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Supporting Information

π-Expanded Azaullazines: Synthesis of Quinolino-Azaullazines by Povarov Reaction and Cycloisomerisation

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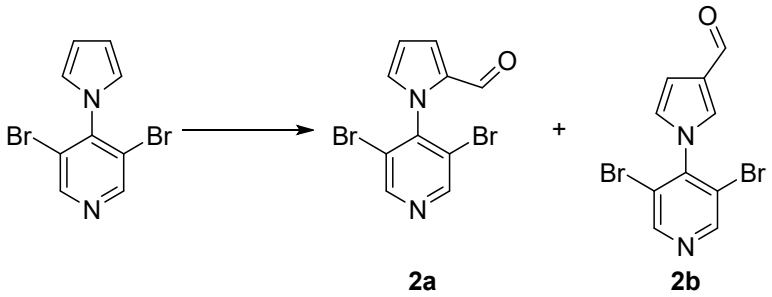
Optimization of Vilsmeier-Haack reaction

Table 1: Optimization of Vilsmeier-Haack reaction

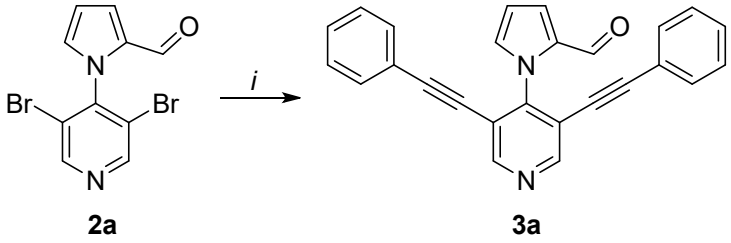


entry	solvent	eq. $POCl_3$	*T* [°C]	*t* [h]	yield[a] 2a [%]	yield[a] 2b [%]
1	DCE	1.2	reflux	3	25	27
2	DCE	2.0	reflux	3	21	23
3[b]	DMF	2.0	r.t.	12	13	29
4[b]	**DMF**	**2.0**	**100**	**3**	**33**	**62**

[a] isolated yield, [b]argon atmosphere

Optimization of Sonogashira reaction

*Table 2: Optimization of sonogashira reaction for **3a**; i: phenylacetylene (3 eq.), [Pd] (0.05 eq.), ligand (0.1 eq.), CuI (0.05 eq), base (6 eq), solvent, T, 24 h.*



entry	[Pd]	Ligand	base	solvent	*T* [°C]	yield 3a [%][a]
1[b]	$PdCl_2(PPh_3)_2$	CataCXium A	NEt_3	acetonitrile	70	51
2	$PdCl_2(PPh_3)_2$	CataCXium A	NEt_3	1,4-dioxane	90	72
3	$PdCl_2(PPh_3)_2$	XPhos	NEt_3	1,4-dioxane	90	55
4	$PdCl_2(CH_3CN)_2$	CataCXium A	NEt_3	1,4-dioxane	90	41
5	**$PdCl_2(PPh_3)_2$**	**CataCXium A**	**HNiPr$_2$**	**1,4-dioxane**	**90**	**80**

[a] isolated yield, [b] conditions of Langer et al.[1]

X-Ray

*Table 3: 11-fluoro-5,13-di-p-tolylindolizino[6,5,4,3-ija]quinolino[2,3-c][1,6]naphthyridine (**5d**)*

Chem. Formula	$C_{32}H_{22}N_3F$ + 0.88 CH_2Cl_2
Form. Wght [g mol^{-1}]	566.49
colour	red
Crsyt. system	monoklinic
Space group (Hall group)	C 2/c (-C 2yc)
a [Å]	25.9576(15)
b [Å]	14.7451(9)
c [Å]	14.1378(8)
α [°]	90
β [°]	96.669(2)
γ [°]	90
V [Å^3]	5374.6(5)
Z	8
N_{ref}	9911
θ_{max} [°]	29.000
h,k,l$_{max}$	35,20,19
ρ_x[g cm^{-3}]	1.400
μ [mm^{-1}]	0.256
$\lambda_{MoK\alpha}$ [A]	0.71073
T [K]	123
F(000)	2345.0
N_{par}	386
R	0.0516(5117)
wR_2	0.1401(7148)
S	1.051

UV-vis-Data

*Table 4: detailed Spectroscopic Data of **5a**, **5c**, **5d**, **5h**, **5j**, **5k** and **5l** in DCM (c = 10^{-5} M) at 20 °C*

	5a	**5c**	**5d**	**5h**	**5j**	**5k**	**5l**
$\lambda_{1,abs}$ [nm]	471	503	477	470	477	482	480
$\varepsilon_{\lambda1}$ [10^4 L·mol^{-1}cm^{-1}]	1.1	0.7	0.8	1.6	0.8	0.7	0.9
$\lambda_{2,abs}$ [nm]	448	480	454	447	477	455	455
$\varepsilon_{\lambda2}$ [10^4 L·mol^{-1}cm^{-1}]	1.0	0.7	0.8	1.3	0.8	0.7	0.9
$\lambda_{3,abs}$ [nm]	362	377	359	447	360	354	360
$\varepsilon_{\lambda3}$ [10^4 L·mol^{-1}cm^{-1}]	1.2	0.7	1.0	1.3	1.0	2.2	1.2
$\lambda_{4,abs}$ [nm]	344	354	342	385	343	321	342
$\varepsilon_{\lambda4}$ [10^4 L·mol^{-1}cm^{-1}]	1.7	1.0	1.5	0.8	1.4	2.5	1.6
$\lambda_{5,abs}$ [nm]	335	320	315	312	314	306	315
$\varepsilon_{\lambda5}$ [10^4 L·mol^{-1}cm^{-1}]	1.6	2.7	1.7	4.6	1.6	2.4	1.8
$\lambda_{6,abs}$ [nm]	301	268	299	285	300	261	299
$\varepsilon_{\lambda6}$ [10^4 L·mol^{-1}cm^{-1}]	3.8	1.9	2.9	5.1	2.5	4.4	2.8
$\lambda_{7,abs}$ [nm]	289		287		264		254
$\varepsilon_{\lambda7}$ [10^4 L·mol^{-1}cm^{-1}]	4.2		3.1		4.6		5.1
$\lambda_{8,abs}$ [nm]	262		264				
$\varepsilon_{\lambda8}$ [10^4 L·mol^{-1}cm^{-1}]	4.6		4.2				
$\lambda_{1,em}$ [nm]	511	533	522	504	522	533	522

	5	9	5	5	4	9	4
$E_g^{opt,a}$ [eV]	2.5	2.4	2.5	2.5	2.5	2.5	2.5
	6	2	3	9	3	0	3
Φ^b	0.2	0.1	0.2	0.3	0.2	0.2	0.2
	6	9	7	5	5	0	8

[a] determined from the intersection of the normalized absorption and emission spectra.

[b] Fluorescence standard: quinine hemisulfate monohydrate in 0.05 M H_2SO_4 (Φ = 0.52).[2]

*Table 5: Quantuum yields and $\lambda_{max,em}$ of solvatochromism measurements for **5a**, **5c** and **5k***

	Cyclohexane		DCM		Acetonitrile		Ethanol	
	Φ^a	$\lambda_{max,em}$ [nm]	Φ^a	$\lambda_{max\,em}$ [nm]	Φ^a	$\lambda_{max,em}$ [nm]	Φ^a	$\lambda_{max,em}$ [nm]
5a	0.26	483	0.26	515	0.22	530	0.27	525
5c	0.30	514	0.19	538	0.15	547	0.20	551
5k	0.16	494	0.20	540	0.01	563	<0.01	553

[a]: Fluorescence standard: quinine hemisulfate monohydrate in 0.05 M H_2SO_4 (Φ = 0.52).[2]

Cyclic voltammetry

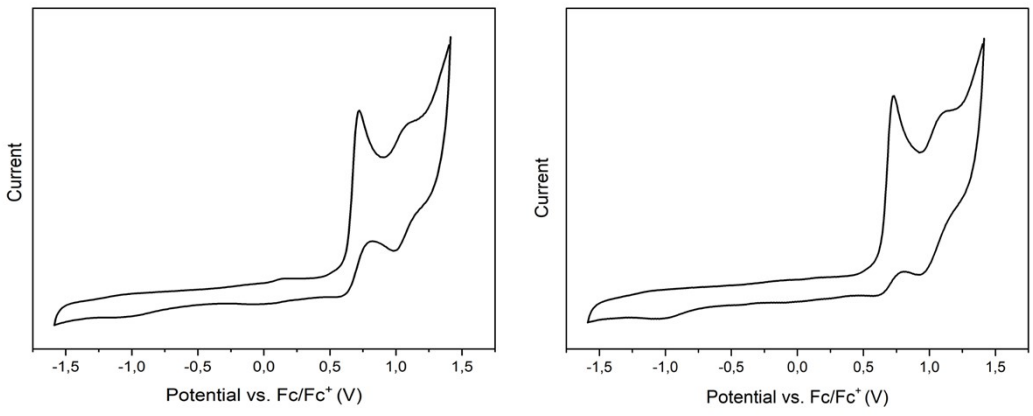


Figure S1: Cyclic voltammograms of **5a**. Measured in DCM with 0.25 M n-Bu_4NPF_6 as a supporting electrolyte, glassy carbon working electrode, and Pt counter-electrode with ferrocene as standard at a scan rate of 100 mV/s (left) and 200 mV/s (right).

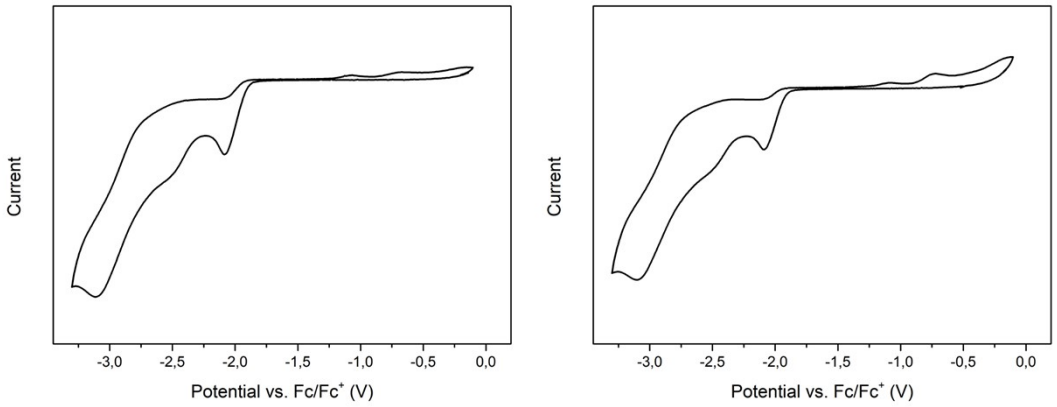


Figure S2*:* Cyclic voltammograms of **5a**. Measured in THF with 0.25 M n-Bu_4NPF_6 as a supporting electrolyte, glassy carbon working electrode, and Pt counter-electrode with ferrocene as standard at a scan rate of 100 mV/s (left) and 200 mV/s (right).

DFT Calculations

Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) calculations were performed with Gaussian09.[3] The ground and excited state structures as well as TD-DFT calculations were performed using the B3LYP, functional and the 6-31G(d,p) basis set. The solvent effects have been considered by using the integral equation formalism variant (IEFPCM) model. NICS2BC were calculated with the B3LYP functional coupled with Grimme's D3[4] empirical dispersion correction and 6-311G(d,p) basis set. Nucleus independent chemical shifts (NICS) were calculated using the gauge including atomic orbitals (GIAO) method at the same level of theory. The bond current maps were generated using the BC-Wizard.[5]

Cartesian coordinates of the optimized ground-states (S_0)

S_o: 5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (**5a**)

E = -1473.83 Hartree

Symbol	X	Y	Z
C	-0.696132	-0.821044	-0.231599
C	0.716544	-0.740026	-0.175463
C	1.548990	-1.879442	-0.234299
N	1.335677	0.479233	-0.082879
C	0.674723	1.689353	-0.104058
C	2.717832	0.677957	-0.036079
C	1.648706	2.685858	-0.070997
C	2.910965	2.064011	-0.031643
H	1.445276	3.746150	-0.076407
H	3.870092	2.558564	-0.013500
C	2.974916	-1.718203	-0.156817
H	3.590029	-2.612099	-0.160724
C	3.566398	-0.482780	-0.051615
C	-1.492306	0.431611	-0.141244
C	-0.767721	1.693139	-0.137844
C	-2.889056	0.512981	-0.055526
C	-3.517520	1.799644	-0.048002
C	-2.690448	2.965493	-0.116362
N	-1.340089	2.890227	-0.139748
C	-3.787325	-0.676072	0.075387
C	-3.954393	-1.301515	1.318891

C	-4.512987	-1.161633	-1.021468
C	-4.806932	-2.396370	1.452743
H	-3.405762	-0.935001	2.181521
C	-5.360832	-2.260408	-0.880446
H	-4.400528	-0.687757	-1.992232
C	-5.524071	-2.897496	0.357284
H	-4.916043	-2.870122	2.424918
H	-5.903757	-2.628146	-1.747210
C	-4.928378	1.979259	0.032059
C	-5.482906	3.239460	0.017656
H	-6.560759	3.355001	0.076114
C	-4.658396	4.388873	-0.071070
H	-5.110864	5.375881	-0.083118
C	-3.291559	4.254649	-0.133521
H	-2.633535	5.115624	-0.190883
H	-5.569449	1.108773	0.100722
C	5.040907	-0.337700	0.031954
C	5.879736	-1.099887	-0.798720
C	5.642599	0.536091	0.952097
C	7.265118	-0.992550	-0.708648
H	5.439285	-1.763600	-1.536642
C	7.030289	0.636207	1.038731
H	5.021500	1.125457	1.618797
C	7.868369	-0.124951	0.213307
H	7.889089	-1.585628	-1.372468
H	7.469676	1.315677	1.764428
C	0.894227	-3.114338	-0.369121
H	1.480095	-4.031209	-0.409193
C	-1.187791	-2.128540	-0.410751
H	-2.246863	-2.302158	-0.522471
N	-0.427330	-3.235920	-0.472196
C	-6.465935	-4.067183	0.513459
H	-7.467350	-3.729082	0.807371
H	-6.571791	-4.622567	-0.422652
H	-6.118283	-4.759539	1.285587
C	9.371092	-0.032083	0.325032
H	9.680046	0.906788	0.792680

H	9.771945	-0.850382	0.935949
H	9.849802	-0.099582	-0.656674

S_o: *N*,*N*-dimethyl-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridin-11-amine (**5c**)

E = -1607.81 Hartree

Symbol	X	Y	Z
C	-0.101742	1.121894	-0.221066
C	-1.495422	0.873836	-0.166936
C	-2.456521	1.908986	-0.203223
N	-1.967565	-0.411122	-0.096678
C	-1.168945	-1.533383	-0.135824
C	-3.319015	-0.771771	-0.053162
C	-2.018386	-2.637817	-0.119088
C	-3.346603	-2.169777	-0.070857
H	-1.690789	-3.666260	-0.140444
H	-4.240334	-2.775012	-0.059910
C	-3.853943	1.580426	-0.128429
H	-4.569531	2.396098	-0.112729
C	-4.296284	0.282138	-0.046592
C	0.838564	-0.029193	-0.156197
C	0.264575	-1.364263	-0.167886
C	2.236914	0.055590	-0.084181
C	3.018464	-1.147655	-0.093253
C	2.323470	-2.395960	-0.163564
N	0.977381	-2.484593	-0.181994
C	2.990080	1.341748	0.046416
C	3.126250	1.959308	1.297574
C	3.626663	1.925745	-1.058446
C	3.854601	3.140897	1.431845
H	2.655271	1.513183	2.168675
C	4.349814	3.110132	-0.917866
H	3.547169	1.454412	-2.033754
C	4.472473	3.742872	0.327082
H	3.945366	3.602036	2.412012
H	4.828875	3.548263	-1.789718

C	4.434194	-1.149269	-0.022921
C	5.174263	-2.335002	-0.055357
C	4.453747	-3.574921	-0.131878
H	4.992829	-4.513782	-0.143468
C	3.085446	-3.596143	-0.183038
H	2.545291	-4.536211	-0.232479
H	4.941052	-0.199441	0.055093
C	-5.743500	-0.034883	0.040223
C	-6.672804	0.642052	-0.766854
C	-6.232015	-0.993557	0.943474
C	-8.035889	0.371416	-0.670693
H	-6.319680	1.369166	-1.491938
C	-7.597116	-1.257825	1.035890
H	-5.540408	-1.521140	1.592160
C	-8.525918	-0.581375	0.233501
H	-8.730442	0.902665	-1.316471
H	-7.947145	-2.000848	1.747961
C	-1.952063	3.214618	-0.312544
H	-2.642138	4.056592	-0.335866
C	0.231399	2.482589	-0.369697
H	1.262579	2.781992	-0.473526
N	-0.653800	3.493851	-0.409360
C	5.228248	5.042383	0.469236
H	6.031295	5.121011	-0.269313
H	4.563601	5.902178	0.319598
H	5.667868	5.142165	1.465834
C	-10.006200	-0.852371	0.354899
H	-10.199094	-1.872132	0.700031
H	-10.473747	-0.170632	1.076322
H	-10.518353	-0.711756	-0.601449
N	6.555343	-2.333387	-0.023710
C	7.291534	-3.580167	0.141411
H	8.359598	-3.363943	0.122018
H	7.063522	-4.085641	1.090693
H	7.083412	-4.279017	-0.676041
C	7.260599	-1.077560	0.181529
H	7.028279	-0.618717	1.153972

H	8.334507	-1.257512	0.135048
H	7.008040	-0.353387	-0.601280

S_o: 5,13-diphenylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (**5i**)

E = -1395.19 Hartree

Symbol	X	Y	Z
C	-0.514879	-1.016078	-0.183975
C	0.887306	-0.824942	-0.131763
C	1.804851	-1.898048	-0.166212
N	1.410033	0.440166	-0.067274
C	0.657649	1.594862	-0.112009
C	2.772561	0.746032	-0.027068
C	1.551741	2.664095	-0.101534
C	2.858363	2.142626	-0.051674
H	1.267031	3.705135	-0.128177
H	3.776479	2.710096	-0.044142
C	3.214241	-1.625605	-0.094591
H	3.896727	-2.469061	-0.078785
C	3.707482	-0.346077	-0.018176
C	-1.405559	0.172754	-0.118562
C	-0.780816	1.486453	-0.141518
C	-2.804163	0.147978	-0.031620
C	-3.530850	1.381493	-0.047166
C	-2.796271	2.606339	-0.138108
N	-1.444159	2.635245	-0.163720
C	-3.608394	-1.104299	0.126614
C	-3.731077	-1.702275	1.389332
C	-4.289992	-1.666244	-0.963296
C	-4.501762	-2.853949	1.553632
H	-3.216167	-1.266076	2.240057
C	-5.056673	-2.820945	-0.797295
H	-4.208497	-1.203879	-1.942481
H	-4.586007	-3.308836	2.536015
H	-5.572268	-3.251188	-1.650597
C	-4.951489	1.452725	0.031236
C	-5.601607	2.665878	-0.004728

H	-6.685165	2.698850	0.052619
C	-4.868315	3.873796	-0.114235
H	-5.395784	4.822474	-0.142737
C	-3.495223	3.844601	-0.176562
H	-2.905899	4.752763	-0.250005
H	-5.524162	0.537157	0.115606
C	5.167121	-0.085144	0.063072
C	6.060365	-0.794520	-0.757544
C	5.690123	0.847565	0.975411
C	7.435166	-0.579692	-0.667323
H	5.670025	-1.502436	-1.482240
C	7.065530	1.059943	1.065344
H	5.017598	1.390176	1.631618
H	8.109005	-1.132368	-1.315235
H	7.451772	1.778280	1.782363
C	1.247424	-3.182429	-0.273555
H	1.902280	-4.051980	-0.294773
C	-0.903950	-2.361005	-0.334347
H	-1.946259	-2.618084	-0.442148
N	-0.060723	-3.407679	-0.372668
C	7.942956	0.348714	0.244085
H	9.013366	0.517700	0.312517
C	-5.162108	-3.418909	0.460426
H	-5.758634	-4.316999	0.588415

S_o: 4,4'-(11-fluorindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine-5,13-diyl)bis(*N,N*-dimethylaniline) (**5k**)

E = -1762.38 Hartree

Symbol	X	Y	Z
C	-0.722862	-0.604255	-0.389556
C	0.690164	-0.605934	-0.311400
C	1.459685	-1.784555	-0.427947
N	1.374808	0.570100	-0.143863
C	0.781790	1.815768	-0.127800
C	2.764822	0.688032	-0.071740
C	1.808815	2.753841	-0.042875

C	3.033781	2.060463	-0.010528
H	1.665012	3.823398	-0.009366
H	4.018174	2.500096	0.037636
C	2.889299	-1.709406	-0.311354
H	3.451489	-2.636814	-0.348268
C	3.551488	-0.517172	-0.128761
C	-1.449934	0.681908	-0.228061
C	-0.657761	1.900431	-0.179095
C	-2.840948	0.825043	-0.121279
C	-3.399308	2.144931	-0.078920
C	-2.512015	3.267254	-0.127143
N	-1.167553	3.125269	-0.149080
C	-3.784340	-0.323576	0.009547
C	-3.869662	-1.045718	1.209144
C	-4.648877	-0.693842	-1.030783
C	-4.758522	-2.102752	1.362445
H	-3.226653	-0.775694	2.042154
C	-5.538655	-1.754826	-0.897997
H	-4.619900	-0.149627	-1.970698
C	-5.613510	-2.500140	0.304444
H	-4.788871	-2.619002	2.313592
H	-6.180062	-1.999017	-1.735298
C	-4.797160	2.389587	0.023768
C	-5.254173	3.681390	0.035617
C	-4.399773	4.800654	-0.038495
C	-3.044646	4.587501	-0.114346
H	-2.344711	5.414919	-0.158801
H	-5.502849	1.571620	0.086456
C	5.024992	-0.459908	-0.014478
C	5.844311	-1.273673	-0.816204
C	5.672577	0.377885	0.910217
C	7.228267	-1.260844	-0.706379
H	5.387924	-1.913308	-1.566173
C	7.055509	0.400385	1.037698
H	5.081754	1.010691	1.564726
C	7.879725	-0.427427	0.236355
H	7.805570	-1.893915	-1.368316

H	7.495432	1.062426	1.772725
C	0.737811	-2.967832	-0.656161
H	1.271280	-3.912923	-0.744880
C	-1.285050	-1.864181	-0.673033
H	-2.350079	-1.963327	-0.819563
N	-0.585888	-3.005729	-0.797833
N	-6.479302	-3.567578	0.438823
N	9.254509	-0.425978	0.371943
C	-6.649473	-4.200365	1.738512
H	-7.353454	-5.026958	1.642499
H	-5.702827	-4.612103	2.106332
H	-7.036454	-3.506349	2.499012
C	-7.455440	-3.840526	-0.605425
H	-8.028777	-4.726962	-0.334201
H	-8.159414	-3.008605	-0.754314
H	-6.964325	-4.043930	-1.563774
C	10.073234	-1.166503	-0.576969
H	9.971303	-0.793608	-1.606898
H	11.120398	-1.082331	-0.285985
H	9.813564	-2.230764	-0.575001
C	9.895680	0.580726	1.205650
H	9.554276	0.511187	2.244468
H	10.972678	0.413013	1.201188
H	9.705527	1.605054	0.853079
H	-4.825417	5.798043	-0.025404
F	-6.585072	3.910891	0.127015

S_o: 5,14-diphenylbenzo[j]naphtho[2,1,8-def][2,7]phenanthroline (**6)**

E = -1417.28 Hartree

Symbol	X	Y	Z
C	-1.371352	0.591479	-0.154293
C	-5.143237	-0.236516	0.110806
C	-5.691663	0.413067	1.230444
C	-6.019961	-0.815086	-0.821734
C	-7.073270	0.481700	1.409019
H	-5.030963	0.849807	1.973107

C	-7.402098	-0.744808	-0.643381
H	-5.611627	-1.311464	-1.697052
C	-7.933769	-0.095482	0.472197
H	-7.477155	0.981055	2.284813
H	-8.062614	-1.193805	-1.379346
H	-9.009240	-0.039607	0.611304
C	3.611828	-1.250520	0.205585
C	3.469055	-1.901135	1.440231
C	4.457623	-1.811170	-0.764098
C	4.141643	-3.097281	1.691547
H	2.825688	-1.469128	2.200767
C	5.125010	-3.011226	-0.512703
H	4.580043	-1.312548	-1.721032
C	4.967183	-3.658250	0.714675
H	4.020502	-3.590493	2.651353
H	5.768238	-3.438527	-1.276074
H	5.486918	-4.591283	0.909946
C	-2.408256	3.190767	-0.066705
H	-2.808869	4.199722	-0.046161
C	-1.027913	2.997530	-0.133512
H	-0.347459	3.839474	-0.154062
C	-3.275832	2.106974	-0.030569
H	-4.344936	2.277321	0.006934
C	-2.786257	0.786192	-0.063404
C	-3.668994	-0.371101	-0.064255
C	-3.130342	-1.615643	-0.244971
H	-3.780231	-2.485829	-0.263868
C	-0.496506	1.706459	-0.178244
C	0.961185	1.495535	-0.219789
C	0.574868	-0.968155	-0.374534
C	0.957415	-2.283953	-0.678561
H	1.994640	-2.522983	-0.859803
C	-1.182151	-3.102466	-0.614355
H	-1.846456	-3.963329	-0.680220
C	-1.722246	-1.825846	-0.382033
C	-0.827456	-0.728153	-0.286247
C	1.515139	0.160625	-0.210439

C	2.907025	0.047724	-0.035480
C	3.704679	1.232072	-0.010885
C	3.045574	2.494654	-0.150245
C	3.811953	3.694136	-0.173395
H	3.276496	4.630766	-0.289323
C	5.178150	3.650655	-0.038817
H	5.758855	4.567914	-0.054564
C	5.835641	2.405800	0.137160
H	6.913998	2.382472	0.260466
C	5.121497	1.230438	0.156897
H	5.638811	0.289088	0.294435
N	0.114628	-3.326823	-0.792975
N	1.701139	2.596435	-0.216610

S_o: 5,13-diphenylindolizino[6,5,4,3-ija]quinolino[2,3-c]quinoline (**7)**

E = -1379.16 Hartree

Symbol	X	Y	Z
C	-0.517709	-1.029364	-0.217404
C	0.891098	-0.849481	-0.158103
C	1.822505	-1.917998	-0.196846
N	1.414366	0.423925	-0.083323
C	0.662438	1.578391	-0.129378
C	2.772930	0.737663	-0.031290
C	1.552799	2.653102	-0.108327
C	2.857644	2.136638	-0.050053
H	1.262243	3.692622	-0.132308
H	3.775629	2.704206	-0.033368
C	3.228525	-1.625218	-0.111352
H	3.918084	-2.463258	-0.096822
C	3.715163	-0.345233	-0.021671
C	-1.402101	0.166361	-0.138240
C	-0.773870	1.477544	-0.162956
C	-2.800857	0.150631	-0.036332
C	-3.522719	1.388429	-0.050245
C	-2.783370	2.608930	-0.154100
N	-1.431715	2.630550	-0.186168

C	-3.618145	-1.091334	0.142470
C	-3.725254	-1.682143	1.410007
C	-4.334312	-1.645931	-0.929186
C	-4.513315	-2.818605	1.596566
H	-3.184259	-1.251790	2.247406
C	-5.118109	-2.785831	-0.741640
H	-4.266170	-1.189070	-1.912014
H	-4.585203	-3.266879	2.583050
H	-5.660418	-3.209571	-1.581628
C	-4.942174	1.468812	0.041944
C	-5.586898	2.685107	0.003758
H	-6.669750	2.723569	0.071459
C	-4.848817	3.888293	-0.121347
H	-5.371349	4.839719	-0.151735
C	-3.476433	3.850627	-0.195421
H	-2.882584	4.755014	-0.279522
H	-5.519813	0.557610	0.138341
C	5.172801	-0.077617	0.074501
C	6.077993	-0.776494	-0.742184
C	5.683626	0.851031	0.997984
C	7.451005	-0.556351	-0.637147
H	5.697947	-1.481247	-1.475448
C	7.057104	1.069479	1.102570
H	5.002111	1.386558	1.650763
H	8.133512	-1.101601	-1.282405
H	7.432882	1.784937	1.828092
C	1.318948	-3.224956	-0.320593
H	2.011711	-4.060613	-0.348229
C	-0.947218	-2.358513	-0.382508
H	-1.996241	-2.577819	-0.488674
C	-0.047930	-3.428875	-0.427927
H	-0.437145	-4.434634	-0.551617
C	-5.207510	-3.376513	0.520814
H	-5.818271	-4.262377	0.666156
C	7.946081	0.368043	0.285273
H	9.015015	0.541549	0.365130

S_o: indolizino[6,5,4,3-ija]quinolino[2,3-c][1,6]naphthyridine (**5´**)

E = -933.29 Hartree

Symbol	X	Y	Z
C	-0.835300	1.307174	0.000032
C	-1.965756	0.469853	0.000002
C	-3.278301	0.984379	-0.000030
N	-1.798269	-0.889174	-0.000002
C	-0.582688	-1.545502	0.000020
C	-2.846842	-1.807338	-0.000035
C	-0.861527	-2.909483	0.000018
C	-2.259497	-3.074065	-0.000032
H	-0.109029	-3.680783	0.000039
H	-2.799736	-4.007599	-0.000054
C	-4.384806	0.061898	-0.000062
H	-5.392214	0.460815	-0.000086
C	-4.170580	-1.284923	-0.000065
C	0.621187	-0.752503	0.000051
C	0.499111	0.690766	0.000063
H	-4.998419	-1.982998	-0.000091
C	-3.384377	2.384875	-0.000029
H	-4.368218	2.847008	-0.000053
C	-1.108419	2.680769	0.000026
H	-0.296527	3.400119	0.000039
N	-2.339051	3.207773	-0.000003
C	2.922989	0.765207	0.000026
C	2.924102	-0.667349	0.000033
C	5.348015	-0.647012	-0.000040
H	6.293827	-1.177037	-0.000079
C	5.346069	0.770722	-0.000068
H	6.288074	1.306756	-0.000119
N	1.781750	-1.390851	0.000084
C	1.673735	1.416192	0.000081
C	4.159737	1.461260	-0.000032
H	4.151265	2.546385	-0.000050
H	1.655486	2.500282	-0.000012
C	4.169319	-1.350522	0.000023

H	4.147455	-2.433566	0.000004

S_o: benzo[j]naphtho[2,1,8-def][2,7]phenanthroline (**6´**)

E = -955.38086

Symbol	X	Y	Z
C	-1.816986	0.731861	0.000020
C	-1.761139	3.528451	-0.000141
H	-1.732257	4.612197	-0.000231
C	-0.564958	2.809455	-0.000055
H	0.390330	3.316711	-0.000037
C	-2.981765	2.871497	-0.000120
H	-3.908024	3.436079	-0.000208
C	-3.036318	1.467562	-0.000017
C	-4.284158	0.755424	0.000041
C	-4.322695	-0.601708	0.000077
H	-5.270388	-1.129364	0.000139
C	-0.575502	1.414969	0.000020
C	0.674292	0.641970	0.000054
C	-0.674308	-1.475738	-0.000004
C	-0.821733	-2.865339	-0.000010
H	0.048235	-3.512710	-0.000110
C	-3.103772	-2.773164	0.000049
H	-4.047038	-3.314708	0.000086
C	-3.111454	-1.368081	0.000062
C	-1.860271	-0.699755	0.000038
C	0.624007	-0.796621	-0.000020
C	1.834497	-1.470544	-0.000092
C	3.050931	-0.769059	-0.000063
C	2.986207	0.660943	0.000075
C	4.198128	1.403921	0.000168
H	4.125882	2.484677	0.000295
C	5.407305	0.756883	0.000095
H	6.327993	1.329330	0.000176
C	5.470953	-0.661341	-0.000080
H	6.437657	-1.151599	-0.000157
C	4.320700	-1.407548	-0.000154

H	4.363311	-2.491783	-0.000276
N	-1.998290	-3.506651	-0.000022
N	1.811024	1.323635	0.000129
H	1.866749	-2.553460	-0.000150
H	-5.203352	1.331528	0.000058

S_o: indolizino[6,5,4,3-ija]quinolino[2,3-c]quinoline (**7´**)

E = -917.25 Hartree

Symbol	X	Y	Z
C	-0.837539	1.308314	-0.000314
C	-1.972614	0.468872	0.000071
C	-3.300181	0.960711	0.000206
N	-1.791859	-0.896872	0.000219
C	-0.572508	-1.545576	-0.000399
C	-2.827006	-1.827998	0.000536
C	-0.836178	-2.914269	-0.000435
C	-2.229092	-3.091820	0.000105
H	-0.073705	-3.675676	-0.000812
H	-2.763388	-4.028825	0.000226
C	-4.387531	0.014467	0.000640
H	-5.401087	0.397965	0.000762
C	0.498599	0.689597	-0.000045
C	0.626740	-0.752017	-0.000415
C	2.924729	0.769875	0.000507
C	2.930053	-0.662401	-0.000374
N	1.789955	-1.387988	-0.000692
C	4.159430	1.469491	0.001120
C	5.348325	0.783097	0.000768
H	6.288719	1.322054	0.001245
C	5.354493	-0.634702	-0.000204
H	6.301964	-1.161845	-0.000512
C	4.177767	-1.341522	-0.000756
H	4.158838	-2.424491	-0.001458
H	4.147554	2.554726	0.001834
C	-3.473741	2.354022	-0.000186
H	-4.478980	2.760136	-0.000048

C	-1.074583	2.688080	-0.000975
H	-0.242220	3.379838	-0.001759
C	-2.372977	3.198808	-0.000860
H	-2.519856	4.272607	-0.001327
C	-4.156610	-1.328504	0.000816
H	-4.974311	-2.038470	0.001089
C	1.672962	1.416137	0.000650
H	1.654569	2.500029	0.001328

Cartesian coordinates of the optimized excited-states (S_1)

S_1: 5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (**5a**)

E = -1473.75 Hartree

Symbol	X	Y	Z
C	-0.708756	-0.783012	-0.370260
C	0.702667	-0.726689	-0.297384
C	1.537153	-1.857501	-0.441815
N	1.321483	0.476831	-0.103472
C	0.649232	1.677811	-0.062833
C	2.698577	0.678485	-0.017222
C	1.631335	2.698831	0.056706
C	2.877281	2.095723	0.083905
H	1.411462	3.754722	0.107489
H	3.834585	2.592170	0.150616
C	2.943722	-1.692020	-0.325193
H	3.573152	-2.574325	-0.395629
C	3.547488	-0.444263	-0.099259
C	-1.494969	0.436177	-0.181559
C	-0.784694	1.685736	-0.131155
C	-2.921527	0.507736	-0.085965
C	-3.540383	1.805856	-0.082235
C	-2.703377	2.982790	-0.132636
N	-1.342957	2.905197	-0.115794
C	-3.778455	-0.692079	0.121134
C	-3.676219	-1.447570	1.302060
C	-4.728663	-1.102764	-0.832929

C	-4.478703	-2.572859	1.512944
H	-2.957506	-1.152183	2.062930
C	-5.525129	-2.228280	-0.620608
H	-4.827408	-0.544089	-1.760625
C	-5.417762	-2.986328	0.558112
H	-4.370251	-3.137660	2.436892
H	-6.239420	-2.526735	-1.385871
C	-4.943279	2.010499	0.007799
C	-5.498457	3.287848	-0.011303
H	-6.577849	3.401080	0.055083
C	-4.677096	4.426092	-0.108247
H	-5.116692	5.419881	-0.127496
C	-3.296586	4.268795	-0.159087
H	-2.632735	5.128069	-0.207645
H	-5.600334	1.152180	0.092198
C	5.016057	-0.320138	0.037742
C	5.876602	-1.018617	-0.829773
C	5.591550	0.475265	1.043928
C	7.259799	-0.914188	-0.697990
H	5.460729	-1.625172	-1.630059
C	6.977931	0.568784	1.173120
H	4.954086	1.000794	1.749370
C	7.838801	-0.121435	0.307088
H	7.901347	-1.452924	-1.391883
H	7.395885	1.184574	1.966204
C	0.885077	-3.090220	-0.699556
H	1.464609	-4.004439	-0.806569
C	-1.198853	-2.081256	-0.701605
H	-2.254670	-2.232924	-0.873788
N	-0.437384	-3.178288	-0.849762
C	-6.299379	-4.192243	0.789103
H	-7.335467	-3.892551	0.996335
H	-6.323622	-4.845079	-0.091686
H	-5.949649	-4.784947	1.640766
C	9.339063	-0.037812	0.460292
H	9.631660	0.822684	1.070383
H	9.734466	-0.939212	0.947393

H	9.835359	0.046980	-0.513124

S_1: *N*,*N*-dimethyl-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridin-11-amine (**5c**)

E = -1607.73 Hartree

Symbol	X	Y	Z
C	-0.084517	1.085984	-0.417698
C	-1.482560	0.858671	-0.327744
C	-2.446440	1.881279	-0.459429
N	-1.945937	-0.411305	-0.127024
C	-1.126936	-1.527909	-0.097757
C	-3.284267	-0.777998	-0.020559
C	-1.980977	-2.650515	0.036324
C	-3.294753	-2.196532	0.084197
H	-1.642312	-3.675166	0.087966
H	-4.184263	-2.804088	0.170177
C	-3.829163	1.545991	-0.321019
H	-4.558518	2.349197	-0.380307
C	-4.268797	0.246594	-0.092423
C	0.846590	-0.029464	-0.232102
C	0.285609	-1.366740	-0.182431
C	2.259266	0.073606	-0.121214
C	3.039824	-1.143742	-0.117874
C	2.355048	-2.408082	-0.189713
N	1.002210	-2.506533	-0.182006
C	2.964419	1.366172	0.102778
C	2.765182	2.089659	1.291949
C	3.865201	1.899538	-0.837954
C	3.424779	3.299639	1.521715
H	2.084152	1.699154	2.044568
C	4.521346	3.109870	-0.605811
H	4.038068	1.368576	-1.771214
C	4.311159	3.837743	0.576886
H	3.248069	3.832849	2.453963
H	5.204199	3.497553	-1.359765
C	4.440852	-1.158398	-0.009016

C	5.197923	-2.360052	-0.034391
C	4.503633	-3.600098	-0.163044
H	5.041034	-4.539465	-0.196284
C	3.122396	-3.602334	-0.226829
H	2.581381	-4.542351	-0.297849
H	4.956411	-0.214831	0.095640
C	-5.711587	-0.064502	0.054434
C	-6.659256	0.507433	-0.812458
C	-6.180224	-0.914901	1.072494
C	-8.020869	0.237699	-0.665692
H	-6.326734	1.150557	-1.623356
C	-7.542814	-1.177965	1.214903
H	-5.476979	-1.355282	1.774029
C	-8.490819	-0.607322	0.350878
H	-8.728464	0.685942	-1.359997
H	-7.875110	-1.834670	2.016354
C	-1.948533	3.178185	-0.729580
H	-2.633510	4.016686	-0.836429
C	0.244627	2.432451	-0.750335
H	1.274369	2.711735	-0.922308
N	-0.644370	3.426077	-0.895488
C	4.998860	5.163645	0.809707
H	6.033982	5.147828	0.449441
H	4.483573	5.975181	0.278051
H	5.011928	5.425269	1.873173
C	-9.967289	-0.876605	0.527128
H	-10.150420	-1.907180	0.851153
H	-10.400156	-0.214898	1.289706
H	-10.518399	-0.707661	-0.403961
N	6.566304	-2.322157	0.068338
C	7.340428	-3.559277	0.045845
H	8.398860	-3.321042	0.143923
H	7.054979	-4.219887	0.874254
H	7.192953	-4.101187	-0.896942
C	7.273444	-1.051634	0.205133
H	6.967387	-0.521969	1.115749
H	8.343816	-1.245584	0.264065

H	7.087548	-0.398396	-0.656327

S_1: 4,4'-(11-fluorindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine-5,13-diyl)bis(*N,N*-dimethylaniline) (**5k**)

E = -1762.31 Hartree

Symbol	X	Y	Z
C	-0.708962	-0.551678	-0.480672
C	0.706496	-0.559902	-0.418551
C	1.480846	-1.729440	-0.602466
N	1.382348	0.606619	-0.201498
C	0.765262	1.838175	-0.130933
C	2.773728	0.742860	-0.128887
C	1.785344	2.800222	-0.012760
C	3.014437	2.133699	-0.016104
H	1.622528	3.865673	0.057075
H	3.989923	2.596447	0.030716
C	2.895612	-1.639960	-0.503273
H	3.470098	-2.556573	-0.593191
C	3.565870	-0.432847	-0.240403
C	-1.439998	0.695859	-0.253504
C	-0.676104	1.910035	-0.177157
C	-2.863700	0.819840	-0.140152
C	-3.427977	2.136115	-0.083084
C	-2.547893	3.280972	-0.108179
N	-1.186597	3.145925	-0.118352
C	-3.774777	-0.348211	0.019099
C	-3.757323	-1.133130	1.185193
C	-4.721761	-0.697432	-0.958642
C	-4.616424	-2.216438	1.364067
H	-3.054822	-0.888940	1.979230
C	-5.587275	-1.778253	-0.801726
H	-4.779947	-0.114004	-1.874983
C	-5.551616	-2.582804	0.365089
H	-4.553666	-2.776077	2.290127
H	-6.290767	-1.993408	-1.597592
C	-4.824811	2.383496	0.030020

C	-5.290800	3.684701	0.057371
C	-4.466928	4.806220	-0.005823
C	-3.089859	4.584971	-0.081813
H	-2.398256	5.422399	-0.109910
H	-5.533265	1.566207	0.090997
C	5.018703	-0.421986	-0.061500
C	5.854054	-1.298991	-0.794953
C	5.651872	0.448689	0.856559
C	7.228466	-1.290441	-0.652192
H	5.416671	-1.973222	-1.525245
C	7.023971	0.461258	1.024731
H	5.047912	1.098816	1.480928
C	7.864999	-0.400778	0.262175
H	7.818651	-1.965482	-1.259292
H	7.450549	1.127486	1.764018
C	0.770381	-2.922035	-0.881086
H	1.306072	-3.859314	-1.016340
C	-1.260117	-1.814279	-0.842878
H	-2.323085	-1.907996	-1.012389
N	-0.556176	-2.945530	-1.022467
N	-6.386338	-3.683611	0.514973
N	9.221520	-0.381896	0.408290
C	-6.503167	-4.310287	1.825833
H	-7.181692	-5.162011	1.752068
H	-5.533562	-4.689039	2.167108
H	-6.893068	-3.619955	2.591951
C	-7.499166	-3.858605	-0.409986
H	-8.030291	-4.777492	-0.155466
H	-8.215475	-3.021295	-0.374606
H	-7.140260	-3.959469	-1.440013
C	10.061569	-1.305670	-0.352284
H	9.953472	-1.142214	-1.431425
H	11.104163	-1.140703	-0.083629
H	9.808085	-2.348753	-0.127763
C	9.855446	0.550238	1.339384
H	9.554833	0.346398	2.374781
H	10.936915	0.441476	1.268488

H	9.597107	1.587392	1.095982
H	-4.889876	5.805231	0.017221
F	-6.648070	3.882532	0.159051

TD-DFT calculations

*Calculated TD-DFT transitions of compound **5a** at B3LYP/6-31+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	*f*	Configuration	CI coefficent
S_1	2.6490	468.04	0.2388	HOMO → LUMO	0.96875
S_2	3.2153	385.61	0.0385	HOMO → LUMO+1	0.65070
				HOMO → LUMO+2	0.22908
S_3	3.3892	365.82	0.0024	HOMO-2 → LUMO	0.30006
				HOMO-1 → LUMO	-0.41862
				HOMO → LUMO+1	-0.15248
				HOMO → LUMO+2	0.43751
S_4	3.5515	349.11	0.2832	HOMO-3 → LUMO	-0.14844
				HOMO-2 → LUMO	0.17587
				HOMO-1 → LUMO	0.53739
				HOMO → LUMO+2	0.36715

*Calculated TD-DFT transitions of compound **5c** at B3LYP/6-31+G(d,p) level (IEFPCM).*

S_n	E (eV)	λ (nm)	*f*	Configuration	CI coefficent
S_1	2.4433	507.45	0.2953	HOMO → LUMO	0.70022
S_2	3.0007	413.18	0.0165	HOMO-1 → LUMO	-0.14216
				HOMO-1 → LUMO+2	0.11581
				HOMO → LUMO+1	0.66492
				HOMO → LUMO+2	0.10556
S_3	3.0987	400.12	0.0124	HOMO-1 → LUMO	0.68343
				HOMO → LUMO+1	0.13660
S_4	3.3446	370.69	0.1809	HOMO-2 → LUMO	-0.33396
				HOMO → LUMO+1	-0.10178
				HOMO → LUMO+2	0.60089

*Calculated TD-DFT transitions of compound **5k** at B3LYP/6-31+G(d,p) level (IEFPCM).*

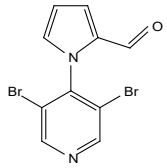
S_n	E (eV)	λ (nm)	*f*	Configuration	CI coefficent
S_1	2.4735	501.26	0.0774	HOMO-1 → LUMO	0.22514
				HOMO → LUMO	0.65804

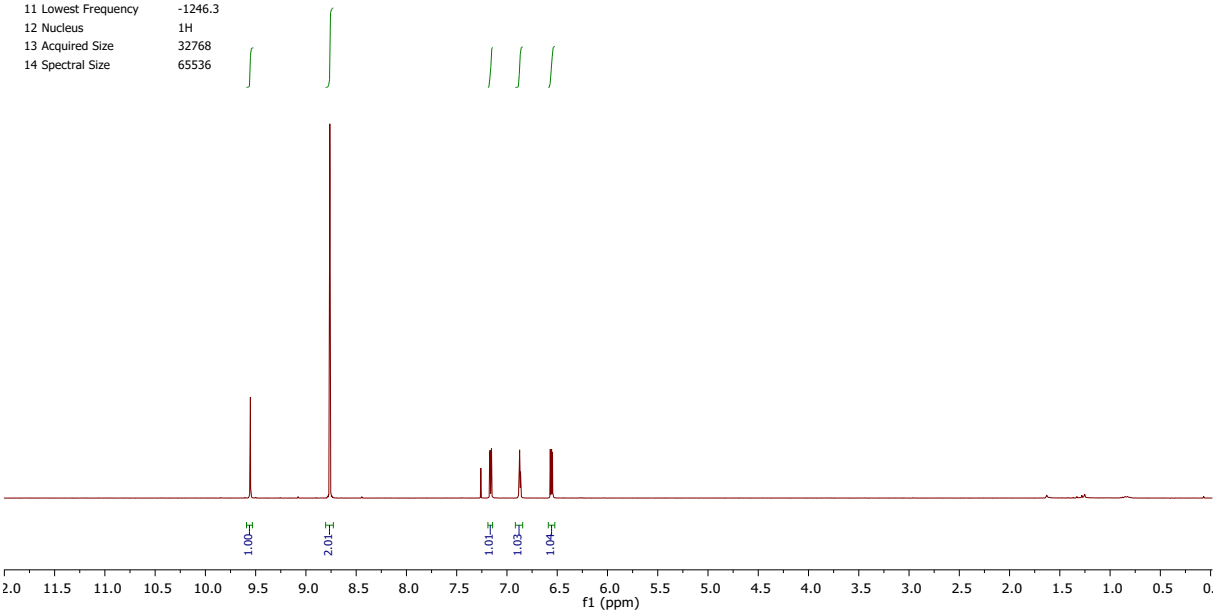
S_2	2.5462	486.93	0.0742	HOMO-1 → LUMO	0.66692
				HOMO → LUMO	-0.22012
S_3	2.8240	439.03	0.2604	HOMO-2 → LUMO	0.69059
				HOMO → LUMO	0.10885
S_4	3.1871	389.02	0.1266	HOMO-2 → LUMO+1	-0.22829
				HOMO → LUMO+1	0.63678
				HOMO → LUMO+2	0.10078

1H-, 13C- and 19F-NMR Spectra

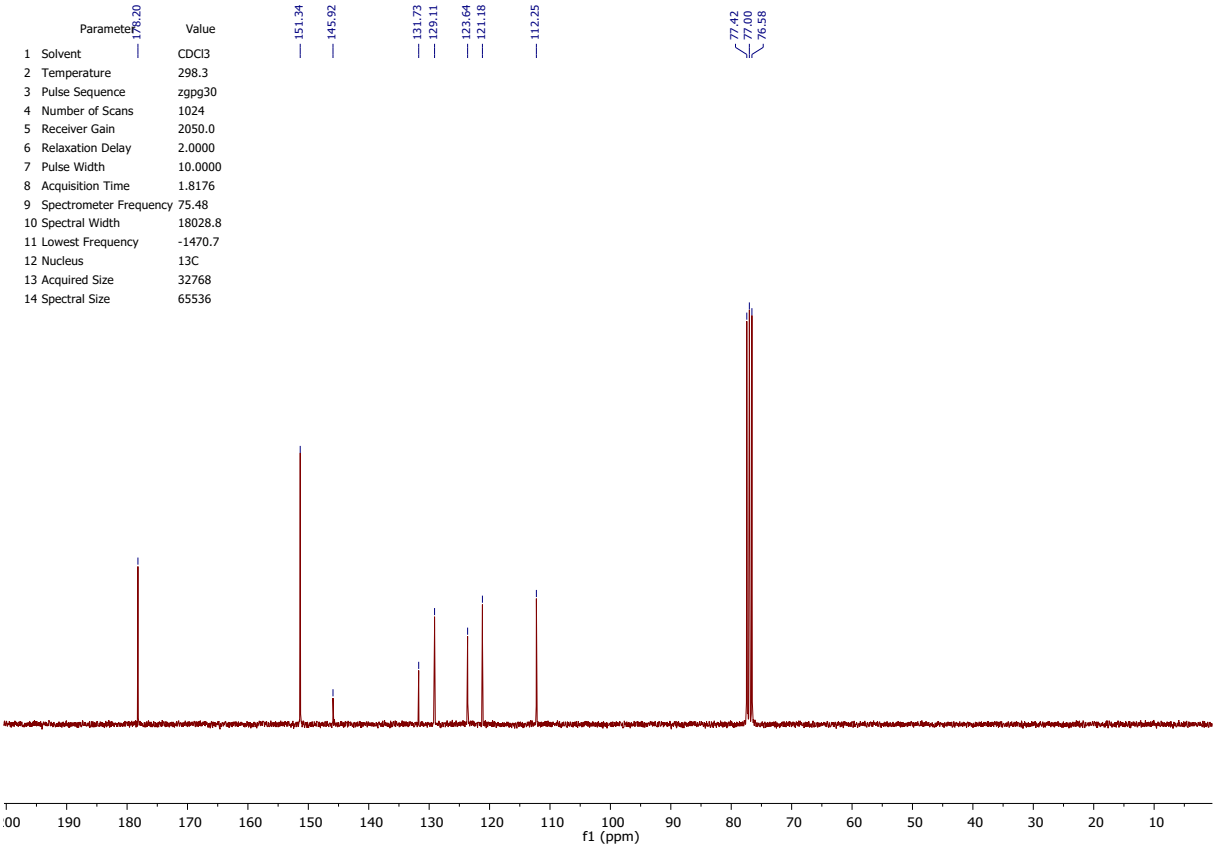
1-(3,5-Dibromopyridin-4-yl)-1*H*-pyrrol-2-carbaldehyd (2a)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362.0
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



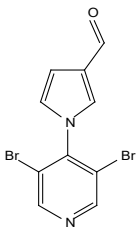


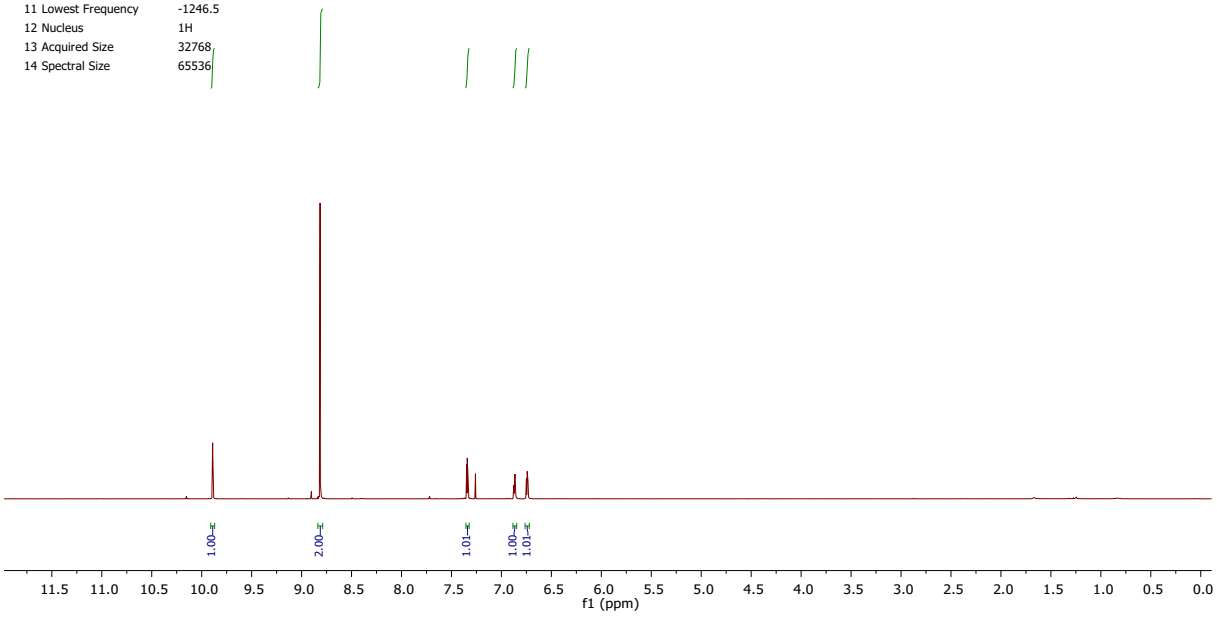
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.3
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1470.7
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

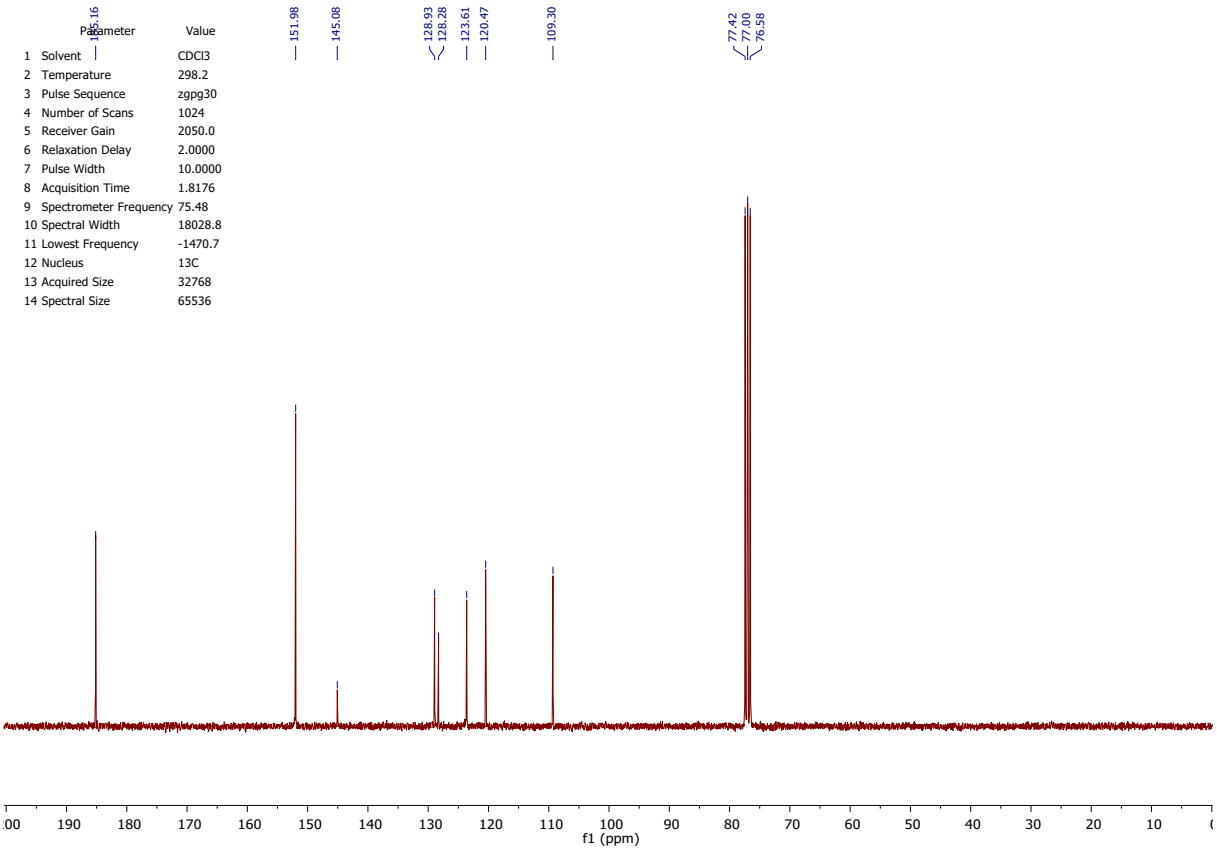


1-(3,5-Dibromopyridin-4-yl)-1*H*-pyrrol-3-carbaldehyd (2b)

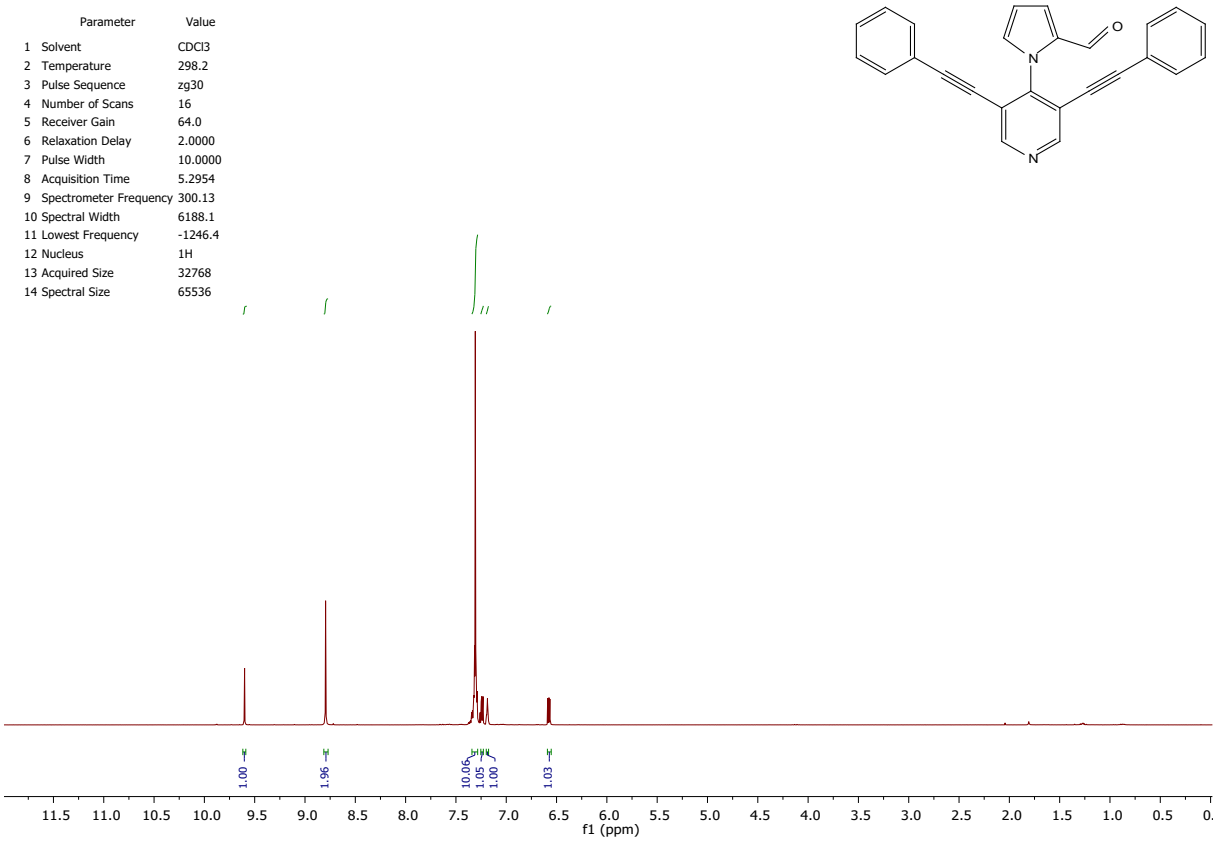
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	362.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.5
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

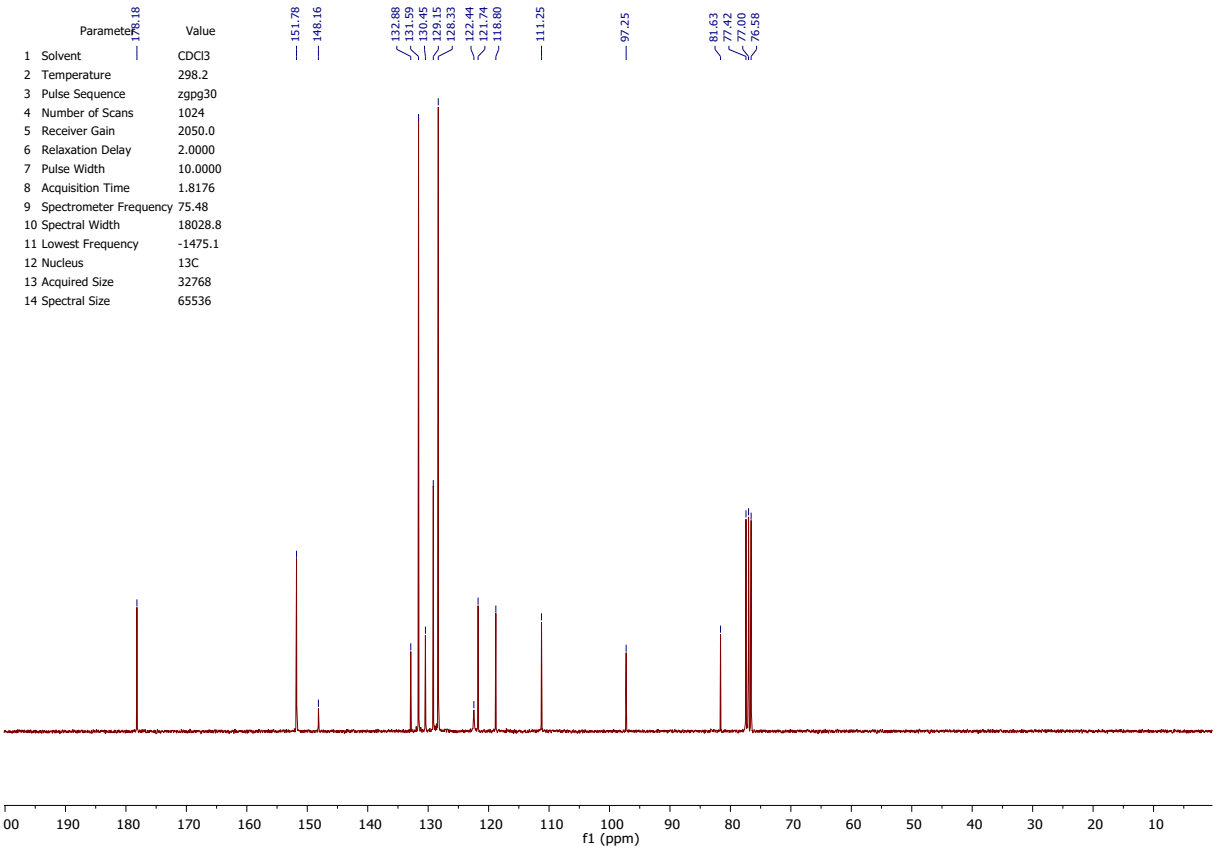






1-(3,5-bis(phenylethynyl)pyridin-4-yl)-1*H*-pyrrole-2-carbaldehyde (3a)

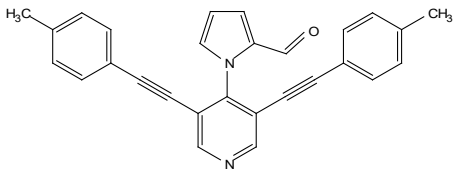


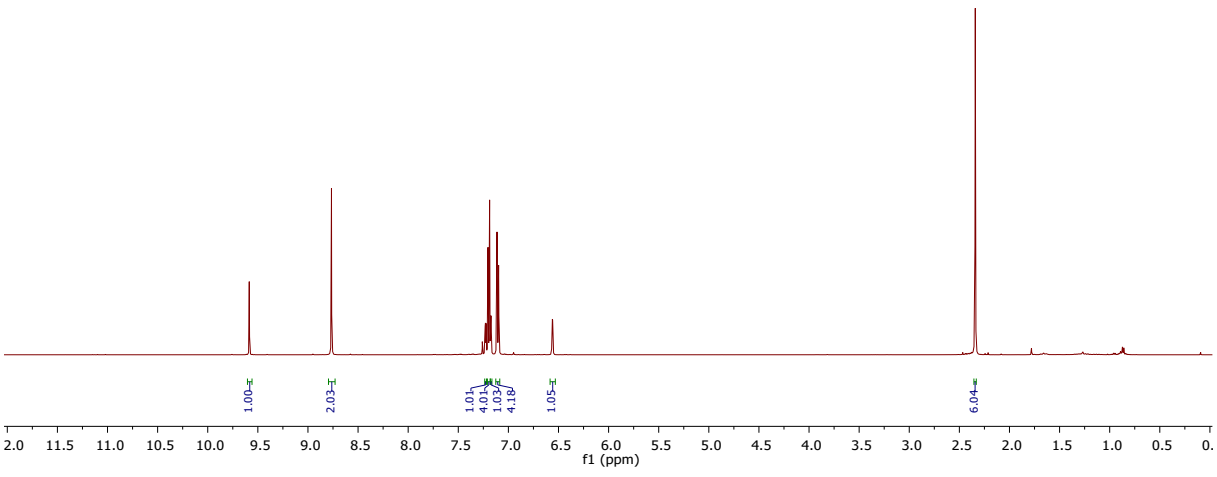


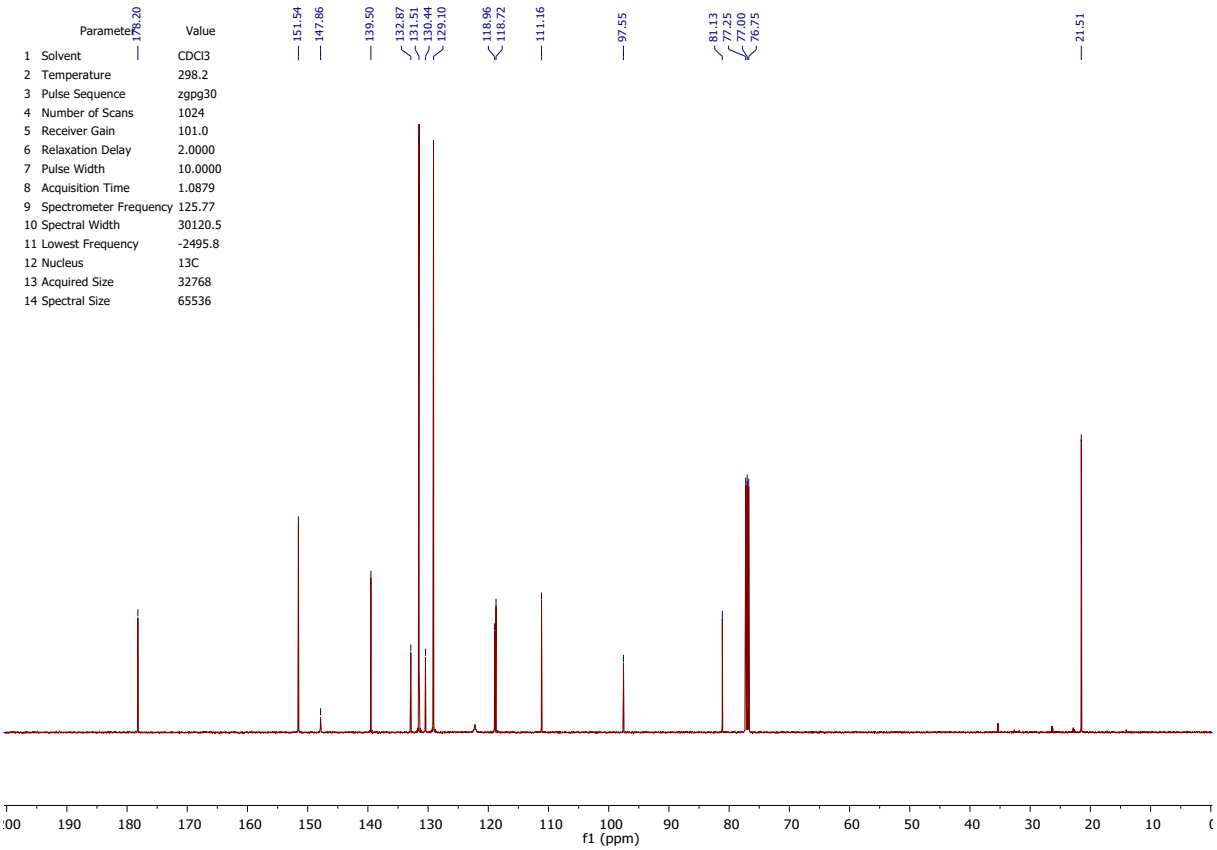
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zgpg30
4 Number of Scans	1024
5 Receiver Gain	2050.0
6 Relaxation Delay	2.0000
7 Pulse Width	10.0000
8 Acquisition Time	1.8176
9 Spectrometer Frequency	75.48
10 Spectral Width	18028.8
11 Lowest Frequency	-1475.1
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

1-(3,5-bis(*p*-tolylethynyl)pyridin-4-yl)-1*H*-pyrrole-2-carbaldehyde (3b)

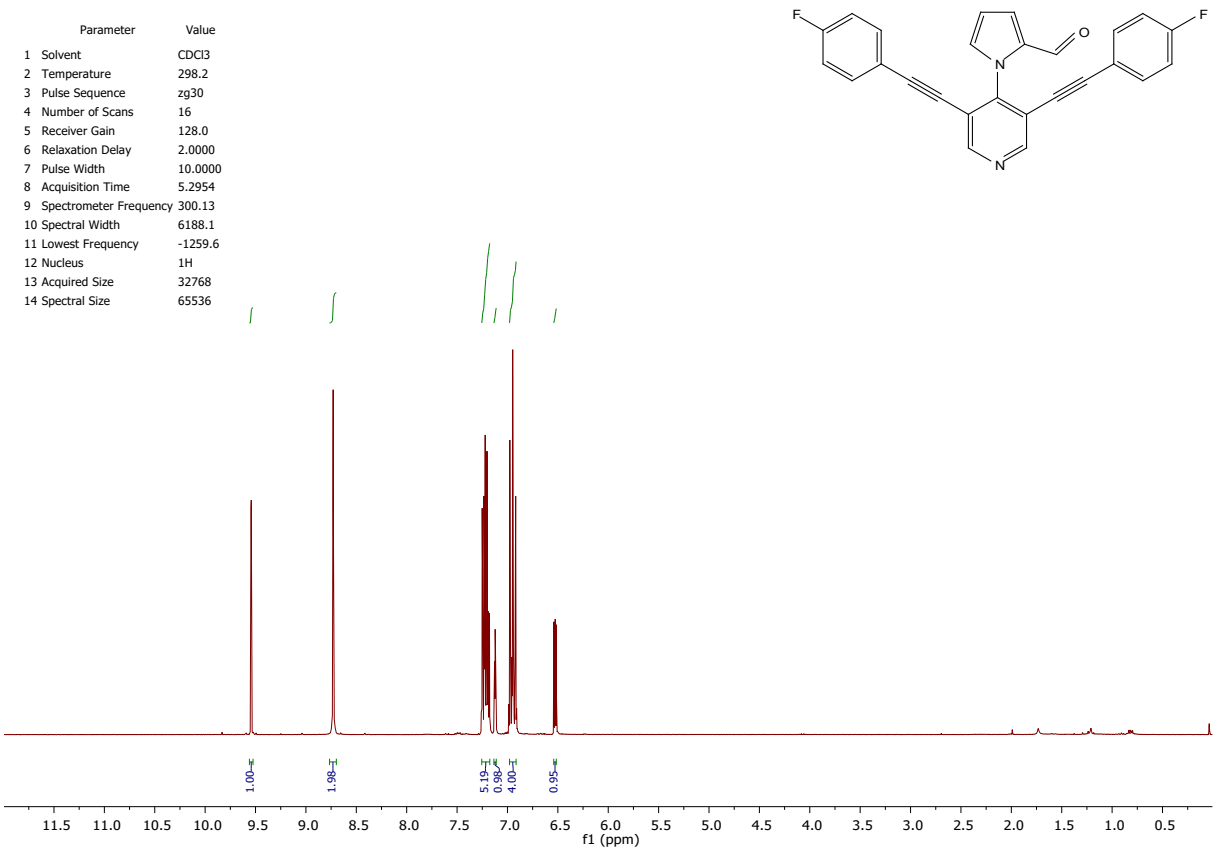
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.1
3 Pulse Sequence	zg30
4 Number of Scans	16
5 Receiver Gain	101.0
6 Relaxation Delay	1.0000
7 Pulse Width	8.0000
8 Acquisition Time	3.2768
9 Spectrometer Frequency	500.13
10 Spectral Width	10000.0
11 Lowest Frequency	-1923.8
12 Nucleus	1H
13 Acquired Size	32768
14 Spectral Size	65536



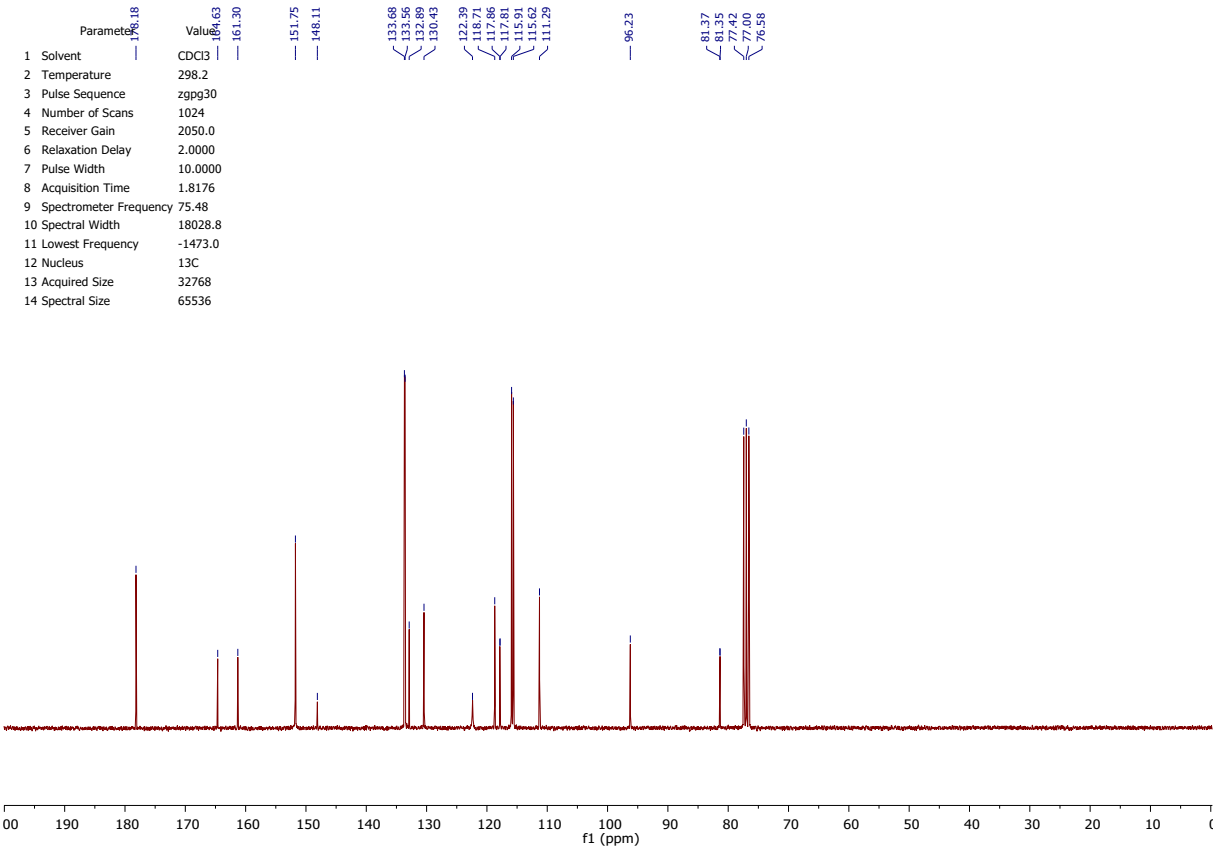




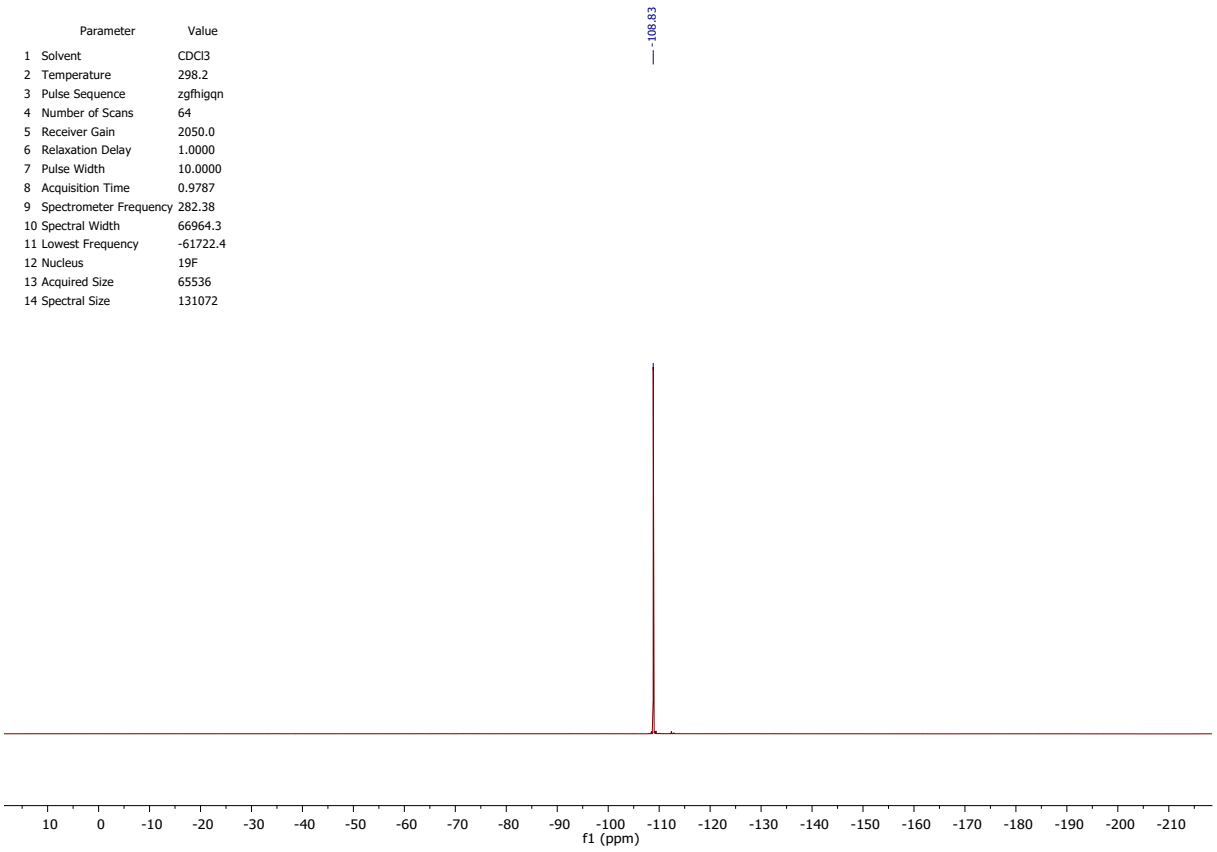
1-(3,5-bis((4-fluorphenyl)ethynyl)pyridin-4-yl)-1*H*-pyrrole-2-carbaldehyde (3c)



	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1473.0
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

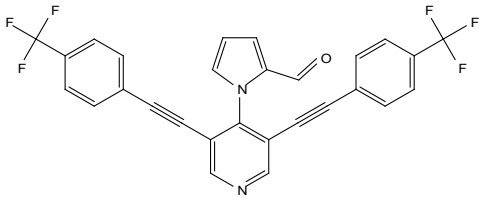


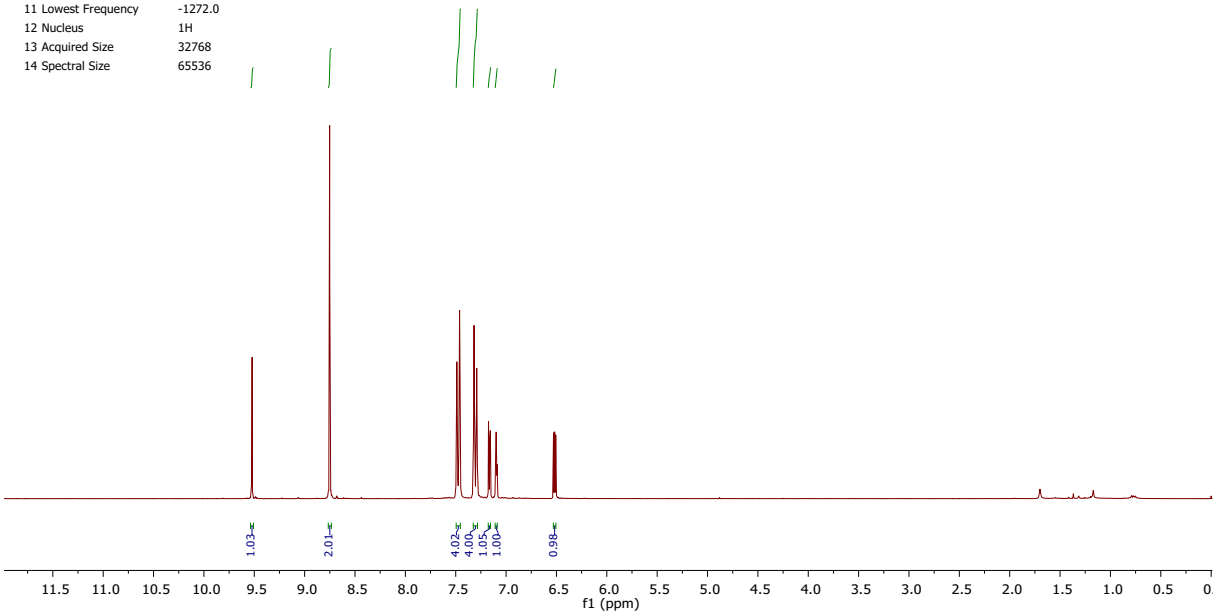
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



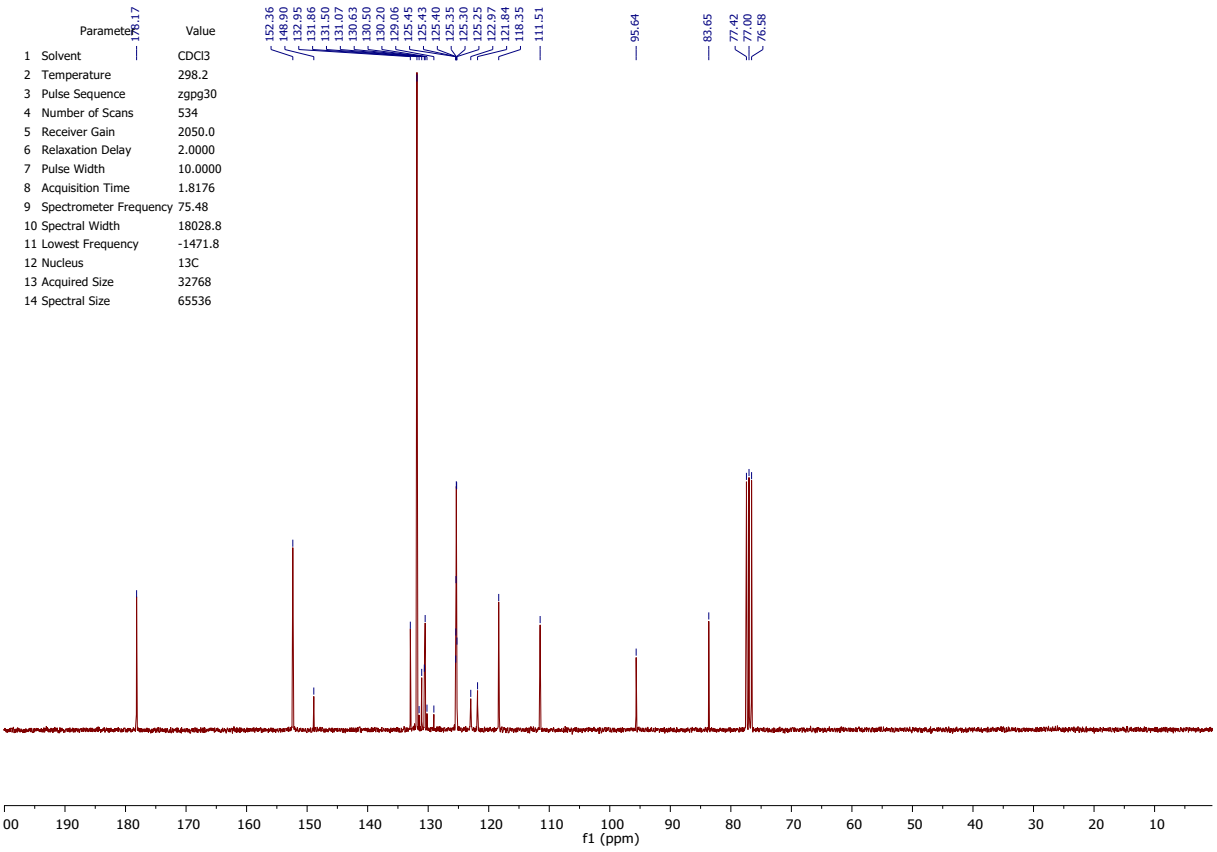
1-(3,5-bis((4-(trifluoromethyl)phenyl)ethynyl)pyridin-4-yl)-1*H*-pyrrole-2-carbaldehyde (3d)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	71.8
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	-1272.0
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

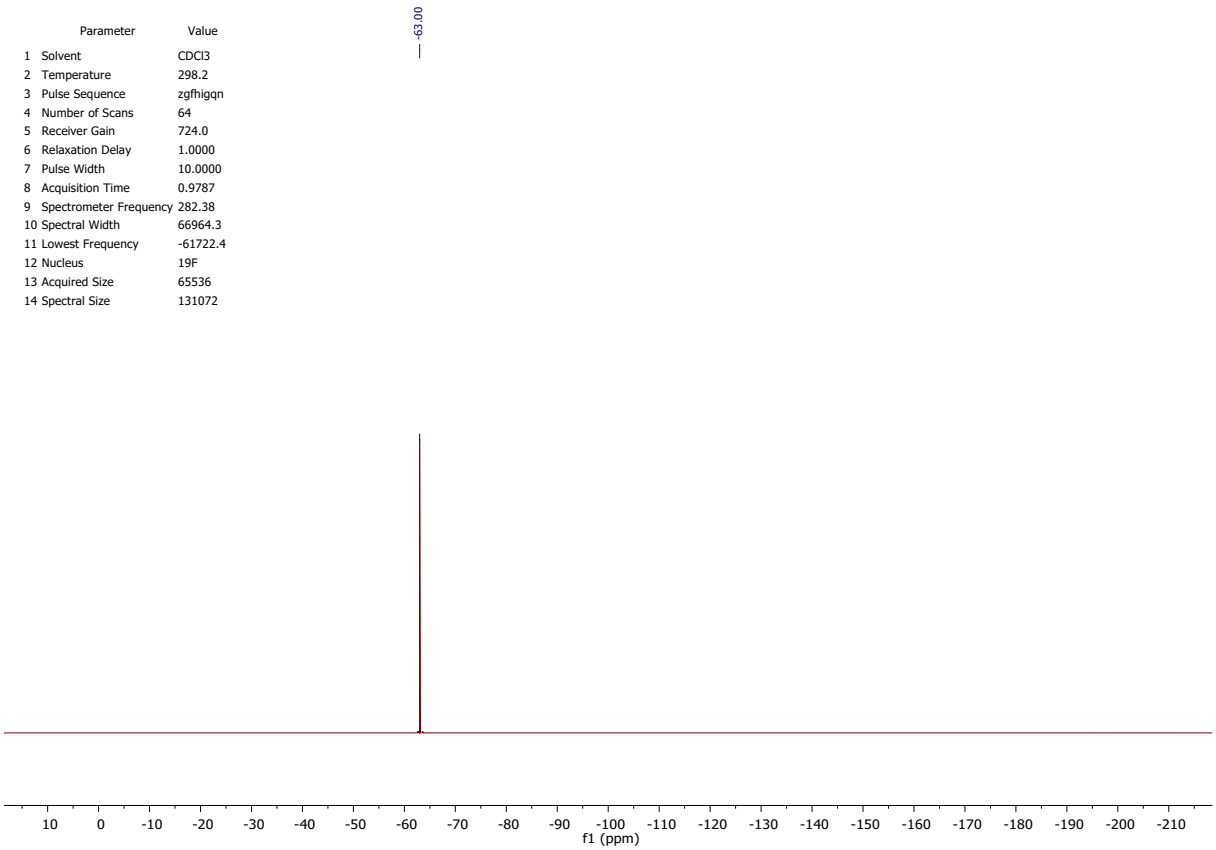




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	534
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1471.8
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

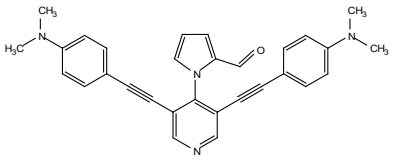


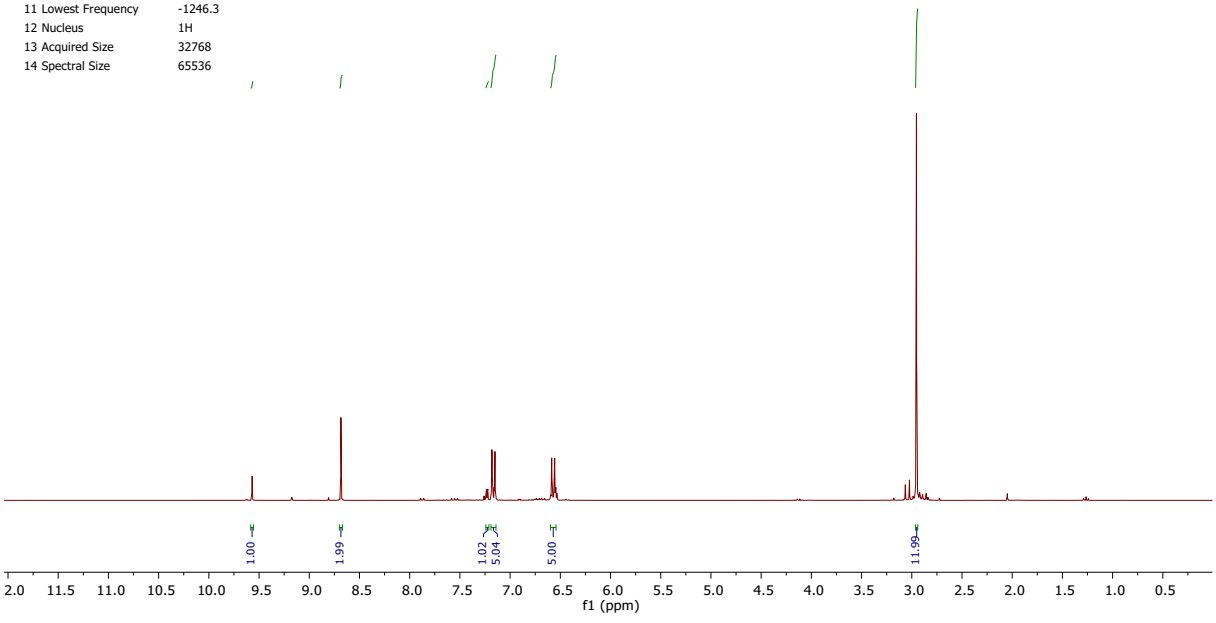
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	724.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



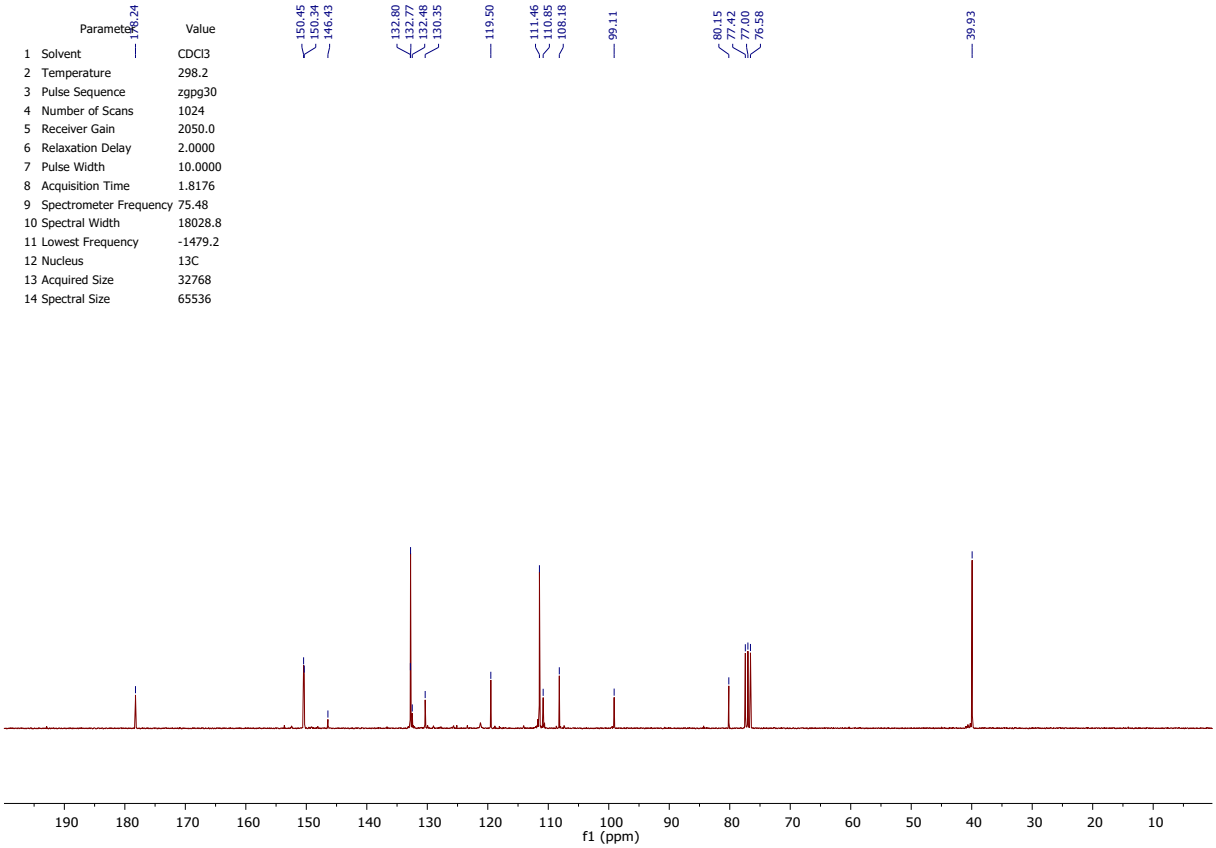
1-(3,5-bis((4-(dimethylamino)phenyl)ethynyl)pyridin-4-yl)-1*H*-pyrrole-2-carbaldehyde (3e)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	45.2
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



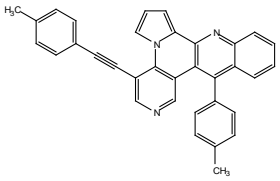


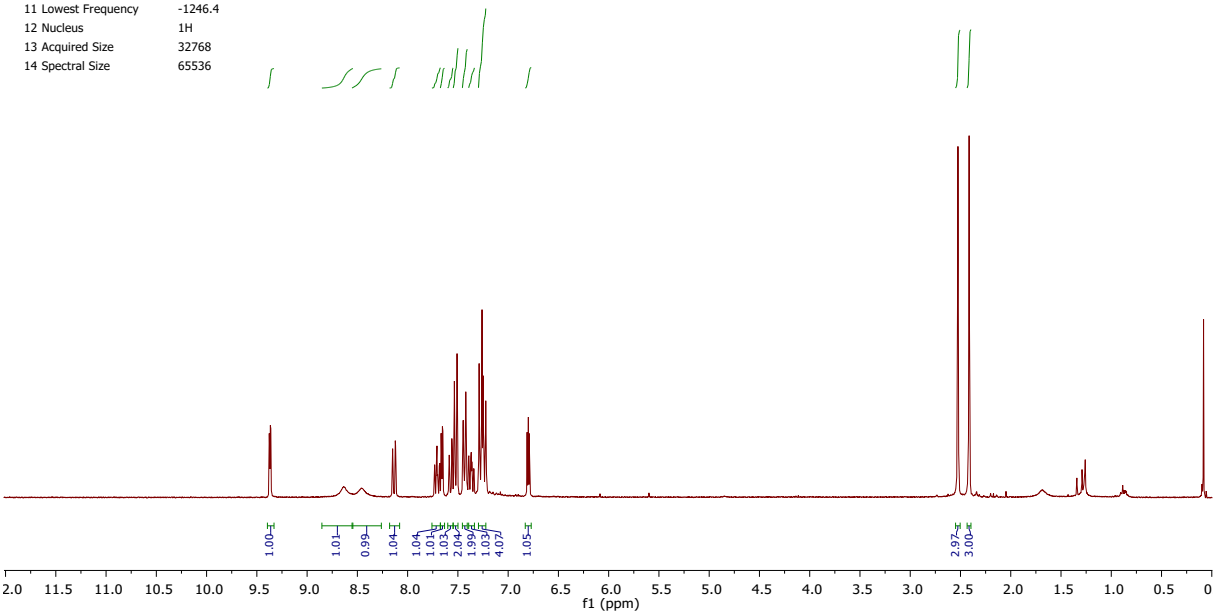
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1479.2
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



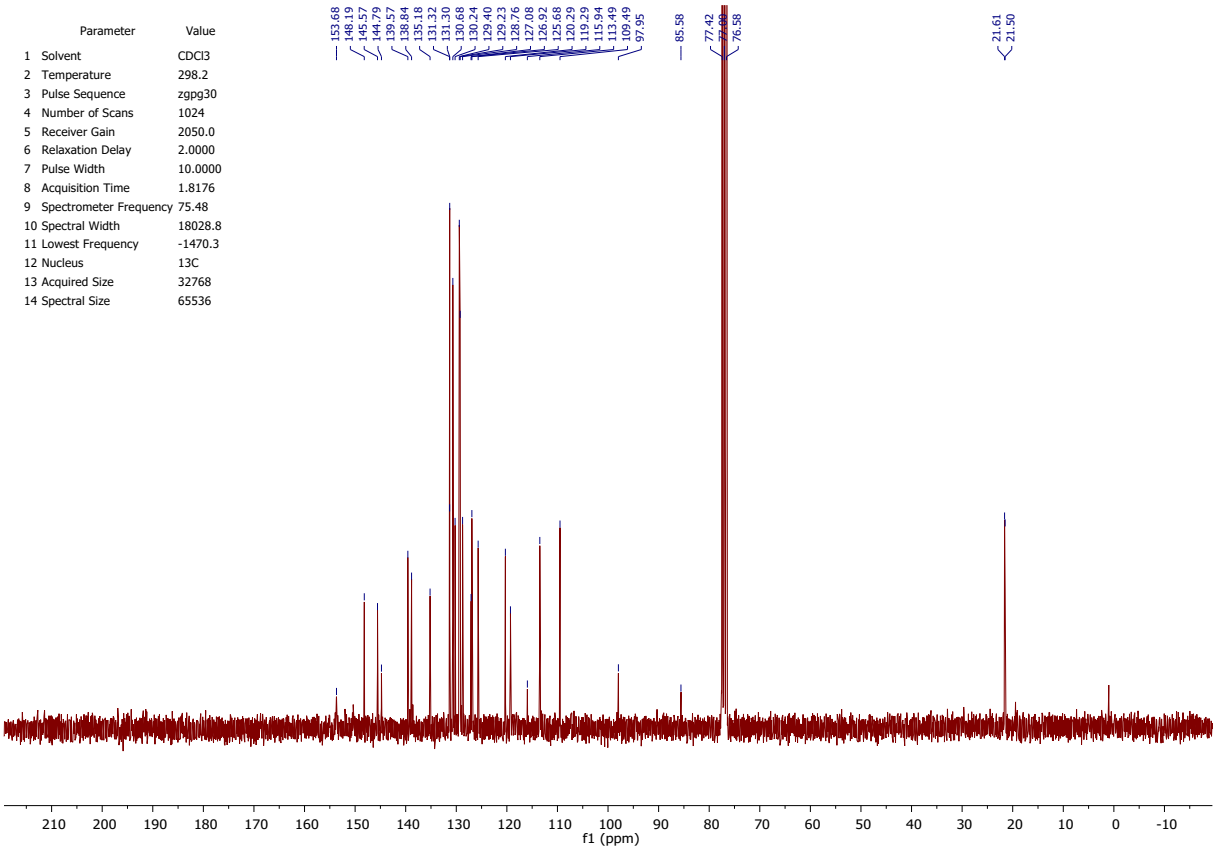
14-(*p*-Tolyl)-4-(*p*-tolylethinyl)pyrrolo[1,2-*a*]chinolino[2,3-*c*][1,6]naphthyridin (4)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	203.0
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



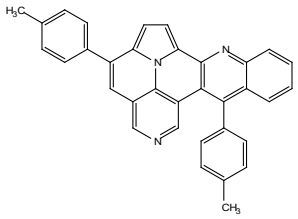


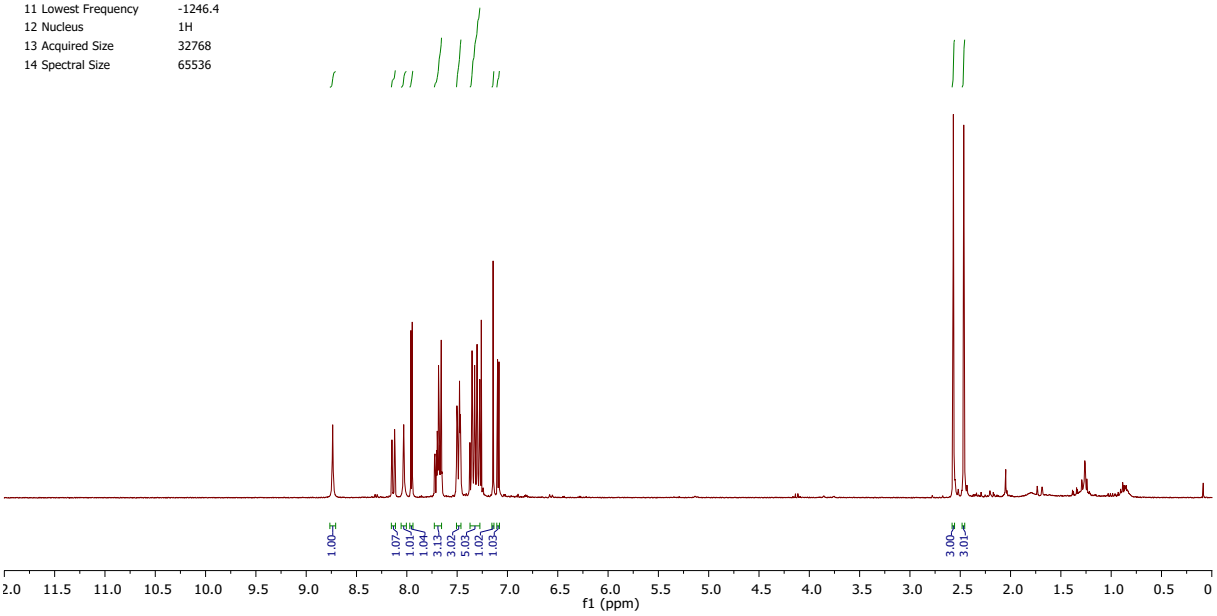
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1470.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



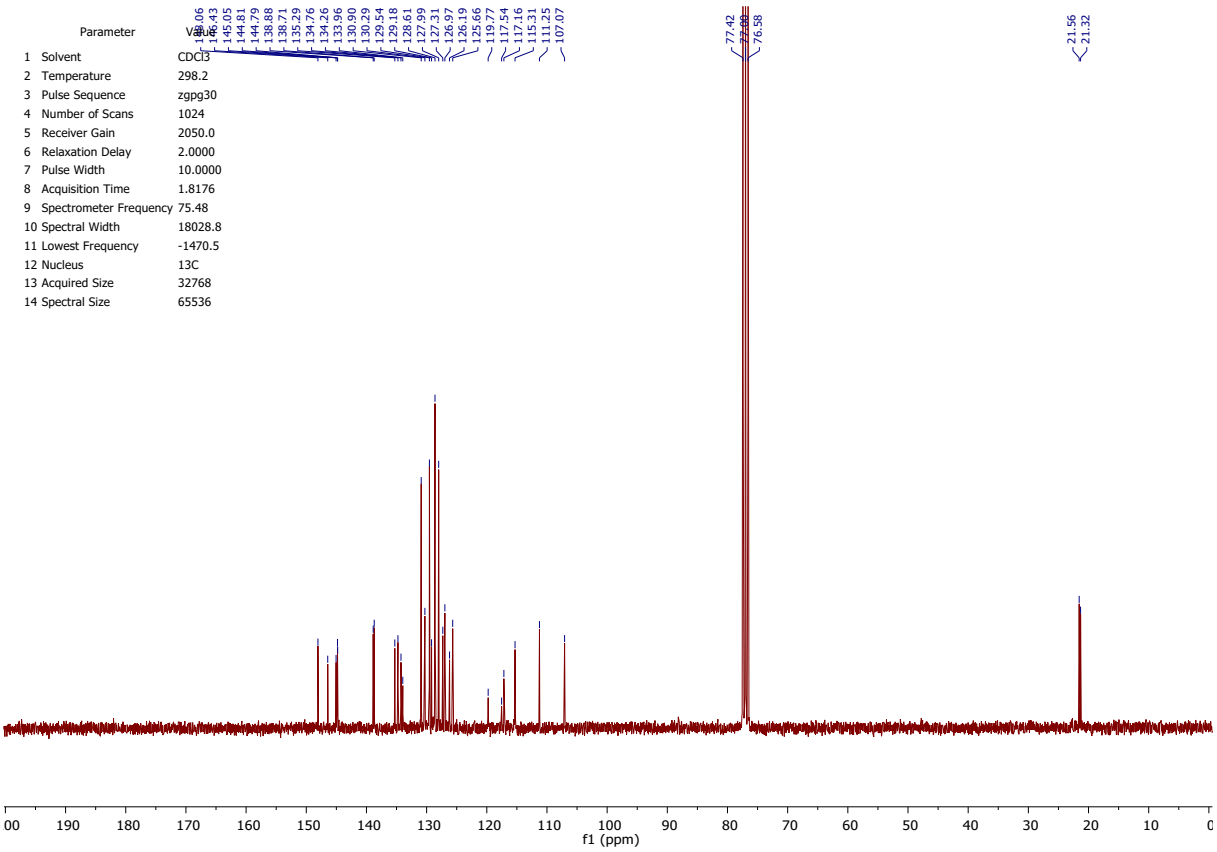
5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5a)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	181.0
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



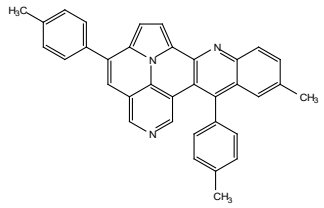


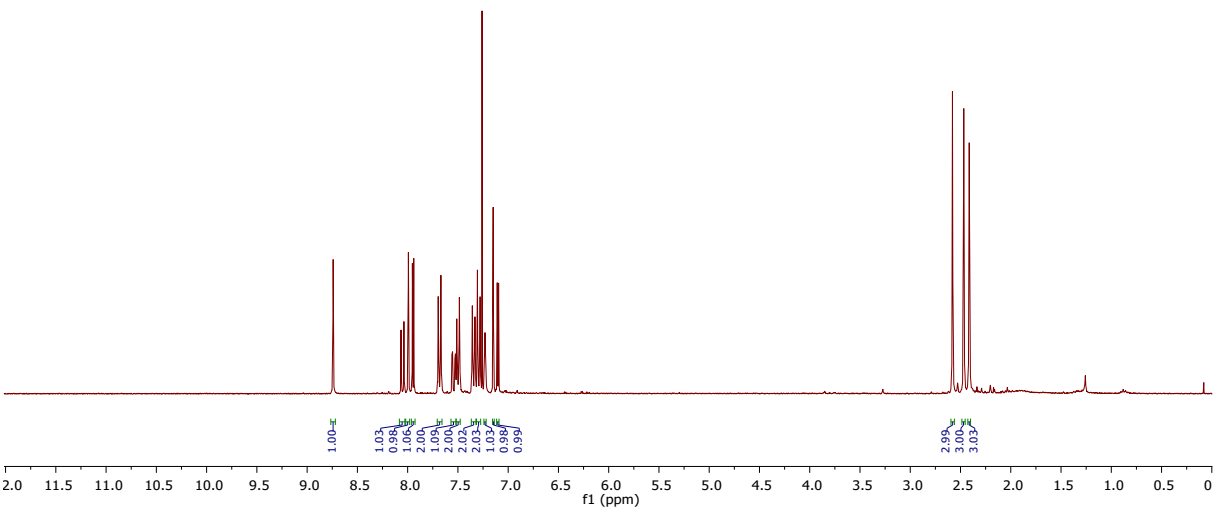
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1470.5
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



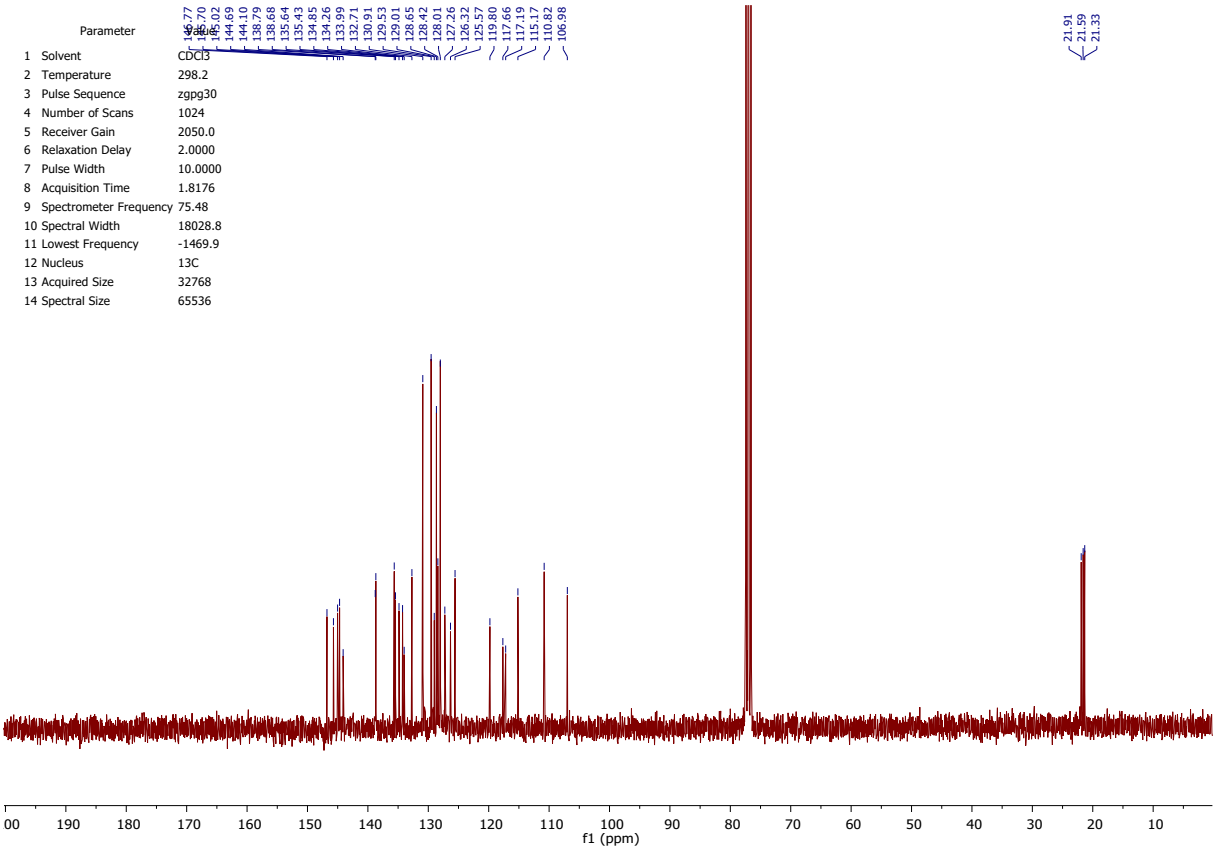
11-methyl-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5b)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	256.0
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



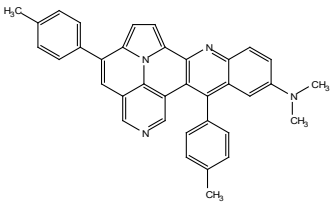


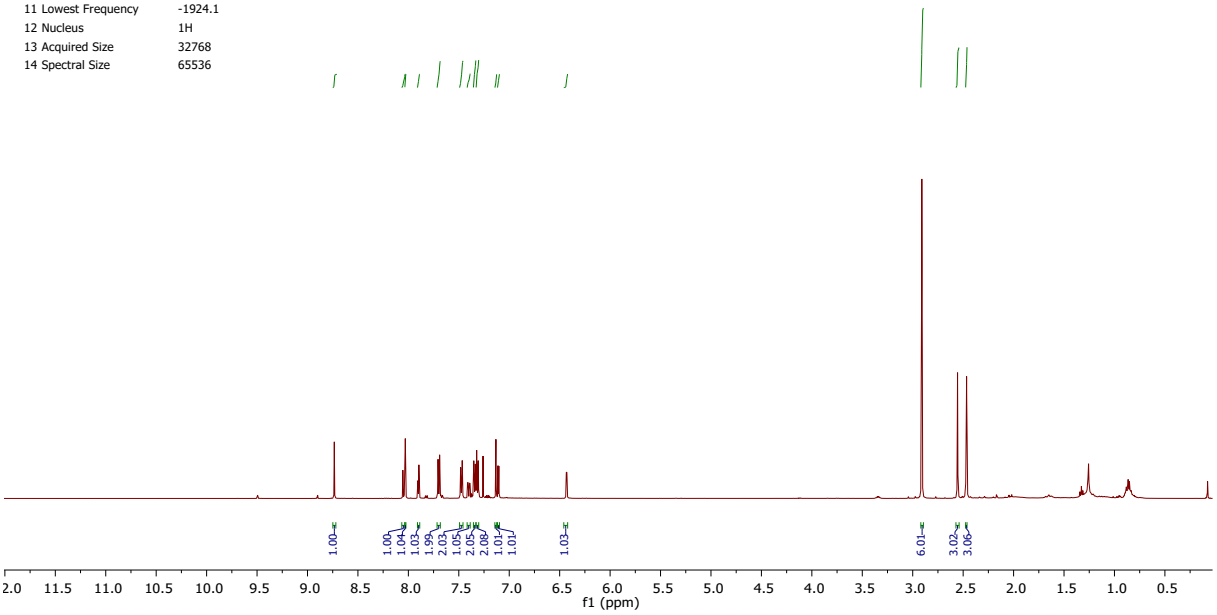
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1469.9
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

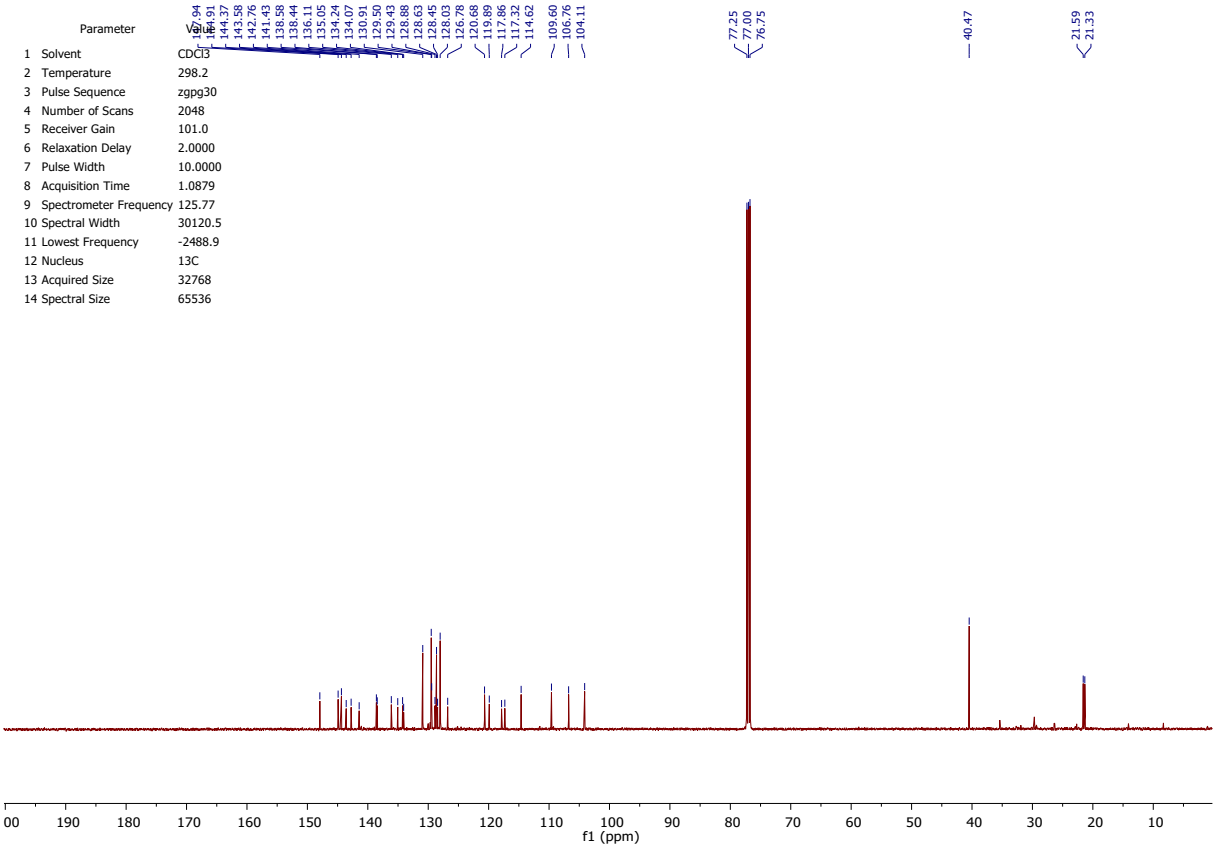


N,*N*-dimethyl-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridin-11-amine (5c)

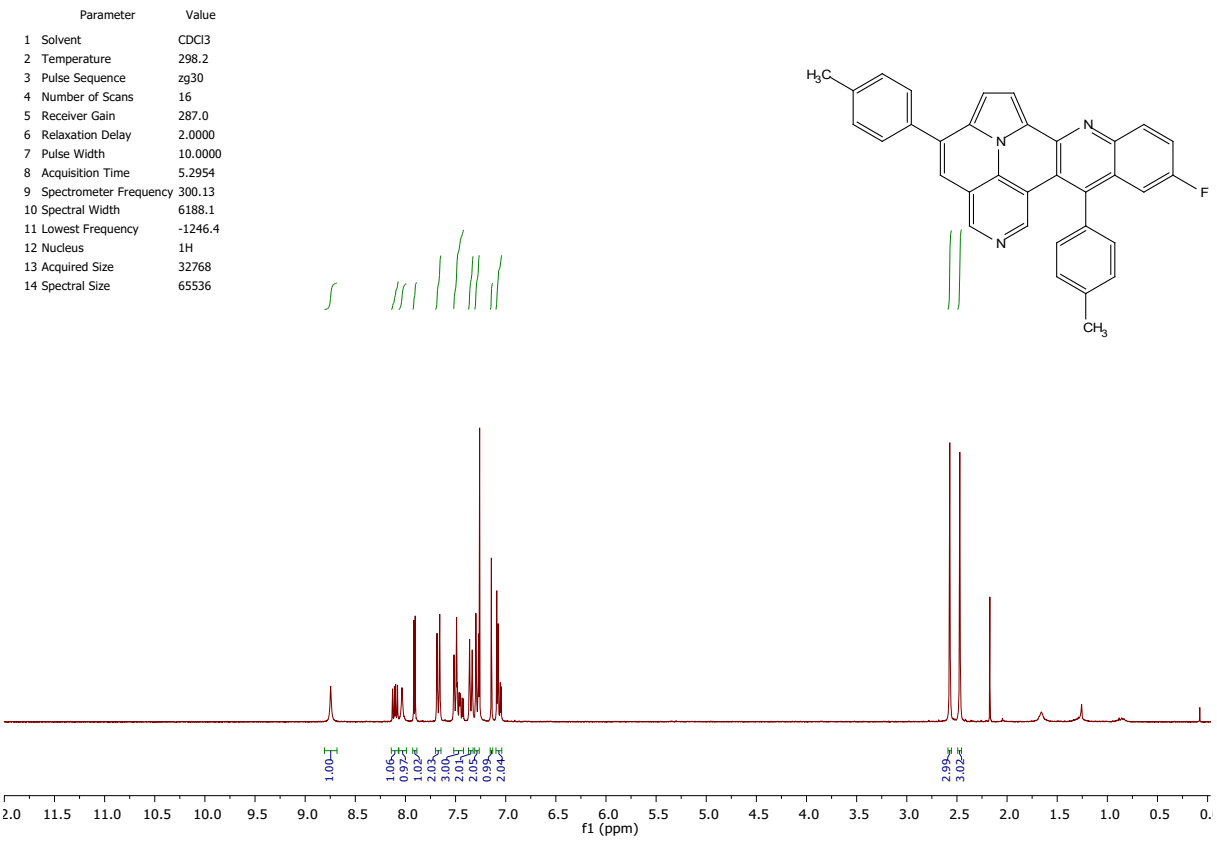
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	32
5	Receiver Gain	101.0
6	Relaxation Delay	1.0000
7	Pulse Width	8.0000
8	Acquisition Time	3.2768
9	Spectrometer Frequency	500.13
10	Spectral Width	10000.0
11	Lowest Frequency	-1924.1
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

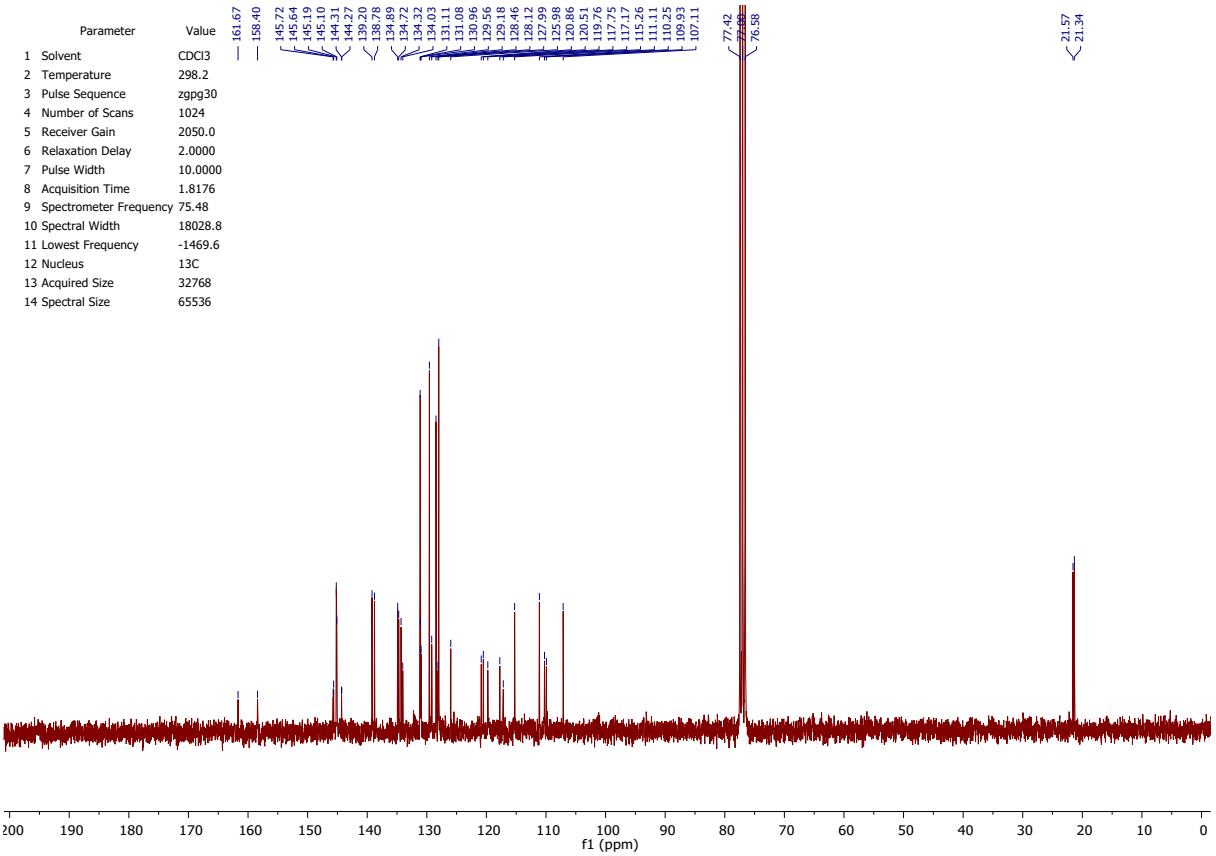


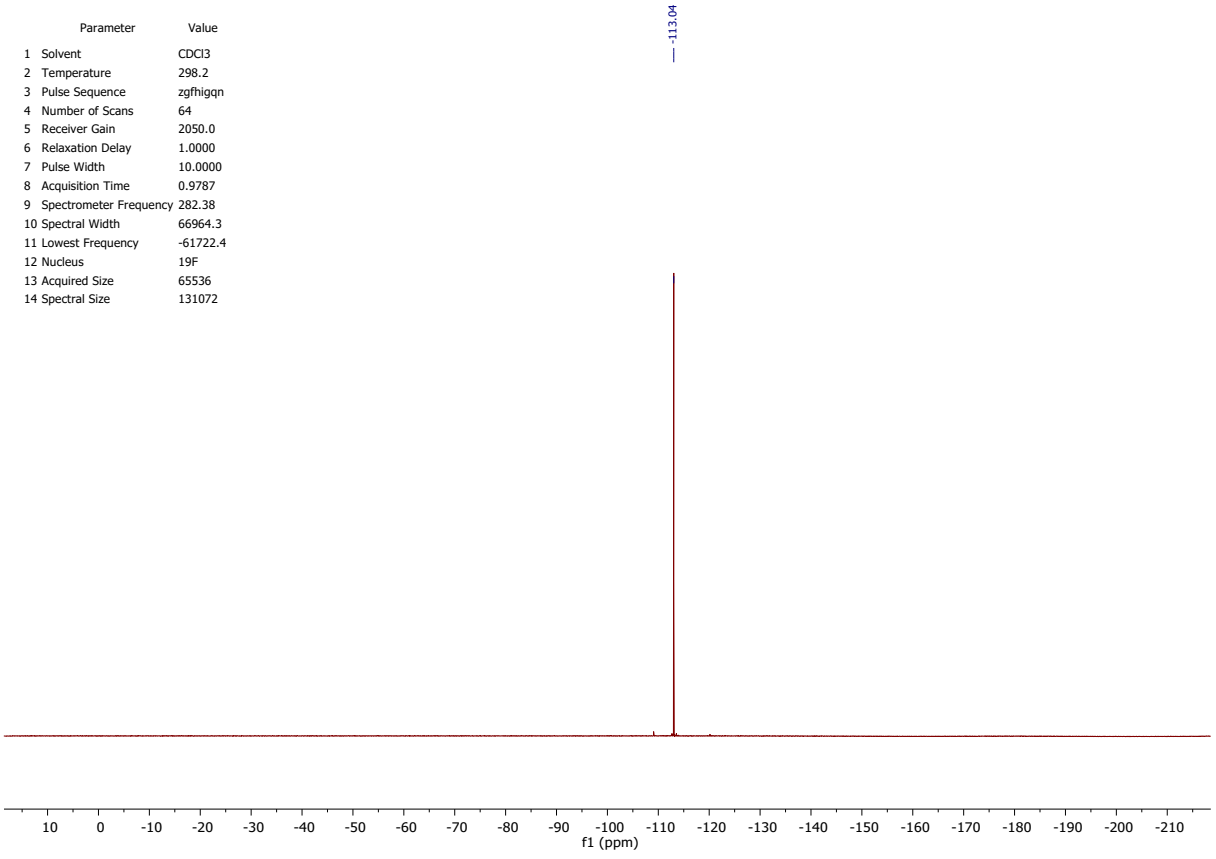




11-fluoro-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5d)

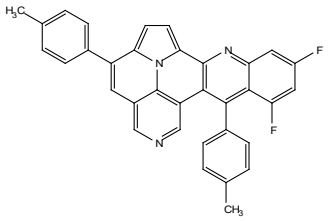


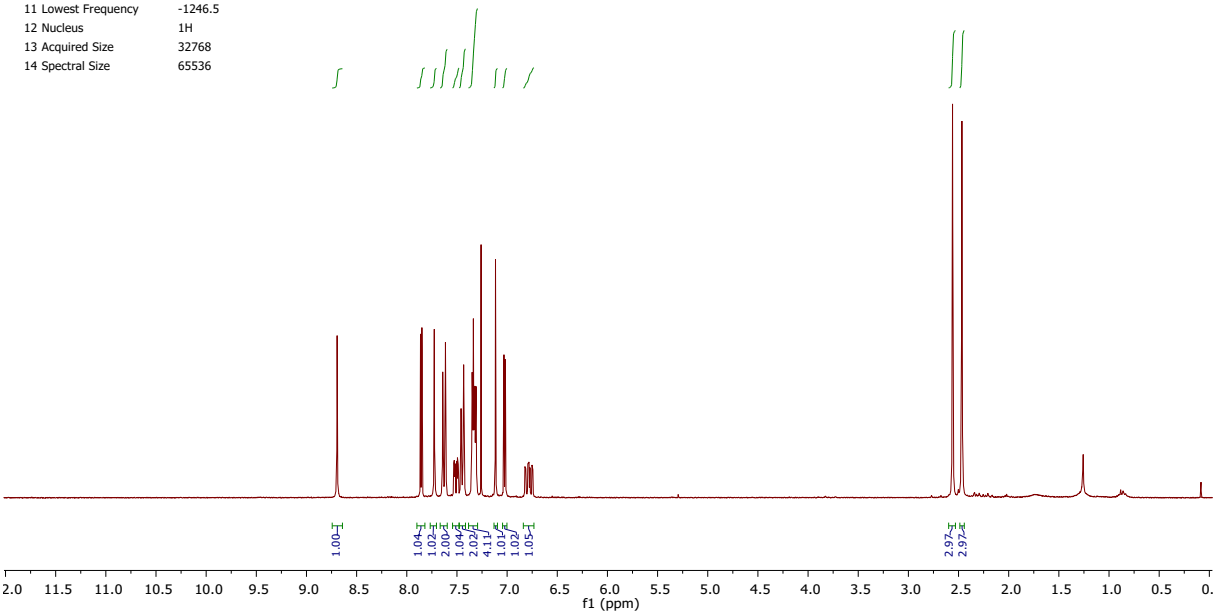




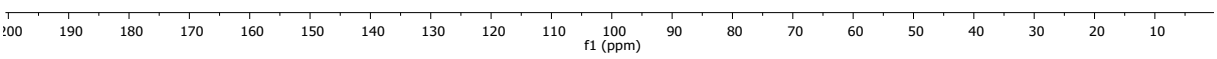
10,12-difluor-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5e)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	203.0
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	-1246.5
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536

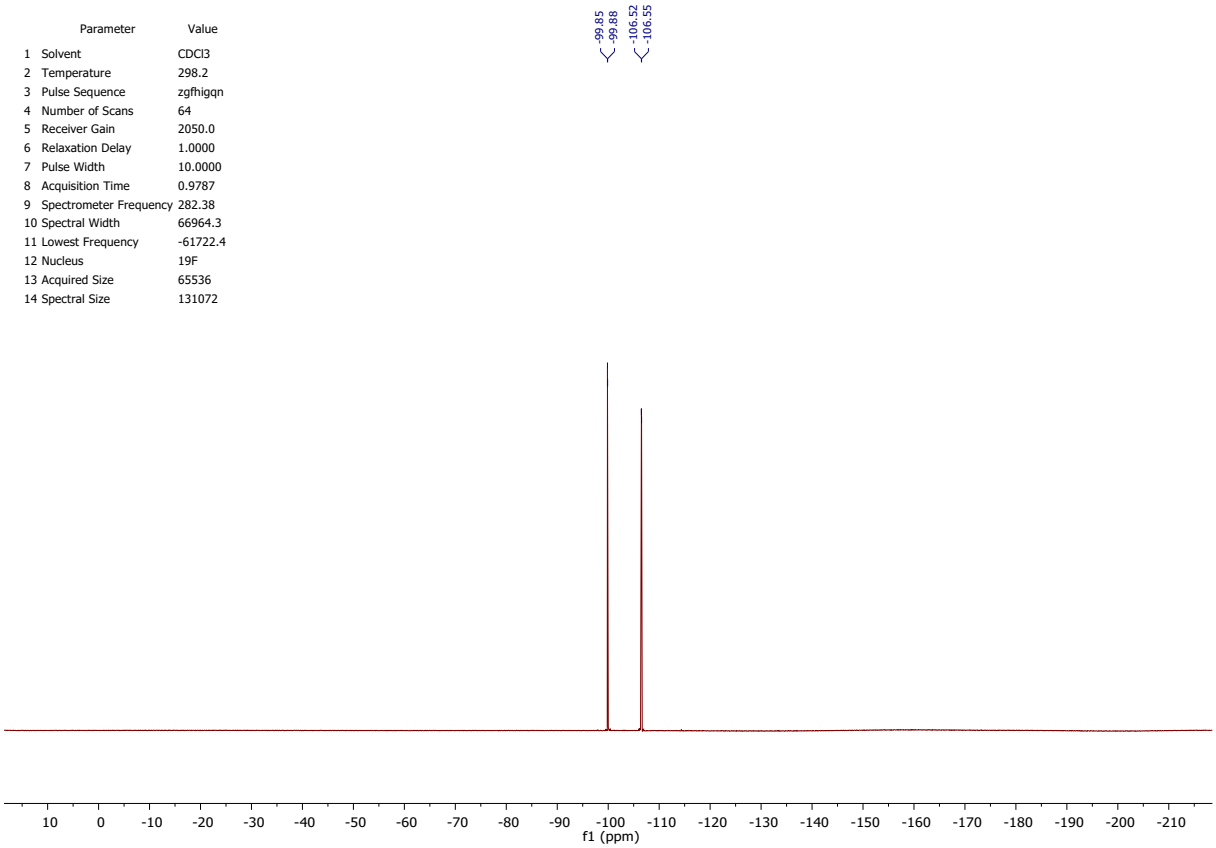




	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.1
3	Pulse Sequence	zgpg30
4	Number of Scans	4096
5	Receiver Gain	101.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2490.2
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

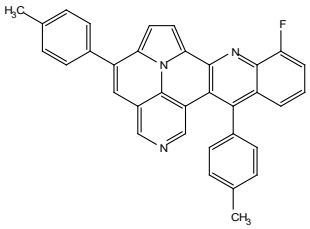


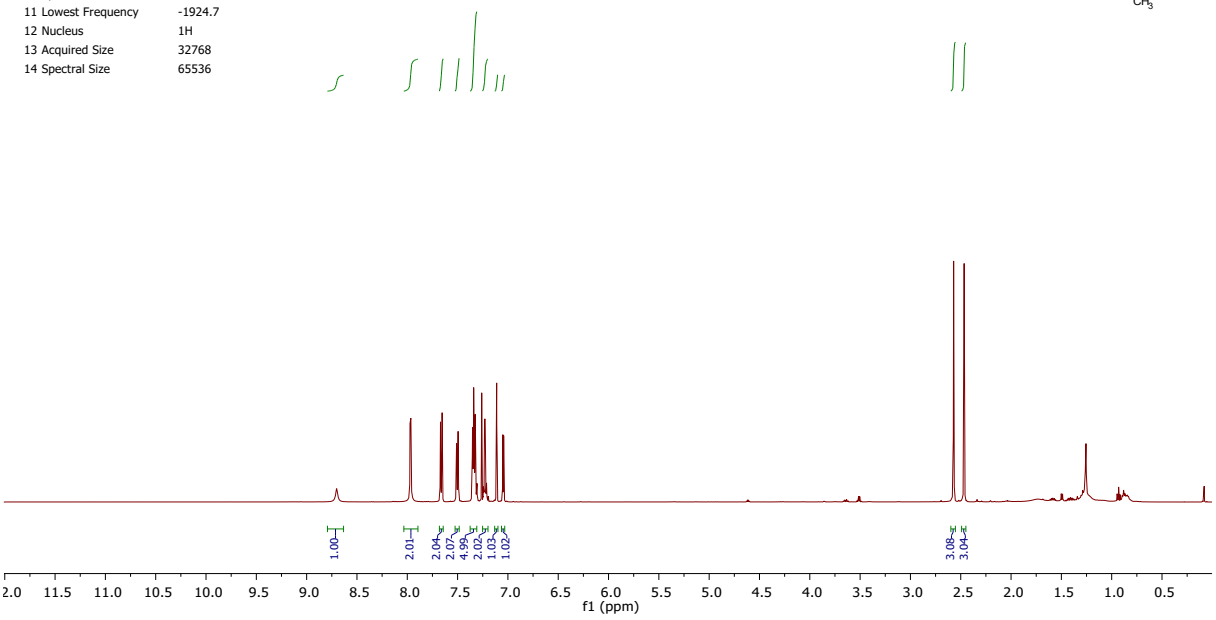
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



9-fluor-5,13-di-*p*-tolylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5f)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101.0
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	-1924.7
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	2048
5	Receiver Gain	101.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.0879
9	Spectrometer Frequency	125.77
10	Spectral Width	30120.5
11	Lowest Frequency	-2490.2
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

158.34
156.30
146.29
146.26
145.13
144.01
143.75
139.09
138.79
138.54
138.44
135.05
134.61
134.24
133.92
130.96
129.56
129.30
128.95
128.94
128.49
127.98
125.87
124.74
124.68
122.72
122.69
119.68
117.93
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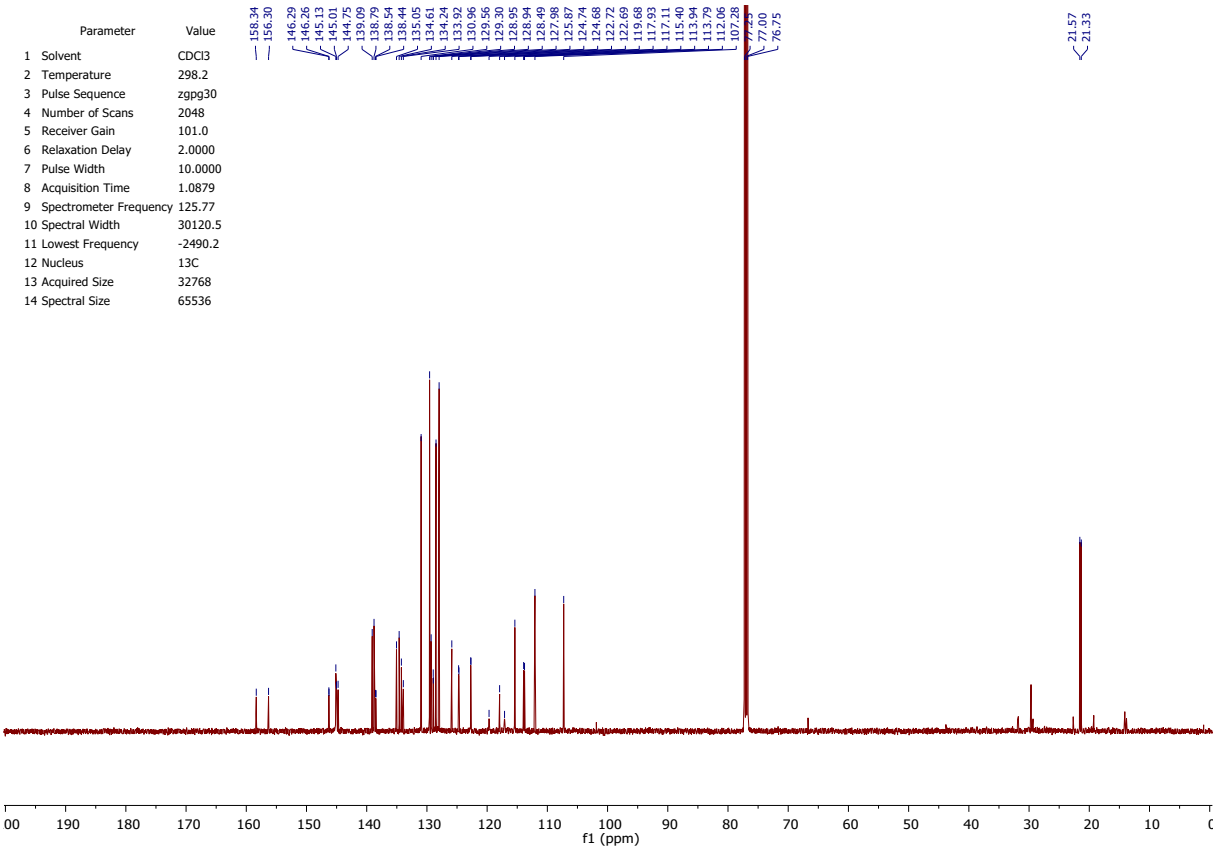
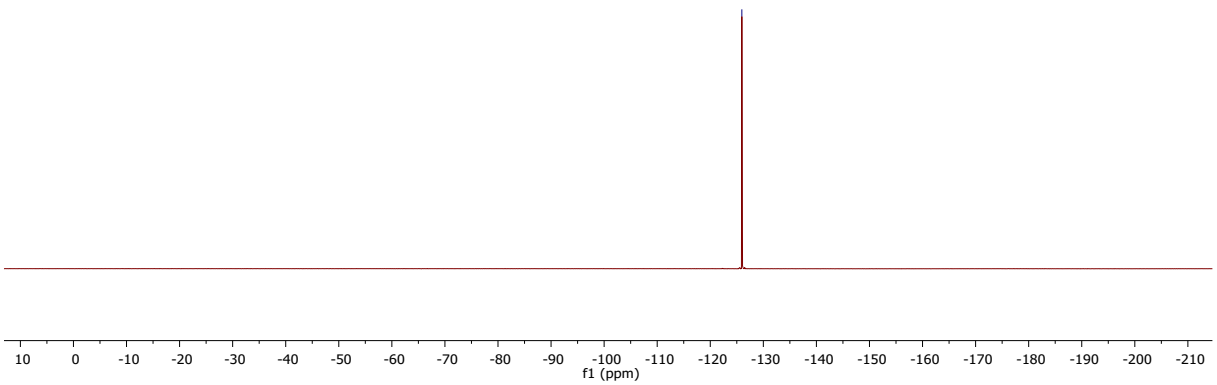
113.94
113.79
112.06
107.28
77.25
77.00
76.75
21.57
21.33



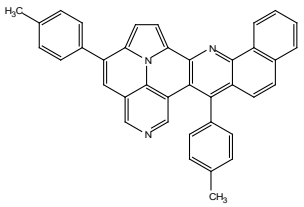
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072

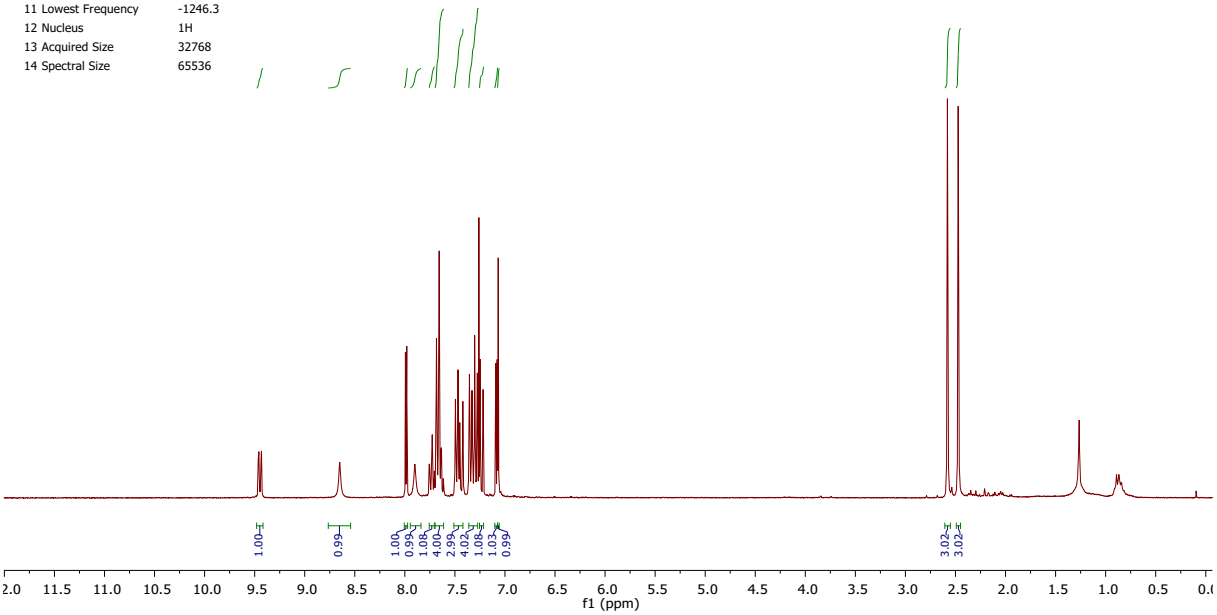
-125.95



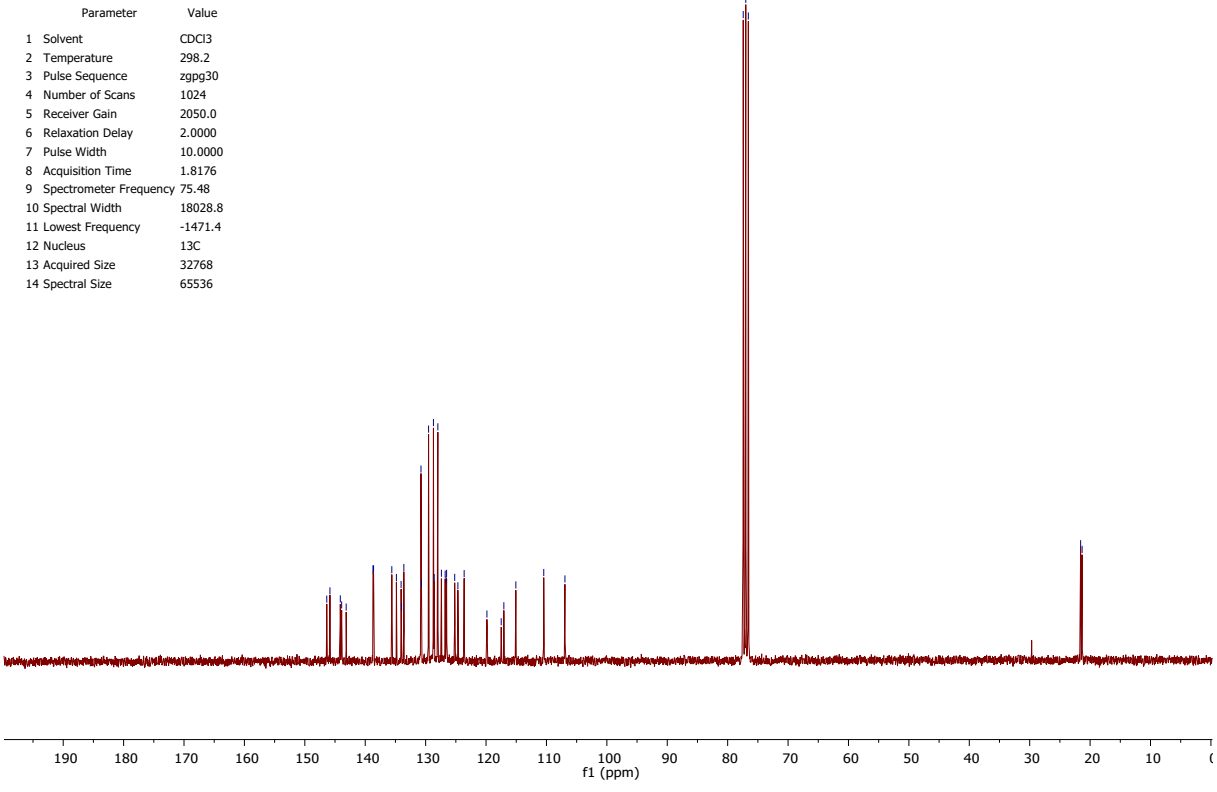
5,15-di-*p*-tolylbenzo[7,8]quinolino[2,3-*c*]indolizino[6,5,4,3-*ija*][1,6]naphthyridine (5h)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	144.0
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



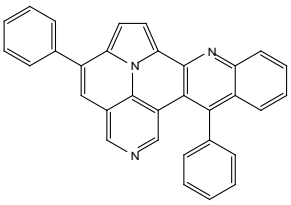


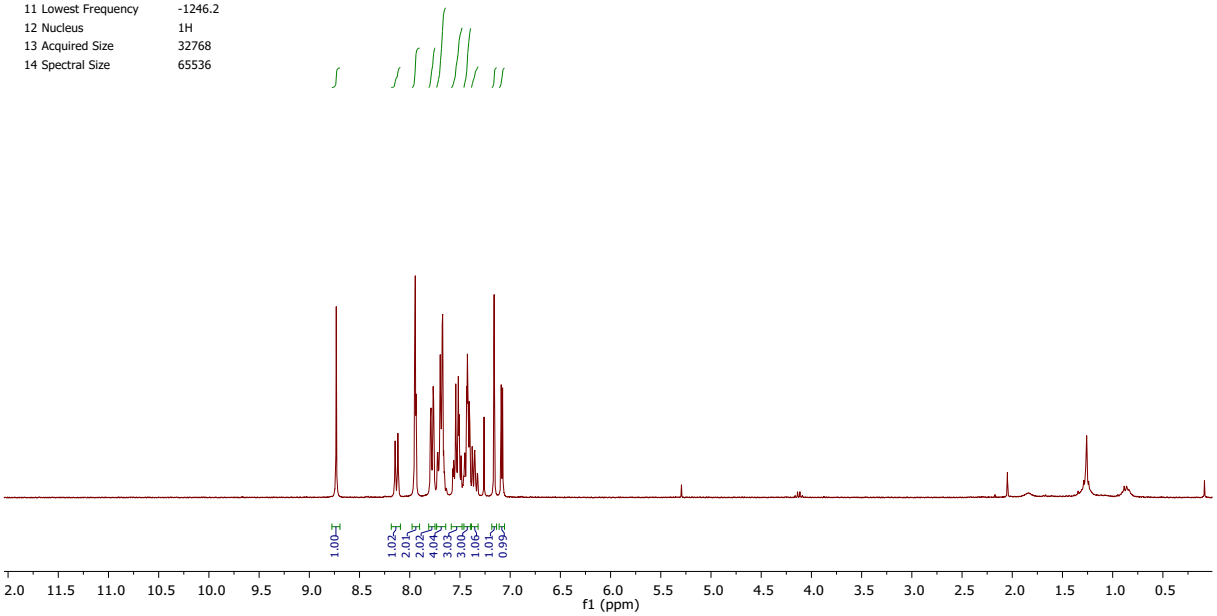
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1471.4
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



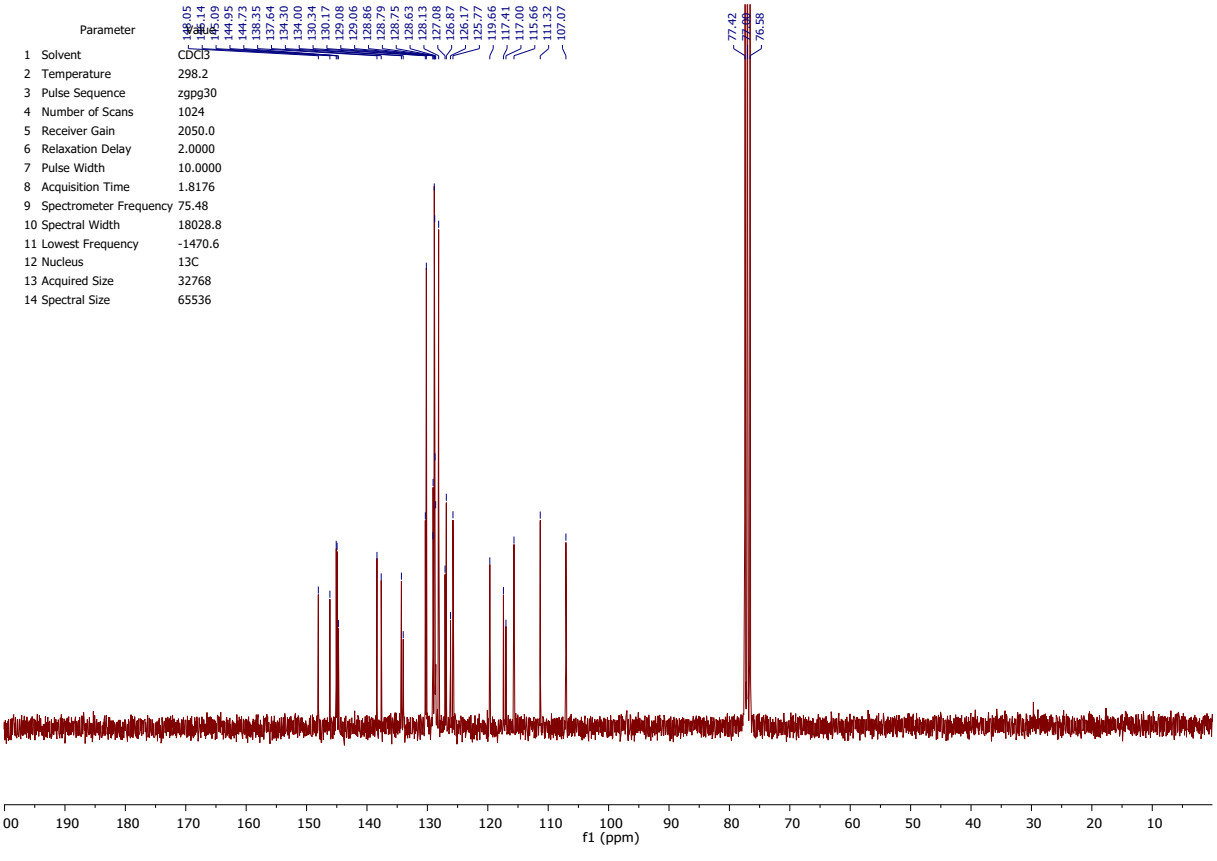
5,13-diphenylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5i)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	203.0
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



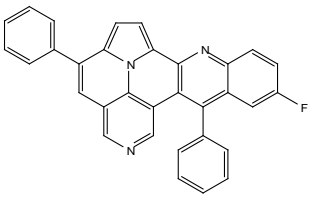


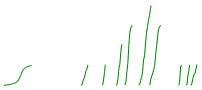
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgpg30
4	Number of Scans	1024
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1470.6
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

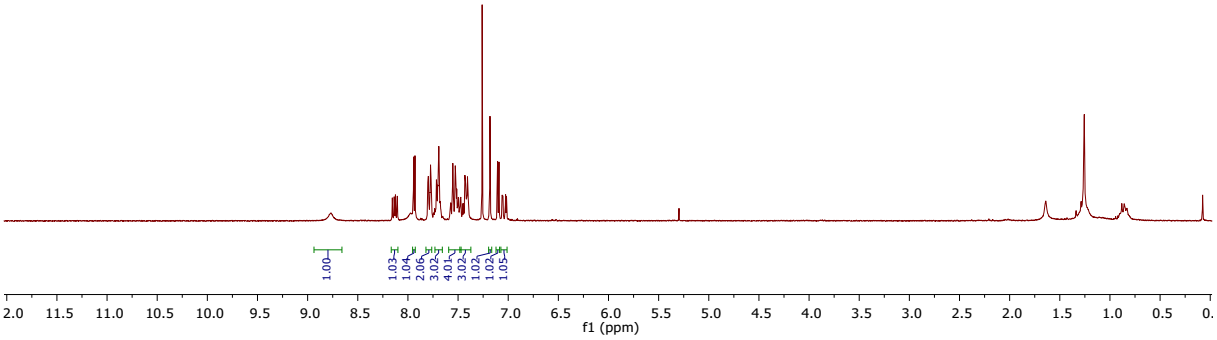


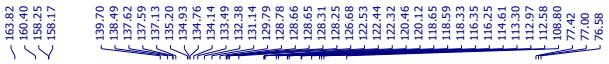
11-fluor-5,13-diphenylindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5j)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	322.0
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

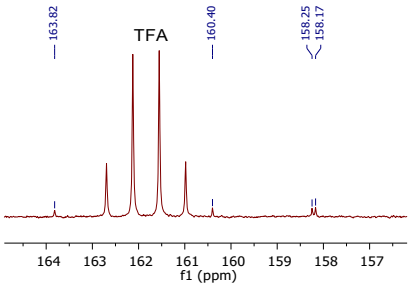


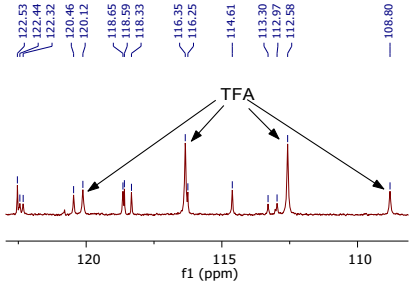


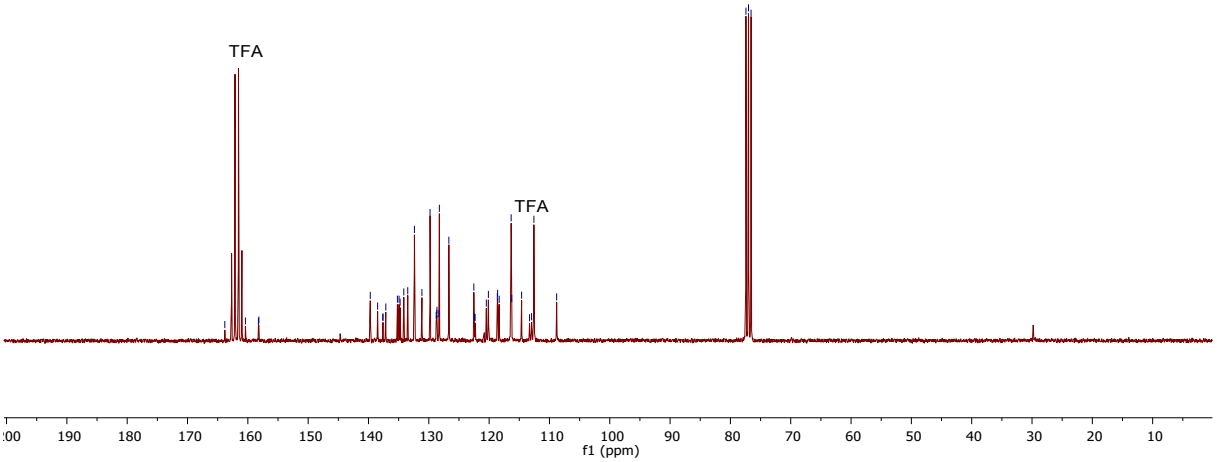




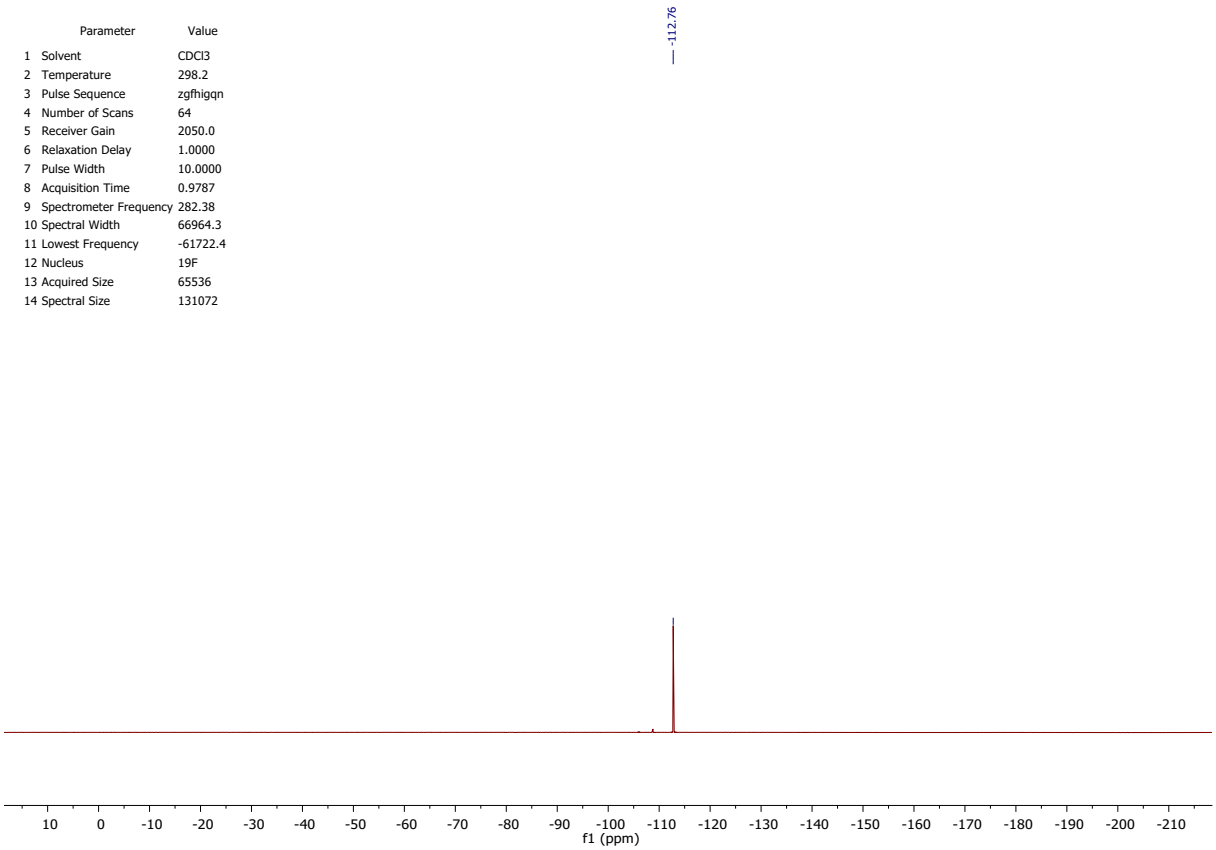
	Parameter	Value
1	Solvent	CDCl3/TFA
2	Temperature	298.7
3	Pulse Sequence	zgpg30
4	Number of Scans	2048
5	Receiver Gain	2050.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	1.8176
9	Spectrometer Frequency	75.48
10	Spectral Width	18028.8
11	Lowest Frequency	-1456.1
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536





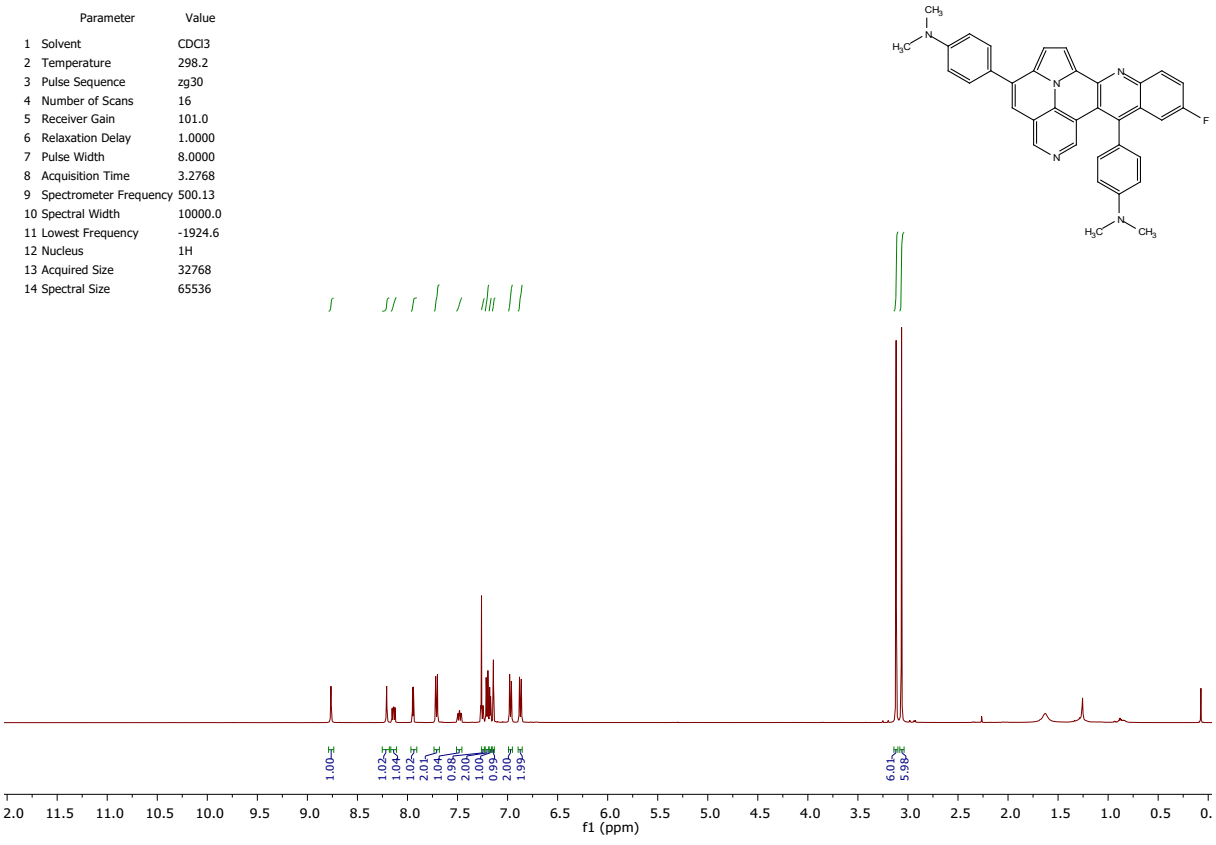


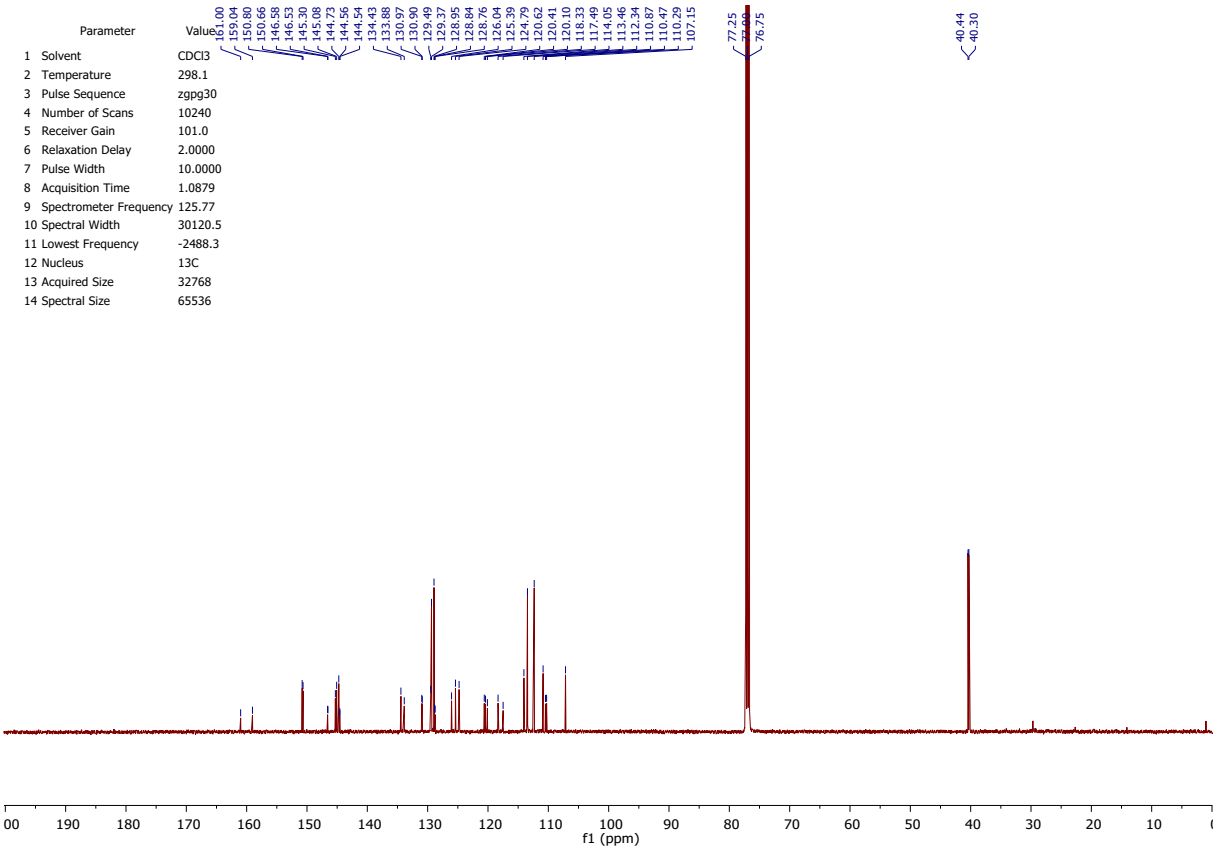
	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	2050.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



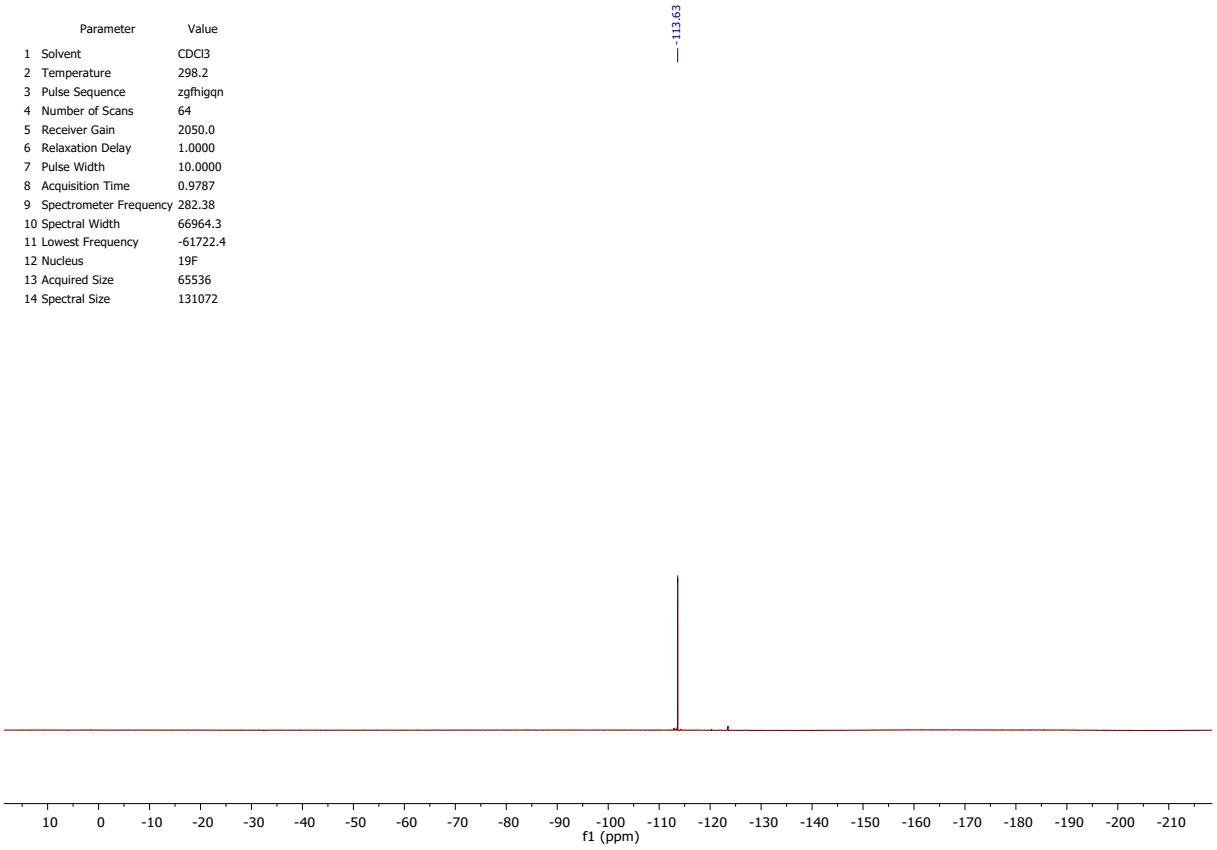
4,4'-(11-fluorindolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine-5,13-diyl)bis(*N*,*N*-dimethylaniline) (5k)

	Parameter	Value
1	Solvent	CDCl3
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	101.0
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	-1924.6
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536





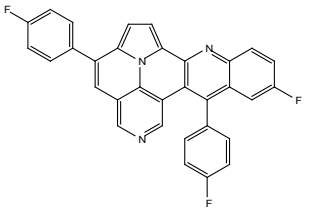
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.1
3 Pulse Sequence	zgpg30
4 Number of Scans	10240
5 Receiver Gain	101.0
6 Relaxation Delay	2.0000
7 Pulse Width	10.0000
8 Acquisition Time	1.0879
9 Spectrometer Frequency	125.77
10 Spectral Width	30120.5
11 Lowest Frequency	-2488.3
12 Nucleus	13C
13 Acquired Size	32768
14 Spectral Size	65536

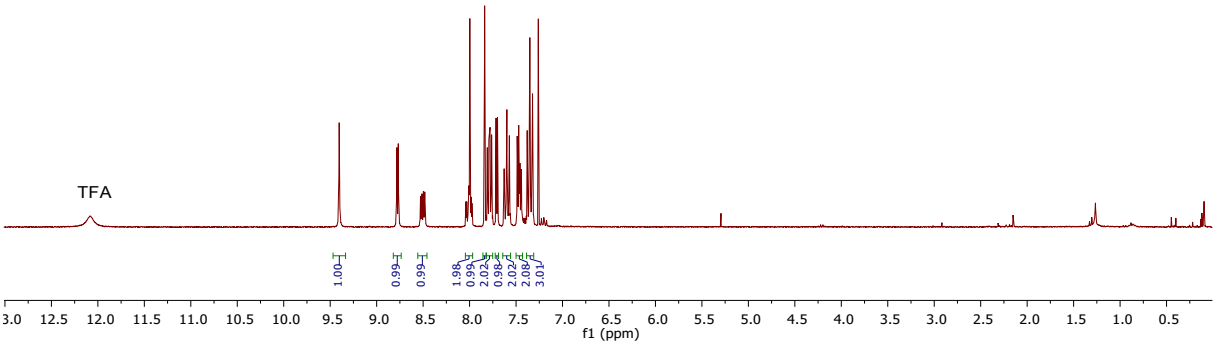


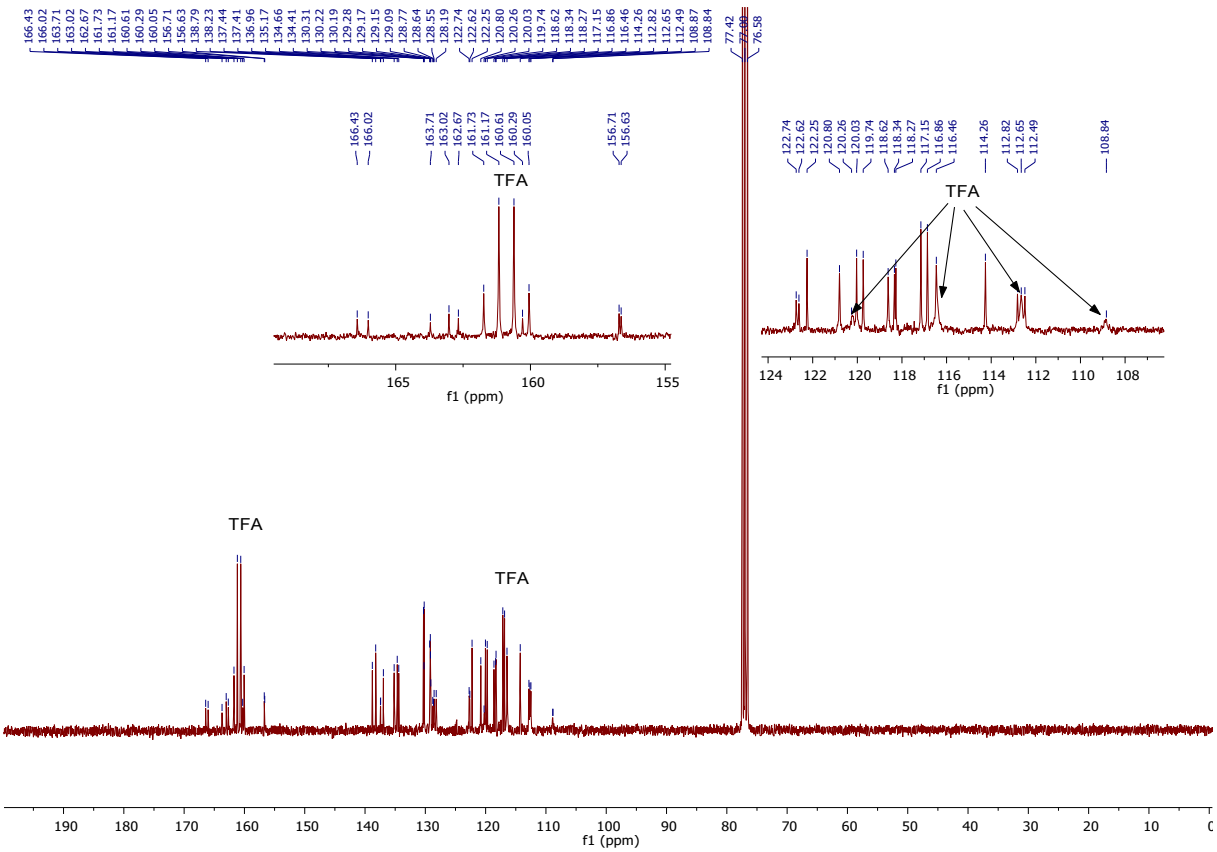
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.2
3 Pulse Sequence	zgfhigqn
4 Number of Scans	64
5 Receiver Gain	2050.0
6 Relaxation Delay	1.0000
7 Pulse Width	10.0000
8 Acquisition Time	0.9787
9 Spectrometer Frequency	282.38
10 Spectral Width	66964.3
11 Lowest Frequency	-61722.4
12 Nucleus	19F
13 Acquired Size	65536
14 Spectral Size	131072

11-fluor-5,13-bis(4-fluorphenyl)indolizino[6,5,4,3-*ija*]quinolino[2,3-*c*][1,6]naphthyridine (5l)

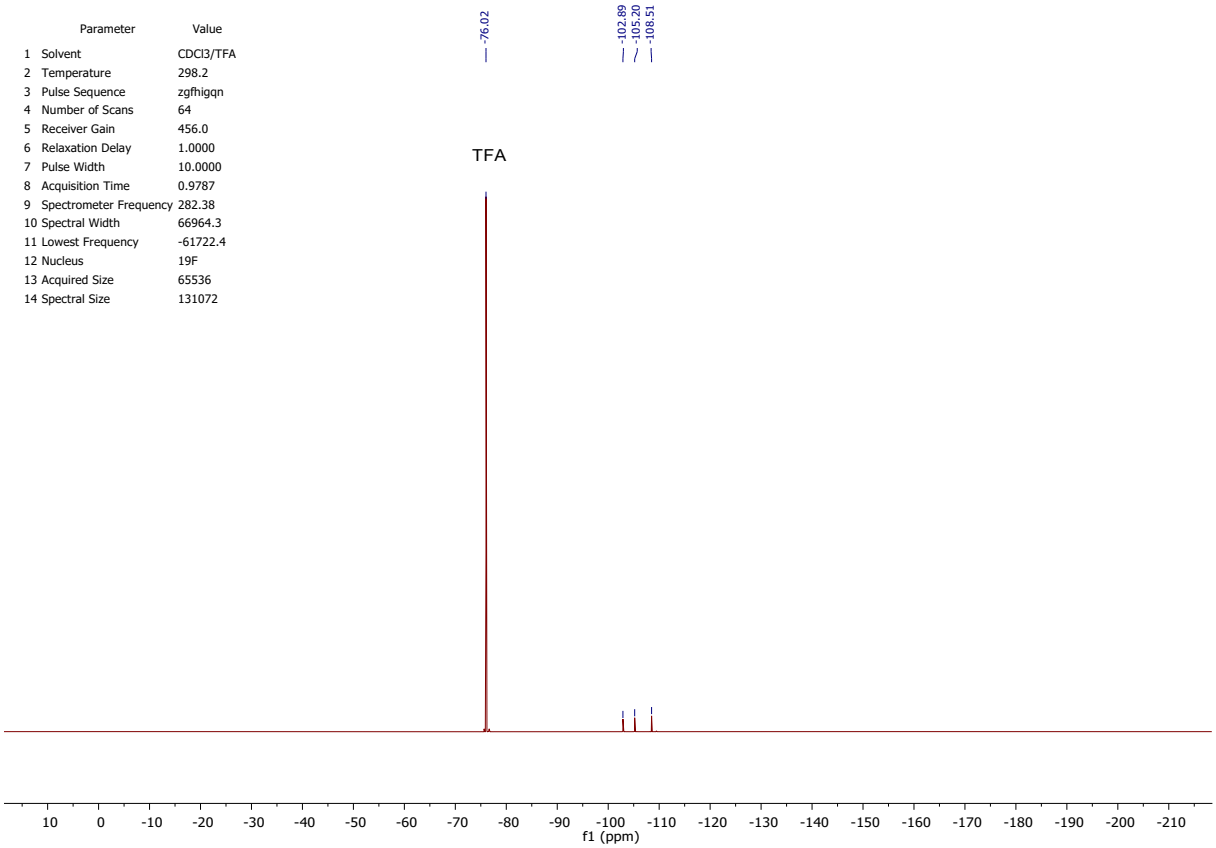
	Parameter	Value
1	Solvent	CDCl3/TFA
2	Temperature	298.2
3	Pulse Sequence	zg30
4	Number of Scans	16
5	Receiver Gain	287.0
6	Relaxation Delay	2.0000
7	Pulse Width	10.0000
8	Acquisition Time	5.2954
9	Spectrometer Frequency	300.13
10	Spectral Width	6188.1
11	Lowest Frequency	-1246.3
12	Nucleus	1H
13	Acquired Size	32768
14	Spectral Size	65536







	Parameter	Value
1	Solvent	CDCl3/TFA
2	Temperature	298.2
3	Pulse Sequence	zgfhigqn
4	Number of Scans	64
5	Receiver Gain	456.0
6	Relaxation Delay	1.0000
7	Pulse Width	10.0000
8	Acquisition Time	0.9787
9	Spectrometer Frequency	282.38
10	Spectral Width	66964.3
11	Lowest Frequency	-61722.4
12	Nucleus	19F
13	Acquired Size	65536
14	Spectral Size	131072



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