Electronic Supplementary Information (ESI)

Synthesis, electronic properties and packing modes of conjugated systems based on 2,5-di(cyanovinyl)furan or thiophene and imino-perfluorophenyl moieties

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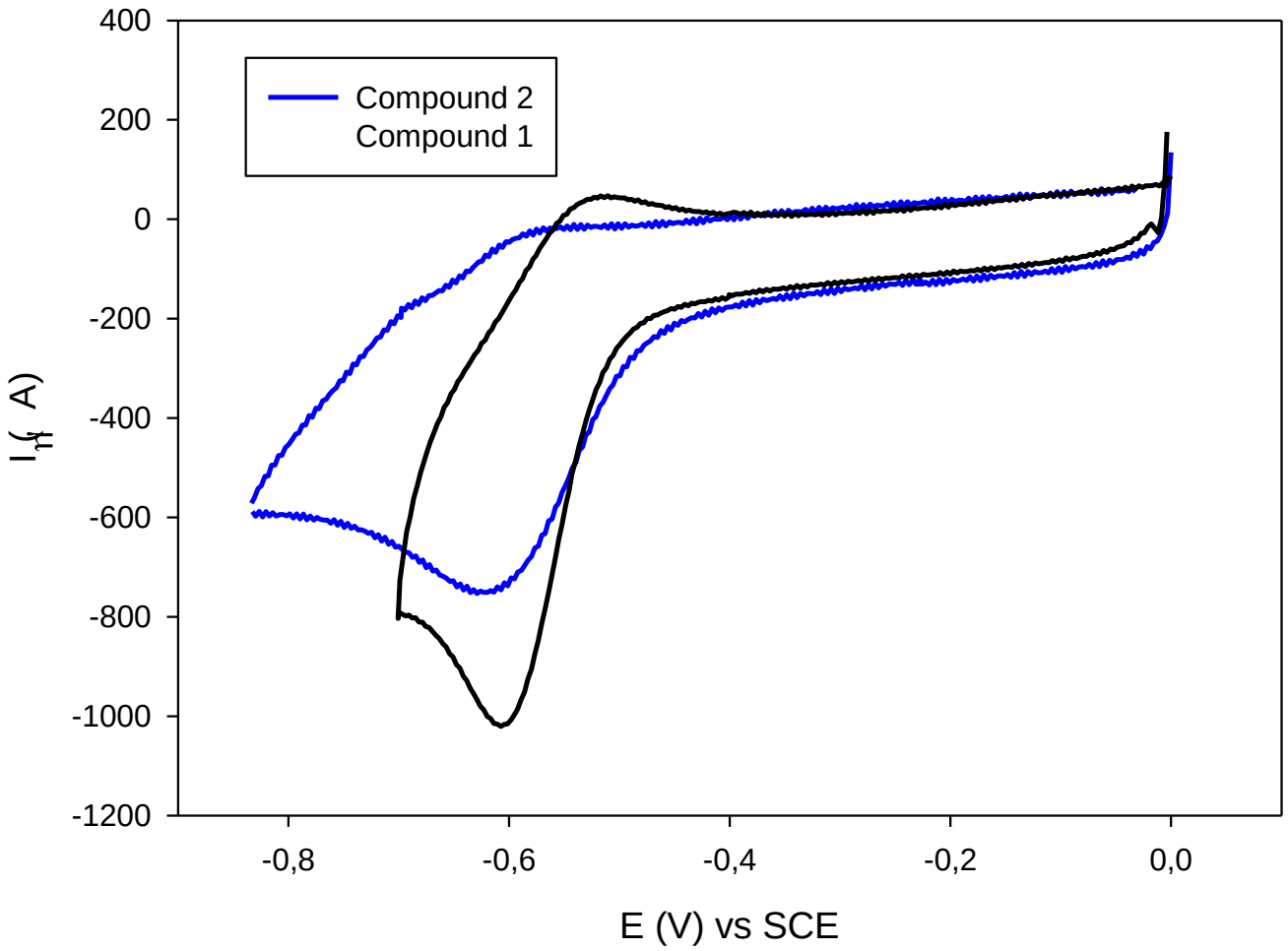


Fig. S1 : CV of compounds **1** and **2** at 2.10^{-5} mol L^{-1} in 0.1 M Bu_4NPF_6/ CH_2Cl_2, scan rate 100mVs^{-1}

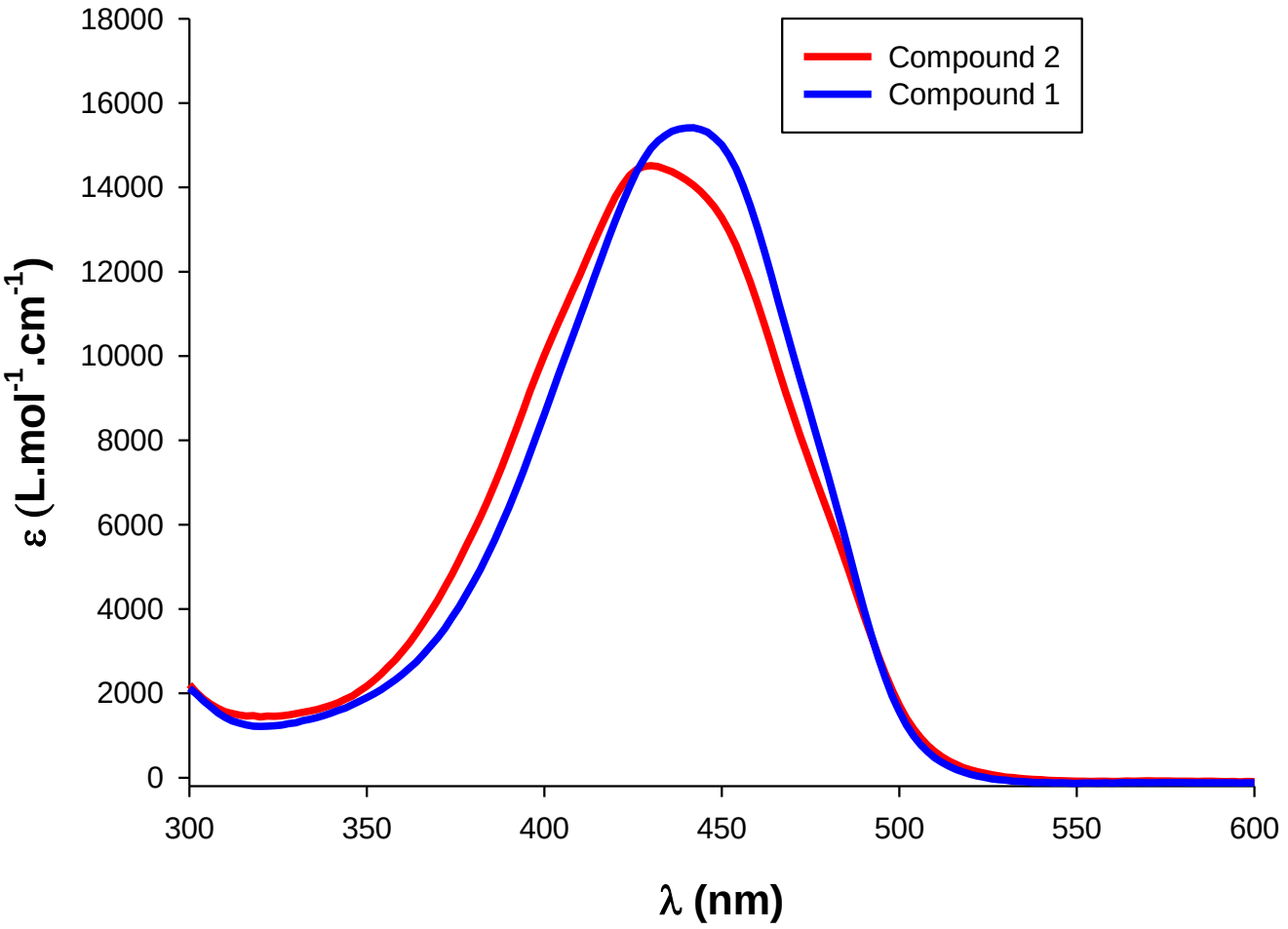
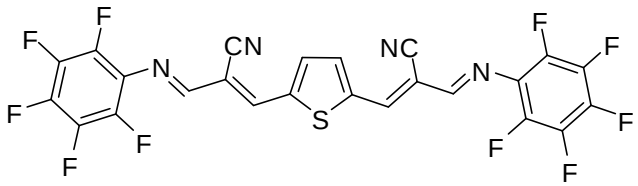
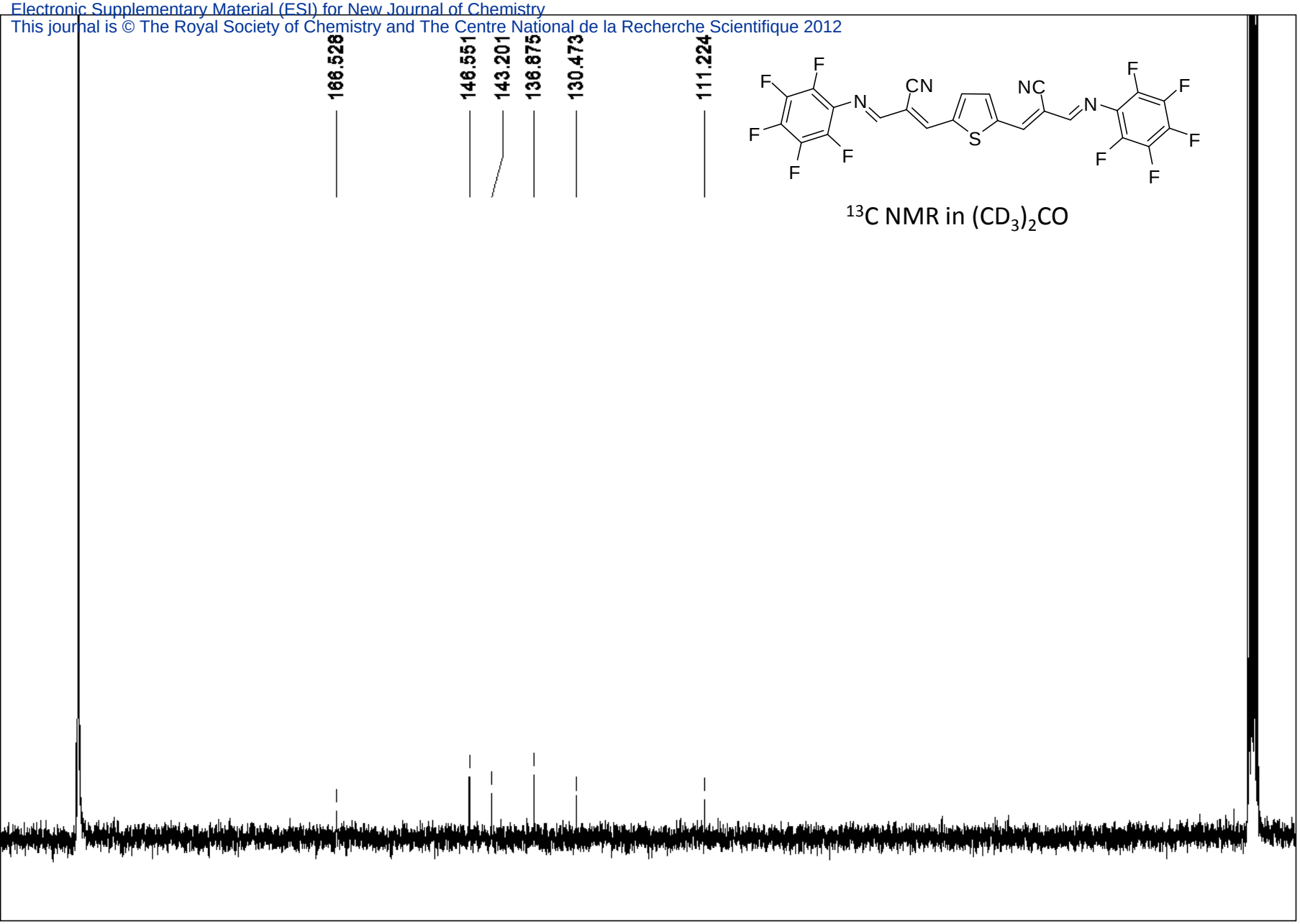
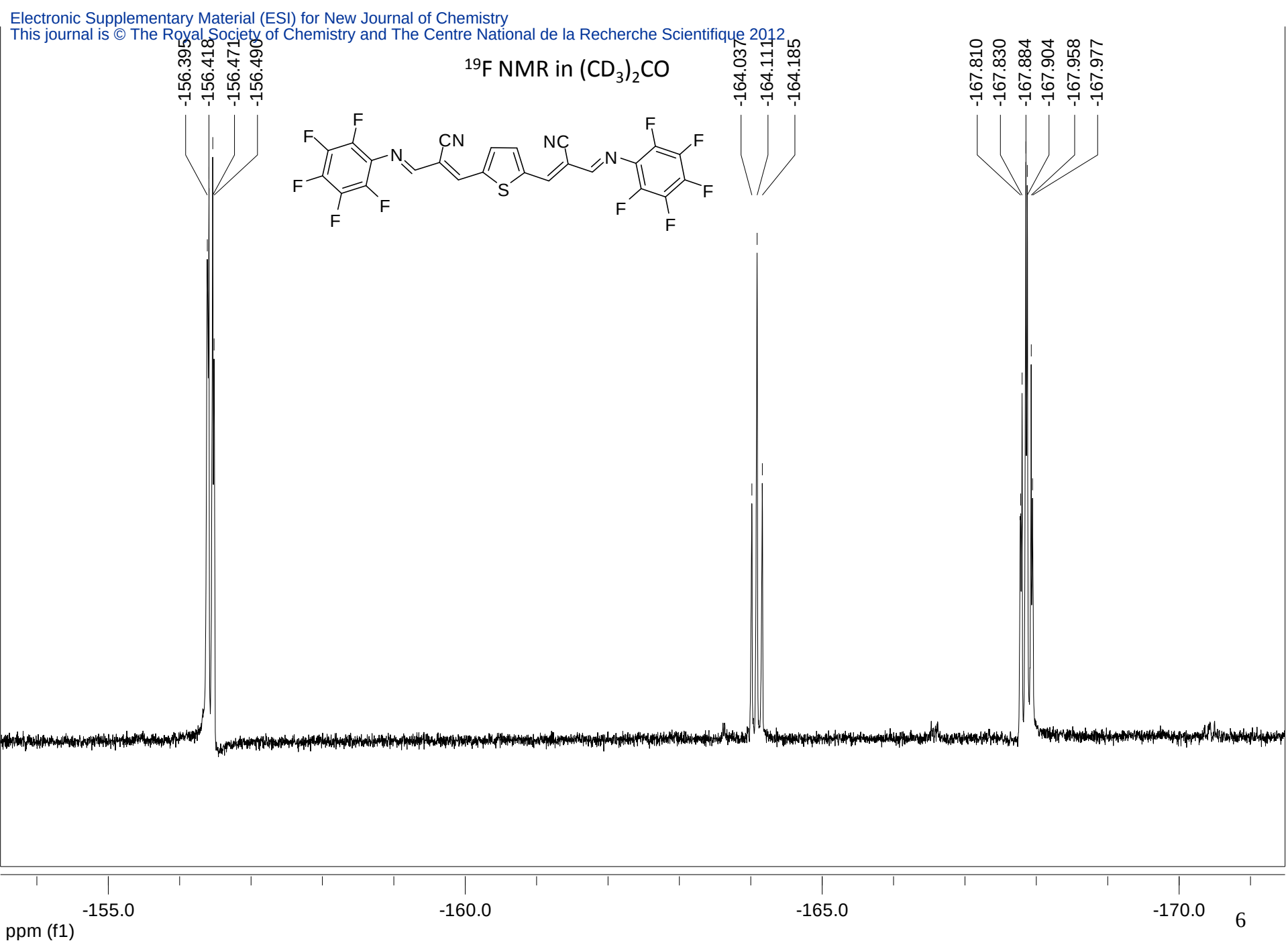


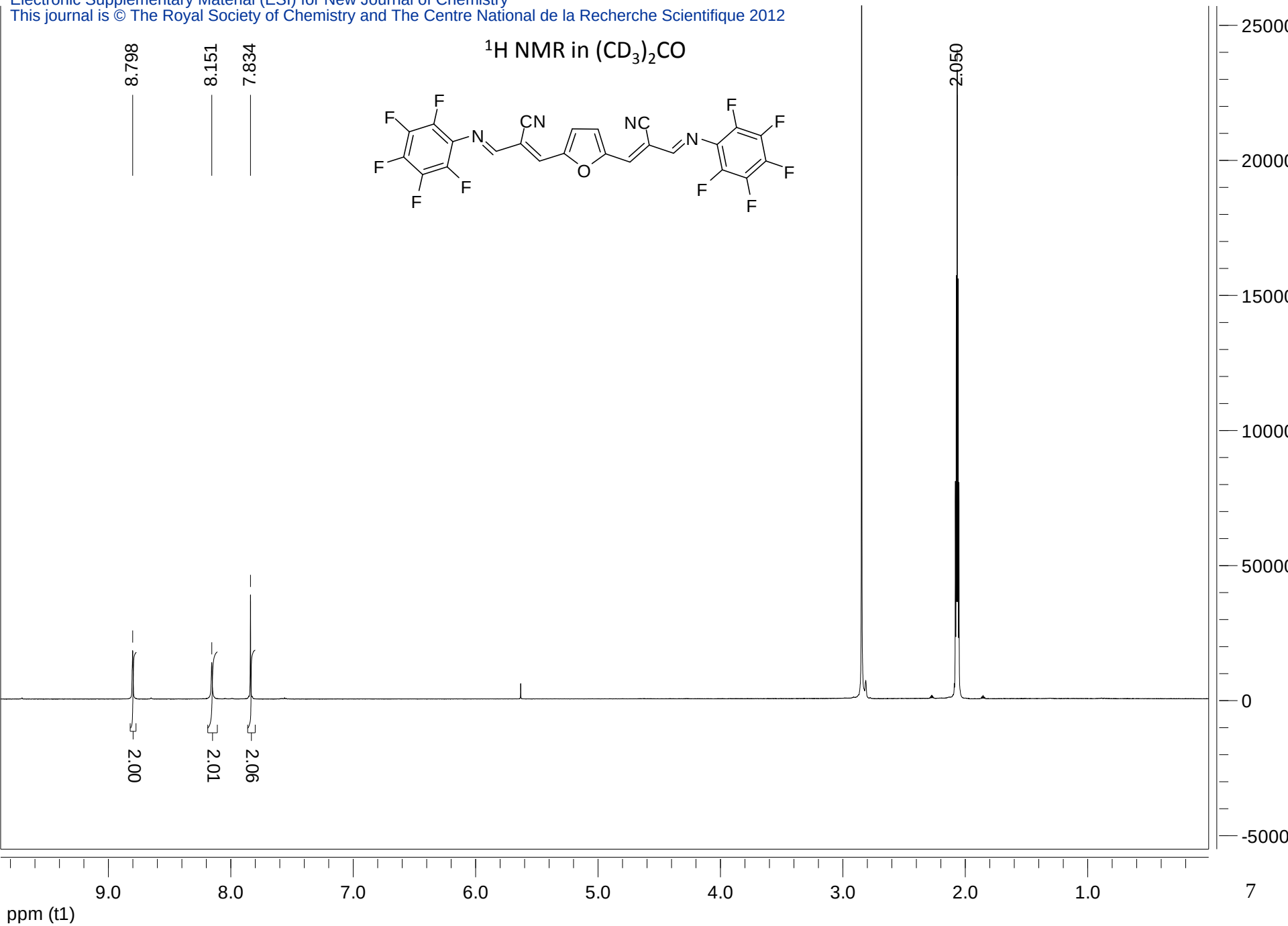
Fig. S2 : UV-Vis absorption spectra of compounds **1** and **2** at 10^{-5} mol L^{-1} in CH_2Cl_2

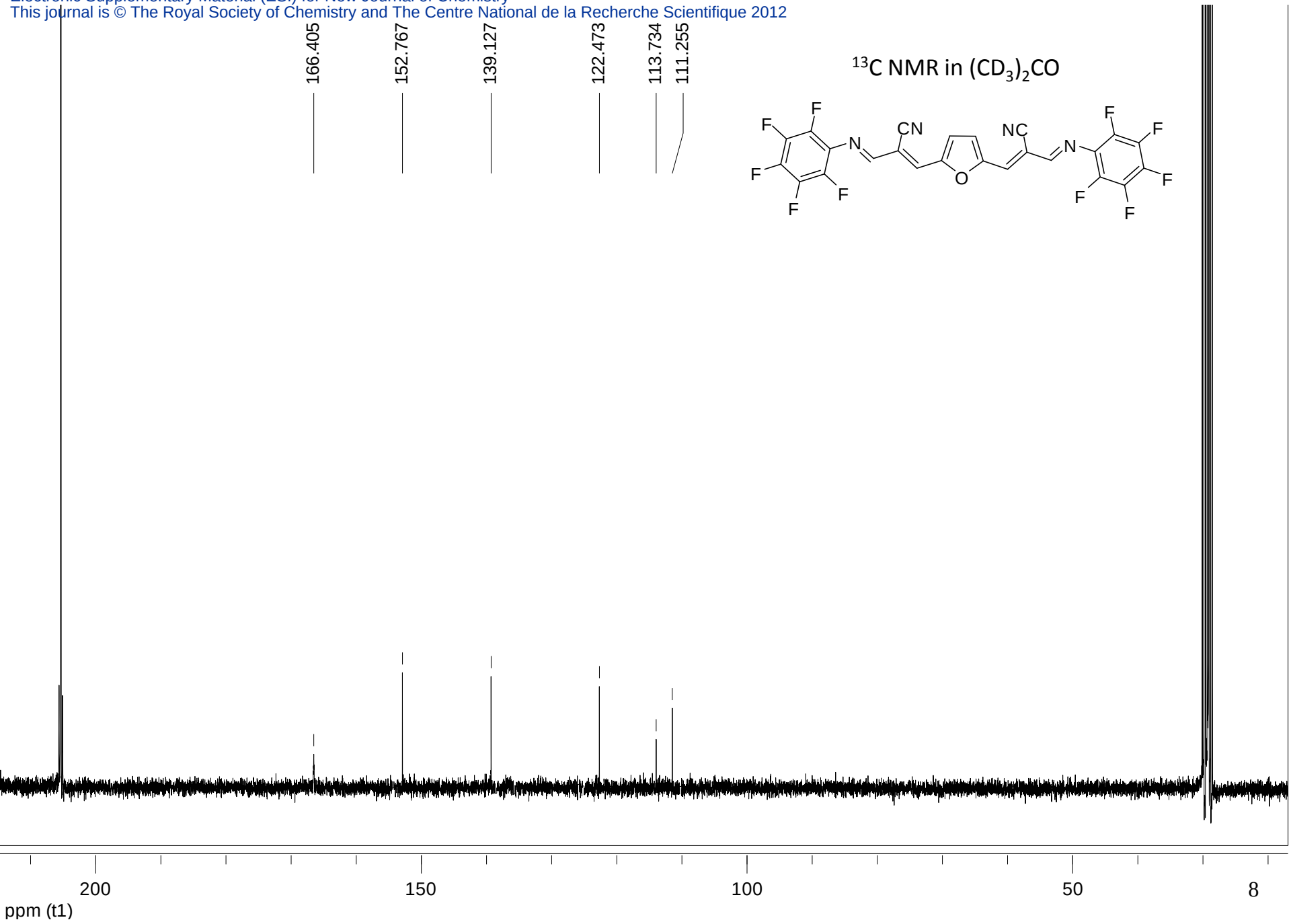
^{1}H NMR in $(CD_3)_2CO$

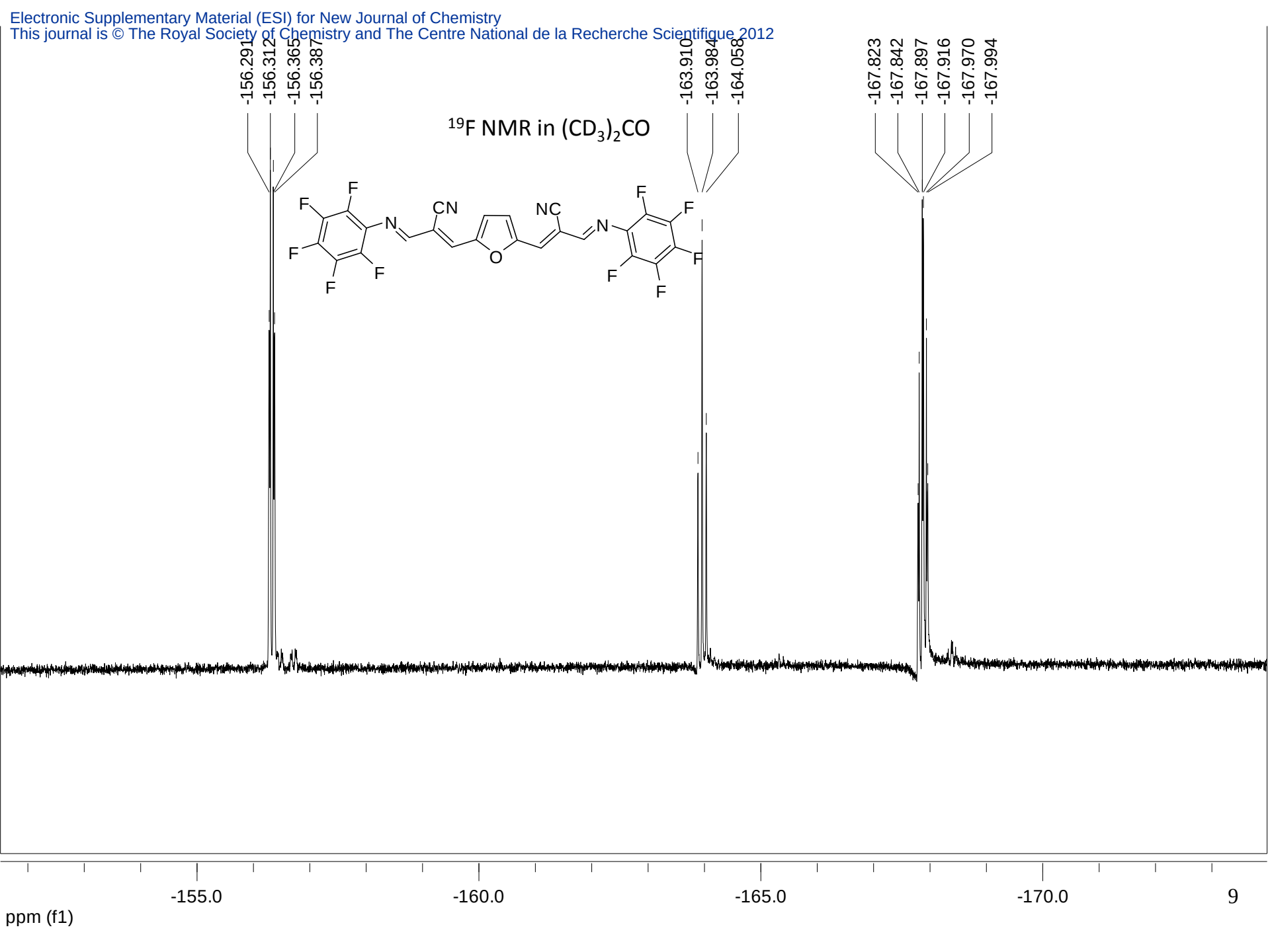












Computational data

Theoretical calculations were performed at the *ab initio density functional level with the Gaussian 09 package. Becke's three-parameter gradient-corrected functional (B3LYP) with a polarized 6-31G (d,p) basis was used for full geometry optimization of compounds **1** and **2.***

Table S1: Atom Coordinates of 1

Row	Symbol	X	Y	Z
1	C	1.2599020	0.3800430	-0.0070910
2	C	0.6991920	1.6555020	-0.0042640
3	C	-0.6992630	1.6555280	0.0036940
4	C	-1.2600160	0.3800850	0.0068520
5	S	-0.0000880	-0.8309330	0.0001300
6	C	2.6208060	-0.0642190	-0.0153220
7	C	3.7792620	0.6625300	-0.0218790
8	C	3.7961520	2.0898960	-0.0162850
9	N	3.7735260	3.2445660	-0.0104660
10	C	5.0605290	-0.0338700	-0.0303280
11	N	6.1605830	0.6200890	-0.0489510
12	C	7.4056890	0.0052960	-0.0166760
13	C	8.4785620	0.7000110	-0.6054170
14	C	9.7761680	0.2104710	-0.5689310
15	C	10.0494900	-0.9847020	0.0869920
16	C	9.0166400	-1.6875450	0.6965690
17	C	7.7198200	-1.2000930	0.6349590
18	F	6.7567600	-1.9029450	1.2574680
19	F	9.2764080	-2.8313430	1.3368160
20	F	11.2950920	-1.4569480	0.1291550
21	F	10.7674760	0.8843020	-1.1568960
22	F	8.2524520	1.8508960	-1.2349020
23	H	1.2909000	2.5587010	-0.0079560
24	H	-1.2909410	2.5587480	0.0071250
25	H	2.7570590	-1.1424070	-0.0163990
26	H	4.9968820	-1.1243320	-0.0320890
27	C	-2.6209570	-0.0640460	0.0152340
28	H	-2.7573300	-1.1422200	0.0168220
29	C	-3.7793350	0.6628270	0.0214830
30	C	-5.0606700	-0.0334580	0.0303330
31	H	-4.9971170	-1.1239340	0.0325460
32	N	-6.1606940	0.6205330	0.0488100
33	C	-7.4057540	0.0055690	0.0168070
34	C	-7.7198880	-1.1993560	-0.6356750
35	C	-8.4784920	0.6995990	0.6065360
36	C	-9.0166470	-1.6869980	-0.6971690
37	C	-9.7760150	0.2098330	0.5701950
38	C	-10.0493800	-0.9848560	-0.0865950
39	F	-8.2523090	1.8500280	1.2368740
40	F	-10.7672030	0.8829840	1.1591440
41	F	-11.2949120	-1.4573140	-0.1286110
42	F	-9.2764560	-2.8303240	-1.3382500
43	F	-6.7569280	-1.9014860	-1.2591490
44	C	-3.7961100	2.0901890	0.0152580
45	N	-3.7733590	3.2448540	0.0087980

Table S2: Atom Coordinates of 2

Row	Symbol	X	Y	Z
1	C	-1.1058000	1.2752870	0.0064720
2	C	-0.7014040	2.6028190	0.0043990
3	C	0.7014830	2.6028730	-0.0041030
4	C	1.1059170	1.2753450	-0.0063610
5	C	-2.3500840	0.5853870	0.0129110
6	C	-3.6159230	1.1005050	0.0214930
7	C	-3.8566710	2.5076400	0.0219600
8	N	-3.9970510	3.6540150	0.0212450
9	C	-4.7614120	0.2007450	0.0241240
10	N	-5.9559190	0.6613280	0.0423840
11	C	-7.0779300	-0.1567270	0.0016520
12	C	-8.2561550	0.3404500	0.5889380
13	C	-9.4503150	-0.3643980	0.5439090
14	C	-9.5124400	-1.5849120	-0.1193550
15	C	-8.3722780	-2.0966730	-0.7280630
16	C	-7.1785500	-1.3944250	-0.6577550
17	F	-6.1075870	-1.9176030	-1.2807960
18	F	-8.4294280	-3.2641480	-1.3754990
19	F	-10.6584530	-2.2633740	-0.1691350
20	F	-10.5444440	0.1253240	1.1315840
21	F	-8.2335170	1.5096890	1.2249750
22	H	-1.3511800	3.4621350	0.0083130
23	H	1.3511620	3.4622550	-0.0078640
24	H	-2.2583880	-0.4964240	0.0096190
25	H	-4.5157330	-0.8632870	0.0215460
26	C	2.3502590	0.5855480	-0.0129440
27	H	2.2586700	-0.4962750	-0.0098820
28	C	3.6160790	1.1007270	-0.0214310
29	C	4.7616060	0.2010460	-0.0242740
30	H	4.5160070	-0.8630150	-0.0219380
31	N	5.9560830	0.6616730	-0.0424210
32	C	7.0780280	-0.1565010	-0.0017990
33	C	7.1785720	-1.3938570	0.6582620
34	C	8.2561260	0.3401410	-0.5897190
35	C	8.3721930	-2.0962710	0.7286110
36	C	9.4501750	-0.3649080	-0.5446540
37	C	9.5122720	-1.5850420	0.1192910
38	F	8.2334780	1.5090350	-1.2264050
39	F	10.5442040	0.1242840	-1.1329610
40	F	10.6581720	-2.2637110	0.1691040
41	F	8.4293520	-3.2634100	1.3766620
42	F	6.1076500	-1.9164650	1.2818360
43	C	3.8567310	2.5078740	-0.0215730
44	N	3.9970240	3.6542580	-0.0203190
45	O	0.0000970	0.4703840	-0.0000300