Electronic Supplementary Material (ESI) for RSC Advances.

A new efficient domino approach for the synthesis of pyrazolyl-phthalazine-diones. Antiradical activity of novel phenolic products

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Contents

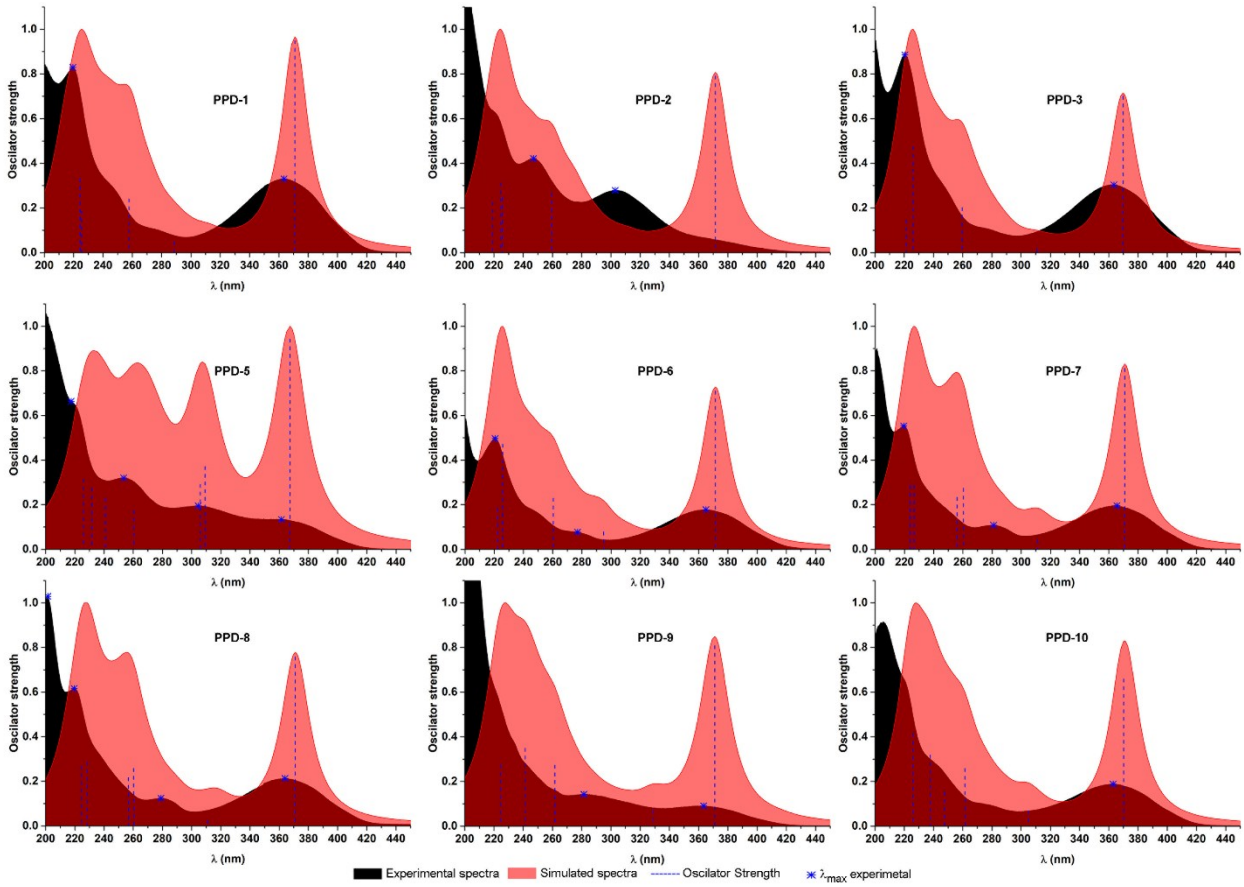


Figure S1. Experimental and simulated UV-Vis spectra of all **PPDs** except **PPD-4**.

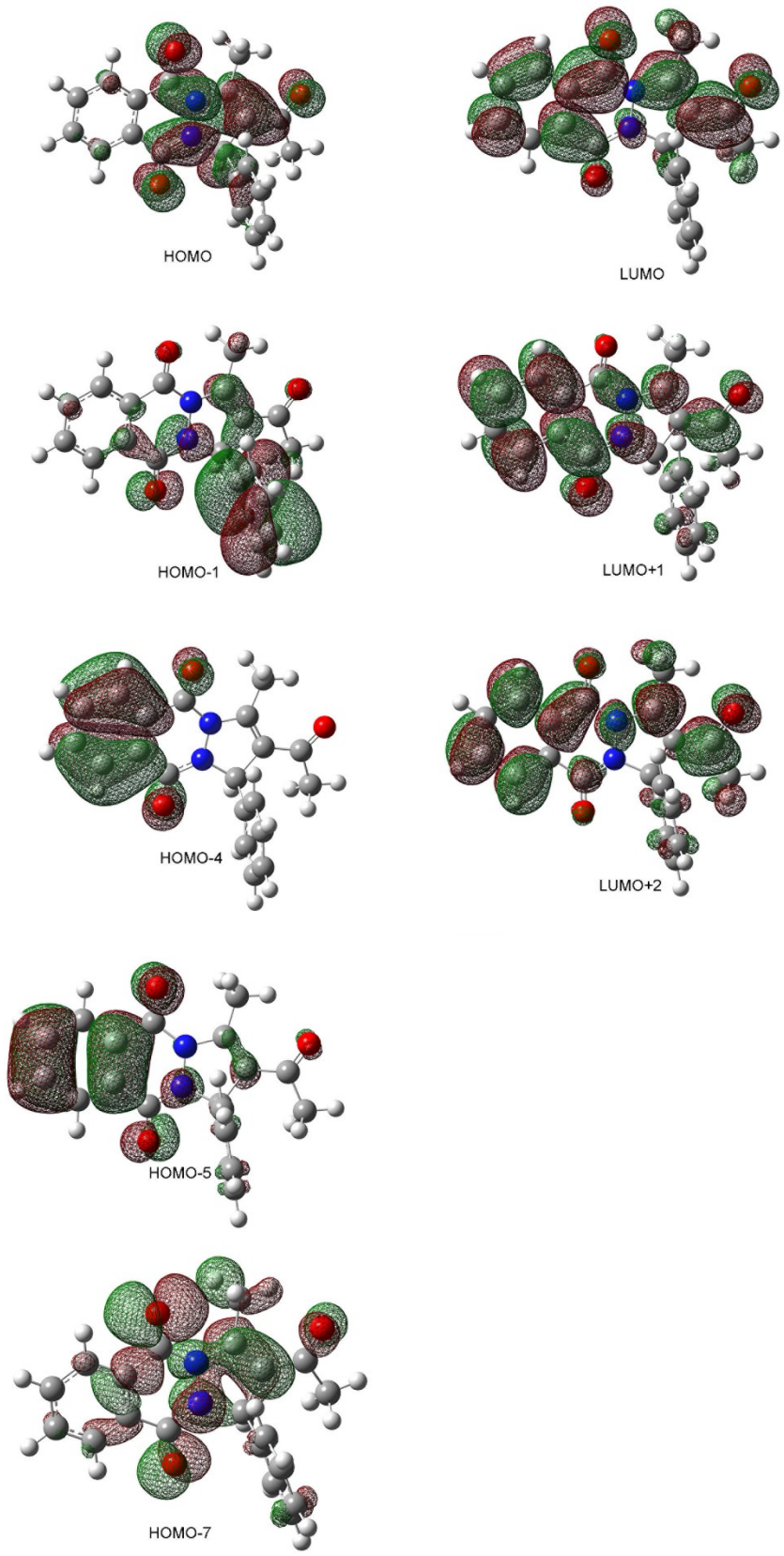


Figure S2. Kohn–Sham orbitals of **PPD-1**.

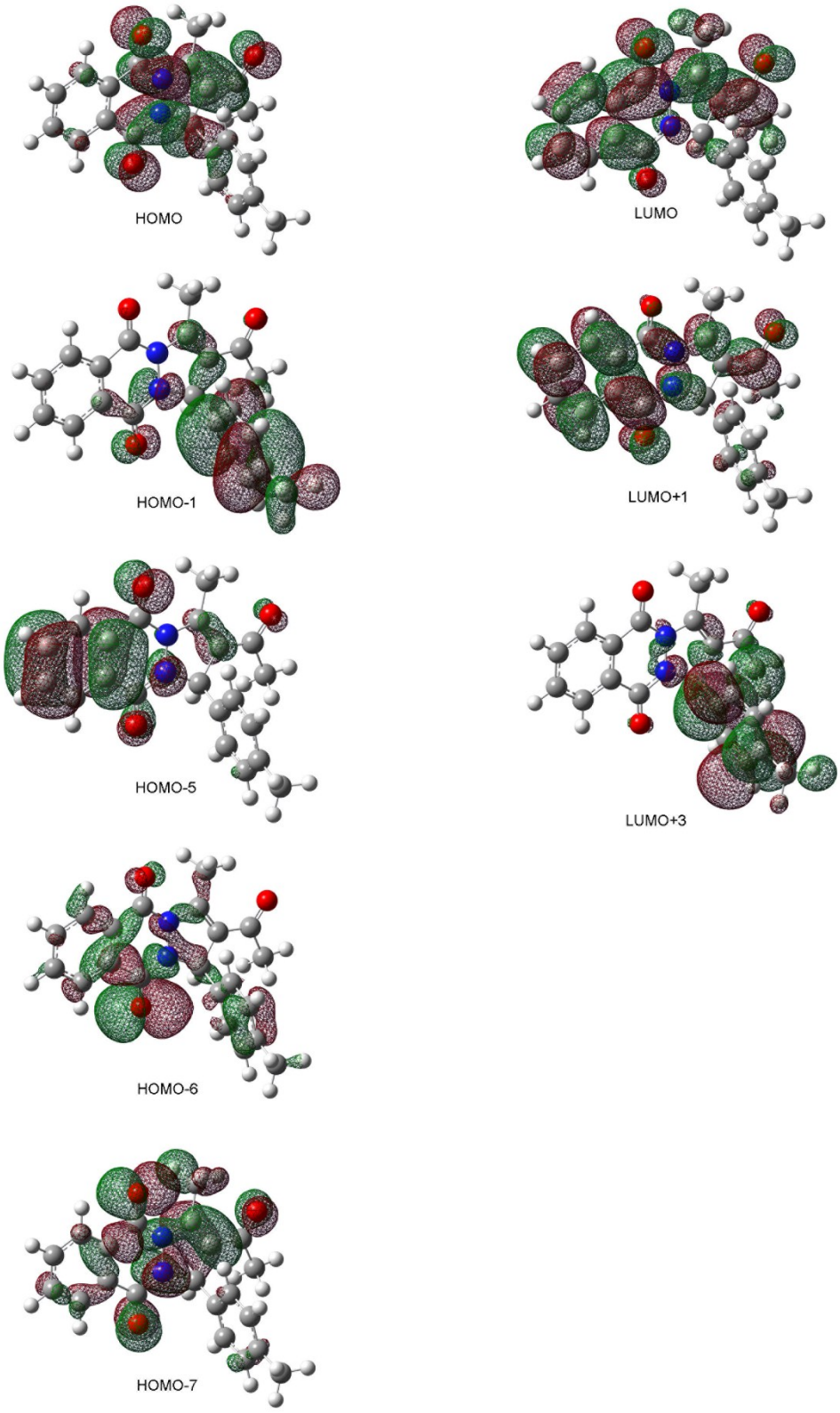


Figure S3. Kohn–Sham orbitals of **PPD-2**.

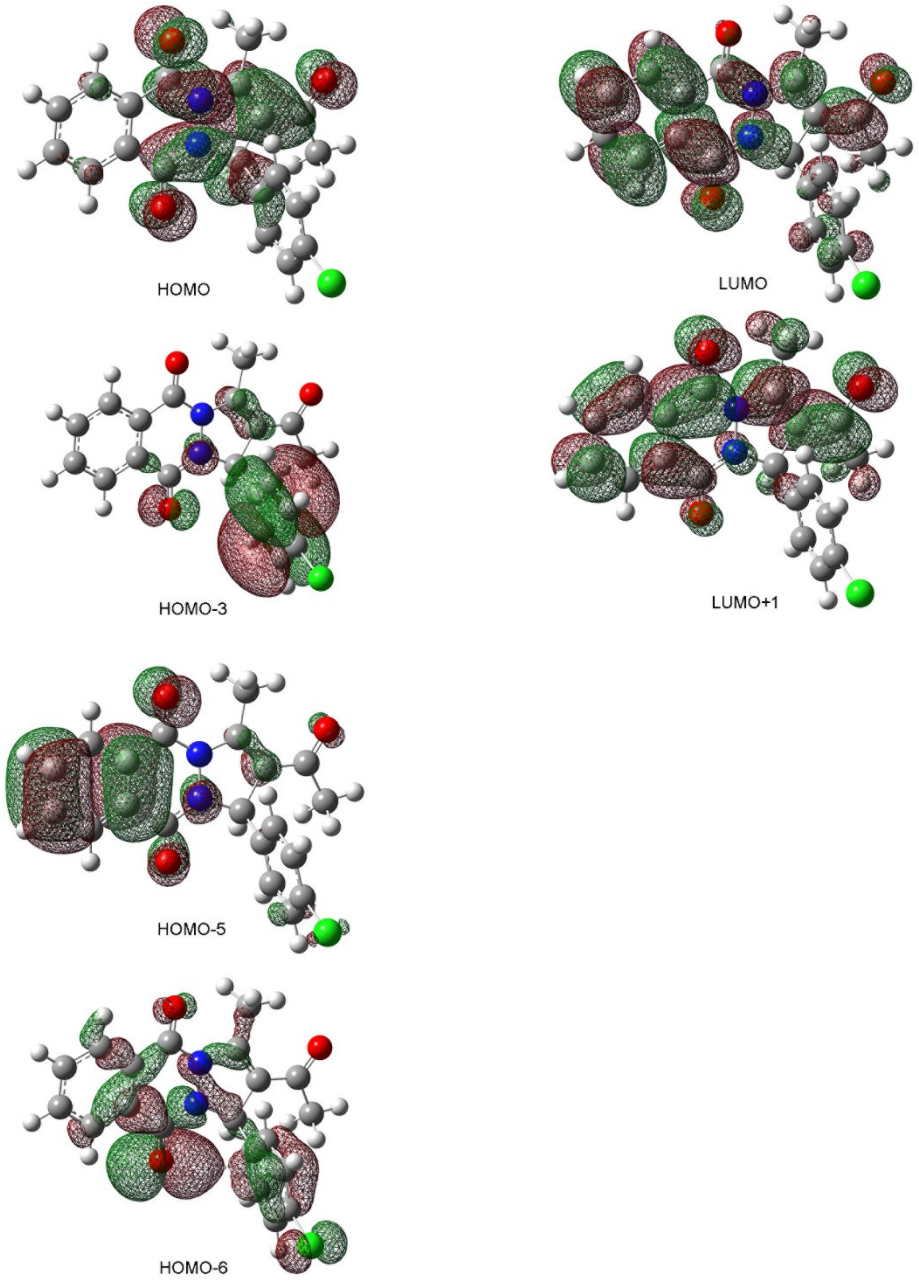


Figure S4. Kohn–Sham orbitals of **PPD-3**.

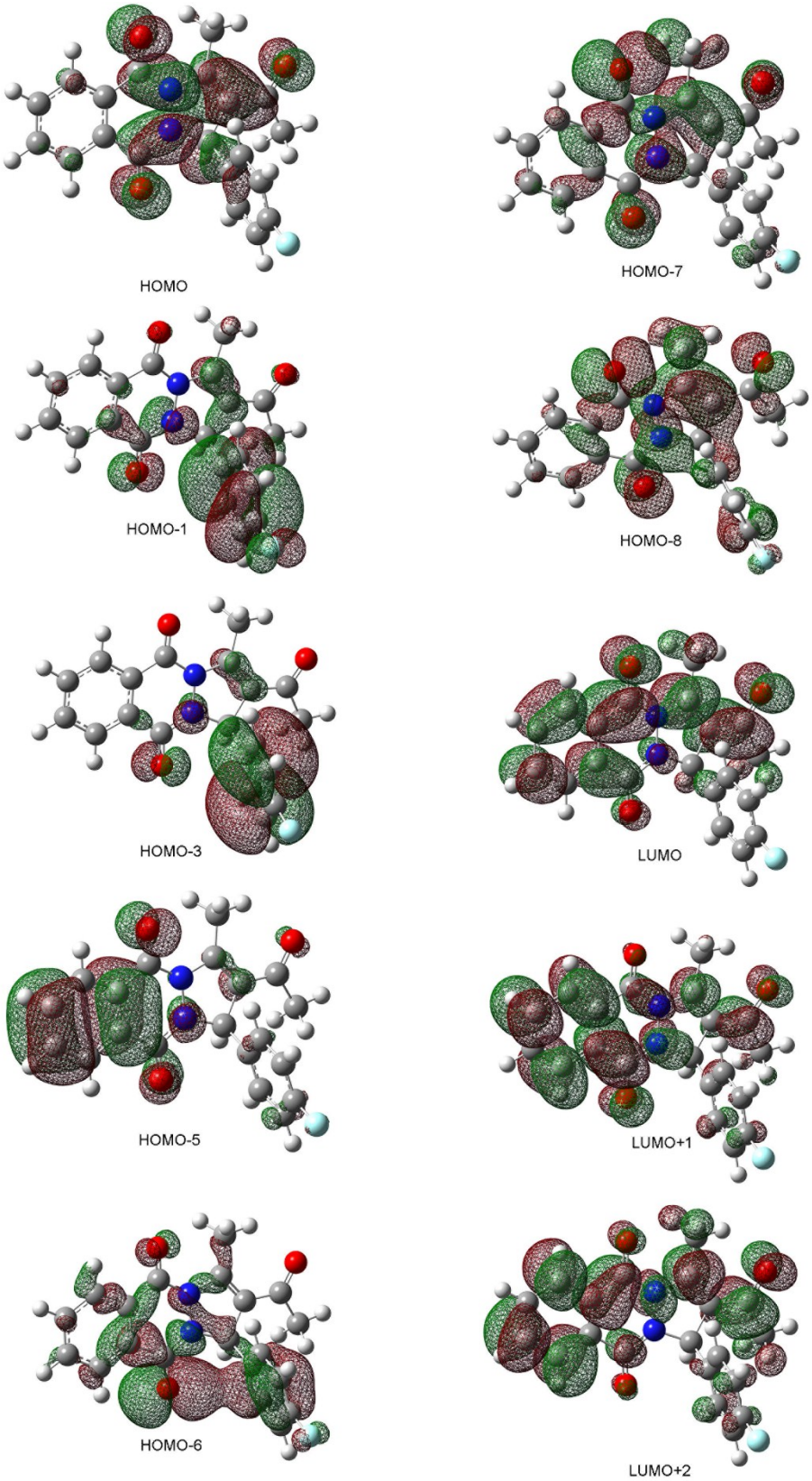


Figure S5. Kohn–Sham orbitals of **PPD-4**.

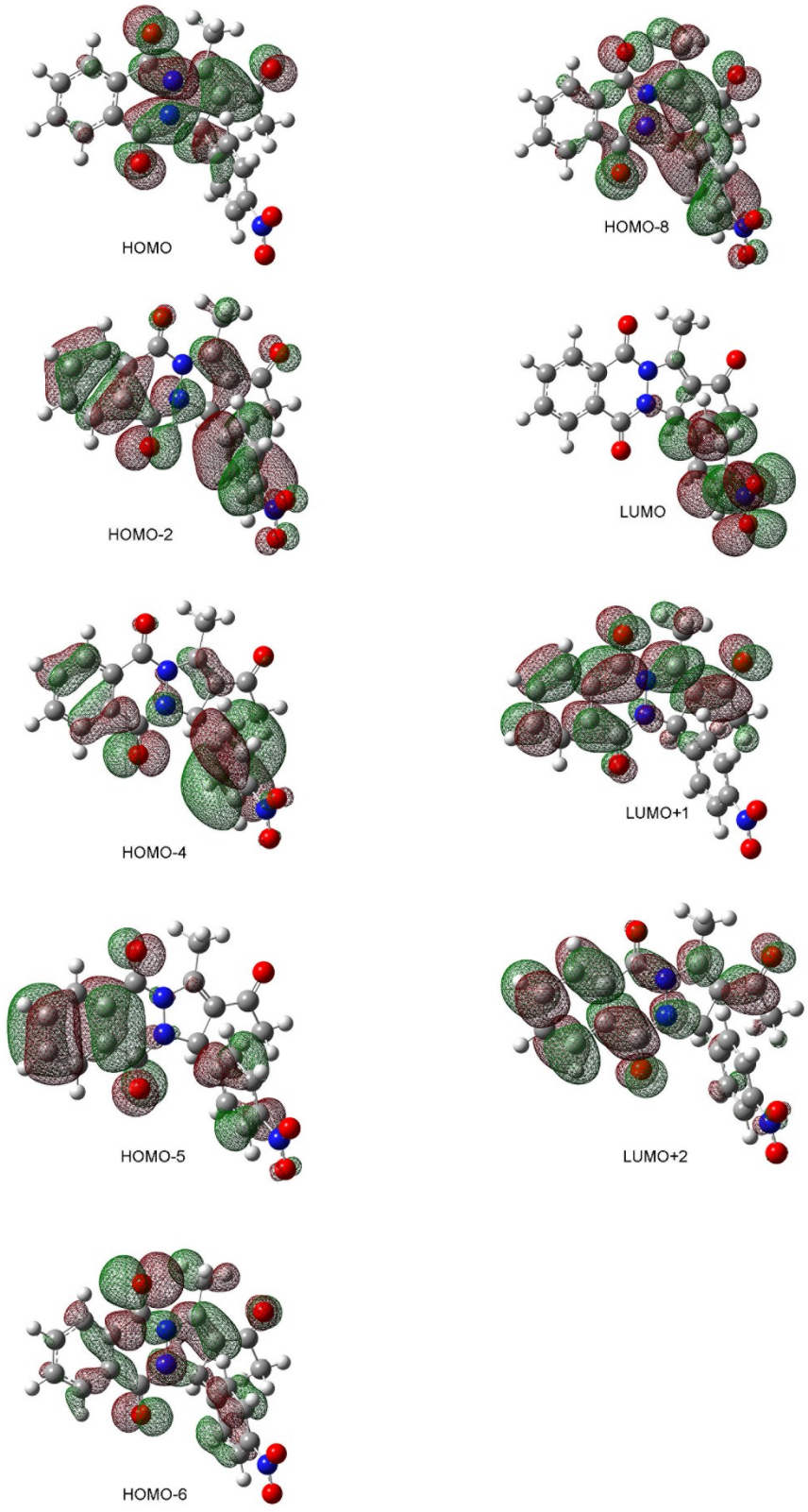


Figure S6. Kohn–Sham orbitals of **PPD-5**.

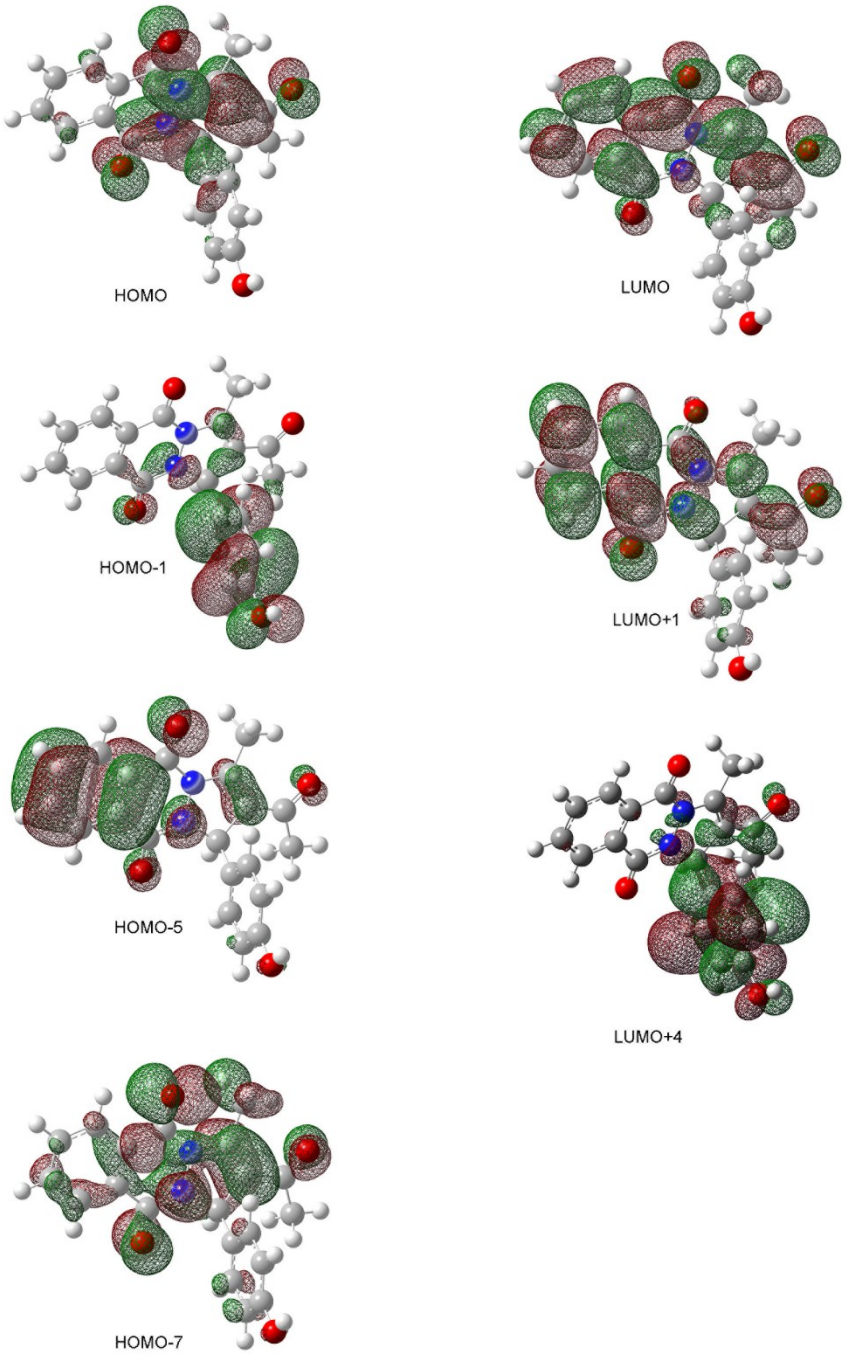


Figure S7. Kohn–Sham orbitals of **PPD-6**.

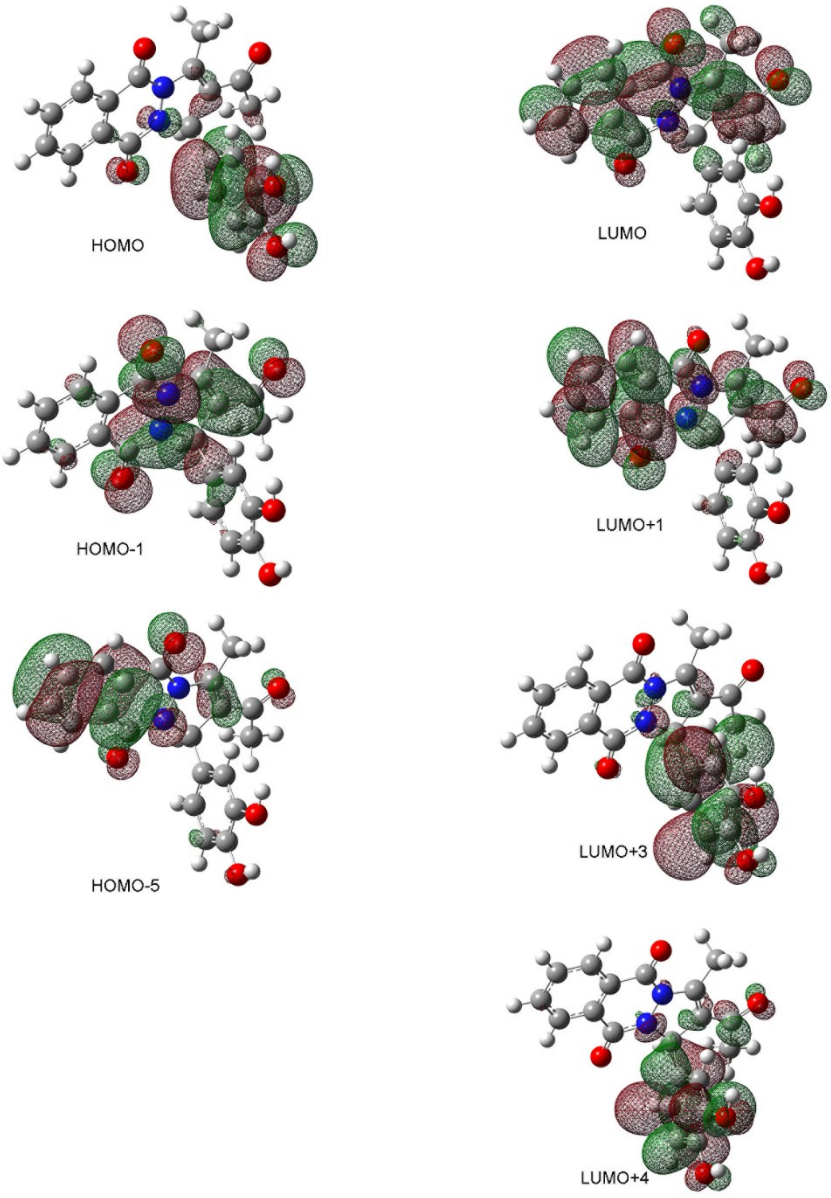


Figure S8. Kohn–Sham orbitals of **PPD-7**.

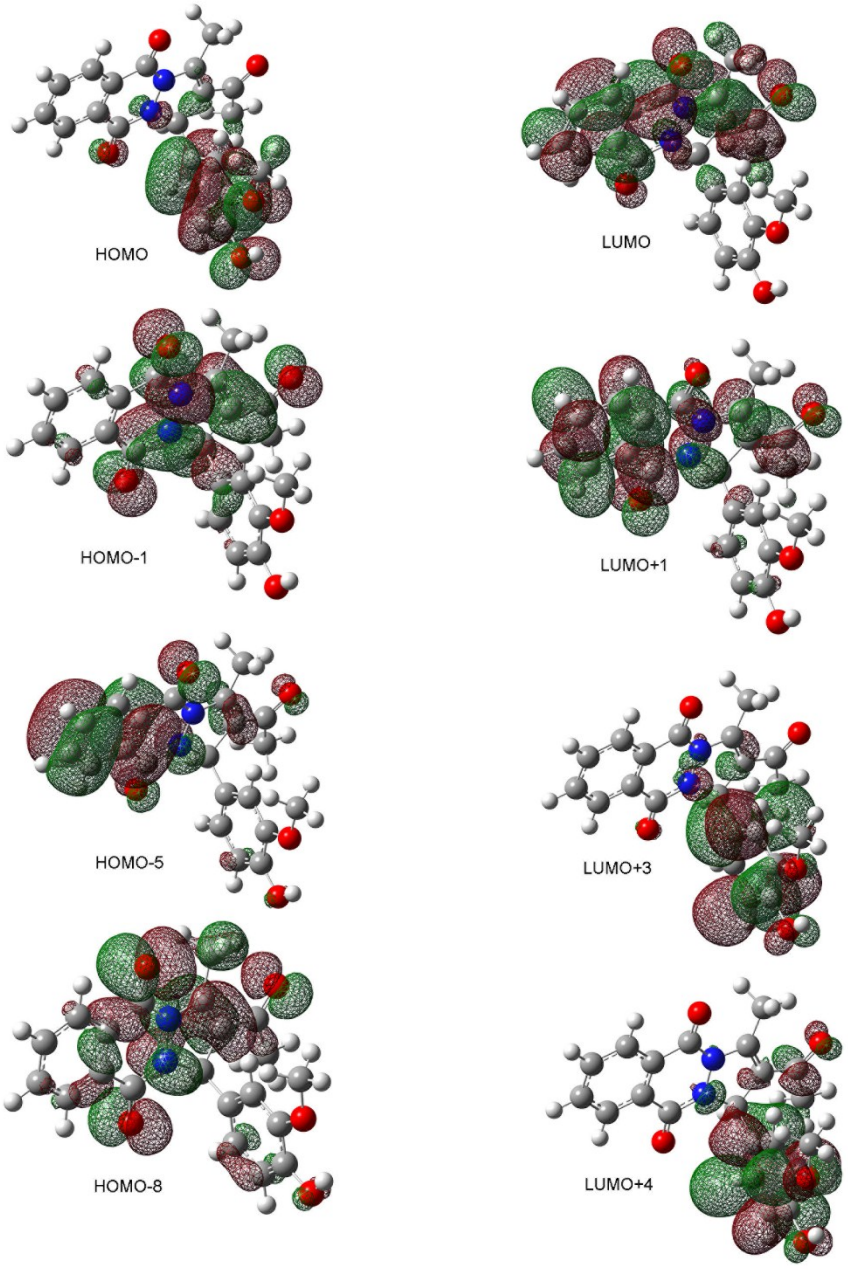


Figure S9. Kohn–Sham orbitals of **PPD-8**.

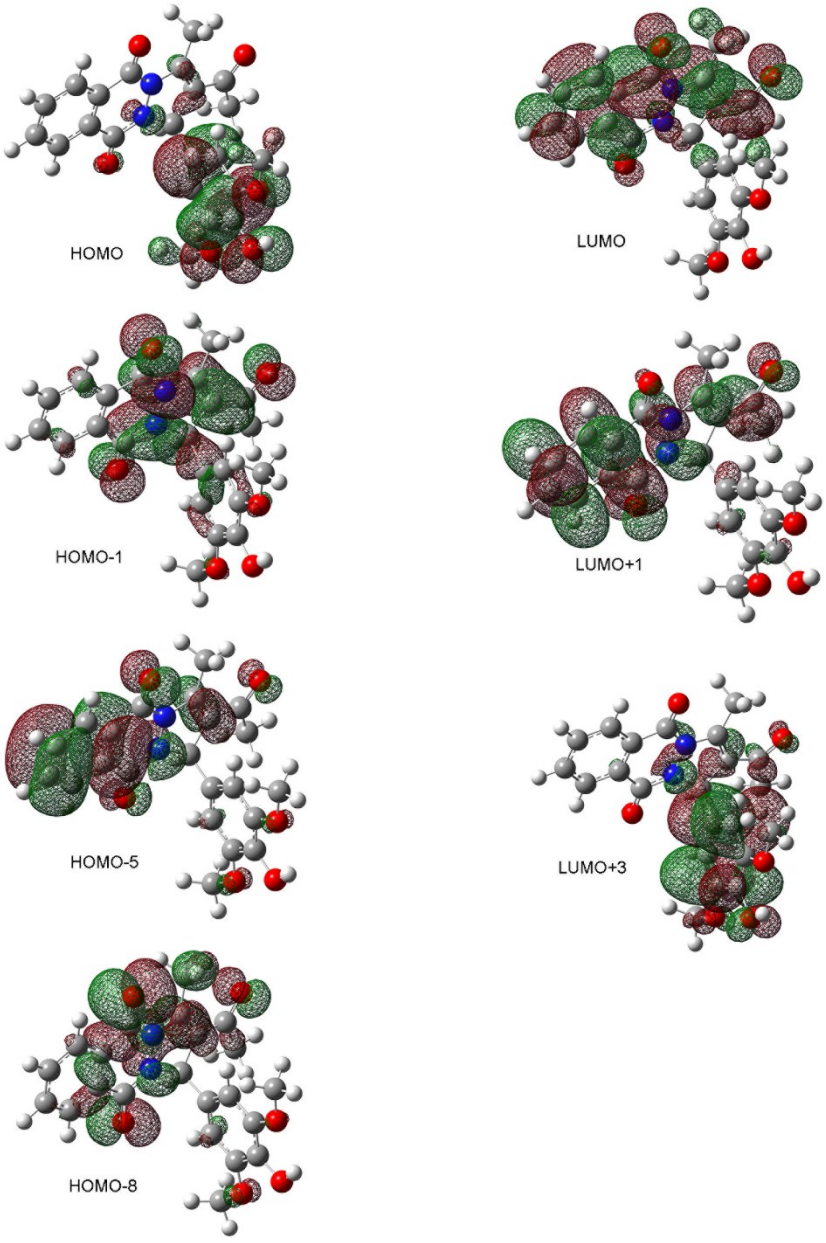


Figure S10. Kohn–Sham orbitals of **PPD-9**.

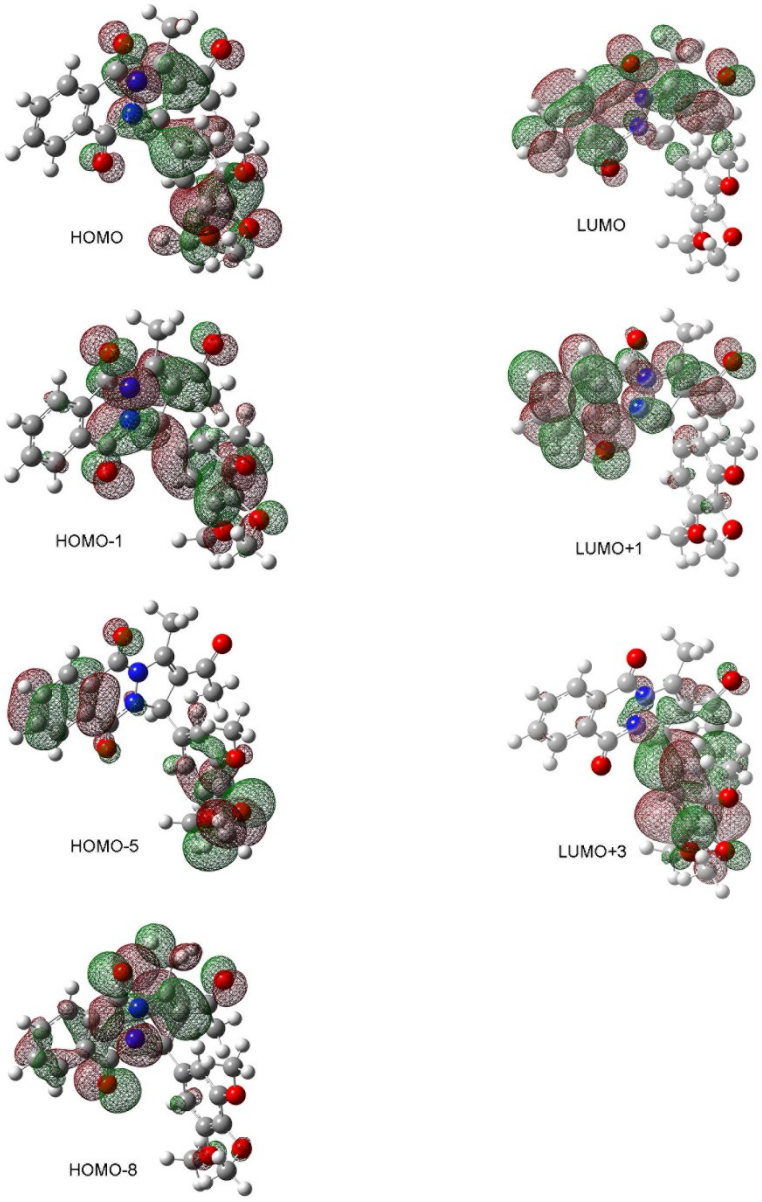


Figure S11. Kohn–Sham orbitals of **PPD-10**.

Table S1. Electron transitions responsible for the appearance of bands in UV-Vis spectra

PPD-1			PPD-2			PPD-3			PPD-4			PPD-5		
λ(nm)	transition		λ(nm)	transition		λ(nm)	transition		λ(nm)	transition		λ(nm)	transition	
370.9	HOMO	LUMO	371.5	HOMO	LUMO	369.7	HOMO	LUMO	370.0	HOMO	LUMO	367.4	HOMO	LUMO+1
288.2	HOMO	LUMO+2	259.7	HOMO-6	LUMO	310.7	HOMO	LUMO+1	310.2	HOMO	LUMO+1	309.1	HOMO-2	LUMO
257.7	HOMO-4	LUMO		HOMO-5	LUMO	259.6	HOMO-6	LUMO	258.8	HOMO-5	LUMO		HOMO	LUMO+2
225.5	HOMO-7	LUMO+1	225.5	HOMO-7	LUMO+1		HOMO-5	LUMO		HOMO-1	LUMO+1	306.0	HOMO	LUMO+2
224.5	HOMO-5	LUMO+1		HOMO-5	LUMO+1	226.1	HOMO-5	LUMO+1	243.9	HOMO-8	LUMO	260.1	HOMO-6	LUMO+1
			224.6	HOMO-5	LUMO+1	221.5	HOMO-3	LUMO+1		HOMO-6	LUMO	240.8	HOMO-8	LUMO+1
			219.2	HOMO-1	LUMO+3					HOMO-6	LUMO+1		HOMO-6	LUMO+1
									225.5	HOMO-7	LUMO+1	231.4	HOMO-4	LUMO+2
										HOMO-5	LUMO+1		HOMO-2	LUMO+2
									224.6	HOMO-8	LUMO+1	225.8	HOMO-5	LUMO+2
										HOMO-7	LUMO+1			
										HOMO-3	LUMO+2			
PPD-6			**PPD-7**			**PPD-8**			**PPD-9**			**PPD-10**		
λ(nm)	transition		λ(nm)	transition		λ(nm)	transition		λ(nm)	transition		λ(nm)	transition	
371.5	HOMO	LUMO	370.8	HOMO-1	LUMO	371.1	HOMO-1	LUMO	371.1	HOMO-1	LUMO	370.2	HOMO-1	LUMO
294.8	HOMO-1	LUMO+1	311.2	HOMO	LUMO+1	310.9	HOMO-1	LUMO +1	328.9	HOMO	LUMO+1	304.6	HOMO	LUMO+1
260.4	HOMO-5	LUMO	260.4	HOMO-5	LUMO	260.3	HOMO-8	LUMO	261.6	HOMO-8	LUMO	261.4	HOMO-8	LUMO
225.8	HOMO-7	LUMO+1	256.0	HOMO	LUMO+3		HOMO-5	LUMO		HOMO-5	LUMO		HOMO-5	LUMO
	HOMO-5	LUMO+1	226.6	HOMO	LUMO+4	256.5	HOMO	LUMO+3	241.4	HOMO	LUMO+3	247.7	HOMO-8	LUMO
222.4	HOMO-1	LUMO+4	224.0	HOMO-5	LUMO+1	228.8	HOMO	LUMO+4	224.5	HOMO-8	LUMO+1	237.9	HOMO	LUMO+3
						224.2	HOMO-5	LUMO +1		HOMO-5	LUMO+1	225.7	HOMO-8	LUMO+1
													HOMO-5	LUMO+1

Table S2. Energies (a.u.) of orbitals of investigated **PPDss**

PPD-1		**PPD-2**		**PPD-3**		**PPD-4**		**PPD-5**	
Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital
-0.05335	LUMO+2	-0.02842	LUMO+3	-0.06709	LUMO+1	-0.05389	LUMO+2	-0.0678	LUMO+2
-0.06618	LUMO+1	-0.06577	LUMO+1	-0.09482	LUMO	-0.06664	LUMO+1	-0.09633	LUMO+1
-0.09395	LUMO	-0.09362	LUMO	-0.2359	HOMO	-0.09459	LUMO	-0.1168	LUMO
-0.23457	HOMO	-0.23405	HOMO	-0.27793	HOMO-3	-0.23557	HOMO	-0.23819	HOMO
-0.28327	HOMO-4	-0.25238	HOMO-1	-0.28801	HOMO-5	-0.26156	HOMO-1	-0.282	HOMO-2
-0.28756	HOMO-5	-0.28714	HOMO-5	-0.29507	HOMO-6	-0.27765	HOMO-3	-0.28684	HOMO-4
-0.29726	HOMO-7	-0.2931	HOMO-6			-0.28793	HOMO-5	-0.2902	HOMO-5
		-0.29653	HOMO-7			-0.29527	HOMO-6	-0.29998	HOMO-6
						-0.29786	HOMO-7	-0.30797	HOMO-8
						-0.30192	HOMO-8		

PPD-6		**PPD-7**		**PPD-8**		**PPD-9**		**PPD-10**	
Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital	Energy (a.u.)	Orbital
-0.0194	LUMO+4	-0.01028	LUMO+4	-0.00995	LUMO+4	-0.0192	LUMO+3	-0.02571	LUMO+3
-0.06554	LUMO+1	-0.02826	LUMO+3	-0.02546	LUMO+3	-0.06557	LUMO+1	-0.06607	LUMO+1
-0.09363	LUMO	-0.06563	LUMO+1	-0.06562	LUMO+1	-0.09364	LUMO	-0.0939	LUMO
-0.23409	HOMO	-0.09382	LUMO	-0.09363	LUMO	-0.22233	HOMO	-0.23389	HOMO
-0.24049	HOMO-1	-0.23144	HOMO	-0.22796	HOMO	-0.23427	HOMO-1	-0.23473	HOMO-1
-0.28692	HOMO-5	-0.23446	HOMO-1	-0.23423	HOMO-1	-0.28639	HOMO-5	-0.28646	HOMO-5
-0.29625	HOMO-7	-0.28704	HOMO-5	-0.28697	HOMO-5	-0.29907	HOMO-8	-0.29623	HOMO-8
				-0.29993	HOMO-8				

Table S3. Interaction of the examined and reference compounds with the stable radical DPPH

Compound	DPPH scavenging ability (%)						IC_{50} (μM)
	50 μM		100 μM		150 μM		
	20 min	60 min	20 min	60 min	20 min	60 min	
PPD-1	3.1±0.6	5.7±0.3	7.7±0.9	10.0±0.3	11.7±1.0	12.8±1.6	–
PPD-2	0.5±1.1	1.5±1.0	1.3±0.7	1.4±1.2	1.3±0.4	1.3±1.1	–
PPD-3	0.3±0.4	2.3±0.3	2.6±0.4	3.3±0.3	3.8±0.4	5.6±0.4	–
PPD-4	5.0±0.5	5.8±0.2	5.6±0.2	8.4±0.5	6.1±0.7	10.1±1.5	–
PPD-5	1.1±0.5	1.9±0.5	1.4±0.7	1.7±1.1	2.4±0.5	2.9±1.2	–
PPD-6	5.7±0.4	9.2±1.3	6.1±0.1	9.7±1.0	7.3±1.7	12.4±2.7	–
PPD-7	98.4±0.4	95.9±0.4	–	–	–	–	4.1±0.2
PPD-8	34.6±0.5	42.7±0.6	36.5±0.6	43.7±0.4	52.1±0.1	54.1±0.5	135.6±0.9
PPD-9	62.4±0.5	75.7±1.5	79.6±2.1	89.7±2.1	–	–	14.6±2.4
PPD-10	4.8±0.5	4.2±0.9	5.8±1.1	5.2±3.0	7.7±0.8	7.0±2.3	–
NDGA	–	–	–	–	–	–	1.80±0.01

Results represent mean values ± standard deviation (SD) of three independent measurements.

Table S4. Calculated thermodynamical parameters (kJ mol^{-1}) of antioxidant mechanisms for **PPDs-7-9** and reaction enthalpies (kJ mol^{-1}) for the reactions of these compounds with the selected radicals in water.

	HAT	SET-PT		SPLET		HAT	SET-PT		SPLET		HAT	SET-PT		SPLET	
			PPD-7					**PPD-8**					**PPD-9**		
	thermodynamical parameters (kJ mol^{-1})														
	BDE	IP	PDE	PA	ETE	BDE	IP	PDE	PA	ETE	BDE	IP	PDE	PA	ETE
	331	450	31	139	341	338	443	44	155	333	319	430	38	155	313
	330		30	138	341										
	reaction enthalpies (kJ mol^{-1})														
Radical	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$^{\bullet}OCH_3$	-97	88	-185	-77	-21	-91	82	-172	-61	-29	-110	69	-178	-61	-49
	-99		-186	-78	-21										
$^{\bullet}OC(CH_3)_3$	-107	88	-195	-86	-20	-100	82	-182	-71	-29	-119	69	-188	-70	-49
	-108		-196	-87	-20										
$^{\bullet}OH$	-168	8	-175	-67	-101	-161	1	-162	-51	-110	-180	-12	-168	-51	-129
	-169		-176	-68	-101										
$^{\bullet}OOH$	-30	108	-138	-30	0	-23	102	-125	-15	-9	-42	89	-132	-14	-29
	-31		-140	-31	0										
$^{\bullet}OOCH_3$	-23	118	-141	-32	9	-16	111	-128	-17	1	-35	98	-134	-16	-19
	-24		-142	-33	9										
$^{\bullet}OO\text{-}CH{=}CH_2$	-22	96	-119	-10	-12	-15	90	-106	5	-21	-35	77	-112	6	-41
	-23		-120	-11	-12										
DPPH	7	90	-84	25	-18	13	84	-71	40	-27	-6	71	-77	41	-46
	5		-85	24	-18										
$O_2^{\bullet-}$	41	263	-222	41	0	48	257	-209	56	-9	29	244	-215	57	-29
	40		-223	40	0										

Table S5. Calculated thermodynamical parameters (kJ mol^{-1}) of antioxidant mechanisms for **PPDs-7-9** and reaction enthalpies (kJ mol^{-1}) for the reactions of these compounds with the selected radicals in benzene.

	HAT	SET-PT		SPLET		HAT	SET-PT		SPLET		HAT	SET-PT		SPLET	
			PPD-7					**PPD-8**					**PPD-9**		
	thermodynamical parameters (kJ mol^{-1})														
	BDE	IP	PDE	PA	ETE	BDE	IP	PDE	PA	ETE	BDE	IP	PDE	PA	ETE
	317	608	98	381	326	342	601	130	426	305	328	590	127	435	282
	316		96	378	327										
	reaction enthalpies (kJ mol^{-1})														
Radical	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}	ΔH_{BDE}	ΔH_{IP}	ΔH_{PDE}	ΔH_{PA}	ΔH_{ETE}
$^{\bullet}OCH_3$	-99	340	-439	-156	57	-74	333	-407	-110	37	-88	321	-410	-102	14
	-100		-441	-159	59										
$^{\bullet}OC(CH_3)_3$	-108	328	-436	-154	46	-83	321	-404	-108	25	-97	309	-407	-100	2
	-110		-438	-156	47										
$^{\bullet}OH$	-31	377	-408	-125	94	-6	369	-375	-79	73	-21	358	-378	-71	51
	-33		-409	-128	95										
$^{\bullet}OOH$	-168	292	-460	-177	9	-143	285	-428	-131	-11	-157	273	-431	-123	-34
	-169		-462	-180	11										
$^{\bullet}OOCH_3$	-23	380	-402	-119	97	3	372	-370	-74	76	-12	361	-373	-65	54
	-24		-404	-122	98										
$^{\bullet}OO\text{-}CH{=}CH_2$	-24	332	-356	-73	50	1	325	-324	-27	29	-13	313	-327	-19	6
	-25		-358	-76	51										
DPPH	-3	233	-236	46	-50	22	226	-204	92	-71	7	214	-207	100	-93
	-5		-238	44	-49										
$O_2^{\bullet-}$	65	863	-798	-29	94	90	856	-766	17	73	76	844	-769	25	51
	64		-800	-32	94										

Table S6. Crystallographic data and structure refinement for **PPD-4**

Empirical formula	$C_{40}\ H_{30}\ F_2\ N_4\ O_6$
Formula weight	700.68
Color, crystal shape	Yellow, needle
Crystal size (mm^3)	0.12 x 0.25 x 0.47
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	*Pbca*
Unit cell dimensions	
a (Å)	22.7947(13)
b (Å)	7.8451(4)
c (Å)	37.255(2)
V ($Å^3$)	6662.3(6)
Z	8
Z'	16
D_{calc} (Mg/m^3)	1.397
μ (mm^{-1})	0.103
F(000)	2912
ϑ range for data collection (°)	2.80-29.17
Reflections collected	28282
Independent reflections, R_{int}	7874, 0.0471
Completeness to ϑ = 26.00°	99.9 %
Data / restraints / parameters	7874 / 0 / 473
Goodness-of-fit	1.030
Final R_1/wR_2 indices [$I > 2\sigma(I)$]	0.0615, 0.1176
Final R_1/wR_2 indices (all data)	0.1427, 0.1465
Largest diff. peak and hole (e $Å^{-3}$)	0.345, −0.181

Spectral characterization of compounds PPD-1-3 and PPD-5

2-Acetyl-3-methyl-1-phenyl-1H-pyrazolo[1,2-b]phthalazine-5,10-dione (PPD-1)

Yellow crystals – Mp 285-287 °C (ref. 288-290 °C;[1] ^{1}H NMR (200 MHz, $CDCl_3$) δ: 2.09 (s, 3H), 3.08 (d, *J* = 1.4 Hz, 3H), 6.50 (q, *J* = 1.4, 1H), 7.43-7.30 (m, 3H), 7.48 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.84-7.79 (m, 2H), 8.22-8.26 (m, 1H), 8.36-8.32 (m, 1H); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 14.5, 30.6, 66.1, 119.0, 127.3, 128.0, 128.3, 128.9, 129.1, 129.6, 133.4, 134.1, 136.5, 146.2, 154.2, 156.3, 193.3; IR (cm^{-1}): 3370, 2922, 2851, 1647, 1602, 1516, 1419, 1354, 1318, 1290, 1275, 1105, 961, 697; $C_{20}H_{16}N_2O_3$ (FW = 332.36): C, 72.28; N, 8.43; H, 4.85%; found: C, 72.01; N, 8.46; H, 4.87%.

2-Acetyl-3-methyl-1-(p-tolyl)-1H-pyrazolo[1,2-b]phthalazine-5,10-dione (PPD-2)

Yellow powder – Mp 169-171 °C; ^{1}H NMR (200 MHz, $CDCl_3$) δ: 2.08 (s, 3H), 2.31 (s, 3H), 3.07 (d, *J* = 1.5 Hz, 3H), 6.46 (q, *J* = 1.4, 1H), 7.15 (s, 1H), 7.18 (s, 1H), 7.39-7.31 (m, 2H), 7.82-7.77 (m, 2H), 8.26-8.17 (m, 1H), 8.37-8.28 (m, 1H); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 14.4, 21.2, 30.6, 65.9, 118.9, 127.3, 128.2, 128.9, 129.5, 133.3, 134.0, 139.0, 146.0, 154.1, 156.2, 193.5; IR (cm^{-1}): 3315, 2922, 1663, 1618, 1466, 1408, 1351, 1317, 1114, 1012, 831, 699, 559, 526; $C_{21}H_{18}N_2O_3$ (FW = 346.39): C, 72.82; N, 8.09; H, 5.24%; found: C, 72.53; N, 8.11; H, 5.22%;

2-Acetyl-1-(4-chlorophenyl)-3-methyl-1H-pyrazolo[1,2-b]phthalazine-5,10-dione (PPD-3)

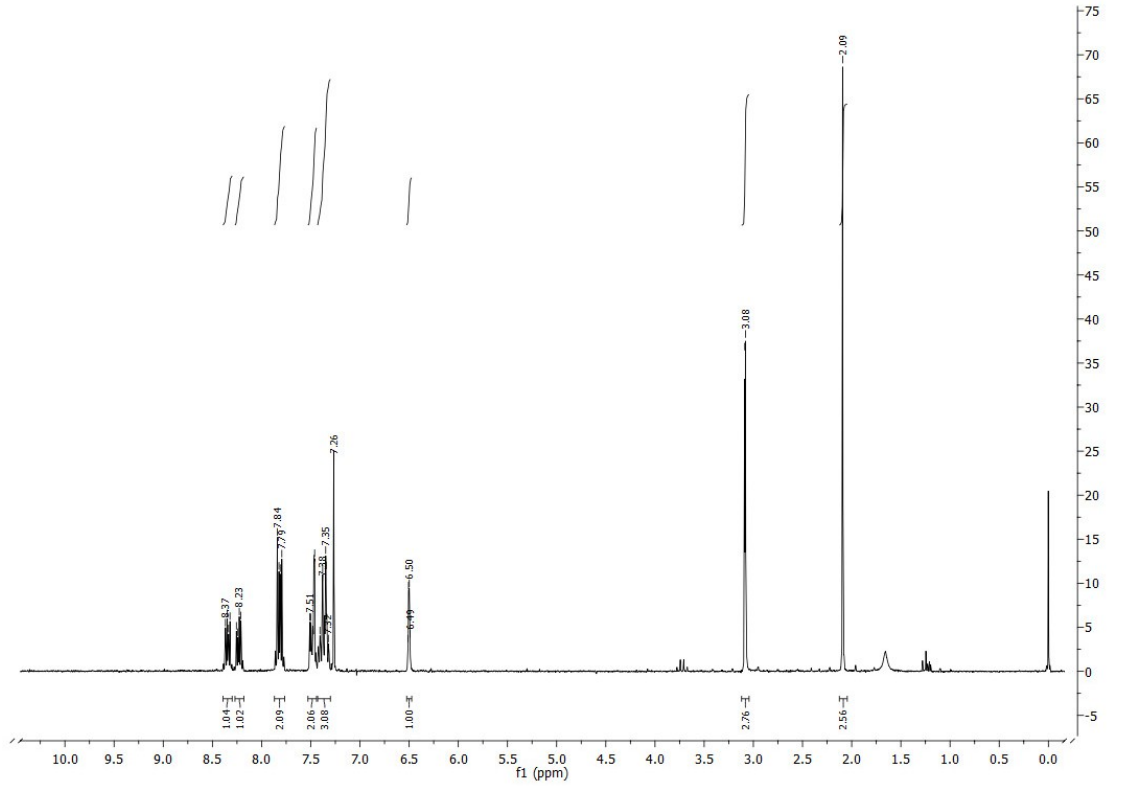
Yellow powder – Mp 173-174 °C (ref. 178-180 °C;[1] ^{1}H NMR (200 MHz, $CDCl_3$) δ: 2.13 (s, 3H), 3.07 (d, *J* = 1.5 Hz, 3H), 6.47 (q, *J* = 1.4, 1H), 7.37-7.31 (m, 2H), 7.47-7.38 (m, 2H), 7.89-7.76 (m, 2H), 8.26-8.21 (m, 1H), 8.36-8.32 (m, 1H); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 14.6, 30.6, 65.5, 118.9, 127.4, 128.1, 128.8, 129.1, 129.6, 133.5, 134.3, 135.1, 146.3, 154.3, 156.3, 192.9; IR (cm^{-1}): 3448, 2922, 2191, 1687, 1653, 1604, 1414, 1359, 1320, 1273, 1110, 821, 697, 614; $C_{20}H_{15}ClN_2O_3$ (FW = 366.08): C, 65.49; N, 7.64; H, 4.12%; found: C, 65.55; N, 7.67; H, 4.14%;

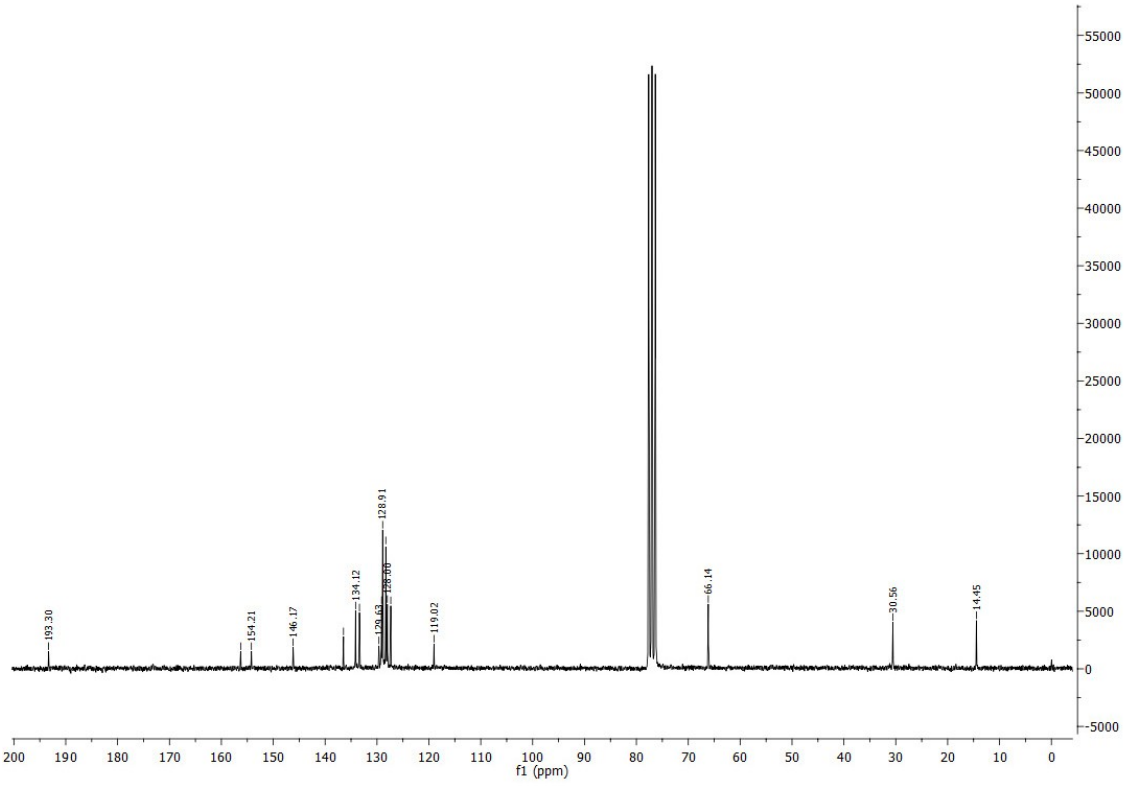
2-Acetyl-3-methyl-1-(4-nitrophenyl)-1H-pyrazolo[1,2-b]phthalazine-5,10-dione (PPD-5)

Yellow powder – Mp 211-214 °C (ref. 215-217 °C;[1] ^{1}H NMR (200 MHz, $CDCl_3$) δ: 2.24 (s, 3H), 3.11 (d, *J* = 0.5 Hz, 3H), 6.59-6.54 (m, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.92-7.81 (m, 2H), 8.28-8.16 (m, 3H), 8.39-8.36 (m, 1H); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 14.8, 30.6, 65.3, 119.3, 124.0, 127.4, 128.2, 128.4, 129.0, 129.5, 133.8, 134.5, 143.7, 146.3, 148.1, 154.3, 156.3, 192.1;IR (cm^{-1}): 3436, 3075, 2922, 2850, 1689, 1648, 1603, 1516, 1470, 1414, 1355, 1321, 1292, 1108, 1015, 959, 876, 820, 694, 594; $C_{20}H_{15}N_3O_5$ (FW = 377.36): C, 63.66; N, 11.14; H, 4.01%; found: C, 63.43; N, 11.16; H, 4.03%;

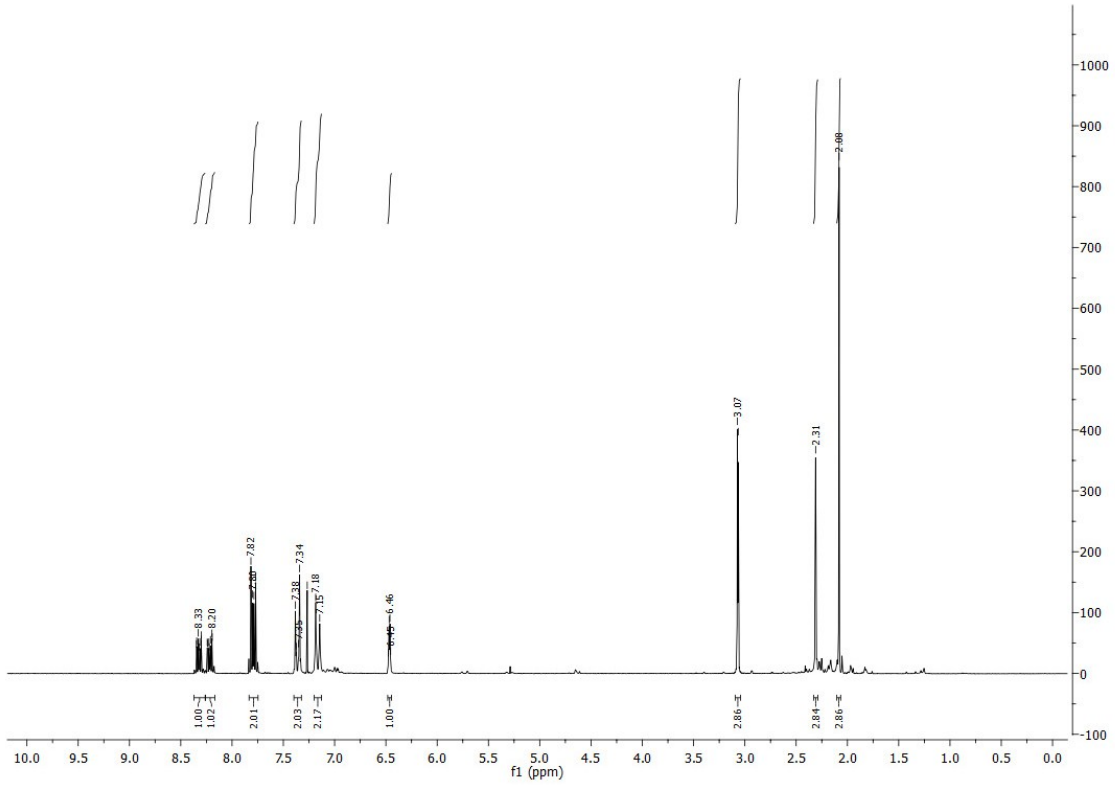
^{1}H and ^{13}C NMR spectra of **PPD-1-10**

PPD-1





PPD-2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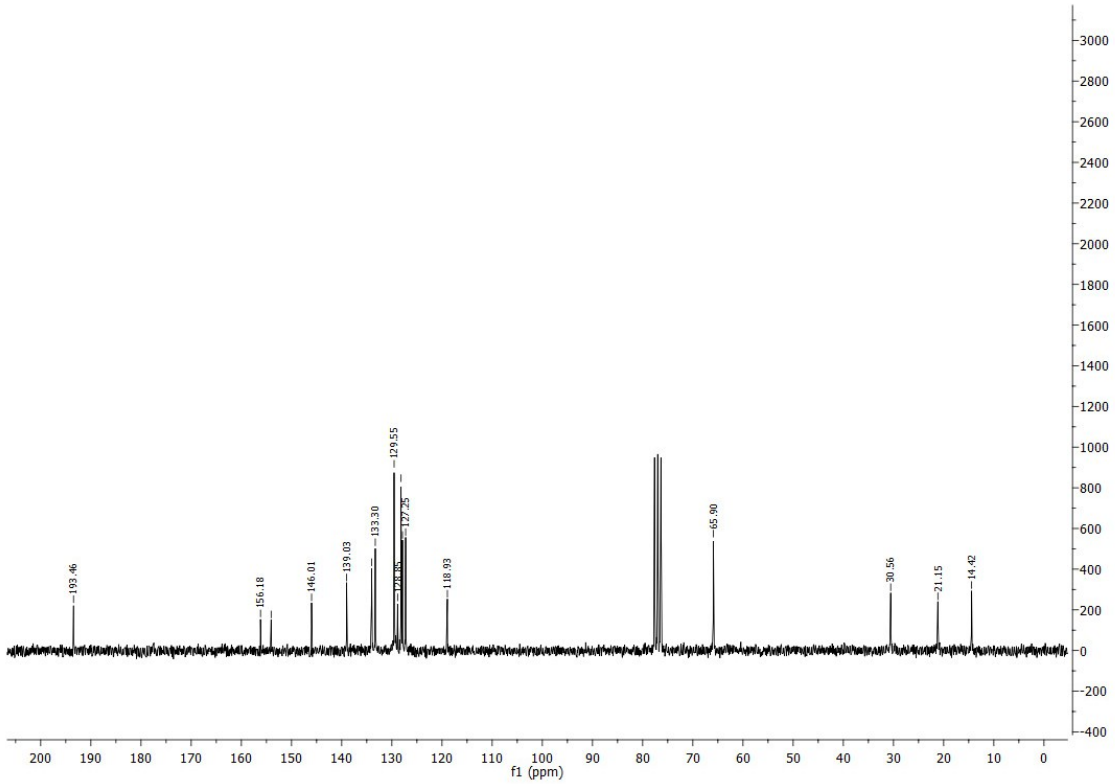
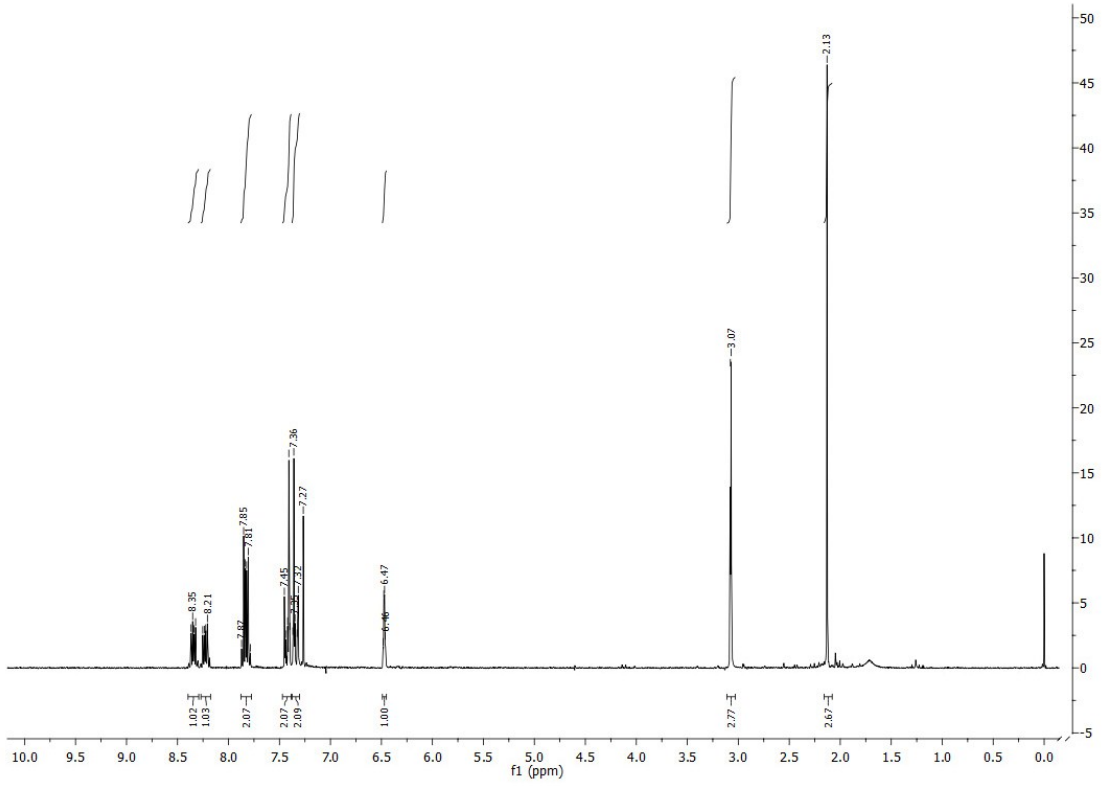
8.20
7.82
7.34
7.18
6.46
3.07
2.31
2.00
1.00
1.02
2.01
2.03
2.17
1.00
2.86
2.84
2.86
f1 (ppm)


193.46
156.18
146.01
139.03
133.30
129.55
127.25
118.93
65.90
30.56
21.15
14.42
f1 (ppm)

PPD-3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8.21
7.87
7.85
7.81
7.45
7.36
7.32
7.27
6.47
6.46
3.07
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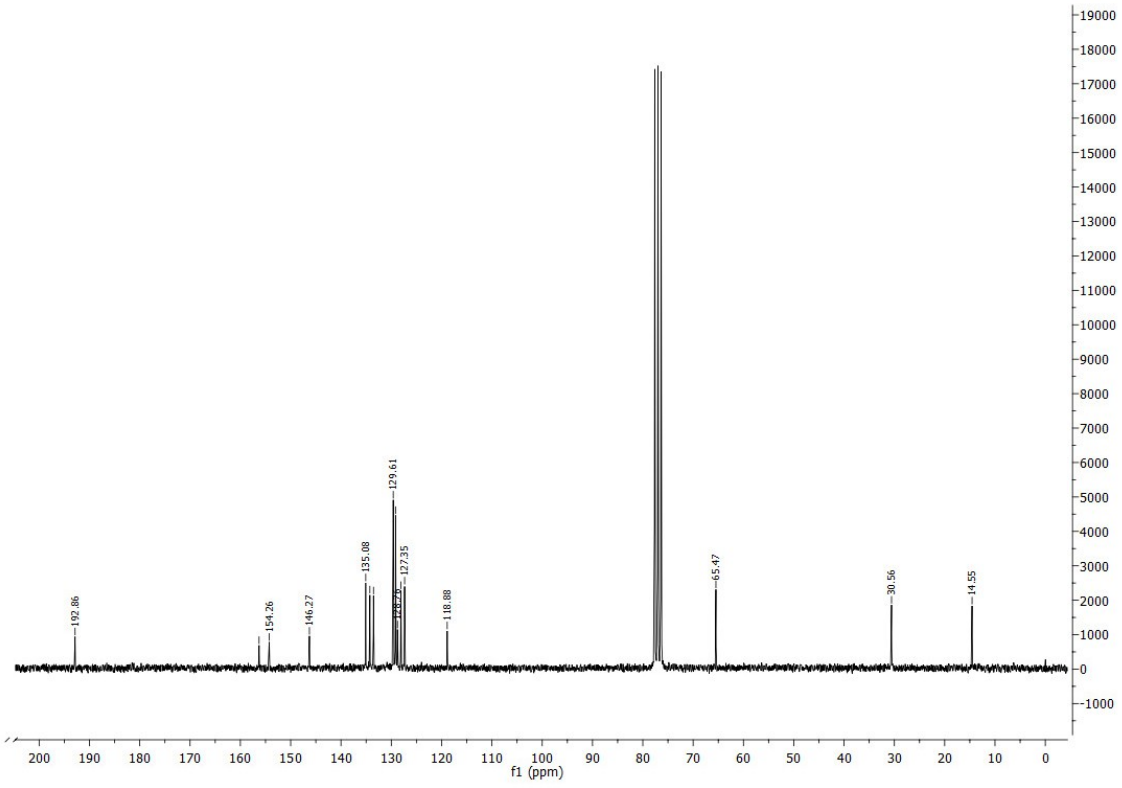
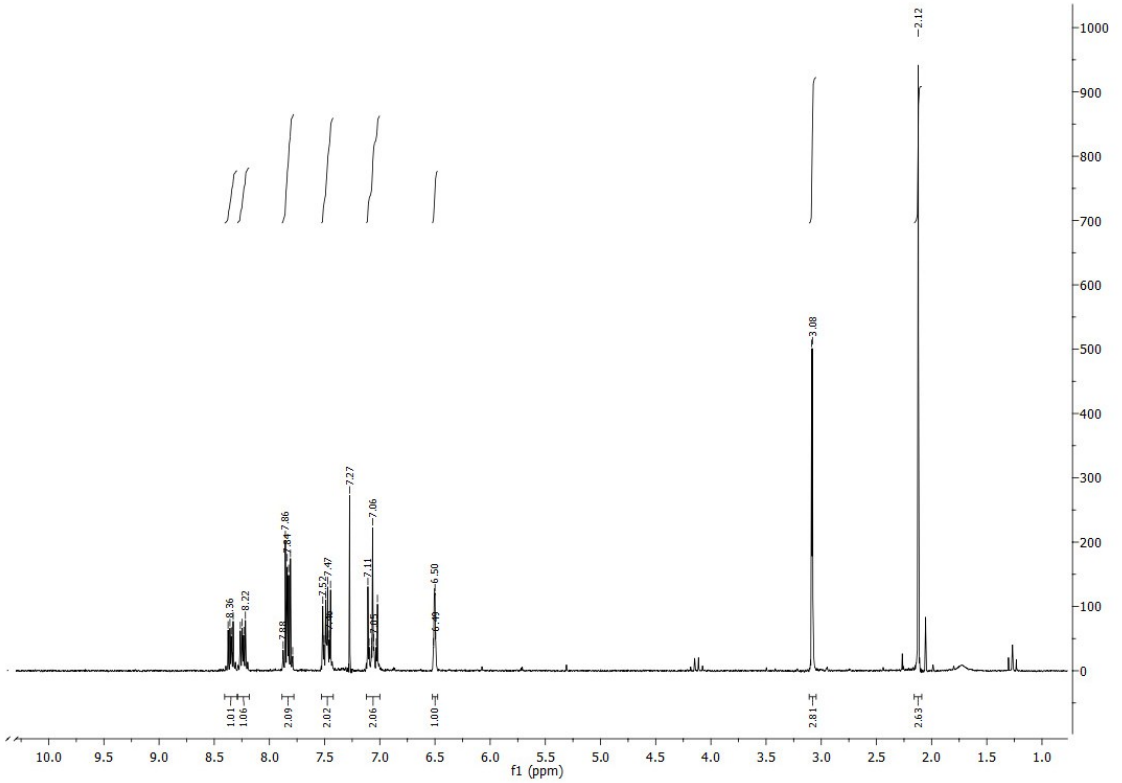
2.07
2.09
1.00
2.77
2.67
f1 (ppm)


192.86
154.26
146.27
135.08
129.61
127.35
118.88
65.47
30.56
14.55
f1 (ppm)

PPD-4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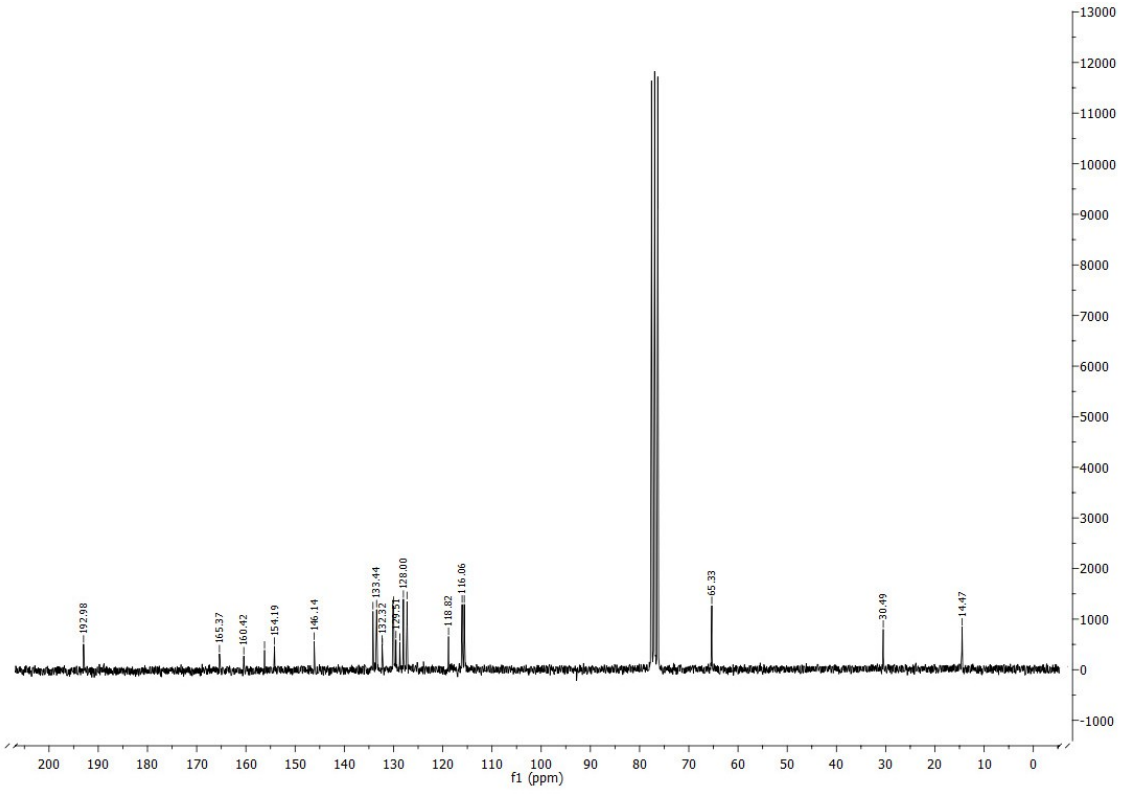
8.22
7.86
7.52
7.47
7.27
7.06
6.50
3.08
2.12
1.01
1.06
2.09
2.02
2.06
1.00
2.81
2.63
f1 (ppm)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160.42
154.19
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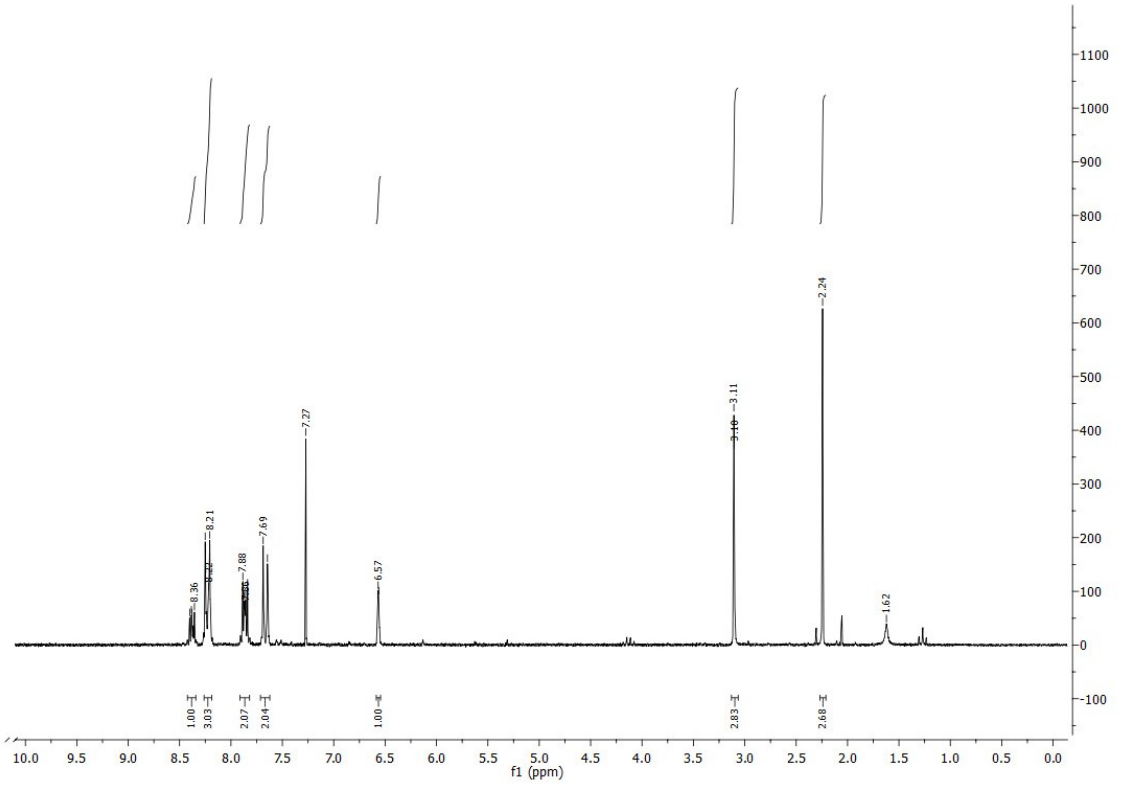
133.44
132.32
129.51
128.00
118.82
116.06
65.33
30.49
14.47
f1 (ppm)

PPD-5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7.27
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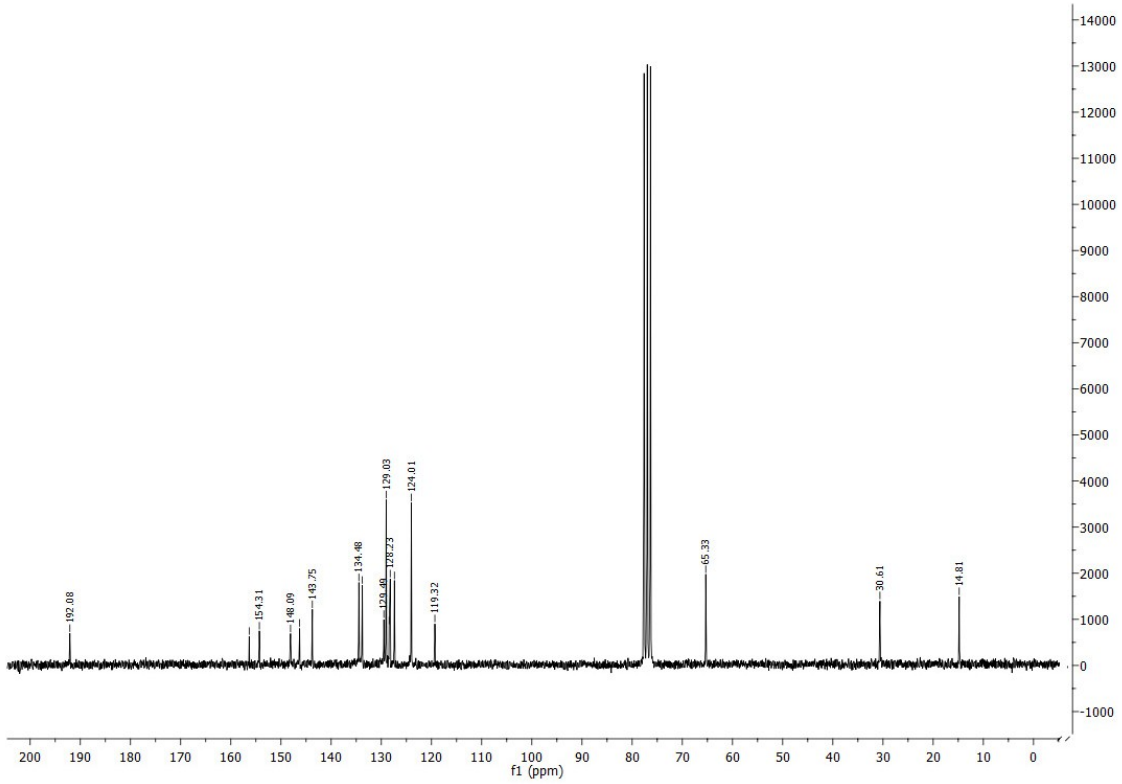
3.03
2.07
2.04
1.00
2.83
2.68
f1 (ppm)


192.08
154.31
148.09
143.75
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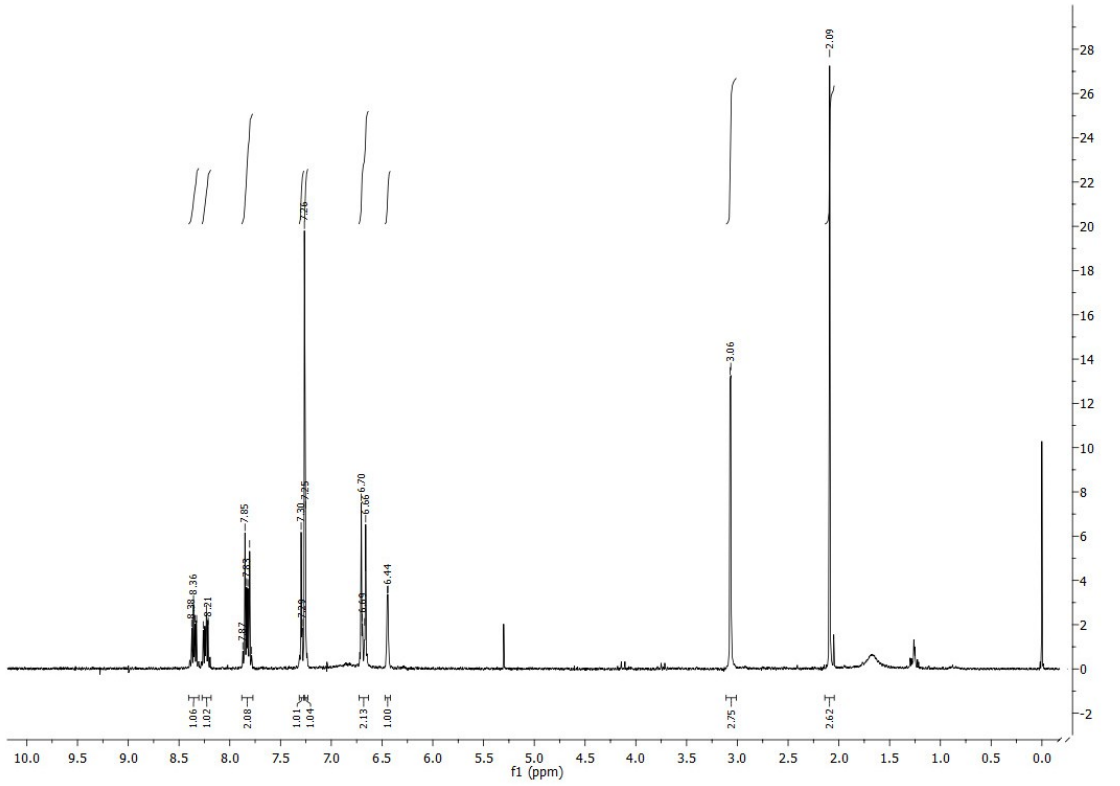
129.00
124.01
119.32
65.33
30.61
14.81
f1 (ppm)

PPD-6


8.38
8.36
8.21
7.85
7.26
6.70
6.44
3.06
2.09
1.06
1.02
2.08
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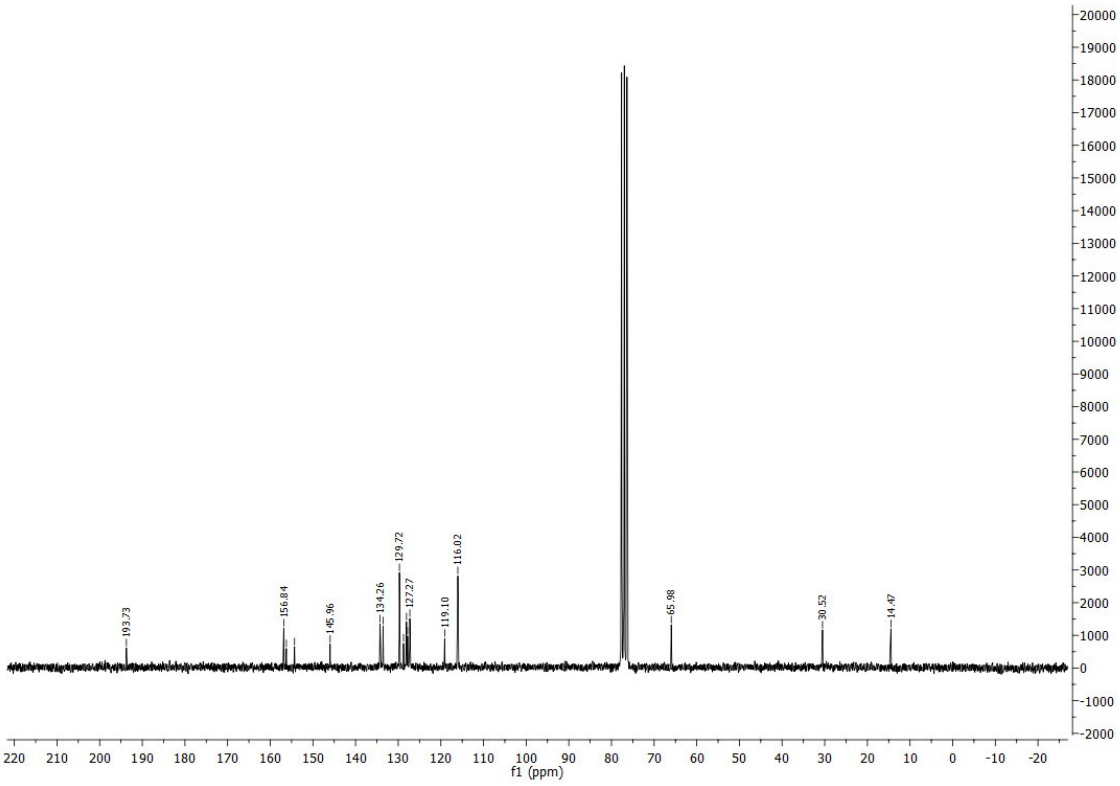
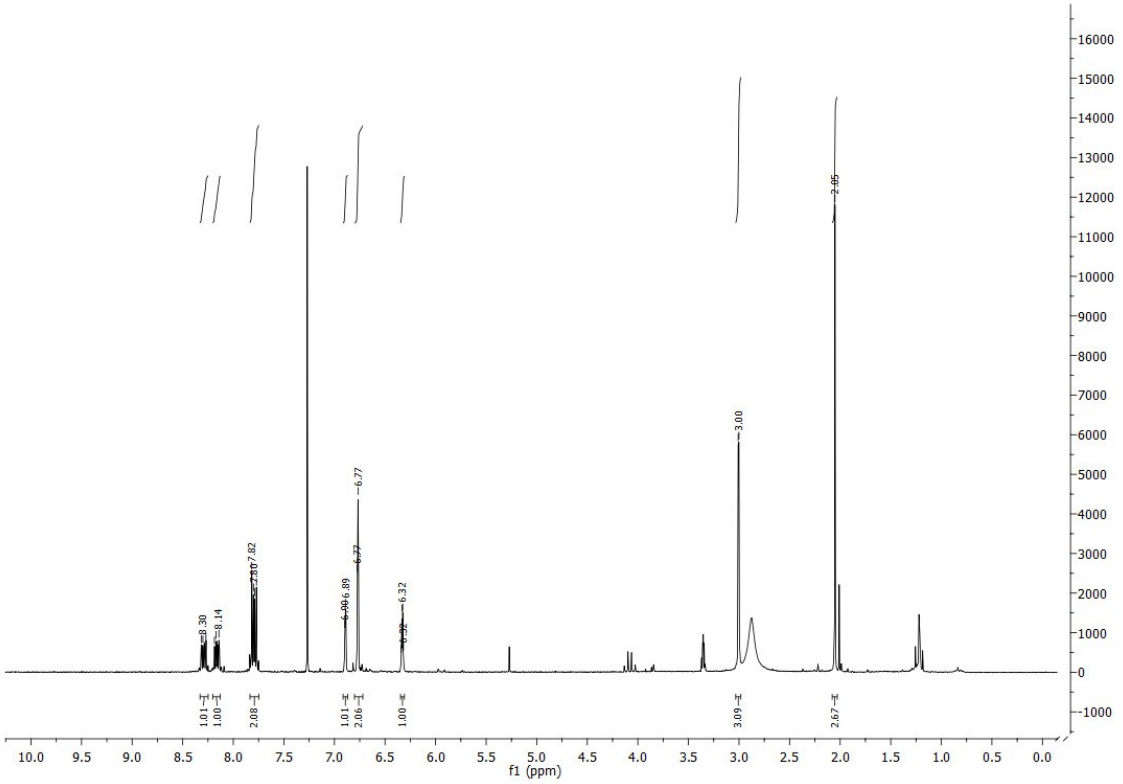
2.13
1.00
2.75
2.62
f1 (ppm)


193.73
156.84
145.96
134.26
129.72
127.27
119.10
116.02
65.98
30.52
14.47
f1 (ppm)

PPD-7


8.30
8.14
7.82
6.89
6.77
6.72
6.32
3.00
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1.01
1.00
2.08
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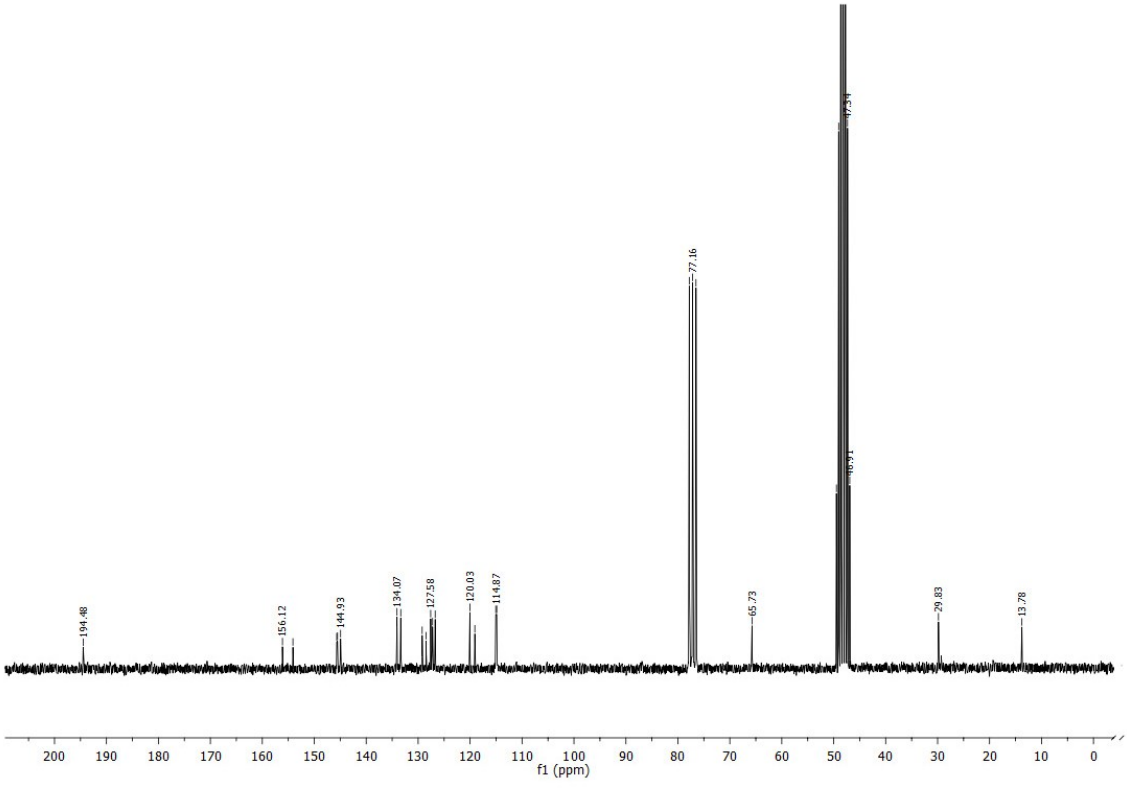
2.06
1.00
3.09
2.67
f1 (ppm)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77.16
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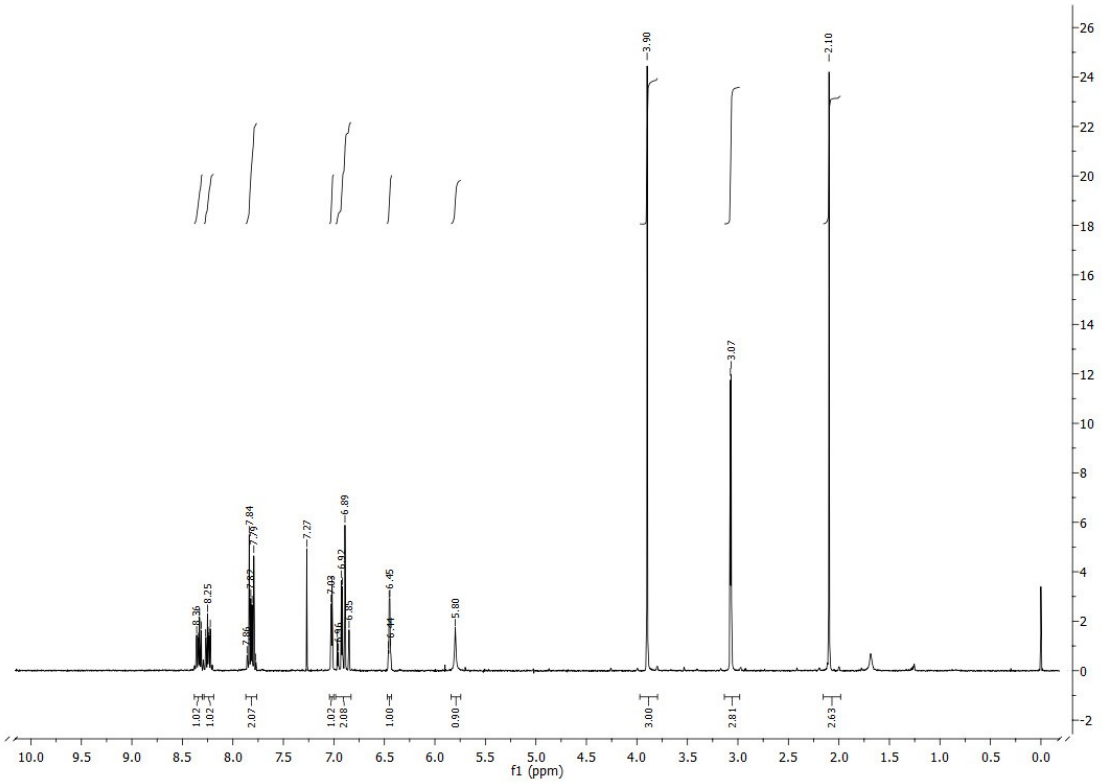
29.83
13.78
f1 (ppm)

PPD-8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3.07
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8.25
7.84
7.79
7.27
6.89
6.92
6.85
6.45
6.44
5.80
1.02
1.02
2.07
1.02
2.08
1.00
0.90
3.00
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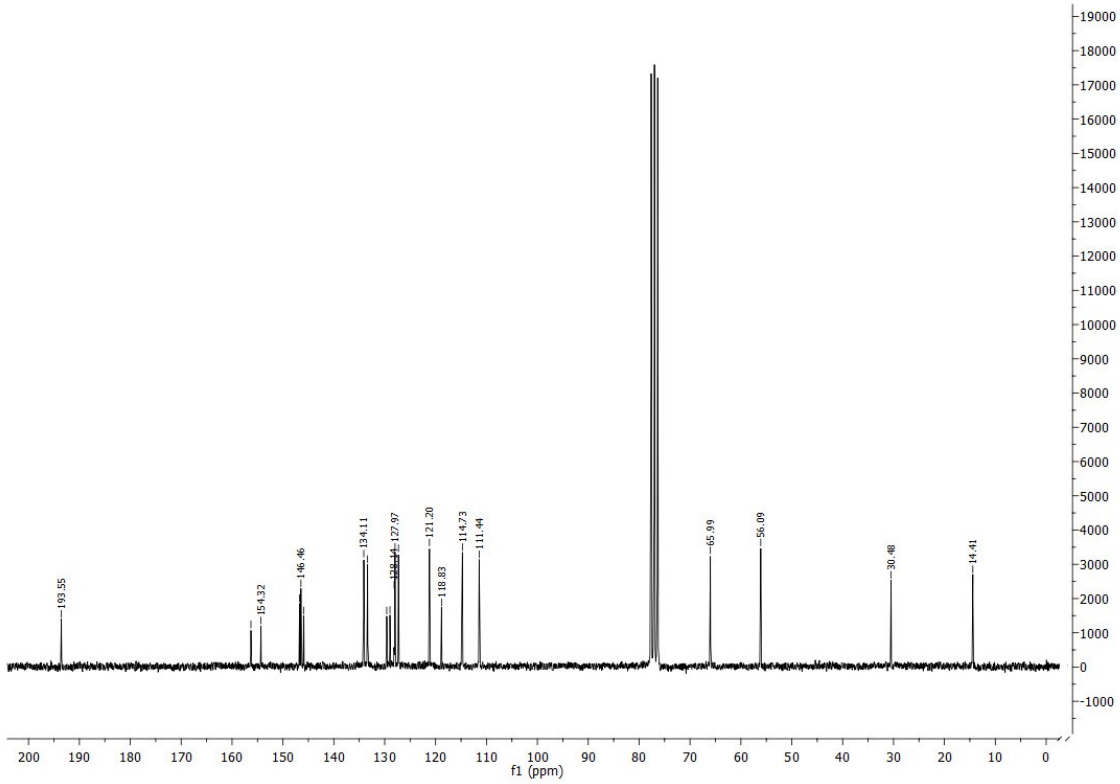
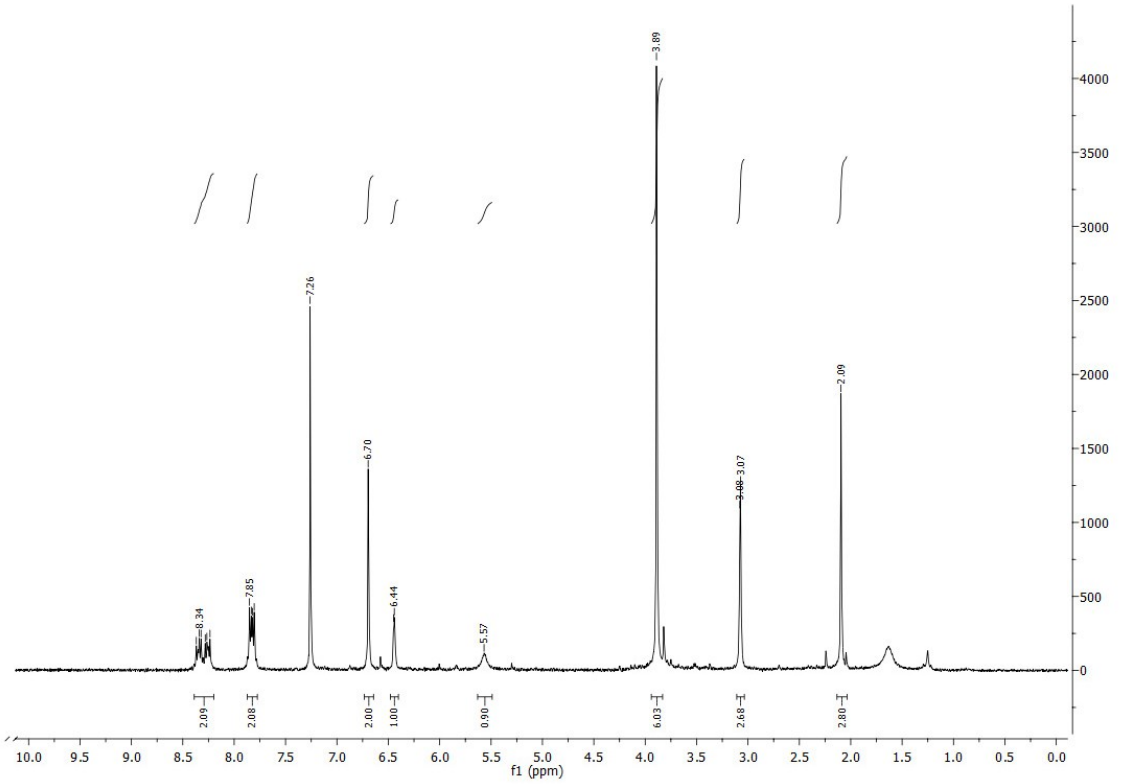
2.63
f1 (ppm)


193.55
154.32
146.46
134.11
128.44
127.97
121.20
118.83
114.73
111.44
65.99
56.09
30.48
14.41
f1 (ppm)

PPD-9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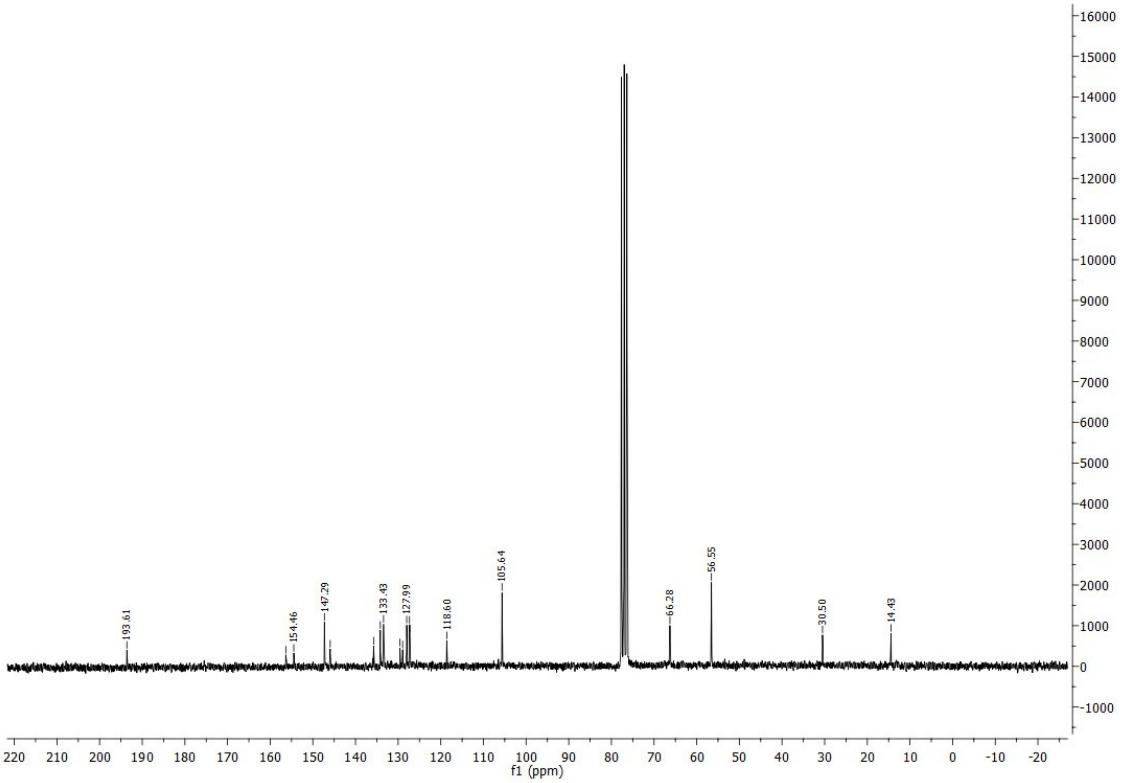
7.85
7.26
6.70
6.44
5.57
3.89
3.07
2.09
2.09
2.08
2.00
1.00
0.90
6.03
2.68
2.80
f1 (ppm)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133.43
127.99
118.60
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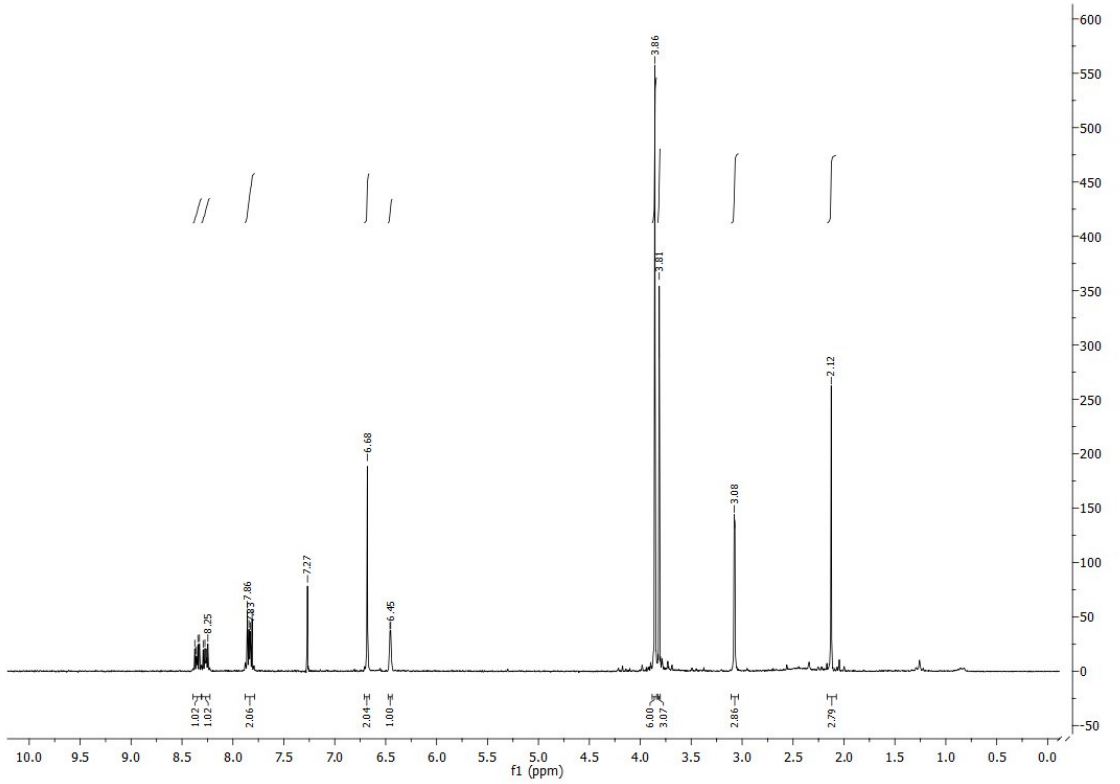
56.55
30.50
14.48
f1 (ppm)

PPD-10


3.86
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7.27
7.86
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1.02
2.06
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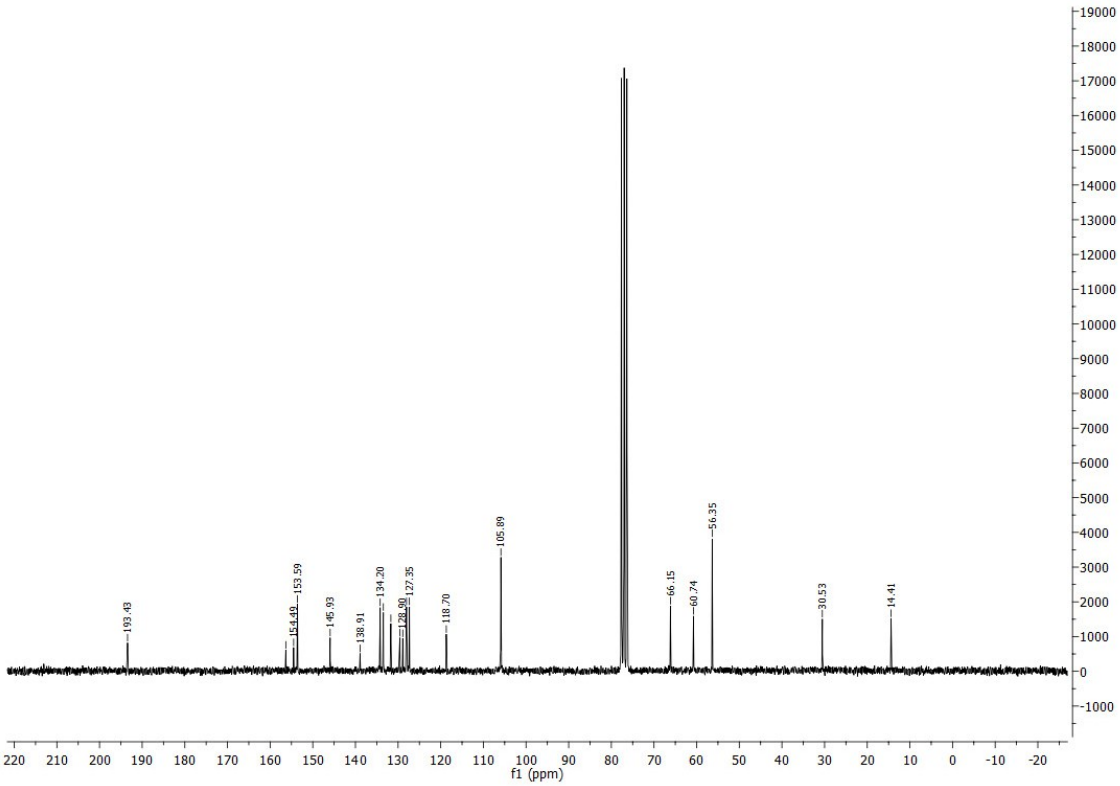
6.00
3.07
2.86
2.79
f1 (ppm)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138.91
134.20
128.90
127.35
118.70
105.89
66.15
60.74
56.35
30.53
14.41
f1 (ppm)

Reference

[1] Kiasat AR, Noorizadeh S, Ghahremani M (2013) Saghanejad SJ, Experimental and theoretical study on one-pot, three-component route to 2H-indazolo[2,1-b]phthalazine-triones catalyzed by nano-alumina sulforic acid. J Mol Struct 1036:216–225. doi:10.1016/j.molstruc.2012.11.014