
Supporting Information

Novel Dihydro-1,3,2H-benzoxazine Derived from Furfurylamine: Crystal Structure, Hirshfeld Surface Analysis, Photo-physical Property, and Computational Study

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1. Characterization Results

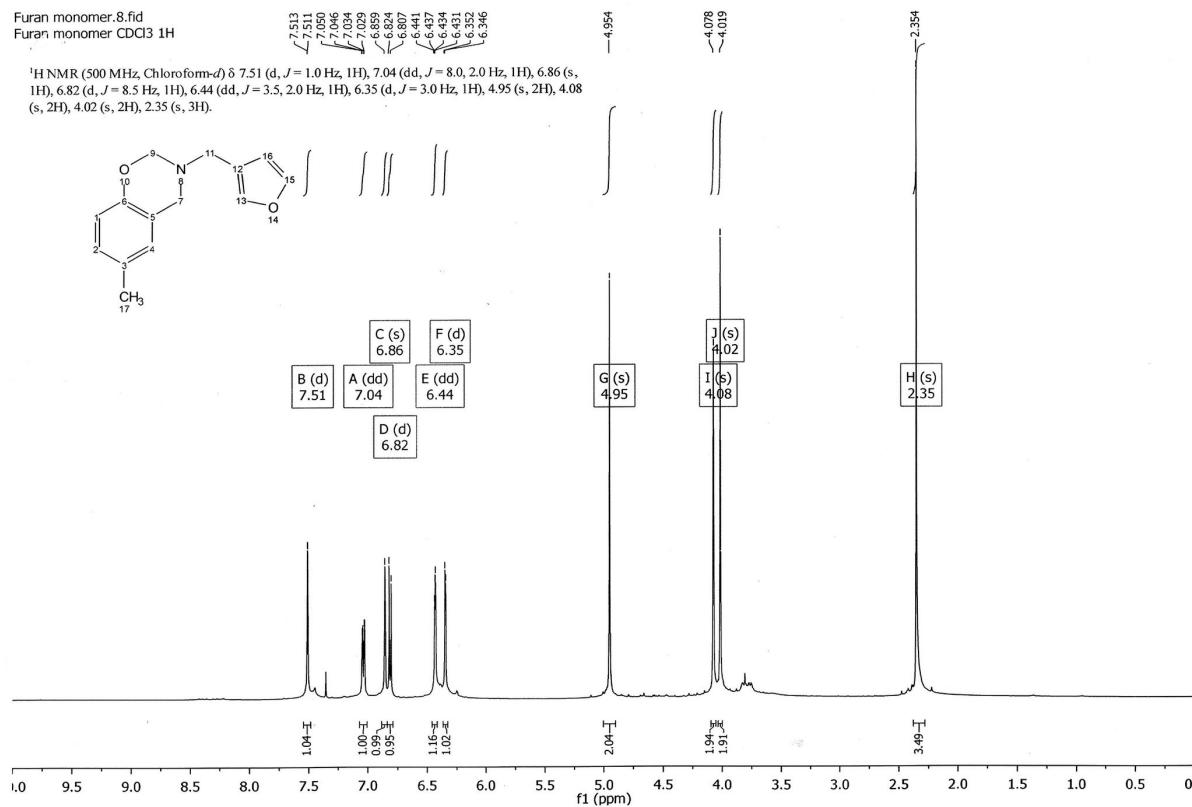


Figure S1. ¹H-NMR spectrum of the benzoxazine (I).

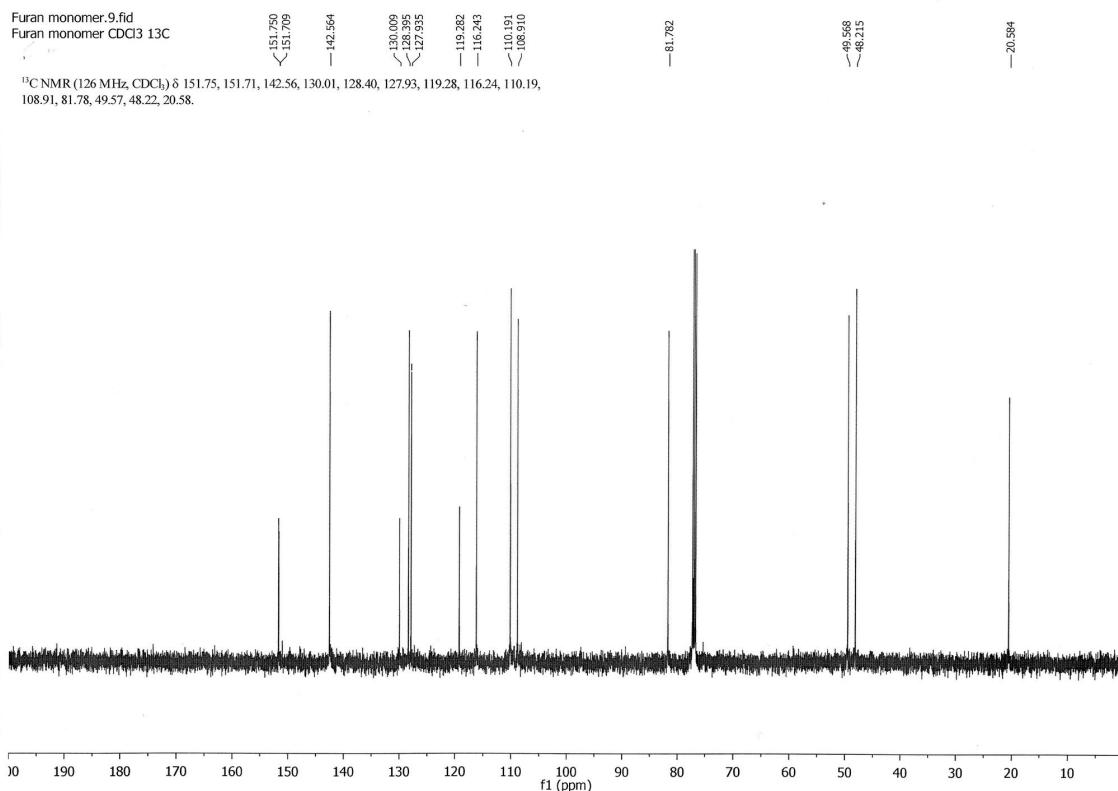


Figure S2. ¹³C-NMR spectrum of the benzoxazine (I).

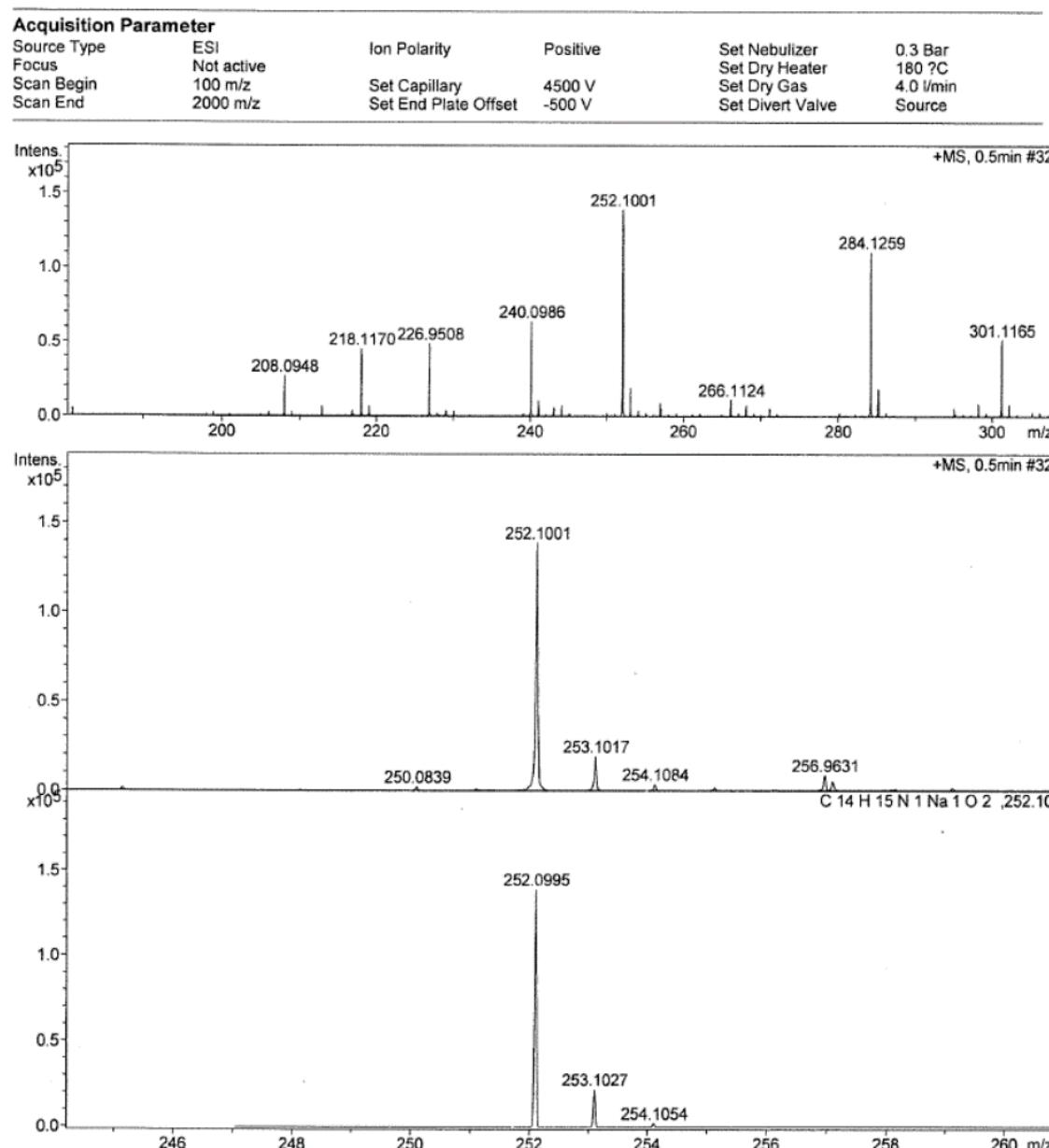


Figure S3. ESI-MS spectrum of the benzoxazine (I).

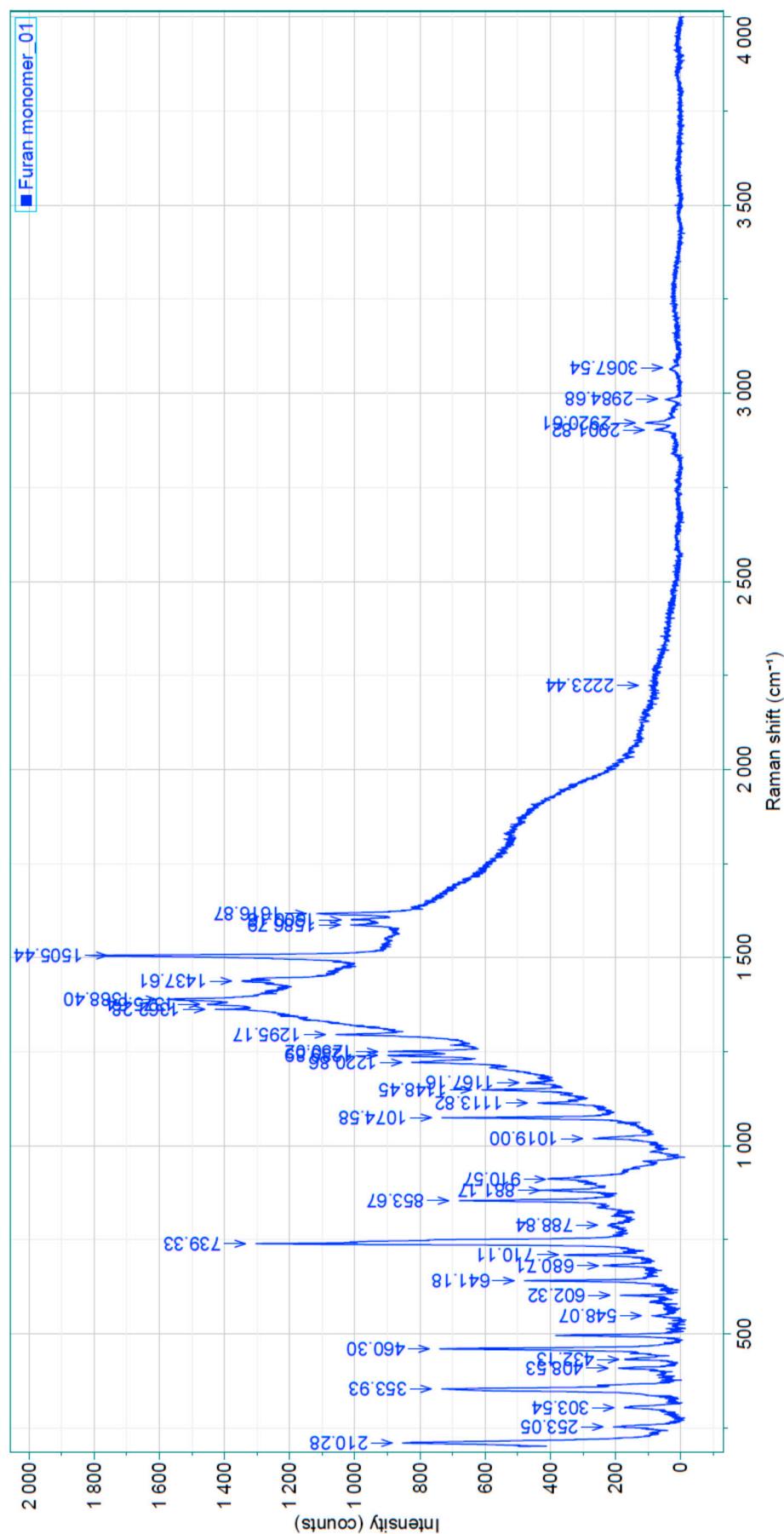


Figure S4. Raman spectrum of the benzoxazine (I).

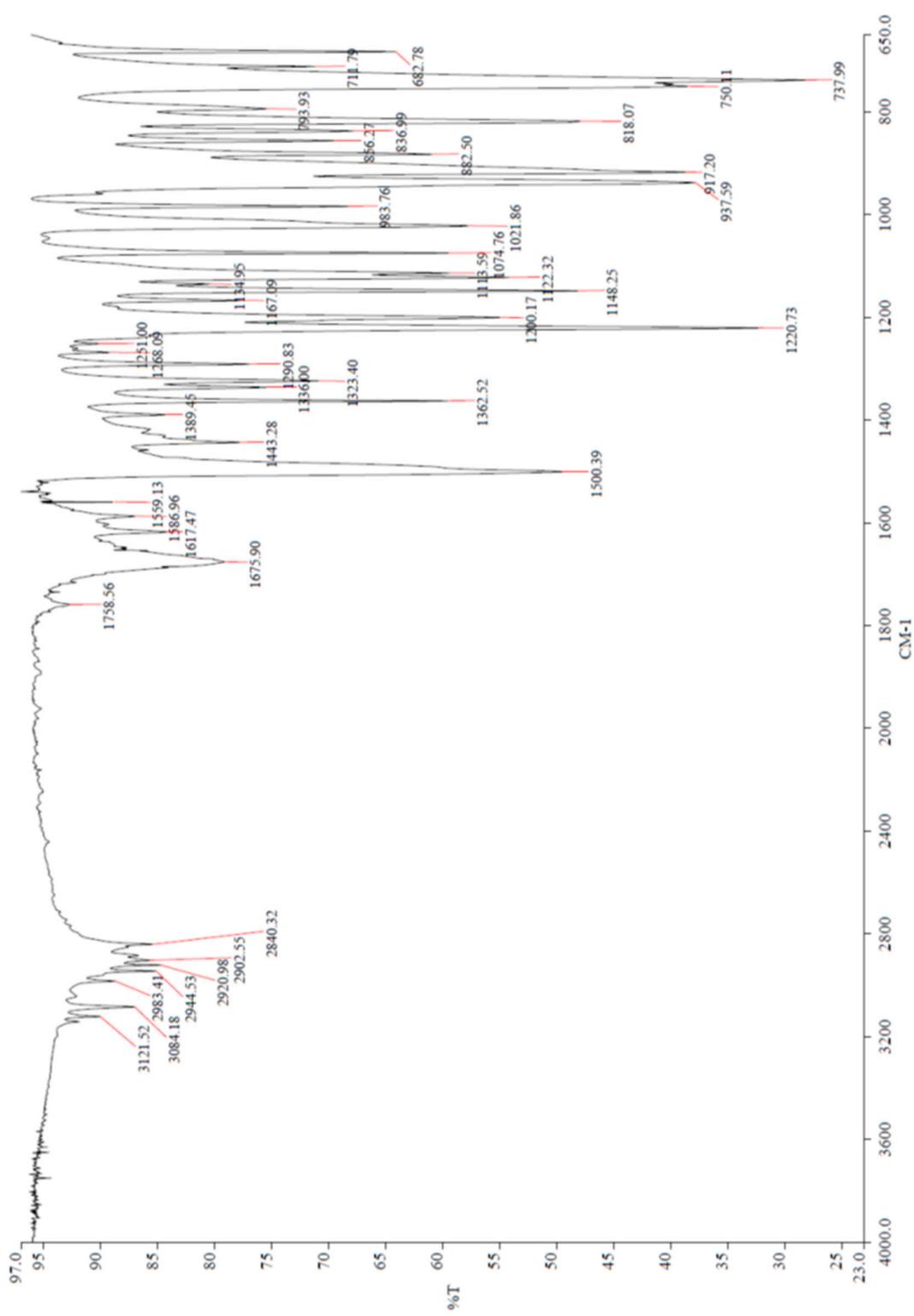


Figure S5. FT-IR spectrum of the benzoxazine (I).

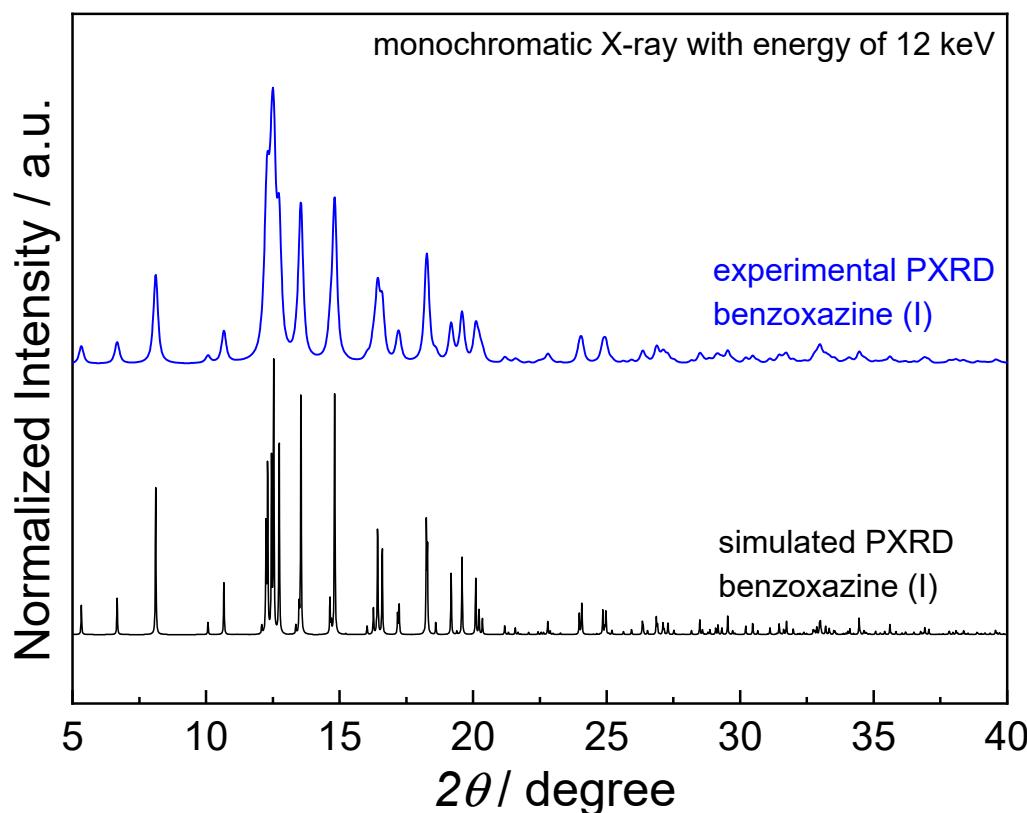


Figure S6. Comparing powder X-ray diffraction pattern (PXRD) of the benzoxazine (I), 3-[(furan-2-yl)methyl]-6-methyl-3,4-dihydro-2*H*-1,3-benzoxazine, measured by using a monochromatic synchrotron X-ray with an energy of 12 keV (wavelength 1.0332 Å) plotted in blue color with respect to the simulated PXRD from cif file collected from single crystal X-ray crystallography (black plot). The result indicates the well-matching between the experimental and the simulated PXRD data, highlighting the high purity of the obtained compound and the well-defined solving of the single crystal structure.

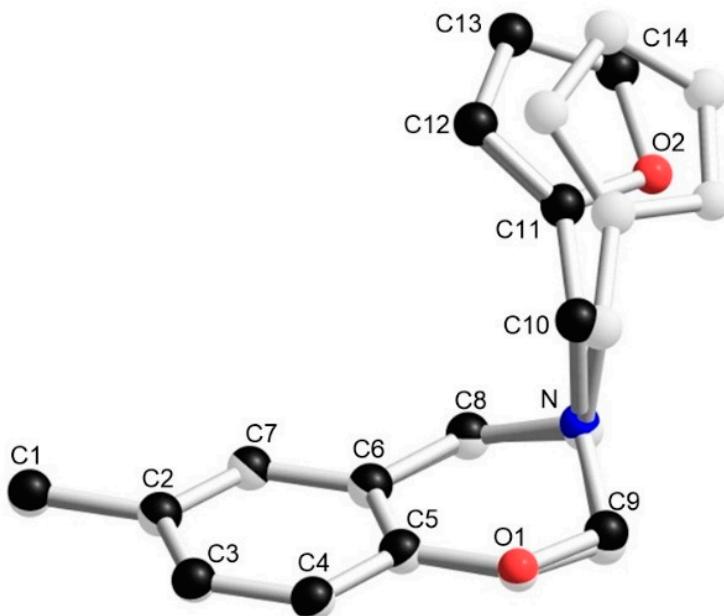


Figure S7. Superimposition of the X-ray (with atom labels) and gas-phase optimized (white color) structures of the benzoxazine (I).

2. Computational Study

Table S1. Selected bond lengths, bond angles, and dihedral angles of the optimized ground state structures of the benzoxazine (I) in gas phase compared with that in solid crystals.

Parameter	Single Crystal	Gas Phase
Bond Length (Å)		
C1–C2	1.508	1.510
C2–C3	1.399	1.403
C3–C4	1.385	1.388
C4–C5	1.393	1.398
C5–C6	1.397	1.400
C6–C7	1.395	1.398
C2–C7	1.388	1.394
C6–C8	1.513	1.518
C8–N1	1.470	1.470
C9–N1	1.437	1.428
C9–O1	1.453	1.452
C5–O1	1.381	1.372
C10–N1	1.475	1.474
C10–C11	1.490	1.490
C11–C12	1.339	1.363
C12–C13	1.426	1.434
C13–C14	1.343	1.358
C14–O2	1.376	1.362
C11–O2	1.376	1.369
Bond Angle (°)		
C1–C2–C3	119.9	120.8
C1–C2–C7	122.3	121.6
C2–C3–C4	121.5	121.3
C3–C4–C5	119.5	120.0
C4–C5–C6	120.5	120.2
C5–C6–C7	118.5	118.5
C6–C7–C2	122.2	122.4
C7–C2–C3	117.7	117.6
C7–C6–C8	122.7	122.2
C4–C5–O1	117.0	117.5
C5–O1–C9	115.0	114.5
O1–C9–N1	114.6	114.2
C6–C8–N1	111.6	112.0
C8–N1–C9	108.6	109.6
C8–N1–C10	112.9	114.2
C9–N1–C10	112.1	113.6
N1–C10–C11	111.8	113.0
C10–C11–C12	132.9	132.9
C10–C11–O2	116.7	117.6
O2–C11–C12	110.5	109.5
C11–C12–C13	106.8	106.8
C12–C13–C14	106.4	105.9
C13–C14–O2	110.5	110.5
C14–O2–C11	105.8	107.3
Dihedral angle (°)		

C1–C2–C3–C4		-177.1	179.9
C1–C2–C7–C6		178.0	-179.9
C7–C2–C3–C4		1.1	-0.4
C4–C5–C6–C7		1.5	-0.7
C3–C4–C5–O1		177.7	179.2
C7–C6–C5–O1		-176.7	-179.1
C7–C6–C8–N1		155.5	162.2
C4–C5–O1–C9		171.6	168.1
C5–O1–C9–N1		41.0	43.4
C6–C8–N1–C9		51.2	46.5
C6–C8–N1–C10		-73.7	-82.3
O1–C9–N1–C10		63.4	66.7
C9–N1–C10–C11		174.0	163.2
C8–N1–C10–C11		-63.0	-70.0
N1–C10–C11–C12		114.8	116.4
N1–C10–C11–O2		-63.4	-65.1

Table S2. Selected bond lengths and dihedral angles of the optimized ground state (GS) and excited state (ES) structures of the benzoxazine (I) in different solvents (dioxane, chloroform, EtOAc, THF and DCM).

Solvent	Dioxane		Chloroform		EtOAc		THF		DCM	
Bond Length (Å)	GS	ES	GS	ES	GS	ES	GS	ES	GS	ES
C1–C2	1.510	1.495	1.510	1.494	1.510	1.494	1.510	1.494	1.510	1.494
C2–C3	1.403	1.413	1.403	1.413	1.403	1.413	1.403	1.414	1.403	1.414
C3–C4	1.388	1.411	1.389	1.411	1.389	1.411	1.389	1.411	1.389	1.411
C4–C5	1.398	1.425	1.398	1.428	1.398	1.428	1.398	1.429	1.398	1.429
C5–C6	1.400	1.420	1.400	1.420	1.400	1.420	1.400	1.420	1.400	1.420
C6–C7	1.399	1.427	1.399	1.427	1.399	1.427	1.399	1.427	1.399	1.427
C2–C7	1.395	1.428	1.395	1.429	1.395	1.429	1.395	1.429	1.395	1.430
C6–C8	1.518	1.497	1.518	1.497	1.518	1.497	1.518	1.497	1.518	1.497
C8–N	1.470	1.468	1.471	1.469	1.471	1.469	1.471	1.469	1.471	1.469
C9–N	1.428	1.413	1.428	1.412	1.428	1.411	1.428	1.411	1.428	1.411
C9–O1	1.455	1.481	1.457	1.486	1.457	1.487	1.457	1.487	1.457	1.488
C5–O1	1.373	1.344	1.373	1.342	1.373	1.341	1.373	1.341	1.373	1.341
C10–N1	1.475	1.475	1.476	1.475	1.476	1.476	1.476	1.476	1.476	1.476
C10–C11	1.490	1.489	1.490	1.489	1.490	1.489	1.490	1.489	1.490	1.489
C11–C12	1.362	1.363	1.362	1.363	1.362	1.363	1.362	1.363	1.362	1.363
C12–C13	1.435	1.434	1.435	1.434	1.435	1.434	1.436	1.434	1.436	1.434
C13–C14	1.358	1.359	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.358
C14–O2	1.363	1.363	1.364	1.364	1.364	1.364	1.365	1.365	1.365	1.365
C11–O2	1.371	1.370	1.371	1.371	1.371	1.371	1.372	1.371	1.372	1.371
Dihedral Angle (°)										
C1–C2–C3–C4	180.0	-177.3	180.0	-177.4	180.0	-177.5	180.0	-177.5	180.0	-177.5
C1–C2–C7–C6	180.0	170.6	180.0	170.2	180.0	170.1	180.0	170.0	180.0	169.9
C7–C2–C3–C4	-0.4	1.4	-0.4	1.4	-0.4	1.4	-0.4	1.4	-0.4	1.4
C4–C5–C6–C7	-0.8	-8.1	-0.7	-8.1	-0.7	-8.2	-0.7	-8.2	-0.7	-8.2
C3–C4–C5–O1	179.2	-178.5	179.2	-179.1	179.2	-179.2	179.2	-179.3	179.2	-179.4
C7–C6–C5–O1	-179.1	171.9	-179.1	172.0	-179.1	172.0	-179.1	172.0	-179.1	171.9

Table S3. Selected bond lengths and dihedral angles of the optimized ground state (GS) and excited state (ES) structures of the benzoxazine (I) in different solvents (EtOH, MeOH, ACN, DMF and water).

Solvent	EtOH		MeOH		ACN		DMF		Water	
Bond Length (Å)	GS	ES								
C1–C2	1.510	1.494	1.510	1.494	1.510	1.494	1.510	1.494	1.510	1.494
C2–C3	1.403	1.414	1.403	1.414	1.403	1.414	1.403	1.414	1.403	1.414
C3–C4	1.389	1.411	1.389	1.411	1.389	1.411	1.389	1.411	1.389	1.411
C4–C5	1.398	1.430	1.398	1.430	1.398	1.430	1.398	1.430	1.398	1.430
C5–C6	1.400	1.420	1.400	1.420	1.400	1.420	1.400	1.420	1.400	1.420
C6–C7	1.399	1.427	1.399	1.427	1.399	1.427	1.399	1.427	1.399	1.427
C2–C7	1.396	1.430	1.396	1.430	1.396	1.430	1.396	1.430	1.396	1.430
C6–C8	1.518	1.497	1.518	1.497	1.518	1.497	1.518	1.497	1.518	1.497
C8–N1	1.472	1.469	1.472	1.469	1.472	1.469	1.472	1.469	1.472	1.469
C9–N1	1.428	1.411	1.428	1.411	1.428	1.411	1.428	1.411	1.428	1.411
C9–O1	1.458	1.490	1.458	1.490	1.458	1.490	1.458	1.490	1.458	1.491
C5–O1	1.374	1.340	1.374	1.339	1.374	1.339	1.374	1.339	1.374	1.339
C10–N1	1.477	1.476	1.477	1.476	1.477	1.476	1.477	1.476	1.477	1.476
C10–C11	1.490	1.489	1.490	1.489	1.490	1.489	1.490	1.489	1.490	1.489
C11–C12	1.362	1.362	1.362	1.362	1.362	1.362	1.362	1.362	1.362	1.362
C12–C13	1.436	1.435	1.436	1.435	1.436	1.435	1.436	1.435	1.436	1.435
C13–C14	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.358
C14–O2	1.365	1.365	1.365	1.365	1.365	1.365	1.365	1.365	1.365	1.365
C11–O2	1.372	1.372	1.372	1.372	1.372	1.372	1.372	1.372	1.372	1.372
Dihedral Angle (°)										
C1–C2–C3–C4	180.0	-177.6	180.0	-177.6	180.0	-177.6	180.0	-177.6	180.0	-177.7
C1–C2–C7–C6	180.0	169.7	180.0	169.6	180.0	169.6	180.0	169.6	180.0	169.5
C7–C2–C3–C4	-0.4	1.3	-0.4	1.3	-0.4	1.3	-0.4	1.3	-0.4	1.3
C4–C5–C6–C7	-0.7	-8.2	-0.7	-8.2	-0.7	-8.2	-0.7	-8.2	-0.7	-8.2
C3–C4–C5–O1	179.2	-179.8	179.2	-179.9	179.2	-179.9	179.2	-179.9	179.1	180.0
C7–C6–C5–O1	-179.1	172.0	-179.1	172.0	-179.1	172.0	-179.1	171.9	-179.1	172.0

3. Cartesian Coordinates

Cartesian coordinates of the optimized structures of the benzoxazine (I) at ground state (PCM/B3LYP/6-311+G(d)) and excited state (PCM/TD-B3LYP/6-311+G(d))

Dioxane

Ground state			Excited state				
C	-2.135985	0.510807	0.460442	C	-2.175545	0.473106	0.471549
C	-0.756986	0.387226	0.268337	C	-0.770006	0.412144	0.243251
C	0.018792	1.519322	-0.010727	C	0.015161	1.554644	-0.066825
C	-0.620345	2.759943	-0.106593	C	-0.662978	2.783063	-0.325442
C	-1.996173	2.907881	0.068451	C	-2.056674	2.878138	-0.031271
C	-2.742127	1.755672	0.358740	C	-2.795831	1.734639	0.346284
H	-2.715329	-0.378758	0.684435	H	-2.727385	-0.442218	0.641770
H	-0.014633	3.638362	-0.320065	H	-0.097854	3.676641	-0.567750
H	-3.815855	1.834136	0.506384	H	-3.864730	1.828736	0.505842
C	-2.666690	4.256673	-0.040730	C	-2.718506	4.216384	-0.101033
H	-3.426868	4.264902	-0.828486	H	-3.802053	4.149990	0.010374
H	-3.169914	4.533054	0.891449	H	-2.336903	4.885035	0.683267
H	-1.945901	5.044235	-0.271565	H	-2.491072	4.711293	-1.054440
C	1.517565	1.365825	-0.199435	C	1.507534	1.450275	-0.113895
O	-0.207376	-0.863918	0.397068	O	-0.210596	-0.806748	0.339181
C	1.162903	-0.972902	-0.079630	C	1.201118	-0.896874	-0.099116
H	1.510299	-1.932027	0.300375	H	1.526199	-1.865701	0.272931
H	1.133368	-0.995333	-1.173246	H	1.178835	-0.889129	-1.191081
N	2.013346	0.092824	0.344517	N	1.997190	0.161737	0.391820
H	1.776107	1.405408	-1.264031	H	1.870396	1.577682	-1.151973
H	2.056297	2.186809	0.278392	H	1.985375	2.257782	0.455856
C	2.259768	0.110463	1.798707	C	2.259284	0.126514	1.842612
H	1.392813	0.471136	2.369609	H	1.405399	0.497847	2.425625
H	2.431587	-0.925502	2.106975	H	2.405058	-0.921877	2.120585
C	3.434678	0.943998	2.178717	C	3.458572	0.920891	2.227352
C	3.568146	2.071795	2.931190	C	3.635479	2.003450	3.036183
C	4.967659	2.387298	2.960910	C	5.040872	2.287307	3.044728
H	2.765211	2.613372	3.409569	H	2.856837	2.536887	3.561310
C	5.582341	1.427373	2.222719	C	5.615768	1.356682	2.239053
H	5.444975	3.215812	3.462433	H	5.548646	3.078274	3.575890
H	6.608296	1.236219	1.952822	H	6.629842	1.160822	1.930572
O	4.667918	0.539039	1.740273	O	4.670455	0.513728	1.734796

Chloroform

Ground state			Excited state		
C	-2.137609	0.509916	0.458826	C	-2.176751
C	-0.758066	0.387616	0.268491	C	-0.767969
C	0.017172	1.520201	-0.010085	C	0.016771
C	-0.622973	2.760439	-0.107259	C	-0.661955
C	-1.999503	2.907364	0.066267	C	-2.055539
C	-2.745103	1.754527	0.356064	C	-2.795622
H	-2.717659	-0.379419	0.682460	H	-2.728838
H	-0.017587	3.639011	-0.320263	H	-0.095731
H	-3.819003	1.831911	0.502467	H	-3.864154
C	-2.670835	4.255800	-0.043783	C	-2.715594
H	-3.432431	4.262066	-0.830086	H	-3.797283
H	-3.173185	4.532496	0.888701	H	-2.319351
H	-1.950658	5.043211	-0.276567	H	-2.500638
C	1.516152	1.368722	-0.198272	C	1.509437
O	-0.206751	-0.863261	0.398434	O	-0.209973
C	1.165137	-0.971518	-0.079093	C	1.210092
H	1.512897	-1.930131	0.301307	H	1.530696
H	1.134418	-0.993595	-1.172350	H	1.192628
N	2.013829	0.095651	0.345543	N	1.999955
H	1.773937	1.409256	-1.262782	H	1.871344
H	2.052764	2.190604	0.280087	H	1.985918
C	2.259508	0.113674	1.800605	C	2.257841
H	1.393727	0.478183	2.370303	H	1.402252
H	2.427702	-0.922435	2.110078	H	2.404878
C	3.436562	0.944531	2.180189	C	3.454356
C	3.574248	2.070020	2.935010	C	3.627537
C	4.974906	2.382363	2.963177	C	5.032479
H	2.773447	2.612858	3.415480	H	2.846853
C	5.587033	1.423444	2.221588	C	5.611696
H	5.454585	3.208818	3.465907	H	5.537111
H	6.612205	1.231138	1.949421	H	6.626757
O	4.669023	0.537685	1.738135	O	4.668685

EtOAc

Ground state			Excited state		
C	-2.137861	0.509640	0.458477	C	-2.178242
C	-0.758219	0.387707	0.268413	C	-0.768741
C	0.016858	1.520387	-0.010139	C	0.017229
C	-0.623545	2.760534	-0.107520	C	-0.660278
C	-2.000220	2.907180	0.065802	C	-2.053850
C	-2.745699	1.754187	0.355543	C	-2.795469
H	-2.718039	-0.379650	0.682086	H	-2.731393
H	-0.018275	3.639161	-0.320431	H	-0.092830
H	-3.819624	1.831305	0.501768	H	-3.863858
C	-2.671771	4.255529	-0.044320	C	-2.712115
H	-3.434022	4.261257	-0.829969	H	-3.793563
H	-3.173543	4.532394	0.888409	H	-2.312856
H	-1.951816	5.042868	-0.277921	H	-2.498383
C	1.515870	1.369357	-0.198325	C	1.509846
O	-0.206462	-0.863123	0.398658	O	-0.212420
C	1.165698	-0.971237	-0.079006	C	1.209179
H	1.513601	-1.929672	0.301598	H	1.527714
H	1.134824	-0.993338	-1.172185	H	1.192402
N	2.014050	0.096349	0.345643	N	1.999126
H	1.773369	1.409881	-1.262849	H	1.871863
H	2.052021	2.191538	0.279964	H	1.986776
C	2.259214	0.114752	1.800969	C	2.256739
H	1.393645	0.480500	2.370062	H	1.401198
H	2.426265	-0.921345	2.111050	H	2.403802
C	3.436847	0.944856	2.180495	C	3.453114
C	3.575642	2.069679	2.936002	C	3.626332
C	4.976612	2.381074	2.963922	C	5.031260
H	2.775387	2.612910	3.416918	H	2.845706
C	5.588047	1.422414	2.221462	C	5.610630
H	5.456932	3.206930	3.467039	H	5.535781
H	6.613007	1.229719	1.948755	H	6.625646
O	4.669094	0.537401	1.737634	O	4.667545

THF

Ground state			Excited state		
C	-2.138103	0.509381	0.458102	C	-2.178549
C	-0.758357	0.387797	0.268343	C	-0.768678
C	0.016549	1.520616	-0.010101	C	0.016577
C	-0.624119	2.760654	-0.107657	C	-0.661775
C	-2.000928	2.907006	0.065418	C	-2.054899
C	-2.746271	1.753843	0.355034	C	-2.795937
H	-2.718331	-0.379926	0.681618	H	-2.731226
H	-0.018979	3.639367	-0.320431	H	-0.094698
H	-3.820230	1.830694	0.501052	H	-3.863994
C	-2.672700	4.255259	-0.044746	C	-2.713143
H	-3.435485	4.260551	-0.829861	H	-3.794047
H	-3.174005	4.532248	0.888186	H	-2.310413
H	-1.952952	5.042566	-0.279001	H	-2.502940
C	1.515610	1.370042	-0.198173	C	1.509205
O	-0.206209	-0.862953	0.398801	O	-0.212160
C	1.166203	-0.970850	-0.078972	C	1.210650
H	1.514226	-1.929183	0.301692	H	1.528965
H	1.135183	-0.992876	-1.172093	H	1.193822
N	2.014197	0.097041	0.345799	N	1.999583
H	1.772991	1.410734	-1.262679	H	1.869801
H	2.051310	2.192420	0.280224	H	1.986365
C	2.259043	0.115574	1.801324	C	2.257758
H	1.393670	0.482217	2.370034	H	1.402332
H	2.425223	-0.920551	2.111737	H	2.405602
C	3.437177	0.944995	2.180837	C	3.453773
C	3.576878	2.069648	2.936364	C	3.626755
C	4.978134	2.380071	2.964224	C	5.031547
H	2.777049	2.613537	3.417227	H	2.846080
C	5.589008	1.421128	2.221675	C	5.611227
H	5.458994	3.205614	3.467346	H	5.535770
H	6.613838	1.227811	1.948902	H	6.626212
O	4.669273	0.536668	1.737779	O	4.668327

DCM

Ground state			Excited state		
C	-2.138273	0.509168	0.457798	C	-2.179020
C	-0.758448	0.387865	0.268274	C	-0.768757
C	0.016316	1.520803	-0.010076	C	0.016746
C	-0.624564	2.760750	-0.107747	C	-0.661458
C	-2.001475	2.906861	0.065142	C	-2.054380
C	-2.746703	1.753560	0.354645	C	-2.795808
H	-2.718524	-0.380166	0.681229	H	-2.731933
H	-0.019533	3.639540	-0.320401	H	-0.093994
H	-3.820689	1.830196	0.500502	H	-3.863698
C	-2.673423	4.255038	-0.045026	C	-2.711835
H	-3.436668	4.259991	-0.829682	H	-3.792552
H	-3.174306	4.532137	0.888092	H	-2.307324
H	-1.953848	5.042319	-0.279840	H	-2.502698
C	1.515415	1.370586	-0.198062	C	1.509390
O	-0.205993	-0.862818	0.398888	O	-0.212720
C	1.166603	-0.970532	-0.078965	C	1.211084
H	1.514725	-1.928791	0.301733	H	1.528574
H	1.135479	-0.992490	-1.172045	H	1.194958
N	2.014319	0.097589	0.345910	N	1.999507
H	1.772711	1.411406	-1.262555	H	1.869936
H	2.050774	2.193114	0.280418	H	1.986558
C	2.258897	0.116219	1.801593	C	2.257255
H	1.393659	0.483546	2.369990	H	1.401720
H	2.424401	-0.919929	2.112259	H	2.405114
C	3.437419	0.945099	2.181112	C	3.453073
C	3.577813	2.069705	2.936530	C	3.625833
C	4.979299	2.379324	2.964399	C	5.030606
H	2.778305	2.614189	3.417239	H	2.845036
C	5.589743	1.420044	2.221941	C	5.610602
H	5.460574	3.204667	3.467456	H	5.534605
H	6.614482	1.226160	1.949214	H	6.625649
O	4.669405	0.535996	1.738037	O	4.667824

DMF

Ground state			Excited state		
C	-2.139013	0.508047	0.456120	C	-2.183004
C	-0.758805	0.388175	0.267722	C	-0.771064
C	0.015215	1.521779	-0.009998	C	0.017792
C	-0.626759	2.761252	-0.108035	C	-0.657413
C	-2.004137	2.906099	0.063958	C	-2.049740
C	-2.748743	1.752049	0.352729	C	-2.795139
H	-2.719218	-0.381552	0.678991	H	-2.738456
H	-0.022320	3.640509	-0.319957	H	-0.086956
H	-3.822866	1.827604	0.497807	H	-3.862187
C	-2.676978	4.253894	-0.045934	C	-2.701844
H	-3.442883	4.257236	-0.827940	H	-3.781805
H	-3.175247	4.531646	0.888359	H	-2.288638
H	-1.958365	5.041034	-0.283876	H	-2.496290
C	1.514534	1.373354	-0.197380	C	1.510209
O	-0.204891	-0.862128	0.398883	O	-0.219475
C	1.168564	-0.968783	-0.079073	C	1.208732
H	1.517172	-1.926736	0.301696	H	1.520545
H	1.137198	-0.990374	-1.171990	H	1.195694
N	2.014852	0.100375	0.346506	N	1.996932
H	1.771685	1.414960	-1.261756	H	1.870496
H	2.048161	2.196528	0.281735	H	1.989290
C	2.258171	0.119254	1.802878	C	2.251835
H	1.393578	0.489728	2.369879	H	1.396550
H	2.420496	-0.917050	2.114579	H	2.396424
C	3.438584	0.945410	2.182532	C	3.449049
C	3.582142	2.070714	2.936130	C	3.623547
C	4.984752	2.376049	2.964553	C	5.029234
H	2.784021	2.618826	3.414941	H	2.843362
C	5.593224	1.413982	2.224082	C	5.608451
H	5.467996	3.200865	3.466601	H	5.534316
H	6.617658	1.216711	1.952578	H	6.623529
O	4.670115	0.531690	1.740685	O	4.663917

ACN

Ground state			Excited state		
C	-2.139009	0.508071	0.456177	C	-2.181388
C	-0.758807	0.388171	0.267753	C	-0.769356
C	0.015225	1.521761	-0.009992	C	0.017770
C	-0.626730	2.761241	-0.108037	C	-0.659297
C	-2.004099	2.906113	0.063974	C	-2.051775
C	-2.748716	1.752080	0.352778	C	-2.795437
H	-2.719214	-0.381518	0.679075	H	-2.735446
H	-0.022280	3.640486	-0.319982	H	-0.090206
H	-3.822835	1.827657	0.497878	H	-3.862637
C	-2.676930	4.253909	-0.045963	C	-2.705920
H	-3.442609	4.257326	-0.828192	H	-3.785792
H	-3.175467	4.531558	0.888217	H	-2.293707
H	-1.958265	5.041087	-0.283624	H	-2.501167
C	1.514541	1.373306	-0.197379	C	1.510351
O	-0.204918	-0.862138	0.398916	O	-0.215914
C	1.168524	-0.968814	-0.079048	C	1.212513
H	1.517123	-1.926771	0.301722	H	1.525768
H	1.137151	-0.990414	-1.171967	H	1.199674
N	2.014834	0.100328	0.346511	N	1.998999
H	1.771699	1.414901	-1.261756	H	1.870511
H	2.048194	2.196471	0.281727	H	1.988186
C	2.258191	0.119206	1.802868	C	2.253701
H	1.393595	0.489631	2.369902	H	1.397779
H	2.420570	-0.917095	2.114554	H	2.399743
C	3.438578	0.945407	2.182507	C	3.449721
C	3.582093	2.070695	2.936139	C	3.622526
C	4.984685	2.376101	2.964536	C	5.027818
H	2.783954	2.618744	3.414995	H	2.841477
C	5.593181	1.414085	2.224018	C	5.608512
H	5.467905	3.200923	3.466599	H	5.531678
H	6.617616	1.216873	1.952479	H	6.623937
O	4.670111	0.531767	1.740619	O	4.665270

EtOH

Ground state			Excited state		
C	-2.138862	0.508288	0.456538	C	-2.181276
C	-0.758735	0.388119	0.267898	C	-0.769533
C	0.015443	1.521574	-0.010015	C	0.017493
C	-0.626306	2.761141	-0.108009	C	-0.659566
C	-2.003597	2.906257	0.064188	C	-2.052225
C	-2.748333	1.752377	0.353161	C	-2.795717
H	-2.719089	-0.381240	0.679569	H	-2.735312
H	-0.021746	3.640291	-0.320118	H	-0.090600
H	-3.822425	1.828154	0.498414	H	-3.863096
C	-2.676251	4.254129	-0.045829	C	-2.706971
H	-3.441375	4.257854	-0.828611	H	-3.786981
H	-3.175352	4.531633	0.888096	H	-2.296038
H	-1.957387	5.041335	-0.282843	H	-2.501541
C	1.514698	1.372762	-0.197601	C	1.510082
O	-0.205093	-0.862263	0.399019	O	-0.215809
C	1.168160	-0.969184	-0.079016	C	1.211735
H	1.516685	-1.927192	0.301739	H	1.525620
H	1.136765	-0.990871	-1.171960	H	1.198222
N	2.014773	0.099784	0.346341	N	1.998761
H	1.771781	1.414139	-1.262025	H	1.870556
H	2.048715	2.195839	0.281280	H	1.987726
C	2.258313	0.118689	1.802607	C	2.254304
H	1.393577	0.488565	2.369835	H	1.398668
H	2.421266	-0.917568	2.114163	H	2.400487
C	3.438332	0.945417	2.182219	C	3.450534
C	3.581298	2.070417	2.936409	C	3.623807
C	4.983690	2.376643	2.964661	C	5.029039
H	2.782939	2.617701	3.415786	H	2.843092
C	5.592529	1.415313	2.223542	C	5.609160
H	5.466541	3.201486	3.467042	H	5.533240
H	6.616998	1.218797	1.951631	H	6.624351
O	4.669937	0.532760	1.739892	O	4.665678

MeOH

Ground state				Excited state		
C	-2.138937	0.508137	0.456325	C	-2.181345	0.464052
C	-0.758765	0.388155	0.267812	C	-0.769376	0.402943
C	0.015314	1.521693	-0.010031	C	0.017736	1.547380
C	-0.626573	2.761200	-0.108058	C	-0.659323	2.776581
C	-2.003920	2.906151	0.064044	C	-2.051820	2.876085
C	-2.748572	1.752176	0.352927	C	-2.795449	1.731048
H	-2.719150	-0.381427	0.679289	H	-2.735399	-0.451418
H	-0.022092	3.640411	-0.320074	H	-0.090257	3.674245
H	-3.822681	1.827815	0.498092	H	-3.862675	1.829803
C	-2.676688	4.253976	-0.045914	C	-2.706044	4.218642
H	-3.442241	4.257473	-0.828270	H	-3.785944	4.160492
H	-3.175343	4.531608	0.888208	H	-2.294062	4.882132
H	-1.957967	5.041148	-0.283440	H	-2.501140	4.715508
C	1.514594	1.373101	-0.197557	C	1.510315	1.439156
O	-0.204937	-0.862180	0.399002	O	-0.215886	-0.812986
C	1.168410	-0.968969	-0.079033	C	1.212375	-0.909657
H	1.517005	-1.926931	0.301746	H	1.525745	-1.874287
H	1.137005	-0.990624	-1.171958	H	1.199405	-0.915994
N	2.014852	0.100138	0.346401	N	1.998972	0.154003
H	1.771649	1.414544	-1.261970	H	1.870488	1.556267
H	2.048404	2.196270	0.281376	H	1.988156	2.251357
C	2.258189	0.119114	1.802759	C	2.253800	0.128986
H	1.393525	0.489427	2.369770	H	1.397907	0.503943
H	2.420706	-0.917156	2.114489	H	2.399893	-0.916835
C	3.438456	0.945483	2.182391	C	3.449831	0.929332
C	3.581831	2.070559	2.936365	C	3.622665	2.016099
C	4.984368	2.376221	2.964704	C	5.027943	2.305273
H	2.783651	2.618311	3.415495	H	2.841644	2.549249
C	5.592948	1.414537	2.223834	C	5.608583	1.373939
H	5.467477	3.200985	3.466968	H	5.531829	3.100605
H	6.617373	1.217575	1.952079	H	6.623986	1.180883
O	4.669997	0.532223	1.740231	O	4.665336	0.524320
						1.738201

H₂O

Ground state			Excited state		
C	-2.139077	0.507828	0.455888	C	-2.181547
C	-0.758818	0.388226	0.267623	C	-0.769151
C	0.015061	1.521932	-0.010073	C	0.017942
C	-0.627109	2.761316	-0.108150	C	-0.659326
C	-2.004564	2.905934	0.063765	C	-2.051632
C	-2.749044	1.751764	0.352460	C	-2.795364
H	-2.719253	-0.381815	0.678714	H	-2.735521
H	-0.022789	3.640657	-0.319974	H	-0.090189
H	-3.823186	1.827126	0.497452	H	-3.862386
C	-2.677563	4.253664	-0.046055	C	-2.705402
H	-3.443992	4.256708	-0.827539	H	-3.785073
H	-3.175298	4.531554	0.888475	H	-2.291718
H	-1.959135	5.040770	-0.284622	H	-2.501737
C	1.514392	1.373782	-0.197474	C	1.510539
O	-0.204616	-0.862015	0.398946	O	-0.215848
C	1.168913	-0.968532	-0.079070	C	1.213596
H	1.517652	-1.926401	0.301756	H	1.526272
H	1.137506	-0.990127	-1.171961	H	1.201584
N	2.015011	0.100852	0.346518	N	1.999284
H	1.771396	1.415351	-1.261868	H	1.870544
H	2.047788	2.197135	0.281561	H	1.988293
C	2.257930	0.119976	1.803061	C	2.253222
H	1.393405	0.491173	2.369627	H	1.397093
H	2.419564	-0.916318	2.115146	H	2.399049
C	3.438696	0.945618	2.182739	C	3.449105
C	3.582888	2.070880	2.936227	C	3.621621
C	4.985719	2.375389	2.964764	C	5.026977
H	2.785060	2.619606	3.414809	H	2.840351
C	5.593776	1.412944	2.224460	C	5.608084
H	5.469345	3.200010	3.466767	H	5.530601
H	6.618120	1.215053	1.953059	H	6.623669
O	4.670111	0.531105	1.740973	O	4.664961



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