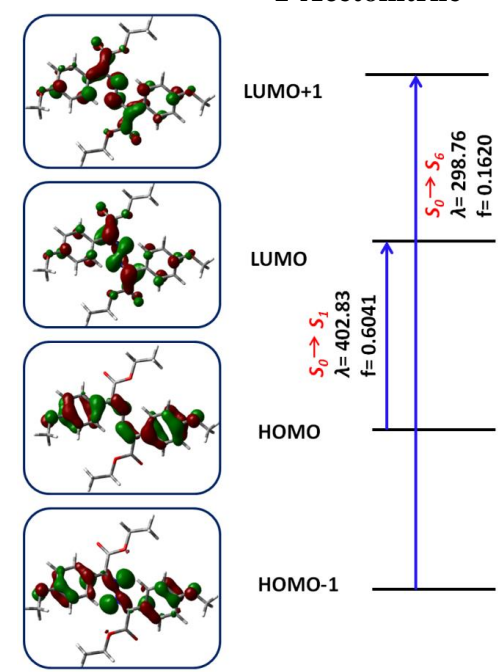


1-Methanol

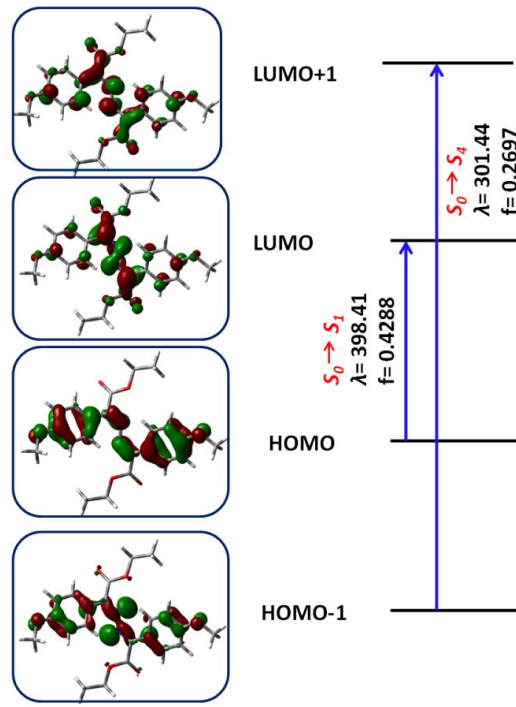
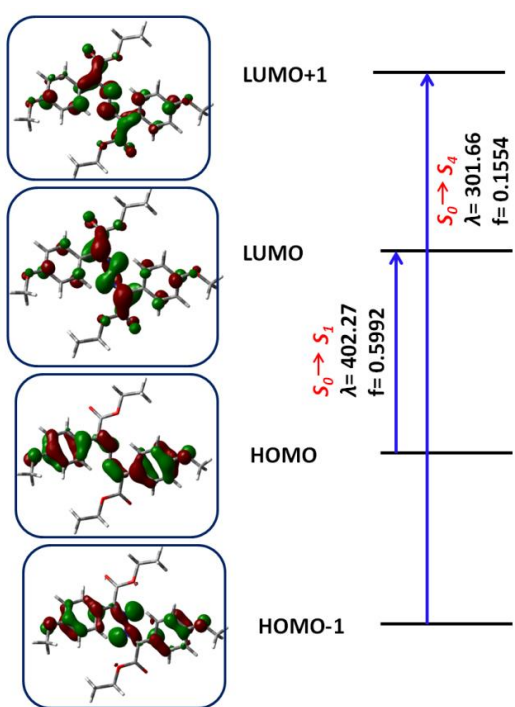


1-DCM

1-Acetonitrile

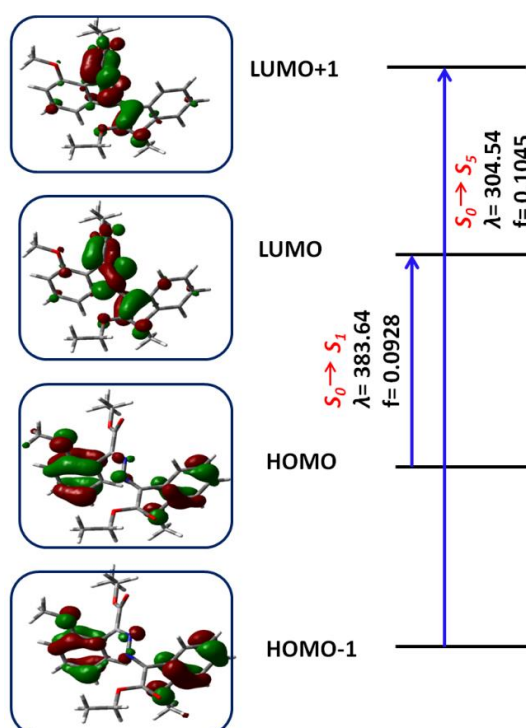
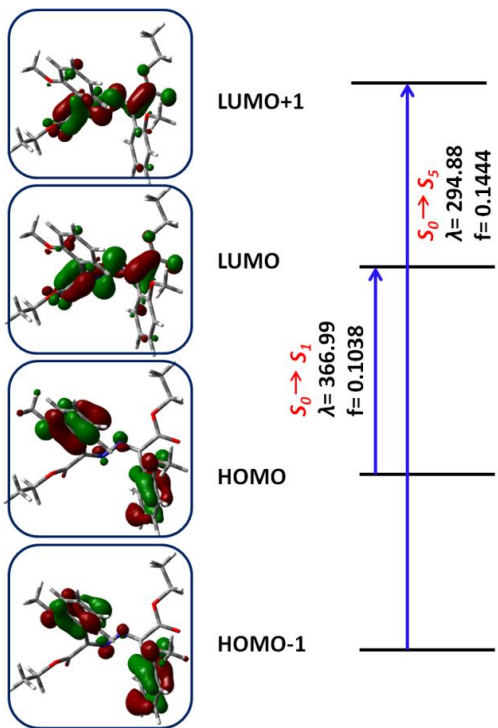


1-DMSO



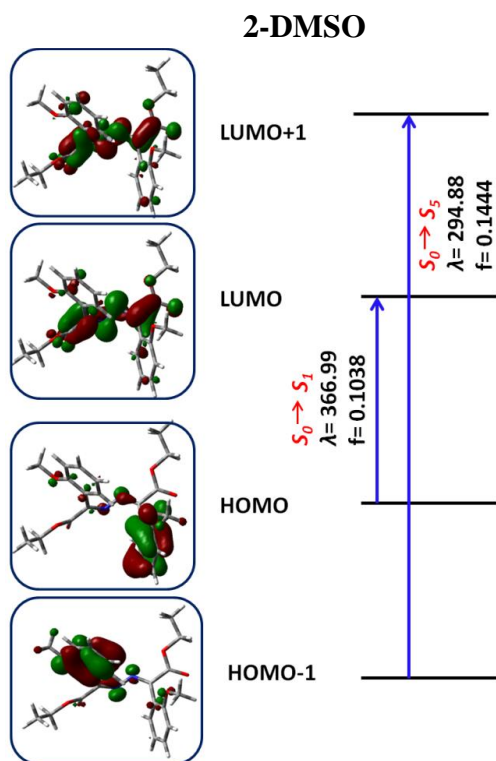
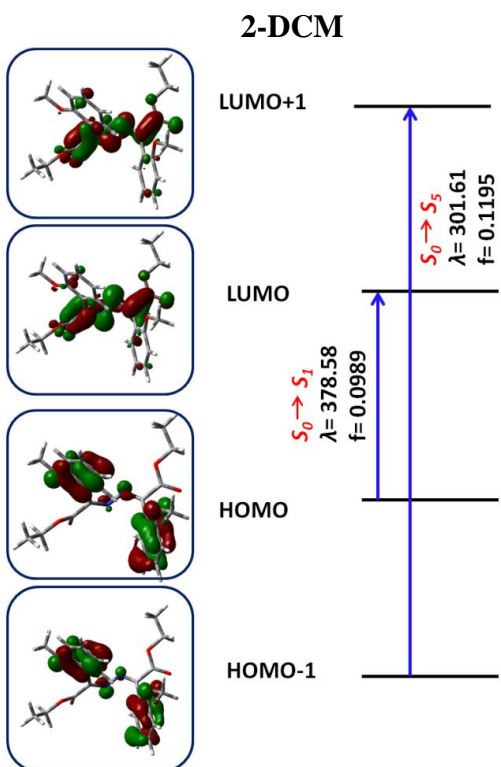
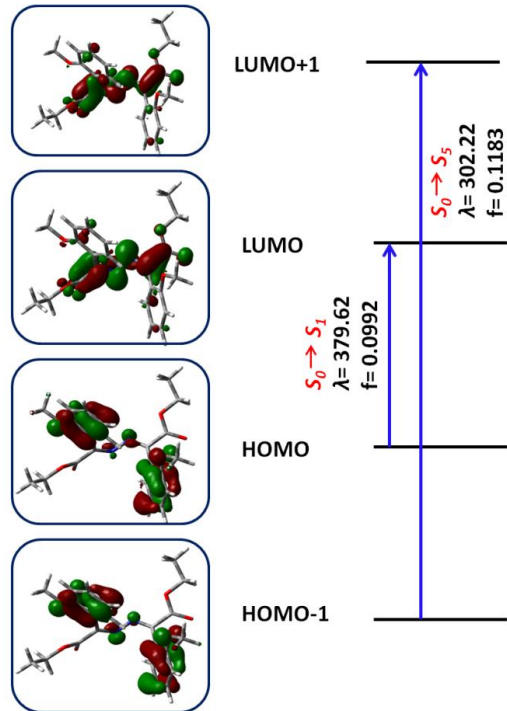
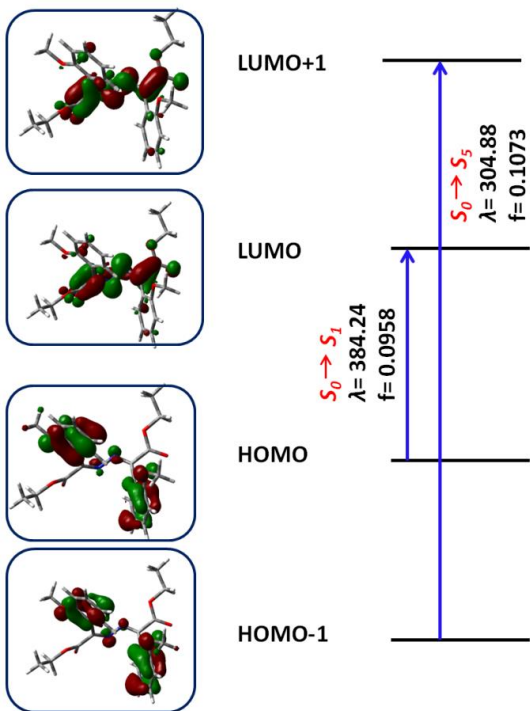
1-THF

1-Hexane



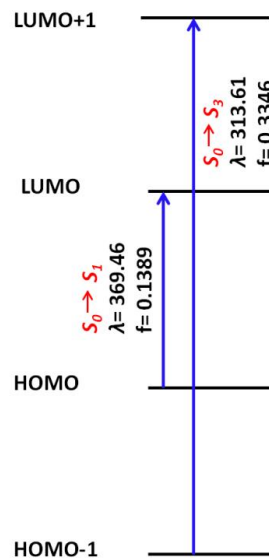
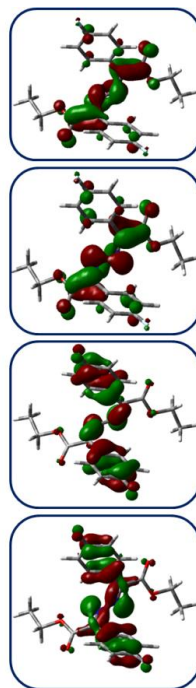
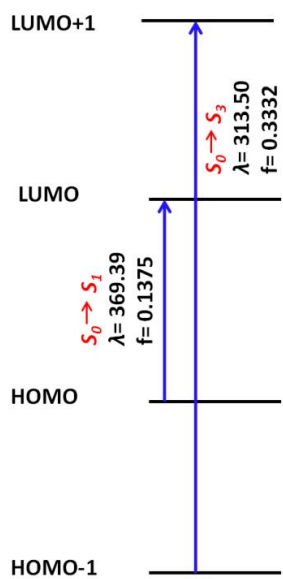
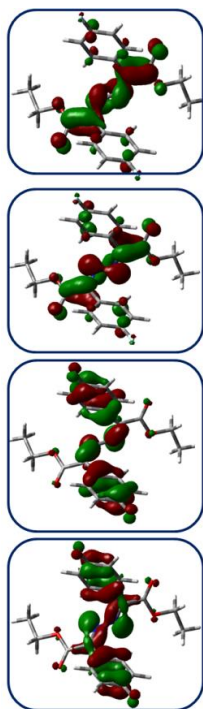
2-Methanol

2-Acetonitrile

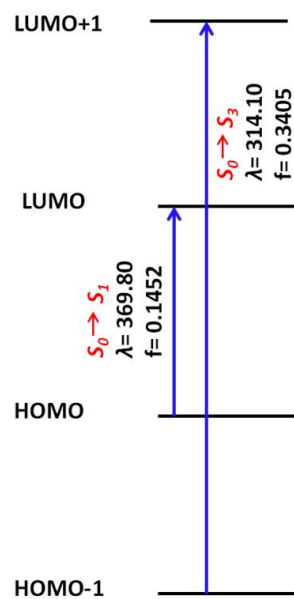
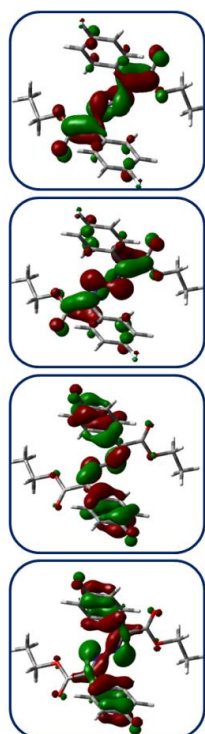


2-THF

2 Hexane

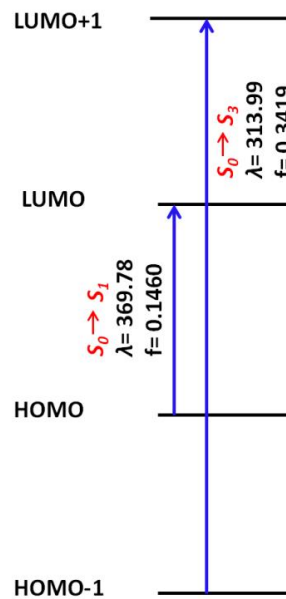
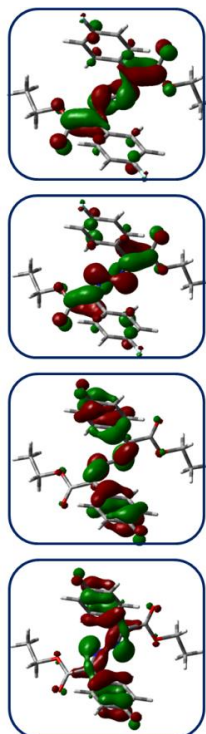


3-Methanol

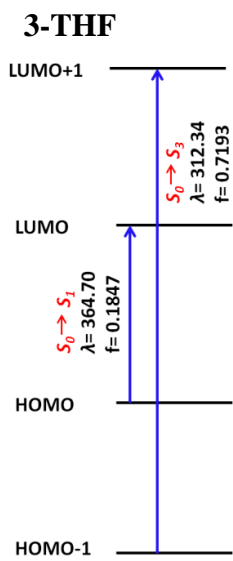
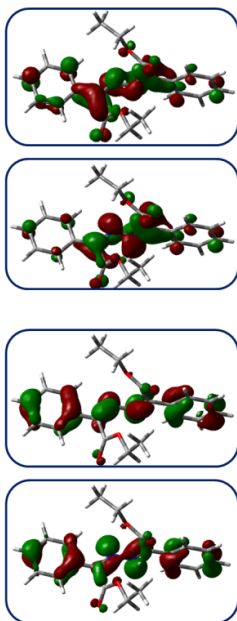
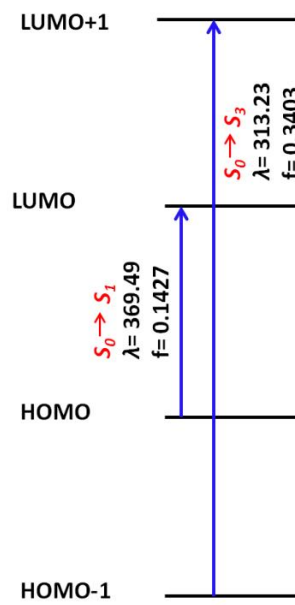
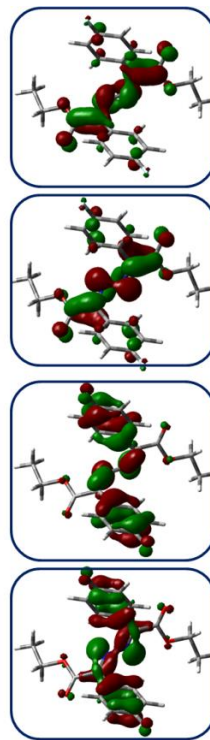
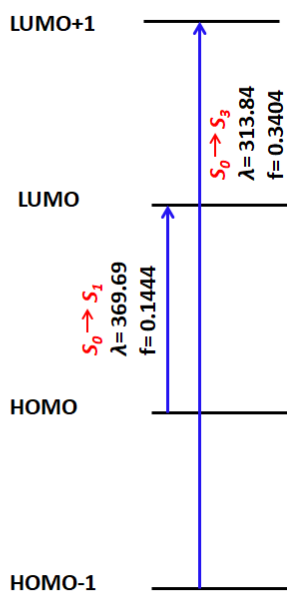
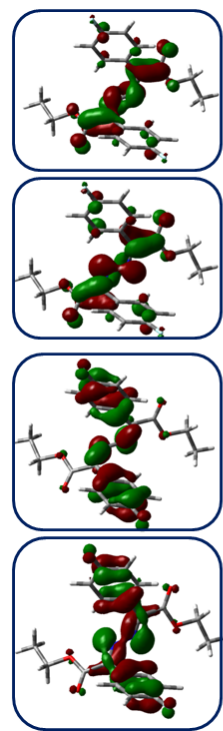


3-DMSO

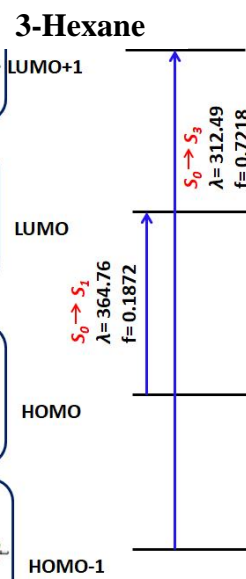
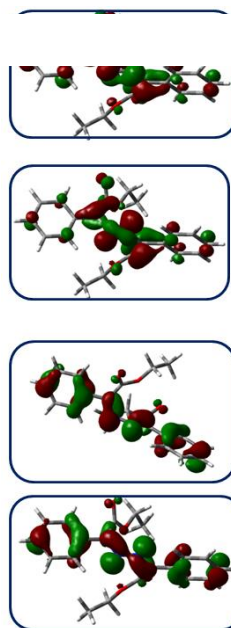
3-Acetonitrile



3-DCM



4-Methanol



4-CH₃CN

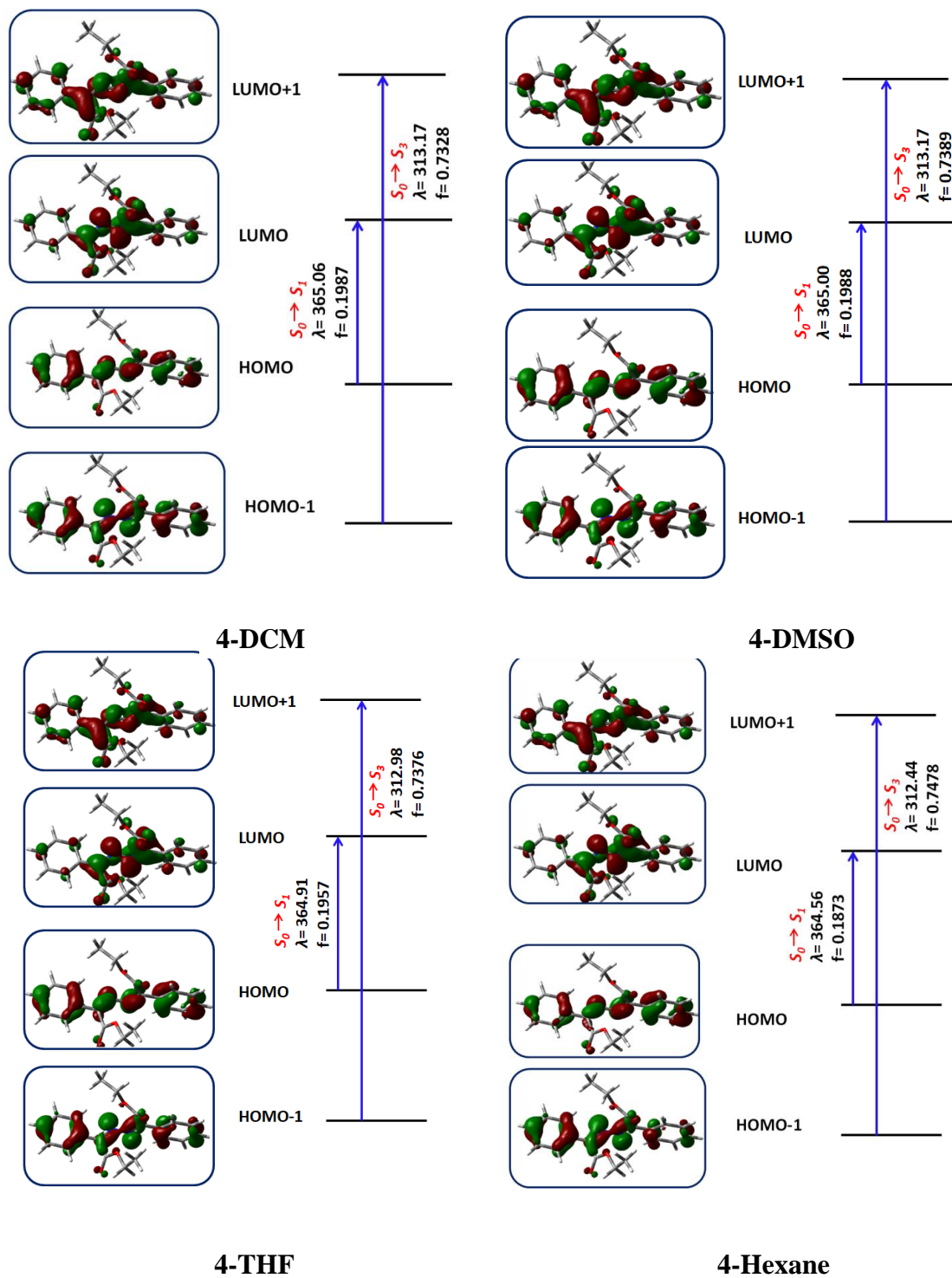


Fig. S6. Possible transitions from TD-DFT calculation for the compounds in different solvent system.

Table S2. Cartesian coordinates of all the systems.

1-CH3OH

0 1

C	1.40997837	1.20390454	0.00000000
C	0.14252337	0.80057054	0.63866300
C	-0.01871863	-0.47121346	1.22356600
C	-0.96216063	1.68596854	0.69817000
C	-1.21566463	-0.85385546	1.82623400
H	0.79447437	-1.18219746	1.21272200
C	-2.15382263	1.31065954	1.29336300
H	-0.88301463	2.66617354	0.24723500
C	-2.29544163	0.03613054	1.86526100
H	-1.28824563	-1.84218246	2.26548000
H	-2.99959863	1.99033054	1.32567000
N	2.40224037	0.45762754	-0.38798700
N	2.27997437	-0.87796646	-0.43325700
C	3.26785637	-1.65116146	-0.08939100
C	4.53125537	-1.29744046	0.58707200
C	5.61717837	-2.19671546	0.61802900
C	4.70302837	-0.05365146	1.24152000
C	6.81524337	-1.87842046	1.25155500
H	5.53193137	-3.15072046	0.11501400
C	5.89218937	0.26753254	1.87553900
H	3.90275137	0.67177654	1.25147000
C	6.96260337	-0.63915246	1.88817200
H	7.62410537	-2.60006346	1.23745000
H	6.01428037	1.22158454	2.37857400

C	2.99908437	-3.09322346	-0.47053500
O	3.80279537	-3.84433646	-0.98862900
C	1.67655237	2.66980154	-0.27810300
O	0.87598337	3.44893554	-0.75783800
C	3.31238637	4.37849154	-0.22971300
H	3.21876637	4.53995954	-1.30836600
O	2.92874237	3.01513554	0.06763700
C	4.73851637	4.56236154	0.25401000
H	4.80890837	4.40318754	1.33505400
H	5.41243137	3.85778554	-0.24320500
H	5.07632537	5.58094054	0.03353600
O	1.73882937	-3.45456546	-0.17088400
C	1.35356637	-4.78938246	-0.57377900
H	1.46509137	-4.87291346	-1.65953400
C	-0.08227163	-4.99783846	-0.12999100
H	-0.17015763	-4.91834046	0.95870300
H	-0.74212363	-4.25295646	-0.58567100
H	-0.42303763	-5.99469146	-0.43066200
C	9.19466437	-1.11052346	2.59636700
H	8.93964237	-2.04644946	3.11006100
H	9.57682837	-1.34132646	1.59362700
H	9.96440537	-0.58474446	3.16398200
C	-3.70571263	-1.50746846	3.01925900
H	-4.72898263	-1.50212846	3.39874400
H	-3.59535763	-2.31341646	2.28219600
H	-3.01058963	-1.68098646	3.85098600
O	-3.50325963	-0.23185846	2.42956900
O	8.08312637	-0.22840646	2.53991800

H	2.03832837	-5.50904746	-0.11361200
H	2.61391637	5.05778754	0.26948200

1- CH3CN

0 1

C	-0.73752715	0.11930586	0.00000000
C	-2.00498215	-0.28402814	0.63866300
C	-2.16622415	-1.55581214	1.22356600
C	-3.10966615	0.60136986	0.69817000
C	-3.36317015	-1.93845414	1.82623400
H	-1.35303115	-2.26679614	1.21272200
C	-4.30132815	0.22606086	1.29336300
H	-3.03052015	1.58157486	0.24723500
C	-4.44294715	-1.04846814	1.86526100
H	-3.43575115	-2.92678114	2.26548000
H	-5.14710415	0.90573186	1.32567000
N	0.25473485	-0.62697114	-0.38798700
N	0.13246885	-1.96256514	-0.43325700
C	1.12035085	-2.73576014	-0.08939100
C	2.38374985	-2.38203914	0.58707200
C	3.46967285	-3.28131414	0.61802900
C	2.55552285	-1.13825014	1.24152000
C	4.66773785	-2.96301914	1.25155500
H	3.38442585	-4.23531914	0.11501400
C	3.74468385	-0.81706614	1.87553900
H	1.75524585	-0.41282214	1.25147000
C	4.81509785	-1.72375114	1.88817200
H	5.47659985	-3.68466214	1.23745000
H	3.86677485	0.13698586	2.37857400

C	0.85157885	-4.17782214	-0.47053500
O	1.65528985	-4.92893514	-0.98862900
C	-0.47095315	1.58520286	-0.27810300
O	-1.27152215	2.36433686	-0.75783800
C	1.16488085	3.29389286	-0.22971300
H	1.07126085	3.45536086	-1.30836600
O	0.78123685	1.93053686	0.06763700
C	2.59101085	3.47776286	0.25401000
H	2.66140285	3.31858886	1.33505400
H	3.26492585	2.77318686	-0.24320500
H	2.92881985	4.49634186	0.03353600
O	-0.40867615	-4.53916414	-0.17088400
C	-0.79393915	-5.87398114	-0.57377900
H	-0.68241415	-5.95751214	-1.65953400
C	-2.22977715	-6.08243714	-0.12999100
H	-2.31766315	-6.00293914	0.95870300
H	-2.88962915	-5.33755514	-0.58567100
H	-2.57054315	-7.07929014	-0.43066200
C	7.04715885	-2.19512214	2.59636700
H	6.79213685	-3.13104814	3.11006100
H	7.42932285	-2.42592514	1.59362700
H	7.81689985	-1.66934314	3.16398200
C	-5.85321815	-2.59206714	3.01925900
H	-6.87648815	-2.58672714	3.39874400
H	-5.74286315	-3.39801514	2.28219600
H	-5.15809515	-2.76558514	3.85098600
O	-5.65076515	-1.31645714	2.42956900
O	5.93562085	-1.31300514	2.53991800

H	-0.10917715	-6.59364614	-0.11361200
H	0.46641085	3.97318886	0.26948200

1-DMSO

0 1

C	-0.95893600	1.53809500	-0.73178900
C	-2.22639100	1.13476100	-0.09312600
C	-2.38763300	-0.13702300	0.49177700
C	-3.33107500	2.02015900	-0.03361900
C	-3.58457900	-0.51966500	1.09444500
H	-1.57444000	-0.84800700	0.48093300
C	-4.52273700	1.64485000	0.56157400
H	-3.25192900	3.00036400	-0.48455400
C	-4.66435600	0.37032100	1.13347200
H	-3.65716000	-1.50799200	1.53369100
H	-5.36851300	2.32452100	0.59388100
N	0.03332600	0.79181800	-1.11977600
N	-0.08894000	-0.54377600	-1.16504600
C	0.89894200	-1.31697100	-0.82118000
C	2.16234100	-0.96325000	-0.14471700
C	3.24826400	-1.86252500	-0.11376000
C	2.33411400	0.28053900	0.50973100
C	4.44632900	-1.54423000	0.51976600
H	3.16301700	-2.81653000	-0.61677500
C	3.52327500	0.60172300	1.14375000
H	1.53383700	1.00596700	0.51968100
C	4.59368900	-0.30496200	1.15638300
H	5.25519100	-2.26587300	0.50566100
H	3.64536600	1.55577500	1.64678500

C	0.63017000	-2.75903300	-1.20232400
O	1.43388100	-3.51014600	-1.72041800
C	-0.69236200	3.00399200	-1.00989200
O	-1.49293100	3.78312600	-1.48962700
C	0.94347200	4.71268200	-0.96150200
H	0.84985200	4.87415000	-2.04015500
O	0.55982800	3.34932600	-0.66415200
C	2.36960200	4.89655200	-0.47777900
H	2.43999400	4.73737800	0.60326500
H	3.04351700	4.19197600	-0.97499400
H	2.70741100	5.91513100	-0.69825300
O	-0.63008500	-3.12037500	-0.90267300
C	-1.01534800	-4.45519200	-1.30556800
H	-0.90382300	-4.53872300	-2.39132300
C	-2.45118600	-4.66364800	-0.86178000
H	-2.53907200	-4.58415000	0.22691400
H	-3.11103800	-3.91876600	-1.31746000
H	-2.79195200	-5.66050100	-1.16245100
C	6.82575000	-0.77633300	1.86457800
H	6.57072800	-1.71225900	2.37827200
H	7.20791400	-1.00713600	0.86183800
H	7.59549100	-0.25055400	2.43219300
C	-6.07462700	-1.17327800	2.28747000
H	-7.09789700	-1.16793800	2.66695500
H	-5.96427200	-1.97922600	1.55040700
H	-5.37950400	-1.34679600	3.11919700
O	-5.87217400	0.10233200	1.69778000
O	5.71421200	0.10578400	1.80812900

H	-0.33058600	-5.17485700	-0.84540100
H	0.24500200	5.39197800	-0.46230700

1-DCM

0 1

C	-0.95893600	1.53809500	-0.73178900
C	-2.22639100	1.13476100	-0.09312600
C	-2.38763300	-0.13702300	0.49177700
C	-3.33107500	2.02015900	-0.03361900
C	-3.58457900	-0.51966500	1.09444500
H	-1.57444000	-0.84800700	0.48093300
C	-4.52273700	1.64485000	0.56157400
H	-3.25192900	3.00036400	-0.48455400
C	-4.66435600	0.37032100	1.13347200
H	-3.65716000	-1.50799200	1.53369100
H	-5.36851300	2.32452100	0.59388100
N	0.03332600	0.79181800	-1.11977600
N	-0.08894000	-0.54377600	-1.16504600
C	0.89894200	-1.31697100	-0.82118000
C	2.16234100	-0.96325000	-0.14471700
C	3.24826400	-1.86252500	-0.11376000
C	2.33411400	0.28053900	0.50973100
C	4.44632900	-1.54423000	0.51976600
H	3.16301700	-2.81653000	-0.61677500
C	3.52327500	0.60172300	1.14375000
H	1.53383700	1.00596700	0.51968100
C	4.59368900	-0.30496200	1.15638300
H	5.25519100	-2.26587300	0.50566100
H	3.64536600	1.55577500	1.64678500

C	0.63017000	-2.75903300	-1.20232400
O	1.43388100	-3.51014600	-1.72041800
C	-0.69236200	3.00399200	-1.00989200
O	-1.49293100	3.78312600	-1.48962700
C	0.94347200	4.71268200	-0.96150200
H	0.84985200	4.87415000	-2.04015500
O	0.55982800	3.34932600	-0.66415200
C	2.36960200	4.89655200	-0.47777900
H	2.43999400	4.73737800	0.60326500
H	3.04351700	4.19197600	-0.97499400
H	2.70741100	5.91513100	-0.69825300
O	-0.63008500	-3.12037500	-0.90267300
C	-1.01534800	-4.45519200	-1.30556800
H	-0.90382300	-4.53872300	-2.39132300
C	-2.45118600	-4.66364800	-0.86178000
H	-2.53907200	-4.58415000	0.22691400
H	-3.11103800	-3.91876600	-1.31746000
H	-2.79195200	-5.66050100	-1.16245100
C	6.82575000	-0.77633300	1.86457800
H	6.57072800	-1.71225900	2.37827200
H	7.20791400	-1.00713600	0.86183800
H	7.59549100	-0.25055400	2.43219300
C	-6.07462700	-1.17327800	2.28747000
H	-7.09789700	-1.16793800	2.66695500
H	-5.96427200	-1.97922600	1.55040700
H	-5.37950400	-1.34679600	3.11919700
O	-5.87217400	0.10233200	1.69778000
O	5.71421200	0.10578400	1.80812900

H	-0.33058600	-5.17485700	-0.84540100
H	0.24500200	5.39197800	-0.46230700

1-THF

0 1

C	-0.95893600	1.53809500	-0.73178900
C	-2.22639100	1.13476100	-0.09312600
C	-2.38763300	-0.13702300	0.49177700
C	-3.33107500	2.02015900	-0.03361900
C	-3.58457900	-0.51966500	1.09444500
H	-1.57444000	-0.84800700	0.48093300
C	-4.52273700	1.64485000	0.56157400
H	-3.25192900	3.00036400	-0.48455400
C	-4.66435600	0.37032100	1.13347200
H	-3.65716000	-1.50799200	1.53369100
H	-5.36851300	2.32452100	0.59388100
N	0.03332600	0.79181800	-1.11977600
N	-0.08894000	-0.54377600	-1.16504600
C	0.89894200	-1.31697100	-0.82118000
C	2.16234100	-0.96325000	-0.14471700
C	3.24826400	-1.86252500	-0.11376000
C	2.33411400	0.28053900	0.50973100
C	4.44632900	-1.54423000	0.51976600
H	3.16301700	-2.81653000	-0.61677500
C	3.52327500	0.60172300	1.14375000
H	1.53383700	1.00596700	0.51968100
C	4.59368900	-0.30496200	1.15638300
H	5.25519100	-2.26587300	0.50566100
H	3.64536600	1.55577500	1.64678500

C	0.63017000	-2.75903300	-1.20232400
O	1.43388100	-3.51014600	-1.72041800
C	-0.69236200	3.00399200	-1.00989200
O	-1.49293100	3.78312600	-1.48962700
C	0.94347200	4.71268200	-0.96150200
H	0.84985200	4.87415000	-2.04015500
O	0.55982800	3.34932600	-0.66415200
C	2.36960200	4.89655200	-0.47777900
H	2.43999400	4.73737800	0.60326500
H	3.04351700	4.19197600	-0.97499400
H	2.70741100	5.91513100	-0.69825300
O	-0.63008500	-3.12037500	-0.90267300
C	-1.01534800	-4.45519200	-1.30556800
H	-0.90382300	-4.53872300	-2.39132300
C	-2.45118600	-4.66364800	-0.86178000
H	-2.53907200	-4.58415000	0.22691400
H	-3.11103800	-3.91876600	-1.31746000
H	-2.79195200	-5.66050100	-1.16245100
C	6.82575000	-0.77633300	1.86457800
H	6.57072800	-1.71225900	2.37827200
H	7.20791400	-1.00713600	0.86183800
H	7.59549100	-0.25055400	2.43219300
C	-6.07462700	-1.17327800	2.28747000
H	-7.09789700	-1.16793800	2.66695500
H	-5.96427200	-1.97922600	1.55040700
H	-5.37950400	-1.34679600	3.11919700
O	-5.87217400	0.10233200	1.69778000
O	5.71421200	0.10578400	1.80812900

H	-0.33058600	-5.17485700	-0.84540100
H	0.24500200	5.39197800	-0.46230700

1-Hexane

0 1

C	-0.95893600	1.53809500	-0.73178900
C	-2.22639100	1.13476100	-0.09312600
C	-2.38763300	-0.13702300	0.49177700
C	-3.33107500	2.02015900	-0.03361900
C	-3.58457900	-0.51966500	1.09444500
H	-1.57444000	-0.84800700	0.48093300
C	-4.52273700	1.64485000	0.56157400
H	-3.25192900	3.00036400	-0.48455400
C	-4.66435600	0.37032100	1.13347200
H	-3.65716000	-1.50799200	1.53369100
H	-5.36851300	2.32452100	0.59388100
N	0.03332600	0.79181800	-1.11977600
N	-0.08894000	-0.54377600	-1.16504600
C	0.89894200	-1.31697100	-0.82118000
C	2.16234100	-0.96325000	-0.14471700
C	3.24826400	-1.86252500	-0.11376000
C	2.33411400	0.28053900	0.50973100
C	4.44632900	-1.54423000	0.51976600
H	3.16301700	-2.81653000	-0.61677500
C	3.52327500	0.60172300	1.14375000
H	1.53383700	1.00596700	0.51968100
C	4.59368900	-0.30496200	1.15638300
H	5.25519100	-2.26587300	0.50566100
H	3.64536600	1.55577500	1.64678500

C	0.63017000	-2.75903300	-1.20232400
O	1.43388100	-3.51014600	-1.72041800
C	-0.69236200	3.00399200	-1.00989200
O	-1.49293100	3.78312600	-1.48962700
C	0.94347200	4.71268200	-0.96150200
H	0.84985200	4.87415000	-2.04015500
O	0.55982800	3.34932600	-0.66415200
C	2.36960200	4.89655200	-0.47777900
H	2.43999400	4.73737800	0.60326500
H	3.04351700	4.19197600	-0.97499400
H	2.70741100	5.91513100	-0.69825300
O	-0.63008500	-3.12037500	-0.90267300
C	-1.01534800	-4.45519200	-1.30556800
H	-0.90382300	-4.53872300	-2.39132300
C	-2.45118600	-4.66364800	-0.86178000
H	-2.53907200	-4.58415000	0.22691400
H	-3.11103800	-3.91876600	-1.31746000
H	-2.79195200	-5.66050100	-1.16245100
C	6.82575000	-0.77633300	1.86457800
H	6.57072800	-1.71225900	2.37827200
H	7.20791400	-1.00713600	0.86183800
H	7.59549100	-0.25055400	2.43219300
C	-6.07462700	-1.17327800	2.28747000
H	-7.09789700	-1.16793800	2.66695500
H	-5.96427200	-1.97922600	1.55040700
H	-5.37950400	-1.34679600	3.11919700
O	-5.87217400	0.10233200	1.69778000
O	5.71421200	0.10578400	1.80812900

H	-0.33058600	-5.17485700	-0.84540100
H	0.24500200	5.39197800	-0.46230700

2- CH3OH

0 1

C	-2.58134502	1.03036875	0.00000000
C	-2.26291002	-0.28487125	0.35297700
C	-2.54395102	-1.32608825	-0.53476500
C	-3.14564202	-1.06884025	-1.76556700
C	-3.45388702	0.24578775	-2.11709900
C	-3.16084802	1.30793975	-1.25532000
H	-1.80995302	-0.50498325	1.31281200
H	-2.29530702	-2.34520525	-0.25057500
H	-3.36844502	-1.88088725	-2.45093200
H	-3.92057902	0.45957075	-3.07327200
C	-3.42670202	2.71351475	-1.66848100
C	-2.25054502	3.65619375	-1.69959200
C	-1.52962202	5.88852575	-1.93509800
H	-0.91088402	5.81314075	-1.03452000
H	-0.90054502	5.61811375	-2.78972200
C	-2.14498902	7.26674975	-2.09217500
H	-2.77453602	7.51312575	-1.23114600
H	-1.35375902	8.02068575	-2.17058100
H	-2.76262102	7.31703575	-2.99444000
C	-6.68515402	2.51878775	-1.54724200
C	-7.82341702	1.64336575	-2.01853200
O	-1.09886602	3.27726675	-1.62562500
O	-2.61483802	4.94168175	-1.83544100
N	-4.55539302	3.18337075	-2.07318900

N	-5.61716002	2.39561375	-2.25560200
C	-9.78885402	0.52747375	-1.32896900
H	-9.42551902	-0.40893925	-1.76468500
H	-10.38431202	1.03684075	-2.09425300
C	-10.57632502	0.29549175	-0.05249800
H	-11.45032702	-0.33098025	-0.26251700
H	-9.96150902	-0.21042025	0.69888300
H	-10.92402202	1.24342075	0.37089500
O	-7.95739402	1.21909675	-3.14389600
O	-8.65678602	1.35723675	-0.99569200
C	-6.85310202	3.39959375	-0.36288400
C	-7.93401102	4.31154675	-0.32694800
C	-5.96134402	3.36945475	0.71372500
C	-8.11137902	5.15120375	0.77574700
C	-6.13628202	4.20673375	1.81766700
H	-5.13126102	2.67163075	0.69705600
C	-7.21096102	5.09172975	1.84342400
H	-8.93640602	5.85336675	0.80863200
H	-5.43735102	4.16314475	2.64740300
H	-7.35767902	5.74969375	2.69597700
C	-1.62118802	1.94724975	1.99249300
H	-2.10663002	1.28147375	2.71831000
H	-0.62453802	1.55855975	1.75040300
H	-1.52684502	2.94385375	2.42745900
C	-9.84480302	5.19771475	-1.46716500
H	-10.55485302	4.98993775	-0.65587500
H	-9.52345802	6.24558375	-1.40770800
H	-10.33074002	5.02341675	-2.42858000

O	-2.40867902	2.10730575	0.82218700
O	-8.73635702	4.31352775	-1.42864700

2- CH3CN

0 1

C	-2.64642095	0.79175704	0.00000000
C	-2.32798595	-0.52348296	0.35297700
C	-2.60902695	-1.56469996	-0.53476500
C	-3.21071795	-1.30745196	-1.76556700
C	-3.51896295	0.00717604	-2.11709900
C	-3.22592395	1.06932804	-1.25532000
H	-1.87502895	-0.74359496	1.31281200
H	-2.36038295	-2.58381696	-0.25057500
H	-3.43352095	-2.11949896	-2.45093200
H	-3.98565495	0.22095904	-3.07327200
C	-3.49177795	2.47490304	-1.66848100
C	-2.31562095	3.41758204	-1.69959200
C	-1.59469795	5.64991404	-1.93509800
H	-0.97595995	5.57452904	-1.03452000
H	-0.96562095	5.37950204	-2.78972200
C	-2.21006495	7.02813804	-2.09217500
H	-2.83961195	7.27451404	-1.23114600
H	-1.41883495	7.78207404	-2.17058100
H	-2.82769695	7.07842404	-2.99444000
C	-6.75022995	2.28017604	-1.54724200
C	-7.88849295	1.40475404	-2.01853200
O	-1.16394195	3.03865504	-1.62562500
O	-2.67991395	4.70307004	-1.83544100
N	-4.62046895	2.94475904	-2.07318900

N	-5.68223595	2.15700204	-2.25560200
C	-9.85392995	0.28886204	-1.32896900
H	-9.49059495	-0.64755096	-1.76468500
H	-10.44938795	0.79822904	-2.09425300
C	-10.64140095	0.05688004	-0.05249800
H	-11.51540295	-0.56959196	-0.26251700
H	-10.02658495	-0.44903196	0.69888300
H	-10.98909795	1.00480904	0.37089500
O	-8.02246995	0.98048504	-3.14389600
O	-8.72186195	1.11862504	-0.99569200
C	-6.91817795	3.16098204	-0.36288400
C	-7.99908695	4.07293504	-0.32694800
C	-6.02641995	3.13084304	0.71372500
C	-8.17645495	4.91259204	0.77574700
C	-6.20135795	3.96812204	1.81766700
H	-5.19633695	2.43301904	0.69705600
C	-7.27603695	4.85311804	1.84342400
H	-9.00148195	5.61475504	0.80863200
H	-5.50242695	3.92453304	2.64740300
H	-7.42275495	5.51108204	2.69597700
C	-1.68626395	1.70863804	1.99249300
H	-2.17170595	1.04286204	2.71831000
H	-0.68961395	1.31994804	1.75040300
H	-1.59192095	2.70524204	2.42745900
C	-9.90987895	4.95910304	-1.46716500
H	-10.61992895	4.75132604	-0.65587500
H	-9.58853395	6.00697204	-1.40770800
H	-10.39581595	4.78480504	-2.42858000

O	-2.47375495	1.86869404	0.82218700
O	-8.80143295	4.07491604	-1.42864700

2-DMSO

0 1

C	2.68033800	-1.68128600	0.82796900
C	2.99877300	-2.99652600	1.18094600
C	2.71773200	-4.03774300	0.29320400
C	2.11604100	-3.78049500	-0.93759800
C	1.80779600	-2.46586700	-1.28913000
C	2.10083500	-1.40371500	-0.42735100
H	3.45173000	-3.21663800	2.14078100
H	2.96637600	-5.05686000	0.57739400
H	1.89323800	-4.59254200	-1.62296300
H	1.34110400	-2.25208400	-2.24530300
C	1.83498100	0.00186000	-0.84051200
C	3.01113800	0.94453900	-0.87162300
C	3.73206100	3.17687100	-1.10712900
H	4.35079900	3.10148600	-0.20655100
H	4.36113800	2.90645900	-1.96175300
C	3.11669400	4.55509500	-1.26420600
H	2.48714700	4.80147100	-0.40317700
H	3.90792400	5.30903100	-1.34261200
H	2.49906200	4.60538100	-2.16647100
C	-1.42347100	-0.19286700	-0.71927300
C	-2.56173400	-1.06828900	-1.19056300
O	4.16281700	0.56561200	-0.79765600
O	2.64684500	2.23002700	-1.00747200
N	0.70629000	0.47171600	-1.24522000

N	-0.35547700	-0.31604100	-1.42763300
C	-4.52717100	-2.18418100	-0.50100000
H	-4.16383600	-3.12059400	-0.93671600
H	-5.12262900	-1.67481400	-1.26628400
C	-5.31464200	-2.41616300	0.77547100
H	-6.18864400	-3.04263500	0.56545200
H	-4.69982600	-2.92207500	1.52685200
H	-5.66233900	-1.46823400	1.19886400
O	-2.69571100	-1.49255800	-2.31592700
O	-3.39510300	-1.35441800	-0.16772300
C	-1.59141900	0.68793900	0.46508500
C	-2.67232800	1.59989200	0.50102100
C	-0.69966100	0.65780000	1.54169400
C	-2.84969600	2.43954900	1.60371600
C	-0.87459900	1.49507900	2.64563600
H	0.13042200	-0.04002400	1.52502500
C	-1.94927800	2.38007500	2.67139300
H	-3.67472300	3.14171200	1.63660100
H	-0.17566800	1.45149000	3.47537200
H	-2.09599600	3.03803900	3.52394600
C	3.64049500	-0.76440500	2.82046200
H	3.15505300	-1.43018100	3.54627900
H	4.63714500	-1.15309500	2.57837200
H	3.73483800	0.23219900	3.25542800
C	-4.58312000	2.48606000	-0.63919600
H	-5.29317000	2.27828300	0.17209400
H	-4.26177500	3.53392900	-0.57973900
H	-5.06905700	2.31176200	-1.60061100

O	2.85300400	-0.60434900	1.65015600
O	-3.47467400	1.60187300	-0.60067800

2-DCM

0 1

C	2.68033800	-1.68128600	0.82796900
C	2.99877300	-2.99652600	1.18094600
C	2.71773200	-4.03774300	0.29320400
C	2.11604100	-3.78049500	-0.93759800
C	1.80779600	-2.46586700	-1.28913000
C	2.10083500	-1.40371500	-0.42735100
H	3.45173000	-3.21663800	2.14078100
H	2.96637600	-5.05686000	0.57739400
H	1.89323800	-4.59254200	-1.62296300
H	1.34110400	-2.25208400	-2.24530300
C	1.83498100	0.00186000	-0.84051200
C	3.01113800	0.94453900	-0.87162300
C	3.73206100	3.17687100	-1.10712900
H	4.35079900	3.10148600	-0.20655100
H	4.36113800	2.90645900	-1.96175300
C	3.11669400	4.55509500	-1.26420600
H	2.48714700	4.80147100	-0.40317700
H	3.90792400	5.30903100	-1.34261200
H	2.49906200	4.60538100	-2.16647100
C	-1.42347100	-0.19286700	-0.71927300
C	-2.56173400	-1.06828900	-1.19056300
O	4.16281700	0.56561200	-0.79765600
O	2.64684500	2.23002700	-1.00747200
N	0.70629000	0.47171600	-1.24522000

N	-0.35547700	-0.31604100	-1.42763300
C	-4.52717100	-2.18418100	-0.50100000
H	-4.16383600	-3.12059400	-0.93671600
H	-5.12262900	-1.67481400	-1.26628400
C	-5.31464200	-2.41616300	0.77547100
H	-6.18864400	-3.04263500	0.56545200
H	-4.69982600	-2.92207500	1.52685200
H	-5.66233900	-1.46823400	1.19886400
O	-2.69571100	-1.49255800	-2.31592700
O	-3.39510300	-1.35441800	-0.16772300
C	-1.59141900	0.68793900	0.46508500
C	-2.67232800	1.59989200	0.50102100
C	-0.69966100	0.65780000	1.54169400
C	-2.84969600	2.43954900	1.60371600
C	-0.87459900	1.49507900	2.64563600
H	0.13042200	-0.04002400	1.52502500
C	-1.94927800	2.38007500	2.67139300
H	-3.67472300	3.14171200	1.63660100
H	-0.17566800	1.45149000	3.47537200
H	-2.09599600	3.03803900	3.52394600
C	3.64049500	-0.76440500	2.82046200
H	3.15505300	-1.43018100	3.54627900
H	4.63714500	-1.15309500	2.57837200
H	3.73483800	0.23219900	3.25542800
C	-4.58312000	2.48606000	-0.63919600
H	-5.29317000	2.27828300	0.17209400
H	-4.26177500	3.53392900	-0.57973900
H	-5.06905700	2.31176200	-1.60061100

O	2.85300400	-0.60434900	1.65015600
O	-3.47467400	1.60187300	-0.60067800

2-THF

0 1

C	2.68033800	-1.68128600	0.82796900
C	2.99877300	-2.99652600	1.18094600
C	2.71773200	-4.03774300	0.29320400
C	2.11604100	-3.78049500	-0.93759800
C	1.80779600	-2.46586700	-1.28913000
C	2.10083500	-1.40371500	-0.42735100
H	3.45173000	-3.21663800	2.14078100
H	2.96637600	-5.05686000	0.57739400
H	1.89323800	-4.59254200	-1.62296300
H	1.34110400	-2.25208400	-2.24530300
C	1.83498100	0.00186000	-0.84051200
C	3.01113800	0.94453900	-0.87162300
C	3.73206100	3.17687100	-1.10712900
H	4.35079900	3.10148600	-0.20655100
H	4.36113800	2.90645900	-1.96175300
C	3.11669400	4.55509500	-1.26420600
H	2.48714700	4.80147100	-0.40317700
H	3.90792400	5.30903100	-1.34261200
H	2.49906200	4.60538100	-2.16647100
C	-1.42347100	-0.19286700	-0.71927300
C	-2.56173400	-1.06828900	-1.19056300
O	4.16281700	0.56561200	-0.79765600
O	2.64684500	2.23002700	-1.00747200
N	0.70629000	0.47171600	-1.24522000

N	-0.35547700	-0.31604100	-1.42763300
C	-4.52717100	-2.18418100	-0.50100000
H	-4.16383600	-3.12059400	-0.93671600
H	-5.12262900	-1.67481400	-1.26628400
C	-5.31464200	-2.41616300	0.77547100
H	-6.18864400	-3.04263500	0.56545200
H	-4.69982600	-2.92207500	1.52685200
H	-5.66233900	-1.46823400	1.19886400
O	-2.69571100	-1.49255800	-2.31592700
O	-3.39510300	-1.35441800	-0.16772300
C	-1.59141900	0.68793900	0.46508500
C	-2.67232800	1.59989200	0.50102100
C	-0.69966100	0.65780000	1.54169400
C	-2.84969600	2.43954900	1.60371600
C	-0.87459900	1.49507900	2.64563600
H	0.13042200	-0.04002400	1.52502500
C	-1.94927800	2.38007500	2.67139300
H	-3.67472300	3.14171200	1.63660100
H	-0.17566800	1.45149000	3.47537200
H	-2.09599600	3.03803900	3.52394600
C	3.64049500	-0.76440500	2.82046200
H	3.15505300	-1.43018100	3.54627900
H	4.63714500	-1.15309500	2.57837200
H	3.73483800	0.23219900	3.25542800
C	-4.58312000	2.48606000	-0.63919600
H	-5.29317000	2.27828300	0.17209400
H	-4.26177500	3.53392900	-0.57973900
H	-5.06905700	2.31176200	-1.60061100

O	2.85300400	-0.60434900	1.65015600
O	-3.47467400	1.60187300	-0.60067800

2-Hexane

0 1

C	2.68033800	-1.68128600	0.82796900
C	2.99877300	-2.99652600	1.18094600
C	2.71773200	-4.03774300	0.29320400
C	2.11604100	-3.78049500	-0.93759800
C	1.80779600	-2.46586700	-1.28913000
C	2.10083500	-1.40371500	-0.42735100
H	3.45173000	-3.21663800	2.14078100
H	2.96637600	-5.05686000	0.57739400
H	1.89323800	-4.59254200	-1.62296300
H	1.34110400	-2.25208400	-2.24530300
C	1.83498100	0.00186000	-0.84051200
C	3.01113800	0.94453900	-0.87162300
C	3.73206100	3.17687100	-1.10712900
H	4.35079900	3.10148600	-0.20655100
H	4.36113800	2.90645900	-1.96175300
C	3.11669400	4.55509500	-1.26420600
H	2.48714700	4.80147100	-0.40317700
H	3.90792400	5.30903100	-1.34261200
H	2.49906200	4.60538100	-2.16647100
C	-1.42347100	-0.19286700	-0.71927300
C	-2.56173400	-1.06828900	-1.19056300
O	4.16281700	0.56561200	-0.79765600
O	2.64684500	2.23002700	-1.00747200
N	0.70629000	0.47171600	-1.24522000

N	-0.35547700	-0.31604100	-1.42763300
C	-4.52717100	-2.18418100	-0.50100000
H	-4.16383600	-3.12059400	-0.93671600
H	-5.12262900	-1.67481400	-1.26628400
C	-5.31464200	-2.41616300	0.77547100
H	-6.18864400	-3.04263500	0.56545200
H	-4.69982600	-2.92207500	1.52685200
H	-5.66233900	-1.46823400	1.19886400
O	-2.69571100	-1.49255800	-2.31592700
O	-3.39510300	-1.35441800	-0.16772300
C	-1.59141900	0.68793900	0.46508500
C	-2.67232800	1.59989200	0.50102100
C	-0.69966100	0.65780000	1.54169400
C	-2.84969600	2.43954900	1.60371600
C	-0.87459900	1.49507900	2.64563600
H	0.13042200	-0.04002400	1.52502500
C	-1.94927800	2.38007500	2.67139300
H	-3.67472300	3.14171200	1.63660100
H	-0.17566800	1.45149000	3.47537200
H	-2.09599600	3.03803900	3.52394600
C	3.64049500	-0.76440500	2.82046200
H	3.15505300	-1.43018100	3.54627900
H	4.63714500	-1.15309500	2.57837200
H	3.73483800	0.23219900	3.25542800
C	-4.58312000	2.48606000	-0.63919600
H	-5.29317000	2.27828300	0.17209400
H	-4.26177500	3.53392900	-0.57973900
H	-5.06905700	2.31176200	-1.60061100

O	2.85300400	-0.60434900	1.65015600
O	-3.47467400	1.60187300	-0.60067800

3- CH3OH

0 1

C	0.04338395	0.44468546	0.00000000
C	-0.71981905	1.32249246	0.92287300
C	-2.10821405	1.49950746	0.76586800
C	-0.07232405	1.99877646	1.97473200
C	-2.82424305	2.33509946	1.61843200
H	-2.63516605	0.98359246	-0.02859400
C	-0.78330105	2.82147446	2.84372900
H	0.99593995	1.89054346	2.10919400
C	-2.15027505	2.98134946	2.64896500
H	-3.89184205	2.48589146	1.49763600
H	-0.29202305	3.34071446	3.65979100
N	-0.39445705	-0.60627354	-0.61340800
N	-1.64672005	-1.01381454	-0.61339700
C	-2.08454505	-2.06477054	0.00002800
C	-1.32132405	-2.94256054	0.92290600
C	-1.96879605	-3.61877654	1.97482200
C	0.06705695	-3.11962754	0.76584800
C	-1.25781005	-4.44145954	2.84382600
H	-3.03705005	-3.51049754	2.10933400
C	0.78309495	-3.95520654	1.61841900
H	0.59399495	-2.60376854	-0.02865900
C	0.10914995	-4.60138854	2.64901000
H	-1.74907105	-4.96064654	3.65993100
H	1.85068295	-4.10604254	1.49758200

C	-3.52171905	-2.41128854	-0.31694300
O	-4.03814205	-3.47681754	-0.04200600
C	1.48055995	0.79118046	-0.31699200
O	1.99700995	1.85669446	-0.04204700
C	3.49458995	0.07063946	-1.31840300
H	3.50131095	0.94007546	-1.98350300
O	2.12739995	-0.21073954	-0.93689700
C	4.04133895	-1.17173254	-1.99569900
H	4.02424295	-2.02907654	-1.31502700
H	3.45339195	-1.42430454	-2.88370700
H	5.07791195	-0.99842554	-2.30477400
O	-4.16858105	-1.40938154	-0.93684500
C	-5.53575305	-1.69080254	-1.31838100
H	-5.54243605	-2.56025554	-1.98345900
C	-6.08251605	-0.44845954	-1.99572000
H	-6.06545705	0.40890146	-1.31506800
H	-5.49455405	-0.19589454	-2.88371900
H	-7.11907805	-0.62179954	-2.30481500
F	-2.84266005	3.78029846	3.48392100
F	0.80154395	-5.40032954	3.48396700
H	4.06236495	0.33668646	-0.42090200
H	-6.10354305	-1.95684154	-0.42088700

3- CH3CN

0 1

C	-1.60520615	0.63991322	0.00000000
C	-2.36840915	1.51772022	0.92287300
C	-3.75680415	1.69473522	0.76586800
C	-1.72091415	2.19400422	1.97473200

C	-4.47283315	2.53032722	1.61843200
H	-4.28375615	1.17882022	-0.02859400
C	-2.43189115	3.01670222	2.84372900
H	-0.65265015	2.08577122	2.10919400
C	-3.79886515	3.17657722	2.64896500
H	-5.54043215	2.68111922	1.49763600
H	-1.94061315	3.53594222	3.65979100
N	-2.04304715	-0.41104578	-0.61340800
N	-3.29531015	-0.81858678	-0.61339700
C	-3.73313515	-1.86954278	0.00002800
C	-2.96991415	-2.74733278	0.92290600
C	-3.61738615	-3.42354878	1.97482200
C	-1.58153315	-2.92439978	0.76584800
C	-2.90640015	-4.24623178	2.84382600
H	-4.68564015	-3.31526978	2.10933400
C	-0.86549515	-3.75997878	1.61841900
H	-1.05459515	-2.40854078	-0.02865900
C	-1.53944015	-4.40616078	2.64901000
H	-3.39766115	-4.76541878	3.65993100
H	0.20209285	-3.91081478	1.49758200
C	-5.17030915	-2.21606078	-0.31694300
O	-5.68673215	-3.28158978	-0.04200600
C	-0.16803015	0.98640822	-0.31699200
O	0.34841985	2.05192222	-0.04204700
C	1.84599985	0.26586722	-1.31840300
H	1.85272085	1.13530322	-1.98350300
O	0.47880985	-0.01551178	-0.93689700
C	2.39274885	-0.97650478	-1.99569900

H	2.37565285	-1.83384878	-1.31502700
H	1.80480185	-1.22907678	-2.88370700
H	3.42932185	-0.80319778	-2.30477400
O	-5.81717115	-1.21415378	-0.93684500
C	-7.18434315	-1.49557478	-1.31838100
H	-7.19102615	-2.36502778	-1.98345900
C	-7.73110615	-0.25323178	-1.99572000
H	-7.71404715	0.60412922	-1.31506800
H	-7.14314415	-0.00066678	-2.88371900
H	-8.76766815	-0.42657178	-2.30481500
F	-4.49125015	3.97552622	3.48392100
F	-0.84704615	-5.20510178	3.48396700
H	2.41377485	0.53191422	-0.42090200
H	-7.75213315	-1.76161378	-0.42088700

3-DMSO

0 1

C	1.06395800	1.25473100	-0.59824400
C	0.30075500	2.13253800	0.32462900
C	-1.08764000	2.30955300	0.16762400
C	0.94825000	2.80882200	1.37648800
C	-1.80366900	3.14514500	1.02018800
H	-1.61459200	1.79363800	-0.62683800
C	0.23727300	3.63152000	2.24548500
H	2.01651400	2.70058900	1.51095000
C	-1.12970100	3.79139500	2.05072100
H	-2.87126800	3.29593700	0.89939200
H	0.72855100	4.15076000	3.06154700
N	0.62611700	0.20377200	-1.21165200

N	-0.62614600	-0.20376900	-1.21164100
C	-1.06397100	-1.25472500	-0.59821600
C	-0.30075000	-2.13251500	0.32466200
C	-0.94822200	-2.80873100	1.37657800
C	1.08763100	-2.30958200	0.16760400
C	-0.23723600	-3.63141400	2.24558200
H	-2.01647600	-2.70045200	1.51109000
C	1.80366900	-3.14516100	1.02017500
H	1.61456900	-1.79372300	-0.62690300
C	1.12972400	-3.79134300	2.05076600
H	-0.72849700	-4.15060100	3.06168700
H	2.87125700	-3.29599700	0.89933800
C	-2.50114500	-1.60124300	-0.91518700
O	-3.01756800	-2.66677200	-0.64025000
C	2.50113400	1.60122600	-0.91523600
O	3.01758400	2.66674000	-0.64029100
C	4.51516400	0.88068500	-1.91664700
H	4.52188500	1.75012100	-2.58174700
O	3.14797400	0.59930600	-1.53514100
C	5.06191300	-0.36168700	-2.59394300
H	5.04481700	-1.21903100	-1.91327100
H	4.47396600	-0.61425900	-3.48195100
H	6.09848600	-0.18838000	-2.90301800
O	-3.14800700	-0.59933600	-1.53508900
C	-4.51517900	-0.88075700	-1.91662500
H	-4.52186200	-1.75021000	-2.58170300
C	-5.06194200	0.36158600	-2.59396400
H	-5.04488300	1.21894700	-1.91331200

H	-4.47398000	0.61415100	-3.48196300
H	-6.09850400	0.18824600	-2.90305900
F	-1.82208600	4.59034400	2.88567700
F	1.82211800	-4.59028400	2.88572300
H	5.08293900	1.14673200	-1.01914600
H	-5.08296900	-1.14679600	-1.01913100

3-DCM

0 1

C	1.06395800	1.25473100	-0.59824400
C	0.30075500	2.13253800	0.32462900
C	-1.08764000	2.30955300	0.16762400
C	0.94825000	2.80882200	1.37648800
C	-1.80366900	3.14514500	1.02018800
H	-1.61459200	1.79363800	-0.62683800
C	0.23727300	3.63152000	2.24548500
H	2.01651400	2.70058900	1.51095000
C	-1.12970100	3.79139500	2.05072100
H	-2.87126800	3.29593700	0.89939200
H	0.72855100	4.15076000	3.06154700
N	0.62611700	0.20377200	-1.21165200
N	-0.62614600	-0.20376900	-1.21164100
C	-1.06397100	-1.25472500	-0.59821600
C	-0.30075000	-2.13251500	0.32466200
C	-0.94822200	-2.80873100	1.37657800
C	1.08763100	-2.30958200	0.16760400
C	-0.23723600	-3.63141400	2.24558200
H	-2.01647600	-2.70045200	1.51109000

C	1.80366900	-3.14516100	1.02017500
H	1.61456900	-1.79372300	-0.62690300
C	1.12972400	-3.79134300	2.05076600
H	-0.72849700	-4.15060100	3.06168700
H	2.87125700	-3.29599700	0.89933800
C	-2.50114500	-1.60124300	-0.91518700
O	-3.01756800	-2.66677200	-0.64025000
C	2.50113400	1.60122600	-0.91523600
O	3.01758400	2.66674000	-0.64029100
C	4.51516400	0.88068500	-1.91664700
H	4.52188500	1.75012100	-2.58174700
O	3.14797400	0.59930600	-1.53514100
C	5.06191300	-0.36168700	-2.59394300
H	5.04481700	-1.21903100	-1.91327100
H	4.47396600	-0.61425900	-3.48195100
H	6.09848600	-0.18838000	-2.90301800
O	-3.14800700	-0.59933600	-1.53508900
C	-4.51517900	-0.88075700	-1.91662500
H	-4.52186200	-1.75021000	-2.58170300
C	-5.06194200	0.36158600	-2.59396400
H	-5.04488300	1.21894700	-1.91331200
H	-4.47398000	0.61415100	-3.48196300
H	-6.09850400	0.18824600	-2.90305900
F	-1.82208600	4.59034400	2.88567700
F	1.82211800	-4.59028400	2.88572300
H	5.08293900	1.14673200	-1.01914600
H	-5.08296900	-1.14679600	-1.01913100

3-THF

0 1

C	1.06395800	1.25473100	-0.59824400
C	0.30075500	2.13253800	0.32462900
C	-1.08764000	2.30955300	0.16762400
C	0.94825000	2.80882200	1.37648800
C	-1.80366900	3.14514500	1.02018800
H	-1.61459200	1.79363800	-0.62683800
C	0.23727300	3.63152000	2.24548500
H	2.01651400	2.70058900	1.51095000
C	-1.12970100	3.79139500	2.05072100
H	-2.87126800	3.29593700	0.89939200
H	0.72855100	4.15076000	3.06154700
N	0.62611700	0.20377200	-1.21165200
N	-0.62614600	-0.20376900	-1.21164100
C	-1.06397100	-1.25472500	-0.59821600
C	-0.30075000	-2.13251500	0.32466200
C	-0.94822200	-2.80873100	1.37657800
C	1.08763100	-2.30958200	0.16760400
C	-0.23723600	-3.63141400	2.24558200
H	-2.01647600	-2.70045200	1.51109000
C	1.80366900	-3.14516100	1.02017500
H	1.61456900	-1.79372300	-0.62690300
C	1.12972400	-3.79134300	2.05076600
H	-0.72849700	-4.15060100	3.06168700
H	2.87125700	-3.29599700	0.89933800
C	-2.50114500	-1.60124300	-0.91518700
O	-3.01756800	-2.66677200	-0.64025000
C	2.50113400	1.60122600	-0.91523600

O	3.01758400	2.66674000	-0.64029100
C	4.51516400	0.88068500	-1.91664700
H	4.52188500	1.75012100	-2.58174700
O	3.14797400	0.59930600	-1.53514100
C	5.06191300	-0.36168700	-2.59394300
H	5.04481700	-1.21903100	-1.91327100
H	4.47396600	-0.61425900	-3.48195100
H	6.09848600	-0.18838000	-2.90301800
O	-3.14800700	-0.59933600	-1.53508900
C	-4.51517900	-0.88075700	-1.91662500
H	-4.52186200	-1.75021000	-2.58170300
C	-5.06194200	0.36158600	-2.59396400
H	-5.04488300	1.21894700	-1.91331200
H	-4.47398000	0.61415100	-3.48196300
H	-6.09850400	0.18824600	-2.90305900
F	-1.82208600	4.59034400	2.88567700
F	1.82211800	-4.59028400	2.88572300
H	5.08293900	1.14673200	-1.01914600
H	-5.08296900	-1.14679600	-1.01913100

3-Hexane

0 1

C	1.06395800	1.25473100	-0.59824400
C	0.30075500	2.13253800	0.32462900
C	-1.08764000	2.30955300	0.16762400
C	0.94825000	2.80882200	1.37648800
C	-1.80366900	3.14514500	1.02018800
H	-1.61459200	1.79363800	-0.62683800
C	0.23727300	3.63152000	2.24548500

H	2.01651400	2.70058900	1.51095000
C	-1.12970100	3.79139500	2.05072100
H	-2.87126800	3.29593700	0.89939200
H	0.72855100	4.15076000	3.06154700
N	0.62611700	0.20377200	-1.21165200
N	-0.62614600	-0.20376900	-1.21164100
C	-1.06397100	-1.25472500	-0.59821600
C	-0.30075000	-2.13251500	0.32466200
C	-0.94822200	-2.80873100	1.37657800
C	1.08763100	-2.30958200	0.16760400
C	-0.23723600	-3.63141400	2.24558200
H	-2.01647600	-2.70045200	1.51109000
C	1.80366900	-3.14516100	1.02017500
H	1.61456900	-1.79372300	-0.62690300
C	1.12972400	-3.79134300	2.05076600
H	-0.72849700	-4.15060100	3.06168700
H	2.87125700	-3.29599700	0.89933800
C	-2.50114500	-1.60124300	-0.91518700
O	-3.01756800	-2.66677200	-0.64025000
C	2.50113400	1.60122600	-0.91523600
O	3.01758400	2.66674000	-0.64029100
C	4.51516400	0.88068500	-1.91664700
H	4.52188500	1.75012100	-2.58174700
O	3.14797400	0.59930600	-1.53514100
C	5.06191300	-0.36168700	-2.59394300
H	5.04481700	-1.21903100	-1.91327100
H	4.47396600	-0.61425900	-3.48195100
H	6.09848600	-0.18838000	-2.90301800

O	-3.14800700	-0.59933600	-1.53508900
C	-4.51517900	-0.88075700	-1.91662500
H	-4.52186200	-1.75021000	-2.58170300
C	-5.06194200	0.36158600	-2.59396400
H	-5.04488300	1.21894700	-1.91331200
H	-4.47398000	0.61415100	-3.48196300
H	-6.09850400	0.18824600	-2.90305900
F	-1.82208600	4.59034400	2.88567700
F	1.82211800	-4.59028400	2.88572300
H	5.08293900	1.14673200	-1.01914600
H	-5.08296900	-1.14679600	-1.01913100

4- CH3OH

0 1

C	-1.41373803	-0.01597444	0.00000000
C	-0.43590503	0.86944556	-0.46653300
C	0.91274197	0.55336356	-0.34372600
C	1.31294297	-0.66044144	0.24764000
C	0.32487997	-1.54456044	0.71157100
C	-1.02700903	-1.22069244	0.58632300
H	-2.46711703	0.23332056	-0.09530900
H	-0.72758803	1.80959256	-0.92717000
H	1.67582897	1.23556956	-0.70321600
H	0.60968197	-2.49418144	1.14924000
H	-1.77835803	-1.91829444	0.94624700
C	2.75548997	-0.96324544	0.38661900
C	3.19254397	-2.21037644	1.12925700
C	4.61171197	-3.00393944	2.86884400
H	3.80476197	-3.68014844	3.16519800

H	5.28008797	-3.55097144	2.19608100
C	5.34839897	-2.41537744	4.05691600
H	4.65320097	-1.91197044	4.73656400
H	5.85240597	-3.21575244	4.60986300
H	6.09364097	-1.68432644	3.73114300
O	2.83566897	-3.33581144	0.85248600
O	4.03666497	-1.89627544	2.12417200
N	3.61491097	-0.15972244	-0.14001200
C	5.45738197	0.99500756	1.73897800
C	7.24673097	-0.09519344	0.20779700
C	8.29475197	0.35069056	1.03163200
C	7.56962597	-0.78170044	-0.97918500
C	9.62345997	0.11172556	0.67678500
H	8.07315997	0.86754256	1.95669100
C	8.89497397	-1.01848544	-1.32548900
H	6.76501397	-1.12150244	-1.62208500
C	9.93116597	-0.57219244	-0.49853600
H	10.41938597	0.46240256	1.32830100
H	9.12200897	-1.54936244	-2.24618100
H	10.96694597	-0.75584944	-0.77125300
C	5.81887397	0.15271456	0.53165100
N	4.92230297	-0.41139944	-0.20475700
C	4.00325897	2.66730856	2.57557700
H	3.69056197	1.98587956	3.37242400
O	5.97554997	0.87224956	2.83196700
O	4.49058597	1.87710256	1.46145700
C	2.85644297	3.51576656	2.06076400
H	2.04930597	2.88574056	1.67387500

H	2.45740897	4.12974356	2.87562600
H	3.19121697	4.18194956	1.25916400
H	4.83013297	3.27365656	2.95897200

4-CH3CN

0 1

C	-0.40734825	-0.12779553	0.00000000
C	0.57048475	0.75762447	-0.46653300
C	1.91913175	0.44154247	-0.34372600
C	2.31933275	-0.77226253	0.24764000
C	1.33126975	-1.65638153	0.71157100
C	-0.02061925	-1.33251353	0.58632300
H	-1.46072725	0.12149947	-0.09530900
H	0.27880175	1.69777147	-0.92717000
H	2.68221875	1.12374847	-0.70321600
H	1.61607175	-2.60600253	1.14924000
H	-0.77196825	-2.03011553	0.94624700
C	3.76187975	-1.07506653	0.38661900
C	4.19893375	-2.32219753	1.12925700
C	5.61810175	-3.11576053	2.86884400
H	4.81115175	-3.79196953	3.16519800
H	6.28647775	-3.66279253	2.19608100
C	6.35478875	-2.52719853	4.05691600
H	5.65959075	-2.02379153	4.73656400
H	6.85879575	-3.32757353	4.60986300
H	7.10003075	-1.79614753	3.73114300
O	3.84205875	-3.44763253	0.85248600
O	5.04305475	-2.00809653	2.12417200
N	4.62130075	-0.27154353	-0.14001200

C	6.46377175	0.88318647	1.73897800
C	8.25312075	-0.20701453	0.20779700
C	9.30114175	0.23886947	1.03163200
C	8.57601575	-0.89352153	-0.97918500
C	10.62984975	-0.00009553	0.67678500
H	9.07954975	0.75572147	1.95669100
C	9.90136375	-1.13030653	-1.32548900
H	7.77140375	-1.23332353	-1.62208500
C	10.93755575	-0.68401353	-0.49853600
H	11.42577575	0.35058147	1.32830100
H	10.12839875	-1.66118353	-2.24618100
H	11.97333575	-0.86767053	-0.77125300
C	6.82526375	0.04089347	0.53165100
N	5.92869275	-0.52322053	-0.20475700
C	5.00964875	2.55548747	2.57557700
H	4.69695175	1.87405847	3.37242400
O	6.98193975	0.76042847	2.83196700
O	5.49697575	1.76528147	1.46145700
C	3.86283275	3.40394547	2.06076400
H	3.05569575	2.77391947	1.67387500
H	3.46379875	4.01792247	2.87562600
H	4.19760675	4.07012847	1.25916400
H	5.83652275	3.16183547	2.95897200

4-DMSO

01

C	-5.68633100	0.28721700	-0.94904700
C	-4.70849800	1.17263700	-1.41558000
C	-3.35985100	0.85655500	-1.29277300

C	-2.95965000	-0.35725000	-0.70140700
C	-3.94771300	-1.24136900	-0.23747600
C	-5.29960200	-0.91750100	-0.36272400
H	-6.73971000	0.53651200	-1.04435600
H	-5.00018100	2.11278400	-1.87621700
H	-2.59676400	1.53876100	-1.65226300
H	-3.66291100	-2.19099000	0.20019300
H	-6.05095100	-1.61510300	-0.00280000
C	-1.51710300	-0.66005400	-0.56242800
C	-1.08004900	-1.90718500	0.18021000
C	0.33911900	-2.70074800	1.91979700
H	-0.46783100	-3.37695700	2.21615100
H	1.00749500	-3.24778000	1.24703400
C	1.07580600	-2.11218600	3.10786900
H	0.38060800	-1.60877900	3.78751700
H	1.57981300	-2.91256100	3.66081600
H	1.82104800	-1.38113500	2.78209600
O	-1.43692400	-3.03262000	-0.09656100
O	-0.23592800	-1.59308400	1.17512500
N	-0.65768200	0.14346900	-1.08905900
C	1.18478900	1.29819900	0.78993100
C	2.97413800	0.20799800	-0.74125000
C	4.02215900	0.65388200	0.08258500
C	3.29703300	-0.47850900	-1.92823200
C	5.35086700	0.41491700	-0.27226200
H	3.80056700	1.17073400	1.00764400
C	4.62238100	-0.71529400	-2.27453600
H	2.49242100	-0.81831100	-2.57113200

C	5.65857300	-0.26900100	-1.44758300
H	6.14679300	0.76559400	0.37925400
H	4.84941600	-1.24617100	-3.19522800
H	6.69435300	-0.45265800	-1.72030000
C	1.54628100	0.45590600	-0.41739600
N	0.64971000	-0.10820800	-1.15380400
C	-0.26933400	2.97050000	1.62653000
H	-0.58203100	2.28907100	2.42337700
O	1.70295700	1.17544100	1.88292000
O	0.21799300	2.18029400	0.51241000
C	-1.41615000	3.81895800	1.11171700
H	-2.22328700	3.18893200	0.72482800
H	-1.81518400	4.43293500	1.92657900
H	-1.08137600	4.48514100	0.31011700
H	0.55754000	3.57684800	2.00992500

4-DCM

0 1

C	-5.68633100	0.28721700	-0.94904700
C	-4.70849800	1.17263700	-1.41558000
C	-3.35985100	0.85655500	-1.29277300
C	-2.95965000	-0.35725000	-0.70140700
C	-3.94771300	-1.24136900	-0.23747600
C	-5.29960200	-0.91750100	-0.36272400
H	-6.73971000	0.53651200	-1.04435600
H	-5.00018100	2.11278400	-1.87621700
H	-2.59676400	1.53876100	-1.65226300
H	-3.66291100	-2.19099000	0.20019300
H	-6.05095100	-1.61510300	-0.00280000

C	-1.51710300	-0.66005400	-0.56242800
C	-1.08004900	-1.90718500	0.18021000
C	0.33911900	-2.70074800	1.91979700
H	-0.46783100	-3.37695700	2.21615100
H	1.00749500	-3.24778000	1.24703400
C	1.07580600	-2.11218600	3.10786900
H	0.38060800	-1.60877900	3.78751700
H	1.57981300	-2.91256100	3.66081600
H	1.82104800	-1.38113500	2.78209600
O	-1.43692400	-3.03262000	-0.09656100
O	-0.23592800	-1.59308400	1.17512500
N	-0.65768200	0.14346900	-1.08905900
C	1.18478900	1.29819900	0.78993100
C	2.97413800	0.20799800	-0.74125000
C	4.02215900	0.65388200	0.08258500
C	3.29703300	-0.47850900	-1.92823200
C	5.35086700	0.41491700	-0.27226200
H	3.80056700	1.17073400	1.00764400
C	4.62238100	-0.71529400	-2.27453600
H	2.49242100	-0.81831100	-2.57113200
C	5.65857300	-0.26900100	-1.44758300
H	6.14679300	0.76559400	0.37925400
H	4.84941600	-1.24617100	-3.19522800
H	6.69435300	-0.45265800	-1.72030000
C	1.54628100	0.45590600	-0.41739600
N	0.64971000	-0.10820800	-1.15380400
C	-0.26933400	2.97050000	1.62653000
H	-0.58203100	2.28907100	2.42337700

O	1.70295700	1.17544100	1.88292000
O	0.21799300	2.18029400	0.51241000
C	-1.41615000	3.81895800	1.11171700
H	-2.22328700	3.18893200	0.72482800
H	-1.81518400	4.43293500	1.92657900
H	-1.08137600	4.48514100	0.31011700
H	0.55754000	3.57684800	2.00992500

4-THF

0 1

C	-5.68633100	0.28721700	-0.94904700
C	-4.70849800	1.17263700	-1.41558000
C	-3.35985100	0.85655500	-1.29277300
C	-2.95965000	-0.35725000	-0.70140700
C	-3.94771300	-1.24136900	-0.23747600
C	-5.29960200	-0.91750100	-0.36272400
H	-6.73971000	0.53651200	-1.04435600
H	-5.00018100	2.11278400	-1.87621700
H	-2.59676400	1.53876100	-1.65226300
H	-3.66291100	-2.19099000	0.20019300
H	-6.05095100	-1.61510300	-0.00280000
C	-1.51710300	-0.66005400	-0.56242800
C	-1.08004900	-1.90718500	0.18021000
C	0.33911900	-2.70074800	1.91979700
H	-0.46783100	-3.37695700	2.21615100
H	1.00749500	-3.24778000	1.24703400
C	1.07580600	-2.11218600	3.10786900
H	0.38060800	-1.60877900	3.78751700
H	1.57981300	-2.91256100	3.66081600

H	1.82104800	-1.38113500	2.78209600
O	-1.43692400	-3.03262000	-0.09656100
O	-0.23592800	-1.59308400	1.17512500
N	-0.65768200	0.14346900	-1.08905900
C	1.18478900	1.29819900	0.78993100
C	2.97413800	0.20799800	-0.74125000
C	4.02215900	0.65388200	0.08258500
C	3.29703300	-0.47850900	-1.92823200
C	5.35086700	0.41491700	-0.27226200
H	3.80056700	1.17073400	1.00764400
C	4.62238100	-0.71529400	-2.27453600
H	2.49242100	-0.81831100	-2.57113200
C	5.65857300	-0.26900100	-1.44758300
H	6.14679300	0.76559400	0.37925400
H	4.84941600	-1.24617100	-3.19522800
H	6.69435300	-0.45265800	-1.72030000
C	1.54628100	0.45590600	-0.41739600
N	0.64971000	-0.10820800	-1.15380400
C	-0.26933400	2.97050000	1.62653000
H	-0.58203100	2.28907100	2.42337700
O	1.70295700	1.17544100	1.88292000
O	0.21799300	2.18029400	0.51241000
C	-1.41615000	3.81895800	1.11171700
H	-2.22328700	3.18893200	0.72482800
H	-1.81518400	4.43293500	1.92657900
H	-1.08137600	4.48514100	0.31011700
H	0.55754000	3.57684800	2.00992500

4-Hexane

0 1

C	-5.68633100	0.28721700	-0.94904700
C	-4.70849800	1.17263700	-1.41558000
C	-3.35985100	0.85655500	-1.29277300
C	-2.95965000	-0.35725000	-0.70140700
C	-3.94771300	-1.24136900	-0.23747600
C	-5.29960200	-0.91750100	-0.36272400
H	-6.73971000	0.53651200	-1.04435600
H	-5.00018100	2.11278400	-1.87621700
H	-2.59676400	1.53876100	-1.65226300
H	-3.66291100	-2.19099000	0.20019300
H	-6.05095100	-1.61510300	-0.00280000
C	-1.51710300	-0.66005400	-0.56242800
C	-1.08004900	-1.90718500	0.18021000
C	0.33911900	-2.70074800	1.91979700
H	-0.46783100	-3.37695700	2.21615100
H	1.00749500	-3.24778000	1.24703400
C	1.07580600	-2.11218600	3.10786900
H	0.38060800	-1.60877900	3.78751700
H	1.57981300	-2.91256100	3.66081600
H	1.82104800	-1.38113500	2.78209600
O	-1.43692400	-3.03262000	-0.09656100
O	-0.23592800	-1.59308400	1.17512500
N	-0.65768200	0.14346900	-1.08905900
C	1.18478900	1.29819900	0.78993100
C	2.97413800	0.20799800	-0.74125000
C	4.02215900	0.65388200	0.08258500
C	3.29703300	-0.47850900	-1.92823200

C	5.35086700	0.41491700	-0.27226200
H	3.80056700	1.17073400	1.00764400
C	4.62238100	-0.71529400	-2.27453600
H	2.49242100	-0.81831100	-2.57113200
C	5.65857300	-0.26900100	-1.44758300
H	6.14679300	0.76559400	0.37925400
H	4.84941600	-1.24617100	-3.19522800
H	6.69435300	-0.45265800	-1.72030000
C	1.54628100	0.45590600	-0.41739600
N	0.64971000	-0.10820800	-1.15380400
C	-0.26933400	2.97050000	1.62653000
H	-0.58203100	2.28907100	2.42337700
O	1.70295700	1.17544100	1.88292000
O	0.21799300	2.18029400	0.51241000
C	-1.41615000	3.81895800	1.11171700
H	-2.22328700	3.18893200	0.72482800
H	-1.81518400	4.43293500	1.92657900
H	-1.08137600	4.48514100	0.31011700
H	0.55754000	3.57684800	2.00992500