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Experimental and Theoretical Study of Antioxidative Properties of Some Salicylaldehyde and Vanillic Schiff Bases

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Table S1 Interaction of the examined and reference compounds with the stable free radical DPPH, after 30 and 60 minutes

	1		**2**		**3**		**4**		**5**		**6**		**7**		**8**		**9**		**10**		**NDGA**	
	Inhibition of DPPH %																					
Concentration umol/ml	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**	**30`**	**30`**	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**	**30`**	**60`**
300	64.6	79.1	5.6	9.0	5.8	12.3	6.6	8.4	7.3	9.2	33.1	34.1	/	/	/	/	76.8	84.2	82.1	85.8	/	/
250	61.9	76.9	5.1	8.5	5.7	9.9	5.8	7.5	5.6	7.6	27.9	29.0	/	/	/	/	73.5	79.7	78.1	84.1	/	/
200	54.3	67.0	3.5	7.4	5.2	8.1	5.7	7.7	5.5	7.4	26.3	27.5	/	/	/	/	66.6	76.6	72.0	73.1	/	/
150	48.4	58.3	4.2	7.3	4.9	7.2	5.2	7.1	4.3	7.1	21.4	22.6	/	/	/	/	59.3	68.2	65.6	74.0	/	/
100	41.1	53.0	3.1	6.3	4.8	6.8	5.5	6.5	3.7	4.4	18.0	19.3	92.1	93.1	91.9	95.6	48.2	58.0	53.9	60.6	96.2	96.2
50	30.4	38.0	2.2	6.1	4.2	6.4	4.6	5.6	2.4	4.1	9.8	11.3	77.2	80.1	91.5	93.9	34.6	43.3	39.1	51.0	94.8	95.9
10	14.0	28.3	0.1	3.4	2.7	5.9	3.7	5.5	0.8	2.8	7.5	9.0	30.0	40.2	79.7	88.4	10.5	43.0	13.7	23.1	90.1	91.4

Table S2. Some selected structural parameters: bond lengths and bond angles for (**1**)

	EXP	Molecule			Radical cation			RadicalA			RadicalB			Anion A			Anion B		
		water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol
O(2)-C(2)	1.316	1.344	1.341	1.344	1.329	1.321	1.329	1.239	1.23562	1.239	1.341	1.338	1.341	1.267	1.253	1.266	1.346	1.343	1.346
O(4')-C(4')	1.353	1.364	1.364	1.364	1.315	1.318	1.315	1.363	1.36297	1.363	1.245	1.241	1.245	1.370	1.376	1.370	1.278	1.263	1.278
N(1)-C(1')	1.416	1.411	1.411	1.411	1.352	1.350	1.352	1.407	1.40462	1.407	1.381	1.383	1.381	1.408	1.400	1.408	1.404	1.393	1.403
N(1)-C(7)	1.288	1.280	1.279	1.280	1.310	1.316	1.311	1.276	1.27446	1.276	1.291	1.290	1.291	1.284	1.442	1.284	1.282	1.285	1.282
C(1)-C(2)	1.422	1.410	1.410	1.410	1.424	1.431	1.424	1.469	1.46967	1.469	1.413	1.412	1.413	1.448	1.454	1.448	1.411	1.412	1.411
C(2)-C(3)	1.385	1.394	1.395	1.394	1.396	1.398	1.396	1.455	1.45556	1.455	1.394	1.395	1.395	1.440	1.448	1.441	1.394	1.394	1.394
C(3)-C(4)	1.359	1.385	1.384	1.385	1.379	1.376	1.379	1.364	1.36421	1.364	1.384	1.383	1.384	1.374	1.370	1.374	1.387	1.388	1.387
C(4)-C(5)	1.391	1.396	1.397	1.396	1.407	1.413	1.407	1.410	1.40984	1.410	1.399	1.399	1.399	1.407	1.411	1.407	1.395	1.394	1.395
C(5)-C(6)	1.366	1.383	1.382	1.383	1.370	1.365	1.370	1.397	1.39496	1.397	1.379	1.379	1.379	1.379	1.378	1.379	1.385	1.386	1.385
C(6)-C(1)	1.397	1.401	1.401	1.401	1.416	1.421	1.416	1.383	1.38471	1.383	1.405	1.405	1.405	1.410	1.410	1.410	1.400	1.399	1.400
C(1)-C(7)	1.422	1.455	1.454	1.455	1.418	1.409	1.417	1.458	1.45723	1.458	1.443	1.443	1.443	1.448	1.442	1.448	1.458	1.458	1.458
C(1')-C(6')	1.380	1.396	1.396	1.396	1.428	1.428	1.428	1.398	1.39813	1.398	1.419	1.418	1.419	1.399	1.401	1.399	1.401	1.406	1.401
C(1')-C(2')	1.393	1.395	1.394	1.395	1.429	1.428	1.429	1.398	1.39719	1.398	1.420	1.419	1.420	1.398	1.399	1.398	1.404	1.409	1.405
C(2')-C(3')	1.373	1.389	1.389	1.389	1.360	1.362	1.360	1.388	1.38806	1.388	1.362	1.363	1.362	1.391	1.392	1.391	1.380	1.374	1.380
C(3')-C(4')	1.387	1.391	1.390	1.391	1.419	1.417	1.419	1.392	1.39122	1.392	1.452	1.453	1.452	1.389	1.387	1.389	1.433	1.443	1.434
C(4')-C(5')	1.390	1.392	1.392	1.392	1.417	1.414	1.417	1.393	1.39251	1.393	1.451	1.452	1.451	1.392	1.391	1.392	1.430	1.437	1.430
C(5')-C(6')	1.372	1.385	1.384	1.385	1.359	1.360	1.359	1.384	1.38292	1.384	1.361	1.361	1.361	1.386	1.385	1.386	1.381	1.376	1.381
O(4')-H(4')		0.961	0.960	0.961	0.967	0.965	0.966	0.961	0.96025	0.961				0.961	0.959	0.961			
O(2)-H(2)		0.993	0.989	0.992	0.985	0.985	0.985				0.987	0.985	0.987				1.000	1.003	1.000
D_{ii} (O2-H--N1)		1.718	1.740	1.719	1.766	1.765	1.766				1.748	1.763	1.749				1.681	1.672	1.681
Angles	EXP	Molecule			Radical cation			RadicalA			RadicalB			Anion A			Anion B		
		water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol
C(7)-N(1)-C(1')	126.4	120.1	119.9	120.1	122.5	122.6	122.5	118.1	118.3	118.1	121.3	121.1	121.3	116.8	117.0	116.8	123.1	124.8	123.1
O(2)-C(2)-C(1)	120.5	121.6	121.9	121.7	122.4	122.4	122.4	123.3	123.3	123.3	122.0	122.2	122.0	124.4	124.6	124.4	119.0	121.1	121.2
C(3)-C(2)-C(1)	118.6	119.6	119.5	119.6	119.3	119.3	119.3	117.0	116.8	117.0	119.5	119.4	119.5	115.0	114.5	114.9	119.8	119.8	119.8
O(2)-C(2)-C(3)	120.9	118.7	118.6	118.7	118.3	118.3	118.3	119.8	119.9	119.8	118.5	122.2	118.5	120.6	120.9	120.6	119.0	119.0	119.0
C(2)-C(3)-C(4)	121.3	120.1	120.1	120.1	119.9	119.8	119.9	121.8	121.8	121.8	120.0	120.1	120.1	123.1	123.2	123.1	120.2	120.4	120.2
C(3)-C(4)-C(5)	121.0	121.0	121.0	121.0	121.7	121.9	121.7	119.8	119.9	119.8	121.2	121.2	121.2	121.1	121.3	121.1	120.7	120.5	120.7
C(4)-C(5)-C(6)	119.0	119.1	119.0	119.0	119.1	119.2	119.1	120.6	120.6	120.6	119.0	119.0	119.0	117.9	117.7	117.9	119.2	119.2	119.2

C(5)-C(6)-C(1)	121.6	121.1	121.2	121.1	120.9	120.8	120.9	121.9	121.9	121.9	121.1	121.2	121.1	123.0	123.2	123.0	121.3	121.6	121.3
C(6)-C(1)-C(7)	120.8	119.4	119.3	119.4	118.6	118.8	118.7	117.1	117.4	117.1	119.0	119.0	119.0	115.2	115.5	115.2	119.8	120.0	119.8
C(2)-C(1)-C(7)	120.7	121.5	121.5	121.5	122.2	122.1	122.2	124.1	123.7	124.1	121.9	121.8	121.9	124.8	124.4	124.8	121.4	121.4	121.4
C(2)-C(1)-C(6)	118.6	119.1	119.2	119.1	119.2	119.0	119.1	118.8	118.9	118.8	119.2	119.2	119.2	120.0	120.1	120.0	118.8	118.5	118.8
N(1)-C(7)-C(1)	122.4	121.9	122.2	121.9	121.7	121.8	121.7	124.9	124.5	124.8	121.9	122.2	121.9	128.4	128.5	128.4	121.4	121.2	121.4
C(2')-C(1')-C(6')	118.6	119.1	119.0	119.1	119.2	118.8	119.2	118.8	118.8	118.8	119.7	119.7	119.7	118.1	117.8	118.1	117.7	117.4	117.7
N(1)-C(1')-C(2')	124.0	123.0	122.8	123.0	124.1	124.6	124.2	123.7	123.7	123.7	123.3	123.1	123.2	123.2	123.4	123.2	124.9	125.5	124.9
N(1)-C(1')-C(6')	117.4	117.9	118.1	117.9	116.7	116.5	116.7	117.5	117.5	117.5	117.0	117.2	117.0	118.7	118.7	118.7	117.4	117.1	117.4
C(1')-C(2')-C(3')	120.6	120.4	120.4	120.4	120.2	120.3	120.2	120.6	120.5	120.6	120.3	120.3	120.3	121.0	121.0	121.0	121.0	121.2	121.1
C(2')-C(3')-C(4')	120.4	119.9	119.9	119.9	119.6	119.7	119.6	119.9	119.9	119.9	121.3	121.3	121.3	119.9	120.0	119.9	122.6	122.7	122.6
O(4')-C(4')-C(5')	117.8	117.5	117.5	117.5	116.8	116.8	116.8	117.5	117.4	117.5	121.7	121.7	121.7	117.6	117.8	117.7	122.8	123.1	122.8
O(4')-C(4')-C(3')	123.0	122.4	122.5	122.4	122.2	122.3	122.2	122.4	122.4	122.4	121.4	121.4	121.4	122.5	122.4	122.5	122.3	122.3	122.3
C(3')-C(4')-C(5')	119.2	120.1	120.1	120.1	121.0	120.9	121.0	120.1	120.1	120.1	116.9	116.8	116.9	119.9	119.8	119.9	114.9	114.6	114.9
C(4')-C(5')-C(6')	119.9	119.7	119.8	119.7	119.2	119.2	119.2	119.7	119.7	119.7	120.9	121.0	120.9	119.8	119.8	119.8	122.0	121.9	122.0
C(1')-C(6')-C(5')	121.3	120.7	120.8	120.7	120.8	121.0	120.8	120.9	120.9	120.9	120.8	120.8	120.8	121.2	121.4	121.2	121.8	122.2	121.8
τ (C1'-N1-C7-C1)	176.5	177.7	177.6	177.7	-172.1	-172.5	-172.1	178.8	178.7	178.8	176.2	176.2	176.2	177.0	176.7	177.0	178.1	180.0	178.1
τ (C7-N1-C1'-C6')	169.0	145.5	143.4	145.4	-159.9	-162.9	-160.1	146.9	146.7	146.8	152.2	150.5	152.1	139.4	139.1	139.4	163.4	180.0	163.7
τ (C6-C1-C7-N1)	-178.9	179.8	179.4	179.8	-179.5	-179.3	-179.5	165.4	164.0	165.4	179.7	179.5	179.7	175.7	176.2	175.7	179.6	180.0	179.6

Table S3. Some selected structural parameters: bond lengths and bond angles for (**7**)

	EXP		Molecule			Radical cation			RadicalA			RadicalB			Anion A			Anion B		
	A	B	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol
C(1')-C(6')	1.388	1.384	1.402	1.401	1.402	1.449	1.450	1.449	1.404	1.410	1.408	1.468	1.468	1.468	1.407	1.411	1.407	1.441	1.448	1.441
C(1)-C(2)	1.422	1.420	1.410	1.409	1.410	1.427	1.426	1.428	1.469	1.475	1.474	1.412	1.412	1.412	1.450	1.456	1.450	1.412	1.414	1.412
C(2)-C(3)	1.403	1.411	1.395	1.394	1.395	1.397	1.395	1.397	1.455	1.457	1.456	1.395	1.396	1.395	1.442	1.448	1.442	1.395	1.397	1.395
C(6')-C(5')	1.377	1.379	1.389	1.388	1.389	1.399	1.402	1.399	1.389	1.391	1.389	1.448	1.449	1.448	1.386	1.386	1.386	1.430	1.439	1.431
N(1)-C(7)	1.288	1.284	1.280	1.282	1.280	1.312	1.315	1.313	1.275	1.276	1.275	1.286	1.284	1.286	1.288	1.286	1.288	1.280	1.279	1.280
C(1')-C(2')	1.378	1.373	1.394	1.394	1.401	1.418	1.412	1.418	1.397	1.399	1.398	1.387	1.387	1.387	1.395	1.394	1.395	1.397	1.398	1.397
C(1)-C(6)																				
C(4')-C(5')	1.401	1.400	1.401	1.402	1.394	1.418	1.420	1.418	1.382	1.388	1.385	1.403	1.403	1.403	1.413	1.411	1.413	1.399	1.398	1.399
C(3)-C(4)	1.369	1.361	1.390	1.389	1.390	1.370	1.367	1.371	1.390	1.386	1.388	1.363	1.364	1.363	1.393	1.394	1.393	1.381	1.376	1.381
O(2)-H(2)	1.359	1.347	1.385	1.384	1.385	1.378	1.378	1.378	1.365	1.362	1.363	1.363	1.383	1.384	1.372	1.369	1.372	1.387	1.386	1.387
O(6')-H(6')			0.984	0.982	0.984	0.974	0.973	0.974				0.990	0.986	0.990				1.013	1.011	1.013
D_H (O2-H--N1)			0.965	0.964	0.965	0.972	0.971	0.972	0.976	0.976	0.976				0.973	0.981	0.974			
D_H (O6'-H--N1)			1.777	1.786	1.777	1.860	1.859	1.861				1.728	1.762	1.730				1.627	1.660	1.628
Angles	EXP		Molecule			Radical cation			RadicalA			RadicalB			Anion A			Anion B		
	A	B	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol	water	benzene	methanol
C(6')-C(1')-N(1)	117.1	116.8	117.7	116.8	117.7	115.7	115.2	115.7	118.3	112.4	112.4	116.3	116.4	116.3	114.4	112.7	114.4	115.5	114.9	115.5
C(2)-C(1)-C(7)	120.9	120.6	121.3	121.9	121.3	122.1	122.8	122.0	124.2	123.5	123.6	121.5	121.5	121.5	124.8	123.4	124.7	120.8	120.8	120.8
O(6')-C(6')-C(1')	117.3	117.8	117.4	120.9	117.4	122.6	119.8	116.0	117.7	119.5	119.1	121.3	116.4	121.3	118.4	118.0	118.4	122.6	122.9	122.6
O(2)-C(2)-C(1)	121.3	121.7	121.7	122.0	121.7	116.0	122.5	122.6	123.3	123.8	123.7	122.0	122.5	122.0	124.5	124.6	124.5	121.3	121.9	121.3
N(1)-C(7)-C(1)	123.2	122.9	121.5	123.0	121.5	121.0	123.7	121.0	125.0	122.6	122.8	121.6	122.0	121.7	127.9	126.3	124.5	120.3	120.2	120.3
C(7)-N(1)-C(1')	127.2	127.0	120.3	119.4	120.3	122.7	121.3	122.7	117.6	124.2	123.6	120.9	120.9	120.9	118.8	121.2	127.9	124.0	125.3	124.0
C(3)-C(2)-C(1)	116.8	116.0	119.5	119.6	119.5	119.2	119.5	119.2	117.0	116.7	116.8	119.4	119.3	119.4	114.9	114.4	114.9	119.5	119.2	119.5
C(5')-C(6')-C(1')	119.5	119.1	120.2	120.2	120.2	120.6	121.0	120.6	120.2	120.4	120.6	117.1	116.9	117.1	121.2	121.0	121.2	114.9	114.5	114.8

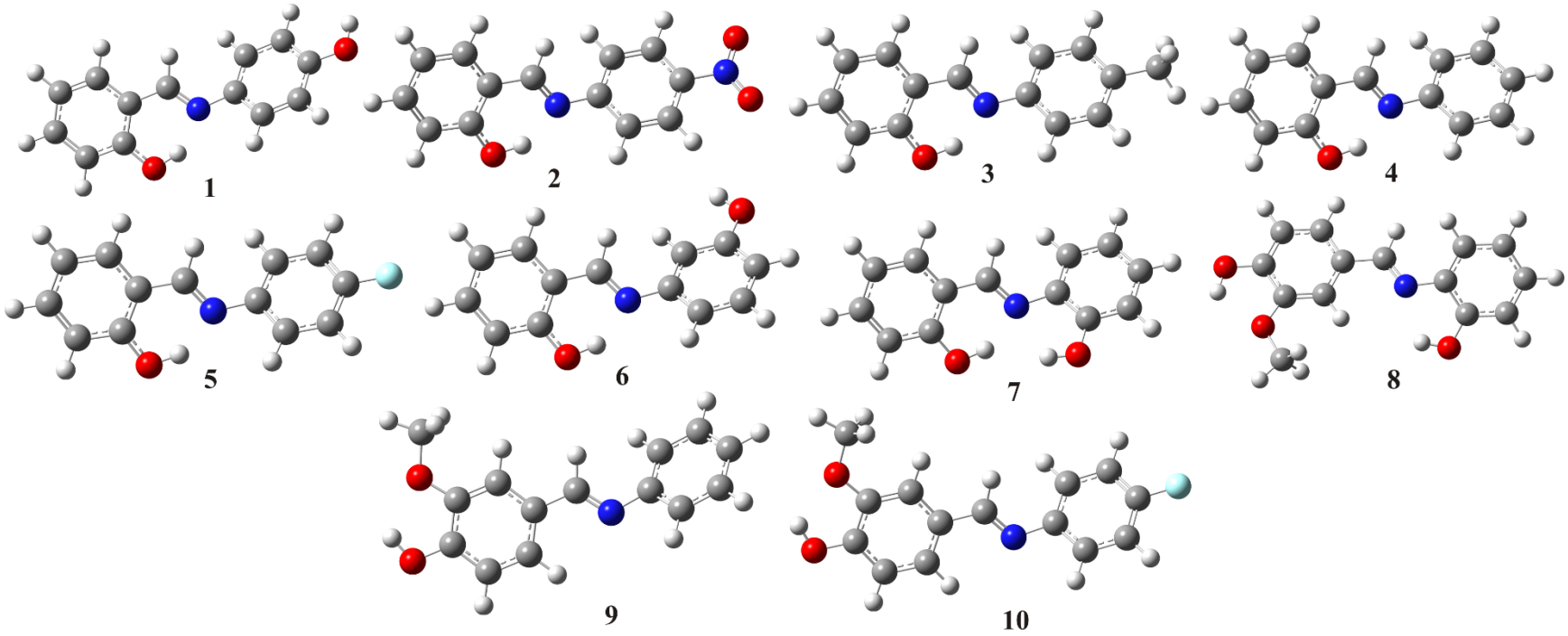


Fig. S1. Optimized geometries of the investigated Schiff bases. Each compound is presented with its most stable isomer

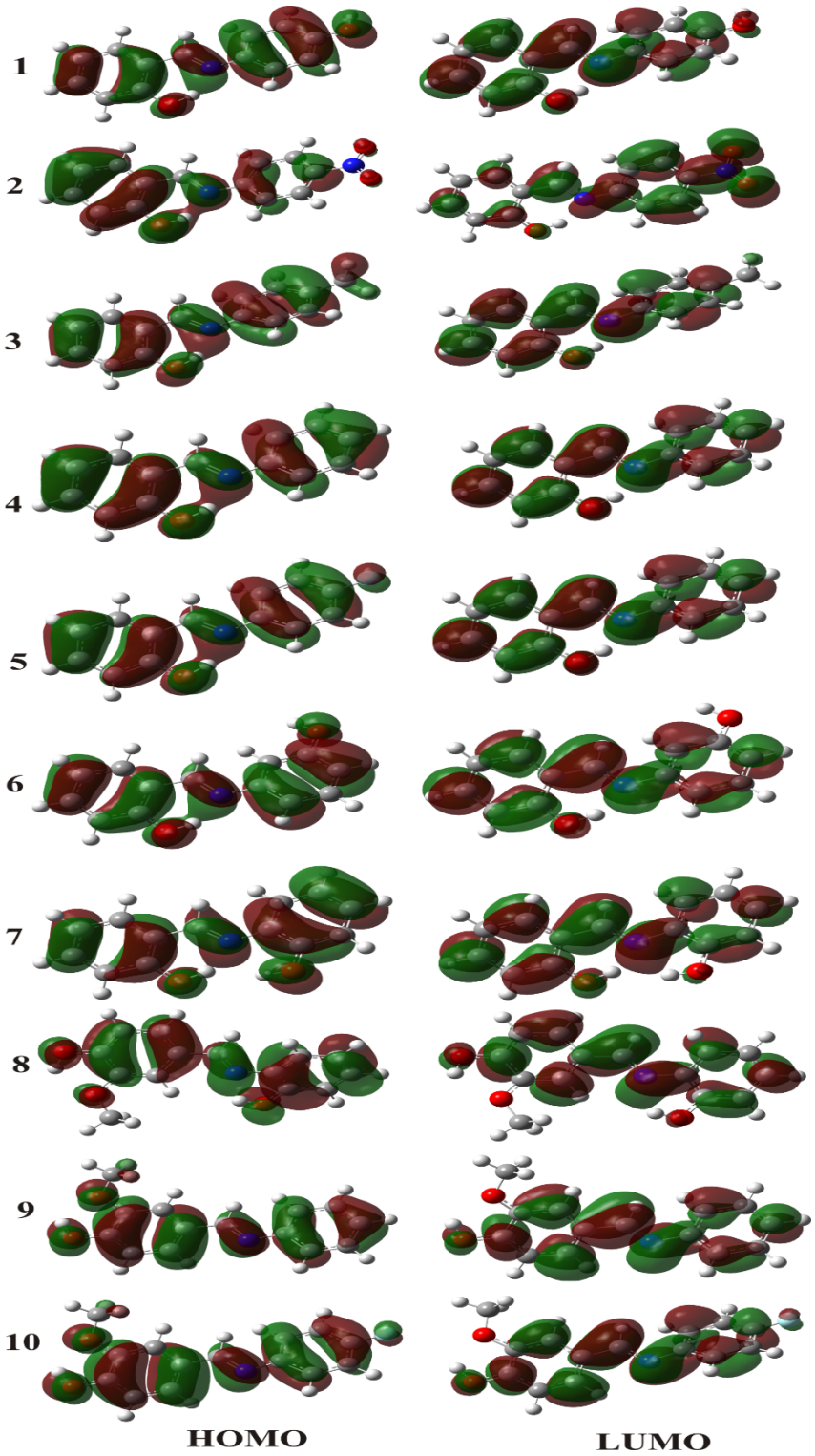


Fig. S2. HOMOs and LUMOs of the investigated Schiff base in methanol

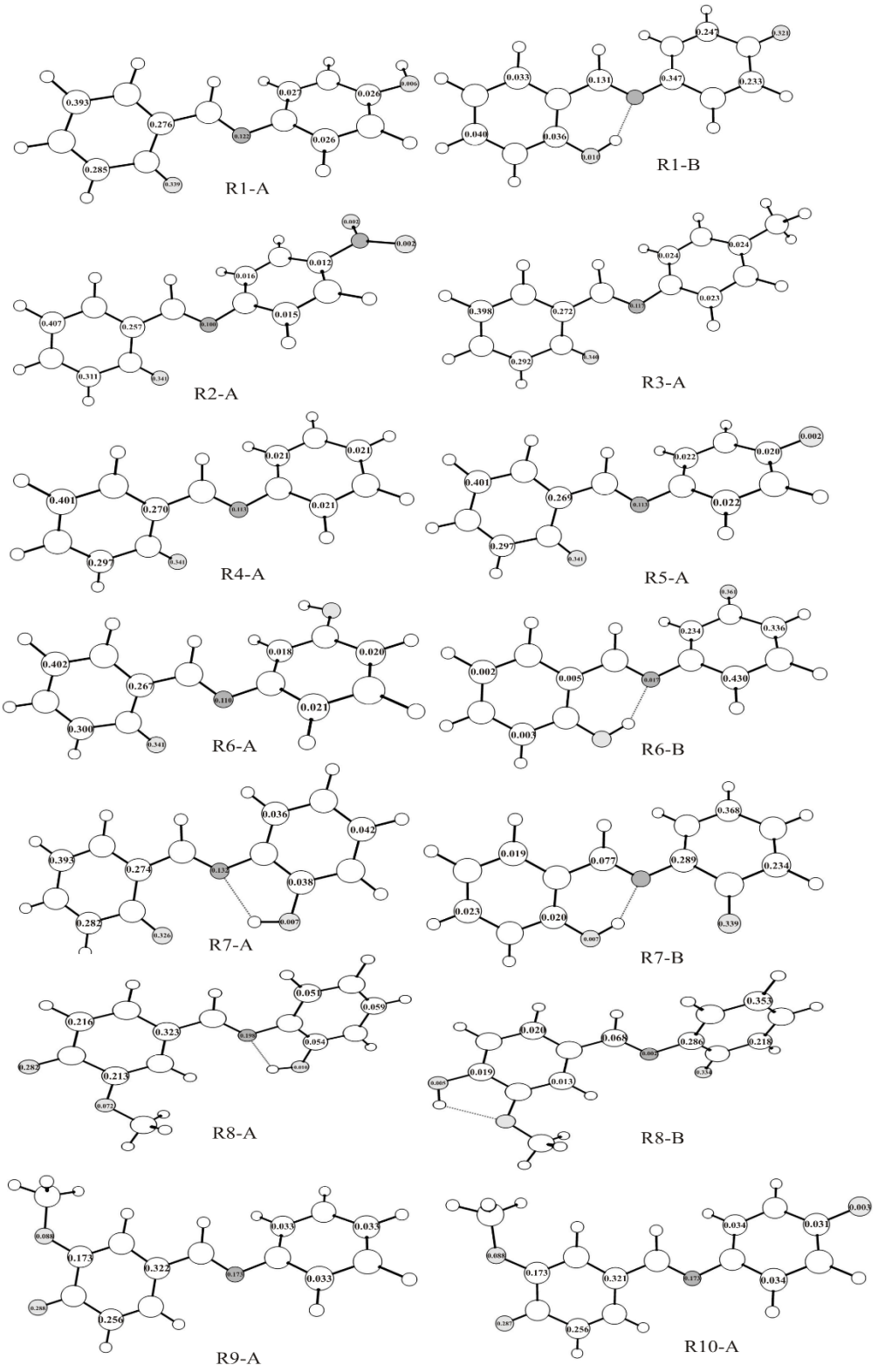


Fig. S3. Spin density distribution in all radicals issued from the investigated Schiff bases in methanol

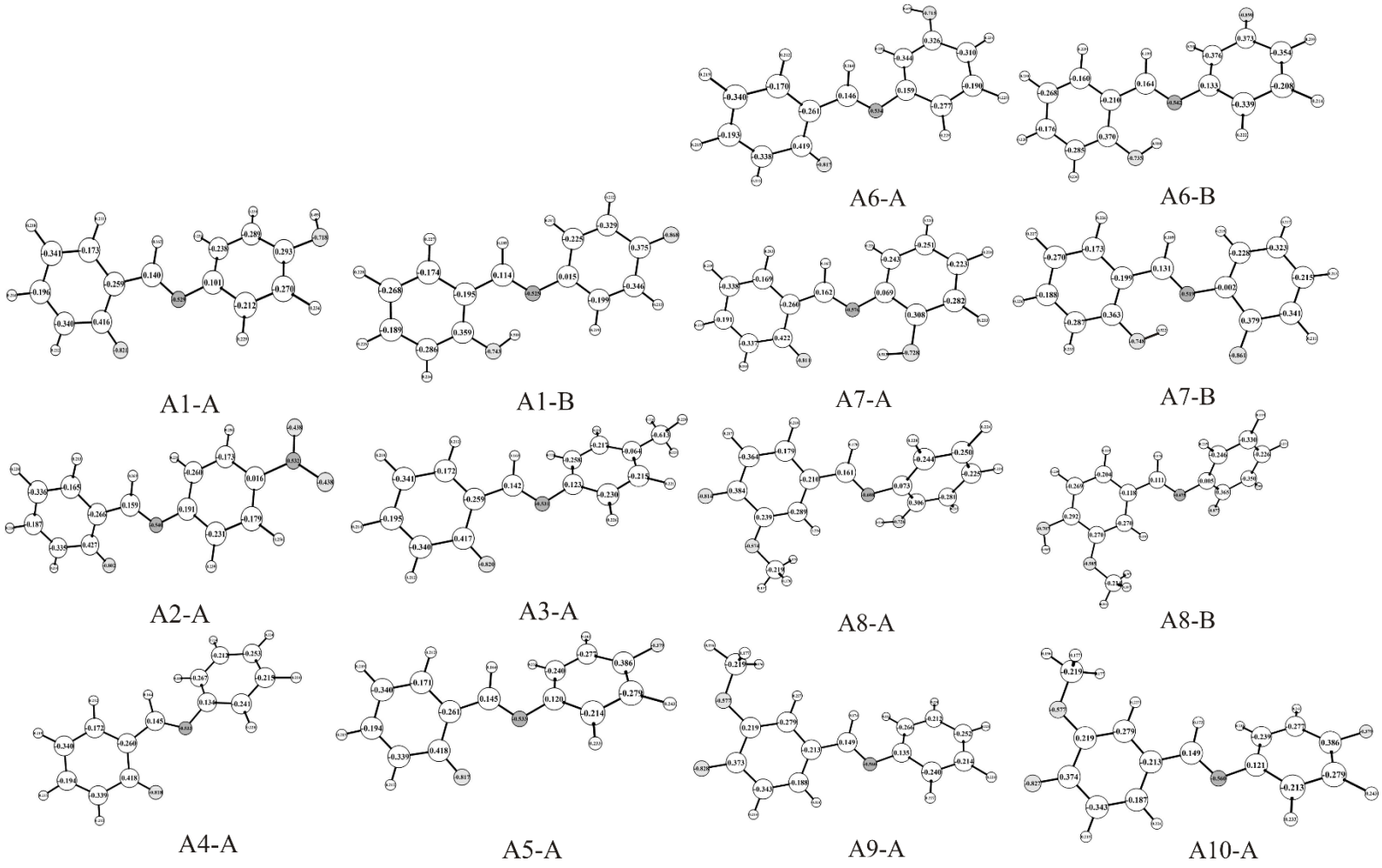
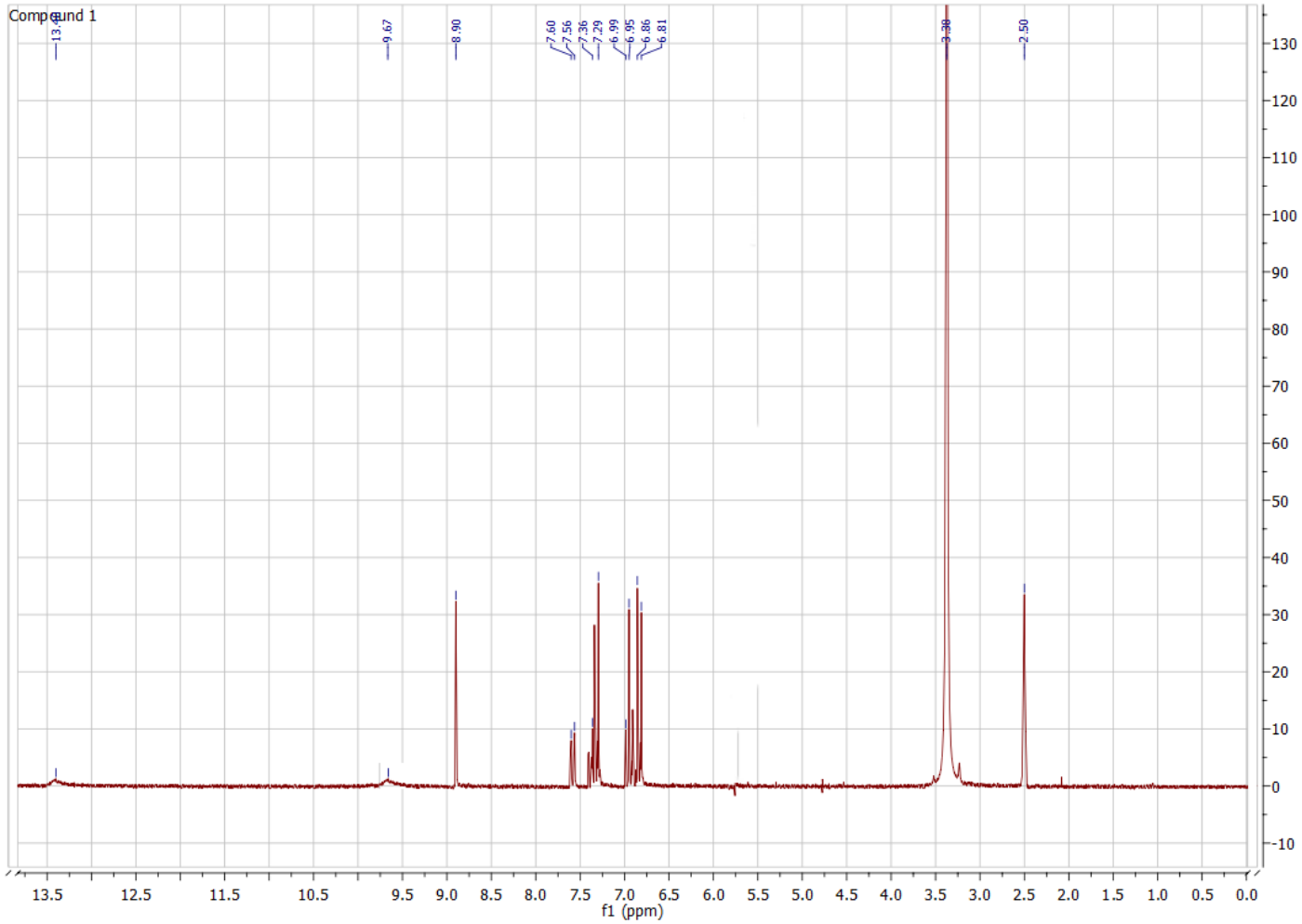
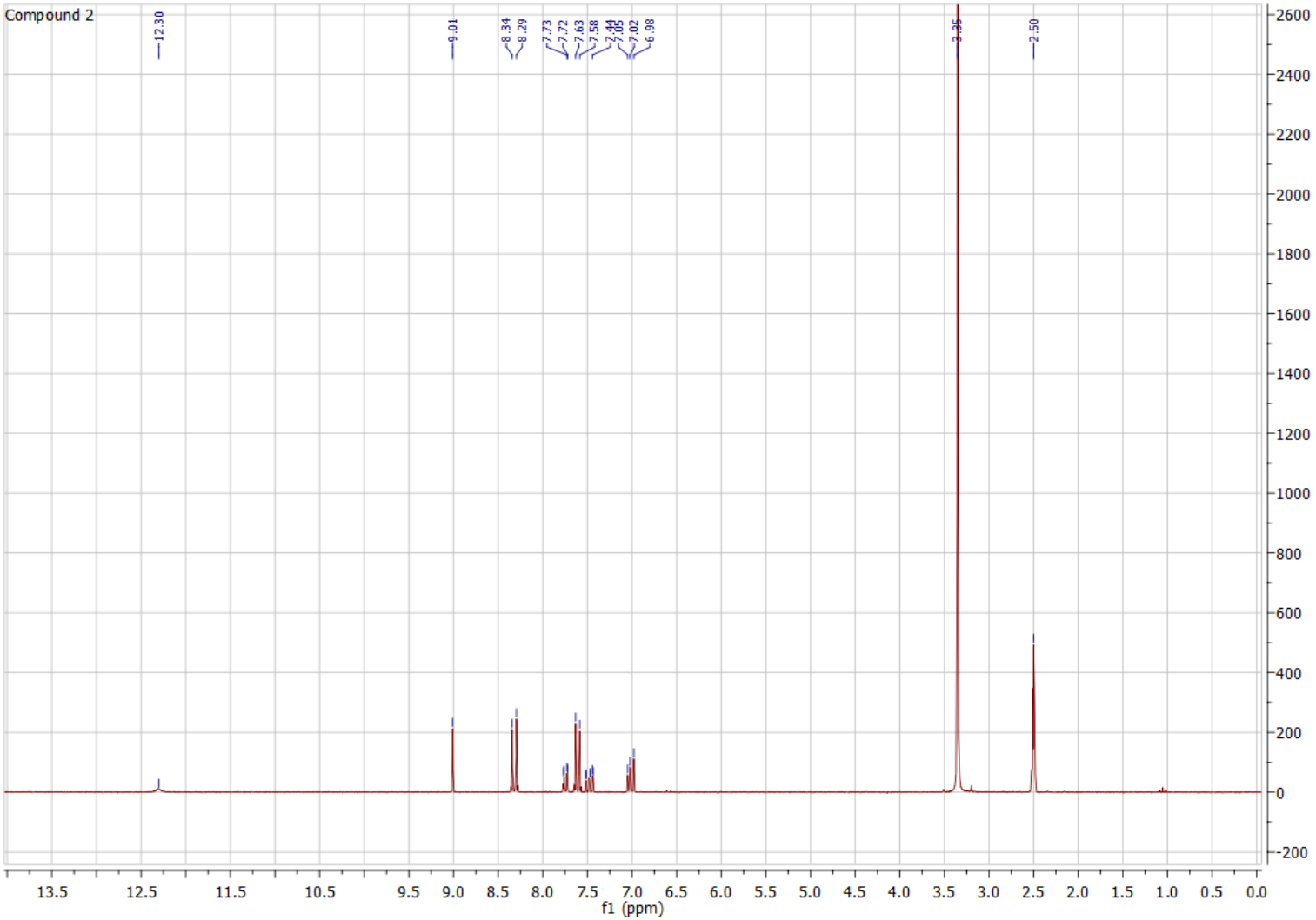


Fig. S4. Charge distribution in all anions issued from the investigated Schiff bases in methanol

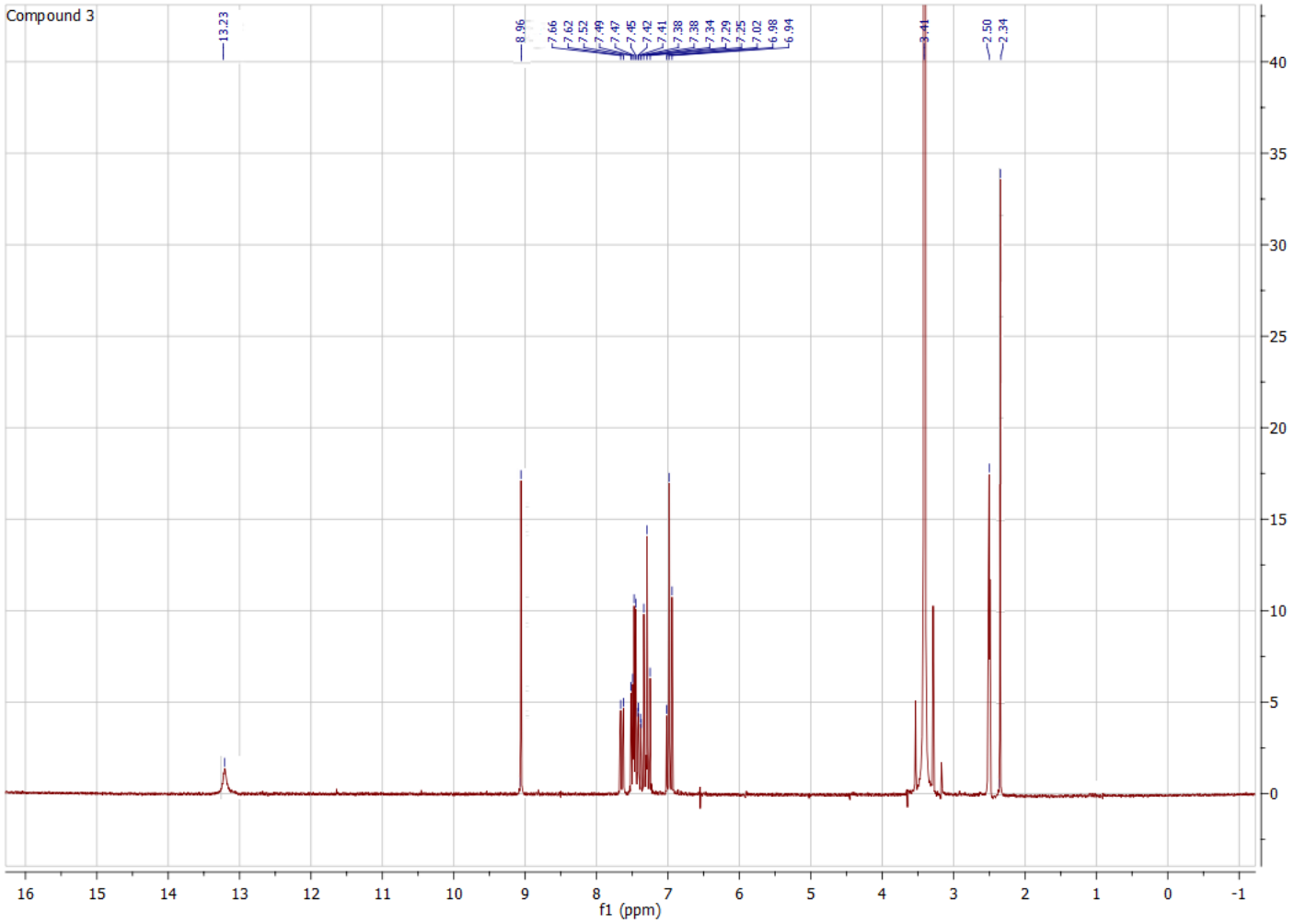
[1]H NMR spectra and Mp of the compounds **1-10**



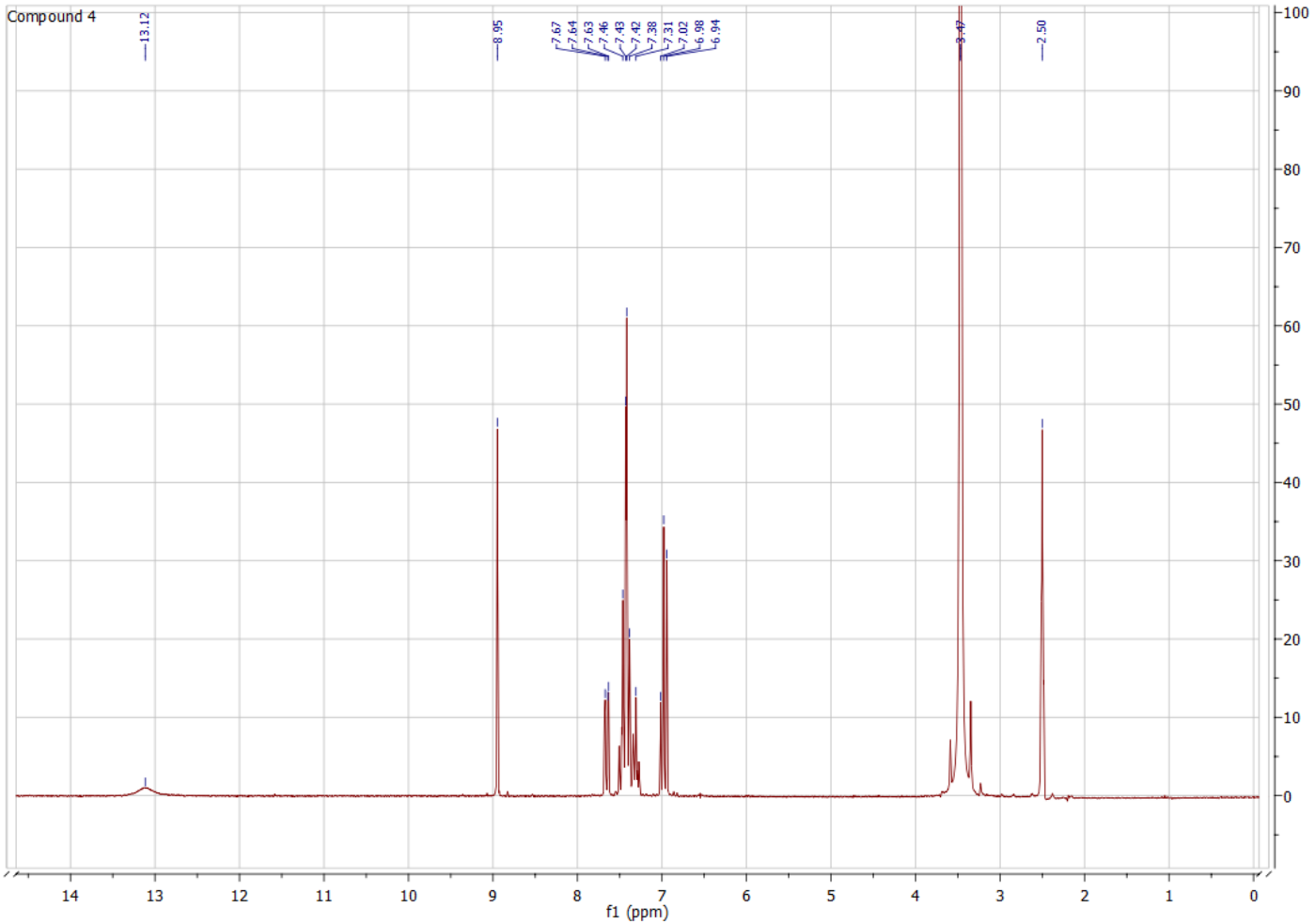
Compound **1** ((*E*)-2-((4-hydroxyphenylimino)methyl)phenol): orange crystals Mp - 137-140 °C



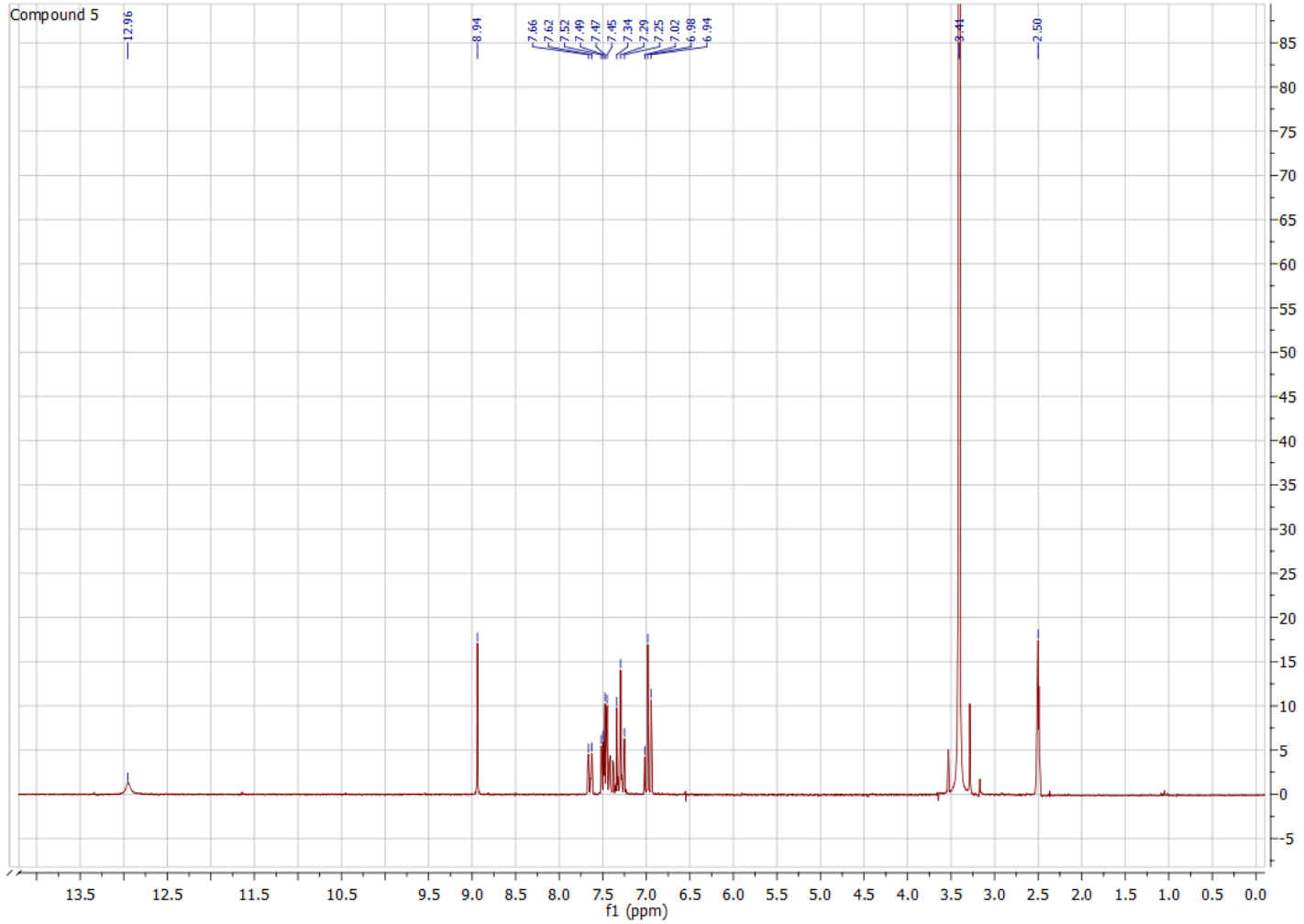
Compound **2** ((*E*)-2-((4-nitrophenylimino)methyl)phenol) orange powder - Mp 156-158 °C



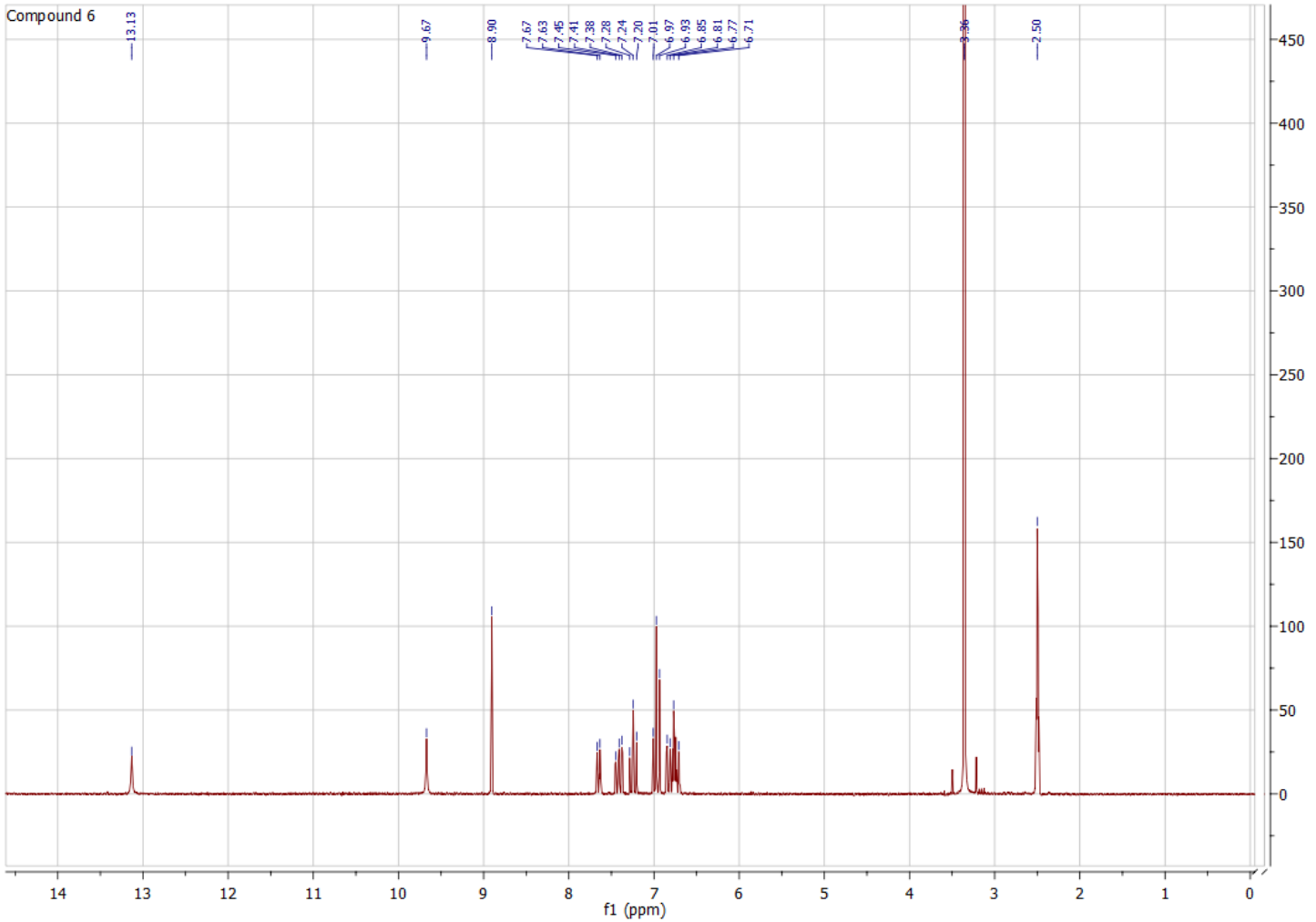
Compound **3** ((*E*)-2-((*p*-tolylimino)methyl)phenol): yellow crystals - Mp 91-93 °C/lit. Mp 90-91.5°C [1]



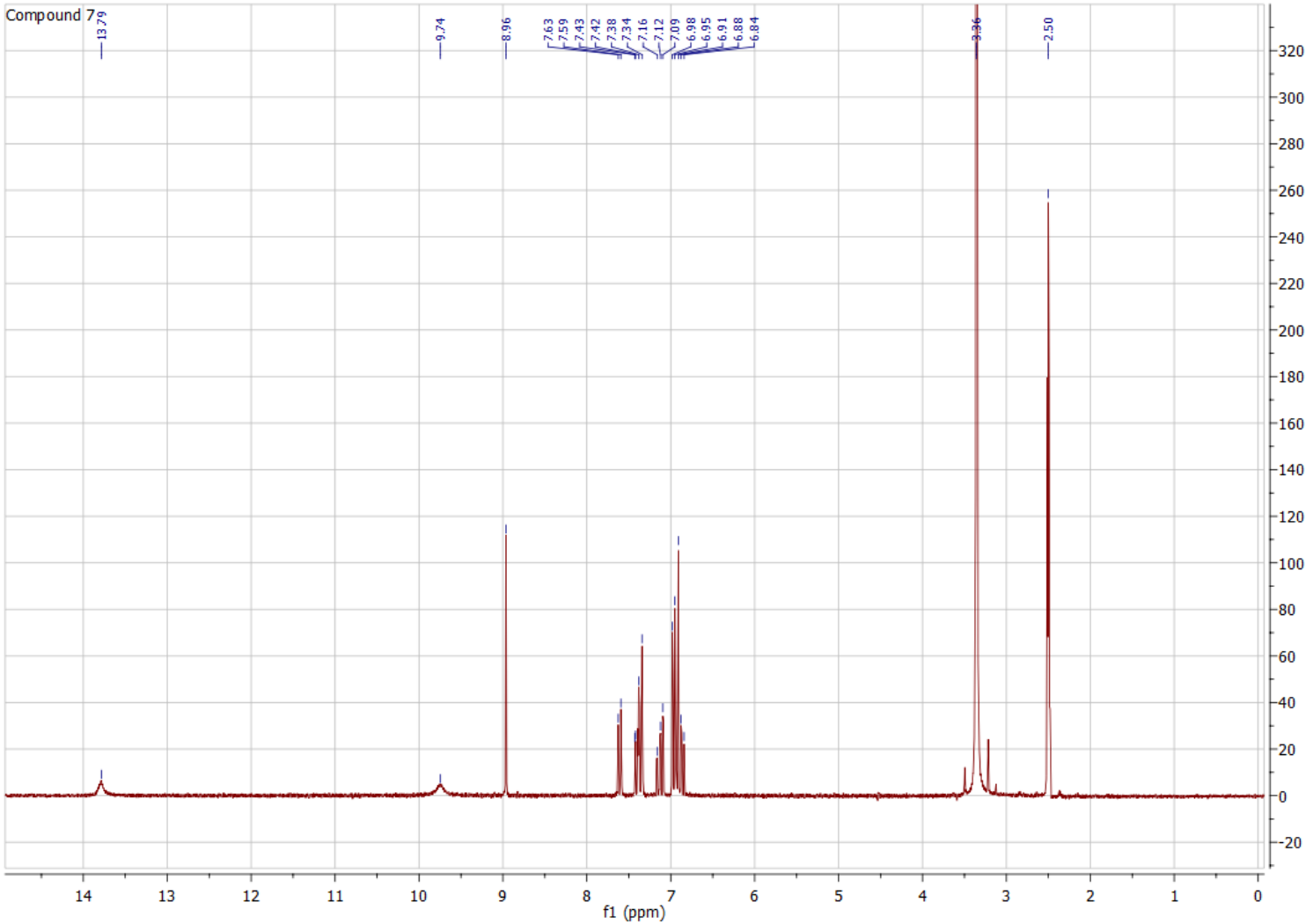
Compound **4** ((*E*)-2-((phenylimino)methyl)phenol): yellow crystals - Mp 50-51°C



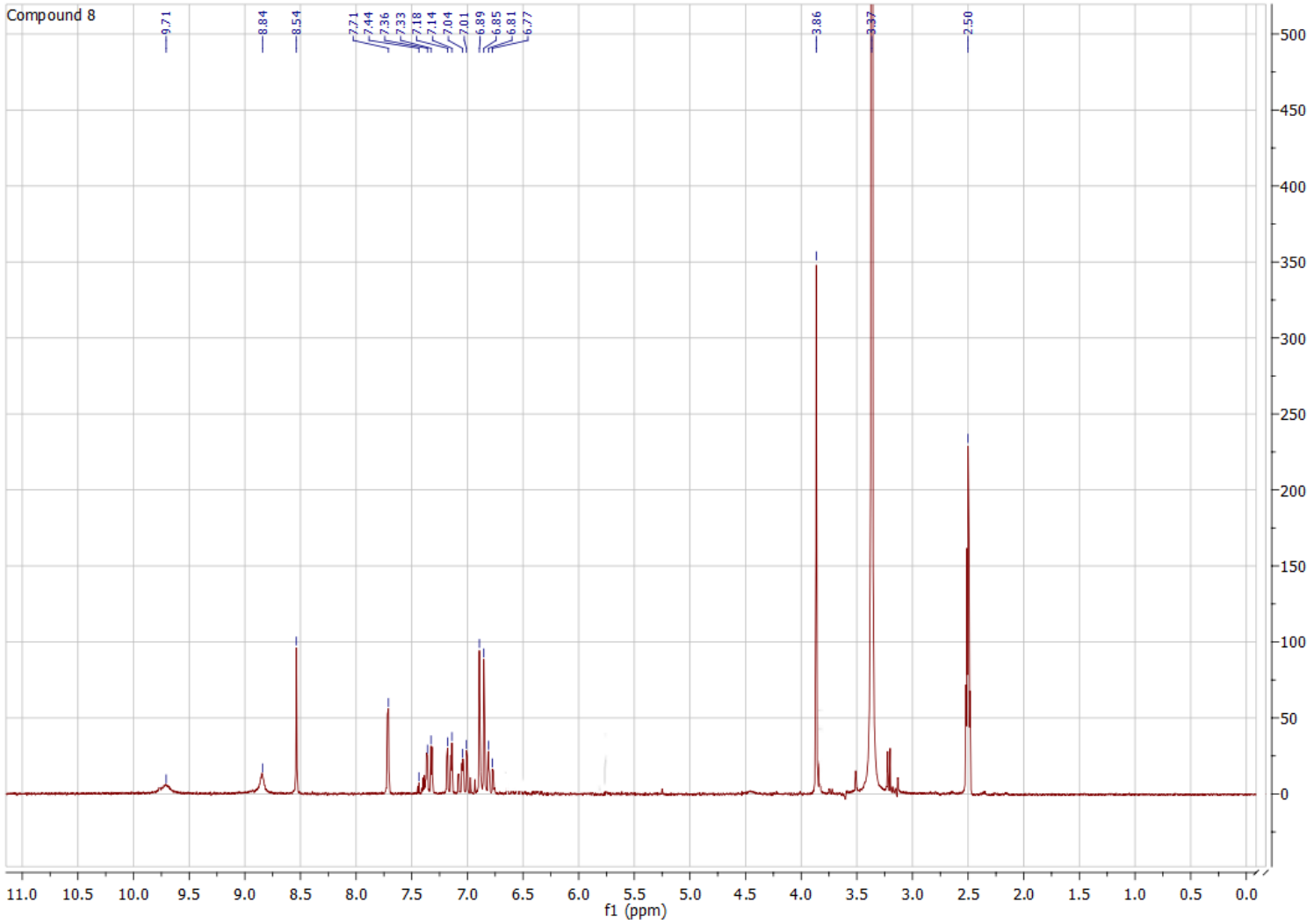
Compound **5** ((*E*)-2-((4-fluorophenylimino)methyl)phenol): yellow crystals - Mp 77-79 °C



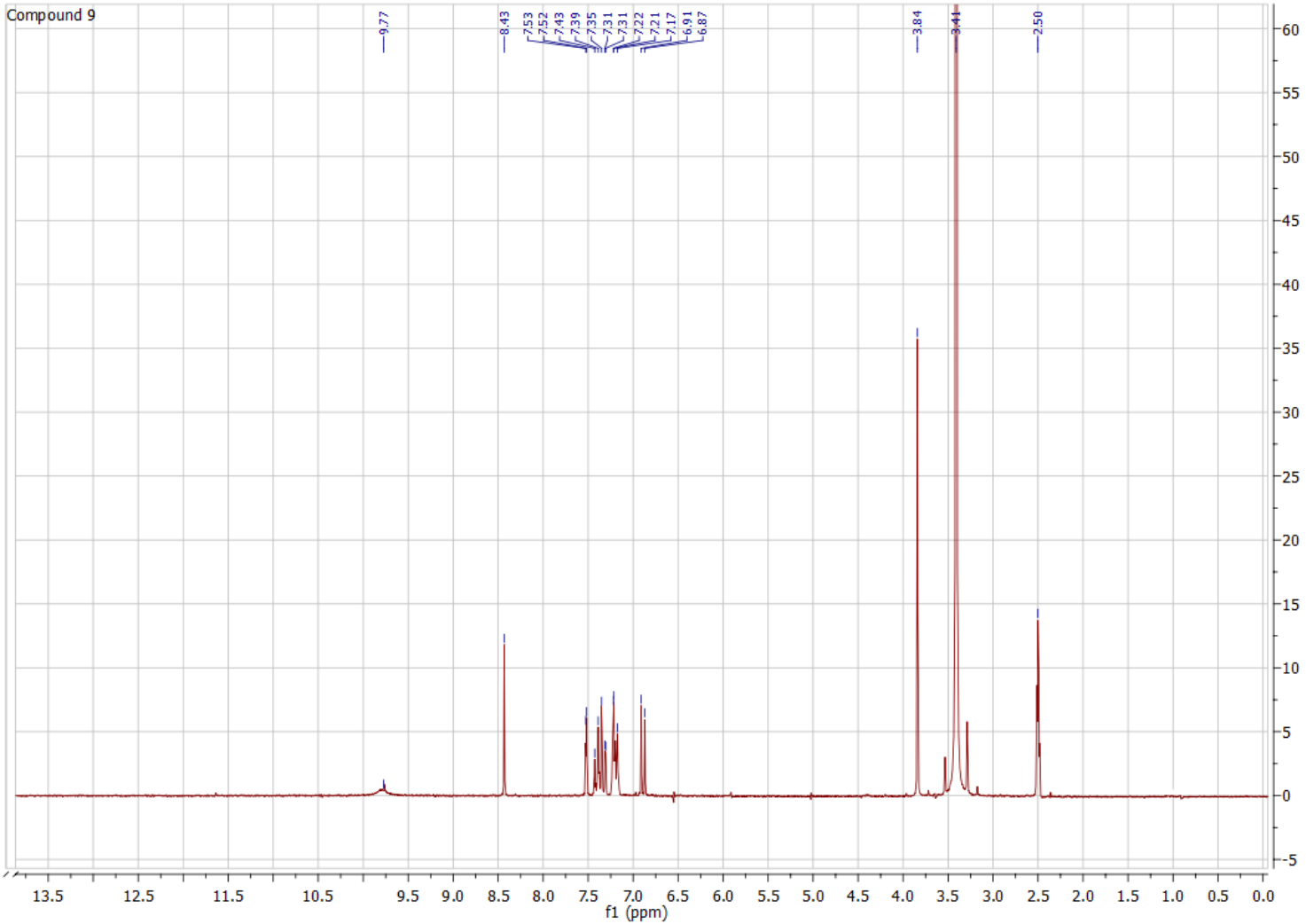
Compound **6** ((*E*)-2-((3-hydroxyphenylimino)methyl)phenol) yellow-orange crystals - Mp 123-125 °C



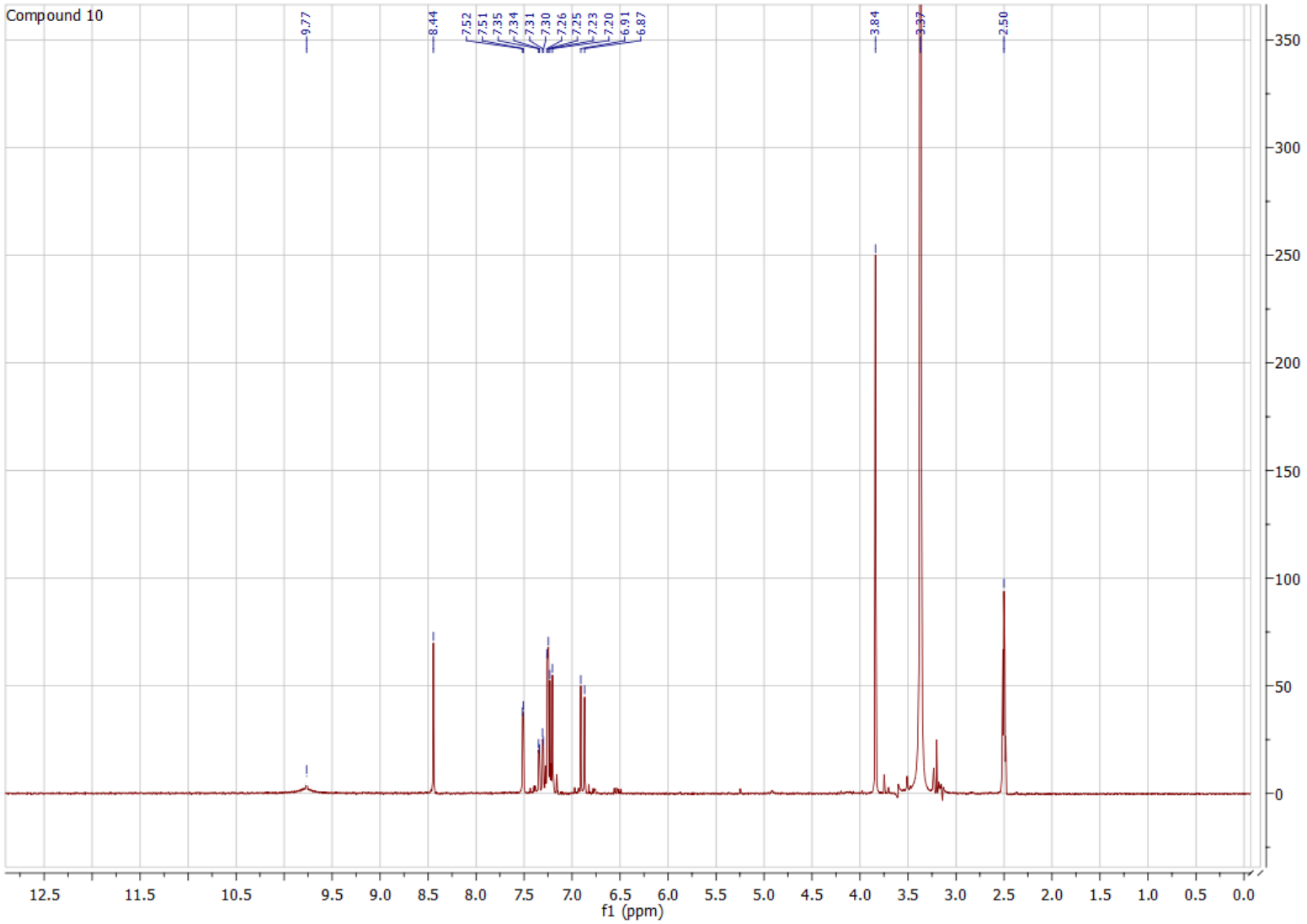
Compound **7** ((*E*)-2-((2-hydroxyphenylimino)methyl)phenol): orange crystals - Mp 182-184 °C/lit. <186°C [2]

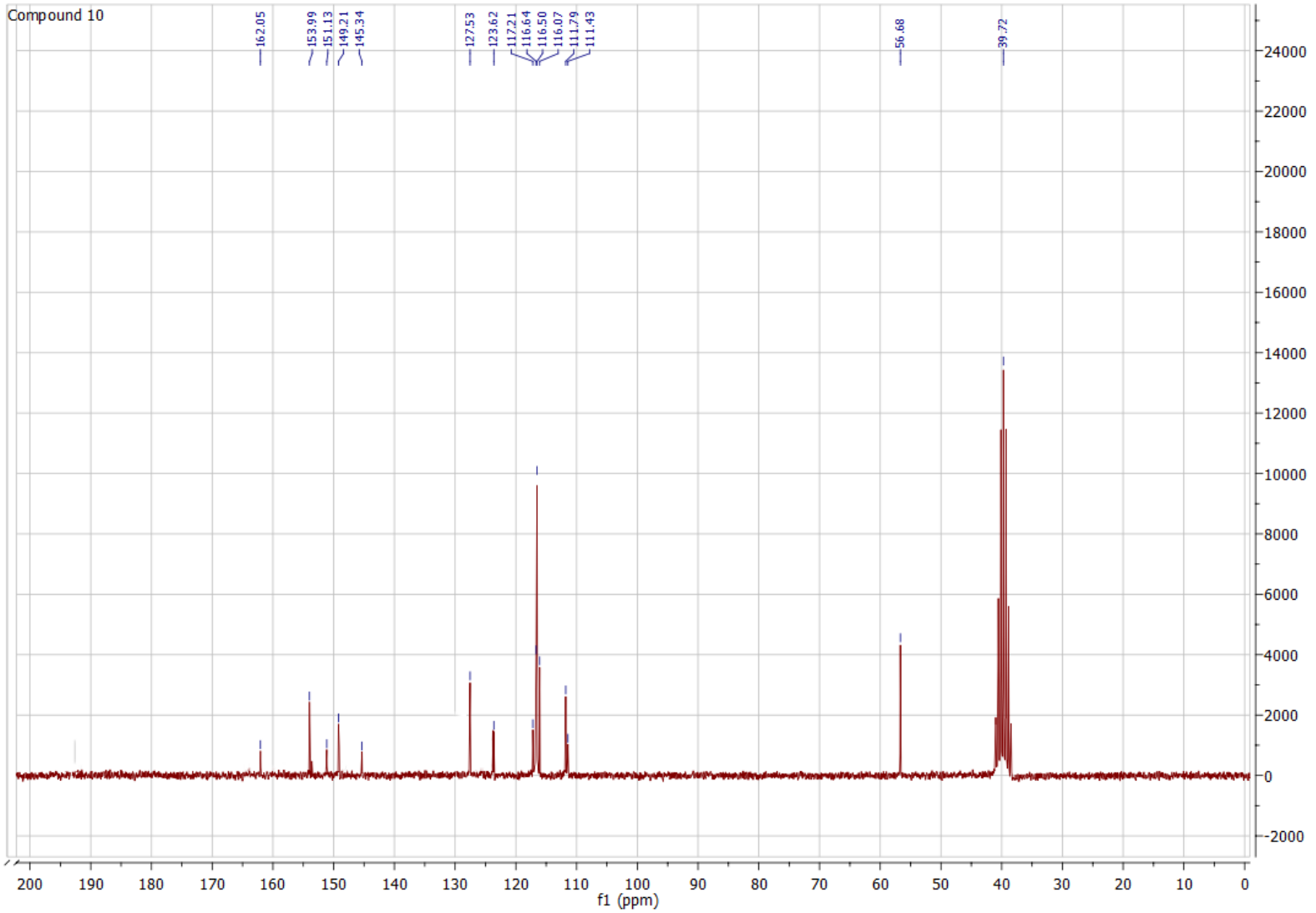


Compound **8** ((*E*)-4-((2-hydroxyphenylimino)methyl)-2-methoxyphenol): brown crystals - Mp 86-88 °C/lit. 88°C [3]



Compound **9** ((*E*)-2-methoxy-4-((phenylimino)methyl)phenol**)**: colourless crystals - Mp 144-146 °C/lit. 141°C [4]


Compound 10
9.77
8.44
7.52
7.51
7.35
7.34
7.31
7.30
7.26
7.25
7.23
7.20
6.91
6.87
3.84
3.37
2.50
f1 (ppm)



Compound **10** ((*E*)-4-((4-fluorophenylimino)methyl)-2-methoxyphenol) colourless crystals - Mp 144-146 °C

References

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