Supporting information

Sterically Hindered Catechol-derived Schiff bases: Design, Synthesis, SAR Analysis and Mechanisms of the Antioxidant Activity

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[b]*Cologne University of Applied Sciences, Campusplatz 1, 51379 Leverkusen, Germany;*
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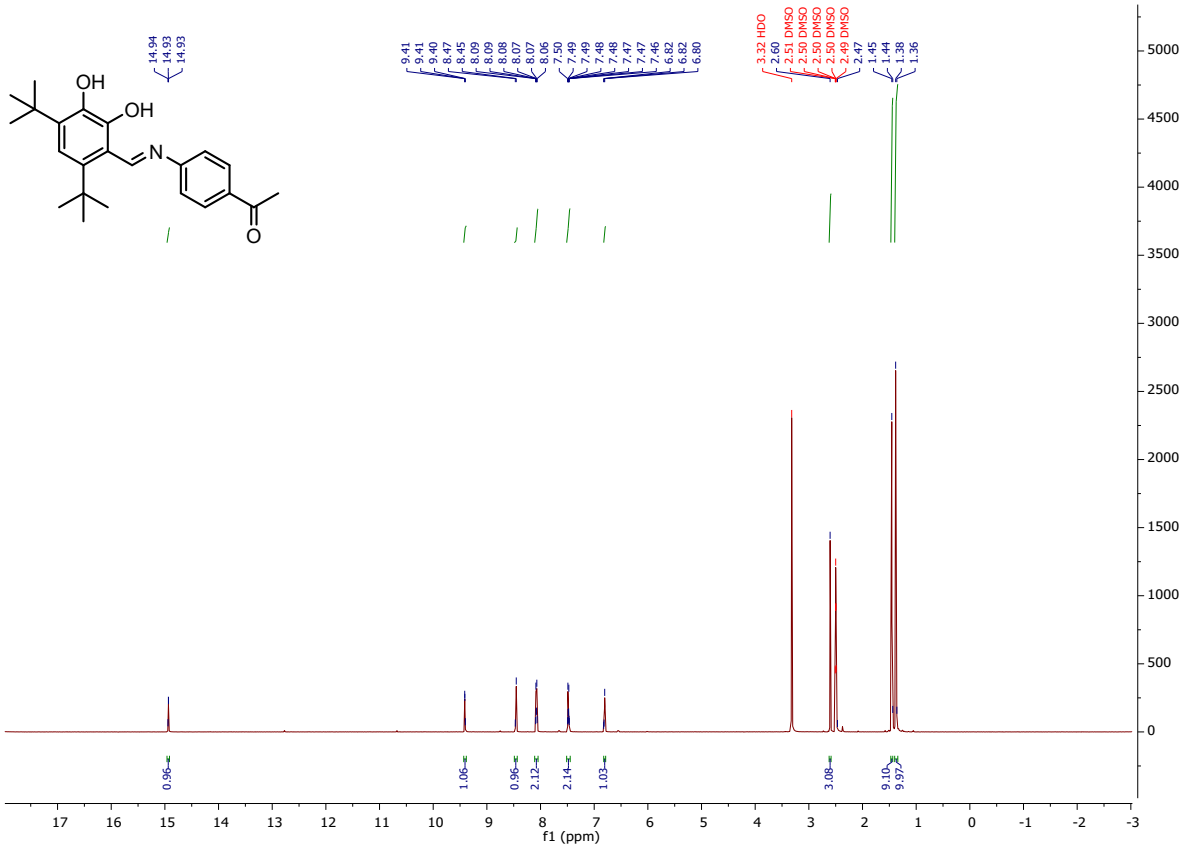
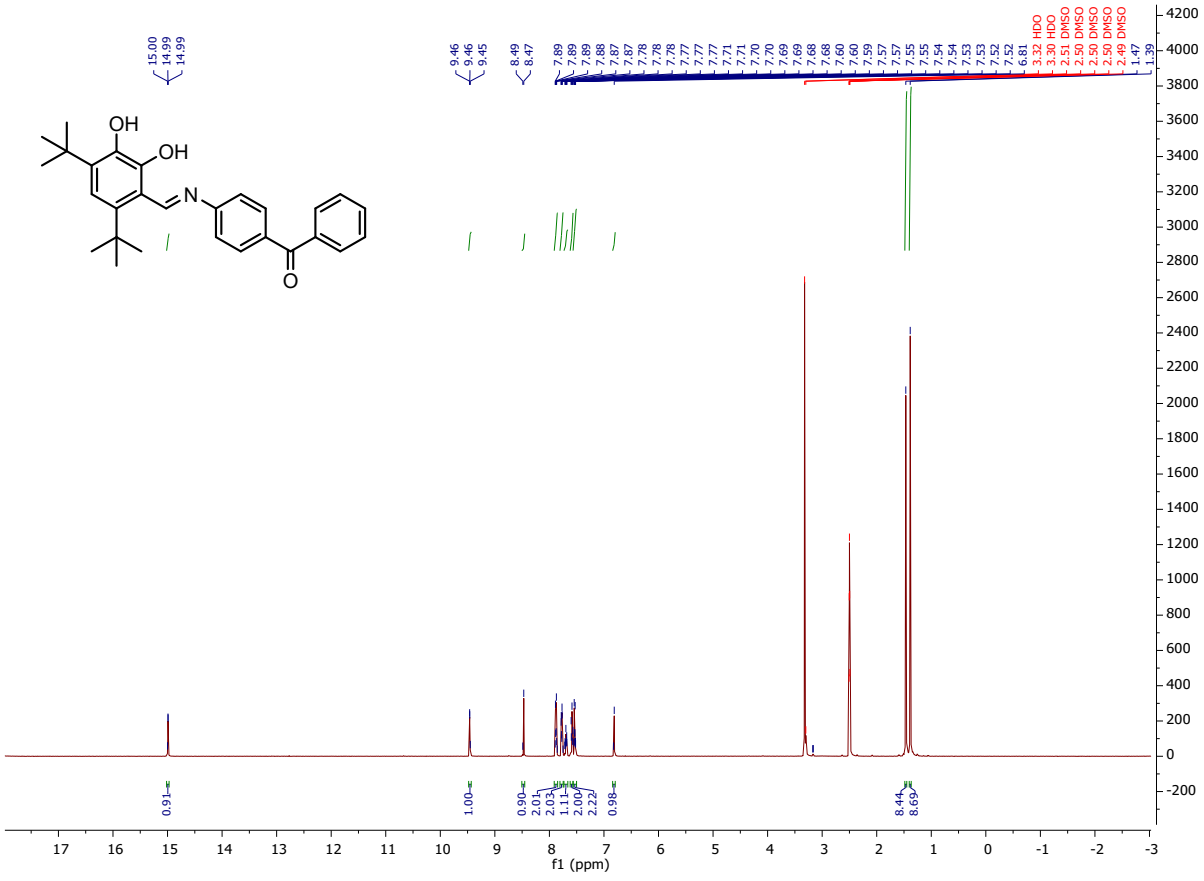
NMR spectra

1-(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)ethan-1-one



(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)(phenyl)methanone



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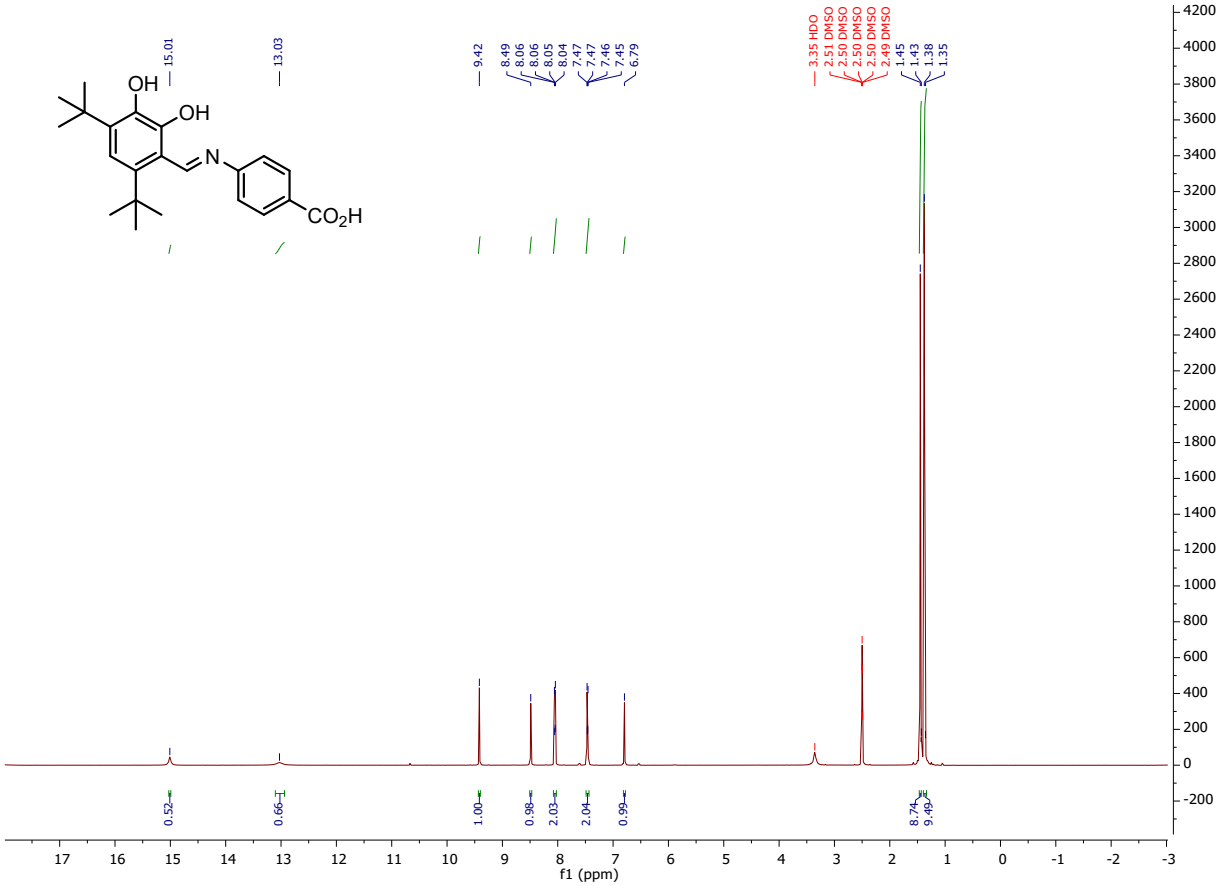

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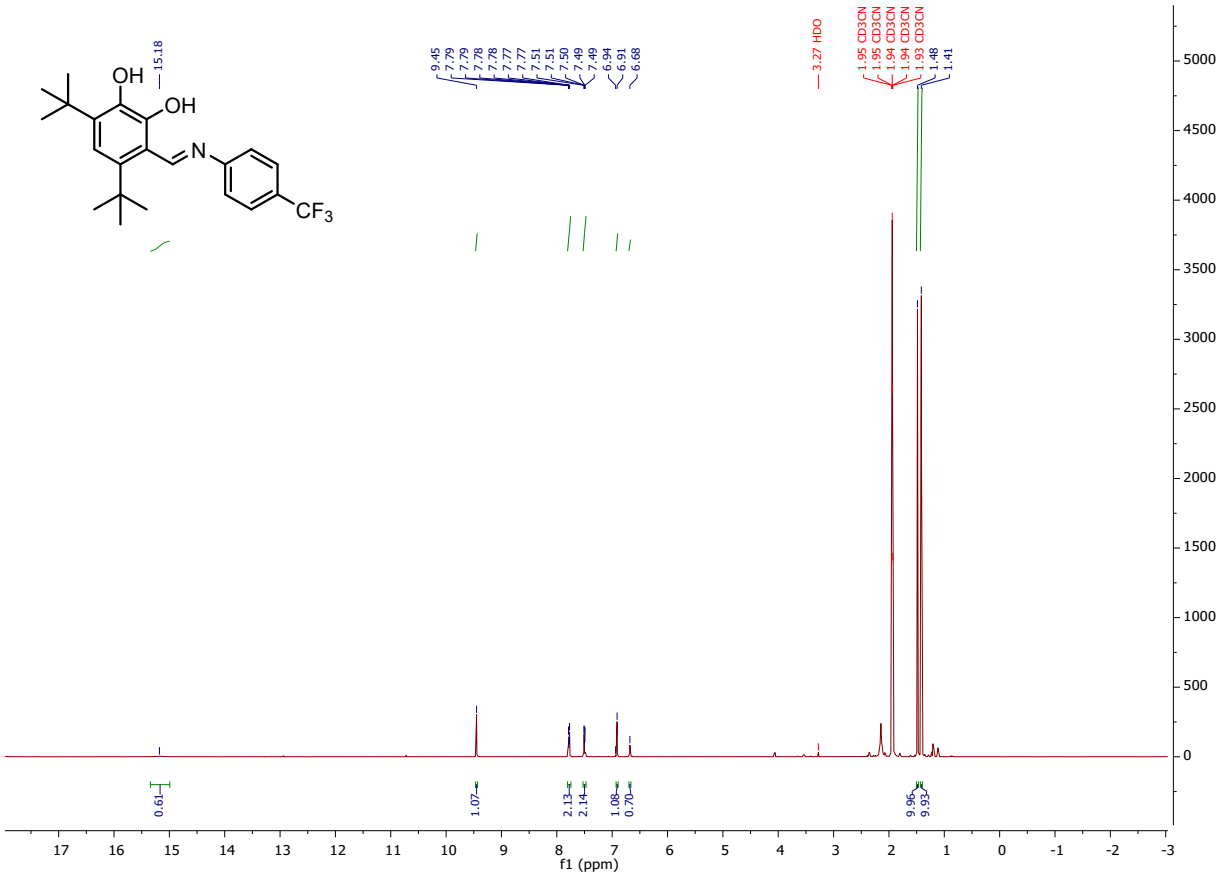

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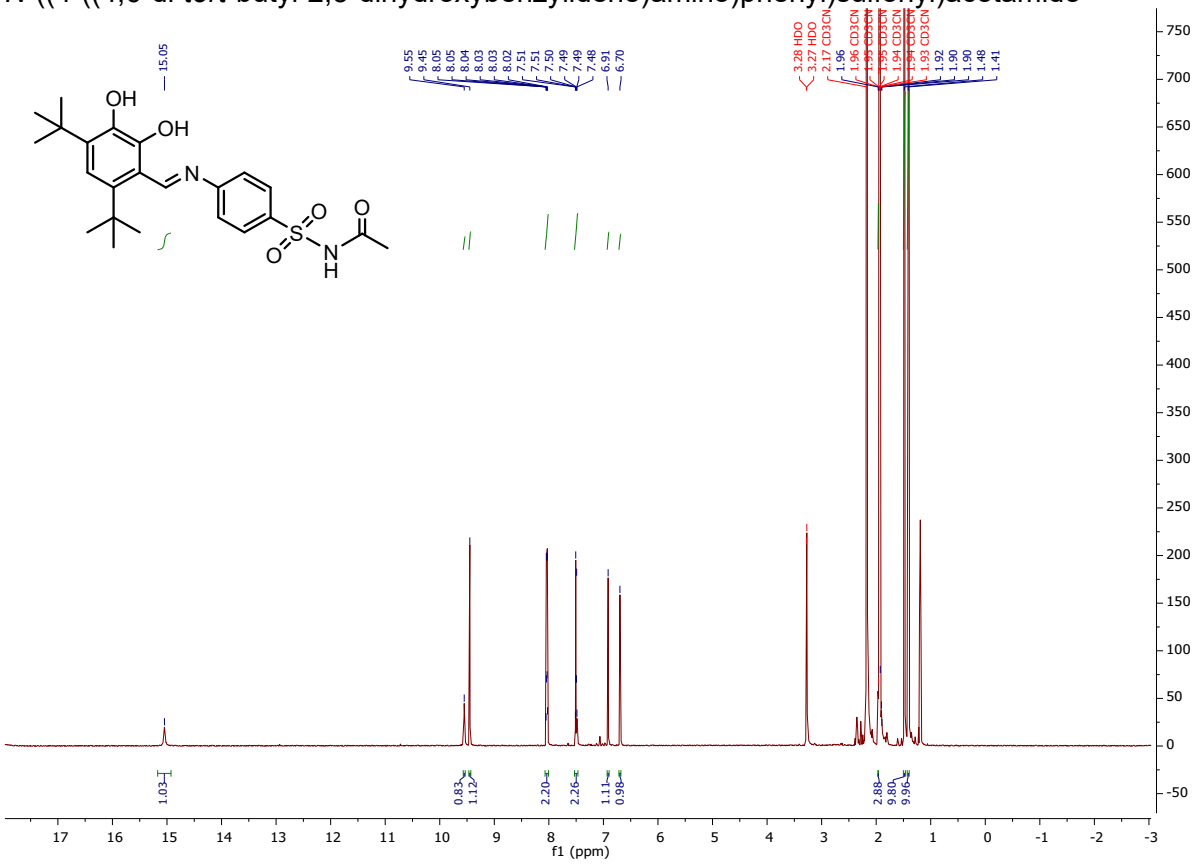

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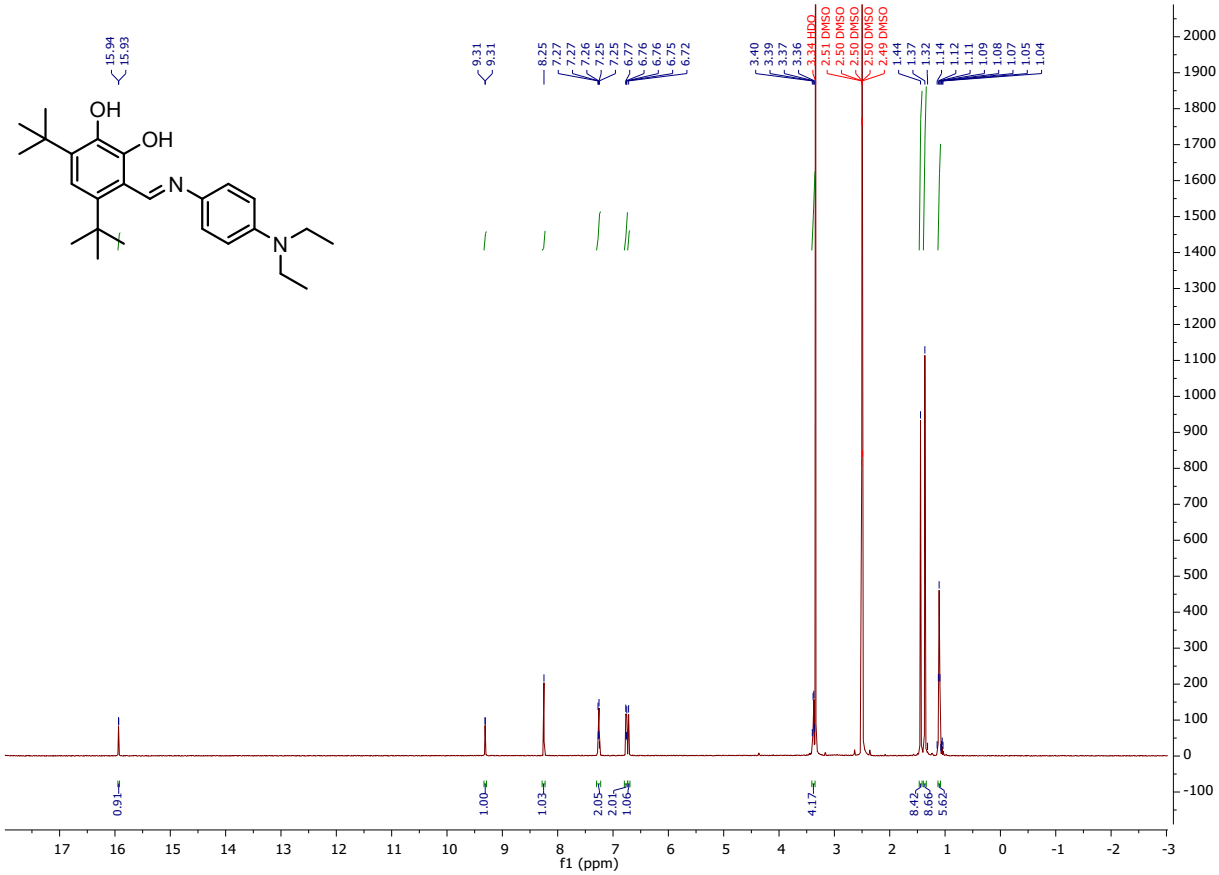

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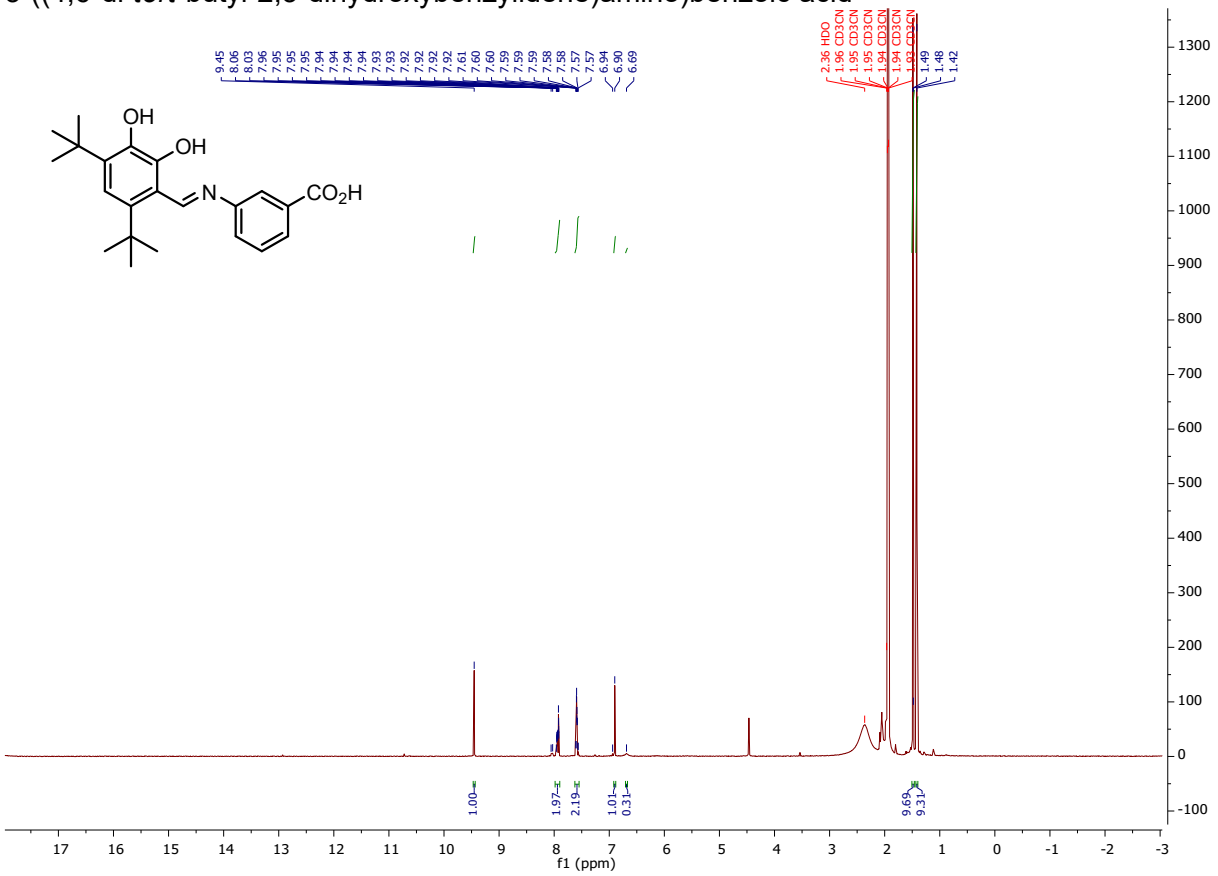

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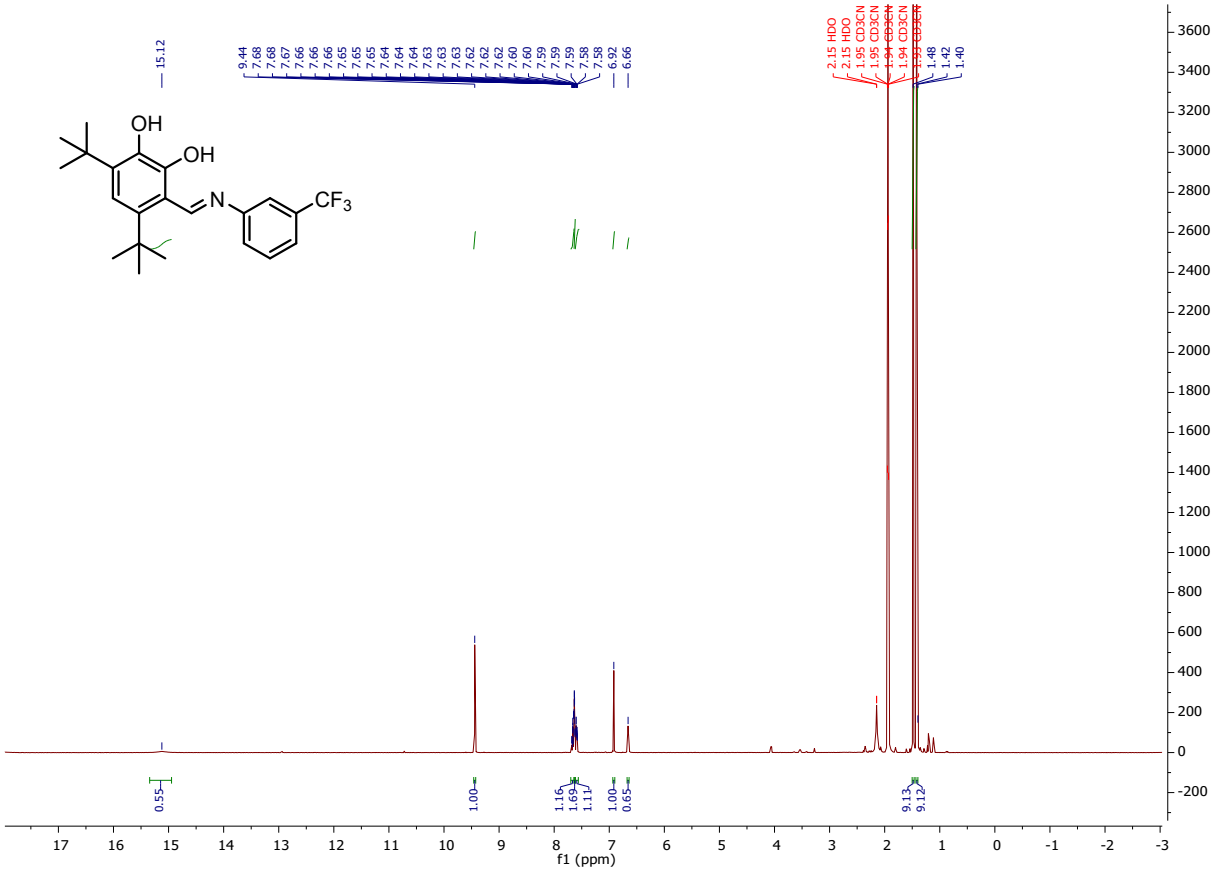

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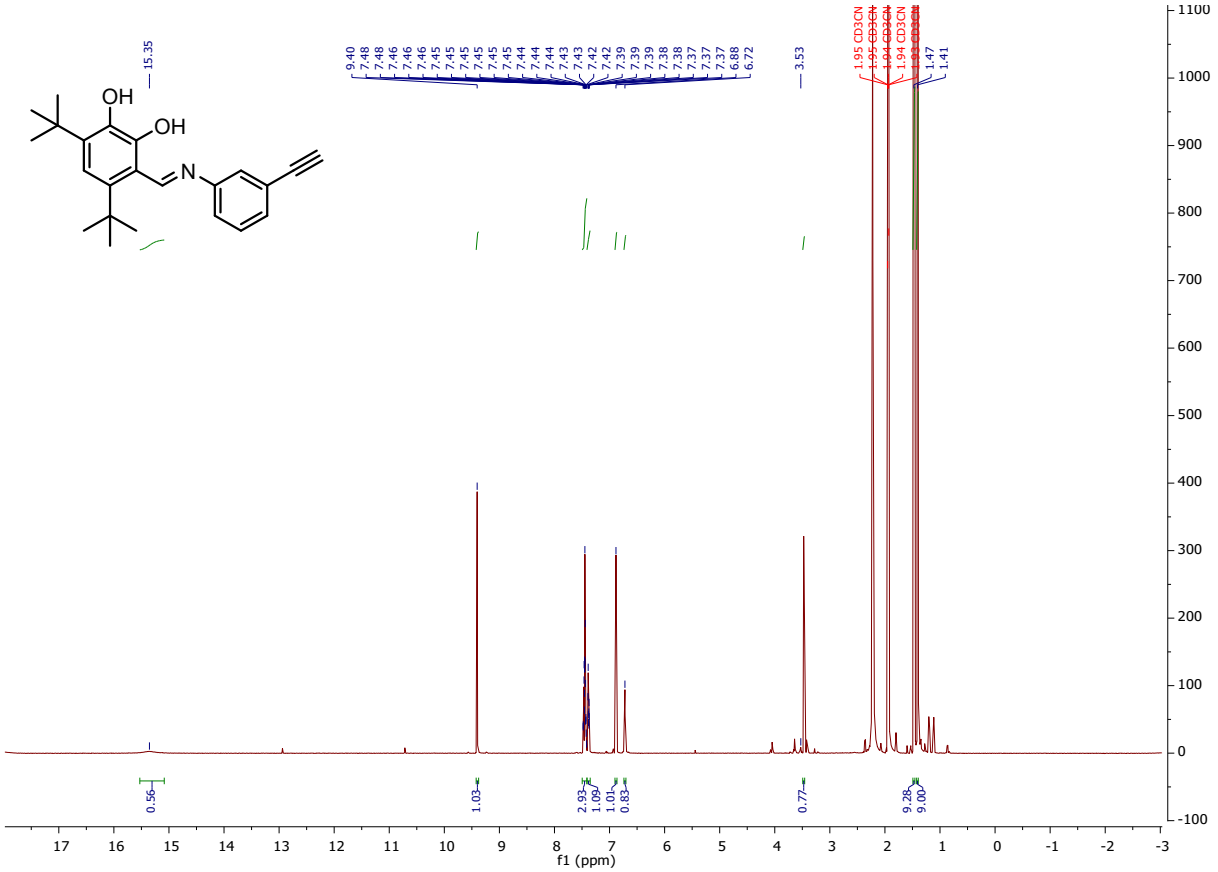

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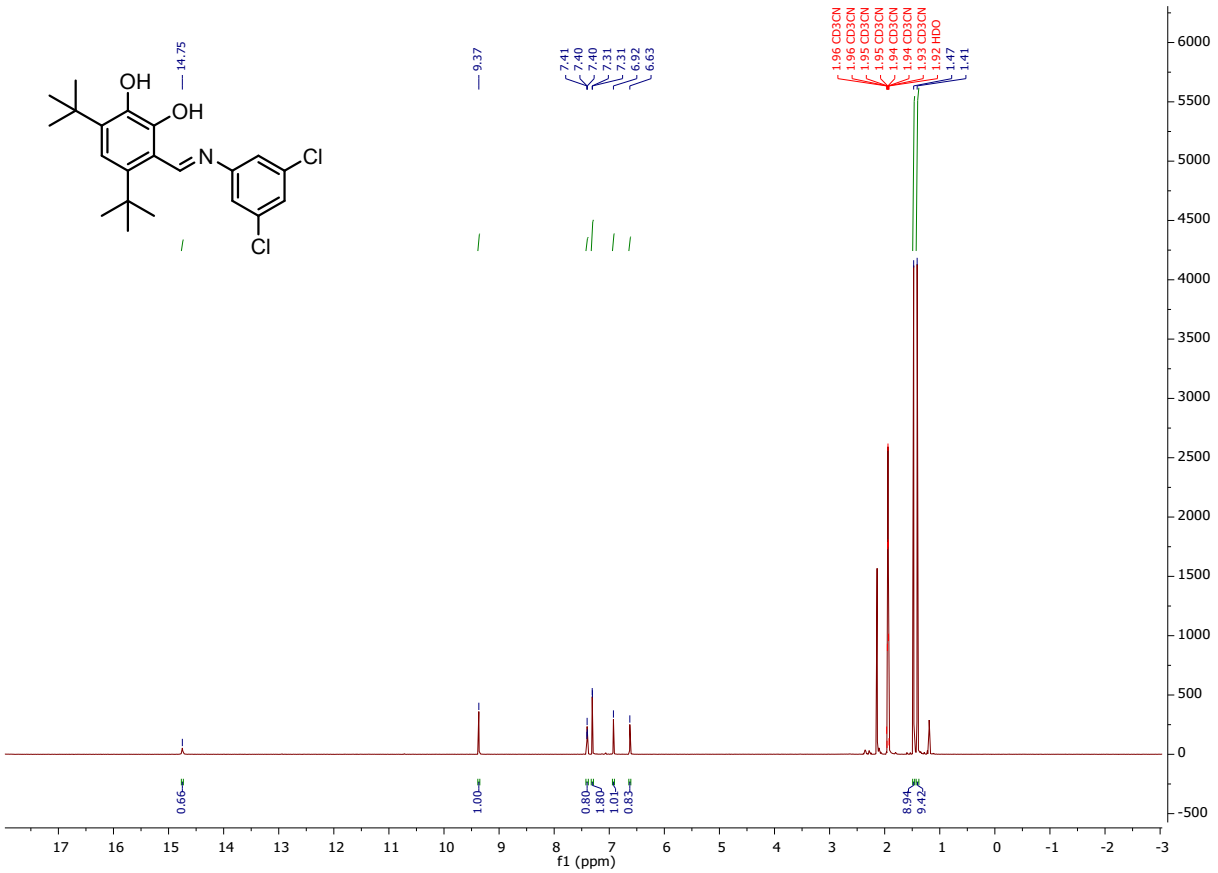
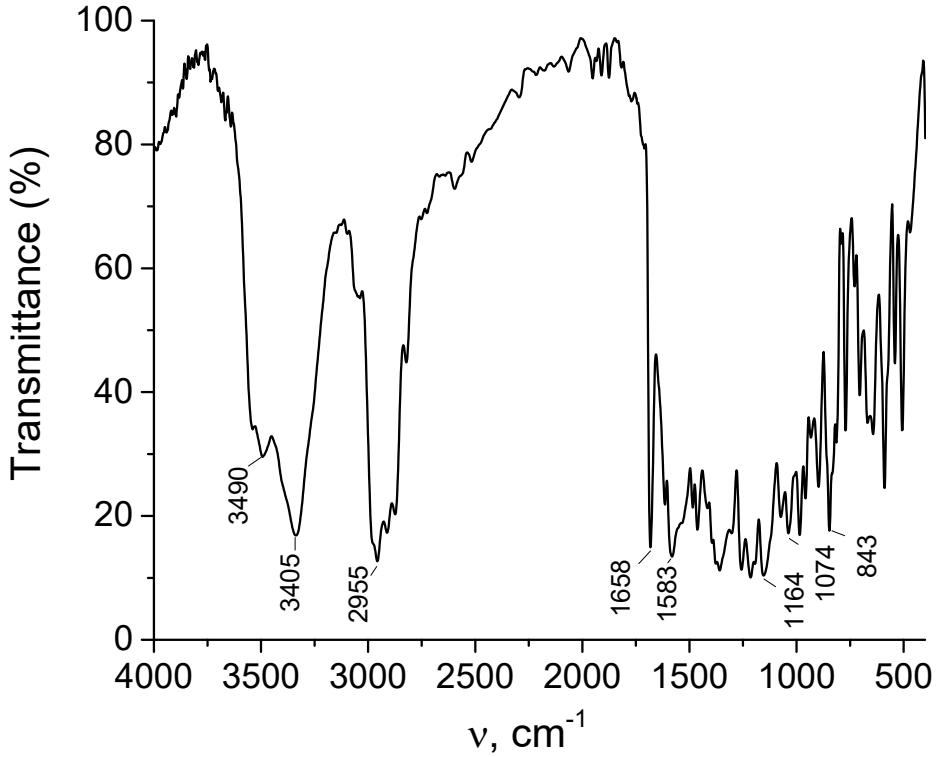
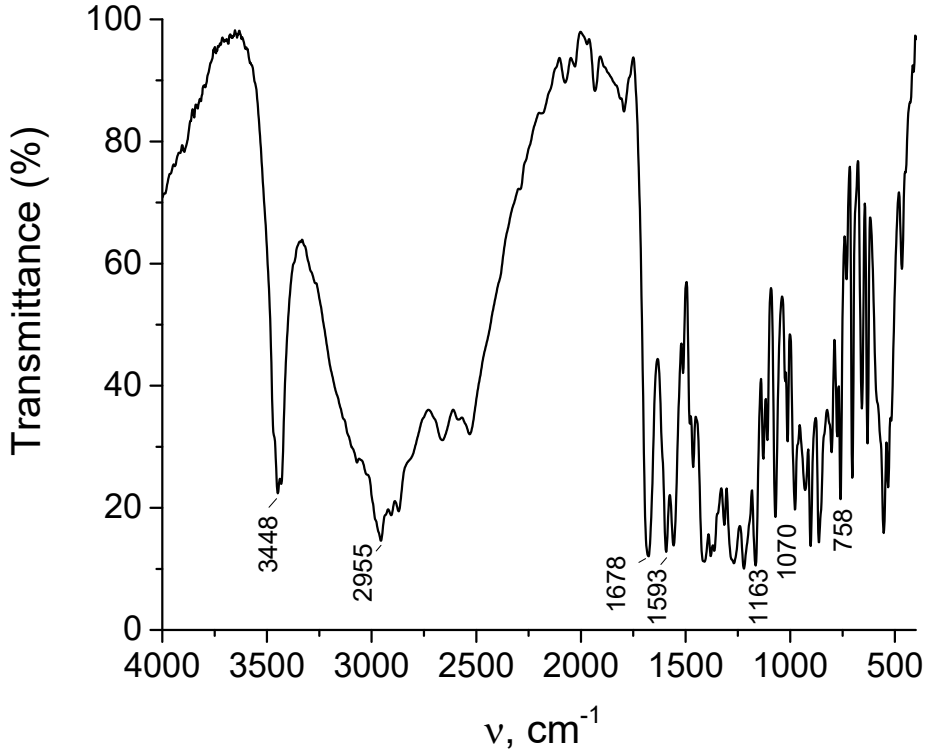


FT-IR spectra

1-(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)ethan-1-one



4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid



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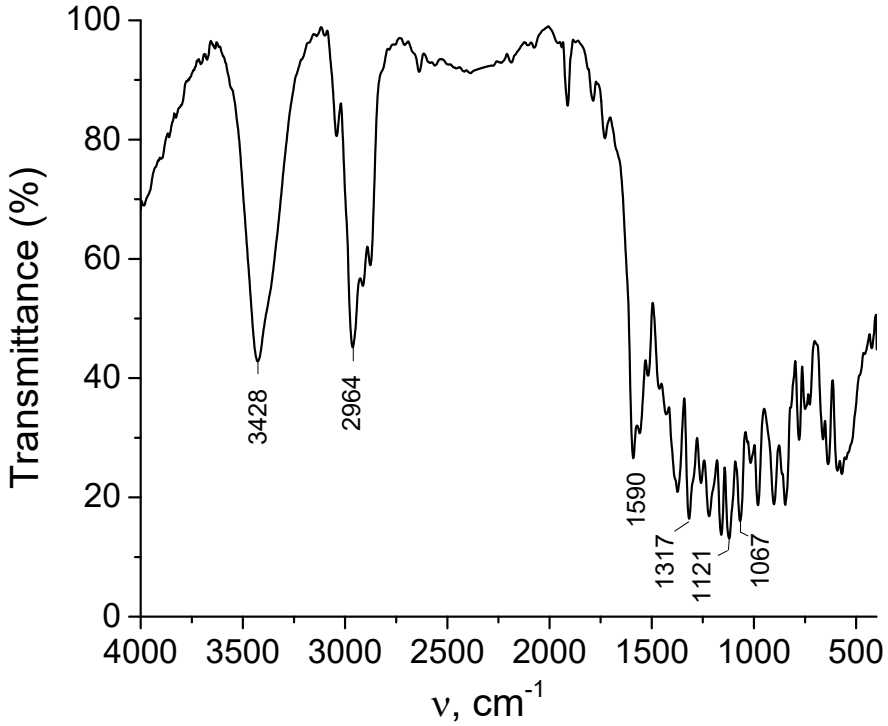

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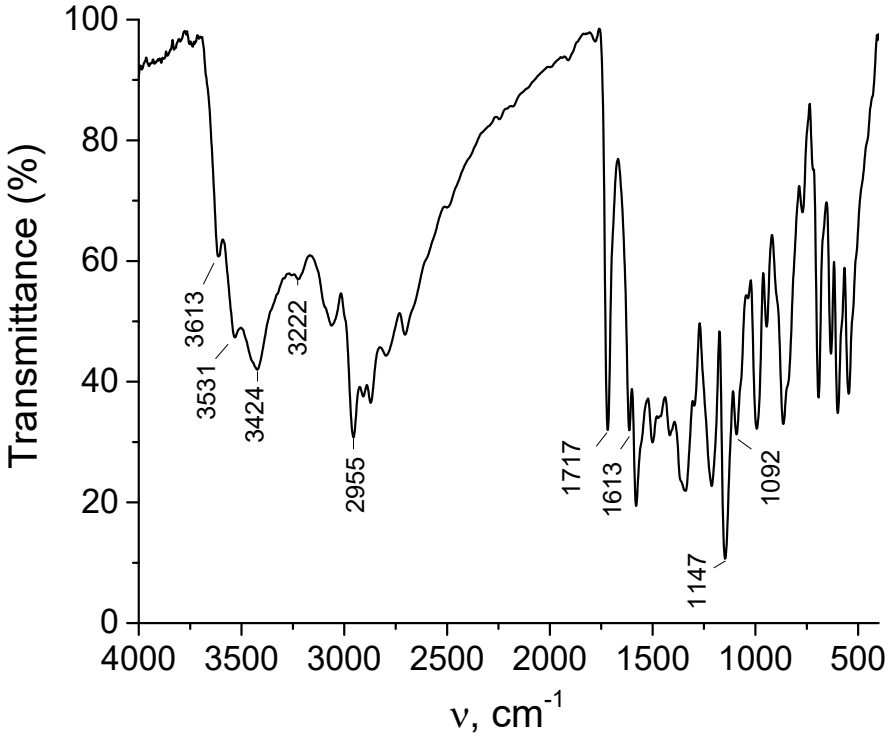
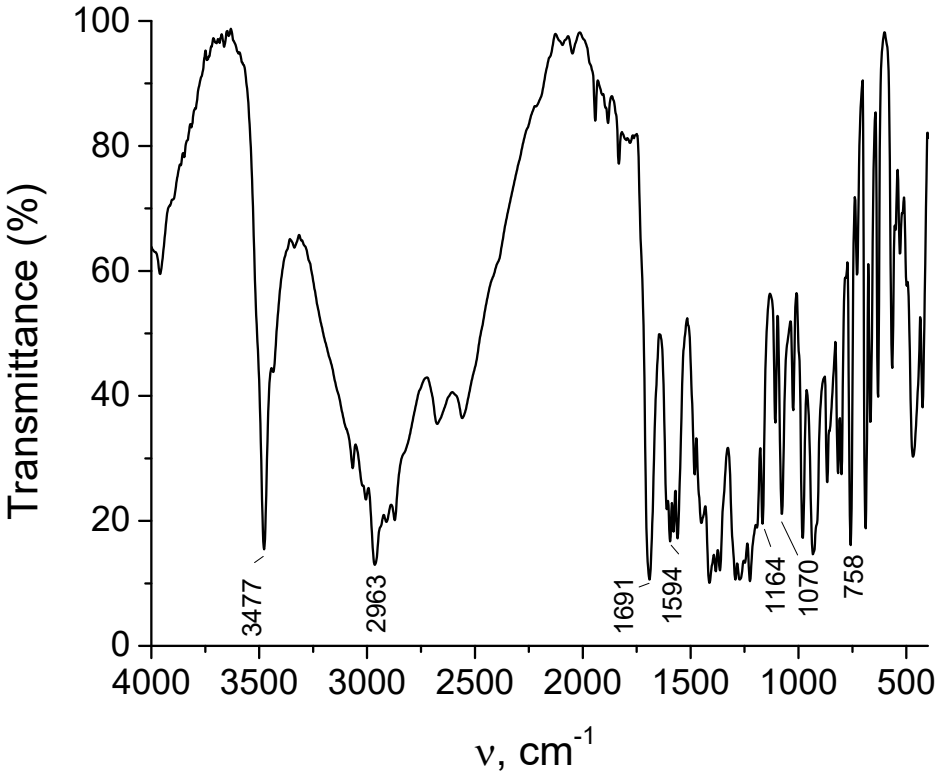


3-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid



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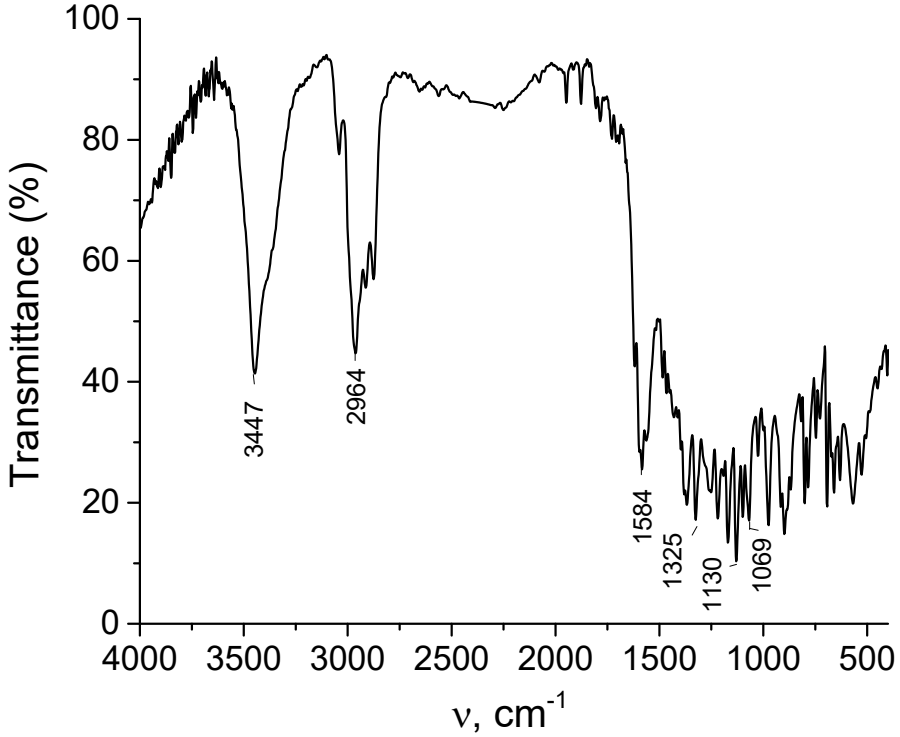

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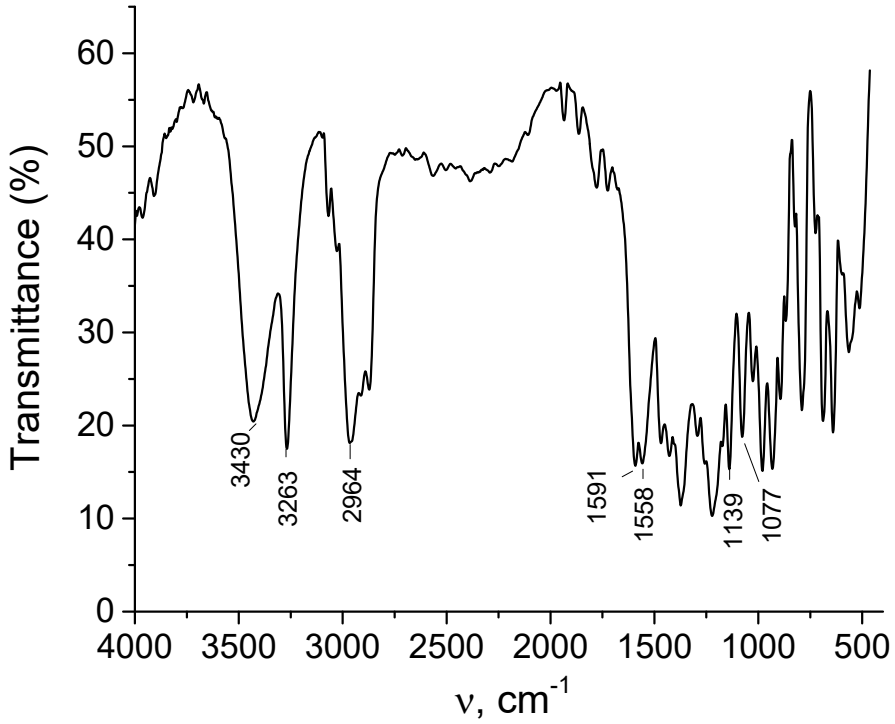

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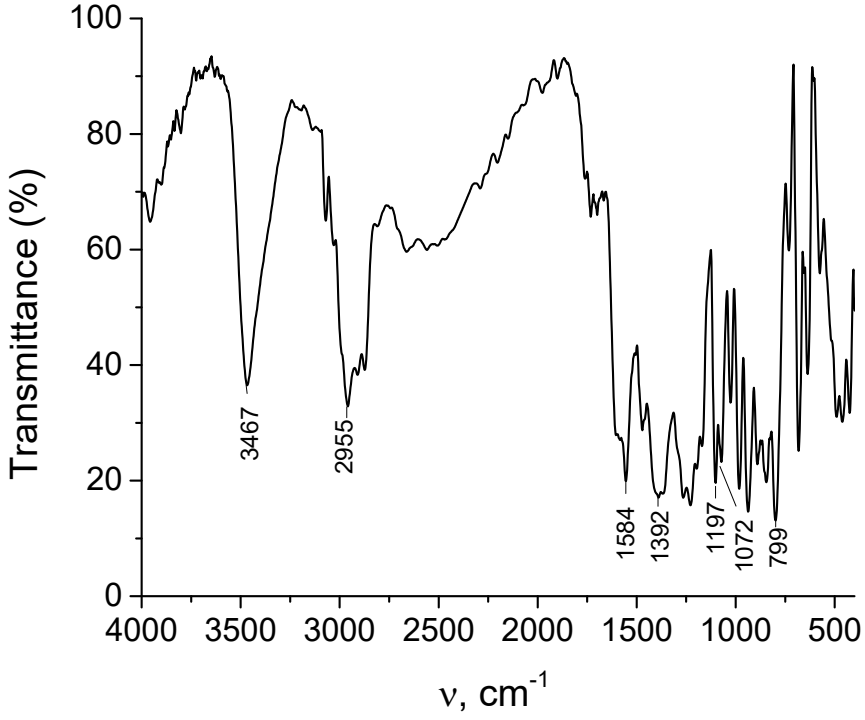
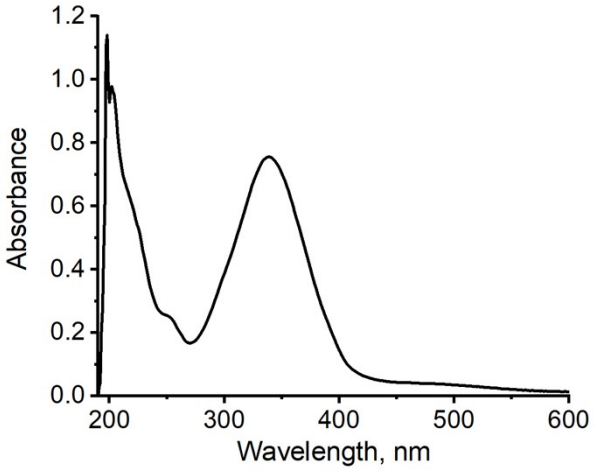
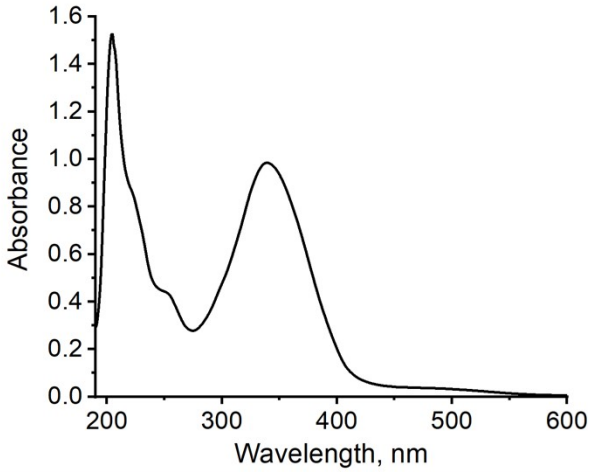


UV-vis spectra

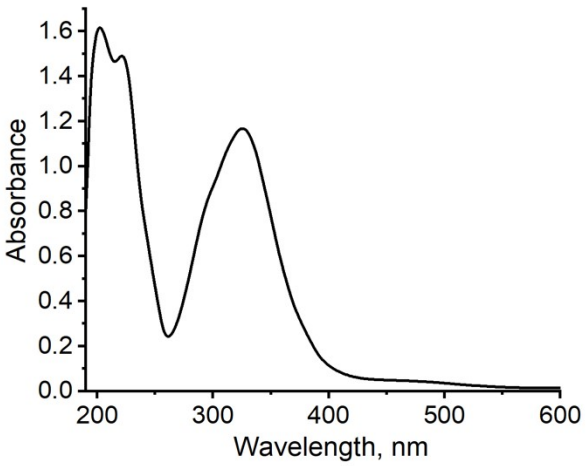
1-(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)ethan-1-one



(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)(phenyl)methanone



4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid



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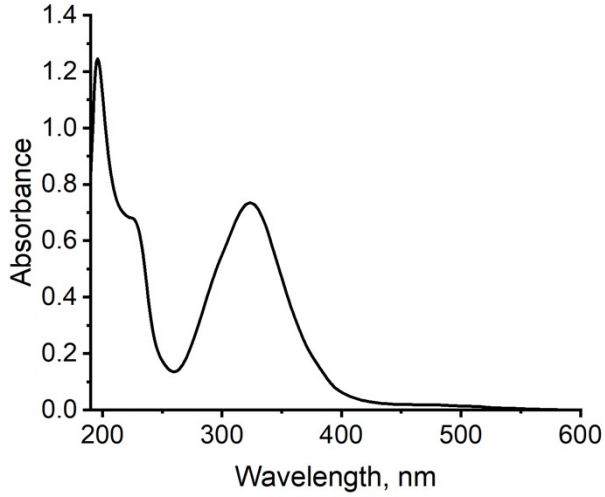
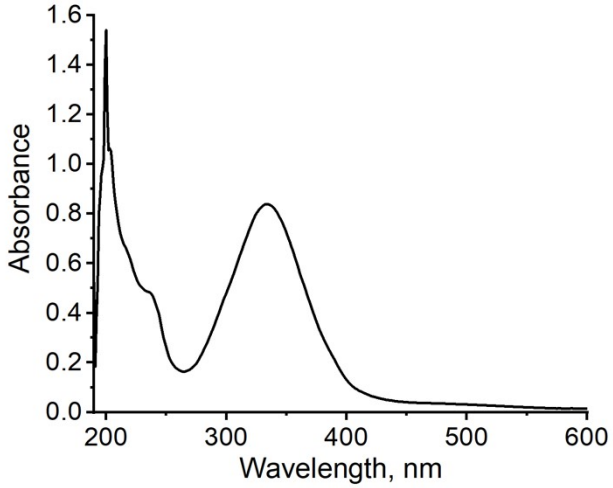
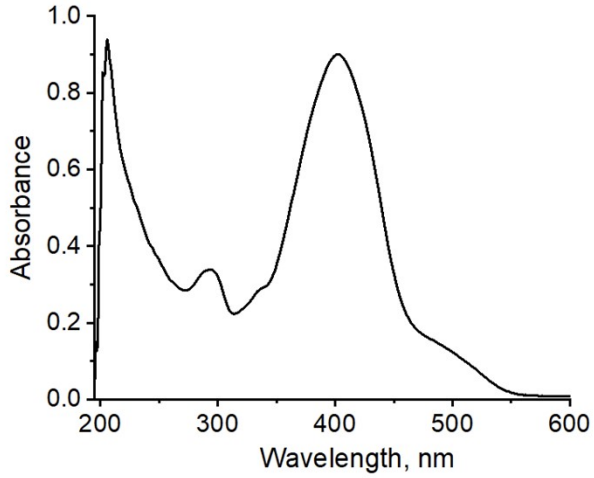


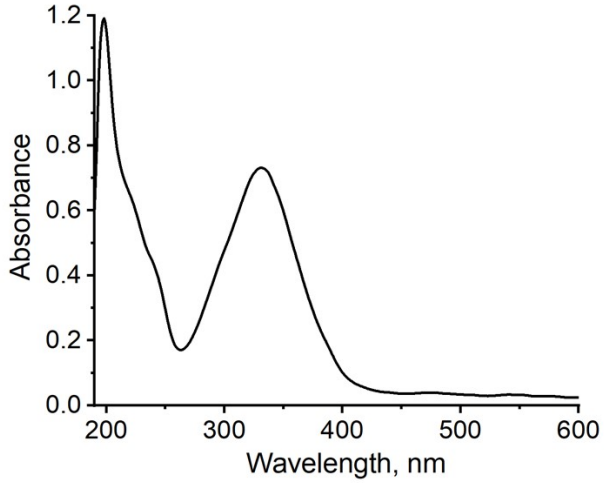
N-((4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)sulfonyl)acetamide



4,6-di-*tert*-butyl-3-(((4-(diethylamino)phenyl)imino)methyl)catechol



3-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid



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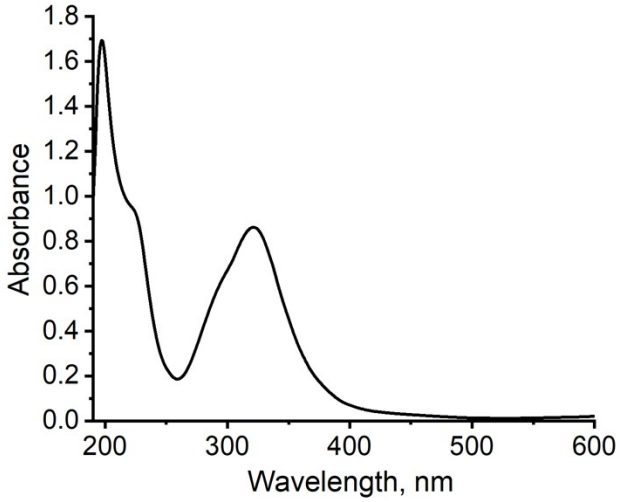
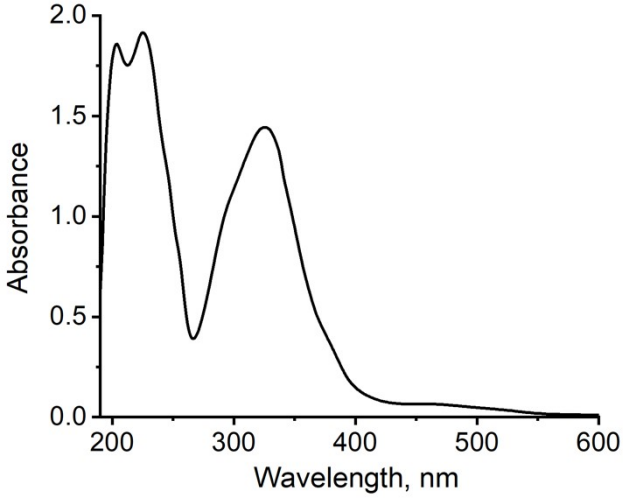
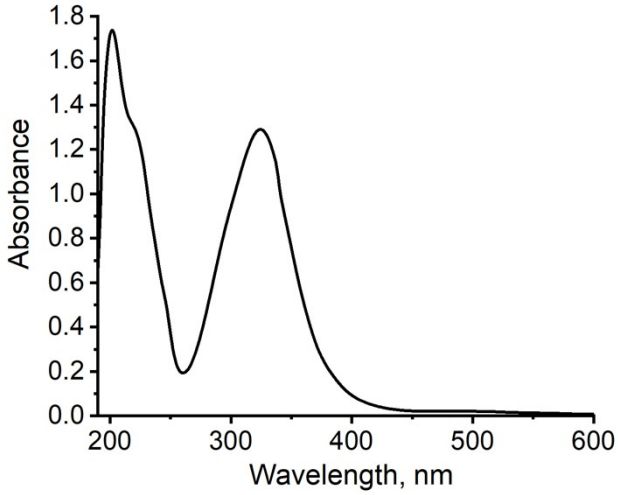




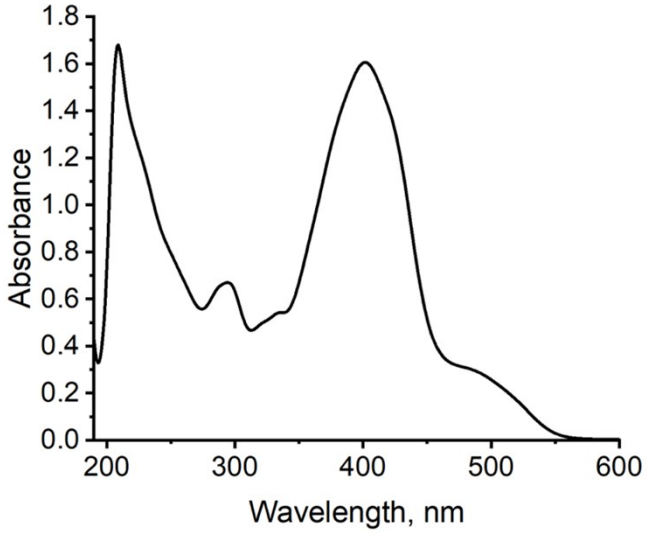
(*E*)-4,6-di-*tert*-butyl-3-(((3-ethynylphenyl)imino)methyl)catechol

4,6-di-*tert*-butyl-3-(((3,5-dichlorophenyl)imino)methyl)catechol



Tautomeric studies

UV-Vis spectrum of the 60 mM solution of the compound **16** (4,6-di-*tert*-butyl-3-(((4-(diethylamino)phenyl)imino)methyl)catechol) in ethanol.



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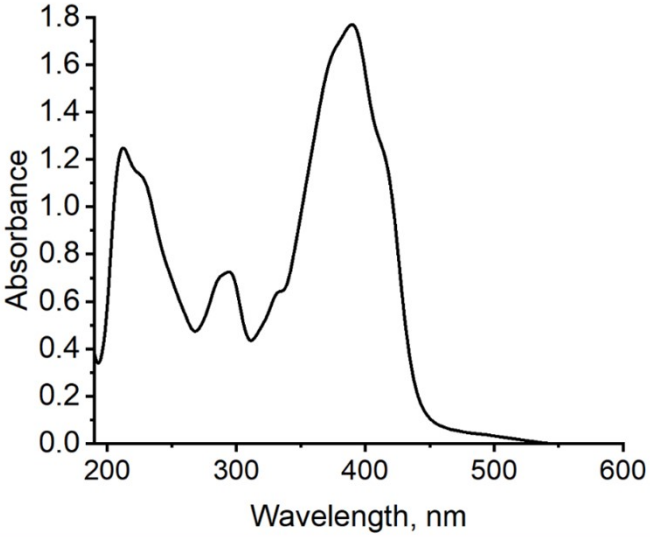
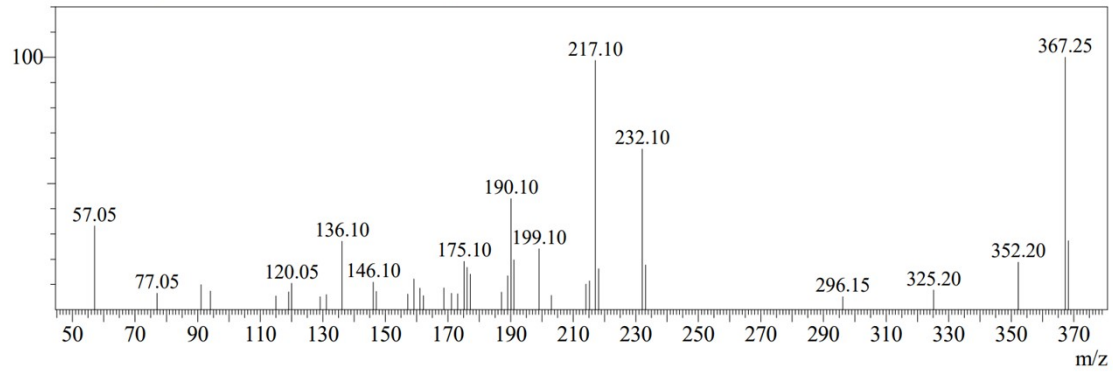


EI-MS spectra

EI-MS spectrum of the compound **7**



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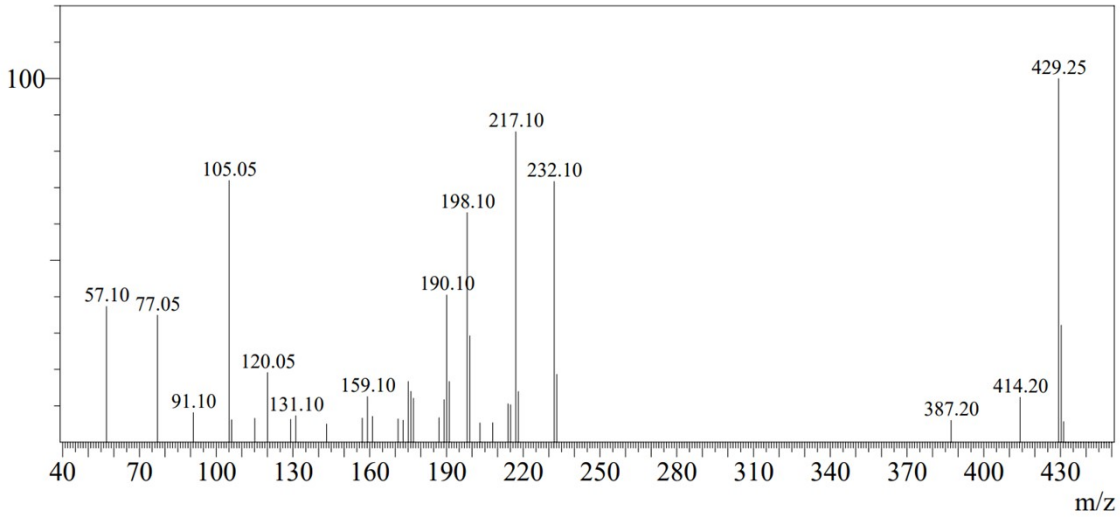
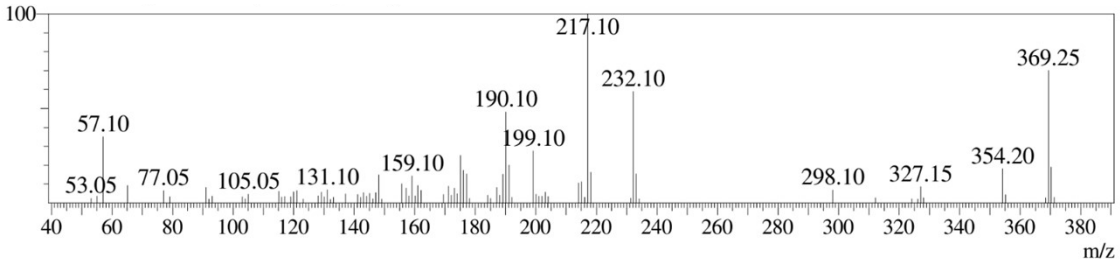


EI-MS spectrum of the compound **9**



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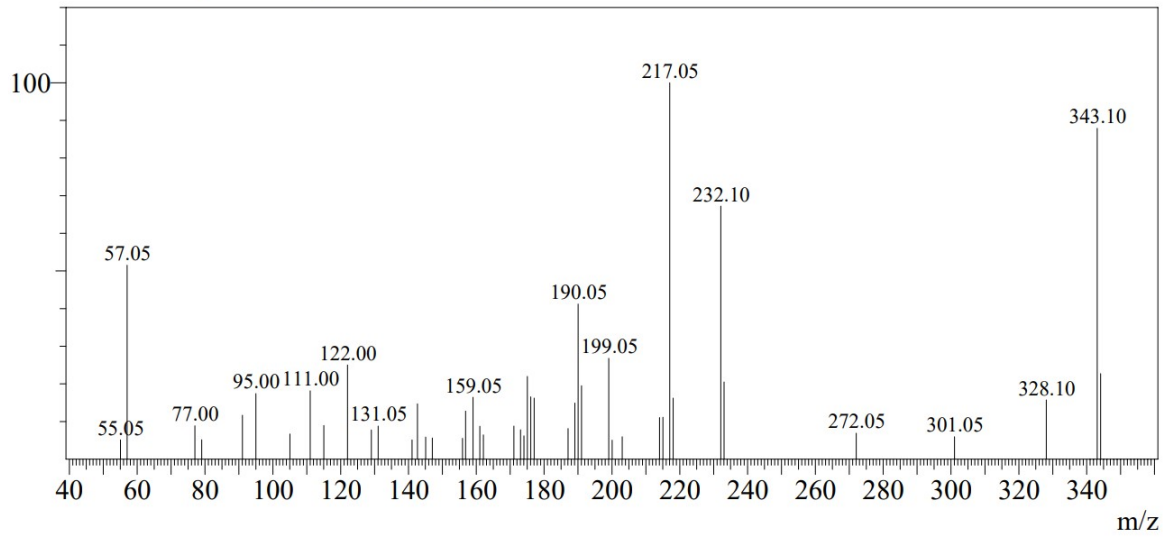

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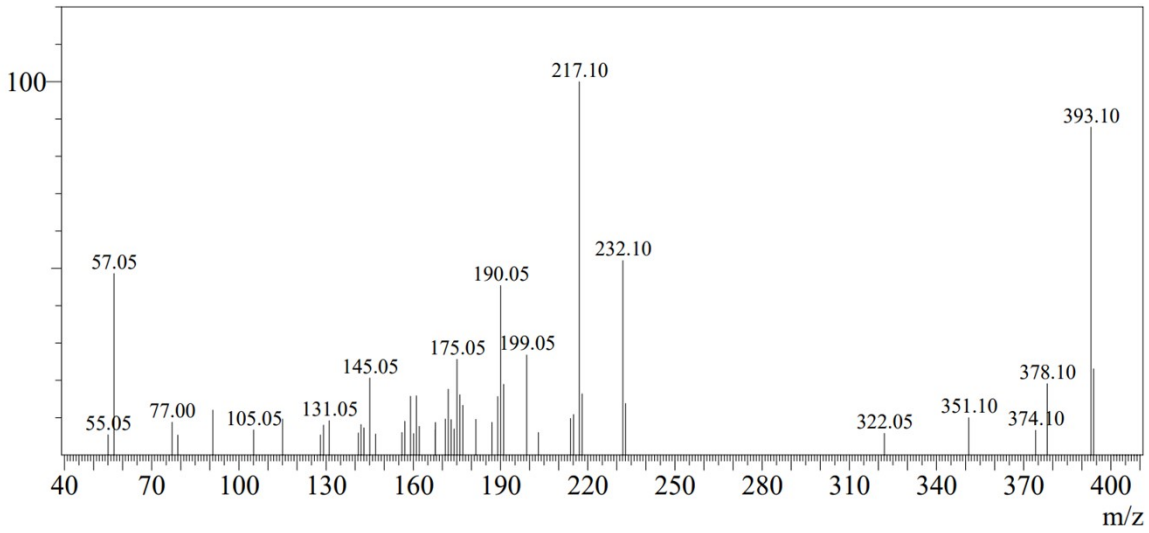
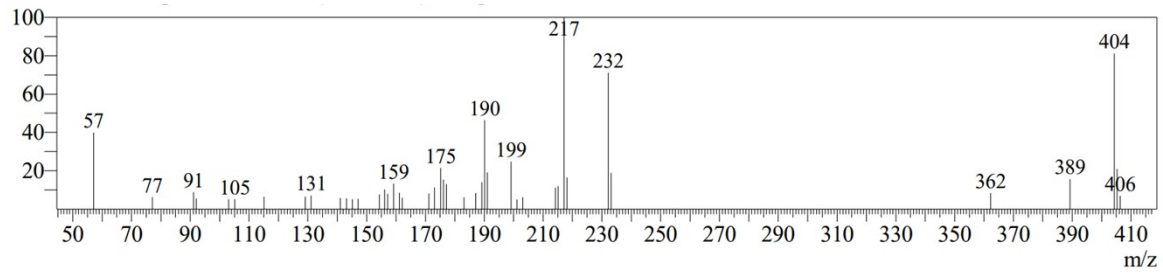
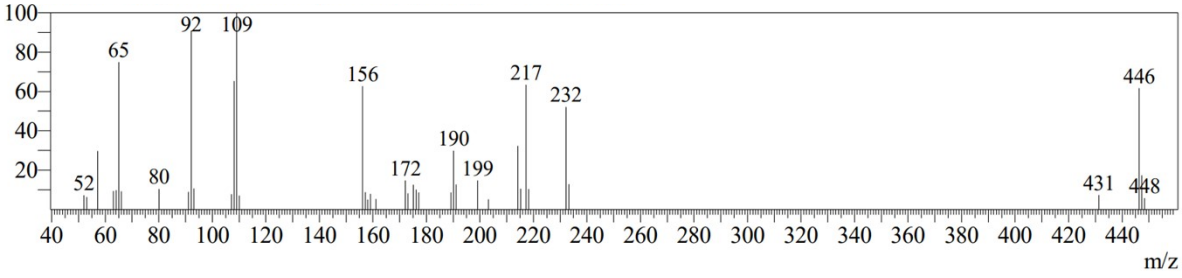


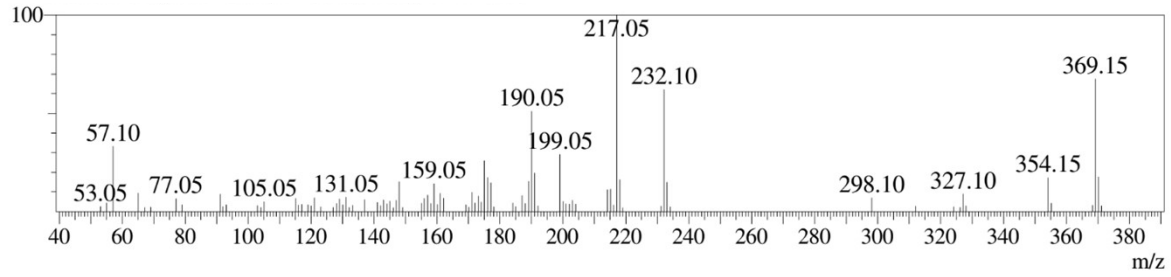
EI-MS spectrum of the compound **14**



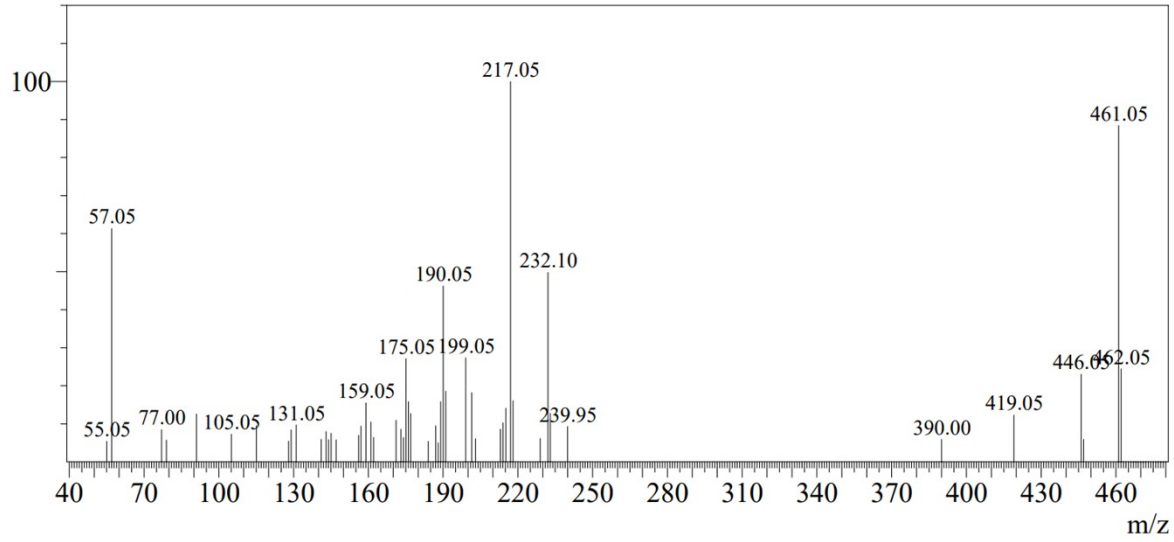
EI-MS spectrum of the compound **15**



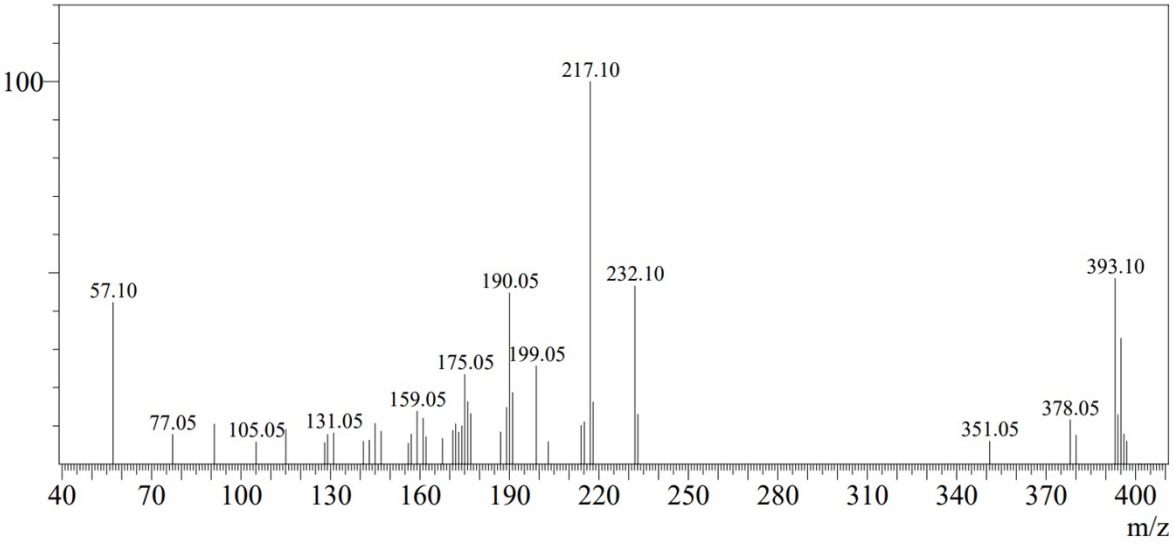
EI-MS spectrum of the compound **20**



EI-MS spectrum of the compound **22**

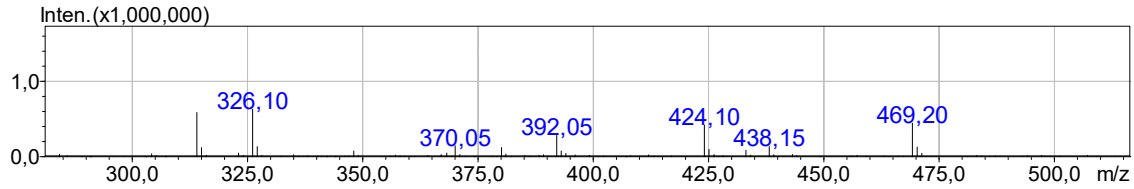


EI-MS spectrum of the compound **24**



ESI-MS spectra of adducts of the Schiff bases and DPPH radical

ESI (+)



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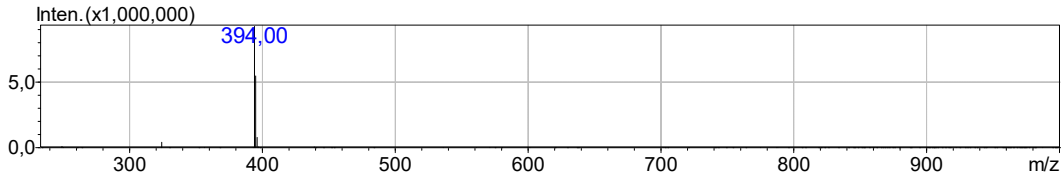
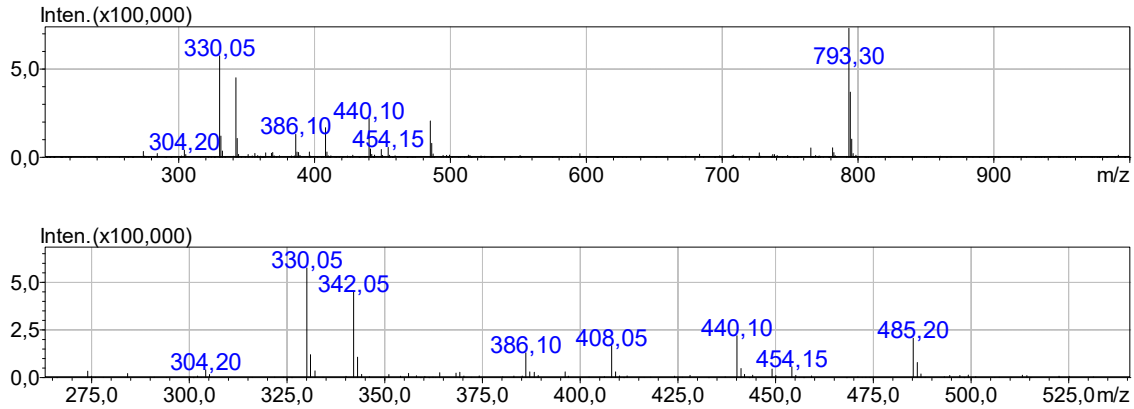


Figure S1. EI-MS spectrum of the reaction mixture of the compound **1** and DPPH (*m/z* = 326.1, $[C_{21}H_{27}NO_2+H]^+$ (compound **1**); 324.1 $[C_{21}H_{25}NO_2+H]^+$ (respective quinone)); (*m/z* = 394.0, $DPPH^-$).

ESI (+)



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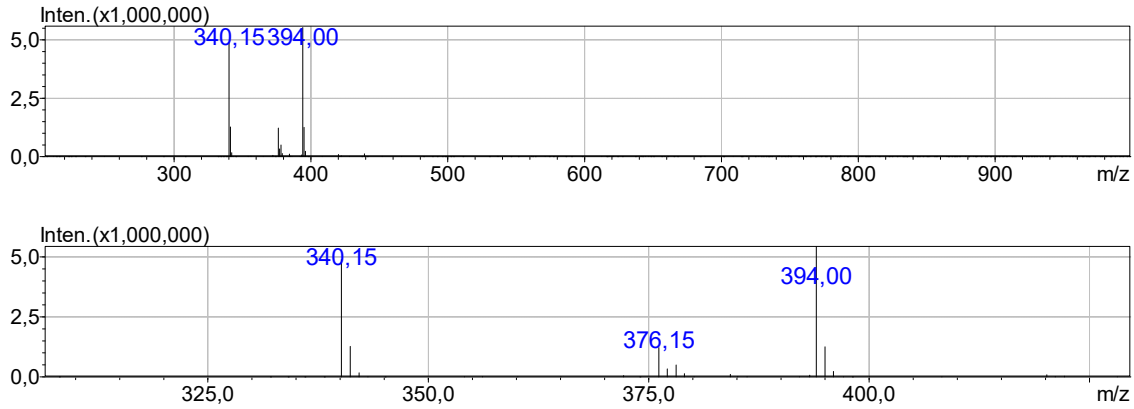
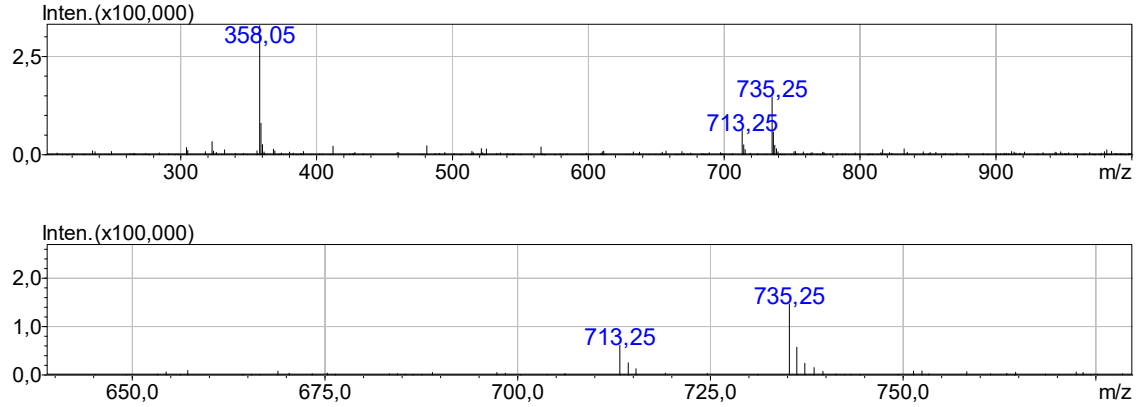


Figure S2. EI-MS spectrum of the reaction mixture of the compound **4** and DPPH (m/z 340 and m/z 342 corresponding to the ions $[C_{21}H_{27}NO_3–H]^-$, $[M–H]^-$ and $[C_{21}H_{27}NO_3+H]^+$, [M+H]+).

ESI (+)



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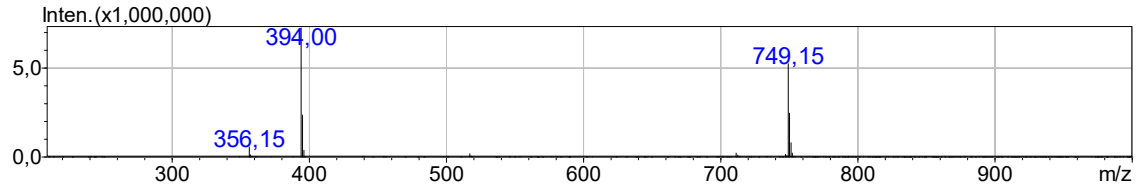
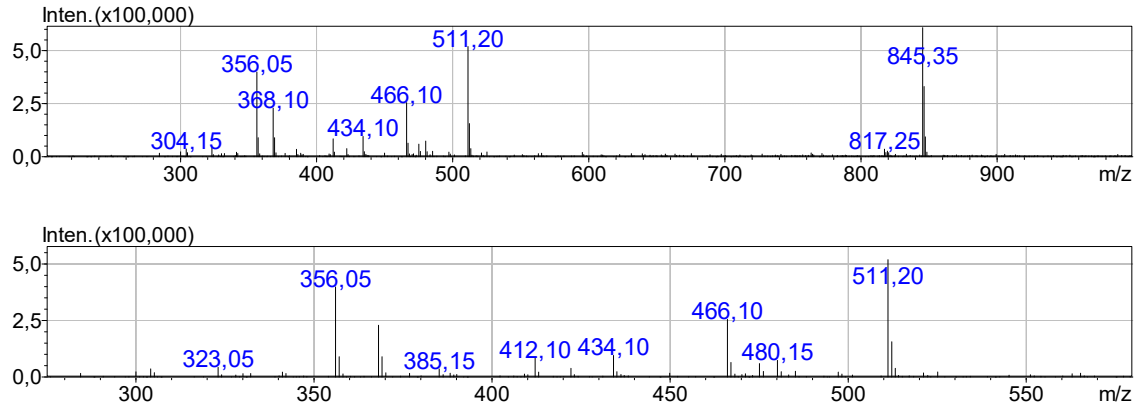


Figure S3. EI-MS spectrum of the reaction mixture of the compound **5** and DPPH (m/z 713 and 735 corresponding to the ions $[C_{42}H_{52}N_2O_4S_2+H]^+$ and $[C_{42}H_{52}N_2O_4S_2+Na]^+$ (calculated *m/z* are 713 and 735, respectively), and an adduct with the DPPH radical with m/z 749, which is assigned to $[C_{39}H_{38}N_6O_8S–H]^–$, $[M+DPPH–H]^–$ (calculated m/z 749)).

ESI (+)



ESI (-)

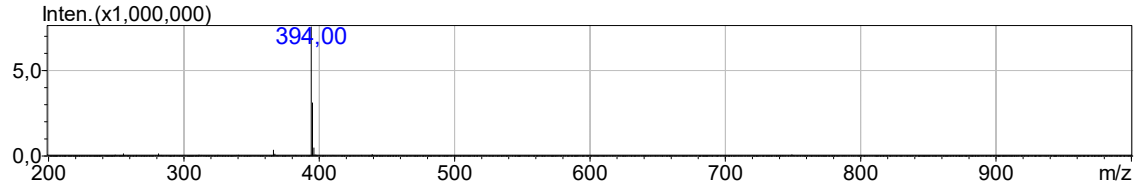
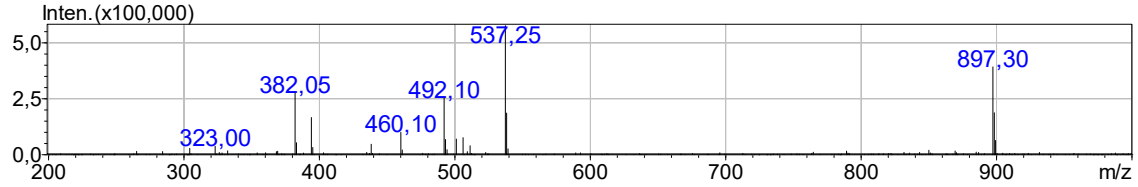


Figure S4. EI-MS spectrum of the reaction mixture of the compound **7** and DPPH (*m/z* 368 $[C_{23}H_{29}NO_3+H]^+$; (*m/z* = 394.0, $DPPH^–$).

ESI (+)



ESI (-)

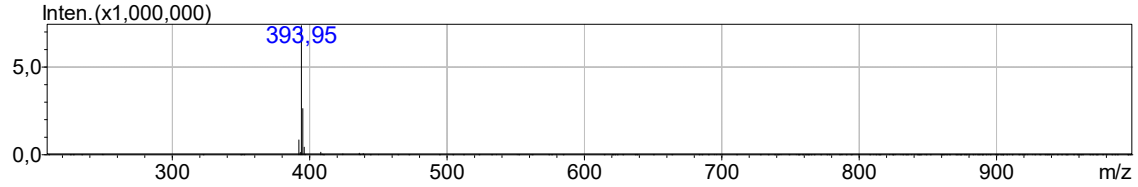
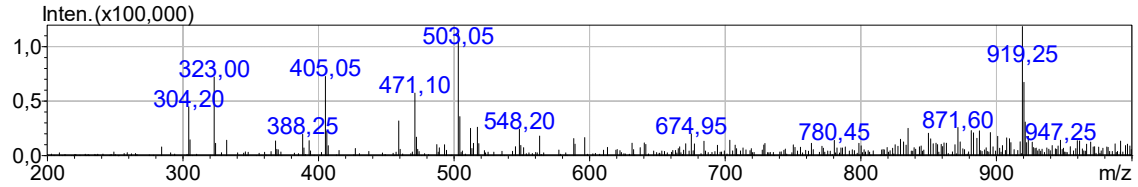


Figure S5. EI-MS spectrum of the reaction mixture of the compound **13** and DPPH (m/z 394 $[C_{22}H_{26}F_3NO_2+H]^+$).

ESI (+)



ESI (-)

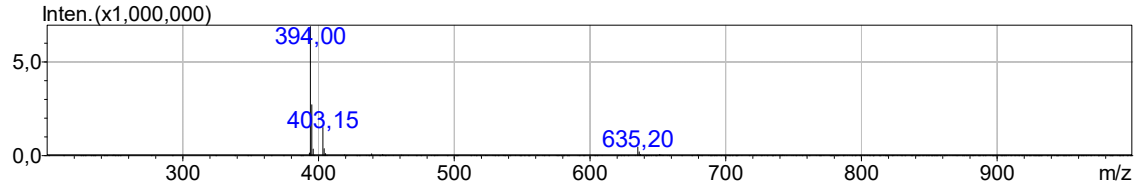
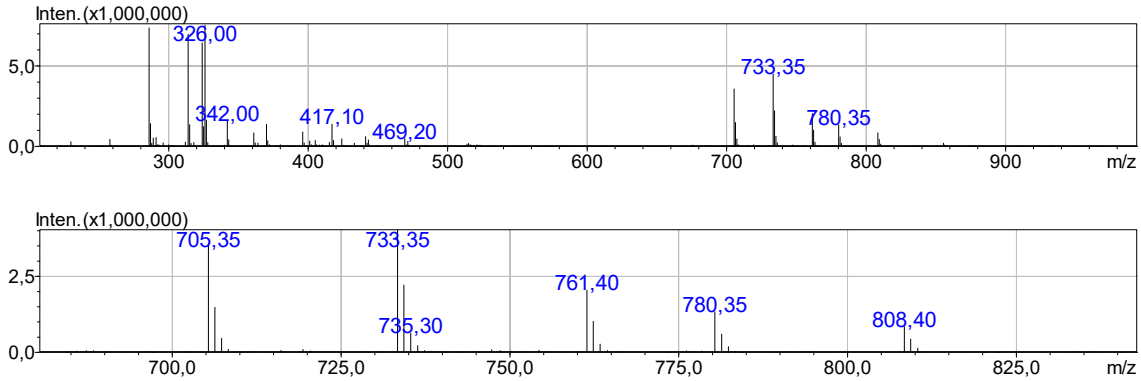


Figure S6. EI-MS spectrum of the reaction mixture of the compound **14** and DPPH (*m/z* = 405, $[C_{21}H_{28}N_2O_4S+H]^+$, m/z = 403.3, $[C_{21}H_{28}N_2O_4S–H]^–$).

ESI-MS spectra of adducts of the Schiff bases and ABTS cation radical

ESI (+)



ESI (-)

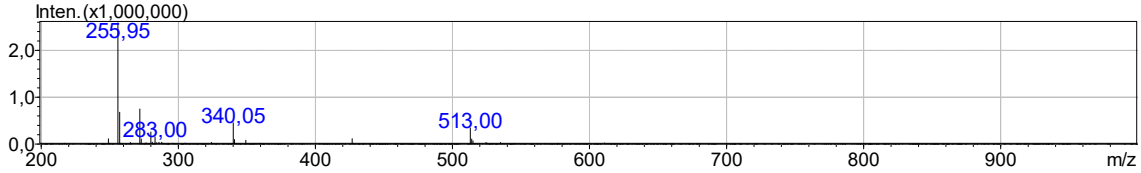
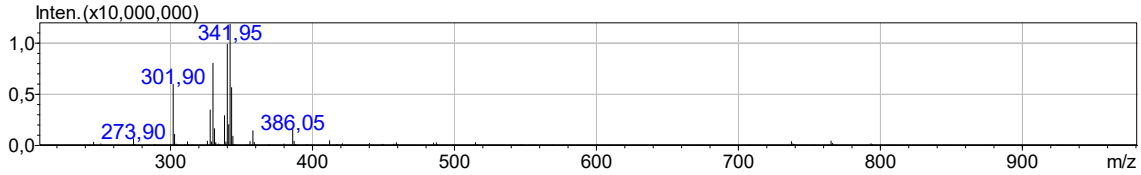


Figure S7. ESI-MS spectrum of the reaction mixture of the compound **1** and ABTS: *m/z* 326.1, $[C_{21}H_{27}NO_2+H]^+$ (compound **1**); *m/z* 324.1 $[C_{21}H_{25}NO_2+H]^+$ (the respective quinone); *m/z* 256 (negative mode) appeared in the ESI-MS spectra of the reaction mixtures, which could be assigned to 3-ethyl-2-imino-1,3-benzothiazoline-6-sulfonate.

ESI (+)



ESI (-)

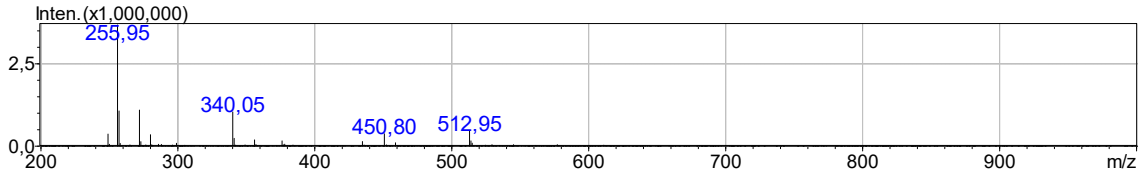
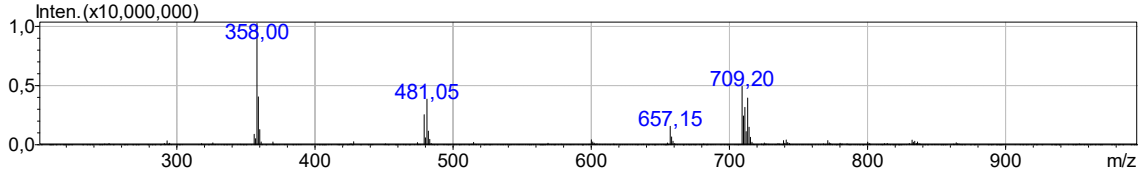
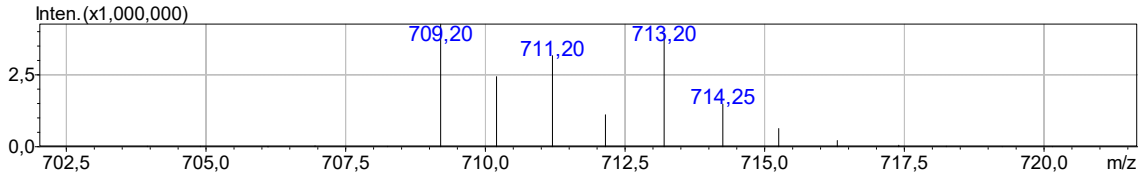


Figure S8. ESI-MS spectrum of the reaction mixture of the compound **4** and ABTS: m/z 340 and m/z 342, corresponding to the ions $[C_{21}H_{27}NO_3–H]^–$, $[M–H]^–$ and $[C_{21}H_{27}NO_3+H]^+$, [M+H]+.

ESI (+)





ESI (-)

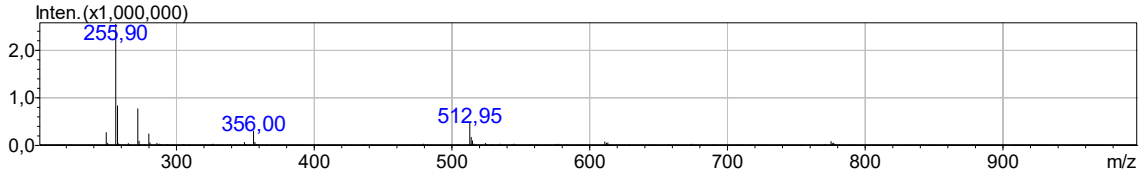
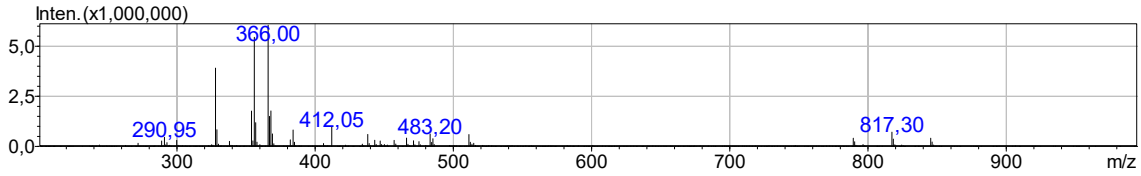


Figure S9. ESI-MS spectrum of the reaction mixture of the compound **5** and ABTS: disulfides (*m/z* 713 $[C_{42}H_{52}N_2O_4S_2+H]^+$, $[M+H]^+$) that could be further oxidized by ABTS, resulting in the respective quinone molecules (*m/z* 709 $[C_{42}H_{48}N_2O_4S_2+H]^+$).

ESI (+)



ESI (-)

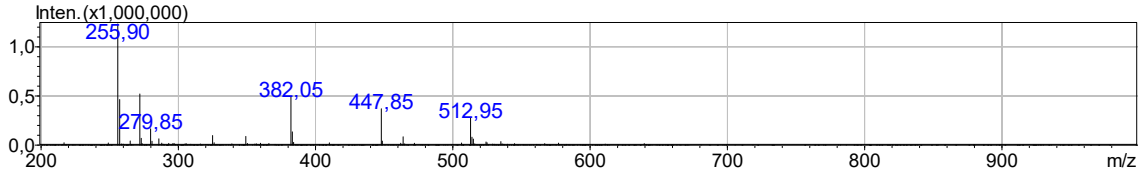
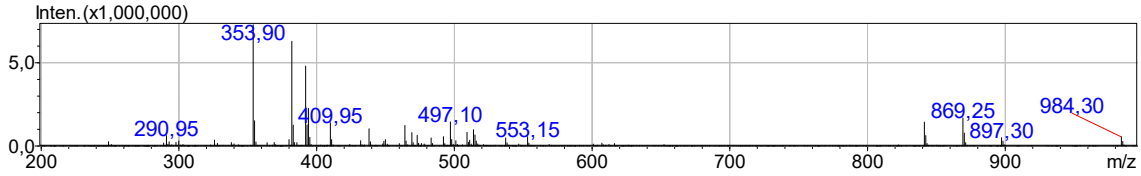


Figure S10. ESI-MS spectrum of the reaction mixture of the compound **7** and ABTS: *m/z* 366 $[C_{23}H_{27}NO_3+H]^+$, quinone.

ESI (+)



ESI (-)

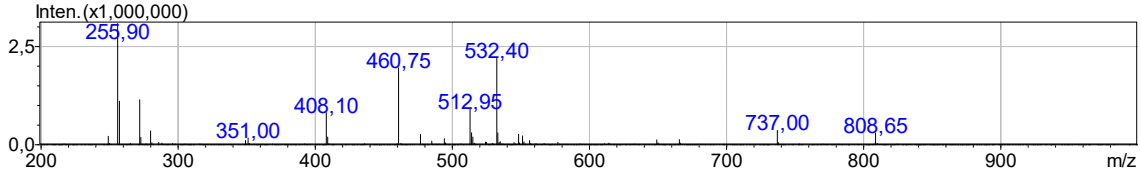
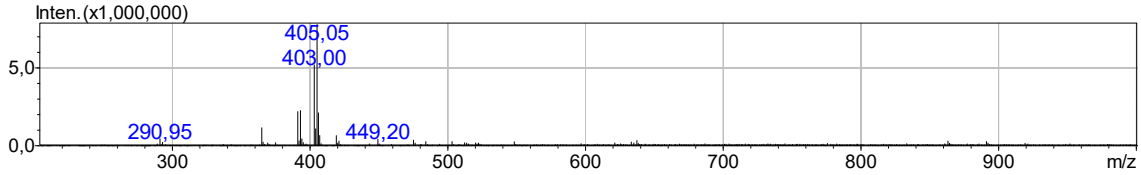


Figure S11. EI-MS spectrum of the reaction mixture of the compound **13** and ABTS: *m/z* 394 $[C_{22}H_{24}F_3NO_2+H]^+$, quinone.

ESI (+)



ESI (-)

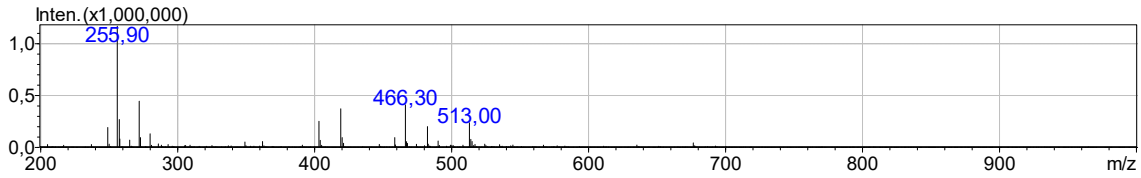


Figure S12. EI-MS spectrum of the reaction mixture of the compound **14** and ABTS: *m/z* 405, $[C_{21}H_{28}N_2O_4S+H]^+$; *m/z* 403 $[C_{21}H_{26}N_2O_4S+H]^+$ (quinone).

UV-Vis spectra of adducts of the Schiff bases with the ABTS cation radical

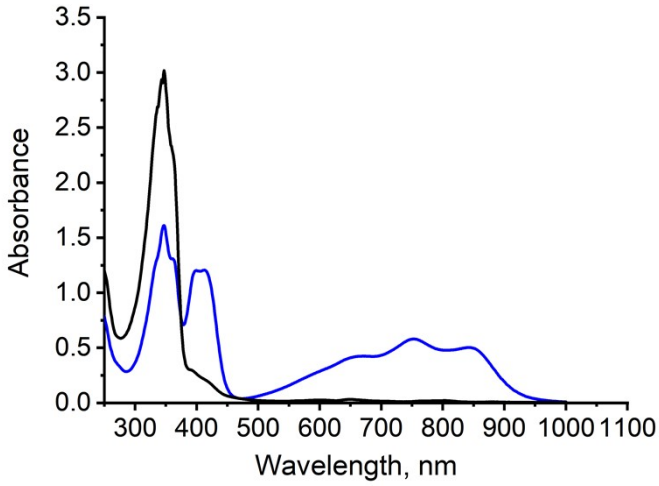


Figure S13. UV-Vis spectrum of the reaction mixture of the compound **1** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

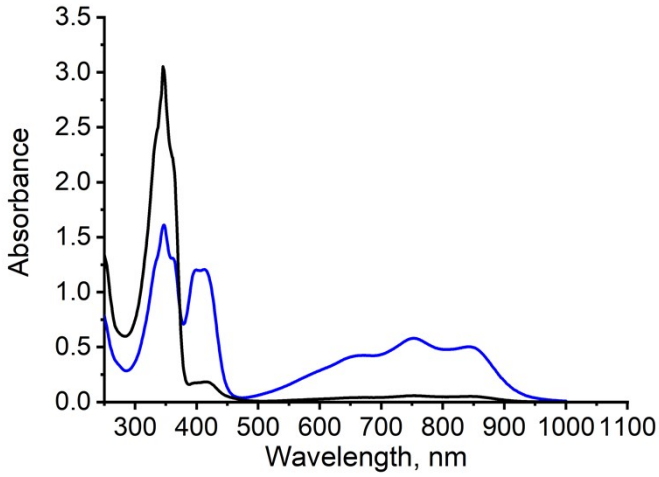


Figure S14. UV-Vis spectrum of the reaction mixture of the compound **4** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

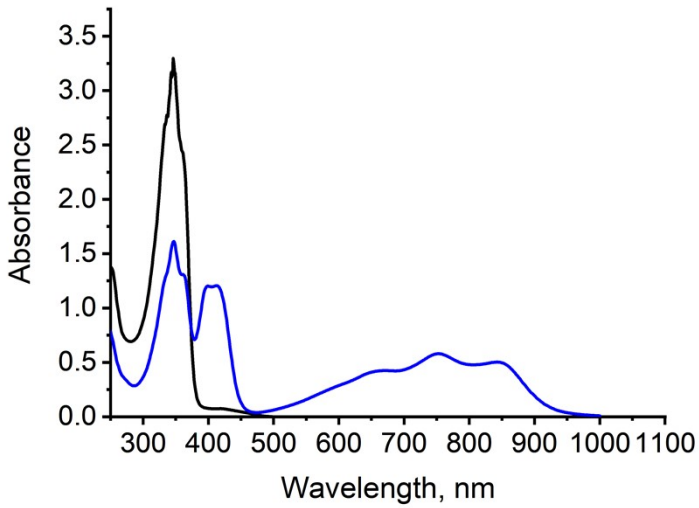


Figure S15. UV-Vis spectrum of the reaction mixture of the compound **7** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

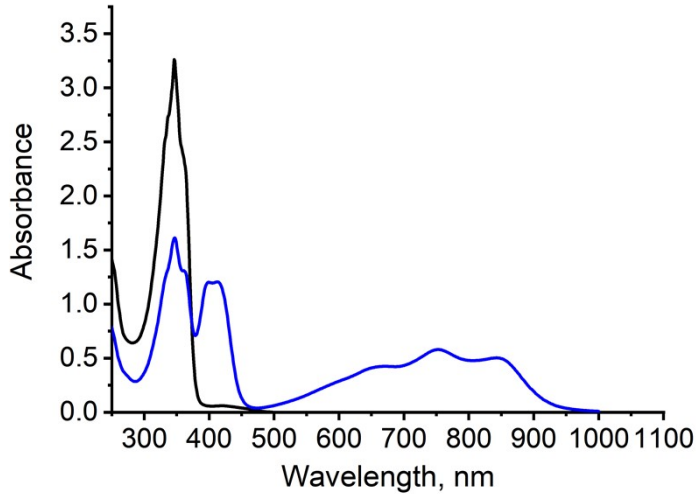


Figure S16. UV-Vis spectrum of the reaction mixture of the compound **9** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

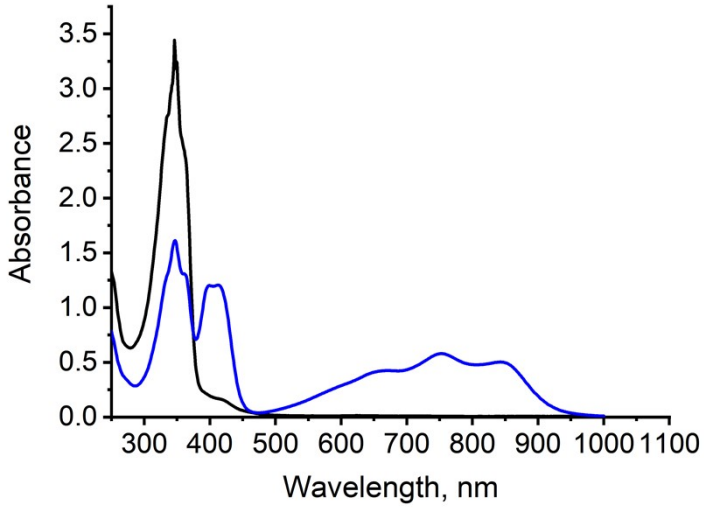


Figure S17. UV-Vis spectrum of the reaction mixture of the compound **14** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

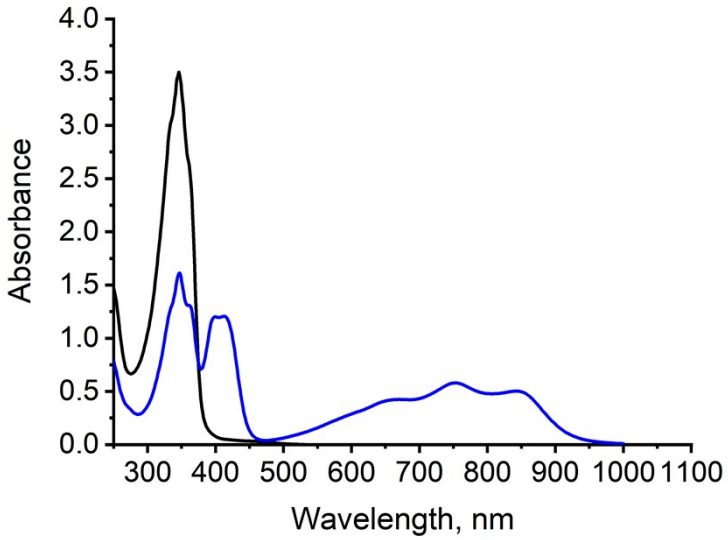


Figure S18. UV-Vis spectrum of the reaction mixture of the compound **19** and ABTS (blue – UV-Vis spectrum of the ABTS cation radical before addition of an antioxidant).

Correlation analysis

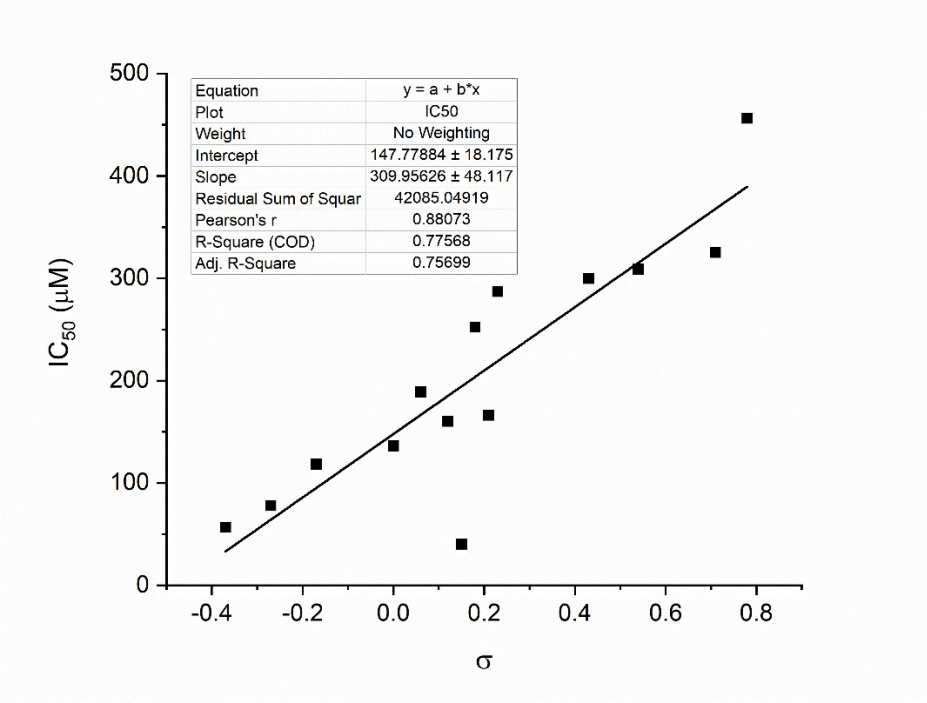


Figure S19. Antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in hexane medium versus Hammett constant (σ).

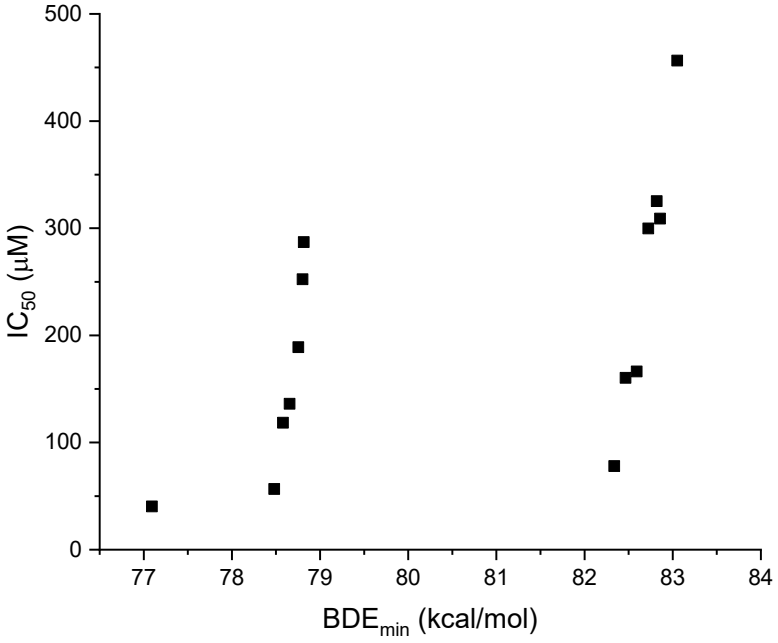


Figure S20. Antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in hexane medium versus lowest BDE calculated *in vacuo* (kcal/mol).

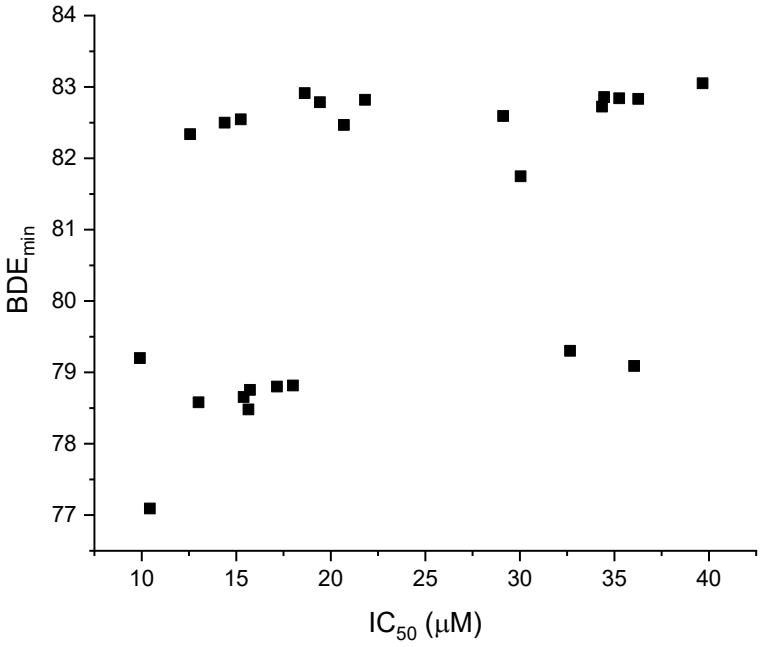


Figure S21. Lowest BDE (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

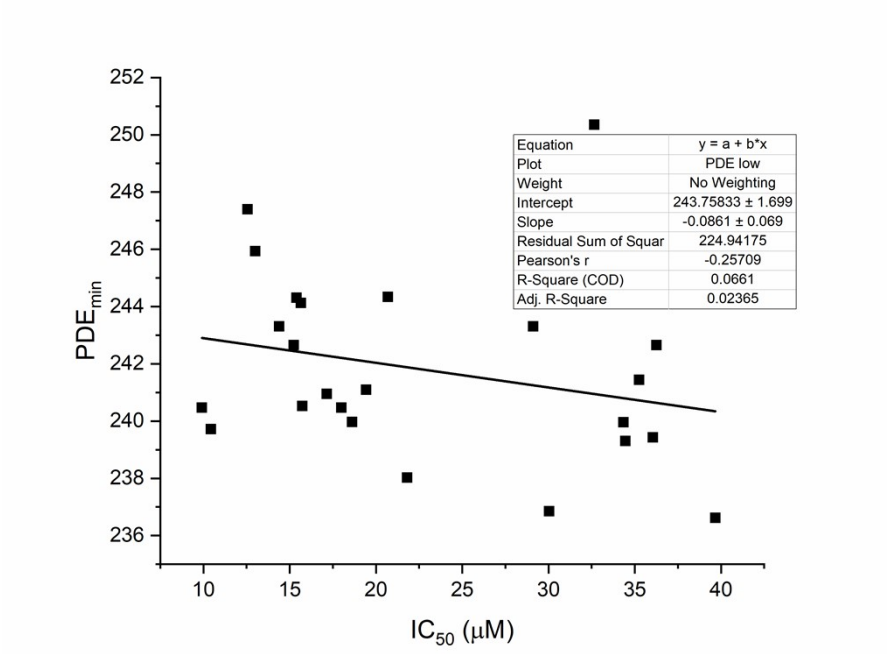


Figure S22. Lowest PDE calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

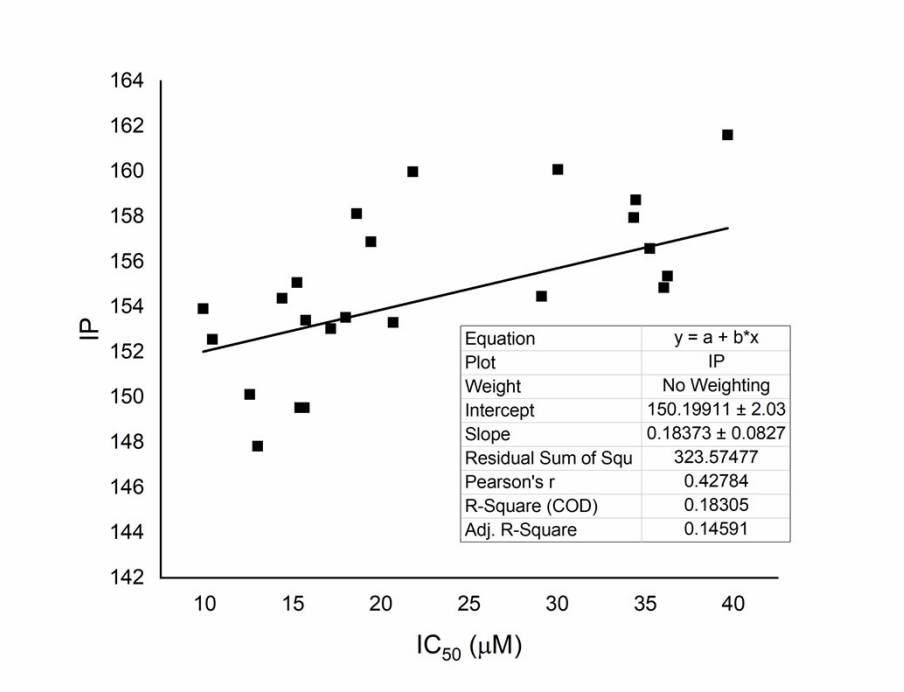


Figure S23. Lowest IP calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

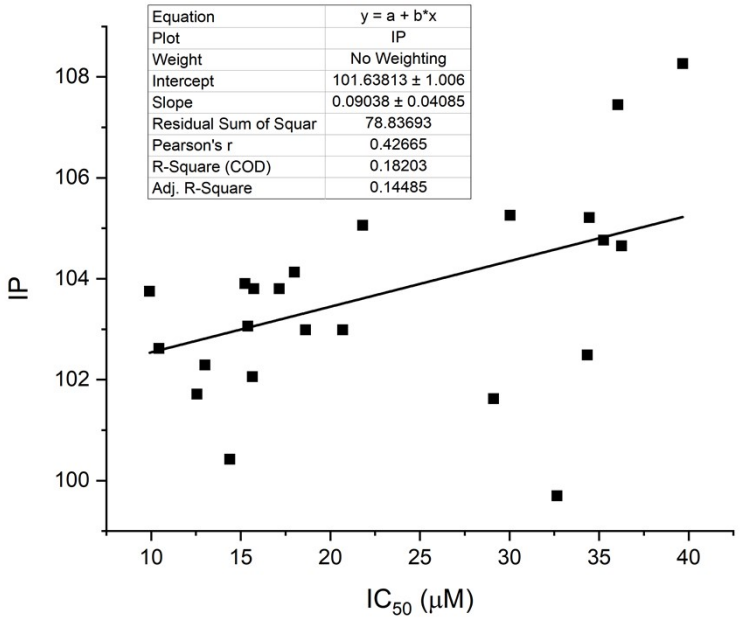


Figure S24. Lowest IP calculated in ethanol (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

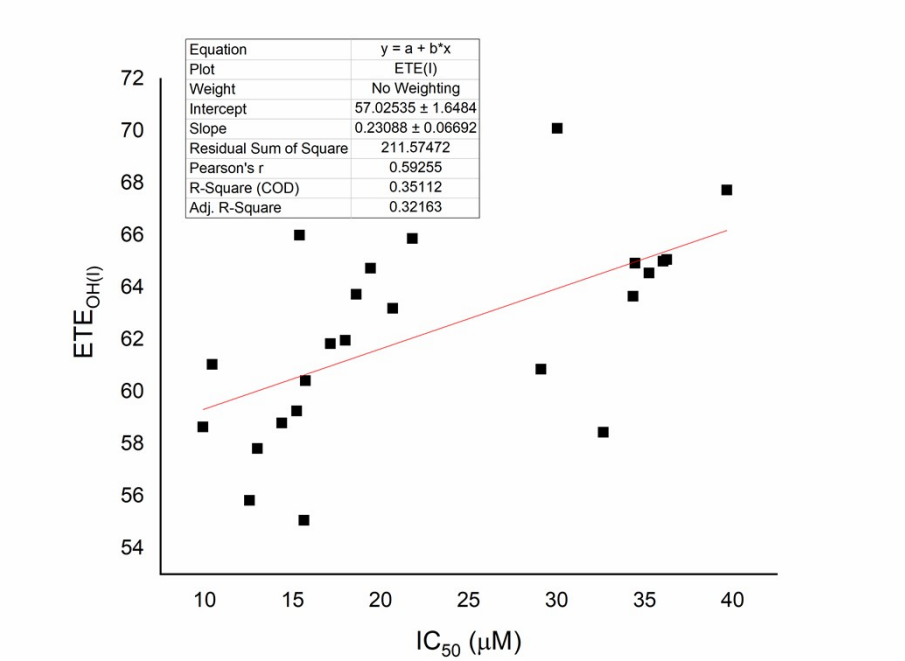


Figure S25. $ETE_{OH(I)}$ calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) for the series of Schiff bases in the DPPH assay in ethanol.

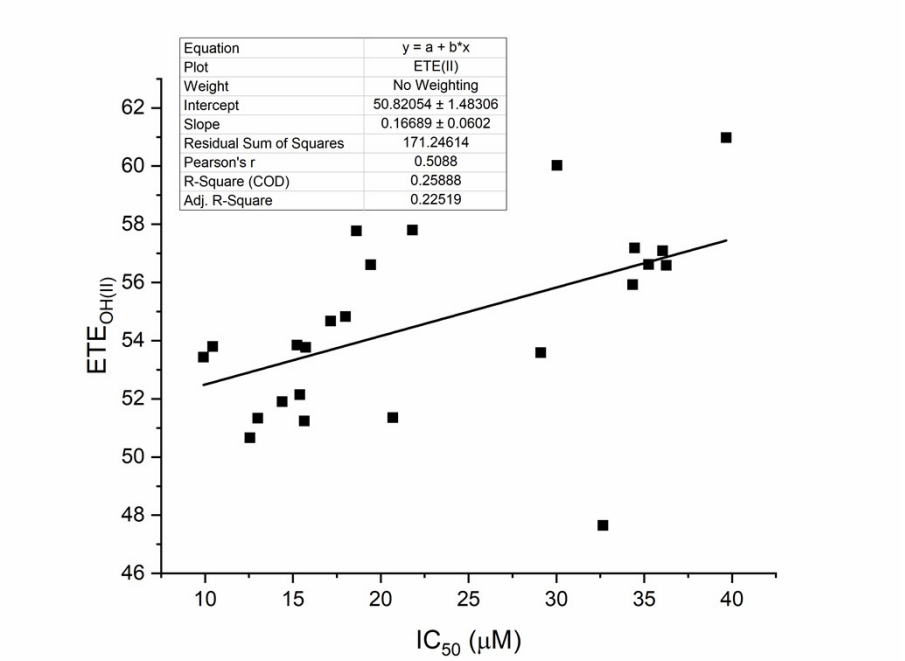


Figure S26. $ETE_{OH(II)}$ calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

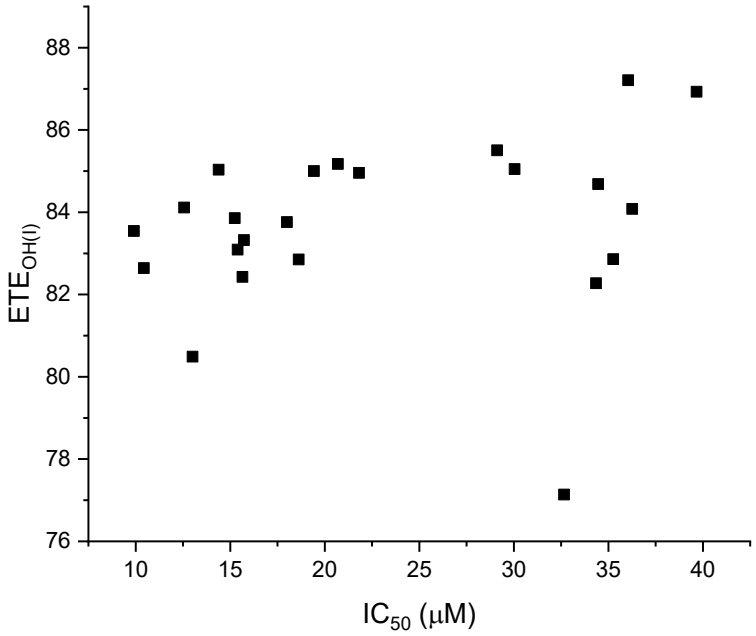


Figure S27. $ETE_{OH(I)}$ calculated in ethanol (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

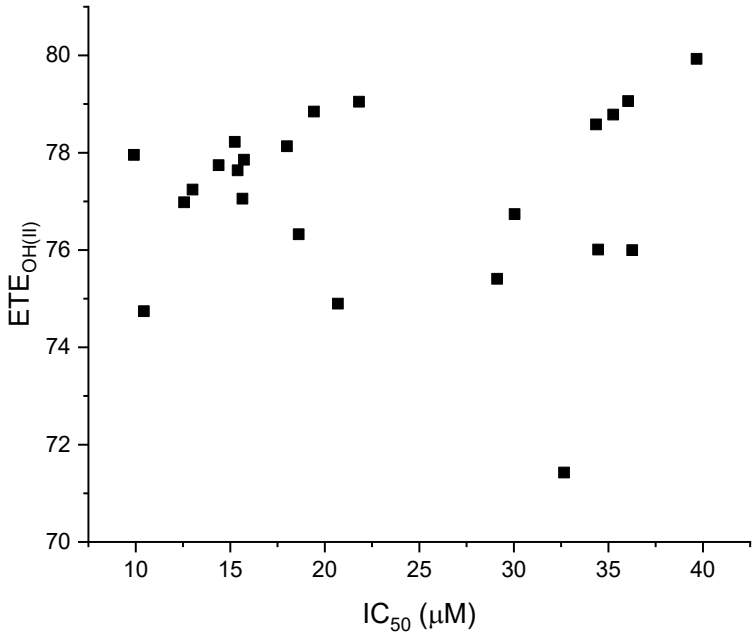


Figure S28. $ETE_{OH(II)}$ calculated in ethanol (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the DPPH assay in ethanol.

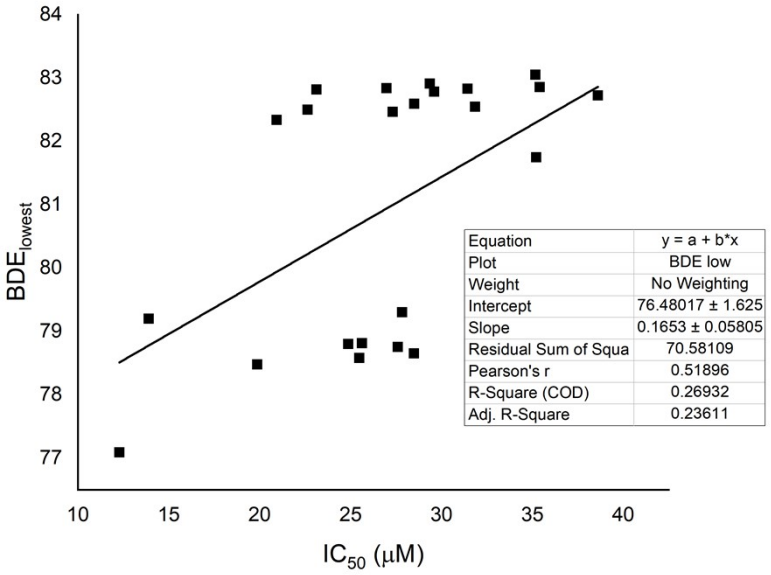


Figure S29. Lowest BDE calculated in ethanol (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the ABTS assay in ethanol.

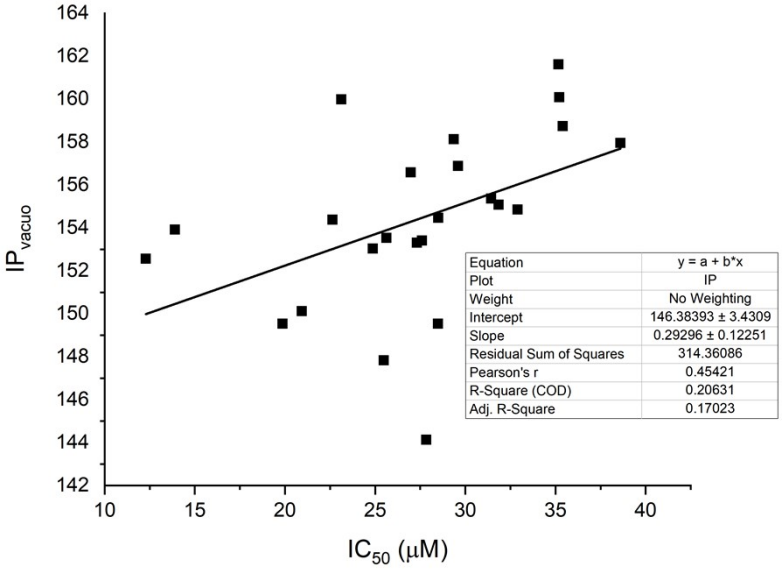


Figure S30. Lowest IP calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the ABTS assay in ethanol.

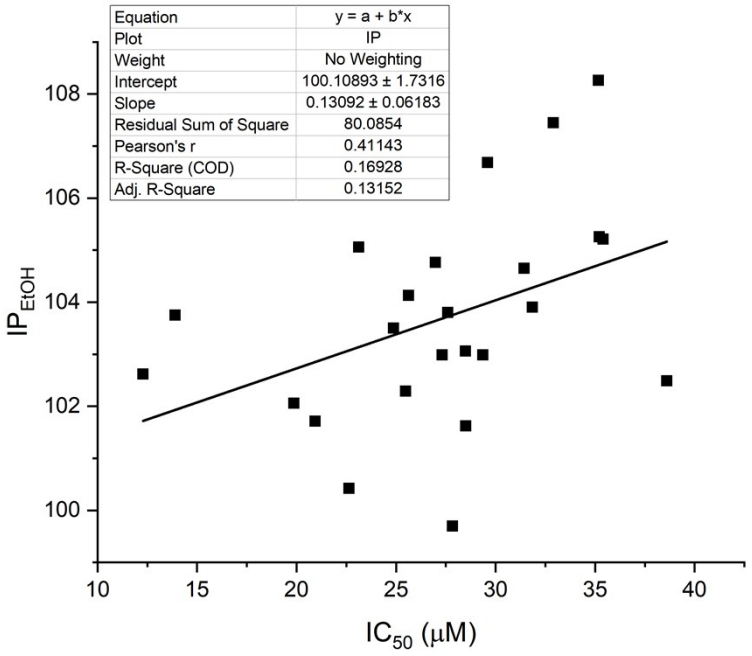


Figure S31. Lowest IP calculated in ethanol (kcal/mol) versus antioxidant activity (IC_{50}) of the Schiff bases in the ABTS assay in ethanol.

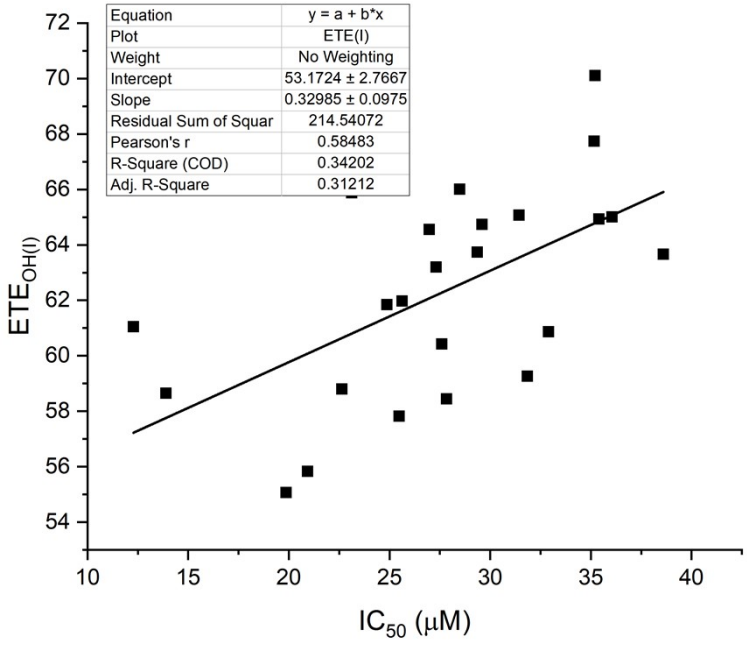


Figure S32. $ETE_{OH(I)}$ calculated *in vacuo* (kcal/mol) versus antioxidant activity (IC_{50}) for the series of Schiff bases in the ABTS assay in ethanol.

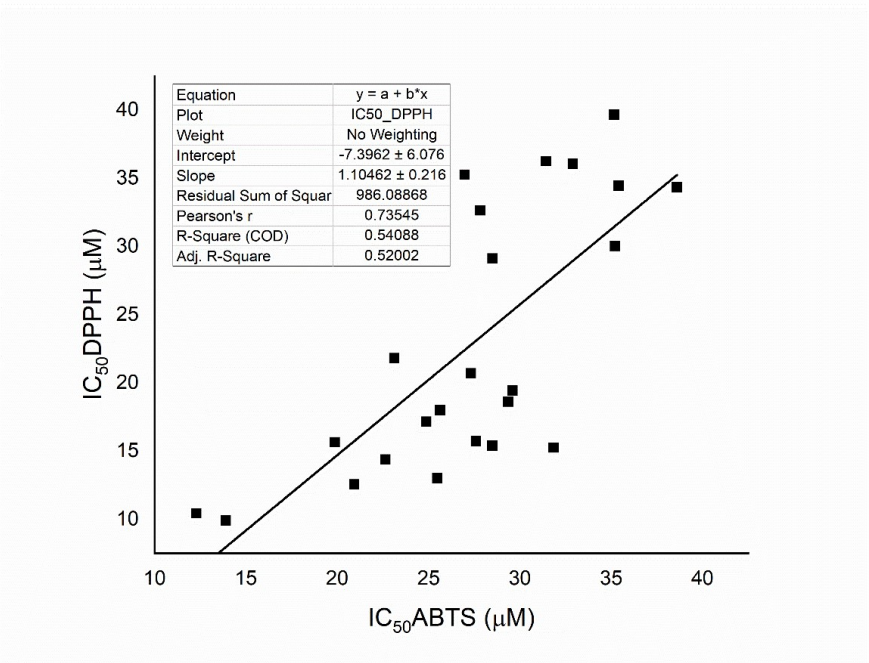


Figure S33. DPPH scavenging activity versus ABTS scavenging activity of the Schiff bases in ethanol.

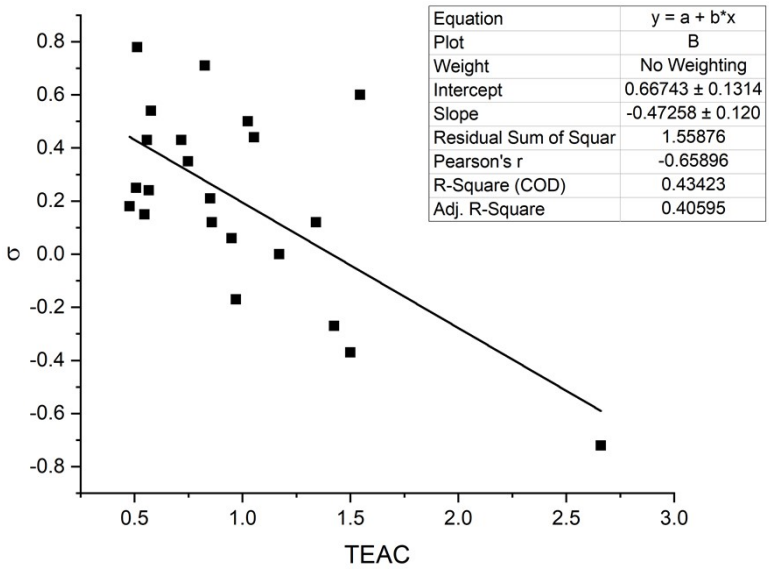


Figure S34. Hammett constant (σ) versus $TEAC_{FRAP}$ of the Schiff bases in ethanol.

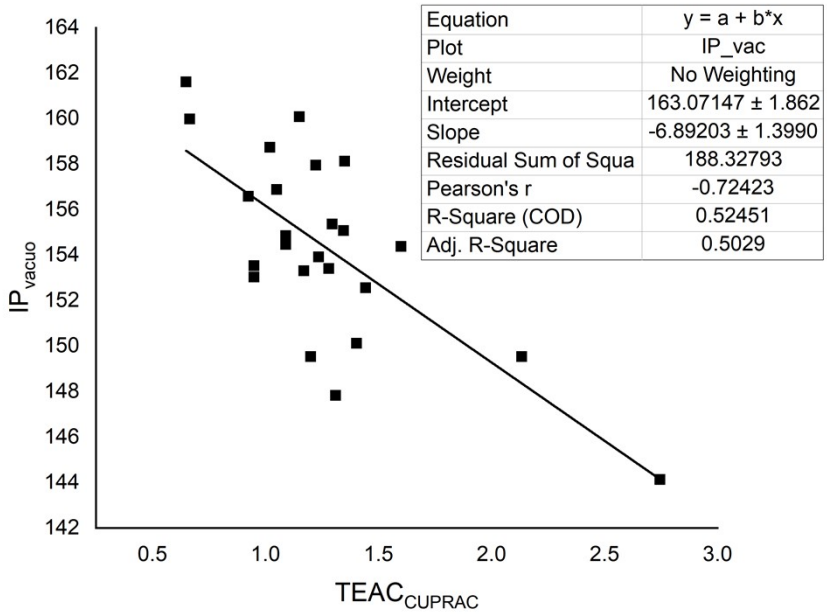


Figure S35. IP calculated *in vacuo* (kcal/mol) versus $TEAC_{CUPRAC}$ of the Schiff bases in ethanol.

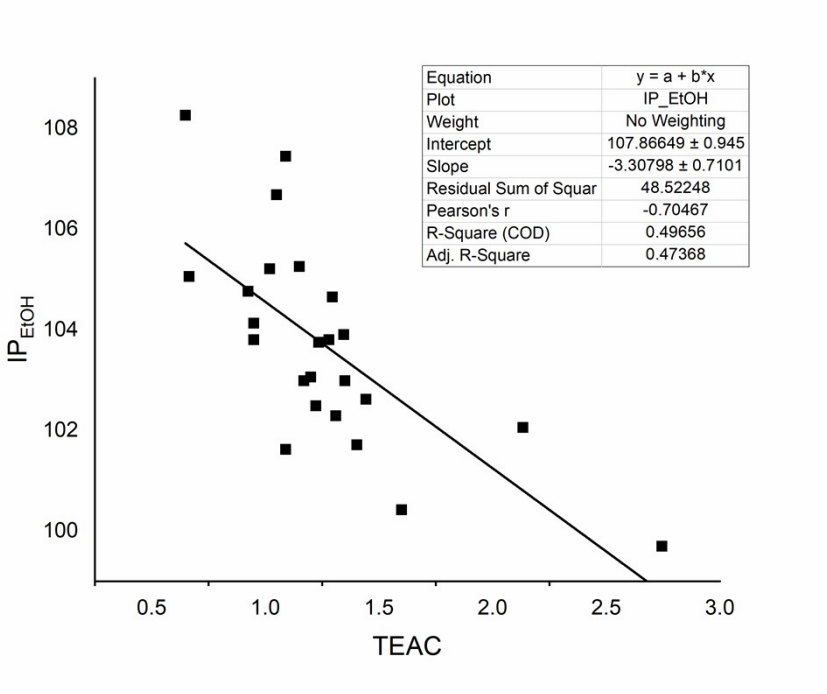


Figure S36. IP calculated in ethanol (kcal/mol) versus $TEAC_{CUPRAC}$ of the Schiff bases in ethanol.

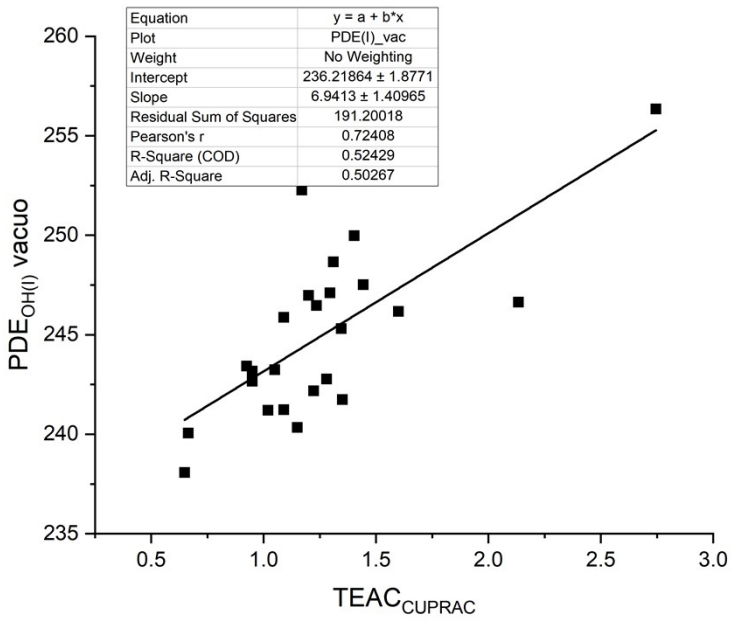


Figure S37. $PDE_{OH(I)}$ calculated *in vacuo* (kcal/mol) versus $TEAC_{CUPRAC}$ of the Schiff bases in ethanol.

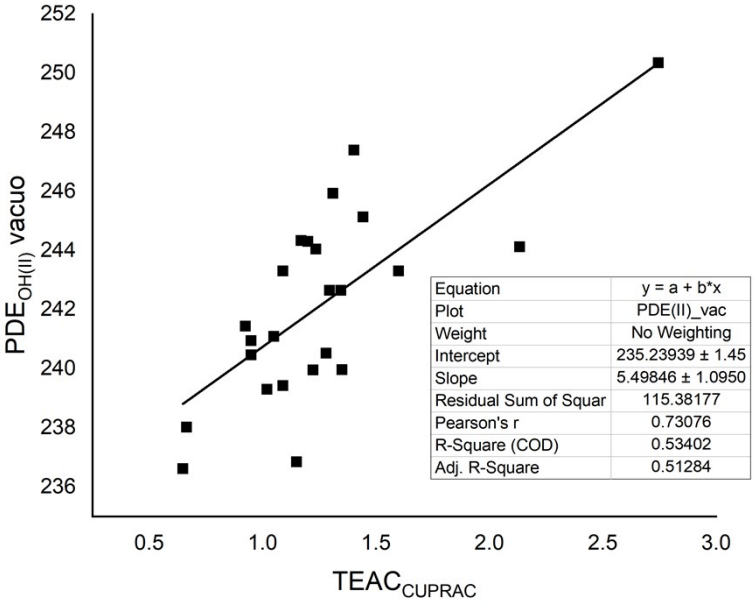


Figure S38. $PDE_{OH(II)}$ calculated *in vacuo* (kcal/mol) versus $TEAC_{CUPRAC}$ of the Schiff bases in ethanol.

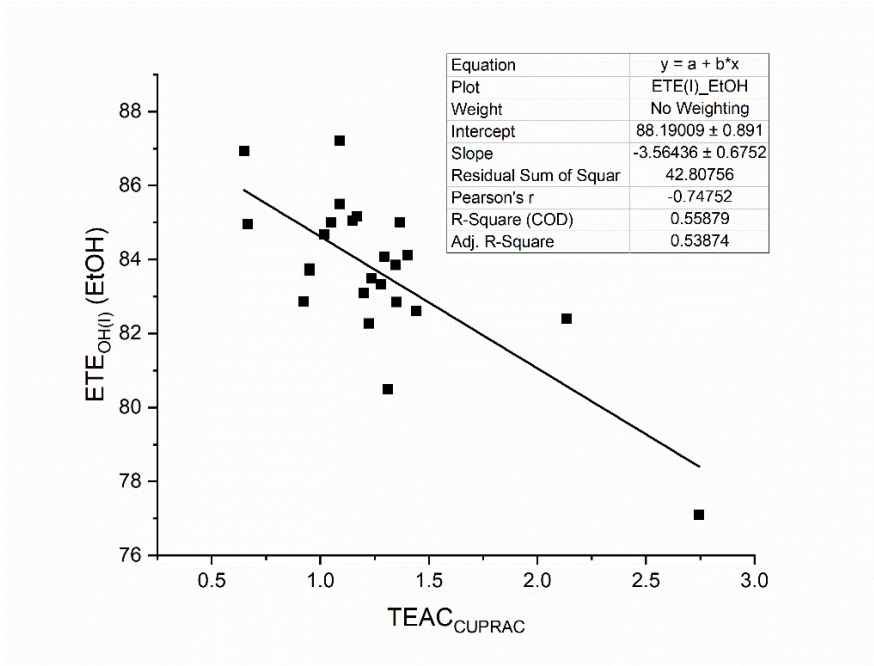


Figure S39. $ETE_{OH(I)}$ calculated in ethanol (kcal/mol) versus antioxidant activity ($TEAC_{CUPRAC}$) of the Schiff bases in ethanol.

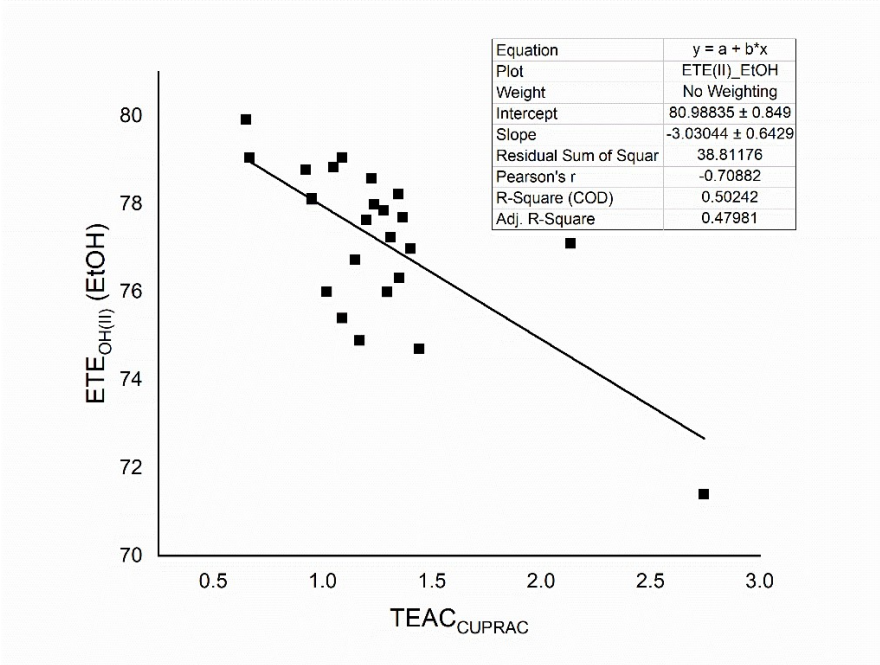


Figure S40. $ETE_{OH(II)}$ calculated in ethanol (kcal/mol) versus antioxidant activity ($TEAC_{CUPRAC}$) of the Schiff bases in ethanol.

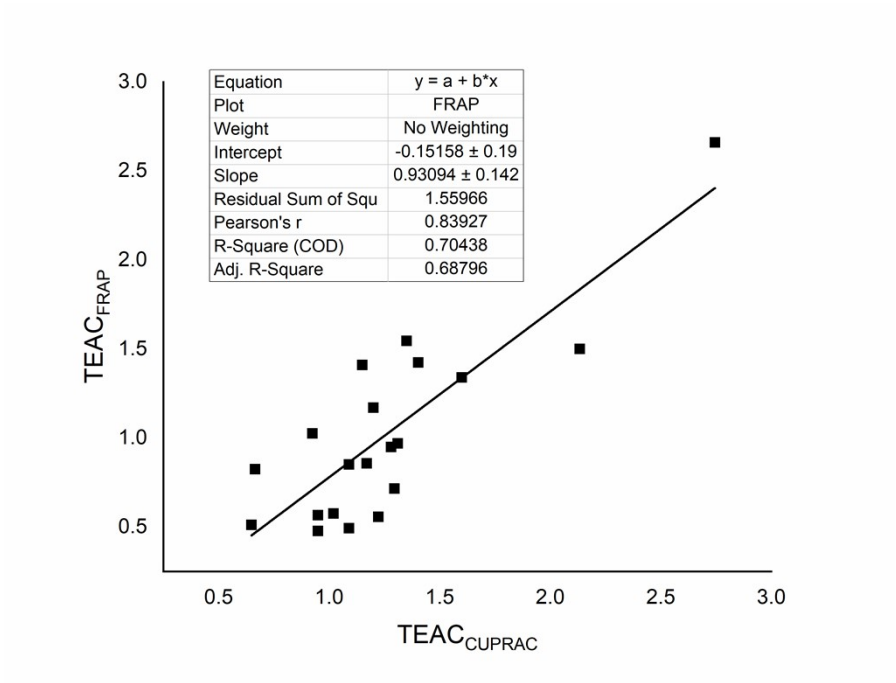


Figure S41. TEAC coefficients obtained in the FRAP assay versus TEAC coefficients obtained in the CUPRAC assay for the Schiff bases in ethanol.

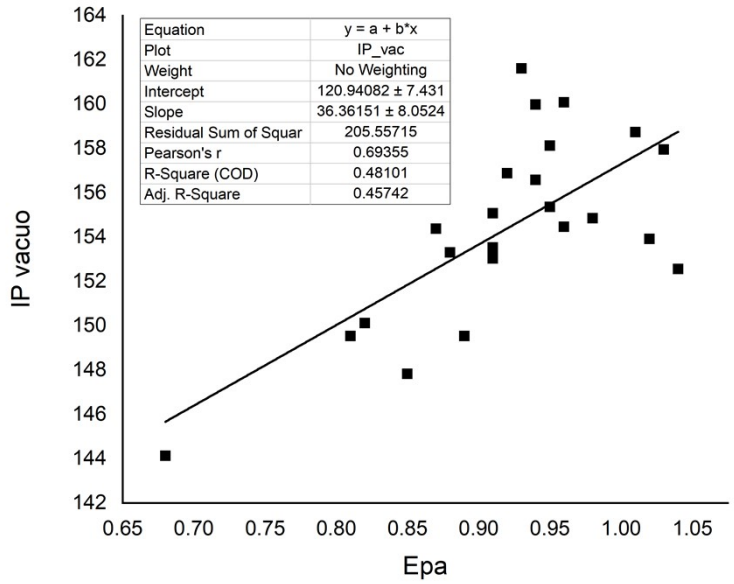


Figure S42. E_{pa}[1] values versus IP calculated *in vacuo* (kcal/mol).

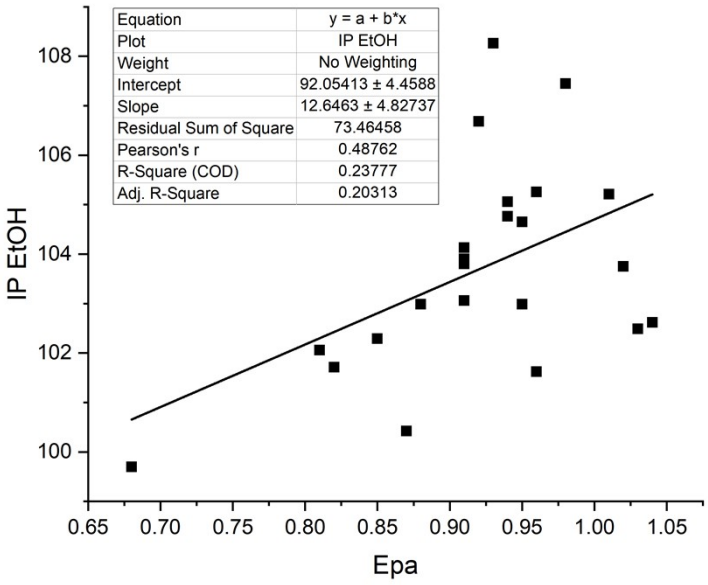
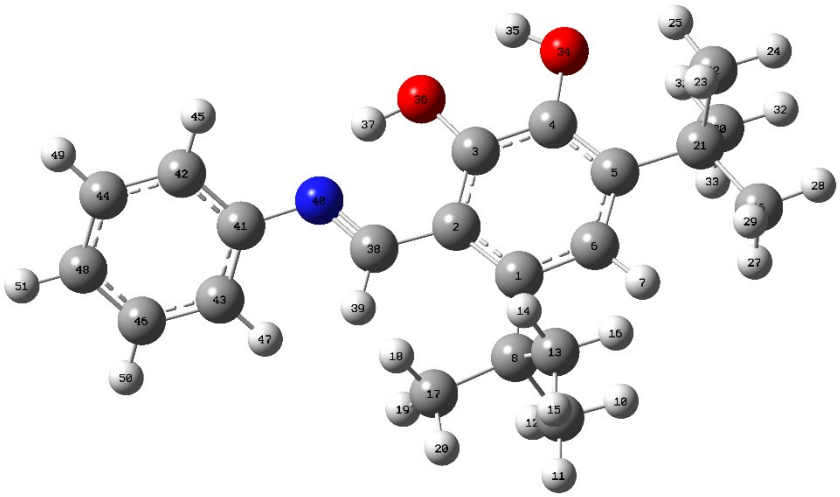


Figure S43. $E_{pa}{}^{1}$ values versus IP calculated in ethanol (kcal/mol).

Cartesian coordinates of the Schiff bases

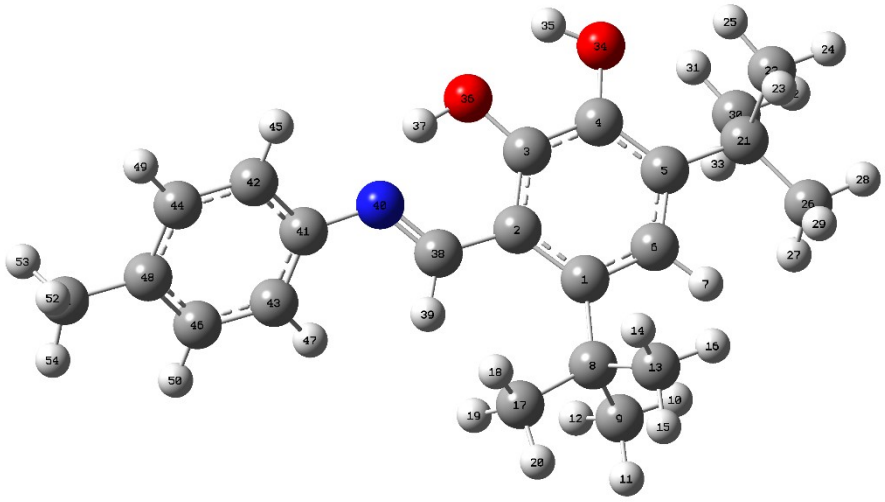
(E)-4,6-di-*tert*-butyl-3-((phenylimino)methyl)benzene-1,2-diol (Compound **1**)



Tag	Symbol	X	Y	Z
1	C	0.8617030	1.1499690	-0.0773480
2	C	-0.0756150	0.0676540	-0.0749820
3	C	0.4407910	-1.2576680	-0.0574840
4	C	1.8120480	-1.5322720	0.0072050
5	C	2.7387490	-0.4907690	0.0474480
6	C	2.2143030	0.8103560	-0.0046590
7	H	2.9283660	1.6172670	0.0057600
8	C	0.5916460	2.6856860	-0.1833390
9	C	1.1430690	3.3834040	1.0859930
10	H	2.2123090	3.2147080	1.2211700
11	H	0.9812080	4.4640520	1.0216860
12	H	0.6329700	3.0172170	1.9814670
13	C	1.3341750	3.2284570	-1.4339990
14	H	0.9515200	2.7581010	-2.3440820
15	H	1.1793560	4.3084040	-1.5198650
16	H	2.4089320	3.0499900	-1.3951510
17	C	-0.8692960	3.1574300	-0.3359620
18	H	-1.3677670	2.7169610	-1.2023500
19	H	-1.4678960	2.9743240	0.5591070
20	H	-0.8630640	4.2403020	-0.4877000
21	C	4.2526360	-0.7598220	0.1332400
22	C	4.7088590	-1.5721030	-1.1034690
23	H	4.5131710	-1.0151390	-2.0245580
24	H	5.7856970	-1.7598700	-1.0461550
25	H	4.1970300	-2.5314600	-1.1666780
26	C	5.0773820	0.5412230	0.1682220
27	H	4.8334600	1.1608810	1.0357100
28	H	6.1387200	0.2880350	0.2352400
29	H	4.9413880	1.1408410	-0.7361910
30	C	4.5669100	-1.5492080	1.4276870
31	H	4.0487880	-2.5070160	1.4512710
32	H	5.6429600	-1.7385340	1.4936800
33	H	4.2716580	-0.9750530	2.3109090
34	O	2.1906870	-2.8453350	0.0344910

35	H	1.3769870	-3.3711320	0.0017780
36	O	-0.3438760	-2.3581460	-0.0837310
37	H	-1.3003780	-2.0421740	-0.1334140
38	C	-1.5237760	0.2074810	-0.0433370
39	H	-1.9453030	1.1980550	0.0579910
40	N	-2.3259750	-0.8053990	-0.1188200
41	C	-3.7192710	-0.6347630	0.0055330
42	C	-4.5542800	-1.4404580	-0.7809430
43	C	-4.2977880	0.2667040	0.9113630
44	C	-5.9364960	-1.3156560	-0.6941140
45	H	-4.1020650	-2.1496050	-1.4645460
46	C	-5.6830280	0.3801080	0.9991140
47	H	-3.6646010	0.8505450	1.5695800
48	C	-6.5079750	-0.4034270	0.1938960
49	H	-6.5704070	-1.9364800	-1.3172550
50	H	-6.1185420	1.0736260	1.7099550
51	H	-7.5856280	-0.3151730	0.2679000

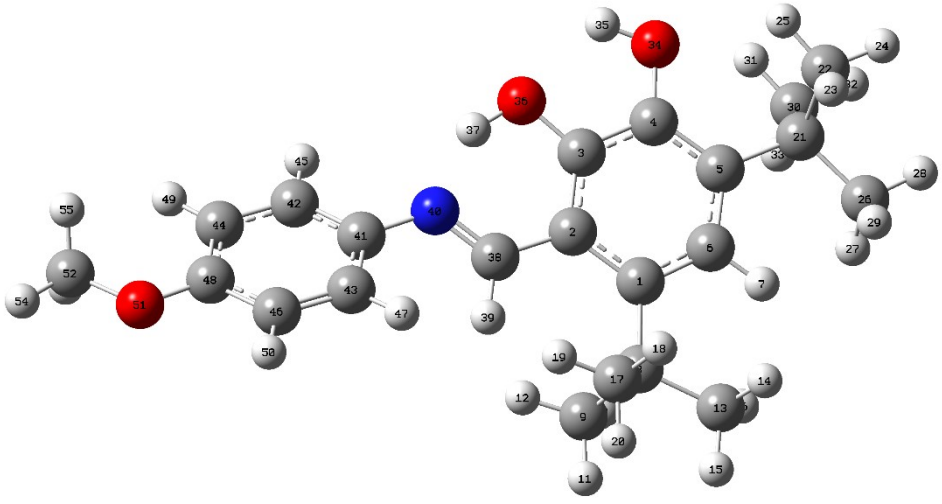
(E)-4,6-di-*tert*-butyl-3-((p-tolylimino)methyl)benzene-1,2-diol (Compound **2**)



Tag	Symbol	X	Y	Z
1	C	1.2345390	1.1525260	-0.0788170
2	C	0.2856940	0.0805000	-0.0832780
3	C	0.7881950	-1.2500250	-0.0624370
4	C	2.1560670	-1.5391000	0.0105350
5	C	3.0937180	-0.5077160	0.0561770
6	C	2.5832680	0.7987360	0.0016850
7	H	3.3056050	1.5982080	0.0168980
8	C	0.9818350	2.6913390	-0.1837300
9	C	1.5344200	3.3809820	1.0895550
10	H	2.6010170	3.2003200	1.2299730
11	H	1.3847400	4.4634750	1.0262890
12	H	1.0157270	3.0188490	1.9817390
13	C	1.7363770	3.2282060	-1.4296880
14	H	1.3529150	2.7637700	-2.3424790
15	H	1.5941350	4.3100140	-1.5143260
16	H	2.8088520	3.0375060	-1.3859710
17	C	-0.4730510	3.1794330	-0.3423600
18	H	-0.9714680	2.7475690	-1.2130710

19	H	-1.0782760	2.9989390	0.5487580
20	H	-0.4543450	4.2627980	-0.4898100
21	C	4.6041560	-0.7930320	0.1501330
22	C	5.0583870	-1.6097590	-1.0843600
23	H	4.8740290	-1.0502010	-2.0062220
24	H	6.1327460	-1.8096390	-1.0211830
25	H	4.5361270	-2.5632650	-1.1509320
26	C	5.4426300	0.4990680	0.1900010
27	H	5.2007130	1.1210200	1.0564120
28	H	6.5008760	0.2345750	0.2624720
29	H	5.3176860	1.1004180	-0.7148580
30	C	4.9030730	-1.5862020	1.4458700
31	H	4.3742770	-2.5382460	1.4662550
32	H	5.9766440	-1.7873310	1.5175630
33	H	4.6093290	-1.0091600	2.3277220
34	O	2.5201500	-2.8564420	0.0398790
35	H	1.7004660	-3.3725940	0.0019990
36	O	-0.0080870	-2.3420700	-0.0940510
37	H	-0.9612870	-2.0142670	-0.1493170
38	C	-1.1618040	0.2350640	-0.0637820
39	H	-1.5743230	1.2299390	0.0314440
40	N	-1.9728220	-0.7703500	-0.1429700
41	C	-3.3657540	-0.5889500	-0.0308640
42	C	-4.2036420	-1.4082740	-0.8004880
43	C	-3.9523750	0.3352390	0.8425660
44	C	-5.5834210	-1.2731450	-0.7272800
45	H	-3.7543180	-2.1377770	-1.4645800
46	C	-5.3386380	0.4547330	0.9138400
47	H	-3.3280410	0.9374540	1.4928300
48	C	-6.1803470	-0.3384430	0.1298550
49	H	-6.2109540	-1.9095920	-1.3434850
50	H	-5.7719310	1.1709670	1.6047100
51	C	-7.6823160	-0.2172290	0.2159370
52	H	-8.1246510	-0.0539700	-0.7713830
53	H	-8.1311940	-1.1282980	0.6249000
54	H	-7.9779120	0.6153550	0.8573950

(E)-4,6-di-*tert*-butyl-3-(((4-methoxyphenyl)imino)methyl)benzene-1,2-diol (Compound **3**)



Tag	Symbol	X	Y	Z
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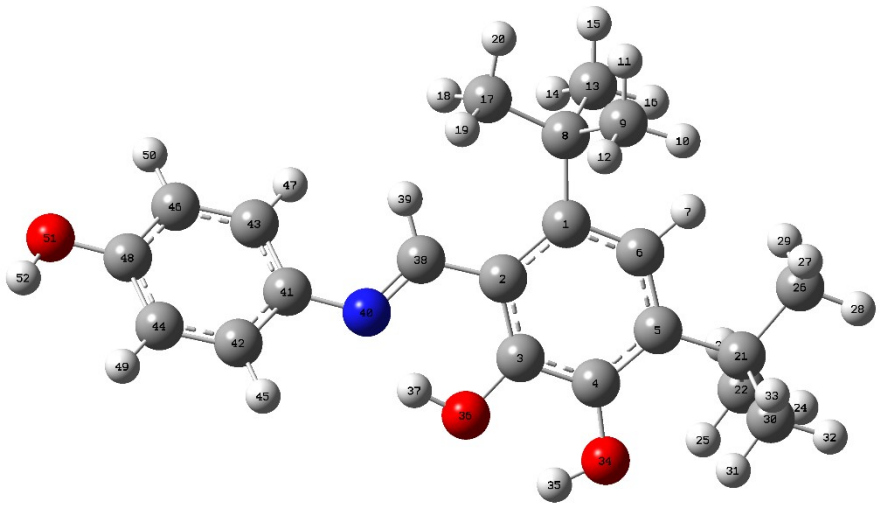
3	C	1.1464940	-1.2268340	-0.0520690
4	C	2.5155830	-1.5348990	-0.0662690
5	C	3.4677860	-0.5204470	-0.0143870
6	C	2.9789620	0.8002510	0.0536480
7	H	3.7150200	1.5828120	0.0972420
8	C	1.2587300	2.6665720	0.1528370
9	C	0.4481080	2.9670500	1.4403820
10	H	1.0319340	2.6954320	2.3240930
11	H	0.2264110	4.0371270	1.5001620
12	H	-0.4995470	2.4332960	1.5023210
13	C	2.5069120	3.5758230	0.2264590
14	H	3.1392380	3.4828160	-0.6597470
15	H	2.1811720	4.6174980	0.2874010
16	H	3.1149900	3.3708390	1.1108240
17	C	0.4893150	3.1181070	-1.1155290
18	H	1.1034390	2.9571250	-2.0056980
19	H	-0.4511230	2.5908520	-1.2719210
20	H	0.2602140	4.1864970	-1.0534110
21	C	4.9767850	-0.8295380	-0.0284010
22	C	5.3435850	-1.5763090	-1.3343190
23	H	5.1133520	-0.9600690	-2.2084980
24	H	6.4165250	-1.7928410	-1.3484760
25	H	4.8032690	-2.5176500	-1.4256770
26	C	5.8366450	0.4475760	0.0354900
27	H	5.6622880	1.0171070	0.9526060
28	H	6.8930280	0.1664160	0.0208400
29	H	5.6612860	1.1060230	-0.8198320
30	C	5.3415510	-1.7023220	1.1974270
31	H	4.8006050	-2.6477610	1.1940070
32	H	6.4143740	-1.9197770	1.1914250
33	H	5.1103020	-1.1757580	2.1281240
34	O	2.8592750	-2.8569430	-0.1308990
35	H	2.0313720	-3.3601460	-0.1561920
36	O	0.3291830	-2.3019780	-0.1029190
37	H	-0.6170370	-1.9543980	-0.0742760
38	C	-0.7695350	0.3055840	0.0065830
39	H	-1.1462190	1.3230750	0.0383520
40	N	-1.6105890	-0.6771750	-0.0191060
41	C	-3.0000980	-0.4578690	-0.0782200
42	C	-3.8403600	-1.3980680	0.5240160
43	C	-3.5897390	0.6305230	-0.7456910
44	C	-5.2253940	-1.2477190	0.5090150
45	H	-3.3955150	-2.2505780	1.0241460
46	C	-4.9662190	0.7831830	-0.7743710
47	H	-2.9693340	1.3435400	-1.2760460
48	C	-5.7968080	-0.1493790	-0.1398800
49	H	-5.8410650	-1.9907330	0.9976080
50	H	-5.4248400	1.6119070	-1.3003650
51	O	-7.1365220	0.0915710	-0.2258580
52	C	-8.0341310	-0.8346760	0.3719560
53	H	-7.8767860	-0.9024610	1.4538600
54	H	-9.0330930	-0.4483390	0.1770610

55	H	-7.9367700	-1.8300940	-0.0746650

(E)-4,6-di-*tert*-butyl-3-(((4-hydroxyphenyl)imino)methyl)benzene-1,2-diol (Compound **5**)



Tag	Symbol	X	Y	Z
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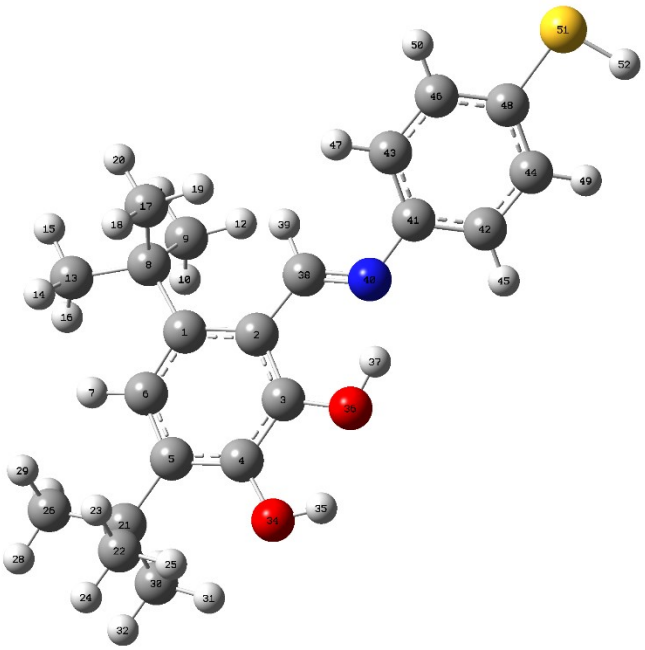
3	C	-0.7717370	-1.2462970	-0.0606490
4	C	-2.1384660	-1.5402350	0.0107460
5	C	-3.0800880	-0.5122690	0.0543650
6	C	-2.5740300	0.7957350	0.0002230
7	H	-3.2990910	1.5927850	0.0136540
8	C	-0.9791820	2.6939640	-0.1835010
9	C	-1.7321080	3.2266140	-1.4322490
10	H	-2.8038880	3.0314000	-1.3915630
11	H	-1.5941480	4.3089340	-1.5175170
12	H	-1.3439690	2.7628860	-2.3434310
13	C	-1.5380240	3.3829550	1.0874020
14	H	-1.0206280	3.0236850	1.9814930
15	H	-1.3921790	4.4659290	1.0234340
16	H	-2.6043410	3.1985260	1.2249300
17	C	0.4742240	3.1876800	-0.3383820
18	H	1.0771720	3.0109060	0.5550720
19	H	0.9770980	2.7565930	-1.2069200
20	H	0.4518030	4.2707610	-0.4873020
21	C	-4.5896410	-0.8029630	0.1458330
22	C	-4.8880670	-1.5965440	1.4414240
23	H	-4.5978560	-1.0180540	2.3234950
24	H	-5.9610480	-1.8014400	1.5113940
25	H	-4.3559230	-2.5466970	1.4631740
26	C	-5.4327300	0.4861910	0.1835810
27	H	-5.3082700	1.0875260	-0.7213560
28	H	-6.4901820	0.2180610	0.2543340
29	H	-5.1944830	1.1094230	1.0500870
30	C	-5.0388960	-1.6219140	-1.0889980
31	H	-4.5130050	-2.5735260	-1.1542480
32	H	-6.1126210	-1.8257370	-1.0275280
33	H	-4.8550550	-1.0620970	-2.0108120
34	O	-2.4978550	-2.8590030	0.0402520

35	H	-1.6761350	-3.3720130	0.0046420
36	O	0.0289560	-2.3356900	-0.0908940
37	H	0.9806130	-2.0030610	-0.1433870
38	C	1.1735880	0.2458850	-0.0575610
39	H	1.5801950	1.2426980	0.0414410
40	N	1.9885290	-0.7566850	-0.1367990
41	C	3.3810470	-0.5767340	-0.0235670
42	C	4.2161690	-1.4357750	-0.7478430
43	C	3.9743920	0.3857160	0.8089810
44	C	5.5991460	-1.3110730	-0.6817570
45	H	3.7668340	-2.1948250	-1.3773680
46	C	5.3555100	0.5085410	0.8865920
47	H	3.3528830	1.0212510	1.4290050
48	C	6.1742640	-0.3346120	0.1339340
49	H	6.2306190	-1.9783000	-1.2609830
50	H	5.8146170	1.2408230	1.5396700
51	O	7.5279150	-0.1679480	0.2502170
52	H	7.9853360	-0.8176980	-0.2934940

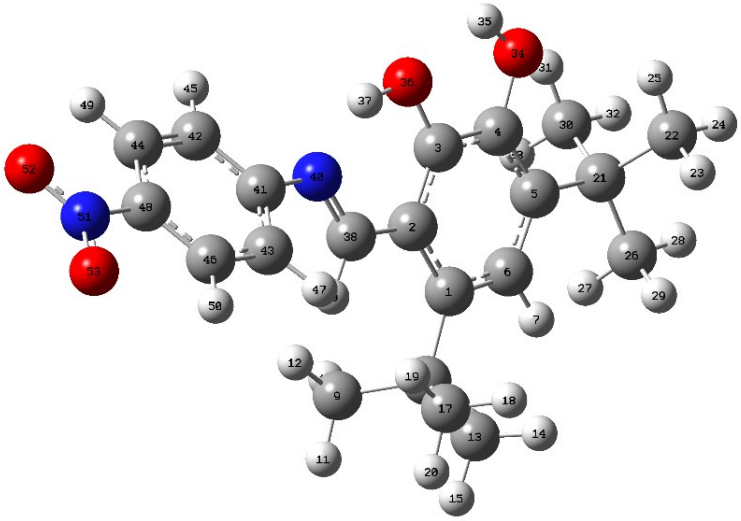
(E)-4,6-di-*tert*-butyl-3-(((3-mercaptophenyl)imino)methyl)benzene-1,2-diol (Compound **5**)



Tag	Symbol	X	Y	Z
1	C	1.5936460	1.1599200	0.0700770
2	C	0.6619740	0.0715290	0.0295490
3	C	1.1771440	-1.2458800	-0.0308190
4	C	2.5547490	-1.5114280	-0.0640810
5	C	3.4750460	-0.4670470	-0.0331100
6	C	2.9465500	0.8385910	0.0354170
7	H	3.6588370	1.6435080	0.0637560
8	C	1.1713650	2.6515890	0.1521870
9	C	0.3685430	2.9327000	1.4489960
10	H	0.9703720	2.6802640	2.3262520
11	H	0.1177300	3.9962510	1.5086270
12	H	-0.5632920	2.3733260	1.5241670
13	C	2.3922180	3.5985900	0.2061710
14	H	3.0151440	3.5219320	-0.6882050

15	H	2.0357000	4.6300020	0.2682270
16	H	3.0179520	3.4154020	1.0829480
17	C	0.3723320	3.0741170	-1.1077850
18	H	0.9780840	2.9250660	-2.0057020
19	H	-0.5557570	2.5208550	-1.2479400
20	H	0.1147380	4.1360550	-1.0480900
21	C	4.9925670	-0.7286960	-0.0688640
22	C	5.3619250	-1.4726340	-1.3757450
23	H	5.0984180	-0.8701820	-2.2501250
24	H	6.4408300	-1.6548550	-1.4056060
25	H	4.8508060	-2.4313960	-1.4523510
26	C	5.8126660	0.5752100	-0.0269130
27	H	5.6351100	1.1453620	0.8891910
28	H	6.8768990	0.3269910	-0.0564470
29	H	5.6036080	1.2218650	-0.8836520
30	C	5.4035340	-1.5808860	1.1568990
31	H	4.8935990	-2.5433040	1.1681320
32	H	6.4825270	-1.7637580	1.1355170
33	H	5.1699540	-1.0555100	2.0876640
34	O	2.9394980	-2.8217820	-0.1256350
35	H	2.1289150	-3.3527900	-0.1345170
36	O	0.3935790	-2.3462440	-0.0622670
37	H	-0.5617820	-2.0317370	-0.0187900
38	C	-0.7824890	0.2281130	0.0459270
39	H	-1.1902200	1.2337980	0.0735320
40	N	-1.5957170	-0.7790120	0.0433310
41	C	-2.9891110	-0.5925190	-0.0028100
42	C	-3.8018350	-1.5138830	0.6707710
43	C	-3.6077400	0.4376820	-0.7264540
44	C	-5.1843710	-1.3840820	0.6667290
45	H	-3.3328610	-2.3243150	1.2166430
46	C	-4.9921500	0.5581750	-0.7485380
47	H	-3.0085560	1.1263350	-1.3106670
48	C	-5.7952190	-0.3458830	-0.0453900
49	H	-5.7858460	-2.0986360	1.2169850
50	H	-5.4494920	1.3484990	-1.3332750
51	S	-7.5640540	-0.1084910	-0.0942680
52	H	-7.8992180	-1.2855560	0.4686470

(E)-4,6-di-*tert*-butyl-3-(((4-nitrophenyl)imino)methyl)benzene-1,2-diol (Compound **6**)



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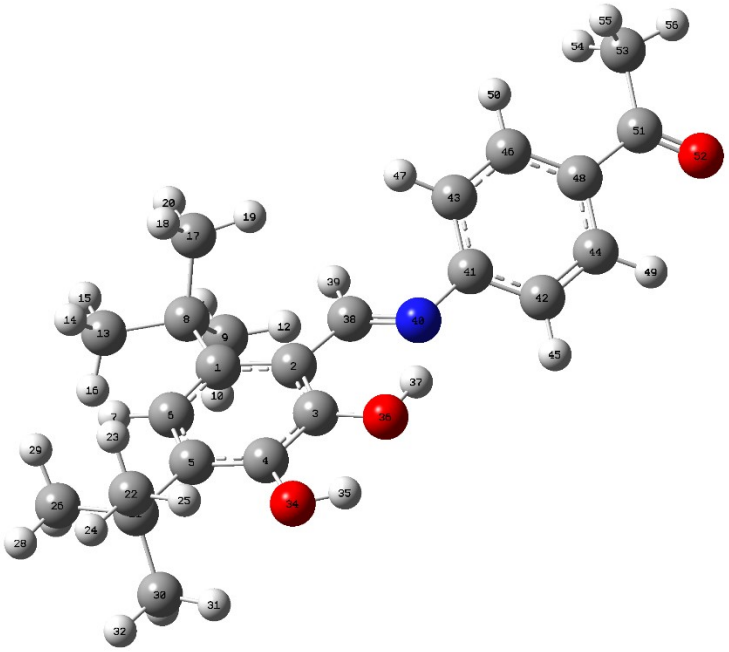
3	C	1.4099070	-1.2534790	-0.0518240
4	C	2.7881550	-1.5137700	-0.0914950
5	C	3.7035180	-0.4653460	-0.0437940
6	C	3.1707480	0.8380990	0.0496390
7	H	3.8812910	1.6438470	0.0905160
8	C	1.3919740	2.6439930	0.2048710
9	C	0.5954070	2.8993500	1.5110020
10	H	1.2006050	2.6293680	2.3805720
11	H	0.3459180	3.9614990	1.5925880
12	H	-0.3373880	2.3404330	1.5800780
13	C	2.6112860	3.5923040	0.2696720
14	H	3.2298570	3.5330100	-0.6289810
15	H	2.2529400	4.6214840	0.3515990
16	H	3.2414460	3.3954320	1.1402170
17	C	0.5856110	3.0873070	-1.0433600
18	H	1.1843540	2.9508630	-1.9478660
19	H	-0.3458890	2.5401750	-1.1860510
20	H	0.3314400	4.1486080	-0.9653040
21	C	5.2219110	-0.7189110	-0.0883080
22	C	5.5904000	-1.4379510	-1.4094840
23	H	5.3210380	-0.8220200	-2.2725560
24	H	6.6701570	-1.6125890	-1.4453120
25	H	5.0856500	-2.3986400	-1.5013710
26	C	6.0361100	0.5878220	-0.0252650
27	H	5.8591890	1.1407890	0.9014110
28	H	7.1010590	0.3444220	-0.0618110
29	H	5.8229040	1.2486160	-0.8700880
30	C	5.6391610	-1.5908620	1.1215920
31	H	5.1355050	-2.5565400	1.1166670
32	H	6.7189840	-1.7666440	1.0943580
33	H	5.4050780	-1.0836540	2.0622000
34	O	3.1801610	-2.8192130	-0.1769170
35	H	2.3757320	-3.3588580	-0.1932820

36	O	0.6315630	-2.3557120	-0.1027990
37	H	-0.3228940	-2.0548450	-0.0470340
38	C	-0.5485480	0.2170020	0.0598010
39	H	-0.9560250	1.2217230	0.1127380
40	N	-1.3665200	-0.7896680	0.0432900
41	C	-2.7525120	-0.5944650	0.0004560
42	C	-3.5672260	-1.4840530	0.7211410
43	C	-3.3563840	0.4146710	-0.7705010
44	C	-4.9458910	-1.3470840	0.7100250
45	H	-3.0984240	-2.2719690	1.2977370
46	C	-4.7367570	0.5540880	-0.7920010
47	H	-2.7446640	1.0682990	-1.3801400
48	C	-5.5165030	-0.3241250	-0.0451590
49	H	-5.5838810	-2.0163760	1.2704360
50	H	-5.2164410	1.3208280	-1.3847740
51	N	-6.9818110	-0.1781080	-0.0672340
52	O	-7.6439630	-0.9704910	0.5934680
53	O	-7.4549000	0.7292740	-0.7428870

1-(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)ethan-1-one (Compound **7**)



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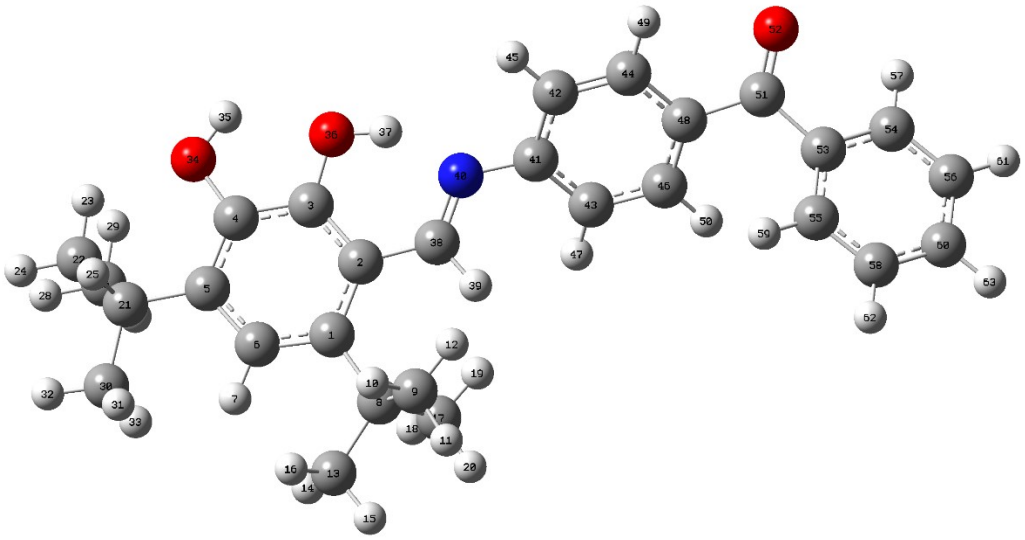
4	C	2.8203770	-1.5049680	-0.1045710
5	C	3.7310050	-0.4528430	-0.0541170
6	C	3.1917740	0.8466650	0.0497780
7	H	3.8977390	1.6563840	0.0931650
8	C	1.4028500	2.6410400	0.2244720
9	C	0.6091270	2.8823590	1.5349030
10	H	1.2198530	2.6115630	2.4003790
11	H	0.3516290	3.9421380	1.6242270
12	H	-0.3184630	2.3150230	1.6034170
13	C	2.6163740	3.5965230	0.2917270

14	H	3.2323200	3.5471370	-0.6093560
15	H	2.2519600	4.6229840	0.3821280
16	H	3.2508370	3.3972920	1.1586180
17	C	0.5891980	3.0881550	-1.0176130
18	H	1.1869120	2.9642850	-1.9246670
19	H	-0.3374580	2.5333870	-1.1619200
20	H	0.3262240	4.1467510	-0.9300480
21	C	5.2505240	-0.6991960	-0.1063020
22	C	5.6173060	-1.4084070	-1.4331460
23	H	5.3423340	-0.7879470	-2.2912320
24	H	6.6975910	-1.5792630	-1.4742790
25	H	5.1151380	-2.3700830	-1.5291760
26	C	6.0589840	0.6108680	-0.0386060
27	H	5.8829950	1.1572320	0.8921610
28	H	7.1250380	0.3729320	-0.0811380
29	H	5.8386540	1.2758830	-0.8782920
30	C	5.6772130	-1.5765150	1.0962520
31	H	5.1769160	-2.5439490	1.0877630
32	H	6.7576610	-1.7481150	1.0633810
33	H	5.4450490	-1.0758440	2.0408490
34	O	3.2173360	-2.8088420	-0.2000360
35	H	2.4134600	-3.3496660	-0.2151290
36	O	0.6676620	-2.3583720	-0.1116760
37	H	-0.2894440	-2.0593410	-0.0507680
38	C	-0.5281310	0.2039490	0.0703290
39	H	-0.9439770	1.2049840	0.1300300
40	N	-1.3361600	-0.8083480	0.0484870
41	C	-2.7273530	-0.6251600	0.0143710
42	C	-3.5327440	-1.5243430	0.7331370
43	C	-3.3443830	0.3814360	-0.7438460
44	C	-4.9103880	-1.3910990	0.7274180
45	H	-3.0540090	-2.3128720	1.3019460
46	C	-4.7292600	0.5027910	-0.7524980
47	H	-2.7419500	1.0444380	-1.3536380
48	C	-5.5333180	-0.3741150	-0.0133480
49	H	-5.5356210	-2.0725170	1.2912120
50	H	-5.1792730	1.2836790	-1.3534840
51	C	-7.0276970	-0.2816740	0.0091540
52	O	-7.6881260	-1.0640490	0.6681820
53	C	-7.7078050	0.8058530	-0.8030400
54	H	-7.3753200	1.7985860	-0.4857160
55	H	-7.4732350	0.7045460	-1.8667900
56	H	-8.7842410	0.7241800	-0.6623890

(4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)(phenyl)methanone (Compound **8**)



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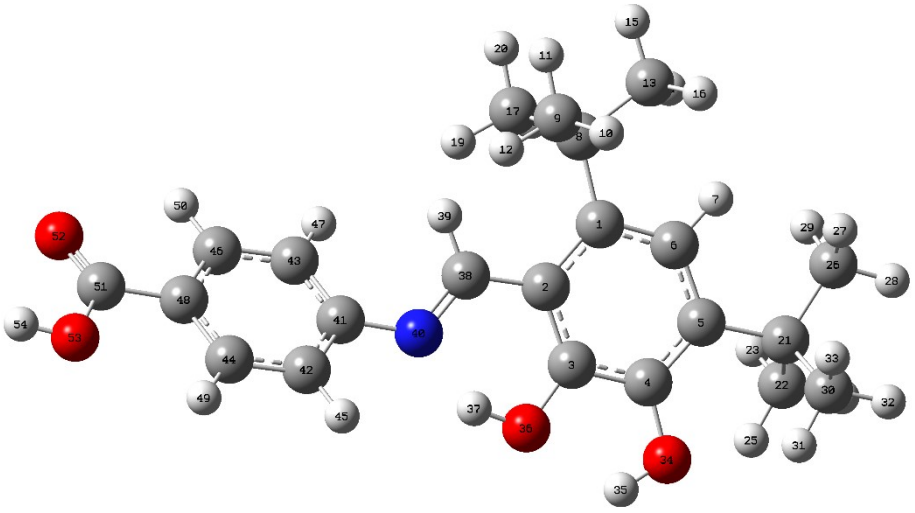
3	C	2.8248030	-1.2698080	-0.0609350
4	C	4.2235740	-1.3572230	-0.1367350
5	C	5.0041640	-0.2047980	-0.1021600
6	C	4.3170090	1.0218130	0.0138010
7	H	4.9227520	1.9095150	0.0434060
8	C	2.3319250	2.5921570	0.2227940
9	C	1.5431490	2.7434420	1.5496750
10	H	2.2003520	2.5522340	2.4022750
11	H	1.1625100	3.7652760	1.6418530
12	H	0.6919690	2.0693350	1.6398440
13	C	3.4243790	3.6853420	0.2621770
14	H	4.0225670	3.7055880	-0.6519160
15	H	2.9424630	4.6616230	0.3585160
16	H	4.0963000	3.5668350	1.1155440
17	C	1.4445460	2.9337800	-1.0021370
18	H	2.0331240	2.8773640	-1.9217760
19	H	0.5877790	2.2719910	-1.1248370
20	H	1.0595640	3.9540850	-0.9112310
21	C	6.5408730	-0.2698860	-0.1838760
22	C	7.0911580	-1.0913480	1.0079170
23	H	6.7089570	-2.1112490	1.0058400
24	H	8.1835340	-1.1335940	0.9543800
25	H	6.8191540	-0.6224240	1.9581760
26	C	6.9633600	-0.9301840	-1.5193160
27	H	6.6015050	-0.3456880	-2.3703720
28	H	8.0552700	-0.9732140	-1.5809670
29	H	6.5755280	-1.9440380	-1.6086880
30	C	7.1901260	1.1264700	-0.1275890
31	H	6.9684630	1.6476810	0.8078600
32	H	8.2758590	1.0162930	-0.1907180
33	H	6.8769710	1.7613720	-0.9610840
34	O	4.7698520	-2.6050700	-0.2431840
35	H	4.0351250	-3.2368740	-0.2440360
36	O	2.1873370	-2.4594760	-0.1013630
37	H	1.2025550	-2.2751840	-0.0210400

38	C	0.7003060	-0.0575080	0.1122590
39	H	0.1698970	0.8869290	0.1847560
40	N	0.0184390	-1.1588180	0.1045730
41	C	-1.3855420	-1.1435270	0.1046170
42	C	-2.0578410	-2.1490770	0.8187980
43	C	-2.1389820	-0.2062580	-0.6181620
44	C	-3.4415920	-2.1892750	0.8401630
45	H	-1.4735520	-2.8860160	1.3572940
46	C	-3.5285810	-0.2436500	-0.5817970
47	H	-1.6378860	0.5269490	-1.2392030
48	C	-4.2004090	-1.2276300	0.1546310
49	H	-3.9619280	-2.9692800	1.3824480
50	H	-4.0913340	0.4759390	-1.1637420
51	C	-5.6915220	-1.3639040	0.1617840
52	O	-6.2047510	-2.4594080	0.3285430
53	C	-6.5601160	-0.1556400	-0.0369730
54	C	-7.8069500	-0.3327000	-0.6523600
55	C	-6.2074530	1.1141600	0.4378040
56	C	-8.6707130	0.7439320	-0.8158710
57	H	-8.0820580	-1.3234000	-0.9933490
58	C	-7.0848500	2.1873280	0.2947910
59	H	-5.2608680	1.2594860	0.9440210
60	C	-8.3118940	2.0065350	-0.3404670
61	H	-9.6269000	0.6001770	-1.3061940
62	H	-6.8113280	3.1625520	0.6815030
63	H	-8.9897150	2.8444380	-0.4596590

3-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid (Compound **9**)



Tag	Symbol	X	Y	Z
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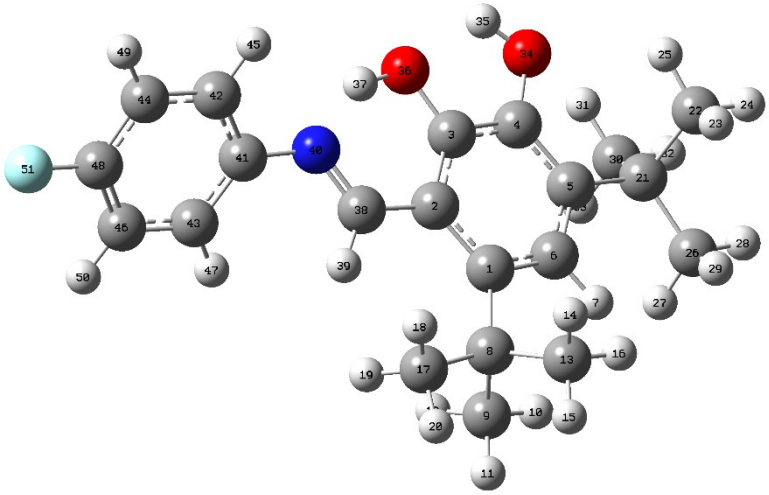
4	C	2.8007390	-1.5151810	-0.0936460
5	C	3.7208170	-0.4714260	-0.0402160
6	C	3.1931820	0.8335920	0.0541940

7	H	3.9064340	1.6367780	0.0994100
8	C	1.4200590	2.6456400	0.2066090
9	C	0.6201920	2.9011680	1.5106360
10	H	1.2227160	2.6291530	2.3815030
11	H	0.3720840	3.9637110	1.5926880
12	H	-0.3133520	2.3432710	1.5760210
13	C	2.6421550	3.5899230	0.2770600
14	H	3.2635740	3.5299380	-0.6196220
15	H	2.2868370	4.6201980	0.3594870
16	H	3.2688910	3.3894540	1.1493110
17	C	0.6188650	3.0939720	-1.0431110
18	H	1.2209800	2.9590770	-1.9456670
19	H	-0.3126270	2.5483610	-1.1905720
20	H	0.3660800	4.1555600	-0.9630510
21	C	5.2382810	-0.7322930	-0.0797530
22	C	5.6084150	-1.4498320	-1.4012000
23	H	5.3455550	-0.8301340	-2.2635990
24	H	6.6873710	-1.6306610	-1.4335790
25	H	5.0982310	-2.4072640	-1.4974630
26	C	6.0585280	0.5703530	-0.0106740
27	H	5.8805990	1.1218820	0.9166770
28	H	7.1225850	0.3222470	-0.0441620
29	H	5.8509100	1.2342210	-0.8544780
30	C	5.6474150	-1.6091580	1.1292150
31	H	5.1380480	-2.5718590	1.1203900
32	H	6.7264090	-1.7910580	1.1051910
33	H	5.4128770	-1.1028090	2.0702000
34	O	3.1861470	-2.8231830	-0.1809130
35	H	2.3773280	-3.3563330	-0.2016900
36	O	0.6400040	-2.3481410	-0.1141940
37	H	-0.3145230	-2.0393010	-0.0628200
38	C	-0.5321030	0.2265050	0.0499910
39	H	-0.9381620	1.2317320	0.1044550
40	N	-1.3499010	-0.7782500	0.0254470
41	C	-2.7387350	-0.5810030	-0.0174370
42	C	-3.5551000	-1.4756970	0.6913640
43	C	-3.3406230	0.4378300	-0.7756550
44	C	-4.9342710	-1.3318580	0.6794020
45	H	-3.0875780	-2.2716160	1.2586990
46	C	-4.7206700	0.5748710	-0.7917990
47	H	-2.7270000	1.0975560	-1.3775510
48	C	-5.5305400	-0.3018080	-0.0607380
49	H	-5.5560950	-2.0179680	1.2392560
50	H	-5.1923990	1.3533920	-1.3788220
51	C	-6.9996140	-0.1095810	-0.1141630
52	O	-7.5661260	0.7568940	-0.7404060
53	O	-7.6824570	-1.0206520	0.6281100
54	H	-8.6224520	-0.8111400	0.5278690

(E)-4,6-di-*tert*-butyl-3-(((4-fluorophenyl)imino)methyl)benzene-1,2-diol (Compound **10**)



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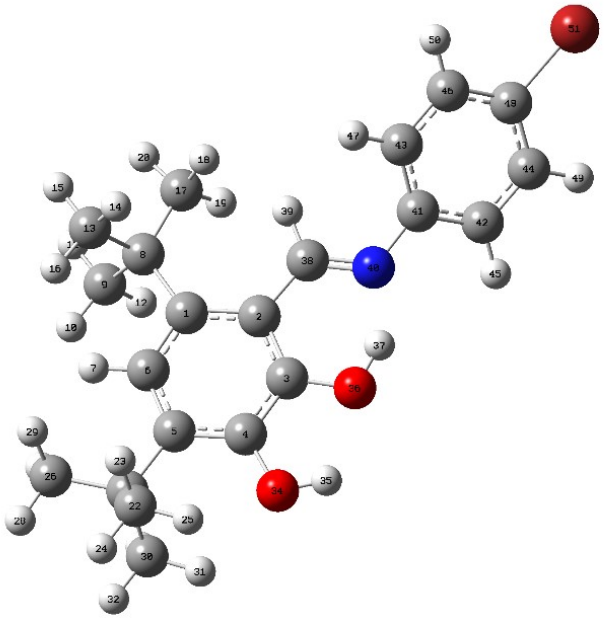
4	C	2.1397730	-1.5389820	0.0048300
5	C	3.0749840	-0.5054460	0.0575030
6	C	2.5623790	0.8003480	0.0038650
7	H	3.2833780	1.6009080	0.0224810
8	C	0.9578120	2.6899590	-0.1893060
9	C	1.5021300	3.3834490	1.0852990
10	H	2.5685220	3.2059000	1.2311530
11	H	1.3500210	4.4653600	1.0190960
12	H	0.9801660	3.0219020	1.9758210
13	C	1.7177140	3.2257490	-1.4325910
14	H	1.3399440	2.7588850	-2.3465000
15	H	1.5736640	4.3070190	-1.5199330
16	H	2.7903210	3.0375310	-1.3829850
17	C	-0.4974880	3.1738440	-0.3577100
18	H	-0.9919750	2.7335210	-1.2265050
19	H	-1.1057320	3.0008570	0.5329620
20	H	-0.4804600	4.2558200	-0.5144750
21	C	4.5855940	-0.7876410	0.1570760
22	C	5.0468400	-1.5996900	-1.0779570
23	H	4.8648050	-1.0381150	-1.9990370
24	H	6.1214450	-1.7965230	-1.0108170
25	H	4.5278780	-2.5546150	-1.1493500
26	C	5.4208690	0.5062720	0.2044190
27	H	5.1736520	1.1253120	1.0714140
28	H	6.4792610	0.2438450	0.2812210
29	H	5.2991850	1.1097660	-0.6994510
30	C	4.8804070	-1.5838900	1.4519240
31	H	4.3543450	-2.5375150	1.4672010
32	H	5.9541330	-1.7822410	1.5277540
33	H	4.5813210	-1.0102390	2.3341760
34	O	2.5073990	-2.8549650	0.0314630
35	H	1.6904870	-3.3749070	-0.0105320
36	O	-0.0223110	-2.3459030	-0.1093830
37	H	-0.9744730	-2.0227340	-0.1661330

38	C	-1.1791750	0.2312470	-0.0642990
39	H	-1.5899640	1.2255010	0.0463750
40	N	-1.9919290	-0.7725110	-0.1541050
41	C	-3.3832530	-0.5895400	-0.0328870
42	C	-4.2233760	-1.3917230	-0.8182330
43	C	-3.9602690	0.3188480	0.8671990
44	C	-5.6054850	-1.2632070	-0.7432800
45	H	-3.7771070	-2.1074520	-1.4981870
46	C	-5.3436900	0.4489180	0.9560600
47	H	-3.3287950	0.9020870	1.5267670
48	C	-6.1409720	-0.3398370	0.1424650
49	H	-6.2639840	-1.8687450	-1.3533460
50	H	-5.8026730	1.1371140	1.6549650
51	F	-7.4887830	-0.2179310	0.2281210

(E)-4,6-di-*tert*-butyl-3-(((4-iodophenyl)imino)methyl)benzene-1,2-diol (Compound **11**)



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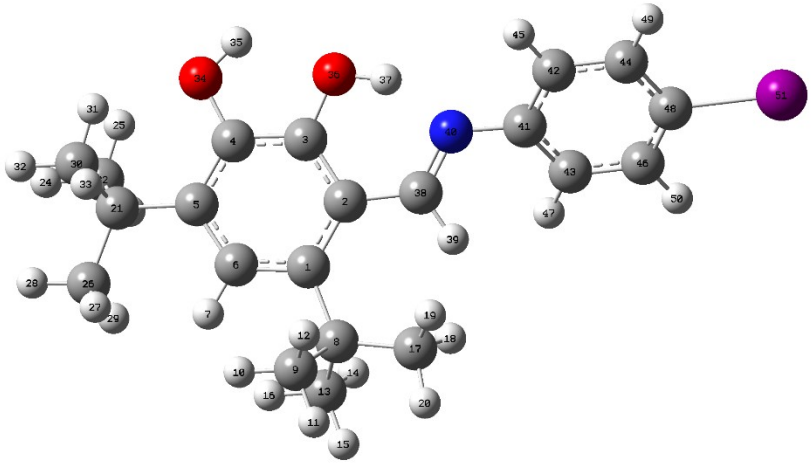
3	C	1.7868780	-1.2496890	0.0784630
4	C	3.1519660	-1.5458590	-0.0124980
5	C	4.0935540	-0.5185660	-0.0732340
6	C	3.5905160	0.7908450	-0.0140010
7	H	4.3169210	1.5862680	-0.0397490
8	C	2.0018440	2.6920000	0.1931830
9	C	2.7758320	3.2237510	1.4293790
10	H	3.8465350	3.0272520	1.3712300
11	H	2.6407430	4.3061900	1.5162350
12	H	2.4020280	2.7611750	2.3470890
13	C	2.5409450	3.3792680	-1.0871630
14	H	2.0085940	3.0205880	-1.9726670
15	H	2.3977540	4.4623740	-1.0212370
16	H	3.6046240	3.1933540	-1.2418970
17	C	0.5517240	3.1876080	0.3716630
18	H	-0.0659610	3.0132720	-0.5122410
19	H	0.0621210	2.7572480	1.2481620

20	H	0.5782450	4.2704090	0.5210470
21	C	5.6011660	-0.8108040	-0.1875750
22	C	5.8781030	-1.6076680	-1.4859920
23	H	5.5742730	-1.0312360	-2.3648040
24	H	6.9497250	-1.8128470	-1.5723260
25	H	5.3458110	-2.5578700	-1.4970470
26	C	6.4446670	0.4775030	-0.2415250
27	H	6.3354750	1.0809320	0.6639770
28	H	7.5004750	0.2079540	-0.3283190
29	H	6.1937810	1.0990190	-1.1056860
30	C	6.0685370	-1.6272340	1.0423050
31	H	5.5439030	-2.5787250	1.1177730
32	H	7.1410760	-1.8312010	0.9646670
33	H	5.8991710	-1.0653650	1.9656120
34	O	3.5105210	-2.8640550	-0.0440820
35	H	2.6909720	-3.3790650	0.0059680
36	O	0.9860360	-2.3380200	0.1226760
37	H	0.0369620	-2.0097990	0.1914040
38	C	-0.1528760	0.2478840	0.0990080
39	H	-0.5582730	1.2457040	0.0024590
40	N	-0.9722940	-0.7506810	0.1947760
41	C	-2.3620470	-0.5558860	0.0948730
42	C	-3.1990010	-1.3500420	0.8906800
43	C	-2.9451210	0.3571430	-0.7958570
44	C	-4.5806510	-1.2088420	0.8345830
45	H	-2.7519180	-2.0705750	1.5653910
46	C	-4.3284030	0.4986150	-0.8646890
47	H	-2.3197540	0.9365430	-1.4649610
48	C	-5.1362230	-0.2803620	-0.0425090
49	H	-5.2178610	-1.8177010	1.4628180
50	H	-4.7707980	1.1983790	-1.5620760
51	Br	-7.0417710	-0.0901440	-0.1357210

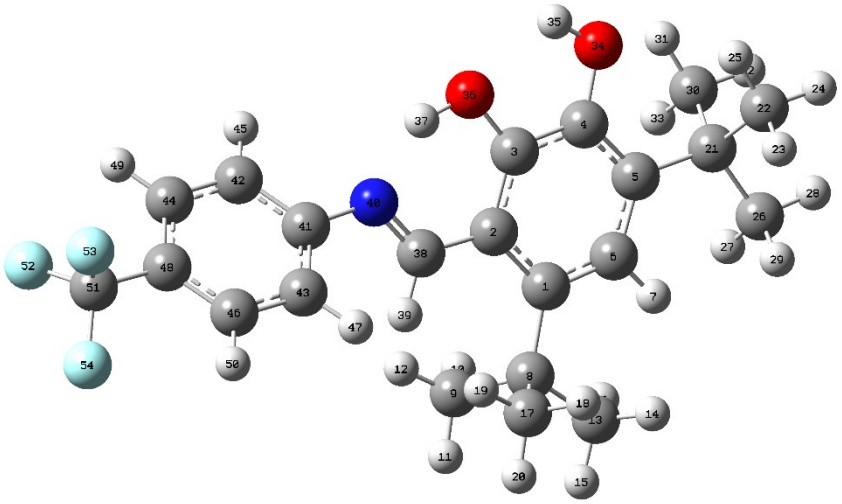
(E)-4,6-di-*tert*-butyl-3-(((4-iodophenyl)imino)methyl)benzene-1,2-diol (Compound **12**)



Tag	Symbol	X	Y	Z
1	C	2.8531280	1.1516510	0.0843240
2	C	1.8985180	0.0840920	0.1046880
3	C	2.3929340	-1.2498240	0.0774140
4	C	3.7576510	-1.5467730	-0.0166240

5	C	4.6997990	-0.5200720	-0.0781140
6	C	4.1977040	0.7895950	-0.0169360
7	H	4.9245480	1.5845780	-0.0437720
8	C	2.6108650	2.6917920	0.1933920
9	C	3.3865130	3.2228760	1.4288380
10	H	4.4569760	3.0253590	1.3695820
11	H	3.2524940	4.3054400	1.5158890
12	H	3.0132080	2.7605860	2.3468950
13	C	3.1494180	3.3785450	-1.0874720
14	H	2.6161220	3.0200720	-1.9724910
15	H	3.0069220	4.4617390	-1.0215200
16	H	4.2128570	3.1920380	-1.2430600
17	C	1.1614550	3.1889420	0.3729680
18	H	0.5423270	3.0129730	-0.5096130
19	H	0.6728650	2.7610110	1.2512390
20	H	1.1891050	4.2720590	0.5198830
21	C	6.2070080	-0.8132670	-0.1953730
22	C	6.4810860	-1.6094380	-1.4948280
23	H	6.1763020	-1.0320880	-2.3726970
24	H	7.5523810	-1.8155160	-1.5831180
25	H	5.9478890	-2.5591400	-1.5056820
26	C	7.0513780	0.4744400	-0.2498740
27	H	6.9442610	1.0772520	0.6562860
28	H	8.1068300	0.2041720	-0.3387880
29	H	6.7993760	1.0968050	-1.1130970
30	C	6.6759350	-1.6309240	1.0330850
31	H	6.1507010	-2.5820690	1.1087670
32	H	7.7481900	-1.8356420	0.9534390
33	H	6.5085770	-1.0695900	1.9570840
34	O	4.1152180	-2.8652130	-0.0501940
35	H	3.2953250	-3.3795890	0.0009880
36	O	1.5915410	-2.3376900	0.1222310
37	H	0.6426970	-2.0087920	0.1936660
38	C	0.4541270	0.2487820	0.1070520
39	H	0.0487360	1.2471350	0.0165850
40	N	-0.3652720	-0.7497600	0.2025920
41	C	-1.7554490	-0.5535910	0.1107790
42	C	-2.5889790	-1.3494130	0.9076730
43	C	-2.3426710	0.3629770	-0.7729140
44	C	-3.9712270	-1.2061350	0.8590570
45	H	-2.1398470	-2.0732280	1.5776910
46	C	-3.7267250	0.5054240	-0.8334630
47	H	-1.7210500	0.9447450	-1.4436520
48	C	-4.5342220	-0.2742360	-0.0105800
49	H	-4.5992590	-1.8199970	1.4915240
50	H	-4.1650260	1.2105270	-1.5279360
51	I	-6.6533990	-0.0604140	-0.1022090

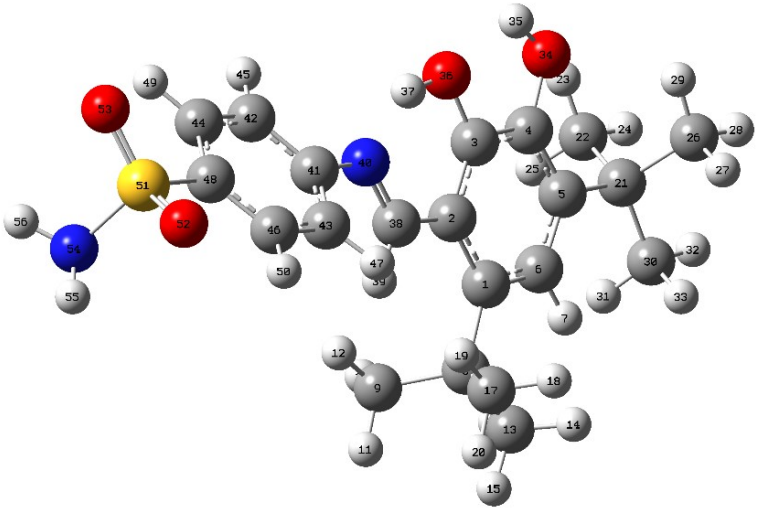
4,6-di-*tert*-butyl-3-(((4-(trifluoromethyl)phenyl)imino)methyl)catechol (Compound **13**)



Tag	Symbol	X	Y	Z
1	C	2.1941400	1.1570070	0.0729090
2	C	1.2598460	0.0695020	0.0375910
3	C	1.7710830	-1.2501180	-0.0262170
4	C	3.1478120	-1.5191090	-0.0661760
5	C	4.0698700	-0.4759840	-0.0406770
6	C	3.5449910	0.8315730	0.0303630
7	H	4.2599390	1.6341630	0.0541720
8	C	1.7761650	2.6497370	0.1574500
9	C	0.9845590	2.9338290	1.4605310
10	H	1.5914820	2.6782860	2.3332960
11	H	0.7394370	3.9984290	1.5222860
12	H	0.0500890	2.3796510	1.5429140
13	C	3.0005590	3.5927330	0.2012680
14	H	3.6163100	3.5134010	-0.6977990
15	H	2.6478150	4.6252140	0.2650600
16	H	3.6322490	3.4086160	1.0735200
17	C	0.9686950	3.0741310	-1.0965640
18	H	1.5650210	2.9189600	-1.9996810
19	H	0.0349540	2.5278720	-1.2270870
20	H	0.7189780	4.1377970	-1.0370500
21	C	5.5866330	-0.7399850	-0.0851630
22	C	5.9468000	-1.4849630	-1.3941040
23	H	5.6790070	-0.8826460	-2.2672350
24	H	7.0252610	-1.6679270	-1.4299870
25	H	5.4348490	-2.4434860	-1.4673820
26	C	6.4090930	0.5625830	-0.0483420
27	H	6.2382420	1.1333430	0.8686480
28	H	7.4725240	0.3121870	-0.0838150
29	H	6.1968320	1.2092870	-0.9042420
30	C	6.0027520	-1.5923930	1.1388370
31	H	5.4924420	-2.5545070	1.1531890
32	H	7.0813500	-1.7760100	1.1113780
33	H	5.7750680	-1.0665560	2.0707660
34	O	3.5308020	-2.8290290	-0.1292430
35	H	2.7215300	-3.3618110	-0.1334310
36	O	0.9858030	-2.3486900	-0.0539900
37	H	0.0325620	-2.0382940	-0.0028930
38	C	-0.1810700	0.2312360	0.0636630

39	H	-0.5845250	1.2385780	0.0971100
40	N	-1.0013040	-0.7714800	0.0667520
41	C	-2.3905820	-0.5693470	0.0284410
42	C	-3.2053960	-1.4333560	0.7746450
43	C	-2.9942720	0.4241220	-0.7575920
44	C	-4.5845990	-1.2832870	0.7682610
45	H	-2.7389860	-2.2100550	1.3685860
46	C	-4.3764740	0.5685330	-0.7696760
47	H	-2.3840620	1.0629280	-1.3846900
48	C	-5.1753340	-0.2773470	-0.0003980
49	H	-5.2031510	-1.9442630	1.3624940
50	H	-4.8335150	1.3364780	-1.3813400
51	C	-6.6712930	-0.1558010	-0.0558530
52	F	-7.2586220	-0.5297300	1.1041260
53	F	-7.2107730	-0.9381040	-1.0278170
54	F	-7.0738610	1.1092460	-0.3171280

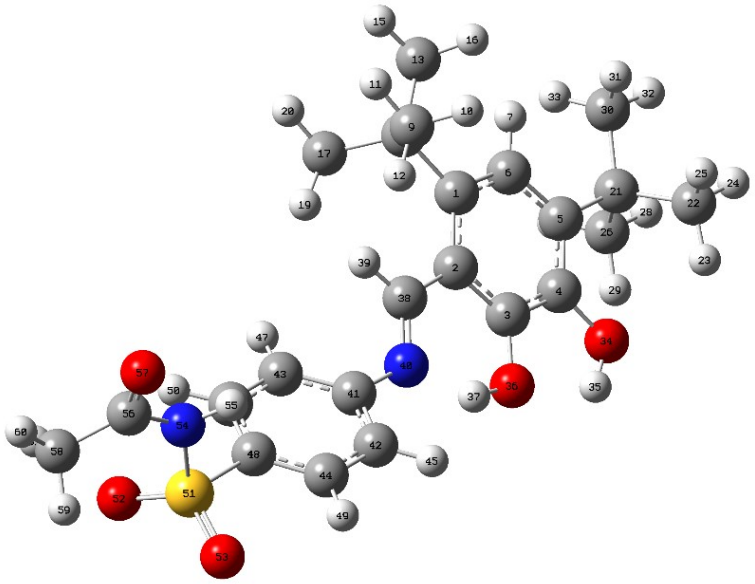
(E)-4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzenesulfonamide (Compound **14**)



Tag	Symbol	X	Y	Z
1	C	2.4677810	1.1560190	0.0672800
2	C	1.5452530	0.0587420	0.0209590
3	C	2.0709310	-1.2556380	-0.0362590
4	C	3.4508150	-1.5103110	-0.0585770
5	C	4.3615210	-0.4576000	-0.0218000
6	C	3.8222400	0.8445720	0.0419000
7	H	4.5285190	1.6545160	0.0740470
8	C	2.0332470	2.6443890	0.1447080
9	C	1.2238700	2.9222020	1.4382600
10	H	1.8232430	2.6738880	2.3183070
11	H	0.9674810	3.9844130	1.4956150
12	H	0.2940650	2.3588550	1.5106780
13	C	3.2471310	3.6001970	0.2009170
14	H	3.8740580	3.5255200	-0.6907790
15	H	2.8829230	4.6290600	0.2584530
16	H	3.8705220	3.4243930	1.0808210
17	C	1.2357080	3.0583740	-1.1190980

18	H	1.8436260	2.9076360	-2.0151890
19	H	0.3090500	2.5025180	-1.2591740
20	H	0.9746790	4.1195850	-1.0644340
21	C	5.8813710	-0.7058030	-0.0469960
22	C	6.2907530	-1.5532000	1.1827620
23	H	5.7905280	-2.5206650	1.1911660
24	H	7.3714860	-1.7254200	1.1691660
25	H	6.0456490	-1.0293620	2.1114010
26	C	6.2657480	-1.4477650	-1.3507720
27	H	6.0025600	-0.8489320	-2.2276800
28	H	7.3464480	-1.6192940	-1.3729500
29	H	5.7649560	-2.4117000	-1.4296900
30	C	6.6897160	0.6052650	-0.0006330
31	H	6.5013670	1.1746750	0.9137710
32	H	7.7560420	0.3659000	-0.0224880
33	H	6.4816440	1.2492850	-0.8595770
34	O	3.8482290	-2.8160500	-0.1161720
35	H	3.0448500	-3.3574950	-0.1313890
36	O	1.2977320	-2.3622160	-0.0735960
37	H	0.3407060	-2.0622660	-0.0351170
38	C	0.1029930	0.2056190	0.0305170
39	H	-0.3110190	1.2086780	0.0616410
40	N	-0.7072150	-0.8055430	0.0227440
41	C	-2.0972800	-0.6172240	-0.0297190
42	C	-2.9098360	-1.5043650	0.6929290
43	C	-2.7010280	0.3774230	-0.8159870
44	C	-4.2910140	-1.3728490	0.6733660
45	H	-2.4407280	-2.2908510	1.2716810
46	C	-4.0843200	0.5091920	-0.8448970
47	H	-2.0902280	1.0205790	-1.4380160
48	C	-4.8683450	-0.3577830	-0.0884940
49	H	-4.9196680	-2.0604920	1.2248690
50	H	-4.5551660	1.2577480	-1.4697630
51	S	-6.6526990	-0.1816080	-0.1167750
52	O	-7.0083900	0.5336190	-1.3405930
53	O	-7.2328370	-1.4763520	0.2325760
54	N	-6.9723650	0.8665480	1.1771070
55	H	-7.4064570	1.7183970	0.8364100
56	H	-7.5522930	0.4007900	1.8677420

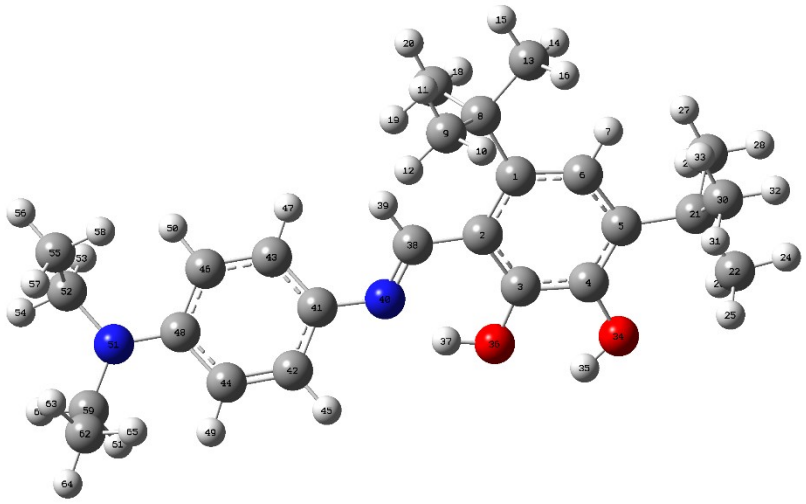
N-((4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)phenyl)sulfonyl)acetamide (Compound **15**)



Tag	Symbol	X	Y	Z
1	C	-3.1658150	1.1802980	0.0293100
2	C	-2.3267100	0.0163340	0.0073270
3	C	-2.9479160	-1.2564020	-0.0515250
4	C	-4.3425390	-1.4087060	-0.0793470
5	C	-5.1727640	-0.2909530	-0.0514500
6	C	-4.5388580	0.9687440	0.0011350
7	H	-5.1837100	1.8287250	0.0189350
8	C	-2.6231090	2.6338830	0.0791090
9	C	-1.7621410	2.9503540	-1.1715900
10	H	-2.3546350	2.8167900	-2.0806530
11	H	-1.4276330	3.9915590	-1.1391230
12	H	-0.8741050	2.3266440	-1.2698960
13	C	-3.7632860	3.6779880	0.0735890
14	H	-4.4172110	3.5811710	0.9434850
15	H	-3.3246830	4.6784740	0.1048950
16	H	-4.3741130	3.6171770	-0.8302070
17	C	-1.8314150	2.8888020	1.3879780
18	H	-2.4707900	2.7117390	2.2569160
19	H	-0.9492580	2.2591970	1.5013030
20	H	-1.4958120	3.9295320	1.4239120
21	C	-6.7066450	-0.4257760	-0.0799980
22	C	-7.1412700	-1.1418090	-1.3825680
23	H	-6.7131400	-2.1404930	-1.4568700
24	H	-8.2315730	-1.2328410	-1.4069170
25	H	-6.8325340	-0.5670640	-2.2607240
26	C	-7.1804020	-1.2364020	1.1515410
27	H	-6.8989220	-0.7294790	2.0792210
28	H	-8.2709000	-1.3269530	1.1357840
29	H	-6.7544580	-2.2386810	1.1640960
30	C	-7.4156650	0.9417410	-0.0396980
31	H	-7.1609220	1.5650520	-0.9013180
32	H	-8.4966980	0.7817300	-0.0609680
33	H	-7.1859930	1.4994850	0.8724480
34	O	-4.8360010	-2.6808720	-0.1349110
35	H	-4.0764680	-3.2821630	-0.1464690

36	O	-2.2586330	-2.4170560	-0.0860190
37	H	-1.2827260	-2.1896870	-0.0825880
38	C	-0.8799140	0.0571700	0.0396730
39	H	-0.3954540	1.0269590	0.0975220
40	N	-0.1423710	-1.0081810	-0.0185670
41	C	1.2529450	-0.9269800	0.0810640
42	C	2.0215480	-1.8059490	-0.6977200
43	C	1.9023500	-0.0476920	0.9662920
44	C	3.4079120	-1.7799520	-0.6332130
45	H	1.5153420	-2.5021170	-1.3552970
46	C	3.2879840	-0.0197500	1.0407550
47	H	1.3190960	0.5848910	1.6243150
48	C	4.0301840	-0.8784680	0.2306680
49	H	4.0058750	-2.4595530	-1.2274320
50	H	3.7904220	0.6412350	1.7360790
51	S	5.8155830	-0.8506310	0.3301720
52	O	6.2332740	-0.4912810	1.6801240
53	O	6.3303800	-2.0579750	-0.3072650
54	N	6.1483570	0.5075440	-0.6667940
55	H	5.6255960	0.5038780	-1.5378400
56	C	7.3314000	1.2731430	-0.7590080
57	O	7.4677630	1.9833870	-1.7303900
58	C	8.3299030	1.1807010	0.3632960
59	H	8.7600170	0.1762620	0.4064220
60	H	9.1180720	1.9058430	0.1715580
61	H	7.8571720	1.3657160	1.3281580

4,6-di-*tert*-butyl-3-(((4-(diethylamino)phenyl)imino)methyl)catechol (Compound **16**)



Tag	Symbol	X	Y	Z
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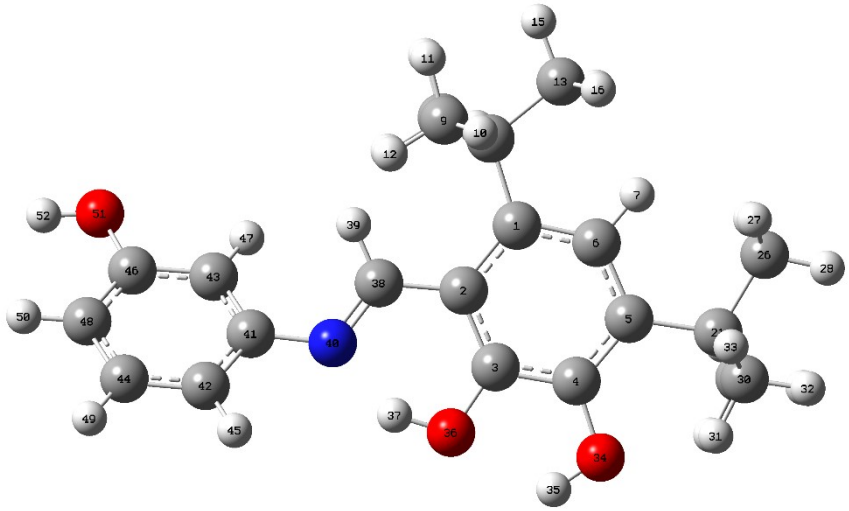
2	C	1.5719500	0.0375520	-0.0150580
3	C	2.0775530	-1.2764850	-0.1180940
4	C	3.4576770	-1.5689570	-0.1182370
5	C	4.3859450	-0.5403170	-0.0080260
6	C	3.8603660	0.7690130	0.1024480
7	H	4.5846030	1.5614650	0.1922640
8	C	2.1097400	2.6024470	0.2410830
9	C	1.2673970	2.8354820	1.5221960
10	H	1.8399570	2.5427140	2.4065560

11	H	1.0198710	3.8973750	1.6184070
12	H	0.3318220	2.2779530	1.5438030
13	C	3.3379830	3.5310690	0.3765620
14	H	3.9894020	3.4852070	-0.4995470
15	H	2.9914280	4.5634710	0.4721600
16	H	3.9318920	3.3017400	1.2646530
17	C	1.3562870	3.0890010	-1.0238070
18	H	1.9924630	2.9789740	-1.9062580
19	H	0.4327330	2.5461420	-1.2217200
20	H	1.1004920	4.1485190	-0.9230330
21	C	5.9240230	-0.6950480	0.0082980
22	C	6.4327900	-2.1453330	-0.1202040
23	H	6.1158840	-2.6094840	-1.0543220
24	H	7.5270510	-2.1317340	-0.0991250
25	H	6.0842350	-2.7762340	0.6975590
26	C	6.5224260	0.1094270	-1.1720030
27	H	6.2776620	1.1724130	-1.1186430
28	H	7.6130420	0.0179050	-1.1697110
29	H	6.1529810	-0.2726890	-2.1275660
30	C	6.4713700	-0.1302710	1.3423850
31	H	6.0654880	-0.6847880	2.1928950
32	H	7.5616060	-0.2233860	1.3666950
33	H	6.2241350	0.9244750	1.4808850
34	O	3.7958120	-2.8878940	-0.2291920
35	H	2.9619230	-3.3786910	-0.2882830
36	O	1.2808940	-2.3623630	-0.2264950
37	H	0.3253070	-2.0290190	-0.2041140
38	C	0.1269050	0.2086780	-0.0389930
39	H	-0.2715560	1.2160180	0.0258050
40	N	-0.6913070	-0.7910090	-0.1224470
41	C	-2.0834860	-0.6149890	-0.2034350
42	C	-2.9094610	-1.6419220	0.2697520
43	C	-2.7103960	0.5108880	-0.7555030
44	C	-4.2912910	-1.5396930	0.2377180
45	H	-2.4481440	-2.5278420	0.6918560
46	C	-4.0925690	0.6188960	-0.8043130
47	H	-2.1159280	1.3089350	-1.1859230
48	C	-4.9348370	-0.4048680	-0.3098980
49	H	-4.8702030	-2.3566470	0.6441020
50	H	-4.5151510	1.5076810	-1.2511760
51	N	-6.3167730	-0.3136890	-0.3876310
52	C	-6.9642950	0.8874850	-0.9092220
53	H	-6.4501490	1.2074070	-1.8213840
54	H	-7.9712370	0.6002720	-1.2213440
55	C	-7.0551370	2.0606850	0.0770580
56	H	-7.5198530	2.9245960	-0.4082060
57	H	-7.6588200	1.7971190	0.9484930
58	H	-6.0671730	2.3614930	0.4319670
59	C	-7.1711170	-1.3939530	0.0994260
60	H	-8.1212680	-1.3215370	-0.4361050
61	H	-6.7356980	-2.3533680	-0.1954370
62	C	-7.4396440	-1.3840910	1.6111800
63	H	-7.9738360	-0.4795340	1.9111890
64	H	-8.0532520	-2.2464280	1.8898540
65	H	-6.5098840	-1.4298220	2.1822510

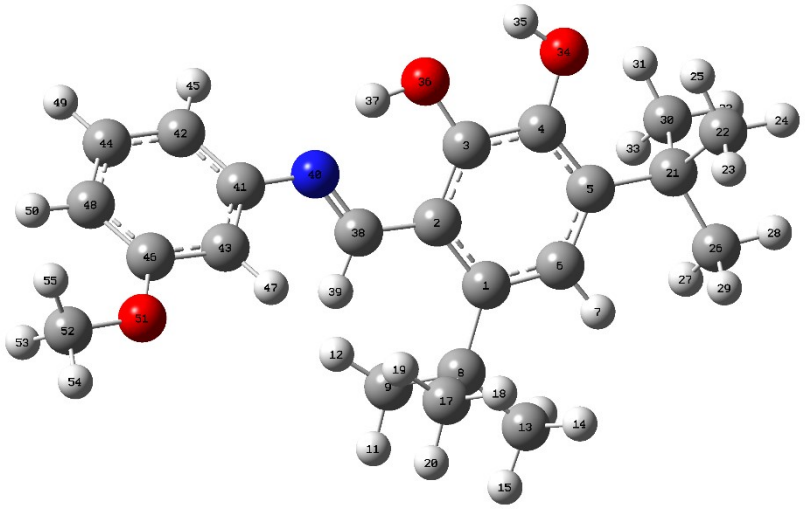
(E)-4,6-di-*tert*-butyl-3-(((3-hydroxyphenyl)imino)methyl)benzene-1,2-diol (Compound **17**)



Tag	Symbol	X	Y	Z
1	C	1.1122210	1.1335790	0.1326760
2	C	0.2435680	-0.0051350	0.0796400
3	C	0.8305610	-1.2883260	-0.0368310
4	C	2.2198750	-1.4726750	-0.1124440
5	C	3.0795050	-0.3782790	-0.0704970
6	C	2.4797110	0.8921310	0.0537140
7	H	3.1454580	1.7356220	0.0903780
8	C	0.6075930	2.5949340	0.2727200
9	C	-0.1754960	2.7893900	1.5973230
10	H	0.4623860	2.5448550	2.4510770
11	H	-0.4842890	3.8345060	1.6970530
12	H	-1.0723330	2.1761260	1.6767940
13	C	1.7735110	3.6087180	0.3270240
14	H	2.3760740	3.5953470	-0.5843550
15	H	1.3603930	4.6153760	0.4304350
16	H	2.4315280	3.4355670	1.1819940
17	C	-0.2476740	3.0077880	-0.9529060
18	H	0.3411430	2.9202650	-1.8700090
19	H	-1.1467340	2.4072860	-1.0866730
20	H	-0.5633060	4.0508920	-0.8538720
21	C	4.6079610	-0.5505770	-0.1532060
22	C	4.9831570	-1.2316070	-1.4922910
23	H	4.6625920	-0.6186030	-2.3398560
24	H	6.0694130	-1.3509220	-1.5552090
25	H	4.5247560	-2.2151070	-1.5866840
26	C	5.3534130	0.7965470	-0.0899980
27	H	5.1685520	1.3269750	0.8482450
28	H	6.4288690	0.6111660	-0.1544270
29	H	5.0847510	1.4561780	-0.9197860
30	C	5.0998540	-1.4149580	1.0336200
31	H	4.6460590	-2.4051100	1.0265680
32	H	6.1865590	-1.5343680	0.9791200
33	H	4.8619440	-0.9329280	1.9864830
34	O	2.6766760	-2.7562320	-0.2260870
35	H	1.8974090	-3.3323200	-0.2316060

36	O	0.1106320	-2.4302780	-0.0849490
37	H	-0.8599990	-2.1737520	-0.0054860
38	C	-1.2063960	0.0667660	0.1389180
39	H	-1.6719670	1.0447820	0.2114010
40	N	-1.9593310	-0.9852970	0.1245400
41	C	-3.3633950	-0.8758560	0.1291540
42	C	-4.0946760	-1.8399230	0.8392000
43	C	-4.0390100	0.1261790	-0.5767420
44	C	-5.4815090	-1.7689360	0.8663050
45	H	-3.5635080	-2.6205820	1.3691720
46	C	-5.4314820	0.1796260	-0.5457630
47	H	-3.5044300	0.8463880	-1.1832840
48	C	-6.1613430	-0.7633410	0.1793950
49	H	-6.0465630	-2.5066480	1.4245110
50	H	-7.2460370	-0.7221100	0.1949810
51	O	-6.0282550	1.1817490	-1.2632570
52	H	-6.9855210	1.1100230	-1.1884720

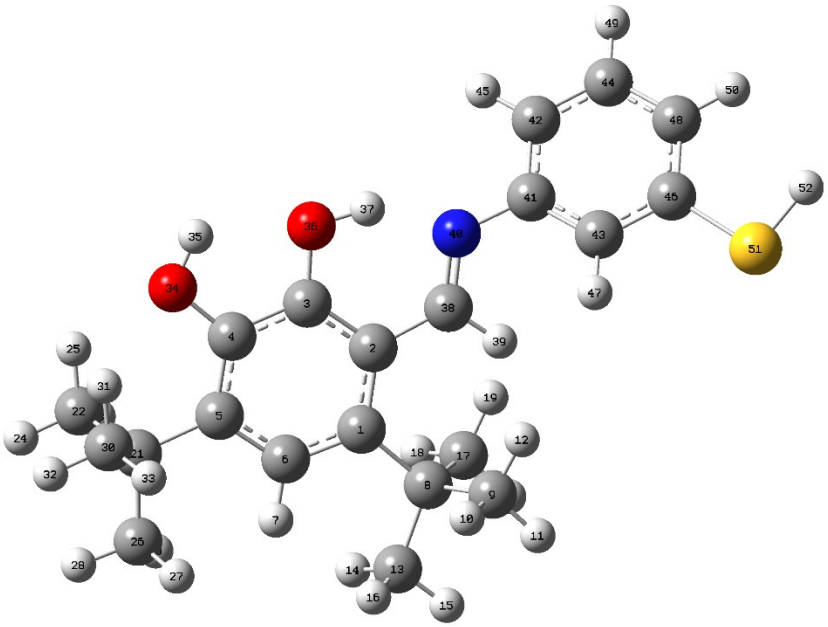
(E)-4,6-di-*tert*-butyl-3-(((3-methoxyphenyl)imino)methyl)benzene-1,2-diol (Compound **18**)



Tag	Symbol	X	Y	Z
1	C	1.3951380	1.1227800	0.1743870
2	C	0.5645910	-0.0437220	0.1190810
3	C	1.1912190	-1.3025230	-0.0453330
4	C	2.5832920	-1.4367710	-0.1644140
5	C	3.4062080	-0.3146670	-0.1197480
6	C	2.7673150	0.9309360	0.0510240
7	H	3.4046530	1.7960100	0.0887720
8	C	0.8453780	2.5621630	0.3637410
9	C	0.0977280	2.6992130	1.7156560
10	H	0.7707350	2.4603960	2.5436880
11	H	-0.2457460	3.7297840	1.8483430
12	H	-0.7729560	2.0511640	1.8085950
13	C	1.9768510	3.6148010	0.4063430
14	H	2.5508740	3.6429820	-0.5229650
15	H	1.5327570	4.6037870	0.5458510
16	H	2.6667340	3.4458610	1.2366670
17	C	-0.0614970	2.9722340	-0.8252240
18	H	0.5002800	2.9235770	-1.7619820

19	H	-0.9445240	2.3453980	-0.9437540
20	H	-0.4072880	4.0020930	-0.6933030
21	C	4.9367860	-0.4322600	-0.2473790
22	C	5.2983130	-1.0690760	-1.6116850
23	H	4.9345100	-0.4481080	-2.4356730
24	H	6.3858780	-1.1497060	-1.7059570
25	H	4.8707480	-2.0652550	-1.7173850
26	C	5.6378320	0.9378770	-0.1715680
27	H	5.4610390	1.4396230	0.7838520
28	H	6.7167770	0.7912210	-0.2691950
29	H	5.3242400	1.6070480	-0.9776320
30	C	5.4897660	-1.3062380	0.9050390
31	H	5.0695030	-2.3109430	0.8863040
32	H	6.5780210	-1.3869710	0.8190860
33	H	5.2616360	-0.8546510	1.8750630
34	O	3.0797420	-2.7009640	-0.3215390
35	H	2.3202000	-3.3029020	-0.3190300
36	O	0.5094730	-2.4673540	-0.1007810
37	H	-0.4669990	-2.2460260	0.0122660
38	C	-0.8851060	-0.0243190	0.2228580
39	H	-1.3823550	0.9343140	0.3341260
40	N	-1.6009320	-1.1013930	0.2030090
41	C	-3.0079850	-1.0416630	0.2507570
42	C	-3.6848760	-2.0440070	0.9648860
43	C	-3.7385870	-0.0559850	-0.4152630
44	C	-5.0695070	-2.0197920	1.0298770
45	H	-3.1124430	-2.8144320	1.4662760
46	C	-5.1359990	-0.0468540	-0.3494870
47	H	-3.2485730	0.6936310	-1.0240480
48	C	-5.8109570	-1.0287330	0.3800280
49	H	-5.5929430	-2.7859060	1.5908110
50	H	-6.8904650	-1.0430420	0.4377070
51	O	-5.7465520	0.9574430	-1.0436820
52	C	-7.1669300	1.0214510	-1.0404320
53	H	-7.5583320	1.1633370	-0.0273630
54	H	-7.4263620	1.8847490	-1.6509210
55	H	-7.6082200	0.1206320	-1.4801310

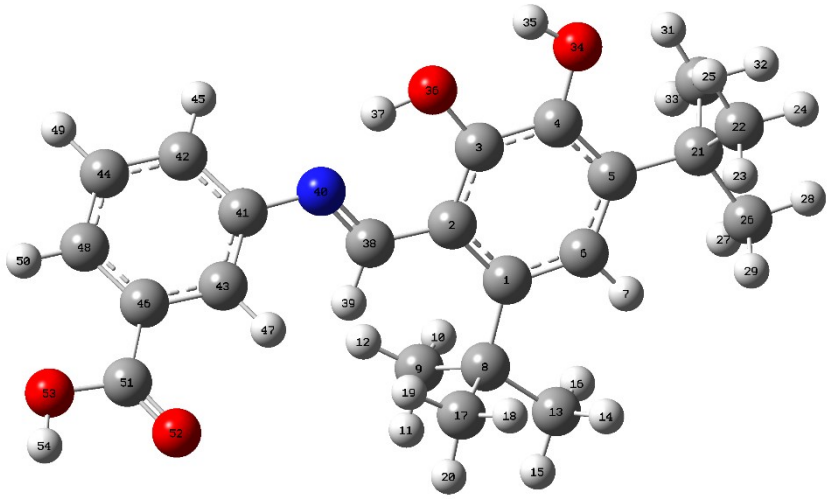
(E)-4,6-di-*tert*-butyl-3-(((4-mercaptophenyl)imino)methyl)benzene-1,2-diol (Compound **19**)



Tag	Symbol	X	Y	Z
1	C	1.3419030	1.1066590	-0.2051120
2	C	0.5207500	-0.0660310	-0.1338040
3	C	1.1569010	-1.3169560	0.0544890
4	C	2.5492980	-1.4377730	0.1822500
5	C	3.3629380	-0.3094970	0.1224580
6	C	2.7146800	0.9278640	-0.0722310
7	H	3.3452640	1.7972450	-0.1215780
8	C	0.7815200	2.5381280	-0.4216180
9	C	-0.1331730	2.9618030	0.7565660
10	H	0.4249200	2.9337810	1.6963180
11	H	-0.4865000	3.9863460	0.6053620
12	H	-1.0119430	2.3303140	0.8826300
13	C	1.9049750	3.5987060	-0.4778760
14	H	2.5995210	3.4208670	-1.3024030
15	H	1.4537860	4.5815480	-0.6363410
16	H	2.4748520	3.6476470	0.4531010
17	C	0.0385500	2.6461200	-1.7787750
18	H	0.7167500	2.3981970	-2.5998250
19	H	-0.8271140	1.9903080	-1.8645930
20	H	-0.3119940	3.6715670	-1.9305970
21	C	4.8937910	-0.4118450	0.2589200
22	C	5.4593000	-1.3005400	-0.8760790
23	H	5.2317070	-0.8675910	-1.8546810
24	H	6.5477690	-1.3700450	-0.7839490
25	H	5.0479910	-2.3085200	-0.8420150
26	C	5.5835210	0.9627650	0.1628160
27	H	5.2608840	1.6428590	0.9560570
28	H	6.6631610	0.8268980	0.2676090
29	H	5.4069960	1.4466850	-0.8018020
30	C	5.2542060	-1.0221890	1.6355900
31	H	4.8351760	-2.0202700	1.7563720
32	H	6.3419440	-1.0914140	1.7360710
33	H	4.8811870	-0.3905420	2.4472290
34	O	3.0560740	-2.6943760	0.3629250

35	H	2.3028000	-3.3039770	0.3675220
36	O	0.4846800	-2.4865500	0.1261450
37	H	-0.4918620	-2.2776340	0.0042020
38	C	-0.9274840	-0.0592070	-0.2444260
39	H	-1.4299960	0.8945660	-0.3729690
40	N	-1.6372130	-1.1408520	-0.2126740
41	C	-3.0429880	-1.0884200	-0.2676760
42	C	-3.7140400	-2.0913430	-0.9800090
43	C	-3.7832810	-0.1056910	0.4027810
44	C	-5.1014970	-2.0742040	-1.0524810
45	H	-3.1369420	-2.8613370	-1.4770590
46	C	-5.1782120	-0.0977510	0.3272650
47	H	-3.2719650	0.6269010	1.0163450
48	C	-5.8411290	-1.0813840	-0.4122490
49	H	-5.6195190	-2.8430160	-1.6147110
50	H	-6.9225420	-1.0840290	-0.4802730
51	S	-6.0407670	1.2050700	1.1959220
52	H	-7.2807600	0.6996170	1.0505810

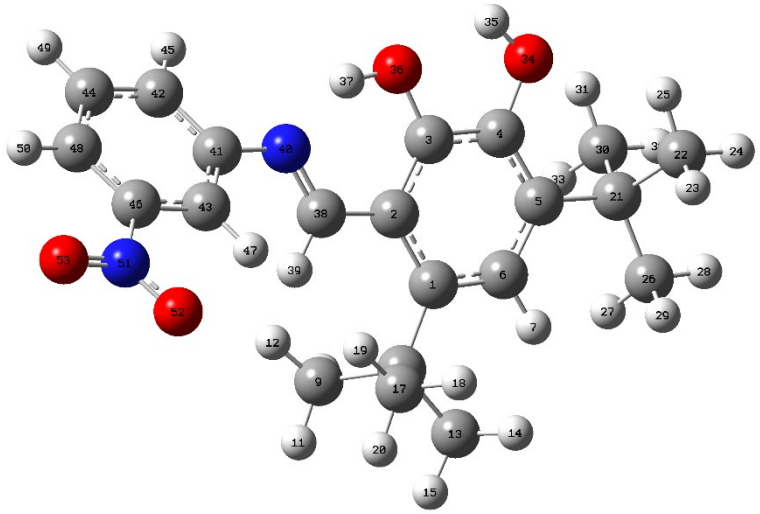
4-((4,6-di-*tert*-butyl-2,3-dihydroxybenzylidene)amino)benzoic acid (Compound **20**)



Tag	Symbol	X	Y	Z
1	C	-1.5258770	1.0879180	-0.2481540
2	C	-0.7316670	-0.1023120	-0.1579680
3	C	-1.3943410	-1.3326470	0.0723490
4	C	-2.7869330	-1.4170490	0.2226800
5	C	-3.5744200	-0.2713910	0.1442750
6	C	-2.9001640	0.9448180	-0.0917150
7	H	-3.5108600	1.8273720	-0.1544600
8	C	-0.9353930	2.4999490	-0.5078850
9	C	-0.2106980	2.5570400	-1.8780260
10	H	-0.9064910	2.3053850	-2.6831330
11	H	0.1614420	3.5698470	-2.0597400
12	H	0.6384390	1.8793630	-1.9600560
13	C	-2.0350620	3.5846200	-0.5749160
14	H	-2.5896260	3.6699070	0.3626600
15	H	-1.5635970	4.5523440	-0.7640000
16	H	-2.7457030	3.4030520	-1.3848600

17	C	0.0061840	2.9309020	0.6462190
18	H	-0.5378720	2.9368080	1.5945430
19	H	0.8745410	2.2860130	0.7752320
20	H	0.3782960	3.9438580	0.4658730
21	C	-5.1050380	-0.3332060	0.3050730
22	C	-5.4591820	-0.8972410	1.7029990
23	H	-5.0588460	-0.2532890	2.4915980
24	H	-6.5466240	-0.9369020	1.8209330
25	H	-5.0628270	-1.9017660	1.8451020
26	C	-5.7634830	1.0544630	0.1811330
27	H	-5.5893940	1.5081160	-0.7985170
28	H	-6.8444020	0.9472330	0.3041790
29	H	-5.4138170	1.7475950	0.9512630
30	C	-5.7080430	-1.2384270	-0.7971220
31	H	-5.3202780	-2.2547340	-0.7414430
32	H	-6.7963250	-1.2791740	-0.6875720
33	H	-5.4849840	-0.8375620	-1.7903290
34	O	-3.3207730	-2.6558370	0.4438540
35	H	-2.5825310	-3.2833210	0.4555230
36	O	-0.7484340	-2.5156510	0.1659320
37	H	0.2302770	-2.3330850	0.0272190
38	C	0.7135390	-0.1315080	-0.2886100
39	H	1.2342280	0.8076400	-0.4479750
40	N	1.4002190	-1.2281400	-0.2370460
41	C	2.8054730	-1.2069570	-0.3101410
42	C	3.4474630	-2.2652550	-0.9718980
43	C	3.5845840	-0.2105290	0.2857630
44	C	4.8337710	-2.3014630	-1.0684970
45	H	2.8407140	-3.0466020	-1.4147300
46	C	4.9785460	-0.2531310	0.1922390
47	H	3.1296920	0.5902870	0.8550280
48	C	5.6089090	-1.2981500	-0.4911140
49	H	5.3138330	-3.1196130	-1.5927410
50	H	6.6880920	-1.3268560	-0.5561590
51	C	5.7461360	0.8362370	0.8536030
52	O	5.2555140	1.7612060	1.4586110
53	O	7.0890440	0.7007860	0.7131050
54	H	7.4944610	1.4509540	1.1721500

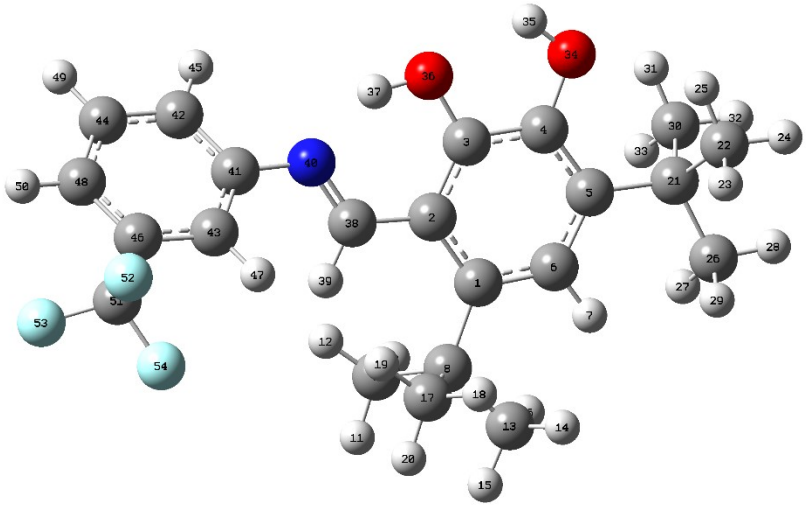
(E)-4,6-di-*tert*-butyl-3-(((3-nitrophenyl)imino)methyl)benzene-1,2-diol (Compound **21**)



Tag	Symbol	X	Y	Z
1	C	1.5133150	1.0875840	0.2429770
2	C	0.7149020	-0.1010650	0.1565820
3	C	1.3735380	-1.3357570	-0.0660090
4	C	2.7659010	-1.4262710	-0.2125760
5	C	3.5569550	-0.2825380	-0.1378960
6	C	2.8867260	0.9377440	0.0904590
7	H	3.5010830	1.8178860	0.1504270
8	C	0.9278280	2.5031330	0.4950150
9	C	0.1998850	2.5696850	1.8630680
10	H	0.8917740	2.3168330	2.6710710
11	H	-0.1663020	3.5853790	2.0398890
12	H	-0.6540620	1.8980090	1.9460340
13	C	2.0322330	3.5831120	0.5599470
14	H	2.5896000	3.6616870	-0.3764920
15	H	1.5646700	4.5537270	0.7432550
16	H	2.7396970	3.4022040	1.3727480
17	C	-0.0084340	2.9332910	-0.6638130
18	H	0.5377030	2.9318430	-1.6108710
19	H	-0.8799800	2.2922470	-0.7921030
20	H	-0.3759290	3.9488060	-0.4892940
21	C	5.0876280	-0.3500300	-0.2945410
22	C	5.4429940	-0.9223520	-1.6888770
23	H	5.0465380	-0.2813420	-2.4817740
24	H	6.5305200	-0.9653480	-1.8037620
25	H	5.0446650	-1.9266160	-1.8269030
26	C	5.7501990	1.0361460	-0.1761060
27	H	5.5757590	1.4953630	0.8008720
28	H	6.8309190	0.9245160	-0.2960980
29	H	5.4050080	1.7265220	-0.9506950
30	C	5.6846270	-1.2515360	0.8140640
31	H	5.2949830	-2.2672800	0.7622210
32	H	6.7730060	-1.2952020	0.7077780
33	H	5.4598550	-0.8452480	1.8046500
34	O	3.2969500	-2.6669550	-0.4259880
35	H	2.5588380	-3.2943460	-0.4372290
36	O	0.7236740	-2.5168750	-0.1554520
37	H	-0.2528350	-2.3338100	-0.0194190

38	C	-0.7282120	-0.1220630	0.2841520
39	H	-1.2426230	0.8215980	0.4374550
40	N	-1.4234850	-1.2151890	0.2393780
41	C	-2.8259520	-1.1825300	0.3079080
42	C	-3.4815860	-2.2283410	0.9774440
43	C	-3.5927810	-0.1834120	-0.3038140
44	C	-4.8686550	-2.2561820	1.0691580
45	H	-2.8825720	-3.0092530	1.4307120
46	C	-4.9772430	-0.2397190	-0.1986900
47	H	-3.1387100	0.6106360	-0.8796680
48	C	-5.6390900	-1.2560620	0.4801610
49	H	-5.3564520	-3.0653050	1.5993320
50	H	-6.7186340	-1.2590410	0.5282620
51	N	-5.7767460	0.8224350	-0.8544130
52	O	-5.1709280	1.7058470	-1.4486030
53	O	-6.9951430	0.7564580	-0.7595620

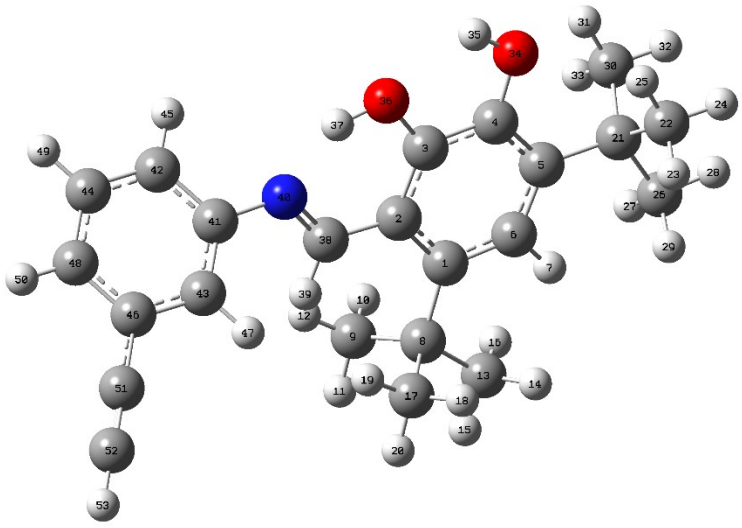
4,6-di-*tert*-butyl-3-(((3-(trifluoromethyl)phenyl)imino)methyl)catechol (Compound **22**)



Tag	Symbol	X	Y	Z
1	C	1.7926280	1.0752300	0.2763690
2	C	1.0174270	-0.1289390	0.2026030
3	C	1.6955700	-1.3470670	-0.0479270
4	C	3.0851020	-1.4064330	-0.2340400
5	C	3.8538200	-0.2470010	-0.1722480
6	C	3.1645140	0.9566030	0.0846700
7	H	3.7612870	1.8494010	0.1349530
8	C	1.1844480	2.4758510	0.5563520
9	C	0.4939790	2.5158710	1.9446310
10	H	1.2141870	2.2732480	2.7307190
11	H	0.1096640	3.5215260	2.1399530
12	H	-0.3412340	1.8235580	2.0459580
13	C	2.2661650	3.5795660	0.5987060
14	H	2.7950450	3.6772630	-0.3523640
15	H	1.7829450	4.5382970	0.8031200
16	H	3.0002330	3.4081320	1.3896500
17	C	0.2063150	2.8940400	-0.5719200
18	H	0.7256330	2.9132140	-1.5338080
19	H	-0.6527820	2.2329280	-0.6808500
20	H	-0.1795010	3.8992890	-0.3778340

21	C	5.3805800	-0.2809890	-0.3725010
22	C	5.7080560	-0.8337650	-1.7814340
23	H	5.2759230	-0.1943810	-2.5568510
24	H	6.7925520	-0.8533160	-1.9276120
25	H	5.3264070	-1.8448220	-1.9172250
26	C	6.0171270	1.1178560	-0.2603270
27	H	5.8603900	1.5652340	0.7251170
28	H	7.0962180	1.0302930	-0.4113540
29	H	5.6357950	1.8071060	-1.0188240
30	C	6.0277470	-1.1790360	0.7103820
31	H	5.6573490	-2.2020720	0.6606490
32	H	7.1133410	-1.1994670	0.5727610
33	H	5.8231700	-0.7857650	1.7105630
34	O	3.6355160	-2.6342180	-0.4726660
35	H	2.9098150	-3.2761590	-0.4674130
36	O	1.0689130	-2.5412540	-0.1284770
37	H	0.0919950	-2.3791320	0.0363360
38	C	-0.4226080	-0.1831880	0.3686240
39	H	-0.9546500	0.7470220	0.5433300
40	N	-1.0928260	-1.2910000	0.3331990
41	C	-2.4947550	-1.2927720	0.4390440
42	C	-3.1048270	-2.3405810	1.1432540
43	C	-3.3014700	-0.3202470	-0.1664000
44	C	-4.4871970	-2.3904870	1.2747740
45	H	-2.4770770	-3.1001140	1.5940970
46	C	-4.6872140	-0.3836810	-0.0331800
47	H	-2.8533680	0.4666730	-0.7593490
48	C	-5.2896510	-1.4129170	0.6895620
49	H	-4.9451480	-3.1972050	1.8349300
50	H	-6.3667860	-1.4522560	0.7876940
51	C	-5.5448080	0.6304550	-0.7417970
52	F	-5.8907450	0.2170020	-1.9877900
53	F	-6.6996430	0.8731930	-0.0824540
54	F	-4.9154710	1.8189250	-0.8933960

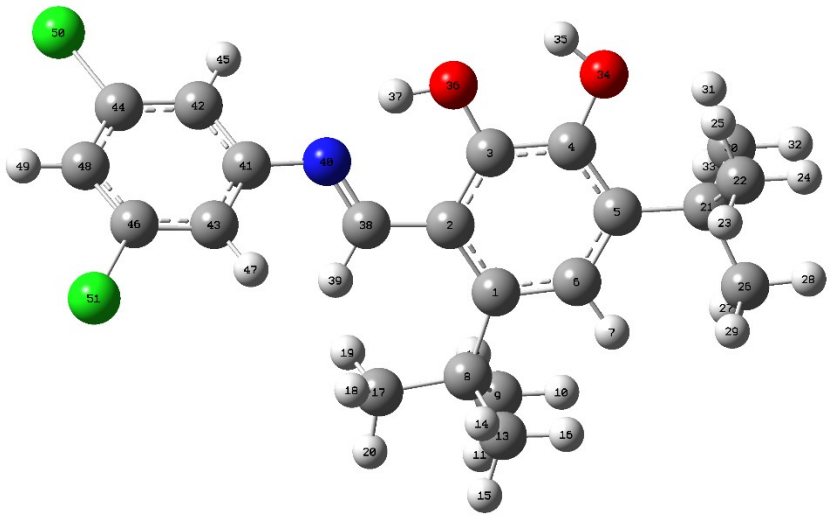
(*E*)-4,6-di-*tert*-butyl-3-(((3-ethynylphenyl)imino)methyl)catechol (Compound **23**)



Tag	Symbol	X	Y	Z
1	C	-1.2282210	1.1118030	-0.2057930

2	C	-0.4051330	-0.0588850	-0.1232540
3	C	-1.0397540	-1.3096330	0.0716140
4	C	-2.4323120	-1.4321360	0.1955940
5	C	-3.2477490	-0.3057450	0.1252010
6	C	-2.6010590	0.9313780	-0.0761440
7	H	-3.2330730	1.7992210	-0.1337180
8	C	-0.6699230	2.5428280	-0.4302560
9	C	0.0785380	2.6425820	-1.7850310
10	H	-0.5957330	2.3876160	-2.6071620
11	H	0.4278530	3.6675580	-1.9426520
12	H	0.9457560	1.9877650	-1.8626390
13	C	-1.7956030	3.6003410	-0.4993770
14	H	-2.3693140	3.6553570	0.4289010
15	H	-1.3460540	4.5829520	-0.6637860
16	H	-2.4864560	3.4143770	-1.3252220
17	C	0.2385820	2.9772730	0.7487730
18	H	-0.3238000	2.9551810	1.6861290
19	H	1.1182810	2.3489500	0.8838000
20	H	0.5902390	4.0014660	0.5914250
21	C	-4.7788310	-0.4097400	0.2576490
22	C	-5.1425300	-1.0107280	1.6375640
23	H	-4.7732270	-0.3725540	2.4457880
24	H	-6.2304570	-1.0811280	1.7350470
25	H	-4.7221980	-2.0071850	1.7669200
26	C	-5.4705770	0.9629420	0.1493760
27	H	-5.2917130	1.4401820	-0.8181420
28	H	-6.5503150	0.8259590	0.2516090
29	H	-5.1517400	1.6493000	0.9387520
30	C	-5.3392710	-1.3076170	-0.8726400
31	H	-4.9263390	-2.3146050	-0.8300600
32	H	-6.4278820	-1.3783740	-0.7832750
33	H	-5.1095100	-0.8813320	-1.8536580
34	O	-2.9375550	-2.6882010	0.3836560
35	H	-2.1834500	-3.2966360	0.3956580
36	O	-0.3656070	-2.4774700	0.1540520
37	H	0.6109000	-2.2675320	0.0356440
38	C	1.0434750	-0.0497510	-0.2275580
39	H	1.5441580	0.9045400	-0.3595450
40	N	1.7555710	-1.1295580	-0.1846670
41	C	3.1618380	-1.0737680	-0.2322770
42	C	3.8385250	-2.0827530	-0.9323980
43	C	3.9006880	-0.0847390	0.4261930
44	C	5.2270890	-2.0734070	-1.0045400
45	H	3.2607150	-2.8567940	-1.4234060
46	C	5.3025300	-0.0782780	0.3614300
47	H	3.3979610	0.6667100	1.0221230
48	C	5.9642150	-1.0798630	-0.3670540
49	H	5.7406790	-2.8506560	-1.5587100
50	H	7.0459010	-1.0773880	-0.4144430
51	C	6.0460690	0.9328880	1.0435130
52	C	6.6738500	1.7868410	1.6164960
53	H	7.2284920	2.5383270	2.1231410

4,6-di-*tert*-butyl-3-(((3,5-dichlorophenyl)imino)methyl)catechol (Compound **24**)



Tag	Symbol	X	Y	Z
1	C	-1.9246010	1.0921820	-0.3542130
2	C	-0.9558410	0.0604460	-0.1305680
3	C	-1.4321990	-1.2438540	0.1816160
4	C	-2.7936750	-1.5342520	0.3269950
5	C	-3.7494250	-0.5323550	0.1571060
6	C	-3.2644530	0.7401710	-0.1856880
7	H	-4.0022710	1.5101830	-0.3390290
8	C	-1.7003000	2.5729590	-0.8004530
9	C	-2.4752320	2.8063460	-2.1254040
10	H	-3.5436860	2.6136480	-2.0273470
11	H	-2.3532770	3.8442360	-2.4497080
12	H	-2.0911150	2.1569760	-2.9170160
13	C	-2.2553480	3.5186280	0.2947730
14	H	-1.7229520	3.3729780	1.2389290
15	H	-2.1264210	4.5620530	-0.0092200
16	H	-3.3173100	3.3562040	0.4841730
17	C	-0.2559220	3.0365170	-1.0824550
18	H	0.3587440	3.0789780	-0.1804630
19	H	0.2454590	2.4254390	-1.8365510
20	H	-0.2965390	4.0561250	-1.4748460
21	C	-5.2536650	-0.8149450	0.3259620
22	C	-5.5290270	-1.3135860	1.7658980
23	H	-5.2391070	-0.5553490	2.4992770
24	H	-6.5984570	-1.5101160	1.8902630
25	H	-4.9847980	-2.2309740	1.9860480
26	C	-6.1150080	0.4414210	0.0939670
27	H	-6.0083710	0.8338000	-0.9212270
28	H	-7.1674570	0.1814740	0.2338830
29	H	-5.8788520	1.2405050	0.8022610
30	C	-5.7004410	-1.8868500	-0.6983060
31	H	-5.1637680	-2.8246220	-0.5611700
32	H	-6.7709260	-2.0835420	-0.5834460
33	H	-5.5306620	-1.5380210	-1.7212070
34	O	-3.1354510	-2.8182150	0.6439780
35	H	-2.3101590	-3.3214350	0.7134350
36	O	-0.6163000	-2.3026900	0.3830250
37	H	0.3277160	-1.9871440	0.2521200
38	C	0.4832800	0.2481890	-0.1464780

39	H	0.8699890	1.2515340	-0.2616210
40	N	1.3221070	-0.7314850	-0.0168410
41	C	2.7041220	-0.4868030	0.0566630
42	C	3.5629410	-1.4033430	-0.5653260
43	C	3.2403810	0.6007250	0.7614320
44	C	4.9333480	-1.1972540	-0.5055310
45	H	3.1498480	-2.2514840	-1.0943320
46	C	4.6191320	0.7670070	0.8024340
47	H	2.5965700	1.2841000	1.2984110
48	C	5.4900530	-0.1154970	0.1728850
49	H	6.5604270	0.0250450	0.2197080
50	Cl	6.0057620	-2.3349400	-1.3049300
51	Cl	5.2876440	2.1268180	1.6925000