Photophysics of Shiff Base: A Theoretical exploration of the excited-state deactivation mechanisms of N-salicilydenemethylfurylamine(SMFA)

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Electronic Supplementary Information:

This supplementary material section contains 4 Tables:

Table SM1: The ground state xyz coordinates of the optimized geometry of the SMFA at the MP2/cc-pVDZ and CC2/ cc-pVDZ level.

Table SM2: The ground state xyz coordinates and the optimized geometry of 16 rotamers of the ground isomers of SMFA.

Table SM3: The charge distributions in the ground and the first excited states of the SMFA.

Table SM4: Selected Bonds lengths (Å), Bond angles, and dihedral angles (deg) of the S_0 and S1 geometry optimized of SMFA (Enol and Cis-keto Forms).

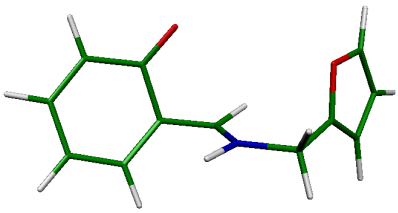
Table SM1:

Enol form of the SMFA (5a, 0.00 eV)			
S0 (Mp2 optimized)			
N	-0.31691	1.36366	-0.05114
C	3.84087	0.33357	0.05321
C	4.17536	-1.02519	0.01372
C	2.49178	0.74410	0.02318
C	1.47179	-0.24852	-0.04721
C	3.17054	-2.01173	-0.05634
C	1.83015	-1.61623	-0.08632
O	2.21628	2.06208	0.06262
C	0.05607	0.12160	-0.08261
H	-0.67396	-0.70757	-0.13997
H	1.22187	2.12208	0.03295
H	4.61192	1.10828	0.10788
H	5.23034	-1.31880	0.03805
H	3.43587	-3.07266	-0.08698
H	1.03098	-2.36533	-0.14050
C	-1.75444	1.68685	-0.09389
C	-2.69568	0.53232	-0.12958
C	-3.34826	-0.12846	-1.15375
C	-4.04586	-1.22586	-0.54930
C	-3.75941	-1.15585	0.79766
O	-2.94179	-0.09751	1.06293
H	-3.32556	0.15069	-2.20708
H	-4.67882	-1.96728	-1.03535
H	-4.05811	-1.75211	1.65736
H	-1.92224	2.31536	-0.98523
H	-1.96637	2.31728	0.78689
S1 (CC2 optimized)			
N	1.20346	-3.41089	0.44065
C	-0.90567	0.13697	-0.77087
C	-0.83881	0.54873	-2.14764
C	-0.13830	-0.92446	-0.34127
C	0.69909	-1.66928	-1.24237
C	-0.04437	-0.15030	-3.04287
C	0.71009	-1.27079	-2.59345
O	-0.15578	-1.28220	1.03099
C	1.50852	-2.74611	-0.73817
H	2.41590	-3.07023	-1.26360
H	0.33078	-3.07219	0.87720
H	-1.52461	0.68449	-0.05167
H	-1.43970	1.40544	-2.47292
H	-0.00117	0.13906	-4.09827
H	1.31546	-1.84662	-3.30464
C	2.29224	-3.54806	1.43789
C	2.54999	-2.25005	2.12302
C	3.32702	-1.14921	1.81175
C	2.94818	-0.11474	2.73357
C	1.95953	-0.65567	3.52822
O	1.70782	-1.95637	3.17314
H	4.07100	-1.09468	1.01680
H	3.34933	0.89639	2.80239
H	1.37946	-0.27591	4.36688
H	3.19520	-3.88288	0.90075
H	2.00443	-4.32318	2.16691
Trans-keto (MP2/cc-pVDZ)			

N	-0.47083	-1.49605	0.38624
C	3.84077	0.86658	0.84011
C	4.28960	0.41096	-0.37481
C	2.52009	0.49944	1.37625
C	1.71842	-0.39227	0.48939
C	3.48537	-0.45759	-1.20470
C	2.23627	-0.84212	-0.78000
O	2.11683	0.90908	2.47826
C	0.45740	-0.71682	0.96940
H	0.19113	-0.30541	1.95253
H	-0.32164	-1.79015	-0.57607
H	4.45469	1.52279	1.46613
H	5.28315	0.70989	-0.72979
H	3.87564	-0.80342	-2.16667
H	1.63504	-1.50677	-1.41432
C	-1.85844	-1.54455	0.85656
C	-2.73705	-0.55270	0.16968
C	-3.28260	0.65895	0.54368
C	-3.97765	1.15712	-0.60851
C	-3.79622	0.21445	-1.59672
O	-3.04622	-0.82965	-1.13546
H	-3.18999	1.12711	1.52336
H	-4.53815	2.08645	-0.70091
H	-4.12684	0.14069	-2.63046
H	-1.85520	-1.33977	1.93824
H	-2.24413	-2.56669	0.70425

Geometry of CI-1 point (qualitative)

N	-0.33203	-0.89546	-1.04009
C	3.43044	1.08255	0.42274
C	4.29319	-0.00181	0.35626
C	1.98486	0.93425	0.33625
C	1.54025	-0.46722	0.41601
C	3.81219	-1.33935	0.24379
C	2.43871	-1.55688	0.22029
O	1.16486	1.87514	0.18318
C	0.13943	-0.57760	0.14577
H	-0.60313	-0.11594	0.81324
H	0.37009	-1.18591	-1.72767
H	3.81514	2.10757	0.47956
H	5.37546	0.17478	0.39238
H	4.51110	-2.17933	0.18997
H	2.04115	-2.58013	0.16146
C	-1.75414	-1.00809	-1.42764
C	-2.66051	-0.38577	-0.43134
C	-3.46798	-0.90546	0.56370
C	-4.04347	0.22259	1.23360
C	-3.53779	1.33785	0.59823
O	-2.70134	0.97829	-0.41531
H	-3.62098	-1.96285	0.77959
H	-4.73727	0.21897	2.07298
H	-3.67309	2.40759	0.74125
H	-2.01189	-2.07359	-1.54571
H	-1.85147	-0.51333	-2.40752



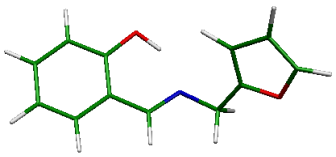
Geometry of CI-2 point (qualitative)

N	-1.38053	-0.74100	-0.44445	
C	-0.53798	0.50665	3.54320	
C	0.79029	0.44298	3.97849	
C	-0.90845	-0.04199	2.29626	
C	0.10684	-0.61160	1.46953	
C	1.79028	-0.14660	3.17369	
C	1.44351	-0.68105	1.93150	
O	-2.18754	0.00582	1.89697	
C	-0.22012	-0.99864	0.10075	
H	0.68037	-1.06210	-0.55578	
H	-2.16192	-0.34855	0.94246	
H	-1.31901	0.96188	4.16006	
H	1.05486	0.86477	4.95420	
H	2.82680	-0.18572	3.52177	
H	2.20282	-1.13214	1.28198	
C	-1.50063	0.25807	-1.51768	
C	-0.33720	0.34971	-2.44877	
C	0.71240	1.24094	-2.56602	
C	1.55800	0.73481	-3.60851	
C	0.96499	-0.43345	-4.03723	
O	-0.18189	-0.67780	-3.34120	
H	0.84808	2.14603	-1.97408	
H	2.48017	1.16821	-3.99363	
H	1.22202	-1.16549	-4.80000	
H	-1.60971	1.22265	-0.99217	
H	-2.43136	0.06772	-2.07762	

Table SM2

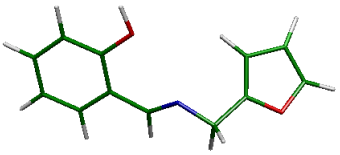
1a (0.02eV)

N	0.23307	-1.83110	1.64421
C	-1.73371	-1.19866	-2.09911
C	-0.95002	-0.80684	-3.19062
C	-1.14627	-1.43108	-0.83817
C	0.26198	-1.26196	-0.69451
C	0.44320	-0.63730	-3.05353
C	1.03785	-0.86973	-1.81049
O	-1.93935	-1.81090	0.18358
C	0.91734	-1.52761	0.58453
H	2.02478	-1.47143	0.61077
H	-1.33818	-1.86663	0.97746
H	-2.81544	-1.33430	-2.19415
H	-1.42986	-0.63044	-4.15927
H	1.05157	-0.33179	-3.90985
H	2.12034	-0.75040	-1.68202
C	0.96580	-2.15827	2.85842
C	0.62310	-3.56604	3.24219
C	-0.21042	-4.50890	2.67837
C	-0.11982	-5.66843	3.52219
C	0.75923	-5.33799	4.52921
O	1.21674	-4.05886	4.36888
H	-0.80974	-4.36832	1.78008
H	-0.63406	-6.62144	3.40438
H	1.14786	-5.87399	5.39223
H	0.65143	-1.46536	3.66021
H	2.06199	-2.04673	2.72501

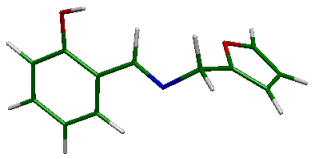
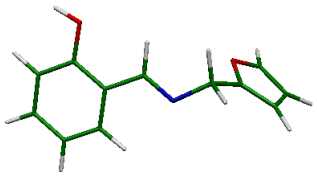


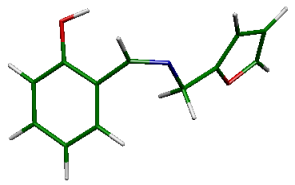
1b (0.6 eV)

N	0.98729	-3.08653	0.80463
C	-1.50854	-1.51795	-2.46656
C	-1.14353	-0.26187	-2.97350
C	-0.83544	-2.08642	-1.36805
C	0.23577	-1.37440	-0.76515
C	-0.09350	0.45569	-2.37825
C	0.57534	-0.10425	-1.28215
O	-1.19884	-3.29709	-0.85844
C	1.00835	-1.86574	0.39121
H	1.63791	-1.09355	0.88708
H	-2.33563	-2.07297	-2.92742
H	-1.68571	0.15230	-3.82976
H	0.19649	1.43868	-2.76079
H	1.39368	0.44570	-0.80285
C	1.78664	-3.36372	1.99091
C	0.86296	-3.88145	3.05147
C	-0.48222	-4.18274	3.04038
C	-0.79185	-4.64960	4.36380
C	0.38853	-4.59698	5.07176
O	1.40318	-4.13073	4.28204
H	-1.13623	-4.07649	2.17647
H	-1.75570	-4.98178	4.74821
H	0.66054	-4.84038	6.09651
H	2.33981	-2.47415	2.36551

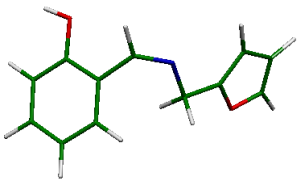


2a (0.5 eV)

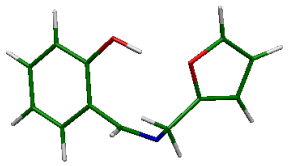
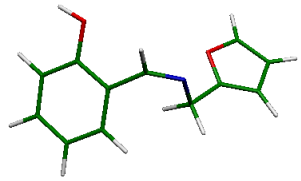
N	2.61750	-2.39581	-0.17983	
C	-1.55433	-0.59515	-1.90800	
C	-0.95764	-0.30528	-3.14039	
C	-0.79683	-1.16175	-0.86627	
C	0.58164	-1.42615	-1.05883	
C	0.40834	-0.58340	-3.34996	
C	1.16551	-1.13734	-2.31470	
O	-1.47104	-1.41989	0.29992	
C	1.41849	-1.96440	0.02895	
H	0.99567	-1.96195	1.05835	
H	-2.61555	-0.39981	-1.72655	
H	-1.56156	0.13420	-3.94117	
H	0.87600	-0.35968	-4.31369	
H	2.23085	-1.35484	-2.43577	
C	3.35134	-2.81732	1.01628	
C	4.40097	-1.80982	1.34849	
C	5.77936	-1.80330	1.27390	
C	6.20109	-0.50712	1.72188	
C	5.04517	0.17697	2.03129	
O	3.94880	-0.60352	1.81068	
H	6.40292	-2.63003	0.93515	
H	7.21762	-0.12457	1.80498	
H	4.84663	1.17931	2.40474	
H	3.85049	-3.77684	0.80435	
2b (0.43 eV)				
N	2.53938	-1.79258	0.23434	
C	-1.57332	-0.74820	-2.12029	
C	-0.87525	-0.52371	-3.31641	
C	-0.87982	-1.10489	-0.95004	
C	0.52858	-1.23813	-0.97395	
C	0.52519	-0.65448	-3.35016	
C	1.21522	-1.00857	-2.18458	
O	-1.52066	-1.33656	0.24060	
C	1.26076	-1.60913	0.25357	
H	0.66188	-1.72125	1.17671	
H	-2.66558	-0.64744	-2.09235	
H	-1.42892	-0.24622	-4.21938	
H	1.07214	-0.47842	-4.28152	
H	2.30389	-1.11668	-2.17270	
C	3.14194	-2.11175	1.53159	
C	3.97337	-0.96530	2.00305	
C	5.33218	-0.76163	2.13691	
C	5.49388	0.57726	2.62686	
C	4.21901	1.08670	2.75028	
O	3.29075	0.16056	2.37717	
H	6.11045	-1.48840	1.90630	
H	6.42153	1.09987	2.85711	
H	3.82625	2.04723	3.07703	
H	3.80496	-2.98391	1.40696	
H	2.37465	-2.35879	2.29550	
H	-2.46625	-1.19189	0.09053	
3a (0.69 eV)				

N	2.83960	-1.58988	-0.22555	
C	-1.75140	-0.70291	-1.62890	
C	-1.47465	-0.23925	-2.92231	
C	-0.72110	-1.23968	-0.83814	
C	0.59937	-1.31273	-1.34203	
C	-0.16624	-0.30263	-3.43661	
C	0.86022	-0.83816	-2.64697	
O	-1.05733	-1.67610	0.41531	
C	1.64493	-1.98511	-0.52342	
H	1.36677	-2.97539	-0.11776	
H	-2.76019	-0.65535	-1.20777	
H	-2.28471	0.17864	-3.52895	
H	0.04924	0.05375	-4.44841	
H	1.87501	-0.92639	-3.04912	
C	3.26625	-0.26650	-0.67797	
C	4.09060	0.34668	0.41157	
C	4.63405	-0.15178	1.57639	
C	5.33461	0.94420	2.18693	
C	5.16423	2.02032	1.34459	
O	4.40824	1.66765	0.26135	
H	4.53149	-1.17603	1.92828	
H	5.89103	0.94346	3.12361	
H	5.49592	3.05587	1.37308	
H	2.42907	0.40750	-0.94607	
H	3.88710	-0.39371	-1.58618	
H	-0.23651	-1.82447	0.90853	

3b (0.68 eV)

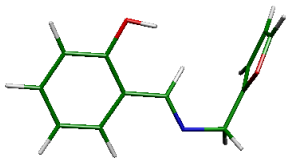
N	2.83211	-1.57457	-0.23425	
C	-1.76829	-0.83323	-1.70495	
C	-1.47271	-0.25081	-2.94803	
C	-0.74141	-1.38775	-0.92249	
C	0.60068	-1.34854	-1.37101	
C	-0.14892	-0.22211	-3.41589	
C	0.87530	-0.77003	-2.62768	
O	-0.96762	-1.97280	0.29408	
C	1.64909	-1.99762	-0.53683	
H	1.37176	-2.97578	-0.11360	
H	-2.80257	-0.85842	-1.33988	
H	-2.28196	0.17619	-3.54918	
H	0.08398	0.21739	-4.39042	
H	1.90420	-0.78031	-3.00095	
C	3.24522	-0.24419	-0.67594	
C	4.08662	0.35708	0.40737	
C	4.61368	-0.14426	1.57807	
C	5.34527	0.93726	2.17818	
C	5.20753	2.00910	1.32439	
O	4.44258	1.66744	0.24390	
H	4.47761	-1.16106	1.93966	
H	5.90038	0.93034	3.11568	
H	5.57018	3.03452	1.34239	
H	2.40158	0.43236	-0.91700	
H	3.85330	-0.34804	-1.59600	
H	-1.92391	-1.96305	0.44880	

4a (0.55eV)

N	3.35084	-1.76373	-1.04946	
C	-1.15759	-0.27520	-0.90319	
C	-1.48241	-0.04894	-2.24857	
C	0.04350	-0.92125	-0.55890	
C	0.92234	-1.35640	-1.57874	
C	-0.60374	-0.45707	-3.26785	
C	0.58930	-1.11304	-2.92790	
O	0.29375	-1.13962	0.76908	
C	2.13566	-2.16629	-1.23274	
H	1.97495	-3.25323	-1.12570	
H	-1.82053	0.04625	-0.09390	
H	-2.42023	0.45746	-2.49973	
H	-0.84987	-0.27520	-4.31860	
H	1.27291	-1.45801	-3.71217	
C	3.58590	-0.31516	-1.12706	
C	3.88728	0.19544	0.24299	
C	4.96276	0.83066	0.82531	
C	4.60146	1.07867	2.19352	
C	3.33173	0.57206	2.34969	
O	2.88692	0.03484	1.17155	
H	5.89644	1.08537	0.32522	
H	5.19804	1.56357	2.96516	
H	2.64021	0.51510	3.18756	
H	2.73087	0.23990	-1.56084	
H	4.47445	-0.14176	-1.75544	
H	1.25727	-1.08982	0.89601	
		4b (0.71 eV)		
N	-4.75044	-1.19697	-2.68171	
C	-0.00484	-1.92845	-1.81045	
C	0.50251	-0.89318	-2.61240	
C	-1.38828	-2.03802	-1.58962	
C	-2.28286	-1.11868	-2.18663	
C	-0.37087	0.03929	-3.19527	
C	-1.75296	-0.07818	-2.97729	
O	-1.94277	-3.01967	-0.81369	
C	-3.73729	-1.23130	-1.87944	
H	-3.98050	-1.36041	-0.81248	
H	0.67725	-2.65525	-1.35189	
H	1.58250	-0.81750	-2.77524	
H	0.02109	0.85607	-3.80885	
H	-2.43917	0.66186	-3.40262	
C	-4.50289	-1.14141	-4.12900	
C	-5.36153	-2.15082	-4.81479	
C	-6.48999	-2.06590	-5.60534	
C	-6.84610	-3.41292	-5.94832	
C	-5.90584	-4.21475	-5.33768	
O	-5.00086	-3.46091	-4.65142	
H	-6.99692	-1.14582	-5.89440	
H	-7.68138	-3.75106	-6.56043	
H	-5.75234	-5.29115	-5.30063	
H	-3.44370	-1.31038	-4.40133	
H	-4.79947	-0.14312	-4.49632	
H	-1.21684	-3.54658	-0.44778	
		5a (0.00 eV)		

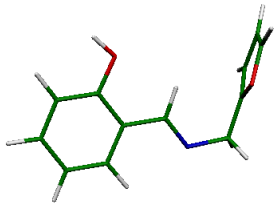
N	-0.31691	1.36366	-0.05114	
C	3.84087	0.33357	0.05321	
C	4.17536	-1.02519	0.01372	
C	2.49178	0.74410	0.02318	
C	1.47179	-0.24852	-0.04721	
C	3.17054	-2.01173	-0.05634	
C	1.83015	-1.61623	-0.08632	
O	2.21628	2.06208	0.06262	
C	0.05607	0.12160	-0.08261	
H	-0.67396	-0.70757	-0.13997	
H	1.22187	2.12208	0.03295	
H	4.61192	1.10828	0.10788	
H	5.23034	-1.31880	0.03805	
H	3.43587	-3.07266	-0.08698	
H	1.03098	-2.36533	-0.14050	
C	-1.75444	1.68685	-0.09389	
C	-2.69568	0.53232	-0.12958	
C	-3.34826	-0.12846	-1.15375	
C	-4.04586	-1.22586	-0.54930	
C	-3.75941	-1.15585	0.79766	
O	-2.94179	-0.09751	1.06293	
H	-3.32556	0.15069	-2.20708	
H	-4.67882	-1.96728	-1.03535	
H	-4.05811	-1.75211	1.65736	
H	-1.92224	2.31536	-0.98523	
H	-1.96637	2.31728	0.78689	
		5b (0.60 eV)		
N	-3.64278	-2.05960	-2.53670	
C	0.30365	-1.56741	-0.62450	
C	1.28034	-0.89885	-1.37749	
C	-0.99150	-1.78641	-1.13292	
C	-1.31574	-1.32132	-2.43580	
C	0.97198	-0.43430	-2.66600	
C	-0.31501	-0.65086	-3.17510	
O	-1.94095	-2.43500	-0.40398	
C	-2.62970	-1.48320	-3.08819	
H	-2.67338	-1.05427	-4.11010	
H	-1.52447	-2.67087	0.43948	
H	0.54537	-1.93050	0.38277	
H	2.27775	-0.74478	-0.95290	
H	1.72367	0.08859	-3.26469	
H	-0.57163	-0.29495	-4.17984	
C	-4.88749	-2.13434	-3.32436	
C	-4.87743	-1.56465	-4.70389	
C	-5.23833	-0.33622	-5.22623	
C	-4.89485	-0.36711	-6.61845	
C	-4.34171	-1.61057	-6.83954	
O	-4.32344	-2.34198	-5.68928	
H	-5.69696	0.48044	-4.66888	
H	-5.03798	0.41560	-7.36261	
H	-3.94423	-2.10495	-7.72361	
H	-5.67108	-1.62570	-2.73600	
H	-5.17009	-3.20098	-3.36588	
		6a (0.48eV)		

N	1.98284	-0.86379	0.82911	
C	-1.26370	-1.75270	-2.67411	
C	-0.86033	-0.61584	-3.38358	
C	-0.66070	-2.07600	-1.44405	
C	0.35141	-1.23848	-0.91231	
C	0.15847	0.21406	-2.87313	
C	0.75376	-0.09993	-1.64872	
O	-1.11752	-3.21320	-0.82953	
C	0.96445	-1.52801	0.39728	
H	0.49905	-2.32233	1.01551	
H	-0.53104	-3.41301	-0.08638	
H	-2.04435	-2.41761	-3.05597	
H	-1.33879	-0.37955	-4.33984	
H	0.47800	1.10137	-3.42830	
H	1.54162	0.52466	-1.21730	
C	2.50928	-1.20559	2.16337	
C	1.86501	-2.34777	2.87463	
C	0.85244	-2.43482	3.81251	
C	0.59204	-3.83237	4.00351	
C	1.45987	-4.49399	3.16043	
O	2.23220	-3.60651	2.47042	
H	0.36392	-1.59135	4.30025	
H	-0.13130	-4.29414	4.67464	
H	1.65259	-5.54653	2.96245	
H	2.42598	-0.29971	2.78875	
H	3.58780	-1.40364	2.03678	



6b (0.43eV)

N	-2.71839	-1.25288	-4.41326	
C	0.03944	-1.05664	-0.43315	
C	0.95375	-0.19987	-1.06433	
C	-1.09472	-1.51857	-1.12484	
C	-1.32003	-1.12077	-2.46402	
C	0.73868	0.20148	-2.39543	
C	-0.39079	-0.25908	-3.08305	
O	-2.01403	-2.35697	-0.54718	
C	-2.51268	-1.60755	-3.18933	
H	-3.19000	-2.27569	-2.63136	
H	-1.71627	-2.52899	0.35797	
H	0.20497	-1.37102	0.60504	
H	1.83204	0.15175	-0.51304	
H	1.44985	0.86998	-2.89045	
H	-0.59015	0.03269	-4.11847	
C	-3.92198	-1.77201	-5.08554	
C	-4.82712	-2.66000	-4.29913	
C	-4.95048	-4.03286	-4.19207	
C	-5.95260	-4.27581	-3.19532	
C	-6.35954	-3.03157	-2.76303	
O	-5.68492	-2.04716	-3.42208	
H	-4.38653	-4.76785	-4.76617	
H	-6.32912	-5.23519	-2.84235	
H	-7.09396	-2.69740	-2.03312	
H	-3.58140	-2.31777	-5.98280	
H	-4.48550	-0.89426	-5.44838	



7a(0.61 eV)

N	3.57516	-1.66829	1.26569	
C	6.67255	-4.25097	-1.29333	
C	7.61886	-4.58855	-0.31366	
C	5.68029	-3.29561	-1.01670	
C	5.63250	-2.67231	0.25104	
C	7.57019	-3.98548	0.95595	
C	6.58037	-3.02995	1.23186	
O	4.79037	-2.98074	-2.01169	
C	4.62952	-1.59711	0.52026	
H	4.80868	-0.62171	0.03603	
H	3.94002	-2.81015	-1.57273	
H	6.68141	-4.71661	-2.28377	
H	8.38996	-5.33234	-0.54061	
H	8.30545	-4.24975	1.72249	
H	6.54760	-2.53473	2.20922	
C	3.29733	-2.98912	1.88302	
C	3.22756	-4.09876	0.87961	
C	2.46395	-4.27174	-0.26430	
C	2.89660	-5.50418	-0.85537	
C	3.88346	-5.99169	-0.02373	
O	4.08050	-5.15448	1.03296	
H	1.67831	-3.59939	-0.61206	
H	2.53618	-5.97144	-1.77099	
H	4.50422	-6.88472	-0.04281	
H	2.33642	-2.89111	2.41259	
H	4.06523	-3.24528	2.63341	
		7b(0.66eV)		
N	9.20351	-4.42886	-3.20436	
C	6.41813	-2.03606	-0.22058	
C	6.86337	-2.54388	1.01134	
C	6.77381	-2.67744	-1.41968	
C	7.60995	-3.81467	-1.39193	
C	7.67111	-3.69189	1.05106	
C	8.03808	-4.32096	-0.14967	
O	6.35386	-2.25261	-2.65039	
C	8.02771	-4.46436	-2.67065	
H	7.26376	-5.03953	-3.21931	
H	5.96036	-1.37483	-2.53363	
H	5.77902	-1.14490	-0.25293	
H	6.57348	-2.03876	1.93866	
H	8.01112	-4.09587	2.00966	
H	8.66968	-5.21655	-0.13296	
C	10.22420	-3.61209	-2.50403	
C	9.78838	-2.20265	-2.23931	
C	9.28771	-1.21155	-3.06370	
C	9.00757	-0.08872	-2.21950	
C	9.36586	-0.47770	-0.94375	
O	9.84896	-1.75038	-0.94806	
H	9.11995	-1.30483	-4.13598	
H	8.60793	0.88388	-2.50694	
H	9.35314	0.02174	0.02278	
H	11.12009	-3.61903	-3.14562	
H	10.50886	-4.07321	-1.54201	
		8a(.060 eV)		

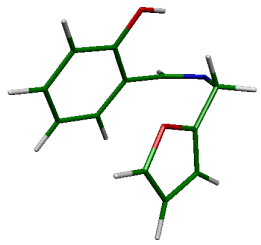
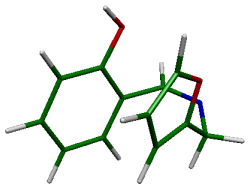
N	3.84564	-1.75379	1.55272	
C	6.52410	-3.34607	-1.77224	
C	7.11264	-4.55027	-1.36194	
C	5.87206	-2.52659	-0.83607	
C	5.81120	-2.91216	0.52264	
C	7.06989	-4.93867	-0.00977	
C	6.43625	-4.11021	0.92684	
O	5.30571	-1.36734	-1.30156	
C	5.10673	-2.04748	1.51299	
H	5.72516	-1.59162	2.30599	
H	5.02118	-0.85606	-0.52605	
H	6.55806	-3.01926	-2.81609	
H	7.61429	-5.18374	-2.10119	
H	7.53212	-5.87691	0.31236	
H	6.39138	-4.40046	1.98246	
C	2.95550	-2.41917	0.56742	
C	3.09242	-3.90979	0.54622	
C	2.90762	-4.87881	1.51616	
C	3.27804	-6.12572	0.91613	
C	3.65430	-5.82360	-0.37694	
O	3.53697	-4.48760	-0.61122	
H	2.55995	-4.70063	2.53366	
H	3.26746	-7.11697	1.36834	
H	4.00217	-6.42248	-1.21581	
H	3.13455	-2.03566	-0.45293	
H	1.92829	-2.13974	0.84979	
		8b(0.67 eV)		
N	9.17433	-4.53126	-3.16716	
C	6.43861	-2.15524	-0.11829	
C	7.14193	-2.38866	1.07524	
C	6.72709	-2.91118	-1.26609	
C	7.74230	-3.89156	-1.23017	
C	8.12804	-3.38765	1.13157	
C	8.41845	-4.13700	-0.02042	
O	6.08510	-2.73751	-2.46210	
C	8.09272	-4.64471	-2.47116	
H	7.36046	-5.38420	-2.83529	
H	5.49240	-1.97728	-2.36402	
H	5.66235	-1.38095	-0.15894	
H	6.90873	-1.79158	1.96306	
H	8.66228	-3.58463	2.06644	
H	9.18563	-4.91947	0.00717	
C	10.15616	-3.50522	-2.74597	
C	9.58731	-2.14819	-2.47311	
C	9.68954	-1.26427	-1.41462	
C	8.90870	-0.11689	-1.77097	
C	8.39328	-0.38740	-3.02229	
O	8.80860	-1.60865	-3.46036	
H	10.22948	-1.44311	-0.48556	
H	8.74360	0.78795	-1.18658	
H	7.75607	0.16974	-3.70623	
H	10.89786	-3.44146	-3.55976	
H	10.69841	-3.83591	-1.84209	

Table SM3:

		S0	S1

Part (1)	C2	-0.30793	-0.27539
	C3	-0.14929	-0.28593
	C4	0.48685	0.52334
	C5	-0.24719	-0.14233
	C6	-0.28799	-0.09379
	C7	-0.14047	-0.28575
	O8	-0.79326	-0.74233
	C9	0.23068	0.12184
	H10	0.18872	0.1893
	H11	0.54422	0.54771
	H12	0.23326	0.23467
	H13	0.22132	0.22088
	H14	0.22175	0.22021
	H15	0.21849	0.22339
	Sum	0.41916	0.45582
	Transferred Charged		**+0.03666**
Part (2)	N1	-0.63532	-0.66045
	C16	-0.20253	-0.20301
	C17	0.3306	0.33666
	C18	-0.30941	-0.31223
	C19	-0.3294	-0.32884
	C20	0.18936	0.18739
	O21	-0.58603	-0.58639
	H22	0.23567	0.23453
	H23	0.2344	0.23288
	H24	0.20746	0.20602
	H25	0.22016	0.21549
	H26	0.22587	0.22214
	Sum	-0.41917	-0.45581
	Transferred Charged		-0.03664

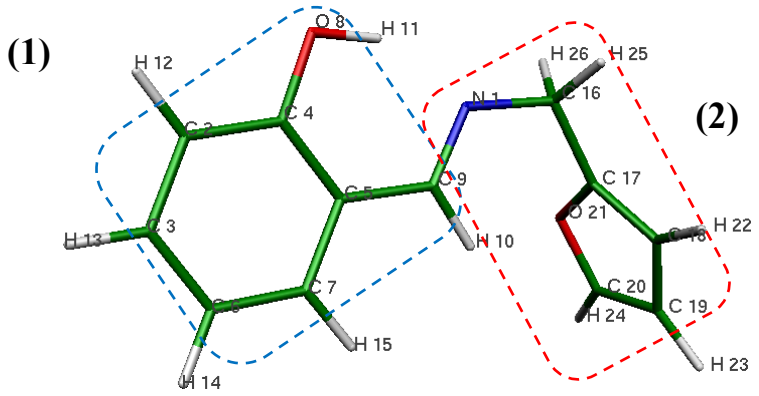


Table SM4:

S_0-enol (5a)		S_1-keto
Distance		
H1-O1	0.997	1.861
O1-C1	1.357	1.418
C1-C6	1.410	1.378
C6-C5	1.403	1.439
C5-C4	1.412	1.386
C4-C3	1.400	1.424
C3-C2	1.416	1.409
C2-C7	1.464	1.438
C7-N1	1.300	1.387
N1-C8	1.479	1.483
C8-C9	1.490	1.490
C9-O2	1.378	1.378
O2-C12	1.371	1.372
C12-C11	1.381	1.379
C11-C10	1.436	1.436
Angle		
H1-O1-C1	106.116	99.173
O1-C1-C6	118.569	119.270
C1-C6-C5	120.291	119.525
C2-C3-C 6	120.727	120.027
C5-C4-C3	119.225	119.788
C4-C3-C2	120.934	121.420
C2-C1-C6	119.433	121.851
C1-C2-C7	121.521	119.722
C2-C7-N1	121.585	122.198
C7-N1-C8	118.864	117.022
N1-C8-C9	115.806	110.832
C8-C9-C10	133.693	133.398
C8-C9-O2	116.452	115.491
C9-O2-C12	107.316	106.695
C12-C11-C10	106.048	106.046
Dihedral		
H1-O1-C1-C2	0.164	-25.690
C1-C2-C7-N1	-1.00	22.996
C2-C7-N1-C8	179.683	-129.167
N1-C8-C9-C10	-94.765	-85.204