Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 85 (11) S533–S541 (2020)
Supplementary material

SUPPLEMENTARY MATERIAL TO

DFT study and NBO analysis of solvation/substituent effects of 3-phenylbenzo[*d*]thiazole-2(3*H*)-imine derivatives

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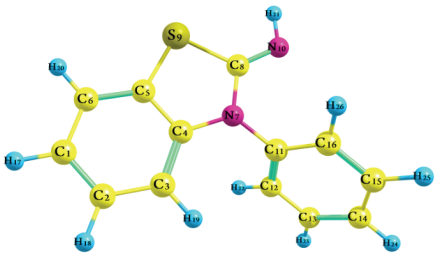
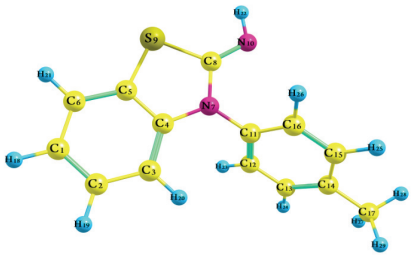
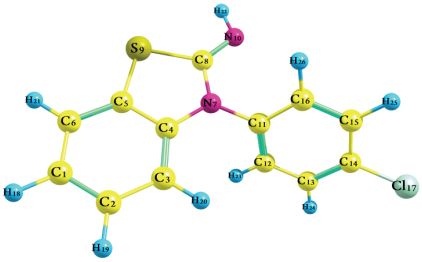
J. Serb. Chem. Soc. 85 (11) (2020) 1445–1462



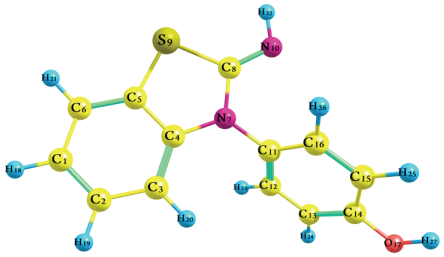
3-phenylbenzo[*d*]thiazol-2(3*H*)-imine [**R=H**]



3-(*p*-tolyl)benzo[*d*]thiazol-2(3*H*)-imine [**R=CH$_3$**]



3-(4-chlorophenyl)benzo[*d*]thiazol- yl)phenol [**R=OH**]4-(2-iminobenzo[*d*]thiazol-3(2*H*)- 2(3*H*)-imine [**R=Cl**]



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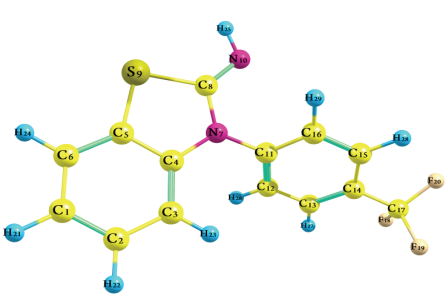
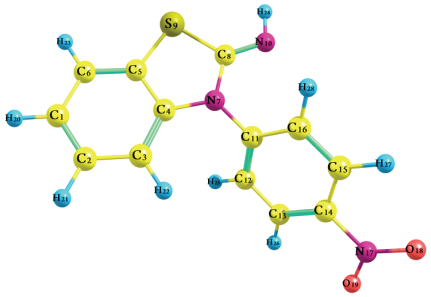
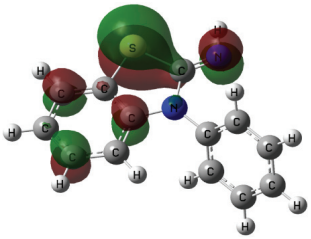


3-(4-(trifluoromethyl)phenyl)benzo[*d*]thiazol--2(3*H*)-imine [**R=CF$_3$**]

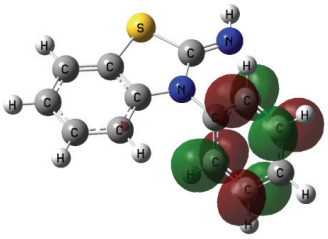


3-(4-nitrophenyl)benzo[*d*]thiazol-2(3*H*)-imine [**R=NO$_2$**]

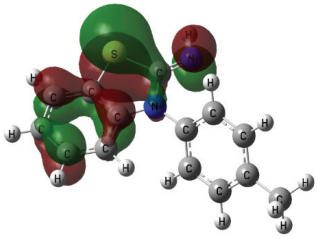
Fig. S-1. The optimized molecular structure of the compounds **1**–**6**.



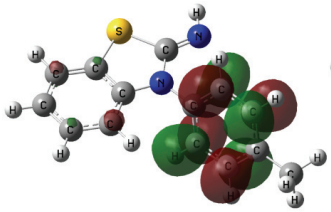
HOMO (R=H): E = –7.0096 eV



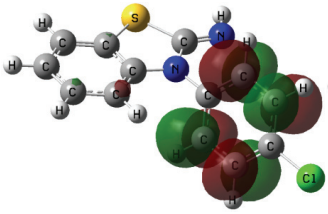
LUMO (R=H): E = –0.1510 eV



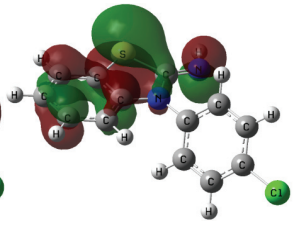
HOMO (R=CH$_3$): E = –6.9487 eV



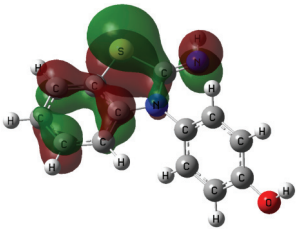
LUMO (R=CH$_3$): E = –0.1524 eV



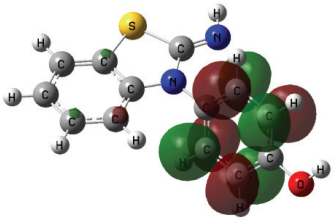
HOMO (R=Cl); E = –7.1438 eV



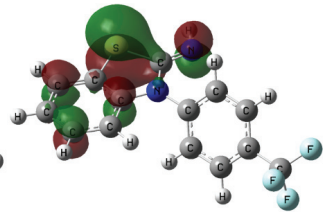
LUMO (R=Cl); E = –0.3023 eV



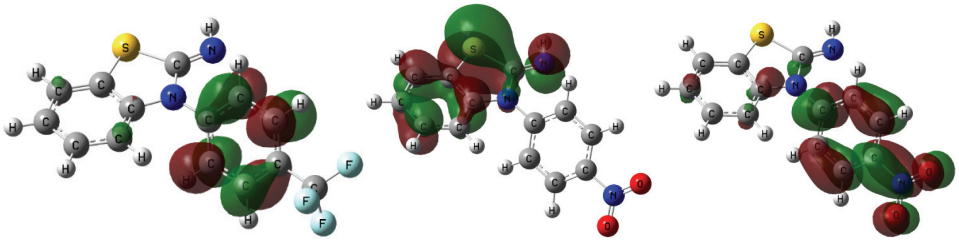
HOMO (R=OH); E = –6.9539 eV



LUMO (R=OH); E = –0.2171 eV



HOMO (R=CF$_3$); E = –7.2788 eV



LUMO (R=CF_3); E = –0.6332 eV HOMO (R=NO_2); E = –7.4243 eV LUMO (R=NO_2); E = –1.7755 eV

Fig. S-2. The shapes of the HOMO and LUMO orbitals of compounds **1**–**6** at the M06-2x/6-311++G** level of theory.

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

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
			R=H			
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
			R=CH_3			
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

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
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
			R=Cl			
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

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
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
			R=OH			
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
			R=CF_3			
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

Atom	No	Natural charge	Natural population			
			Core	Valence	Rydberg	Total
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
			$R=NO_2$			
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

Distance, Å	Phase	*NICS* / ppm							
		Compound **1** (R= H)				Compound **2** (R= 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
		Compound **3** (R= Cl)				Compound **4** (R= OH)			
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

Distance, Å	Phase	*NICS* / ppm							
		Compound **1** (R= H)				Compound **2** (R= 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)
	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

Distance, Å	Phase	*NICS* / ppm							
		Compound **1** (R= H)				Compound **2** (R= 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)
		Compound **5** (R= CF_3)				Compound **6** (R= NO_2)			
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