Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information (SI)

Synthesis, linear and nonlinear optical properties of thermally stable ferrocene-diketopyrrolopyrrole dyads

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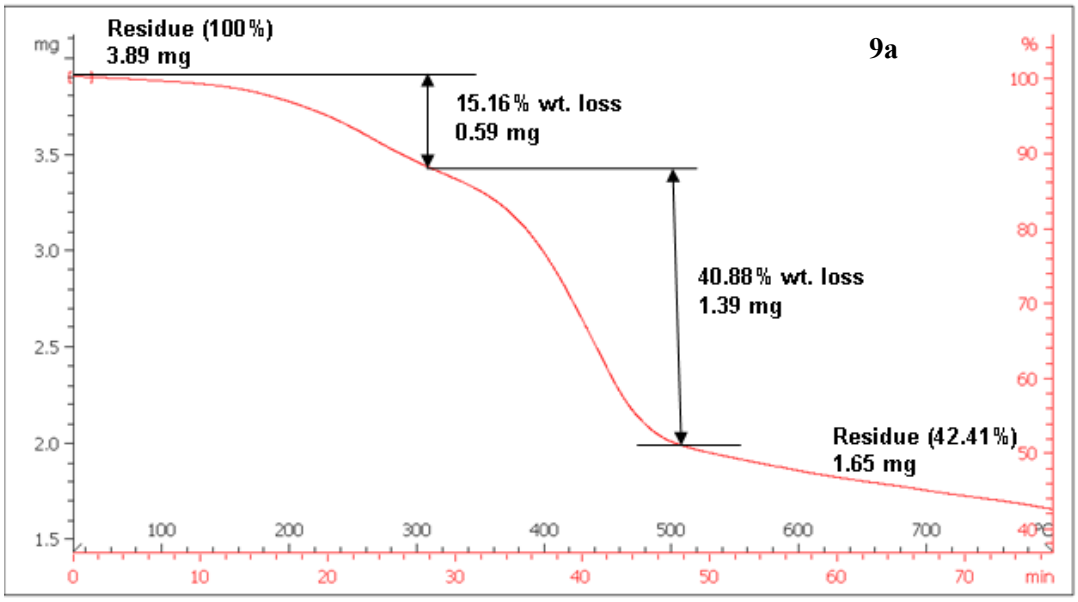
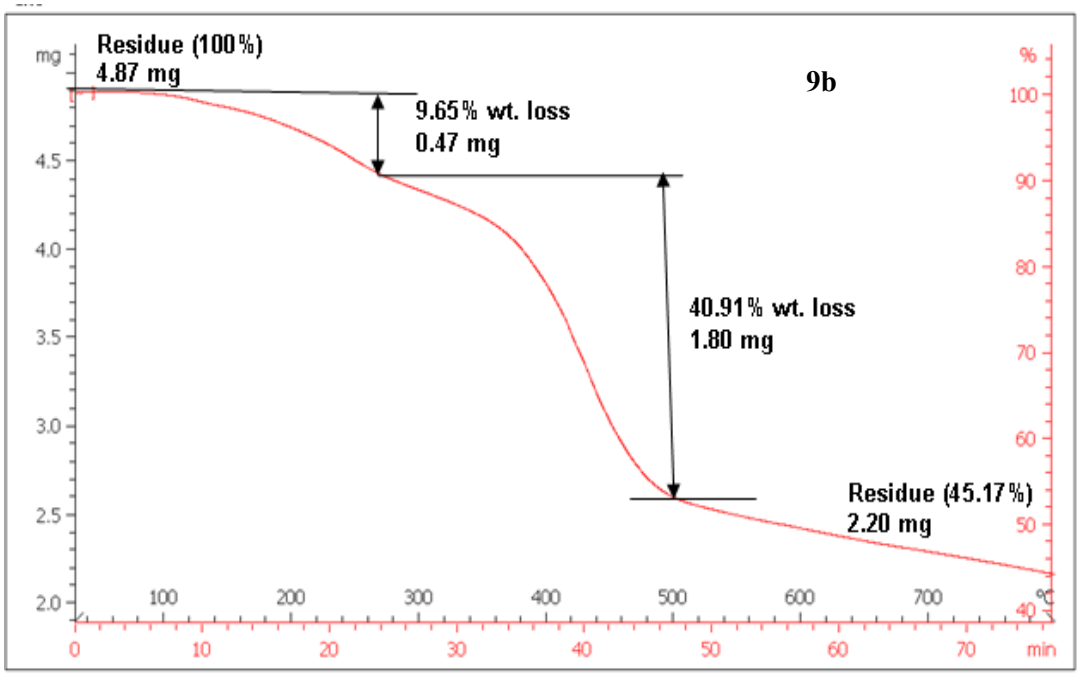
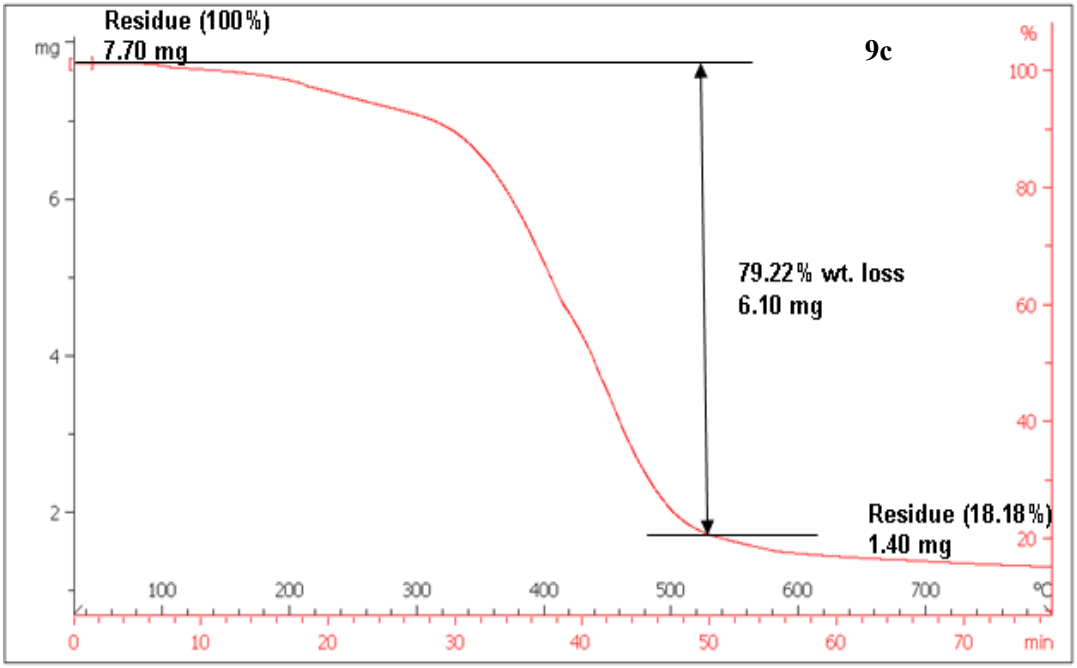
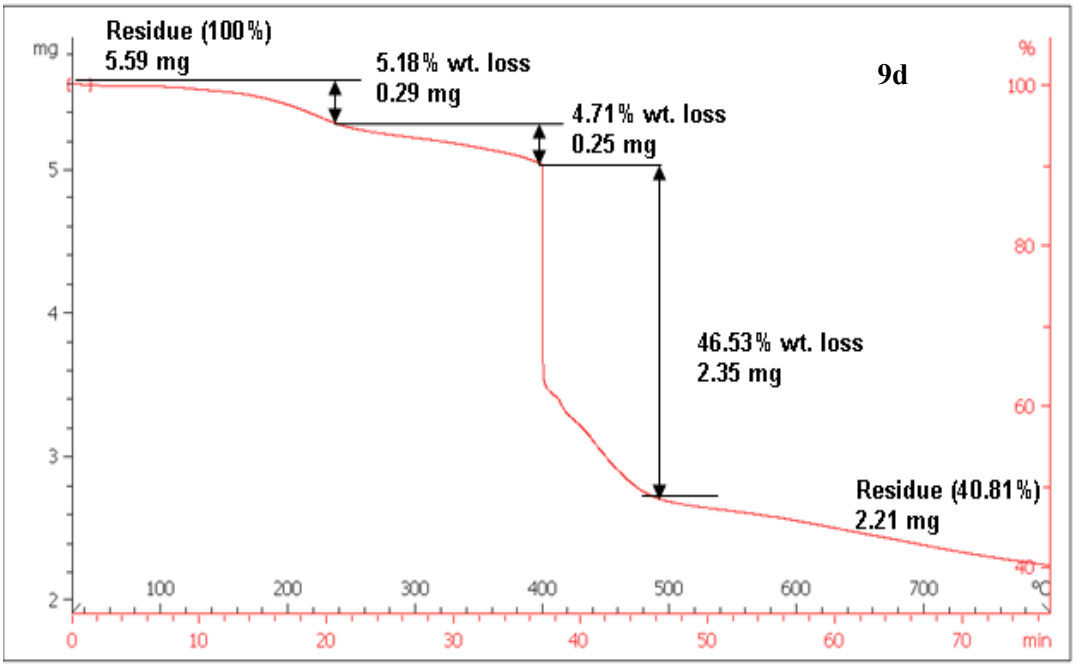
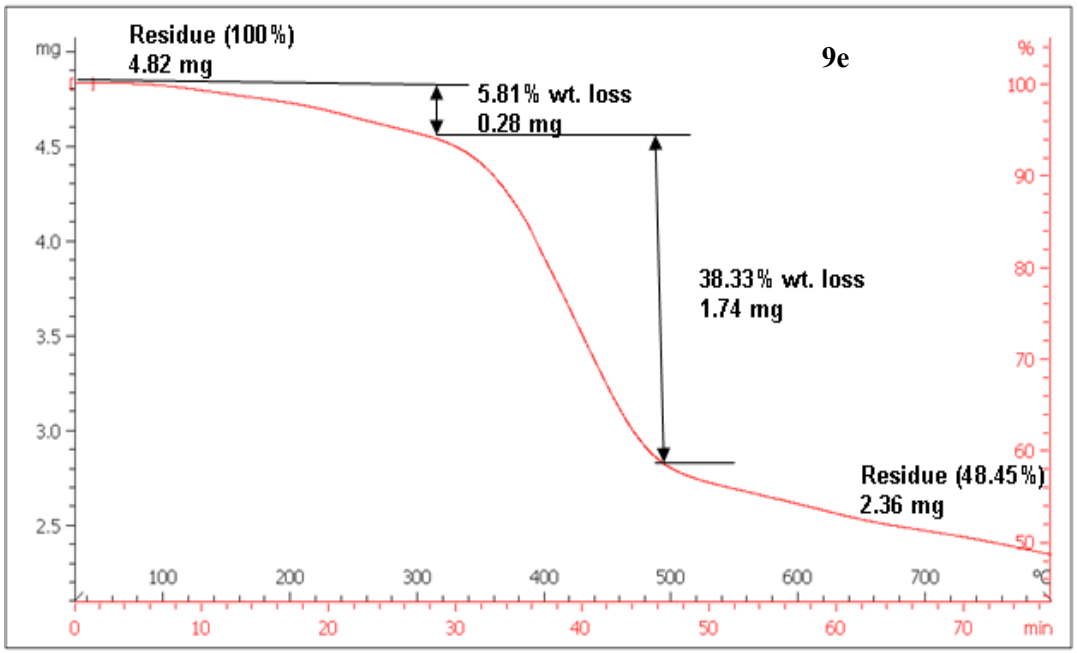
Thermogravimetric curves






Residue (100%)
7.70 mg
9c
79.22% wt. loss
6.10 mg
Residue (18.18%)
1.40 mg
mg
%
min
°C


Residue (100%)
5.59 mg
5.18% wt. loss
0.29 mg
4.71% wt. loss
0.25 mg
9d
46.53% wt. loss
2.35 mg
Residue (40.81%)
2.21 mg
mg
%
min
°C



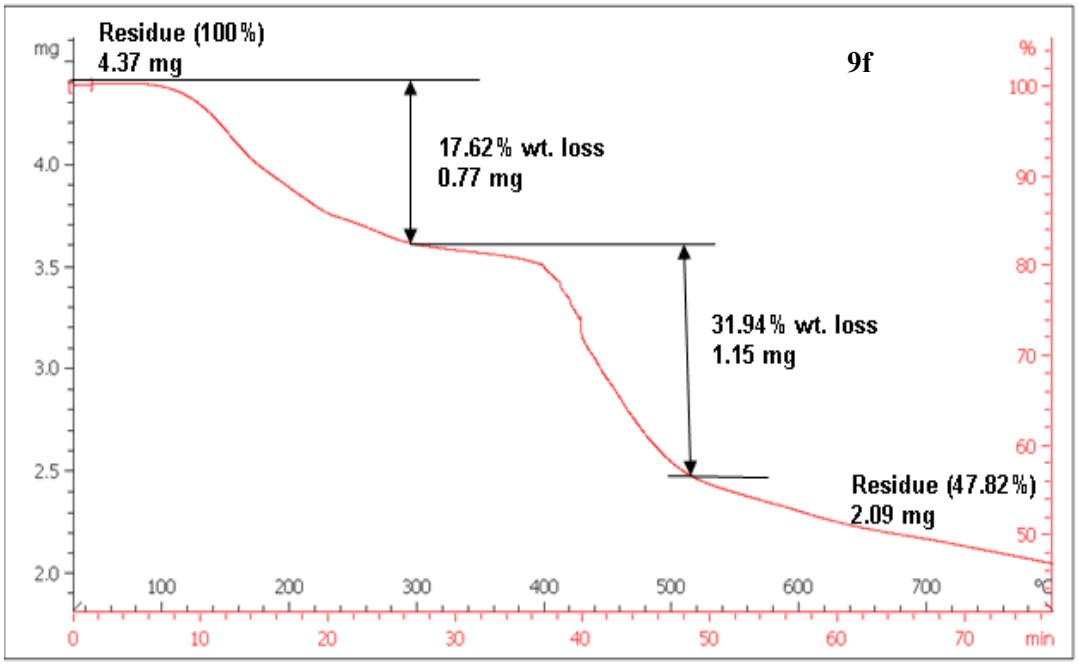
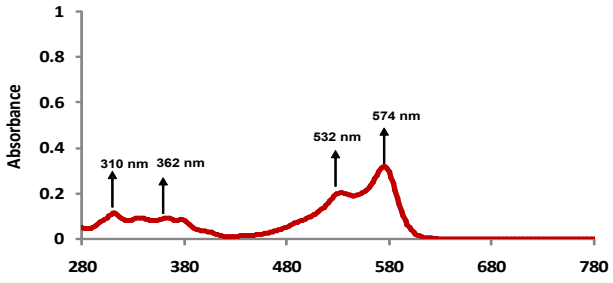
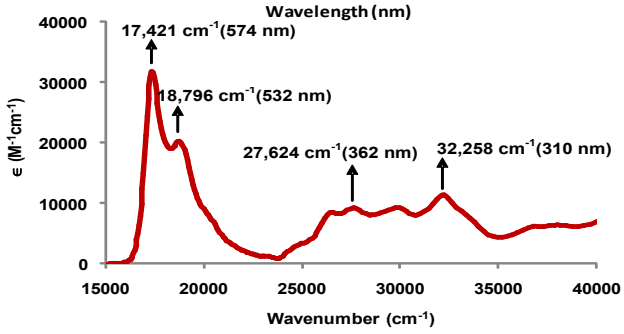


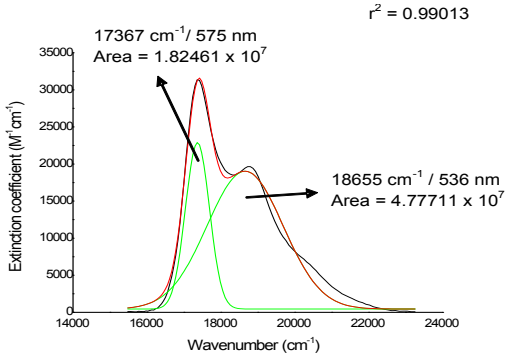
Figure S1: Thermogravimetric (TGA) curves of dyads **9a- 9f**.

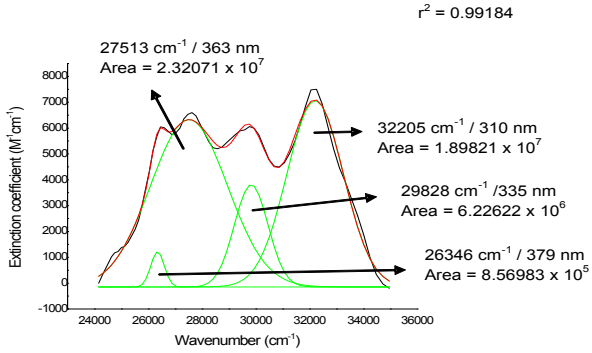
Absorbance vs wavelength (nm)/ Extinction coefficient ($M^{-1}cm^{-1}$) vs wavenumber (cm^{-1})	Resolved peaks after band fitting

5

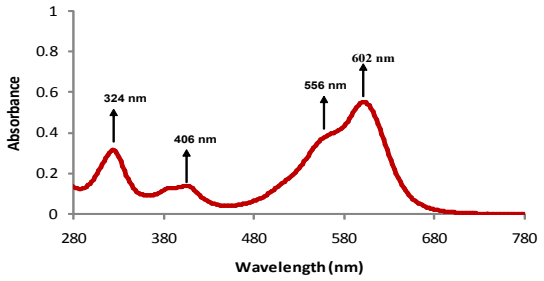


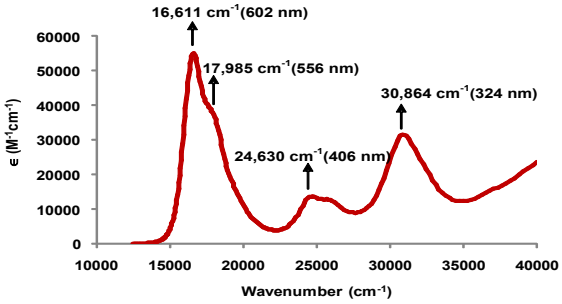


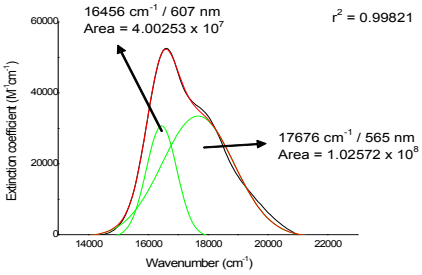


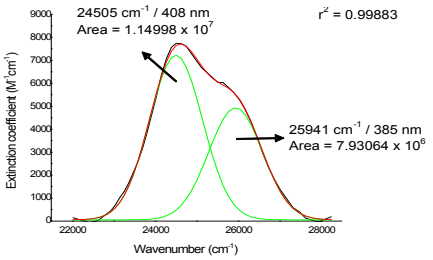


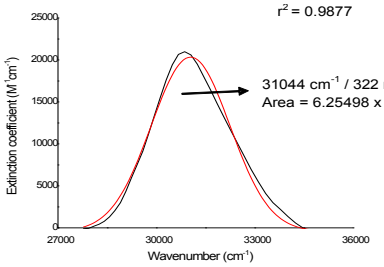
9a



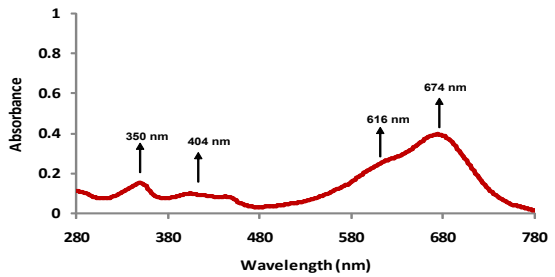


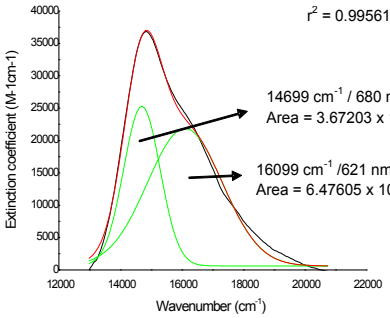


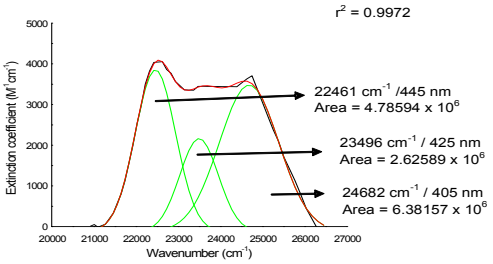


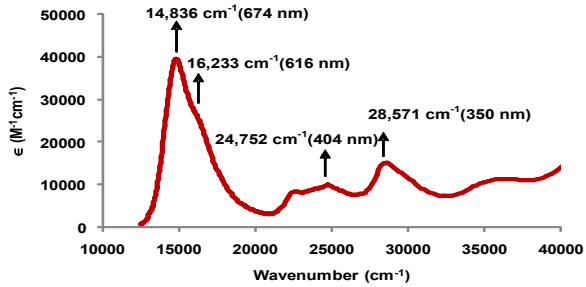


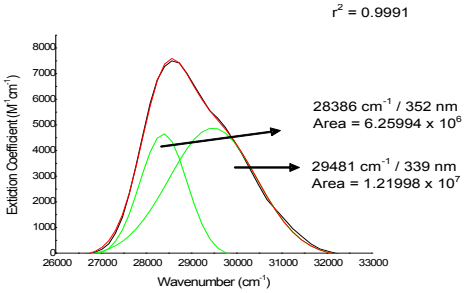
9b


Absorbance
Wavelength (nm)
350 nm
404 nm
616 nm
674 nm

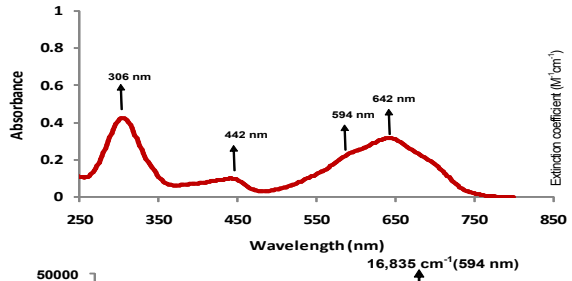

r² = 0.99561
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)
14699 cm-1 / 680 nm
Area = 3.67203 x 10⁷
16099 cm-1 /621 nm
Area = 6.47605 x 10⁷

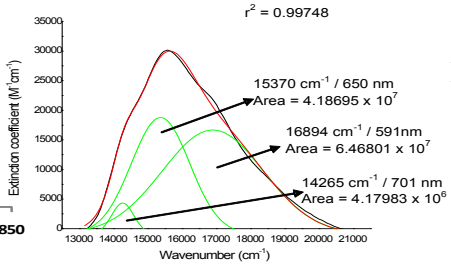

r² = 0.9972
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)
22461 cm-1 /445 nm
Area = 4.78594 x 10⁶
23496 cm-1 / 425 nm
Area = 2.62589 x 10⁶
24682 cm-1 / 405 nm
Area = 6.38157 x 10⁶

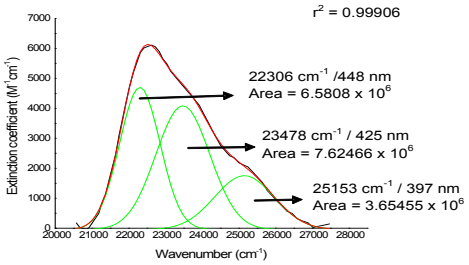

ε (M-1cm-1)
Wavenumber (cm-1)
14,836 cm-1(674 nm)
16,233 cm-1(616 nm)
24,752 cm-1(404 nm)
28,571 cm-1(350 nm)

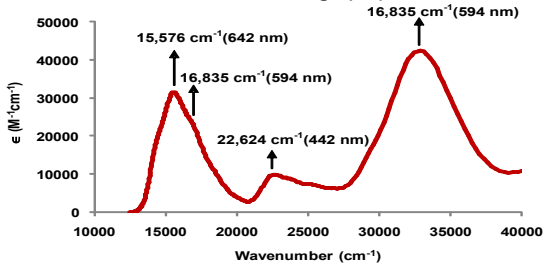

r² = 0.9991
Extiction Coefficient (M-1cm-1)
Wavenumber (cm-1)
28386 cm-1 / 352 nm
Area = 6.25994 x 10⁶
29481 cm-1 / 339 nm
Area = 1.21998 x 10⁷

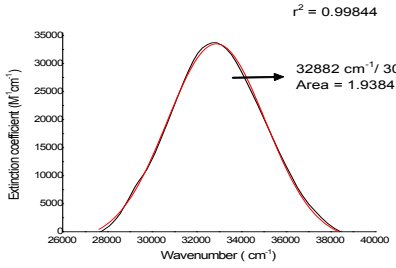
9c


Absorbance
Wavelength (nm)
306 nm
442 nm
594 nm
642 nm

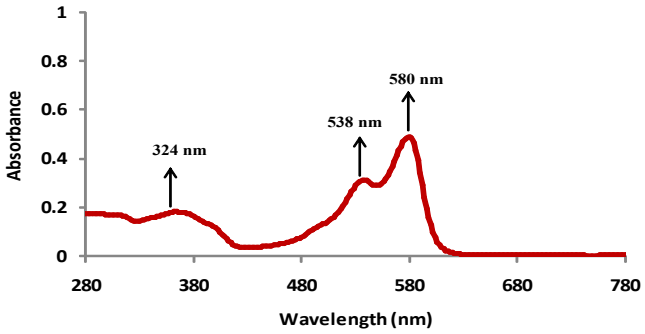

r² = 0.99748
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)
15370 cm-1 / 650 nm
Area = 4.18695 x 10⁷
16894 cm-1 / 591nm
Area = 6.46801 x 10⁷
14265 cm-1 / 701 nm
Area = 4.17983 x 10⁶

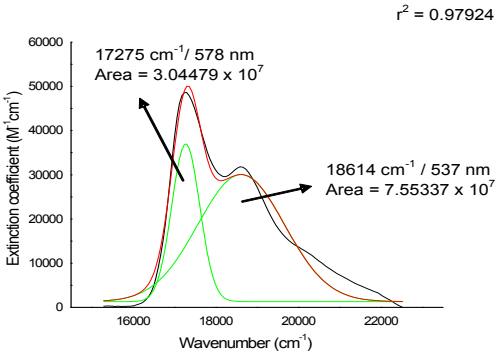

r² = 0.99906
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)
22306 cm-1 /448 nm
Area = 6.5808 x 10⁶
23478 cm-1 / 425 nm
Area = 7.62466 x 10⁶
25153 cm-1 / 397 nm
Area = 3.65455 x 10⁶

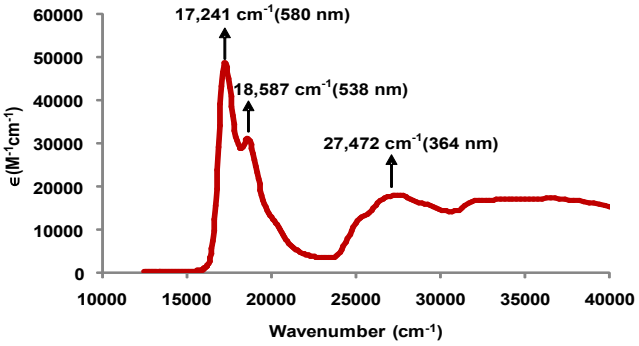

ε (M-1cm-1)
Wavenumber (cm-1)
15,576 cm-1(642 nm)
16,835 cm-1(594 nm)
22,624 cm-1(442 nm)
16,835 cm-1(594 nm)

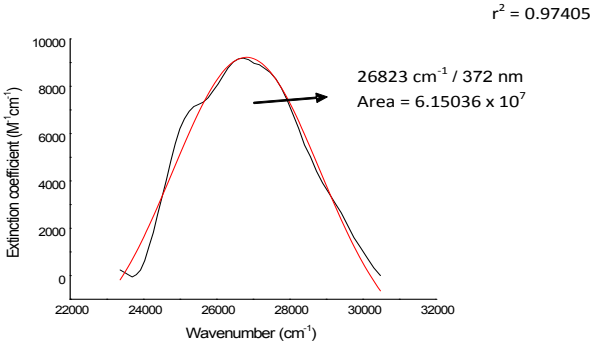

r² = 0.99844
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)
32882 cm-1/ 304 nm
Area = 1.93841 x 10⁸

9d

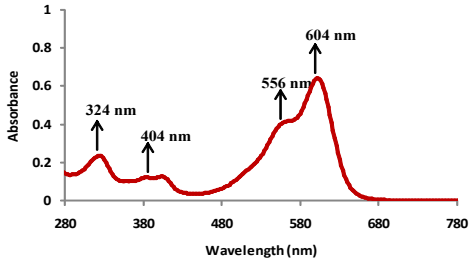

Absorbance
Wavelength (nm)
324 nm
538 nm
580 nm

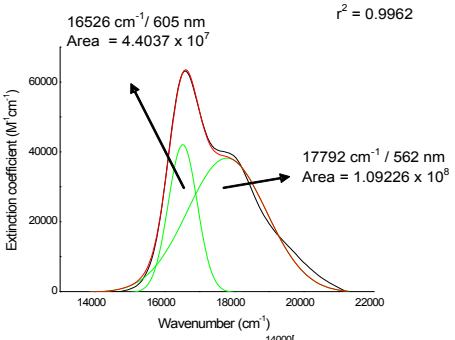

r2 = 0.97924
17275 cm-1/ 578 nm
Area = 3.04479 x 10^7
18614 cm-1 / 537 nm
Area = 7.55337 x 10^7
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)

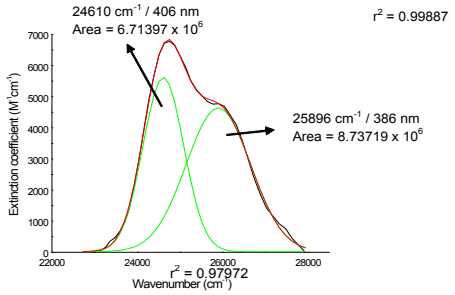

ε (M-1cm-1)
Wavenumber (cm-1)
17,241 cm-1(580 nm)
18,587 cm-1(538 nm)
27,472 cm-1(364 nm)

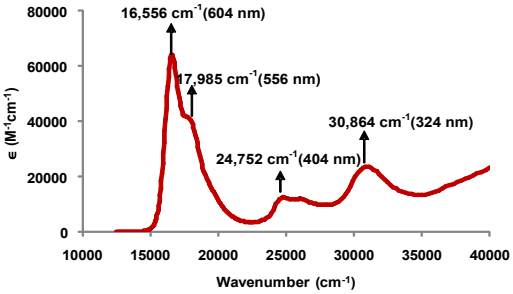

r2 = 0.97405
26823 cm-1 / 372 nm
Area = 6.15036 x 10^7
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)

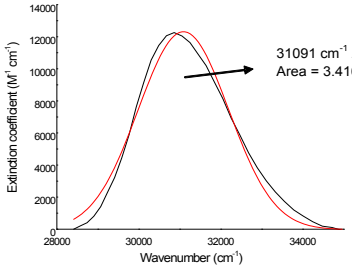
9e


Absorbance
Wavelength (nm)
324 nm
404 nm
556 nm
604 nm


r2 = 0.9962
16526 cm-1/ 605 nm
Area = 4.4037 x 10^7
17792 cm-1 / 562 nm
Area = 1.09226 x 10^8
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)


r2 = 0.99887
24610 cm-1 / 406 nm
Area = 6.71397 x 10^6
25896 cm-1 / 386 nm
Area = 8.73719 x 10^6
r2 = 0.97972
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)


ε (M-1cm-1)
Wavenumber (cm-1)
16,556 cm-1(604 nm)
17,985 cm-1(556 nm)
24,752 cm-1(404 nm)
30,864 cm-1(324 nm)


31091 cm-1 / 321 nm
Area = 3.416 x 10^7
Extinction coefficient (M-1cm-1)
Wavenumber (cm-1)

9f

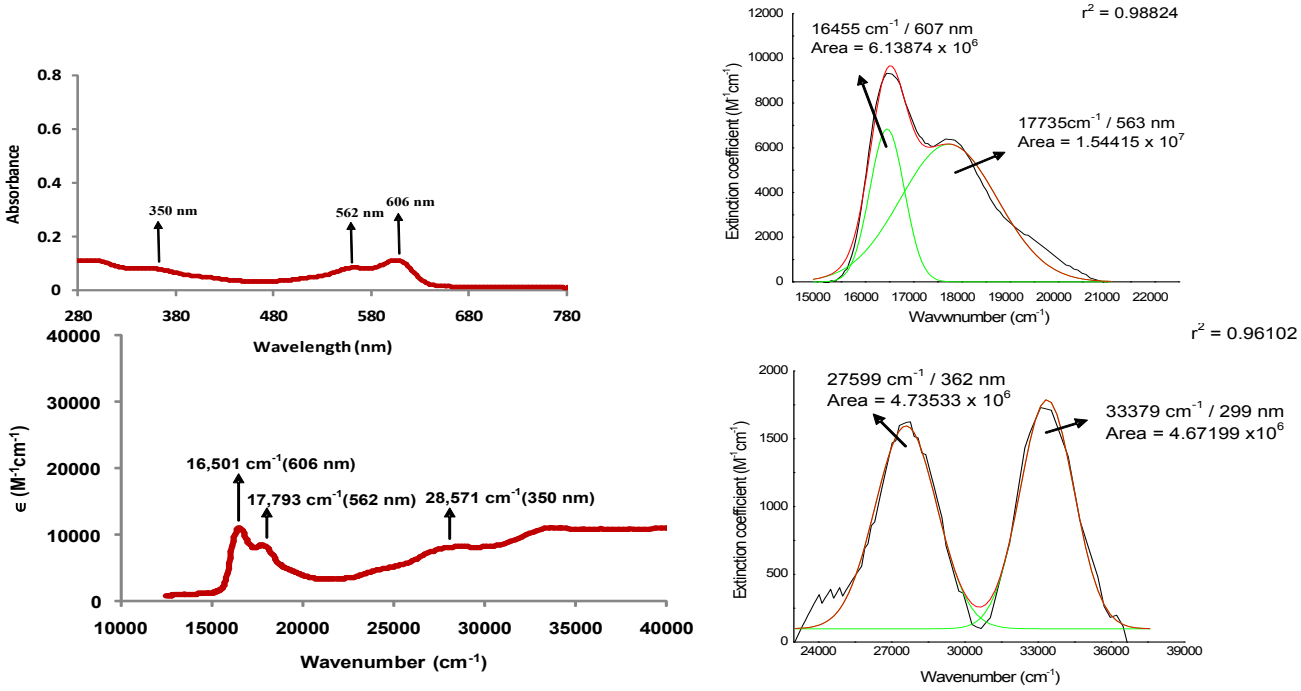


Figure S2: UV-visible absorption spectra of dyads **5** & **9a-9f** recorded at 1 x 10^{-5} M in dichloromethane and the resolved peaks after band fitting.

Table S1: Comparison of experimentally (UV-visible) and theoretically (TD-DFT) calculated absorption bands and assignment of electronic transitions for the dyads **5** & **9a-9f**.

Compound	Transition	CI coefficient	E(eV)/ λ_{theor} [a] in nm	Oscillator strength	Assignment	λ_{exp} [b] in nm
5	1A- H->L	0.71112(101%)	2.1427/ 549.69	0.7791	Intra-ligand CT	574
	---	---	---	---	---	532(sh)
	6A- H-2->L	0.61141(75%)	3.4065/ 345.76	0.3441	Intra-ligand CT	362
	H-5->L	-0.22299(10%)			Intra-ligand CT	
	19A- H-5->L+1	0.57452(66%)	4.6966/ 250.78	0.0012	Intra-ligand CT	310
	H-9->L	0.26882(14%)			Intra-ligand CT	
	20A-H-11->L	0.59307(70%)	4.7223/ 249.42	0.0054	Intra-ligand CT	310
	H-12->L	0.34694(24%)			Intra-ligand CT	
9a	1A- H->L	0.56950(65%)	1.8460/ 638.05	0.7374	MLCT or D-A transition	602
	H-2->L	0.26672(14%)			MLCT or D-A transition	
	---	---	---	---	---	556(sh)
	9A- H-5->L	0.49985(50%)	2.9185/ 403.57	0.0835	LMCT + L-A transition	406
	H->L+1	0.43130(37%)			Weak MLCT + π-π* + L-A transition	
	19A- H-7->L	0.52993(56%)	3.6226/ 325.13	0.0718	Intra-ligand CT	324
	H->L+2	-0.37339(28%)			weak LMCT + π-π*	
9b	1A- H->L	0.66701(89%)	1.6606/ 709.28	1.21	Weak MLCT + D-A transition	674
	---	---	---	---	---	616(sh)
	---	---	---	---	---	404(br)
	14A- H-5->L	0.48018(46%)	3.1816/ 370.20	0.2611	A-D transition	350
	H-9->L	0.38911(30%)			L-A transition	
9c	1A- H->L	0.69872(98%)	1.6284/ 723.31	1.765	D-A transition	642
	---	---	---	---	---	594(sh)
	---	---	---	---	---	442(br)

	9A- H-3->L	0.60188(72%)	2.6407/ 446.03	0.0875	D-A transition	306
	H->L+1	-0.35520(25%)			D-A transition	
	10A- H-4->L	0.67032(90%)	2.7299/ 431.45	0.1472	D-A transition	306
9d	1A- H->L	0.48499(47%)	1.9916/ 591.40	0.6832	MLCT	580
	H-1->L	-0.23980(12%)			MLCT	
	---	---	---	---	---	538(sh)
	21A- H->L+2	0.57876(67%)	3.8794/ 303.61	0.074	Intra-ligand CT + π-π*	324
	H-7->L	-0.26890(14%)			Weak Intra-ligand CT	
9e	1A- H->L	0.18514(71%)	1.8978/ 620.63	1.2559	MLCT	604
	---	---	---	---	---	556 (sh)
	15A- H-6->L	0.67118(90%)	3.0220/ 389.75	0.2909	MLCT	404
	30A- H->L+2	0.30767(58%)	3.7841/ 311.26	0.4928	LMCT + π-π*	324
	H-1->L+1	0.12894(19%)			MLCT + π-π*	
9f	1A- H->L	0.67811(92%)	1.8670/ 630.87	2.1192	MLCT + Intra-ligand CT	606
	---	---	---	---	---	562 (sh)
	24A- H->L+2	0.61119(75%)	3.3803/ 348.44	0.1944	LMCT + π-π*	350

[a] Calculated from TD-DFT using B3LYP/6-31G and applying correction factor of 0.95. [b] recorded at 1x 10^{-5} M in dichloromethane. MLCT: Metal to ligand charge transfer. D- Donor. A-Acceptor.

Table S2: UV-visible data of **5** & **9a-9f** in various solvents.[a]

Solvent / Compound	Hexane	Toluene	Diethyl ether	DCM	THF	Methanol	ACN	DMF	DMSO
5	570	578 (65500)	568	574 (31600)	570 (30400)	570	566	572	574
	526	534 (40000)	524	532 (20200)	528 (19100)	544	526	530	530
	358	362 (18300)	358	362 (9200)	360 (6300)	358	360	362	366
	310	310 (22600)	308	310 (11400)	308 (8400)	---	308	308	---
9a	594	604 (50400)	592	602 (55000)	594 (41300)	568	590	594	596
	552	556 (33900)	554	556 (37300)	550 (27200)	522	550	552	552
	400	404 (13400)	400	406 (13700)	402 (9600)	380	400	384	412
	320	324 (36000)	320	324 (31500)	320 (18300)	316	320	322	320
9b	672	678 (68600)	662	674 (39500)	658 (43600)	648	650	652	650
	614	614 (41500)	602	616 (25800)	598 (28100)	594	590	584	580
	396	416 (14700)	396	404 (10000)	444 (9700)	400	392	400	392
	348	350	346	350	348	344	344	348	348

		(24100)		(15100)	(18200)				
9c	638	644 (32500)	636	642 (31500)	634 (39300)	630	630	632	602
	598	596 (24900)	426	594 (23800)	588 (37800)	582	586	436	596
	442	436 (12300)	---	442 (9900)	438 (20100)	432	434	---	342
	---	302 (59500)	---	304 (42300)	312 (60300)	---	---	308	---
9d	570	580 (62000)	570	580 (48700)	576 (75900)	572	572	578	580
	530	538 (41400)	530	538 (31100)	534 (49500)	532	532	538	540
	360	364 (35000)	360	364 (18100)	360 (31300)	362	360	362	364
	308	312 (46100)	306	324 (14400)	310 (29900)	---	---	---	---
9e	590	602 (90800)	592	604 (63800)	598 (84,000)	594	590	592	592
	554	558 (56800)	542	556 (40400)	558 (53,200)	542	542	554	---
	---	402 (16100)	398	404 (12500)	400 (17800)	---	---	---	---
	318	324 (30600)	320	324 (23500)	322 (33400)	326	320	318	---
9f	574	606 (38400)	570	606 (11000)	602 (25400)	604	570	582	580

	522	562 (25500)	532	562 (8400)	560 (17600)	558	528	536	532
	364	364 (18500)	---	350 (8200)	364 (11800)	---	---	---	---

[a] Absorption wavelength (nm) at room temperature (c ≈ 1 x 10^{-5} M) and molar extinction coefficient between brackets (M^{-1} cm^{-1}).

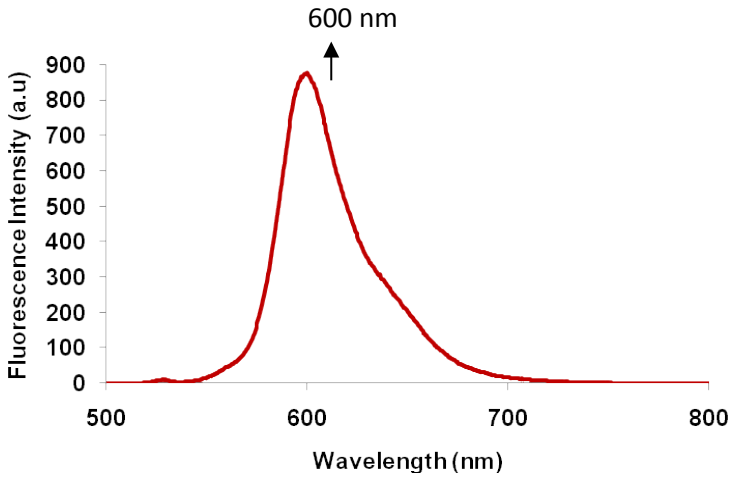


Figure S3: Emission spectra of **5** at 1 x 10^{-5} in DCM at λ_{ex} = 530 nm.

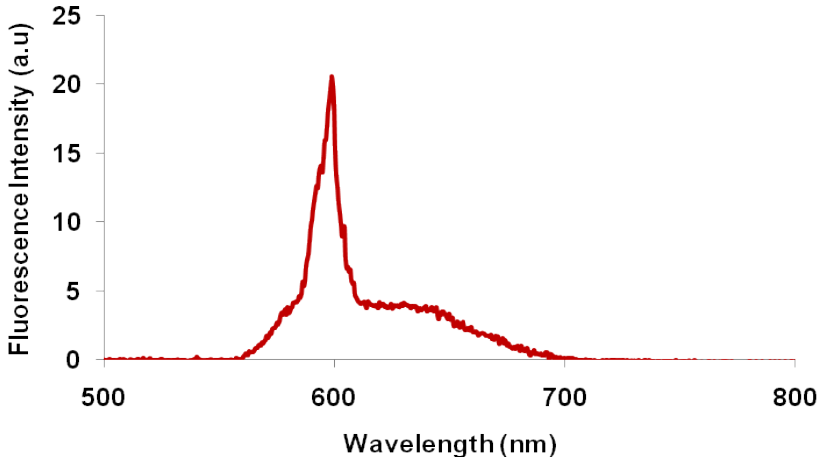


Figure S4: Emission spectra of **9a** at 1 x 10^{-5} in DCM at λ_{ex} = 600 nm.

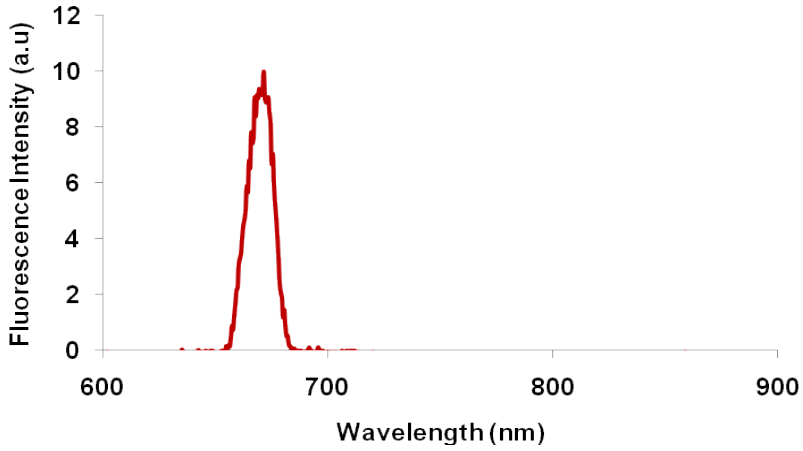


Figure S5: Emission spectra of **9b** at 1 x 10^{-5} in DCM at λ_{ex} = 674 nm.

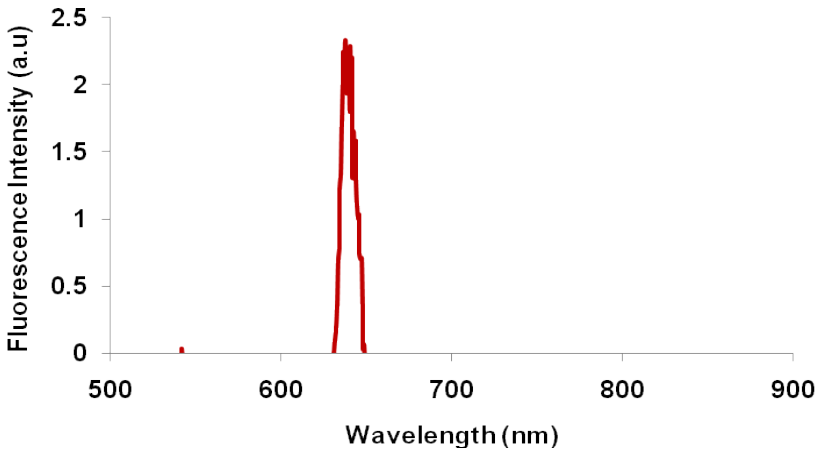


Figure S6: Emission spectra of **9c** at 1 x 10^{-5} in DCM at λ_{ex} = 642 nm.

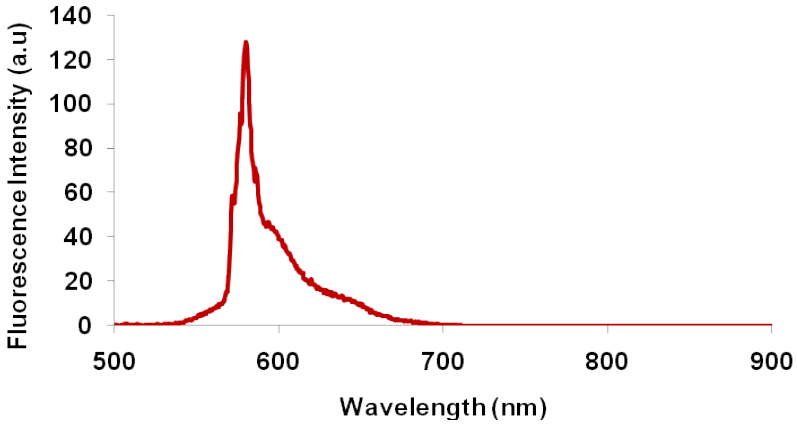


Figure S7: Emission spectra of **9d** at 1 x 10^{-5} in DCM at λ_{ex} = 580 nm.

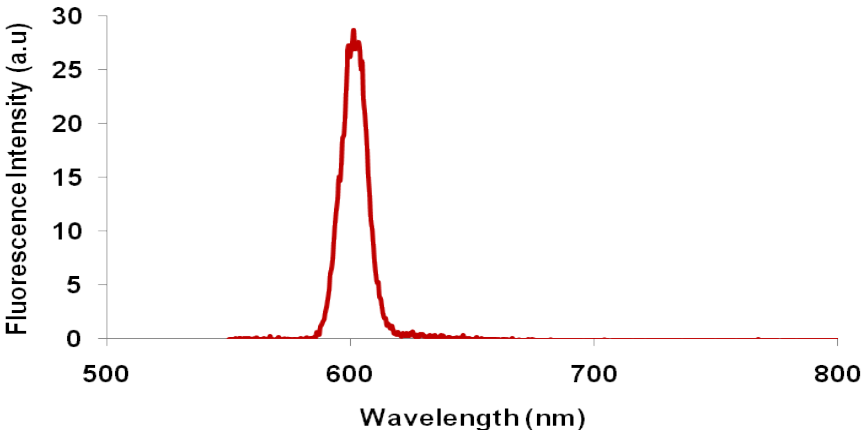


Figure S8: Emission spectra of **9e** at 1 x 10^{-5} in DCM at λ_{ex} = 604 nm.

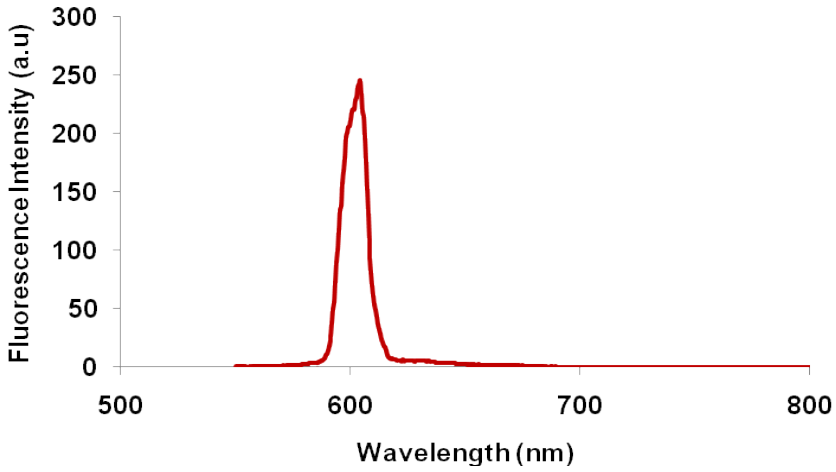


Figure S9: Emission spectra of **9f** at 1 x 10^{-5} in DCM at λ_{ex} = 606 nm.

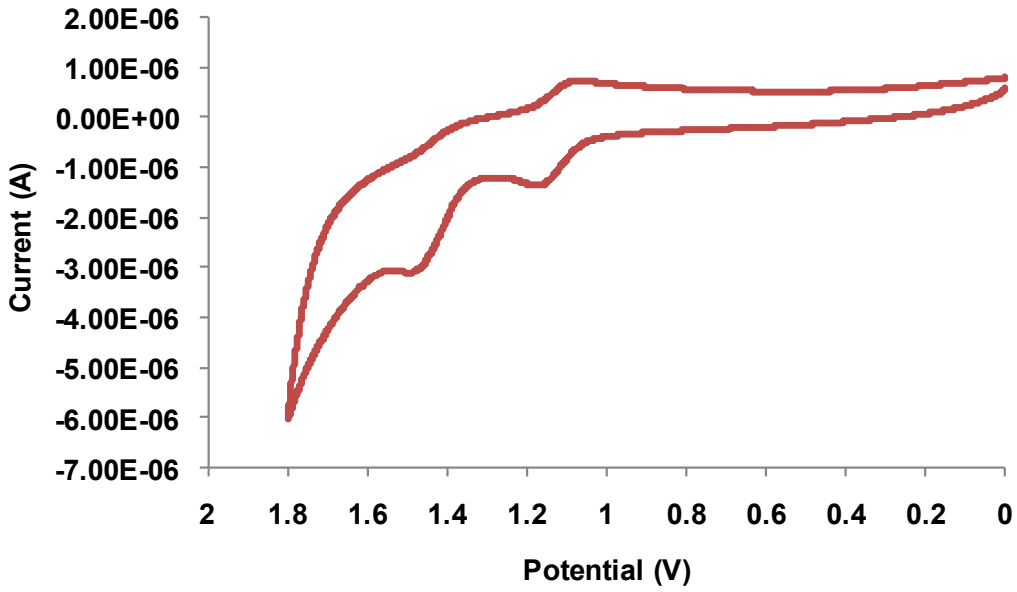


Figure S10: Cyclic voltammogram of **5** (1 x 10^{-4} M in dichloromethane).

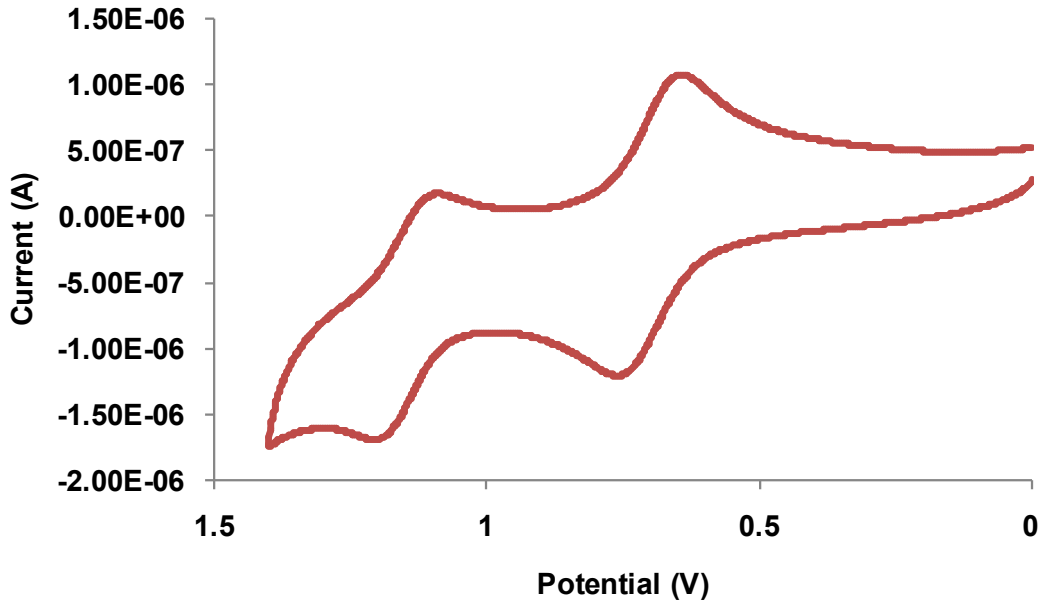


Figure S11: Cyclic voltammogram of **9a** (1 x 10^{-4} M in dichloromethane).

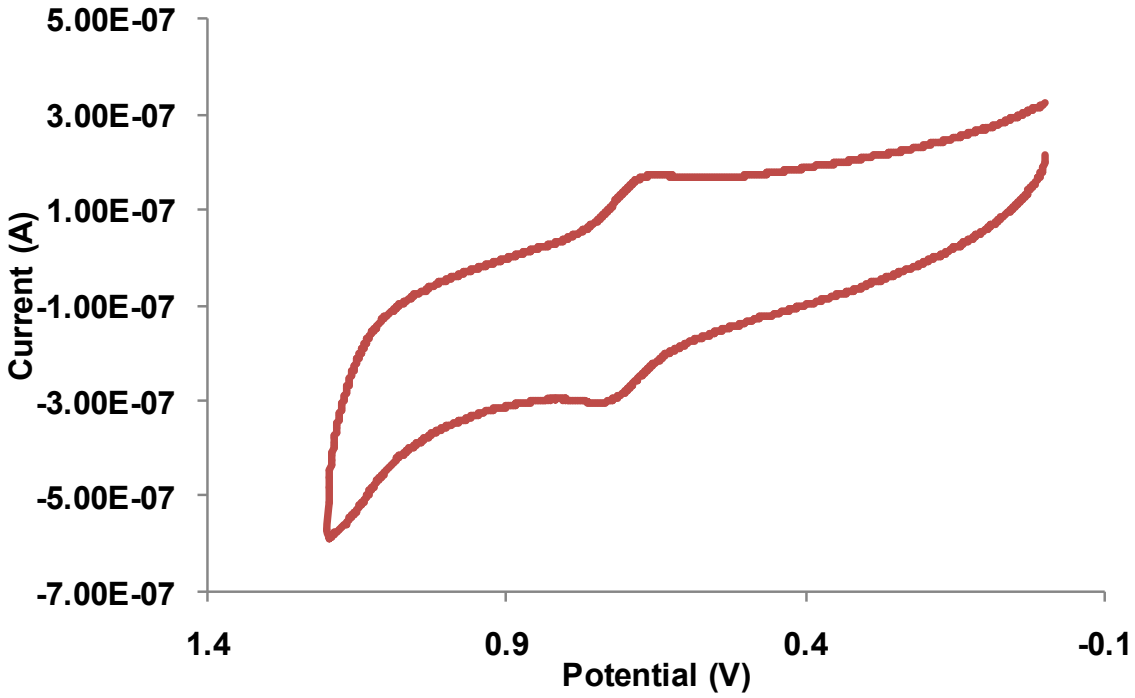


Figure S12: Cyclic voltammogram of **9b** (1 x 10^{-4} M in dichloromethane).

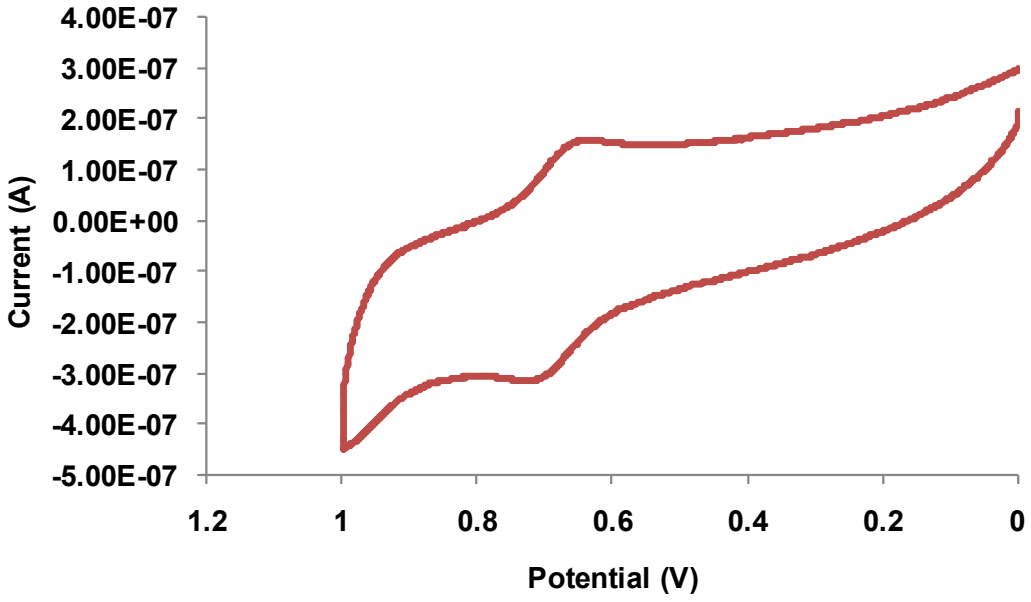


Figure S13: Cyclic voltammogram of **9c** (1 x 10^{-4} M in dichloromethane).

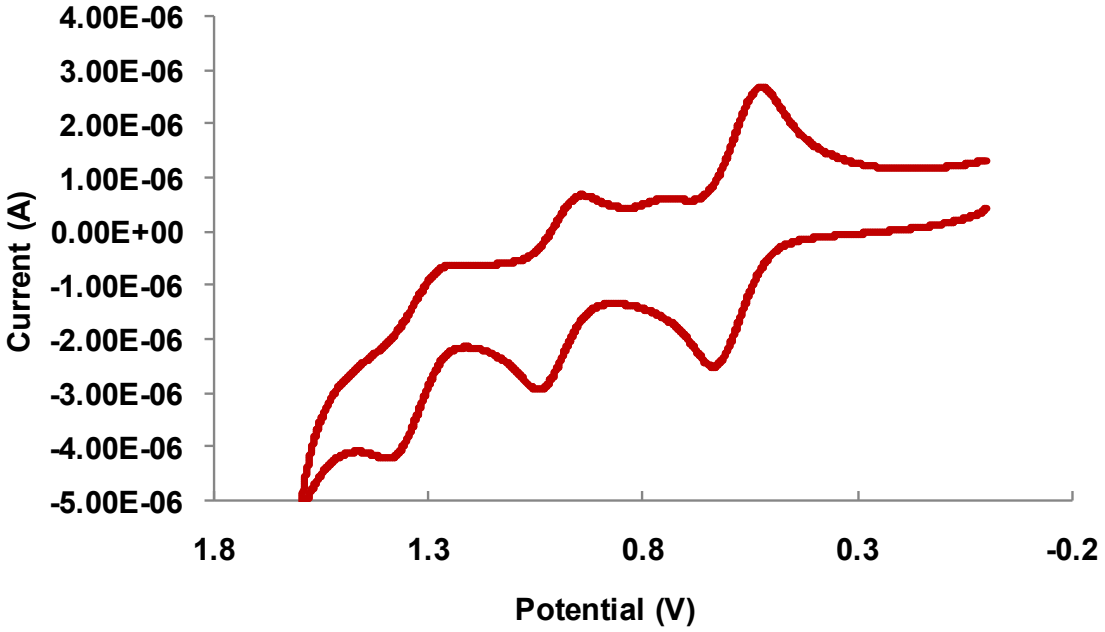


Figure S14: Cyclic voltammogram of **9d** (1 x 10^{-4} M in dichloromethane).

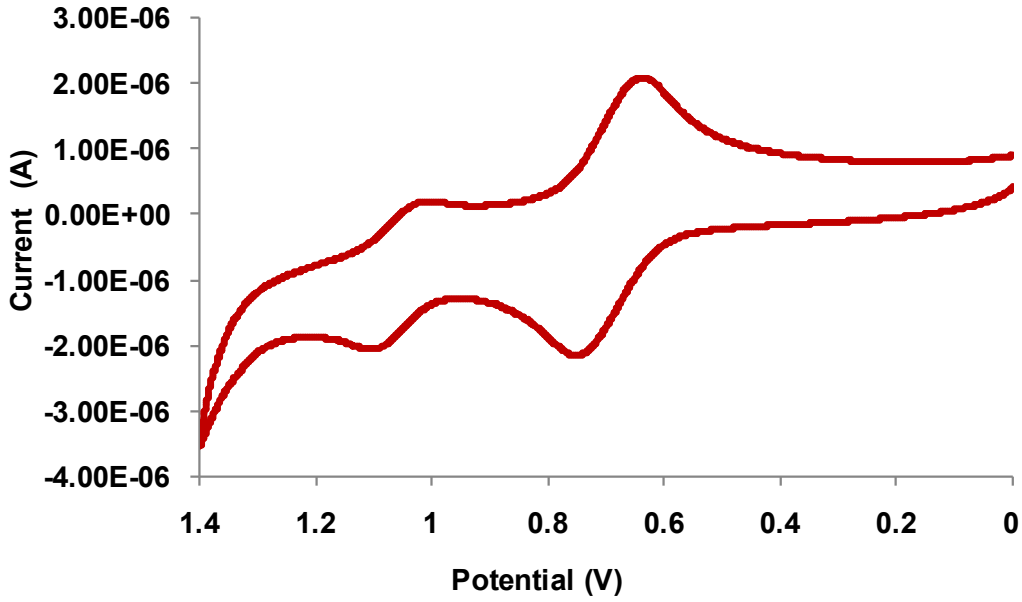


Figure S15: Cyclic voltammogram of **9e** (1 x 10^{-4} M in dichloromethane).

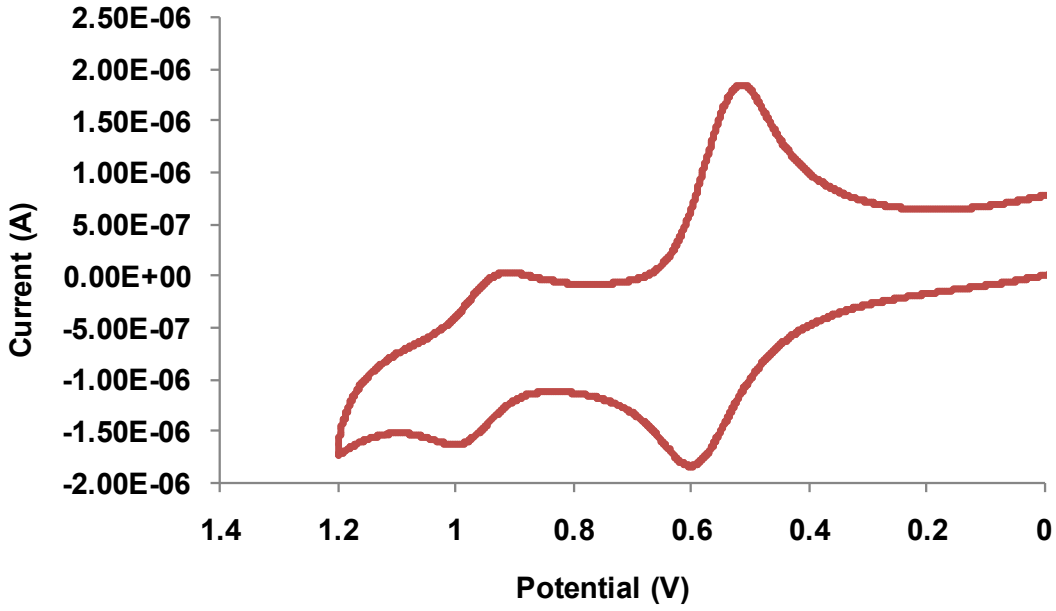


Figure S16: Cyclic voltammogram of **9f** (1 x 10^{-4} M in dichloromethane).

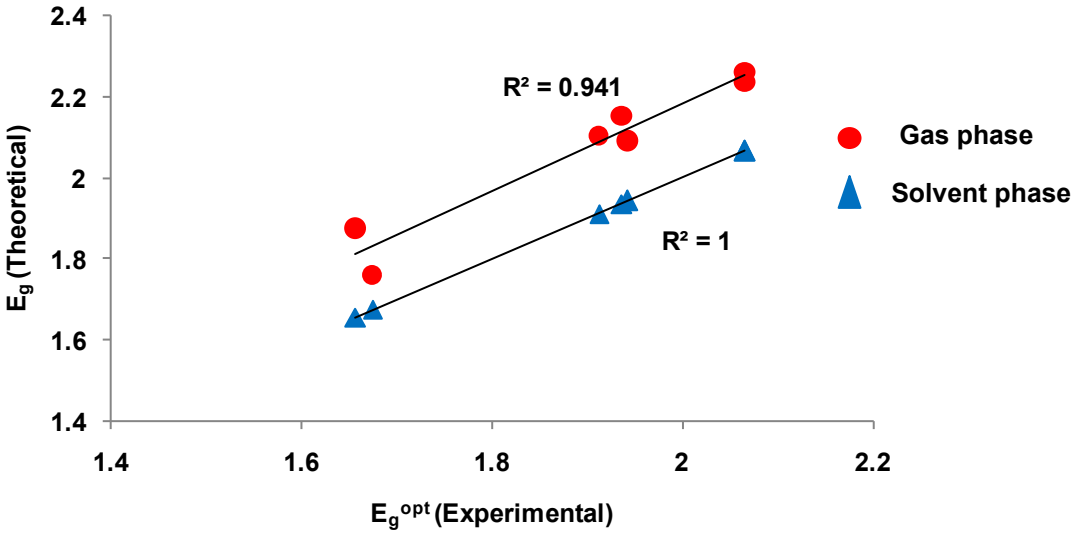


Figure S17: Linear correlation between the optical gap E_g^{opt}, determined from UV/CV and TD-DFT for the dyads **9a-9f** & **5**.

Table S3: Energies of the Frontier Orbitals HOMO-n to LUMO+n (n=0, 1, 2, 3, 4, 5 & 6) obtained from TD-DFT carried out at B3LYP/6-31G level in dichloromethane as solvent medium.

Compound	5	9a	9b	9c	9d	9e	9f
HOMO-6	-7.80232	-7.09809	-7.02434	-6.88366	-6.85182	-6.33318	-6.11249
HOMO-5	-7.46517	-6.94244	-6.90924	-6.60883	-6.82434	-6.18841	-5.94813
HOMO-4	-7.43986	-6.62679	-6.64856	-6.34243	-6.42597	-5.63847	-5.47384
HOMO-3	-7.27687	-6.35494	-6.38460	-6.10324	-6.04688	-5.62486	-5.47139
HOMO-2	-7.04339	-5.67874	-5.70242	-5.65425	-5.47855	-5.62296	-5.44636
HOMO-1	-6.98815	-5.67112	-5.69425	-5.63357	-5.44445	-5.56581	-5.39656
HOMO	-5.51656	-5.30839	-5.34214	-5.14023	-5.17315	-5.05125	-5.06077
LUMO	-3.24713	-3.22591	-3.48496	-3.31679	-2.94237	-2.90889	-2.97828
LUMO+1	-2.01609	-2.06017	-2.47079	-2.57310	-1.69608	-1.60465	-1.85173
LUMO+2	-1.00491	-1.26260	-1.44274	-1.50315	-0.98069	-0.96682	-1.38533
LUMO+3	-0.57307	-0.62477	-0.72137	-0.93716	-0.44980	-0.54286	-0.82559
LUMO+4	0.05523	-0.47238	-0.49470	-0.53878	-0.34667	-0.42721	-0.35619
LUMO+5	0.76681	-0.16435	-0.47892	-0.45388	-0.27646	-0.41905	-0.32599
LUMO+6	1.35512	0.16490	-0.21605	-0.25986	-0.22041	-0.20435	-0.28272

Table S4: Energies of the Frontier Orbitals HOMO-n to LUMO+n (n=0, 1, 2, 3, 4, 5 & 6) obtained from TD-DFT carried out at B3LYP/6-31G level in gas phase.

Compound	5	9a	9b	9c	9d	9e	9f
HOMO-6	-7.68041	-7.08067	-7.04856	-6.80012	-6.75931	-6.15004	-5.97317
HOMO-5	-7.34490	-6.85808	-6.87876	-6.73264	-6.65781	-6.06351	-5.85317
HOMO-4	-7.27088	-6.75650	-6.85019	-6.32501	-6.47440	-5.62894	-5.49425
HOMO-3	-7.26190	-6.35005	-6.47386	-6.10950	-5.97453	-5.62677	-5.49289
HOMO-2	-7.10217	-5.79983	-5.89453	-5.77670	-5.52853	-5.60962	-5.44064
HOMO-1	-7.01183	-5.77316	-5.87330	-5.73589	-5.46595	-5.54677	-5.40091
HOMO	-5.48717	-5.20853	-5.34948	-5.07601	-4.99301	-4.79628	-4.82267
LUMO	-3.22808	-3.10427	-3.47543	-3.31788	-2.75705	-2.64494	-2.73256
LUMO+1	-1.99024	-1.94643	-2.47215	-2.54807	-1.59431	-1.40873	-1.70261
LUMO+2	-1.00382	-1.20464	-1.49281	-1.49172	-0.85960	-0.83484	-1.26832
LUMO+3	-0.75457	-0.61987	-0.80709	-0.97933	-0.43647	-0.45689	-0.67593
LUMO+4	-0.00013	-0.59184	-0.69062	-0.58177	-0.36898	-0.42531	-0.33334
LUMO+5	0.75130	-0.19456	-0.34830	-0.562187	-0.28925	-0.40925	-0.31456
LUMO+6	1.30206	0.15156	-0.28762	-0.16925	-0.24299	-0.13932	-0.25034

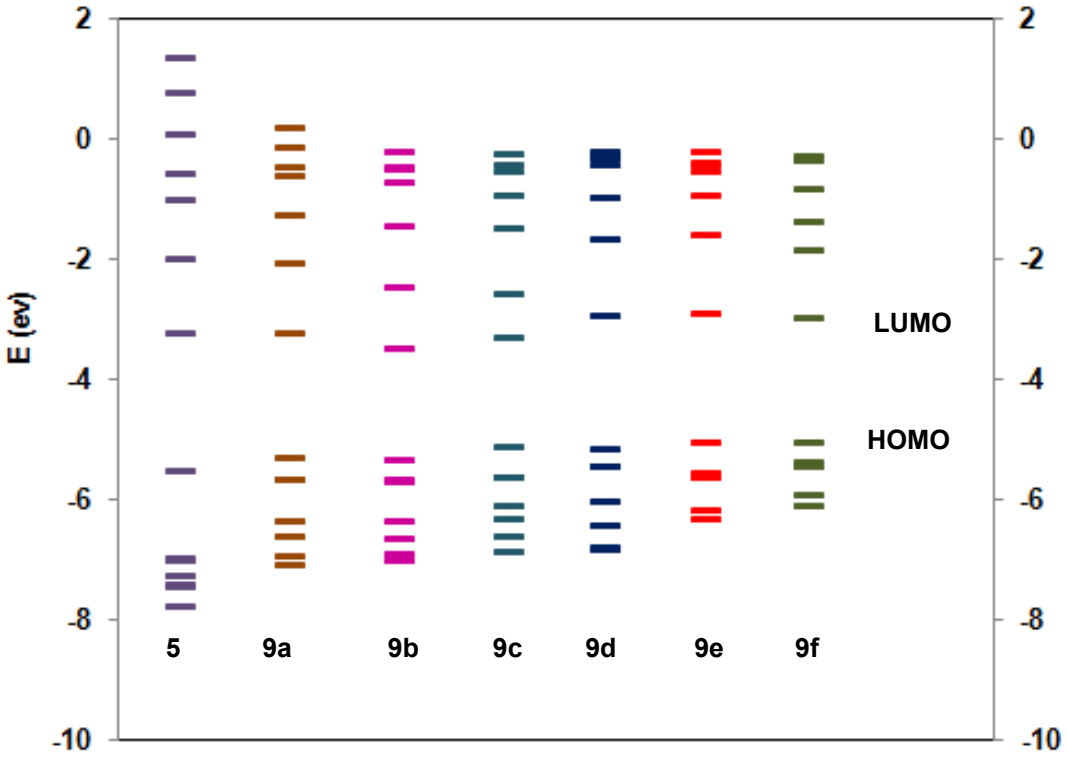


Figure S18: B3LYP/6-31G predicted energy level diagram for the dyads **5** & **9a-9f**.

Frontier Molecular Orbitals

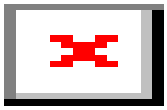
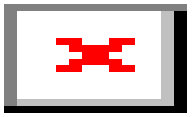
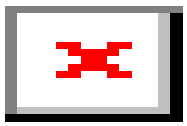
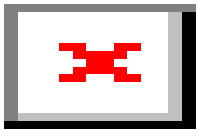
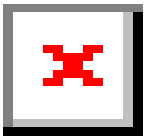
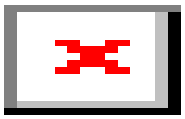
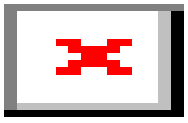
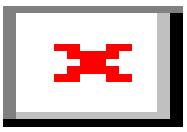
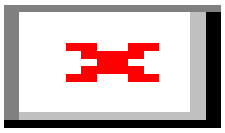
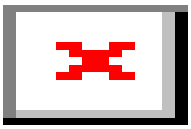
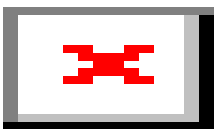
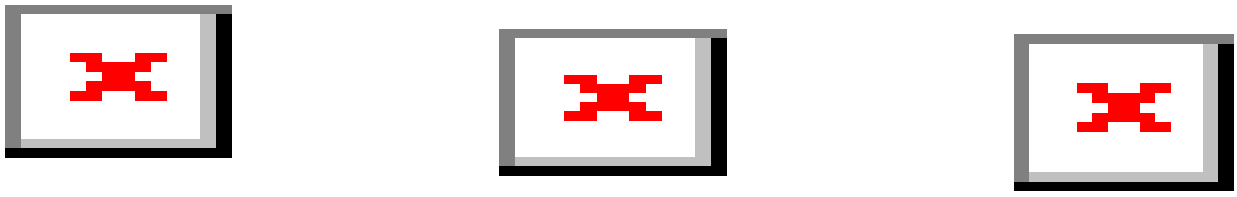
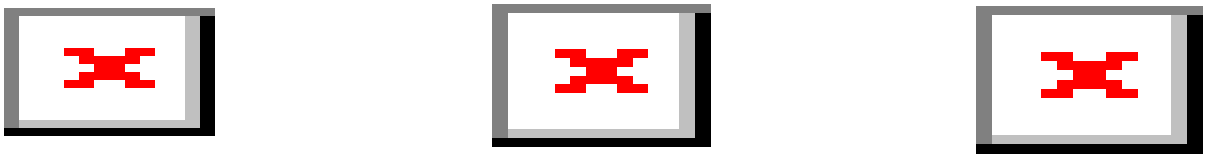
	5	9a	9b	9c
LUMO				
HOMO				
HOMO-2				
HOMO-3				
HOMO-4				

Figure S19: Contour Surfaces of frontier molecular orbitals involved in electronic transitions of the dyads **5**& **9a- 9c**, obtained from TD-DFT calculations using dichloromethane as solvent at an iso-surface value of 0.02 au.

9d	9e	9f



LUMO



HOMO

Figure S20: Contour Surfaces of frontier molecular orbitals involved in electronic transitions of the dyads **9d- 9f**, obtained from TD-DFT calculations using dichloromethane as solvent at an iso-surface value of 0.02 au.

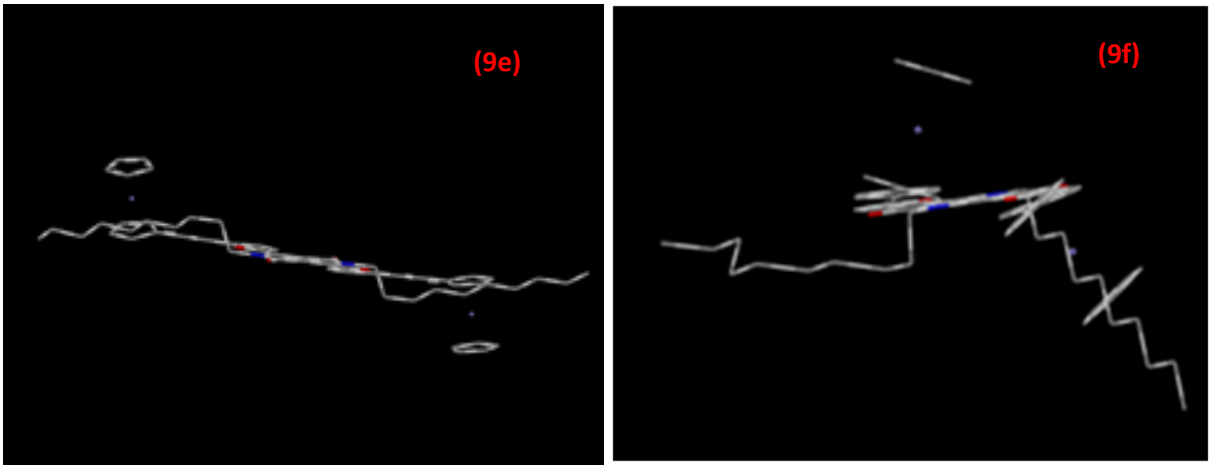


Figure S21. Gaussian optimized structures of **9e** & **9f** depicting their non-centrosymmetric nature in one of the possible minimum energy optimized structures.

Table S5. Cartesian coordinates from the optimized structure of **5** at B3LYP/6-31G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.657374	-1.156551	-0.173254
2	6	0	1.141984	-2.437340	-0.260245
3	1	0	0.087208	-2.676152	-0.275889
4	6	0	2.249860	-3.337842	-0.334424
5	6	0	3.382131	-2.571893	-0.289321
6	8	0	3.066015	-1.231763	-0.185379
7	1	0	2.211060	-4.411320	-0.415200
8	6	0	1.015385	0.112938	-0.104115
9	6	0	-0.362085	0.334653	-0.116135
10	6	0	0.662445	2.418987	0.019875

11	6	0	-0.606885	1.731566	-0.042743
12	6	0	-1.623872	-0.356552	-0.184325
13	6	0	-1.984031	1.950450	-0.060673
14	8	0	-1.922857	-1.571651	-0.260744
15	8	0	0.967878	3.630266	0.097406
16	7	0	1.641549	1.360254	-0.017197
17	7	0	-2.605865	0.698733	-0.149455
18	6	0	-2.628547	3.222602	-0.010707
19	6	0	-4.340363	4.678657	0.028315
20	6	0	-3.171209	5.412460	0.090275
21	6	0	3.081112	1.666188	0.027477
22	1	0	3.150246	2.669936	0.457422
23	1	0	3.561069	0.960868	0.706675
24	6	0	3.751410	1.641647	-1.357988
25	1	0	3.583765	0.662569	-1.822430
26	1	0	3.263767	2.391457	-1.994222
27	6	0	5.268354	1.920469	-1.301199
28	1	0	5.651994	1.914319	-2.331538
29	1	0	5.444196	2.936818	-0.917166
30	6	0	6.078272	0.911190	-0.460214
31	1	0	5.847621	1.047600	0.606904
32	1	0	5.772614	-0.115733	-0.704098
33	6	0	7.598850	1.054071	-0.655316
34	1	0	7.900227	2.089814	-0.434646
35	1	0	7.845834	0.881889	-1.714294
36	6	0	8.418785	0.089831	0.221188
37	1	0	8.178895	0.271137	1.280286
38	1	0	8.108323	-0.945376	0.010760

39	6	0	9.939048	0.218226	0.017234
40	1	0	10.245467	1.254897	0.225875
41	1	0	10.180944	0.034046	-1.040933
42	6	0	10.759878	-0.739784	0.899344
43	1	0	10.514532	-0.559544	1.957489
44	1	0	10.459264	-1.777737	0.687466
45	6	0	12.280942	-0.603753	0.702863
46	1	0	12.580357	0.433374	0.914782
47	1	0	12.526129	-0.783467	-0.354451
48	6	0	13.092657	-1.563077	1.587967
49	1	0	12.838876	-2.608732	1.372402
50	1	0	14.170206	-1.440869	1.427899
51	1	0	12.889906	-1.384786	2.651588
52	6	0	-4.041207	0.376514	-0.160284
53	1	0	-4.561295	1.101474	-0.789711
54	1	0	-4.107575	-0.608858	-0.627836
55	6	0	-4.660420	0.342706	1.249333
56	1	0	-4.142102	-0.420658	1.845064
57	1	0	-4.484577	1.309628	1.736540
58	6	0	-6.175174	0.052161	1.232953
59	1	0	-6.563946	0.182972	2.252886
60	1	0	-6.683713	0.807775	0.613870
61	6	0	-6.555254	-1.356805	0.736573
62	1	0	-6.232172	-1.491948	-0.305879
63	1	0	-6.007202	-2.106714	1.326979
64	6	0	-8.066627	-1.638261	0.831120
65	1	0	-8.608433	-0.883469	0.243345
66	1	0	-8.393445	-1.509654	1.874827

67	6	0	-8.448551	-3.052627	0.353740
68	1	0	-8.152770	-3.173030	-0.699980
69	1	0	-7.856748	-3.784774	0.922800
70	6	0	-9.945443	-3.399189	0.503559
71	1	0	-10.074613	-4.472080	0.306924
72	1	0	-10.250255	-3.238384	1.549694
73	6	0	-10.879363	-2.595972	-0.423314
74	1	0	-10.751295	-1.522443	-0.228088
75	1	0	-10.575370	-2.758809	-1.469434
76	6	0	-12.375800	-2.945270	-0.272375
77	1	0	-12.673074	-2.807817	0.778089
78	1	0	-12.965597	-2.222762	-0.853970
79	6	0	-12.743636	-4.368186	-0.727606
80	1	0	-12.240897	-5.132392	-0.123983
81	1	0	-13.823187	-4.540666	-0.644821
82	1	0	-12.458858	-4.529633	-1.775268
83	8	0	-4.019546	3.314559	-0.034948
84	6	0	-2.085943	4.501188	0.066511
85	1	0	-3.118389	6.488056	0.146792
86	1	0	-1.027550	4.718663	0.101044
87	6	0	-5.741863	5.028372	0.018019
88	1	0	-6.436542	4.175371	-0.038867
89	8	0	-6.154506	6.203368	0.069491
90	35	0	5.222233	-2.995618	-0.361954

Table S6. Cartesian coordinates from the optimized structure of **9a** at B3LYP/6-31G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-7.350669	-2.767934	0.375082
2	6	0	-0.022007	-0.630723	-0.312040
3	6	0	0.375534	-1.961091	-0.318207
4	1	0	1.401466	-2.294293	-0.236098
5	6	0	-0.792323	-2.749639	-0.455008
6	6	0	-1.880174	-1.892496	-0.530877
7	6	0	-3.250948	-2.105433	-0.679740
8	6	0	-4.438310	-2.350294	-0.834540
9	6	0	-5.809942	-2.629292	-1.004016
10	6	0	-6.417727	-3.945698	-1.052500
11	1	0	-5.898907	-4.876705	-0.887195
12	6	0	-7.797475	-3.783662	-1.385911
13	1	0	-8.516012	-4.579720	-1.503333
14	6	0	-8.062876	-2.381737	-1.542360
15	1	0	-9.014684	-1.943023	-1.797726
16	6	0	-6.849567	-1.665104	-1.308488
17	1	0	-6.708187	-0.597746	-1.366541
18	6	0	-6.559398	-2.460208	2.277454
19	1	0	-5.519494	-2.284862	2.505044
20	6	0	-7.203665	-3.740209	2.212064
21	1	0	-6.736901	-4.695142	2.395573
22	6	0	-8.582058	-3.525387	1.872888
23	1	0	-9.333627	-4.290722	1.758766
24	6	0	-8.788414	-2.112603	1.729207

25	1	0	-9.722107	-1.629567	1.487542
26	6	0	-7.537739	-1.453819	1.979780
27	1	0	-7.365830	-0.389324	1.959008
28	8	0	-1.416927	-0.568330	-0.440393
29	1	0	-0.843824	-3.825759	-0.498754
30	6	0	0.754514	0.554711	-0.205992
31	6	0	2.148282	0.613275	-0.092964
32	6	0	1.371490	2.805899	-0.085391
33	6	0	2.549671	1.972740	-0.019410
34	6	0	3.321367	-0.220504	-0.026512
35	6	0	3.938811	2.032297	0.090524
36	8	0	3.485494	-1.464154	-0.050179
37	8	0	1.208306	4.047216	-0.055709
38	7	0	0.281059	1.872137	-0.207640
39	7	0	4.412639	0.714544	0.091506
40	6	0	4.719563	3.221438	0.196688
41	6	0	6.579589	4.470218	0.390208
42	6	0	5.502890	5.335166	0.337594
43	6	0	-1.106511	2.360826	-0.243773
44	1	0	-1.045663	3.376374	-0.646988
45	1	0	-1.677579	1.738755	-0.932837
46	6	0	-1.757474	2.399167	1.152100
47	1	0	-1.878630	1.373294	1.524158
48	1	0	-1.069880	2.914482	1.834812
49	6	0	-3.116682	3.126608	1.167538
50	1	0	-3.444466	3.223795	2.212553
51	1	0	-2.981148	4.153080	0.793817
52	6	0	-4.234618	2.434959	0.363023

53	1	0	-3.961512	2.387062	-0.701216
54	1	0	-4.332858	1.391990	0.701098
55	6	0	-5.591531	3.150620	0.499766
56	1	0	-5.490088	4.190097	0.152202
57	1	0	-5.863132	3.209176	1.565134
58	6	0	-6.731482	2.466495	-0.275677
59	1	0	-6.462158	2.407871	-1.341805
60	1	0	-6.832583	1.427159	0.075457
61	6	0	-8.087470	3.181703	-0.133329
62	1	0	-7.990226	4.217376	-0.492906
63	1	0	-8.350220	3.250764	0.933551
64	6	0	-9.231345	2.486123	-0.893188
65	1	0	-8.972026	2.420102	-1.961242
66	1	0	-9.327314	1.448586	-0.535169
67	6	0	-10.588841	3.197845	-0.745499
68	1	0	-10.493571	4.233198	-1.104302
69	1	0	-10.846267	3.265768	0.321819
70	6	0	-11.725506	2.494519	-1.504263
71	1	0	-11.863671	1.466971	-1.144081
72	1	0	-12.677600	3.022909	-1.378870
73	1	0	-11.510093	2.443807	-2.579061
74	6	0	5.801538	0.233949	0.139941
75	1	0	6.358663	0.836902	0.859891
76	1	0	5.736621	-0.791363	0.512273
77	6	0	6.492846	0.262752	-1.236440
78	1	0	5.956049	-0.412911	-1.915853
79	1	0	6.409264	1.274328	-1.652289
80	6	0	7.981941	-0.131711	-1.170799

81	1	0	8.429051	0.035278	-2.161265
82	1	0	8.505990	0.548634	-0.481277
83	6	0	8.248305	-1.589936	-0.748571
84	1	0	7.864148	-1.766531	0.266523
85	1	0	7.687754	-2.266827	-1.411031
86	6	0	9.743669	-1.957396	-0.788028
87	1	0	10.297641	-1.265100	-0.137944
88	1	0	10.128141	-1.797337	-1.807500
89	6	0	10.023654	-3.412912	-0.366934
90	1	0	9.673248	-3.566574	0.665511
91	1	0	9.419914	-4.082083	-0.997686
92	6	0	11.505020	-3.836053	-0.468761
93	1	0	11.567375	-4.922486	-0.318921
94	1	0	11.865457	-3.644547	-1.491669
95	6	0	12.437473	-3.129174	0.534920
96	1	0	12.371715	-2.042188	0.389736
97	1	0	12.081186	-3.326729	1.558178
98	6	0	13.919757	-3.547549	0.426160
99	1	0	14.266226	-3.377705	-0.604276
100	1	0	14.520084	-2.883503	1.063983
101	6	0	14.198015	-5.006702	0.827250
102	1	0	13.685062	-5.716051	0.167826
103	1	0	15.270435	-5.229918	0.780489
104	1	0	13.860654	-5.201008	1.853550
105	8	0	6.107935	3.151117	0.303670
106	6	0	4.325844	4.556015	0.215387
107	1	0	5.570912	6.410496	0.382852
108	1	0	3.301505	4.894727	0.147225

109	6	0	8.006283	4.654401	0.508653
110	1	0	8.598180	3.725233	0.518889
111	8	0	8.549337	5.773737	0.593815

Table S7. Cartesian coordinates from the optimized structure of **9b** at B3LYP/6-31G

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	26	0	-8.038829	-2.591082	0.469602
2	6	0	-0.582066	-0.900592	-0.253986
3	6	0	-0.278718	-2.256272	-0.219769
4	1	0	0.721928	-2.657417	-0.128513
5	6	0	-1.498222	-2.964185	-0.331788
6	6	0	-2.524269	-2.034890	-0.433766
7	6	0	-3.905490	-2.157307	-0.580134
8	6	0	-5.106473	-2.325031	-0.734195
9	6	0	-6.492045	-2.516748	-0.905823
10	6	0	-7.177355	-3.793793	-0.980904
11	1	0	-6.714989	-4.757240	-0.835095
12	6	0	-8.544048	-3.542666	-1.311864
13	1	0	-9.308535	-4.291926	-1.445794
14	6	0	-8.725088	-2.124372	-1.439691
15	1	0	-9.649002	-1.625204	-1.686343
16	6	0	-7.472140	-1.485886	-1.190407
17	1	0	-7.268064	-0.427713	-1.225673
18	6	0	-7.237416	-2.343186	2.376574
19	1	0	-6.191699	-2.212283	2.607435
20	6	0	-7.930909	-3.596042	2.291750

21	1	0	-7.501923	-4.571015	2.461480
22	6	0	-9.299643	-3.322451	1.956095
23	1	0	-10.080435	-4.056059	1.830571
24	6	0	-9.450740	-1.900747	1.833989
25	1	0	-10.365075	-1.378318	1.600336
26	6	0	-8.175503	-1.294990	2.094358
27	1	0	-7.962383	-0.237734	2.089956
28	8	0	-1.969934	-0.744671	-0.383162
29	1	0	-1.625473	-4.034791	-0.342797
30	6	0	0.276067	0.227728	-0.186535
31	6	0	1.673386	0.188570	-0.077873
32	6	0	1.055285	2.429021	-0.139035
33	6	0	2.171933	1.514261	-0.048555
34	6	0	2.782946	-0.727383	0.007287
35	6	0	3.564433	1.476347	0.051978
36	8	0	2.853331	-1.979787	0.019546
37	8	0	0.984664	3.678437	-0.150767
38	7	0	-0.100241	1.574272	-0.229553
39	7	0	3.940162	0.127143	0.089757
40	6	0	4.425615	2.607229	0.117702
41	6	0	6.376519	3.736995	0.267575
42	6	0	5.345031	4.670505	0.185014
43	6	0	-1.448585	2.161374	-0.294693
44	1	0	-1.313171	3.149595	-0.744853
45	1	0	-2.061663	1.550909	-0.957343
46	6	0	-2.099051	2.314648	1.093430
47	1	0	-2.291195	1.320296	1.517539
48	1	0	-1.380225	2.817418	1.752812

49	6	0	-3.405413	3.133203	1.058114
50	1	0	-3.716508	3.334873	2.093068
51	1	0	-3.202291	4.115260	0.604397
52	6	0	-4.575499	2.459727	0.314827
53	1	0	-4.300259	2.268181	-0.732530
54	1	0	-4.771428	1.474447	0.764900
55	6	0	-5.862177	3.305680	0.345972
56	1	0	-5.665887	4.278968	-0.129097
57	1	0	-6.128013	3.523195	1.391911
58	6	0	-7.059090	2.634413	-0.350823
59	1	0	-6.786801	2.395304	-1.390839
60	1	0	-7.271045	1.672779	0.143413
61	6	0	-8.334739	3.496591	-0.347564
62	1	0	-8.126079	4.451388	-0.853661
63	1	0	-8.598343	3.750429	0.690669
64	6	0	-9.537762	2.815783	-1.024703
65	1	0	-9.273089	2.555646	-2.061445
66	1	0	-9.752512	1.863815	-0.513299
67	6	0	-10.810458	3.682792	-1.030938
68	1	0	-10.596763	4.631600	-1.544496
69	1	0	-11.072394	3.946521	0.004351
70	6	0	-12.007749	2.993139	-1.704048
71	1	0	-12.263827	2.057478	-1.190598
72	1	0	-12.896971	3.633846	-1.693060
73	1	0	-11.784885	2.748247	-2.750273
74	6	0	5.290001	-0.454637	0.135625
75	1	0	5.896593	0.112768	0.844770
76	1	0	5.150852	-1.467264	0.522105

77	6	0	5.970603	-0.497455	-1.245620
78	1	0	5.358590	-1.109626	-1.921581
79	1	0	5.993882	0.517809	-1.660254
80	6	0	7.407197	-1.055833	-1.192890
81	1	0	7.866323	-0.923841	-2.183021
82	1	0	8.008302	-0.451097	-0.495575
83	6	0	7.506448	-2.541725	-0.796225
84	1	0	7.119354	-2.688823	0.222518
85	1	0	6.858850	-3.135498	-1.459030
86	6	0	8.945055	-3.088320	-0.865445
87	1	0	9.591053	-2.479917	-0.216440
88	1	0	9.330783	-2.963841	-1.889350
89	6	0	9.044917	-4.572591	-0.465083
90	1	0	8.697347	-4.692813	0.572815
91	1	0	8.348226	-5.151089	-1.089747
92	6	0	10.456862	-5.181965	-0.601056
93	1	0	10.381620	-6.267464	-0.450648
94	1	0	10.814836	-5.037863	-1.632572
95	6	0	11.496301	-4.603010	0.379230
96	1	0	11.577141	-3.518123	0.226006
97	1	0	11.136609	-4.743736	1.410765
98	6	0	12.905007	-5.221461	0.246459
99	1	0	13.254098	-5.100884	-0.790017
100	1	0	13.601488	-4.645993	0.872370
101	6	0	12.986328	-6.704769	0.646342
102	1	0	12.369980	-7.336902	-0.003027
103	1	0	14.016975	-7.073131	0.582584
104	1	0	12.642427	-6.851094	1.678508

105	8	0	5.802953	2.446625	0.225971
106	6	0	4.125241	3.968628	0.091427
107	1	0	5.464929	5.741863	0.191506
108	6	0	7.787655	3.756202	0.376712
109	1	0	3.126969	4.375884	0.012820
110	6	0	8.619427	4.853832	0.438482
111	6	0	10.031292	4.674681	0.547534
112	6	0	8.126579	6.190986	0.397504
113	7	0	11.192698	4.517175	0.637344
114	7	0	7.681438	7.278643	0.360607
115	1	0	8.257918	2.778661	0.414548

Table S8. Cartesian coordinates from the optimized structure of **9c** at B3LYP/6-31G

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	26	0	10.163696	2.042507	0.443574
2	6	0	2.561559	1.205790	-0.283952
3	6	0	2.414496	2.586560	-0.303148
4	1	0	1.466187	3.102967	-0.238428
5	6	0	3.708644	3.146765	-0.428380
6	6	0	4.622012	2.104540	-0.485266
7	6	0	6.009779	2.062884	-0.622783
8	6	0	7.222451	2.091569	-0.772279
9	6	0	8.622039	2.130995	-0.938513
10	6	0	9.438807	3.327720	-1.010893
11	1	0	9.079907	4.334473	-0.866427
12	6	0	10.773286	2.933934	-1.335197

13	1	0	11.613108	3.598310	-1.465425
14	6	0	10.803860	1.504342	-1.462029
15	1	0	11.670741	0.910144	-1.705344
16	6	0	9.488521	1.002396	-1.219006
17	1	0	9.174094	-0.028413	-1.255268
18	6	0	9.332347	1.799989	2.337885
19	1	0	8.279700	1.706681	2.555015
20	6	0	10.073994	3.026685	2.276455
21	1	0	9.679946	4.015058	2.453088
22	6	0	11.435144	2.705264	1.952336
23	1	0	12.244457	3.410042	1.843517
24	6	0	11.533388	1.280345	1.813638
25	1	0	12.429886	0.726280	1.583637
26	6	0	10.233132	0.720585	2.052759
27	1	0	9.979906	-0.327624	2.032022
28	8	0	3.923029	0.888233	-0.392517
29	1	0	3.956725	4.194922	-0.478004
30	6	0	1.580213	0.182608	-0.187666
31	6	0	0.196565	0.378620	-0.108675
32	6	0	0.559724	-1.917877	-0.080686
33	6	0	-0.446364	-0.883938	-0.046375
34	6	0	-0.808307	1.412757	-0.081688
35	6	0	-1.828477	-0.689283	0.015574
36	8	0	-0.740623	2.664604	-0.111894
37	8	0	0.491126	-3.169123	-0.049388
38	7	0	1.805163	-1.199503	-0.173860
39	7	0	-2.053797	0.693345	-0.000394
40	6	0	-2.815303	-1.710171	0.087668

41	6	0	-4.898282	-2.583201	0.198593
42	6	0	-3.991229	-3.637819	0.170863
43	6	0	3.080853	-1.931625	-0.189135
44	1	0	2.837460	-2.926897	-0.573806
45	1	0	3.757933	-1.437747	-0.886006
46	6	0	3.713605	-2.060750	1.209703
47	1	0	4.022785	-1.067912	1.561511
48	1	0	2.943620	-2.426948	1.900730
49	6	0	4.915730	-3.026172	1.240760
50	1	0	5.228285	-3.156833	2.286821
51	1	0	4.589755	-4.018683	0.893643
52	6	0	6.135174	-2.574061	0.413829
53	1	0	5.859505	-2.484243	-0.646946
54	1	0	6.440976	-1.567099	0.736739
55	6	0	7.327202	-3.540935	0.539168
56	1	0	7.014592	-4.543697	0.209473
57	1	0	7.604128	-3.640043	1.600149
58	6	0	8.562738	-3.106218	-0.269062
59	1	0	8.281119	-2.988398	-1.327044
60	1	0	8.889405	-2.112325	0.076809
61	6	0	9.741779	-4.090808	-0.165667
62	1	0	9.413703	-5.083471	-0.510147
63	1	0	10.023220	-4.210844	0.891893
64	6	0	10.977565	-3.657165	-0.974377
65	1	0	10.695845	-3.535528	-2.031810
66	1	0	11.309903	-2.665235	-0.628679
67	6	0	12.153710	-4.646038	-0.875265
68	1	0	11.820141	-5.636722	-1.217627

69	1	0	12.436380	-4.765986	0.181058
70	6	0	13.381711	-4.208622	-1.689438
71	1	0	13.756739	-3.235783	-1.346479
72	1	0	14.200086	-4.932244	-1.599623
73	1	0	13.135011	-4.112901	-2.754393
74	6	0	-3.336345	1.414846	-0.006172
75	1	0	-4.014389	0.931195	0.699612
76	1	0	-3.104005	2.417751	0.359726
77	6	0	-3.976374	1.487488	-1.406332
78	1	0	-3.346305	2.115545	-2.050529
79	1	0	-3.983043	0.481388	-1.843915
80	6	0	-5.418478	2.032432	-1.384394
81	1	0	-5.823974	1.981077	-2.404991
82	1	0	-6.047736	1.366656	-0.773406
83	6	0	-5.562744	3.476066	-0.866017
84	1	0	-5.237112	3.532648	0.183399
85	1	0	-4.887790	4.135593	-1.433295
86	6	0	-7.006414	4.005222	-0.967527
87	1	0	-7.682795	3.315647	-0.444851
88	1	0	-7.319251	3.998649	-2.023522
89	6	0	-7.162843	5.431286	-0.406269
90	1	0	-6.861814	5.439339	0.653207
91	1	0	-6.457982	6.095233	-0.929446
92	6	0	-8.586474	6.015690	-0.530060
93	1	0	-8.545774	7.085249	-0.280954
94	1	0	-8.910841	5.956269	-1.581099
95	6	0	-9.634811	5.321392	0.362432
96	1	0	-9.679687	4.252688	0.117783

97	1	0	-9.308320	5.384857	1.412976
98	6	0	-11.056015	5.912894	0.241402
99	1	0	-11.371850	5.876376	-0.812193
100	1	0	-11.753251	5.264774	0.790698
101	6	0	-11.193445	7.351955	0.768253
102	1	0	-10.572001	8.054902	0.201318
103	1	0	-12.231193	7.700061	0.700097
104	1	0	-10.888979	7.413008	1.821361
105	8	0	-4.169781	-1.382001	0.149169
106	6	0	-2.687246	-3.097306	0.102695
107	1	0	-4.244045	-4.686271	0.197288
108	6	0	-6.311440	-2.435894	0.261931
109	1	0	-1.744874	-3.626100	0.065904
110	1	0	-6.646492	-1.402783	0.279734
111	6	0	-7.222219	-3.454063	0.297412
112	1	0	-6.854361	-4.478306	0.285924
113	6	0	-8.661710	-3.307408	0.355930
114	6	0	-9.471953	-4.585372	0.489253
115	6	0	-9.301150	-2.089821	0.311725
116	6	0	-10.935341	-4.462203	-0.008429
117	1	0	-8.967326	-5.398711	-0.049467
118	6	0	-10.722761	-1.945850	0.401779
119	1	0	-8.721254	-1.181090	0.192136
120	6	0	-11.556607	-3.188891	0.626086
121	1	0	-9.479965	-4.885004	1.550510
122	6	0	-11.327063	-0.695636	0.324115
123	6	0	-10.557251	0.495195	0.160831
124	6	0	-12.741081	-0.541116	0.416460

125	7	0	-9.895876	1.458203	0.027528
126	7	0	-13.909751	-0.429432	0.493637
127	1	0	-12.575308	-3.042152	0.251389
128	1	0	-11.648080	-3.346926	1.713007
129	6	0	-11.740193	-5.697952	0.445932
130	1	0	-12.781429	-5.628597	0.109801
131	1	0	-11.312647	-6.616209	0.025477
132	1	0	-11.742282	-5.793169	1.538716
133	6	0	-10.977831	-4.369898	-1.552390
134	1	0	-10.559649	-5.278519	-2.001932
135	1	0	-12.012232	-4.268356	-1.901089
136	1	0	-10.409149	-3.513532	-1.928659

Table S9. Cartesian coordinates from the optimized structure of **9d** at B3LYP/6-31G

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	26	0	10.855393	-2.497193	-0.881450
2	6	0	9.489356	-2.318173	0.689420
3	6	0	10.280290	-3.519057	0.830406
4	1	0	9.899266	-4.527549	0.863466
5	6	0	11.660367	-3.148283	0.921343
6	1	0	12.491321	-3.825427	1.041937
7	6	0	11.742980	-1.719439	0.828144
8	1	0	12.646009	-1.131491	0.876612
9	6	0	10.414423	-1.206816	0.678651
10	1	0	10.148400	-0.163495	0.616378
11	6	0	9.790361	-2.488039	-2.669278

12	1	0	8.722096	-2.372058	-2.765516
13	6	0	10.492623	-3.730336	-2.518424
14	1	0	10.045871	-4.711754	-2.493299
15	6	0	11.894705	-3.438043	-2.420158
16	1	0	12.687295	-4.161502	-2.310126
17	6	0	12.058573	-2.015193	-2.510698
18	1	0	12.995693	-1.481664	-2.481977
19	6	0	10.757673	-1.427919	-2.664933
20	1	0	10.546543	-0.375571	-2.772965
21	6	0	8.022925	-2.236324	0.639945
22	6	0	7.365444	-1.086672	0.150374
23	6	0	7.222103	-3.305059	1.094259
24	6	0	5.978171	-1.006315	0.112232
25	1	0	7.951390	-0.250126	-0.214981
26	6	0	5.832949	-3.237682	1.055428
27	1	0	7.696254	-4.191445	1.500661
28	6	0	5.180746	-2.085138	0.561694
29	1	0	5.494425	-0.113710	-0.269350
30	1	0	5.238369	-4.071356	1.412934
31	6	0	3.763729	-2.009963	0.517669
32	6	0	2.544182	-1.935890	0.473073
33	6	0	1.150476	-1.890700	0.438988
34	6	0	0.157408	-2.778618	0.823401
35	8	0	0.540826	-0.733604	-0.079398
36	6	0	-1.096173	-2.178639	0.546718
37	1	0	0.325794	-3.751647	1.256672
38	6	0	-0.843787	-0.930257	-0.004813
39	1	0	-2.083568	-2.584942	0.718482

40	6	0	-1.743264	0.075877	-0.457195
41	6	0	-3.137739	0.004018	-0.430777
42	6	0	-2.582297	2.062521	-1.364241
43	6	0	-3.671838	1.202863	-0.977590
44	6	0	-4.228922	-0.859809	-0.058417
45	6	0	-5.064019	1.129281	-0.962737
46	8	0	-4.274543	-2.005145	0.450709
47	8	0	-2.543701	3.202490	-1.886357
48	7	0	-1.400773	1.312676	-1.020551
49	7	0	-5.410475	-0.109753	-0.412594
50	6	0	-5.957619	2.133979	-1.436725
51	6	0	-7.932509	3.075990	-1.889604
52	6	0	-6.978289	3.967442	-2.291722
53	1	0	-7.157717	4.931592	-2.737469
54	6	0	-5.711311	3.370511	-2.004286
55	1	0	-4.725943	3.778999	-2.182951
56	8	0	-7.354172	1.937199	-1.359651
57	35	0	-9.820937	3.131875	-1.930064
58	6	0	-0.065833	1.887687	-1.239536
59	1	0	0.600277	1.103154	-1.603568
60	1	0	-0.198306	2.633714	-2.028886
61	6	0	0.523513	2.556412	0.014385
62	1	0	-0.163569	3.343524	0.352878
63	1	0	0.596114	1.815726	0.820689
64	6	0	1.913273	3.158092	-0.259638
65	1	0	2.589718	2.363295	-0.610070
66	1	0	1.840612	3.888880	-1.079638
67	6	0	2.531284	3.840599	0.974212

68	1	0	1.853206	4.631734	1.328630
69	1	0	2.606394	3.109094	1.793122
70	6	0	3.920477	4.446072	0.704037
71	1	0	4.596818	3.655566	0.342969
72	1	0	3.843540	5.180830	-0.112186
73	6	0	4.544870	5.122017	1.938251
74	1	0	3.867271	5.909751	2.301843
75	1	0	4.625345	4.386065	2.753010
76	6	0	5.931833	5.732081	1.666276
77	1	0	6.608717	4.944896	1.299232
78	1	0	5.850242	6.470186	0.853413
79	6	0	6.559245	6.404560	2.900723
80	1	0	5.882830	7.191175	3.269413
81	1	0	6.643253	5.666648	3.713584
82	6	0	7.945419	7.016841	2.627894
83	1	0	8.620745	6.230747	2.258521
84	1	0	7.860598	7.754466	1.816087
85	6	0	8.564804	7.685430	3.865617
86	1	0	9.548736	8.112980	3.640043
87	1	0	7.924963	8.495809	4.237206
88	1	0	8.692848	6.963038	4.681686
89	6	0	-6.749441	-0.653413	-0.143273
90	1	0	-7.400275	-0.422814	-0.989446
91	1	0	-6.612825	-1.736234	-0.088579
92	6	0	-7.362739	-0.121563	1.166577
93	1	0	-6.764324	-0.486761	2.012141
94	1	0	-7.294151	0.972930	1.170007
95	6	0	-8.838645	-0.529286	1.345701

96	1	0	-9.422662	-0.137049	0.498906
97	1	0	-9.230992	-0.031208	2.244034
98	6	0	-9.077682	-2.046126	1.477226
99	1	0	-8.460390	-2.440252	2.298977
100	1	0	-8.740862	-2.561822	0.566040
101	6	0	-10.554657	-2.400787	1.732632
102	1	0	-10.893956	-1.899789	2.652812
103	1	0	-11.165697	-1.991219	0.915562
104	6	0	-10.798302	-3.916366	1.864212
105	1	0	-10.144870	-4.307951	2.657830
106	1	0	-10.484051	-4.416445	0.934919
107	6	0	-12.257227	-4.308464	2.182666
108	1	0	-12.283723	-5.379516	2.425520
109	1	0	-12.584252	-3.778225	3.090974
110	6	0	-13.254898	-4.020057	1.043305
111	1	0	-13.230789	-2.948836	0.800441
112	1	0	-12.927180	-4.550293	0.135194
113	6	0	-14.712946	-4.416484	1.361663
114	1	0	-15.031599	-3.905056	2.282360
115	1	0	-15.363224	-4.037372	0.560592
116	6	0	-14.939441	-5.930858	1.511115
117	1	0	-14.372862	-6.346381	2.352159
118	1	0	-15.998567	-6.155442	1.684039
119	1	0	-14.628324	-6.464006	0.603445

Table S10. Cartesian coordinates from the optimized structure of **9e** at B3LYP/6-31G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-10.036442	2.139810	-0.246230
2	6	0	-2.446215	1.143053	0.205468
3	6	0	-2.262276	2.516106	0.281967
4	1	0	-1.304030	3.011267	0.203055
5	6	0	-3.537051	3.101952	0.482331
6	6	0	-4.474272	2.082097	0.525422
7	6	0	-5.858326	2.067122	0.707552
8	6	0	-7.064917	2.117250	0.894312
9	6	0	-8.459191	2.181562	1.099245
10	6	0	-9.250277	3.392471	1.205071
11	1	0	-8.875135	4.393634	1.062945
12	6	0	-10.584741	3.021120	1.556609
13	1	0	-11.407957	3.700134	1.714797
14	6	0	-10.640224	1.590964	1.667389
15	1	0	-11.512425	1.010495	1.924576
16	6	0	-9.340473	1.067119	1.387464
17	1	0	-9.045678	0.029982	1.403433
18	6	0	-9.249374	1.933183	-2.163059
19	1	0	-8.201596	1.848823	-2.405917
20	6	0	-9.995232	3.154790	-2.063943
21	1	0	-9.610058	4.147940	-2.233341
22	6	0	-11.346907	2.821328	-1.713152
23	1	0	-12.156771	3.520194	-1.574195
24	6	0	-11.435164	1.393796	-1.595682

25	1	0	-12.323404	0.831416	-1.354015
26	6	0	-10.138217	0.844666	-1.874431
27	1	0	-9.879692	-0.202443	-1.876361
28	8	0	-3.810104	0.854126	0.351348
29	1	0	-3.755343	4.152602	0.588837
30	6	0	-1.496485	0.099055	0.020445
31	6	0	-0.115248	0.261312	-0.115223
32	6	0	-0.541452	-2.022473	-0.230911
33	6	0	0.488664	-1.016552	-0.267255
34	6	0	0.916774	1.266553	-0.144880
35	6	0	1.870547	-0.856491	-0.389149
36	8	0	0.890854	2.517969	-0.054137
37	8	0	-0.514167	-3.273681	-0.322245
38	7	0	-1.760648	-1.275175	-0.044270
39	7	0	2.135939	0.517723	-0.321093
40	6	0	2.825059	-1.899406	-0.557199
41	6	0	4.868637	-2.826989	-0.810059
42	6	0	3.936661	-3.852169	-0.798687
43	6	0	-3.052531	-1.974821	0.005510
44	1	0	-2.817508	-2.990164	0.339967
45	1	0	-3.683332	-1.491622	0.751920
46	6	0	-3.753767	-2.036056	-1.365194
47	1	0	-4.056942	-1.024008	-1.663395
48	1	0	-3.024875	-2.390242	-2.105224
49	6	0	-4.976022	-2.976004	-1.375547
50	1	0	-5.339662	-3.062350	-2.409707
51	1	0	-4.655098	-3.986571	-1.079568
52	6	0	-6.146260	-2.531575	-0.476351

53	1	0	-5.817173	-2.478376	0.571533
54	1	0	-6.450821	-1.510706	-0.753405
55	6	0	-7.358531	-3.476428	-0.571245
56	1	0	-7.047313	-4.492444	-0.283517
57	1	0	-7.686487	-3.542366	-1.620250
58	6	0	-8.548144	-3.045472	0.305270
59	1	0	-8.215812	-2.960550	1.351611
60	1	0	-8.874270	-2.037780	0.001587
61	6	0	-9.746304	-4.009346	0.230888
62	1	0	-9.419954	-5.014593	0.538514
63	1	0	-10.074738	-4.100553	-0.815976
64	6	0	-10.939631	-3.575786	1.101229
65	1	0	-10.611073	-3.480955	2.147832
66	1	0	-11.271293	-2.572064	0.790948
67	6	0	-12.133714	-4.545494	1.032012
68	1	0	-11.801877	-5.547199	1.342440
69	1	0	-12.460668	-4.641373	-0.013963
70	6	0	-13.321283	-4.105540	1.902969
71	1	0	-13.694962	-3.121355	1.592507
72	1	0	-14.153456	-4.815635	1.833787
73	1	0	-13.030408	-4.032525	2.958552
74	6	0	3.434825	1.204746	-0.353978
75	1	0	4.064041	0.733729	-1.111974
76	1	0	3.210460	2.228431	-0.663972
77	6	0	4.147761	1.200894	1.011781
78	1	0	3.534004	1.756552	1.733656
79	1	0	4.214454	0.166596	1.369643
80	6	0	5.565993	1.802303	0.953516

81	1	0	6.046743	1.651090	1.931121
82	1	0	6.167056	1.235509	0.225474
83	6	0	5.619072	3.302753	0.605305
84	1	0	5.208988	3.472500	-0.400848
85	1	0	4.969748	3.858144	1.298994
86	6	0	7.044706	3.882920	0.667058
87	1	0	7.692414	3.311072	-0.013332
88	1	0	7.451679	3.734343	1.679725
89	6	0	7.104180	5.381592	0.314489
90	1	0	6.741926	5.527166	-0.715009
91	1	0	6.400483	5.921536	0.965059
92	6	0	8.501670	6.021938	0.456871
93	1	0	8.397987	7.109693	0.344187
94	1	0	8.874288	5.852091	1.479307
95	6	0	9.544960	5.503344	-0.552618
96	1	0	9.649307	4.415185	-0.441184
97	1	0	9.173500	5.675003	-1.575189
98	6	0	10.941570	6.145848	-0.407383
99	1	0	11.302698	5.992237	0.620622
100	1	0	11.644428	5.610833	-1.061785
101	6	0	10.988232	7.645290	-0.748637
102	1	0	10.366861	8.237808	-0.067644
103	1	0	12.011831	8.032336	-0.681597
104	1	0	10.628933	7.825273	-1.770137
105	8	0	4.190568	-1.603477	-0.660405
106	6	0	2.651833	-3.273503	-0.639691
107	1	0	4.164051	-4.901713	-0.896919
108	6	0	6.259334	-2.789226	-0.927929

109	6	0	7.475730	-2.791158	-1.042865
110	26	0	10.338985	-2.388668	0.271012
111	6	0	10.190353	-0.852430	1.668750
112	6	0	9.382739	-1.967503	2.071865
113	1	0	8.314898	-1.953545	2.224892
114	6	0	10.241237	-3.107013	2.222934
115	1	0	9.934908	-4.095476	2.527211
116	6	0	11.581622	-2.696092	1.912740
117	1	0	12.460059	-3.321360	1.944187
118	6	0	11.550067	-1.302739	1.570260
119	1	0	12.400419	-0.696992	1.298977
120	6	0	9.699989	-1.650000	-1.556788
121	1	0	9.330899	-0.657897	-1.763130
122	6	0	8.882377	-2.777116	-1.151863
123	6	0	9.766274	-3.917212	-1.006601
124	1	0	9.456193	-4.912334	-0.729480
125	6	0	11.093682	-3.492775	-1.323663
126	1	0	11.974675	-4.115304	-1.313915
127	6	0	11.052799	-2.098430	-1.661603
128	1	0	11.897536	-1.493140	-1.951099
129	1	0	9.838267	0.149811	1.481846
130	1	0	1.695028	-3.774765	-0.587777

Table S11. Cartesian coordinates from the optimized structure of **9f** at B3LYP/6-31G

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-14.448485	1.110785	-1.397547
2	6	0	-13.147953	1.357015	0.219633
3	6	0	-14.107926	2.435059	0.163462
4	1	0	-13.876408	3.483507	0.060240
5	6	0	-15.423792	1.879992	0.269174
6	1	0	-16.348031	2.436256	0.268295
7	6	0	-15.296668	0.455668	0.381452
8	1	0	-16.107608	-0.247328	0.489493
9	6	0	-13.902757	0.130075	0.344011
10	1	0	-13.486686	-0.860204	0.440886
11	6	0	-13.318274	1.119578	-3.145154
12	1	0	-12.248562	1.247355	-3.203422
13	6	0	-14.296100	2.168959	-3.184173
14	1	0	-14.090551	3.222638	-3.289254
15	6	0	-15.595520	1.568886	-3.073458
16	1	0	-16.538527	2.092649	-3.082085
17	6	0	-15.420538	0.148493	-2.966635
18	1	0	-16.208952	-0.582724	-2.880810
19	6	0	-14.012748	-0.129327	-3.011142
20	1	0	-13.558585	-1.106746	-2.966592
21	6	0	-11.684131	1.486577	0.226429
22	6	0	-10.847122	0.396130	-0.095254
23	6	0	-11.066885	2.707123	0.571167
24	6	0	-9.462253	0.515441	-0.075528

25	1	0	-11.290367	-0.553628	-0.374844
26	6	0	-9.681831	2.839318	0.588890
27	1	0	-11.682361	3.555949	0.847943
28	6	0	-8.849079	1.744268	0.264929
29	1	0	-8.838351	-0.335354	-0.327090
30	1	0	-9.229821	3.787069	0.860573
31	6	0	-7.435095	1.871164	0.280794
32	6	0	-6.216401	1.969005	0.288648
33	6	0	-4.829811	2.119678	0.308892
34	6	0	-3.988807	3.172003	0.636754
35	8	0	-4.041277	1.017567	-0.070501
36	6	0	-2.652340	2.733789	0.463794
37	1	0	-4.310929	4.147448	0.964901
38	6	0	-2.702483	1.415966	0.030903
39	1	0	-1.739651	3.290793	0.625840
40	6	0	-1.651700	0.512653	-0.294569
41	6	0	-0.283665	0.789347	-0.241317
42	6	0	-0.501252	-1.402517	-0.989915
43	6	0	0.438487	-0.360522	-0.660355
44	6	0	0.654924	1.837401	0.070490
45	6	0	1.806015	-0.077229	-0.624499
46	8	0	0.510595	3.018674	0.467962
47	8	0	-0.358164	-2.577660	-1.405417
48	7	0	-1.790993	-0.806774	-0.744828
49	7	0	1.944431	1.245921	-0.184953
50	6	0	2.855543	-0.967147	-0.988845
51	6	0	4.980368	-1.651943	-1.325665
52	6	0	4.137841	-2.695253	-1.677267

53	1	0	4.458137	-3.657756	-2.043244
54	6	0	2.802910	-2.269581	-1.465539
55	1	0	1.889772	-2.824907	-1.630823
56	8	0	4.194475	-0.567165	-0.894550
57	6	0	-3.020693	-1.589158	-0.932734
58	1	0	-3.776255	-0.952292	-1.396904
59	1	0	-2.751930	-2.386832	-1.631758
60	6	0	-3.560412	-2.198850	0.372596
61	1	0	-2.787819	-2.846065	0.809036
62	1	0	-3.759489	-1.395187	1.092730
63	6	0	-4.848783	-3.006737	0.136417
64	1	0	-5.608386	-2.351682	-0.317468
65	1	0	-4.651366	-3.806833	-0.593472
66	6	0	-5.419657	-3.624518	1.425685
67	1	0	-4.660697	-4.277768	1.882359
68	1	0	-5.615615	-2.823256	2.154487
69	6	0	-6.711598	-4.429442	1.196874
70	1	0	-7.466747	-3.778076	0.729709
71	1	0	-6.513318	-5.236606	0.474833
72	6	0	-7.293219	-5.033751	2.487718
73	1	0	-6.537716	-5.682349	2.957196
74	1	0	-7.494111	-4.225490	3.207766
75	6	0	-8.583653	-5.841350	2.259074
76	1	0	-9.337347	-5.194026	1.784207
77	1	0	-8.381280	-6.652974	1.543061
78	6	0	-9.170517	-6.438810	3.550619
79	1	0	-8.417465	-7.085276	4.027298
80	1	0	-9.375288	-5.627462	4.266346

81	6	0	-10.460069	-7.248321	3.321732
82	1	0	-11.211405	-6.602432	2.843347
83	1	0	-10.254614	-8.059969	2.607983
84	6	0	-11.040482	-7.838987	4.616613
85	1	0	-11.954070	-8.412645	4.421372
86	1	0	-10.320250	-8.510935	5.100250
87	1	0	-11.289426	-7.047220	5.334561
88	6	0	3.174164	2.016590	0.048563
89	1	0	3.881264	1.805662	-0.756425
90	1	0	2.868457	3.063977	-0.012364
91	6	0	3.818684	1.726564	1.417030
92	1	0	3.097862	1.974915	2.207817
93	1	0	4.025184	0.652172	1.488882
94	6	0	5.129220	2.509093	1.639622
95	1	0	5.834978	2.270837	0.828630
96	1	0	5.596582	2.147255	2.566784
97	6	0	4.955450	4.037319	1.737864
98	1	0	4.215018	4.266095	2.519368
99	1	0	4.540873	4.432159	0.799127
100	6	0	6.270647	4.775869	2.050143
101	1	0	6.688307	4.389661	2.993235
102	1	0	7.006835	4.541356	1.267661
103	6	0	6.091052	6.301762	2.165902
104	1	0	5.319231	6.505345	2.922801
105	1	0	5.697568	6.694085	1.215337
106	6	0	7.372266	7.075955	2.542601
107	1	0	7.095700	8.114146	2.771313
108	1	0	7.788774	6.656228	3.471921

109	6	0	8.462650	7.068765	1.452732
110	1	0	8.742152	6.031035	1.224442
111	1	0	8.045291	7.487671	0.523502
112	6	0	9.740779	7.848767	1.829427
113	1	0	10.142809	7.446909	2.771715
114	1	0	10.507057	7.659031	1.064426
115	6	0	9.539560	9.368048	1.964755
116	1	0	8.838637	9.616385	2.769826
117	1	0	10.487700	9.872206	2.186163
118	1	0	9.143649	9.794692	1.034159
119	26	0	14.740066	-2.134603	-0.377749
120	6	0	13.303029	-0.939750	-1.311992
121	6	0	14.102402	-0.158283	-0.397641
122	1	0	13.732677	0.393447	0.452484
123	6	0	15.472215	-0.236856	-0.808265
124	1	0	16.306549	0.249374	-0.327476
125	6	0	15.539213	-1.071741	-1.972764
126	1	0	16.430896	-1.314991	-2.528925
127	6	0	14.211447	-1.510756	-2.280881
128	1	0	13.930105	-2.122842	-3.123327
129	6	0	13.750098	-3.636821	0.667520
130	1	0	12.680668	-3.768524	0.721234
131	6	0	14.548823	-2.853600	1.566019
132	1	0	14.186528	-2.303484	2.420174
133	6	0	15.915966	-2.943380	1.137349
134	1	0	16.762021	-2.472982	1.613390
135	6	0	15.961923	-3.782204	-0.026334
136	1	0	16.848262	-4.051966	-0.578838

137	6	0	14.622745	-4.211058	-0.316682
138	1	0	14.327107	-4.862021	-1.124478
139	6	0	11.838817	-1.067642	-1.309846
140	6	0	11.195447	-2.159281	-1.931975
141	6	0	11.027722	-0.090027	-0.697267
142	6	0	9.809939	-2.272689	-1.942295
143	1	0	11.792270	-2.933569	-2.402332
144	6	0	9.640045	-0.195788	-0.697760
145	1	0	11.492992	0.772995	-0.233757
146	6	0	9.001499	-1.292037	-1.320867
147	1	0	9.336711	-3.120886	-2.425037
148	1	0	9.035556	0.569433	-0.223076
149	6	0	7.586120	-1.406849	-1.322782
150	6	0	6.367133	-1.500370	-1.318392

1

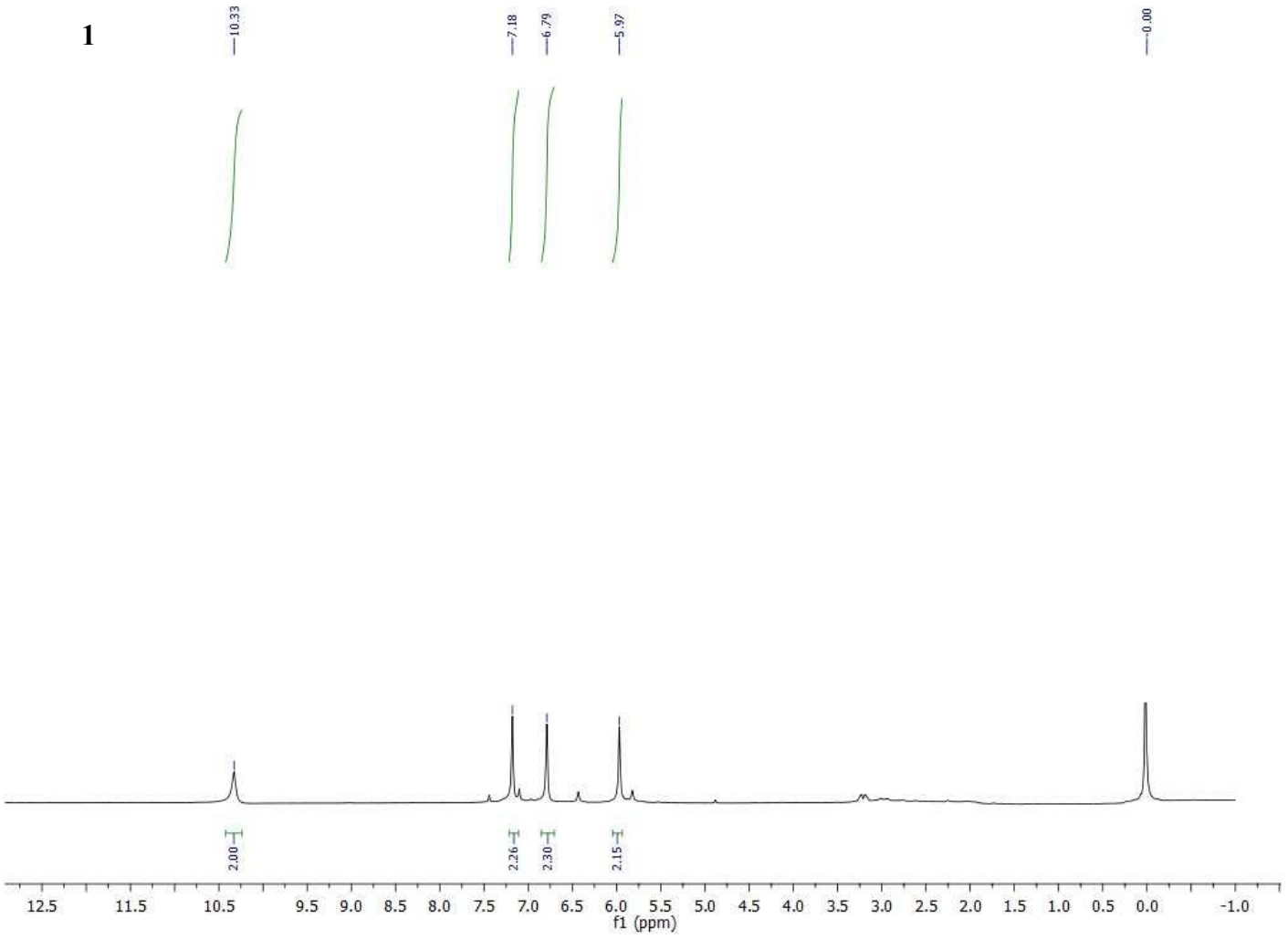


Figure S22: ^{1}H NMR (DMSO-d_6) of **1**.

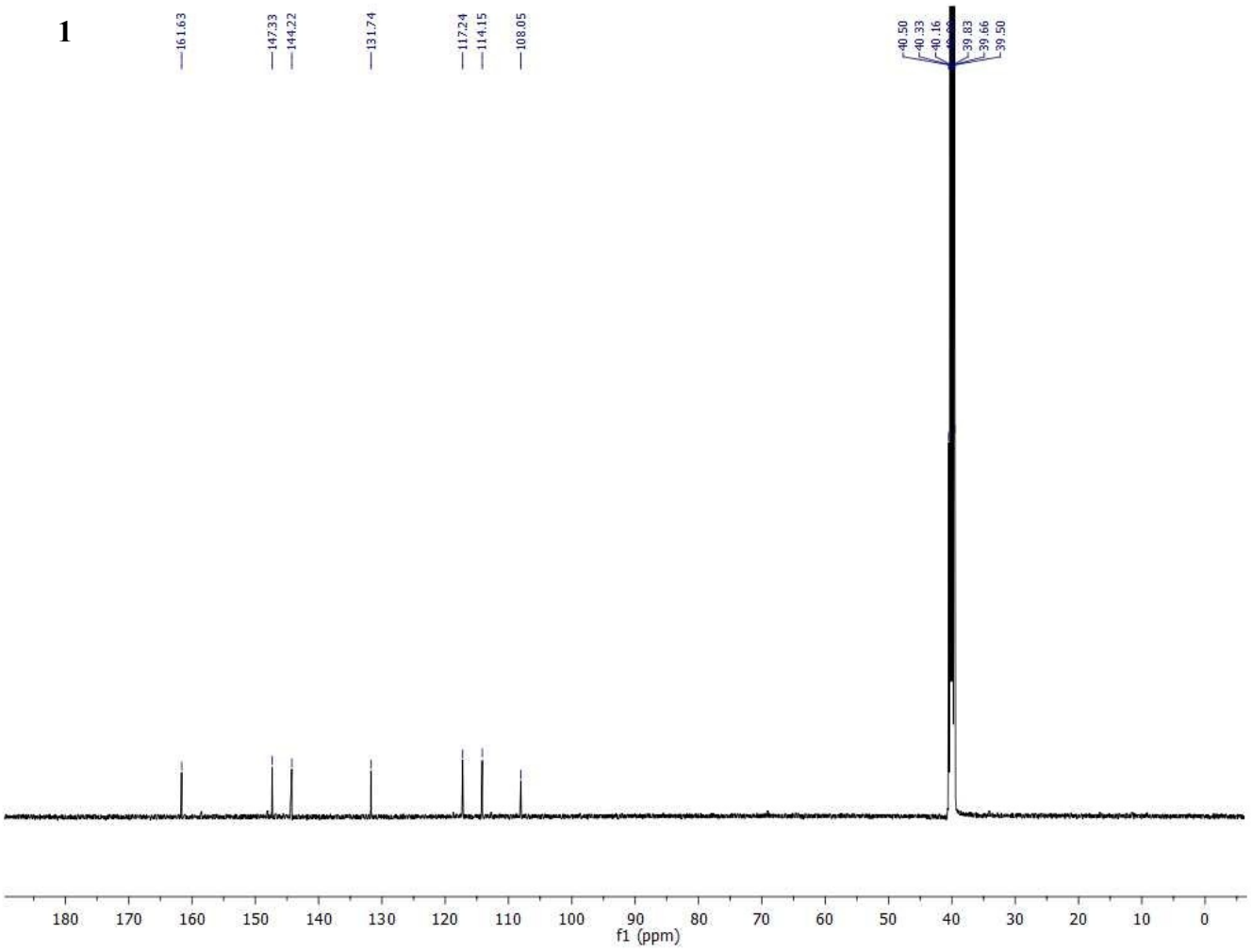


Figure S23: ^{13}C NMR (DMSO-d_6) of **1**.

2

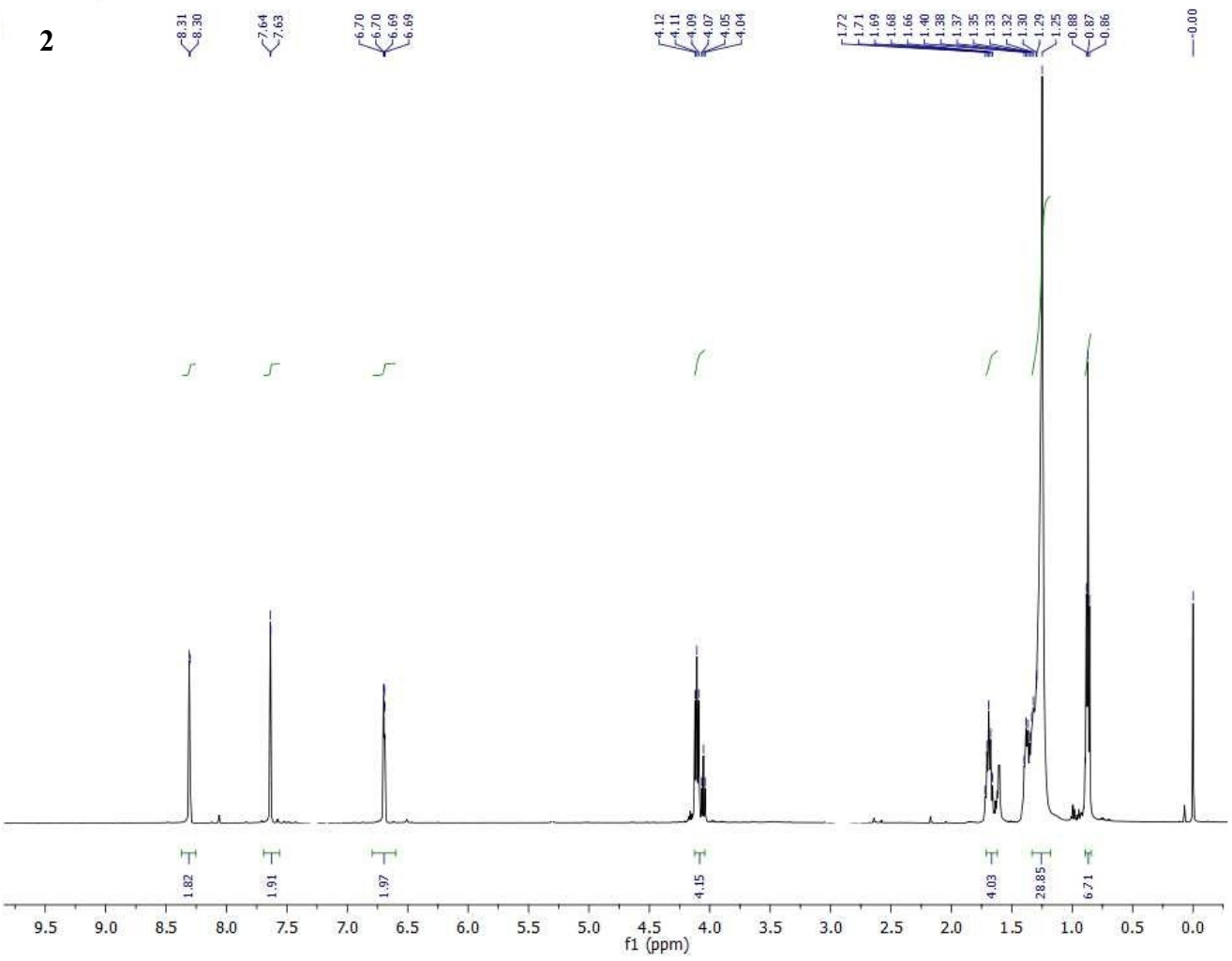


Figure S24: ^{1}H NMR ($CDCl_3$) of **2**.

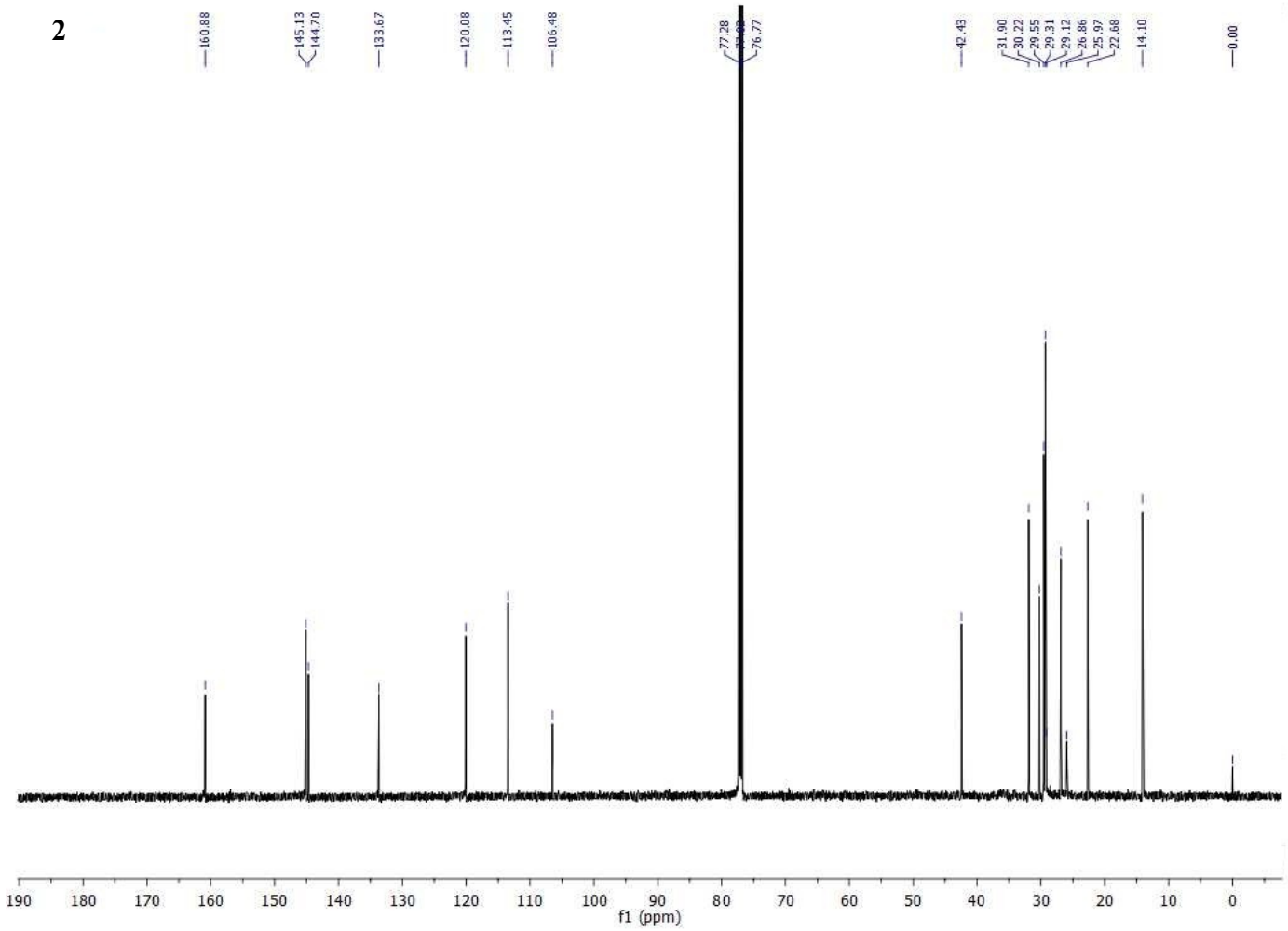


Figure S25: ^{13}C NMR ($CDCl_3$) of **2**.

3

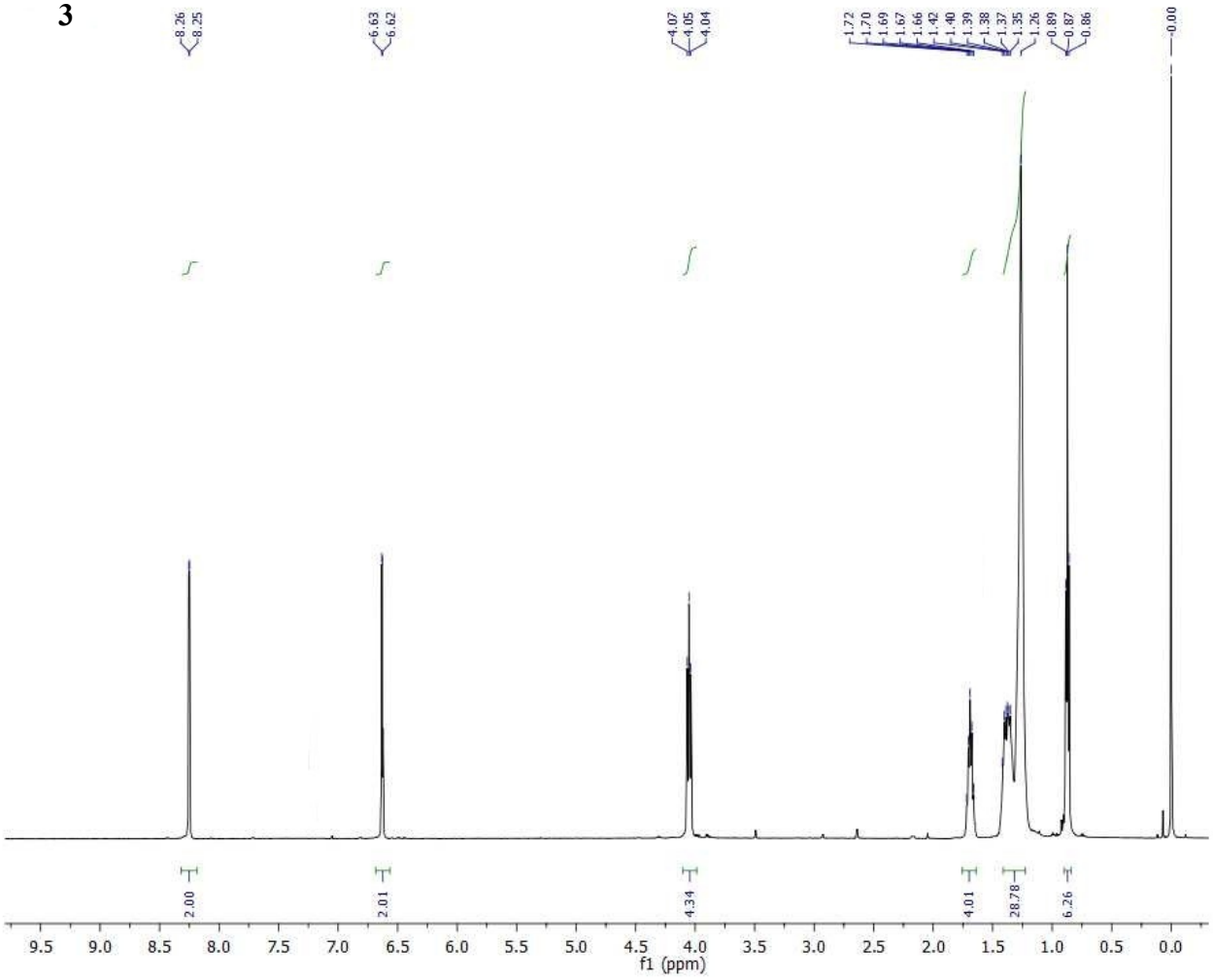


Figure S26: ^{1}H NMR ($CDCl_3$) of **3**.

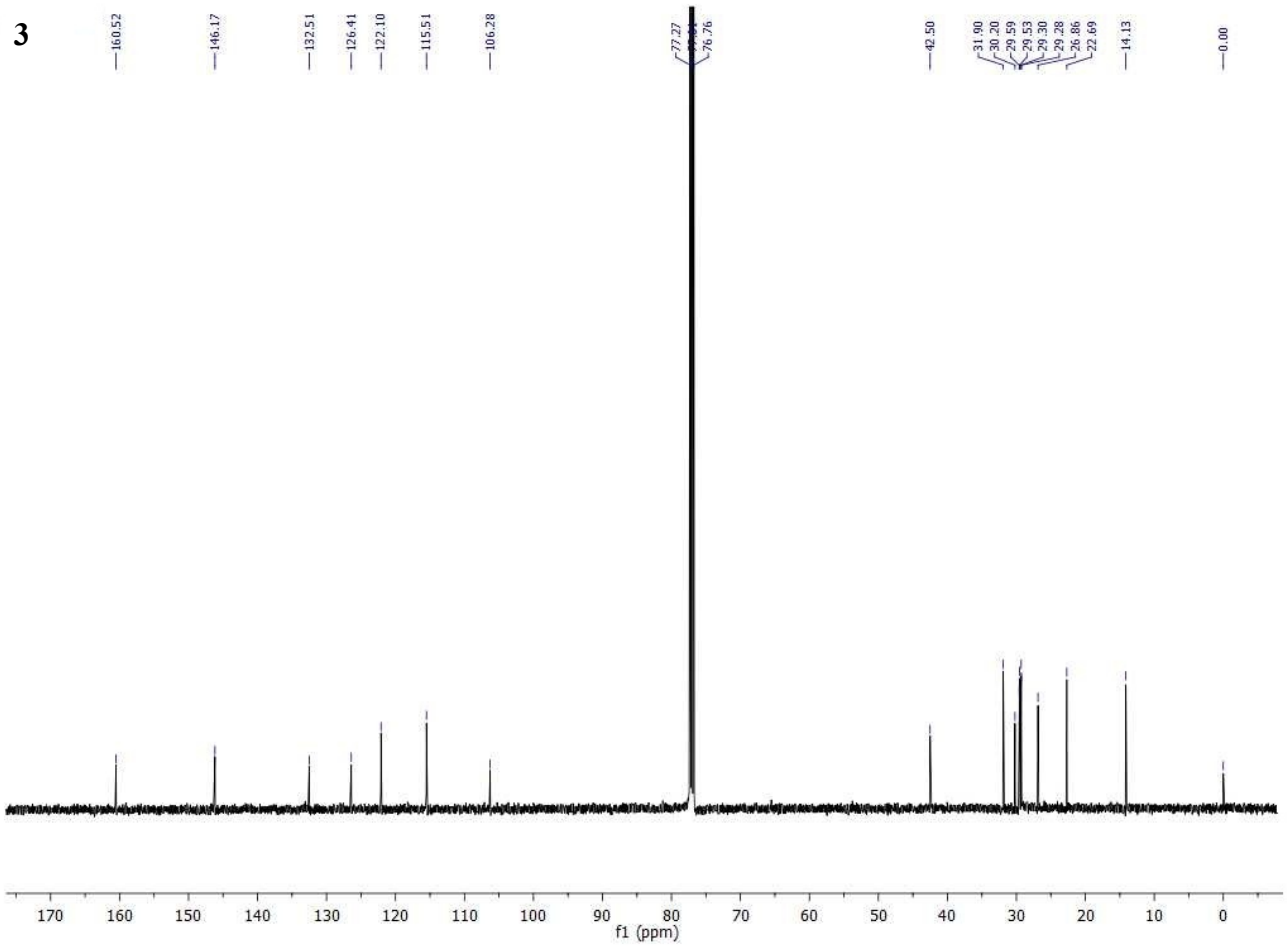


Figure S27: ^{13}C NMR ($CDCl_3$) of **3**.

4

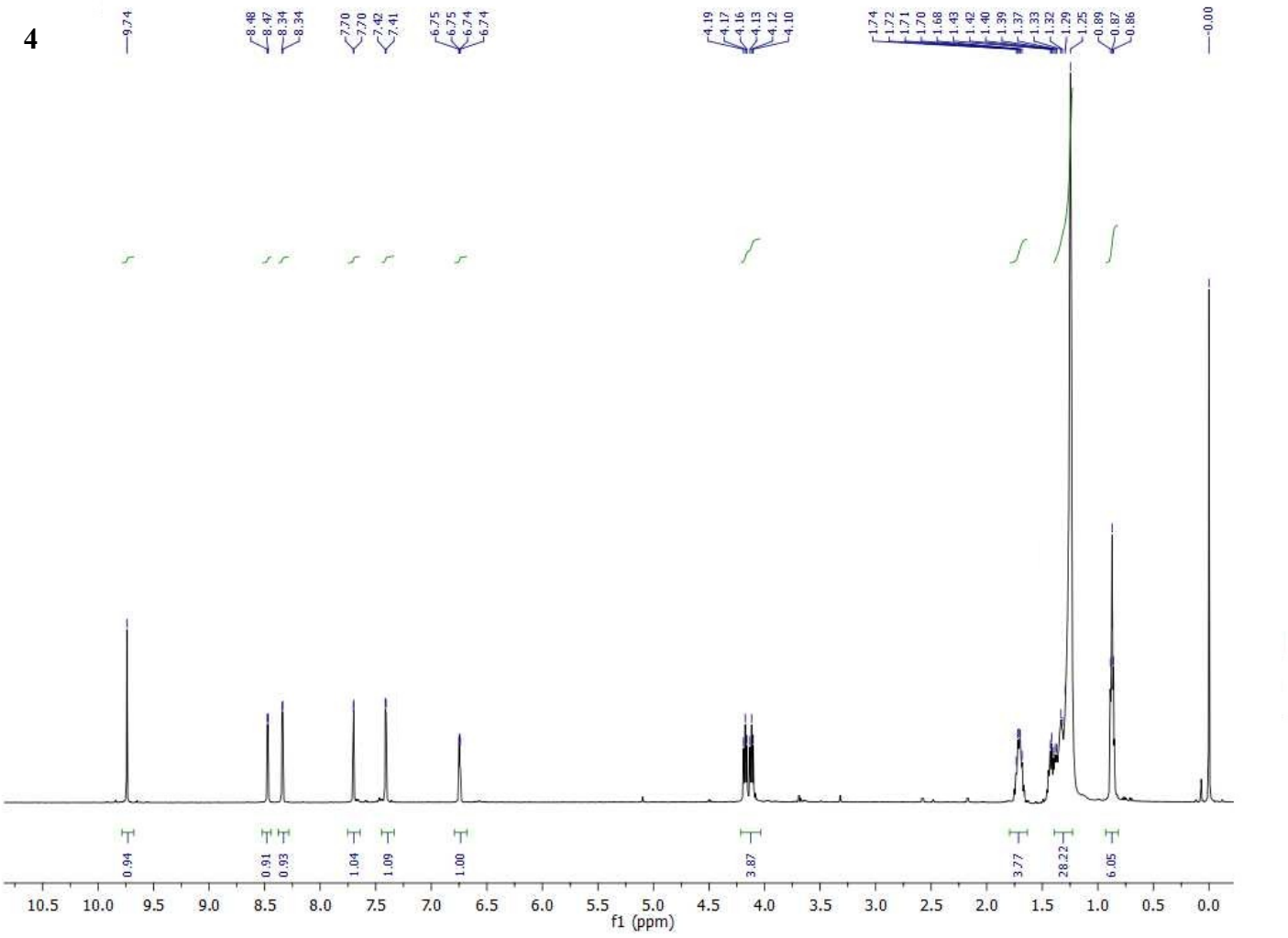


Figure S28: ^{1}H NMR ($CDCl_3$) of **4**.

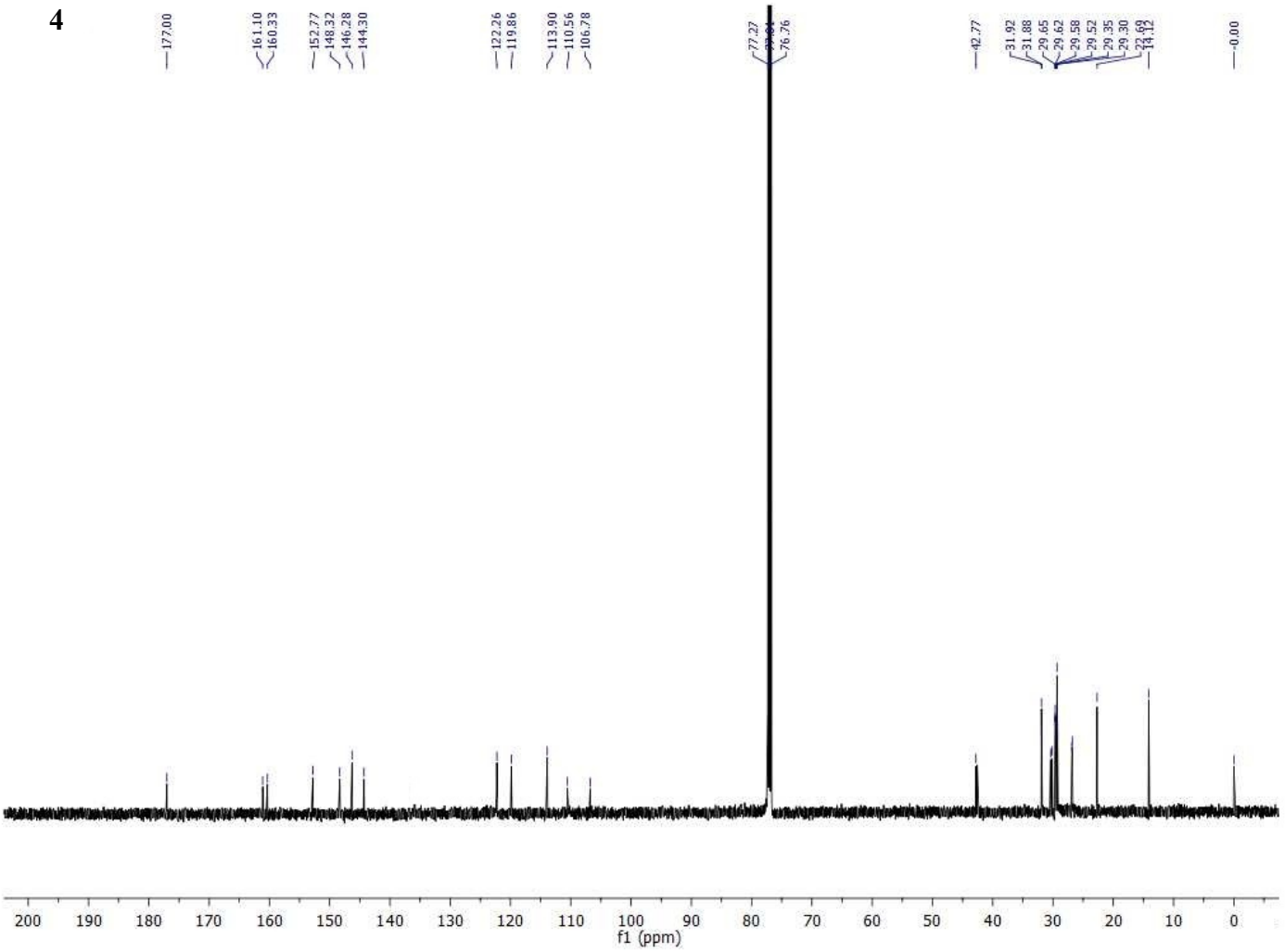


Figure S29: ^{13}C NMR ($CDCl_3$) of **4**.

5

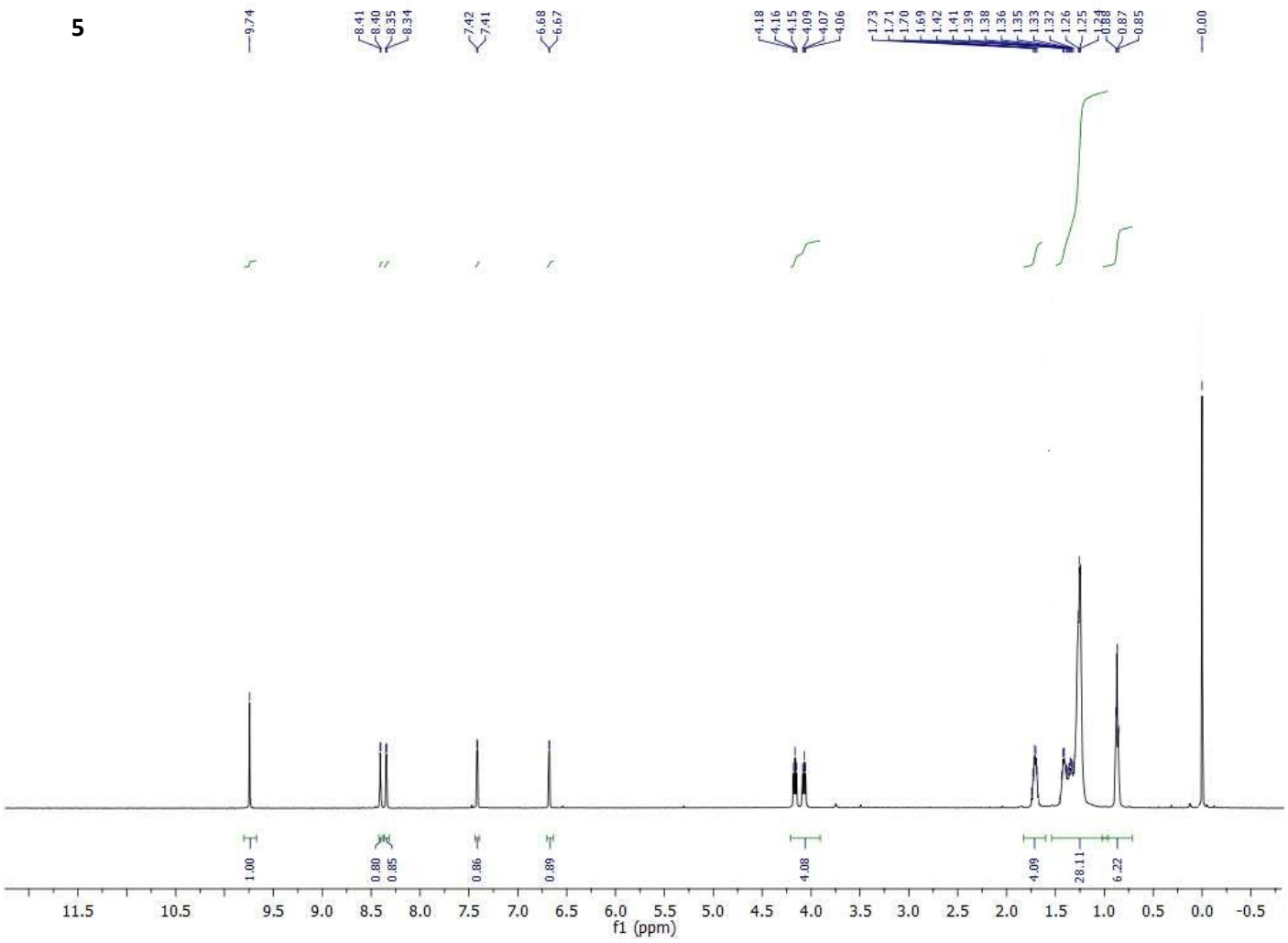


Figure S30: ^{1}H NMR ($CDCl_3$) of **5**.

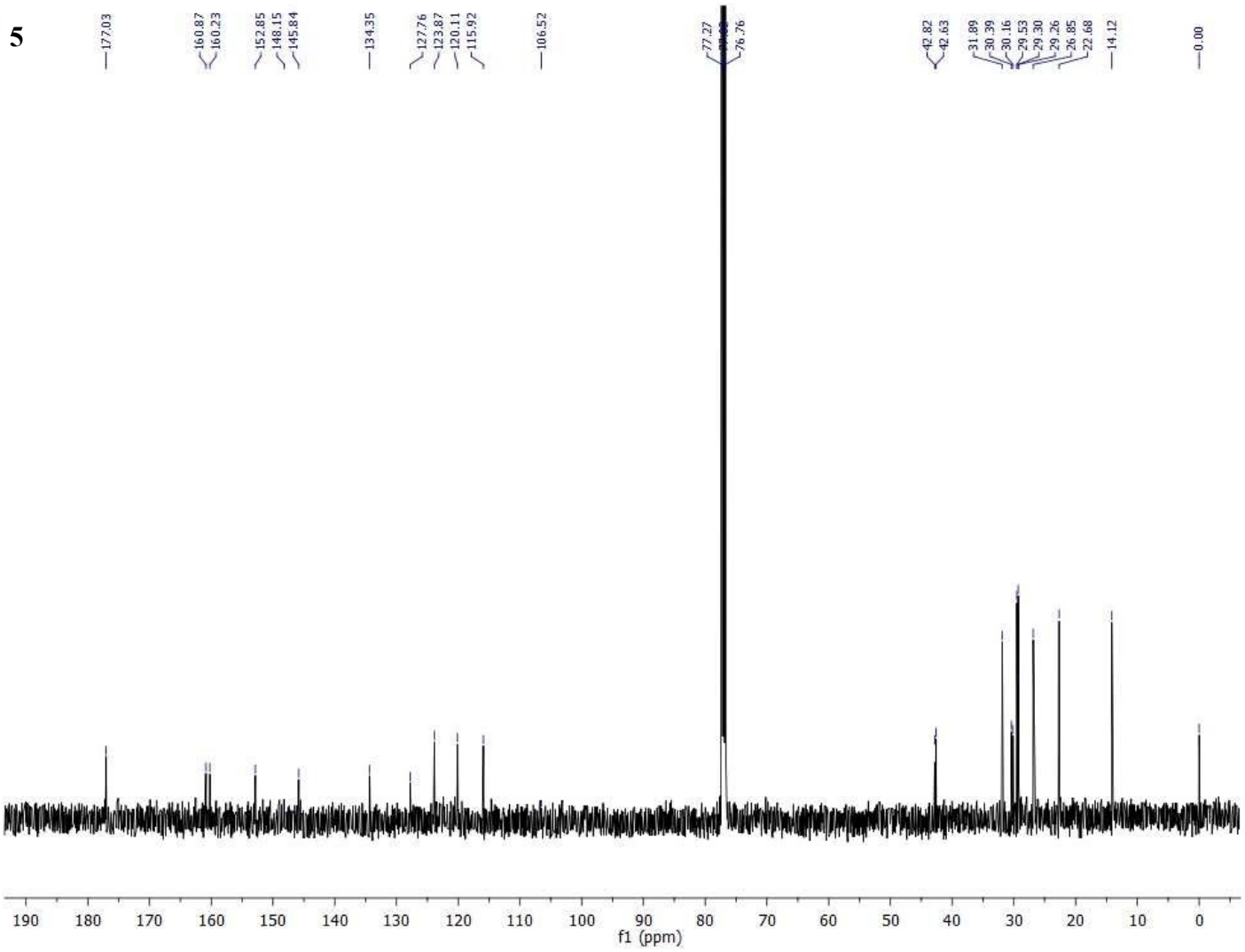


Figure S31: ^{13}C NMR ($CDCl_3$) of **5**.

6b

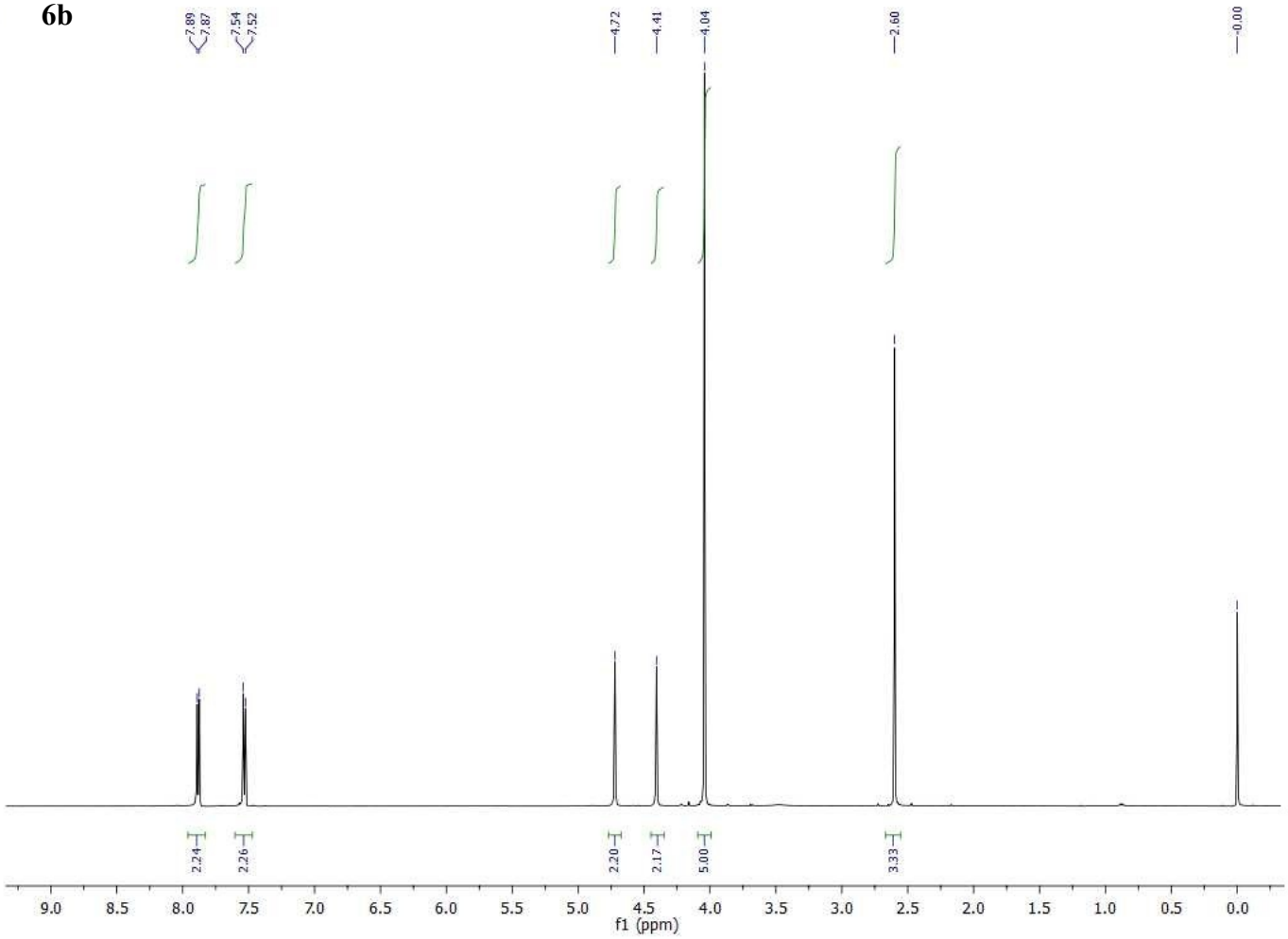


Figure S32: ^{1}H NMR ($CDCl_3$) of **6b**.

6b

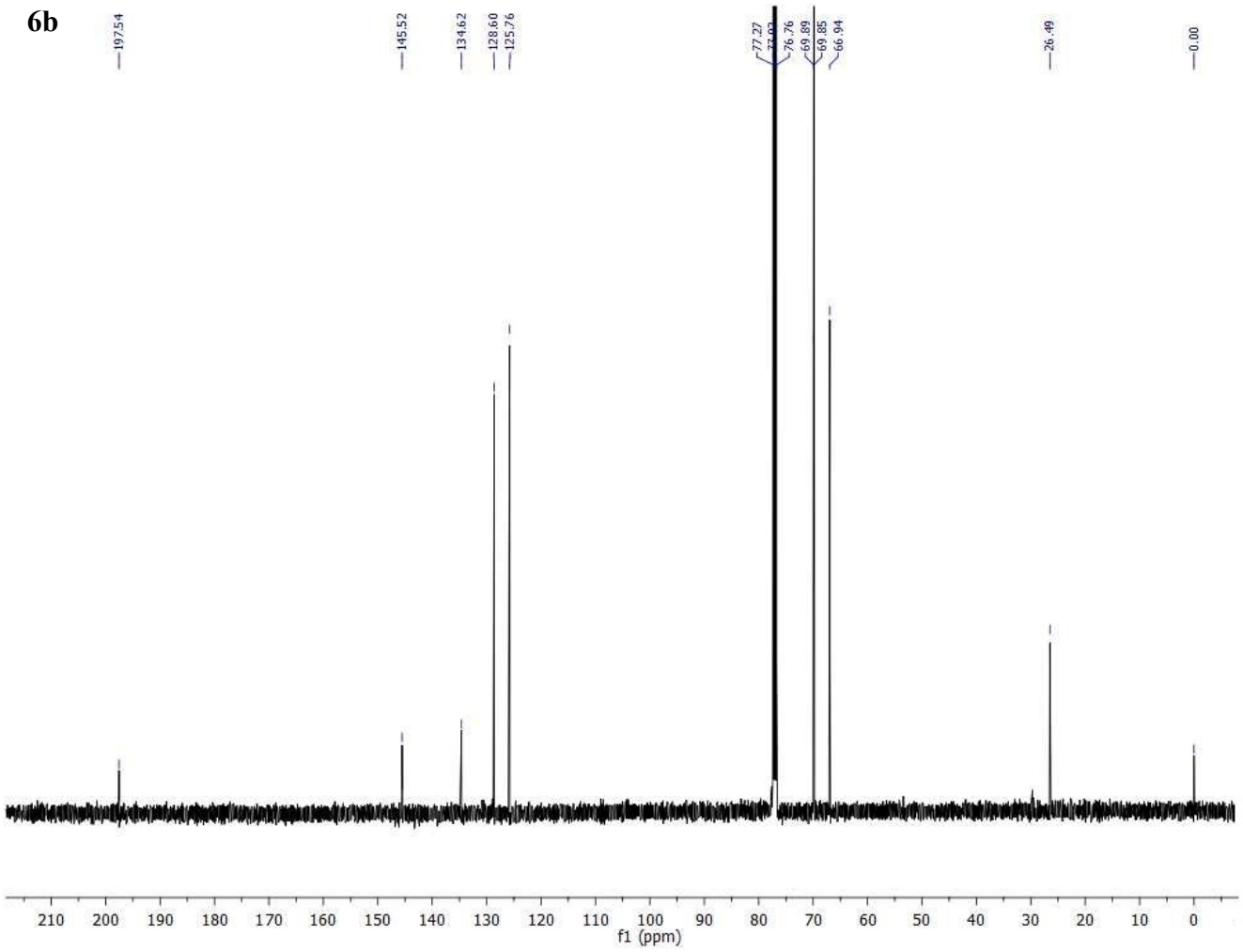


Figure S33: ^{1}H NMR ($CDCl_3$) of **6b**.

7a

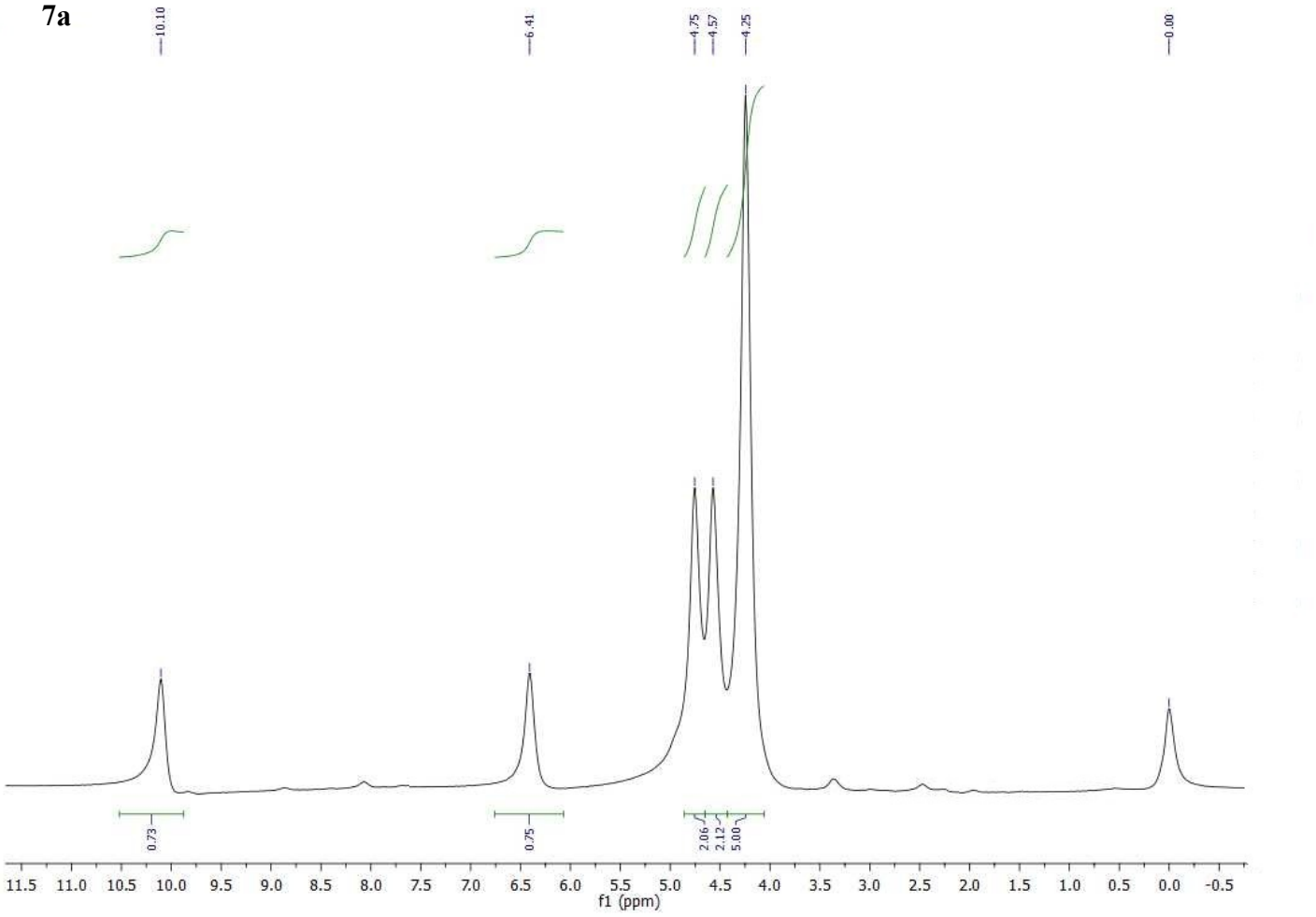


Figure S34: ^{1}H NMR ($CDCl_3$) of **7a**.

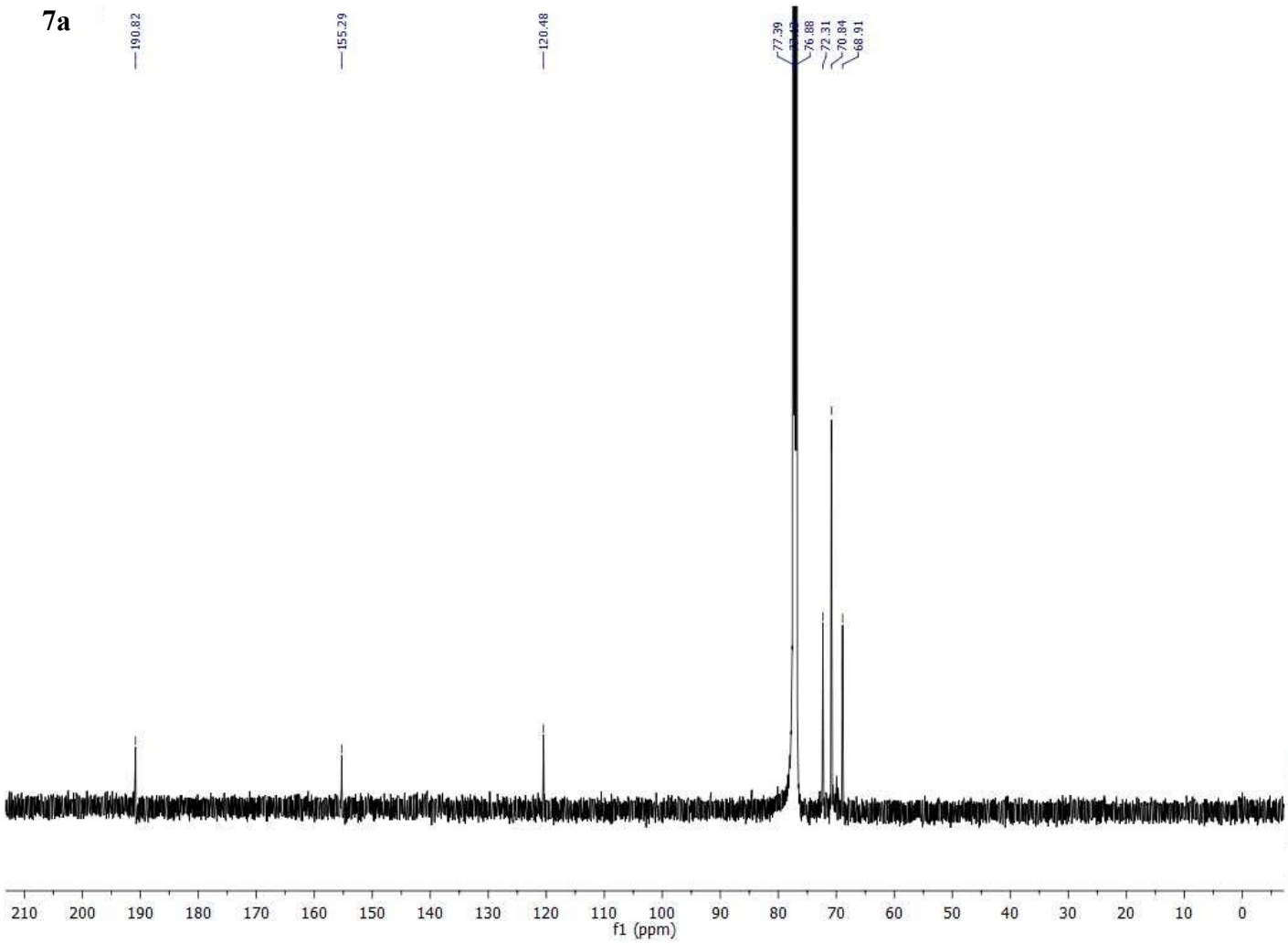


Figure S35: ^{13}C NMR ($CDCl_3$) of **7a**.

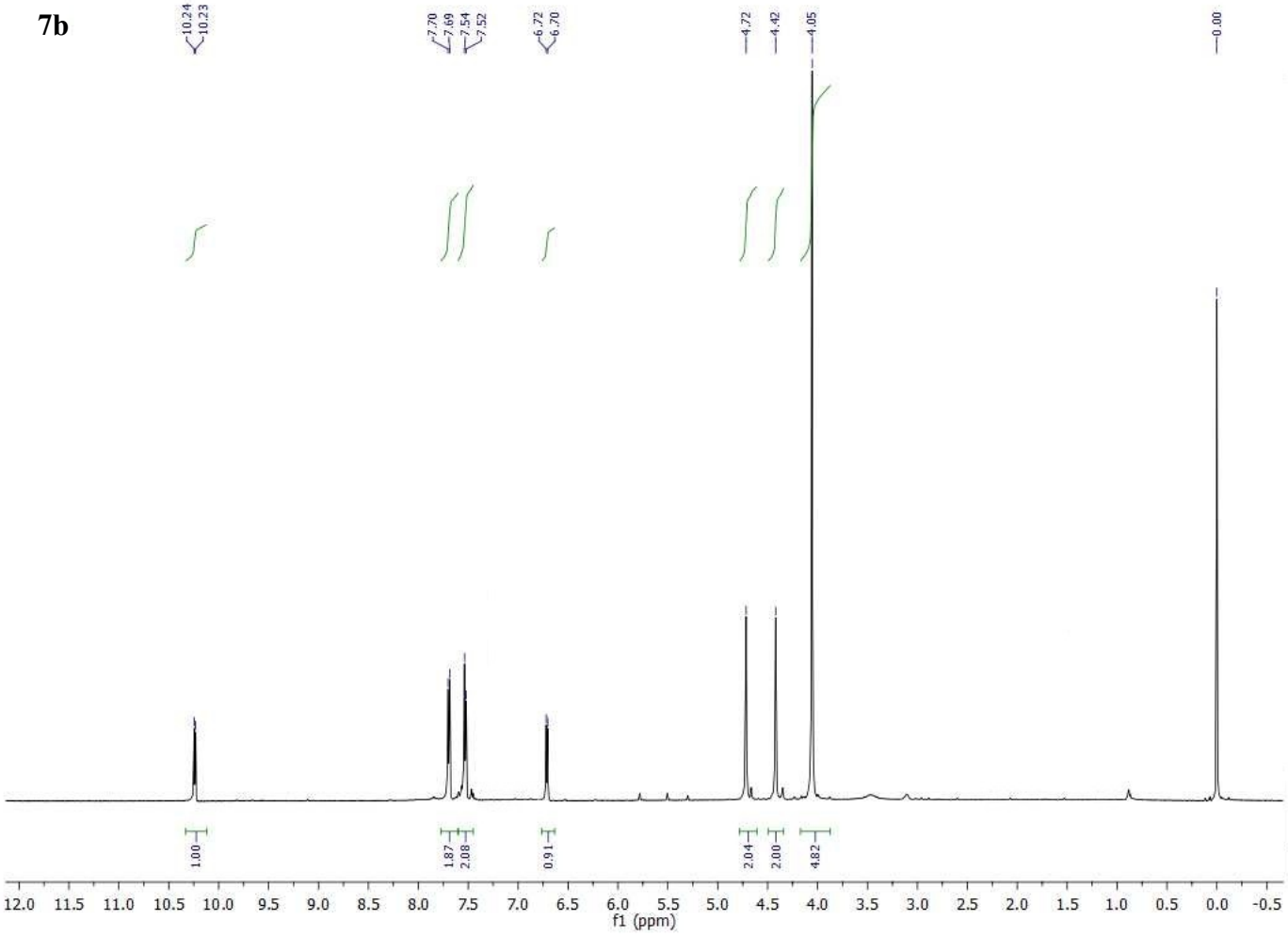


Figure S36: ^{1}H NMR ($CDCl_3$) of **7b**.

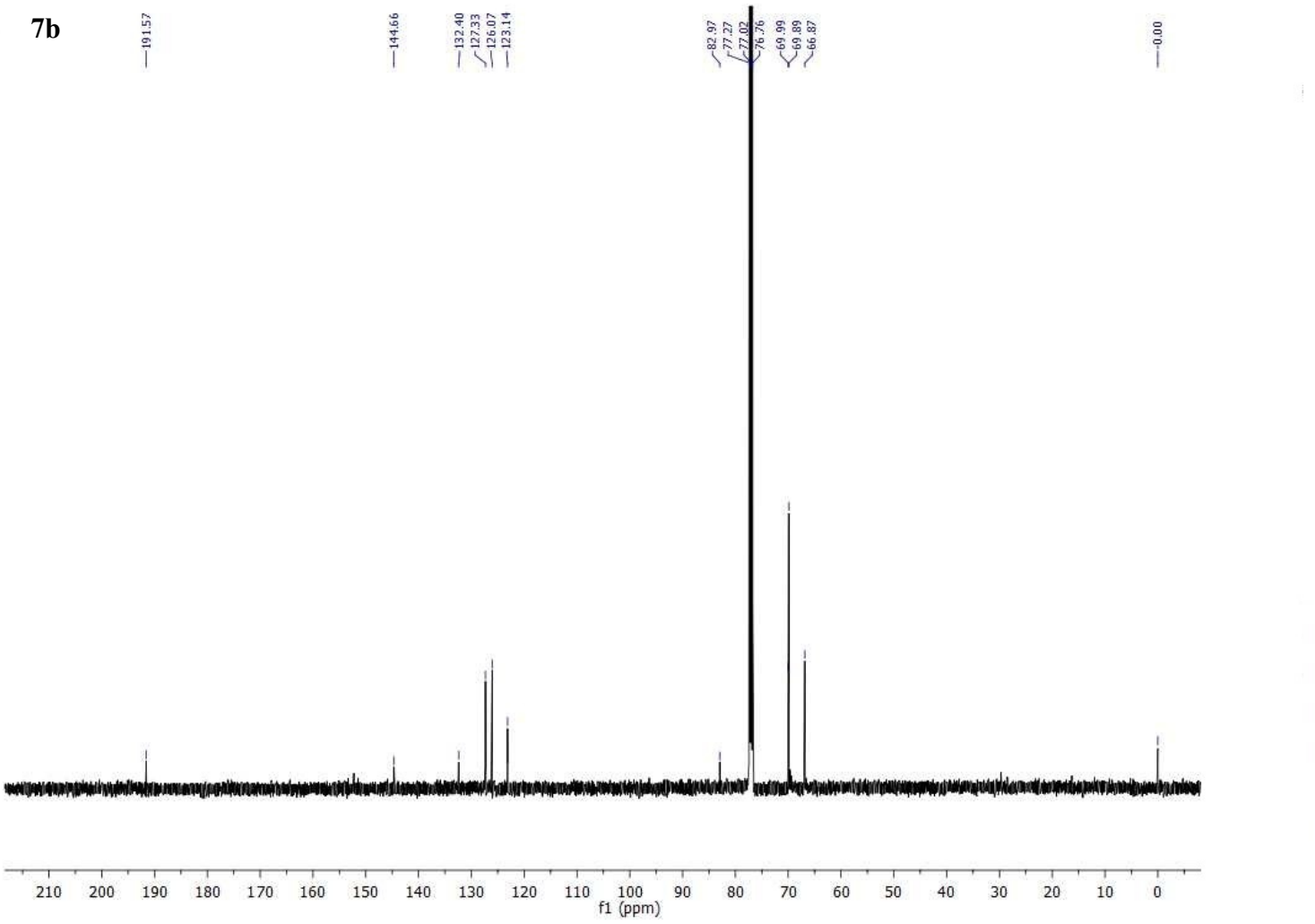


Figure S37: ^{13}C NMR ($CDCl_3$) of **7b**.

8a

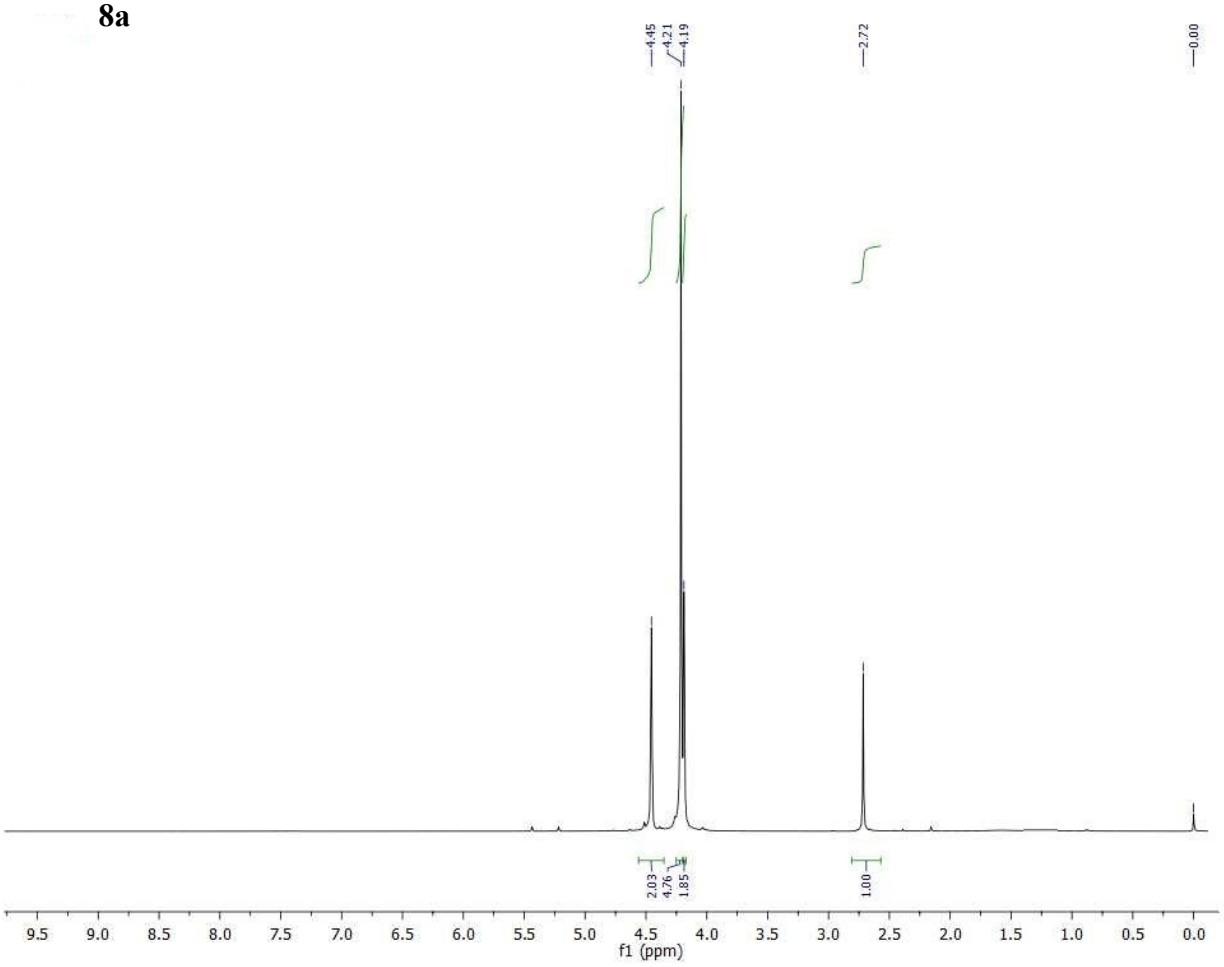


Figure S38: ^{1}H NMR ($CDCl_3$) of **8a**.

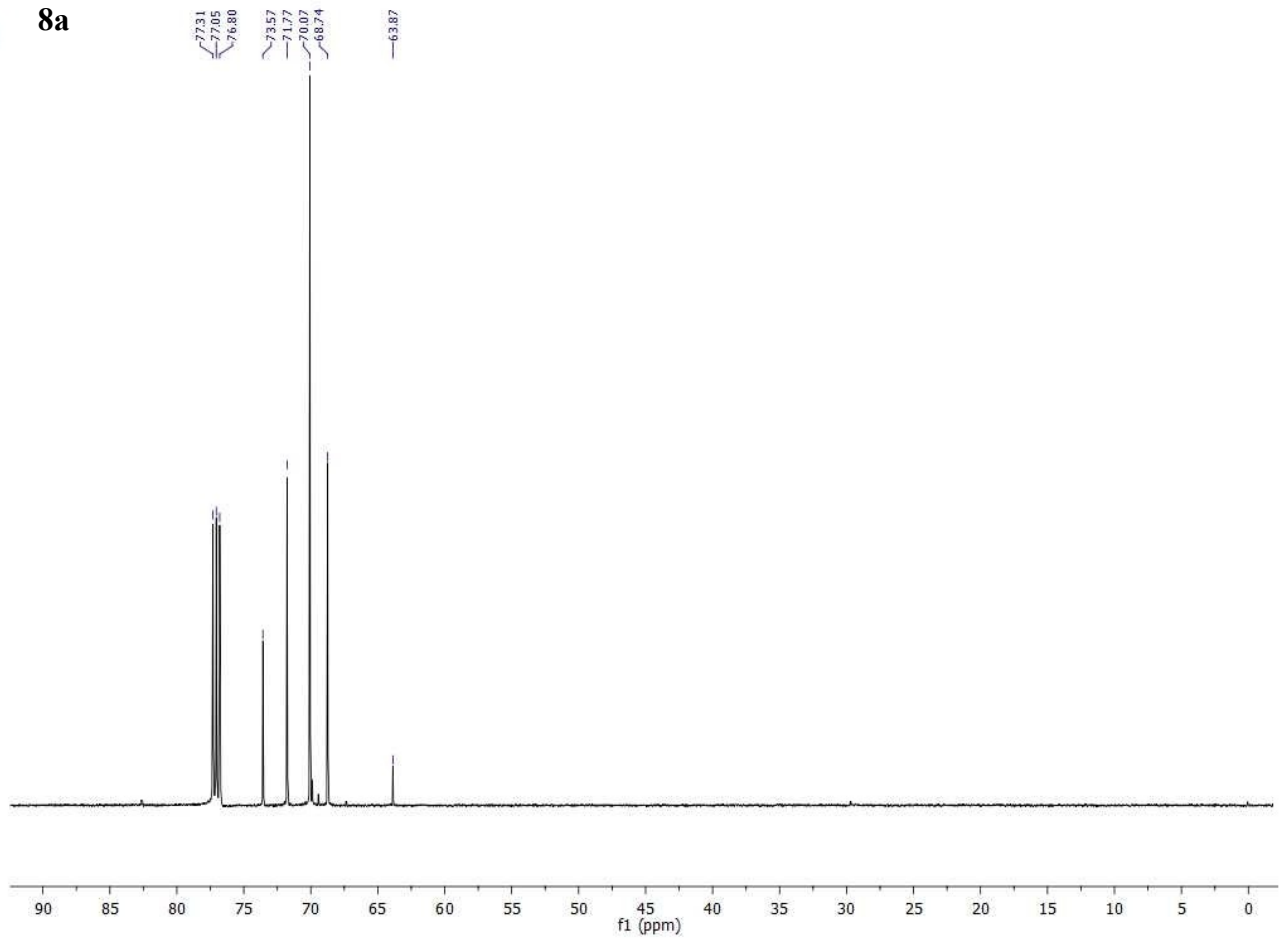


Figure S39: ^{13}C NMR ($CDCl_3$) of **8a**.

8b

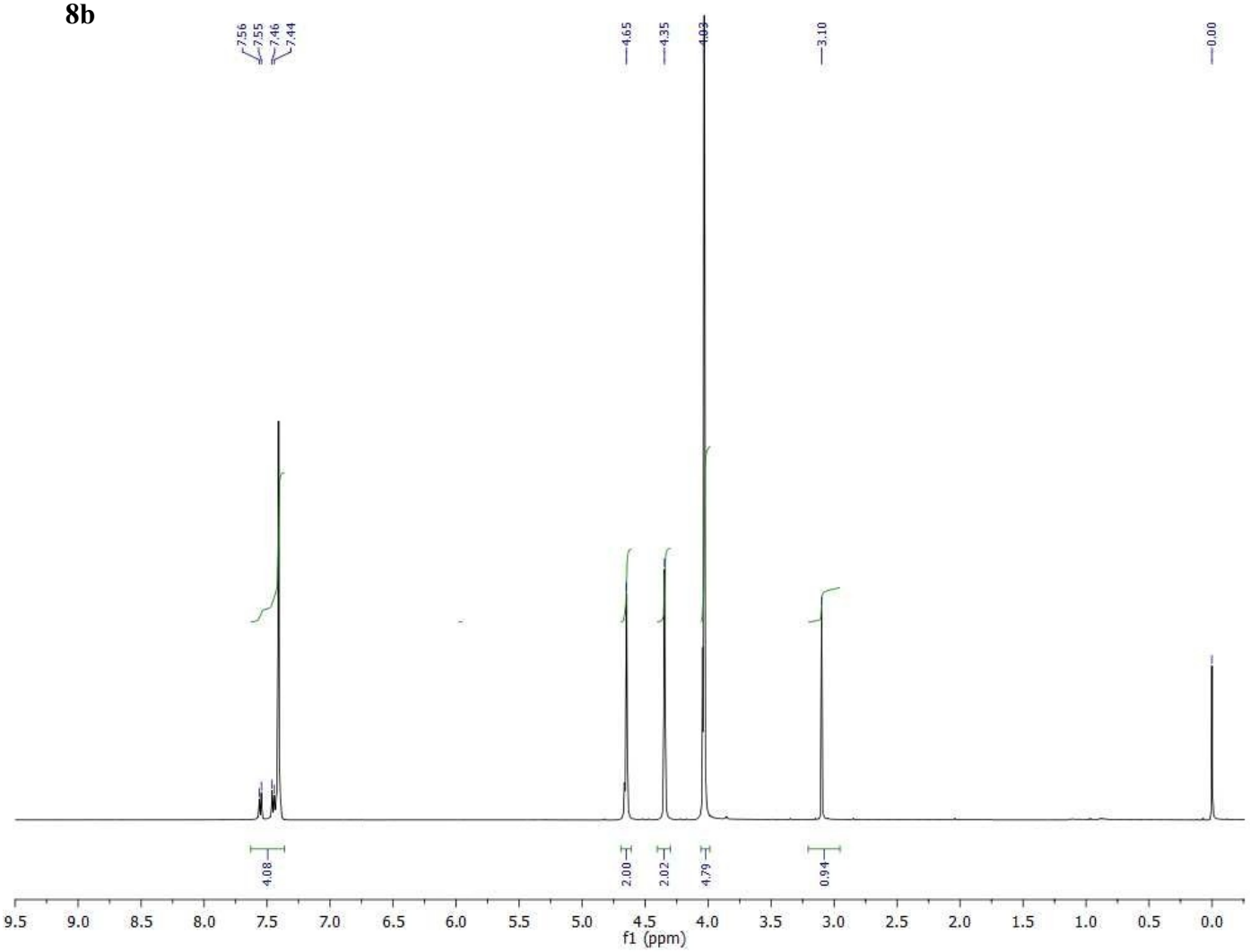


Figure S40: ^{1}H NMR ($CDCl_3$) of **8b**.

8b

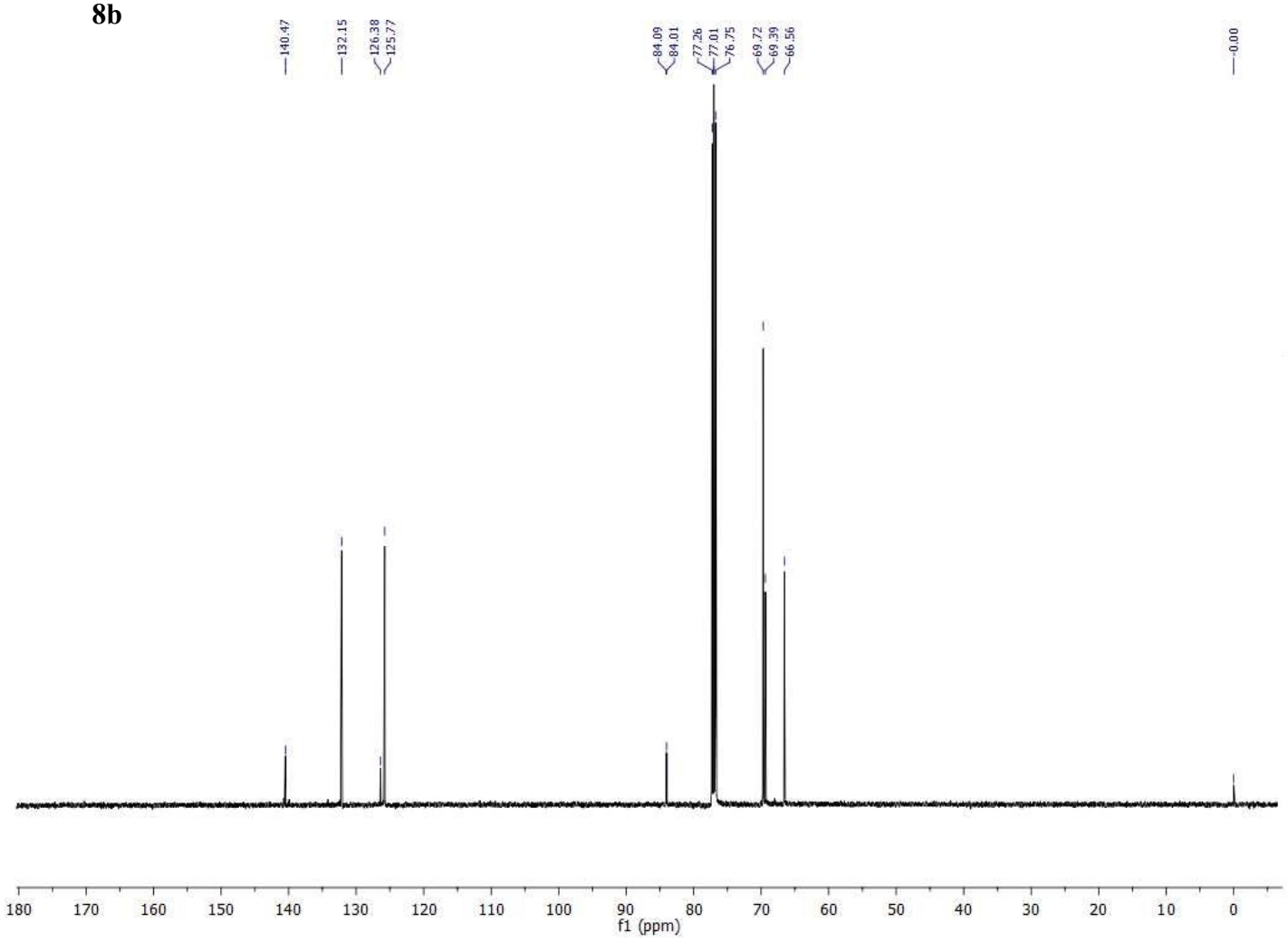


Figure S41: ^{13}C NMR ($CDCl_3$) of **8b**.

9a

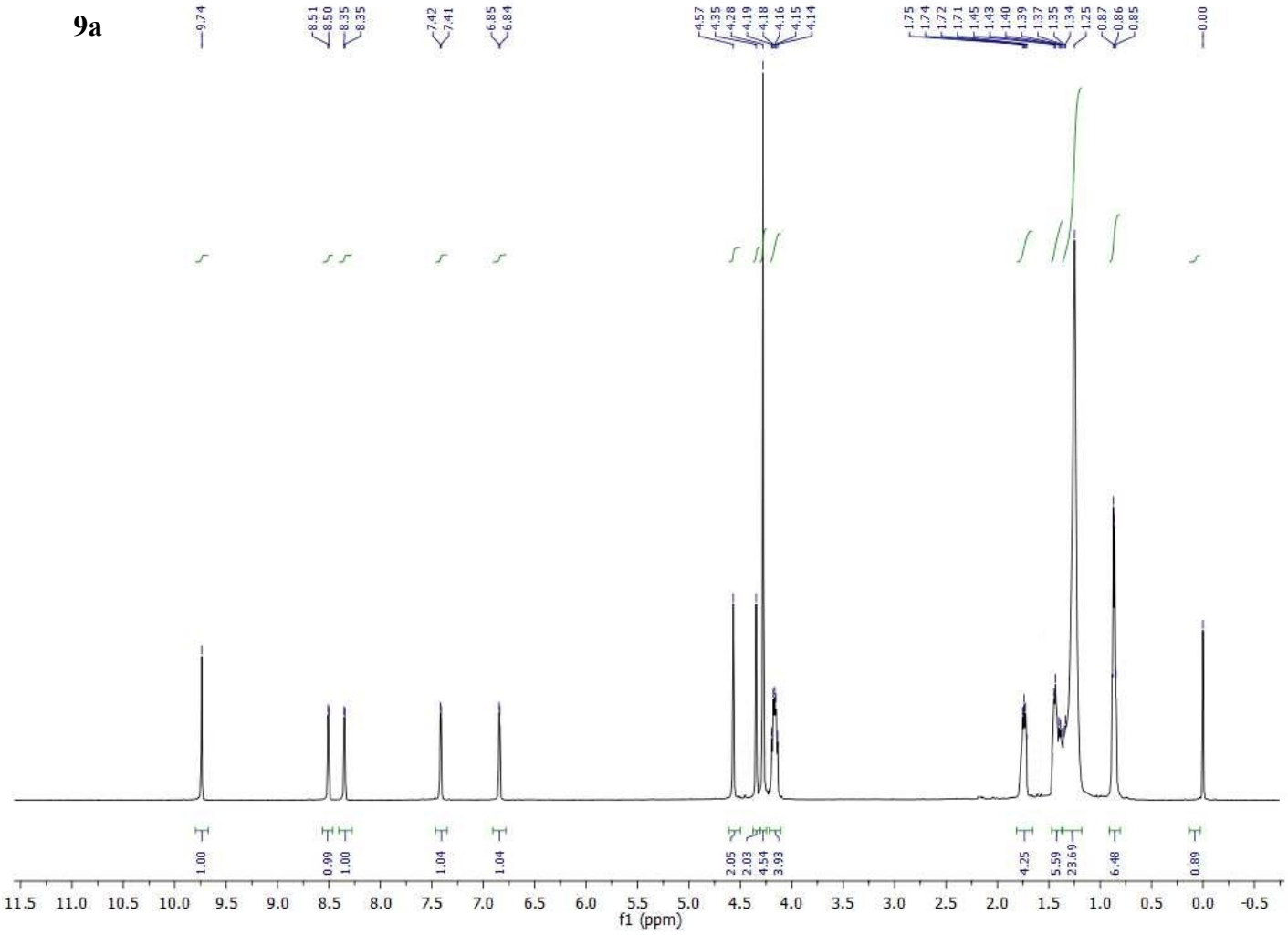


Figure S42: ^{1}H NMR ($CDCl_3$) of **9a**.

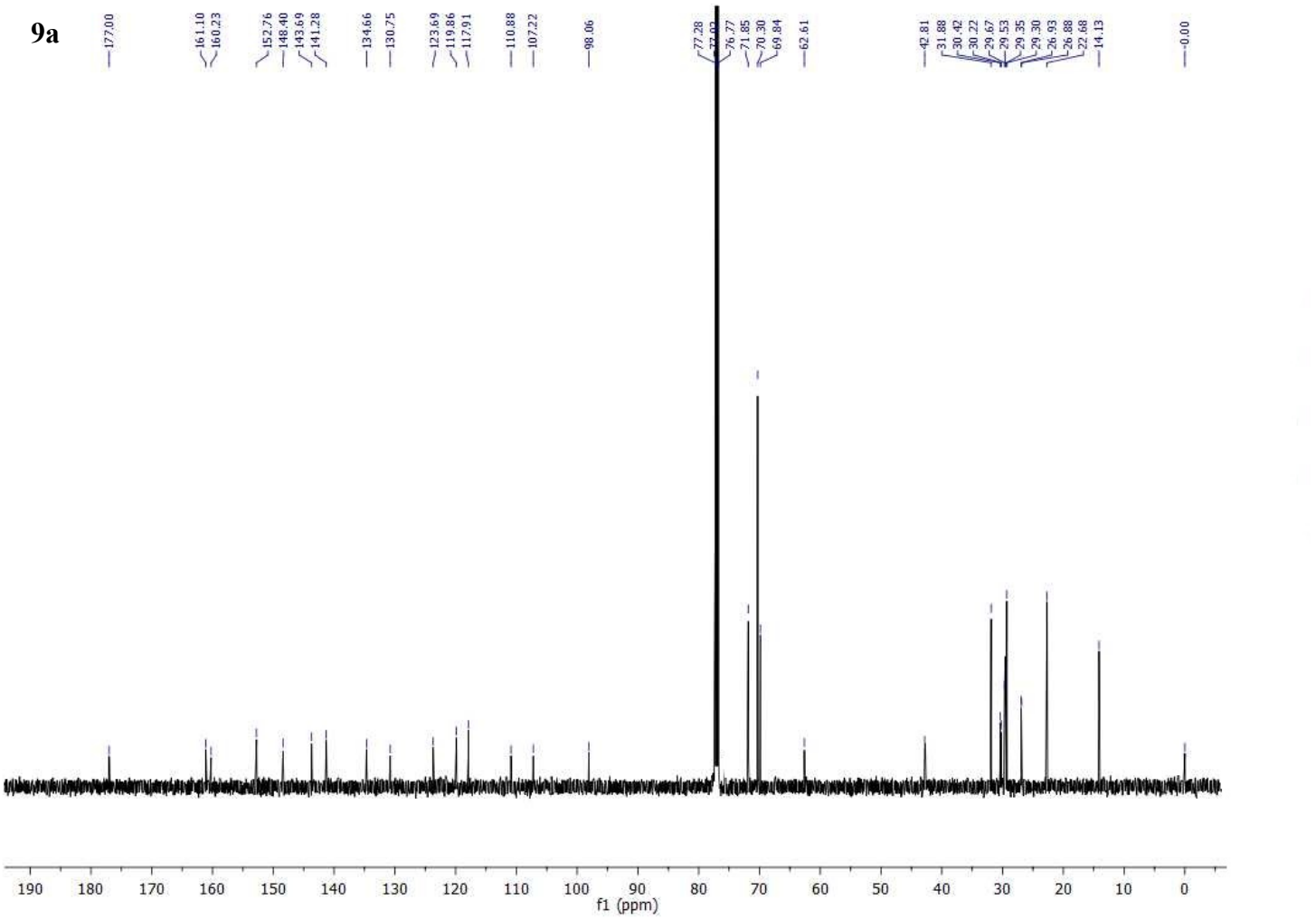


Figure S43: ^{13}C NMR ($CDCl_3$) of **9a**.

9b

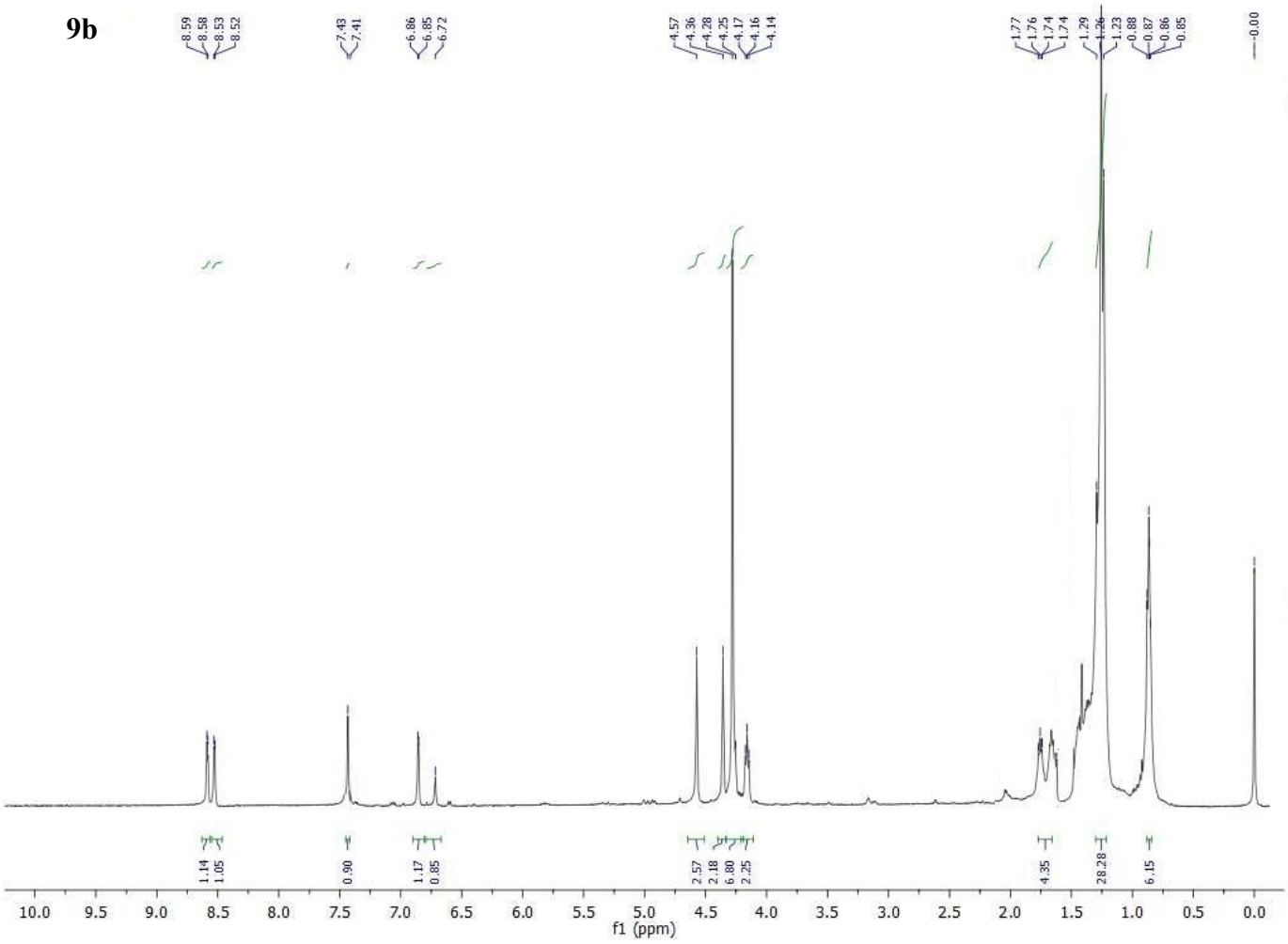


Figure S44: ^{1}H NMR ($CDCl_3$) of **9b**.

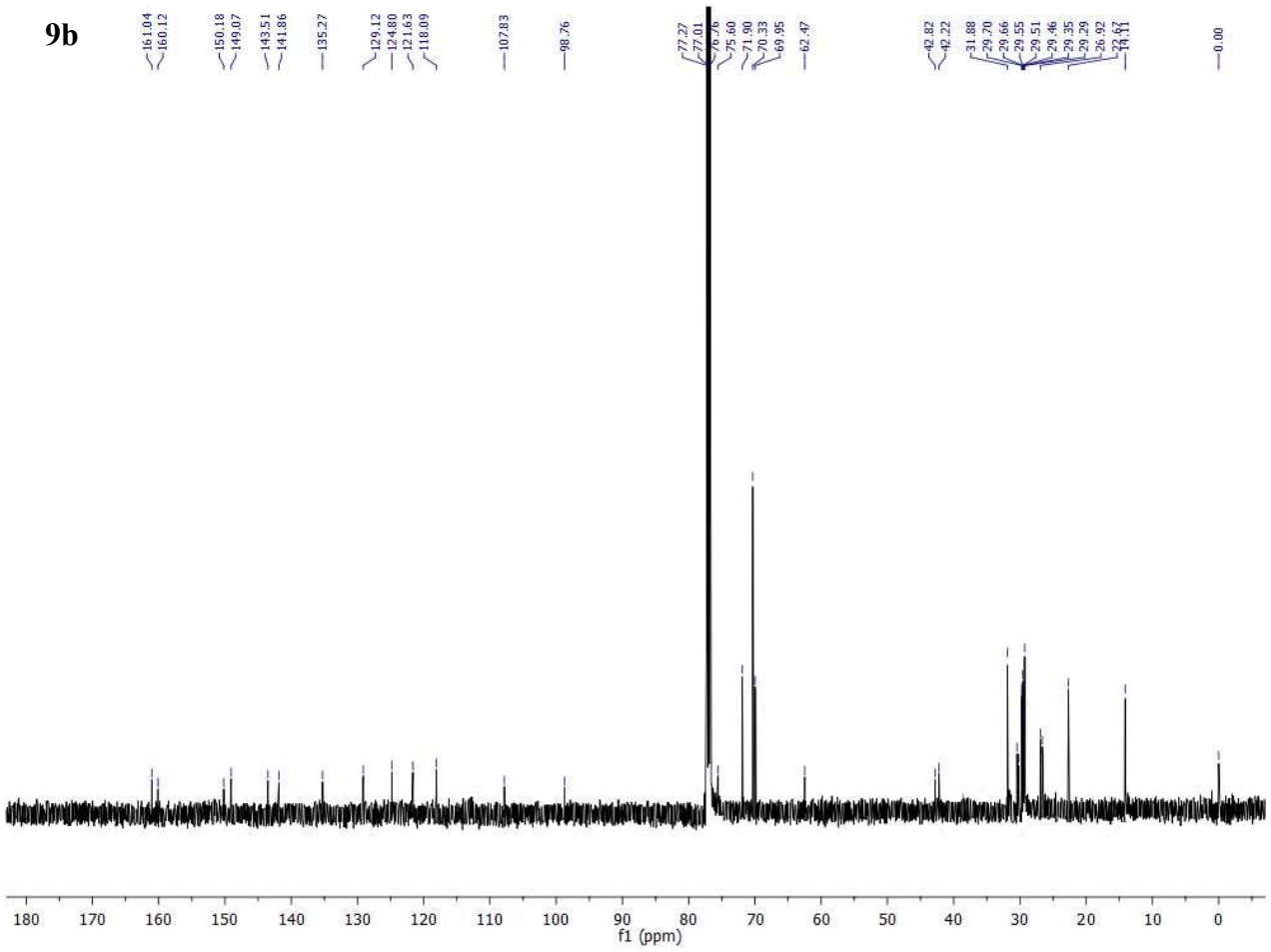


Figure S45: ^{13}C NMR ($CDCl_3$) of **9b**.

9c

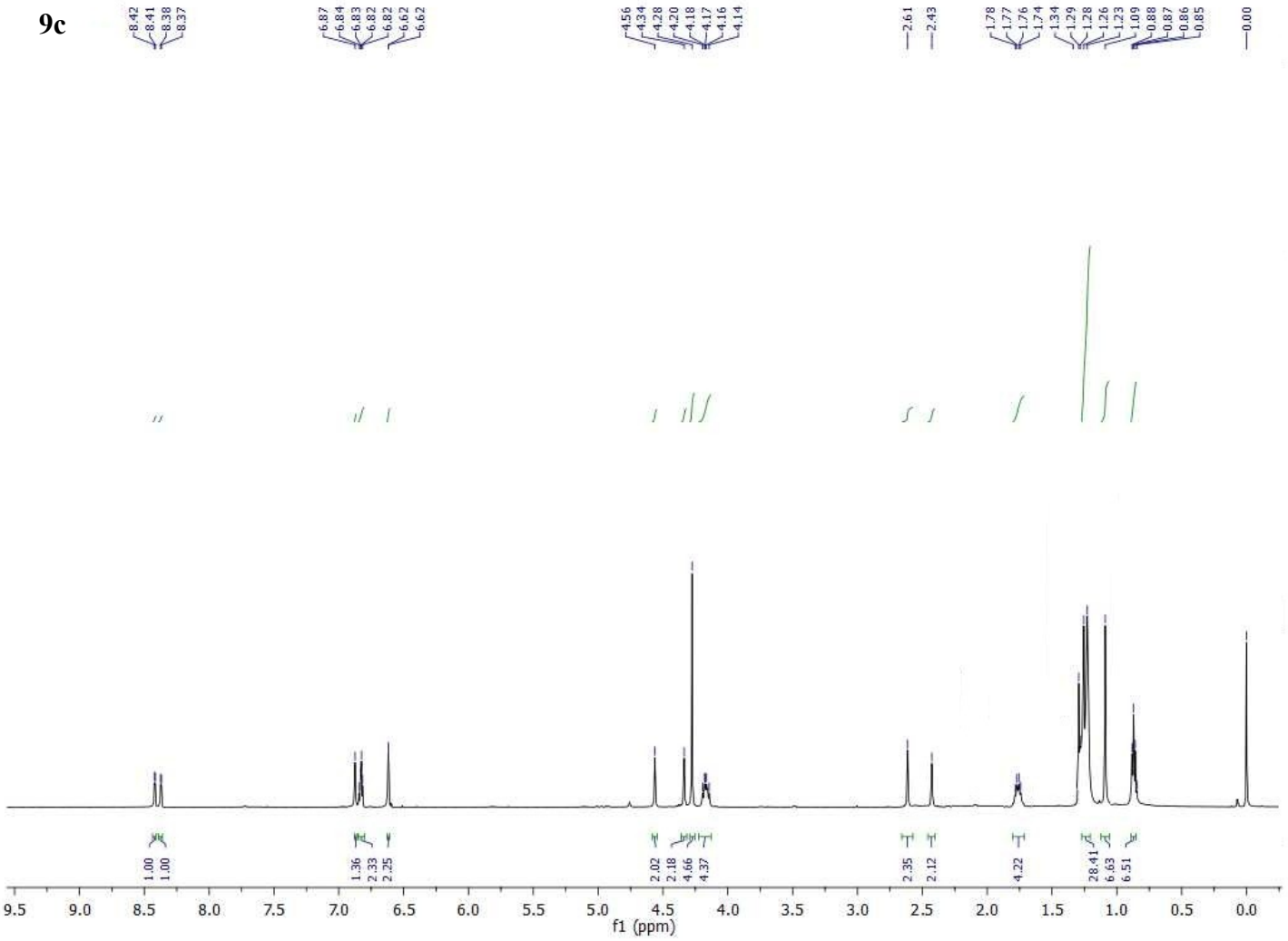


Figure S46: ^{1}H NMR ($CDCl_3$) of **9c**.

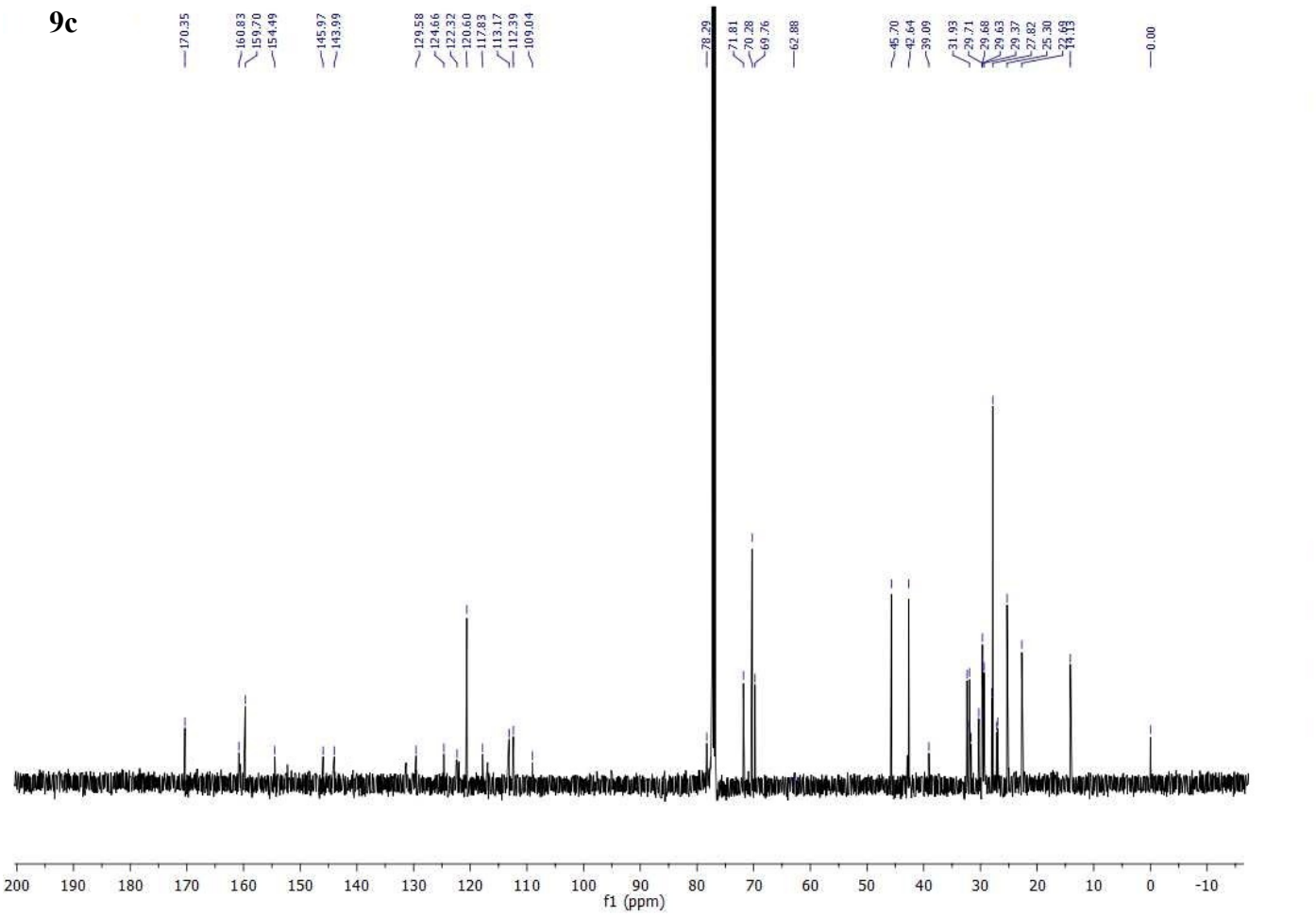


Figure S47: ^{13}C NMR ($CDCl_3$) of **9c**.

9d

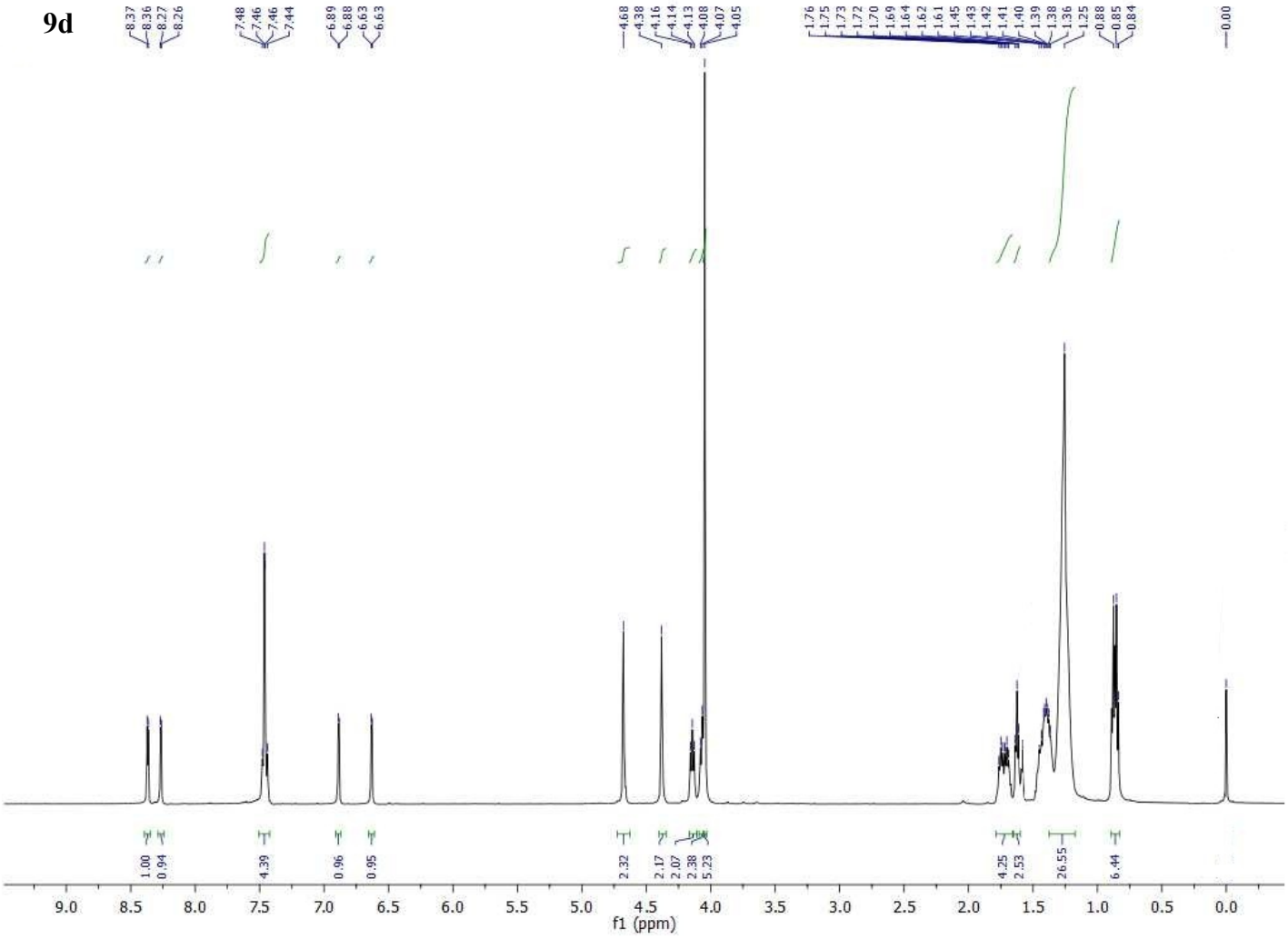


Figure S48: ^{1}H NMR ($CDCl_3$) of **9d**.

9d

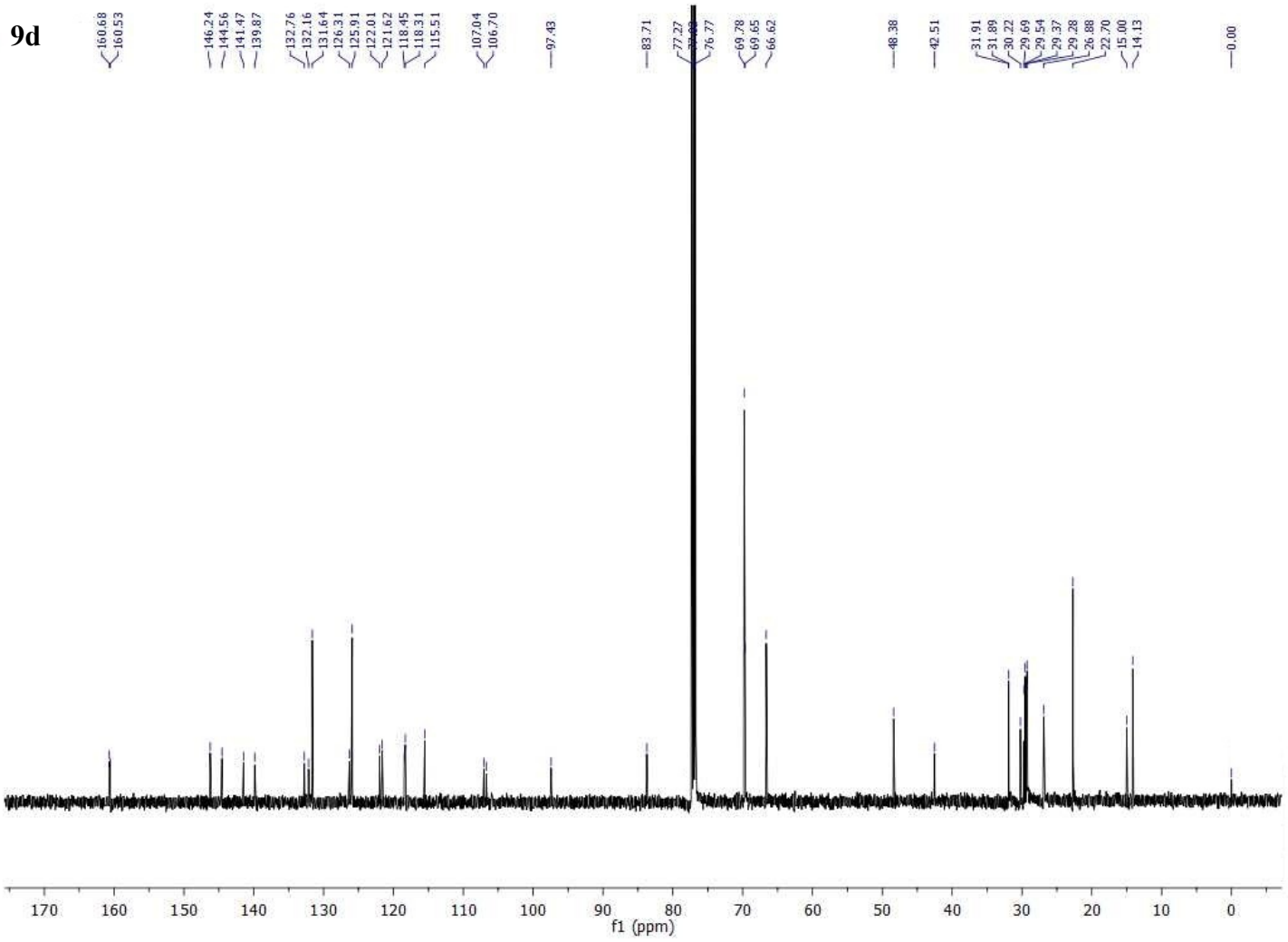


Figure S49: ^{13}C NMR ($CDCl_3$) of **9d**.

9e

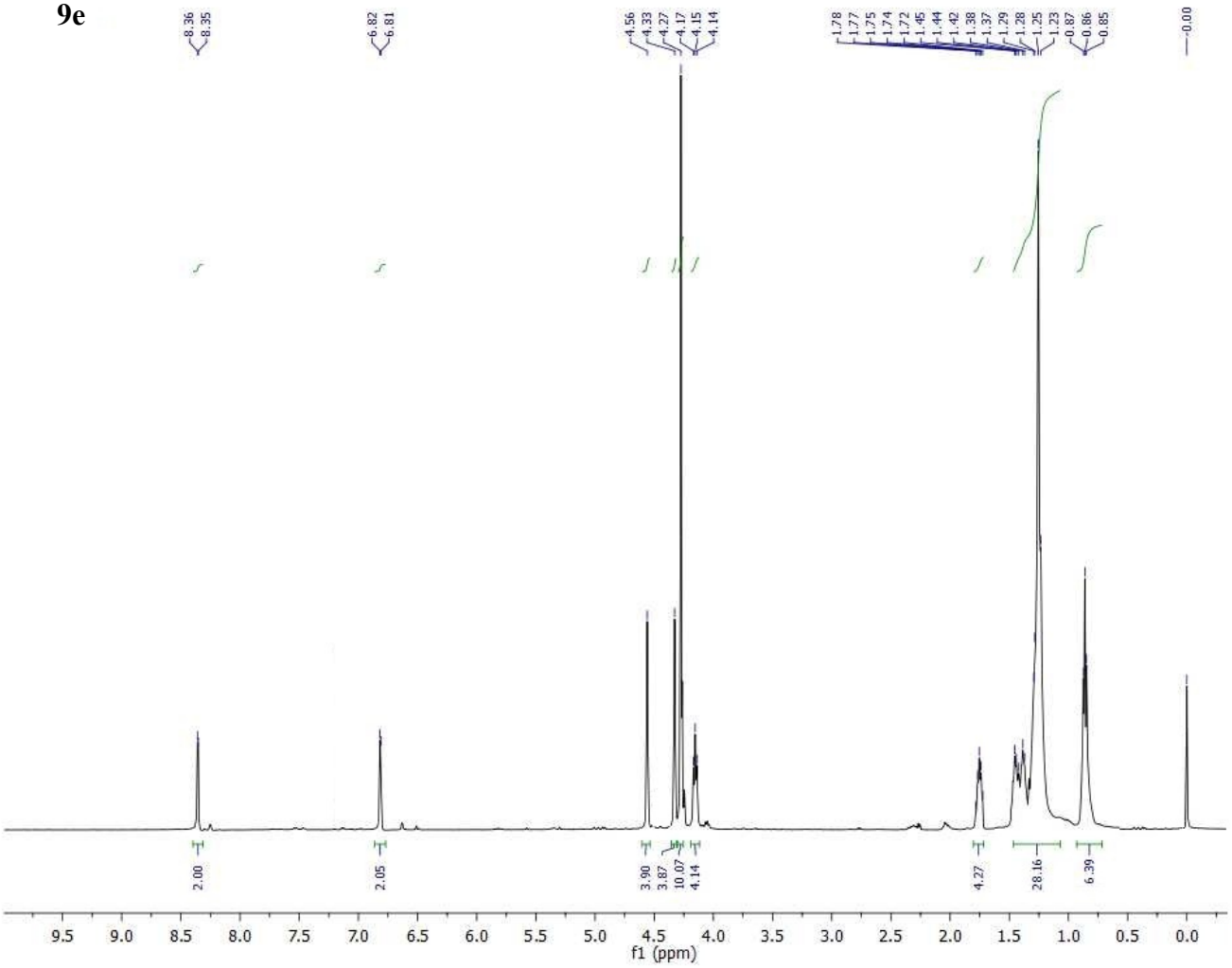


Figure S50: ^{1}H NMR ($CDCl_3$) of **9e**.

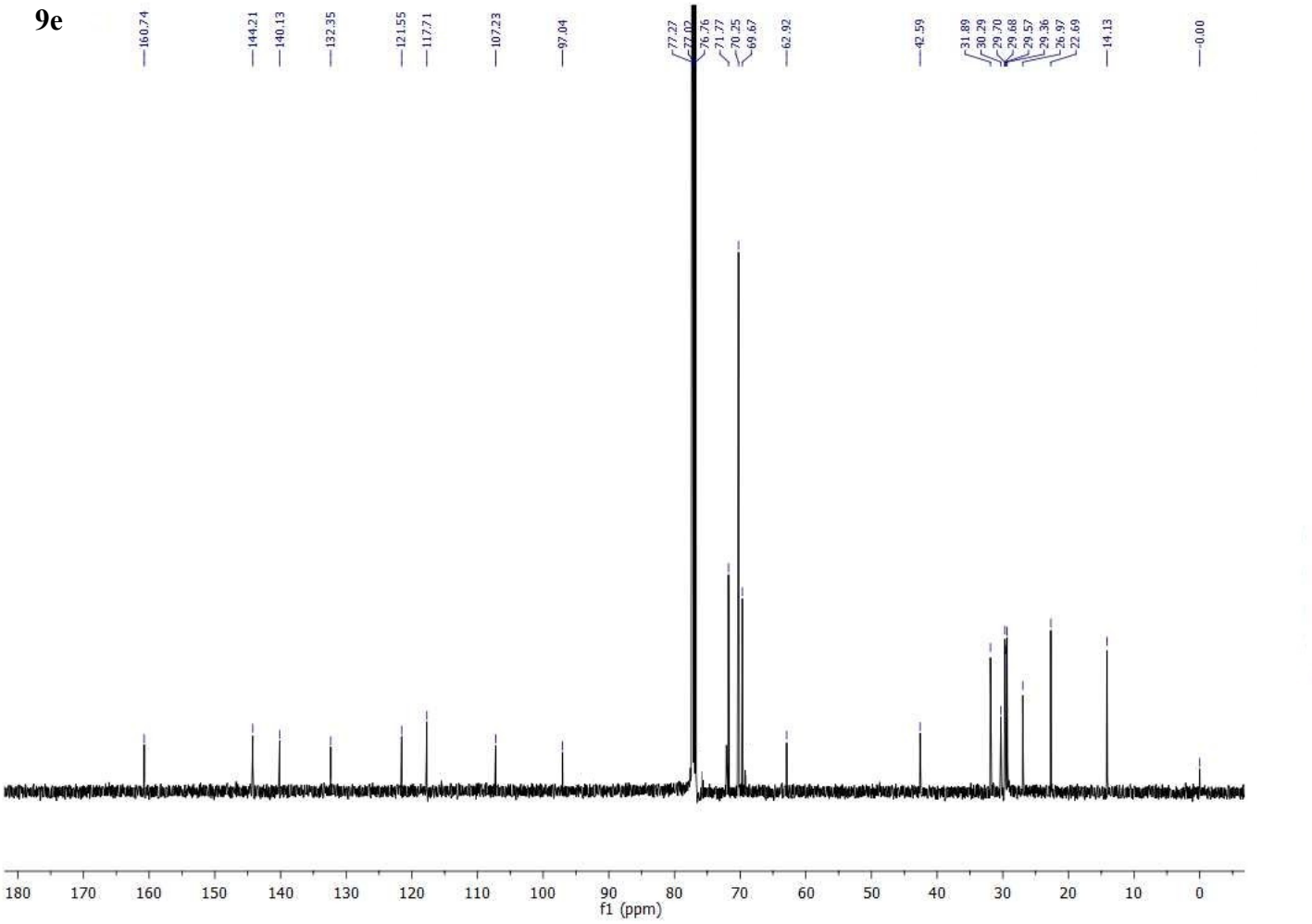


Figure S51: ^{13}C NMR ($CDCl_3$) of **9e**.

9f

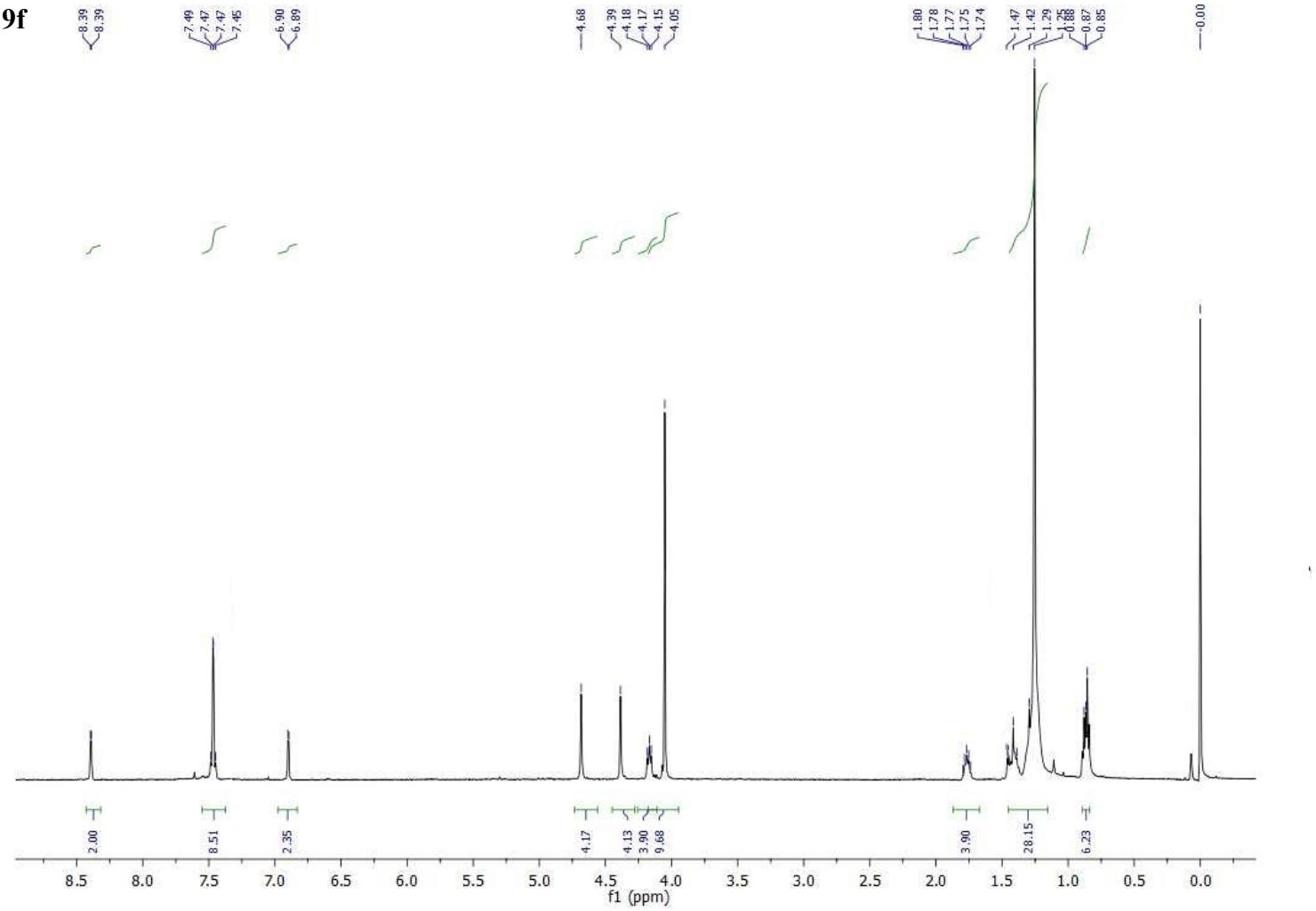


Figure S52: ^{1}H NMR ($CDCl_3$) of **9f**.

9f

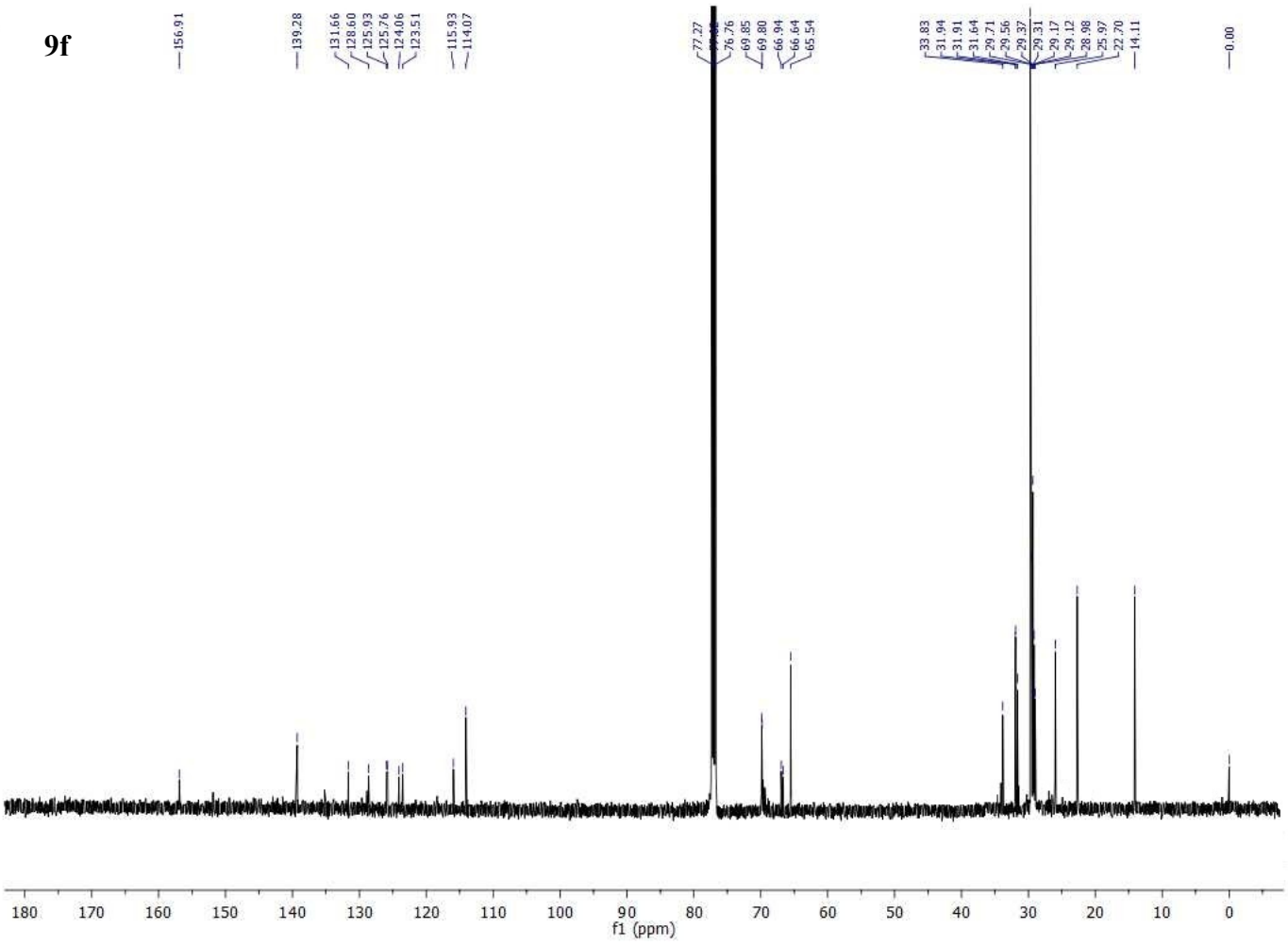


Figure S53: ^{13}C NMR ($CDCl_3$) of **9f**.

Complete Reference 65

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.(complete reference 65).