Supporting Information For:

New Insights into the Dual Fluorescence of Methyl Salicylate: Effects of Intermolecular Hydrogen Bonding and Solvation

Panwang Zhou[a], Mark R. Hoffmann[b], Keli Han[a*], Guozhong He[a]

[a]State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning, China

[b]Department of Chemistry, University of North Dakota, Abbott Hall Room 236, 151 Cornell Street Stop 9024, Grand Forks, ND 58202-9024, USA

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Table S1. Computed vertical excitation (ketoB) and emission energies (from enol, in nm) of MS in different solvents with LR and SS solvation at the PBE0/aug-cc-pVTZ level.

	Abs.		Em.	
	LR	SS	LR	SS
MCH	288	289	404	397
Acetonitrile	286	284	408	394
DMF	286	285	408	393
DMSO	286	285	408	393

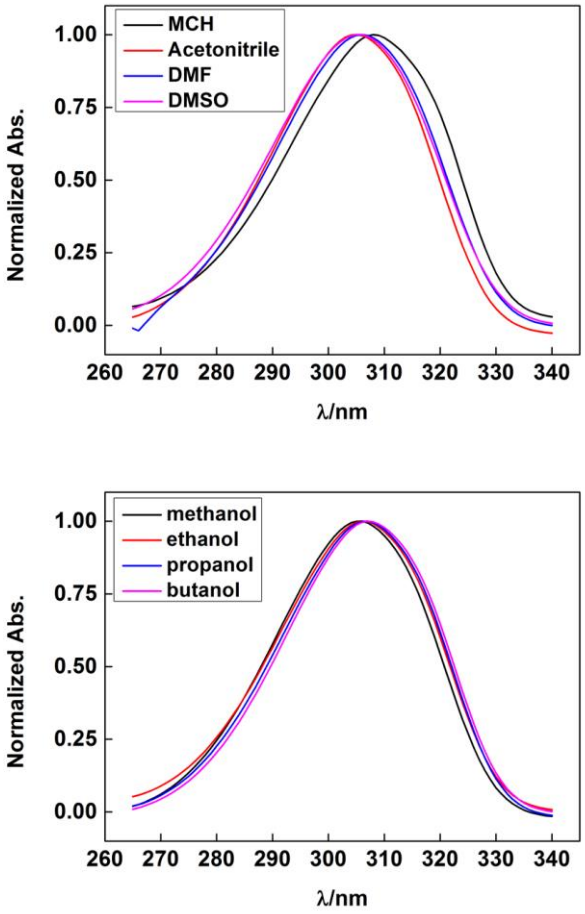

Figure S1. Measured steady-state absorption spectra of MS in different solvents.

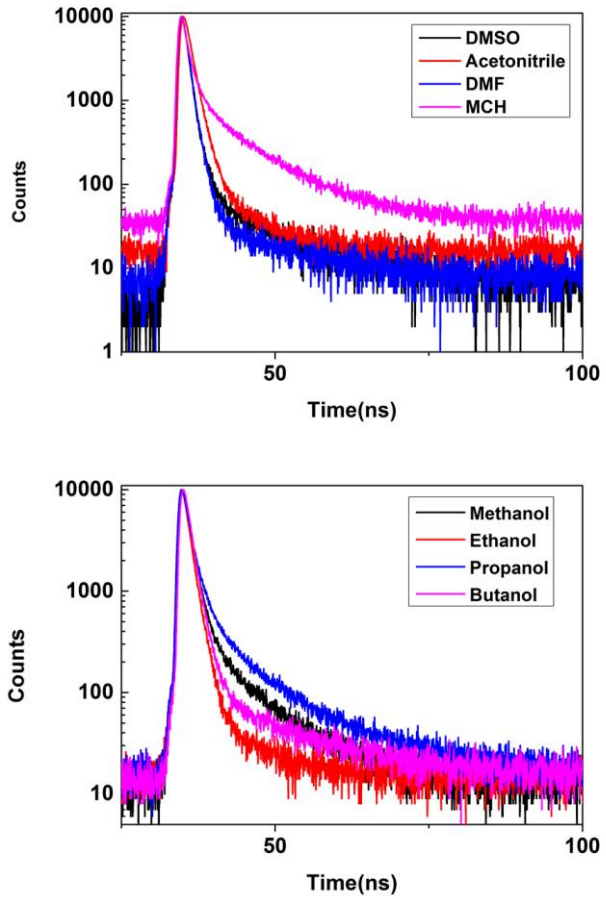

Figure S2. Measured time-resolved fluorescence decays of MS in different solvents from time-correlated single photon counting (TCSPC) data.

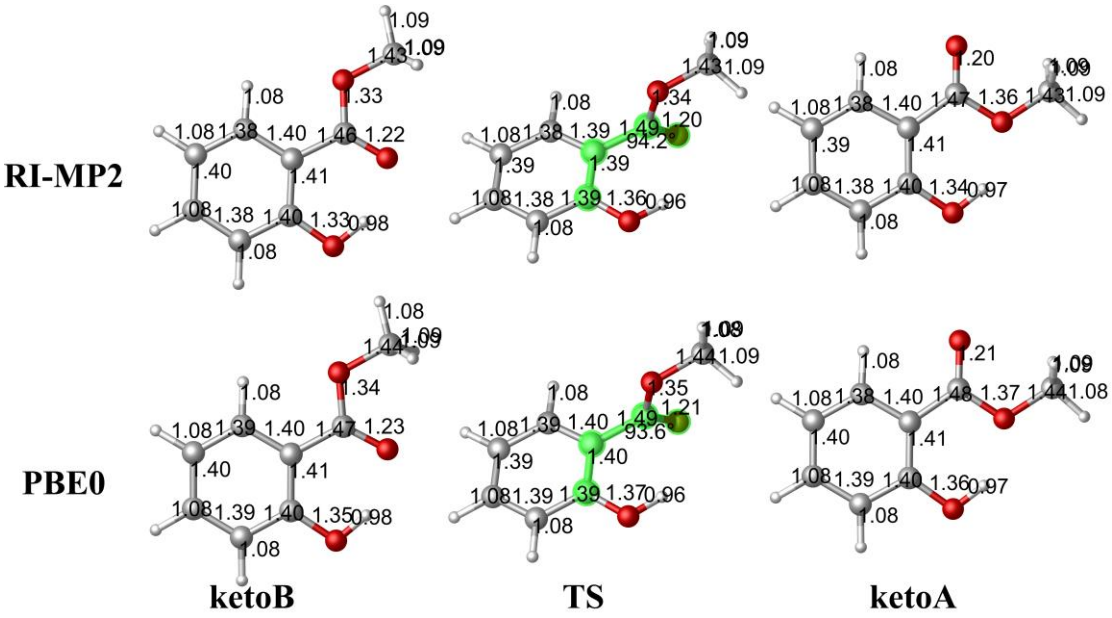

Figure S3. Optimized geometries of ketoB, TS, and ketoA by PBE0/aug-cc-pVTZ and RI-MP2/aug-cc-pVTZ, the bond lengths are given in Å and the bond angles are in degree.

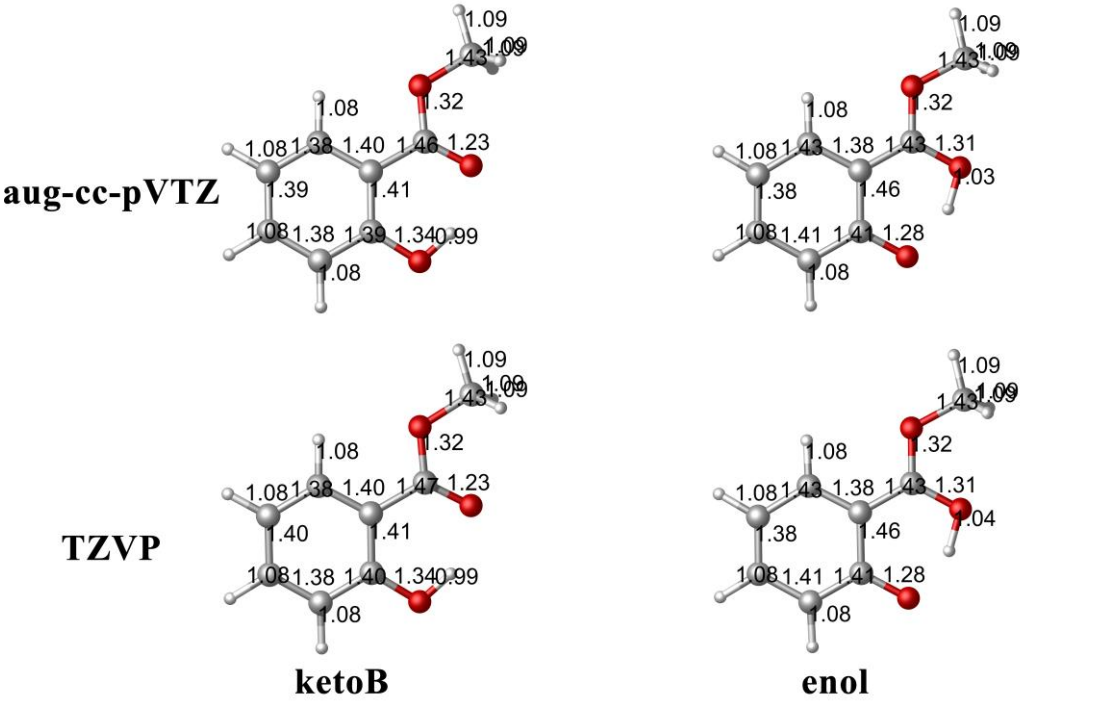

Figure S4. Optimized geometries of ketoB(S_0) and enol (S_1) by PBE0/aug-cc-pVTZ (top) and PBE0/TZVP (bottom), the bond lengths are given in Å.

S0 geometry of ketoA in gas phase, PBE0/aug-cc-pVTZ
Energy = -534.9485965715

C	2.4596942	-1.2657314	0.0012095
C	2.9945597	0.0209352	0.0015752
C	2.1709822	1.1261003	-0.0000548
C	0.7835130	0.9782417	-0.0016119
C	0.2314794	-0.3161382	-0.0020250
C	1.0919223	-1.4195457	-0.0010889
H	3.1085696	-2.1316518	0.0028761
H	4.0690744	0.1609159	0.0032137
H	2.5744533	2.1305755	0.0002784
H	0.6384995	-2.4025616	-0.0021386
O	0.0590542	2.1067933	-0.0028355
H	-0.8794134	1.8634685	-0.0029514
C	-1.2119726	-0.6155747	-0.0022530
O	-1.6964648	-1.7160899	-0.0035833
O	-1.9895629	0.4998834	-0.0000428
C	-3.3977723	0.2666277	0.0019452
H	-3.6859257	-0.2957469	0.8889508
H	-3.8618309	1.2493933	0.0036717
H	-3.6888591	-0.2940945	-0.8851354

S1 geometry of ketoA in gas phase, TD-PBE0/aug-cc-pVTZ
Energy = -534.9396244568

C	2.5025012	-1.2255299	0.0008898
C	3.0633140	0.0435245	-0.0010524
C	2.1817623	1.1354195	-0.0023059
C	0.7902709	0.9401314	-0.0016375
C	0.1902890	-0.3714148	0.0001847
C	1.0939243	-1.4289347	0.0015838
H	3.1432514	-2.0990820	0.0018742
H	4.1332823	0.1894330	-0.0016154
H	2.5366215	2.1583548	-0.0035300
H	0.6949198	-2.4349184	0.0030681
O	0.0308529	2.0188124	-0.0025984
H	-0.9160357	1.7113989	-0.0021416
C	-1.2272690	-0.6389475	0.0009328
O	-1.7525431	-1.7430052	0.0035472
O	-2.0033266	0.5277446	-0.0019824
C	-3.4072437	0.3220383	0.0007252
H	-3.7110884	-0.2324295	0.8888882
H	-3.8599373	1.3113386	-0.0018502
H	-3.7135457	-0.2381339	-0.8829802

S0 geometry of ketoB in gas phase, PBE0/aug-cc-pVTZ
Energy = -534.9551892374

C	-1.9886367	-1.7185270	0.0000893
C	-2.8906217	-0.6541691	-0.0004493
C	-2.4498446	0.6516039	-0.0002244
C	-1.0819105	0.9308246	0.0002918
C	-0.1627180	-0.1380627	0.0006387
C	-0.6374634	-1.4538054	0.0006166
H	-2.3462270	-2.7397694	-0.0000193
H	-3.9560775	-0.8525225	-0.0010940
H	-3.1424923	1.4833259	-0.0005395
H	0.0811392	-2.2623910	0.0009158
O	-0.6969770	2.2060529	0.0003461
H	0.2870890	2.2051720	0.0004375
C	1.2670744	0.1695634	0.0005224
O	1.7188299	1.3061891	0.0001888
O	2.0587561	-0.9001481	0.0005297
C	3.4590396	-0.6325864	-0.0002997
H	3.7407369	-0.0651954	0.8863203
H	3.9429326	-1.6054439	-0.0001827
H	3.7397705	-0.0659096	-0.8876881

S1 geometry of enol in gas phase, TD-PBE0/aug-cc-pVTZ
Energy = -534.9220658626

C	-2.0911399	-1.7115202	-0.0002383
C	-2.9787581	-0.6686763	0.0016170
C	-2.4825476	0.6555794	0.0017711
C	-1.1023509	0.9269451	0.0004337
C	-0.1736134	-0.1848616	-0.0011860
C	-0.6796759	-1.4635540	-0.0022247
H	-2.4386107	-2.7366159	-0.0002639
H	-4.0456698	-0.8480418	0.0030468
H	-3.1531887	1.5058382	0.0041177
H	0.0013592	-2.3057258	-0.0047871
O	-0.6399266	2.1238324	0.0011363
H	0.7698314	1.9094036	-0.0038514
C	1.2273749	0.1215425	-0.0021552
O	1.6733980	1.3455962	-0.0063454
O	2.0979181	-0.8789272	0.0021568
C	3.4784021	-0.5351420	0.0018058
H	3.7317935	0.0482415	0.8878640
H	4.0145458	-1.4802764	0.0063556
H	3.7332578	0.0405646	-0.8888528

S0 geometry of ketoB-methA in gas phase, PBE0/aug-cc-pVTZ
Energy = -650.5997514551

C	-1.7809001	-1.2960358	-1.1421002
C	-2.5723083	-0.1637050	-0.9520326
C	-2.1307740	0.8956118	-0.1867797
C	-0.8724691	0.8404811	0.4100164
C	-0.0634564	-0.2966229	0.2265282
C	-0.5371370	-1.3554510	-0.5543146
H	-2.1400960	-2.1196852	-1.7448135
H	-3.5523761	-0.1098250	-1.4109462
H	-2.7376598	1.7799874	-0.0347067
H	0.0943092	-2.2235623	-0.6874780
O	-0.4665112	1.8827611	1.1475952
H	0.4351913	1.6585673	1.4838946
C	1.2529527	-0.3285297	0.8634014
O	1.6949024	0.5818626	1.5525402
O	1.9478589	-1.4370944	0.6354235
C	3.2367628	-1.4980910	1.2434661
H	3.1513445	-1.4301169	2.3274759
H	3.6514015	-2.4591664	0.9527230
H	3.8671490	-0.6850035	0.8850076
C	-1.5504919	5.1176116	-0.0196027
O	-2.1543588	4.2436974	0.9024189
H	-2.2886251	5.8733330	-0.2895374
H	-1.2378541	4.6039192	-0.9368914
H	-0.6783312	5.6307815	0.4028338
H	-1.5255212	3.5447692	1.1146767

S1 geometry of enol-methA in gas phase, TD-PBE0/aug-cc-pVTZ
Energy = -650.5677469696

C	-1.9549432	-1.4869492	-0.9715667
C	-2.6686903	-0.3216074	-1.0278511
C	-2.0988618	0.8595945	-0.5004314
C	-0.8154147	0.8640939	0.0818972
C	-0.0699587	-0.3715840	0.1365965
C	-0.6478740	-1.5050754	-0.3827368
H	-2.3596378	-2.4097198	-1.3662683
H	-3.6563201	-0.2940175	-1.4681684
H	-2.6337185	1.8021396	-0.5303165
H	-0.1039598	-2.4411092	-0.3467520
O	-0.2882577	1.9335756	0.5657960
H	1.0399601	1.4433646	1.0660991
C	1.2353586	-0.3562685	0.7329302
O	1.7695918	0.7286266	1.2347304

O	1.9308686	-1.4834548	0.7786098
C	3.2191950	-1.4307783	1.3799915
H	3.1472027	-1.1154763	2.4216181
H	3.6108145	-2.4423314	1.3186663
H	3.8695539	-0.7402923	0.8416665
C	-1.5883884	5.3578787	0.3408668
O	-2.1186207	4.0589430	0.3967496
H	-2.4170165	6.0499308	0.1843319
H	-0.8802028	5.4850325	-0.4874668
H	-1.0827301	5.6418196	1.2721936
H	-1.3949460	3.4241529	0.5176112

S0 geometry of ketoB-methB in gas phase, PBE0/aug-cc-pVTZ
Energy = -650.6005558858

C	-1.9020722	-1.9095505	-0.8102004
C	-2.7685972	-0.8621120	-1.1250833
C	-2.4147789	0.4484548	-0.8891193
C	-1.1732449	0.7503892	-0.3273821
C	-0.2912563	-0.3005961	-0.0037823
C	-0.6764761	-1.6228678	-0.2539651
H	-2.1902661	-2.9349395	-1.0003901
H	-3.7367538	-1.0782167	-1.5612528
H	-3.0808366	1.2672034	-1.1286434
H	0.0119213	-2.4180898	-0.0016621
O	-0.8726190	2.0318392	-0.1187098
H	0.0259728	2.0526231	0.2750335
C	1.0075860	0.0206439	0.5830647
O	1.3802650	1.1711594	0.8042122
O	1.7584061	-1.0310848	0.8642840
C	3.0355712	-0.7700054	1.4526440
H	2.9197702	-0.2261133	2.3892032
H	3.4754239	-1.7466715	1.6319379
H	3.6606277	-0.1857715	0.7793008
C	4.1322285	3.6824015	0.9210881
O	4.0044462	2.3319790	1.2950881
H	5.1716535	3.9709523	1.0796706
H	3.5006480	4.3427409	1.5268418
H	3.8924478	3.8451080	-0.1362909
H	3.0937585	2.0497846	1.1482224

S1 geometry of ketoB-methB in gas phase, TD-PBE0/aug-cc-pVTZ
Energy = -650.6005558858

C	-1.9020722	-1.9095505	-0.8102004
C	-2.7685972	-0.8621120	-1.1250833

C	-2.4147789	0.4484548	-0.8891193
C	-1.1732449	0.7503892	-0.3273821
C	-0.2912563	-0.3005961	-0.0037823
C	-0.6764761	-1.6228678	-0.2539651
H	-2.1902661	-2.9349395	-1.0003901
H	-3.7367538	-1.0782167	-1.5612528
H	-3.0808366	1.2672034	-1.1286434
H	0.0119213	-2.4180898	-0.0016621
O	-0.8726190	2.0318392	-0.1187098
H	0.0259728	2.0526231	0.2750335
C	1.0075860	0.0206439	0.5830647
O	1.3802650	1.1711594	0.8042122
O	1.7584061	-1.0310848	0.8642840
C	3.0355712	-0.7700054	1.4526440
H	2.9197702	-0.2261133	2.3892032
H	3.4754239	-1.7466715	1.6319379
H	3.6606277	-0.1857715	0.7793008
C	4.1322285	3.6824015	0.9210881
O	4.0044462	2.3319790	1.2950881
H	5.1716535	3.9709523	1.0796706
H	3.5006480	4.3427409	1.5268418
H	3.8924478	3.8451080	-0.1362909
H	3.0937585	2.0497846	1.1482224

S0 geometry of ketoA in gas phase, RI-MP2/aug-cc-pVTZ
Energy = -534.9485965715

C	2.4596942	-1.2657314	0.0012095
C	2.9945597	0.0209352	0.0015752
C	2.1709822	1.1261003	-0.0000548
C	0.7835130	0.9782417	-0.0016119
C	0.2314794	-0.3161382	-0.0020250
C	1.0919223	-1.4195457	-0.0010889
H	3.1085696	-2.1316518	0.0028761
H	4.0690744	0.1609159	0.0032137
H	2.5744533	2.1305755	0.0002784
H	0.6384995	-2.4025616	-0.0021386
O	0.0590542	2.1067933	-0.0028355
H	-0.8794134	1.8634685	-0.0029514
C	-1.2119726	-0.6155747	-0.0022530
O	-1.6964648	-1.7160899	-0.0035833
O	-1.9895629	0.4998834	-0.0000428
C	-3.3977723	0.2666277	0.0019452
H	-3.6859257	-0.2957469	0.8889508
H	-3.8618309	1.2493933	0.0036717

H -3.6888591 -0.2940945 -0.8851354

S0 geometry of ketoB in gas phase, RI-MP2/aug-cc-pVTZ
Energy = -532.4085472062

C	-1.9912360	-1.7222018	0.0000908
C	-2.9002009	-0.6593520	0.0001481
C	-2.4521072	0.6526495	0.0000006
C	-1.0821104	0.9322345	-0.0001541
C	-0.1626538	-0.1357875	-0.0001945
C	-0.6315575	-1.4576997	-0.0000905
H	-2.3454877	-2.7436899	0.0001594
H	-3.9644746	-0.8563556	0.0002878
H	-3.1428298	1.4851719	0.0000646
H	0.0882698	-2.2638923	-0.0001096
O	-0.7056004	2.2263868	-0.0002210
H	0.2772098	2.2282333	-0.0002390
C	1.2748935	0.1680041	-0.0001998
O	1.7386834	1.3062685	-0.0003091
O	2.0555518	-0.9192735	-0.0000564
C	3.4662668	-0.6355908	0.0002490
H	3.7345413	-0.0678475	0.8874677
H	3.9503254	-1.6053085	0.0002976
H	3.7349157	-0.0677470	-0.8867916

TS geometry of ketoB→ketoA in gas phase, PBE0/aug-cc-pVTZ
Energy = -534.9321152207

C	-2.2554721	-0.0639451	1.4930956
C	-2.9405934	-0.2359172	0.2975353
C	-2.2668690	-0.2137539	-0.9095077
C	-0.8901096	-0.0249079	-0.9348771
C	-0.1933861	0.1359238	0.2617368
C	-0.8849966	0.1231634	1.4674906
H	-2.7845169	-0.0754191	2.4370442
H	-4.0136502	-0.3836050	0.3036125
H	-2.7892793	-0.3362743	-1.8497120
H	-0.3360279	0.2600575	2.3915032
O	-0.2908752	-0.0071556	-2.1506374
H	0.6352404	0.2330074	-2.0705096
C	1.2850119	0.3486755	0.2574633
O	1.8291104	1.4216992	0.2790790
O	1.9481513	-0.8130067	0.2098313
C	3.3721102	-0.7059270	0.2193628
H	3.7104699	-0.2187046	1.1334356
H	3.7446525	-1.7252196	0.1683741

H	3.7202853	-0.1267227	-0.6357752

TS geometry of ketoB→ketoA in gas phase, RIMP2/aug-cc-pVTZ
Energy = -532.3875233563

C	-2.2611316	-0.0669004	1.4991871
C	-2.9476096	-0.2369977	0.2970790
C	-2.2659682	-0.2119569	-0.9144655
C	-0.8858481	-0.0215877	-0.9337836
C	-0.1911313	0.1384401	0.2680398
C	-0.8836401	0.1226358	1.4799540
H	-2.7926755	-0.0812990	2.4405680
H	-4.0193457	-0.3847540	0.2998093
H	-2.7844522	-0.3332232	-1.8560731
H	-0.3335241	0.2573577	2.4026432
O	-0.2789132	-0.0021798	-2.1582175
H	0.6516055	0.2325965	-2.0596000
C	1.2841014	0.3483017	0.2591588
O	1.8414746	1.4267761	0.2672413
O	1.9374004	-0.8294020	0.2187951
C	3.3735635	-0.7053696	0.2151289
H	3.7068441	-0.2002584	1.1181644
H	3.7475722	-1.7218998	0.1779434
H	3.7009333	-0.1383106	-0.6530279

S0 geometry of ketoB in Acetonitrile, PBE0/aug-cc-pVTZ

C	1.985618000	-1.722002000	-0.000036000
C	2.891830000	-0.661521000	-0.000036000
C	2.453862000	0.647005000	-0.000008000
C	1.087500000	0.927430000	0.000030000
C	0.163433000	-0.135961000	0.000024000
C	0.634003000	-1.453184000	-0.000010000
H	2.339498000	-2.744508000	-0.000054000
H	3.956502000	-0.862847000	-0.000053000
H	3.152744000	1.473868000	-0.000002000
H	-0.084821000	-2.261619000	-0.000010000
O	0.699826000	2.207427000	0.000078000
H	-0.286264000	2.197847000	0.000116000
C	-1.268014000	0.174616000	0.000048000
O	-1.709946000	1.318718000	0.000001000
O	-2.057358000	-0.887481000	-0.000010000
C	-3.465179000	-0.634570000	-0.000064000
H	-3.749817000	-0.075000000	-0.890018000
H	-3.936449000	-1.612889000	-0.000102000
H	-3.749893000	-0.075028000	0.889884000

S0 geometry of ketoB in Acetonitrile, PBE0/TZVP

C	1.982724000	-1.726469000	-0.000031000
C	2.892062000	-0.667352000	0.000013000
C	2.456159000	0.642532000	0.000042000
C	1.089676000	0.927445000	0.000029000
C	0.162714000	-0.135151000	-0.000016000
C	0.630940000	-1.454563000	-0.000045000
H	2.334538000	-2.750803000	-0.000053000
H	3.957307000	-0.870944000	0.000026000
H	3.157174000	1.468920000	0.000076000
H	-0.091278000	-2.261352000	-0.000079000
O	0.709849000	2.211333000	0.000056000
H	-0.276391000	2.213958000	0.000036000
C	-1.269390000	0.177536000	-0.000028000
O	-1.708865000	1.322487000	0.000034000
O	-2.060130000	-0.884618000	-0.000041000
C	-3.470488000	-0.634801000	-0.000021000
H	-3.758152000	-0.076467000	-0.890900000
H	-3.938282000	-1.615480000	-0.000036000
H	-3.758134000	-0.076502000	0.890885000

S1 geometry of enol in Acetonitrile, PBE0/aug-cc-pVTZ

C	-2.077780000	-1.707954000	0.000756000
C	-2.982785000	-0.670937000	0.000535000
C	-2.499920000	0.652202000	0.000064000
C	-1.117893000	0.937367000	-0.000150000
C	-0.170897000	-0.171846000	0.000043000
C	-0.672336000	-1.458568000	0.000490000
H	-2.419372000	-2.735157000	0.001137000
H	-4.046953000	-0.863990000	0.000725000
H	-3.179655000	1.495848000	-0.000090000
H	0.008654000	-2.299989000	0.000623000
O	-0.671969000	2.136852000	-0.000525000
H	0.819833000	1.922776000	-0.000970000
C	1.222913000	0.127497000	-0.000234000
O	1.682136000	1.356616000	-0.000966000
O	2.089357000	-0.869430000	0.000229000
C	3.479770000	-0.544420000	-0.000258000
H	3.739808000	0.027922000	0.890299000
H	4.000057000	-1.497526000	0.000213000
H	3.739433000	0.026836000	-0.891622000

S1 geometry of enol in Acetonitrile, PBE0/TZVP

C	-2.079473000	-1.709792000	0.000572000

C	-2.983999000	-0.671903000	0.000696000
C	-2.501510000	0.653018000	0.000430000
C	-1.119417000	0.938637000	-0.000049000
C	-0.172097000	-0.172652000	-0.000121000
C	-0.672567000	-1.459997000	-0.000226000
H	-2.421205000	-2.738007000	0.000927000
H	-4.049403000	-0.864208000	0.001273000
H	-3.182403000	1.496870000	0.000722000
H	0.009892000	-2.301447000	-0.000705000
O	-0.670404000	2.138421000	-0.000258000
H	0.816449000	1.929570000	-0.001620000
C	1.223633000	0.129180000	-0.000364000
O	1.681430000	1.359526000	-0.002149000
O	2.090387000	-0.868929000	0.000950000
C	3.482706000	-0.545291000	0.000180000
H	3.744954000	0.027074000	0.891213000
H	4.000841000	-1.500383000	0.001500000
H	3.744587000	0.024412000	-0.892668000

S0 geometry of ketoB in DMSO, PBE0/aug-cc-pVTZ

C	1.985601000	-1.722020000	-0.000036000
C	2.891841000	-0.661567000	-0.000037000
C	2.453881000	0.646987000	-0.000010000
C	1.087533000	0.927401000	0.000030000
C	0.163431000	-0.135947000	0.000026000
C	0.633976000	-1.453180000	-0.000008000
H	2.339454000	-2.744534000	-0.000054000
H	3.956506000	-0.862909000	-0.000056000
H	3.152828000	1.473802000	-0.000005000
H	-0.084837000	-2.261624000	-0.000008000
O	0.699805000	2.207447000	0.000078000
H	-0.286308000	2.197746000	0.000119000
C	-1.268038000	0.174636000	0.000051000
O	-1.709879000	1.318820000	-0.000001000
O	-2.057338000	-0.887385000	-0.000009000
C	-3.465238000	-0.634663000	-0.000066000
H	-3.749918000	-0.075179000	-0.890053000
H	-3.936357000	-1.613045000	-0.000104000
H	-3.749998000	-0.075207000	0.889914000

S0 geometry of ketoB in DMSO, PBE0/TZVP

C	1.982702000	-1.726493000	-0.000031000
C	2.892075000	-0.667410000	0.000014000
C	2.456186000	0.642506000	0.000042000

C	1.089717000	0.927417000	0.000029000
C	0.162711000	-0.135130000	-0.000016000
C	0.630908000	-1.454553000	-0.000045000
H	2.334481000	-2.750837000	-0.000053000
H	3.957311000	-0.871025000	0.000026000
H	3.157278000	1.468835000	0.000076000
H	-0.091295000	-2.261356000	-0.000080000
O	0.709846000	2.211357000	0.000056000
H	-0.276418000	2.213876000	0.000034000
C	-1.269419000	0.177566000	-0.000028000
O	-1.708809000	1.322594000	0.000035000
O	-2.060111000	-0.884516000	-0.000041000
C	-3.470554000	-0.634899000	-0.000021000
H	-3.758267000	-0.076659000	-0.890935000
H	-3.938192000	-1.615642000	-0.000035000
H	-3.758248000	-0.076693000	0.890921000

S1 geometry of enol in DMSO, PBE0/aug-cc-pVTZ

C	-2.077617000	-1.707907000	0.000759000
C	-2.982828000	-0.670939000	0.000534000
C	-2.500102000	0.652174000	0.000062000
C	-1.118045000	0.937476000	-0.000149000
C	-0.170843000	-0.171715000	0.000046000
C	-0.672248000	-1.458534000	0.000494000
H	-2.419162000	-2.735126000	0.001139000
H	-4.046961000	-0.864149000	0.000720000
H	-3.179940000	1.495745000	-0.000097000
H	0.008726000	-2.299959000	0.000628000
O	-0.672287000	2.136985000	-0.000527000
H	0.820264000	1.922935000	-0.000967000
C	1.222873000	0.127563000	-0.000230000
O	1.682220000	1.356732000	-0.000957000
O	2.089274000	-0.869333000	0.000227000
C	3.479783000	-0.544523000	-0.000262000
H	3.739883000	0.027733000	0.890324000
H	3.999907000	-1.497709000	0.000207000
H	3.739504000	0.026653000	-0.891652000

S1 geometry of enol in DMSO, PBE0/TZVP

C	-2.079307000	-1.709746000	0.000577000
C	-2.984048000	-0.671916000	0.000692000
C	-2.501706000	0.652984000	0.000420000
C	-1.119584000	0.938753000	-0.000053000
C	-0.172046000	-0.172509000	-0.000117000

C	-0.672480000	-1.459956000	-0.000210000
H	-2.420990000	-2.737978000	0.000934000
H	-4.049416000	-0.864393000	0.001261000
H	-3.182713000	1.496754000	0.000699000
H	0.009966000	-2.301409000	-0.000675000
O	-0.670741000	2.138557000	-0.000267000
H	0.816960000	1.929760000	-0.001602000
C	1.223583000	0.129257000	-0.000355000
O	1.681535000	1.359646000	-0.002119000
O	2.090294000	-0.868821000	0.000940000
C	3.482717000	-0.545400000	0.000168000
H	3.745036000	0.026863000	0.891237000
H	4.000678000	-1.500576000	0.001470000
H	3.744661000	0.024229000	-0.892700000

S0 geometry of ketoB in MCH, PBE0/aug-cc-pVTZ

C	1.986100000	-1.721295000	-0.000036000
C	2.891046000	-0.659567000	-0.000016000
C	2.452897000	0.647705000	0.000016000
C	1.085862000	0.928977000	0.000031000
C	0.163460000	-0.136591000	0.000006000
C	0.635045000	-1.453417000	-0.000027000
H	2.341061000	-2.743457000	-0.000057000
H	3.955995000	-0.860301000	-0.000027000
H	3.148772000	1.476861000	0.000036000
H	-0.084542000	-2.261162000	-0.000039000
O	0.701278000	2.206489000	0.000066000
H	-0.283609000	2.203380000	0.000068000
C	-1.266713000	0.173783000	0.000011000
O	-1.713284000	1.313801000	0.000036000
O	-2.058384000	-0.892263000	-0.000031000
C	-3.461855000	-0.630005000	-0.000049000
H	-3.744337000	-0.065981000	-0.888347000
H	-3.940903000	-1.605057000	-0.000086000
H	-3.744372000	-0.066028000	0.888267000

S0 geometry of ketoB in MCH, PBE0/TZVP

C	1.983321000	-1.725448000	-0.000050000
C	2.891086000	-0.664839000	-0.000260000
C	2.454723000	0.643622000	-0.000227000
C	1.087630000	0.928881000	0.000022000
C	0.162745000	-0.136050000	0.000216000
C	0.632152000	-1.454960000	0.000173000
H	2.336518000	-2.749336000	-0.000069000

H	3.956639000	-0.867542000	-0.000447000
H	3.152203000	1.472667000	-0.000359000
H	-0.090974000	-2.260903000	0.000322000
O	0.710598000	2.210355000	0.000141000
H	-0.274416000	2.219247000	0.000459000
C	-1.267929000	0.176059000	0.000401000
O	-1.711950000	1.317132000	-0.000135000
O	-2.060858000	-0.889754000	0.000138000
C	-3.466534000	-0.629818000	-0.000267000
H	-3.751205000	-0.066757000	-0.889573000
H	-3.942525000	-1.607094000	-0.000447000
H	-3.751727000	-0.066821000	0.888912000

S1 geometry of enol in MCH, PBE0/aug-cc-pVTZ

C	-2.085903000	-1.710298000	0.000680000
C	-2.980538000	-0.669952000	0.000611000
C	-2.489612000	0.653903000	0.000153000
C	-1.109036000	0.931273000	-0.000137000
C	-0.172875000	-0.179372000	-0.000104000
C	-0.677230000	-1.461378000	0.000209000
H	-2.431081000	-2.736331000	0.001130000
H	-4.046262000	-0.855546000	0.000925000
H	-3.163314000	1.501922000	0.000148000
H	0.003729000	-2.303339000	0.000109000
O	-0.653405000	2.129177000	-0.000424000
H	0.793684000	1.915052000	-0.001010000
C	1.225061000	0.123784000	-0.000384000
O	1.677094000	1.350059000	-0.001497000
O	2.094041000	-0.874585000	0.000408000
C	3.479157000	-0.538422000	-0.000055000
H	3.735389000	0.038434000	0.889093000
H	4.008326000	-1.487229000	0.000678000
H	3.735174000	0.036949000	-0.890234000

S1 geometry of enol in MCH, PBE0/TZVP

C	-2.087671000	-1.712009000	0.000433000
C	-2.981125000	-0.670411000	0.000798000
C	-2.490678000	0.655013000	0.000769000
C	-1.109920000	0.932265000	0.000114000
C	-0.173990000	-0.180759000	-0.000171000
C	-0.676963000	-1.462955000	-0.000831000
H	-2.432744000	-2.739088000	0.000710000
H	-4.048364000	-0.853791000	0.001655000
H	-3.165653000	1.503096000	0.001444000

H	0.005617000	-2.304743000	-0.001861000
O	-0.651261000	2.130856000	0.000079000
H	0.784776000	1.920460000	-0.002291000
C	1.226626000	0.125243000	-0.000649000
O	1.675417000	1.353072000	-0.003356000
O	2.095532000	-0.874778000	0.001411000
C	3.482244000	-0.539512000	0.000630000
H	3.740419000	0.037849000	0.890094000
H	4.009844000	-1.490023000	0.002477000
H	3.740295000	0.034315000	-0.891155000

S0 geometry of ketoB in DMF, PBE0/aug-cc-pVTZ

C	1.985615000	-1.722005000	-0.000036000
C	2.891832000	-0.661529000	-0.000036000
C	2.453865000	0.647002000	-0.000008000
C	1.087506000	0.927425000	0.000030000
C	0.163433000	-0.135959000	0.000024000
C	0.633998000	-1.453184000	-0.000009000
H	2.339491000	-2.744513000	-0.000054000
H	3.956503000	-0.862857000	-0.000054000
H	3.152759000	1.473857000	-0.000003000
H	-0.084823000	-2.261620000	-0.000010000
O	0.699823000	2.207430000	0.000078000
H	-0.286271000	2.197829000	0.000117000
C	-1.268018000	0.174619000	0.000049000
O	-1.709934000	1.318735000	0.000000000
O	-2.057355000	-0.887464000	-0.000010000
C	-3.465189000	-0.634586000	-0.000065000
H	-3.749834000	-0.075031000	-0.890024000
H	-3.936433000	-1.612916000	-0.000102000
H	-3.749911000	-0.075059000	0.889889000

S0 geometry of ketoB in DMF, PBE0/TZVP

C	1.982720000	-1.726473000	-0.000031000
C	2.892064000	-0.667362000	0.000013000
C	2.456164000	0.642528000	0.000042000
C	1.089683000	0.927440000	0.000029000
C	0.162714000	-0.135147000	-0.000016000
C	0.630934000	-1.454561000	-0.000045000
H	2.334528000	-2.750809000	-0.000053000
H	3.957308000	-0.870958000	0.000026000
H	3.157192000	1.468906000	0.000076000
H	-0.091281000	-2.261353000	-0.000079000
O	0.709849000	2.211337000	0.000056000

H	-0.276395000	2.213944000	0.000035000
C	-1.269395000	0.177541000	-0.000028000
O	-1.708855000	1.322505000	0.000034000
O	-2.060127000	-0.884601000	-0.000041000
C	-3.470499000	-0.634818000	-0.000021000
H	-3.758172000	-0.076500000	-0.890906000
H	-3.938267000	-1.615508000	-0.000036000
H	-3.758154000	-0.076535000	0.890891000

S1 geometry of enol in DMF, PBE0/aug-cc-pVTZ

C	-2.077752000	-1.707946000	0.000758000
C	-2.982792000	-0.670937000	0.000533000
C	-2.499951000	0.652197000	0.000063000
C	-1.117919000	0.937386000	-0.000148000
C	-0.170888000	-0.171823000	0.000044000
C	-0.672321000	-1.458562000	0.000492000
H	-2.419336000	-2.735151000	0.001139000
H	-4.046955000	-0.864018000	0.000721000
H	-3.179704000	1.495830000	-0.000092000
H	0.008666000	-2.299984000	0.000625000
O	-0.672023000	2.136875000	-0.000524000
H	0.819907000	1.922804000	-0.000969000
C	1.222906000	0.127509000	-0.000233000
O	1.682150000	1.356636000	-0.000964000
O	2.089342000	-0.869413000	0.000228000
C	3.479772000	-0.544438000	-0.000259000
H	3.739821000	0.027889000	0.890302000
H	4.000031000	-1.497558000	0.000212000
H	3.739445000	0.026805000	-0.891628000

S1 geometry of enol in DMF, PBE0/TZVP

C	-2.079444000	-1.709784000	0.000573000
C	-2.984007000	-0.671905000	0.000695000
C	-2.501544000	0.653012000	0.000428000
C	-1.119446000	0.938657000	-0.000050000
C	-0.172088000	-0.172627000	-0.000121000
C	-0.672552000	-1.459990000	-0.000223000
H	-2.421168000	-2.738002000	0.000928000
H	-4.049406000	-0.864240000	0.001271000
H	-3.182456000	1.496850000	0.000718000
H	0.009904000	-2.301441000	-0.000700000
O	-0.670462000	2.138445000	-0.000259000
H	0.816537000	1.929603000	-0.001617000
C	1.223624000	0.129193000	-0.000362000

O	1.681448000	1.359546000	-0.002144000
O	2.090371000	-0.868910000	0.000948000
C	3.482708000	-0.545310000	0.000178000
H	3.744968000	0.027038000	0.891217000
H	4.000813000	-1.500416000	0.001494000
H	3.744600000	0.024380000	-0.892674000