

1 **Theoretical investigations on the HOMO-LUMO gap and global**
2 **reactivity descriptors studies, NBO and NICS analyses of 3-**
3 **substituted 3-phenylbenzo[*d*]thiazole-2(3*H*)-imine and its**
4 **derivatives: Solvent and substituent effects**

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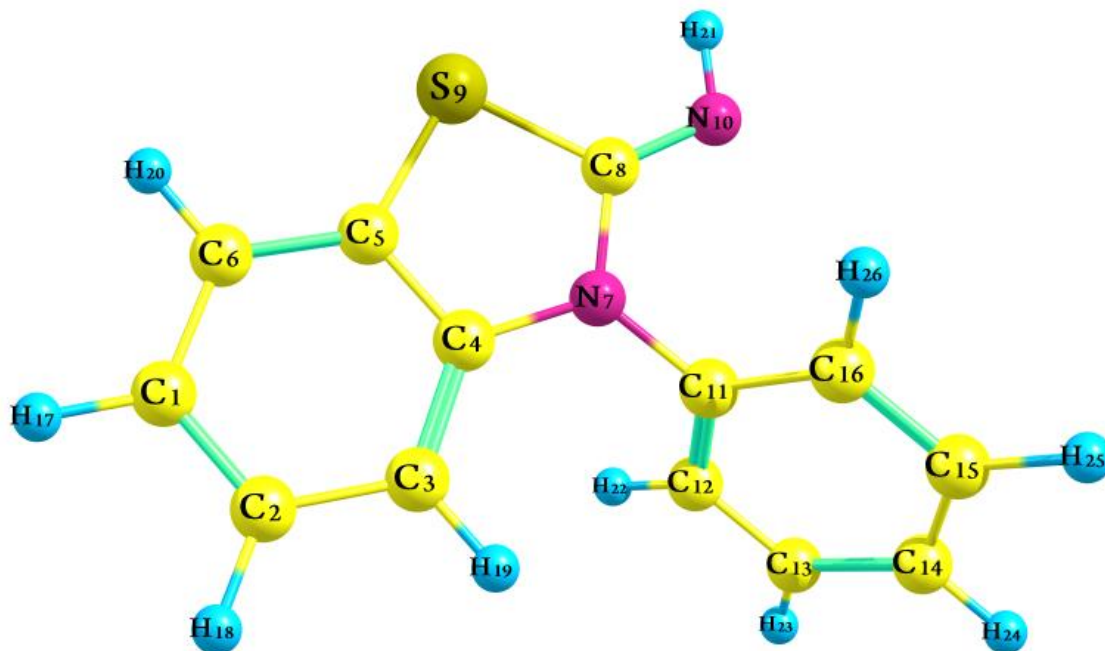
12 **SUPPLEMENTARY MATERIAL**

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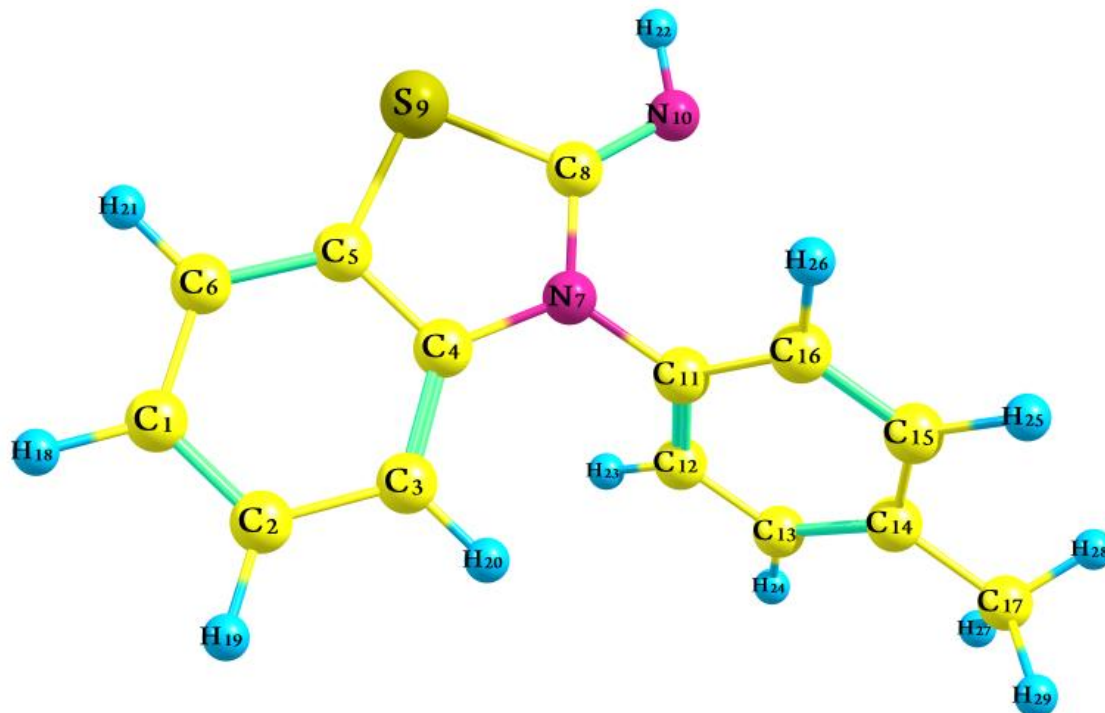
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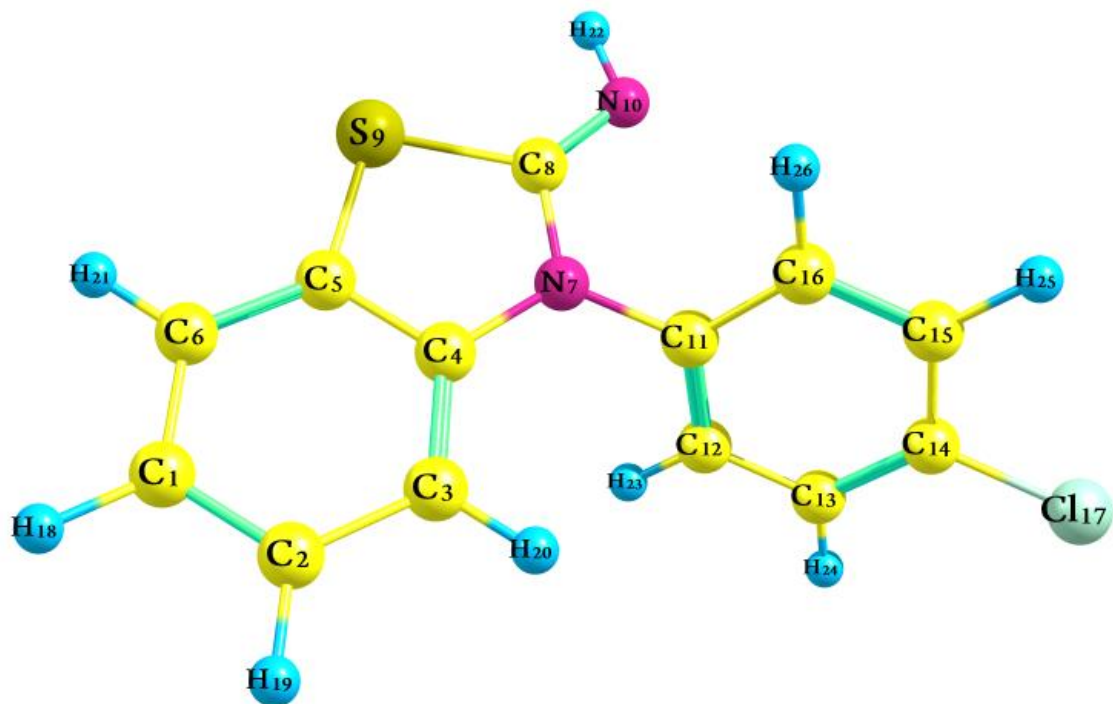
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Fig. S-1a. 3-phenylbenzo[*d*]thiazol-2(3*H*)-imine [X=H]



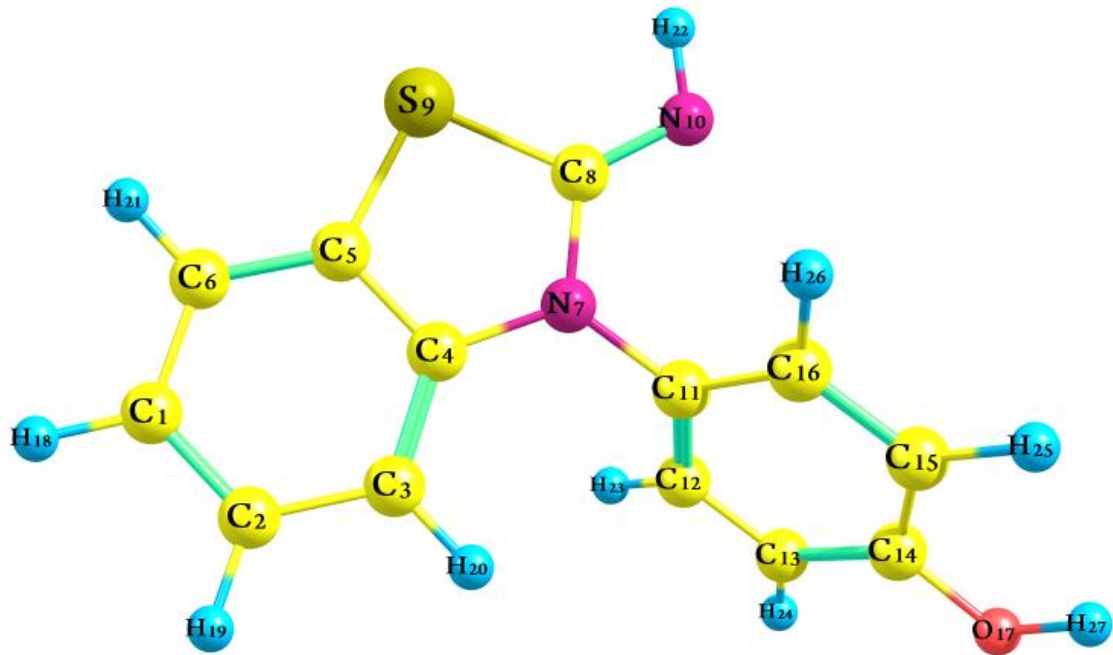
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Fig. S-1b. 3-(*p*-tolyl)benzo[*d*]thiazol-2(3*H*)-imine [X=CH₃]



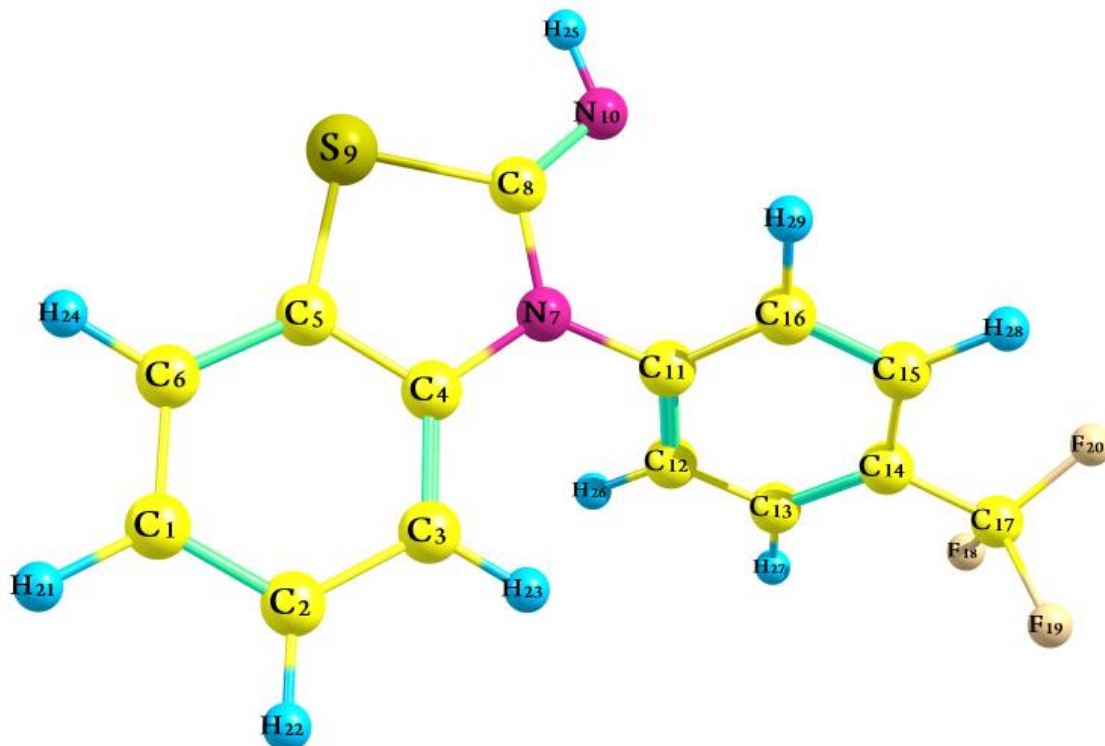
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Fig. S-1c. 3-(4-chlorophenyl)benzo[*d*]thiazol-2(3*H*)-imine [X=Cl]



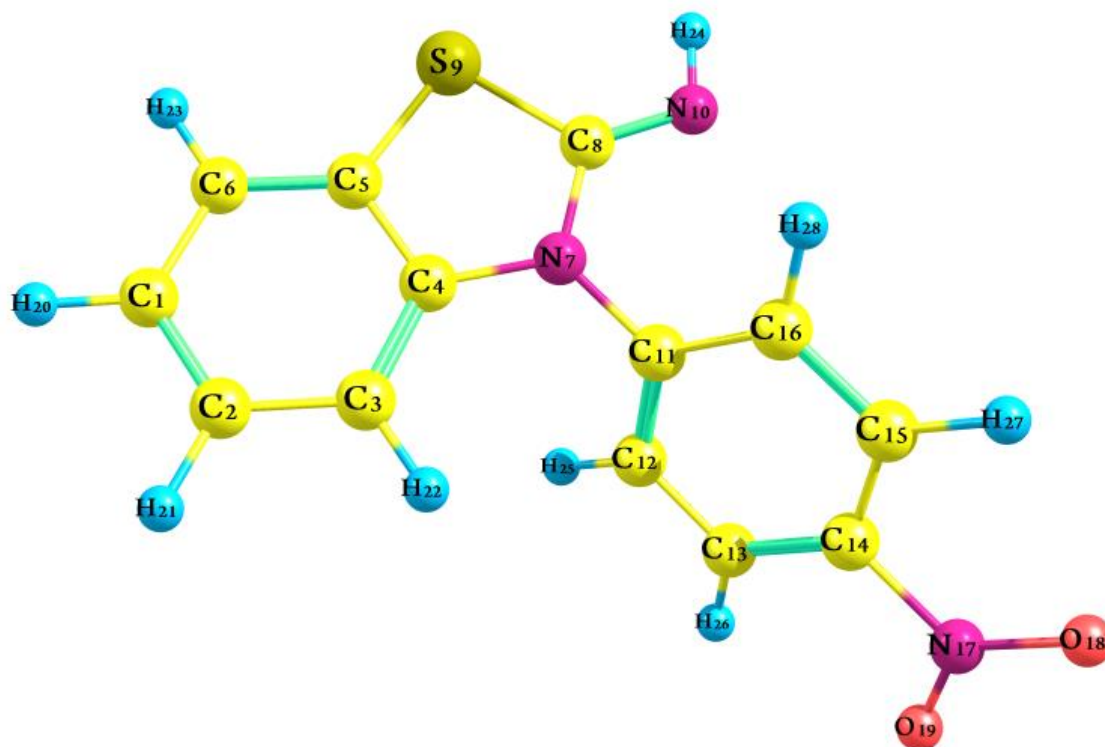
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Fig. S-1d. 4-(2-iminobenzo[*d*]thiazol-3(2*H*)-yl)phenol [X=OH]



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Fig. S-1e. 3-(4-(trifluoromethyl)phenyl)benzo[*d*]thiazol-2(3*H*)-imine [$X=CF_3$]

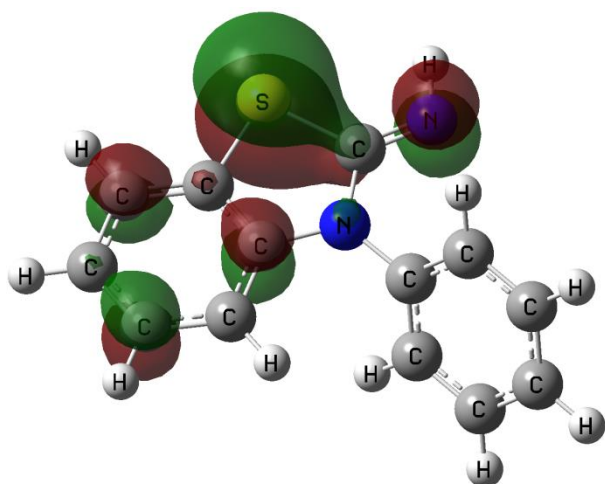


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Fig. S-1f. 3-(4-nitrophenyl)benzo[*d*]thiazol-2(3*H*)-imine [$X=NO_2$]

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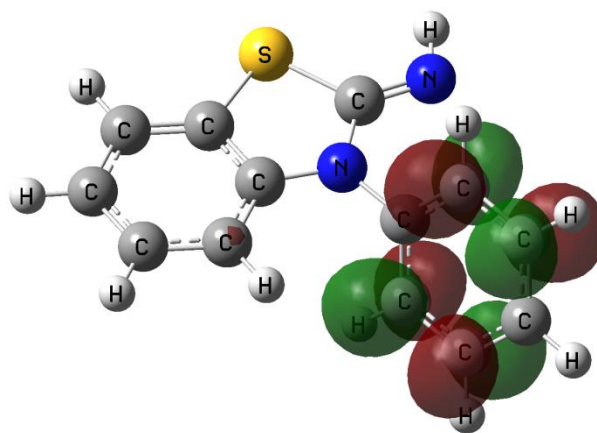
Fig. S-1. The optimized molecular structure of the compounds 1–6.



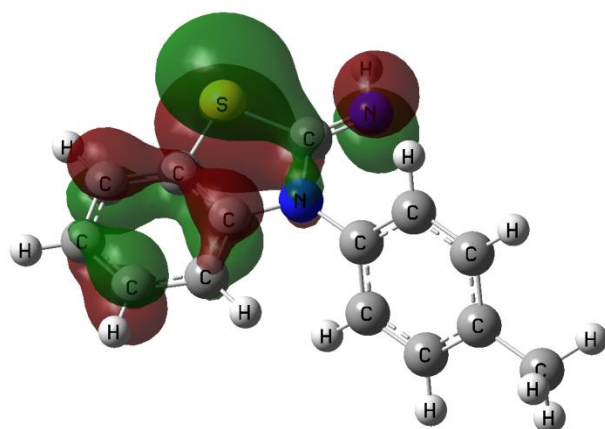
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HOMO (X=H): $E = -7.0096$ eV



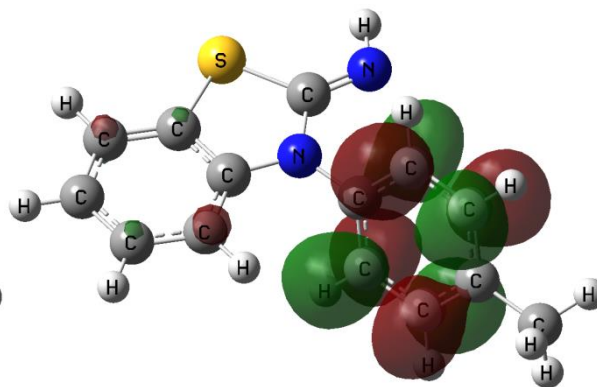
LUMO (X=H): $E = -0.1510$ eV



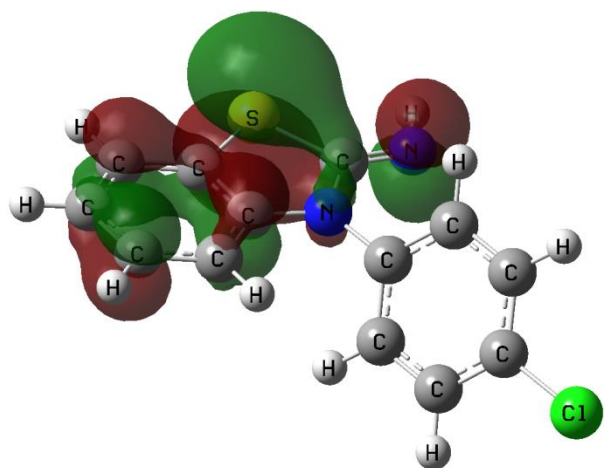
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HOMO (X=CH₃): $E = -6.9487$ eV



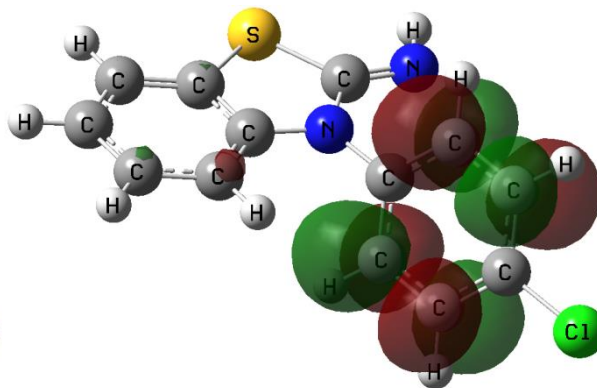
LUMO (X=CH₃): $E = -0.1524$ eV



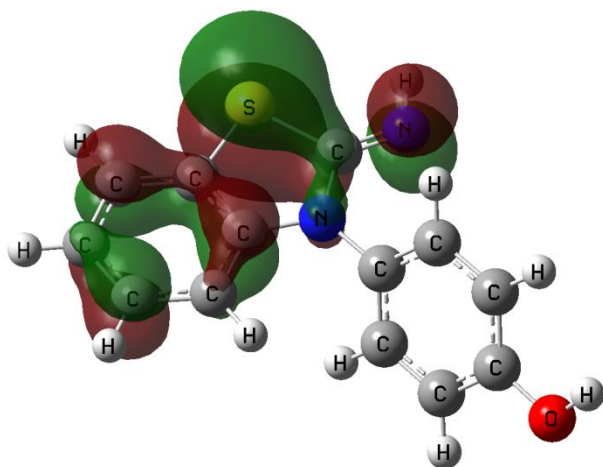
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HOMO (X=Cl): $E = -7.1438$ eV

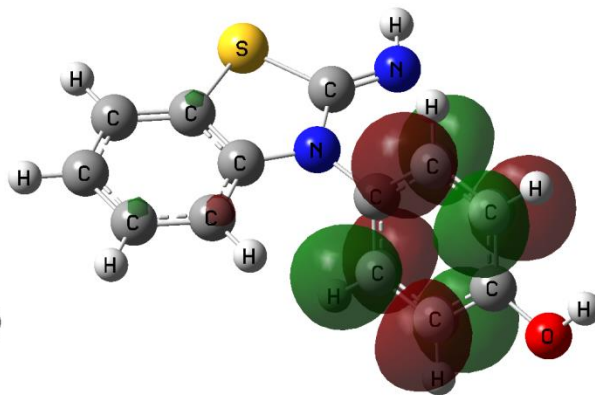


LUMO (X=Cl): $E = -0.3023$ eV

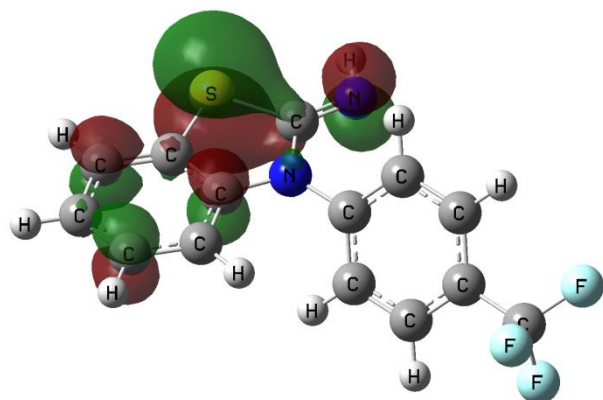


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38 HOMO (X=OH); $E = -6.9539$ eV

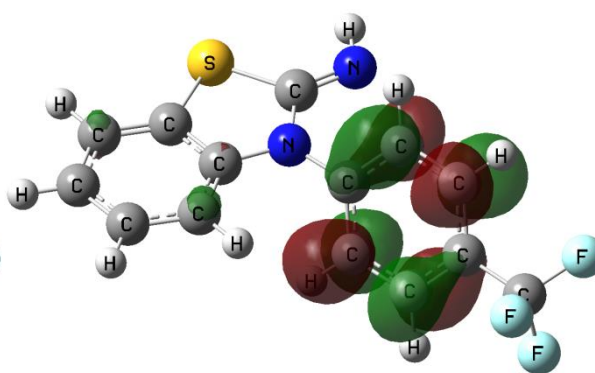


LUMO (X=OH); $E = -0.2171$ eV

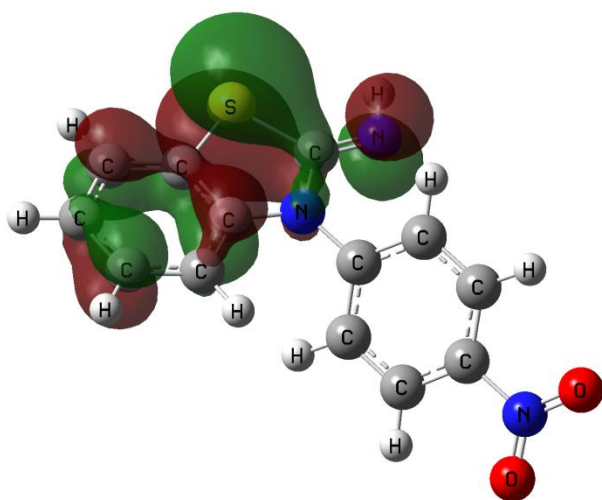


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40 HOMO (X=CF₃); $E = -7.2788$ eV



LUMO (X=CF₃); $E = -0.6332$ eV



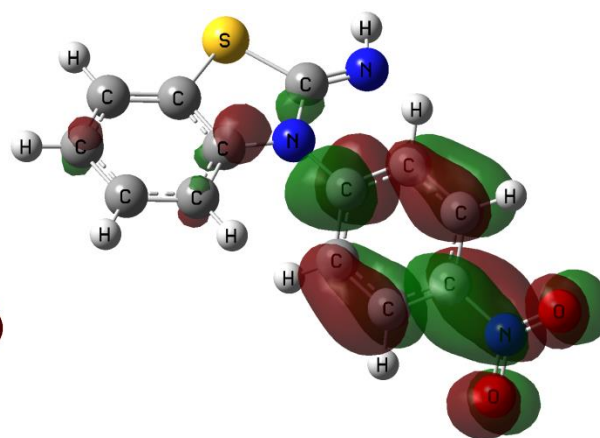
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42 HOMO (X=NO₂); $E = -7.4243$ eV

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44 **Fig. S-2.** The shapes of HOMO and LUMO orbitals of the considered compounds at the

45 M06-2x/6-311++G** level of theory.



LUMO (X=NO₂); $E = -1.7755$ eV

Table S-I. Calculated NBO charges on ring atoms of the 3-substituted 3-phenylbenzo[*d*]thiazole-2(3*H*)-imine and its derivatives

Table S-Ia. Summary of natural population analysis [**X=H**]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.22296	1.99921	4.20621	0.01753	6.22296
C	2	-0.19443	1.99923	4.17818	0.01702	6.19443
C	3	-0.24133	1.99911	4.22807	0.01415	6.24133
C	4	0.17376	1.99892	3.80749	0.01983	5.82624
C	5	-0.20438	1.99882	4.18611	0.01945	6.20438
C	6	-0.20846	1.99908	4.19084	0.01855	6.20846
N	7	-0.51340	1.99916	5.48747	0.02677	7.51340
C	8	0.33961	1.99929	3.62186	0.03924	5.66039
S	9	0.30698	9.99899	5.65736	0.03667	15.69302
N	10	-0.72158	1.99938	5.69661	0.02559	7.72158
C	11	0.15776	1.99899	3.82156	0.02169	5.84224
C	12	-0.21253	1.99909	4.19824	0.0152	6.21253
C	13	-0.20290	1.99921	4.18661	0.01708	6.20290
C	14	-0.20373	1.99921	4.18763	0.01689	6.20373
C	15	-0.19844	1.99921	4.18239	0.01684	6.19844
C	16	-0.18327	1.99908	4.16832	0.01586	6.18327
H	17	0.21462	0.00000	0.78399	0.00139	0.78538
H	18	0.21366	0.00000	0.78492	0.00143	0.78634
H	19	0.23215	0.00000	0.76618	0.00167	0.76785
H	20	0.22069	0.00000	0.77779	0.00152	0.77931
H	21	0.35294	0.00000	0.64442	0.00264	0.64706
H	22	0.22445	0.00000	0.77402	0.00153	0.77555
H	23	0.21352	0.00000	0.78497	0.0015	0.78648
H	24	0.21247	0.00000	0.78613	0.0014	0.78753
H	25	0.21386	0.00000	0.78463	0.00151	0.78614
H	26	0.23094	0.00000	0.76748	0.00158	0.76906

Table S-Ib. Summary of natural population analysis [**X=CH₃**]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.22365	1.99921	4.20688	0.01756	6.22365
C	2	-0.19486	1.99923	4.17861	0.01703	6.19486
C	3	-0.24142	1.99911	4.22812	0.01419	6.24142
C	4	0.17432	1.99892	3.80681	0.01995	5.82568
C	5	-0.20499	1.99883	4.18676	0.01940	6.20499
C	6	-0.20875	1.99908	4.19113	0.01855	6.20875
N	7	-0.51206	1.99916	5.48597	0.02694	7.51206
C	8	0.34003	1.99929	3.62143	0.03925	5.65997
S	9	0.3057	9.99899	5.65856	0.03676	15.69430
N	10	-0.722	1.99938	5.69699	0.02563	7.72200
C	11	0.14786	1.99898	3.83152	0.02164	5.85214
C	12	-0.20329	1.99909	4.18875	0.01545	6.20329
C	13	-0.20406	1.99910	4.18889	0.01607	6.20406
C	14	-0.02914	1.99910	4.01533	0.01471	6.02914
C	15	-0.1987	1.99910	4.18375	0.01585	6.19870
C	16	-0.17451	1.99909	4.15929	0.01614	6.17451
C	17	-0.59855	1.99933	4.58982	0.00940	6.59855
H	18	0.21433	0.00000	0.78428	0.00140	0.78567
H	19	0.2133	0.00000	0.78527	0.00143	0.78670
H	20	0.23211	0.00000	0.76621	0.00168	0.76789
H	21	0.2204	0.00000	0.77807	0.00152	0.77960
H	22	0.35237	0.00000	0.64498	0.00265	0.64763
H	23	0.22345	0.00000	0.77504	0.00151	0.77655
H	24	0.20964	0.00000	0.78875	0.00162	0.79036
H	25	0.21002	0.00000	0.78838	0.00159	0.78998
H	26	0.23004	0.00000	0.76839	0.00157	0.76996
H	27	0.21035	0.00000	0.78821	0.00144	0.78965
H	28	0.21452	0.00000	0.78403	0.00145	0.78548
H	29	0.21756	0.00000	0.78095	0.00148	0.78244

Table S-Ic. Summary of natural population analysis [**X=Cl**]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.22109	1.99921	4.20440	0.01747	6.22109
C	2	-0.19340	1.99923	4.17716	0.01702	6.19340
C	3	-0.24186	1.99911	4.22859	0.01416	6.24186
C	4	0.17195	1.99892	3.80921	0.01991	5.82805
C	5	-0.20450	1.99882	4.18622	0.01946	6.20450
C	6	-0.20733	1.99908	4.18973	0.01852	6.20733
N	7	-0.51398	1.99916	5.48806	0.02675	7.51398
C	8	0.33817	1.99929	3.62324	0.03930	5.66183
S	9	0.31156	9.99898	5.65272	0.03674	15.68844
N	10	-0.72168	1.99938	5.69671	0.02559	7.72168
C	11	0.15530	1.99899	3.82434	0.02138	5.84470
C	12	-0.19563	1.99909	4.18159	0.01495	6.19563
C	13	-0.22392	1.99902	4.20656	0.01834	6.22392
C	14	-0.04327	1.99862	4.02155	0.02311	6.04327
C	15	-0.21928	1.99902	4.20215	0.01811	6.21928
C	16	-0.16629	1.99909	4.15137	0.01583	6.16629
Cl	17	0.01100	9.99963	6.96890	0.02047	16.98900
H	18	0.21554	0.00000	0.78307	0.00139	0.78446
H	19	0.21468	0.00000	0.78390	0.00142	0.78532
H	20	0.23127	0.00000	0.76703	0.00170	0.76873
H	21	0.22148	0.00000	0.77700	0.00151	0.77852
H	22	0.35456	0.00000	0.64283	0.00261	0.64544
H	23	0.22930	0.00000	0.76922	0.00149	0.77070
H	24	0.23032	0.00000	0.76788	0.00180	0.76968
H	25	0.23065	0.00000	0.76756	0.00179	0.76935
H	26	0.23645	0.00000	0.76200	0.00155	0.76355

Table S-Id. Summary of natural population analysis [**X=OH**]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.22360	1.99921	4.20685	0.01755	6.22360
C	2	-0.19449	1.99923	4.17824	0.01703	6.19449
C	3	-0.24189	1.99911	4.22854	0.01423	6.24189
C	4	0.17411	1.99892	3.80697	0.01999	5.82589
C	5	-0.20493	1.99882	4.18669	0.01942	6.20493
C	6	-0.20861	1.99908	4.19098	0.01856	6.20861
N	7	-0.51070	1.99916	5.48458	0.02695	7.51070
C	8	0.33997	1.99929	3.62146	0.03928	5.66003
S	9	0.30587	9.99899	5.65844	0.03671	15.69413
N	10	-0.72398	1.99938	5.69893	0.02567	7.72398
C	11	0.12327	1.99898	3.85598	0.02178	5.87673
C	12	-0.18724	1.99910	4.17325	0.01489	6.18724
C	13	-0.25242	1.99911	4.23610	0.01721	6.25242
C	14	0.32693	1.99883	3.65071	0.02353	5.67307
C	15	-0.28023	1.99911	4.26460	0.01652	6.28023
C	16	-0.16015	1.99910	4.14484	0.01621	6.16015
O	17	-0.68134	1.99976	6.66855	0.01302	8.68134
H	18	0.21448	0.00000	0.78412	0.00140	0.78552
H	19	0.21358	0.00000	0.78499	0.00143	0.78642
H	20	0.23186	0.00000	0.76646	0.00168	0.76814
H	21	0.22049	0.00000	0.77798	0.00152	0.77951
H	22	0.35246	0.00000	0.64489	0.00265	0.64754
H	23	0.22536	0.00000	0.77316	0.00148	0.77464
H	24	0.22770	0.00000	0.77064	0.00165	0.77230
H	25	0.21035	0.00000	0.78779	0.00186	0.78965
H	26	0.23175	0.00000	0.76669	0.00156	0.76825
H	27	0.47143	0.00000	0.52407	0.00450	0.52857

Table S-Ie. Summary of natural population analysis [$\mathbf{X}=\mathbf{CF}_3$]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.21891	1.99921	4.20229	0.01742	6.21891
C	2	-0.19265	1.99922	4.17641	0.01701	6.19265
C	3	-0.24128	1.99911	4.22802	0.01414	6.24128
C	4	0.16989	1.99892	3.81136	0.01983	5.83011
C	5	-0.20340	1.99882	4.18507	0.01951	6.20340
C	6	-0.20667	1.99908	4.18910	0.01849	6.20667
N	7	-0.51524	1.99916	5.48973	0.02635	7.51524
C	8	0.33725	1.99929	3.62415	0.03930	5.66275
S	9	0.31535	9.99898	5.64897	0.03670	15.68465
N	10	-0.72088	1.99937	5.69594	0.02557	7.72088
C	11	0.17962	1.99899	3.80001	0.02137	5.82038
C	12	-0.20752	1.99910	4.19328	0.01514	6.20752
C	13	-0.17722	1.99913	4.16173	0.01636	6.17722
C	14	-0.14892	1.99895	4.13266	0.01731	6.14892
C	15	-0.17262	1.99913	4.15737	0.01612	6.17262
C	16	-0.17642	1.99909	4.16127	0.01605	6.17642
C	17	1.08796	1.99913	2.85246	0.06045	4.91204
F	18	-0.36172	1.99992	7.35506	0.00674	9.36172
F	19	-0.36189	1.99992	7.35526	0.00672	9.36189
F	20	-0.36055	1.99992	7.35384	0.00679	9.36055
H	21	0.21632	0.00000	0.78230	0.00138	0.78368
H	22	0.21558	0.00000	0.78300	0.00142	0.78442
H	23	0.23122	0.00000	0.76711	0.00168	0.76878
H	24	0.22221	0.00000	0.77628	0.00151	0.77779
H	25	0.35600	0.00000	0.64140	0.00260	0.64400
H	26	0.23042	0.00000	0.76807	0.00151	0.76958
H	27	0.23248	0.00000	0.76581	0.00171	0.76752
H	28	0.23267	0.00000	0.76564	0.00170	0.76733
H	29	0.23892	0.00000	0.75948	0.00160	0.76108

Table S-If. Summary of natural population analysis [$X=NO_2$]

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
C	1	-0.21652	1.99921	4.19995	0.01736	6.21652
C	2	-0.19189	1.99922	4.17566	0.01701	6.19189
C	3	-0.24080	1.99911	4.22754	0.01414	6.24080
C	4	0.16800	1.99892	3.81328	0.01980	5.83200
C	5	-0.20311	1.99882	4.18474	0.01955	6.20311
C	6	-0.20578	1.99908	4.18823	0.01847	6.20578
N	7	-0.51537	1.99917	5.49011	0.02609	7.51537
C	8	0.33565	1.99929	3.62569	0.03937	5.66435
S	9	0.32064	9.99898	5.64360	0.03678	15.67936
N	10	-0.71983	1.99937	5.69488	0.02558	7.71983
C	11	0.19328	1.99900	3.78675	0.02096	5.80672
C	12	-0.20947	1.99910	4.19549	0.01488	6.20947
C	13	-0.18653	1.99911	4.16929	0.01814	6.18653
C	14	0.06419	1.99880	3.91641	0.02060	5.93581
C	15	-0.18178	1.99911	4.16482	0.01785	6.18178
C	16	-0.17749	1.99910	4.16247	0.01592	6.17749
N	17	0.52074	1.99949	4.42127	0.05850	6.47926
O	18	-0.38935	1.99980	6.37322	0.01633	8.38935
O	19	-0.39247	1.99980	6.37635	0.01633	8.39247
H	20	0.21728	0.00000	0.78135	0.00137	0.78272
H	21	0.21654	0.00000	0.78205	0.00141	0.78346
H	22	0.23052	0.00000	0.76779	0.00168	0.76948
H	23	0.22303	0.00000	0.77547	0.00150	0.77697
H	24	0.35771	0.00000	0.63971	0.00257	0.64229
H	25	0.23340	0.00000	0.76508	0.00151	0.76660
H	26	0.25303	0.00000	0.74498	0.00198	0.74697
H	27	0.25314	0.00000	0.74489	0.00197	0.74686
H	28	0.24322	0.00000	0.75516	0.00162	0.75678

Table S-II. NICS values (in ppm) as a function of distance (in Å) for the 3-phenylbenzo[*d*]thiazole-2(3*H*)-imine and its derivatives at the M06-2x/6-311++G^{**} level of theory: isotropic chemical shift.

NICS, ppm	Phase	Compound 1 (X= H)				Compound 2 (X= CH ₃)			
		Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)	Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)
2.0	Gas	-4.6217	-1.5146	-4.4537	-10.5900	-4.6796	-1.5846	-4.2576	-10.5218
	Toluene	-4.2950	-1.4442	-4.5894	-10.3286	-4.5955	-1.5935	-4.1854	-10.3744
	Acetone	-4.5285	-1.3832	-4.5325	-10.4442	-4.5771	-1.4834	-4.1710	-10.2315
	Ethanol	-4.5081	-1.4660	-4.5328	-10.5069	-4.5562	-1.4956	-4.2113	-10.2631
1.5	Gas	-7.1722	-2.0861	-7.1897	-16.448	-7.2803	-2.0840	-6.8582	-16.2225
	Toluene	-6.8198	-2.0056	-7.2300	-16.0554	-7.1986	-2.0498	-6.8136	-16.0620
	Acetone	-7.1552	-1.8674	-7.2066	-16.2292	-7.1825	-1.9111	-6.8651	-15.9587
	Ethanol	-7.1078	-1.9474	-7.2317	-16.2869	-7.1425	-1.9225	-6.8546	-15.9196
1.0	Gas	-9.7105	-3.1773	-9.7558	-22.6436	-9.7869	-3.1028	-9.3313	-22.2210
	Toluene	-9.3577	-3.0824	-9.7729	-22.2130	-9.7275	-2.9356	-9.3519	-22.0150
	Acetone	-9.7522	-2.7948	-9.7675	-22.3145	-9.7202	-2.7381	-9.4464	-21.9047
	Ethanol	-9.7070	-2.8572	-9.8098	-22.3740	-9.6871	-2.7460	-9.4012	-21.8343
0.5	Gas	-9.6251	-4.6895	-9.3219	-23.6365	-9.5189	-4.7553	-8.9765	-23.2507
	Toluene	-9.3672	-4.5635	-9.3601	-23.2908	-9.5405	-4.5131	-9.0021	-23.0557
	Acetone	-9.6511	-4.2552	-9.3122	-23.2185	-9.5449	-4.2524	-9.0118	-22.8091
	Ethanol	-9.6485	-4.3077	-9.3255	-23.2817	-9.5463	-4.2510	-8.9992	-22.7965
0.0	Gas	-8.0102	-5.4891	-7.5476	-21.0469	-7.8825	-5.6676	-7.3470	-20.8971
	Toluene	-8.0260	-5.4198	-7.5399	-20.9857	-7.9679	-5.3677	-7.2553	-20.5909
	Acetone	-8.1074	-5.1744	-7.4336	-20.7154	-7.9860	-5.2698	-7.1951	-20.4509
	Ethanol	-8.1045	-5.1636	-7.4340	-20.7021	-7.9891	-5.2555	-7.2011	-20.4457
-0.5	Gas	-9.3195	-4.7736	-9.3764	-23.4695	-9.3556	-4.8678	-9.1387	-23.3621
	Toluene	-9.6110	-4.8469	-9.3544	-23.8123	-9.5149	-4.4802	-8.9907	-22.9858
	Acetone	-9.5762	-4.5207	-9.3241	-23.4210	-9.5540	-4.5705	-8.9850	-23.1095
	Ethanol	-9.5470	-4.4643	-9.3432	-23.3545	-9.5292	-4.5575	-8.9555	-23.0422
-1.0	Gas	-9.3223	-3.0900	-9.7775	-22.1898	-9.4463	-3.1218	-9.4708	-22.0389
	Toluene	-9.6890	-3.1799	-9.8100	-22.6789	-9.5736	-2.8404	-9.2951	-21.7091
	Acetone	-9.5506	-2.9145	-9.7841	-22.2492	-9.6188	-2.9230	-9.3682	-21.9100
	Ethanol	-9.5307	-2.8811	-9.8313	-22.2431	-9.5934	-2.9155	-9.2714	-21.7803
-1.5	Gas	-6.8060	-1.7926	-7.2211	-15.8197	-6.8632	-1.8705	-6.9403	-15.6740
	Toluene	-7.1479	-1.8402	-7.2340	-16.2221	-6.9291	-1.7278	-6.8916	-15.5485
	Acetone	-6.8996	-1.7148	-7.1579	-15.7723	-6.9726	-1.8112	-6.8048	-15.5886
	Ethanol	-6.9128	-1.6737	-7.1805	-15.7670	-6.9857	-1.8015	-6.7372	-15.5244
-2.0	Gas	-4.2921	-1.1560	-4.5723	-10.0204	-4.2886	-1.2338	-4.3525	-9.8749
	Toluene	-4.5971	-1.1743	-4.4791	-10.2505	-4.3248	-1.1589	-4.0689	-9.5526
	Acetone	-4.3068	-1.1244	-4.3748	-9.80600	-4.3612	-1.2565	-4.1913	-9.8090
	Ethanol	-4.3291	-1.0720	-4.3661	-9.7672	-4.3886	-1.2448	-4.1742	-9.8076

Continued Table S-II.

NICS, ppm	Phase	Compound 3 (X= Cl)				Compound 4 (X= OH)			
		Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)	Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)
2.0	Gas	-4.6681	-1.5628	-4.0381	-10.2690	-4.7094	-1.7457	-4.0738	-10.5289
	Toluene	-4.6665	-1.6598	-4.0823	-10.4086	-4.6473	-1.5785	-4.0031	-10.2289
	Acetone	-4.6309	-1.5836	-4.0536	-10.2681	-4.5602	-1.4586	-4.0422	-10.0610
	Ethanol	-4.5402	-1.4353	-4.2966	-10.2721	-4.5821	-1.4760	-4.0298	-10.0879
1.5	Gas	-7.2014	-2.0954	-6.6640	-15.9608	-7.3057	-2.4003	-6.6736	-16.3796
	Toluene	-7.2568	-2.1913	-6.6854	-16.1335	-7.2678	-2.1900	-6.6514	-16.1092
	Acetone	-7.2512	-2.0519	-6.7064	-16.0095	-7.2415	-2.0276	-6.7314	-16.0005
	Ethanol	-7.1267	-2.0341	-7.2034	-16.3642	-7.2516	-2.0512	-6.7240	-16.0268
1.0	Gas	-9.6856	-3.2194	-9.3089	-22.2139	-9.8479	-3.6477	-9.0224	-22.5180
	Toluene	-9.7555	-3.2687	-9.3198	-22.3440	-9.8214	-3.3207	-9.3572	-22.4993
	Acetone	-9.7947	-2.9820	-9.4063	-22.1830	-9.8998	-3.1455	-9.5258	-22.5711
	Ethanol	-9.7166	-3.1670	-9.9286	-22.8122	-9.8857	-3.1751	-9.5096	-22.5704
0.5	Gas	-9.5120	-4.9156	-9.3773	-23.8049	-9.6588	-5.3680	-9.6266	-24.6534
	Toluene	-9.5310	-4.9931	-9.3822	-23.9063	-9.6653	-4.9427	-9.5989	-24.2069
	Acetone	-9.5995	-4.6078	-9.4719	-23.6792	-9.7694	-4.7929	-9.7998	-24.3621
	Ethanol	-9.6751	-4.8435	-9.2333	-23.7519	-9.7504	-4.8212	-9.7707	-24.3423
0.0	Gas	-7.8765	-5.8902	-8.0624	-21.8291	-8.0422	-6.2165	-8.6032	-22.8619
	Toluene	-7.9215	-5.7879	-8.0107	-21.7201	-8.0993	-5.9672	-8.4406	-22.5071
	Acetone	-8.0107	-5.5190	-7.9977	-21.5274	-8.1710	-5.7060	-8.5125	-22.3895
	Ethanol	-8.1428	-5.8223	-7.1347	-21.0998	-8.1589	-5.7133	-8.4852	-22.3574
-0.5	Gas	-9.2556	-5.2727	-9.5289	-24.0572	-9.4764	-5.4703	-9.7847	-24.7314
	Toluene	-9.3926	-4.8301	-9.4502	-23.6729	-9.6168	-5.3942	-9.6601	-24.6711
	Acetone	-9.5688	-4.6444	-9.4202	-23.6334	-9.7630	-4.8805	-9.6745	-24.3180
	Ethanol	-9.5993	-4.9761	-8.3892	-22.9646	-9.7343	-4.8686	-9.7068	-24.3097
-1.0	Gas	-9.3146	-3.4136	-9.4464	-22.1746	-9.5338	-3.6143	-9.4197	-22.5678
	Toluene	-9.4574	-3.0583	-9.3680	-21.8837	-9.6447	-3.5581	-9.3829	-22.5857
	Acetone	-9.6439	-2.9303	-9.3398	-21.9140	-9.8477	-3.1890	-9.3784	-22.4151
	Ethanol	-9.6235	-3.1776	-8.3825	-21.1836	-9.8098	-3.1729	-9.4646	-22.4473
-1.5	Gas	-6.8322	-1.9890	-6.7578	-15.579	-6.9197	-2.0288	-6.7293	-15.6778
	Toluene	-6.8752	-1.8077	-6.7204	-15.4033	-6.9733	-2.0325	-6.6954	-15.7012
	Acetone	-6.9926	-1.7763	-6.6763	-15.4452	-7.1597	-2.0090	-6.6727	-15.8414
	Ethanol	-7.0321	-1.9018	-5.9164	-14.8503	-7.1302	-1.9928	-6.7297	-15.8527
-2.0	Gas	-4.3250	-1.2899	-4.1572	-9.7721	-4.3209	-1.2282	-4.1826	-9.7317
	Toluene	-4.3113	-1.1861	-4.1578	-9.6552	-4.3546	-1.2863	-4.1219	-9.7628
	Acetone	-4.3740	-1.2191	-4.1041	-9.6972	-4.4935	-1.4191	-4.0970	-10.0096
	Ethanol	-4.4458	-1.2972	-3.5713	-9.3143	-4.4758	-1.4024	-4.1087	-9.9869

Continued Table S-II.

NICS, ppm	Phase	Compound 5 (R= CF ₃)				Compound 6 (R= NO ₂)			
		Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)	Ring (6) benzo	Ring (5) thiazole	Ring (6) phenyl	Rings (6+5+6)
2.0	Gas	-4.7764	-1.6698	-4.3416	-10.7878	-4.7860	-1.6952	-4.4284	-10.9096
	Toluene	-4.6909	-1.5222	-4.3154	-10.5285	-4.7806	-1.6872	-4.3765	-10.8443
	Acetone	-4.6578	-1.5445	-4.2791	-10.4814	-4.7183	-1.4753	-4.3726	-10.5662
	Ethanol	-4.7110	-1.6052	-4.2784	-10.5946	-4.7614	-1.6647	-4.3651	-10.7912
1.5	Gas	-7.3988	-2.2247	-7.0312	-16.6547	-7.4891	-2.2215	-7.0933	-16.8039
	Toluene	-7.2081	-2.0835	-6.9915	-16.2831	-7.4679	-2.2036	-7.1223	-16.7938
	Acetone	-7.2033	-2.0777	-6.9553	-16.2363	-7.2514	-1.9962	-7.0993	-16.3469
	Ethanol	-7.3038	-2.1106	-6.9598	-16.3742	-7.4179	-2.1566	-7.0828	-16.6573
1.0	Gas	-9.8903	-3.3930	-9.6912	-22.9745	-10.0383	-3.3860	-9.8248	-23.2491
	Toluene	-9.6709	-3.2519	-9.6516	-22.5744	-10.0074	-3.3465	-9.9034	-23.2573
	Acetone	-9.6767	-3.1077	-9.6472	-22.4316	-9.7023	-3.1225	-9.8662	-22.6910
	Ethanol	-9.7838	-3.0890	-9.6559	-22.5287	-9.9365	-3.2173	-9.8379	-22.9917
0.5	Gas	-9.5401	-5.1370	-9.5681	-24.2452	-9.5849	-5.1226	-10.0049	-24.7124
	Toluene	-9.5060	-4.9890	-9.5554	-24.0504	-9.5880	-5.0746	-10.0145	-24.6771
	Acetone	-9.5103	-4.8049	-9.5971	-23.9123	-9.5044	-4.9364	-9.9870	-24.4278
	Ethanol	-9.5310	-4.7102	-9.6019	-23.8431	-9.5788	-4.8934	-9.9441	-24.4163
0.0	Gas	-7.8398	-6.0651	-8.1246	-22.0295	-7.8252	-6.0740	-8.6750	-22.5742
	Toluene	-7.8940	-5.9687	-8.0934	-21.9561	-7.8684	-6.0226	-8.6578	-22.5488
	Acetone	-7.9521	-5.7006	-8.1007	-21.7534	-7.9199	-5.8775	-8.5944	-22.3918
	Ethanol	-7.9482	-5.7010	-8.0942	-21.7434	-7.9225	-5.8506	-8.5410	-22.3141
-0.5	Gas	-9.2892	-5.4553	-9.9172	-24.6617	-9.3353	-5.6113	-10.0874	-25.0340
	Toluene	-9.2785	-5.3408	-9.8329	-24.4522	-9.3847	-5.5449	-10.1003	-25.0299
	Acetone	-9.4378	-4.7759	-9.7833	-23.9970	-9.3375	-4.9497	-9.9816	-24.2688
	Ethanol	-9.4756	-5.0680	-9.7700	-24.3136	-9.4461	-5.3594	-9.9403	-24.7458
-1.0	Gas	-9.4275	-3.5519	-10.0560	-23.0354	-9.5453	-3.7051	-9.9428	-23.1932
	Toluene	-9.3261	-3.4451	-9.9313	-22.7025	-9.5602	-3.6541	-9.9960	-23.2103
	Acetone	-9.4878	-3.0016	-9.8462	-22.3356	-9.3709	-3.1000	-9.8634	-22.3343
	Ethanol	-9.5420	-3.2870	-9.8434	-22.6724	-9.5639	-3.5248	-9.8354	-22.9241
-1.5	Gas	-6.8642	-1.9845	-7.3348	-16.1835	-6.9204	-2.0799	-7.1695	-16.1698
	Toluene	-6.8310	-1.9733	-7.1842	-15.9885	-6.9216	-2.0511	-7.2112	-16.1839
	Acetone	-6.9114	-1.8002	-7.0990	-15.8106	-6.8397	-1.8647	-7.1235	-15.8279
	Ethanol	-6.9098	-1.8985	-7.1011	-15.9094	-6.9152	-1.9909	-7.1072	-16.0133
-2.0	Gas	-4.2885	-1.2014	-4.6150	-10.1049	-4.2845	-1.2753	-4.5061	-10.0659
	Toluene	-4.3180	-1.2372	-4.4740	-10.0292	-4.2878	-1.2548	-4.5134	-10.056
	Acetone	-4.3423	-1.1925	-4.4077	-9.9425	-4.3149	-1.2554	-4.4633	-10.0336
	Ethanol	-4.3089	-1.1919	-4.4078	-9.9086	-4.2946	-1.2264	-4.4560	-9.9770