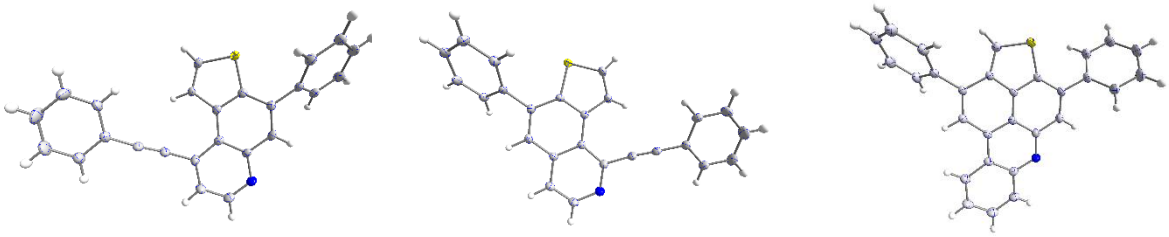
SUPPORTING INFORMATION

Table of Content

Single-crystal X-ray diffraction data

Crystals were obtained by slow evaporation of Hep/CH_2Cl_2 2:1 at 25°C. X-ray single crystal structure analysis was performed on a Bruker Apex Kappa-II CCD-diffractometer.



3a **4a** **8a**

Figure S1. *ORTEPs of crystal structures* ***3a, 4a*** *and* ***8a*** *(drawn with ellipsoids probability of 50%).*

Table S1. *Single crystal X-ray diffraction data of compounds* ***3a, 4a*** *and* ***8a****.*

	3a	**4a**	**8a**
Chem. Formula	$C_{25}H_{15}NS$	$C_{25}H_{15}NS$	$C_{29}H_{17}NS$
Form. Weight [g mol^{-1}]	361.44	361.44	411.50
Crsyt. system	triclinic	triclinic	Triclinic
Space group (Hall group)	P -1(-P 1)	P -1(-P 1)	P -1(-P 1)
a [Å]	7.904(6)	8.0985(9)	8.0321(4)
b [Å]	10.247(7)	10.3014(12)	10.3560(5)
c [Å]	11.533(8)	11.0803(12)	13.1722(6)
α [°]	96.72(2)	96.301(4)	105.953(2)
β [°]	102.06(2)	101.547(3)	95.907(2)
γ [°]	99.58(2)	101.238(4)	108.672(2)
V [Å^3]	889.5(11)	877.60(17)	975.86(8)
Z	2	2	2
N_{ref}	4082(4075)	5128(5119)	5699(5693)
θ_{max} [°]	27.490	29.997	29.999
h,k,l_{max}	10,13,14	11,14,15	11,14,18
D_x[g cm^{-3}]	1.349	1.368	1.400
μ [mm^{-1}]	0.191	0.193	0.184
$\lambda_{MoK\alpha}$ [A]	0.71073	0.71073	0.71073
T [K]	123	123	123

F(000)	376.0	376.0	428.0
N_{par}	244	244	381
R	0.0704(2451)	0.0516(3778)	0.0407(4636)
wR2	0.1397(4075)	0.1255(5119)	0.1168(5693)
S	1.011	1.039	1.052

Optical Properties

Acidochromic studies

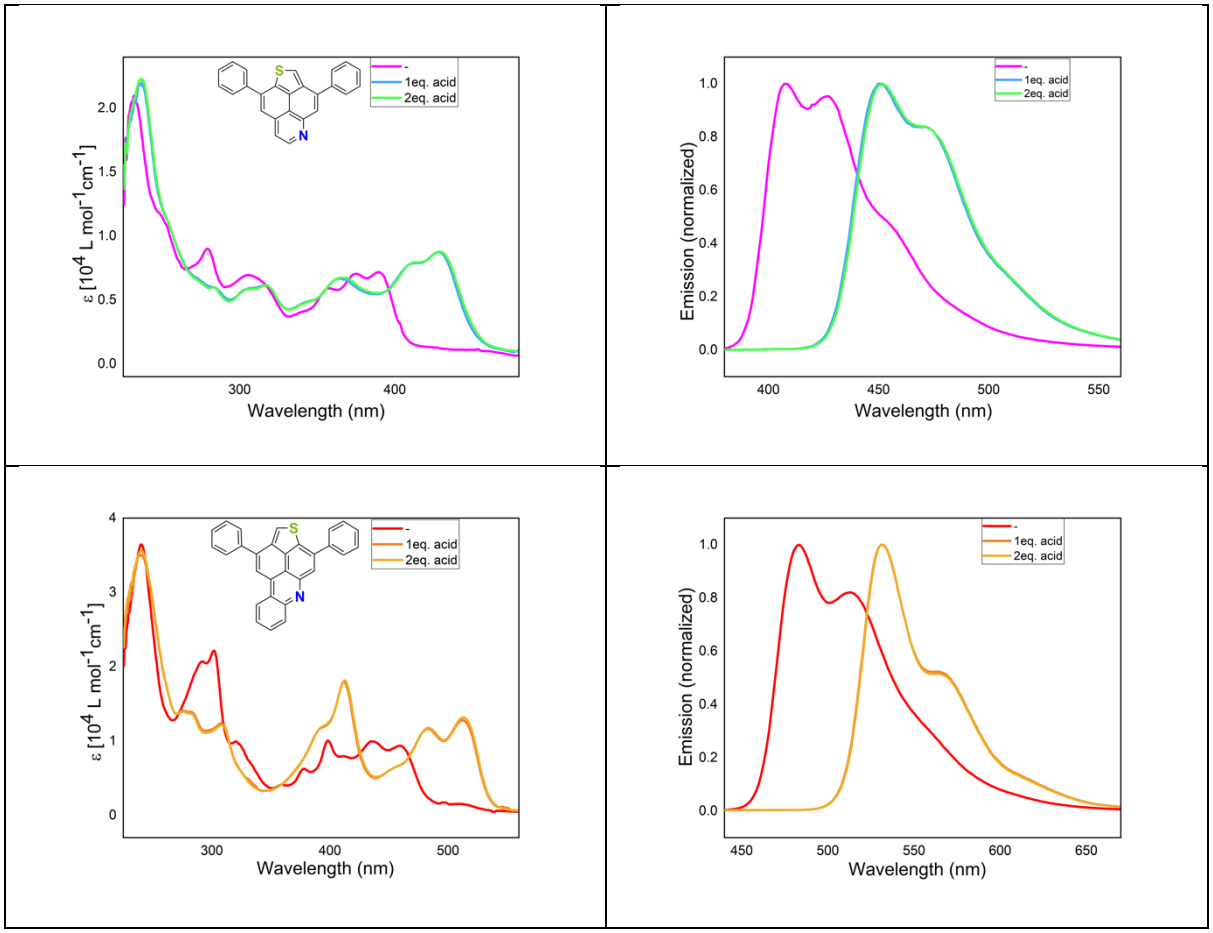


Figure S2. *Absorption and emission spectra of* ***6a*** *and* ***8a*** *in CH_2Cl_2 (c = 10^{-5} M) at 20°C with different concentration of TFA.*

Cyclic voltammetry

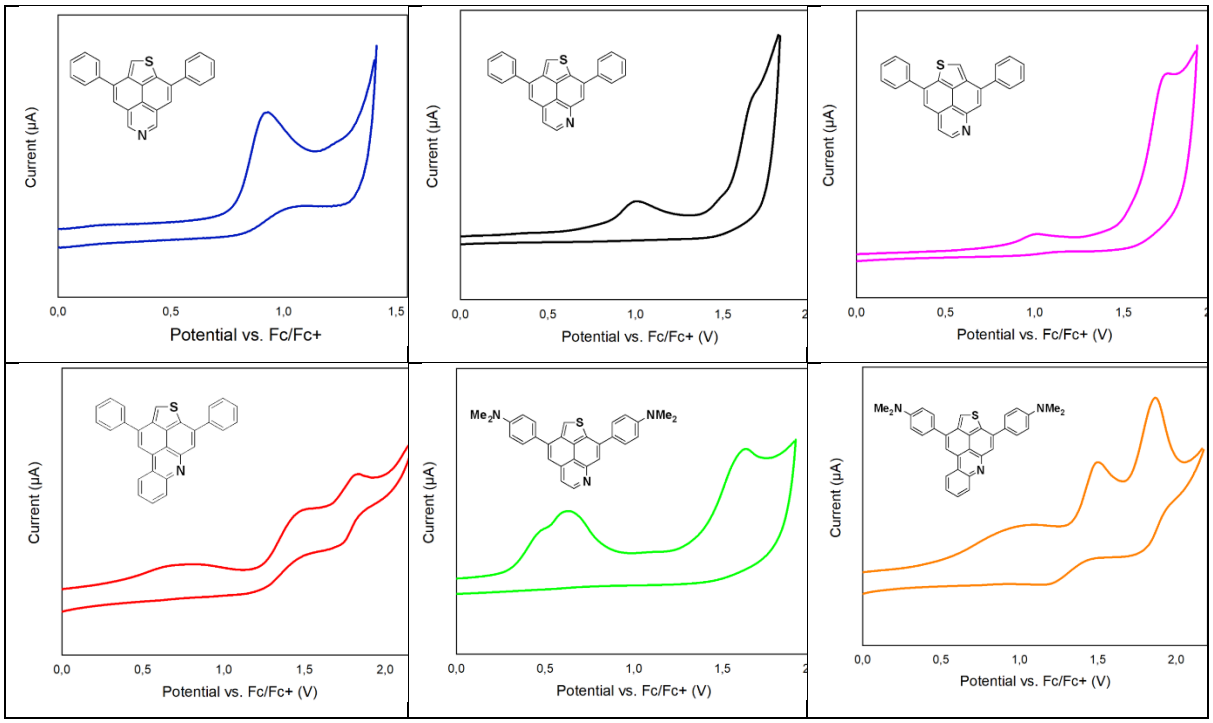
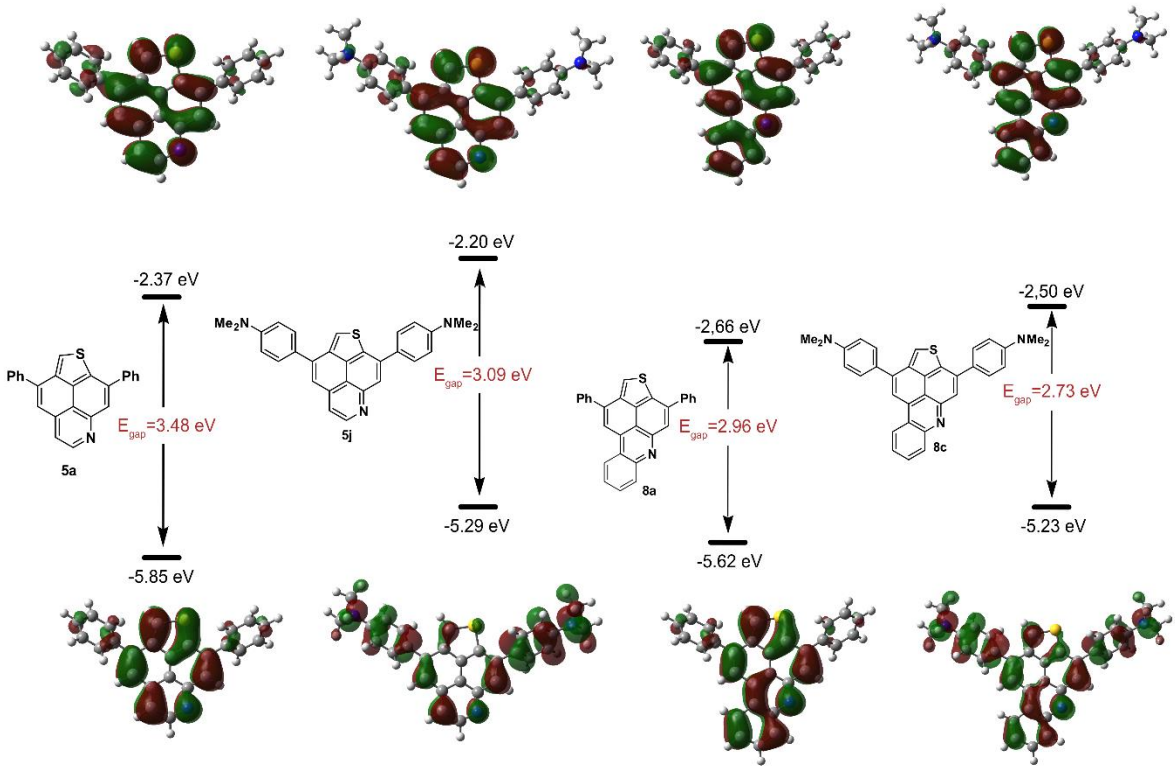


Figure S3. *Cyclic voltammograms of TNP,* ***5a, 6a, 8a, 5j*** *and* ***8c*** *measured in CH_2Cl_2 with 0.1 M n-Bu_4NPF_6 as a supporting electrolyte, glassy carbon working electrode, ANE2 as reference electrode and Pt counter-electrode with ferrocene as standard at a scan rate of 50 mV^{s-1}.*

DFT and TD-DFT Calculations



Scheme S1. *Calculated frontier molecular orbitals and energy levels of* ***5a, 5j, 8a*** *and* ***8c*** *at the B3LYP/6-311+G(d,p) level of theory within IEFPCM of dichloromethane (isovalue = 0.02 a.u.).*

Table S2. *Comparision of optical, electrochemical and calculated band gap.*

	5a	***5j***	***6a***	***8a***	***8c***
$E_{(HOMO)}^{CV}$ [eV][a]	-5.59	-5.10	-5.63	-5.17	-5.20
$E_{(HOMO)}^{calc}$ [eV][b]	-5.68	-5.29	-5.85	-5.62	-5.23
$E_{(LUMO)}^{calc}$ [eV][b]	-2.21	-2.20	-2.33	-2.66	-2.50
E_g^{CV} [eV][c]	3.38	2.61	3.05	2.61	2.33
E_g^{calc} [eV][b]	3.47	3.09	3.52	2.96	2.73
E_g^{opt} [eV][d]	2.91	2.25	2.63	2.25	2.01

a) Calculated using the equation: E(HOMO) = -e[E_{Ox}^{onset} vs. Fc/Fc^{+})+4.80]. b) Calculated DFT energy levels at the B3LYP/6-31G(d,p) level of theory within IEFPCM of dichloromethane. c) Calculated using correction factor: E(LUMO) = 1.16E_g^{opt} - E(HOMO)[cv. 45] d) Estimated from the intersection of normalized absorption and emission spectra. [e] Calculated TD-DFT excitation energies (ΔE) at the CAM-B3LYP/6-31+G(d,p) level of theory within IEFPCM for **5a** and **6a**. [f] Calculated TD-DFT excitation energies (ΔE) at the B3LYP/6-31+G(d,p) level of theory within IEFPCM for **5j**, **8a** and **8c**.

Cartesian coordinates of the optimized ground-state (S_0) and excited-state (S_1) structures

Calculated by (TD-)DFT at the B3LYP/6-311G(d,p) level of theory for ground state in gas phase and within IEFPCM of dichloromethane. The local minima of the optimized geometries were confirmed by frequency calculations, ensuring that no imaginary frequencies are presented. The stated Energy E for the S_0 state is the sum of electronic and zero-point Energies.

Table S3. *Cartesian Coordinates of* ***5a*** *(S_0); E = -1414.931728 Hartree.*

Symbol	X	Y	Z
C	-1.1900513	2.4040533	-0.0015588
C	0.0386239	1.6992679	0.0083882
C	1.2817949	2.3807005	0.0095813
C	1.2126710	3.7737565	0.0023390
C	-2.3997463	1.6443146	0.0034792
C	0.0263423	0.3001766	0.0159655
C	-1.1653025	-0.4196149	0.0407779
C	-2.4226207	0.2588899	0.0279363
C	0.9213687	-1.8280658	0.0127962
C	1.2248368	-0.4846276	-0.0044142
C	2.5002344	0.2195719	-0.0115854
C	2.4928190	1.5909060	0.0044746
H	3.4385329	2.1210592	-0.0176440
H	-3.3317345	2.1965606	0.0113678
H	2.1092864	4.3824659	0.0023365
H	1.5919021	-2.6728341	0.0262845
S	-0.7900318	-2.1306231	0.0318656
C	-3.7154162	-0.4750174	0.0337191
C	-3.9528721	-1.5209858	0.9378792
C	-4.7360402	-0.1175638	-0.8596011
C	-5.1757294	-2.1878507	0.9479441
H	-3.1904914	-1.7957885	1.6571661
C	-5.9568077	-0.7867599	-0.8499026
H	-4.5626076	0.6782153	-1.5747442
C	-6.1809635	-1.8249201	0.0533819
H	-5.3444706	-2.9867974	1.6610140
H	-6.7310536	-0.5006942	-1.5527470
C	3.7847510	-0.5267252	-0.0348052
C	4.8147150	-0.1965326	0.8583265
C	4.0081243	-1.5555196	-0.9629708
C	6.0309828	-0.8738379	0.8249372
H	4.6516153	0.5832817	1.5933518
C	5.2268531	-2.2282761	-0.9984853
H	3.2351646	-1.8103545	-1.6782187
C	6.2415569	-1.8921356	-0.1034680
H	6.8120068	-0.6093478	1.5287703
H	5.3852001	-3.0123119	-1.7303308
H	7.1881713	-2.4196074	-0.1293418
H	-7.1312826	-2.3462625	0.0602288

C	-0.0486406	4.3924432	-0.0056861
H	-0.0986125	5.4783577	-0.0108937
N	-1.2214314	3.7614491	-0.0075917

Table S4. *Cartesian Coordinates of* ***5j*** *(S_0); E = -1682.940739 Hartree.*

Symbol	X	Y	Z
C	1.2080185	2.9825462	0.0127798
C	-0.0242317	2.2839389	-0.0057320
C	-1.2654965	2.9687837	-0.0099065
C	-1.1896311	4.3631177	0.0039871
C	2.4135044	2.2183946	0.0029616
C	-0.0171840	0.8845517	-0.0209353
C	1.1726849	0.1613230	-0.0491002
C	2.4372891	0.8305773	-0.0303041
C	-0.9211316	-1.2392925	-0.0362299
C	-1.2204345	0.1047442	-0.0067135
C	-2.4977393	0.8110138	0.0041170
C	-2.4781564	2.1854627	-0.0073919
H	-3.4203312	2.7216483	0.0228918
H	3.3463157	2.7693183	-0.0056940
H	-2.0837136	4.9757931	0.0024155
H	-1.5937605	-2.0816863	-0.0638367
S	0.7893079	-1.5487473	-0.0525172
C	3.7234422	0.0958593	-0.0364360
C	3.9519781	-1.0033044	-0.8779586
C	4.7849140	0.4894921	0.7928121
C	5.1680697	-1.6707447	-0.9010969
H	3.1745836	-1.3332273	-1.5573982
C	6.0049290	-0.1690444	0.7885898
H	4.6444810	1.3184460	1.4777365
C	6.2413504	-1.2680823	-0.0717845
H	5.2845604	-2.5056354	-1.5775862
H	6.7759400	0.1688429	1.4666036
C	-3.7806118	0.0744126	0.0209880
C	-4.8507979	0.4617074	-0.8005869
C	-4.0021724	-1.0182167	0.8744317
C	-6.0712753	-0.1957939	-0.7792133
H	-4.7155226	1.2831009	-1.4957410
C	-5.2191640	-1.6819834	0.9173617
H	-3.2164728	-1.3410767	1.5475423
C	-6.3002585	-1.2863902	0.0938172
H	-6.8480062	0.1353119	-1.4540637
H	-5.3310481	-2.5090911	1.6042334
N	-7.5181903	-1.9279985	0.1447976
N	7.4602854	-1.9103404	-0.1059338
C	8.4859646	-1.5734682	0.8710292
H	8.1786184	-1.8007857	1.9011362
H	9.3862404	-2.1439622	0.6502171
H	8.7461175	-0.5122563	0.8205124
C	-7.6625355	-3.1513629	0.9212942
H	-8.6961884	-3.4870362	0.8640920
H	-7.0169894	-3.9606889	0.5540119
H	-7.4274443	-2.9816512	1.9761978
C	-8.5581445	-1.5910417	-0.8169135
H	-9.4560056	-2.1592697	-0.5812261

H	-8.8150709	-0.5290442	-0.7648839
H	-8.2669062	-1.8213576	-1.8509257
C	7.6094170	-3.1423731	-0.8675387
H	7.3776491	-2.9846855	-1.9249344
H	8.6436815	-3.4750929	-0.8033963
H	6.9641672	-3.9491631	-0.4937079
N	1.2452016	4.3410537	0.0255014
C	0.0736322	4.9756049	0.0210189
H	0.1277269	6.0616118	0.0314450

Table S5. *Cartesian Coordinates of* ***5j*** *(S_1); E = -1682.569246 Hartree.*

Symbol	X	Y	Z
C	1.1808724	2.9606485	0.0324427
C	-0.0538477	2.2387685	-0.0127236
C	-1.3082469	2.9231693	-0.0087534
C	-1.2421026	4.3459387	0.0414448
C	2.3867821	2.2123220	0.0164656
C	-0.0282972	0.8343401	-0.0665001
C	1.1852074	0.1240253	-0.1054450
C	2.4269585	0.8076236	-0.0535638
C	-0.9029300	-1.3269540	-0.1234949
C	-1.2226846	0.0293858	-0.0771384
C	-2.4852351	0.7297866	-0.0741790
C	-2.4879172	2.1399486	-0.0619631
H	-3.4433772	2.6587478	-0.0425062
H	3.3200352	2.7685322	0.0271168
H	-2.1473334	4.9478941	0.0476871
H	-1.5582143	-2.1826495	-0.1960035
S	0.8376229	-1.6130678	-0.1476597
C	3.7324059	0.1038030	-0.0490706
C	4.0008827	-0.9978611	-0.8825102
C	4.7818032	0.5261105	0.7898834
C	5.2376235	-1.6373132	-0.8905799
H	3.2353538	-1.3561754	-1.5653495
C	6.0227325	-0.1030619	0.8003964
H	4.6163269	1.3568209	1.4712202
C	6.2954867	-1.2019544	-0.0535238
H	5.3786436	-2.4761791	-1.5619862
H	6.7792394	0.2613830	1.4854294
C	-3.7783952	0.0294440	-0.0301049
C	-4.9067864	0.5178687	-0.7430028
C	-3.9712572	-1.1432016	0.7462305
C	-6.1330066	-0.1122523	-0.6966130
H	-4.7992046	1.4017344	-1.3634554
C	-5.1897813	-1.7876164	0.8097449
H	-3.1455967	-1.5311874	1.3323402
C	-6.3165598	-1.2945515	0.0834352
H	-6.9547948	0.2998599	-1.2686372
H	-5.2822647	-2.6710648	1.4288970
N	-7.5225427	-1.9270747	0.1361644
N	7.5388612	-1.8134466	-0.0766219
C	8.5205814	-1.4804626	0.9476296
H	8.1752718	-1.7387815	1.9616652
H	9.4422827	-2.0293638	0.7478556
H	8.7602882	-0.4114424	0.9288834
C	-7.7003162	-3.1316151	0.9495009

H	-8.7267826	-3.4787556	0.8491714
H	-7.0271846	-3.9285860	0.6153117
H	-7.5037937	-2.9198411	2.0063586
C	-8.6709769	-1.4103976	-0.6106936
H	-9.5262671	-2.0617160	-0.4415134
H	-8.9291989	-0.3993344	-0.2764098
H	-8.4561889	-1.3859891	-1.6845500
C	7.7069448	-3.0682894	-0.7982408
H	7.4635556	-2.9465647	-1.8596635
H	8.7510091	-3.3785011	-0.7322567
H	7.0775602	-3.8758539	-0.3908748
N	1.2016799	4.3295033	0.0793880
C	0.0059525	4.9584177	0.0800146
H	0.0573227	6.0468059	0.1167837

Table S6. *Cartesian Coordinates of* ***6a*** *(S_0); E = -1414.931641 Hartree.*

Symbol	X	Y	Z
C	-1.2773947	2.3791593	-0.0087608
C	-0.0310260	1.6997763	-0.0064725
C	1.1941508	2.4078591	0.0037339
C	1.0855970	3.8154910	0.0085400
C	-2.4851140	1.5803552	-0.0038227
C	-0.0192302	0.3005626	-0.0142485
C	-1.2135226	-0.4892374	0.0044443
C	-2.4920786	0.2100682	0.0119463
C	1.1761890	-0.4141400	-0.0401282
C	2.4304107	0.2688390	-0.0263938
C	2.4072666	1.6552197	-0.0006593
H	3.3489088	2.1921631	-0.0099175
H	-3.4211810	2.1260664	0.0164453
H	1.9688315	4.4434352	0.0146118
C	-3.7748164	-0.5392509	0.0350593
C	-3.9916776	-1.5780394	0.9535946
C	-4.8106488	-0.2022414	-0.8488266
C	-5.2086816	-2.2541566	0.9884690
H	-3.2150842	-1.8382171	1.6629981
C	-6.0254277	-0.8820637	-0.8157307
H	-4.6534336	0.5864582	-1.5755673
C	-6.2289857	-1.9109292	0.1026656
H	-5.3613450	-3.0460416	1.7130941
H	-6.8110325	-0.6111915	-1.5120387
C	3.7244255	-0.4630547	-0.0330715
C	4.7373897	-0.1173765	0.8733016
C	3.9692459	-1.4947515	-0.9514873
C	5.9590183	-0.7851307	0.8626724
H	4.5571069	0.6665724	1.5997623
C	5.1932807	-2.1592907	-0.9628130
H	3.2119420	-1.7596734	-1.6797582
C	6.1911200	-1.8086442	-0.0550954
H	6.7275045	-0.5095151	1.5758804
H	5.3687367	-2.9469430	-1.6866722
H	7.1421678	-2.3286092	-0.0628822
H	-7.1744242	-2.4405732	0.1280920
C	-0.1759583	4.3920480	0.0043038
H	-0.2664277	5.4745130	0.0075797
N	-1.3452022	3.7163290	-0.0034681

C	-0.9017110	-1.8311222	-0.0147186
H	-1.5678489	-2.6793685	-0.0297162
S	0.8106918	-2.1264422	-0.0335404

S_0 **8a**

E = -1568.607280 Hartree

Table S7. *Cartesian Coordinates of* ***8a*** *(S_0); E = -1568.607280 Hartree.*

Symbol	X	Y	Z
C	-1.0199210	1.9244626	-0.0030064
C	0.0673215	0.9965080	0.0084341
C	1.4061474	1.4226629	0.0102884
C	-2.3557562	1.3957502	0.0015476
C	-0.2189362	-0.3787578	0.0161272
C	-1.5237626	-0.8593523	0.0418838
C	-2.6367146	0.0452023	0.0279369
C	0.2461621	-2.6447089	0.0133432
C	0.8028892	-1.3802235	-0.0048400
C	2.1828023	-0.9359706	-0.0132383
C	2.4364223	0.4155850	0.0034064
H	3.4706036	0.7336288	-0.0212887
H	-3.1656037	2.1149639	0.0094419
H	0.7420577	-3.6021724	0.0291814
S	-1.4846023	-2.6054638	0.0315505
C	-4.0419585	-0.4385114	0.0349690
C	-4.4681486	-1.4187694	0.9437124
C	-4.9786549	0.0949991	-0.8625351
C	-5.7923148	-1.8505382	0.9540137
H	-3.7702084	-1.8248948	1.6661760
C	-6.3010138	-0.3400947	-0.8528644
H	-4.6618758	0.8413409	-1.5818275
C	-6.7127823	-1.3149422	0.0549016
H	-6.1052574	-2.6011948	1.6708009
H	-7.0085537	0.0786832	-1.5594672
C	3.3039105	-1.9098922	-0.0379626
C	4.3776858	-1.7793866	0.8554462
C	3.3287803	-2.9636415	-0.9647823
C	5.4433179	-2.6750345	0.8241297
H	4.3649845	-0.9827711	1.5904369
C	4.3980413	-3.8550514	-0.9983265
H	2.5214895	-3.0683978	-1.6798974
C	5.4576491	-3.7160272	-0.1028953
H	6.2597864	-2.5625130	1.5284340
H	4.4054640	-4.6556829	-1.7292519
H	6.2872028	-4.4132901	-0.1274807
H	-7.7423025	-1.6539858	0.0616818
N	-0.8175171	3.2443576	-0.0091814
C	2.9108046	3.4367818	0.0108363
H	3.7937466	2.8100313	0.0205617
C	3.0577876	4.8021708	0.0055531
H	4.0492206	5.2398722	0.0099245
C	1.9186799	5.6442992	-0.0056953
H	2.0477522	6.7206644	-0.0099955
C	0.6598399	5.1026272	-0.0105879
H	-0.2266626	5.7253953	-0.0185332
C	0.4630468	3.6911520	-0.0049862
C	1.6244106	2.8349082	0.0052847

Table S8. *Cartesian Coordinates of* ***8a*** *(S_0); E = -1836.616606 Hartree.*

Symbol	X	Y	Z
C	1.2103569	2.4214262	0.0098238
C	0.0068317	1.6508352	-0.0141015
C	-1.2627729	2.2535234	-0.0192990
C	2.4600766	1.7166190	0.0017346
C	0.1029578	0.2493733	-0.0311412
C	1.3315455	-0.4030595	-0.0597329
C	2.5618072	0.3381366	-0.0356792
C	-0.6666898	-1.9311304	-0.0482720
C	-1.0475939	-0.6034221	-0.0174697
C	-2.3591239	0.0212422	-0.0036480
C	-2.4191860	1.3985983	-0.0148033
H	-3.3986078	1.8573952	0.0223019
H	3.3591229	2.3208854	-0.0035328
H	-1.2864397	-2.8127998	-0.0785767
S	1.0534095	-2.1281801	-0.0631056
C	3.8848993	-0.3254765	-0.0382382
C	4.1757005	-1.4129948	-0.8761954
C	4.9218610	0.1294497	0.7913323
C	5.4269362	-2.0116547	-0.8954323
H	3.4198986	-1.7868303	-1.5571868
C	6.1761619	-0.4602203	0.7913803
H	4.7339966	0.9510745	1.4736145
C	6.4746298	-1.5476171	-0.0650095
H	5.5916179	-2.8399881	-1.5699677
H	6.9260878	-0.0780616	1.4695940
C	-3.5979065	-0.7849800	0.0193161
C	-4.6972583	-0.4515984	-0.7880571
C	-3.7488804	-1.8966571	0.8641269
C	-5.8770519	-1.1788086	-0.7633092
H	-4.6169309	0.3824409	-1.4766752
C	-4.9249178	-2.6296862	0.9109888
H	-2.9404060	-2.1796434	1.5280677
C	-6.0340978	-2.2905733	0.0992524
H	-6.6776865	-0.8860957	-1.4279563
H	-4.9827041	-3.4672751	1.5919588
N	-7.2101643	-3.0043357	0.1504679
N	7.7261039	-2.1216352	-0.0936968
C	8.7355445	-1.7134481	0.8729896
H	8.4426128	-1.9378909	1.9076839
H	9.6637373	-2.2402735	0.6600181
H	8.9394939	-0.6409001	0.8027640
C	-7.2788199	-4.2382138	0.9206194
H	-8.2890774	-4.6380597	0.8593335
H	-6.5832070	-5.0029667	0.5497737
H	-7.0562172	-4.0601822	1.9769952
C	-8.2791229	-2.7150340	-0.7948554
H	-9.1373123	-3.3423070	-0.5616019
H	-8.6008880	-1.6720563	-0.7212376
H	-7.9844393	-2.9084390	-1.8352481
C	7.9492437	-3.3393417	-0.8602094
H	7.7187018	-3.1892766	-1.9191998
H	8.9991335	-3.6163477	-0.7874952
H	7.3450549	-4.1811895	-0.4958774
N	1.1891344	3.7582362	0.0256817
C	-2.4784862	4.4549587	-0.0182073

H	-3.4381216	3.9534532	-0.0411355
C	-1.2861579	3.6840242	-0.0068142
C	-0.0195260	4.3738547	0.0170532
C	-0.0244039	5.7991065	0.0321552
H	0.9383803	6.2959802	0.0508498
C	-1.1980850	6.5073731	0.0226271
H	-1.1793071	7.5913802	0.0343095
C	-2.4405947	5.8282356	-0.0039015
H	-3.3638256	6.3959568	-0.0131944

Table S92. *Cartesian Coordinates of* ***8c*** *(S_1); E = -1836.226094 Hartree.*

Symbol	X	Y	Z
C	1.1834763	2.4013268	0.0033256
C	-0.0109990	1.6095913	-0.0408727
C	-1.3015393	2.2121705	-0.0469283
C	2.4354336	1.7233640	-0.0049537
C	0.1056641	0.2113367	-0.0838167
C	1.3594086	-0.4262423	-0.1156964
C	2.5617127	0.3270502	-0.0672061
C	-0.6293050	-1.9975086	-0.1493782
C	-1.0332664	-0.6687009	-0.0971812
C	-2.3424139	-0.0527640	-0.0919347
C	-2.4233765	1.3541607	-0.0913949
H	-3.4142887	1.7954813	-0.0707715
H	3.3321681	2.3365182	0.0066841
H	-1.2323613	-2.8912077	-0.2222656
S	1.1183126	-2.1782940	-0.1594001
C	3.9058637	-0.3008525	-0.0585620
C	4.2462506	-1.3710258	-0.9050490
C	4.9175808	0.1671755	0.8002788
C	5.5180482	-1.9396386	-0.9049947
H	3.5117651	-1.7609519	-1.6048292
C	6.1924009	-0.3917137	0.8182351
H	4.6964352	0.9761049	1.4921975
C	6.5387674	-1.4585613	-0.0482516
H	5.7142410	-2.7581293	-1.5876391
H	6.9172745	0.0048947	1.5194290
C	-3.5852520	-0.8307286	-0.0379070
C	-4.7537362	-0.4085505	-0.7266432
C	-3.6933206	-2.0212088	0.7266569
C	-5.9358783	-1.1193714	-0.6730522
H	-4.7144278	0.4838579	-1.3435678
C	-4.8689706	-2.7417596	0.8015821
H	-2.8408081	-2.3594452	1.3053047
C	-6.0343970	-2.3182498	0.0952036
H	-6.7877606	-0.7583884	-1.2357900
H	-4.8969251	-3.6302005	1.4201445
N	-7.1972155	-3.0287802	0.1554637
N	7.8189720	-1.9959580	-0.0668942
C	8.7511738	-1.6454099	0.9975056
H	8.3959076	-1.9599892	1.9925851
H	9.7089302	-2.1317214	0.8041555
H	8.9286713	-0.5647955	1.0224536
C	-7.2785240	-4.2603190	0.9409540
H	-8.2752823	-4.6845173	0.8329000
H	-6.5470023	-4.9969327	0.5900205

H	-7.0980078	-4.0612201	2.0040259
C	-8.3898215	-2.5676291	-0.5553913
H	-9.2073668	-3.2605104	-0.3636442
H	-8.6898512	-1.5711309	-0.2113959
H	-8.2113251	-2.5296532	-1.6363325
C	8.0520086	-3.2487605	-0.7746726
H	7.8058514	-3.1501097	-1.8375234
H	9.1109398	-3.5036709	-0.7046891
H	7.4643331	-4.0846659	-0.3608985
N	1.1348764	3.7546487	0.0414927
C	-2.5386594	4.4159494	0.0021408
H	-3.4971994	3.9045700	-0.0232449
C	-1.3474517	3.6632543	-0.0035624
C	-0.0836268	4.3643727	0.0356832
C	-0.1059236	5.7882696	0.0730065
H	0.8513272	6.3025963	0.0979009
C	-1.2974411	6.4969549	0.0758888
H	-1.2827777	7.5838575	0.1050523
C	-2.5254181	5.8094998	0.0410961
H	-3.4627014	6.3598006	0.0450547

TD-DFT

Table S3. *Calculated TD-DFT transitions of compound* ***5a*** *at B3LYP/6-311+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	f	Configuration	CI coefficient
S_1	3.20	388	0.3528	HOMO → LUMO	0.68891
S_2	3.60	345	0.2218	HOMO-1 → LUMO	0.67451
				HOMO → LUMO+1	0.13125
				HOMO → LUMO+2	-0.11053
S_3	3.82	324	0.0380	HOMO-2 → LUMO	0.65661
				HOMO → LUMO+1	0.16623
				HOMO → LUMO+2	-0.15601
S_4	3.92	316	0.1430	HOMO-2 → LUMO	-0.14585
				HOMO-1 → LUMO	-0.12676
				HOMO → LUMO+1	0.66034
S_5	4.05	306	0.0013	HOMO-6 → LUMO	0.65316
				HOMO-4 → LUMO	0.14826

Table S4. *Calculated TD-DFT transitions of compound* ***5j*** *at B3LYP/6-311+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	f	Configuration	CI coefficient
S_1	2.62	473	0.2852	HOMO-1 → LUMO	0.68233
				HOMO → LUMO	0.17529
S_2	2.71	458	0.1898	HOMO-1 → LUMO	-0.17193
				HOMO → LUMO	0.67535
S_3	3.33	372	0.1722	HOMO-2 → LUMO	0.68052
S_4	3.73	332	0.0693	HOMO-3 → LUMO	-0.40939
				HOMO-2 → LUMO+1	-0.16498
				HOMO-1 → LUMO+1	-0.10543
				HOMO → LUMO+1	0.49767
				HOMO → LUMO+2	0.15085
S_5	3.83	324	0.5414	HOMO-3 → LUMO	0.47848
				HOMO-2 → LUMO+2	0.10911
				HOMO-1 → LUMO+2	0.13470
				HOMO → LUMO+1	0.44688
				HOMO → LUMO+2	-0.13849
S_6	3.90	318	0.1326	HOMO-1 → LUMO+1	0.68370
				HOMO → LUMO+1	0.11736

Table S5. *Calculated TD-DFT transitions of compound* ***6a*** *at B3LYP/6-311+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	f	Configuration	CI coefficient
S_1	3.20	387	0.3932	HOMO → LUMO	0.69150
S_2	3.67	338	0.1155	HOMO-1 → LUMO	0.60645
				HOMO → LUMO+1	0.32022
S_3	3.82	324	0.1389	HOMO-2 → LUMO	-0.36545
				HOMO-1 → LUMO	-0.27906
				HOMO → LUMO+1	0.52505
S_4	3.89	319	0.0708	HOMO-2 → LUMO	0.54145
				HOMO-1 → LUMO	-0.12988
				HOMO → LUMO+1	0.32581
				HOMO → LUMO+2	-0.25569
S_5	4.24	293	0.0036	HOMO-6 → LUMO	0.67995
				HOMO-5 → LUMO	-0.10402
				HOMO-4 → LUMO	0.11579
S_6	4.24	293	0.0036	HOMO-3 → LUMO	0.66175
				HOMO → LUMO+2	0.16156
				HOMO → LUMO+5	0.12377

Table S6. *Calculated TD-DFT transitions of compound* ***8a*** *at B3LYP/6-311+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	f	Configuration	CI coefficient
S_1	2.67	465	0.3557	HOMO → LUMO	0.69984
S_2	3.3274	373	0.2430	HOMO-1 → LUMO	0.65498
				HOMO → LUMO+2	0.21934
S_3	3.49	355	0.0945	HOMO-2 → LUMO	0.67547
				HOMO → LUMO+1	0.10142
				HOMO → LUMO+2	-0.14747
S_4	3.68	337	0.0921	HOMO-3 → LUMO	0.13734
				HOMO → LUMO+1	0.67192
S_5	3.74	332	0.0012	HOMO-7 → LUMO	0.66669
				HOMO-6 → LUMO	0.10515
				HOMO-5 → LUMO	-0.15102
S_6	3.82	325	0.0257	HOMO-3 → LUMO	0.64480
				HOMO → LUMO+1	-0.12234
				HOMO → LUMO+3	0.19183

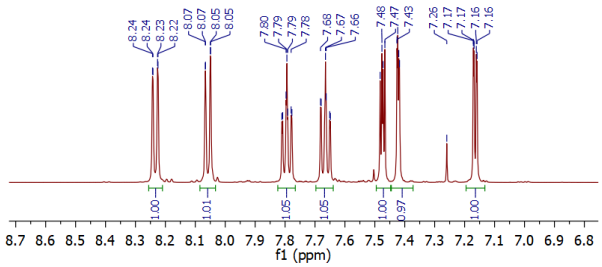
Table S7. *Calculated TD-DFT transitions of compound* ***8c*** *at B3LYP/6-311+G(d,p) level (IEFPCM).*

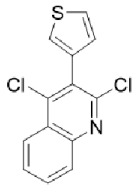
S_n	E (eV)	λ (nm)	f	Configuration	CI coefficient
S_1	2.36	525	0.3593	HOMO-1 → LUMO	0.64203
				HOMO → LUMO	-0.28976
S_2	2.40	517	0.2473	HOMO-1 → LUMO	0.29078
				HOMO → LUMO	0.63661
S_3	2.86	433	0.0779	HOMO-2 → LUMO	0.69498
S_4	3.42	362	0.0901	HOMO-3 → LUMO	0.61136
				HOMO-2 → LUMO+2	0.15467
				HOMO → LUMO+2	-0.29703
S_5	3.61	343	0.2327	HOMO-4 → LUMO	0.10891
				HOMO-2 → LUMO+1	-0.13716
				HOMO → LUMO+1	0.66707
S_6	3.78	329	0.0016	HOMO-8 → LUMO	0.66635
				HOMO-6 → LUMO	-0.11854
				HOMO-5 → LUMO	0.15368

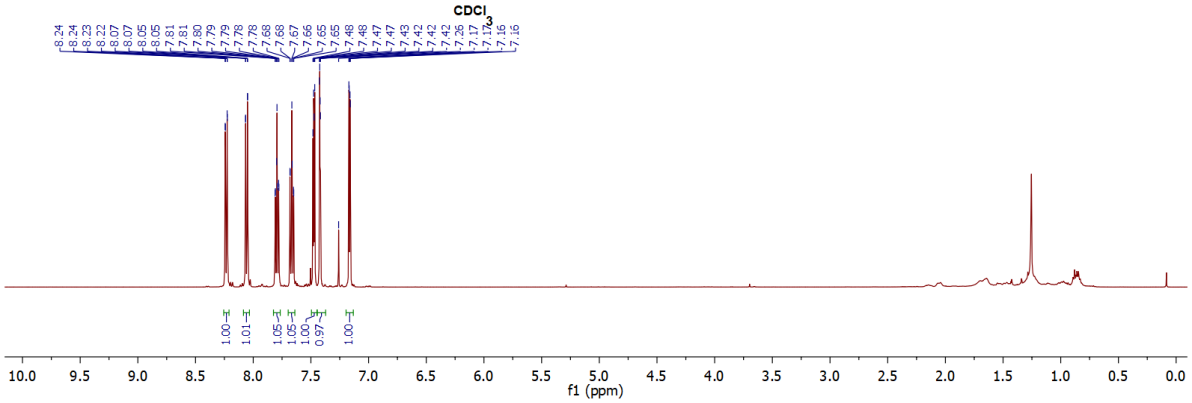
^{1}H-, ^{19}F-, and ^{13}C{1H}-NMR Spectra

2,4-dichloro-3-(thiophen-3-yl)quinoline

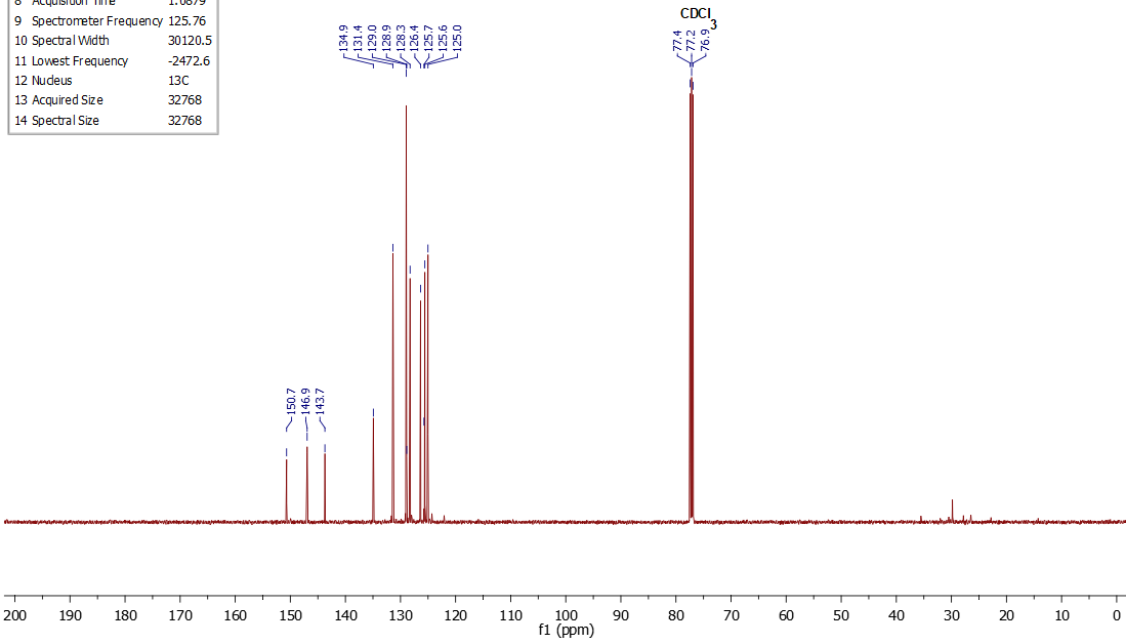
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.0
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





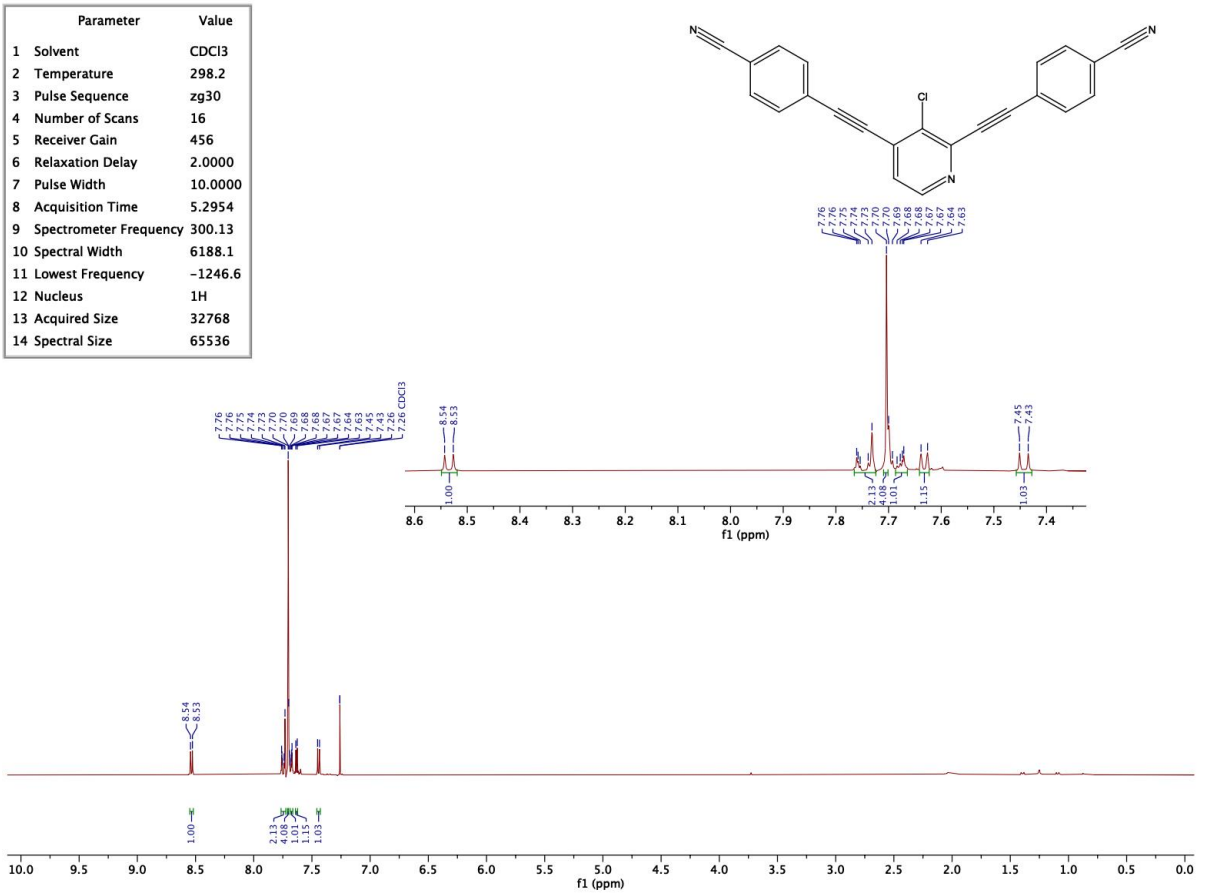


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Number of Scans	512
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2472.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

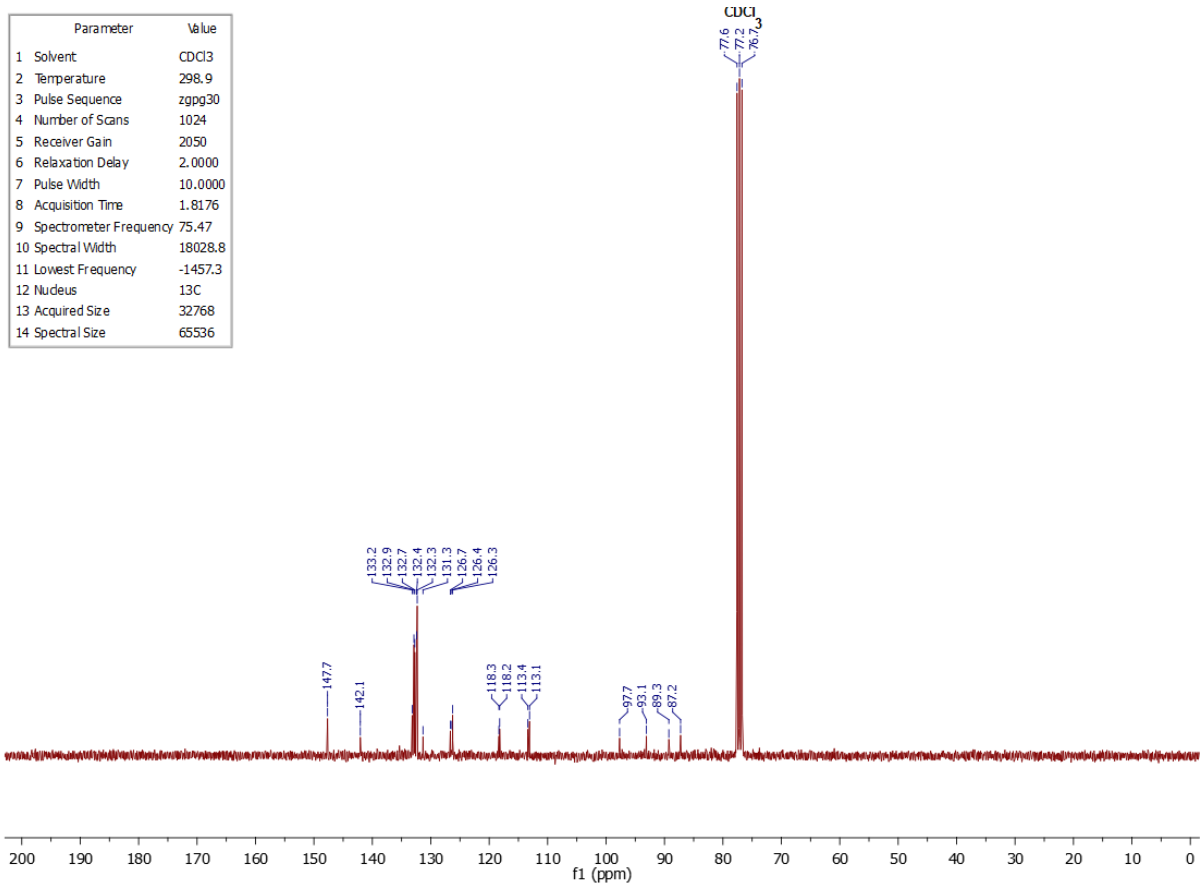


4,4'-((3-chloropyridine-2,4-diyl)bis(ethyne-2,1-diyl))dibenzonitrile

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	456
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

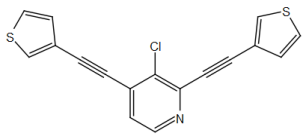


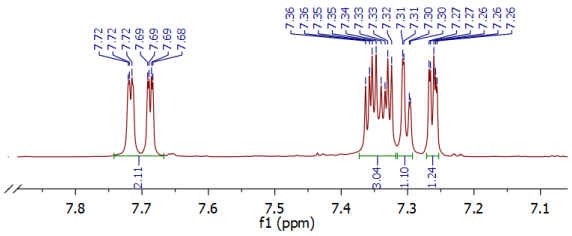
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.9
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1457.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

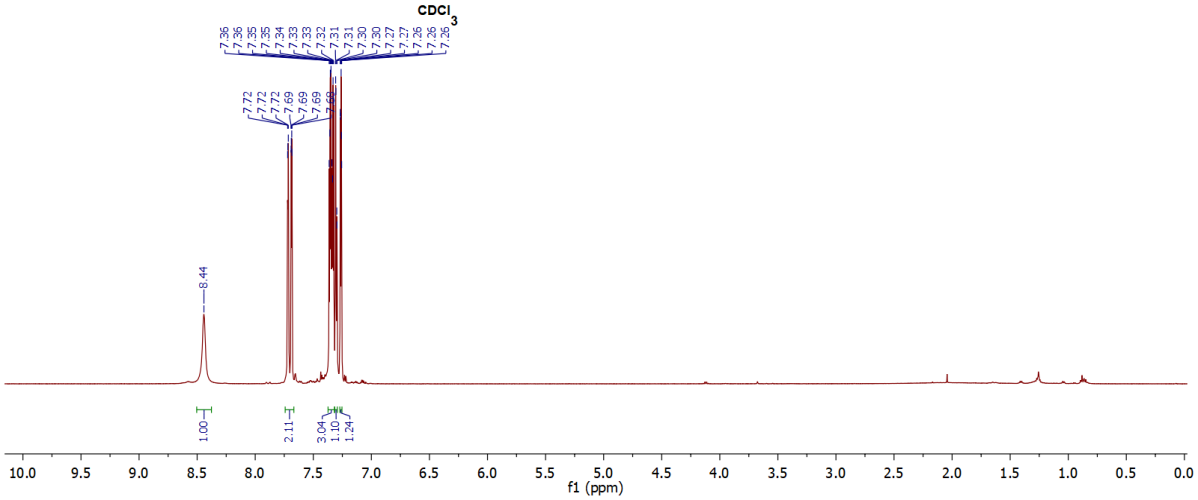


3-chloro-2,4-bis(thiophen-3-ylethynyl)pyridine

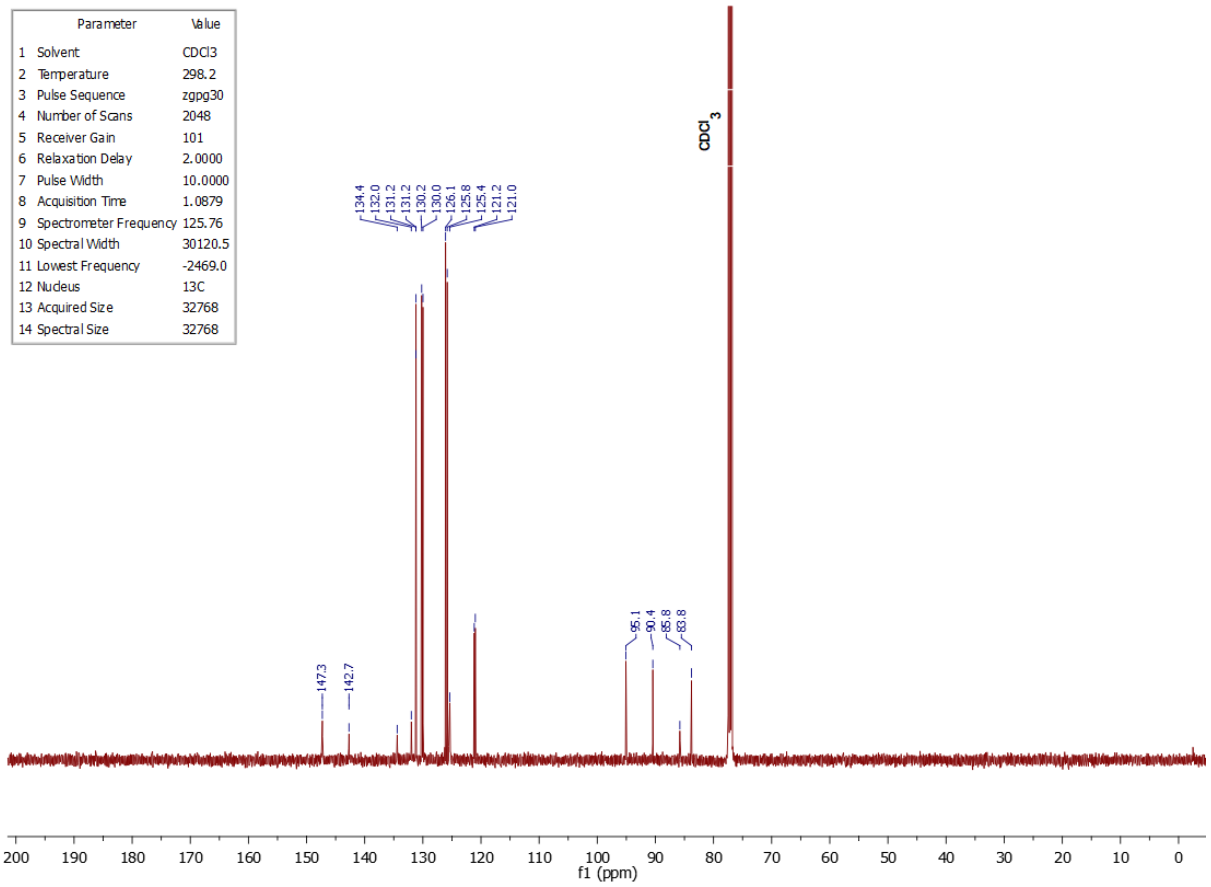
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





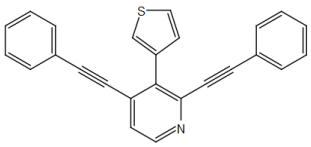


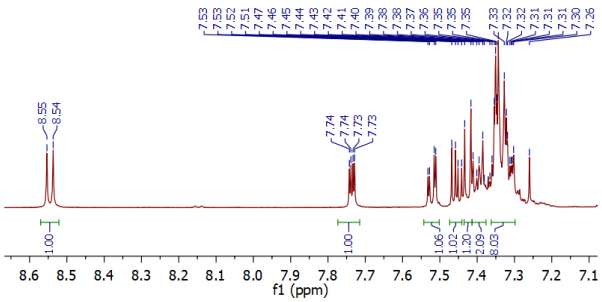
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	2048
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2469.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

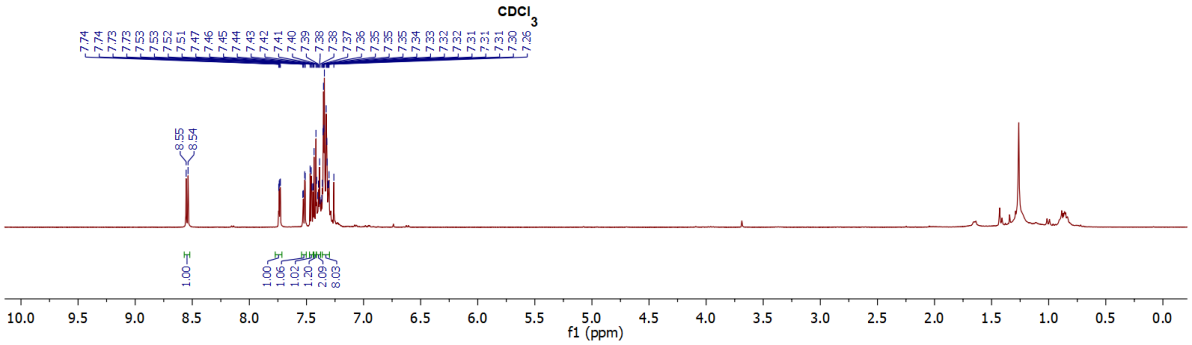


2,4-bis(phenylethynyl)-3-(thiophen-3-yl)pyridine (1a)

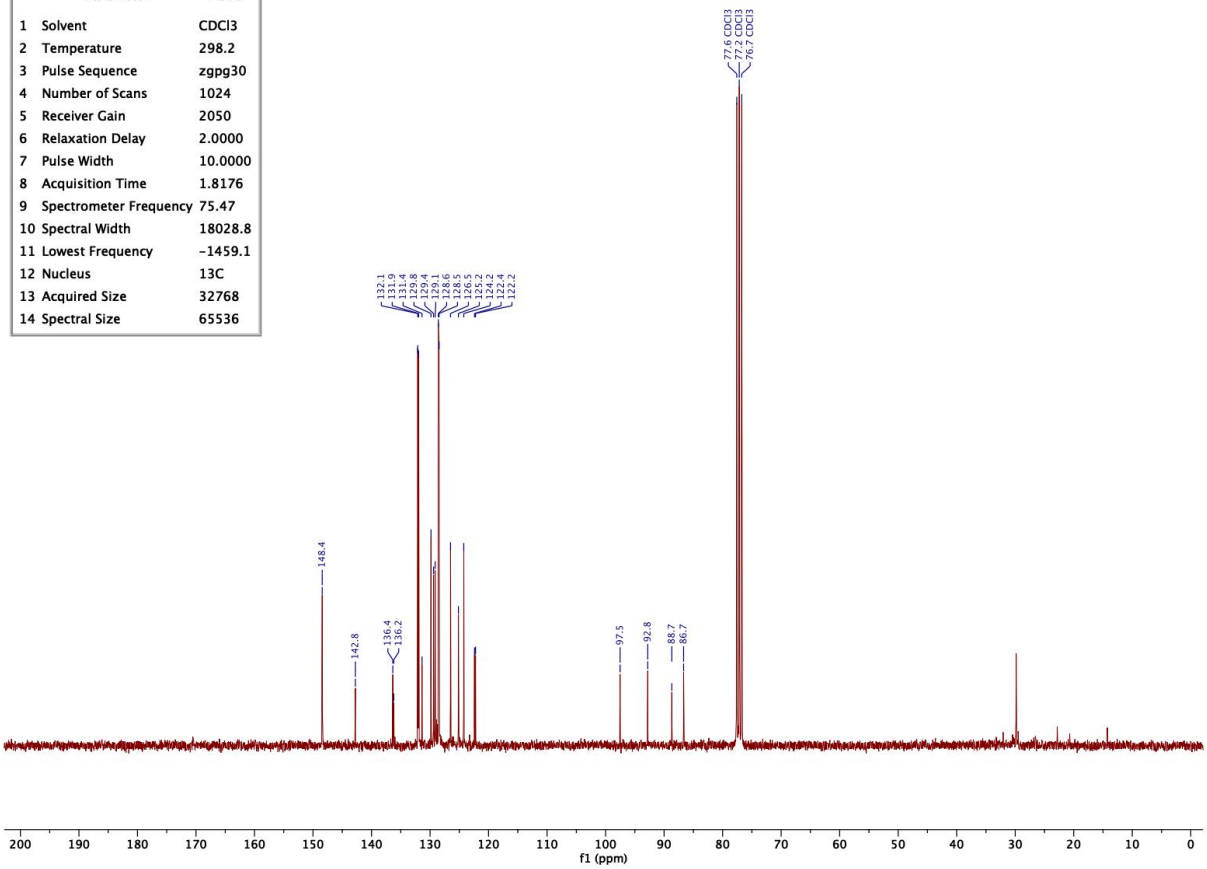
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	161
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.2
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





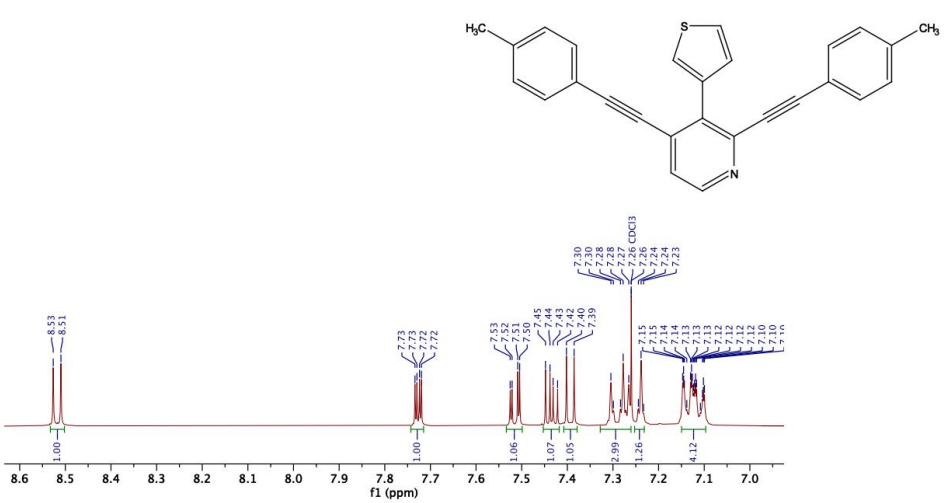


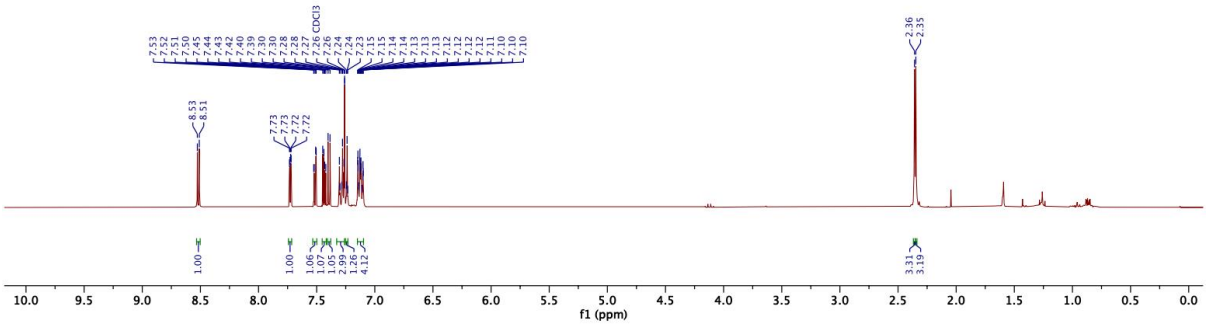
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1459.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



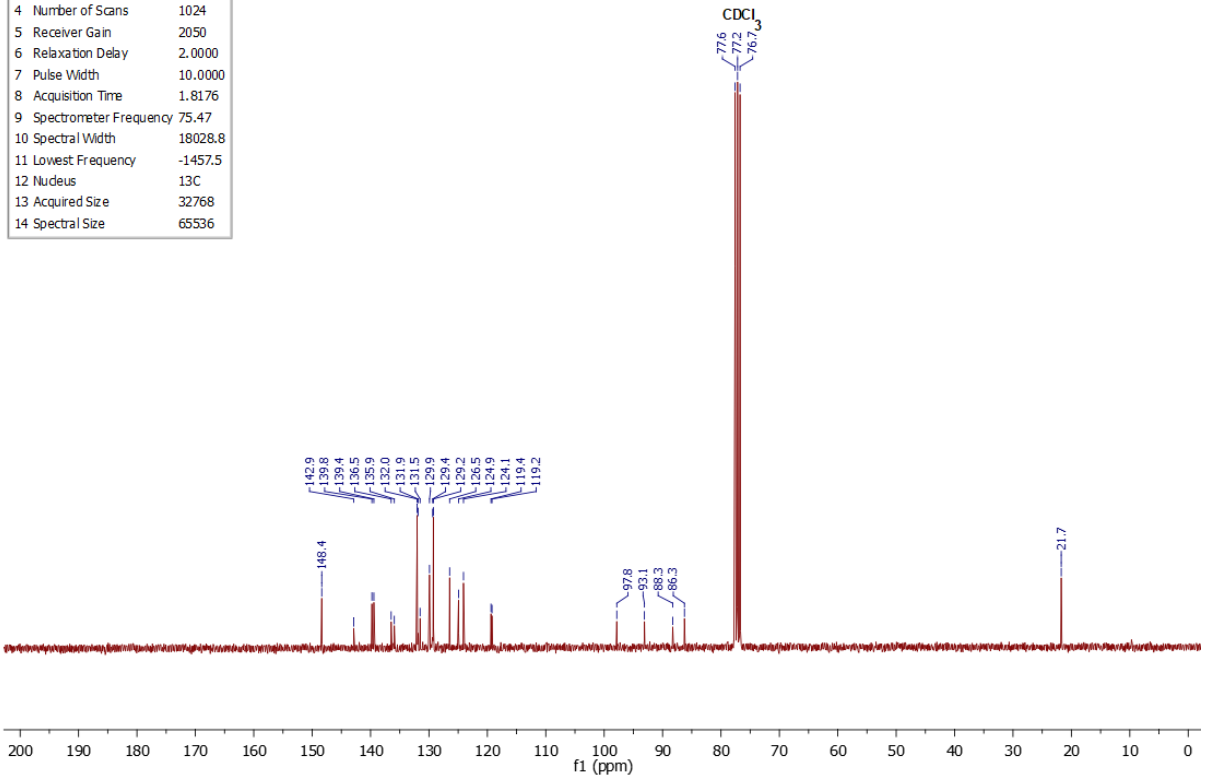
3-(thiophen-3-yl)-2,4-bis(*p*-tolylethynyl)pyridine (1b)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	287
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



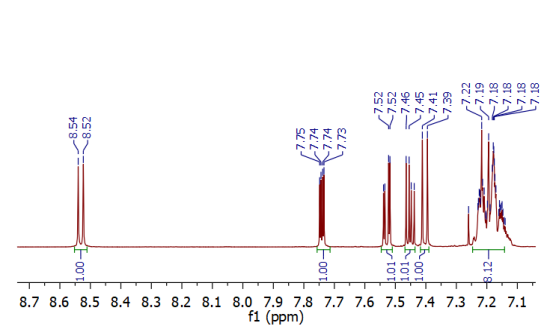


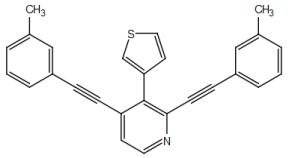
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1457.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

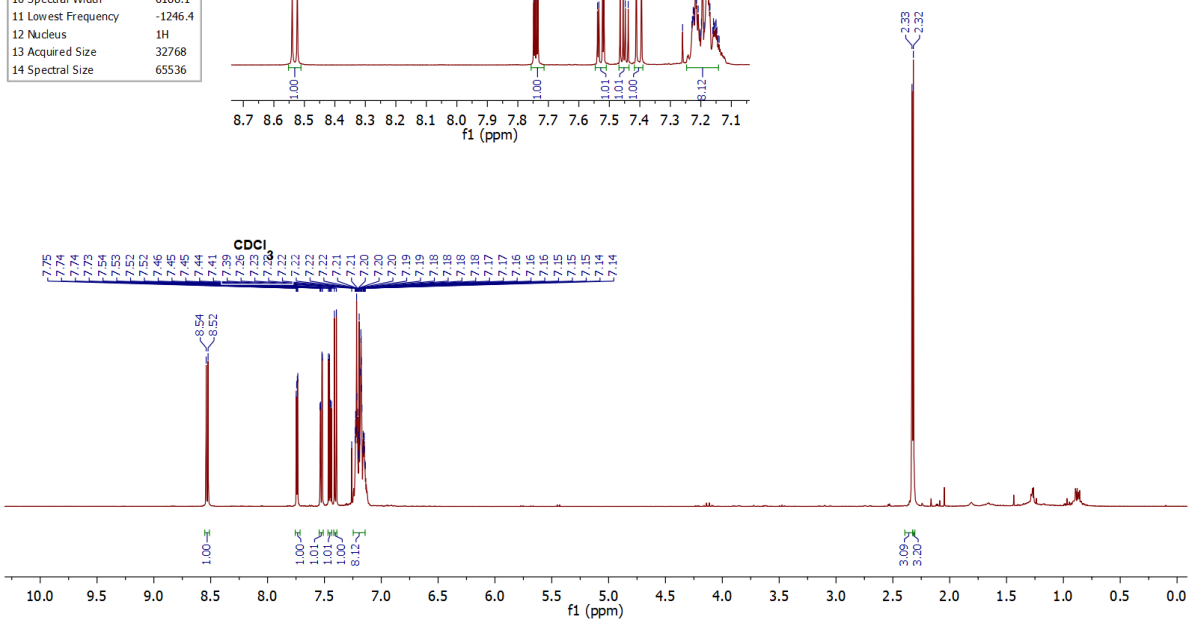


3-(thiophen-3-yl)-2,4-bis(*m*-tolylethynyl)pyridine (1c)

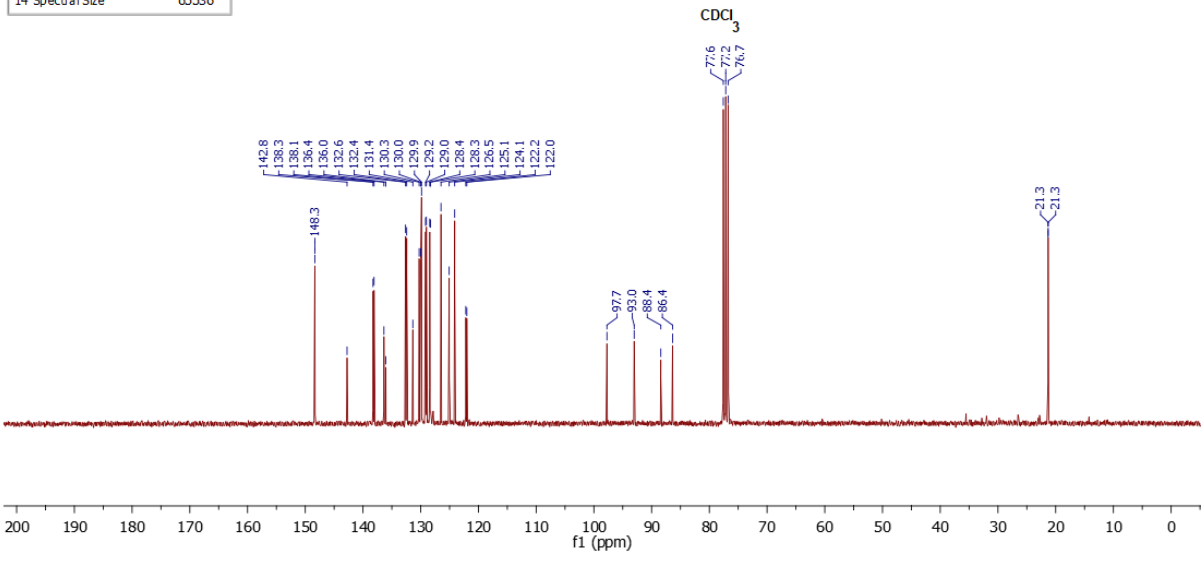
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	64
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



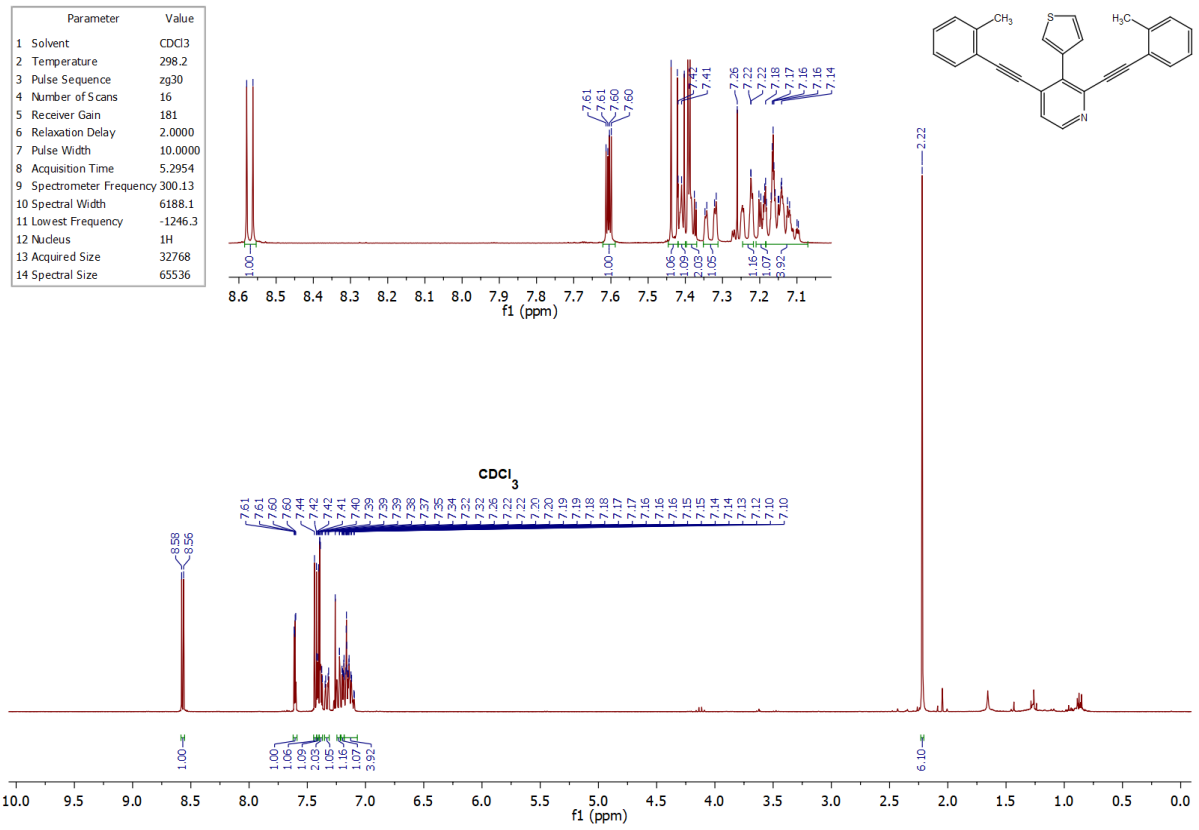


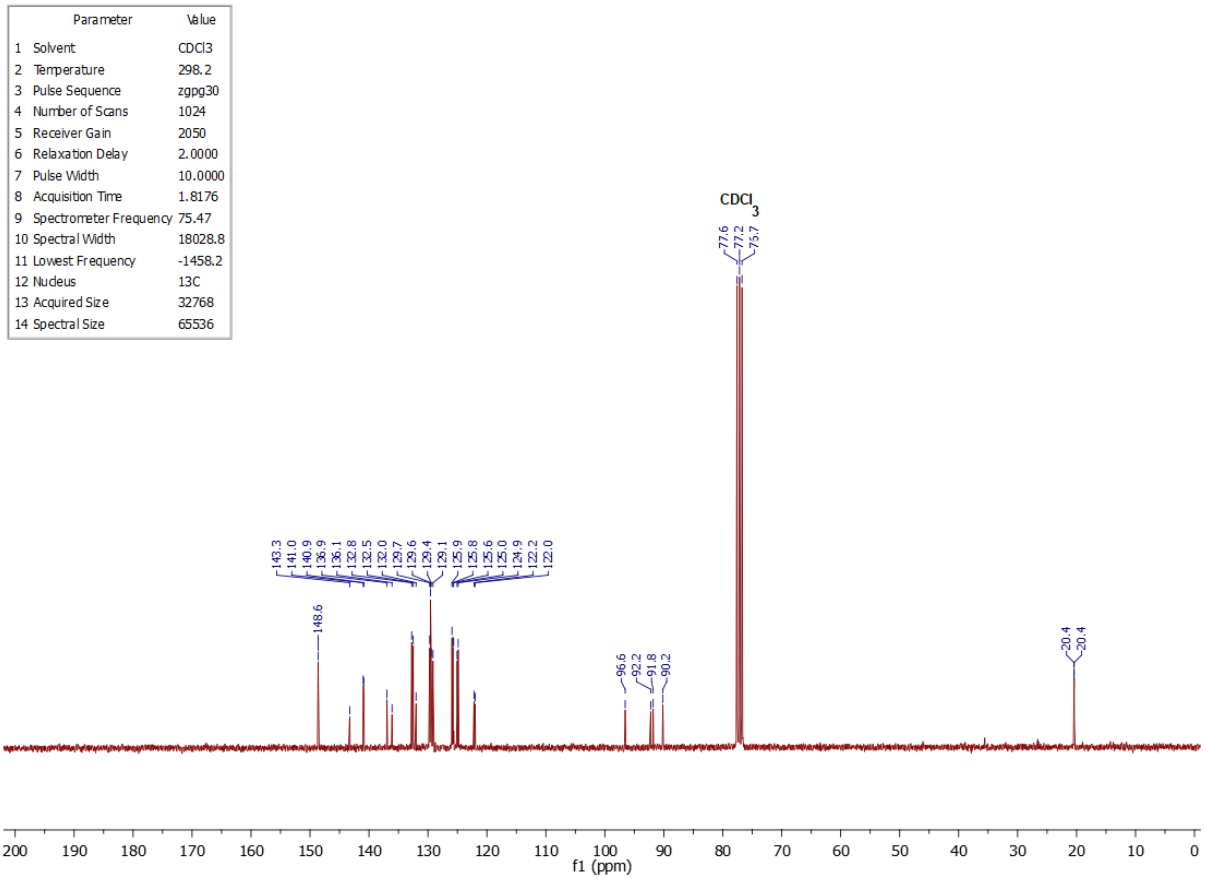


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1462.2
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



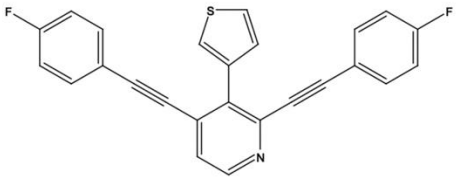
3-(thiophen-3-yl)-2,4-bis(*o*-tolylethynyl)pyridine (1d)

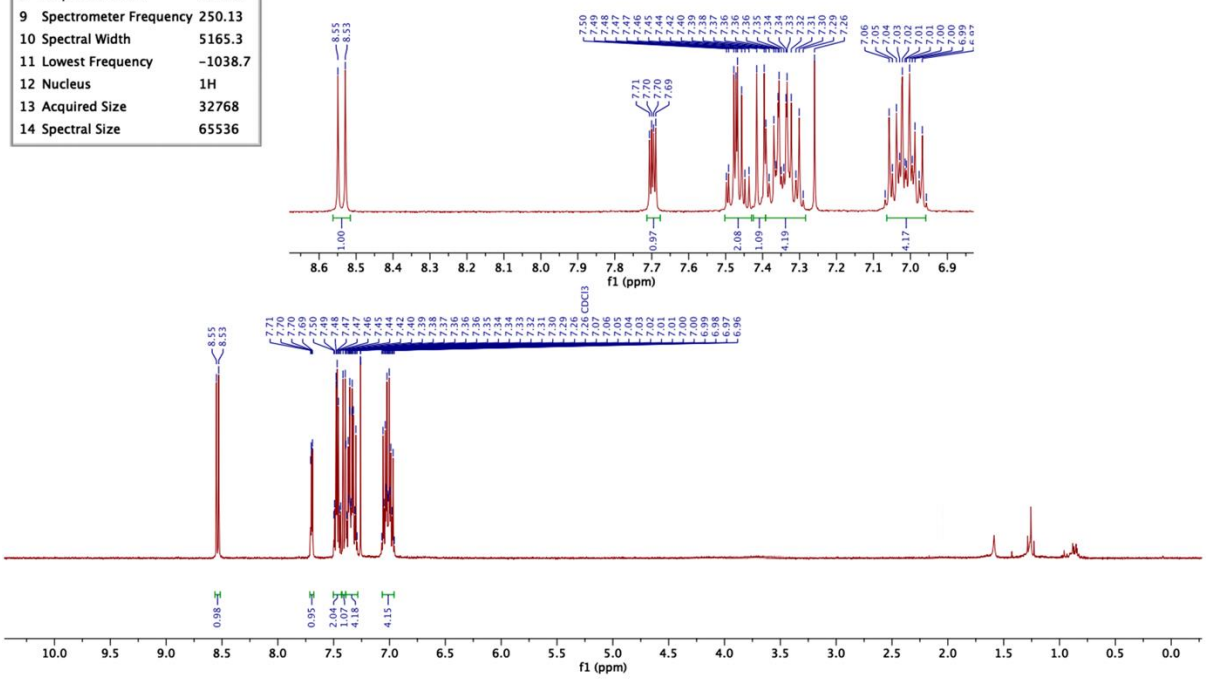




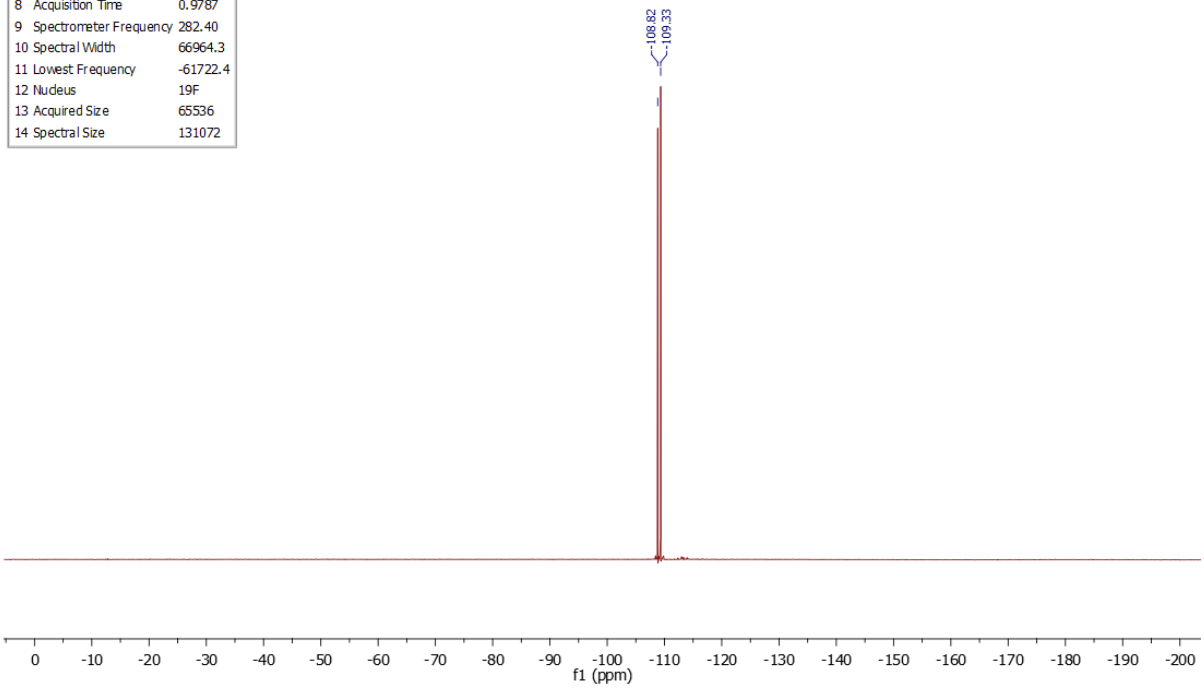
2,4-bis((4-fluorophenyl)ethynyl)-3-(thiophen-3-yl)pyridine (1e)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	812
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.7
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

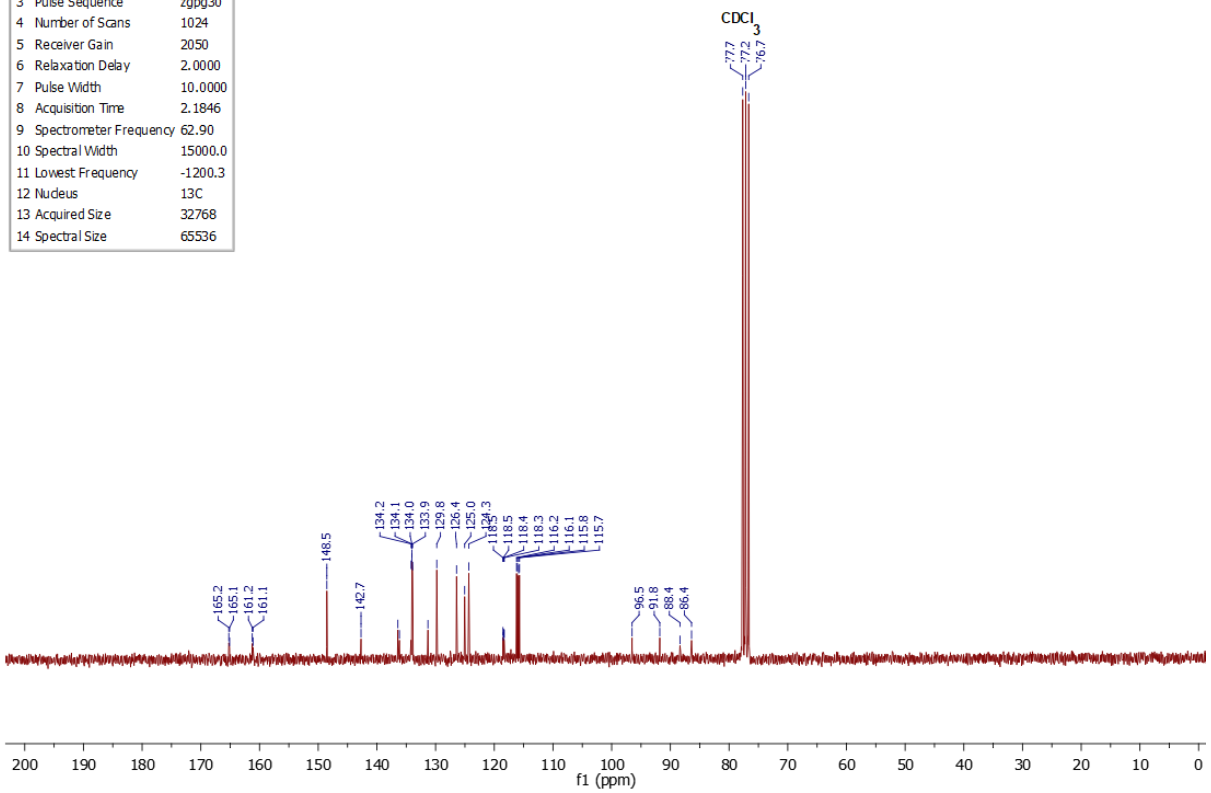




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.40
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

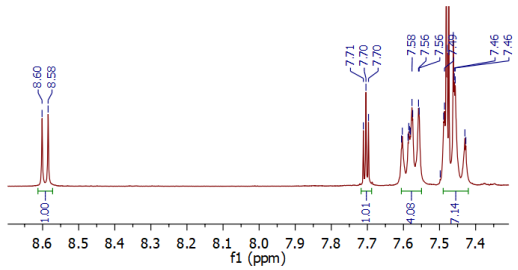


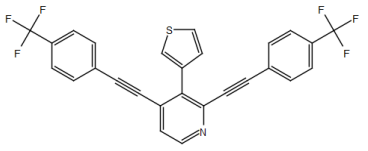
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	297.8
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1200.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

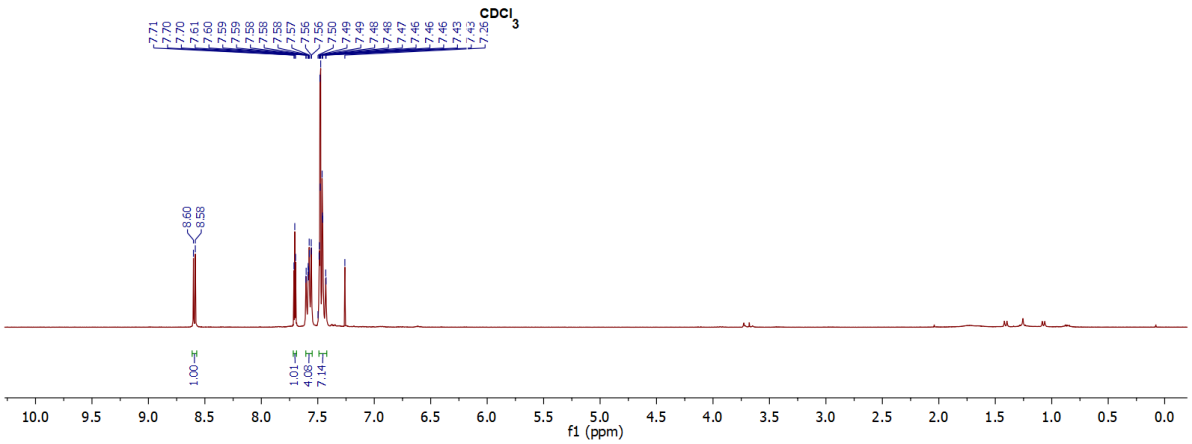


3-(thiophen-3-yl)-2,4-bis((4-(trifluoromethyl)phenyl)ethynyl)pyridine (1f)

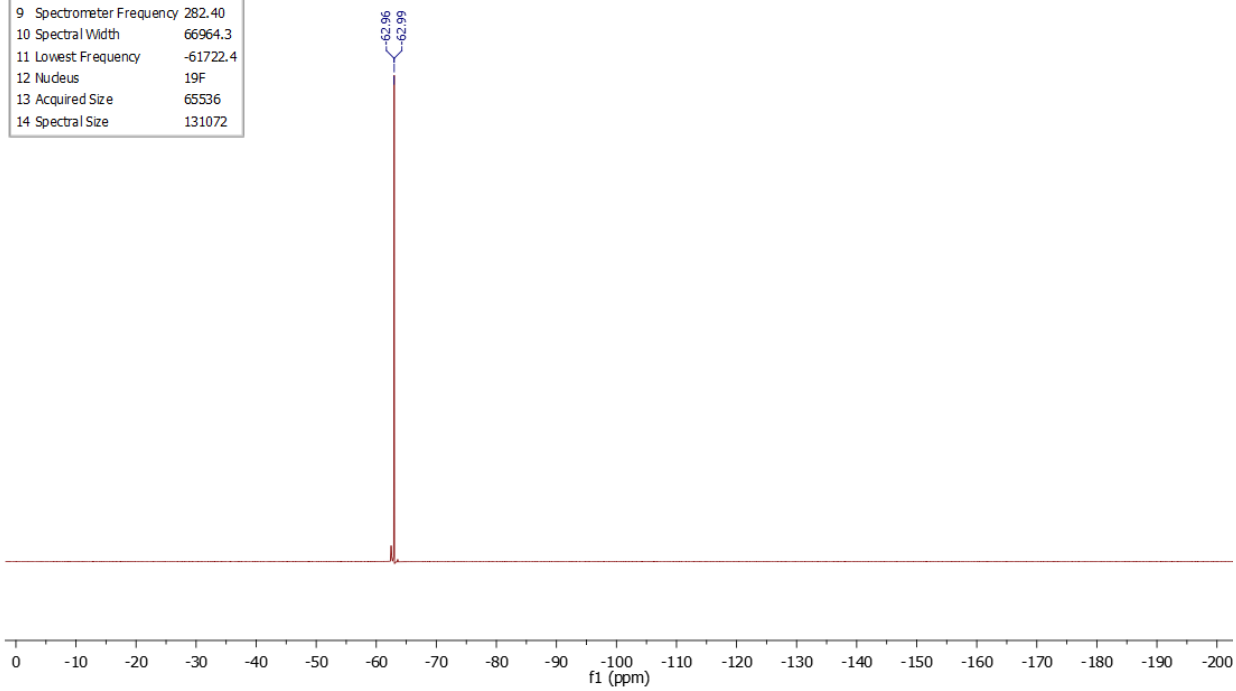
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	181
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.5
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



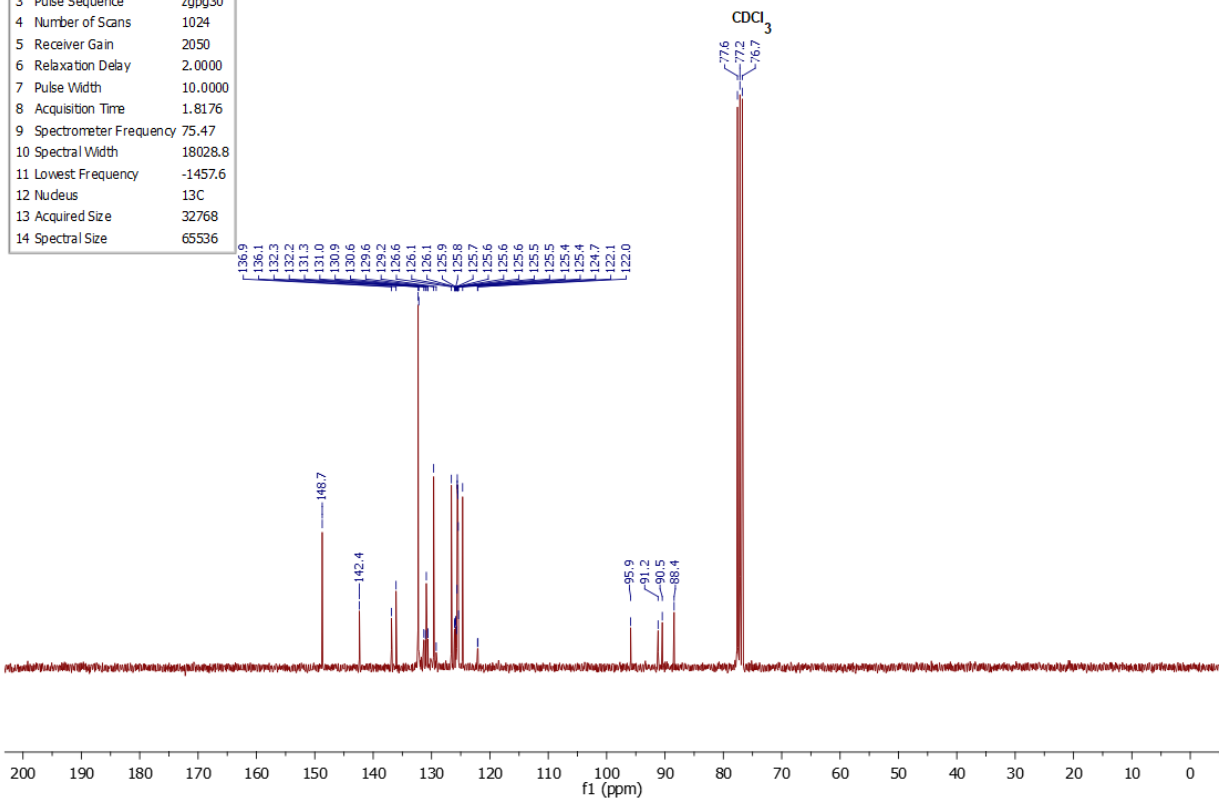




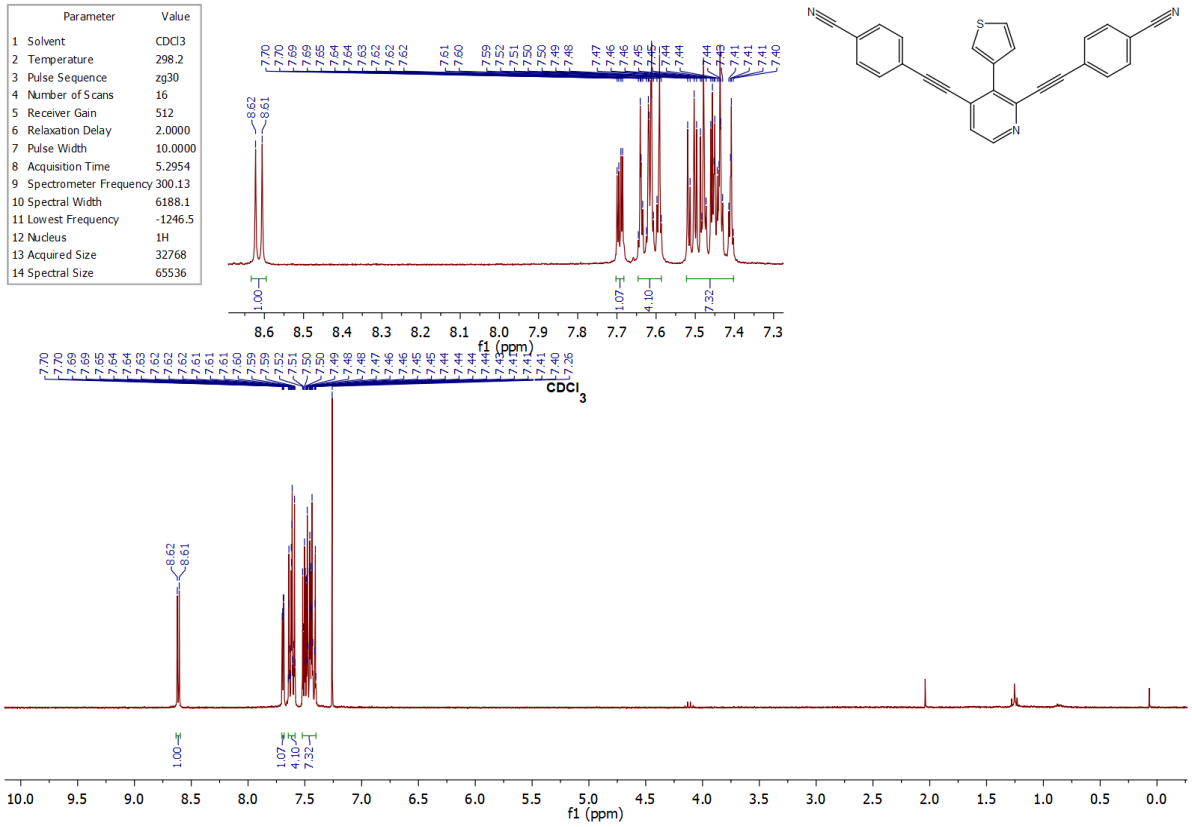
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.7
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	1620
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.40
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

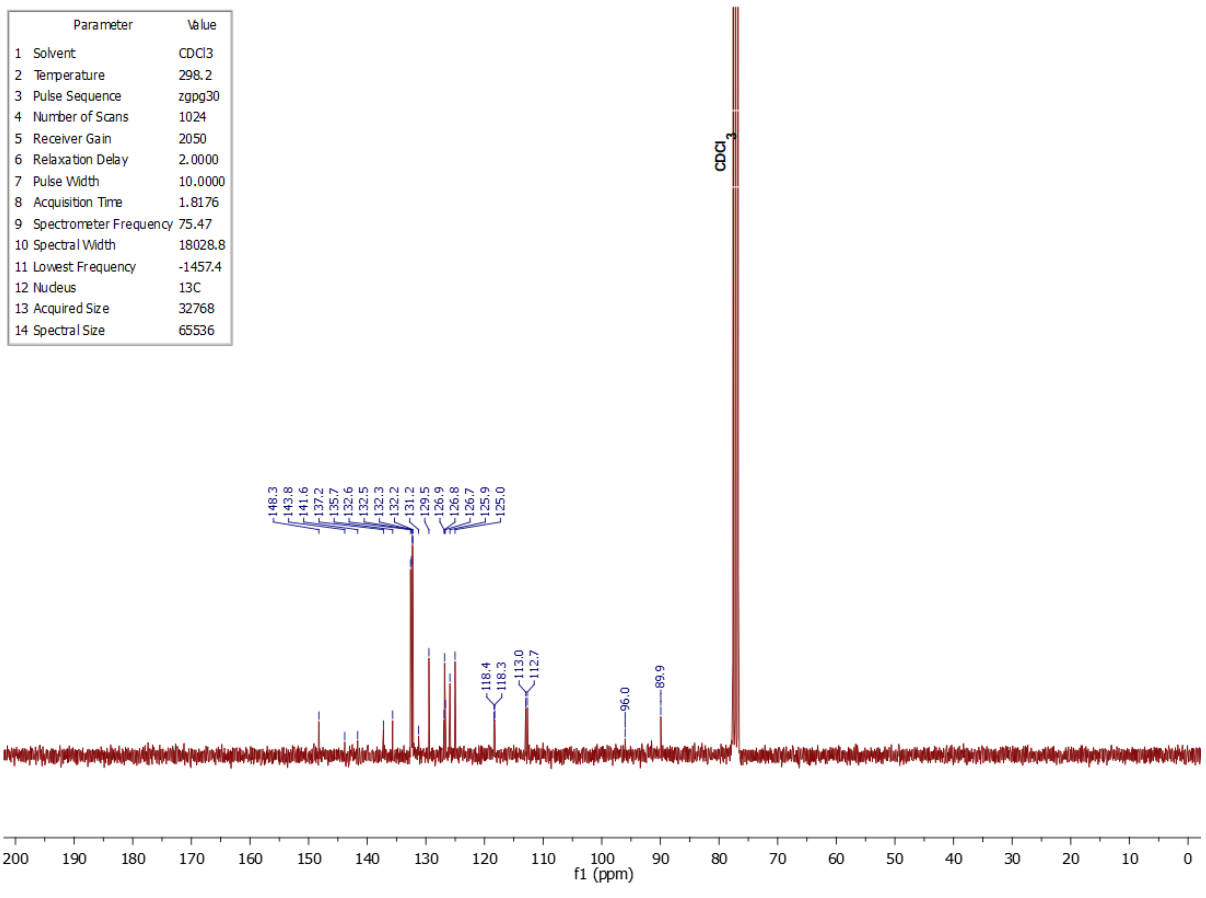


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.7
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1457.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

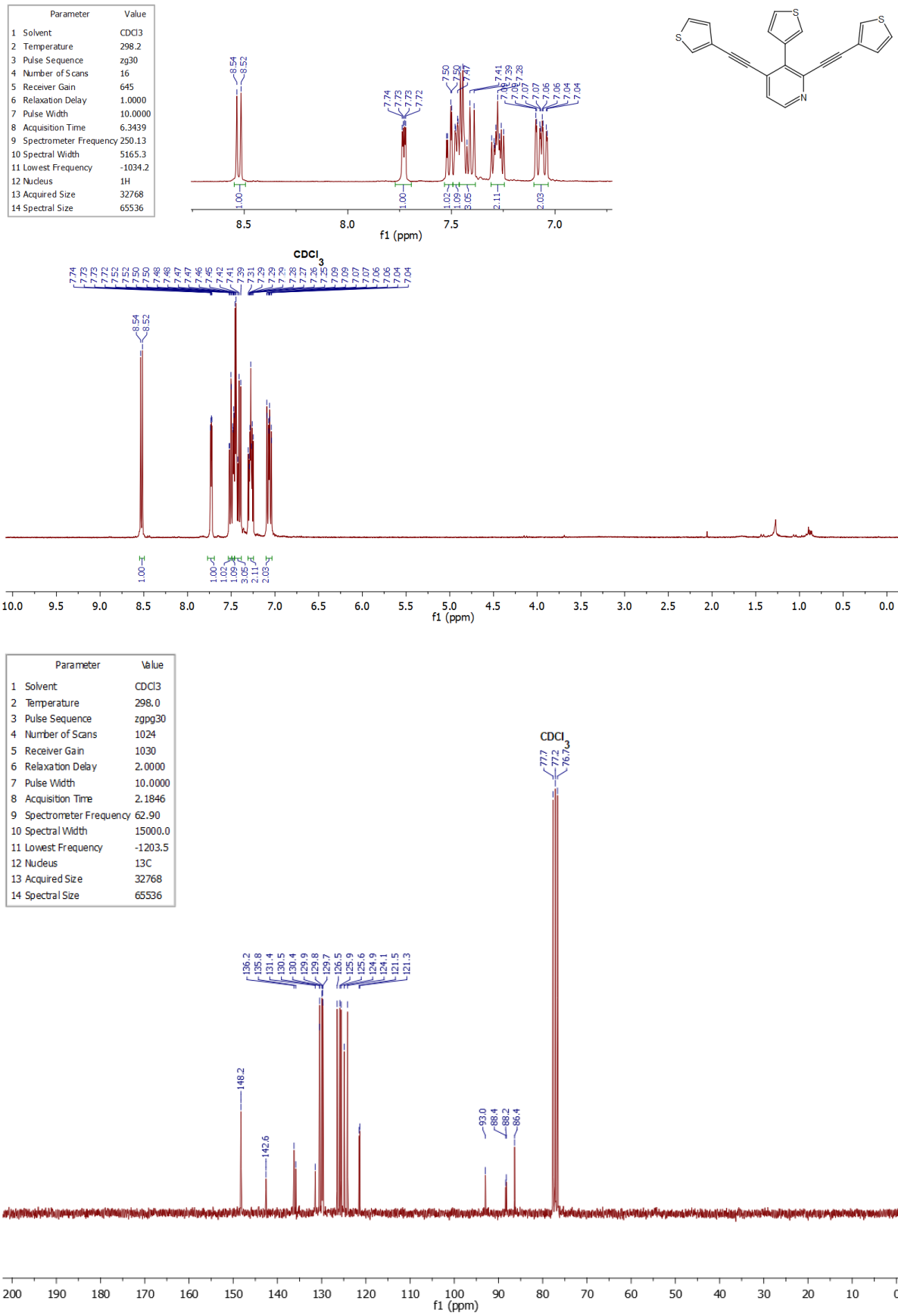


4,4'-((3-(thiophen-3-yl)pyridine-2,4-diyl)bis(ethyne-2,1-diyl))dibenzonitrile (1g)

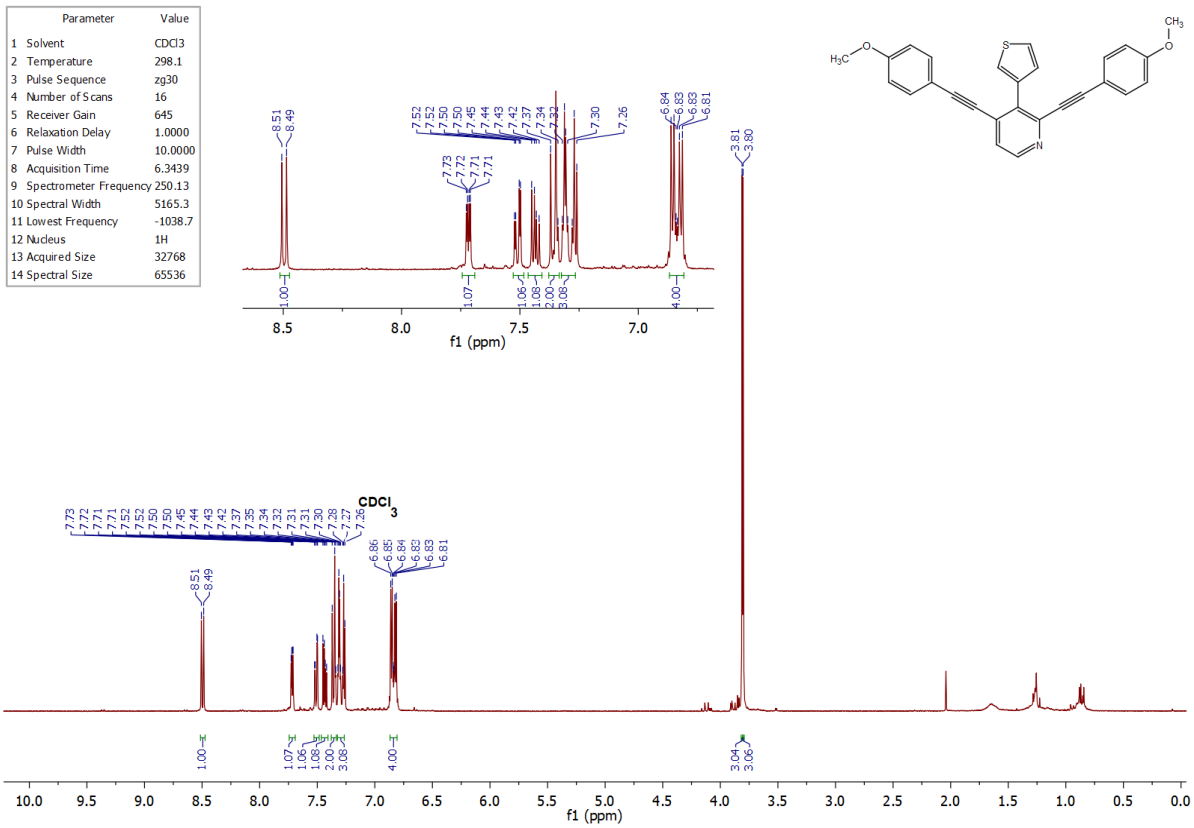


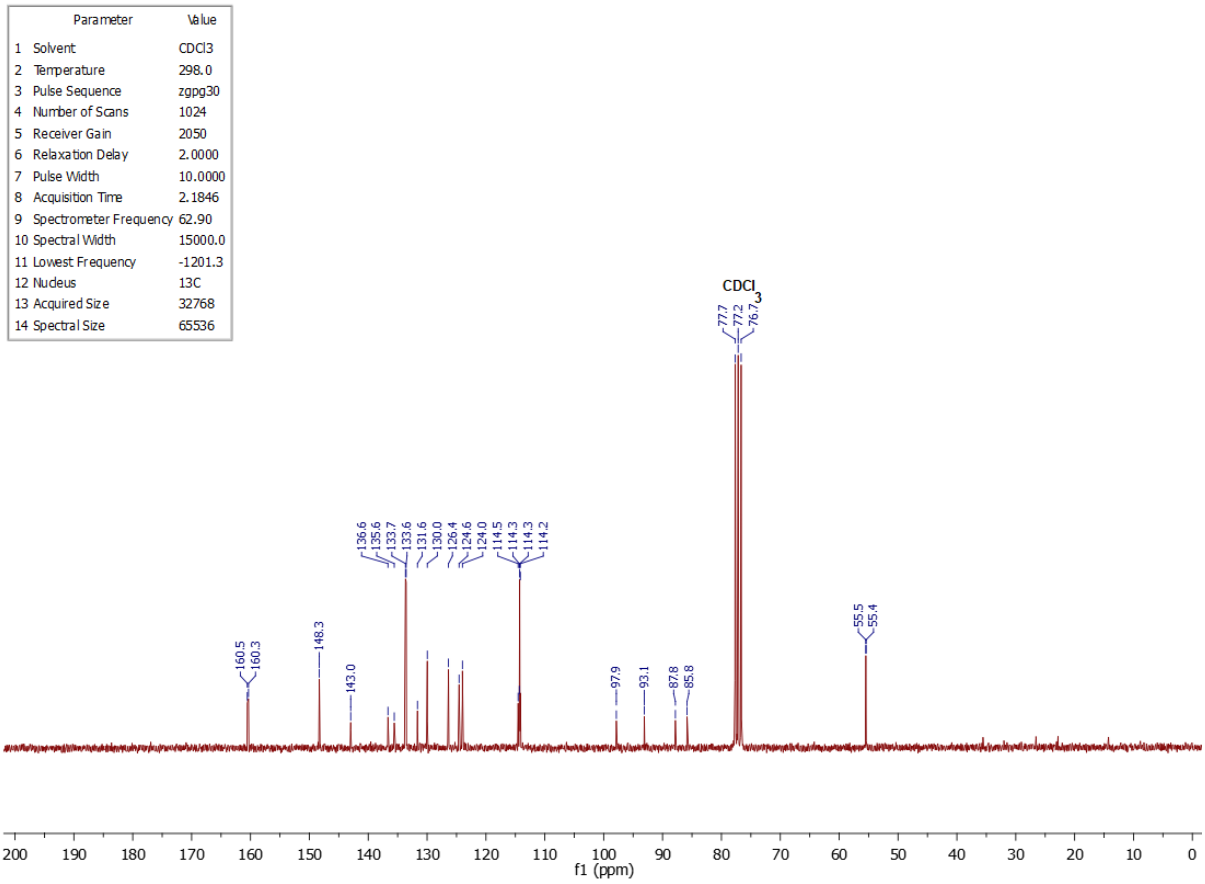


3-(thiophen-3-yl)-2,4-bis(thiophen-3-ylethynyl)pyridine (1h)

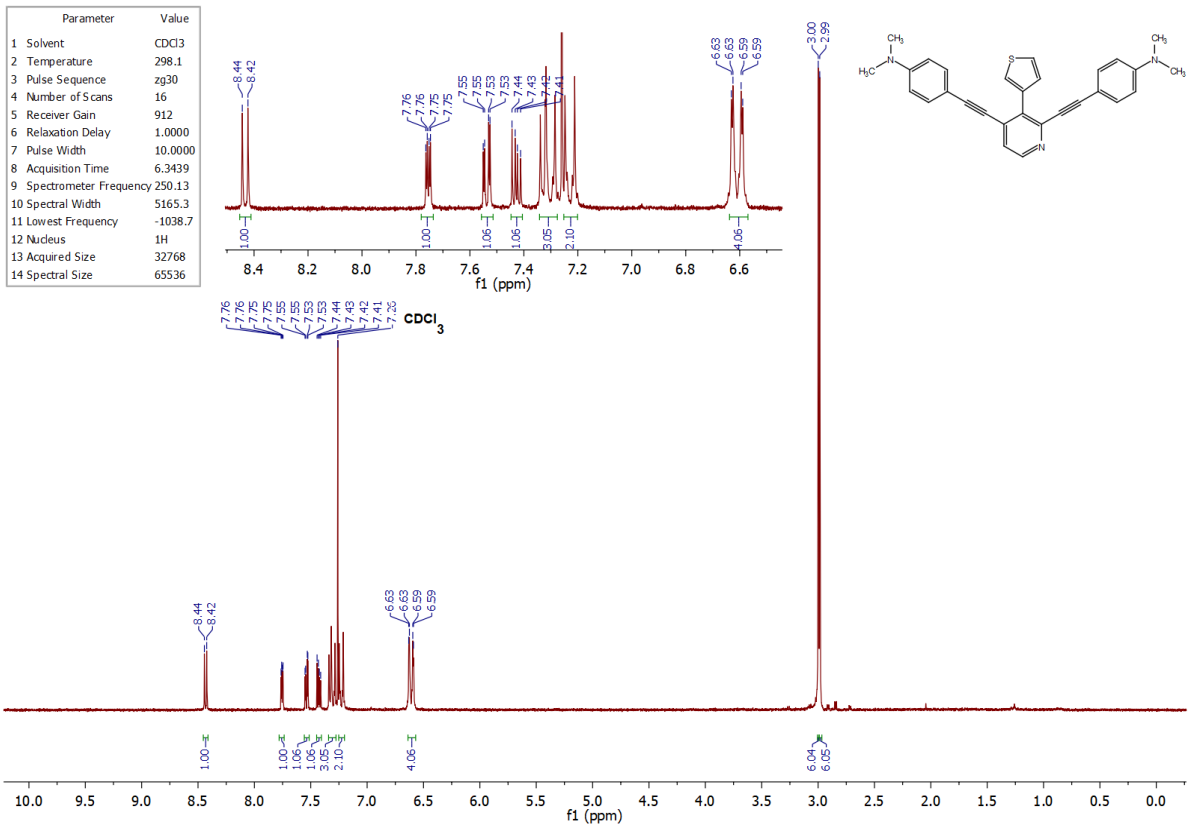


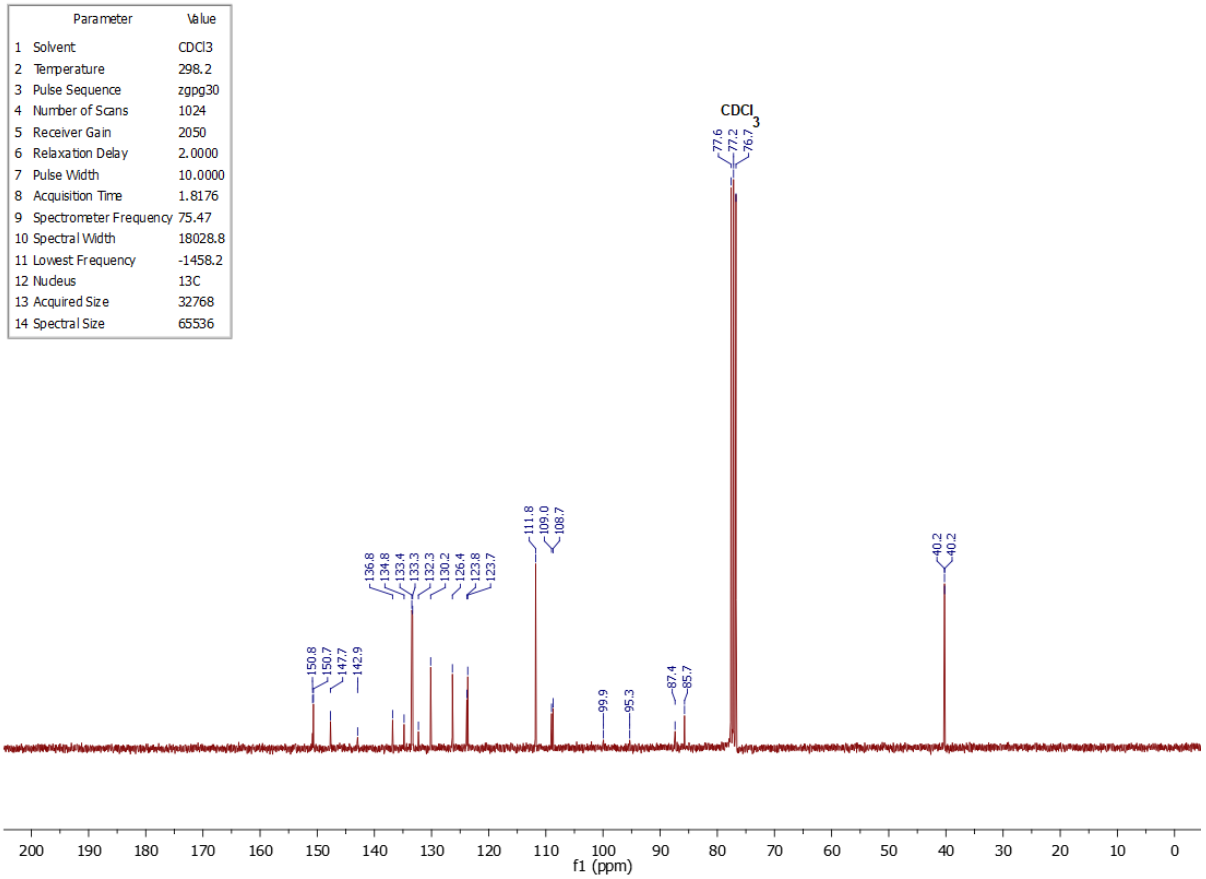
2,4-bis((4-methoxyphenyl)ethynyl)-3-(thiophen-3-yl)pyridine (1i)



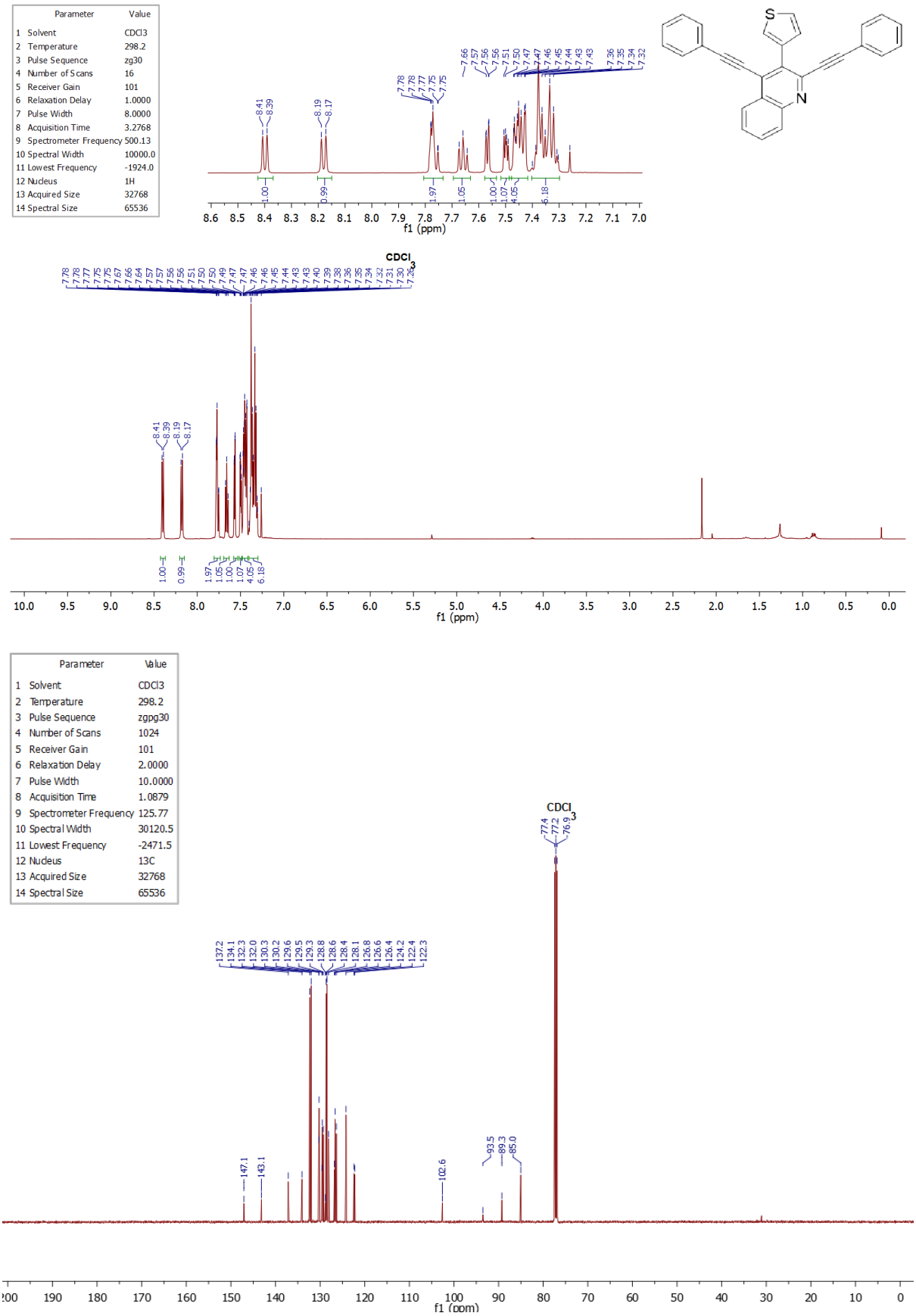


2,4-bis((4-methoxyphenyl)ethynyl)-3-(thiophen-3-yl)pyridine (1j)



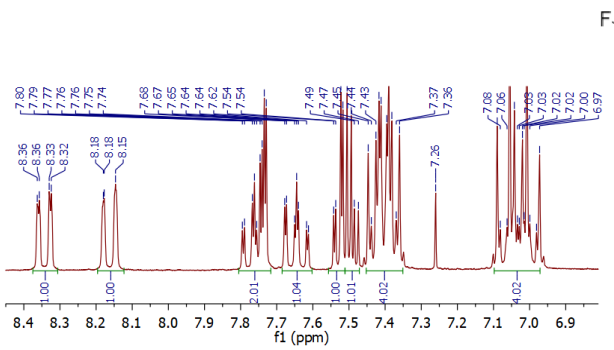


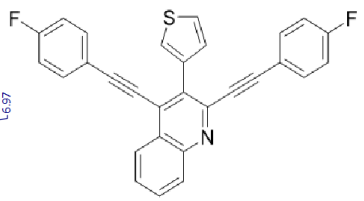
2,4-bis(phenylethynyl)-3-(thiophen-3-yl)quinoline (2a)

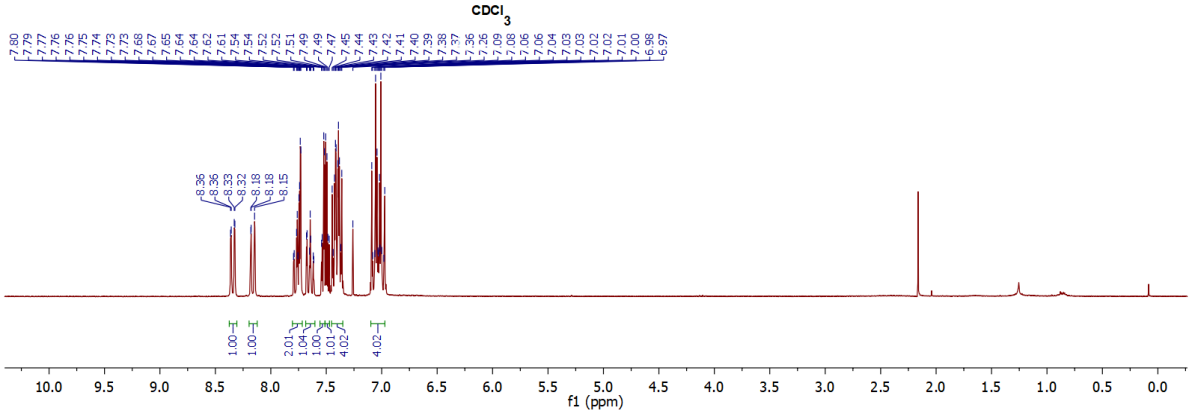


2,4-bis((4-fluorophenyl)ethynyl)-3-(thiophen-3-yl)quinoline (2b)

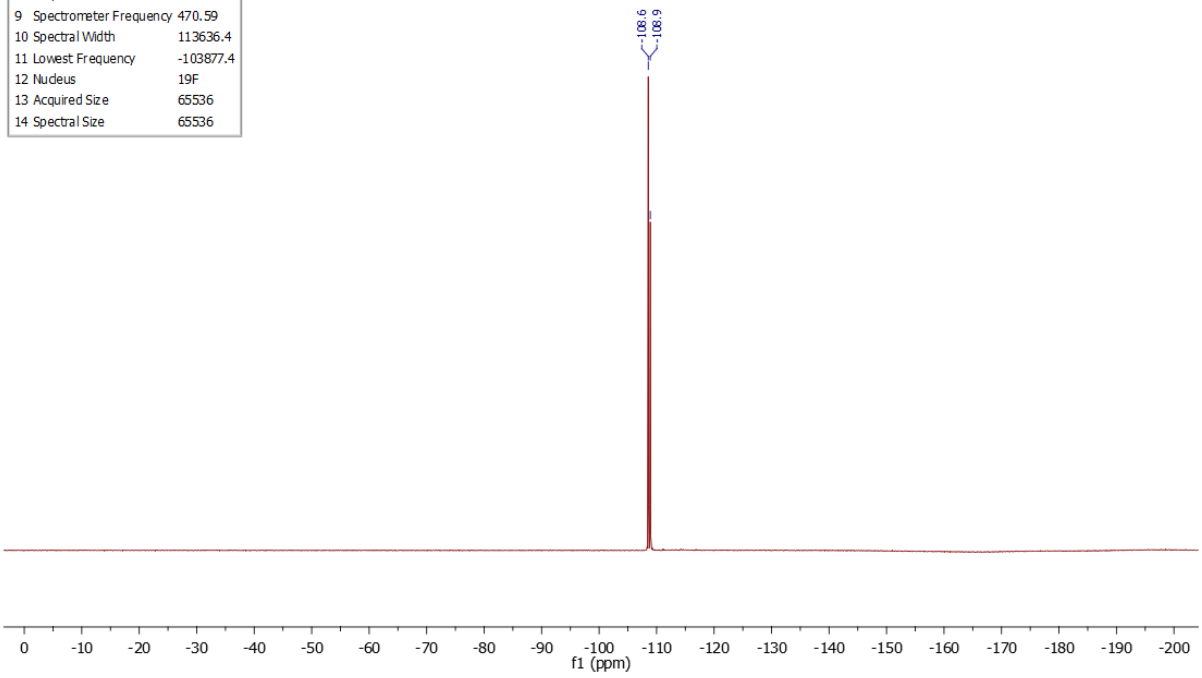
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	575
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



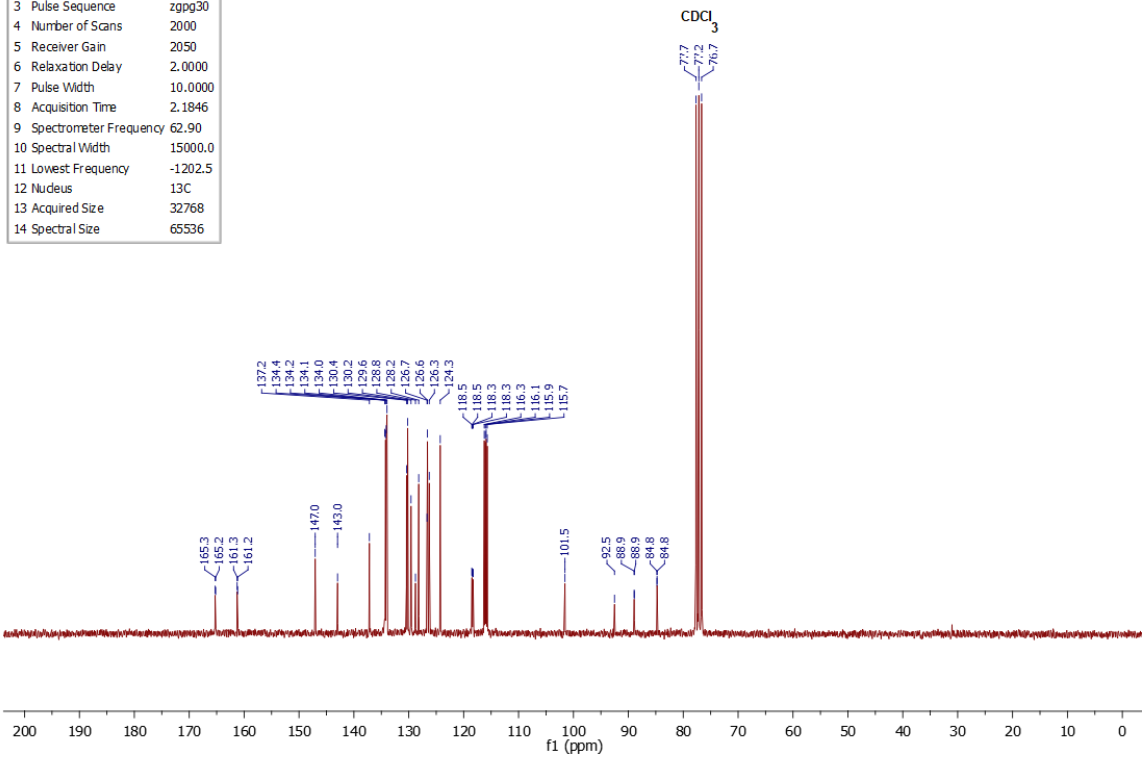




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgig
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	12.0000
8	Acquisition Time	0.5767
9	Spectrometer Frequency	470.59
10	Spectral Width	113636.4
11	Lowest Frequency	-103877.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	65536

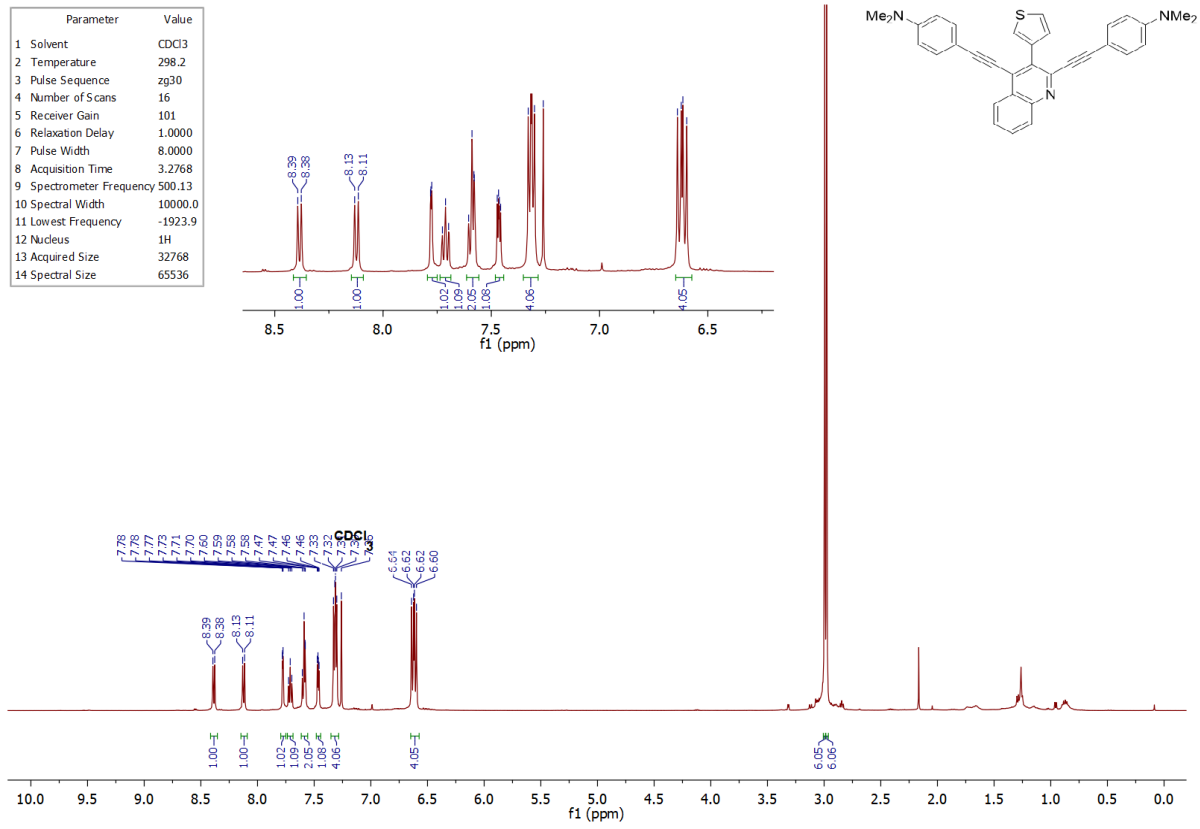


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	2000
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1202.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

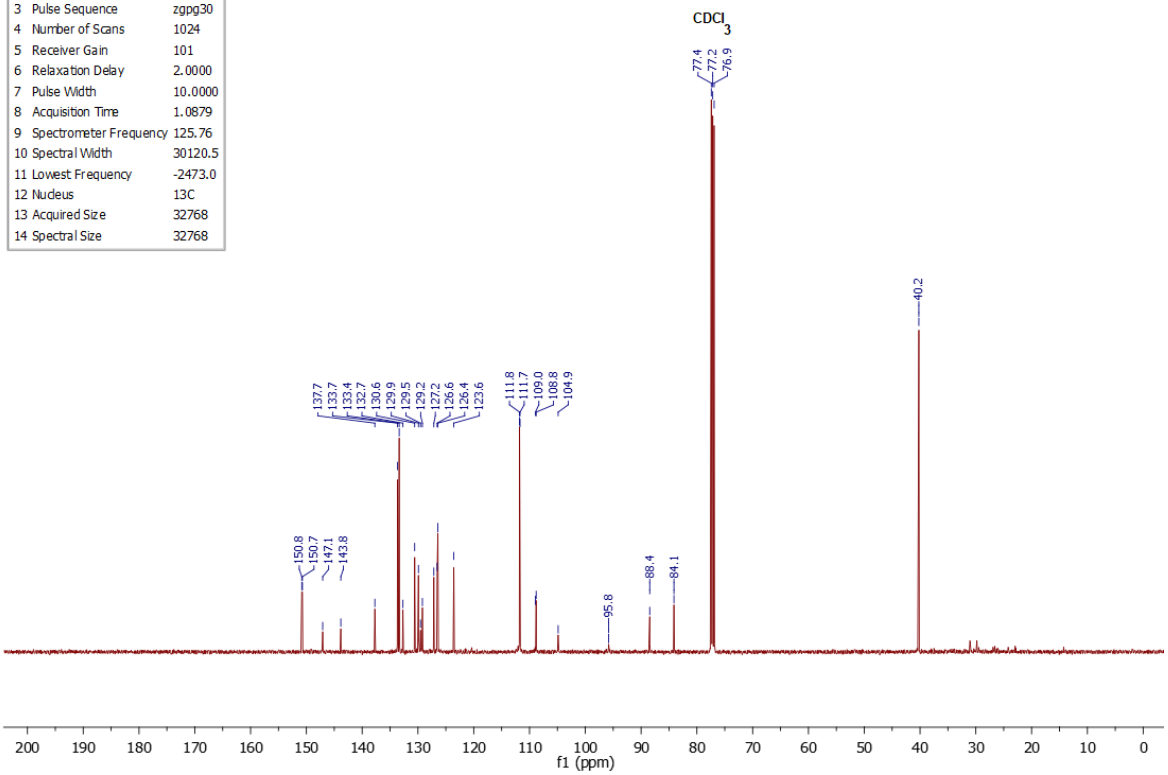


4,4'-((3-(thiophen-3-yl)quinoline-2,4-diyl)bis(ethyne-2,1-diyl))bis(N,N-dimethylaniline) (2c)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.9
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

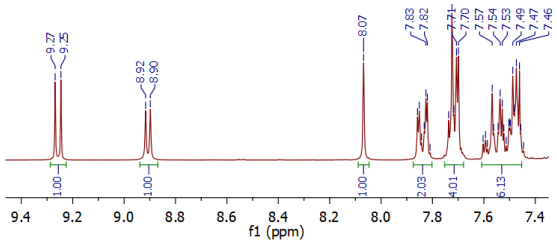


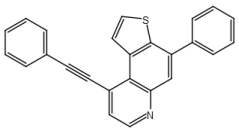
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2473.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

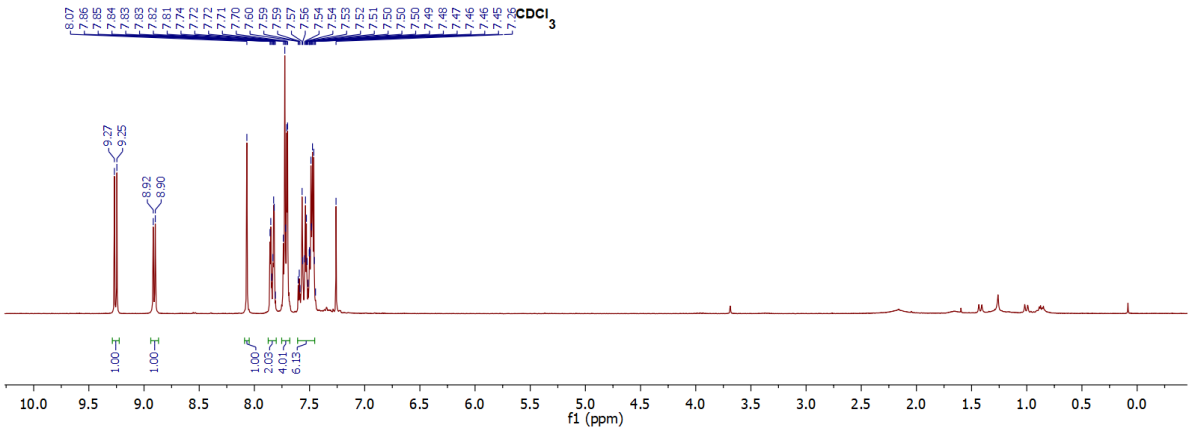


4-phenyl-9-(phenylethynyl)thieno[3,2-*f*]quinoline (3a)

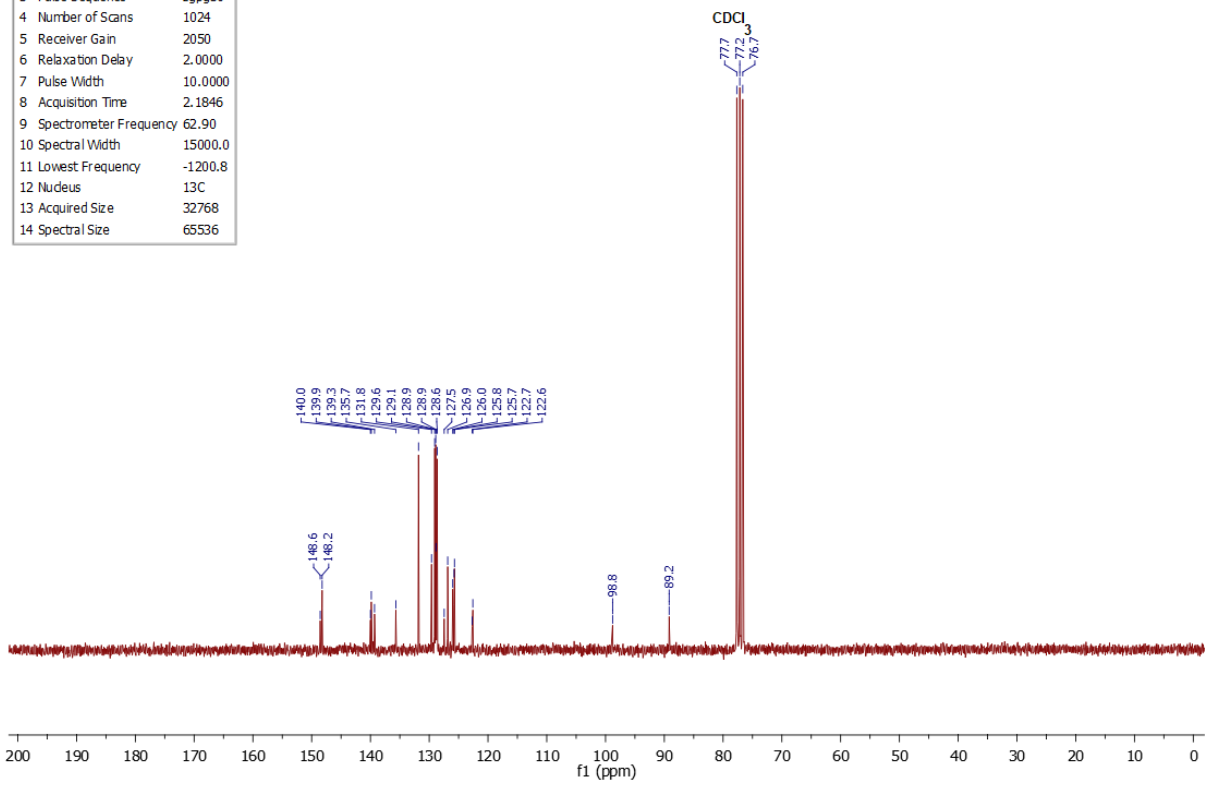
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





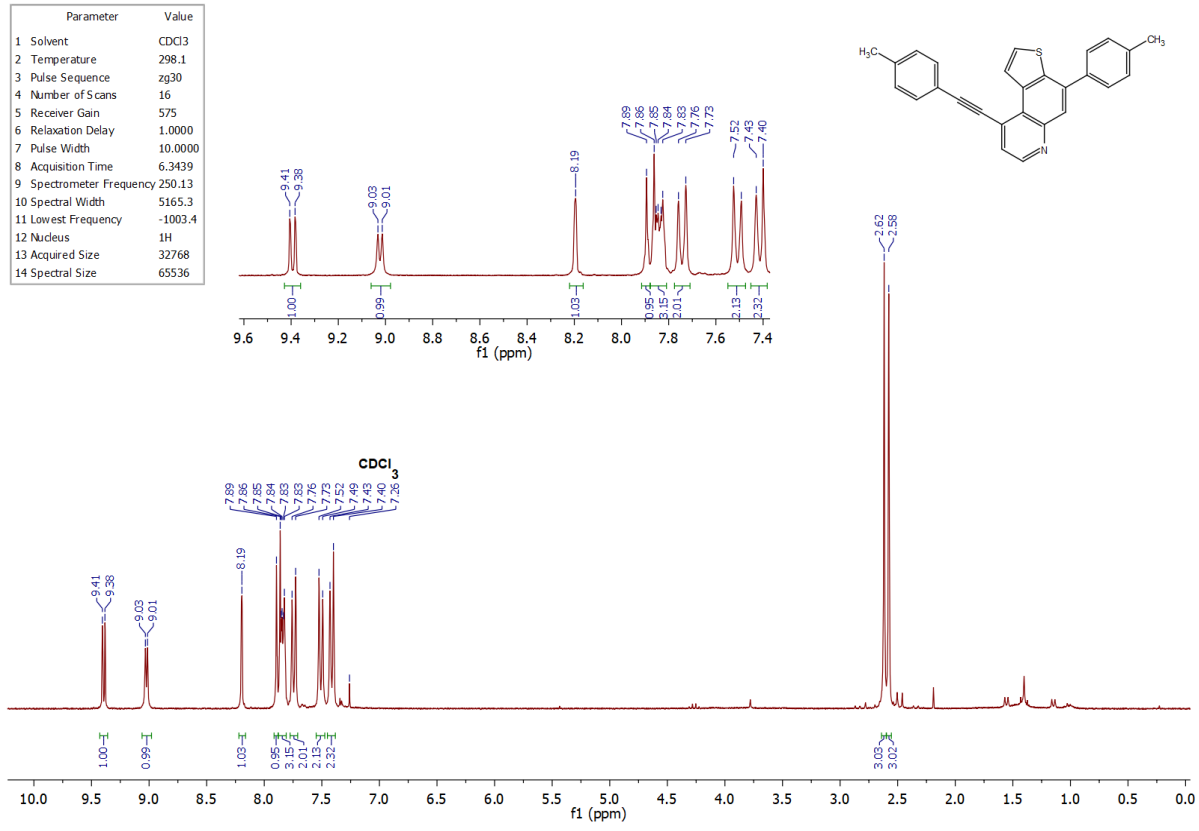


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	297.8
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1200.8
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

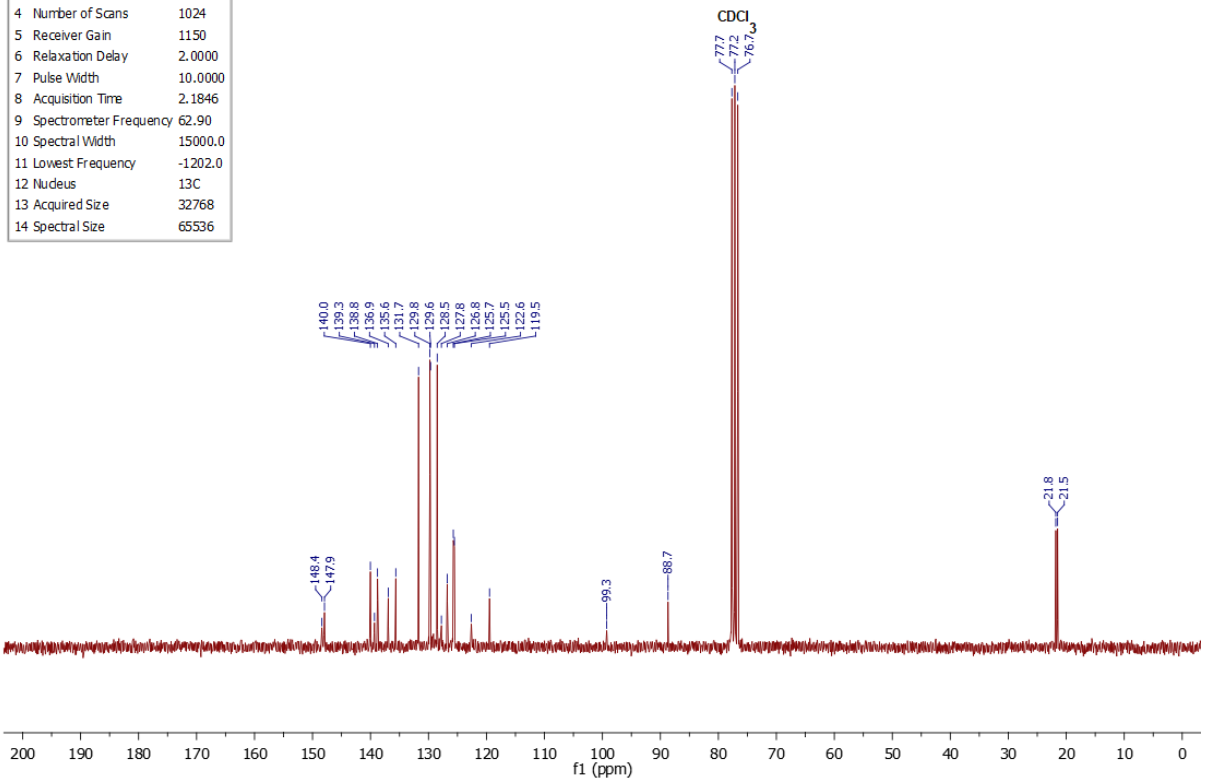


4-(*p*-tolyl)-9-(*p*-tolylethynyl)thieno[3,2-*f*]quinoline (3b)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	575
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1003.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

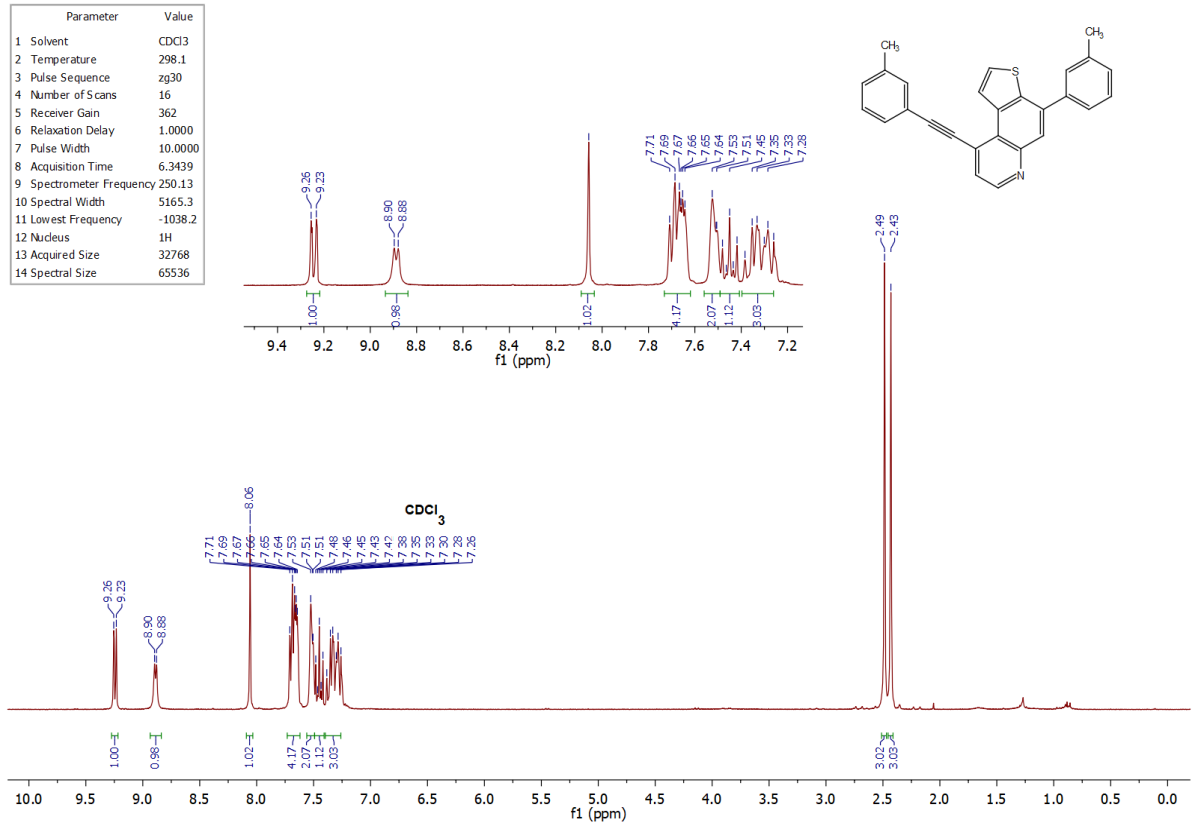


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.0
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	1150
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1202.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

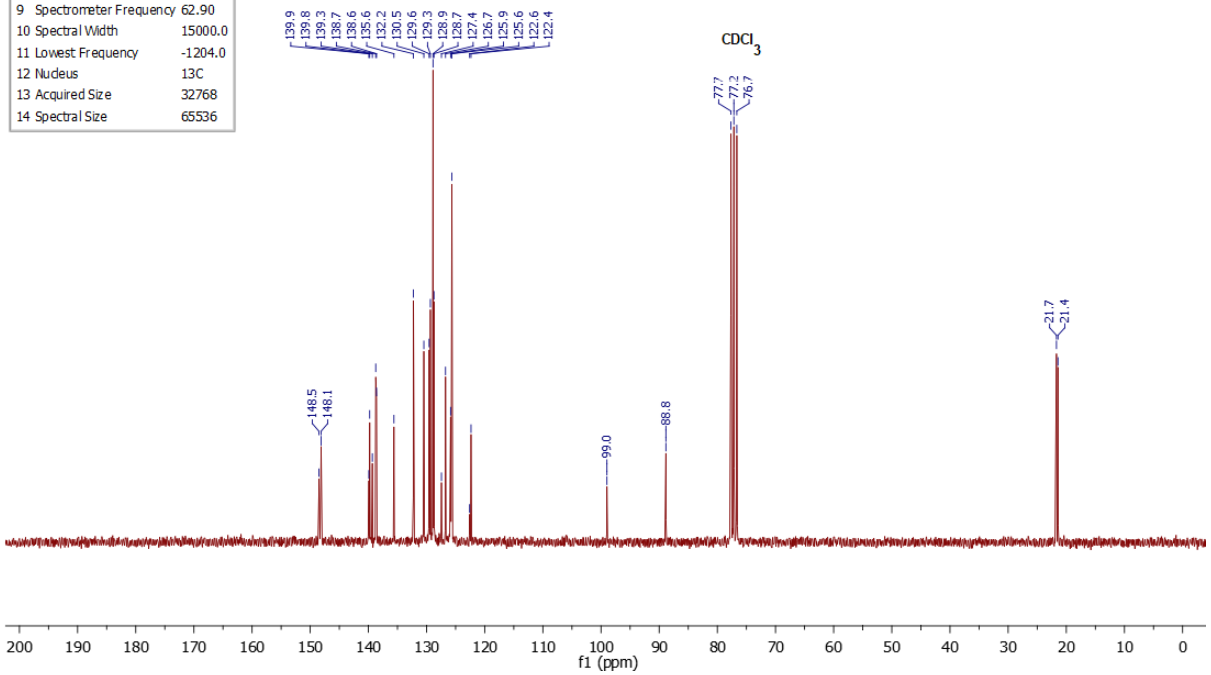


4-(*m*-tolyl)-9-(*m*-tolylethynyl)thieno[3,2-*f*]quinoline (3c)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.2
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

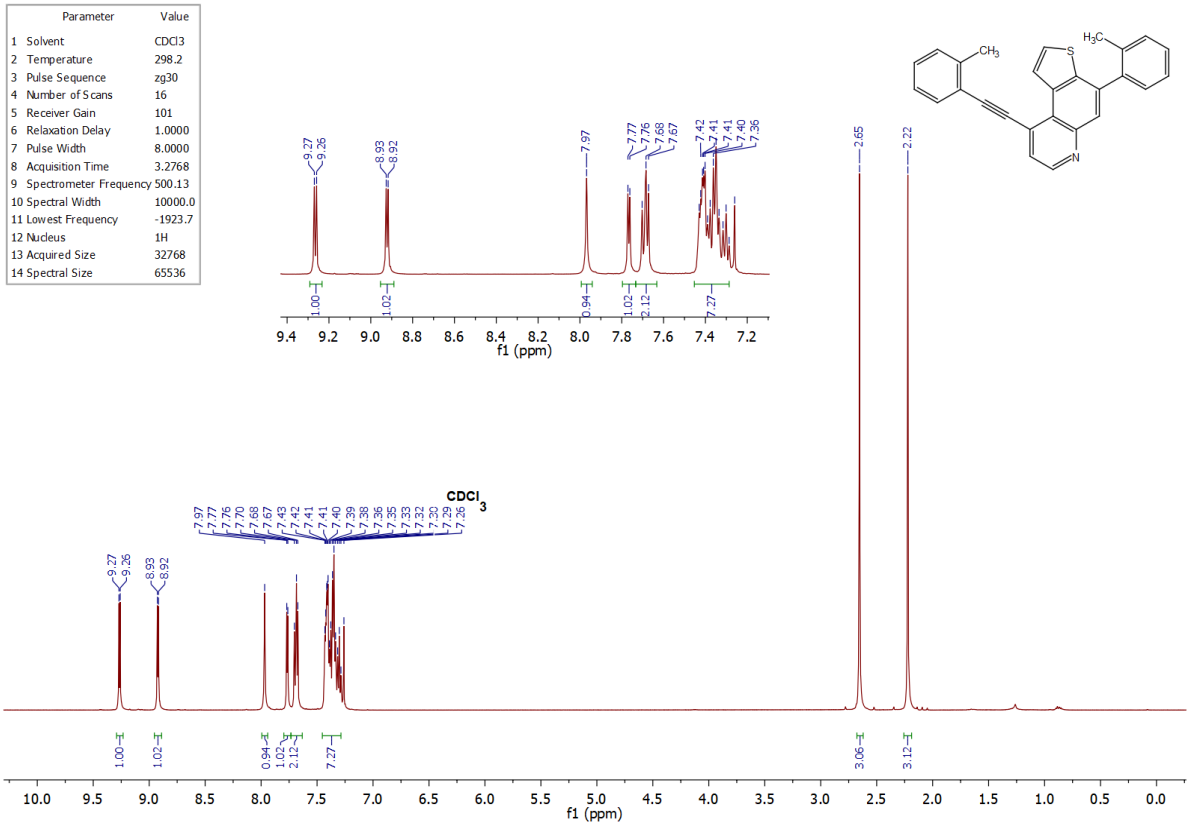


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.0
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	912
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1204.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

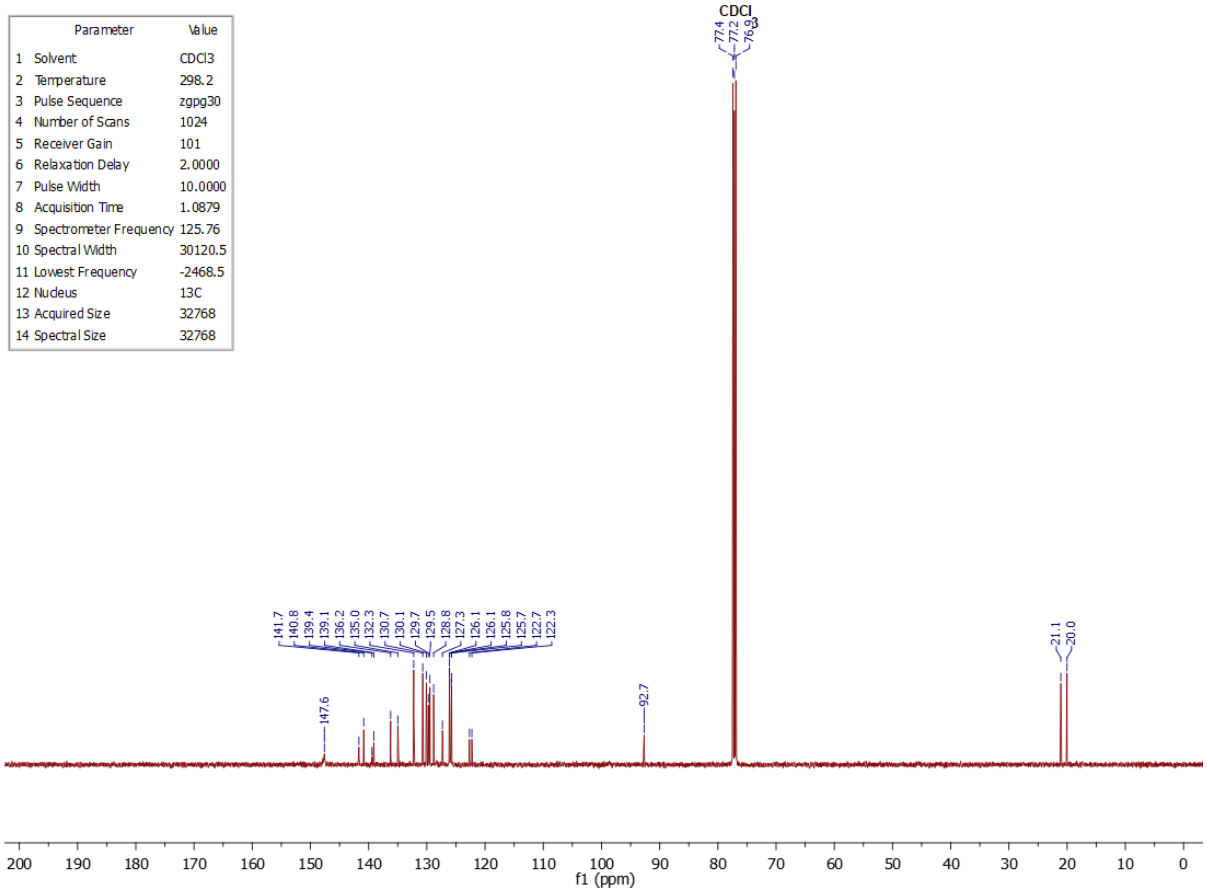


4-(*o*-tolyl)-9-(*o*-tolylethynyl)thieno[3,2-*f*]quinoline (3d)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.7
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

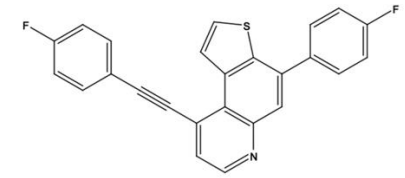


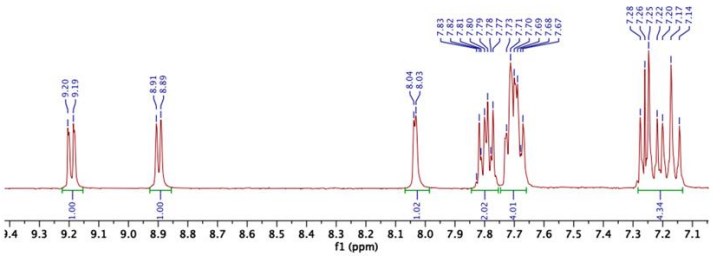
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2468.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

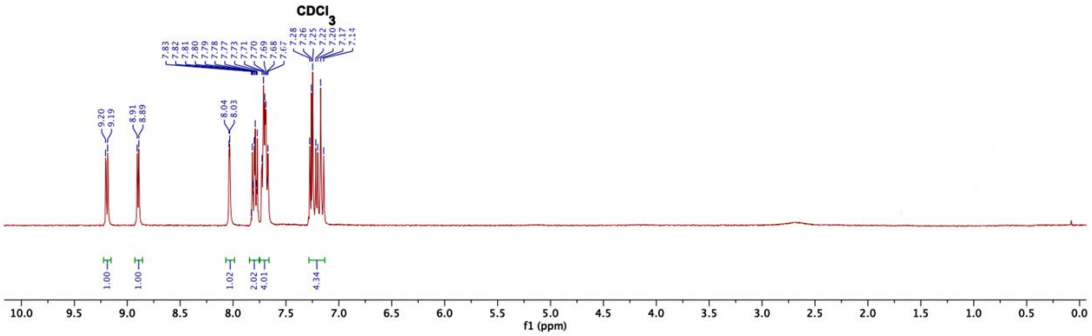


4-(4-fluorophenyl)-9-((4-fluorophenyl)ethynyl)thieno[3,2-*f*]quinoline (3e)

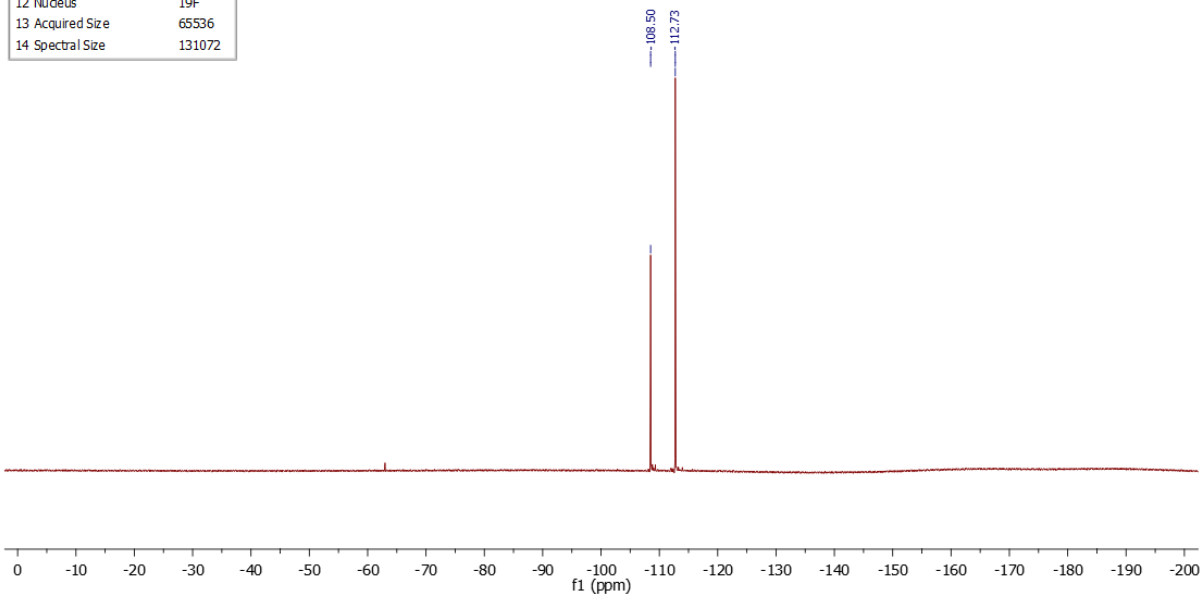
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	203
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.2
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



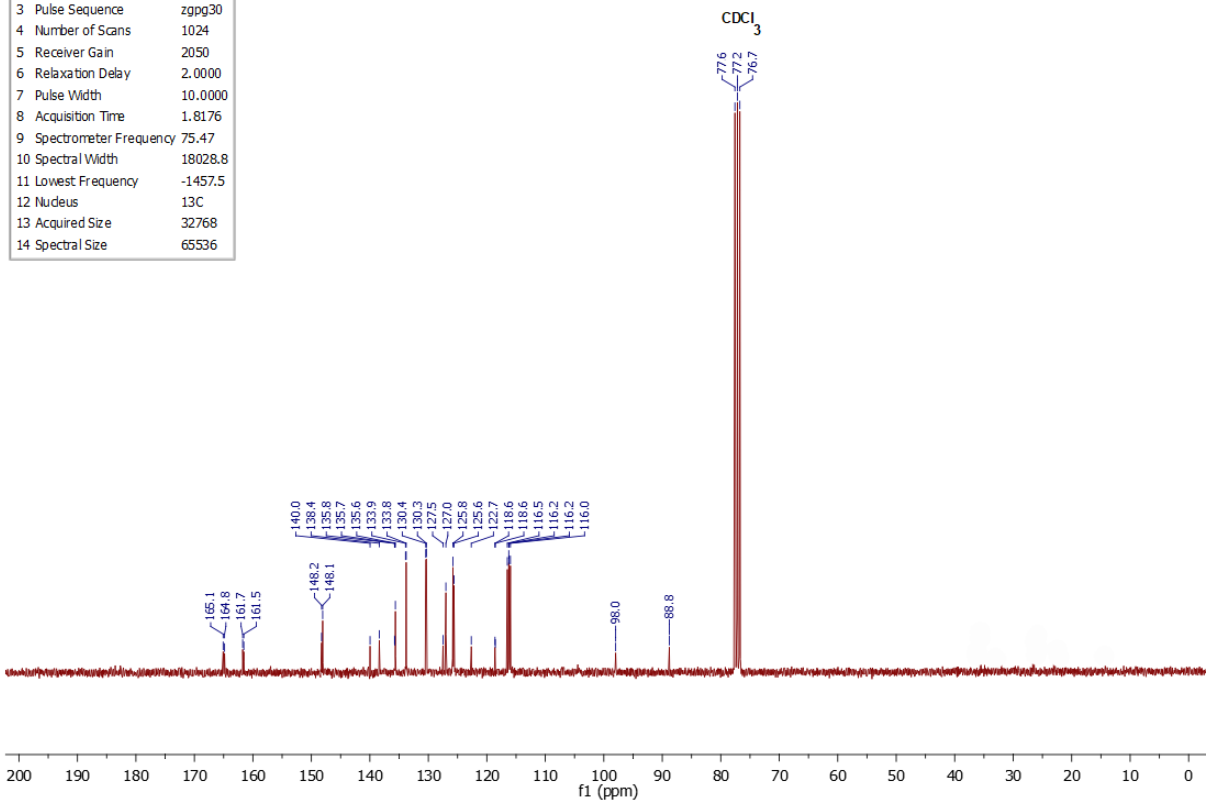




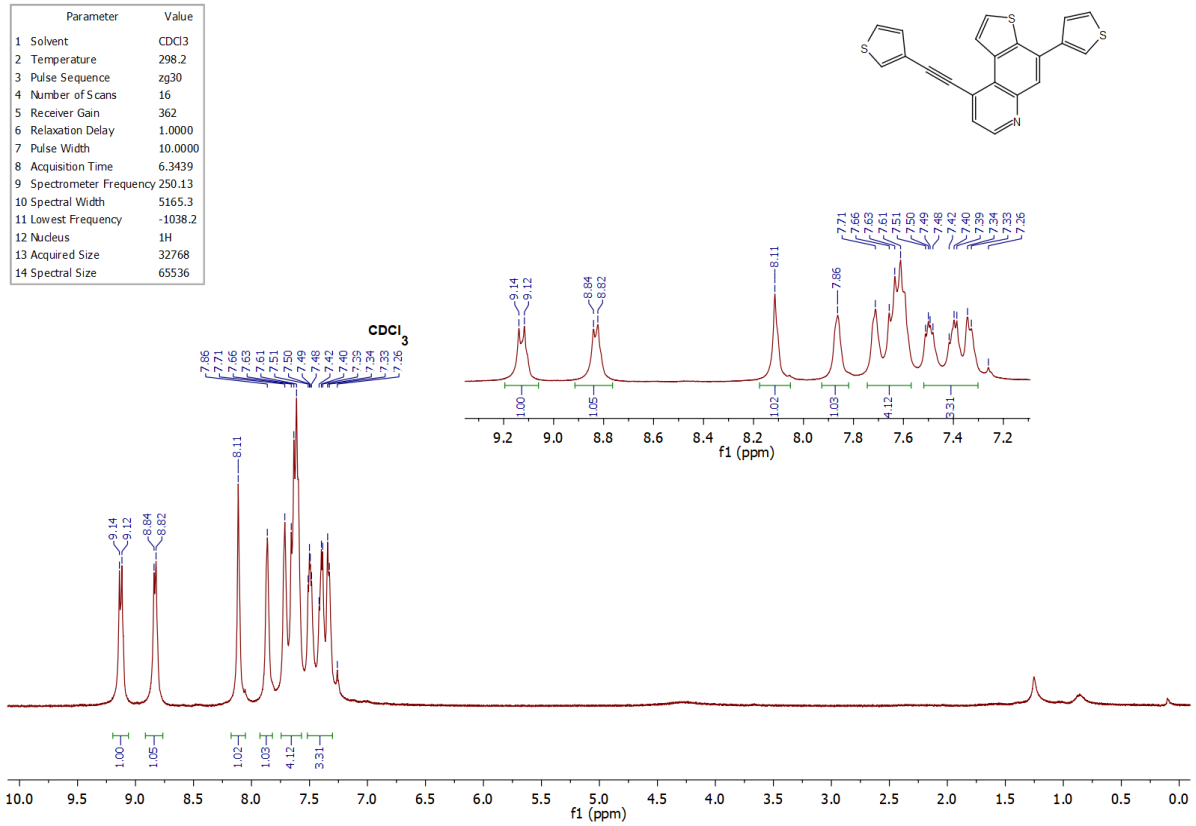
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.40
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

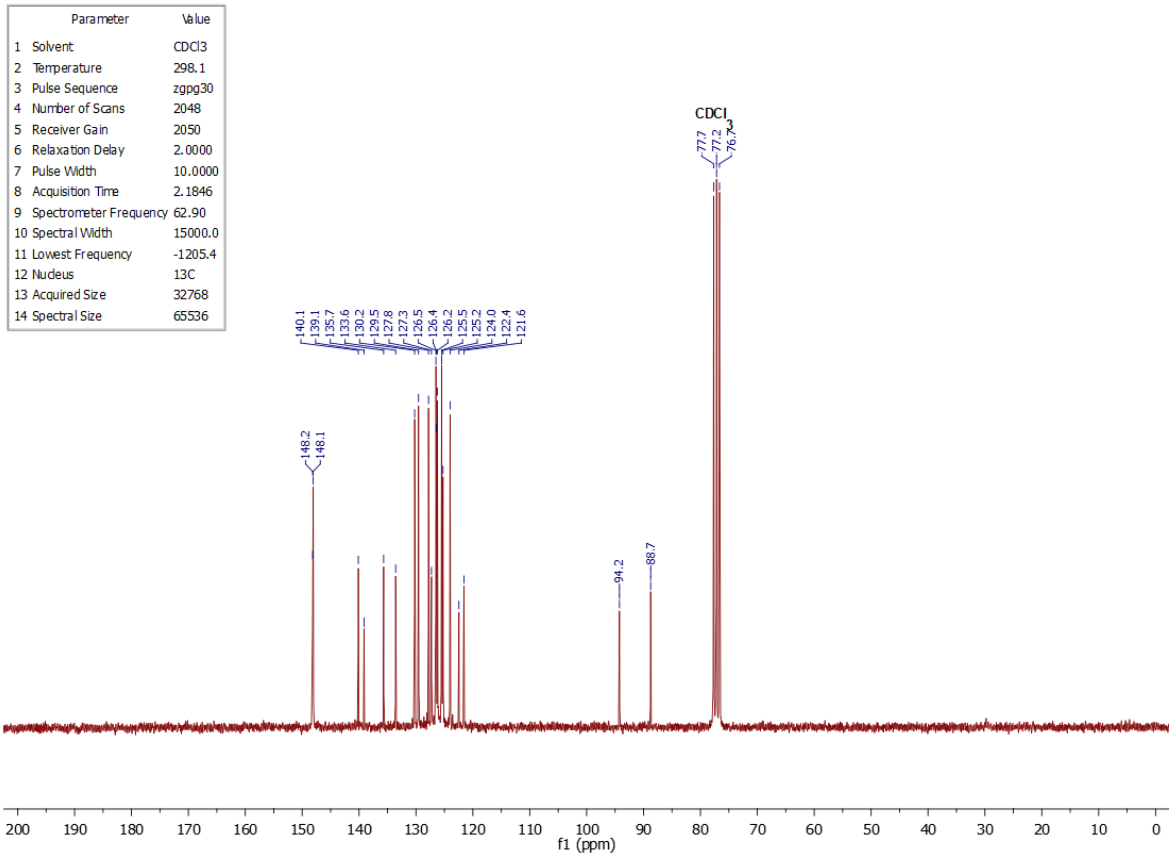


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1457.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

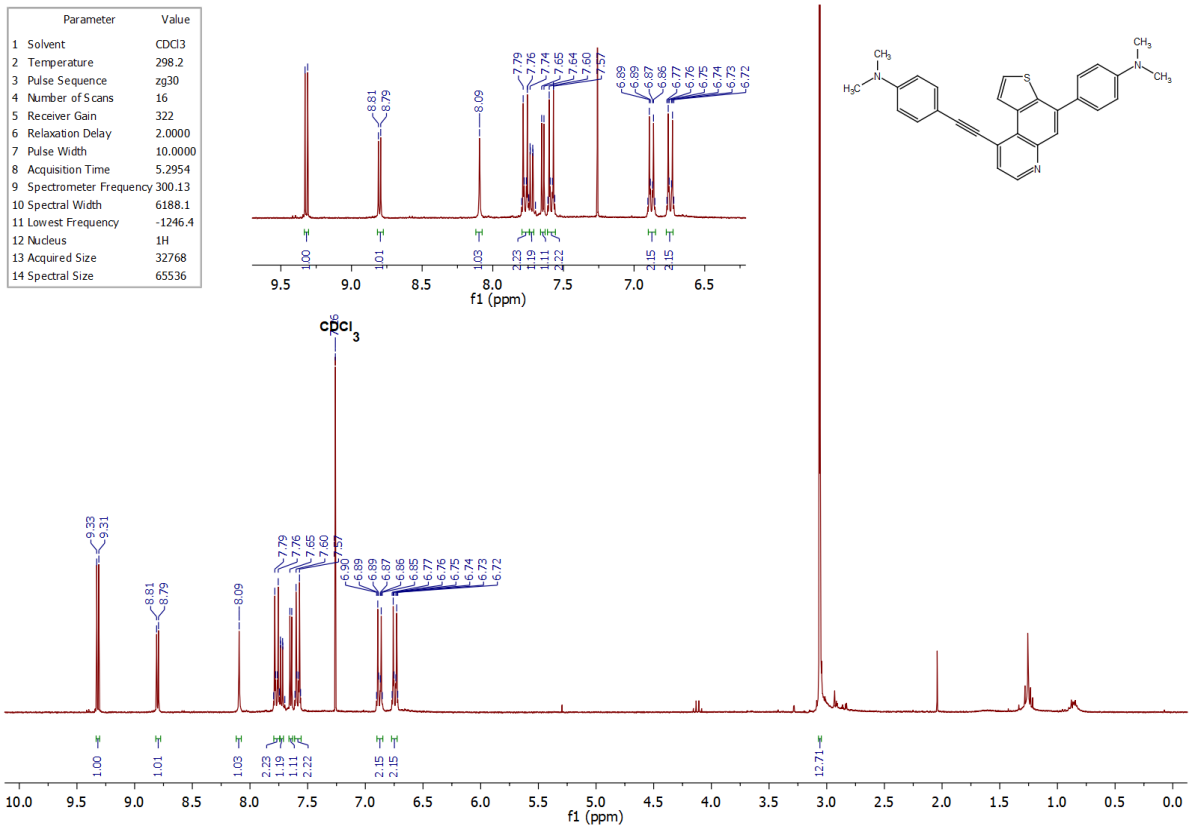


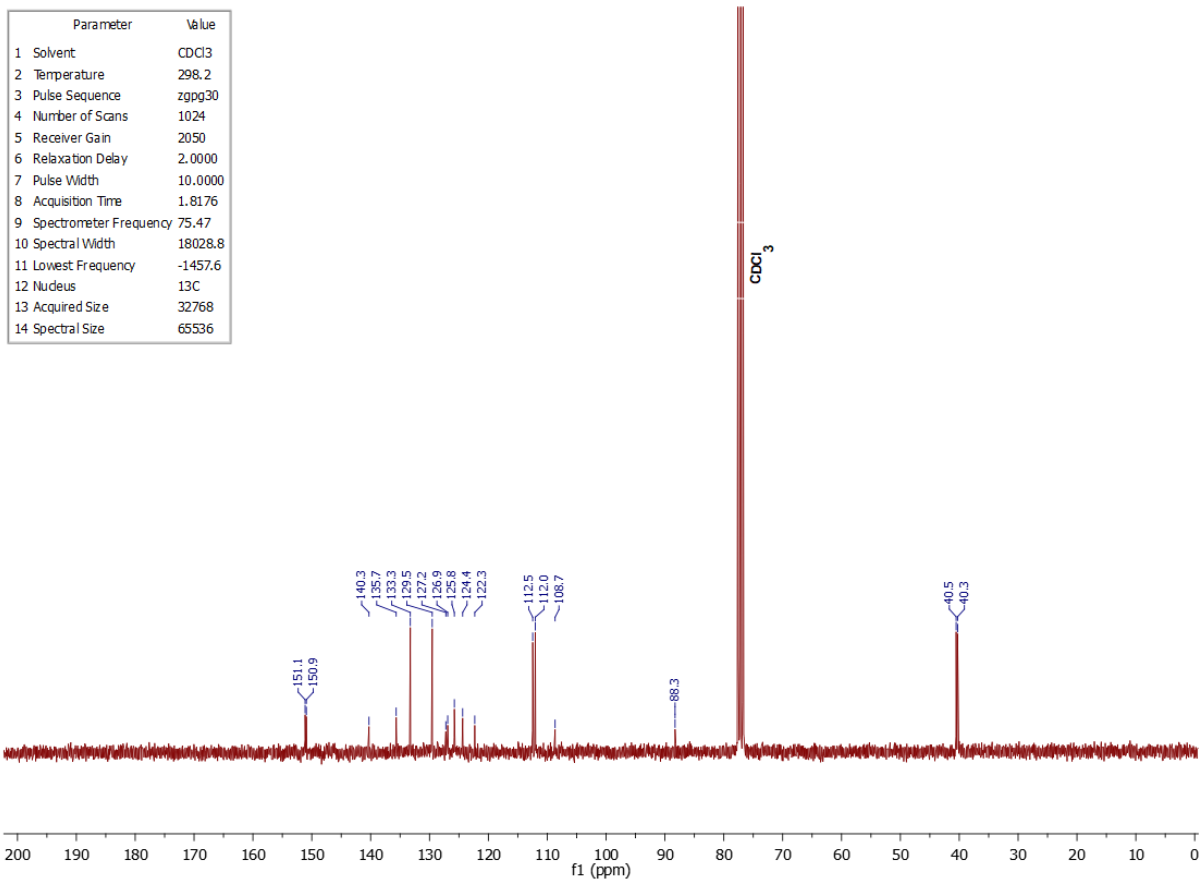
4-(thiophen-3-yl)-9-(thiophen-3-ylethynyl)thieno[3,2-f]quinoline (3h)



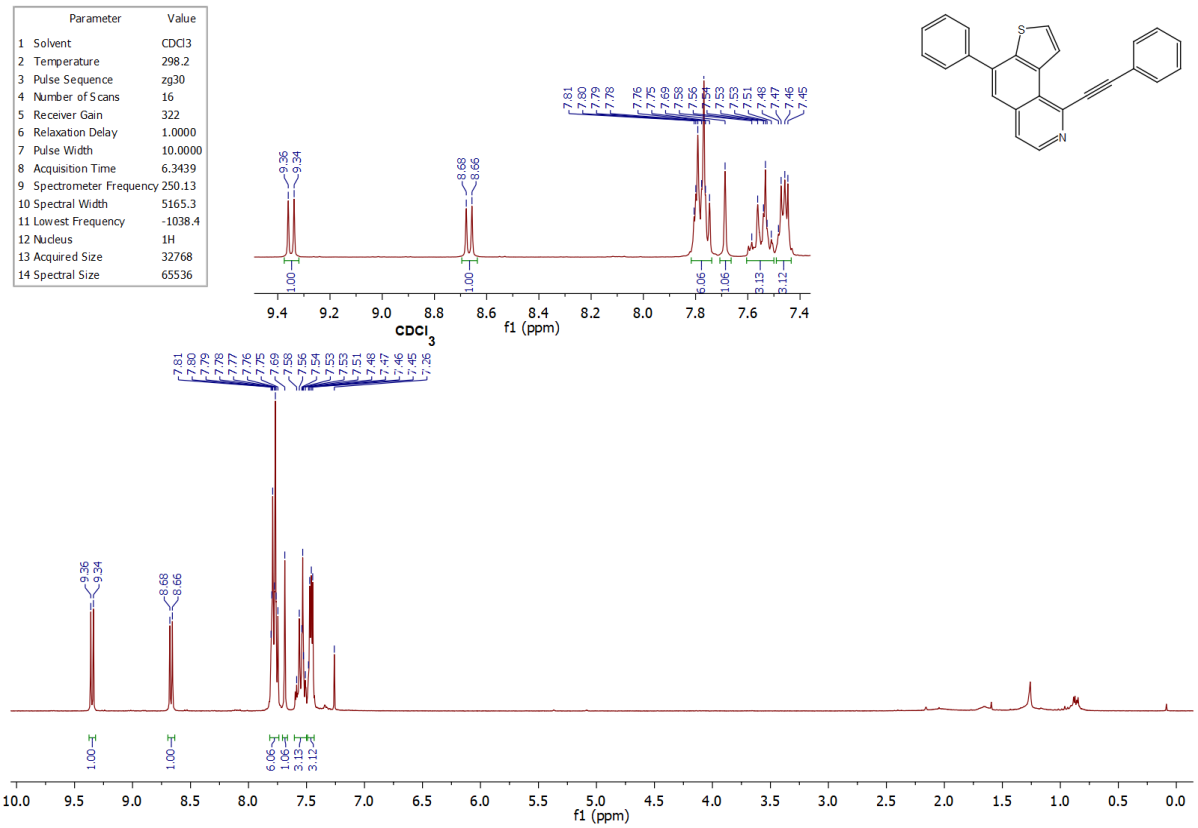


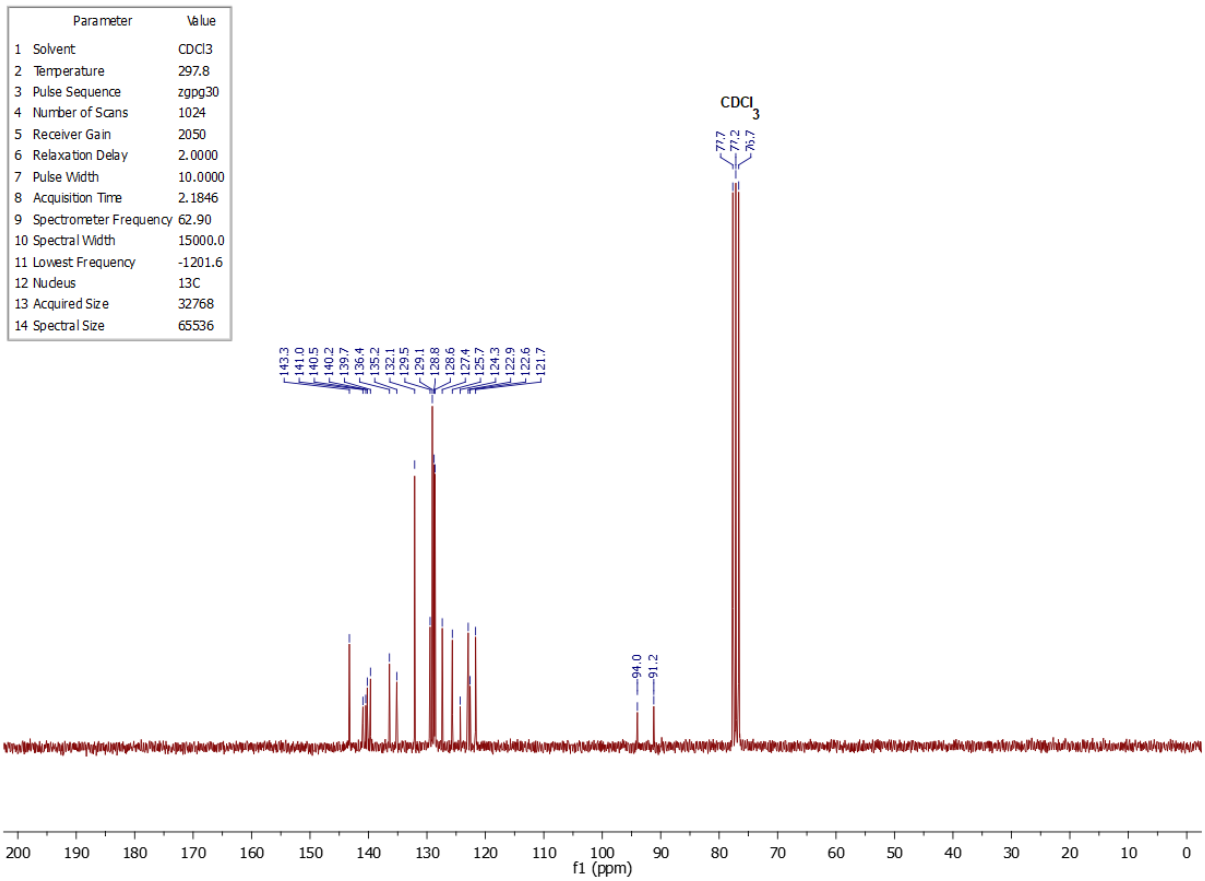
4-(9-((4-(dimethylamino)phenyl)ethynyl)thieno[3,2-*f*]quinolin-4-yl)-N,N-dimethylaniline (3j)





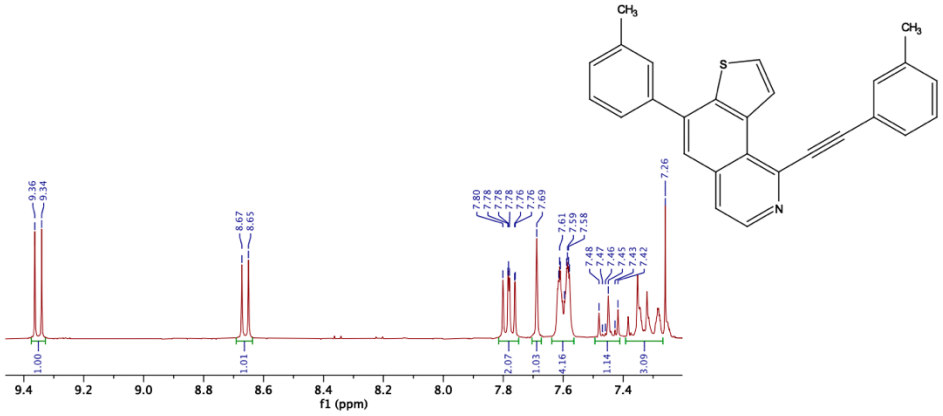
6-phenyl-1-(phenylethynyl)thieno[2,3-*h*]isoquinoline (4a)

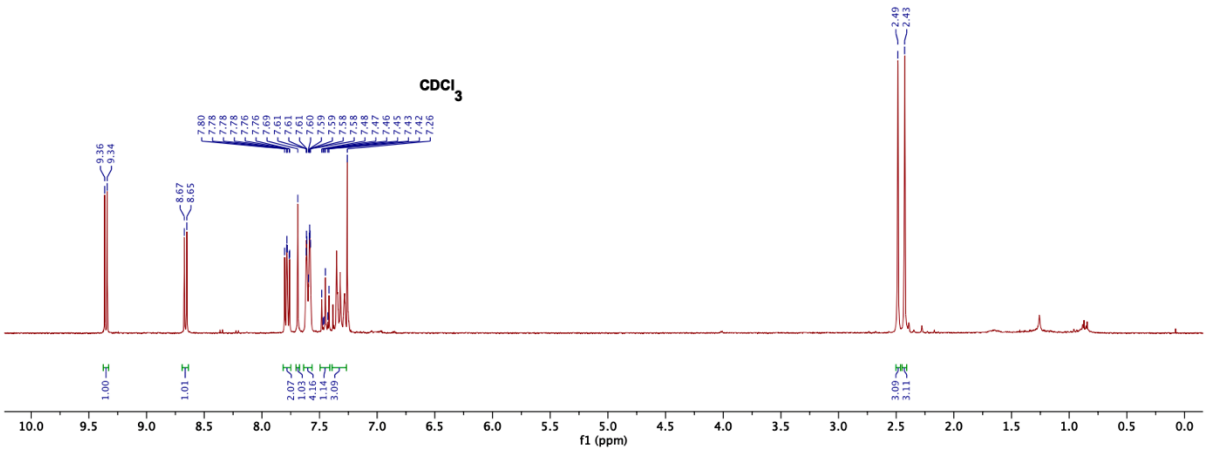




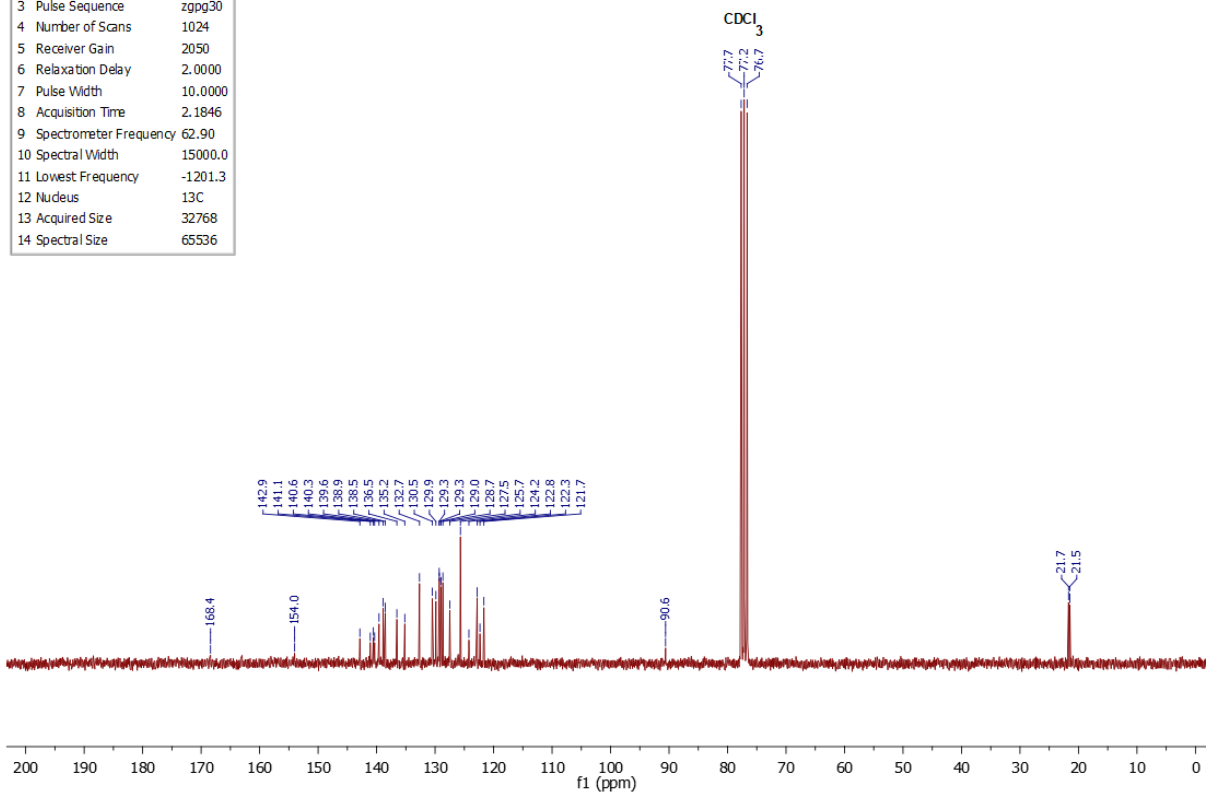
6-(*m*-tolyl)-1-(*m*-tolylethynyl)thieno[2,3-*h*]isoquinoline (4c)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	724
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.7
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



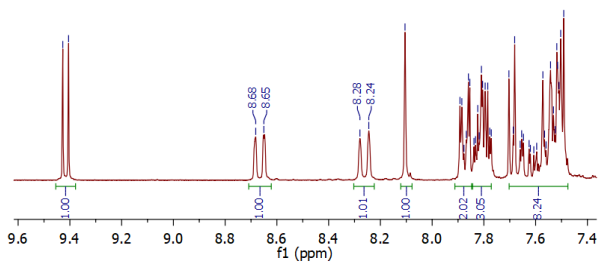


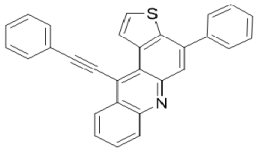
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.0
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1201.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

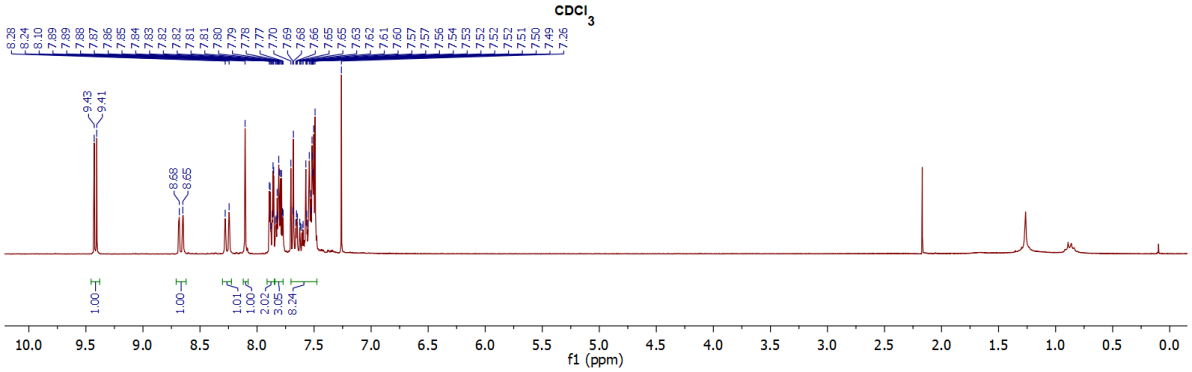


4-phenyl-11-(phenylethynyl)thieno[3,2-*a*]acridine (7a)

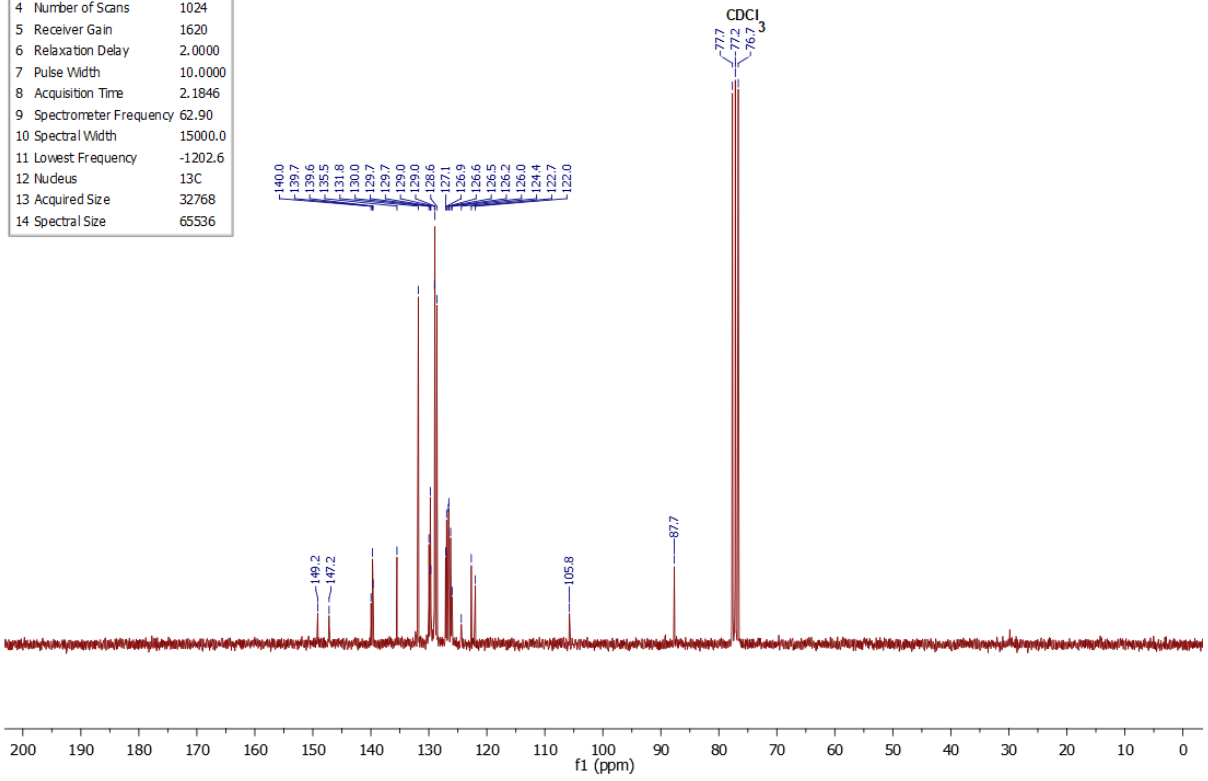
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





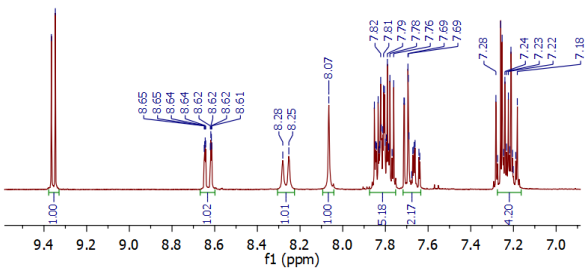


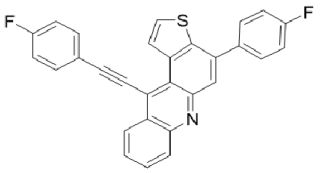
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.0
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	1620
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1202.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

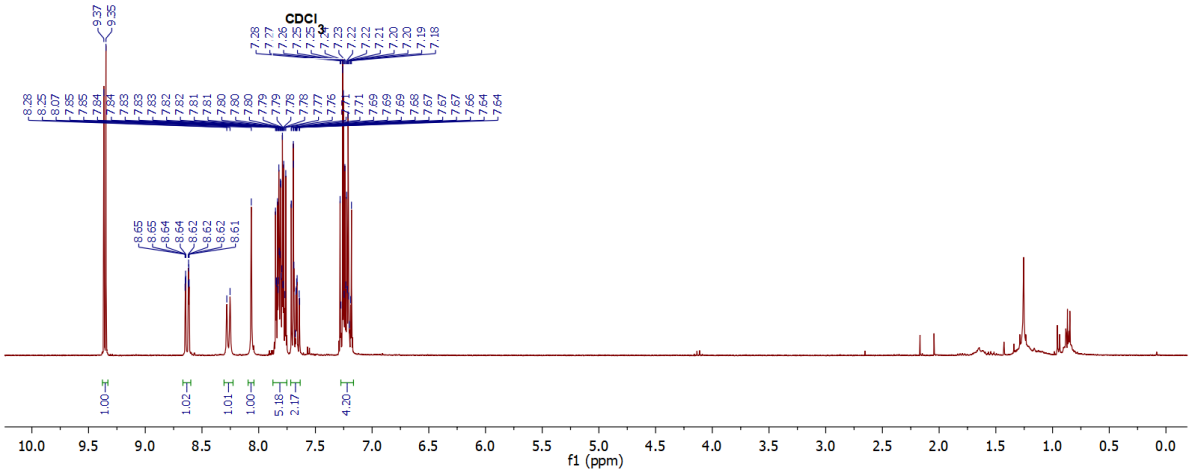


4-(4-fluorophenyl)-11-((4-fluorophenyl)ethynyl)thieno[3,2-*a*]acridine (7b)

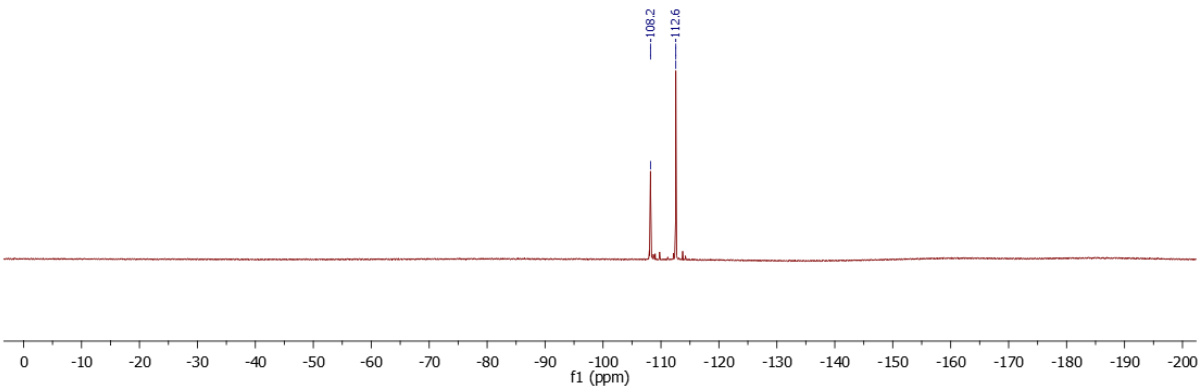
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	228
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	32768



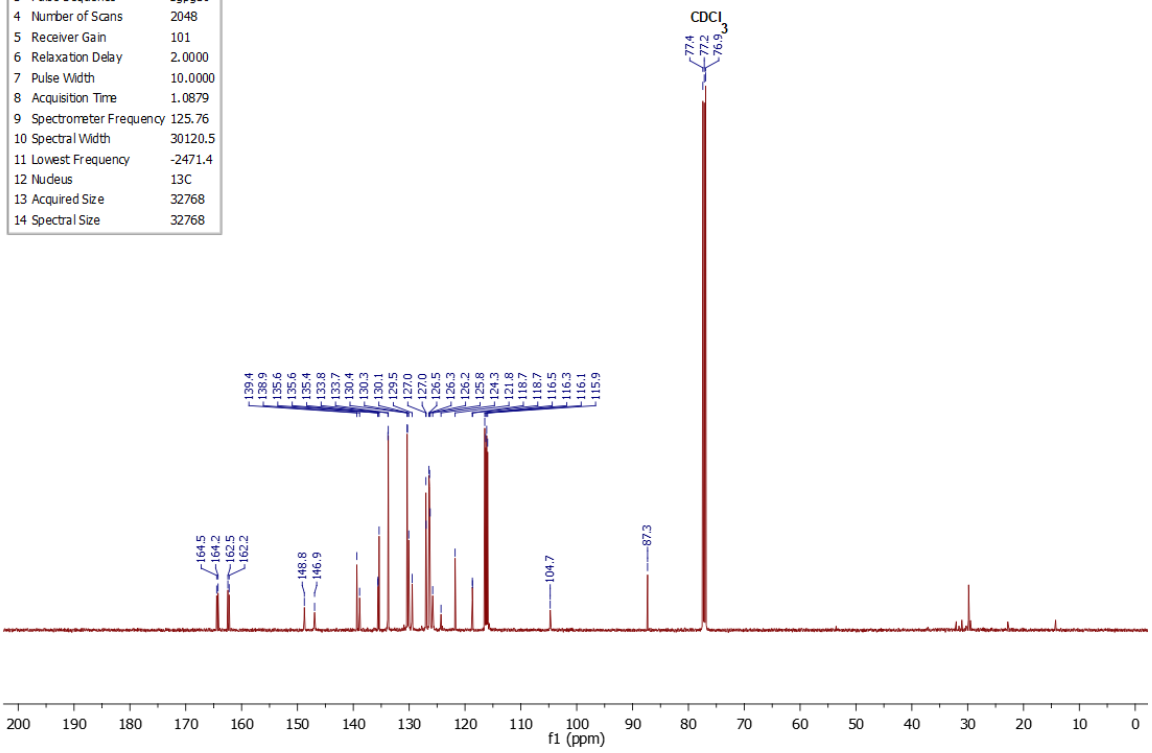




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.40
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	65536

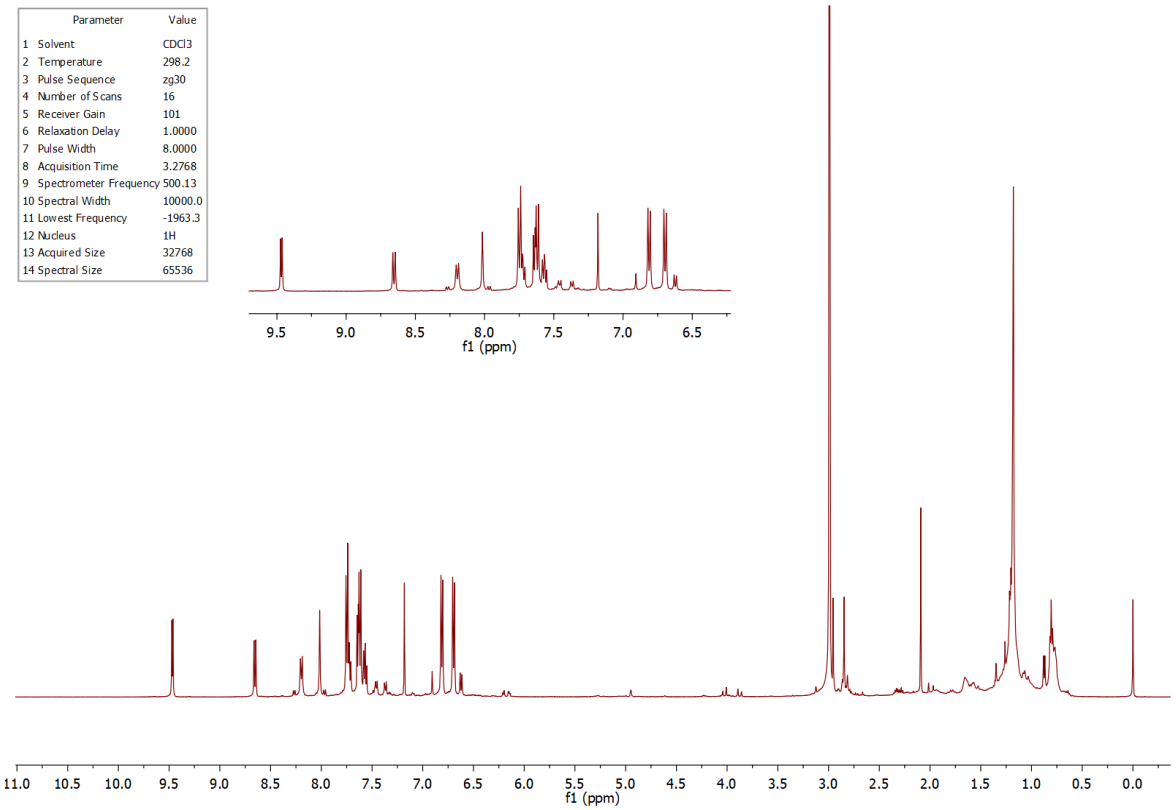


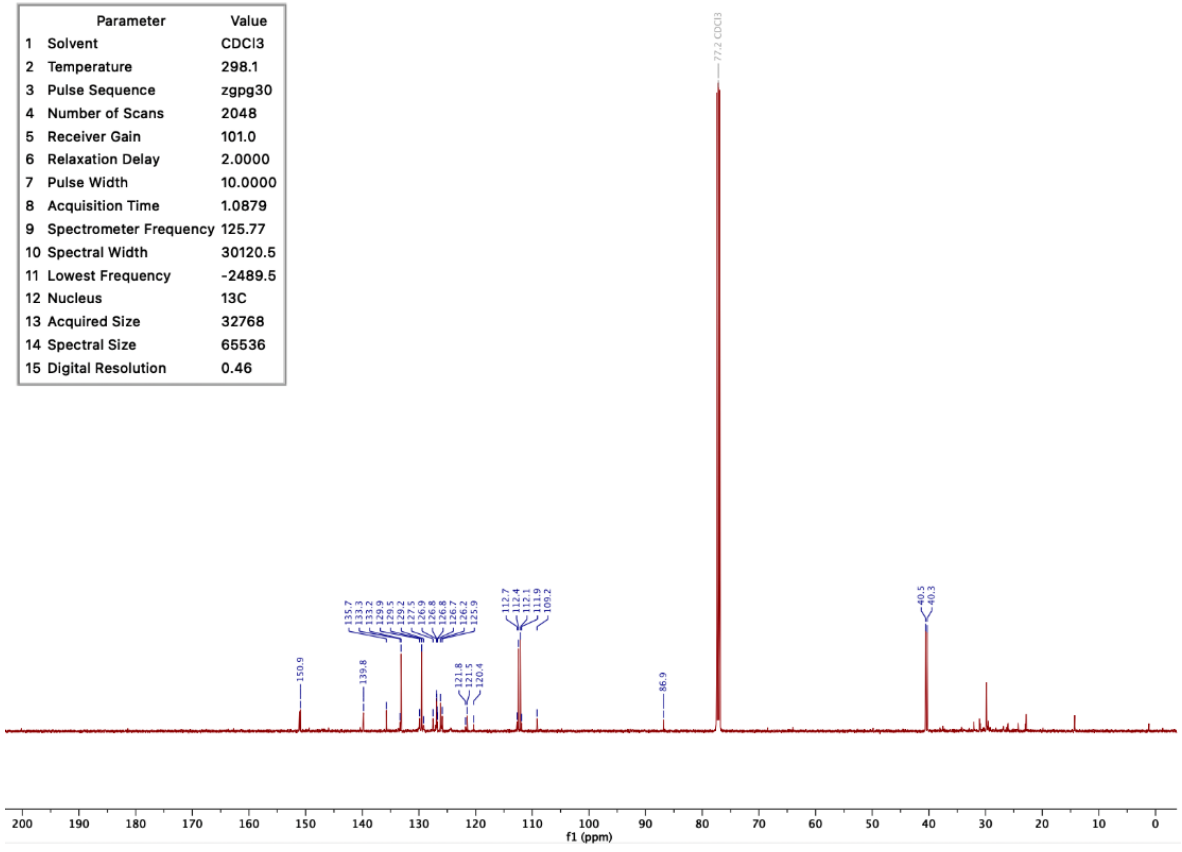
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Number of Scans	2048
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2471.4
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768



4-(11-((4-(dimethylamino)phenyl)ethynyl)thieno[3,2-*a*]acridin-4-yl)-N,N-dimethylaniline (7c)[1]

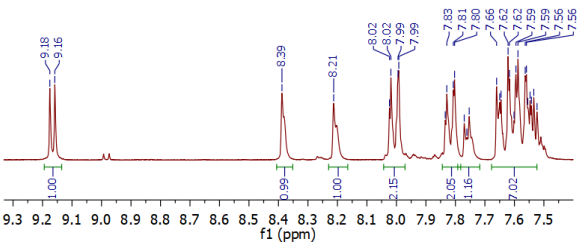
[1] NMR spectrum of **7c** contains small amounts of impurities – as desired product **8c** is available directly from **2c** we did not execute repeated purification

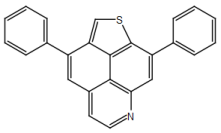


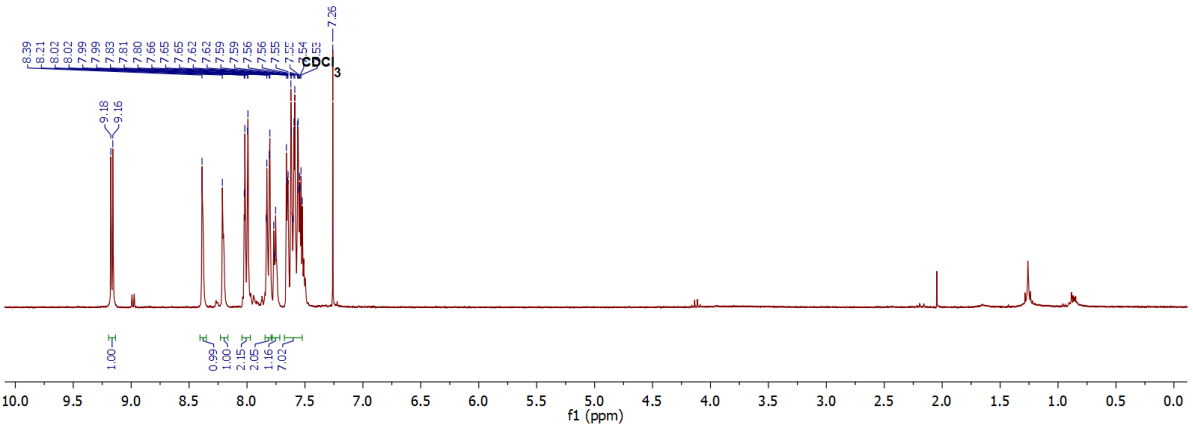


3,9-diphenylthieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5a)

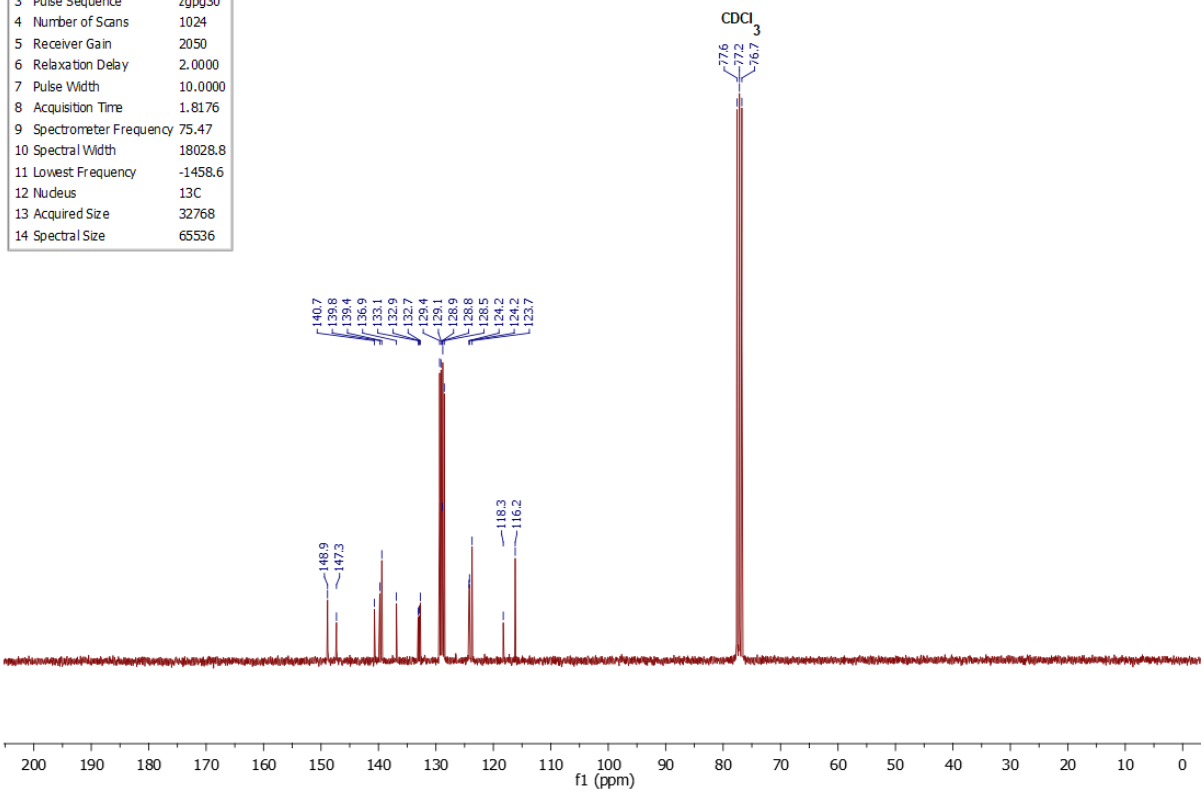
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	287
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



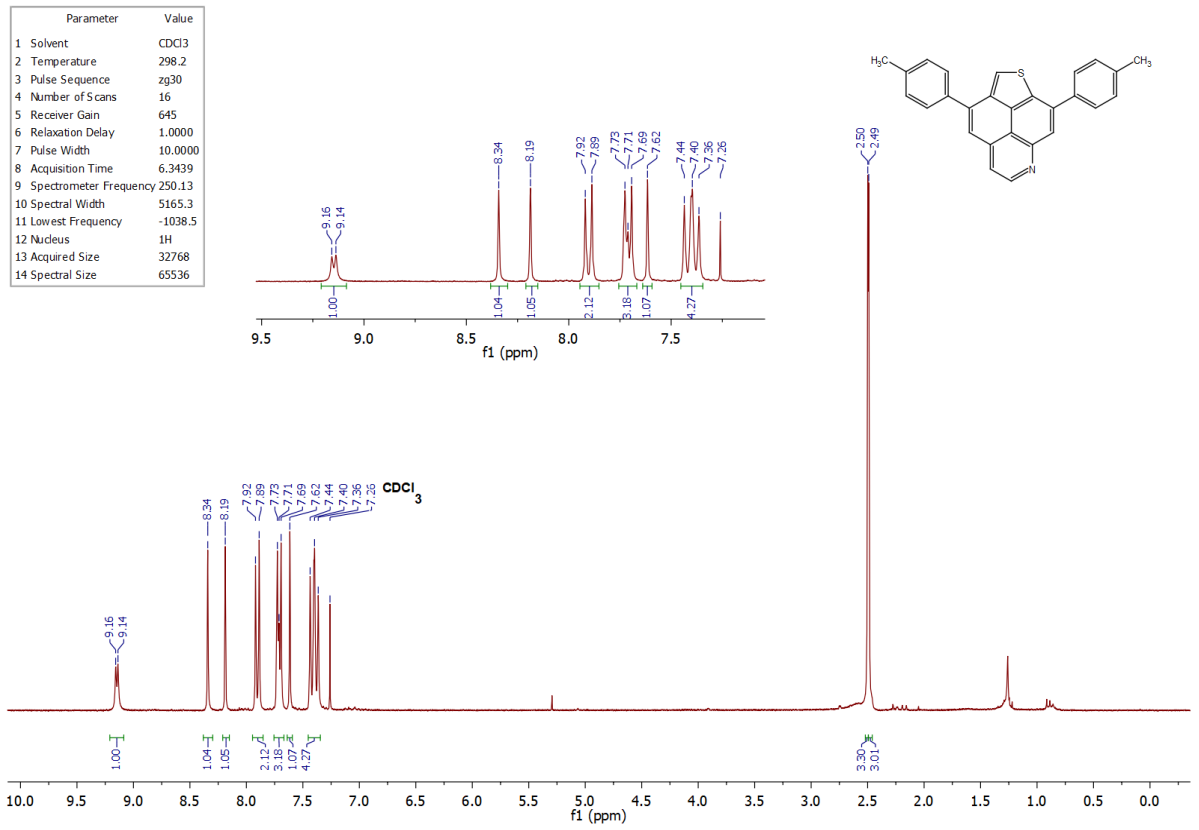


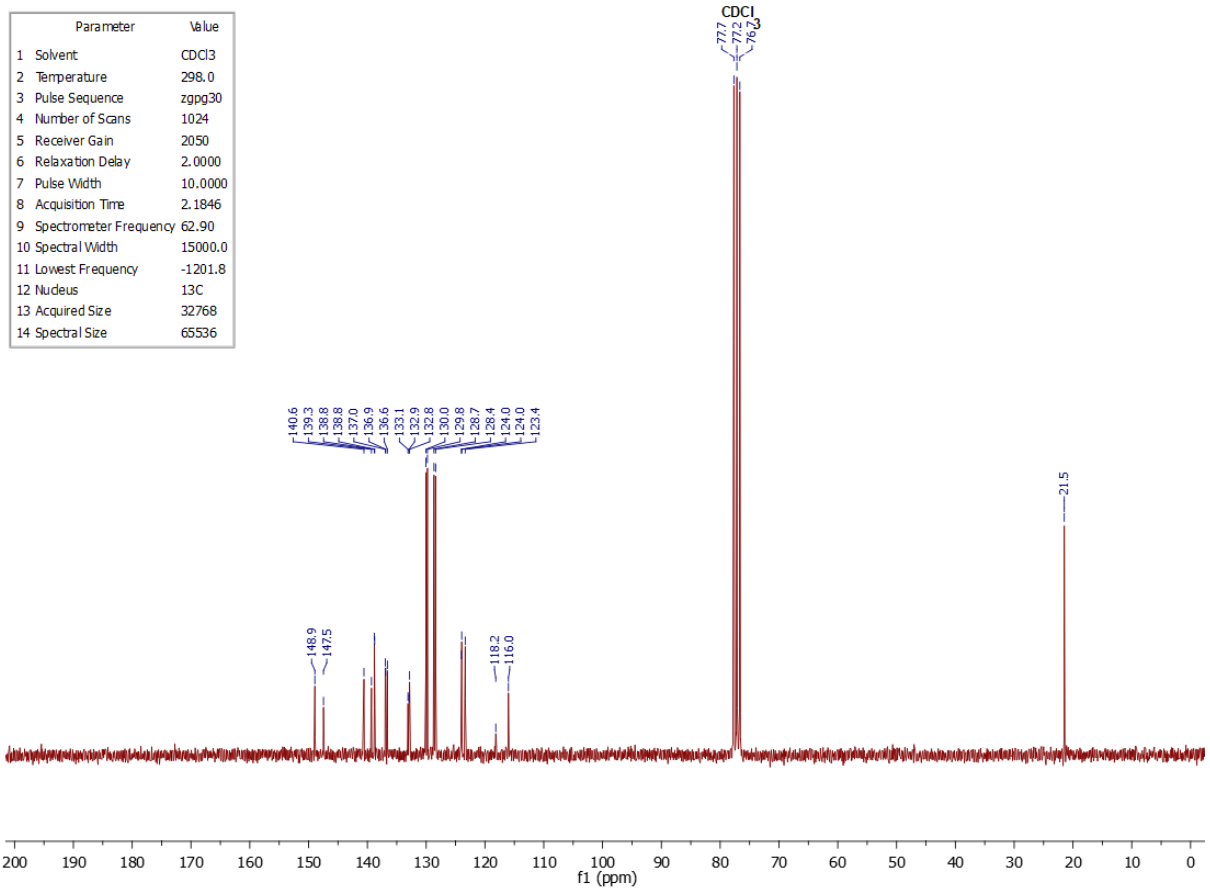


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1458.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

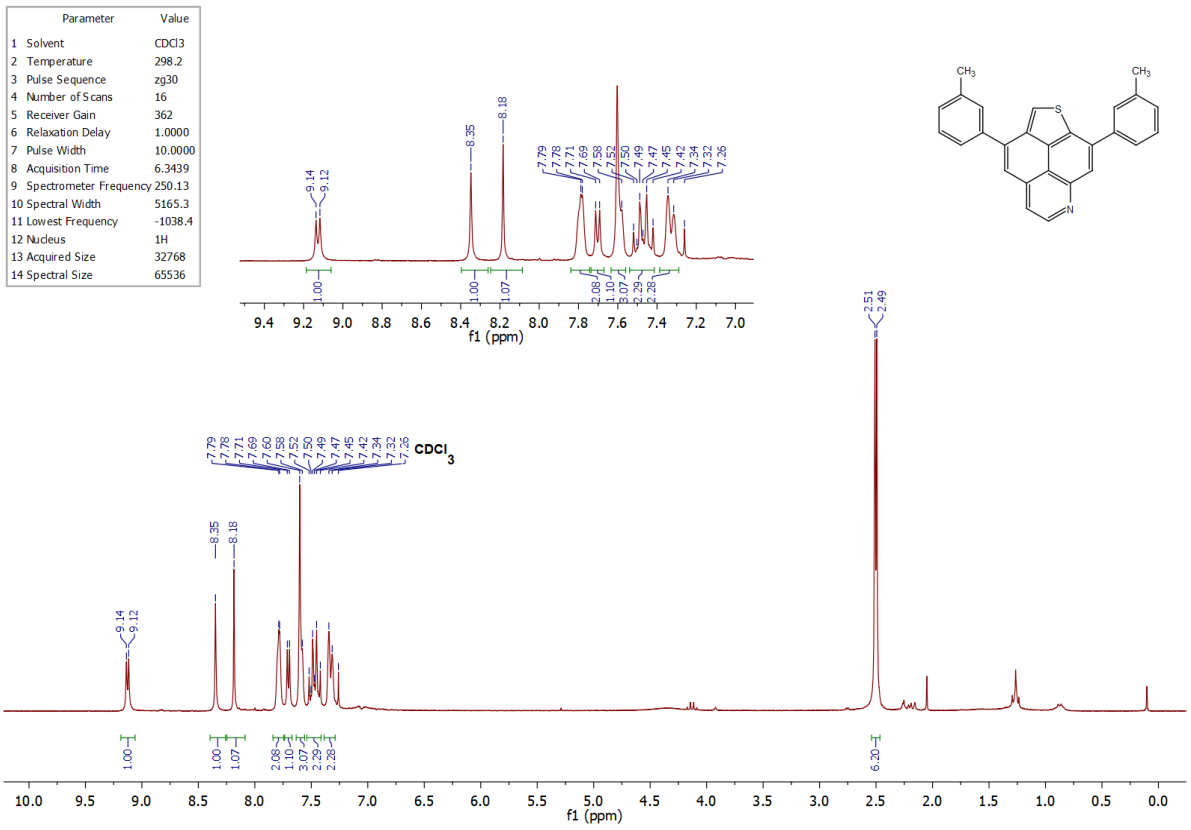


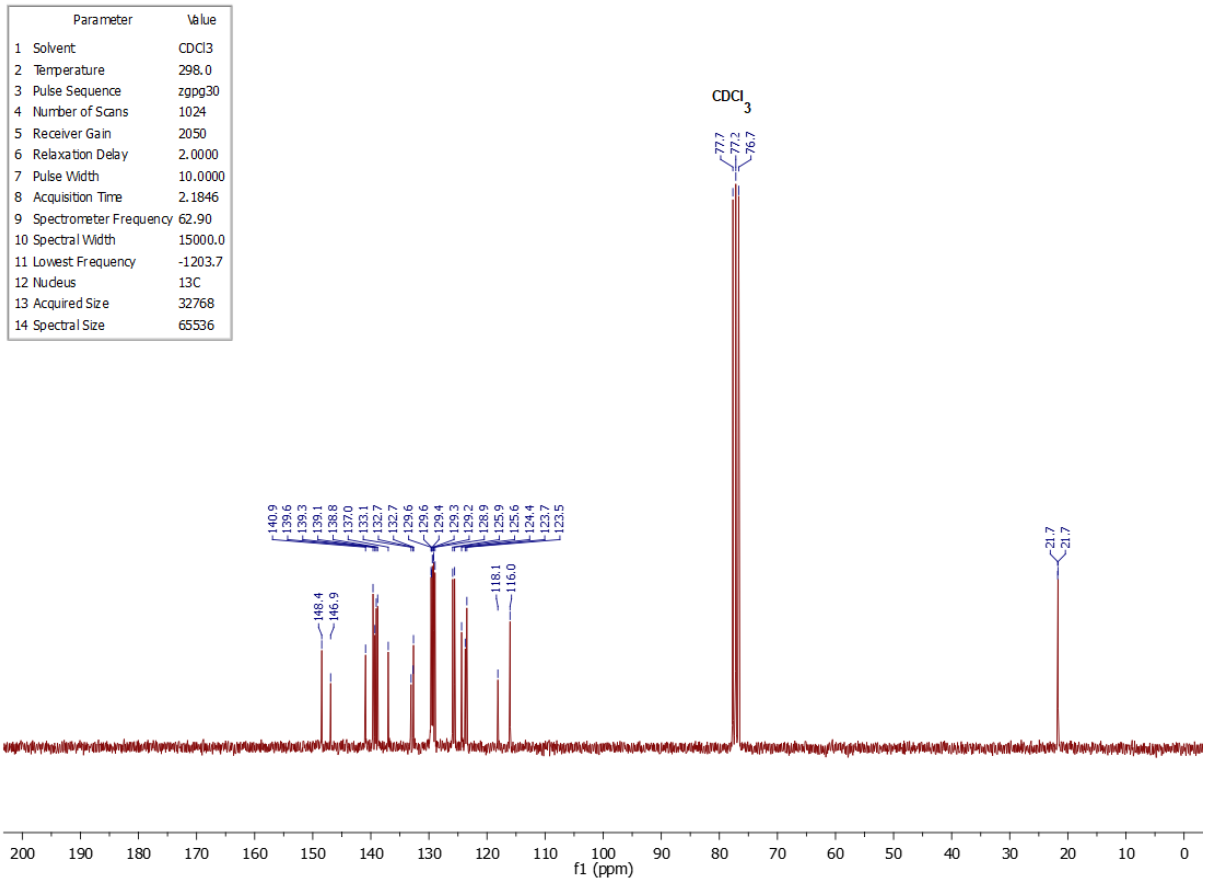
3,9-di-*p*-tolylthieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5b)



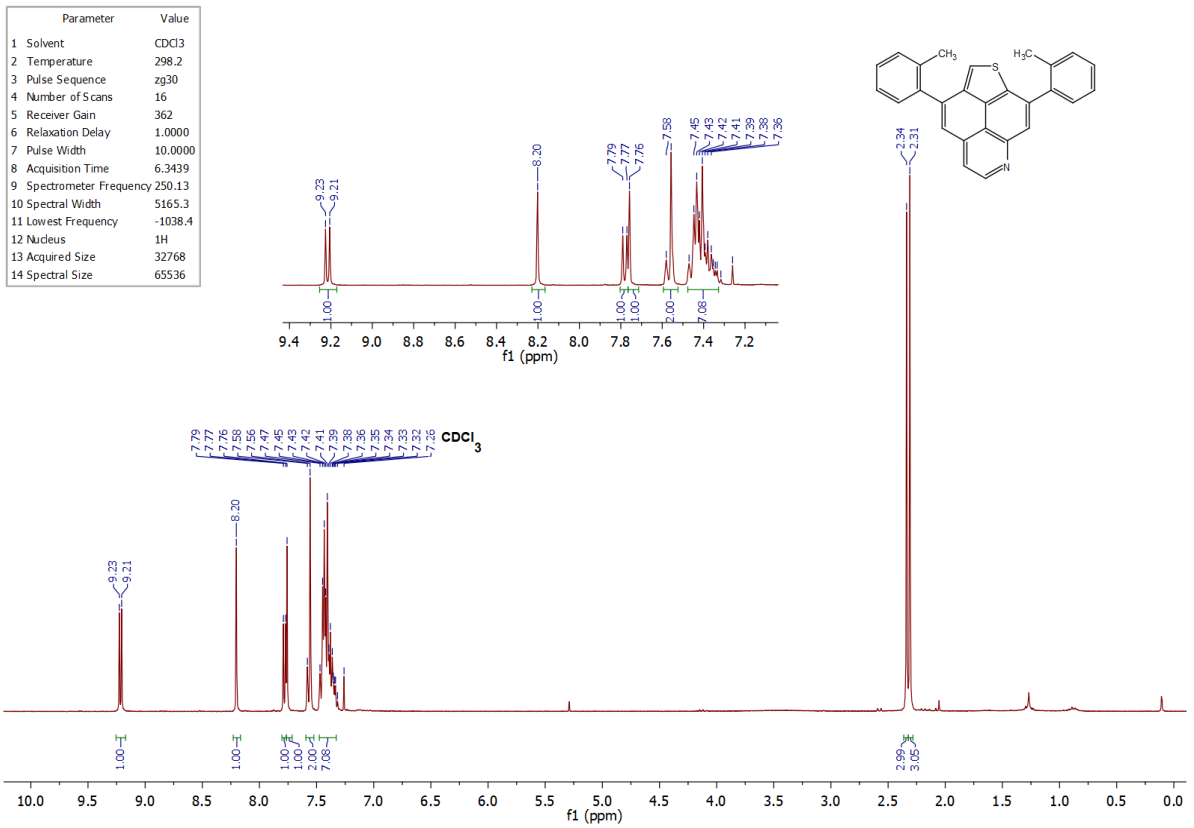


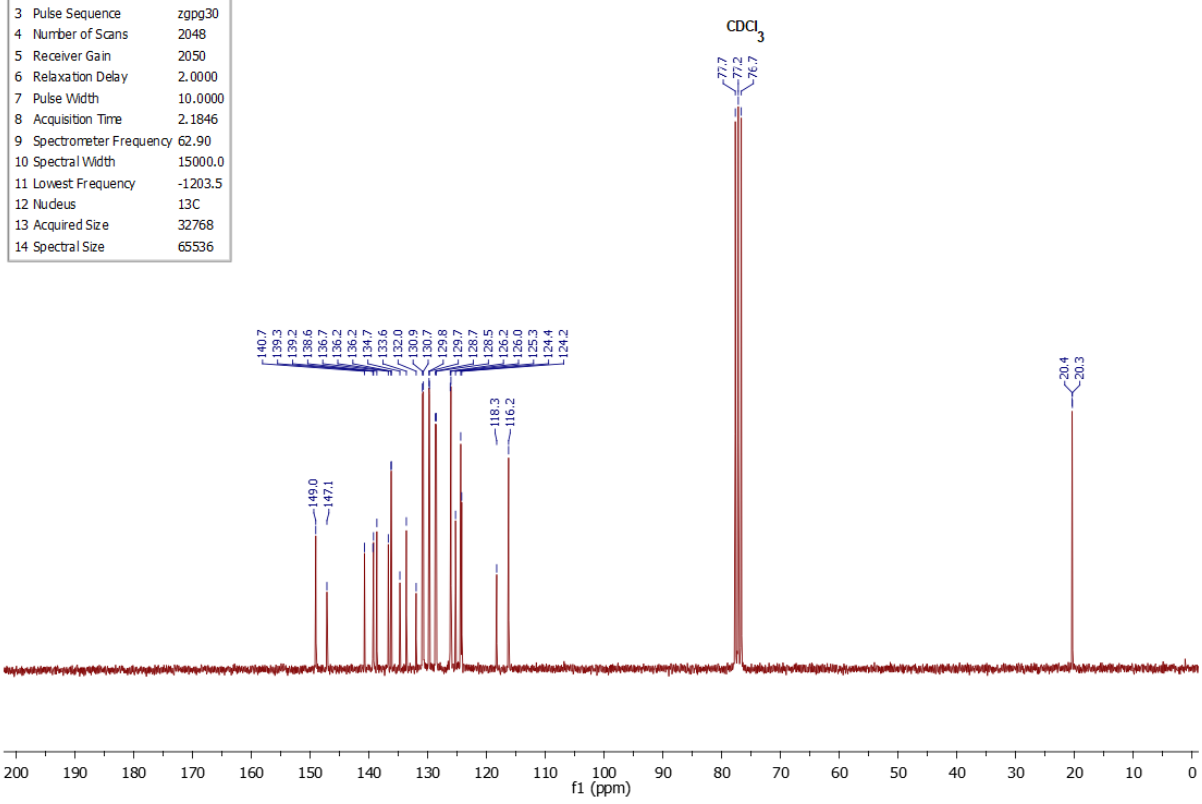
3,9-di-*m*-tolylthieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5c)





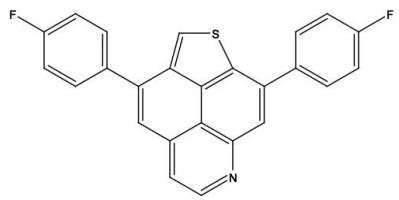
3,9-di-*o*-tolylthieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5d)

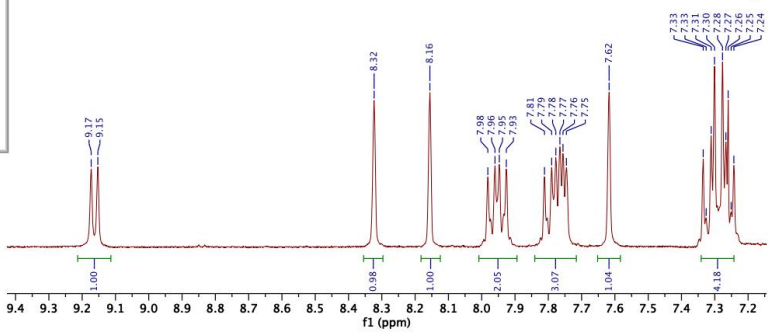


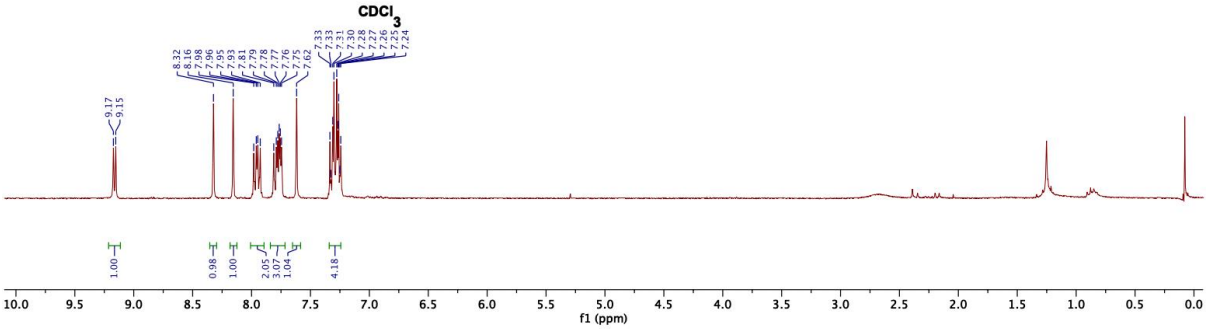


3,9-bis(4-fluorophenyl)thieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5e)

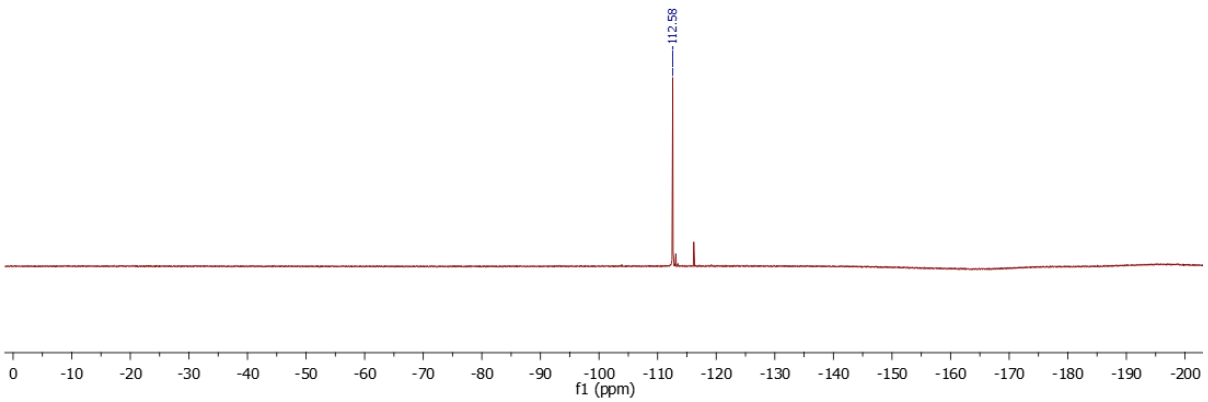
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	645
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



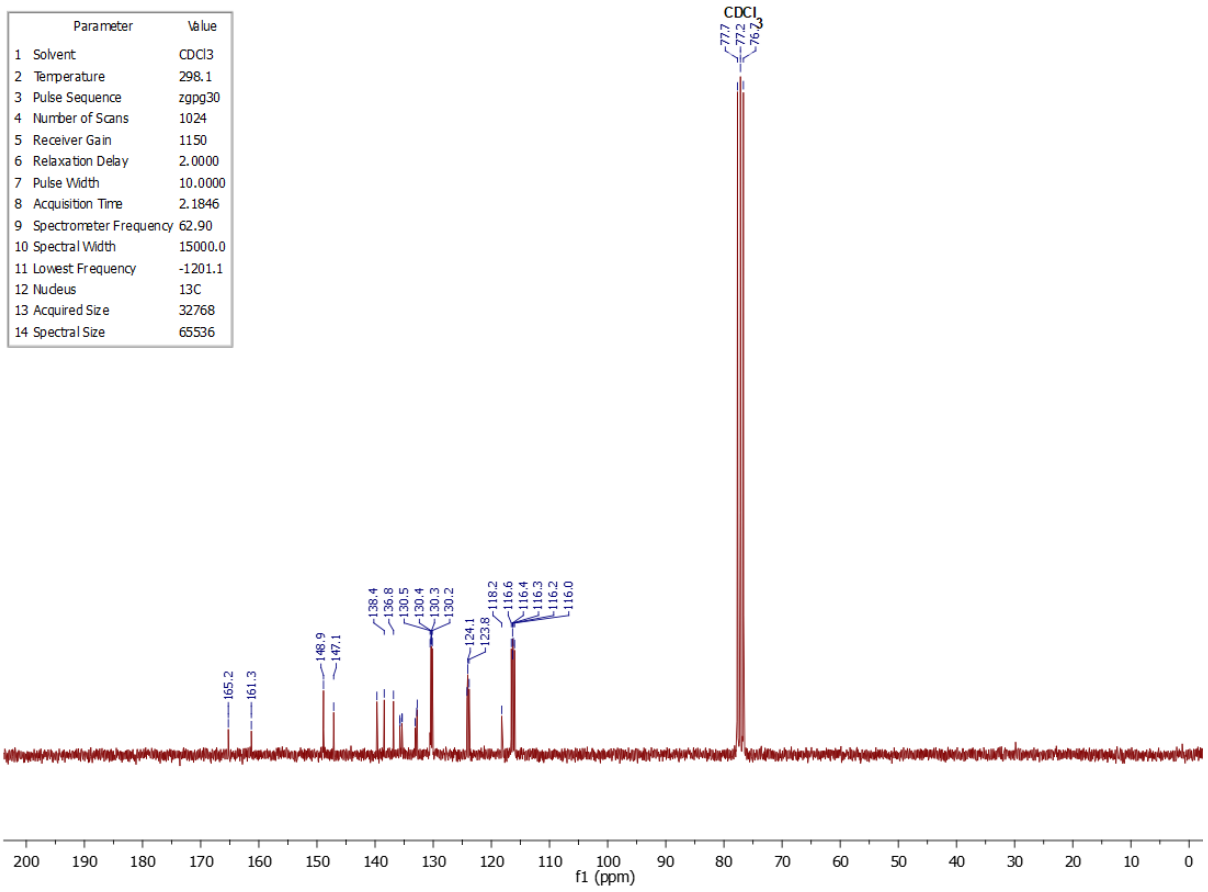




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgig
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	12.0000
8	Acquisition Time	0.5767
9	Spectrometer Frequency	470.59
10	Spectral Width	113636.4
11	Lowest Frequency	-103877.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	65536

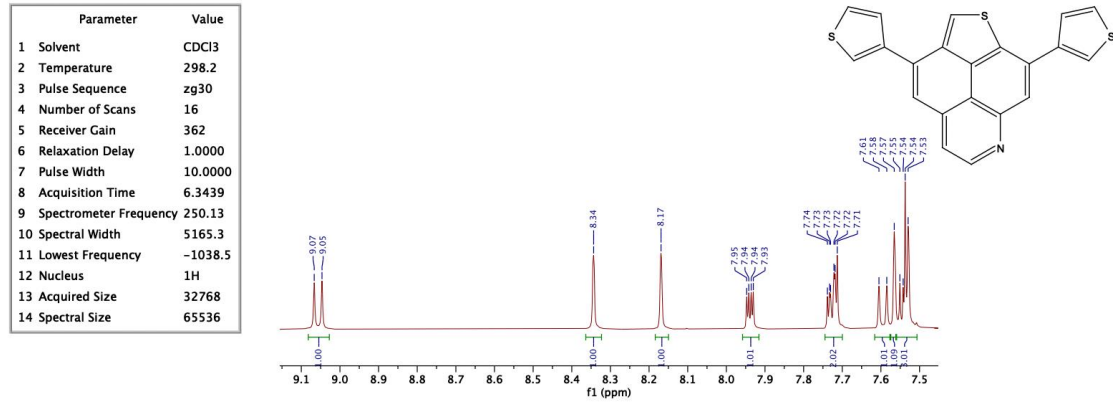


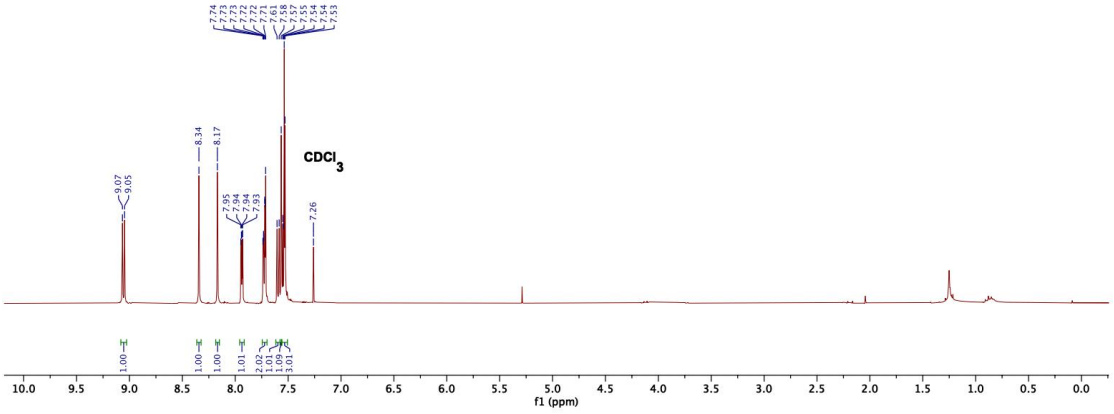
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	1150
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1201.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



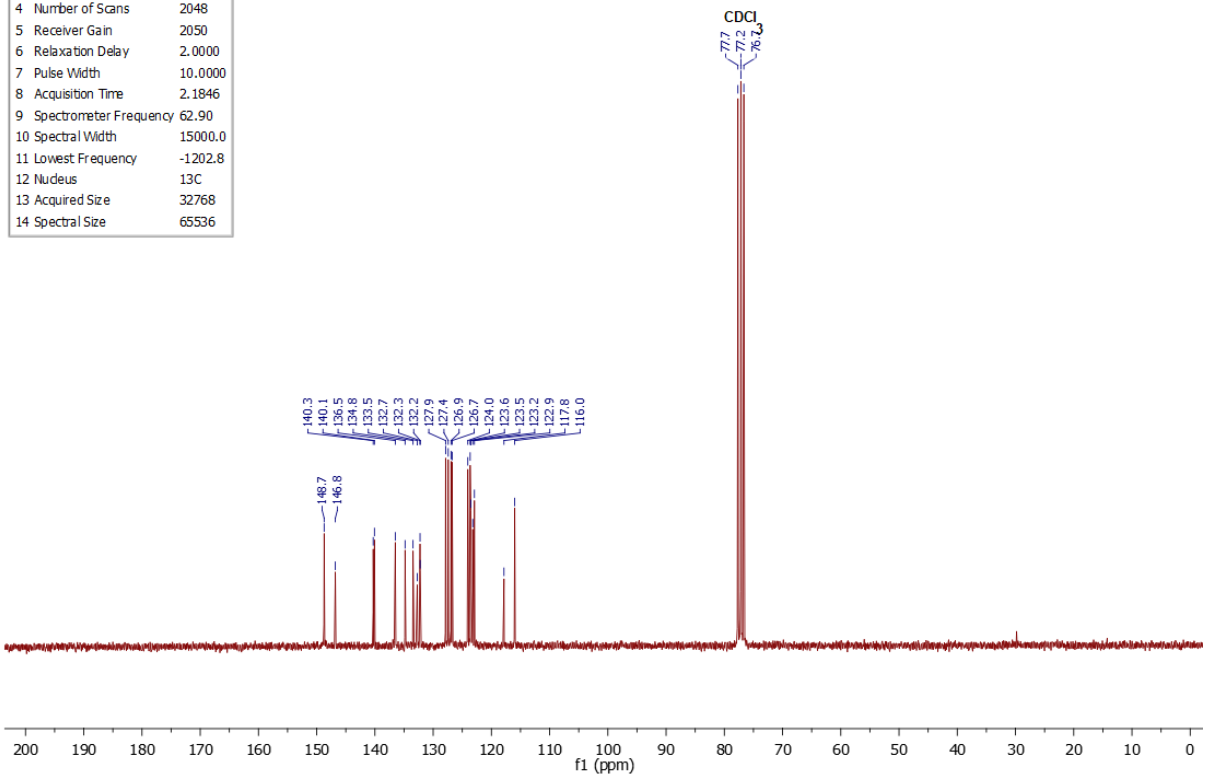
3,9-di(thiophen-3-yl)thieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine (5h)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.5
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



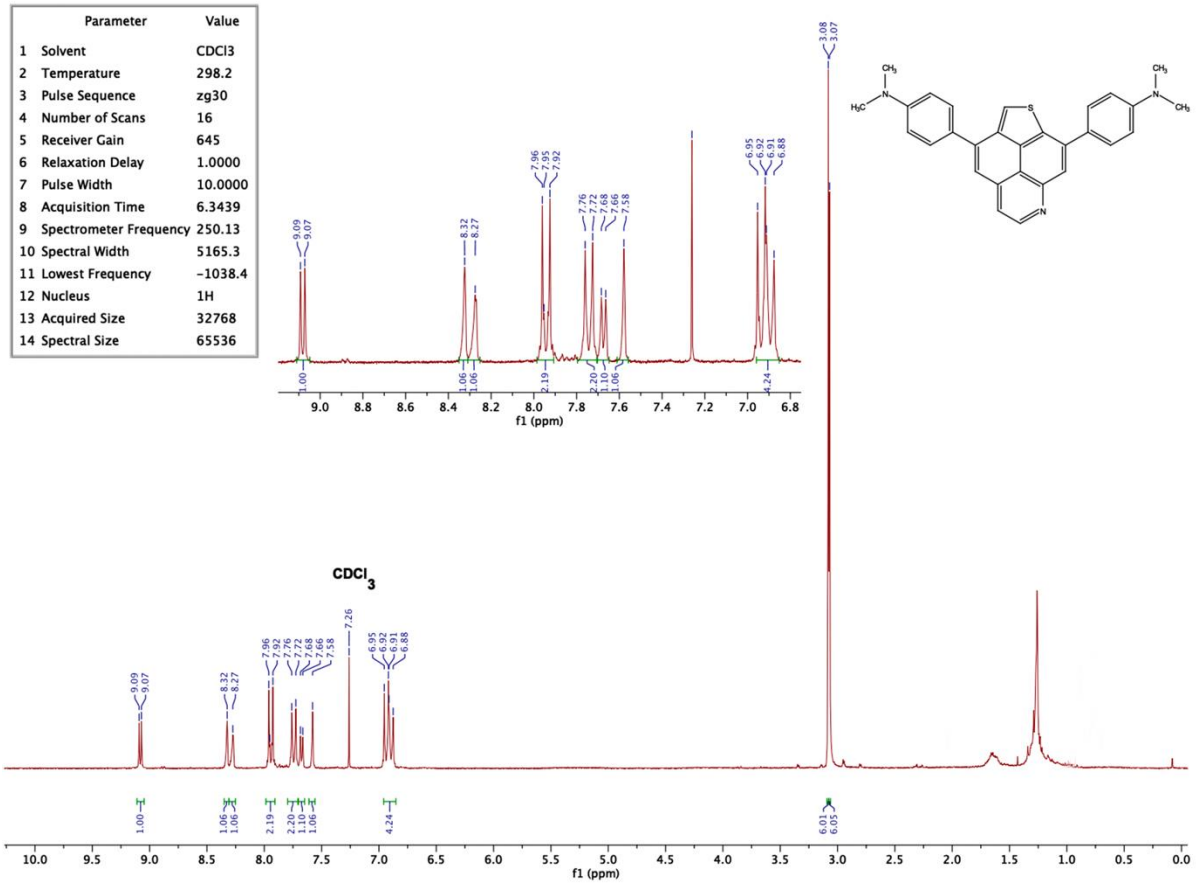


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	2048
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1202.8
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

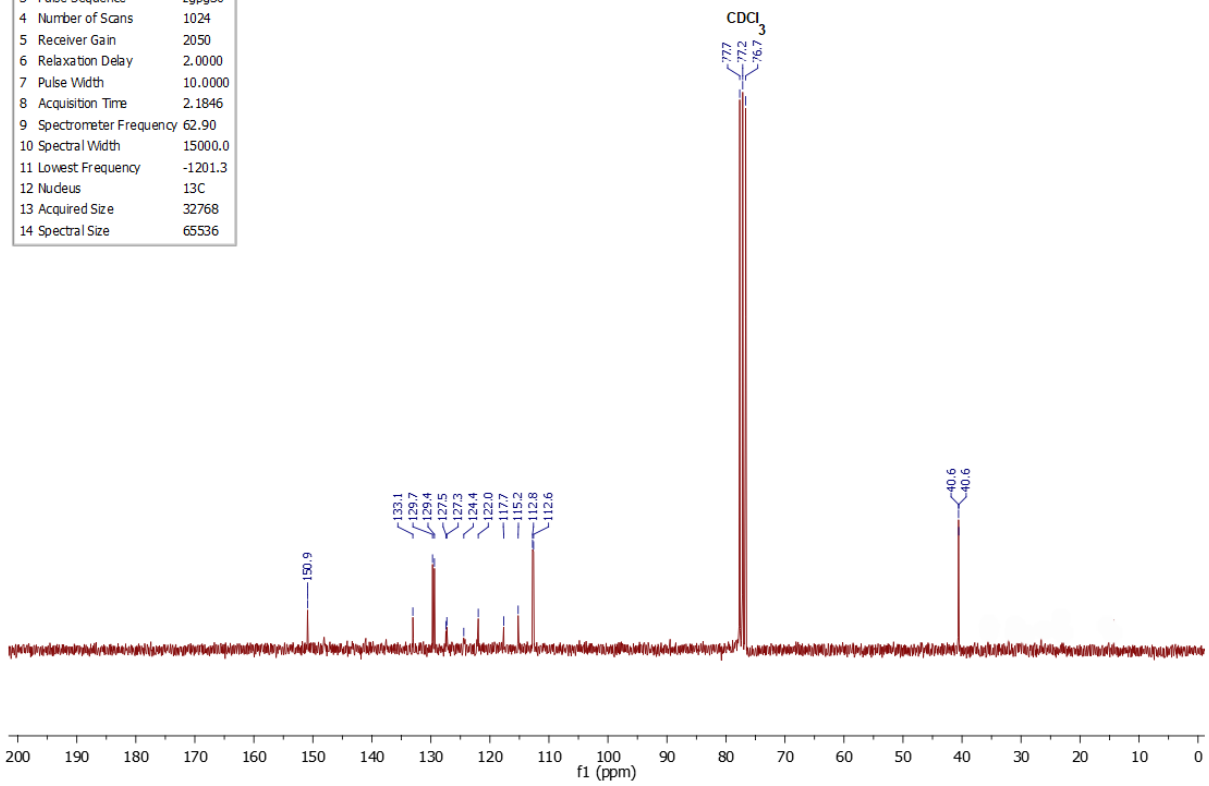


4,4'-(thieno[2',3',4':4,5]naphtho[1,8-*bc*]pyridine-3,9-diyl)bis(N,N-dimethylaniline) (5j)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	645
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	6.3439
9	Spectrometer Frequency	250.13
10	Spectral Width	5165.3
11	Lowest Frequency	-1038.4
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

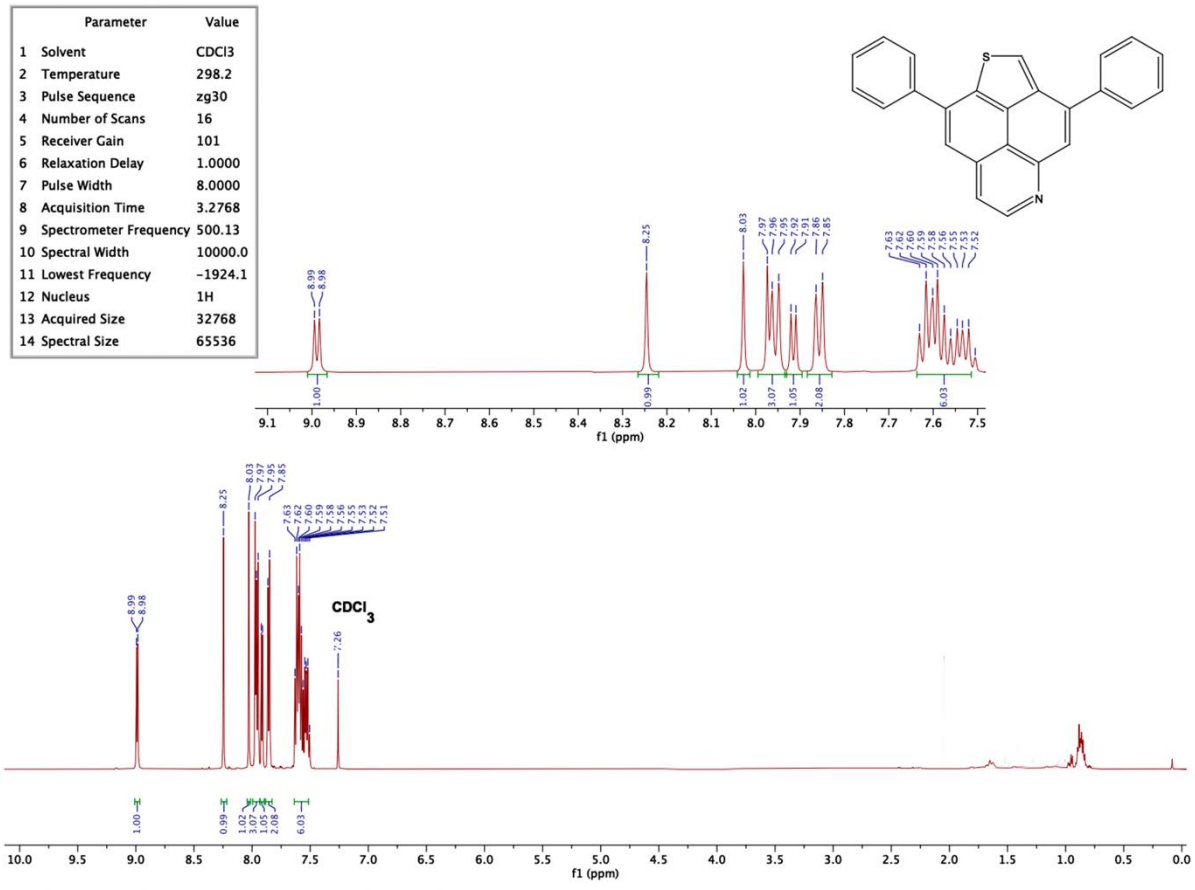


	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	2.1846
9	Spectrometer Frequency	62.90
10	Spectral Width	15000.0
11	Lowest Frequency	-1201.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

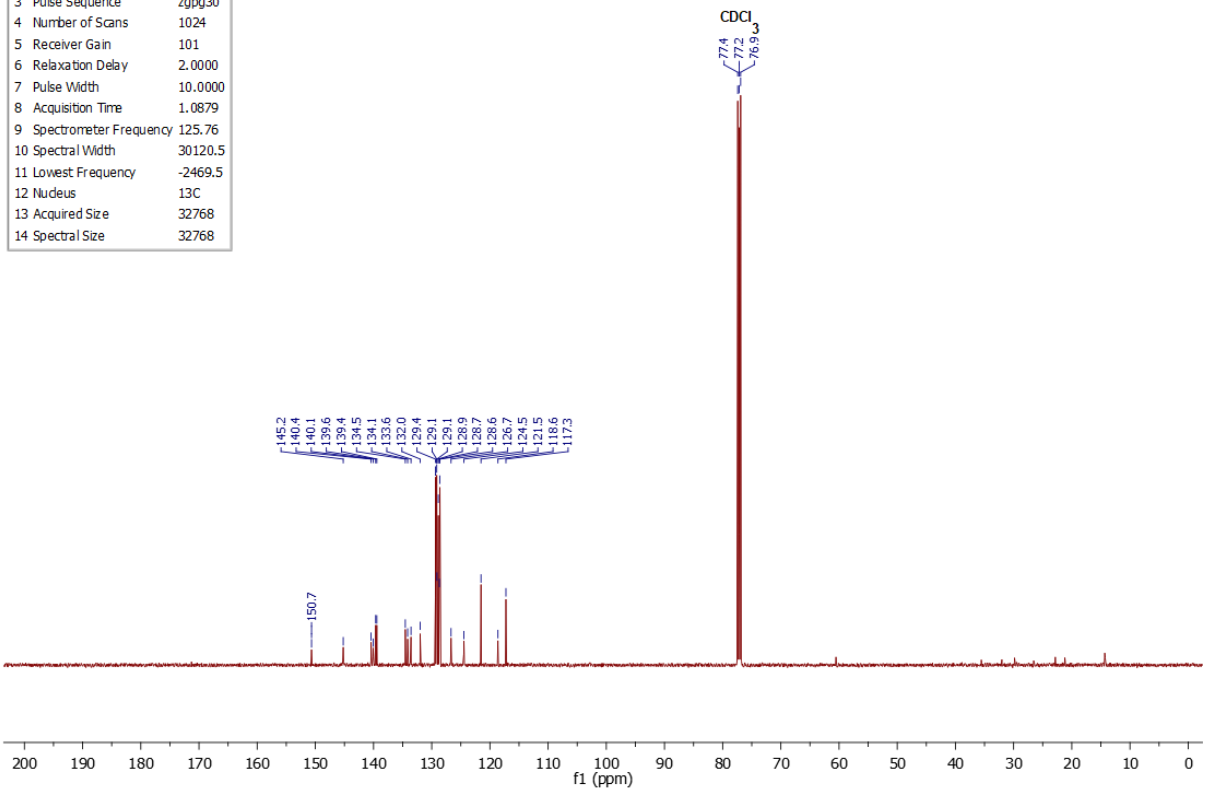


3,9-diphenylthieno[4',3',2':4,5]naphtho[1,8-*bc*]pyridine (6a)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.1
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

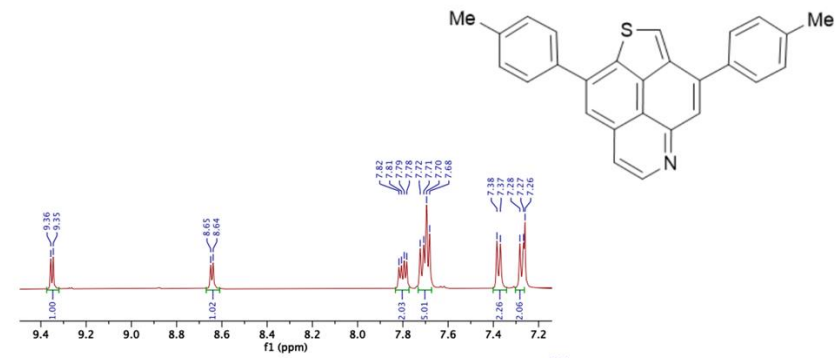


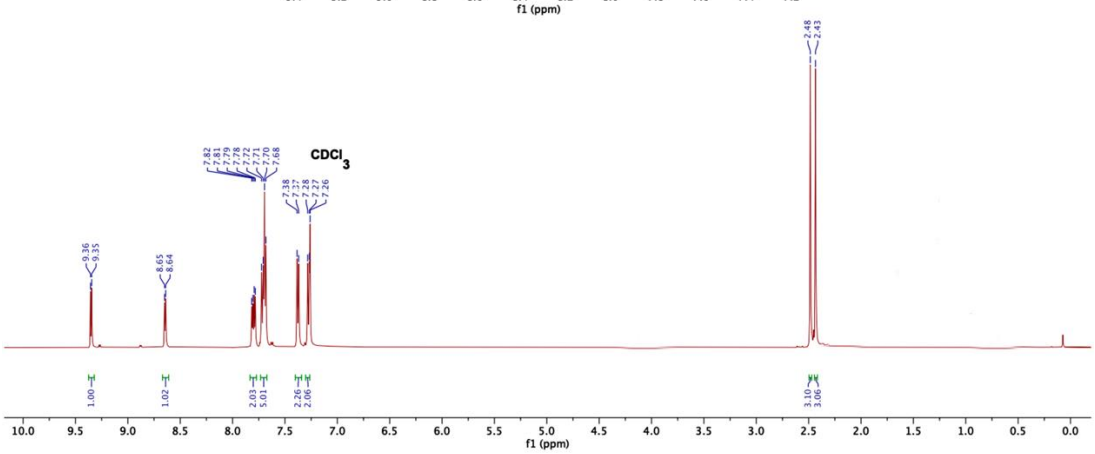
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2469.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768



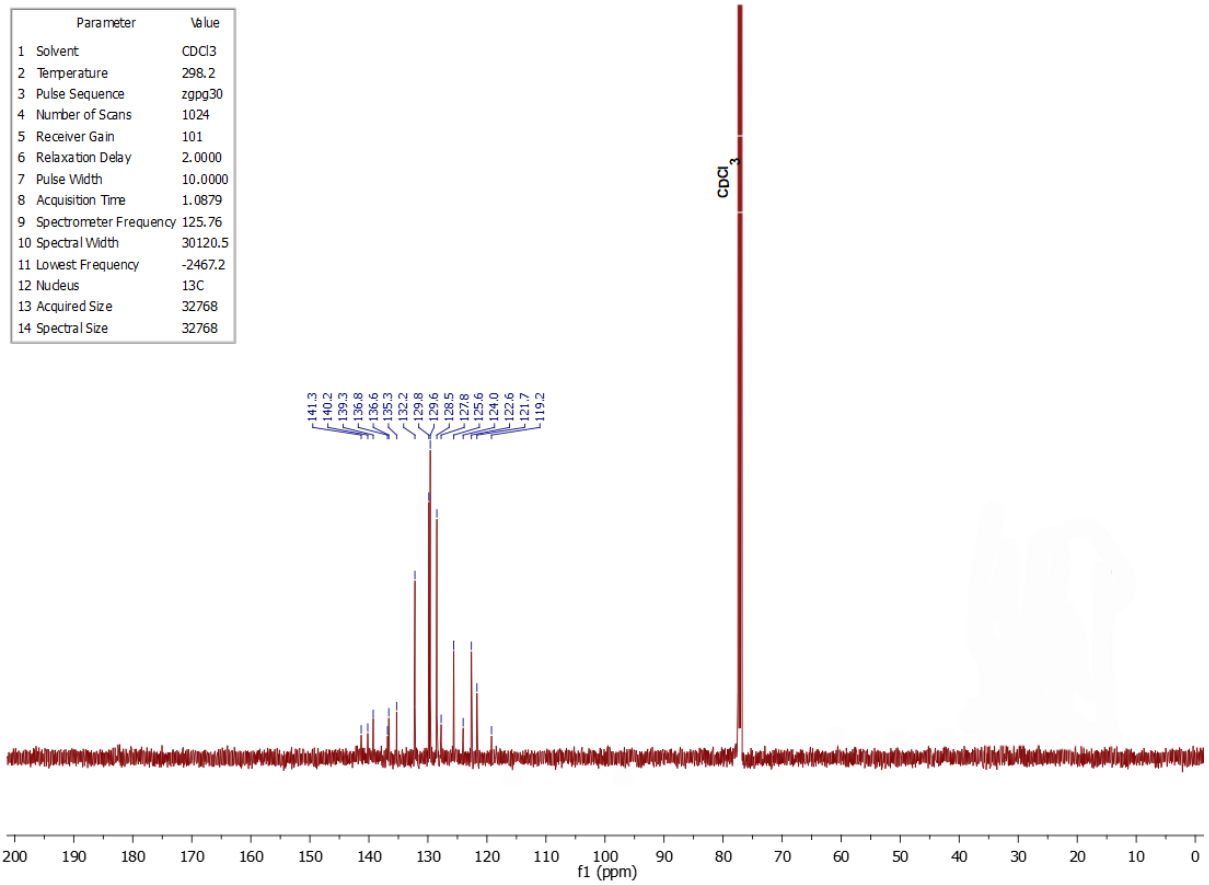
3,9-di-*p*-tolylthieno[4',3',2':4,5]naphtho[1,8-*bc*]pyridine (6b)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.8
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



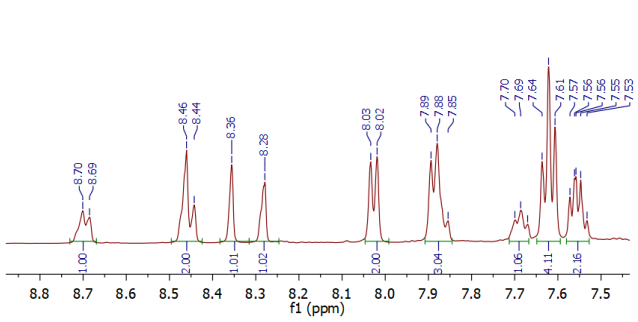


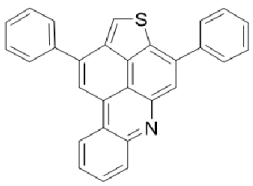
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2467.2
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

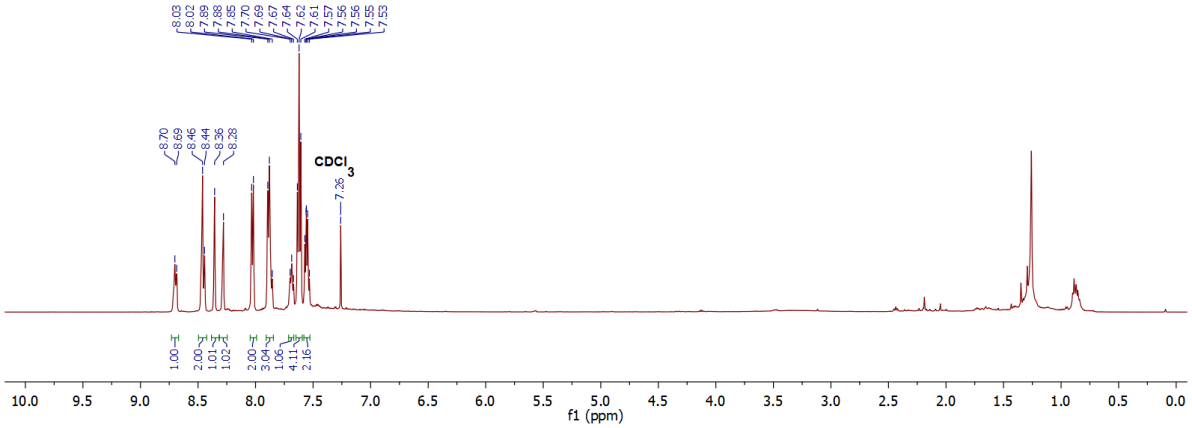


3,11-diphenylthieno[2',3',4':4,5]naphtho[1,8-*bc*]quinoline (8a)

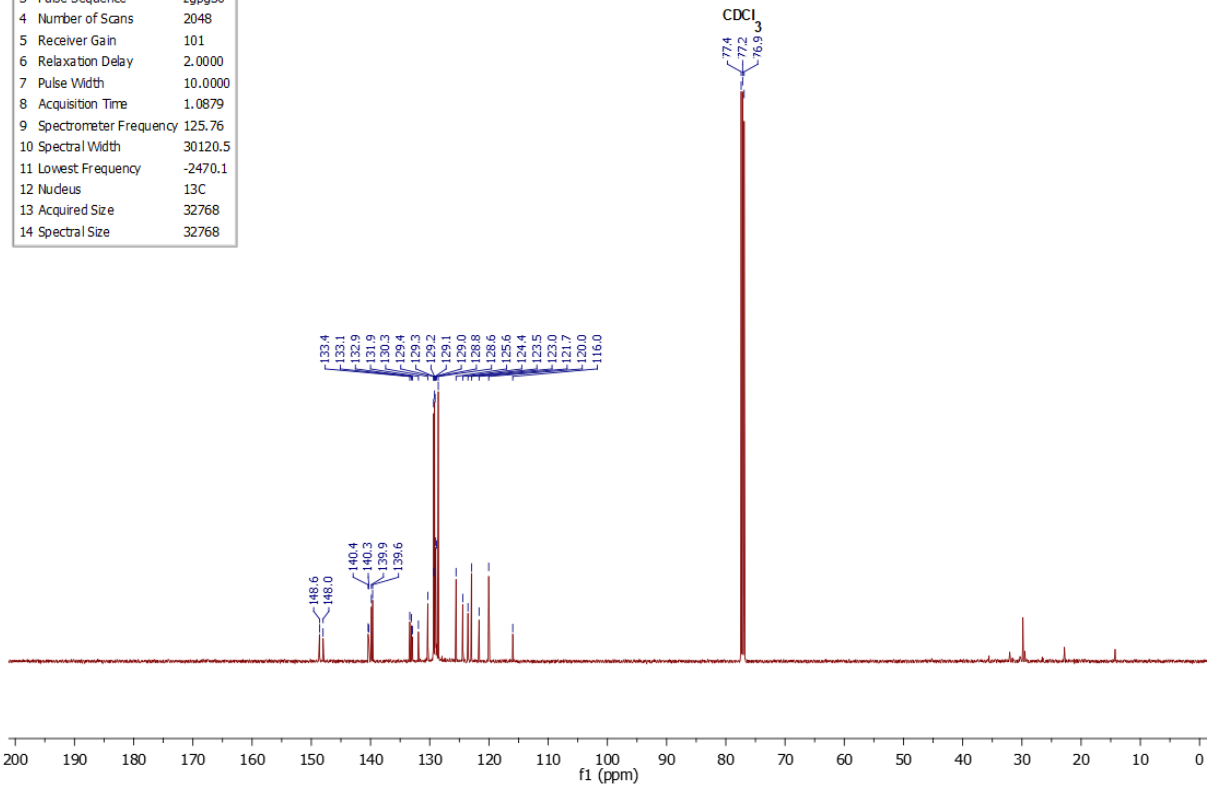
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	32
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1923.9
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





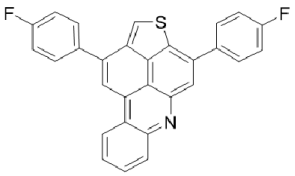


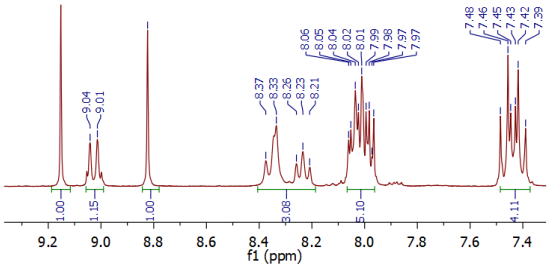
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Number of Scans	2048
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2470.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768

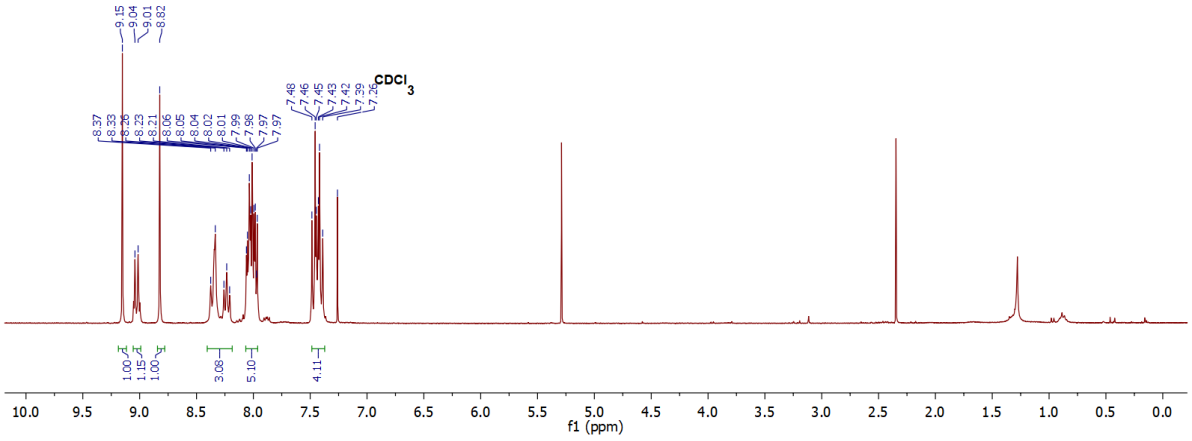


3,11-bis(4-fluorophenyl)thieno[2',3',4':4,5]naphtho[1,8-*bc*]quinoline (8b)

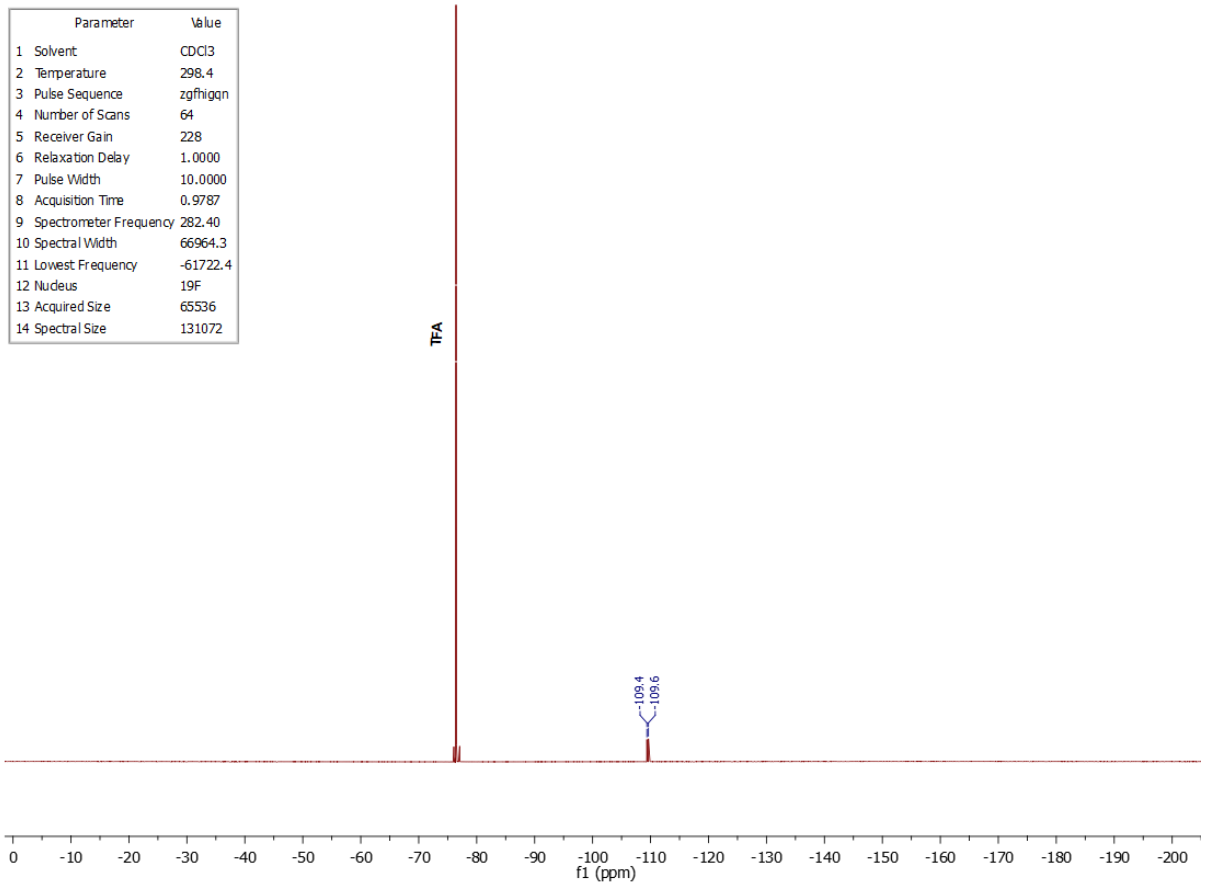
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	32
5	Receiver Gain	72
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	4.3691
9	Spectrometer Frequency	300.13
10	Spectral Width	7500.0
11	Lowest Frequency	-1354.7
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536



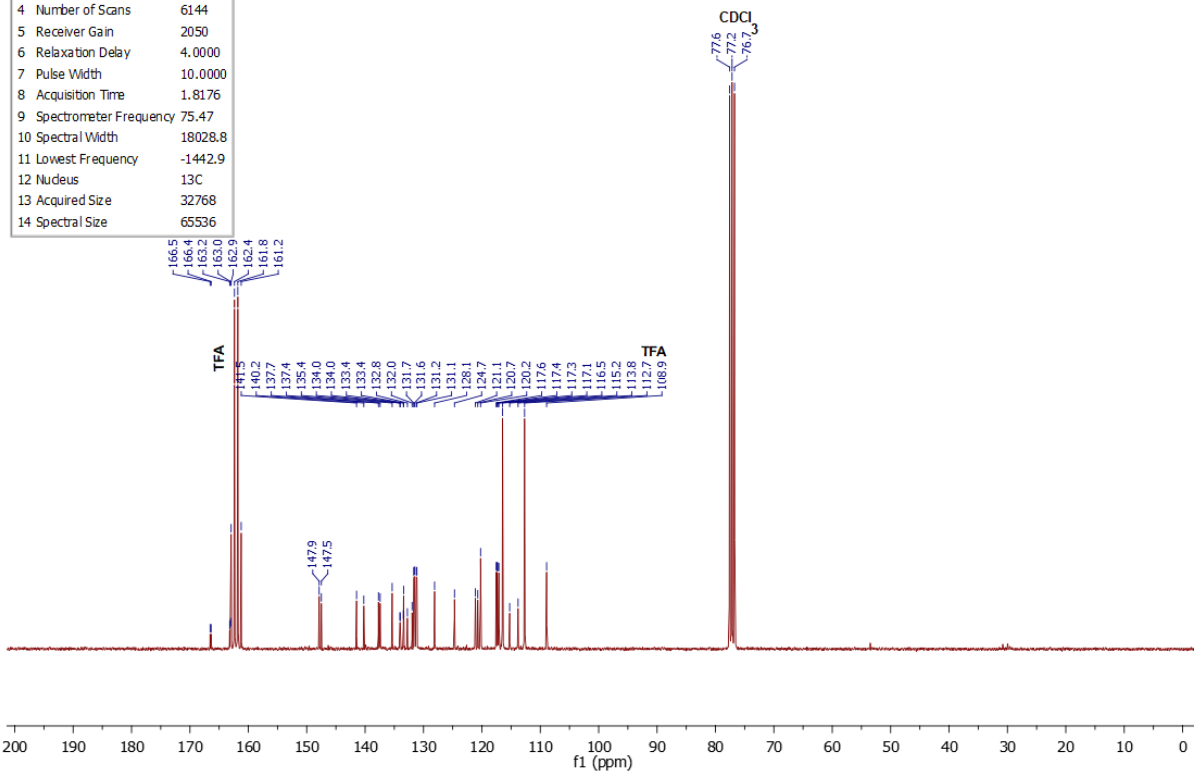




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.4
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	228
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.40
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

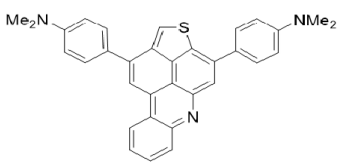


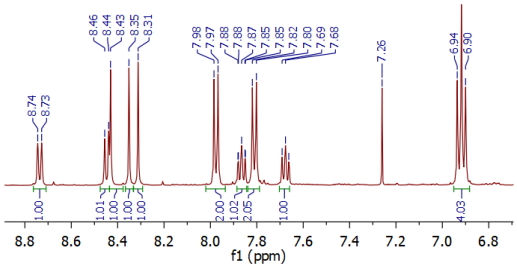
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.8
3	Pulse Sequence	zgpg30
4	Number of Scans	6144
5	Receiver Gain	2050
6	Relaxation Delay	4.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.47
10	Spectral Width	18028.8
11	Lowest Frequency	-1442.9
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

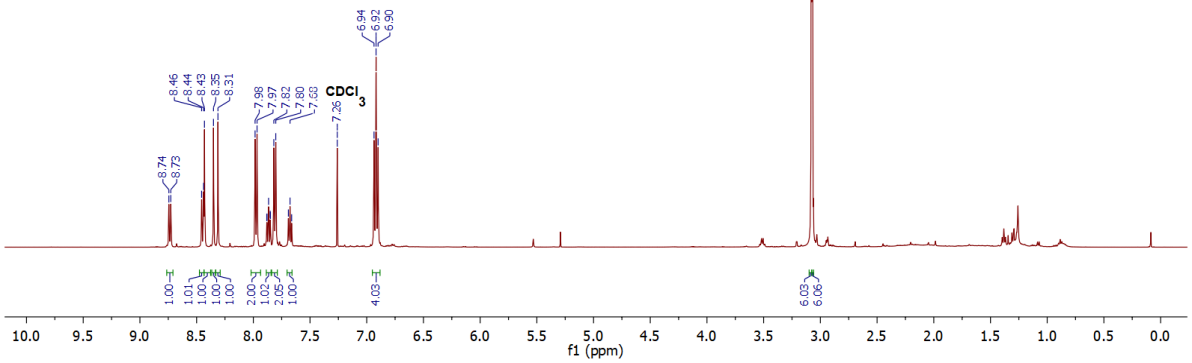


4,4'-(thieno[2',3',4':4,5]naphtho[1,8-*bc*]quinoline-3,11-diyl)bis(N,N-dimethylaniline) (8c)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zg30
4	Number of Scans	64
5	Receiver Gain	101
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1967.0
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536







	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	4096
5	Receiver Gain	101
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.76
10	Spectral Width	30120.5
11	Lowest Frequency	-2470.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	32768