Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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1. Supporting figures and tables

Table S1 Optical Properties of **3a-n** in $CHCl_3$.

Compounds	λ_{abs} (nm)	log ε	λ_{em} (nm)	$\Delta\nu_{St}$ (cm^{-1})[a]	Φ_F[b]	τ (ns)	k_r (s^{-1})	k_d (s^{-1})	k_r/k_d
3a	339	4.45	392	3987	0.22	1.12	$2.0x10^8$	$6.9x10^8$	0.28
3b	342	4.51	445	6767	0.02	0.26	$7.89x10^7$	$3.68x10^9$	0.02
3c	340	4.54	392	3902	0.26	1.12	$2.35x10^8$	$6.57x10^8$	0.36
3d	342	4.54	397	4050	0.11	0.57	$1.83x10^8$	$1.56x10^9$	0.12
3f	342	4.48	400	4239	0.20	0.76	$2.57x10^8$	$1.05x10^9$	0.24
3g	340	4.50	398	4285	0.26	1.27	$2.05x10^8$	$5.83x10^8$	0.35
3h	339	4.46	393	4053	0.23	1.13	$2.04x10^8$	$6.84x10^8$	0.30
3i	340	4.42	392	3900	0.19	1.11	$1.77x10^8$	$7.23x10^8$	0.24
3l	340	4.25	394	4030	0.29	1.22	$2.40x10^8$	$5.77x10^8$	0.41
3m	341	4.49	393	3879	0.07	0.28	$2.47x10^8$	$3.28x10^9$	0.07
3n	341	4.49	393	3879	0.07	0.29	$2.35x10^8$	$3.12x10^9$	0.07

[a] $\Delta\nu = \nu_{abs} - \nu_{em}$, Stokes shift. [b] Fluorescence quantum yields (±5% error) were determined using quinine sulfate as the standard (Φ_F = 0.54 in 0.1 M H_2SO_4).

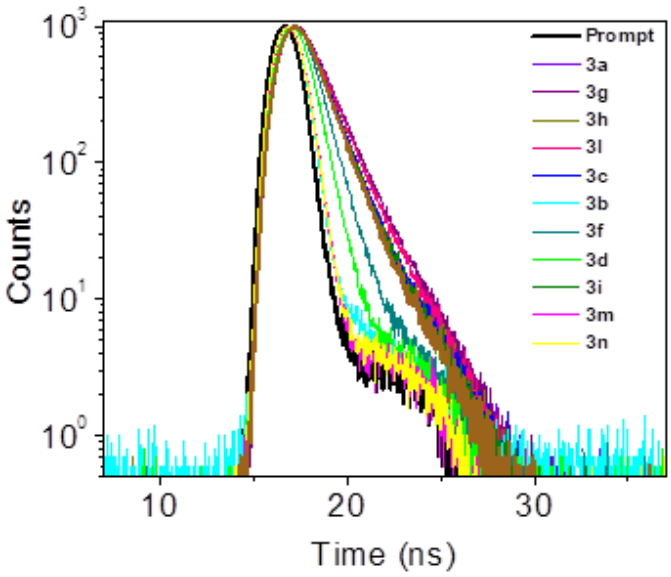

Figure S1. Fluorescent decay profiles of **3a**-**n** in $CHCl_3$ (λ_{ex} = 340 nm).

Cartesian coordinates of optimized geometry of **3a**

6	0.550352000	-3.216872000	-0.344467000
6	-0.711795000	-2.620183000	-0.253001000
6	-0.941705000	-1.246657000	-0.098028000
6	0.201452000	-0.405866000	-0.065873000
6	1.477617000	-1.025016000	-0.077477000
6	1.667631000	-2.411713000	-0.241197000
8	-1.879968000	-3.337700000	-0.278343000
6	-2.381184000	-1.113995000	0.024451000
1	0.634505000	-4.287650000	-0.478511000
6	-4.237631000	-2.720144000	-0.029411000
6	-5.115511000	-1.667872000	0.194428000
6	-2.886316000	-2.419569000	-0.103362000
1	-6.182511000	-1.837974000	0.263941000
6	-4.637414000	-0.354974000	0.350469000
6	-3.278736000	-0.066268000	0.273181000

1	-2.927788000	0.947946000	0.409501000
1	-4.588503000	-3.738783000	-0.134866000
1	2.659247000	-2.837245000	-0.303473000
6	0.487881000	0.999527000	-0.001874000
7	1.794286000	1.205914000	0.066679000
7	2.401380000	-0.005212000	0.036095000
8	-5.577265000	0.613302000	0.584958000
1	-5.136013000	1.464900000	0.669524000
6	3.819353000	-0.072156000	0.065157000
6	4.469118000	-1.081650000	0.779367000
6	4.562533000	0.901938000	-0.606673000
1	3.893533000	-1.802670000	1.344915000
1	4.040237000	1.688324000	-1.134550000
6	5.860910000	-1.130152000	0.792708000
6	5.951267000	0.851798000	-0.572156000
1	6.360449000	-1.914610000	1.349641000
1	6.524076000	1.609974000	-1.093853000
6	6.606819000	-0.167685000	0.117563000
1	7.689708000	-0.205758000	0.135333000
6	-0.410195000	2.171866000	-0.049958000
6	-1.365092000	2.301384000	-1.066517000
6	-0.270049000	3.208941000	0.881525000
1	-1.465406000	1.517309000	-1.808166000
1	0.479459000	3.119032000	1.658350000
6	-2.170623000	3.435567000	-1.140926000
6	-1.078154000	4.339282000	0.808434000
1	-2.897723000	3.525938000	-1.940429000

1	-0.961319000	5.131898000	1.539079000
6	-2.033061000	4.455538000	-0.201083000
1	-2.658562000	5.339234000	-0.260462000

Cartesian coordinates of optimized geometry of **3g**

6	-1.701093000	-3.369665000	0.274743000
6	-0.326649000	-3.120238000	0.200454000
6	0.254485000	-1.850522000	0.083542000
6	-0.629817000	-0.740204000	0.069757000
6	-2.023253000	-1.005698000	0.065751000
6	-2.569095000	-2.298548000	0.193215000
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6	1.680412000	-2.094804000	-0.027174000
1	-2.062244000	-4.384548000	0.380597000
6	3.053928000	-4.130084000	-0.008435000
6	4.178846000	-3.337263000	-0.193635000
6	1.826575000	-3.489857000	0.065997000
1	5.165807000	-3.777538000	-0.259535000
6	4.061430000	-1.941301000	-0.311651000
6	2.823438000	-1.311011000	-0.237373000
1	2.750973000	-0.237022000	-0.345198000
1	3.125894000	-5.207454000	0.069038000
1	-3.637690000	-2.452354000	0.245248000
6	-0.538434000	0.693028000	0.037832000
7	-1.745931000	1.233791000	-0.023633000
7	-2.648786000	0.221582000	-0.023566000
8	5.224511000	-1.244751000	-0.507137000
1	5.024327000	-0.303618000	-0.543330000

6	-4.034048000	0.528128000	-0.056646000
6	-4.920898000	-0.261649000	-0.792520000
6	-4.501797000	1.649554000	0.633899000
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1	-3.795587000	2.261370000	1.178650000
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6	-5.855020000	1.965076000	0.596366000
1	-6.960149000	-0.559520000	-1.382935000
1	-6.213028000	2.836258000	1.133103000
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6	0.634639000	1.587836000	0.094177000
6	1.594901000	1.467408000	1.110772000
6	0.774975000	2.632914000	-0.821773000
1	1.495164000	0.682486000	1.851600000
1	0.031592000	2.751754000	-1.600685000
6	2.662934000	2.347521000	1.194013000
6	1.844447000	3.523713000	-0.751972000
1	3.399519000	2.264945000	1.984211000
1	1.919667000	4.316190000	-1.484253000
6	2.799086000	3.382227000	0.259442000
8	3.883791000	4.190706000	0.422334000
6	4.058251000	5.280800000	-0.473150000
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1	3.216049000	5.979624000	-0.423872000
1	4.965750000	5.787666000	-0.149597000

Cartesian coordinates of optimized geometry of **3b**

6	1.542001000	-3.326264000	-0.462096000
6	0.180540000	-3.031183000	-0.332102000
6	-0.350245000	-1.753031000	-0.108258000
6	0.577843000	-0.679077000	-0.049444000
6	1.959389000	-0.998548000	-0.098293000
6	2.452864000	-2.297954000	-0.327813000
8	-0.794296000	-3.991930000	-0.380595000
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6	-3.222565000	-3.942520000	-0.072618000
6	-4.311675000	-3.132147000	0.215597000
6	-1.978190000	-3.336182000	-0.148370000
1	-5.309913000	-3.544837000	0.288465000
6	-4.143083000	-1.753160000	0.434037000
6	-2.887955000	-1.157455000	0.356117000
1	-2.777177000	-0.098657000	0.547538000
1	-3.332978000	-5.008356000	-0.226119000
1	3.513609000	-2.486129000	-0.415043000
6	0.552070000	0.751369000	0.077689000
7	1.784389000	1.236533000	0.150275000
7	2.638328000	0.193807000	0.057331000
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6	4.904490000	-0.420540000	0.744818000
6	4.538827000	1.559597000	-0.601444000

1	4.509110000	-1.259785000	1.302234000
1	3.848870000	2.222183000	-1.106393000
6	6.273776000	-0.166394000	0.735270000
6	5.906094000	1.810810000	-0.590591000
1	6.942509000	-0.833208000	1.267273000
1	6.291085000	2.682969000	-1.106374000
6	6.779642000	0.946085000	0.067954000
1	7.845260000	1.143000000	0.067354000
6	-0.567925000	1.709680000	0.074536000
6	-1.594916000	1.612856000	-0.880163000
6	-0.577519000	2.782922000	0.976871000
1	-1.576791000	0.805291000	-1.602231000
1	0.223699000	2.866874000	1.700078000
6	-2.612628000	2.553276000	-0.919591000
6	-1.598555000	3.722970000	0.937219000
1	-3.404062000	2.494394000	-1.657692000
1	-1.603554000	4.548333000	1.642620000
6	-2.626649000	3.614365000	-0.005181000
6	-3.713482000	4.617807000	-0.036709000
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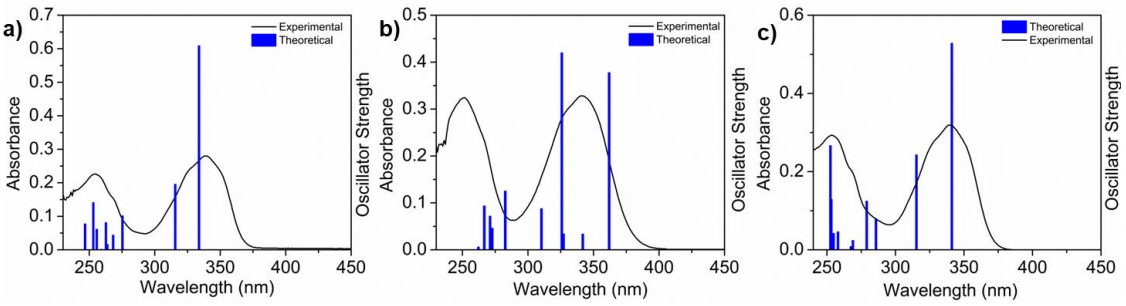


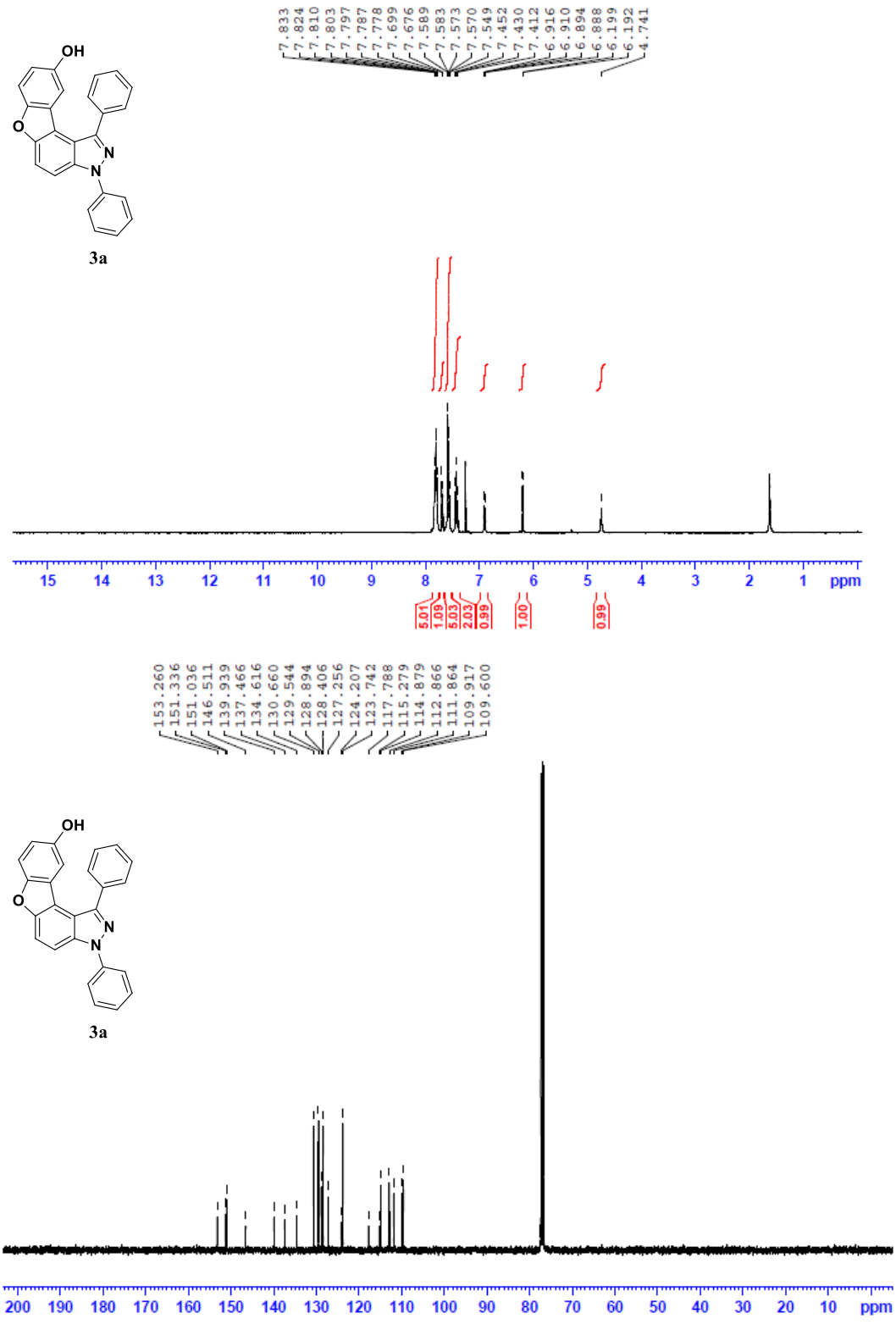
Figure S2. Plot showing the correlation of experimental UV/Vis spectrum with oscillator strength of theoretically generated absorption spectrum of a) **3a**, b) **3b** and c) **3g**.

Table S2 TD-DFT computed representative intense vertical excitations, absorption maximum (λ_{max}), molecular orbital (MO) contributions and oscillator strengths (*f*) of **3a**, **3g** and **3b** in chloroform

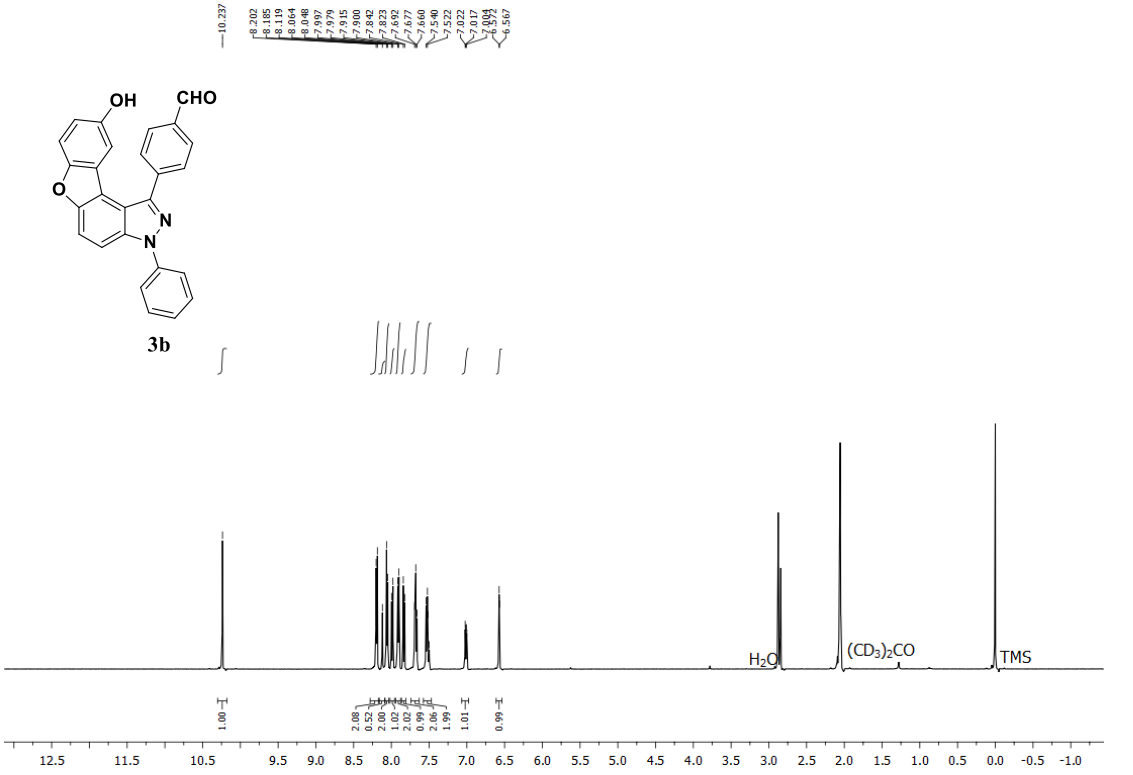
Molecules	Transitions	λ_{max}	λ_{Obs}	MO contribution (%)	Oscillator strength (*f*)
3a	H→L	334	339	96	0.608
3b	H→L	361	342	97	0.377
	H→L+1	326		90	0.419
3g	H→L	341	340	97	0.527

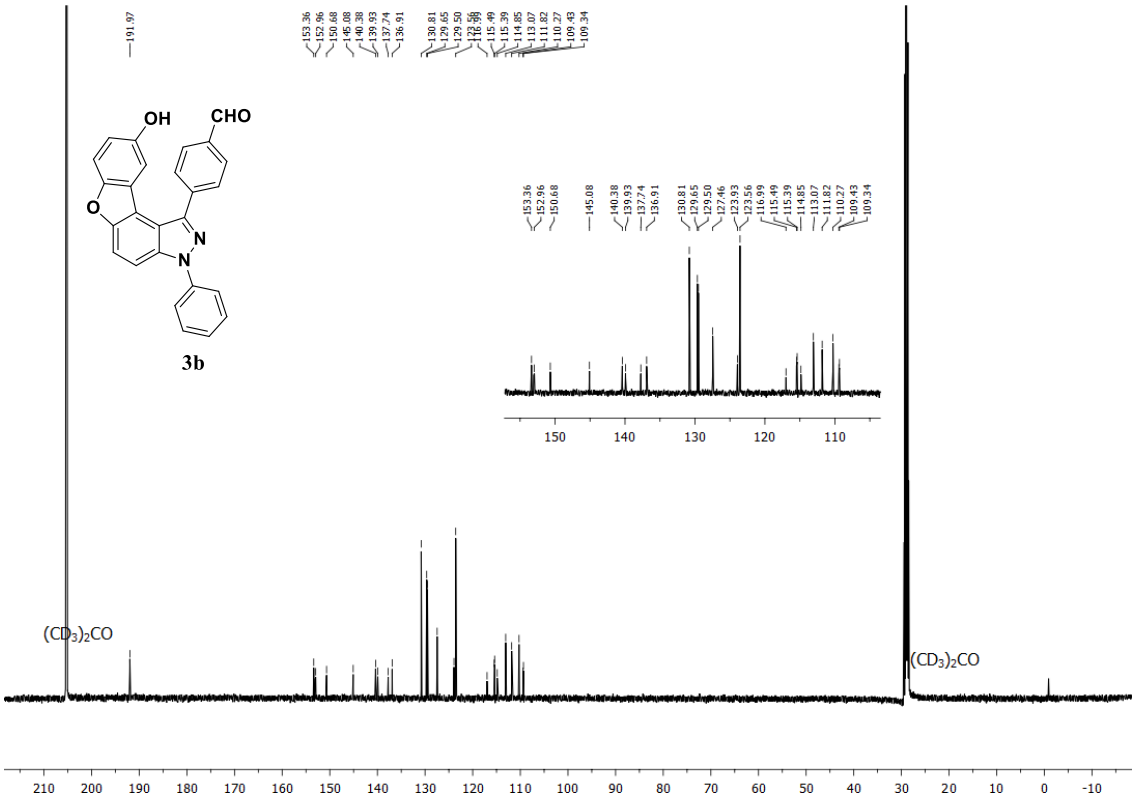
2. ^{1}H and ^{13}C NMR spectra of 1,3-diphenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol

1,3-diphenyl-3*H*-benzofuro[3,2-e]indazol-9-ol (3a)

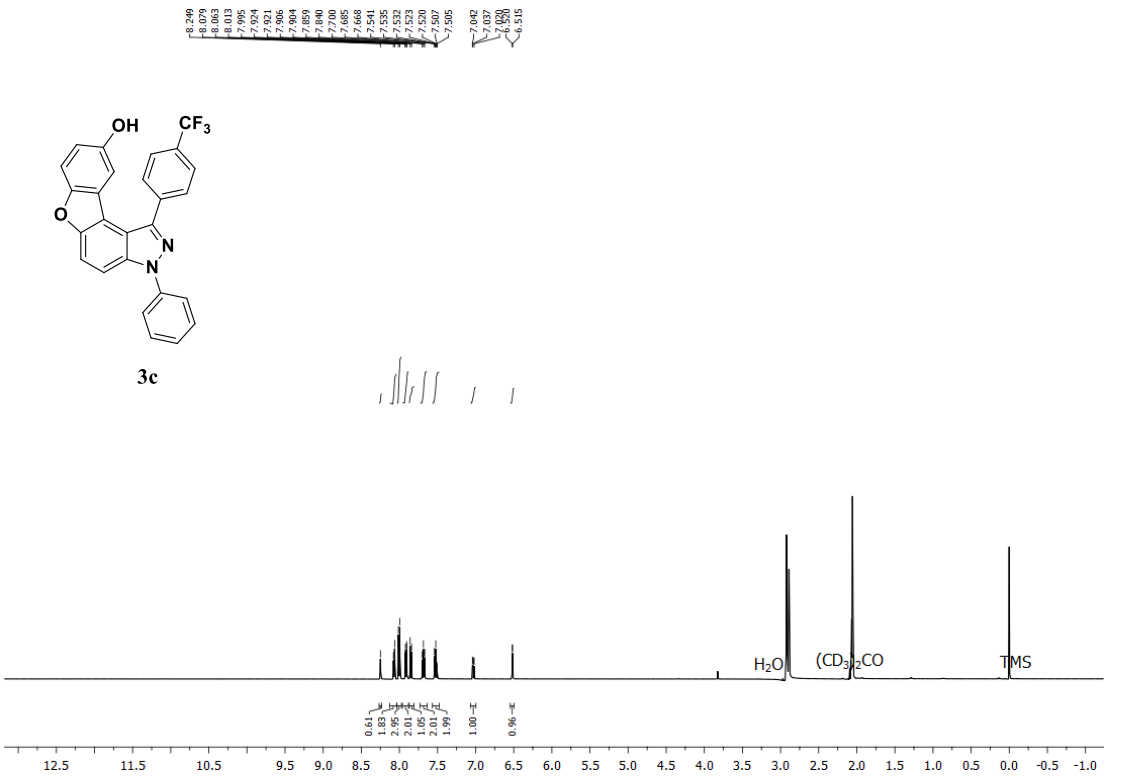


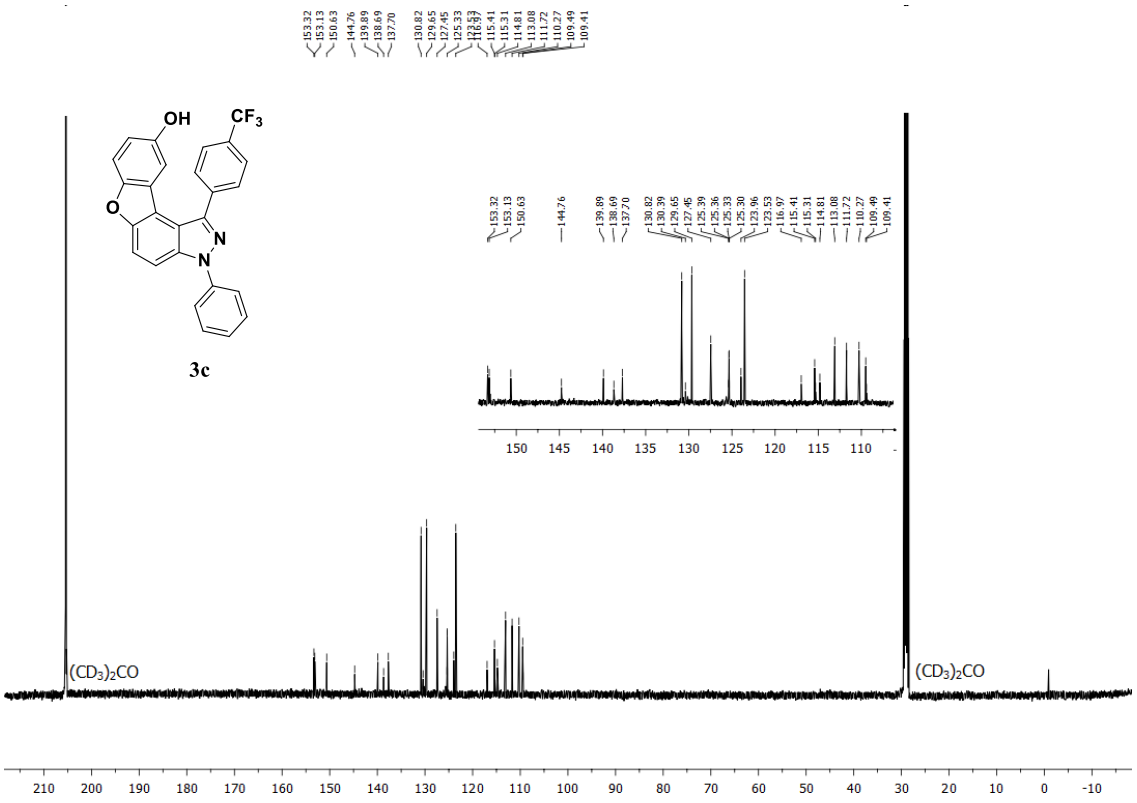
4-(9-hydroxy-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-1-yl)benzaldehyde (3b)



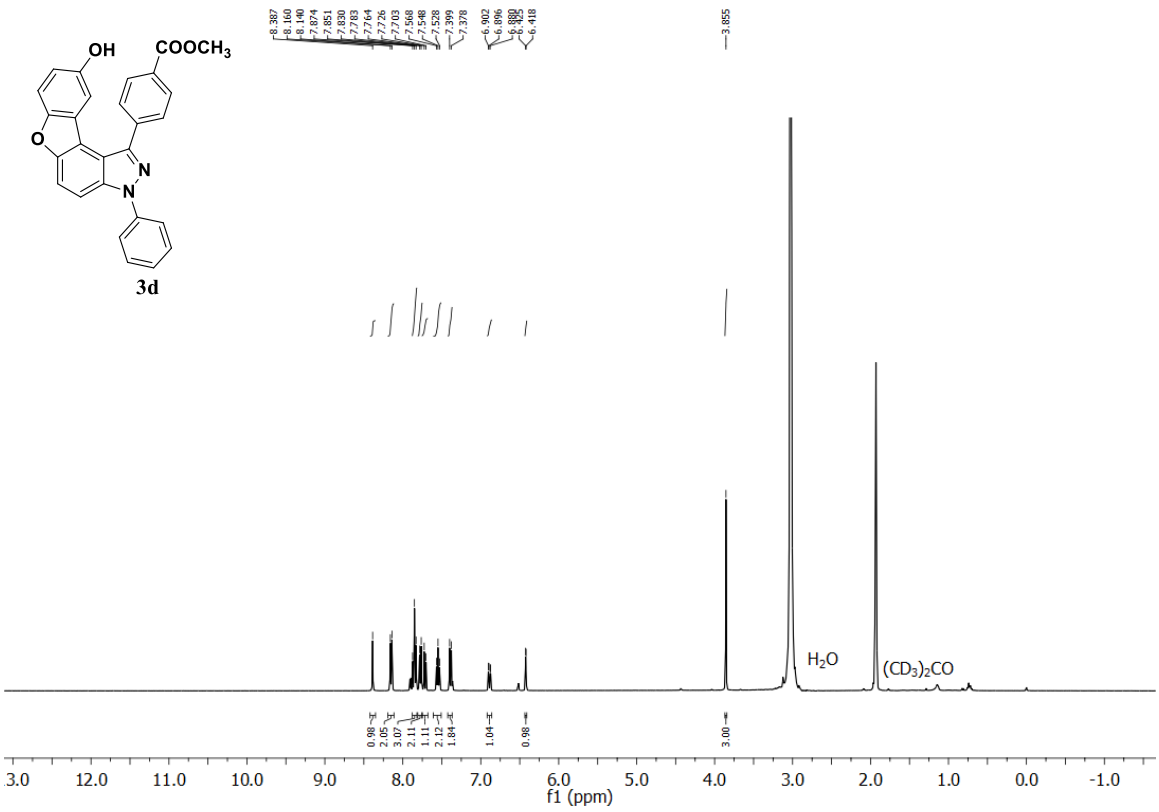


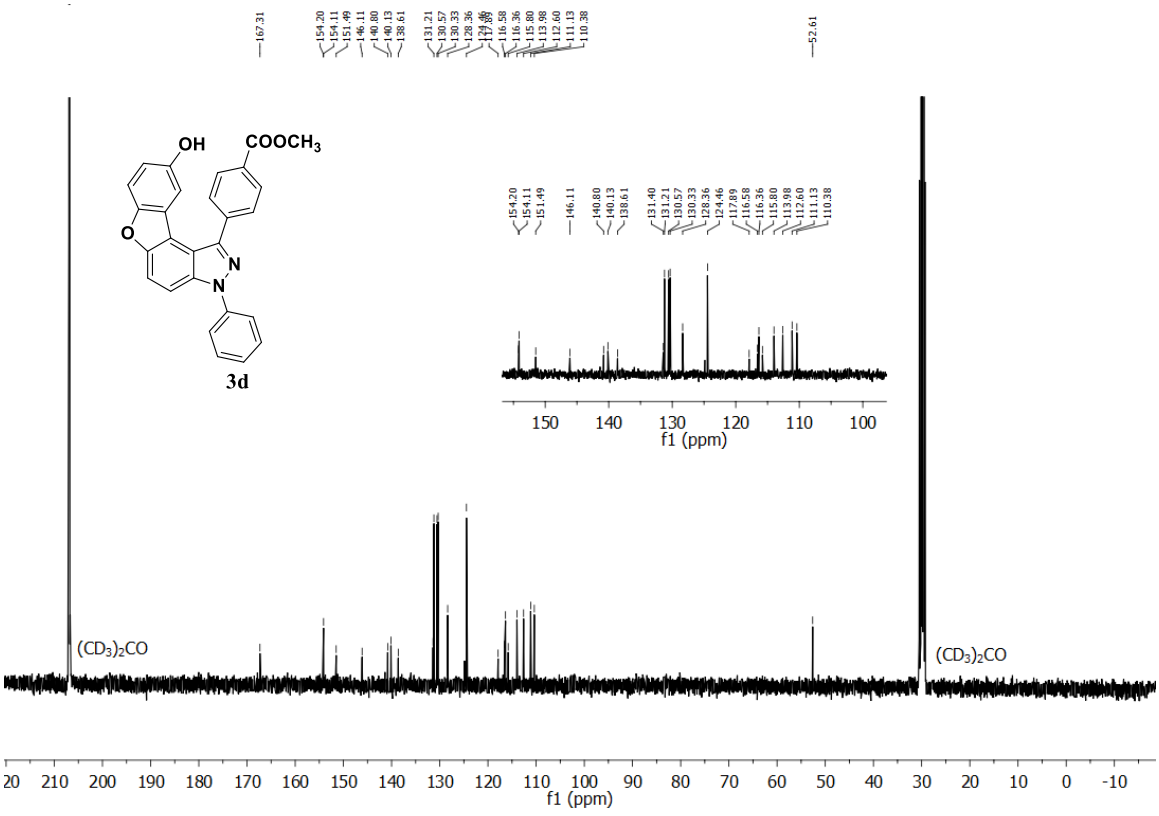
3-phenyl-1-(4-(trifluoromethyl)phenyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3c)



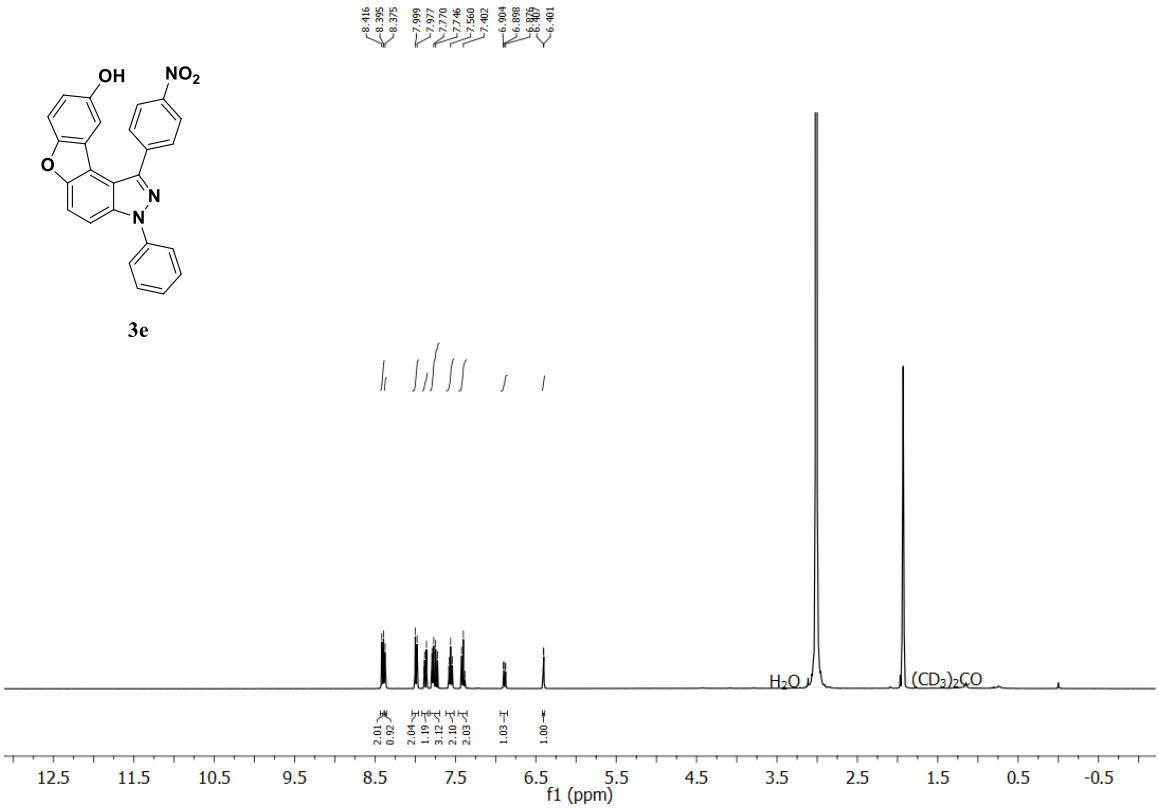


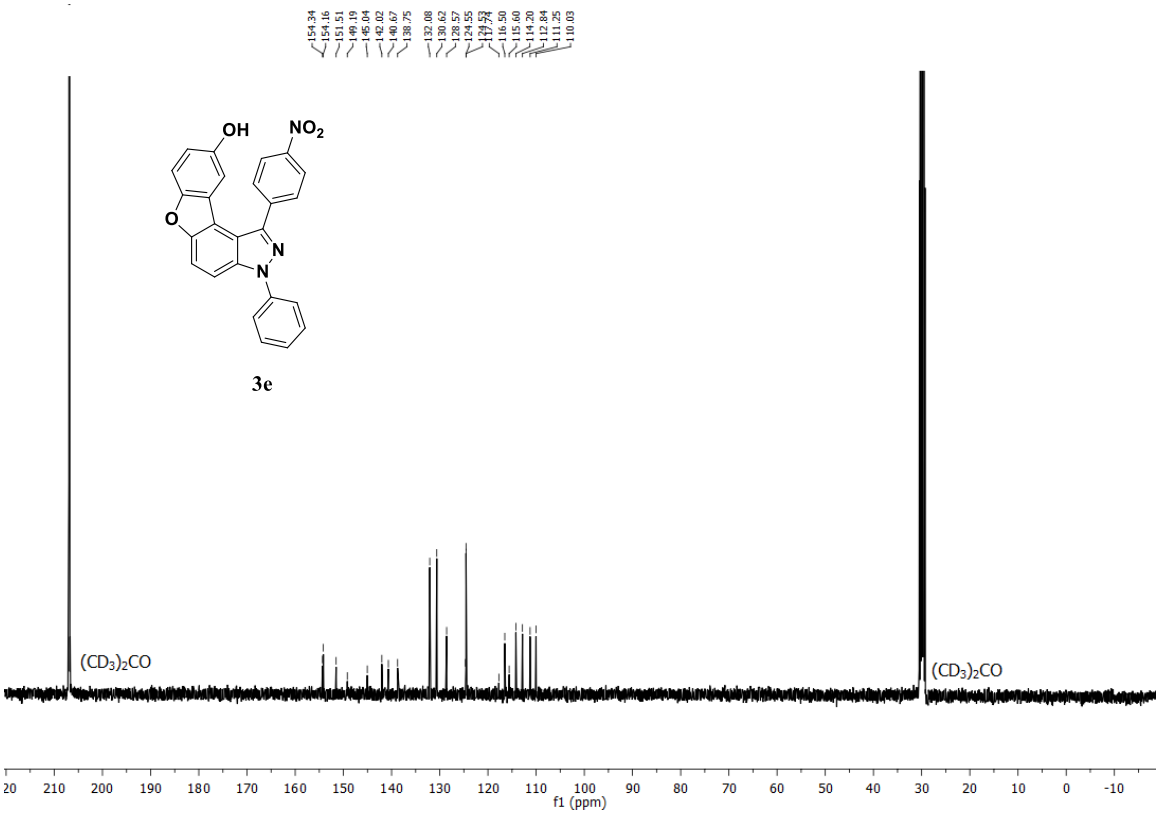
Methyl 4-(9-hydroxy-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-1-yl)benzoate (3d)



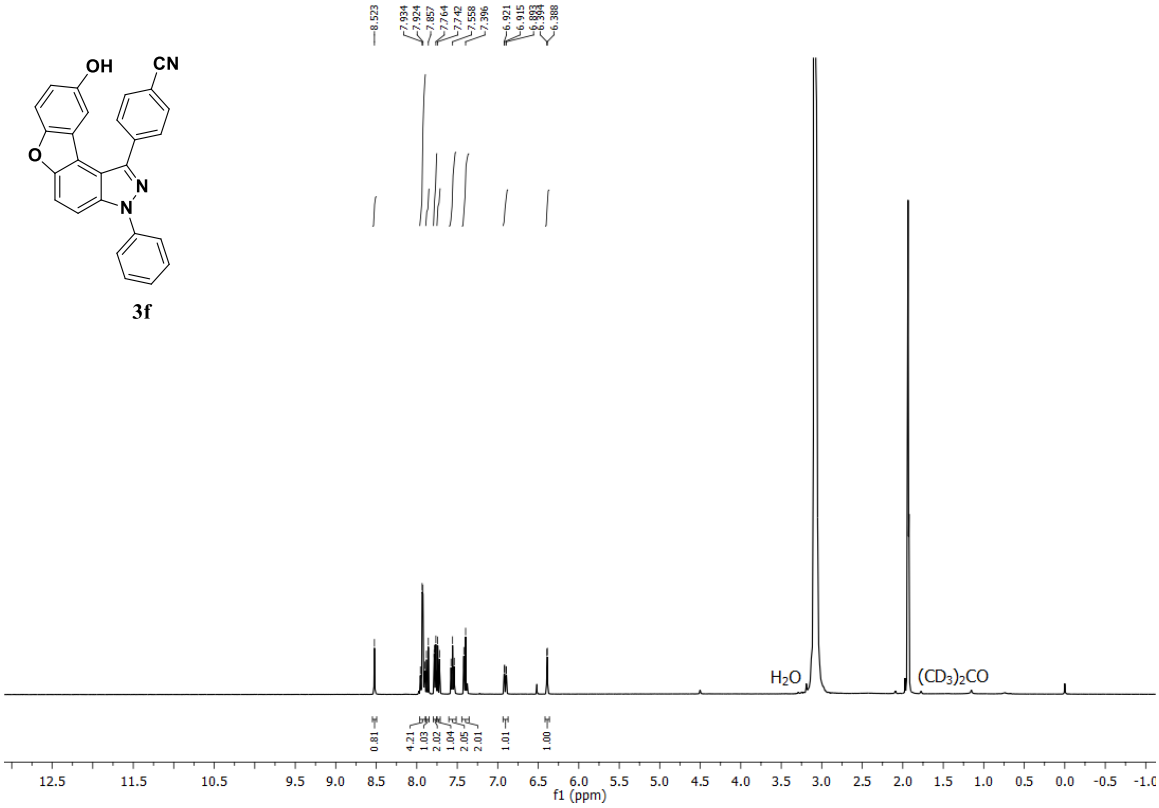


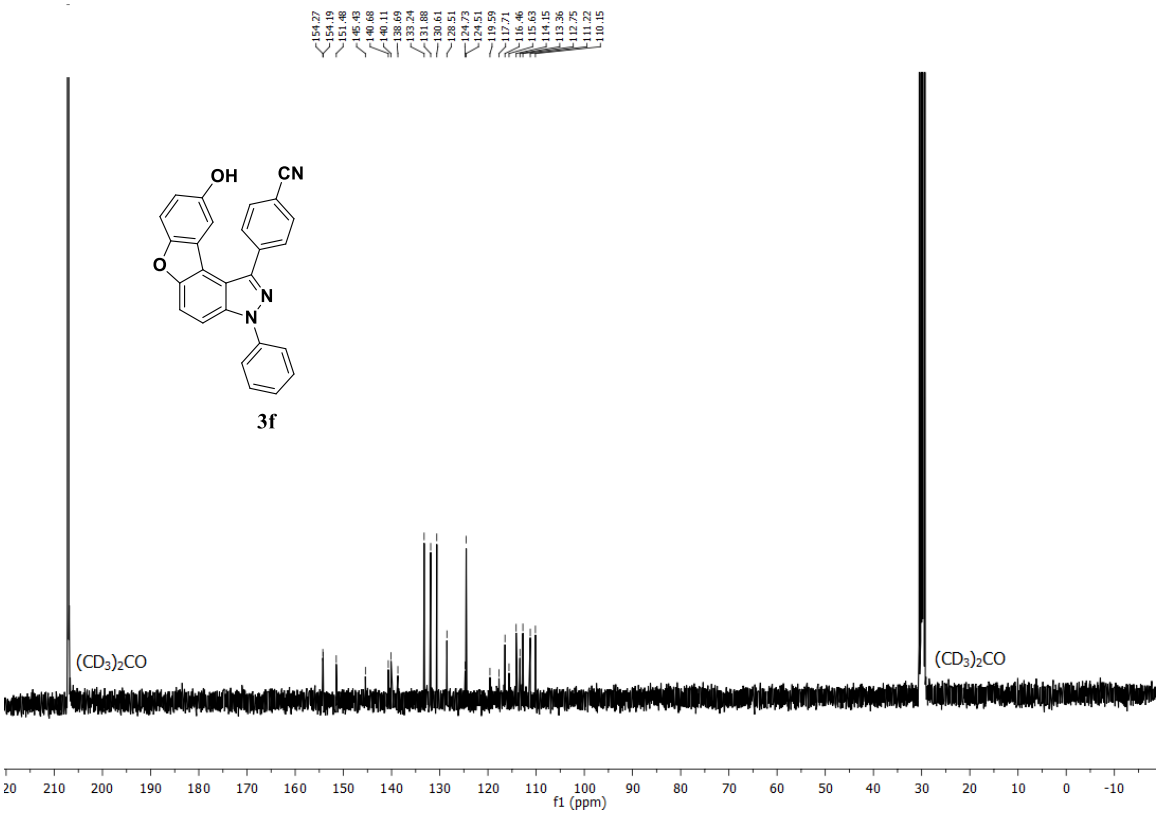
1-(4-nitrophenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3e)



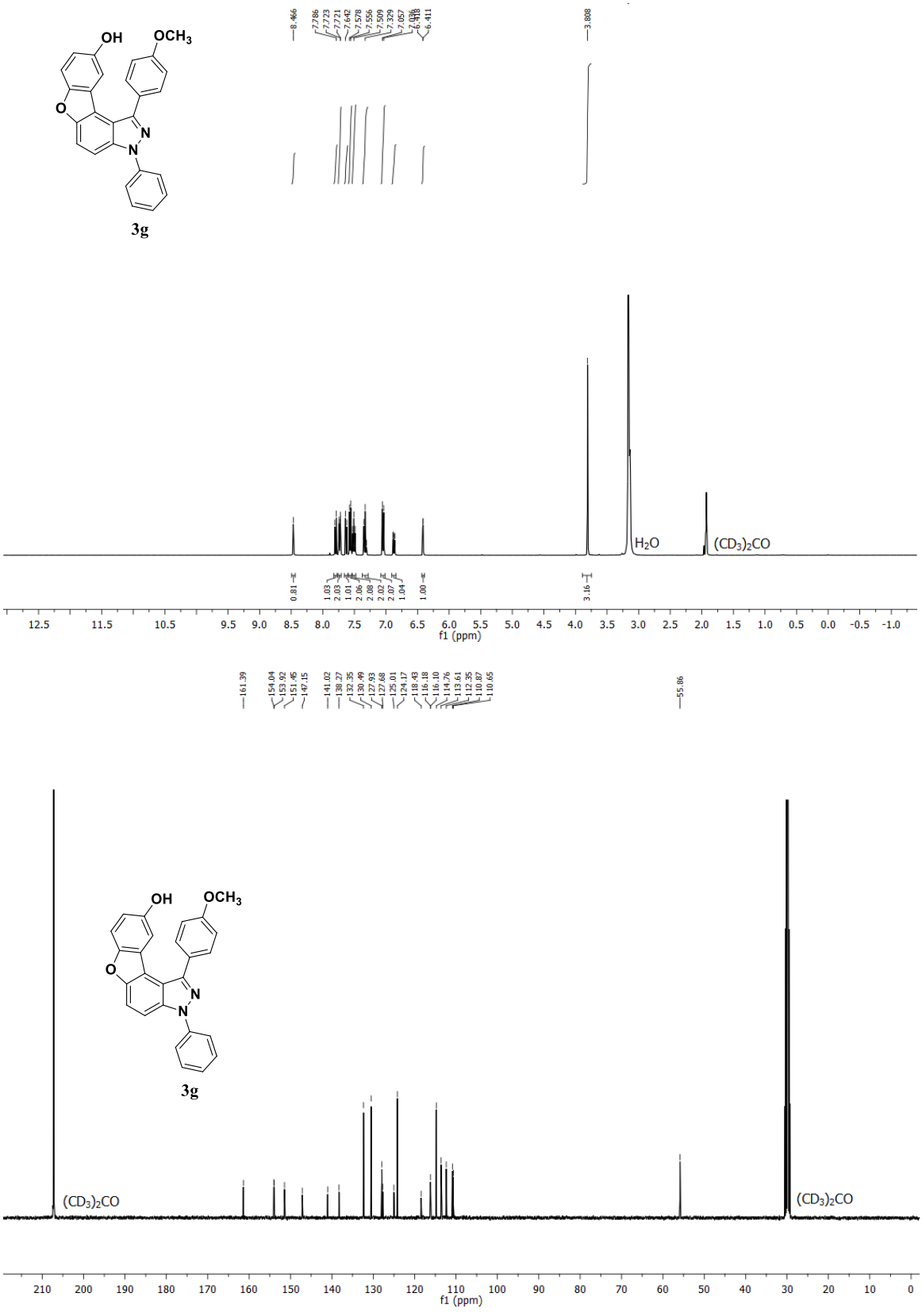


4-(9-hydroxy-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-1-yl)benzonitrile (3f)

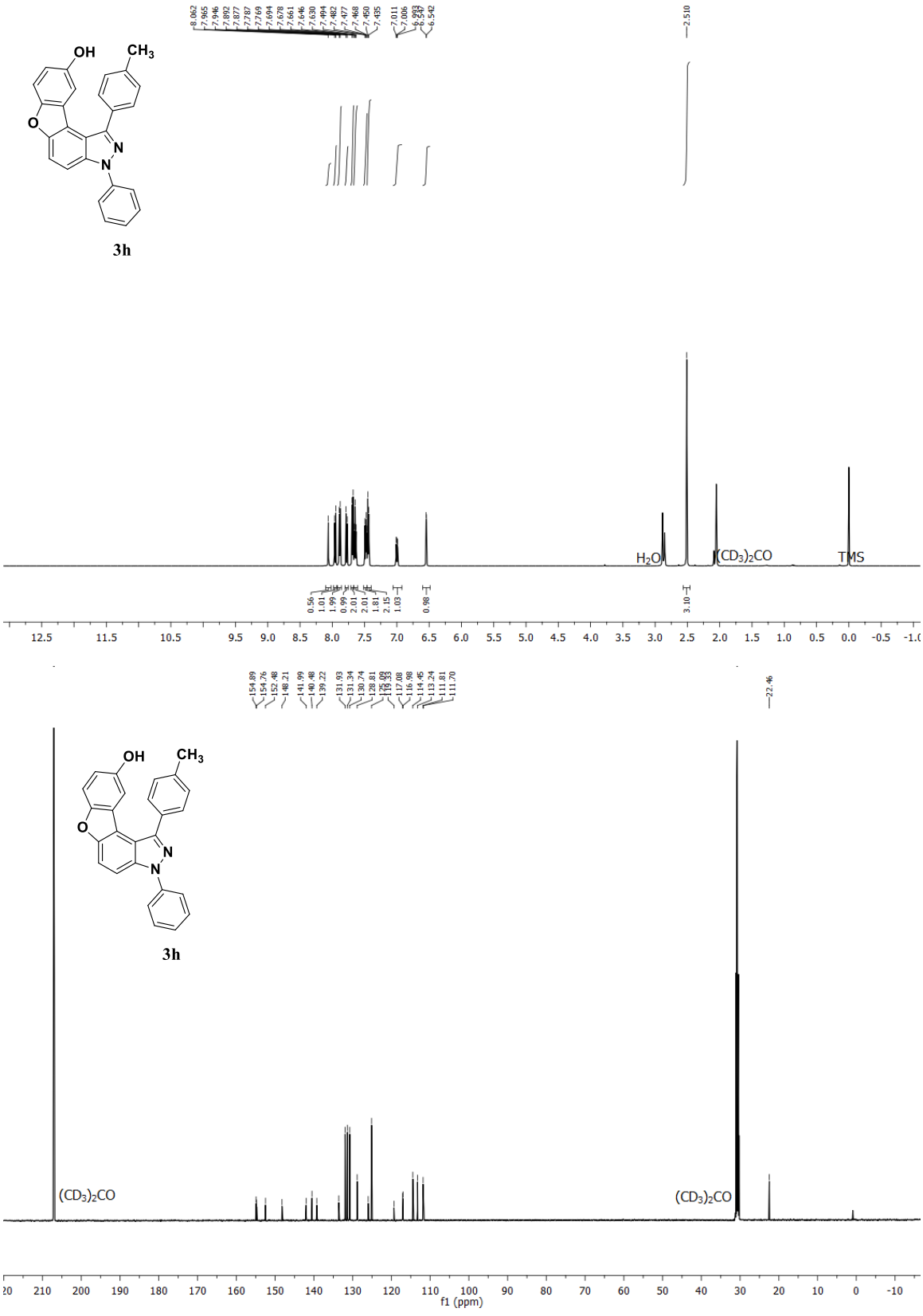




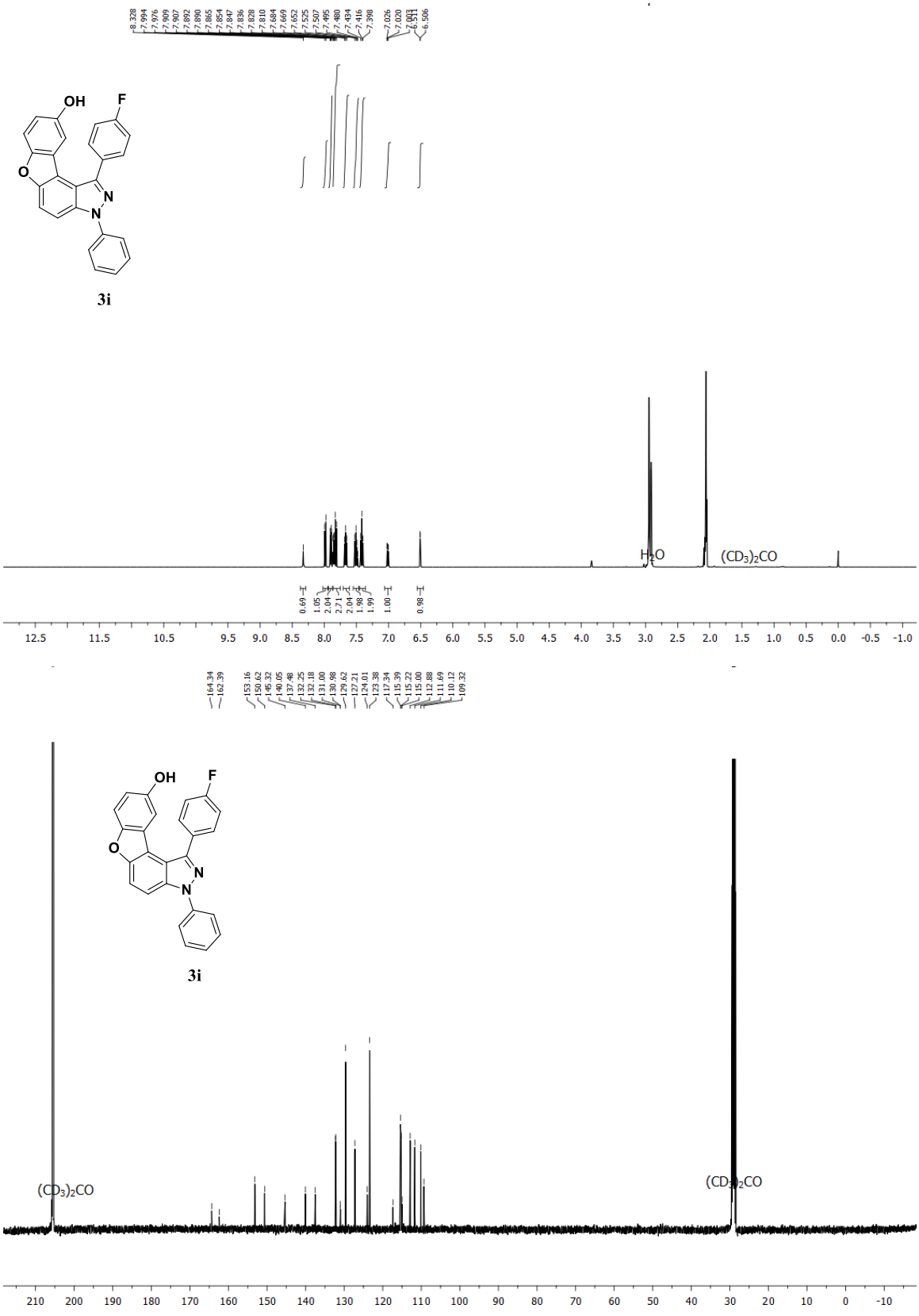
1-(4-methoxyphenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3g)



3-phenyl-1-(p-tolyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3h)

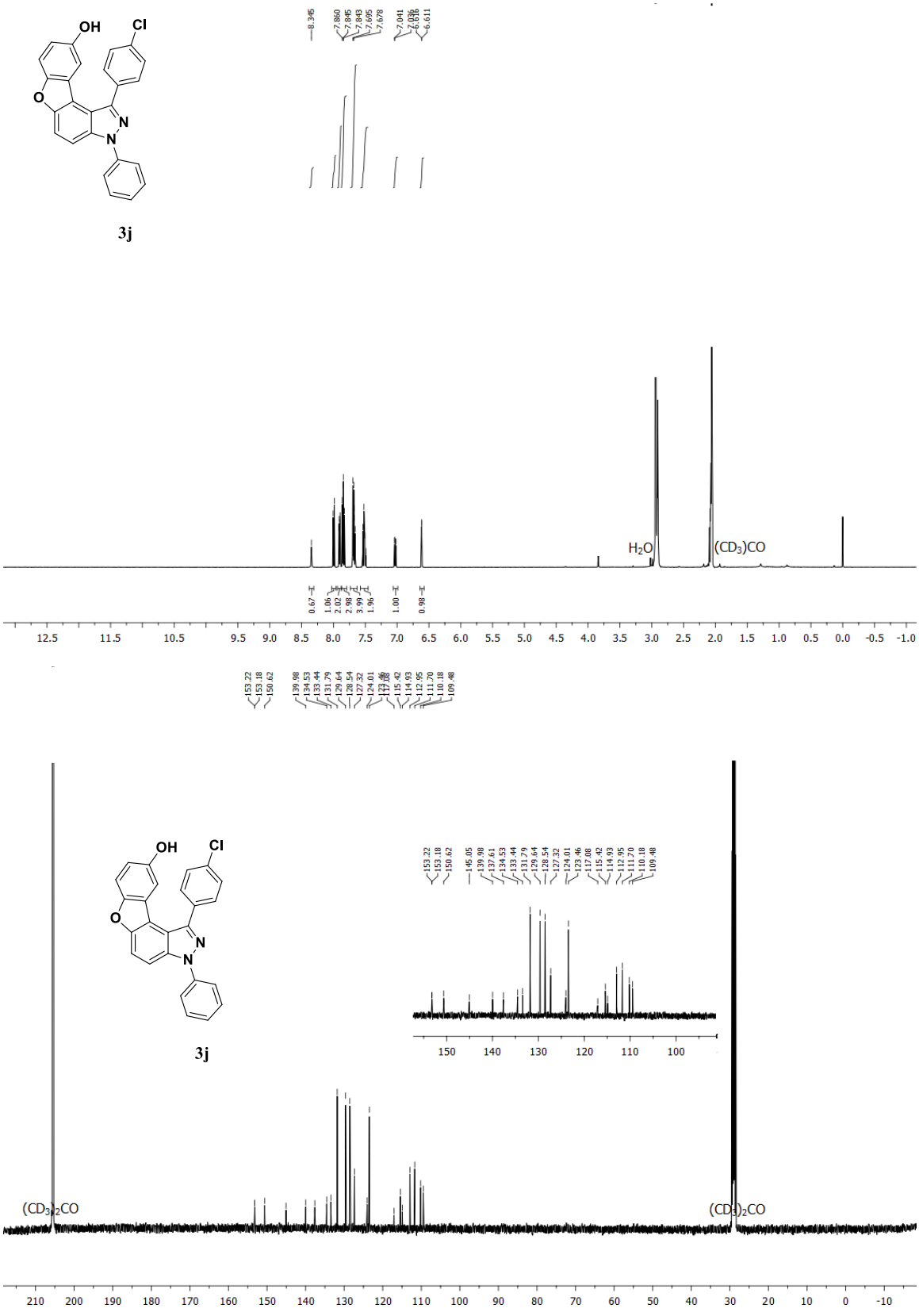


1-(4-fluorophenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3i)

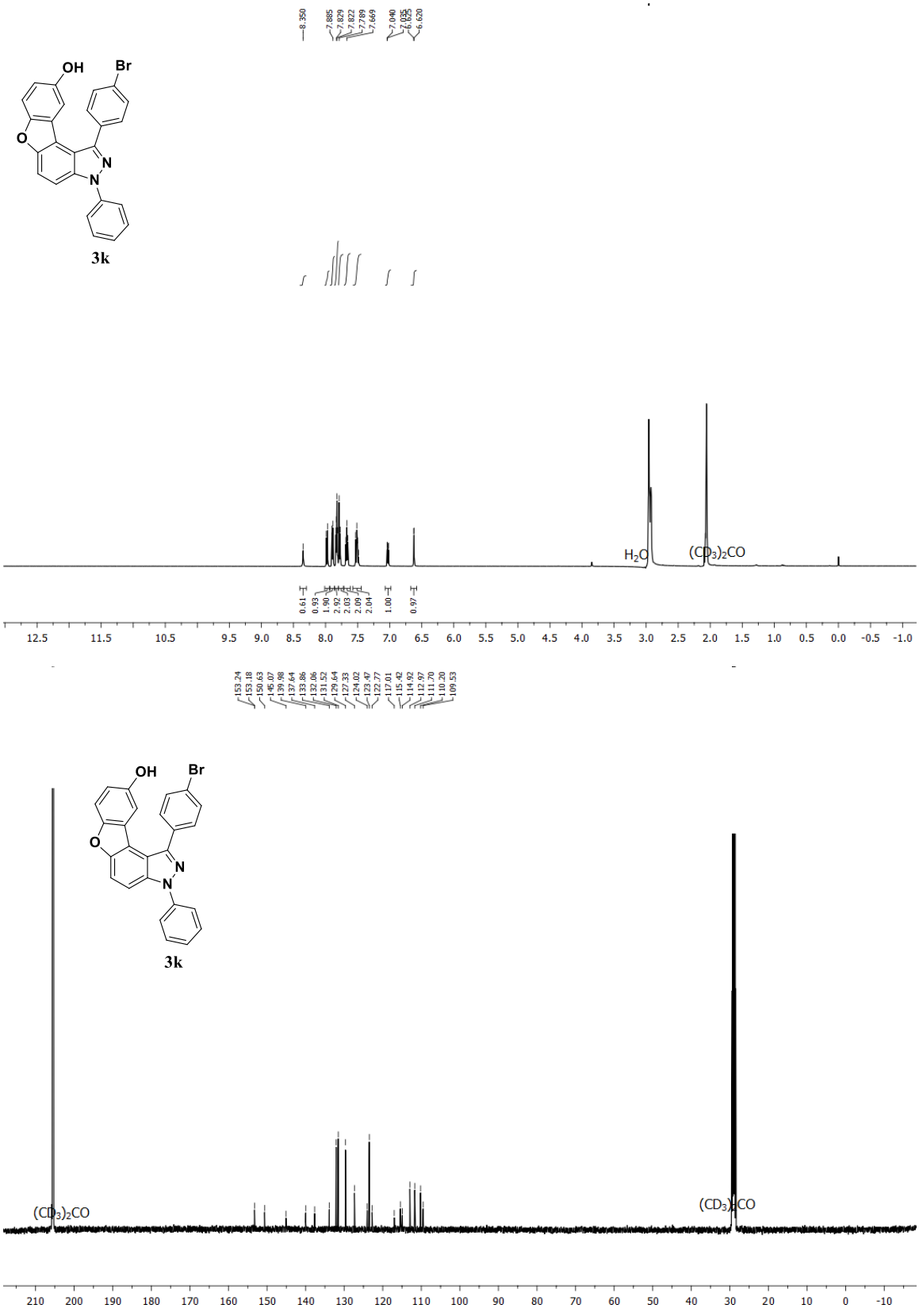


1-(4-chlorophenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3j)

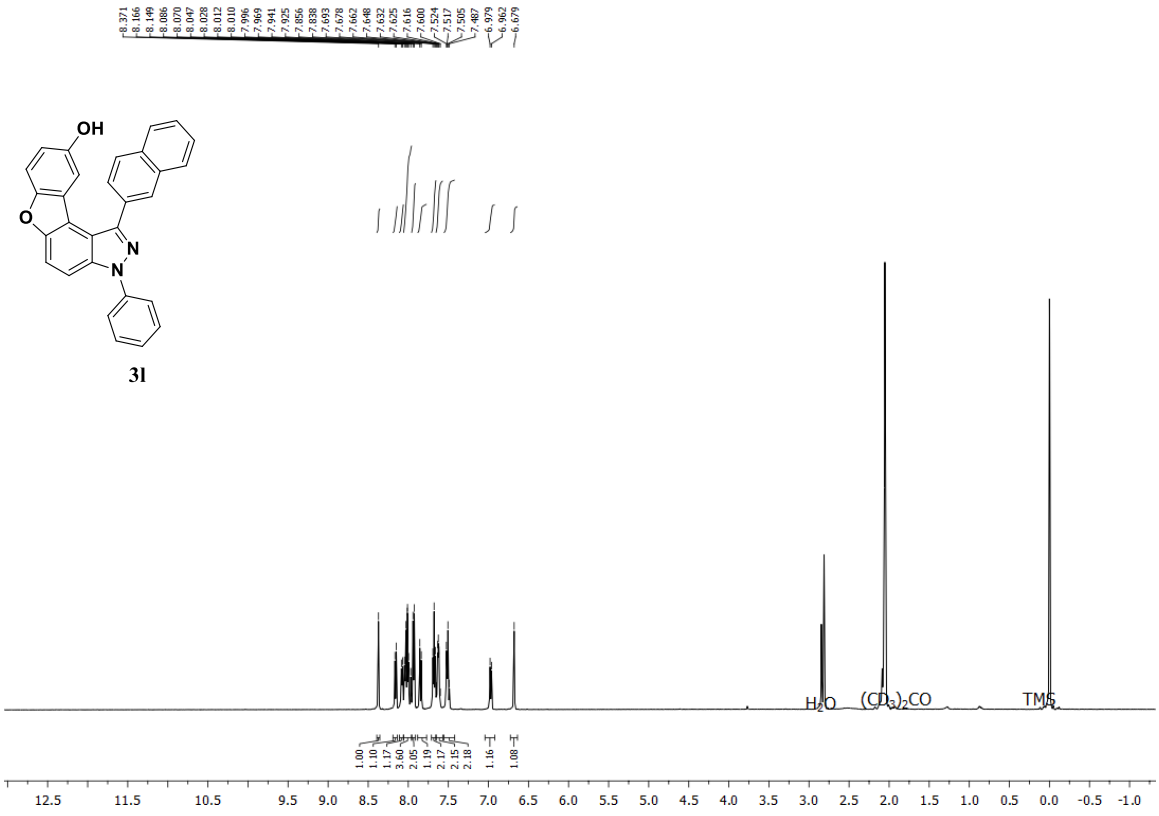
3j

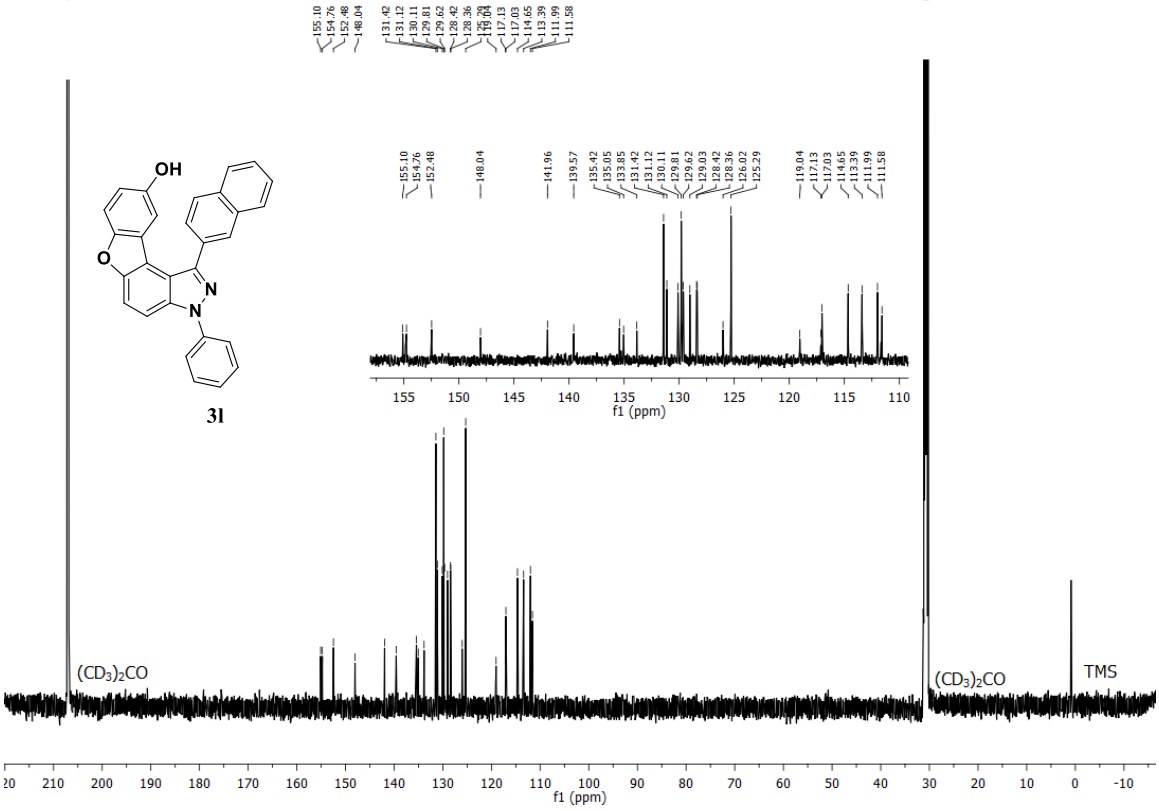


1-(4-bromophenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3k)



1-(naphthalen-1-yl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3l)





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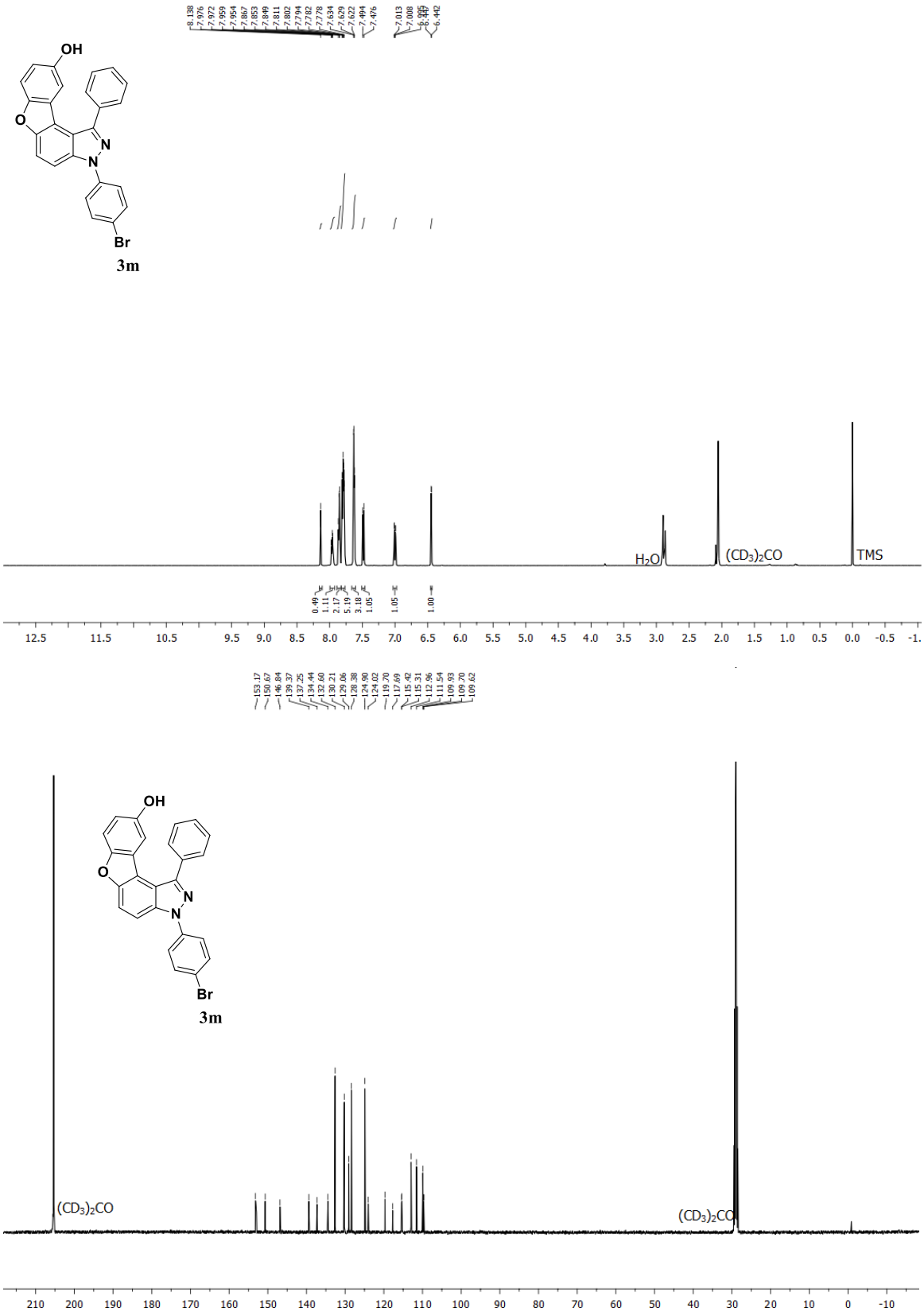
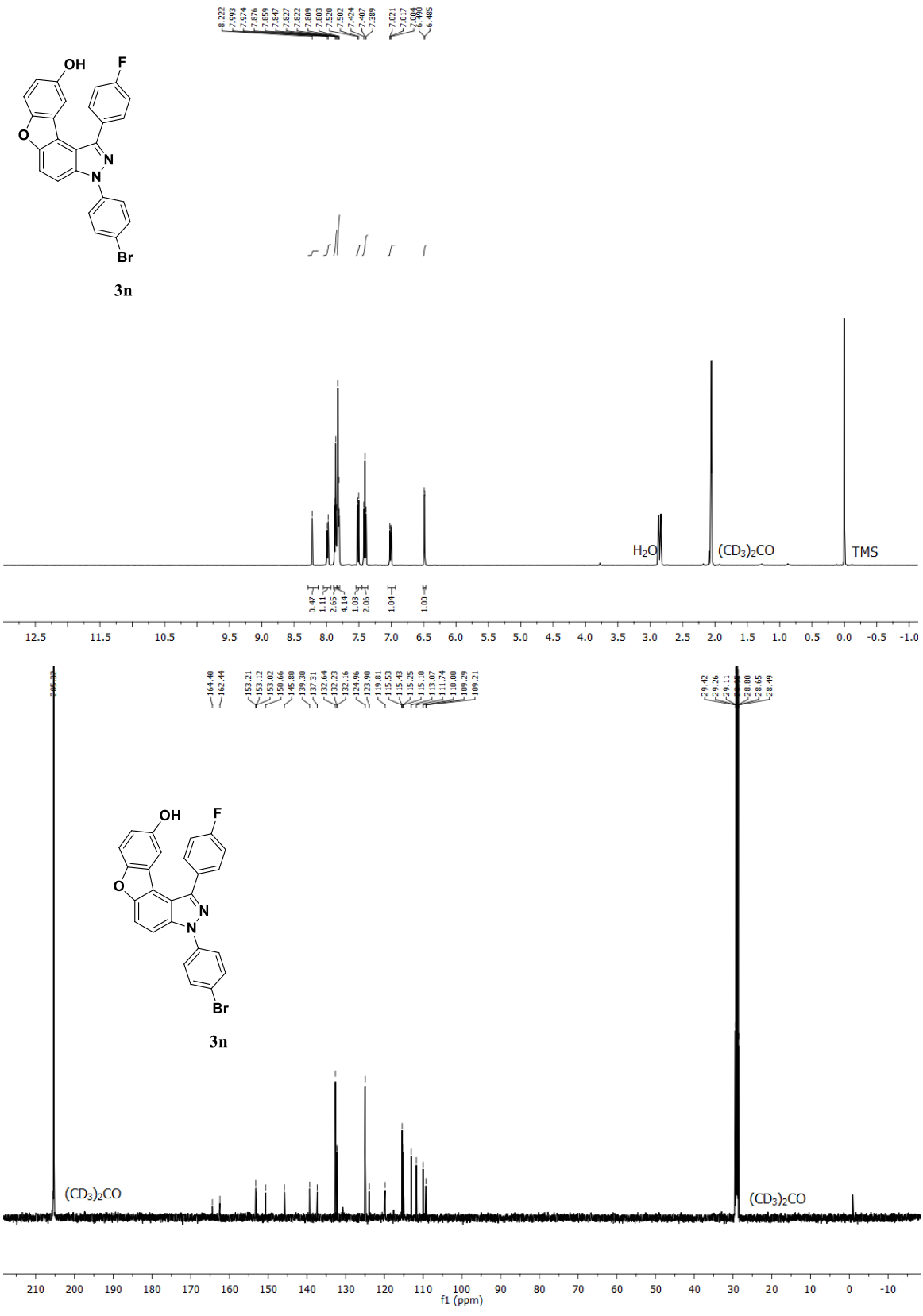
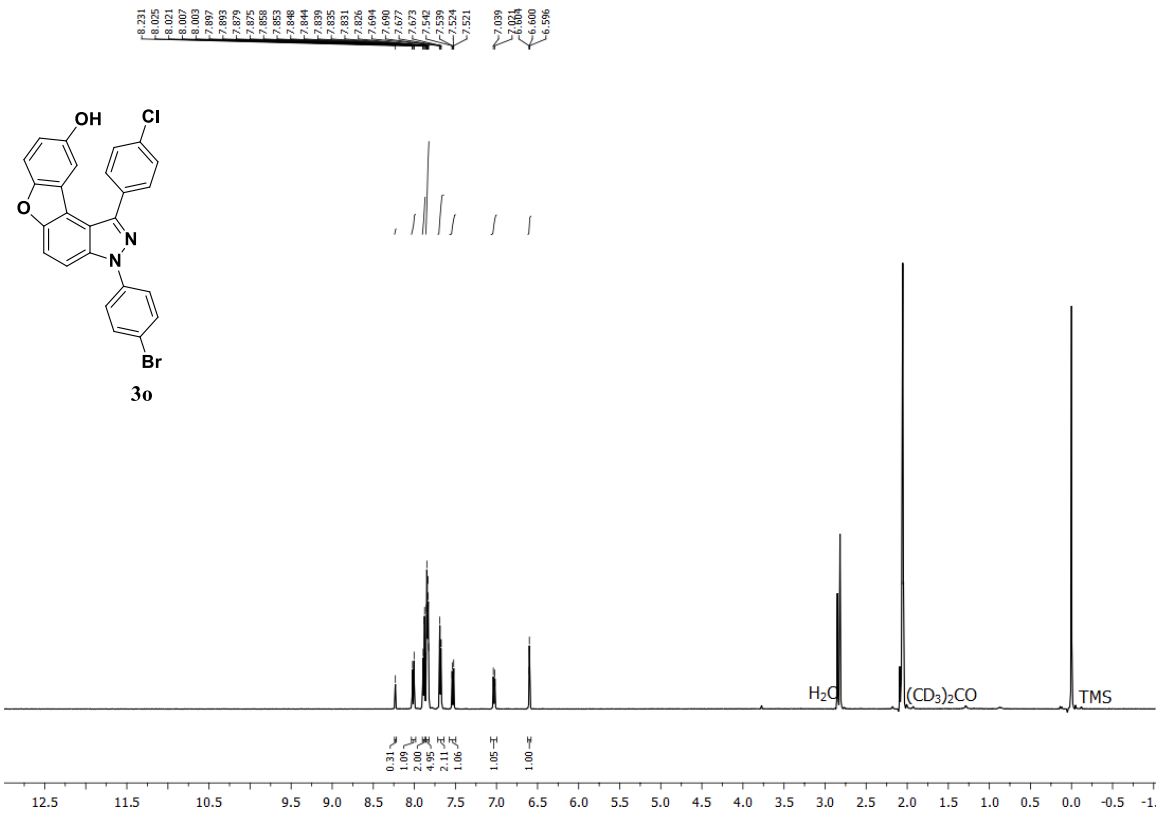
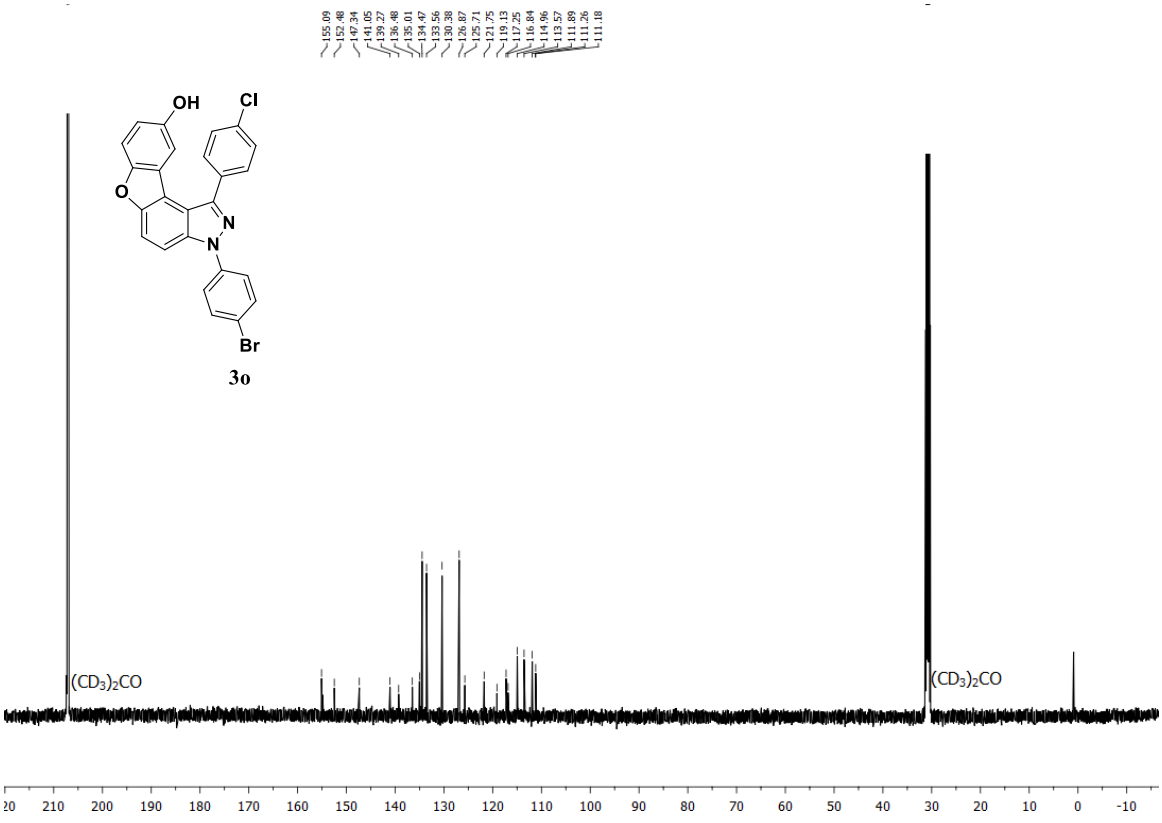


3-(4-bromophenyl)-1-(4-fluorophenyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3n)

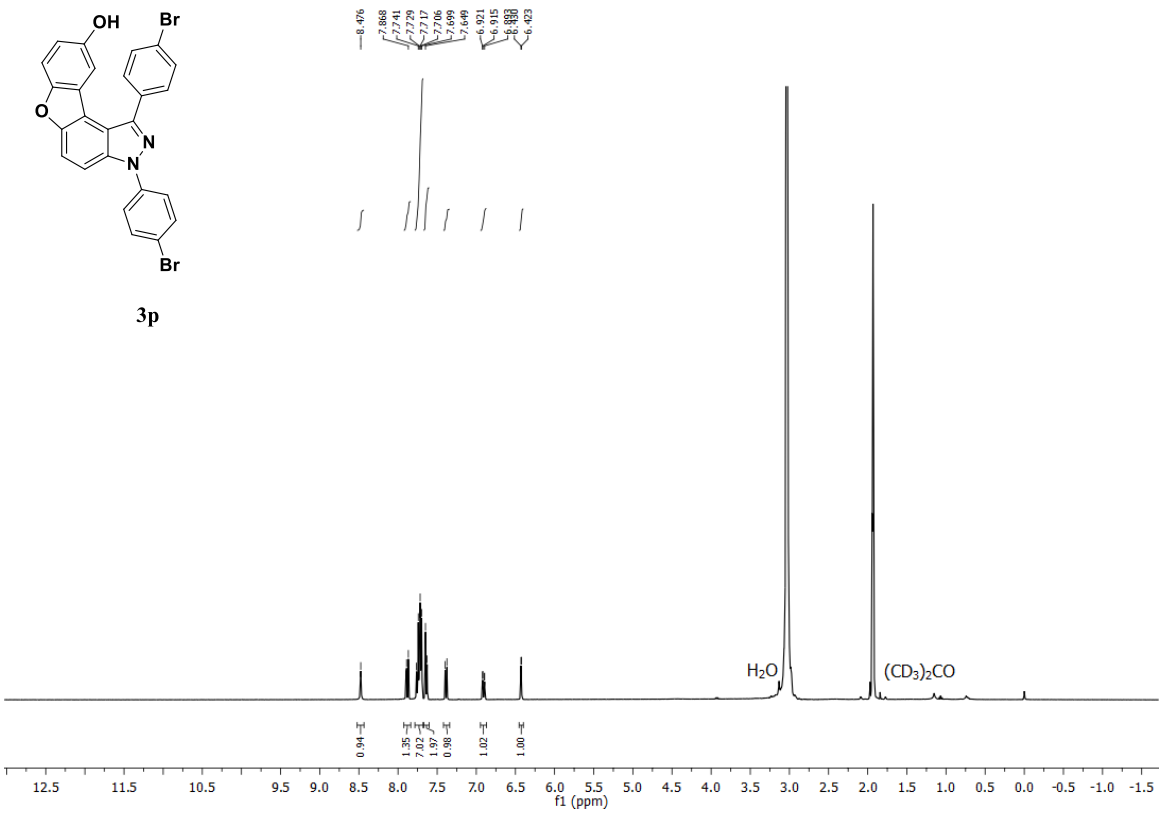


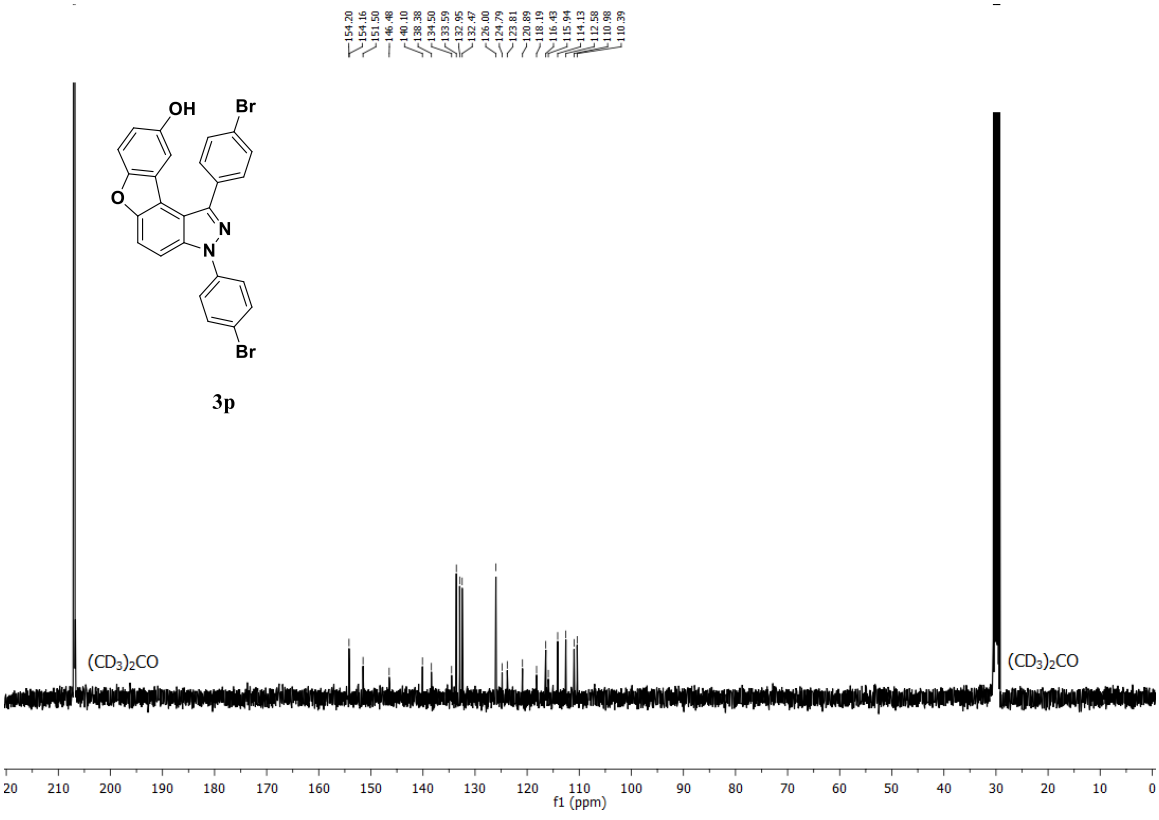
3-(4-bromophenyl)-1-(4-chlorophenyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3o)



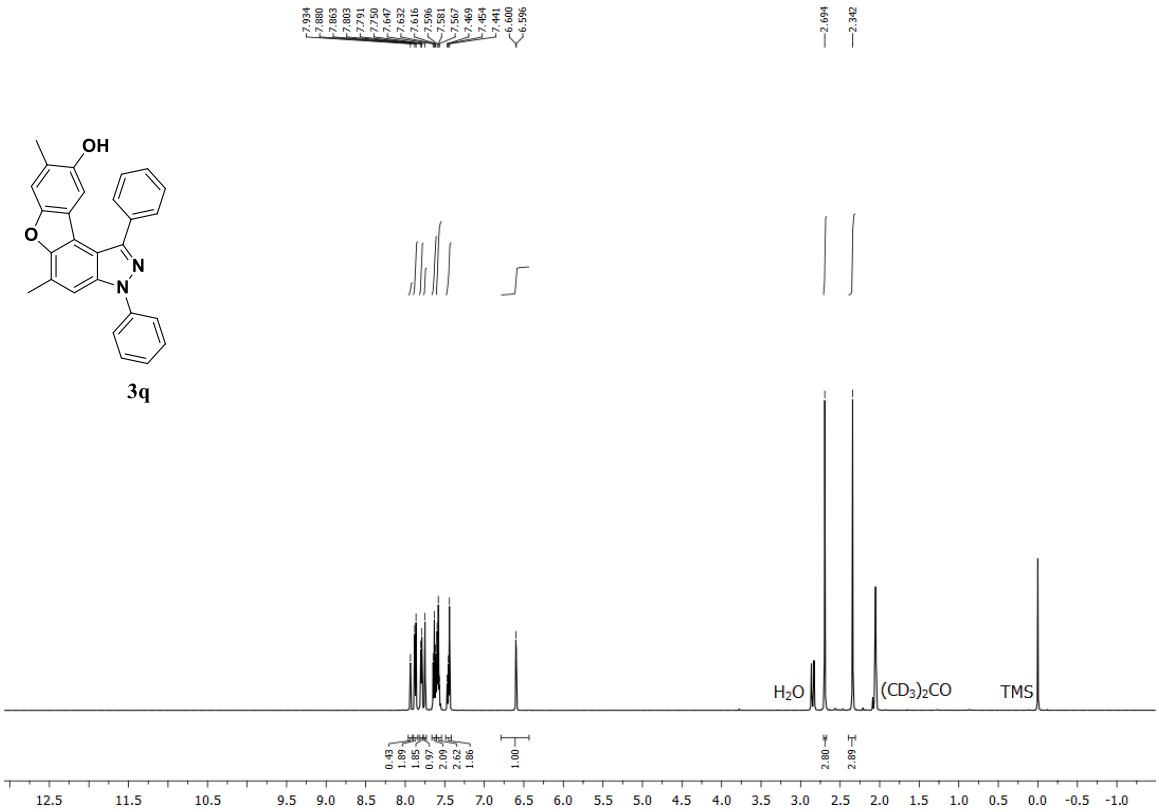


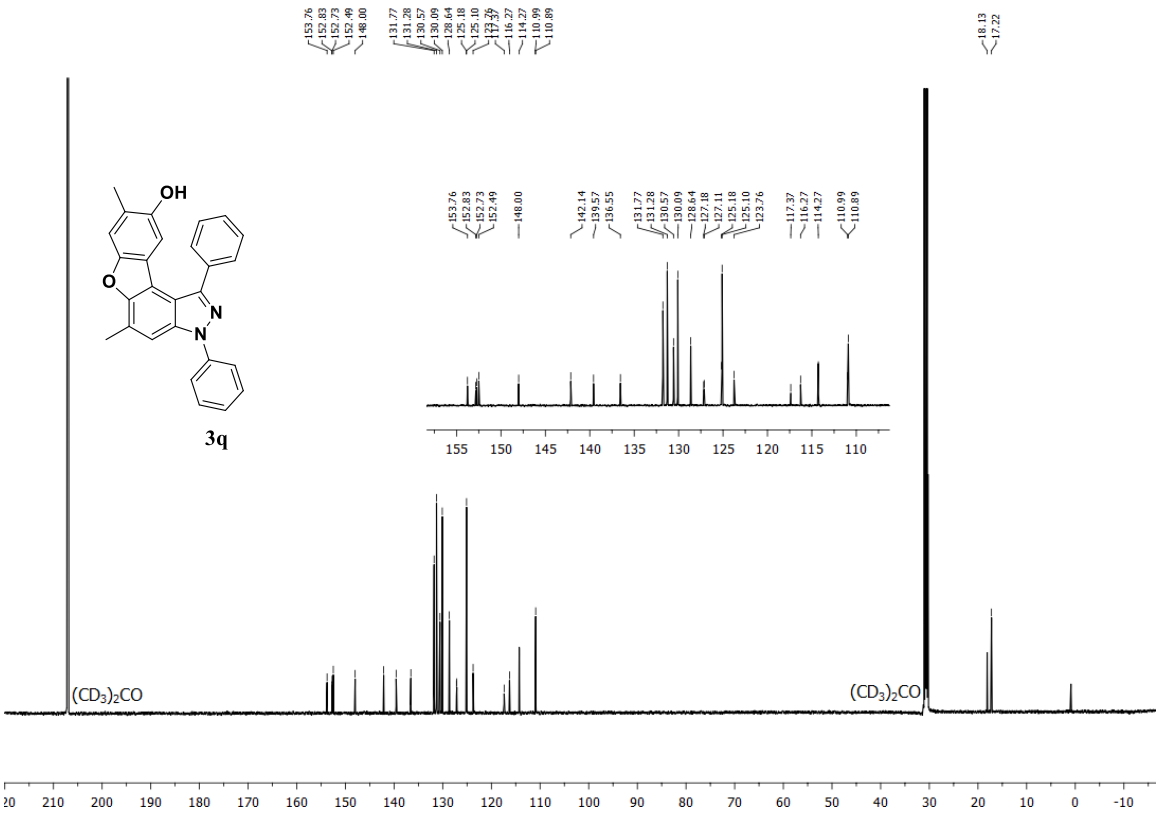
1,3-bis(4-bromophenyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3p)



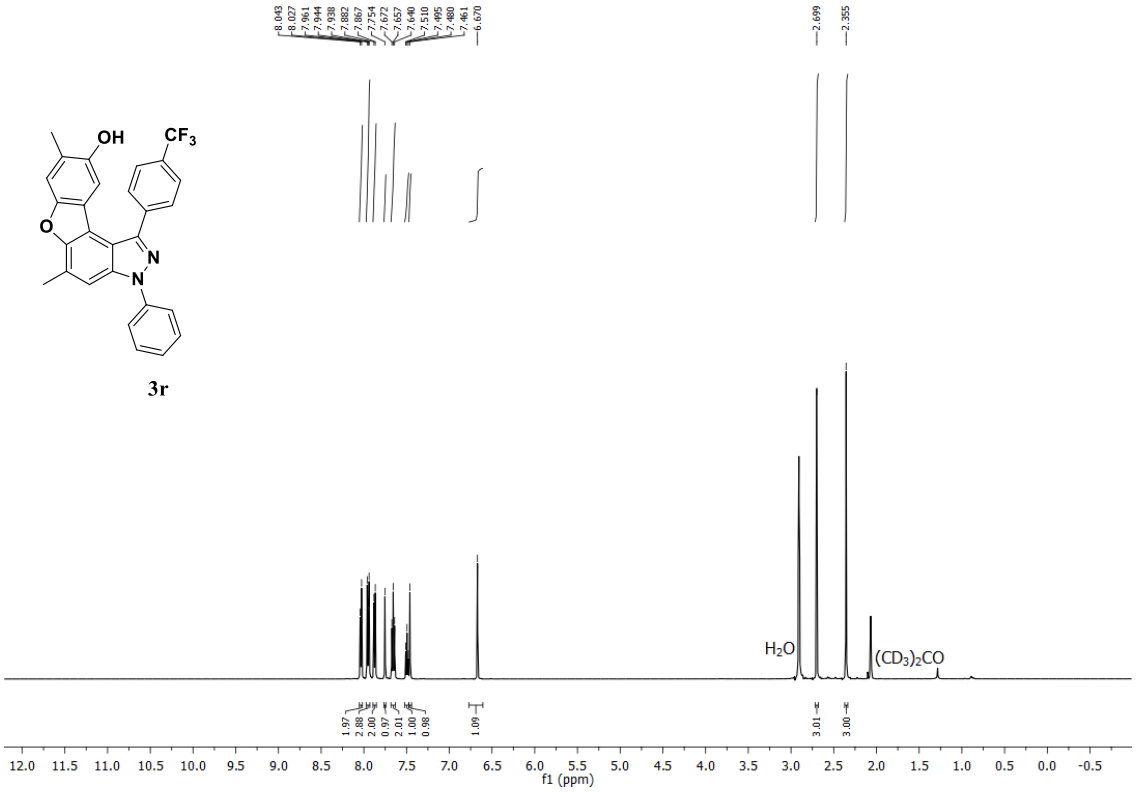


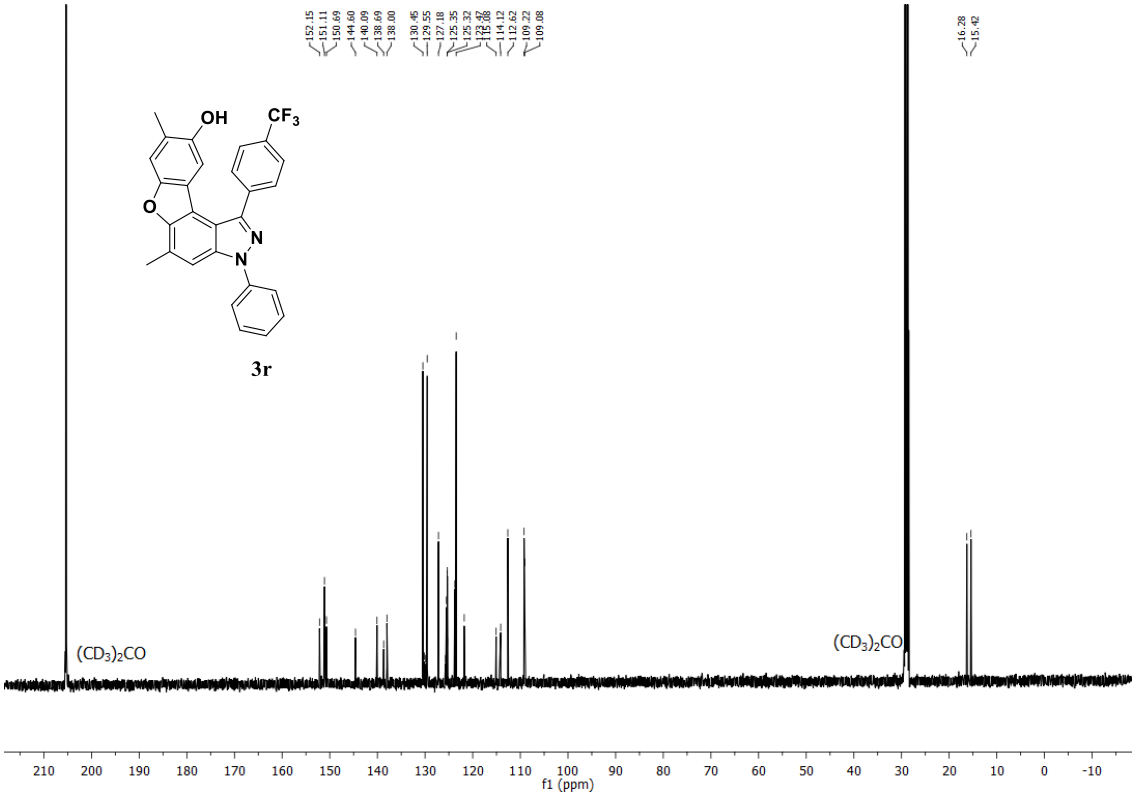
5,8-dimethyl-1,3-diphenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3q)



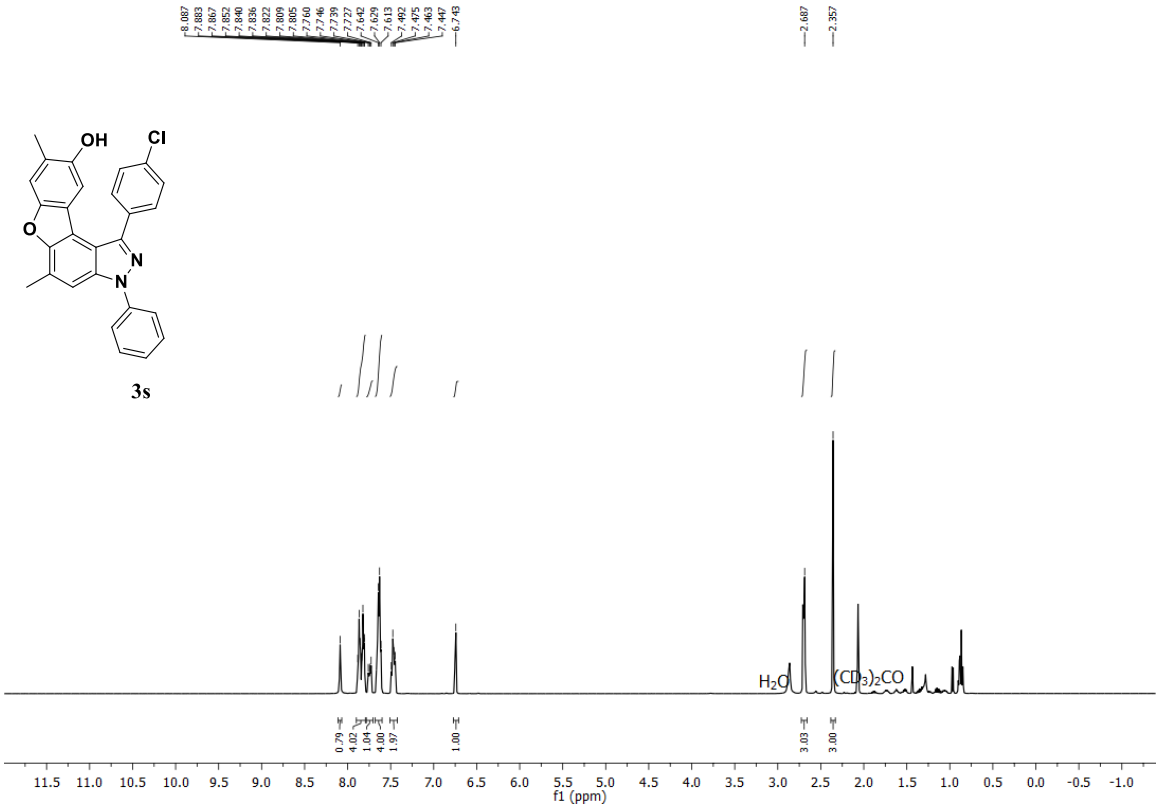


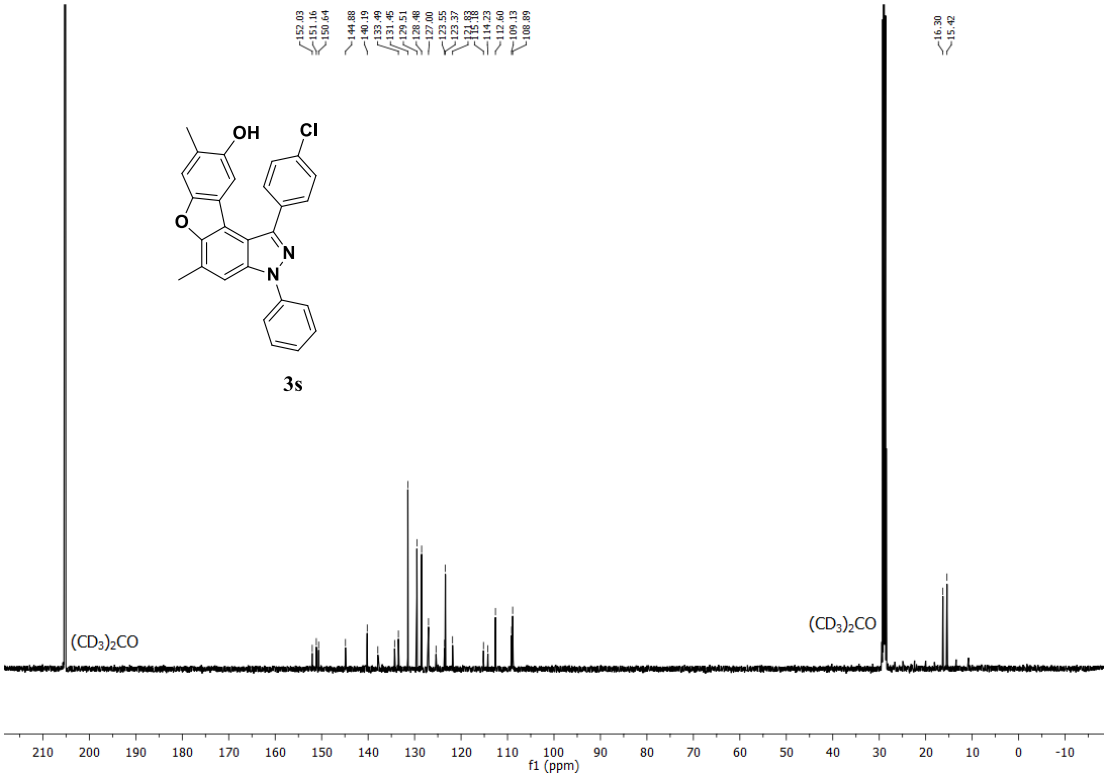
5,8-dimethyl-3-phenyl-1-(4-(trifluoromethyl)phenyl)-3H-benzofuro[3,2-e]indazol-9-ol (3r)



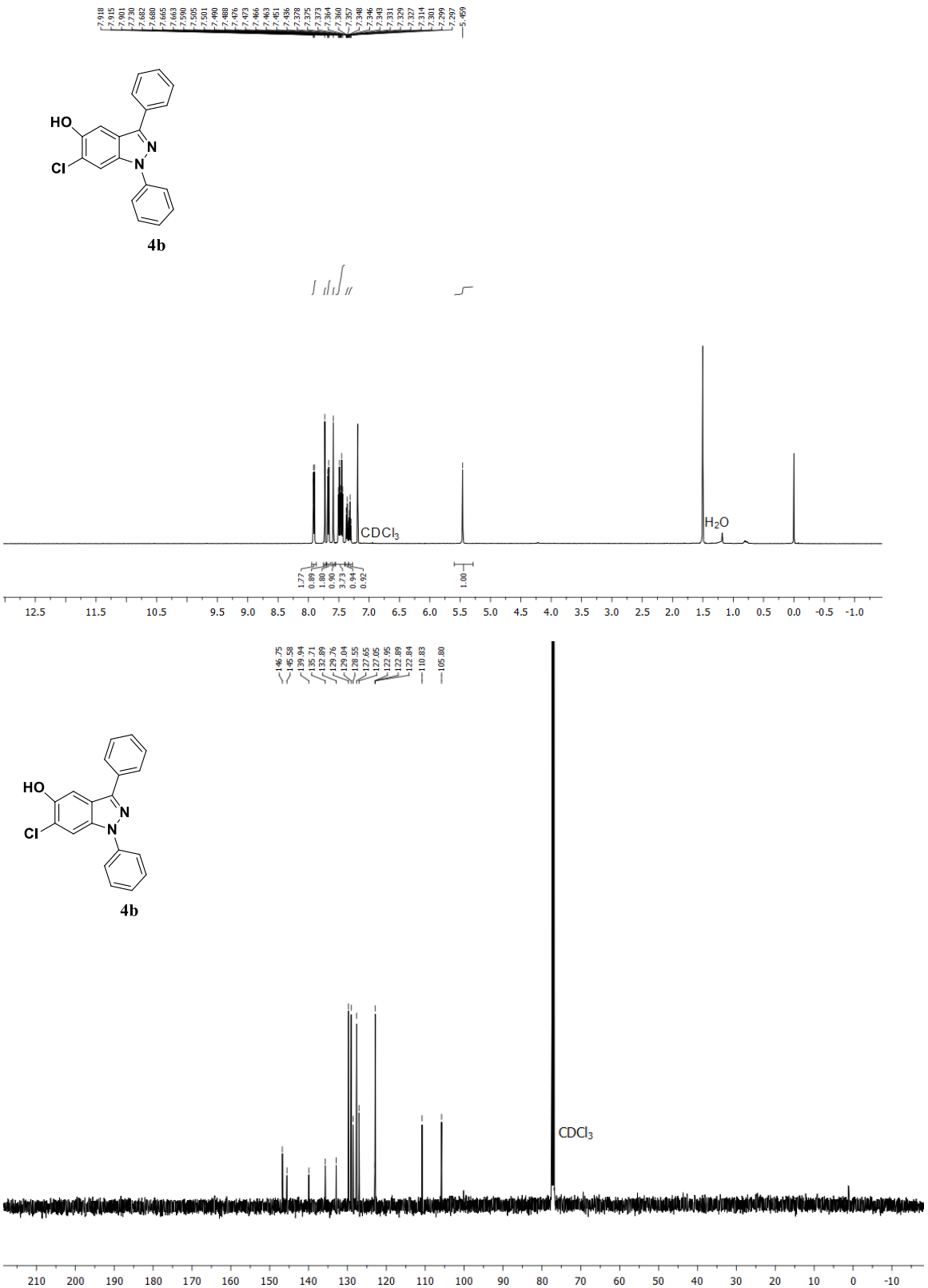


1-(4-chlorophenyl)-5,8-dimethyl-3-phenyl-3H-benzofuro[3,2-*e*]indazol-9-ol (3s)

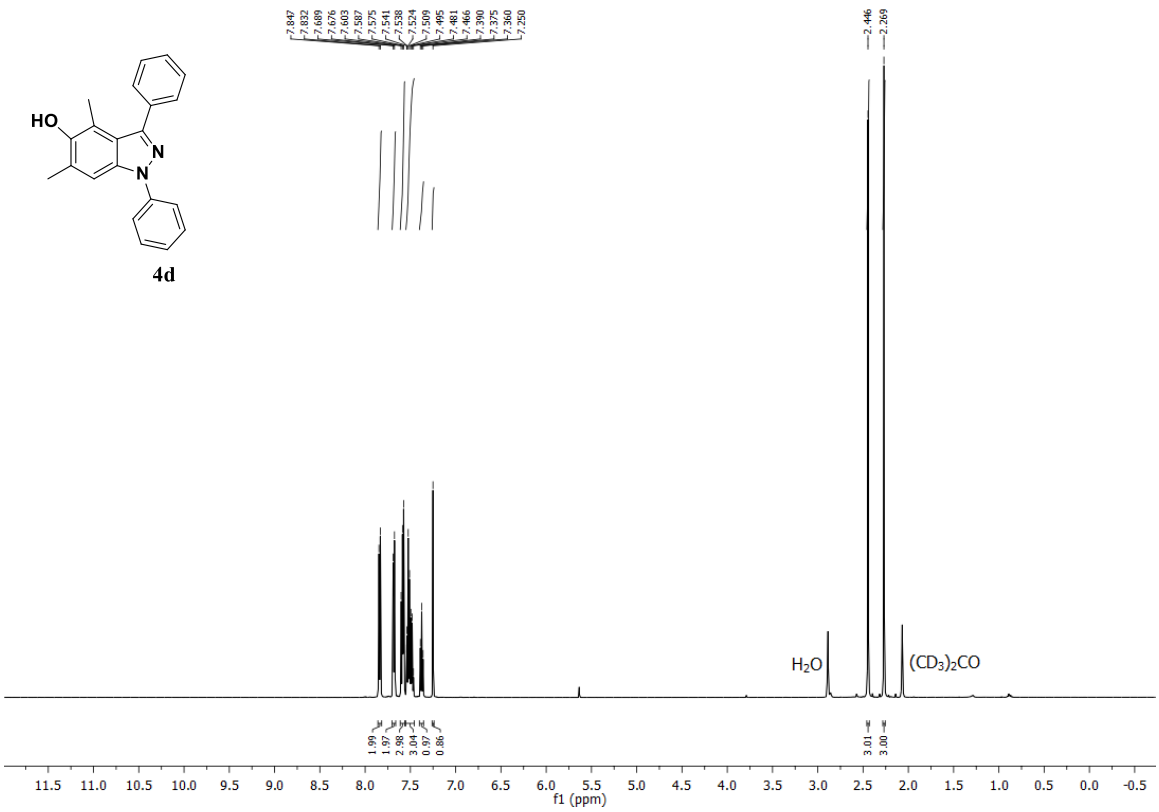


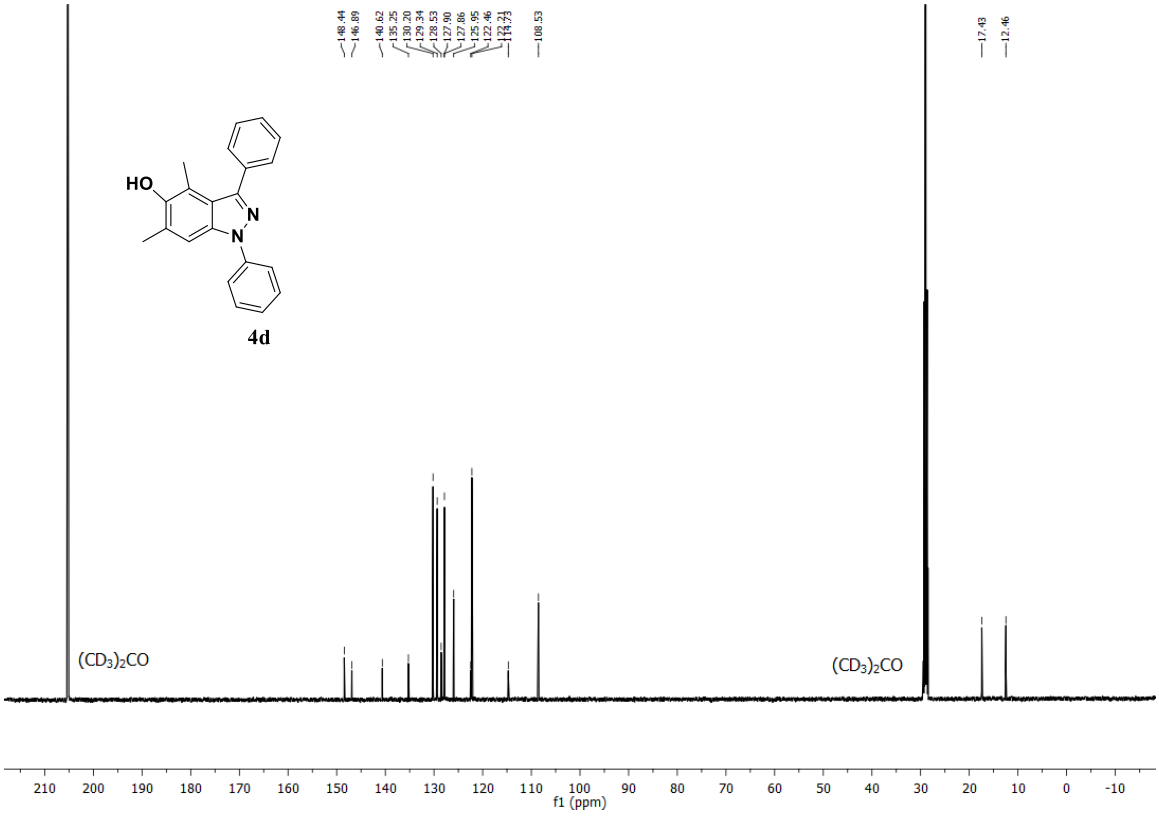


6-chloro-1,3-diphenyl-1*H*-indazol-5-ol (4b)

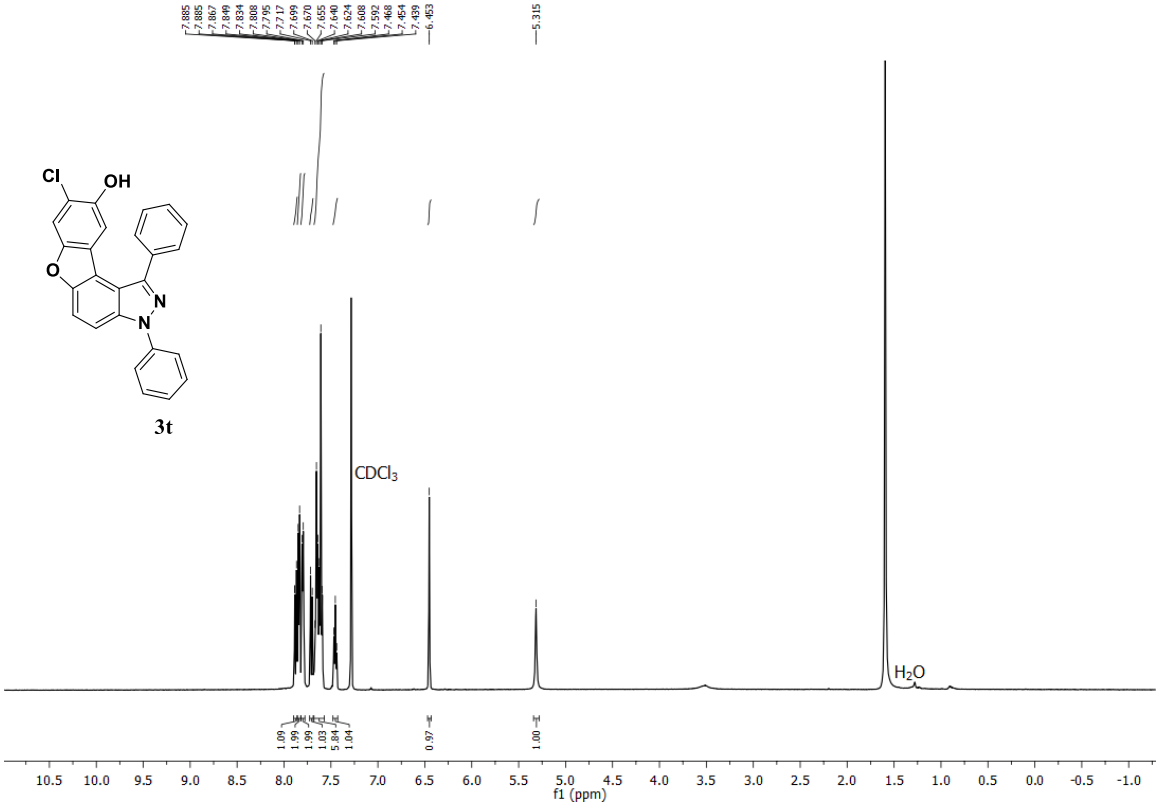


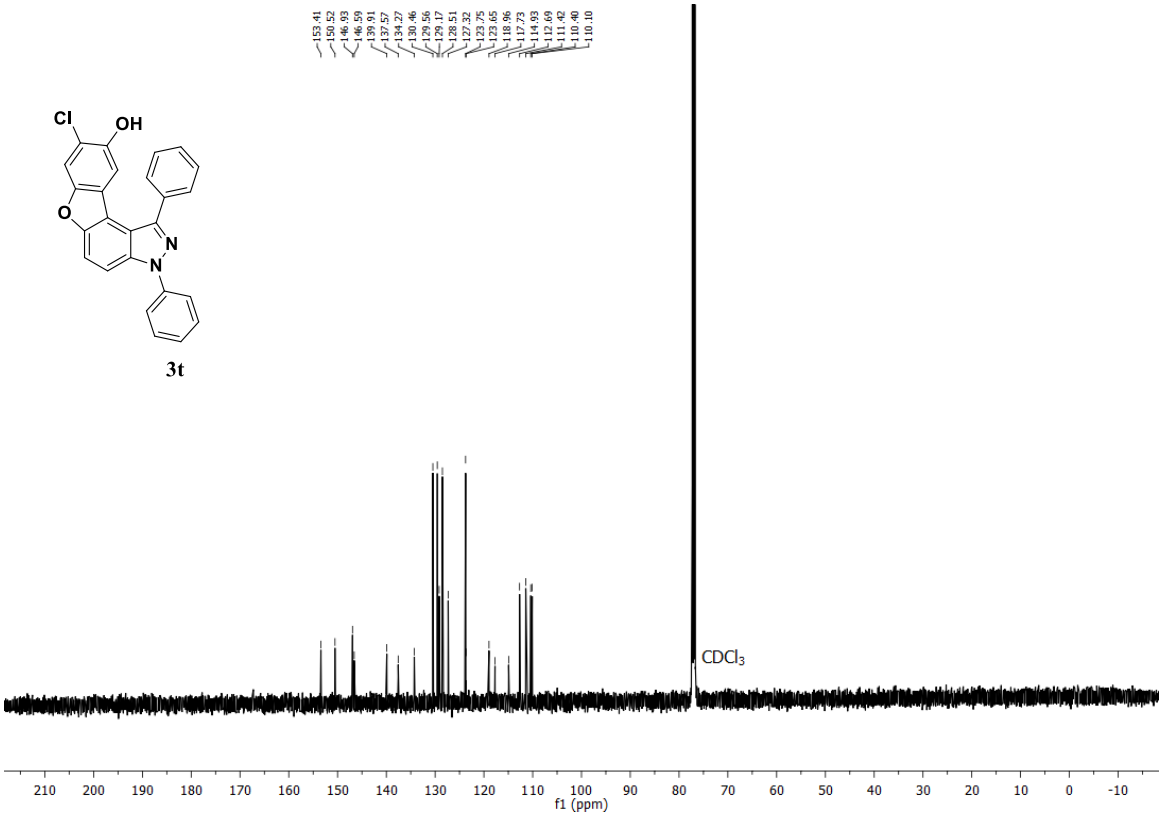
4,6-dimethyl-1,3-diphenyl-1*H*-indazol-5-ol (4d)





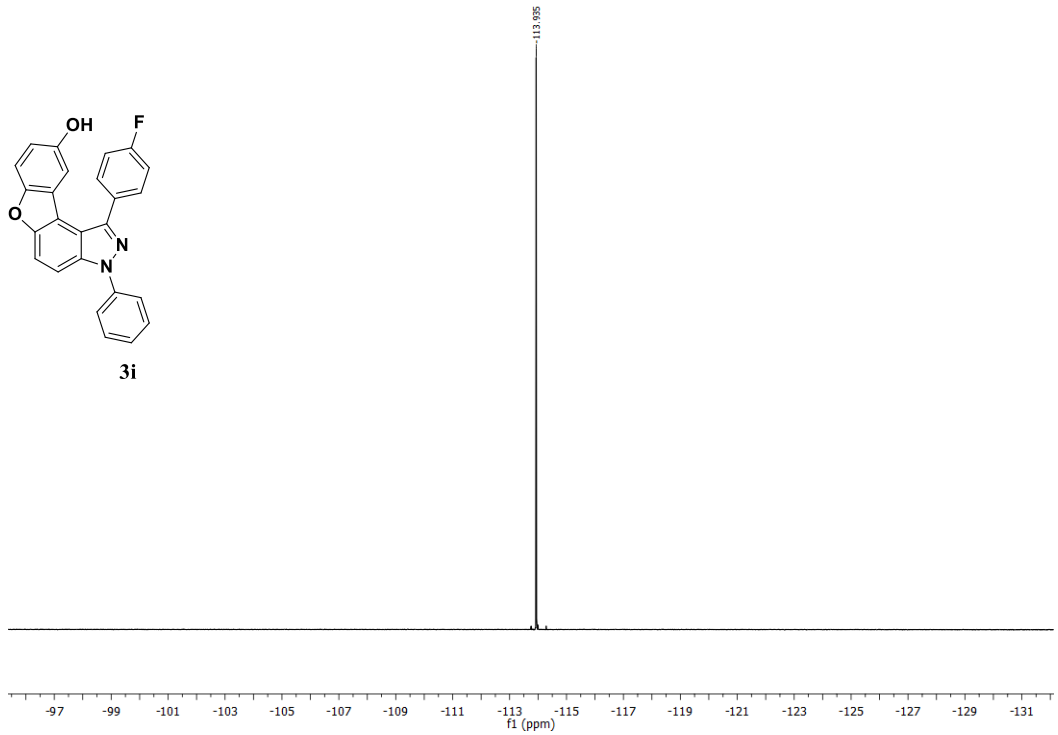
8-chloro-1,3-diphenyl-3H-benzofuro[3,2-e]indazol-9-ol (3t)



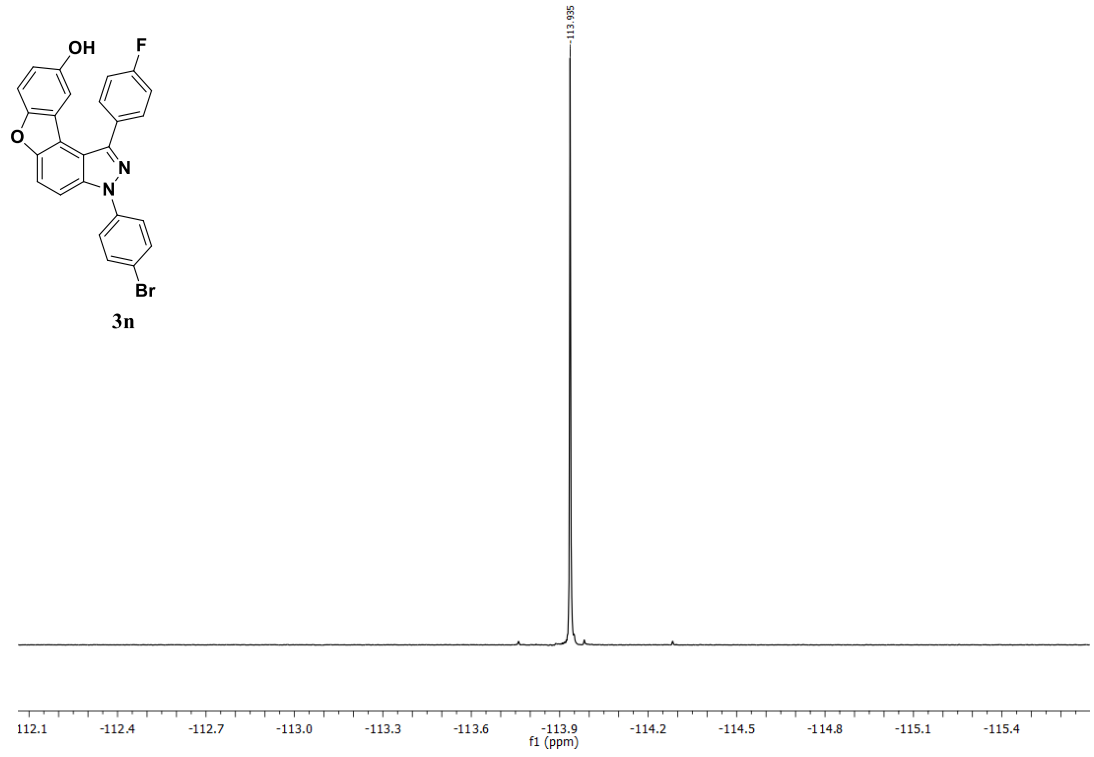


3. ^{19}F Spectrum of 3i and 3n

1-(4-fluorophenyl)-3-phenyl-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3i)



3-(4-bromophenyl)-1-(4-fluorophenyl)-3*H*-benzofuro[3,2-*e*]indazol-9-ol (3n)



4. HRMS Spectrum of the reaction between 1a and 2d