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Supporting Information

Cobalt-Catalyzed Intramolecular Decarbonylative Coupling of Acylindoles and Diarylketones through the Cleavage of C−C Bonds

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1. General information

Commercially available reagents were used without further purification. Solvents were treated prior to use according to the standard methods. All reactions were carried out under an atmosphere of nitrogen using standard Schlenk techniques unless otherwise noted. Flash column chromatography was carried out using silica gel (200–300 mesh) at increased pressure. ^{1}H NMR, ^{13}C NMR spectra were recorded on a WNMR-I spectrometer (400 MHz ^{1}H, 100 MHz ^{13}C) and Bruker AVANCE HD III (600 MHz ^{1}H, 151MHz ^{13}C). The spectra were recorded in $CDCl_3$. The spectra were recorded in $CDCl_3$ as the solvent at room temperature. ^{1}H and ^{13}C chemical shifts are reported in ppm relative to either the residual solvent peak (^{13}C) or TMS (^{1}H) as an internal standard. HRMS were performed on Bruker Daltonics MicroTof-Q II mass spectrometer. **Safety precautions.** The vessels used in this study are glass tubes with screw Teflon caps. Caution should be exercised at all times during the synthesis. Face shield and leather gloves must be worn.

2. Computational studies

Computational Details

The geometries were optimized at the density functional B3LYP[1-3] level of theory. The LANL2DZ type ECP[4] together with the valence basis functions were choosen only for the metal element and 6-31G(d)[5] for the rest. The natures of all intermediates and transition states were confirmed by analytic computation of their vibrational frequencies. Transition-state (TS) structures were verified to connect with reactants and products by following normal modes associated with the corresponding imaginary frequencies.[6] The free energies at 423.15 K (the temperature of corresponding experiments) were obtained after vibrational frequency computations. All frequencies below 50 cm^{-1} were replaced by 50 cm^{-1} when computing vibrational entropies[7] using a Python script written by Rob Paton and Ignacio Funes-Ardoiz[8]. For all species but CO (gas at 1 atm), a factor of RT×ln(34.7) (2.98 kcal mol^{-1}) was added to account for the 1 atm to 1 M standard-state change.

Single-point energies based on the B3LYP geometries were obtained at M06/LANL2TZ(f)(Ni)/6-311+G(d,p) level.[9-12] Solvation effects in 1,4-dioxane were treated by the implicit sol-vation model SMD.[13] All calculations were performed with the Gaussian09 program.[14] The molecule graphs were produced by CYLview (version 1.0 BETA) program.[15]

Finding the catalyst

Starting from the precatalyst $Co_2(CO)_8$ and the ligand NHC, there are several possible candidates for the catalyst depending on how the CO ligands disscociate and NHC coordinates to the metal. We denote these candidates with the general formula $Co_2(CO)_m(NHC)_n$ (m = 0–7, n = 1–2).

First of all, the precatalyst/NHC ratio is 1 based on some experimental evidences although a 1/2 ratio was used in this paper to improve the coordination. The NHC may combine to the Co atom coordinating to the substrate or the other metal atom, and we denote these two situations as mode A and B, respectively. The procatalyst $Co_2(CO)_8$ satisfies the 18e rule, and at least one CO has to be dissociated to create active sites. It requires more than 40 kcal mol $^{-1}$ to generate Co_2 $(CO)_3$(NHC) from $Co_2(CO)_8$ and NHC, thus the complex with $m \leqslant 3$ could not be generated under the experimental conditions. For m = 6–4 with both mode A and B, the free energies along the reaction path were examined. The $Co_2(CO)_4$(NHC) catalyst shows the lowest energy span δ E. The reaction paths for m = 6 and 5 have energy differences between **TS1** and the references (catalyst + substrate) larger than the δE value (Figure S1).

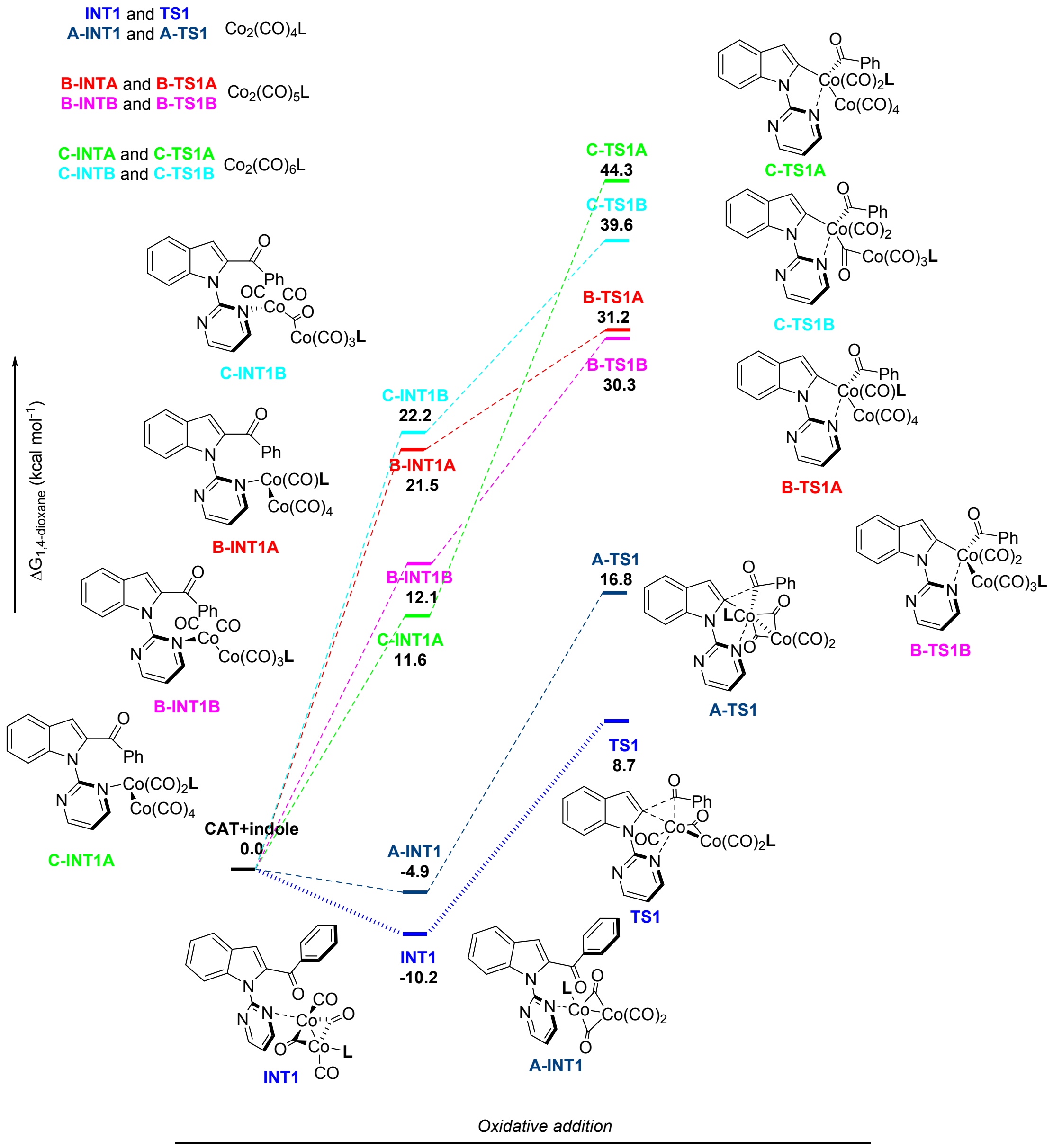
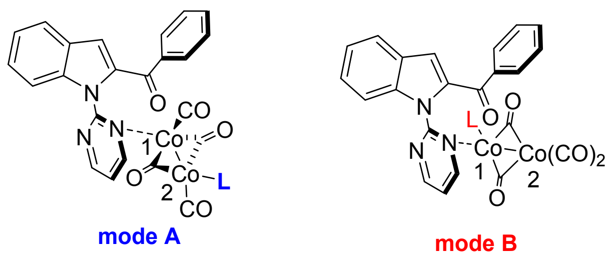


Figure S1 Free engergies of possible candidates for the catalyst

There are two possible coordination modes for this transformation. In mode A, NHC ligand coordinated to the Co2. In mode B, NHC ligand coordinated to the Co1.



An alternative made is NHC ligand coordinated to the Co1 (mode B), which is disfavored by more than 30 kcal mol^{-1} compared to the mode A. The computed activation energy barrier for decarbobylative step is 52.1 kcal mol^{-1}, which is higher than the total activation energy in mode A.

Consequently, mode B could be ruled out at this stage

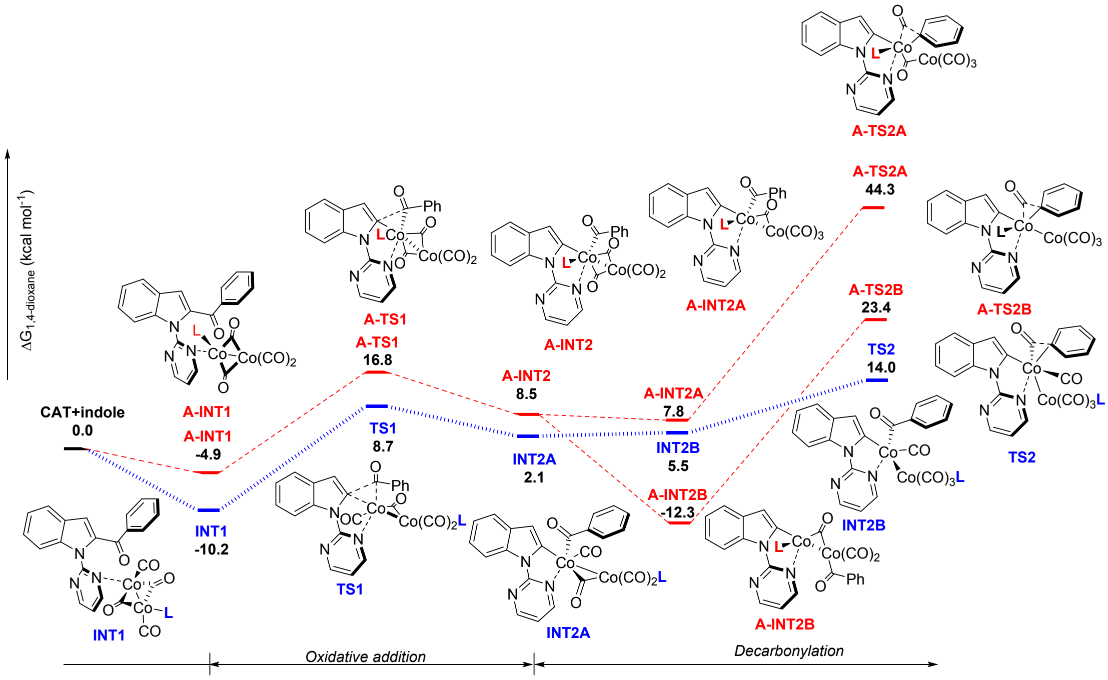


Figure S2 Free engergies of modes A and B.

The DFT-study was conducted (without considering NHC ligand). The result shows the NHC ligand is crucial for the reaction mechanism and the barriers.

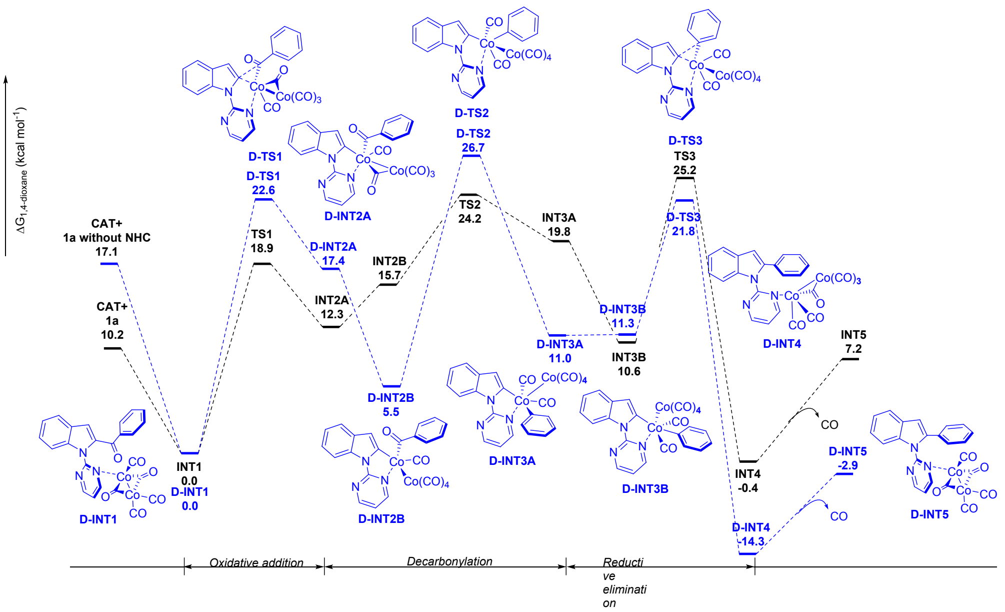


Figure S3 DFT-calculated reaction energy profile of Co-catalyzed decarbonylation (blue: without considering NHC ligand).

M06 single point energies E in Hartrees for all optimized species and free energies G at 423.15 K.

Species	E	G
Indole	-970.886646940	-970.68340794
D-CAT	-856.792844318	-856.819630318
D-INT1	-1827.7354824	-1827.5255174
D-TS1	-1827.70097473	-1827.48956173
D-INT2A	-1827.70740099	-1827.49782299
D-INT2B	-1827.72777575	-1827.51640675
D-TS2	-1827.69315931	-1827.48303431
D-INT3A	-1827.7160514	-1827.5064284
D-INT3B	-1827.71612527	-1827.50687127
D-TS3	-1827.6986544	-1827.4907534
D-INT4	-1827.75650455	-1827.54837155
D-INT5	-1714.42970958	-1714.22571758
C-INT1A	-2865.98321219	-2865.39688219
C-TS1A	-2865.93059654	-2865.34466354
C-INT1B	-2865.96627989	-2865.38343389
C-TS1B	-2865.94038155	-2865.35569955
B-INT1A	-2752.66506340	-2752.0773824
B-TS1A	-2752.64675607	-2752.06184207
B-INT1B	-2752.68782769	-2752.10593169
B-TS1B	-2752.66148876	-2752.07685876
A-INT1	-2639.36876489	-2638.78862489
A-TS1	-2639.33737942	-2638.75399122
A-INT2	-2639.34949217	-2638.76715617
A-INT2A	-2639.35087280	-2638.7683378
A-TS2A	-2639.28931908	-2638.71019708
A-INT2B	-2526.04561554	-2525.46966854
A-TS2B	-2525.99022566	-2525.41277466

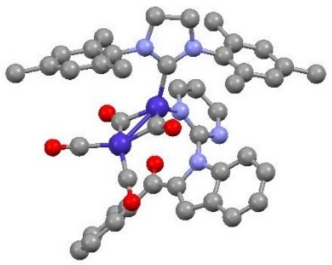
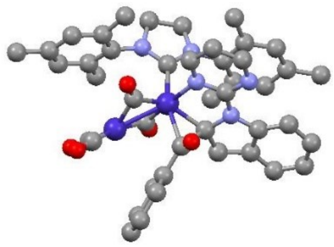
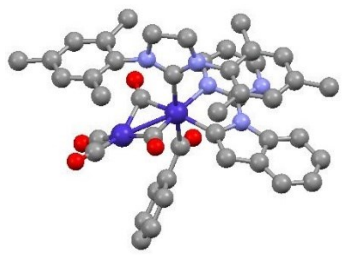
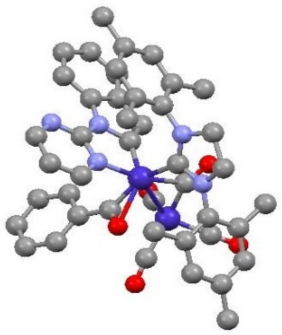
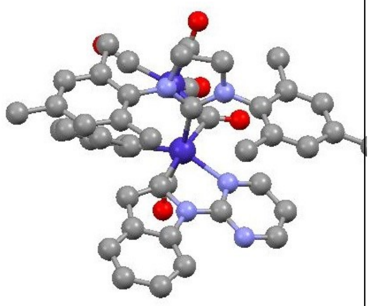
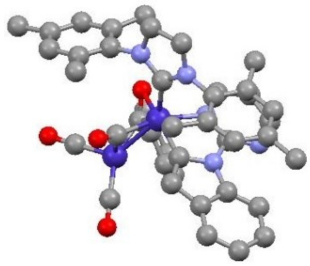
Details of density functional theory (DFT) study on the reaction mechanism

M06 single point energies E in Hartrees for all optimized species and free energies G at 423.15 K.

Species	**E**	**G**
INT1	-2639.37651424	-2638.80010324
TS1	-2639.34844063	-2638.76995912
INT2A	-2639.35877438	-2638.78041638
INT2B	-2639.35369343	-2638.77511443
TS2	-2639.33991110	-2638.7614351
INT3A	-2639.34608012	-2638.76853712
INT3B	-2639.35869006	-2638.78310106
TS3	-2639.33686723	-2638.75992123
INT4	-2639.37735815	-2638.80066115
INT5	-2526.05618035	-2525.48413135

CAT	-1668.44168332	-1668.10515332
Indole	-970.886646940	-970.68340794
Product	-857.580800525	-857.383829525
CO	-113.280672859	-113.304440859
INT3A’	-2526.04013057	-2525.46570757
INT3B’	-2526.04174722	-2525.47093122
TS4	-2526.02285149	-2525.45233249

Structures of intermediates and transition states:

A-INT1	A-TS1	A-INT2
		
A-INT2A	**A-TS2A**	**A-INT2B**
		
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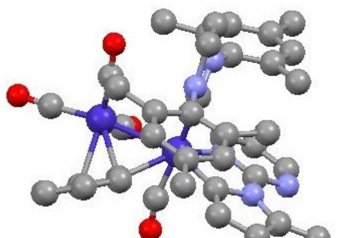
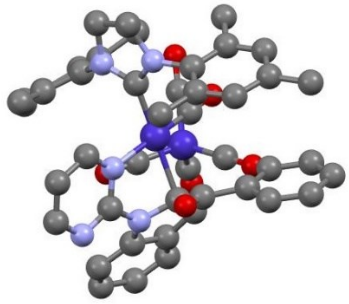
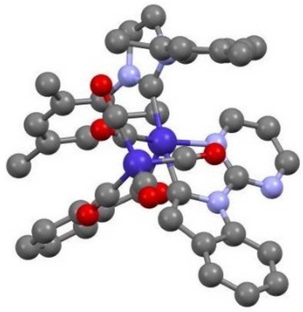
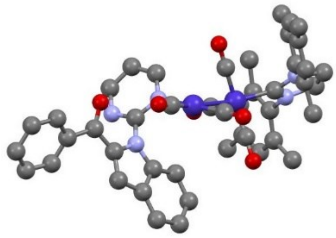
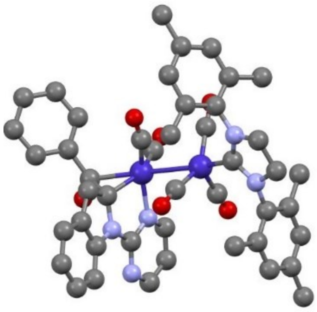
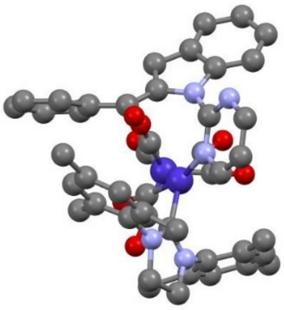
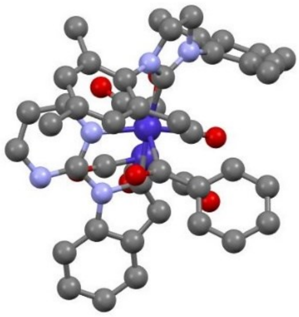
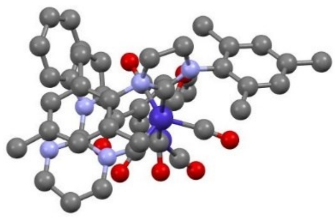
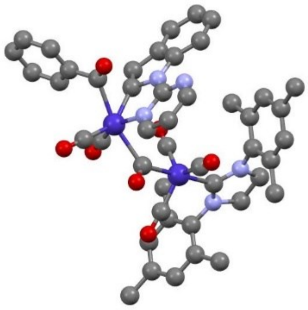
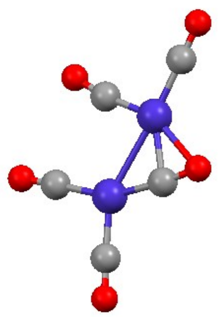
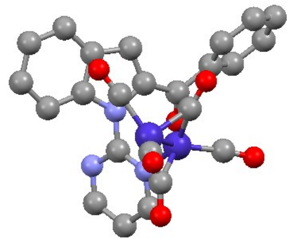
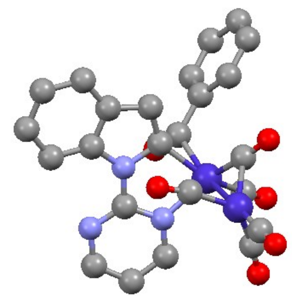
		
B-INT1A	**B-TS1A**	**B-INT1B**

		
B-TS1B 		
C-INT1A 	**C-TS1A** 	**C-INT1B** 
C-TS1B 		
D-CAT	**D-INT1**	**D-TS1**

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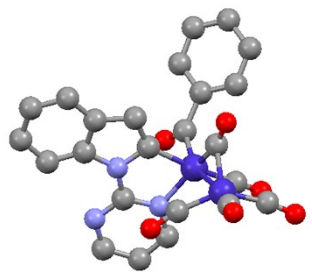
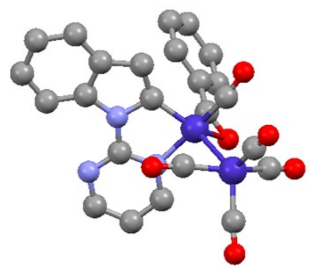
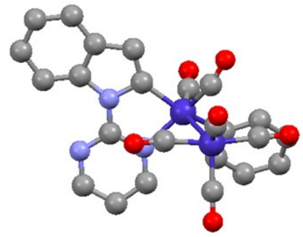

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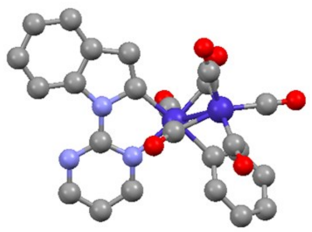
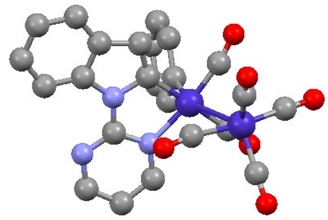
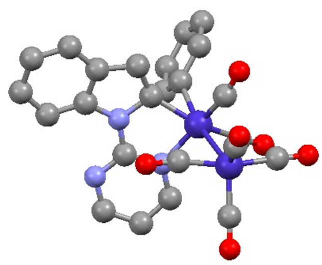

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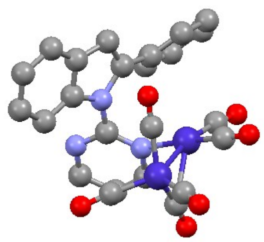
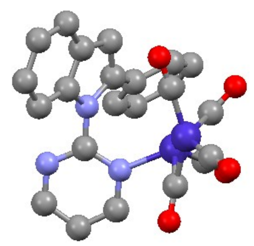

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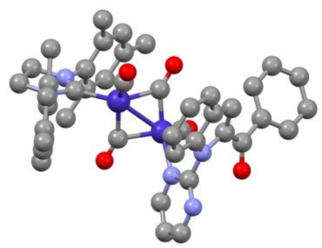
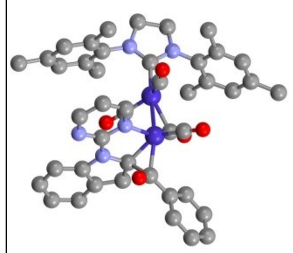
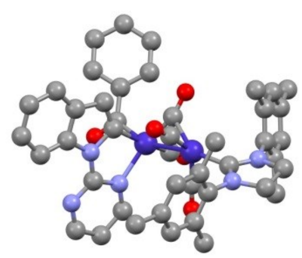

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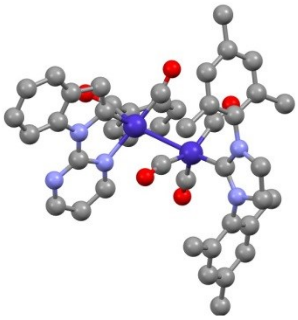	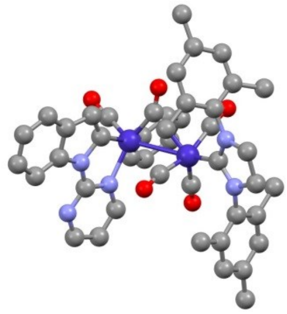	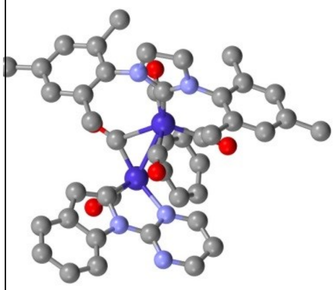
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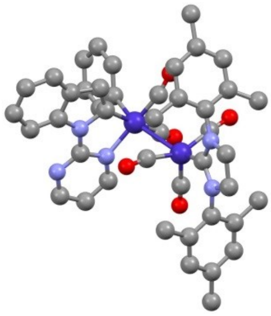	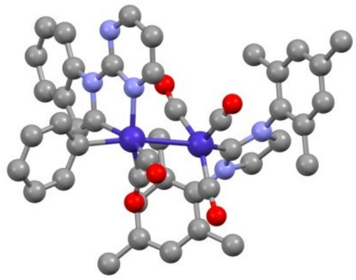	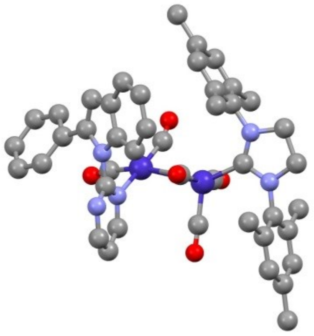
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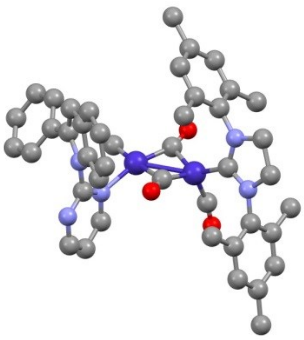	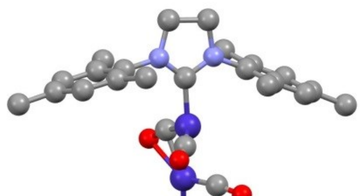	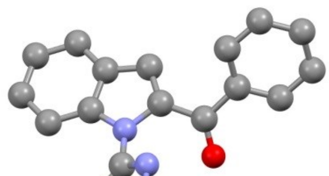
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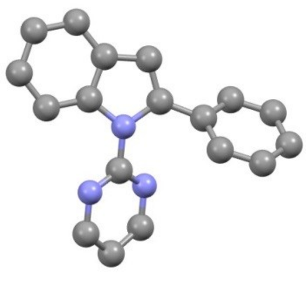	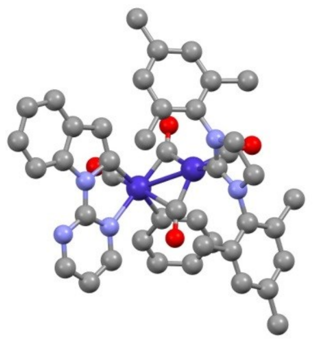	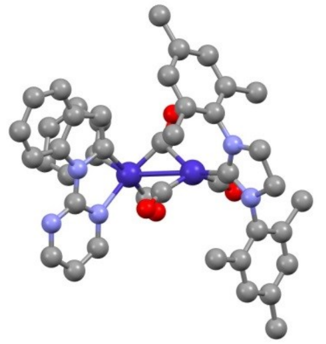
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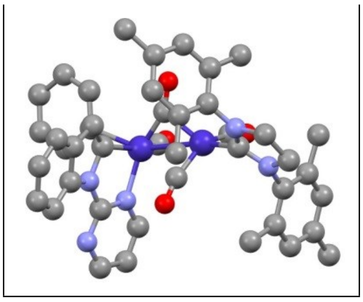

Cartesian Coordinates and Energies.

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Cat, E(M06) = -1668.44168332

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C	2.5956582516	8.4347435418	1.1618820323
O	1.4581763596	8.6190507916	1.2249638876
Co	6.8077868996	7.9292345495	0.3995849095
C	4.676034551	9.0164254974	-0.4437471847
C	6.78539351	7.2844009276	-1.2387415904
C	5.9615203036	7.650721927	1.8999964926
O	4.7007545134	9.6910863691	-1.394738778
O	6.7281840751	6.723132948	-2.249613947
O	5.2042630713	7.3194724848	2.7740604595
C	8.6625179149	7.7644758418	0.7662215993
N	9.3911779814	8.8852519534	0.9580146944
N	9.4750758042	6.6995273923	0.9168886555
C	10.8199589264	8.6184286552	1.2142903283
C	8.8551625614	10.2146547209	0.8517388815
C	10.8518195942	7.0801923484	1.3060679922
C	9.1000747398	5.3147505357	0.8270084434
H	11.1461248963	9.1060503364	2.1384217852
H	11.4346066494	9.0041012689	0.3924254493
C	8.8377164397	10.8597661888	-0.3998763994
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H	11.0668350142	6.7229949538	2.3200730114
H	11.582360912	6.6291976662	0.6281911848
C	9.3365831715	4.6252119544	-0.3788471776
C	8.5773132791	4.655441697	1.9536736489
C	8.321881364	12.1573640463	-0.4667165027
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C	7.8841740794	12.1561154422	1.8941617569
C	8.430278779	10.1756154057	3.3618210696
C	9.0028728424	3.2704686216	-0.4446212754
C	9.9378521692	5.3141704689	-1.5822801433
C	8.261865535	3.2963458349	1.8363173214
C	8.33895593	5.3621460129	3.2676463644

C	7.8330819632	12.8195587584	0.6640166821
H	8.2981592791	12.6614558805	-1.4302943395
H	8.7968456792	9.2675153934	-1.8675772244
H	10.414050503	9.9043169116	-1.5553827843
H	9.2642556692	10.8465787773	-2.5117121391
H	7.5169193242	12.6592463186	2.7859859691
H	7.8652804139	9.2376568518	3.3501616225
H	9.4563043774	9.9347447277	3.6687227304
H	7.9991777677	10.8203713602	4.133161658
C	8.4550072037	2.5889386325	0.6479468655
H	9.1770477187	2.7331301069	-1.3743735812
H	10.946650414	5.6953051651	-1.3778639238
H	9.3291299295	6.1618846467	-1.9103552726
H	10.0163705433	4.6177012871	-2.4220124908
H	7.855443663	2.7793454609	2.7031479531
H	9.0693024505	6.1551805826	3.4545710836
H	7.3480998356	5.8280249886	3.2914799062
H	8.3900039784	4.6517927999	4.0989641004
C	7.2412513143	14.205072729	0.5539003228
C	8.07162486	1.1317093613	0.5373921916
H	7.3586189885	14.767522094	1.4861445708
H	7.7100062781	14.7788658108	-0.2526027349
H	6.1664732762	14.1547757338	0.3355875917
H	8.0736928015	0.6405792458	1.5160354505
H	7.0627802471	1.0212905418	0.1183764761
H	8.7566976749	0.5850184576	-0.1197891813

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Indole (reactant), E(M06) = -970.886646940

C	0.377907	1.900314	1.489574
O	0.478528	1.591755	2.671839
C	-0.858146	2.563557	0.967523
C	-1.217187	2.547650	-0.388832
C	-1.711904	3.179994	1.896689
C	-2.403404	3.151490	-0.808652
H	-0.578828	2.045981	-1.108455
C	-2.888891	3.790595	1.474806
H	-1.428900	3.166453	2.944275
C	-3.236541	3.778460	0.119649
H	-2.678871	3.127219	-1.859524
H	-3.538864	4.274469	2.198894
H	-4.157826	4.251976	-0.209564
C	1.521148	1.700722	0.560165
N	2.481931	0.693639	0.757893

C	2.008364	2.609317	-0.348353
C	2.231902	-0.526258	1.411992
C	3.595687	0.982175	-0.043184
C	3.315364	2.182694	-0.748463
H	1.512689	3.525701	-0.637257
N	0.964173	-0.956390	1.401903
N	3.284401	-1.147717	1.954422
C	4.794832	0.285575	-0.233620
C	4.265591	2.706991	-1.641157
C	0.728056	-2.094806	2.053872
C	3.023756	-2.303740	2.573395
C	5.714086	0.824576	-1.128373
H	5.005452	-0.619798	0.319562
C	5.458754	2.022908	-1.824862
H	4.061856	3.629162	-2.178814
H	-0.305362	-2.437137	2.061141
C	1.738412	-2.828251	2.676314
H	3.880479	-2.816440	3.007338
H	6.658882	0.310800	-1.283972
H	6.206382	2.412630	-2.510041
H	1.536893	-3.758013	3.196313

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INT1, E(M06) = -2639.37651424

Co	-0.6425024442	0.874487486	-0.8895599252
C	-0.8054362607	2.5726761191	-1.3501142966
O	-0.7169442489	3.6692431373	-1.7096740074
C	-3.9923523972	1.6353494214	-0.5616705413
O	-4.2183775265	1.5443894729	-1.7692116597
C	-4.1816758273	2.9323514202	0.1582585374
C	-3.4358699272	3.2958186161	1.2911325675
C	-5.1183784125	3.8350756537	-0.3708303257
C	-3.6424653861	4.5392294292	1.8909702763
H	-2.6670657226	2.6346229993	1.6765094957
C	-5.3309057894	5.0673448984	0.2398891904
H	-5.6697421806	3.5488222561	-1.2607133129
C	-4.5934711599	5.4211027934	1.3745704203
H	-3.0510373788	4.8202050472	2.7580797498
H	-6.0666174155	5.7550832695	-0.1683934207
H	-4.7544998654	6.3860987657	1.848266568
C	-3.6114762492	0.4327028693	0.2055030204
N	-3.2210783741	-0.7453413818	-0.4597121097
C	-3.8580290466	0.1242653985	1.5272742175
C	-2.8512578345	-0.8508431027	-1.8164455972

C	-3.2341831358	-1.7967987981	0.4493840312
C	-3.620935121	-1.2713522712	1.7113436021
H	-4.2265331486	0.8189079996	2.2679593918
N	-1.7752112206	-0.1392457073	-2.2212102825
N	-3.5553949153	-1.6904515106	-2.5655672617
C	-2.9149908304	-3.1482643586	0.2743511876
C	-3.7041296816	-2.1324873042	2.8219929124
C	-1.4928955634	-0.189457702	-3.5365589969
C	-3.2331289876	-1.7625926283	-3.8609101604
C	-3.0068918148	-3.9720566483	1.3890242042
H	-2.6267590003	-3.5400551346	-0.6945264518
C	-3.3980080668	-3.4730406054	2.6511686395
H	-3.9974652115	-1.7460144143	3.7941100429
H	-0.6373760231	0.3901851582	-3.8608783758
C	-2.2200346103	-0.9845816275	-4.4132839196
H	-3.8125659417	-2.4584788936	-4.4636983993
H	-2.7754917625	-5.028536791	1.2850600756
H	-3.4541551349	-4.1522945249	3.496908418
H	-1.9788536032	-1.0169624255	-5.4696128662
C	-0.1466731699	1.0616386003	0.8616710773
O	-0.3790420925	1.6411928648	1.8682390388
Co	1.0823152622	-0.3185654869	0.403322519
C	0.9546791807	-0.0000794074	-1.4206993167
C	0.6031650721	-1.293434171	1.7837362692
O	1.3450037275	-0.1412235122	-2.5342910002
O	0.2224748364	-2.0103006378	2.6096905295
C	2.9877334999	-0.6486570435	0.3799228144
N	3.8988765377	0.3542415961	0.3342048628
N	3.6738920213	-1.8152253003	0.4428756018
C	5.2905657183	-0.1142058625	0.4942995537
C	3.6032703187	1.7605386024	0.3431110475
C	5.1392649816	-1.6361938154	0.3620505122
C	3.1136771998	-3.1363098899	0.504598059
H	5.6776896951	0.1868912893	1.4764127699
H	5.9393048627	0.3187302744	-0.2720126778
C	3.7365977732	2.4900164639	-0.8555067628
C	3.2504951979	2.3958699691	1.547785396
H	5.6415304558	-2.1868853435	1.1627191947
H	5.5137574279	-2.0138333338	-0.5974277179
C	2.773061413	-3.8107595751	-0.6832643477
C	2.9892804531	-3.761916883	1.7594492647
C	3.4660191199	3.8602575479	-0.8297936766
C	4.1557409019	1.8265427807	-2.1469735642
C	2.9896606709	3.7705444351	1.5192817692

C	3.13361716	1.6398201798	2.8509636995
C	2.2538456431	-5.1054533315	-0.5816588575
C	2.9839198407	-3.1848285208	-2.0419777938
C	2.467399936	-5.0581511035	1.8071782427
C	3.4192538868	-3.0727612388	3.0338529489
C	3.0769883147	4.5175694199	0.3424843539
H	3.555139928	4.4281135499	-1.7535371384
H	3.5059224277	0.9829641476	-2.3963357388
H	5.1856972099	1.4483816404	-2.0990822457
H	4.1123704024	2.5418330681	-2.9739464555
H	2.706700388	4.2665420517	2.4452296045
H	2.1712377032	1.1209661223	2.9164362287
H	3.9197015778	0.8855486038	2.9651464618
H	3.199666943	2.328038884	3.6994530846
C	2.0816016167	-5.742490504	0.6512545979
H	1.9832065429	-5.631694653	-1.494804532
H	4.0445910246	-2.967649582	-2.2243611117
H	2.4399732834	-2.2437044241	-2.1571492909
H	2.651808438	-3.8664538253	-2.8312231421
H	2.3570405907	-5.5422019483	2.7752203173
H	4.5133408735	-3.0032021135	3.1056894699
H	3.0228448352	-2.0561888678	3.1021992217
H	3.0703037306	-3.6291015014	3.9085374352
C	2.7422326336	5.9906520425	0.3266181921
C	1.4800487499	-7.1262513936	0.7327613882
H	2.8439268177	6.4365561596	1.3215718059
H	3.3907552645	6.5428090519	-0.3627096715
H	1.7071375782	6.1515144702	-0.0019286545
H	1.8523004903	-7.6753608892	1.6042535418
H	0.386733048	-7.0758946755	0.8231918532
H	1.7049032763	-7.7158873617	-0.1625716693

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TS1, E(M06) = -2639.34844063

Co	-1.3306036375	0.9777515824	-0.8006362308
C	-1.1568137156	2.3605420727	-1.9204612586
O	-1.1018710366	3.2961634982	-2.5948977195
C	-3.4168305955	1.3094552629	-0.5603901613
O	-4.1196668309	0.8705040695	-1.4658228016
C	-3.8661513445	2.5491569552	0.1839850451
C	-3.1106055554	3.2426325641	1.139923215
C	-5.1389936029	3.0407535159	-0.1530667098
C	-3.6205703692	4.389878978	1.7490241584
H	-2.1192244315	2.9041210896	1.4065877595

C	-5.6451725508	4.1882533048	0.4534874836
H	-5.715379673	2.5037138515	-0.8981124203
C	-4.8878193623	4.8681262838	1.4100054769
H	-3.018762465	4.9139803933	2.487154449
H	-6.6320391924	4.5523993649	0.1788364224
H	-5.2797442018	5.7643002091	1.8843578165
C	-2.6185469991	0.0217086956	0.3803417324
N	-2.8697597349	-1.2758969988	-0.1679169005
C	-3.0377858761	-0.0347847493	1.7027644391
C	-2.5342504671	-1.5328190788	-1.4713815791
C	-3.4510469627	-2.1069934405	0.7947317617
C	-3.5512905975	-1.3396842296	1.9873173557
H	-3.0320514044	0.8017811552	2.3867439119
N	-1.7950390766	-0.5551989144	-2.0585396945
N	-2.9256997431	-2.6682937217	-2.0561435299
C	-3.8693236758	-3.4378275756	0.7363796168
C	-4.0933206845	-1.9253206076	3.143116374
C	-1.5013447351	-0.7172681857	-3.3522858784
C	-2.5959611298	-2.8165776777	-3.3405963433
C	-4.4006587234	-3.9927016966	1.9008177094
H	-3.7930989195	-4.0026559509	-0.1827193545
C	-4.5133933554	-3.2492308809	3.0902425331
H	-4.1777530106	-1.3494630611	4.0607338099
H	-0.924721643	0.0756705048	-3.8147793464
C	-1.8900982719	-1.8525837505	-4.0574223884
H	-2.9169817166	-3.744494325	-3.8106281924
H	-4.7422252395	-5.0242735688	1.8836291345
H	-4.9356377863	-3.717433461	3.9752445444
H	-1.6433291984	-1.978057766	-5.1049649926
C	-0.290701134	1.6091713196	0.4830643662
O	0.1199741234	2.3031429977	1.351377869
Co	1.1370073958	0.1888602476	0.0352939812
C	1.2224923991	0.4751470931	-1.692696439
C	0.40852859	-0.9007048351	1.2350594375
O	1.3687512053	0.4816527528	-2.8501818693
O	-0.1035200637	-1.6844392791	1.912568499
C	2.9974417964	-0.3551597281	0.2051310642
N	3.9951058752	0.5525117952	0.3108223524
N	3.5542260413	-1.5862291556	0.2566830456
C	5.3143127405	-0.0610805199	0.5709003619
C	3.835285678	1.9799181592	0.3732023116
C	5.0315592534	-1.5513412164	0.3342317135
C	2.873524001	-2.8504617107	0.196416959
H	5.630808359	0.1511315457	1.6000223113

H	6.0712935177	0.3446683437	-0.1056893727
C	4.1145223903	2.7435291252	-0.7786867247
C	3.4799727957	2.5932338516	1.5878843114
H	5.3895697936	-2.1894710268	1.146726855
H	5.4658411146	-1.918873457	-0.6035678071
C	2.5852710032	-3.4333403614	-1.0510765642
C	2.5841700218	-3.5210987071	1.3999631517
C	3.9947522625	4.1325280876	-0.6962952224
C	4.5315377616	2.095763899	-2.0790486454
C	3.3788305288	3.988630882	1.618024315
C	3.1830087962	1.799009001	2.8385931153
C	1.957149745	-4.683245934	-1.0666401084
C	2.9447968459	-2.7531075916	-2.3510605786
C	1.9557431214	-4.7674248116	1.3306867911
C	2.942744435	-2.9291131351	2.7434002756
C	3.6195097386	4.7747197653	0.489560783
H	4.2008857864	4.7289627485	-1.5824704567
H	3.7643246043	1.4130946935	-2.4572797438
H	5.4580648032	1.5170736554	-1.9735984194
H	4.707592652	2.8567396913	-2.8450207284
H	3.0981631516	4.4702376574	2.5521631491
H	2.127518838	1.5055104986	2.8625925388
H	3.7818710617	0.8856577083	2.9080607635
H	3.3792750692	2.4020328248	3.7309348051
C	1.6234085492	-5.3613483757	0.1094292592
H	1.7269184289	-5.1394177485	-2.0271744598
H	3.9958174417	-2.4411109036	-2.3743977054
H	2.3424910559	-1.8565227719	-2.5225982964
H	2.7830281172	-3.4312264132	-3.1944868944
H	1.7150831832	-5.2839585249	2.2572512312
H	4.0253976308	-2.9655138635	2.9267726418
H	2.6333412268	-1.883123935	2.8240903537
H	2.4575927407	-3.4856081199	3.5502484962
C	3.4605824856	6.2761918431	0.5394975479
C	0.9057827861	-6.6899894756	0.0645933742
H	3.6021965501	6.6608438254	1.5548770497
H	4.1773789167	6.7788326648	-0.1190112367
H	2.4552810084	6.5741326211	0.2140181148
H	1.2094566172	-7.3386925558	0.8933408587
H	-0.1805834808	-6.5514295387	0.1422656447
H	1.1014461595	-7.2210213133	-0.8729806736

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INT2A, E(M06) = -2639.35877438

Co	-1.323790701	0.8964880721	-0.7374232258
C	-0.7318755207	2.2498721882	-1.7771921229
O	-0.4110778744	3.1476387416	-2.4228934143
C	-3.0786118562	1.831710228	-0.7196530063
O	-3.8974836589	1.496357373	-1.5507428808
C	-3.429088117	2.8916498261	0.2894669477
C	-2.4881846803	3.7741399822	0.8305461725
C	-4.7801484458	3.0192223511	0.6554843137
C	-2.8893972312	4.7702670701	1.7227068815
H	-1.4451268754	3.688794472	0.553109418
C	-5.1747815601	3.9961037615	1.5651552129
H	-5.503901094	2.3403856097	0.2160041981
C	-4.2289227854	4.8773415815	2.0991489126
H	-2.1519643487	5.4572506988	2.1295311904
H	-6.2195488854	4.0771539068	1.8541489433
H	-4.536834917	5.644750933	2.8049155208
C	-2.3933664	-0.2767347567	0.3734351254
N	-2.9341179367	-1.3621375931	-0.3717143562
C	-2.8439313356	-0.4105072511	1.6569157732
C	-2.7041799106	-1.4264871237	-1.7145497948
C	-3.7208297597	-2.1822888198	0.460410663
C	-3.6680253403	-1.5947385042	1.7514484708
H	-2.6184317149	0.2657907782	2.4710978454
N	-1.8993632711	-0.4362820295	-2.1925080992
N	-3.2480934302	-2.4015515353	-2.4536968757
C	-4.4405162847	-3.3471802796	0.1990918105
C	-4.362876875	-2.2046641269	2.804014679
C	-1.6681739619	-0.4262006138	-3.5080480923
C	-2.9944807937	-2.3678311247	-3.7617850344
C	-5.1244662082	-3.9322758662	1.2678652682
H	-4.4680068709	-3.7725619735	-0.7952834985
C	-5.0866984547	-3.3693982894	2.5533350419
H	-4.3366017484	-1.7725806358	3.8011683023
H	-1.0292370272	0.3679906242	-3.8781954935
C	-2.2050531752	-1.386644617	-4.3595035452
H	-3.444959329	-3.1627718448	-4.3539821815
H	-5.6973082783	-4.8397177699	1.0957255933
H	-5.6302429298	-3.8490063059	3.3635492791
H	-2.0119022106	-1.3691926394	-5.4253659202
C	-0.3286342647	1.2965026192	0.6960651001
O	-0.0568550024	1.8975110704	1.6783952646
Co	1.1558913419	-0.0102085998	0.1546844479
C	1.1886215444	0.1161391847	-1.5905365114
C	0.5459846198	-1.1244078485	1.4098761314

O	1.3281748728	-0.0211114684	-2.741371557
O	0.1375853121	-1.9451289635	2.1087699762
C	3.0528908299	-0.4413399631	0.2761190815
N	3.9701549675	0.5523783143	0.3037051489
N	3.7114940728	-1.616307233	0.3725268672
C	5.3449094314	0.0688712223	0.5466870309
C	3.6788283302	1.9598874164	0.2915425783
C	5.1828440855	-1.4518645258	0.4049250146
C	3.1406074181	-2.9355874446	0.4126692996
H	5.6766521876	0.3679337184	1.5489020983
H	6.0404856413	0.495035524	-0.1815186764
C	3.8453043298	2.6746523827	-0.914155869
C	3.3090361785	2.611549006	1.4814628036
H	5.6129573873	-2.0082716828	1.2419799361
H	5.6224511148	-1.8384748959	-0.5223791516
C	2.8684838092	-3.6206055101	-0.7857501696
C	2.9427579171	-3.5475359003	1.6652200876
C	3.5902704454	4.0466312317	-0.910487706
C	4.294984198	1.9916060665	-2.1851991034
C	3.0680612302	3.990765227	1.4308060845
C	3.1444758808	1.8817296043	2.7946781319
C	2.3461242934	-4.9155567439	-0.7011119983
C	3.1335099721	-3.0037519254	-2.1390929231
C	2.4185023837	-4.8424834719	1.6952651783
C	3.2882084542	-2.8434046242	2.9572794707
C	3.1909852426	4.7230784666	0.2496052548
H	3.7078851067	4.603649234	-1.8375392559
H	3.626382007	1.1736339229	-2.4694473226
H	5.3032541251	1.5685018368	-2.0876535092
H	4.3209542976	2.7055095578	-3.0136201754
H	2.774349166	4.5009454108	2.3455771636
H	2.0993680267	1.5848810844	2.9357712146
H	3.7573020471	0.9776366431	2.8535353471
H	3.4189862075	2.5330458742	3.6310161745
C	2.1009207479	-5.5393616758	0.5255817559
H	2.128513355	-5.4512219568	-1.6226894714
H	4.1309641507	-2.5527799494	-2.1980020164
H	2.4130598819	-2.2161595898	-2.3777550691
H	3.0669845665	-3.763706143	-2.9235437715
H	2.2483770843	-5.3153142267	2.6599248391
H	4.3747357644	-2.7722740186	3.1035627239
H	2.8876149431	-1.8260452728	2.9893718647
H	2.8809706885	-3.3899154899	3.8125173872
C	2.8922027507	6.2036164411	0.2130711673

C	1.4929299891	-6.9207975268	0.587109602
H	2.9007530059	6.6393581057	1.2172120146
H	3.6216807753	6.7453768827	-0.3995984861
H	1.9017759852	6.3938746194	-0.2204808283
H	1.8394288179	-7.4735279327	1.4668568827
H	0.3983058742	-6.8636952304	0.6489951029
H	1.7391082081	-7.5082183504	-0.3037826774

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INT2B, E(M06) = -2639.35369343

Co	1.4110295921	-0.500968711	0.7432894581
C	2.4221766304	-1.3085243663	2.1539361729
O	3.5954844984	-1.562394283	2.2418375936
C	1.4054439059	-1.8937052719	3.1148735854
C	1.4467050169	-3.2823602871	3.3306598773
C	0.4711937524	-1.1151476369	3.8106559271
C	0.5496667187	-3.8815123937	4.211753734
H	2.194201697	-3.8772553016	2.8138761202
C	-0.4120791627	-1.7180214048	4.7080125086
H	0.4435944082	-0.0406651141	3.6769365348
C	-0.3829905126	-3.0999575694	4.9010815958
H	0.5856622359	-4.9558265962	4.3721769836
H	-1.124376435	-1.1033400753	5.2508890184
H	-1.0789584386	-3.5674634722	5.5922940085
C	3.0027676837	0.0193059815	-0.1276519094
N	3.4747124728	-0.99574336	-0.9994075124
C	3.8386625769	1.091001803	-0.2518268047
C	2.7780863554	-2.1606504357	-1.0825936826
C	4.625076128	-0.5520362335	-1.6809067745
C	4.8645023193	0.7688912905	-1.2225527988
H	3.7648768721	2.0184687257	0.2997771601
N	1.6548893847	-2.1889292527	-0.3031745175
N	3.1943197878	-3.1608033195	-1.867182352
C	5.4337217411	-1.1749733848	-2.6288143631
C	5.9597544794	1.4757174722	-1.7338070043
C	0.9339287443	-3.3186940975	-0.3104514932
C	2.4538535748	-4.2685426898	-1.8611714024
C	6.5187460782	-0.4452593313	-3.121416633
H	5.2266850015	-2.1835476278	-2.9616248427
C	6.779489584	0.8611739549	-2.6796426689
H	6.167486828	2.487445429	-1.3950191777
H	0.0464799616	-3.3291683314	0.3104468299
C	1.301643445	-4.4117885865	-1.0867156699
H	2.8013238614	-5.0758914373	-2.5033653446

H	7.1728309761	-0.9030509089	-3.8585123791
H	7.6333437286	1.4007456805	-3.0811633447
H	0.7118893822	-5.3203867808	-1.0913507163
C	1.2723960696	1.102217953	1.4899892594
O	1.4485483855	2.133028226	1.9803934366
Co	-1.0785037759	0.226013688	0.2351706246
C	-1.3554855273	1.0551351653	1.7864788539
C	-1.7095128826	-1.3946569856	0.585050418
C	-0.0827026791	-0.0091111369	-1.2036949931
O	-1.6689520446	1.5100543736	2.8096200211
O	-2.1022861999	-2.4583814323	0.8420830677
O	0.3554365118	-0.1802774824	-2.2739797851
C	-2.3410913527	1.341185277	-0.7898918757
N	-2.2820554226	2.6851431165	-0.9536656358
N	-3.3913237283	0.8929420281	-1.5215647148
C	-3.2807716642	3.2042831439	-1.9124749365
C	-1.3447455665	3.6065030557	-0.3703362175
C	-4.1673537104	1.978958367	-2.1594133148
C	-3.9376256328	-0.4357285444	-1.5495581306
H	-2.7746406821	3.5506073278	-2.8222498956
H	-3.8257162546	4.0500987788	-1.4843880354
C	-1.7433704662	4.3293941045	0.7747620741
C	-0.1097210028	3.859862195	-0.9920362325
H	-4.3241839933	1.7698452697	-3.2213063053
H	-5.1515117472	2.0652628165	-1.6826065978
C	-4.8033795532	-0.849728373	-0.5190479071
C	-3.682861878	-1.2571668417	-2.6623504162
C	-0.8544356822	5.2574180234	1.319116122
C	-3.1084974306	4.1457430871	1.3978793698
C	0.7432191698	4.8062156299	-0.4086959819
C	0.3331647231	3.1694355059	-2.2603703406
C	-5.3862261159	-2.1160780873	-0.6116146769
C	-5.0865183805	0.0282435664	0.6771647392
C	-4.2889562116	-2.5177956479	-2.7065085038
C	-2.7854688371	-0.8087631393	-3.7923838033
C	0.4008169367	5.5023679072	0.7503463985
H	-1.1509861553	5.8052418537	2.2111876609
H	-3.3748748816	3.091896397	1.5073628279
H	-3.8937571008	4.6237946577	0.7954591765
H	-3.1400614765	4.6030817546	2.3909589747
H	1.7038229199	5.0004830751	-0.8822083621
H	1.1644700919	2.4835064895	-2.0641707983
H	-0.4650989322	2.5847959243	-2.7208049367
H	0.685881878	3.9061524469	-2.9918707137

C	-5.1370050438	-2.968933145	-1.6916101284
H	-6.0510422588	-2.4449668506	0.1845541182
H	-5.4417445982	1.0246691536	0.3875317743
H	-4.1842536462	0.1719084486	1.2817559828
H	-5.8520773089	-0.4245890811	1.31424579
H	-4.0937831701	-3.1614389769	-3.5617647611
H	-3.1796037191	0.0808172293	-4.3008232132
H	-1.7801395073	-0.5606930829	-3.4403223372
H	-2.6940134915	-1.5981681931	-4.5446549131
C	1.3599648822	6.4815510327	1.3853331808
C	-5.7563942281	-4.3461073414	-1.7476181395
H	2.088747958	6.8574388171	0.6596731423
H	0.8328053048	7.3407576781	1.8148804873
H	1.9227611725	6.005777327	2.1991097926
H	-5.755595483	-4.7453755419	-2.7671277186
H	-5.2026022269	-5.0537604491	-1.1166629823
H	-6.7915052277	-4.335922635	-1.388032705

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TS2, E(M06) = -2639.33991110

Co	1.533525	-0.737080	1.173886
C	2.635027	-0.906777	2.507839
O	3.517465	-0.885619	3.268859
C	0.925846	-1.702786	3.030286
C	1.029075	-3.092657	3.200582
C	0.168488	-0.983509	3.970725
C	0.327039	-3.754508	4.211522
H	1.685651	-3.670795	2.555925
C	-0.538846	-1.638120	4.980536
H	0.127768	0.099895	3.922660
C	-0.472064	-3.029248	5.096786
H	0.416827	-4.833472	4.315475
H	-1.134643	-1.059567	5.682545
H	-1.018304	-3.539805	5.885670
C	2.874252	-0.067353	-0.047827
N	3.344561	-1.073885	-0.937669
C	3.612478	1.056348	-0.295818
C	2.741316	-2.294655	-0.930610
C	4.374549	-0.566802	-1.755525
C	4.558277	0.782634	-1.356999
H	3.508981	1.997509	0.228315
N	1.749329	-2.426550	0.000038
N	3.123365	-3.247170	-1.792419
C	5.129715	-1.157219	-2.767287

C	5.535188	1.552329	-2.001663
C	1.072081	-3.582040	-0.005311
C	2.445419	-4.392827	-1.754550
C	6.096371	-0.364980	-3.392359
H	4.968680	-2.188301	-3.052451
C	6.297236	0.971756	-3.014704
H	5.697484	2.587622	-1.712053
H	0.266818	-3.666152	0.714370
C	1.381028	-4.617370	-0.881241
H	2.767769	-5.160194	-2.456552
H	6.702748	-0.796513	-4.184229
H	7.058842	1.561450	-3.518773
H	0.824038	-5.546649	-0.874289
C	0.996344	0.943469	1.450640
O	1.183759	2.044284	1.796770
Co	-0.965426	0.159006	0.358120
C	-1.552207	0.937360	1.849685
C	-1.602623	-1.503761	0.661901
C	0.007048	-0.175473	-1.082511
O	-2.017020	1.406992	2.798209
O	-1.974836	-2.577485	0.872557
O	0.489600	-0.407744	-2.110843
C	-2.144316	1.307428	-0.760709
N	-2.079299	2.648304	-0.907657
N	-3.147780	0.854712	-1.551754
C	-3.038440	3.174959	-1.903619
C	-1.158652	3.572168	-0.298736
C	-3.882297	1.940103	-2.240135
C	-3.676636	-0.479894	-1.631144
H	-2.490357	3.565448	-2.769189
H	-3.624594	3.992583	-1.475398
C	-1.603871	4.336872	0.799346
C	0.108488	3.788583	-0.868978
H	-3.943057	1.742221	-3.313767
H	-4.904678	2.003310	-1.848519
C	-4.582756	-0.925085	-0.648577
C	-3.369485	-1.273752	-2.751788
C	-0.728986	5.272869	1.354599
C	-3.004508	4.209761	1.355450
C	0.940683	4.748464	-0.281689
C	0.611038	3.034003	-2.076835
C	-5.132918	-2.202074	-0.783896
C	-4.954550	-0.068328	0.538711
C	-3.942889	-2.547661	-2.836788

C	-2.473651	-0.778275	-3.863693
C	0.552266	5.487235	0.836596
H	-1.060830	5.853009	2.213241
H	-3.382263	3.186189	1.308560
H	-3.709750	4.848481	0.804376
H	-3.033190	4.528177	2.401582
H	1.925414	4.914848	-0.713943
H	1.363462	2.291720	-1.786147
H	-0.184321	2.504448	-2.606011
H	1.091921	3.720523	-2.782897
C	-4.817020	-3.035124	-1.861950
H	-5.826400	-2.555022	-0.023447
H	-5.235732	0.949704	0.244568
H	-4.120362	0.020965	1.242599
H	-5.800477	-0.505281	1.077425
H	-3.701664	-3.171801	-3.694535
H	-2.980100	-0.024786	-4.482539
H	-1.553586	-0.327606	-3.485344
H	-2.194582	-1.602234	-4.527122
C	1.494209	6.475895	1.481987
C	-5.397409	-4.426583	-1.959555
H	2.205110	6.885750	0.756743
H	0.951467	7.311398	1.937321
H	2.079188	5.994558	2.276573
H	-5.357478	-4.807345	-2.985232
H	-4.841805	-5.129893	-1.325461
H	-6.441653	-4.449968	-1.628581

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INT3A, E(M06) = -2639.34608012

Co	1.553853	-0.818275	1.270325
C	2.943744	-0.832078	2.337457
O	3.853673	-0.791895	3.040174
C	0.792335	-1.802032	2.894863
C	1.169580	-3.135247	3.148913
C	-0.045471	-1.208628	3.857822
C	0.671746	-3.862188	4.236603
H	1.890034	-3.629017	2.500219
C	-0.548155	-1.920859	4.950656
H	-0.316980	-0.162450	3.772443
C	-0.204513	-3.260903	5.139273
H	0.984814	-4.894195	4.383727
H	-1.204495	-1.421070	5.660460
H	-0.593914	-3.818175	5.987672

C	2.776381	-0.097390	-0.105390
N	3.199173	-1.098396	-1.023779
C	3.481683	1.035787	-0.406505
C	2.607771	-2.328368	-0.985812
C	4.155067	-0.576295	-1.918243
C	4.349367	0.776525	-1.535181
H	3.401679	1.976423	0.123731
N	1.690254	-2.485536	0.012648
N	2.934541	-3.262174	-1.888957
C	4.841365	-1.155025	-2.985202
C	5.263557	1.560751	-2.251024
C	1.020158	-3.644763	0.034415
C	2.265585	-4.412946	-1.825946
C	5.746224	-0.348815	-3.680248
H	4.674543	-2.188273	-3.258445
C	5.955787	0.991285	-3.318485
H	5.431879	2.598408	-1.973331
H	0.279941	-3.750143	0.818339
C	1.266069	-4.659130	-0.885685
H	2.542483	-5.165255	-2.562800
H	6.298079	-0.771965	-4.515363
H	6.668960	1.591401	-3.878007
H	0.715312	-5.591741	-0.856824
C	0.967123	0.842993	1.594992
O	1.161015	1.926292	1.990034
Co	-0.962709	0.165209	0.428900
C	-1.618237	0.947805	1.893558
C	-1.633300	-1.503543	0.701751
C	-0.035588	-0.198444	-1.038081
O	-2.129306	1.440428	2.803377
O	-2.033524	-2.572116	0.866018
O	0.405413	-0.447146	-2.078405
C	-2.094170	1.374970	-0.685701
N	-1.993262	2.716058	-0.797961
N	-3.107721	0.966459	-1.486133
C	-2.947360	3.295548	-1.769343
C	-1.030859	3.594426	-0.185788
C	-3.803737	2.085042	-2.162093
C	-3.659371	-0.355541	-1.613533
H	-2.395635	3.721341	-2.615178
H	-3.525840	4.097593	-1.302170
C	-1.425972	4.358625	0.930160
C	0.234925	3.767369	-0.775894
H	-3.838223	1.917167	-3.242058

H	-4.834852	2.155013	-1.796363
C	-4.579662	-0.817272	-0.651631
C	-3.361138	-1.116139	-2.759740
C	-0.498738	5.240884	1.490472
C	-2.824527	4.299589	1.503108
C	1.120153	4.673172	-0.182173
C	0.674550	3.022255	-2.013705
C	-5.145455	-2.082145	-0.829005
C	-4.955206	0.009955	0.555156
C	-3.949228	-2.380014	-2.885387
C	-2.470994	-0.593955	-3.864056
C	0.783786	5.403579	0.959476
H	-0.791073	5.819364	2.364483
H	-3.316554	3.343311	1.315022
H	-3.456250	5.090555	1.074589
H	-2.805396	4.454883	2.585921
H	2.103270	4.806456	-0.629111
H	1.343160	2.194006	-1.753847
H	-0.164201	2.605258	-2.577206
H	1.232808	3.688586	-2.680530
C	-4.832717	-2.886934	-1.929313
H	-5.849253	-2.448074	-0.084466
H	-5.181698	1.049567	0.291584
H	-4.145095	0.035819	1.291370
H	-5.837371	-0.409210	1.047915
H	-3.712830	-2.979573	-3.761789
H	-3.010590	0.114238	-4.508319
H	-1.585769	-0.083094	-3.480734
H	-2.132066	-1.413692	-4.504345
C	1.781307	6.331706	1.611015
C	-5.428060	-4.268054	-2.071309
H	2.494047	6.731606	0.882004
H	1.285133	7.175999	2.101695
H	2.361166	5.802714	2.378608
H	-5.395527	-4.614635	-3.109273
H	-4.877300	-4.997511	-1.463157
H	-6.471194	-4.291562	-1.737123

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INT3B, E(M06) = -2639.35869006

Co	-1.496068	-0.546899	-1.078901
C	-0.687163	-1.121200	-2.630373
O	-0.287783	-1.491991	-3.641092
C	-3.247031	-0.760783	-2.060315

C	-3.650060	-2.025350	-2.513409
C	-4.099737	0.322884	-2.316197
C	-4.863908	-2.205181	-3.187433
H	-3.022607	-2.898531	-2.355004
C	-5.310402	0.148661	-2.992905
H	-3.843265	1.320942	-1.974489
C	-5.701025	-1.117660	-3.431240
H	-5.147272	-3.200428	-3.524007
H	-5.951078	1.009721	-3.171451
H	-6.643348	-1.253578	-3.955774
C	-2.530747	-0.009083	0.459857
N	-2.900002	-1.129072	1.251436
C	-3.099078	1.092287	1.036774
C	-2.408724	-2.350459	0.918489
C	-3.703101	-0.723205	2.334912
C	-3.841304	0.682698	2.210316
H	-3.014092	2.108614	0.675549
N	-1.611806	-2.341802	-0.192269
N	-2.700903	-3.435074	1.646832
C	-4.294657	-1.446648	3.368075
C	-4.602153	1.374561	3.161331
C	-1.066101	-3.511540	-0.554194
C	-2.150998	-4.583082	1.256721
C	-5.048065	-0.730101	4.301575
H	-4.172027	-2.519378	3.438160
C	-5.200411	0.661426	4.199501
H	-4.726389	2.452086	3.087403
H	-0.417578	-3.496754	-1.422536
C	-1.304823	-4.684380	0.151094
H	-2.397627	-5.457704	1.856008
H	-5.524419	-1.264236	5.119200
H	-5.795064	1.189886	4.940309
H	-0.854837	-5.622476	-0.150088
C	-1.279430	1.177435	-1.423361
O	-1.377608	2.302194	-1.650713
Co	1.223204	0.003318	-0.607157
C	1.430891	0.965586	-2.096570
C	1.834184	-1.622003	-1.074733
C	0.391551	-0.379170	0.902426
O	1.653770	1.535579	-3.081059
O	2.166125	-2.691975	-1.370719
O	0.070758	-0.694384	1.976728
C	2.574434	1.055943	0.382101
N	2.515322	2.368550	0.704949

N	3.734726	0.565867	0.881458
C	3.669552	2.832695	1.504231
C	1.471105	3.314765	0.416509
C	4.568275	1.590051	1.549580
C	4.292995	-0.745539	0.697943
H	3.329359	3.149287	2.496883
H	4.147711	3.690042	1.020536
C	1.627143	4.183540	-0.683000
C	0.384754	3.452589	1.300928
H	4.814986	1.277673	2.568772
H	5.508081	1.723552	1.001658
C	5.039747	-1.018490	-0.464450
C	4.177915	-1.692920	1.731292
C	0.634952	5.137777	-0.922491
C	2.850451	4.154386	-1.571871
C	-0.574988	4.432222	1.021239
C	0.216218	2.603106	2.538612
C	5.640409	-2.273812	-0.586734
C	5.181598	0.000152	-1.571003
C	4.796205	-2.936285	1.558772
C	3.417512	-1.396812	3.003224
C	-0.480658	5.271261	-0.090888
H	0.741595	5.797383	-1.781393
H	3.340905	3.179428	-1.576908
H	3.589147	4.898736	-1.242337
H	2.584977	4.398337	-2.604762
H	-1.419352	4.540032	1.699586
H	-0.612893	1.897987	2.417639
H	1.108374	2.018568	2.772427
H	-0.017039	3.234116	3.404145
C	5.524224	-3.250099	0.408029
H	6.212623	-2.494337	-1.485506
H	5.586598	0.953287	-1.208841
H	4.214715	0.217902	-2.037382
H	5.854696	-0.369547	-2.350132
H	4.707102	-3.677559	2.350027
H	3.854769	-0.554948	3.555256
H	2.371590	-1.145308	2.806228
H	3.433758	-2.264733	3.669257
C	-1.560319	6.282484	-0.396408
C	6.156150	-4.611235	0.232835
H	-2.079413	6.602910	0.513133
H	-1.151917	7.172381	-0.887472
H	-2.314672	5.855919	-1.070622

H	6.295783	-5.115635	1.194505
H	5.526827	-5.260035	-0.390409
H	7.132877	-4.540398	-0.258716

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TS3, E(M06) = -2639.33686723

Co	-1.4684887444	-0.5571908121	-1.2515274384
C	-1.0280082437	-0.9767928893	-2.988702353
O	-0.8083952274	-1.2172605059	-4.0915666354
C	-3.5159959512	-0.3922828529	-1.5140643129
C	-4.2870885166	-1.5540341805	-1.726946149
C	-3.96536094	0.797304582	-2.1328150101
C	-5.4348268142	-1.5301600232	-2.5212975892
H	-4.0049571892	-2.4963133324	-1.271456963
C	-5.1052211144	0.8141916753	-2.9295660605
H	-3.4231824336	1.7247582719	-1.9851041739
C	-5.8534558587	-0.3501029651	-3.1343722987
H	-6.0005418819	-2.4487223158	-2.6601480803
H	-5.4116099459	1.7480946679	-3.3954021607
H	-6.7459745636	-0.333337073	-3.7534850705
C	-2.7593444121	-0.2298632763	0.172997202
N	-2.903844789	-1.4007700954	0.9905517349
C	-3.240531558	0.8285264187	0.93440869
C	-2.2980155253	-2.5604299042	0.6067393832
C	-3.5013926342	-1.0672380952	2.2210581589
C	-3.7088780743	0.3389508157	2.1945791227
H	-3.3270115847	1.8476325317	0.5832975385
N	-1.5516988333	-2.4452560662	-0.5292975142
N	-2.4688210868	-3.6872596767	1.30834675
C	-3.8480253756	-1.8524775861	3.3169817012
C	-4.2939009351	0.9597804265	3.3112428809
C	-0.9790644075	-3.5650132857	-0.9923824997
C	-1.8626731399	-4.7776204748	0.8392896828
C	-4.4240966529	-1.2058962041	4.4149966486
H	-3.6778590655	-2.9206783442	3.3119088157
C	-4.6456229644	0.1809558491	4.4104733459
H	-4.4680337926	2.0326490621	3.3126013705
H	-0.3966371467	-3.4663005496	-1.900790707
C	-1.1030871941	-4.7812627599	-0.3313710088
H	-1.9990336653	-5.6864144416	1.4227130367
H	-4.7088074283	-1.792440839	5.2841055556
H	-5.1006601998	0.6519916931	5.2780382026
H	-0.6245366135	-5.6773733123	-0.7073679704
C	-1.011497952	1.1581272014	-1.338491627

O	-1.1004053411	2.3126972251	-1.4465562275
Co	1.2024367222	0.0370321646	-0.6538248108
C	1.5186809421	0.9164562585	-2.1687001555
C	1.7630591258	-1.5893366624	-1.1590439908
C	0.3201134132	-0.4110099143	0.8093340737
O	1.7950839038	1.4304312992	-3.1703608641
O	2.0717884679	-2.6509107303	-1.5070353197
O	-0.0706367469	-0.7575079453	1.8497104546
C	2.5232834712	1.071416665	0.4119102977
N	2.4597908642	2.3619809311	0.8141938974
N	3.6708869713	0.5492663463	0.9120762939
C	3.5631070375	2.7466853086	1.7226490684
C	1.4227765207	3.3307777187	0.5755399787
C	4.4997639517	1.5380996287	1.6361450933
C	4.2261895575	-0.7540967096	0.6719742672
H	3.1683908804	2.9052835481	2.7336308299
H	4.0279844226	3.6791153086	1.3908781139
C	1.6071855159	4.2676961739	-0.4638528745
C	0.3253360887	3.4230011447	1.4480385661
H	4.7942231071	1.1510845992	2.6157004887
H	5.4133895769	1.749950146	1.0673044598
C	4.9990961672	-0.976497173	-0.4837866554
C	4.0803288865	-1.7501671517	1.6546919576
C	0.6410065903	5.257764158	-0.6447737917
C	2.8239495252	4.2362905878	-1.3605003768
C	-0.6148694585	4.4375563999	1.223096431
C	0.1148069818	2.4900637539	2.6180018145
C	5.5919656803	-2.2304487994	-0.6531431503
C	5.1814378752	0.0924497212	-1.5356322084
C	4.6921785213	-2.9893280721	1.4367341643
C	3.2929170455	-1.5088098189	2.9218432953
C	-0.4863541012	5.3528632911	0.1794082719
H	0.7743560746	5.9773051495	-1.449866674
H	2.8701791238	3.3213182672	-1.9571439338
H	3.7590969997	4.3006706579	-0.7899138739
H	2.8060489995	5.0820017922	-2.0544125127
H	-1.4699415678	4.5097122819	1.8927851467
H	-0.7299182289	1.8174437368	2.4340421954
H	0.9856835573	1.8646584581	2.8244042492
H	-0.1176733159	3.0614074345	3.5243723197
C	5.443946477	-3.2534626645	0.2887336705
H	6.1853617168	-2.4112590549	-1.5471197948
H	5.5450318303	1.0359058571	-1.1112922372
H	4.238780306	0.3143261603	-2.0466057629

H	5.9036779827	-0.2314770544	-2.2907671652
H	4.5792821217	-3.7671902193	2.1889149876
H	3.715664407	-0.6897148467	3.5177355604
H	2.250606596	-1.2505598737	2.7138520153
H	3.2969931551	-2.4039188303	3.5511024943
C	-1.5360162992	6.4110911581	-0.0663139558
C	6.0685846322	-4.6102497757	0.0614704995
H	-2.1188012217	6.6167523719	0.8375874808
H	-1.0875300903	7.3521552164	-0.4039026034
H	-2.2403118839	6.0902533398	-0.8451353009
H	6.1923820117	-5.157713107	1.001615258
H	5.4426602701	-5.2263178392	-0.5974325548
H	7.0519666353	-4.525277351	-0.4142300984

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INT4, E(M06) = -2639.37735815

Co	-1.084574	-0.746609	-1.164866
C	-2.024956	-1.353377	-2.534546
O	-2.481229	-1.826852	-3.484552
C	-4.656175	-0.930188	-0.671999
C	-4.974904	-2.300020	-0.686560
C	-5.026649	-0.144754	-1.779236
C	-5.626010	-2.866017	-1.782420
H	-4.749930	-2.918393	0.177502
C	-5.688431	-0.711031	-2.865306
H	-4.771458	0.910821	-1.787714
C	-5.985183	-2.076306	-2.876051
H	-5.867308	-3.925700	-1.772957
H	-5.959028	-0.087696	-3.713198
H	-6.492565	-2.519704	-3.728130
C	-4.065105	-0.279961	0.506775
N	-3.179536	-0.912893	1.410414
C	-4.455359	0.916728	1.054724
C	-2.453020	-2.097432	1.209535
C	-3.066785	-0.111430	2.558970
C	-3.842727	1.053849	2.341426
H	-5.194349	1.576862	0.621627
N	-1.685024	-2.222860	0.101153
N	-2.572054	-3.025249	2.161821
C	-2.339608	-0.306951	3.734858
C	-3.904653	2.038900	3.342274
C	-1.092387	-3.418574	-0.089272
C	-1.922919	-4.177319	1.988262
C	-2.420208	0.681670	4.711006

H	-1.743555	-1.197680	3.887656
C	-3.195430	1.843051	4.520833
H	-4.504407	2.933244	3.194436
H	-0.495346	-3.514797	-0.989046
C	-1.187135	-4.447647	0.836115
H	-2.013448	-4.906480	2.790836
H	-1.875678	0.549958	5.641889
H	-3.239978	2.590274	5.308607
H	-0.685662	-5.394693	0.675343
C	-0.589567	0.641509	-2.100266
O	-0.594507	1.549221	-2.826677
Co	1.457385	-0.222956	-0.894356
C	2.058213	0.082281	-2.555406
C	2.005694	-1.899577	-0.760598
C	0.285079	-0.362947	0.446665
O	2.507057	0.234877	-3.613063
O	2.346157	-3.008734	-0.699007
O	-0.005688	-0.435212	1.594999
C	2.536789	1.140596	0.046749
N	2.237795	2.427314	0.351268
N	3.780135	0.899114	0.537601
C	3.335928	3.149750	1.029267
C	1.065303	3.179129	-0.003843
C	4.366491	2.041223	1.269926
C	4.507980	-0.338219	0.516821
H	2.979124	3.610902	1.954636
H	3.713843	3.947280	0.377961
C	0.996468	3.813842	-1.257146
C	0.063071	3.376585	0.968497
H	4.480199	1.792452	2.331599
H	5.357865	2.283635	0.873858
C	5.447619	-0.562028	-0.505800
C	4.348600	-1.254719	1.573289
C	-0.121768	4.606390	-1.539453
C	2.071802	3.656101	-2.305766
C	-1.041324	4.163738	0.629924
C	0.172677	2.800744	2.360896
C	6.198983	-1.741233	-0.471456
C	5.656732	0.436911	-1.620068
C	5.124216	-2.417573	1.563176
C	3.364590	-1.009180	2.693086
C	-1.157804	4.780547	-0.620259
H	-0.183090	5.093327	-2.510575
H	1.844417	2.816751	-2.971041

H	3.057981	3.466860	-1.871972
H	2.138133	4.556638	-2.925408
H	-1.826697	4.302561	1.369749
H	-0.788485	2.861183	2.878901
H	0.477579	1.752842	2.350574
H	0.903765	3.357306	2.964841
C	6.047308	-2.685558	0.547804
H	6.923850	-1.922536	-1.262376
H	5.903812	1.434627	-1.236536
H	4.762095	0.544412	-2.240588
H	6.478162	0.120951	-2.270366
H	4.999951	-3.134639	2.372222
H	3.622747	-0.115792	3.276860
H	2.346760	-0.864036	2.318994
H	3.355046	-1.856859	3.385380
C	-2.377122	5.601961	-0.970007
C	6.844179	-3.969354	0.543465
H	-2.805480	6.083255	-0.083988
H	-2.139153	6.383056	-1.700117
H	-3.162466	4.973749	-1.411255
H	7.060917	-4.311019	1.561569
H	6.291326	-4.774217	0.041144
H	7.796147	-3.849534	0.015390

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INT5, E(M06) = -2526.05618035

Co	-0.7591006777	-0.8063862999	-1.4168998549
C	-1.8183890934	-1.0156334087	-2.7947446096
O	-2.3937929285	-1.1726111903	-3.7863407732
C	-4.55693134	-0.9385994358	-0.9487309458
C	-4.8274194405	-2.3155400913	-1.0469854422
C	-4.9739670896	-0.0996185926	-1.9979922231
C	-5.4769143856	-2.8342513846	-2.1667339403
H	-4.5694556919	-2.9795202591	-0.2274989144
C	-5.6336496394	-0.6191766145	-3.1081881884
H	-4.7548458701	0.9626265951	-1.9439446732
C	-5.8826418722	-1.9903887948	-3.2020354166
H	-5.6812168113	-3.9004140394	-2.2207025355
H	-5.9387059252	0.0463216677	-3.9110695257
H	-6.3886802879	-2.3968134672	-4.0732172085
C	-3.9755980036	-0.3385478348	0.2604758374
N	-3.0609812463	-0.9877686153	1.1214490758
C	-4.3933268463	0.8185155901	0.8706798413
C	-2.3395939286	-2.1681457035	0.8710736875

C	-2.9615876082	-0.2437172831	2.3083388583
C	-3.7715575261	0.9092005867	2.1565536291
H	-5.1540255244	1.4786452937	0.4770856842
N	-1.5604152675	-2.2463405393	-0.2322522244
N	-2.4852376594	-3.1418318197	1.7745213863
C	-2.2219381598	-0.4800164764	3.4692203084
C	-3.8493775649	1.8411508021	3.2063530672
C	-0.9914337266	-3.4442655032	-0.4792507035
C	-1.8511555679	-4.2924556839	1.5511509991
C	-2.3183488173	0.4567553203	4.4938679066
H	-1.6023233165	-1.3615641429	3.5724011055
C	-3.1235091754	1.6062301319	4.3672231353
H	-4.4741659701	2.7253041682	3.1088262526
H	-0.4007171193	-3.5043256965	-1.3874213398
C	-1.1094545962	-4.5167551087	0.3918804183
H	-1.9606431742	-5.0596986637	2.3150823201
H	-1.7632162635	0.2925040128	5.4133195919
H	-3.178609734	2.3129663624	5.190925252
H	-0.6266579236	-5.4649677221	0.1859708435
C	0.3365333214	0.1815020832	-2.4175713608
O	0.6686199432	0.8338031467	-3.3464264434
Co	1.5327446678	0.1107260628	-0.8767988923
C	2.6373746364	-1.0422159907	-1.6483424969
C	0.3677277188	-0.3356090013	0.3526602117
O	3.2800556264	-1.9527537084	-1.9696032769
O	0.1163860693	-0.6370442468	1.4710385554
C	2.570530914	1.3575357833	0.2021809764
N	2.2617633401	2.6718927824	0.2883077025
N	3.6740913062	1.1494541704	0.9580133593
C	3.2174155188	3.4561583398	1.0962313592
C	1.1507822766	3.317015509	-0.3545327853
C	4.162093752	2.3696601067	1.6367954734
C	4.4114831308	-0.075966752	1.0836533694
H	2.6942927725	3.9975824344	1.8905535622
H	3.7328414312	4.1931092011	0.4684868071
C	1.2903544093	3.7820924077	-1.6750148967
C	-0.0349734537	3.5248895234	0.3755421734
H	4.0936705981	2.2538594741	2.7244548281
H	5.2111723568	2.5534004741	1.3832675828
C	5.4427812481	-0.3465489476	0.1636300459
C	4.1501463403	-0.9399044506	2.1618292938
C	0.2051495044	4.4396083332	-2.2621881837
C	2.5624331877	3.5682818528	-2.4614739217
C	-1.0927981974	4.1831913241	-0.2591139688

C	-0.177289967	3.057126349	1.8046433312
C	6.1848528696	-1.5194247258	0.3232687785
C	5.7488922358	0.5994029026	-0.9742113216
C	4.921694796	-2.1019685546	2.2784618618
C	3.0758880144	-0.6360619896	3.179589156
C	-0.9963915689	4.6415174528	-1.5768408242
H	0.3023869223	4.7968034462	-3.2851430919
H	2.6460230285	2.526288895	-2.78926099
H	3.4576789675	3.8030787433	-1.8746863325
H	2.5711557285	4.1980345225	-3.3563808952
H	-2.0167252573	4.3380140292	0.2937931355
H	-1.2027599627	3.1945715703	2.1580282332
H	0.0691758948	1.9970616725	1.9110835222
H	0.4815356633	3.6164836727	2.4829150387
C	5.935103674	-2.4146885108	1.3684784871
H	6.9767632039	-1.7396031304	-0.3896595423
H	6.1004281752	1.5745313661	-0.6118274944
H	4.8638530967	0.7845593475	-1.591558825
H	6.5310337683	0.1868724473	-1.6182518339
H	4.7246251246	-2.7781283734	3.1078813865
H	3.2554385185	0.3195085942	3.6885814836
H	2.0853078691	-0.5773261395	2.7189356085
H	3.0474881269	-1.4148055172	3.948173686
C	-2.1673983227	5.3174370102	-2.251878063
C	6.731284185	-3.6926628861	1.4974450528
H	-2.8351951369	5.7875742734	-1.5221576492
H	-1.835243847	6.0887060743	-2.9554994494
H	-2.7635135411	4.5934479346	-2.8231333515
H	6.6834911223	-4.0944711886	2.5149818921
H	6.3476132256	-4.4670196394	0.8200733827
H	7.7856987469	-3.5362557198	1.2433858724

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Product, E(M06) = -857.580800525

C	-0.6362584233	-1.0887134941	-0.8102346056
N	-1.4053189216	0.0966734939	-0.7170613876
C	-1.4574475976	-2.1619042028	-0.5919524284
C	-0.8864439109	1.3924362387	-0.5628720162
C	-2.7431755926	-0.2663995654	-0.4500931633
C	-2.7874864864	-1.6805532321	-0.3538905509
H	-1.1524584035	-3.1960463389	-0.6790876635
N	0.3475706152	1.4940617707	-0.0503478258
N	-1.6797846157	2.4089424193	-0.9310993989
C	-3.8864283188	0.5150897647	-0.2594869391

C	-4.0051036946	-2.3217116001	-0.0792500933
C	0.8347028865	2.7292335839	0.0732747061
C	-1.177662721	3.6358165557	-0.7657689224
C	-5.081101385	-0.1462207376	0.019958782
H	-3.8463698697	1.5918320407	-0.3511351281
C	-5.1447549775	-1.5484910486	0.1071733366
H	-4.0493715326	-3.4054381384	-0.0094942357
H	1.8422482239	2.806248942	0.479088316
C	0.1041646883	3.8658901735	-0.2720095021
H	-1.8289550324	4.4600066155	-1.052412035
H	-5.985192014	0.4395385198	0.1626096211
H	-6.0955443999	-2.0296669161	0.3200436007
H	0.5053850823	4.8664160144	-0.1558446733
C	0.76573506	-1.145141849	-1.2583985814
C	1.6548623715	-2.0350970387	-0.6357975453
C	1.2200115279	-0.4031901389	-2.3624480105
C	2.962784962	-2.17647102	-1.0993114205
H	1.3166993865	-2.6029668061	0.2261710493
C	2.5278995973	-0.5422142144	-2.8209910947
H	0.5374835489	0.2699359211	-2.8736552216
C	3.4060352264	-1.4287480761	-2.1914548926
H	3.6380286532	-2.8668072854	-0.6004791184
H	2.8603388819	0.0359390272	-3.6793407577
H	4.4257581853	-1.5364193783	-2.5513102

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INT3A’, E(M06) = -2526.04013057

Co	1.2609403375	-0.9973057578	1.4315095035
C	2.6002765577	-1.1540254074	2.5647271811
O	3.4679504039	-1.2185300543	3.3136342609
C	0.3058965852	-2.3588211736	2.5895858299
C	0.94094442	-3.5679078437	2.9426752407
C	-1.0078227543	-2.1987674734	3.0705126026
C	0.3038295962	-4.5645676878	3.6909727775
H	1.9686712287	-3.7541514514	2.6330029457
C	-1.656273793	-3.1852875935	3.8199799062
H	-1.5526074344	-1.2858982204	2.8552522845
C	-1.0059461109	-4.3795374894	4.1325032135
H	0.8394801742	-5.4800164243	3.9356687061
H	-2.675826896	-3.0154847512	4.1614700274
H	-1.5067619481	-5.1468216639	4.7179054081
C	2.4430129223	0.1380451334	0.323949407
N	3.0278486993	-0.5662961106	-0.7685648967
C	3.0280460649	1.3755650518	0.348271469

C	2.7068307983	-1.8816357831	-0.9679168312
C	3.9679631634	0.2444562892	-1.4327229105
C	3.9831762469	1.4790726925	-0.7316847361
H	2.8140950393	2.1478068405	1.0748351399
N	1.8277072459	-2.3888528744	-0.0630600241
N	3.2443070063	-2.5596264958	-1.9904938622
C	4.776118467	0.009104534	-2.5454279918
C	4.8488624342	2.494322466	-1.1637913398
C	1.4455750201	-3.6578294794	-0.2370305517
C	2.8659509216	-3.8321955576	-2.1223064647
C	5.6237694004	1.0411468398	-2.9553042852
H	4.7452284819	-0.9402896729	-3.0629616254
C	5.6626238853	2.2676956255	-2.2728420411
H	4.8916877107	3.4410091172	-0.6308717394
H	0.7258474529	-4.0355897469	0.4804048264
C	1.95056984	-4.4441100961	-1.2689137465
H	3.313417545	-4.3772618426	-2.9518819888
H	6.2675797362	0.8857440439	-3.8168734686
H	6.3395974546	3.047750307	-2.611861213
H	1.640946629	-5.4745691745	-1.3970634623
C	0.597261023	0.5034111478	2.225129523
O	0.8757804722	1.3249830046	3.0251216981
Co	-0.839636938	0.5607552779	0.7918232879
C	-1.8395337693	1.1719496765	2.106927307
C	-0.6534461277	-0.9932508996	-0.0458268796
O	-2.5712626399	1.4414217363	2.9614002151
O	-0.9460450493	-1.9463603269	-0.6448853362
C	-2.0030882046	1.3370882447	-0.5816466058
N	-1.7906811717	2.6067303594	-0.9963466216
N	-3.1114459382	0.8792801292	-1.2086848191
C	-2.7235938196	3.0349089657	-2.0599912334
C	-0.6876929354	3.4597686573	-0.6432246657
C	-3.768800229	1.9157987027	-2.0375159685
C	-3.754433742	-0.4027406095	-1.0926671982
H	-2.1946626913	3.1014098106	-3.0184955688
H	-3.1407131093	4.019558359	-1.8324261031
C	-0.8883663012	4.4685989484	0.3191022789
C	0.5222758946	3.3529285243	-1.3534650301
H	-4.0019245092	1.5229391081	-3.0302330508
H	-4.7091288065	2.2235025427	-1.5629243236
C	-4.6763463457	-0.6482267718	-0.061991237
C	-3.5228473381	-1.3576211253	-2.1060720563
C	0.1655099603	5.3483151993	0.5814167573
C	-2.2036040561	4.6300403773	1.0460559232

C	1.541183242	4.2649813015	-1.061418124
C	0.7288939314	2.2965696176	-2.4139641788
C	-5.3157409719	-1.8953960322	-0.0291564147
C	-5.0266203691	0.375045394	0.9931082525
C	-4.1887061259	-2.580270249	-2.0305910231
C	-2.5845093638	-1.0802857257	-3.2575437169
C	1.3871969112	5.2620378126	-0.0936421172
H	0.0227083957	6.127377476	1.3270482541
H	-2.4462584893	3.7532401712	1.653505455
H	-3.0408322389	4.7856802347	0.3539565181
H	-2.1663470468	5.4950299983	1.7145766265
H	2.4814954904	4.1827778838	-1.6000638282
H	0.6002975849	1.2897539274	-2.0040673722
H	0.0209297676	2.4072232036	-3.2457553033
H	1.7393559394	2.3578138026	-2.8249062044
C	-5.0800826132	-2.8762299715	-0.9916303485
H	-6.0253306476	-2.0947621948	0.7714516823
H	-4.6594709016	1.3738145532	0.7471896014
H	-4.6020242513	0.1058239422	1.9658837217
H	-6.1137145966	0.4337071772	1.119699874
H	-4.0029632839	-3.3258368459	-2.800797943
H	-3.0080179282	-0.3535129509	-3.9642396988
H	-1.625359635	-0.6832336596	-2.9146707684
H	-2.3863349169	-1.9981049257	-3.8184121068
C	2.5174400232	6.2114594061	0.2289189863
C	-5.7549123038	-4.2255534057	-0.9144207543
H	3.161801853	6.378251898	-0.6406728617
H	2.1415116466	7.1832750248	0.5663792406
H	3.1499164118	5.8115254519	1.0325733144
H	-6.0537490515	-4.5826990037	-1.9063825966
H	-5.0787043514	-4.9785871836	-0.4889909181
H	-6.6475562711	-4.1923152817	-0.2815460914

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INT3B’, E(M06) = -2526.04174722

Co	-1.2800850158	-0.9574806761	-1.1372143673
C	-0.5350320065	-1.9090431182	-2.5033864302
O	-0.135286876	-2.5141804112	-3.393520764
C	-2.9242325095	-1.0380981688	-2.2574561471
C	-3.6868019631	-2.2140389726	-2.3201919369
C	-3.3580042193	0.0618826924	-3.0110629019
C	-4.851205063	-2.2851259629	-3.0943185591
H	-3.3840289237	-3.0988832011	-1.7666867092
C	-4.5171780666	-0.007067476	-3.7887669477

H	-2.8008428157	0.9938414301	-2.9901344802
C	-5.2728930234	-1.1805527523	-3.8332273028
H	-5.4240060892	-3.2102243415	-3.1183691306
H	-4.8311226824	0.8644998462	-4.3599284144
H	-6.1757848815	-1.2329245523	-4.4366263494
C	-2.3825229905	-0.0449839765	0.1492287172
N	-2.8847646123	-0.9298888917	1.1487034274
C	-2.8678194934	1.1980872473	0.4422321663
C	-2.5179476095	-2.2392487921	1.115804327
C	-3.6844225329	-0.2258593296	2.0713814185
C	-3.6820183369	1.1251015891	1.6352441369
H	-2.6720117671	2.092896565	-0.1324728467
N	-1.6729292379	-2.5548407965	0.0906501182
N	-2.9701405395	-3.1046469861	2.034457352
C	-4.3750965561	-0.6447912085	3.2063696267
C	-4.400836115	2.0748067345	2.3731857132
C	-1.2535669026	-3.8233648248	0.0217496188
C	-2.5370333546	-4.3596045374	1.9350045512
C	-5.0826718703	0.3251840026	3.922570031
H	-4.3607061905	-1.6817525923	3.514732774
C	-5.095941541	1.6668663961	3.5116259441
H	-4.4215752179	3.1145303938	2.0555914946
H	-0.5773614788	-4.0611925139	-0.7938089163
C	-1.658402962	-4.7875795354	0.9376625223
H	-2.9104673309	-5.0530587858	2.686719363
H	-5.6332385551	0.0298559099	4.8117291488
H	-5.6593010292	2.3970178694	4.0874480658
H	-1.3108274675	-5.8116327107	0.8733704352
C	-0.5707017883	0.6081966931	-1.6277922659
O	-0.6358438335	1.6920222159	-2.0888437965
Co	1.1148268751	0.2608536788	-0.5369809487
C	1.9664668304	-0.0805009024	-2.0546029231
C	0.4589215796	-0.5673138767	0.8708964913
O	2.533374957	-0.4616188563	-2.9883768434
O	0.2798537662	-1.1514392915	1.8621636057
C	2.5810036451	1.0580800949	0.4669737885
N	2.4593481476	2.2988464696	0.9829035683
N	3.8032488761	0.5841786818	0.7973483282
C	3.6394010538	2.7288699803	1.7619094913
C	1.3106333405	3.1549455699	0.8556999942
C	4.6272117491	1.5732288249	1.5286312816
C	4.401387085	-0.6439779671	0.3480720057
H	3.3714559534	2.8473863489	2.8176206086
H	4.0099738505	3.6910242683	1.3943742082

C	1.2090390846	3.9926141926	-0.2718560857
C	0.3526104467	3.1935148486	1.8861065225
H	5.0075161635	1.140960397	2.4591045994
H	5.485986139	1.8701594636	0.9158380379
C	5.132801676	-0.6588795643	-0.8545424945
C	4.3197331305	-1.7885478908	1.1652584243
C	0.1158717712	4.8575850605	-0.3567854007
C	2.2406428021	3.9639220351	-1.3753595952
C	-0.727312347	4.0722344109	1.7489000412
C	0.47026856	2.3387293389	3.1266371486
C	5.7201391246	-1.8627120585	-1.258823703
C	5.3394438724	0.5832523558	-1.6917041137
C	4.9286091539	-2.9647341768	0.7184652251
C	3.6217932561	-1.7629842257	2.5050575872
C	-0.8666708696	4.9077565741	0.6374416938
H	0.0266473276	5.5039715039	-1.2270640753
H	2.1766014751	3.0338143578	-1.951115015
H	3.2635167288	4.0384414029	-0.9869120789
H	2.0841747655	4.7947992003	-2.069448279
H	-1.4828784445	4.0941639057	2.5308586819
H	0.8208056682	1.3287640386	2.9010133023
H	1.1687146369	2.7783004747	3.8527529368
H	-0.5005820597	2.249622638	3.6222700973
C	5.6197256558	-3.028699142	-0.4962662447
H	6.2722832569	-1.8843994664	-2.1960841246
H	4.5137231344	1.2921881284	-1.5985694074
H	5.4385235582	0.3242349615	-2.749700874
H	6.2607242973	1.1047256007	-1.3965554323
H	4.8658129845	-3.8539347625	1.3421764432
H	3.9915373776	-0.9493689592	3.1410838406
H	2.5418277958	-1.626227849	2.4051238102
H	3.7916090196	-2.702118462	3.0403094582
C	-2.0614753937	5.8219897898	0.4978861212
C	6.230842289	-4.3252019011	-0.9741424366
H	-2.4617415227	6.1118564538	1.475080803
H	-1.8061669466	6.7348387201	-0.0510607325
H	-2.8717600779	5.3275795972	-0.0541163203
H	6.5089639699	-4.9710699489	-0.1345348197
H	5.523487681	-4.8874447545	-1.5980177839
H	7.1265485985	-4.1484427835	-1.5790091002

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TS4, E(M06) = -2526.02285149

Co	-1.180810	-1.326373	-1.012745

C	-0.605604	-2.508389	-2.269574
O	-0.350778	-3.264849	-3.100429
C	-3.156672	-1.298700	-1.561588
C	-3.981511	-2.412186	-1.293778
C	-3.452781	-0.544285	-2.721240
C	-5.037346	-2.755390	-2.139600
H	-3.810274	-3.026316	-0.416331
C	-4.500730	-0.895482	-3.565089
H	-2.855071	0.328356	-2.963134
C	-5.306160	-2.005092	-3.283985
H	-5.649493	-3.621596	-1.898114
H	-4.689305	-0.297024	-4.453721
H	-6.127571	-2.273965	-3.942356
C	-2.589841	-0.360502	-0.080600
N	-2.873327	-0.992422	1.180838
C	-3.065228	0.939217	0.029497
C	-2.286349	-2.188290	1.478107
C	-3.540706	-0.093680	2.035948
C	-3.654398	1.129060	1.318811
H	-3.052025	1.665338	-0.771151
N	-1.414690	-2.628186	0.526931
N	-2.584876	-2.835265	2.611907
C	-4.015805	-0.243318	3.335735
C	-4.276087	2.224774	1.941903
C	-0.816600	-3.804517	0.751476
C	-1.956863	-3.992407	2.817330
C	-4.625332	0.866046	3.931401
H	-3.916261	-1.185009	3.858774
C	-4.755091	2.082568	3.242311
H	-4.383475	3.166830	1.410308
H	-0.132380	-4.146237	-0.018757
C	-1.050016	-4.539776	1.908100
H	-2.196966	-4.505847	3.746765
H	-5.009070	0.778174	4.944102
H	-5.240669	2.923942	3.730449
H	-0.552305	-5.485190	2.087715
C	-0.516502	0.118214	-1.815749
O	-0.556952	1.061655	-2.530123
Co	1.099463	0.183571	-0.591700
C	2.031518	-0.652541	-1.845009
C	0.353674	-0.196979	0.950036
O	2.633191	-1.341538	-2.554759
O	0.090525	-0.481269	2.049164
C	2.479893	1.312855	0.188388

N	2.277058	2.637579	0.357271
N	3.717322	1.020103	0.647128
C	3.422890	3.336312	0.975630
C	1.089662	3.363705	-0.004057
C	4.457874	2.207896	1.127359
C	4.382086	-0.252388	0.582853
H	3.128106	3.770975	1.936749
H	3.768303	4.148881	0.327605
C	0.959662	3.851374	-1.319187
C	0.116941	3.633961	0.976386
H	4.781676	2.062383	2.163030
H	5.350882	2.368482	0.513309
C	5.175060	-0.560522	-0.538475
C	4.295519	-1.132196	1.678647
C	-0.173793	4.602379	-1.637316
C	1.998165	3.563779	-2.377790
C	-1.004831	4.382953	0.603424
C	0.260202	3.160814	2.404340
C	5.837135	-1.792163	-0.564645
C	5.349540	0.405932	-1.687712
C	4.979418	-2.349414	1.604946
C	3.506502	-0.781843	2.918545
C	-1.170878	4.873188	-0.694190
H	-0.283480	4.978756	-2.652103
H	1.934016	2.522173	-2.712004
H	3.018908	3.730764	-2.014589
H	1.842998	4.202689	-3.252277
H	-1.769139	4.582399	1.351033
H	0.634507	2.136139	2.463433
H	0.950459	3.799905	2.972910
H	-0.706401	3.190423	2.915240
C	5.745296	-2.704467	0.489679
H	6.439087	-2.042607	-1.435661
H	4.448238	0.995707	-1.871790
H	5.592804	-0.130898	-2.609099
H	6.172068	1.108566	-1.493585
H	4.915082	-3.035928	2.446553
H	3.806686	0.188929	3.331833
H	2.432515	-0.727089	2.720131
H	3.664892	-1.534354	3.697008
C	-2.403511	5.658060	-1.079033
C	6.441733	-4.043569	0.419649
H	-2.918042	6.054534	-0.197755
H	-2.154665	6.500285	-1.734613

H	-3.119132	5.027478	-1.622708
H	6.664126	-4.432897	1.418776
H	5.814960	-4.787753	-0.089358
H	7.382665	-3.978370	-0.137261

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C-INT1A

Co	-0.370446	0.536298	-0.467918
C	-2.042699	-2.376453	0.406907
O	-3.052151	-1.801615	-0.010539
C	-1.904769	-2.744816	1.848862
C	-0.665317	-2.781448	2.510079
C	-3.081880	-3.016663	2.566880
C	-0.613286	-3.090778	3.871294
H	0.255061	-2.547933	1.984583
C	-3.020435	-3.343719	3.918482
H	-4.031848	-2.973319	2.044081
C	-1.784381	-3.378872	4.573928
H	0.347801	-3.103086	4.377159
H	-3.932348	-3.573699	4.463339
H	-1.736899	-3.629329	5.630396
C	-0.991681	-2.783535	-0.536711
N	-1.014809	-2.333977	-1.879145
C	-0.100930	-3.827944	-0.444452
C	-1.780993	-1.298903	-2.429260
C	-0.149340	-3.141857	-2.629090
C	0.455478	-4.063892	-1.737697
H	0.098371	-4.396894	0.451135
N	-1.661601	-0.029713	-1.939675
N	-2.515744	-1.640153	-3.487414
C	0.190091	-3.097242	-3.984937
C	1.414637	-4.973226	-2.219013
C	-2.439971	0.895430	-2.534539
C	-3.243829	-0.695347	-4.079847
C	1.138127	-4.009961	-4.434034
H	-0.278896	-2.398735	-4.667689
C	1.746544	-4.939005	-3.564171
H	1.891532	-5.674932	-1.541376
H	-2.365413	1.896447	-2.138479
C	-3.265686	0.614384	-3.612574
H	-3.825067	-1.005894	-4.945650
H	1.415804	-4.006053	-5.484202
H	2.488710	-5.627861	-3.956007
H	-3.869832	1.387515	-4.072301

C	0.512534	0.633492	1.062107
O	0.963206	0.616238	2.115012
Co	4.791756	-0.593797	1.319729
C	5.298504	-0.150217	-0.310788
C	6.082554	-1.546443	2.083898
C	4.525316	0.871024	2.257171
C	3.324292	-1.538756	1.239366
O	5.613677	0.158121	-1.391458
O	6.917511	-2.177288	2.587786
O	4.332221	1.854897	2.860344
O	2.316432	-2.139747	1.164048
C	0.987767	-0.399813	-1.219730
O	1.899129	-0.767787	-1.803903
C	-1.268355	2.253946	0.051212
N	-0.511599	3.368296	-0.045747
N	-2.492717	2.619070	0.502296
C	-1.249948	4.604006	0.293212
C	0.865373	3.446502	-0.470285
C	-2.540354	4.048874	0.901492
C	-3.613871	1.782960	0.843891
H	-1.423554	5.192067	-0.616959
H	-0.671384	5.215608	0.989191
C	1.869236	3.609865	0.506227
C	1.181809	3.433417	-1.843590
H	-3.443221	4.529124	0.517939
H	-2.555952	4.115536	1.996284
C	-3.580180	0.989597	2.007194
C	-4.788417	1.876542	0.068823
C	3.200817	3.665841	0.081772
C	1.573498	3.749249	1.982901
C	2.526617	3.511396	-2.213447
C	0.126745	3.346734	-2.923607
C	-4.716486	0.243267	2.332517
C	-2.380421	0.923953	2.920937
C	-5.891589	1.099030	0.431565
C	-4.937124	2.831855	-1.095916
C	3.554667	3.603021	-1.268899
H	3.979968	3.735156	0.835567
H	0.584395	3.372527	2.255338
H	1.624169	4.803787	2.287719
H	2.318437	3.203839	2.569063
H	2.779214	3.495810	-3.271716
H	-0.098659	2.306430	-3.189201
H	-0.814304	3.823434	-2.627911

H	0.476178	3.840814	-3.835626
C	-5.873178	0.264331	1.550930
H	-4.688392	-0.375036	3.226490
H	-1.769342	1.829960	2.884115
H	-1.733942	0.078039	2.666630
H	-2.700813	0.776816	3.957009
H	-6.794483	1.159644	-0.173121
H	-3.978498	3.188591	-1.479462
H	-5.479526	2.358751	-1.921518
H	-5.517628	3.717226	-0.803084
C	5.001966	3.609317	-1.693421
C	-7.064801	-0.594318	1.901393
H	5.394995	2.585319	-1.704028
H	5.123179	4.026002	-2.699297
H	5.619220	4.191377	-1.001382
H	-8.000742	-0.149421	1.547308
H	-6.979489	-1.586598	1.438991
H	-7.146996	-0.744756	2.983044

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C-TS1A

Co	-0.364037	0.099347	-0.122815
C	-1.220645	-0.906988	1.520549
O	-2.179527	-1.607024	1.232794
C	-1.044467	-0.495683	2.970250
C	-0.719723	0.787474	3.413284
C	-1.308338	-1.494837	3.924852
C	-0.627401	1.067152	4.779944
H	-0.561714	1.584542	2.700005
C	-1.202160	-1.220642	5.285021
H	-1.586188	-2.486568	3.582809
C	-0.857917	0.063807	5.719075
H	-0.376139	2.073034	5.105350
H	-1.389983	-2.008902	6.009083
H	-0.775732	0.278850	6.780860
C	0.364398	-1.510486	0.727412
N	0.073722	-2.683874	-0.017600
C	1.356892	-1.848713	1.632682
C	-0.778196	-2.591868	-1.071544
C	0.852816	-3.753030	0.442370
C	1.675593	-3.234301	1.476616
H	1.806857	-1.184563	2.356190
N	-1.186962	-1.319287	-1.348573

N	-1.120154	-3.680303	-1.765599
C	0.916471	-5.087921	0.045047
C	2.594519	-4.075280	2.125245
C	-1.898072	-1.152526	-2.467667
C	-1.866547	-3.486031	-2.850442
C	1.834684	-5.900568	0.709259
H	0.285916	-5.467027	-0.747246
C	2.664996	-5.405719	1.733375
H	3.242658	-3.680882	2.901806
H	-2.143732	-0.132371	-2.720661
C	-2.272300	-2.220313	-3.272686
H	-2.136903	-4.379267	-3.410121
H	1.913185	-6.945426	0.422047
H	3.373136	-6.073526	2.215060
H	-2.847302	-2.070179	-4.177959
C	0.852128	1.039752	0.834918
O	1.747859	1.485096	1.381973
Co	4.443687	-0.409196	-1.037957
C	4.129926	1.125467	-1.841061
C	3.325308	-1.630529	-1.632140
C	6.089742	-0.917530	-1.466625
C	4.371581	-0.293256	0.723181
O	3.916115	2.126716	-2.408877
O	2.562188	-2.417619	-2.040116
O	7.163560	-1.253119	-1.752090
O	4.312834	-0.238435	1.888140
C	0.754755	0.340706	-1.756768
O	1.047439	0.313392	-2.857903
C	-1.745905	1.745164	-0.435780
N	-1.371329	3.052583	-0.418977
N	-3.083724	1.739408	-0.711101
C	-2.447483	3.986941	-0.815183
C	-0.087375	3.636462	-0.132584
C	-3.678042	3.099449	-0.731687
C	-4.047013	0.666489	-0.723009
H	-2.253021	4.355764	-1.830426
H	-2.481663	4.844936	-0.140290
C	0.126094	4.187626	1.149734
C	0.879598	3.776439	-1.148162
H	-4.355931	3.211008	-1.580445
H	-4.253395	3.253037	0.190180
C	-4.538072	0.133407	0.484668
C	-4.636435	0.308556	-1.955016
C	1.375329	4.743884	1.432132

C	-0.958794	4.243957	2.202746
C	2.120768	4.325085	-0.808208
C	0.610524	3.444244	-2.597952
C	-5.512634	-0.867623	0.418811
C	-4.141637	0.664687	1.840630
C	-5.613125	-0.691055	-1.965844
C	-4.308859	1.013417	-3.255251
C	2.399351	4.787995	0.480232
H	1.557207	5.143102	2.427688
H	-1.674392	3.421598	2.125158
H	-1.530529	5.179547	2.124293
H	-0.527028	4.224052	3.208377
H	2.892042	4.370075	-1.571024
H	1.484699	2.971331	-3.053261
H	-0.251938	2.787653	-2.731511
H	0.411135	4.368014	-3.157909
C	-6.046890	-1.313038	-0.791919
H	-5.870768	-1.301525	1.349796
H	-4.914030	1.351488	2.214292
H	-3.194104	1.202913	1.827119
H	-4.044639	-0.149310	2.562358
H	-6.053935	-0.981338	-2.917592
H	-3.353286	1.543896	-3.224101
H	-4.281974	0.308156	-4.093089
H	-5.081490	1.755410	-3.497840
C	3.771100	5.310114	0.830837
C	-7.065340	-2.427617	-0.829356
H	4.198328	5.896872	0.010701
H	3.747363	5.937104	1.728021
H	4.458889	4.477030	1.023539
H	-7.685514	-2.376409	-1.730387
H	-6.572897	-3.408888	-0.824837
H	-7.727589	-2.395392	0.042469

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C-INT1B

Co	-1.891977	-0.668390	1.408234
C	-3.233555	-1.542621	2.241362
O	-3.959968	-2.224234	2.825403
C	-5.176667	0.406528	0.069845
O	-5.407928	1.104491	1.056512
C	-5.969599	-0.835992	-0.189078

C	-5.471124	-1.930526	-0.913257
C	-7.254948	-0.910774	0.371709
C	-6.255545	-3.072291	-1.083532
H	-4.462862	-1.906929	-1.311123
C	-8.039260	-2.045522	0.188446
H	-7.617351	-0.065955	0.948342
C	-7.540723	-3.129395	-0.541532
H	-5.856606	-3.920766	-1.632728
H	-9.036699	-2.090067	0.617441
H	-8.150118	-4.018849	-0.679093
C	-4.167490	0.840232	-0.917940
N	-3.236106	1.841482	-0.603268
C	-4.144694	0.631062	-2.280990
C	-2.937803	2.346201	0.682157
C	-2.633086	2.273556	-1.778694
C	-3.178858	1.515703	-2.849333
H	-4.798443	-0.040156	-2.818489
N	-2.518120	1.482504	1.623767
N	-3.049798	3.667447	0.819610
C	-1.649207	3.247476	-1.989060
C	-2.731719	1.751393	-4.162861
C	-2.323512	2.001934	2.847302
C	-2.808950	4.168071	2.034172
C	-1.231069	3.459886	-3.297377
H	-1.254230	3.834545	-1.168083
C	-1.763562	2.720044	-4.376155
H	-3.141567	1.180300	-4.991538
H	-1.996598	1.304071	3.609994
C	-2.477067	3.357939	3.115224
H	-2.895382	5.248302	2.135094
H	-0.484204	4.224143	-3.495808
H	-1.409766	2.918746	-5.383997
H	-2.312715	3.758446	4.109123
C	-1.839920	-1.578015	-0.047841
O	-1.778758	-2.231992	-1.011217
Co	1.711456	-0.306338	0.694864
C	1.821123	-1.915851	1.513022
C	2.095882	1.076294	1.793284
C	0.866877	0.005445	-0.871729
O	1.808236	-2.876176	2.147819
O	2.212011	1.917727	2.571436
O	0.308949	0.229652	-1.853405
C	-0.078721	-0.301719	1.559397
O	-0.327626	-0.168225	2.751468

C	3.435087	-0.405253	-0.335821
N	3.959301	-1.522408	-0.892793
N	4.186252	0.643324	-0.752798
C	5.089272	-1.250760	-1.808612
C	3.588105	-2.897693	-0.691297
C	5.323433	0.250588	-1.614409
C	4.111890	2.019933	-0.344541
H	4.800902	-1.507678	-2.834716
H	5.955807	-1.861534	-1.539709
C	4.289932	-3.635362	0.287013
C	2.636835	-3.512267	-1.521614
H	5.297453	0.814462	-2.551897
H	6.271550	0.473811	-1.112422
C	4.831328	2.425543	0.800391
C	3.438129	2.954802	-1.147972
C	3.997787	-4.990168	0.434641
C	5.306653	-2.976707	1.190445
C	2.376336	-4.876112	-1.328632
C	1.875205	-2.767473	-2.591668
C	4.822046	3.776469	1.145994
C	5.584042	1.431640	1.654457
C	3.459100	4.300449	-0.756102
C	2.702731	2.570690	-2.410639
C	3.036021	-5.629728	-0.358457
H	4.525816	-5.561262	1.195184
H	4.848031	-2.188357	1.798455
H	6.128140	-2.513247	0.629985
H	5.746429	-3.710056	1.872515
H	1.632579	-5.356286	-1.961068
H	0.848334	-2.564944	-2.266651
H	2.332911	-1.807419	-2.840686
H	1.814558	-3.366105	-3.507471
C	4.133928	4.731102	0.385992
H	5.362943	4.093390	2.035094
H	6.422812	0.974192	1.113950
H	4.935915	0.616801	1.993920
H	5.995960	1.923031	2.540503
H	2.935630	5.029502	-1.371601
H	2.949619	1.561329	-2.746415
H	1.617174	2.601716	-2.264723
H	2.941656	3.269560	-3.220482
C	2.713613	-7.090700	-0.150346
C	4.118736	6.182797	0.803975
H	2.173870	-7.508014	-1.006258

H	3.621910	-7.684803	0.002443
H	2.082617	-7.230018	0.736947
H	3.802373	6.833633	-0.017324
H	3.425108	6.344440	1.639357
H	5.108397	6.514181	1.138505

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C-TS1B

Co	-2.211678	-1.302721	0.971523
C	-2.805038	-2.427945	2.281565
O	-3.188583	-3.173519	3.067277
C	-4.234713	-0.956158	0.248687
O	-4.908418	-0.170522	0.898022
C	-4.917367	-2.082348	-0.494859
C	-4.279570	-3.035723	-1.300934
C	-6.308846	-2.177735	-0.319840
C	-5.009657	-4.050998	-1.917358
H	-3.210219	-2.994758	-1.457129
C	-7.037922	-3.196423	-0.929736
H	-6.799176	-1.437862	0.302956
C	-6.391535	-4.138112	-1.732863
H	-4.494935	-4.777128	-2.541032
H	-8.112771	-3.254167	-0.778156
H	-6.957742	-4.933858	-2.209769
C	-2.760948	-0.146015	-0.520938
N	-2.728806	1.223697	-0.108117
C	-2.865009	-0.118081	-1.909762
C	-2.630388	1.506683	1.224817
C	-2.854930	2.074955	-1.210038
C	-2.920824	1.238827	-2.358946
H	-2.942910	-0.987012	-2.545761
N	-2.367900	0.418463	1.994605
N	-2.772450	2.757103	1.673133
C	-2.905487	3.466513	-1.300828
C	-3.033933	1.827844	-3.630518
C	-2.289221	0.612516	3.316888
C	-2.677558	2.925637	2.991942
C	-3.021894	4.021605	-2.577069
H	-2.870799	4.079678	-0.410459
C	-3.082560	3.214305	-3.728177
H	-3.085973	1.204970	-4.519395
H	-2.065361	-0.263903	3.914840
C	-2.446951	1.872719	3.878313

H	-2.792474	3.946314	3.351843
H	-3.078984	5.102133	-2.679454
H	-3.175844	3.682424	-4.704483
H	-2.371813	2.026102	4.947986
C	-1.391983	-2.539644	0.035731
O	-0.840594	-3.362514	-0.562269
Co	1.550744	-0.297049	0.583882
C	2.405927	-1.683378	1.372497
C	1.213815	1.110911	1.657908
C	0.763848	-0.534853	-1.015624
O	2.833791	-2.575547	1.962131
O	0.940313	1.926859	2.427665
O	0.310670	-0.708976	-2.062702
C	-0.086153	-1.094414	1.615139
O	-0.017074	-1.377545	2.767598
C	3.136807	0.472864	-0.426174
N	4.168690	-0.227876	-0.958423
N	3.274585	1.757030	-0.834072
C	5.082851	0.592819	-1.784502
C	4.555800	-1.593049	-0.725766
C	4.438500	1.980879	-1.720073
C	2.501052	2.912191	-0.467181
H	5.130693	0.188944	-2.801287
H	6.094761	0.569851	-1.366607
C	5.443819	-1.866643	0.335738
C	4.157658	-2.602499	-1.618480
H	4.097063	2.339986	-2.697075
H	5.099153	2.742741	-1.294045
C	2.915797	3.665574	0.651535
C	1.441741	3.344183	-1.282357
C	5.892867	-3.176273	0.505974
C	5.880317	-0.785121	1.296493
C	4.635946	-3.901259	-1.403377
C	3.228462	-2.341623	-2.780275
C	2.217869	4.832372	0.962602
C	4.072504	3.222067	1.516978
C	0.770086	4.520725	-0.924338
C	1.002337	2.603635	-2.523422
C	5.493624	-4.211973	-0.347132
H	6.566710	-3.396447	1.331055
H	5.021280	-0.320552	1.793137
H	6.435657	0.018357	0.796147
H	6.531227	-1.200042	2.071492
H	4.327033	-4.689034	-2.087403

H	2.186882	-2.533256	-2.500720
H	3.276714	-1.307575	-3.132442
H	3.469547	-3.001234	-3.620373
C	1.133036	5.271721	0.193976
H	2.524971	5.410262	1.831700
H	5.016834	3.181263	0.959053
H	3.903589	2.224146	1.935828
H	4.214155	3.915412	2.351061
H	-0.063542	4.847644	-1.541629
H	1.689178	1.800690	-2.798020
H	0.013116	2.155133	-2.382545
H	0.921280	3.293056	-3.371638
C	5.965320	-5.628439	-0.116797
C	0.363624	6.513131	0.580083
H	5.910831	-6.223712	-1.034082
H	6.998921	-5.653880	0.245691
H	5.344626	-6.130033	0.637134
H	-0.082685	6.997493	-0.294761
H	-0.455118	6.267044	1.269181
H	1.004942	7.243942	1.084554

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Co	0.740154	0.447965	0.307089
C	1.731297	-1.499316	1.838223
O	2.429700	-0.872452	2.635830
C	2.328071	-2.646525	1.072492
C	1.769005	-3.263916	-0.058680
C	3.545701	-3.139425	1.576979
C	2.408647	-4.348096	-0.659787
H	0.845503	-2.917154	-0.500605
C	4.175957	-4.228508	0.982019
H	3.973924	-2.658748	2.449384
C	3.607711	-4.838369	-0.140273
H	1.957072	-4.810763	-1.532333
H	5.105654	-4.607112	1.398504
H	4.093498	-5.693377	-0.603080
C	0.254005	-1.182099	1.769008
N	-0.255370	-0.347778	2.826426
C	-0.769507	-2.112080	1.497687
C	0.314958	0.883336	3.094063
C	-1.536373	-0.756722	3.171628
C	-1.874111	-1.856746	2.335040

H	-0.713506	-2.935656	0.802169
N	0.942831	1.461986	2.036882
N	0.182757	1.404401	4.309682
C	-2.440904	-0.241975	4.107592
C	-3.139581	-2.476121	2.447300
C	1.582074	2.611801	2.295810
C	0.801472	2.567302	4.530588
C	-3.672909	-0.877100	4.198328
H	-2.177950	0.589779	4.747830
C	-4.023794	-1.981137	3.384785
H	-3.406024	-3.293691	1.786729
H	2.098027	3.068858	1.462829
C	1.560582	3.205324	3.552954
H	0.686637	2.990506	5.526072
H	-4.393705	-0.513516	4.925650
H	-5.007367	-2.427425	3.490889
H	2.080606	4.136442	3.744126
C	0.334285	-0.460048	-1.124327
O	0.062414	-1.035250	-2.085756
Co	-3.920294	-1.823279	-1.536466
C	-3.759421	-1.002242	-3.089128
C	-3.909589	-0.577435	-0.293569
C	-5.461392	-2.704496	-1.474437
C	-2.594768	-2.949233	-1.321761
O	-3.622547	-0.414231	-4.088345
O	-3.893475	0.263027	0.518982
O	-6.467775	-3.283168	-1.425950
O	-1.690148	-3.678794	-1.153195
C	1.399904	1.880235	-0.801851
N	2.656086	1.964372	-1.300703
N	0.725511	3.004742	-1.140210
C	2.920009	3.271878	-1.945550
C	3.652965	0.920232	-1.344317
C	1.515024	3.885998	-2.031452
C	-0.712260	3.156770	-1.079443
H	3.394973	3.135334	-2.919931
H	3.600342	3.862719	-1.319035
C	4.574825	0.763568	-0.293204
C	3.748161	0.130126	-2.511310
H	1.098752	3.851399	-3.044902
H	1.476021	4.921185	-1.681446
C	-1.291636	3.975440	-0.093324
C	-1.513012	2.535373	-2.063139
C	5.547615	-0.236174	-0.401282

C	4.548835	1.617754	0.950717
C	4.740823	-0.851903	-2.568592
C	2.820748	0.298462	-3.693843
C	-2.686731	4.059780	-0.034285
C	-0.479005	4.798410	0.880654
C	-2.901232	2.638157	-1.949512
C	-0.946394	1.833397	-3.276993
C	5.639547	-1.065870	-1.519690
H	6.254853	-0.362404	0.415600
H	4.240877	2.647138	0.740547
H	5.542848	1.655367	1.407205
H	3.863079	1.197731	1.694903
H	4.811665	-1.466844	-3.462973
H	1.829513	-0.120065	-3.494599
H	2.679031	1.346589	-3.977825
H	3.223448	-0.224383	-4.566193
C	-3.510254	3.368858	-0.925027
H	-3.139334	4.678635	0.738404
H	-0.822333	5.839639	0.875209
H	0.586633	4.798078	0.638821
H	-0.587017	4.433227	1.908469
H	-3.518231	2.116403	-2.676518
H	0.102158	1.554878	-3.165952
H	-1.516849	0.930349	-3.508857
H	-1.020935	2.490961	-4.154277
C	6.666485	-2.170118	-1.589131
C	-5.011177	3.386326	-0.779413
H	6.979252	-2.365372	-2.620326
H	7.558156	-1.928429	-1.000959
H	6.251556	-3.104265	-1.188758
H	-5.510744	3.412883	-1.753738
H	-5.340786	2.473895	-0.267434
H	-5.351495	4.246343	-0.192785

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Co	0.719590	0.236765	0.424396
C	1.591039	-1.560584	0.667148
O	2.403554	-1.414605	1.559480
C	1.766787	-2.627110	-0.375491
C	0.842623	-2.975360	-1.370016
C	2.983662	-3.335079	-0.303988
C	1.123947	-4.003834	-2.268655

H	-0.114681	-2.487027	-1.466159
C	3.261893	-4.358638	-1.204531
H	3.694374	-3.071336	0.470172
C	2.332802	-4.696708	-2.192573
H	0.379759	-4.261467	-3.015864
H	4.199971	-4.902113	-1.126641
H	2.546026	-5.501241	-2.891275
C	-0.256885	-1.205131	1.291639
N	-0.278351	-1.035155	2.708317
C	-1.233417	-2.139897	0.996974
C	0.447176	-0.029662	3.268582
C	-1.256470	-1.864698	3.282323
C	-1.874096	-2.554282	2.209397
H	-1.493421	-2.515660	0.019844
N	1.057916	0.789144	2.363309
N	0.520932	0.089990	4.598151
C	-1.655818	-2.046978	4.605840
C	-2.923979	-3.450221	2.463752
C	1.839751	1.749138	2.869245
C	1.291807	1.069171	5.067816
C	-2.698359	-2.947048	4.831641
H	-1.173921	-1.517405	5.416077
C	-3.327312	-3.639046	3.779991
H	-3.412399	-3.967467	1.643653
H	2.336770	2.386482	2.150695
C	2.003561	1.934207	4.237201
H	1.342842	1.159143	6.151186
H	-3.031861	-3.116047	5.851836
H	-4.140095	-4.323997	4.002420
H	2.637018	2.720785	4.628889
C	-0.002013	-0.025191	-1.154608
O	-0.500204	-0.127493	-2.180483
Co	-4.245248	-0.821485	-1.826122
C	-3.958617	0.404591	-3.057031
C	-3.972013	-0.089239	-0.247864
C	-5.926321	-1.396011	-1.918113
C	-3.142439	-2.156657	-2.078596
O	-3.725363	1.233746	-3.847839
O	-3.772978	0.415955	0.787097
O	-7.021571	-1.776892	-1.979287
O	-2.357316	-3.019858	-2.214673
C	1.636264	1.857351	-0.328229
N	2.913968	1.950410	-0.754359
N	1.062311	3.077532	-0.408997

C	3.293817	3.337678	-1.122503
C	3.841614	0.878187	-1.028004
C	1.962225	4.095132	-1.001289
C	-0.354970	3.354317	-0.292818
H	3.714675	3.360180	-2.131377
H	4.058910	3.708389	-0.430789
C	4.801692	0.508824	-0.070657
C	3.841183	0.299106	-2.316414
H	1.566277	4.418079	-1.969691
H	2.024055	4.971633	-0.349708
C	-0.879634	3.876387	0.904796
C	-1.185141	3.167659	-1.421189
C	5.735663	-0.477828	-0.410593
C	4.850437	1.116364	1.309802
C	4.792731	-0.681410	-2.602906
C	2.857425	0.708375	-3.388379
C	-2.262389	4.063590	0.997965
C	-0.021448	4.295694	2.076500
C	-2.560952	3.358415	-1.270478
C	-0.656194	2.856757	-2.804253
C	5.744568	-1.091777	-1.663310
H	6.478861	-0.766799	0.329369
H	4.588661	2.179505	1.308899
H	5.854135	1.021319	1.735472
H	4.156828	0.597062	1.980424
H	4.792461	-1.133739	-3.592024
H	1.843736	0.359114	-3.170010
H	2.803777	1.795506	-3.516493
H	3.145919	0.279765	-4.352183
C	-3.125496	3.769172	-0.059022
H	-2.673731	4.445269	1.930439
H	-0.303804	5.302833	2.404323
H	1.042900	4.314750	1.830022
H	-0.154066	3.632436	2.938243
H	-3.205610	3.160026	-2.121906
H	0.324328	2.376769	-2.797591
H	-1.350911	2.208597	-3.344774
H	-0.563237	3.785441	-3.384811
C	6.745011	-2.170695	-2.002536
C	-4.621100	3.872970	0.099440
H	7.207812	-1.995613	-2.980548
H	7.542455	-2.229690	-1.255301
H	6.256978	-3.152664	-2.048334
H	-5.103758	4.193327	-0.829544

H	-5.030817	2.889288	0.359501
H	-4.896546	4.573712	0.894834

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Co	-0.824137	1.042088	0.012142
C	-2.256490	2.055783	0.132820
O	-3.123546	2.809371	0.240588
C	-5.412796	0.313327	-0.594185
O	-4.801065	0.826578	-1.532593
C	-6.892237	0.492224	-0.464787
C	-7.457468	1.657422	-1.007754
C	-7.731717	-0.473944	0.111323
C	-8.831789	1.868224	-0.944684
H	-6.799451	2.385658	-1.470706
C	-9.110989	-0.267057	0.158965
H	-7.309264	-1.397104	0.493954
C	-9.661699	0.906220	-0.359730
H	-9.259133	2.779734	-1.353584
H	-9.755087	-1.025433	0.595679
H	-10.735439	1.068490	-0.315772
C	-4.686784	-0.455502	0.430133
N	-3.367171	-0.881888	0.196685
C	-5.004043	-0.705178	1.748856
C	-2.783479	-0.956376	-1.091071
C	-2.880435	-1.469161	1.361266
C	-3.884475	-1.345220	2.359913
H	-5.923726	-0.411513	2.234196
N	-1.679010	-0.216588	-1.331801
N	-3.392957	-1.755025	-1.962571
C	-1.672920	-2.134039	1.603200
C	-3.642342	-1.852234	3.651251
C	-1.215928	-0.247140	-2.599626
C	-2.923490	-1.767422	-3.210527
C	-1.467153	-2.628890	2.884728
H	-0.926039	-2.258680	0.829655
C	-2.435367	-2.484559	3.902570
H	-4.396110	-1.756130	4.428010
H	-0.343189	0.358409	-2.804405
C	-1.828309	-0.997551	-3.591631
H	-3.439762	-2.415929	-3.915068
H	-0.531572	-3.132583	3.108322
H	-2.229297	-2.882726	4.891965

H	-1.449488	-0.992692	-4.607051
C	-0.011957	2.030473	1.199809
O	0.407629	2.752635	1.999794
Co	1.596582	0.023634	-0.048466
C	1.322748	1.324236	-1.208301
C	1.060309	-1.498375	-0.791478
C	1.417613	-0.243890	1.690270
O	1.190035	2.085350	-2.090079
O	0.633659	-2.478831	-1.250586
O	1.333420	-0.499722	2.823086
C	3.574741	0.049703	-0.006279
N	4.378736	1.139413	0.082135
N	4.389839	-1.038303	-0.009543
C	5.818501	0.817939	0.169238
C	4.000702	2.525257	0.126708
C	5.830245	-0.708604	0.029762
C	4.026139	-2.412799	-0.205299
H	6.223244	1.159526	1.128863
H	6.372759	1.323863	-0.627749
C	4.027781	3.276614	-1.062742
C	3.733428	3.135375	1.366803
H	6.316304	-1.210573	0.872573
H	6.320533	-1.047754	-0.890362
C	3.895271	-2.907133	-1.516862
C	3.923658	-3.266204	0.907694
C	3.724653	4.640103	-0.994839
C	4.393694	2.652797	-2.389589
C	3.438584	4.501637	1.382225
C	3.769819	2.355734	2.659059
C	3.622581	-4.265913	-1.691527
C	4.019916	-1.993516	-2.713312
C	3.646516	-4.618925	0.681212
C	4.115832	-2.758734	2.318144
C	3.416908	5.269799	0.213932
H	3.727661	5.222685	-1.913777
H	3.943032	1.665108	-2.514908
H	5.481860	2.535338	-2.491905
H	4.056360	3.284012	-3.216717
H	3.219133	4.976704	2.335851
H	2.986867	1.593985	2.692215
H	4.728475	1.840802	2.799655
H	3.623015	3.022919	3.513355
C	3.485119	-5.137545	-0.606651
H	3.509278	-4.651880	-2.702572

H	5.004489	-1.511268	-2.764636
H	3.271697	-1.193980	-2.675618
H	3.877707	-2.552923	-3.642946
H	3.559762	-5.284698	1.537427
H	5.122330	-2.348484	2.471136
H	3.403599	-1.967687	2.568399
H	3.982612	-3.571451	3.038705
C	3.051679	6.735477	0.256852
C	3.152610	-6.595651	-0.822489
H	3.372711	7.201859	1.194703
H	3.507660	7.287794	-0.571827
H	1.964822	6.872603	0.181715
H	3.473603	-7.210475	0.024957
H	2.070494	-6.739922	-0.940175
H	3.631349	-6.987096	-1.727001

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Co	-1.535543	-0.215979	-1.182864
C	-1.437345	0.238407	-2.930069
O	-1.365030	0.516454	-4.046470
C	-3.679324	-0.494038	-0.987075
O	-4.141810	-1.493959	-1.523855
C	-4.536753	0.760265	-0.931041
C	-4.258740	1.922559	-1.654504
C	-5.739573	0.680443	-0.210152
C	-5.152727	2.996824	-1.639231
H	-3.349226	1.990418	-2.239967
C	-6.623662	1.756721	-0.183102
H	-5.974037	-0.232855	0.329378
C	-6.331239	2.921736	-0.898277
H	-4.921626	3.892328	-2.210018
H	-7.544683	1.683411	0.389525
H	-7.021686	3.760914	-0.881781
C	-2.651725	-0.787650	0.362097
N	-2.435822	-2.179265	0.595955
C	-3.129527	-0.264843	1.564407
C	-1.904746	-2.941490	-0.411077
C	-2.800565	-2.515512	1.898564
C	-3.231536	-1.312881	2.526841
H	-3.427662	0.763919	1.710551
N	-1.408171	-2.212828	-1.447705
N	-1.906140	-4.271628	-0.321218

C	-2.773861	-3.735606	2.577553
C	-3.651924	-1.345950	3.868749
C	-0.979409	-2.907057	-2.509980
C	-1.436734	-4.936746	-1.378956
C	-3.192654	-3.734056	3.906979
H	-2.451292	-4.640285	2.079939
C	-3.627155	-2.556623	4.547622
H	-3.984107	-0.436110	4.361122
H	-0.610774	-2.327433	-3.347349
C	-0.980838	-4.296884	-2.529511
H	-1.435547	-6.021955	-1.298733
H	-3.188874	-4.669096	4.460521
H	-3.947125	-2.600849	5.584925
H	-0.621122	-4.845789	-3.391288
C	-1.314472	1.394255	-0.487078
O	-1.454640	2.442968	-0.010930
Co	1.147438	0.309551	-0.472833
C	1.147549	1.663665	-1.638809
C	1.545292	-1.111109	-1.493220
C	0.429856	-0.267856	1.032604
O	1.187267	2.470227	-2.470822
O	1.797570	-2.003959	-2.189367
O	0.072476	-0.688226	2.058103
C	2.763680	0.883156	0.497333
N	3.010188	2.114641	1.007777
N	3.800344	0.084112	0.861204
C	4.222823	2.167231	1.852103
C	2.222206	3.312547	0.895772
C	4.868441	0.804573	1.588075
C	4.089421	-1.249557	0.408792
H	3.934293	2.302032	2.902067
H	4.859073	3.008966	1.565499
C	2.604213	4.271288	-0.066351
C	1.188814	3.576088	1.810704
H	5.137954	0.272164	2.504556
H	5.765609	0.875879	0.961040
C	4.716800	-1.431499	-0.838821
C	3.856662	-2.334894	1.272593
C	1.895452	5.472141	-0.126632
C	3.761446	4.033735	-1.009415
C	0.514163	4.799264	1.712763
C	0.774575	2.596194	2.881420
C	5.069135	-2.727933	-1.221896
C	4.990753	-0.267890	-1.762608

C	4.225411	-3.613956	0.841057
C	3.239987	-2.148918	2.639335
C	0.839591	5.752893	0.748085
H	2.176761	6.209215	-0.875800
H	3.690396	3.064577	-1.510629
H	4.726841	4.061220	-0.485592
H	3.789569	4.807861	-1.781621
H	-0.292478	5.004985	2.413502
H	-0.126421	2.052177	2.579226
H	1.543565	1.848693	3.089308
H	0.544067	3.121849	3.814784
C	4.824375	-3.833965	-0.402228
H	5.543825	-2.876414	-2.189544
H	5.644888	0.482603	-1.300981
H	4.062848	0.241532	-2.043981
H	5.479631	-0.611145	-2.679079
H	4.042731	-4.459787	1.500495
H	3.855666	-1.505338	3.280934
H	2.247872	-1.693336	2.582737
H	3.138624	-3.113007	3.146642
C	0.064461	7.044932	0.636855
C	5.182651	-5.229489	-0.857521
H	-0.385666	7.326668	1.594634
H	0.703638	7.870382	0.304591
H	-0.751291	6.951353	-0.092090
H	5.319081	-5.906342	-0.007555
H	4.391177	-5.653285	-1.489804
H	6.105383	-5.234916	-1.448213

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A-INT1

Co	0.157556	-0.561473	0.073357
C	-1.533724	-0.702742	0.809368
O	-1.841596	-0.905714	1.935239
C	-2.036189	2.785625	1.271868
O	-1.500753	2.522042	2.350809
C	-3.519085	2.971206	1.196171
C	-4.171301	3.412613	2.359070
C	-4.279963	2.673579	0.055105
C	-5.552230	3.584780	2.371381
H	-3.574760	3.614591	3.242674
C	-5.666427	2.832785	0.075186

H	-3.797301	2.284604	-0.833171
C	-6.303507	3.295671	1.227726
H	-6.045858	3.938682	3.272499
H	-6.247838	2.586745	-0.809189
H	-7.382808	3.423200	1.238876
C	-1.202603	2.991720	0.075923
N	0.166038	2.661292	0.099312
C	-1.469502	3.667511	-1.096978
C	0.849910	2.132462	1.224396
C	0.760845	3.162952	-1.047668
C	-0.251553	3.781254	-1.830178
H	-2.429054	4.074320	-1.379285
N	0.792919	0.797623	1.435917
N	1.507249	3.007388	1.976712
C	2.097435	3.125395	-1.458886
C	0.089760	4.362071	-3.066690
C	1.226872	0.386099	2.643041
C	2.001172	2.565131	3.134615
C	2.403565	3.713804	-2.679254
H	2.864311	2.659434	-0.850759
C	1.411906	4.322886	-3.480140
H	-0.673761	4.831589	-3.680709
H	1.104200	-0.669262	2.854665
C	1.811600	1.251401	3.556303
H	2.540622	3.289691	3.740697
H	3.433659	3.706957	-3.025865
H	1.694420	4.766022	-4.430840
H	2.140590	0.902472	4.528484
Co	-2.053522	-0.618607	-1.003231
C	-0.248794	-0.625959	-1.684451
C	-3.531950	-1.540152	-0.732380
C	-2.607852	0.310109	-2.388793
O	0.304794	-0.555824	-2.733283
O	-4.494945	-2.169347	-0.615860
O	-3.029905	0.976158	-3.236445
C	1.587542	-1.940538	0.035128
N	1.267467	-3.258407	-0.042427
N	2.949119	-1.875389	0.028065
C	2.434904	-4.162721	-0.015533
C	-0.041244	-3.850397	0.001388
C	3.603716	-3.188838	-0.170424
C	3.799781	-0.720667	0.102661
H	2.375776	-4.895491	-0.824795
H	2.461144	-4.711047	0.935297

C	-0.664340	-4.079895	1.240238
C	-0.624608	-4.292572	-1.203179
H	4.059550	-3.230829	-1.167129
H	4.393534	-3.343117	0.570313
C	4.415663	-0.411372	1.331340
C	4.138910	-0.017068	-1.071438
C	-1.914212	-4.709796	1.246813
C	-0.045038	-3.651125	2.550419
C	-1.873538	-4.914306	-1.142504
C	0.067633	-4.113920	-2.534363
C	5.300946	0.671566	1.385469
C	4.214540	-1.259697	2.566795
C	5.041929	1.046366	-0.966877
C	3.592747	-0.411980	-2.421691
C	-2.543601	-5.118320	0.069411
H	-2.409030	-4.877811	2.201109
H	1.049338	-3.658796	2.518524
H	-0.364075	-4.314153	3.361360
H	-0.370554	-2.636908	2.808699
H	-2.338784	-5.243604	-2.069204
H	-0.604309	-4.387758	-3.353296
H	0.388030	-3.081052	-2.693670
H	0.957753	-4.752573	-2.619730
C	5.620007	1.421075	0.251254
H	5.767477	0.919645	2.336907
H	4.966742	-2.059629	2.615711
H	3.233000	-1.738388	2.589387
H	4.328741	-0.661674	3.476264
H	5.308671	1.590825	-1.870427
H	2.501688	-0.370260	-2.462175
H	3.984675	0.249195	-3.200101
H	3.884606	-1.437323	-2.684225
C	-3.921589	-5.735111	0.097308
C	6.558851	2.602083	0.332454
H	-4.047805	-6.476751	-0.699158
H	-4.124366	-6.224505	1.055839
H	-4.687728	-4.962789	-0.048299
H	7.192785	2.671511	-0.558393
H	6.001850	3.545393	0.407169
H	7.211318	2.537097	1.209378

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A-TS1

Co	-0.285357	0.158501	0.291646
C	-1.850894	0.261771	1.360781
O	-2.211100	-0.051275	2.438439
C	0.249054	2.239707	0.843286
O	0.586225	2.384667	2.013040
C	-0.492834	3.392841	0.183237
C	-0.899893	4.413571	1.065163
C	-0.787427	3.548696	-1.182847
C	-1.586403	5.534126	0.604342
H	-0.663676	4.304712	2.116932
C	-1.463265	4.679992	-1.644544
H	-0.488774	2.805394	-1.906473
C	-1.871181	5.675083	-0.755870
H	-1.894125	6.301696	1.309650
H	-1.669525	4.777083	-2.707157
H	-2.400482	6.551830	-1.119450
C	1.385115	1.224498	-0.079593
N	2.433825	0.819513	0.808386
C	2.022349	1.921524	-1.105291
C	2.125624	0.102357	1.933347
C	3.665335	1.318297	0.379539
C	3.423600	1.996441	-0.846007
H	1.526961	2.395123	-1.938397
N	0.839478	-0.331688	1.998124
N	3.069225	-0.115891	2.855297
C	4.945843	1.242858	0.934654
C	4.490668	2.603743	-1.530276
C	0.485185	-0.964781	3.120621
C	2.690701	-0.769036	3.954064
C	5.983115	1.864993	0.239852
H	5.112619	0.736161	1.874491
C	5.764249	2.533783	-0.980530
H	4.314626	3.125720	-2.467031
H	-0.554172	-1.257250	3.190201
C	1.385819	-1.210915	4.153071
H	3.465027	-0.936371	4.700861
H	6.985144	1.841023	0.660408
H	6.599976	3.007201	-1.488559
H	1.079154	-1.721037	5.058619
Co	-2.549476	1.201145	-0.186881
C	-1.101922	0.539020	-1.317259
C	-3.650603	2.073727	0.906651
C	-3.559043	1.327466	-1.622693
O	-0.852845	0.485856	-2.481330

O	-4.387748	2.682718	1.550104
O	-4.282025	1.363553	-2.523556
C	-0.182303	-1.829092	-0.473779
N	-1.256922	-2.642857	-0.676341
N	0.904962	-2.533462	-0.878431
C	-0.902907	-3.998996	-1.153247
C	-2.647209	-2.442431	-0.362926
C	0.582253	-3.858046	-1.463306
C	2.300401	-2.182328	-0.914645
H	-1.503164	-4.267847	-2.026593
H	-1.105977	-4.731707	-0.362123
C	-3.124749	-2.741647	0.926320
C	-3.543723	-2.121742	-1.405011
H	0.794564	-3.847250	-2.538669
H	1.196156	-4.637645	-1.004427
C	3.143466	-2.676525	0.098273
C	2.834100	-1.556180	-2.059266
C	-4.493276	-2.602465	1.182692
C	-2.228567	-3.265956	2.023623
C	-4.901892	-1.998629	-1.098208
C	-3.095968	-1.979425	-2.841936
C	4.524361	-2.485865	-0.027749
C	2.609421	-3.463665	1.272911
C	4.220309	-1.396082	-2.139287
C	1.957555	-1.110495	-3.203825
C	-5.396448	-2.213604	0.192240
H	-4.859249	-2.809289	2.186434
H	-1.176254	-3.043336	1.840048
H	-2.327081	-4.356510	2.115662
H	-2.506728	-2.833156	2.989498
H	-5.592097	-1.728832	-1.894674
H	-3.814513	-1.381525	-3.409760
H	-2.119205	-1.503360	-2.933829
H	-3.038273	-2.963008	-3.329846
C	5.084104	-1.850821	-1.137829
H	5.177666	-2.860562	0.757522
H	2.487416	-4.526187	1.018097
H	1.637318	-3.098126	1.610166
H	3.303724	-3.416321	2.117094
H	4.636864	-0.908632	-3.017979
H	1.138206	-0.468474	-2.874096
H	2.548515	-0.562796	-3.944406
H	1.506547	-1.968615	-3.721154
C	-6.862239	-2.022784	0.503646

C	6.575921	-1.647340	-1.253027
H	-7.492642	-2.289391	-0.351673
H	-7.173557	-2.630392	1.359944
H	-7.076973	-0.974867	0.751448
H	6.921291	-1.794321	-2.282669
H	6.849929	-0.626940	-0.958183
H	7.126406	-2.339947	-0.607588

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A-INT2

Co	-0.201952	0.268330	0.280916
C	-1.846489	0.166197	1.330106
O	-2.213869	-0.210334	2.379350
C	-0.150563	2.185207	1.003700
O	0.255995	2.315244	2.141243
C	-0.682644	3.423130	0.311947
C	-1.212016	4.426527	1.149567
C	-0.653008	3.648403	-1.072638
C	-1.732105	5.599565	0.612283
H	-1.207353	4.261137	2.221700
C	-1.154096	4.837917	-1.606941
H	-0.197558	2.922856	-1.729955
C	-1.704983	5.809300	-0.770803
H	-2.150443	6.356366	1.270661
H	-1.106941	5.003631	-2.679814
H	-2.101477	6.729893	-1.190932
C	1.533649	0.872510	-0.372943
N	2.537804	0.785184	0.631642
C	2.110769	1.496509	-1.446060
C	2.239633	0.203450	1.828880
C	3.742096	1.358966	0.180516
C	3.487055	1.809415	-1.140731
H	1.618428	1.709494	-2.385090
N	0.961586	-0.256163	1.939496
N	3.171949	0.124901	2.787388
C	4.985487	1.514426	0.792101
C	4.517455	2.427815	-1.861323
C	0.621738	-0.811029	3.103915
C	2.800632	-0.431205	3.939640
C	5.993433	2.139816	0.051805
H	5.155180	1.167750	1.802361
C	5.764234	2.589399	-1.258641
H	4.342947	2.781600	-2.874537

H	-0.405595	-1.143907	3.192647
C	1.519004	-0.929396	4.161546
H	3.564579	-0.476829	4.714360
H	6.969630	2.286668	0.506757
H	6.567969	3.074670	-1.806723
H	1.225139	-1.374836	5.104575
Co	-2.493485	1.195316	-0.170260
C	-1.015457	0.638818	-1.347202
C	-3.652851	1.964102	0.940638
C	-3.508358	1.325318	-1.609211
O	-0.783335	0.578308	-2.506172
O	-4.446234	2.487266	1.591218
O	-4.231217	1.380817	-2.506941
C	-0.215077	-1.855276	-0.418185
N	-1.309696	-2.643239	-0.616022
N	0.858546	-2.616370	-0.739488
C	-0.992042	-4.027663	-1.039082
C	-2.706356	-2.400513	-0.369034
C	0.520049	-3.978520	-1.219198
C	2.265764	-2.315130	-0.759343
H	-1.529903	-4.275484	-1.958823
H	-1.308112	-4.732214	-0.261321
C	-3.248895	-2.706159	0.893851
C	-3.546005	-2.057670	-1.449925
H	0.832695	-4.089756	-2.262930
H	1.051112	-4.728109	-0.625232
C	3.068221	-2.738266	0.314636
C	2.841761	-1.799576	-1.938176
C	-4.625503	-2.548011	1.085789
C	-2.408165	-3.252718	2.024633
C	-4.915650	-1.915841	-1.206894
C	-3.027406	-1.920125	-2.863206
C	4.453501	-2.552576	0.225111
C	2.496873	-3.443692	1.523462
C	4.227989	-1.640823	-1.979585
C	2.005700	-1.468359	-3.151078
C	-5.474320	-2.136583	0.055982
H	-5.042706	-2.759512	2.068218
H	-1.357746	-2.969701	1.934270
H	-2.455860	-4.350478	2.047270
H	-2.774992	-2.891537	2.989678
H	-5.563670	-1.630787	-2.032847
H	-3.712972	-1.319353	-3.467567
H	-2.043211	-1.453088	-2.909722

H	-2.952097	-2.905206	-3.345162
C	5.052004	-1.996043	-0.905449
H	5.077341	-2.859350	1.062226
H	2.571587	-4.534816	1.412446
H	1.445718	-3.199705	1.688069
H	3.050988	-3.177458	2.428645
H	4.677886	-1.221593	-2.876574
H	1.152028	-0.833706	-2.905190
H	2.610324	-0.945231	-3.897886
H	1.617877	-2.378765	-3.629848
C	-6.951221	-1.930408	0.297988
C	6.541702	-1.758393	-0.966457
H	-7.541539	-2.173630	-0.592087
H	-7.312402	-2.548169	1.126922
H	-7.164814	-0.884067	0.553414
H	6.940113	-1.963597	-1.966523
H	6.770043	-0.711556	-0.730626
H	7.079361	-2.387585	-0.249192

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A-INT2A

Co	0.262878	0.059859	-0.180046
C	3.244446	2.517537	0.243727
O	4.000622	3.139962	-0.362940
C	0.872129	1.633005	-0.961578
O	1.633075	0.946018	-1.666646
C	0.503594	3.030675	-1.272312
C	1.091565	3.674679	-2.375960
C	-0.464114	3.702898	-0.509651
C	0.718818	4.975240	-2.704639
H	1.839031	3.144160	-2.957489
C	-0.837693	5.002582	-0.846151
H	-0.905472	3.201959	0.345123
C	-0.246327	5.640133	-1.940873
H	1.178808	5.472918	-3.554188
H	-1.586415	5.519308	-0.252579
H	-0.536207	6.655413	-2.198742
C	-1.306163	0.592841	0.780445
N	-2.445101	0.757521	-0.069804
C	-1.716452	0.937959	2.040331
C	-2.313819	0.491831	-1.394542
C	-3.558073	1.202838	0.666676
C	-3.112186	1.317529	2.007320

H	-1.101990	0.924959	2.928458
N	-1.070541	0.057994	-1.737188
N	-3.327597	0.676716	-2.251189
C	-4.864061	1.503377	0.281483
C	-4.017425	1.745341	2.988054
C	-0.833173	-0.163256	-3.032212
C	-3.070281	0.426258	-3.534109
C	-5.744565	1.928535	1.280649
H	-5.174742	1.415785	-0.751411
C	-5.327072	2.046738	2.616153
H	-3.699205	1.844117	4.022699
H	0.176967	-0.467694	-3.281153
C	-1.822499	0.002604	-3.995936
H	-3.898162	0.581312	-4.224003
H	-6.768037	2.178150	1.013609
H	-6.034939	2.382680	3.369619
H	-1.627127	-0.180584	-5.045759
Co	2.173560	1.526888	1.338503
C	3.511812	0.874386	2.283202
C	1.241420	2.727563	2.294269
C	1.192243	0.033016	1.697907
O	4.371858	0.531455	2.975680
O	0.756863	3.507826	2.992370
O	0.928445	-0.751066	2.542521
C	0.421066	-2.083528	-0.079936
N	-0.568848	-3.000061	0.031007
N	1.589666	-2.770788	-0.112714
C	-0.076448	-4.387926	0.198587
C	-1.991316	-2.790519	0.064179
C	1.412207	-4.241626	-0.112429
C	2.926477	-2.266641	-0.282587
H	-0.596379	-5.066020	-0.483592
H	-0.263854	-4.723770	1.225357
C	-2.644151	-2.560846	1.291916
C	-2.724754	-2.961202	-1.125073
H	1.685168	-4.643295	-1.096949
H	2.055432	-4.709852	0.636164
C	3.809688	-2.300160	0.818681
C	3.383154	-1.881114	-1.556330
C	-4.033078	-2.406533	1.280849
C	-1.896487	-2.539042	2.602732
C	-4.114596	-2.799103	-1.082053
C	-2.065643	-3.375573	-2.421276
C	5.122703	-1.861049	0.632096

C	3.400388	-2.833849	2.172785
C	4.707186	-1.447198	-1.688532
C	2.523229	-1.940619	-2.796288
C	-4.785796	-2.502419	0.105765
H	-4.540076	-2.201212	2.220845
H	-0.964270	-1.976839	2.541747
H	-1.653411	-3.561138	2.927701
H	-2.513305	-2.089334	3.386074
H	-4.684151	-2.911357	-2.002431
H	-2.669680	-3.071194	-3.281292
H	-1.068032	-2.945358	-2.537181
H	-1.957181	-4.468137	-2.475816
C	5.588355	-1.411808	-0.607527
H	5.797821	-1.864428	1.484858
H	3.600470	-3.912454	2.246934
H	2.342644	-2.668321	2.381363
H	3.977045	-2.345906	2.964019
H	5.057012	-1.136533	-2.671292
H	1.593334	-2.490676	-2.632175
H	2.266421	-0.927677	-3.122697
H	3.066144	-2.426958	-3.615258
C	-6.278784	-2.277064	0.128951
C	6.999638	-0.896904	-0.766518
H	-6.750058	-2.603986	-0.803705
H	-6.753363	-2.816350	0.957045
H	-6.504066	-1.211756	0.264817
H	7.352706	-1.004638	-1.797615
H	7.058953	0.169093	-0.510233
H	7.697413	-1.427275	-0.109343

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A-TS2A

Co	-0.093644	-0.169540	-0.882085
C	-0.316447	-2.209301	-0.967110
O	-1.344670	-2.781363	-1.164164
C	0.289263	0.130330	-2.553410
O	0.206696	0.424411	-3.681792
C	1.987352	-0.383582	-1.832032
C	2.458897	-1.225419	-2.863533
C	2.938361	0.364556	-1.116883
C	3.818260	-1.296692	-3.178793
H	1.754541	-1.768442	-3.484117

C	4.300811	0.265112	-1.406684
H	2.625898	1.009968	-0.311225
C	4.744772	-0.555153	-2.446583
H	4.145381	-1.934299	-3.995874
H	5.011373	0.844120	-0.822496
H	5.802926	-0.609501	-2.688295
C	-0.021441	1.842368	-0.909111
N	-1.317322	2.407017	-1.099367
C	0.850757	2.897342	-0.885447
C	-2.374770	1.585857	-1.372370
C	-1.247575	3.814045	-1.162824
C	0.123865	4.138490	-1.021491
H	1.922895	2.836902	-0.780469
N	-2.107972	0.253155	-1.283991
N	-3.554121	2.117745	-1.714832
C	-2.232042	4.792752	-1.307889
C	0.513861	5.484694	-1.028776
C	-3.089272	-0.576653	-1.663409
C	-4.514954	1.267141	-2.074094
C	-1.815789	6.125649	-1.311603
H	-3.273053	4.523894	-1.422526
C	-0.460878	6.469200	-1.174541
H	1.562284	5.753222	-0.925805
H	-2.854946	-1.631276	-1.604051
C	-4.327623	-0.110951	-2.092548
H	-5.465631	1.715046	-2.358851
H	-2.558782	6.910308	-1.426458
H	-0.170896	7.516770	-1.184282
H	-5.105877	-0.798397	-2.401531
Co	1.457432	-2.892020	-0.687917
C	1.109586	-3.347834	0.980142
C	1.189593	-4.105728	-1.958810
C	3.279345	-3.098803	-0.539079
O	1.003166	-3.821437	2.034819
O	1.000787	-5.001773	-2.661981
O	4.392687	-3.356094	-0.405353
C	-0.208666	-0.316977	1.335163
N	0.744834	-0.002097	2.258389
N	-1.210935	-0.948715	2.021024
C	0.468705	-0.550792	3.609688
C	1.867071	0.906204	2.194380
C	-0.973044	-1.020701	3.485432
C	-2.594121	-1.174295	1.655414
H	0.610790	0.224021	4.368022

H	1.159915	-1.373805	3.819501
C	3.185694	0.414533	2.225630
C	1.624846	2.292305	2.336577
H	-1.682389	-0.367262	4.007095
H	-1.124922	-2.041327	3.843746
C	-3.098077	-2.484826	1.538923
C	-3.480515	-0.071217	1.658191
C	4.245661	1.330884	2.267967
C	3.504835	-1.057710	2.262958
C	2.715353	3.164499	2.374792
C	0.234700	2.850955	2.504549
C	-4.472784	-2.652355	1.313730
C	-2.249724	-3.726622	1.670598
C	-4.840025	-0.294776	1.434029
C	-3.012000	1.333810	1.948246
C	4.037010	2.708717	2.321362
H	5.262946	0.944480	2.272934
H	2.700149	-1.655097	1.840002
H	3.670323	-1.394063	3.295970
H	4.419157	-1.274530	1.702805
H	2.522888	4.231141	2.467335
H	0.278168	3.919583	2.732715
H	-0.355635	2.729242	1.595265
H	-0.304226	2.355930	3.321464
C	-5.358601	-1.579246	1.240552
H	-4.856759	-3.665399	1.213193
H	-2.860281	-4.558417	2.036865
H	-1.411388	-3.597074	2.355065
H	-1.833726	-4.018114	0.701676
H	-5.513937	0.559404	1.429737
H	-2.170412	1.628621	1.321365
H	-3.821645	2.050924	1.785156
H	-2.687188	1.441928	2.991383
C	5.194475	3.679386	2.333242
C	-6.829737	-1.790939	0.971717
H	5.018812	4.503890	3.033441
H	6.129206	3.185471	2.617647
H	5.346817	4.126536	1.342025
H	-7.449881	-1.123794	1.581082
H	-7.073761	-1.585756	-0.079395
H	-7.132082	-2.821948	1.181574

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A-INT2B

Co	-0.344276	-0.036515	0.048151
C	-3.307872	-1.771410	1.875504
O	-4.426908	-1.734960	2.158410
C	-1.783371	-1.491299	-0.346560
O	-2.069980	-0.449754	-1.008550
C	-1.871855	-2.851334	-0.961831
C	-2.911345	-3.142602	-1.862570
C	-0.963910	-3.866396	-0.611710
C	-3.044794	-4.424247	-2.391550
H	-3.610329	-2.355394	-2.130230
C	-1.101919	-5.149706	-1.144347
H	-0.137462	-3.635154	0.055357
C	-2.142725	-5.431771	-2.031614
H	-3.852467	-4.641673	-3.085964
H	-0.390604	-5.925116	-0.873082
H	-2.248880	-6.430511	-2.446627
C	1.332623	-0.427482	0.911738
N	2.285401	-1.000333	0.011977
C	1.928883	-0.416833	2.144570
C	1.941437	-1.152796	-1.295662
C	3.470452	-1.338369	0.691297
C	3.259014	-0.971983	2.045534
H	1.469748	-0.062329	3.057489
N	0.679816	-0.726201	-1.575780
N	2.786152	-1.694286	-2.183691
C	4.659052	-1.914220	0.246416
C	4.284772	-1.195439	2.974080
C	0.238646	-0.889460	-2.826366
C	2.326209	-1.831685	-3.428386
C	5.664542	-2.125700	1.195312
H	4.790120	-2.187120	-0.792548
C	5.479553	-1.770063	2.541128
H	4.146983	-0.928055	4.018761
H	-0.787011	-0.580286	-2.999112
C	1.042569	-1.446462	-3.816808
H	3.017001	-2.276558	-4.142880
H	6.600886	-2.580763	0.883088
H	6.278243	-1.950344	3.256320
H	0.681564	-1.582612	-4.829273
Co	-1.584745	-1.687417	1.502401
C	-1.093594	0.145271	1.749133
C	-0.730439	-2.312156	2.990842

O	-1.199936	0.801938	2.720351
O	-0.216314	-2.802188	3.895718
C	-0.244457	1.987367	-0.355770
N	0.832875	2.754002	-0.653247
N	-1.335298	2.787339	-0.468672
C	0.502186	4.164669	-0.960506
C	2.229840	2.429245	-0.573226
C	-1.025892	4.164413	-0.912832
C	-2.722930	2.487826	-0.230630
H	0.902362	4.441323	-1.940845
H	0.954539	4.825608	-0.212858
C	2.894108	2.567869	0.662259
C	2.937630	2.133092	-1.750304
H	-1.484473	4.349434	-1.891202
H	-1.434687	4.891305	-0.204453
C	-3.284043	2.806082	1.022051
C	-3.527983	2.024617	-1.286951
C	4.268622	2.328146	0.702223
C	2.158611	2.997195	1.909838
C	4.315088	1.898201	-1.656781
C	2.268447	2.114320	-3.105547
C	-4.643328	2.547057	1.224550
C	-2.491309	3.483905	2.116223
C	-4.882748	1.789362	-1.036202
C	-2.989707	1.828174	-2.684546
C	4.995887	1.975890	-0.440927
H	4.785510	2.408458	1.655672
H	2.824798	2.963157	2.776783
H	1.301753	2.352373	2.120014
H	1.786926	4.027454	1.823795
H	4.866311	1.648765	-2.561239
H	2.766680	1.408279	-3.777046
H	1.214681	1.834992	-3.039594
H	2.319339	3.102244	-3.584979
C	-5.456346	2.021141	0.216562
H	-5.076589	2.769226	2.197645
H	-2.575522	4.577171	2.031099
H	-1.433577	3.221315	2.089747
H	-2.875036	3.205138	3.101640
H	-5.505412	1.410795	-1.844657
H	-1.910235	1.669794	-2.687373
H	-3.457078	0.960769	-3.159793
H	-3.207348	2.703742	-3.312726
C	6.469836	1.661801	-0.348210

C	-6.908759	1.699875	0.480521
H	6.960808	1.740891	-1.323958
H	6.981703	2.336813	0.347000
H	6.619157	0.638675	0.019426
H	-7.501375	1.731877	-0.440052
H	-7.014799	0.692732	0.904669
H	-7.352264	2.401178	1.195879

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A-TS2B

Co	-0.101239	-0.243083	-0.831218
C	-1.737567	-2.405357	-1.751498
O	-2.787892	-2.269771	-2.247397
C	0.281330	-0.355829	-2.531002
O	0.293810	-0.179397	-3.689392
C	1.407761	-1.588709	-1.729117
C	1.316670	-2.699360	-2.619182
C	2.642828	-1.397972	-1.057135
C	2.392974	-3.602306	-2.754475
H	0.523374	-2.750641	-3.354673
C	3.692854	-2.291090	-1.207920
H	2.770447	-0.550455	-0.400632
C	3.568860	-3.409795	-2.049843
H	2.300231	-4.424206	-3.459806
H	4.620305	-2.113982	-0.669333
H	4.402292	-4.095918	-2.174116
C	0.832797	1.454777	-1.018483
N	-0.070156	2.538475	-1.199331
C	2.094705	1.967163	-1.134551
C	-1.403749	2.271060	-1.332157
C	0.636945	3.740703	-1.401125
C	2.010551	3.394071	-1.354867
H	3.017920	1.410975	-1.070767
N	-1.737535	0.964357	-1.135395
N	-2.255883	3.250605	-1.650147
C	0.203402	5.052161	-1.595102
C	2.973290	4.400916	-1.508108
C	-3.018070	0.636797	-1.351174
C	-3.524556	2.893946	-1.856225
C	1.184510	6.034487	-1.746063
H	-0.850920	5.290743	-1.634938
C	2.551329	5.714610	-1.703020

H	4.032219	4.157126	-1.479060
H	-3.283571	-0.399907	-1.213058
C	-3.964714	1.579455	-1.738945
H	-4.207132	3.697815	-2.126017
H	0.879940	7.065712	-1.902653
H	3.288993	6.503402	-1.825888
H	-4.993566	1.293239	-1.918998
Co	-0.294632	-2.963417	-0.944551
C	-0.067592	-3.110627	0.803747
C	-0.428325	-4.687121	-1.298814
O	-0.121470	-3.376317	1.935767
O	-0.557726	-5.819178	-1.496888
C	-0.133457	-0.208538	1.374701
N	0.903713	-0.283677	2.256800
N	-1.273543	-0.309825	2.119672
C	0.480510	-0.402489	3.673692
C	2.302258	0.040479	2.093858
C	-1.027509	-0.576941	3.557985
C	-2.644499	0.011969	1.801764
H	0.767659	0.503302	4.220671
H	0.972800	-1.254820	4.147587
C	3.275422	-0.978183	2.168142
C	2.689832	1.398227	2.088307
H	-1.593524	0.125463	4.176671
H	-1.350388	-1.593305	3.803603
C	-3.607273	-1.001064	1.621998
C	-3.044171	1.363923	1.911036
C	4.627136	-0.612158	2.130916
C	2.925573	-2.442526	2.272631
C	4.052727	1.707758	2.040076
C	1.686366	2.520220	2.191752
C	-4.950713	-0.623524	1.474703
C	-3.263466	-2.469594	1.600812
C	-4.395726	1.684241	1.766782
C	-2.054470	2.464486	2.210428
C	5.039957	0.719210	2.044817
H	5.377480	-1.398365	2.183861
H	2.577684	-2.834359	1.312354
H	2.131694	-2.640877	2.996105
H	3.807132	-3.019676	2.568910
H	4.346653	2.754883	2.017444
H	2.179231	3.488292	2.068254
H	0.912368	2.441643	1.428345
H	1.190886	2.524397	3.171844

C	-5.368187	0.705867	1.536496
H	-5.692043	-1.405937	1.328100
H	-4.177288	-3.070904	1.576441
H	-2.685274	-2.773091	2.478446
H	-2.661246	-2.730312	0.726544
H	-4.697150	2.726409	1.851136
H	-1.295111	2.559988	1.429922
H	-2.566337	3.427313	2.297633
H	-1.519187	2.288229	3.151454
C	6.504777	1.079638	1.964601
C	-6.821242	1.081913	1.364563
H	6.707472	2.044142	2.442465
H	7.131580	0.322086	2.446896
H	6.835810	1.159617	0.920494
H	-7.124525	1.850061	2.085062
H	-7.010726	1.489718	0.362483
H	-7.478057	0.216092	1.495049

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D-CAT

Co	4.7088225578	-2.1285966968	-2.8976703976
C	3.1062843601	-2.4328578727	-2.1486038533
O	2.079202787	-2.6289796399	-1.6761483229
C	4.1526801612	-1.2643901575	-4.2799971494
O	3.6199959978	-0.7077777023	-5.1436685717
Co	6.9666754874	-1.6163613016	-4.1590049728
C	6.5648061273	-2.4407328259	-2.6698840518
C	6.6398613141	-0.7021846745	-5.6793157067
O	6.1819483326	-2.9832120903	-1.675699596
O	6.4624066643	-0.1209711098	-6.6509320229
C	8.7105328197	-1.7186756395	-4.2761760561
O	9.8558365107	-1.8132692091	-4.3043863387

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D-INT1

Co	0.972685419	-0.6668022648	0.353741274
C	0.5441801442	-2.2258261568	1.0960223406
O	0.4322186448	-3.2674476224	1.5751640791
C	-2.3726149952	-0.576617906	1.0303450773
O	-2.1773956402	-0.4835804784	2.2435843185
C	-3.0804498823	-1.7600485499	0.4556724316
C	-2.8513036114	-2.2346683891	-0.8460363724
C	-3.9731341806	-2.4493221477	1.2930166423
C	-3.5170447656	-3.3729742428	-1.3024071069

H	-2.1284625186	-1.7436192903	-1.4882363671
C	-4.6469438585	-3.5746896722	0.8284590097
H	-4.1242613771	-2.0841725598	2.3036552626
C	-4.4203159364	-4.0384224594	-0.4715032164
H	-3.3219621045	-3.7432473831	-2.3048656559
H	-5.3450498114	-4.0947704167	1.4785585456
H	-4.9407501384	-4.9217150401	-0.831904253
C	-1.9651235083	0.5296485301	0.1406675459
N	-1.1243047053	1.5548931167	0.6203188763
C	-2.5253351533	0.9501948272	-1.0481065885
C	-0.3489664961	1.5168665011	1.7940089341
C	-1.1708792307	2.6245003156	-0.2696240761
C	-2.0365613287	2.2607049892	-1.3350383985
H	-3.2626578272	0.400347903	-1.6149088763
N	0.5842110904	0.5425059854	1.8939667964
N	-0.550611409	2.4842949071	2.679876046
C	-0.5051220789	3.855390659	-0.241573072
C	-2.253089638	3.166637381	-2.3909170167
C	1.2588162172	0.4769976374	3.0572190493
C	0.1603599547	2.4334916068	3.8100412127
C	-0.7394424531	4.7275214485	-1.2973967985
H	0.1463290824	4.1286828824	0.5805445928
C	-1.6041981852	4.3903951811	-2.3621090633
H	-2.9119391779	2.902768123	-3.2132853142
H	1.9931083448	-0.3148488665	3.1405656551
C	1.0623039849	1.4055338478	4.0704792647
H	-0.009849082	3.2374925374	4.5224995813
H	-0.2478317195	5.6962329818	-1.3002840829
H	-1.7562932984	5.1020496935	-3.1681469665
H	1.6160615843	1.3442925573	4.9999650988
C	0.9423055923	-1.2067846254	-1.3914044453
O	0.508451478	-1.8322213473	-2.2825977451
Co	2.3388155054	0.1874360383	-1.4676694434
C	2.8356204897	-0.1073744951	0.2913443713
C	1.4519738904	1.1511857484	-2.6814984482
O	3.5999926231	-0.0734096697	1.183588002
O	0.9447315802	1.8510407014	-3.4416538338
C	3.9412615727	0.0709084006	-2.2271272299
O	4.9555889135	-0.0702809177	-2.7536646371

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D-TS1

Co	0.3780011944	-0.8543882109	0.4522591703
C	0.5764820983	-2.3247732388	1.4879759927

O	0.6005339795	-3.2713157033	2.1394303487
C	-1.6893856435	-0.7585688922	0.8389627417
O	-1.9754190114	-0.282583558	1.9251006184
C	-2.5950327241	-1.7770840593	0.191665729
C	-2.3592625276	-2.4190859842	-1.0319452838
C	-3.7565822986	-2.1056158779	0.912697464
C	-3.2641704284	-3.3584103149	-1.5253742172
H	-1.4716133288	-2.1966331825	-1.6074097071
C	-4.656766253	-3.048083388	0.4211436882
H	-3.9351270512	-1.6073380406	1.8589723906
C	-4.4146897208	-3.6782820989	-0.8012988765
H	-3.0644416501	-3.8442115744	-2.4765617659
H	-5.5485805097	-3.2899890851	0.9931502002
H	-5.1153011486	-4.4142297661	-1.1865720559
C	-0.8760110114	0.4915743234	-0.2692830531
N	-0.681709854	1.7261062289	0.4197605488
C	-1.6327996926	0.790829498	-1.3913079746
C	0.0839104605	1.7468664309	1.5539323636
C	-1.3217377494	2.7697131966	-0.2597905692
C	-1.9184494461	2.1942325627	-1.4133234306
H	-1.9987067391	0.0677403121	-2.1058237758
N	0.7031722406	0.5667643695	1.8253963738
N	0.1887103451	2.8598731948	2.2828251379
C	-1.4133483986	4.1344694251	0.0172803996
C	-2.6306380106	3.0113454914	-2.3063526291
C	1.455496235	0.5147792712	2.9313447751
C	0.9516083894	2.7852859114	3.3746134984
C	-2.1248980285	4.9208896635	-0.8885515377
H	-0.9563613686	4.5550293636	0.9025449753
C	-2.7267939794	4.3709145007	-2.0357745792
H	-3.0923301854	2.5840208842	-3.1920992361
H	1.9458053245	-0.430484338	3.1365652201
C	1.6142379874	1.6201525366	3.7591564278
H	1.0319843152	3.6973325613	3.9626375412
H	-2.2186993883	5.9864363852	-0.6981940597
H	-3.2726538981	5.0193212282	-2.7151694456
H	2.2285373031	1.5730863942	4.6500648671
C	0.8066164729	-1.6341529031	-1.0810572782
O	0.9410857268	-2.2638444583	-2.0670091099
Co	2.6412779844	-0.6729083855	-1.1378673715
C	3.2412792765	-1.2900898226	0.4070282683
C	1.9751940116	0.9071704491	-1.6492246727
O	3.7530647386	-1.5366861026	1.4163962719
O	1.6862386033	1.9990159704	-1.8775221151

C	4.1968304498	-0.6355535541	-2.0307064108
O	5.1816299087	-0.6381716139	-2.6221438577

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D-INT2A

Co	-1.5749906457	-0.6329376899	0.7920597228
C	-1.1187563573	-1.9461895115	1.9854701285
O	-0.8774953798	-2.7745336774	2.7403856846
C	-3.4101217707	-1.3787857904	0.7362920214
O	-4.2180534618	-0.8970821925	1.4950132354
C	-3.8046502643	-2.4634663307	-0.2232137203
C	-2.945863777	-3.494572451	-0.6202851212
C	-5.1299231999	-2.4517145606	-0.6923476943
C	-3.4012420178	-4.4997001395	-1.4741728514
H	-1.9274837953	-3.5290681706	-0.2503364286
C	-5.5734597328	-3.4394949813	-1.5669961111
H	-5.7939247382	-1.6585851667	-0.3645288945
C	-4.7102730026	-4.467889936	-1.9576009663
H	-2.730583525	-5.3032037422	-1.7652395562
H	-6.594033907	-3.4131816239	-1.9390781229
H	-5.0585594566	-5.2431228178	-2.6347750719
C	-2.4058625022	0.6348882677	-0.4026093806
N	-2.8955049318	1.7671804436	0.3002921151
C	-2.7190444786	0.8093211024	-1.7218676306
C	-2.7081607128	1.8397277121	1.6470595464
C	-3.5152131242	2.6629338337	-0.5930554487
C	-3.4099260666	2.0709272004	-1.8775687644
H	-2.4903257723	0.1148381936	-2.5191385794
N	-2.0283220494	0.778778853	2.1706050396
N	-3.1639091487	2.8827156912	2.3488252684
C	-4.1318422988	3.895513813	-0.385991821
C	-3.9426543772	2.7443205533	-2.9843334337
C	-1.8005366602	0.7957642292	3.4894359837
C	-2.9211621628	2.872272959	3.6581289443
C	-4.6541903653	4.5436197232	-1.5075916472
H	-4.2002050112	4.3255781975	0.6043103446
C	-4.5617085822	3.9774006283	-2.7892319087
H	-3.8724718195	2.3096446939	-3.9779094593
H	-1.2622015551	-0.0529032434	3.8985842434
C	-2.229749215	1.8412952291	4.2967491233
H	-3.2970779836	3.725796195	4.2191292559
H	-5.1420382457	5.5061901652	-1.3813065482
H	-4.9789873077	4.5095287364	-3.6399138661
H	-2.0372116743	1.8475257413	5.3625683821

C	-0.6818454399	-1.2536593388	-0.6227813258
O	-0.4003687134	-1.6532307398	-1.6906485691
Co	1.0925525815	-0.3237593731	-0.1400030774
C	1.7167939965	-1.7303664253	0.780217071
C	0.4712271559	1.2797439425	0.2947236122
O	2.2032906757	-2.5113573814	1.4750007832
O	0.2802070616	2.3632234464	0.6483083674
C	2.6224476831	0.2161335305	-0.912318839
O	3.5823402261	0.5456367127	-1.4493171952

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D-INT2B

Co	0.5316453367	-0.8391549676	0.475618593
C	0.7708001721	-1.9543407962	1.9589314211
O	-0.2833607043	-2.5359269776	1.7472235836
C	1.6844295548	-2.2381380046	3.0743568003
C	1.3613148861	-3.2873639645	3.9585090437
C	2.8495165078	-1.4837264909	3.2762163202
C	2.2015291481	-3.5747895872	5.0275129685
H	0.4524820817	-3.8564835148	3.7907828356
C	3.6857937975	-1.7771964829	4.3522515951
H	3.084822718	-0.6772997213	2.5905437565
C	3.3641025747	-2.8195819713	5.2244881191
H	1.9542806246	-4.3829170718	5.7099562284
H	4.5878230325	-1.1931888704	4.5096740419
H	4.0187976514	-3.0457029076	6.0618899248
C	2.2552749179	-0.0834065828	0.2621858518
N	3.0590594504	-0.8658142937	-0.6129603899
C	2.9868321627	1.0176461692	0.6099087118
C	2.5123367389	-1.985781916	-1.1632587762
C	4.3029320776	-0.2401166647	-0.8197978823
C	4.2729589432	0.9536701989	-0.0550748032
H	2.6601994353	1.8120709215	1.2684186524
N	1.2258575589	-2.2008369093	-0.7699133913
N	3.1991969098	-2.7718730686	-1.9973960022
C	5.4038357803	-0.6128048638	-1.5885628142
C	5.3932761013	1.7942470233	-0.0652339353
C	0.5985324672	-3.2834869288	-1.2452786594
C	2.5533973088	-3.8417787559	-2.4642348977
C	6.5057367814	0.2451331046	-1.5799322648
H	5.3976420721	-1.5283711282	-2.1657043134
C	6.5015209417	1.4315032539	-0.8287466836
H	5.3948025595	2.7160439463	0.510409424
H	-0.424421287	-3.4235565812	-0.9118261792

C	1.2372867686	-4.157574569	-2.1165911244
H	3.1169903655	-4.475518056	-3.1460864211
H	7.3817729118	-0.0136962857	-2.1679921755
H	7.375379869	2.0771931447	-0.8456032302
H	0.7335489073	-5.0326200003	-2.508463845
C	-0.0574413286	0.5811607128	1.3833819207
O	-0.2632740288	1.4884108753	2.0604971463
Co	-1.650082263	0.0465607441	-0.8093651107
C	-2.2017671356	1.7489831316	-0.5876896291
C	-2.4700960269	-0.8464883855	0.5175253532
C	-0.1234611858	0.2302439894	-1.7105516789
O	-2.5981822026	2.8259302829	-0.4977945556
O	-3.109137015	-1.3820517636	1.3147734969
O	0.7079559129	0.4364887525	-2.4936856857
C	-2.5498695188	-0.7028524743	-2.1523964458
O	-3.1535742322	-1.1573216045	-3.0230305239

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D-TS2

Co	0.2571857412	-0.2416507259	-0.5858291122
C	0.1318068347	-1.404772275	-1.8948937545
O	-0.1137079646	-2.1001979182	-2.784949058
C	1.9771715245	-1.5019502383	-0.962298039
C	2.142434965	-2.7446226686	-0.3281170084
C	3.0227128497	-1.056796613	-1.7907384218
C	3.3413061341	-3.4576699538	-0.4224659986
H	1.3232656772	-3.19355177	0.2248649378
C	4.2235170955	-1.7618503144	-1.8885485387
H	2.9112155182	-0.1481253526	-2.3745035354
C	4.3938045674	-2.96001469	-1.1912894082
H	3.4427048112	-4.4107734667	0.0912407482
H	5.0223310629	-1.3769128273	-2.5174659253
H	5.3262199939	-3.5125080837	-1.2690402308
C	-1.6069451233	0.2717375412	-0.8184285955
N	-2.4557652817	-0.4801428697	0.0431947465
C	-2.4124026884	1.0254410239	-1.6198315708
C	-1.8894771168	-1.2545294645	1.0058517718
C	-3.8075905817	-0.1716746454	-0.215146438
C	-3.7959315792	0.7782808237	-1.2672247057
H	-2.0754892308	1.699317515	-2.396753494
N	-0.5227181695	-1.2814351091	0.970375523
N	-2.6443878676	-1.8974956909	1.9064247298
C	-4.9874936754	-0.6338409285	0.3647159566
C	-5.0136442566	1.2747842161	-1.7478938189

C	0.0976621719	-1.890791615	1.9908309701
C	-1.9991755615	-2.535272048	2.8800700169
C	-6.1870503483	-0.1222569231	-0.1358553448
H	-4.9691048485	-1.3566445848	1.1695795098
C	-6.2009764739	0.8186481032	-1.1774831915
H	-5.0302572273	2.0037028948	-2.5537689151
H	1.1805629955	-1.8494233813	1.9804381142
C	-0.6066207105	-2.5391483396	2.9969058012
H	-2.6234271564	-3.0572927519	3.6029314069
H	-7.1259128497	-0.4618698917	0.2926450377
H	-7.1519055638	1.1963837771	-1.5436097378
H	-0.0966137823	-3.0288012562	3.8174811707
C	0.762210486	1.1898928229	-1.5232764777
O	0.8637586571	1.9487798079	-2.393920076
Co	1.6518146928	1.7549241602	0.748388641
C	3.1648746895	1.6879900109	-0.2371578247
C	2.4112548187	1.0571283489	2.2253226612
C	-0.0126905732	1.4756913736	1.3414508377
O	4.170894751	1.7449458396	-0.7875695783
O	2.8928377034	0.6171995964	3.1727901517
O	-0.9995807312	1.5205922499	1.9414312912
C	1.4658671644	3.5504482151	0.6671547214
O	1.3720534566	4.6947300769	0.6650490543

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D-INT3A

Co	1.6808846593	-1.0184535082	1.2445444658
C	3.1966297294	-1.3010567968	2.1949770543
O	4.1807957302	-1.4998165444	2.7406663752
C	0.5969878376	-1.9440077856	2.6829230702
C	0.8750384705	-1.818341275	4.0553618781
C	-0.4933563658	-2.7625009514	2.3322199748
C	0.1201420822	-2.4861842323	5.0266196566
H	1.6899130189	-1.181814769	4.394874646
C	-1.2513939264	-3.4376475857	3.2954323097
H	-0.7786178074	-2.8771782655	1.2881533264
C	-0.9463802503	-3.3034283514	4.6512229343
H	0.3709565312	-2.3653450178	6.0781007966
H	-2.0888321706	-4.0579447719	2.9828546386
H	-1.5350906989	-3.8226470887	5.4027707221
C	2.768150085	-0.2270090663	-0.213799797
N	3.1135963116	-1.1957135263	-1.1965748242
C	3.294260791	0.9638302367	-0.6227245866
C	2.7606094744	-2.4980721158	-1.0051123465

C	3.8517442304	-0.5932498747	-2.2373303348
C	3.9739334405	0.7750592338	-1.8873550785
H	3.2177099292	1.9025768163	-0.0896676573
N	2.0578091509	-2.7400993692	0.141044985
N	3.1198326061	-3.4342732226	-1.8929223765
C	4.4001788532	-1.1161129846	-3.408035657
C	4.6678051913	1.6394262989	-2.7432523642
C	1.7657841299	-4.0170692413	0.4185970359
C	2.7916462865	-4.6920031791	-1.6045714526
C	5.0861428009	-0.2311904967	-4.2425713024
H	4.2956059978	-2.1640707137	-3.6544461729
C	5.2193613614	1.1278773553	-3.9161657501
H	4.7729871578	2.6919391037	-2.4938498026
H	1.2267091451	-4.1882238211	1.3434676468
C	2.1193597508	-5.0538040462	-0.436690313
H	3.0858477002	-5.4403997854	-2.3381922462
H	5.5241506975	-0.6064751036	-5.1633325252
H	5.7595792086	1.7888662291	-4.5886137027
H	1.8744071839	-6.0832950516	-0.2052330907
C	1.4788176141	0.7050519329	1.995085387
O	2.0923903154	1.5034383897	2.5934489313
Co	-0.3901074713	0.6014925141	1.2863799892
C	-0.8678336827	1.0976022827	2.9801427541
C	-2.0793249637	0.0272345426	0.9357703511
C	0.1954374652	-0.6582208683	-0.051764169
O	-1.2159056945	1.4546854738	4.0114826756
O	-3.1663082266	-0.2626935589	0.7158797898
O	-0.1199818049	-1.0937003488	-1.0877754244
C	-0.1702045477	2.0948275353	0.2754414439
O	-0.1288723571	3.0698234931	-0.3271576442

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D-INT3B

Co	-1.4691460739	-0.6930765864	-1.0535625074
C	-0.5932741348	-1.3507840868	-2.556961581
O	-0.1589524127	-1.8019683321	-3.5162680972
C	-3.2124429168	-0.817711205	-2.0650518877
C	-3.5432908335	-2.0076106284	-2.7283551931
C	-4.127623222	0.2419304106	-2.1222230008
C	-4.7516670775	-2.1386895975	-3.4220033907
H	-2.869785105	-2.8603915522	-2.7217046082
C	-5.3339123904	0.1141455463	-2.8179694961
H	-3.928692405	1.1752969036	-1.6067059522
C	-5.6531571642	-1.0765665448	-3.4709368666

H	-4.9797583416	-3.0754160479	-3.9256624878
H	-6.0260986422	0.952632129	-2.8407918948
H	-6.5915779487	-1.1751140784	-4.0099545073
C	-2.4423419838	-0.0829191605	0.4956172765
N	-2.9292622409	-1.1770010313	1.2579341862
C	-2.8625759744	1.0599824557	1.111118371
C	-2.567589836	-2.4326996398	0.8955606149
C	-3.66321262	-0.7095667498	2.3672752775
C	-3.6309544701	0.7045837365	2.2868997248
H	-2.6612434076	2.071208674	0.78314782
N	-1.7731736738	-2.4819744292	-0.2159058461
N	-2.9672864715	-3.4991605557	1.5985195607
C	-4.3214946034	-1.3888959175	3.3901875121
C	-4.285760271	1.4562023434	3.2700937578
C	-1.3347753585	-3.6909703654	-0.5951808991
C	-2.5263439417	-4.6858539615	1.1905059501
C	-4.966722157	-0.6138489022	4.3565685424
H	-4.3290933712	-2.4700989215	3.4292303024
C	-4.9500290421	0.7885894993	4.297818738
H	-4.2747082821	2.542137458	3.2307793216
H	-0.6885424287	-3.7220104913	-1.4658302199
C	-1.6838166239	-4.8475011853	0.0873482778
H	-2.8591910047	-5.543979652	1.7711863159
H	-5.4911433191	-1.1102980854	5.1682166233
H	-5.4627466751	1.3614602766	5.0658163271
H	-1.3210724404	-5.818400986	-0.2267399526
C	-1.2679983532	1.0218778008	-1.4903474153
O	-1.3559031365	2.1337445647	-1.7672220866
Co	1.2129731019	0.0866367049	-0.6874263602
C	1.4770581986	0.7732221858	-2.3413187917
C	2.5705205999	-1.0815850919	-0.7406797729
C	0.3578692557	-0.7847173602	0.6281272883
O	1.7422289655	1.2297856657	-3.3637634498
O	3.4762324689	-1.7920657239	-0.7473093668
O	0.1856794601	-1.3100536896	1.6496139433
C	1.5248031075	1.5791249992	0.2718849621
O	1.7912330969	2.5112280551	0.889439438

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D-TS3

Co	-0.4927677597	0.7522138293	0.0318310405
C	-1.5697621632	2.0325138031	0.8517994415
O	-2.1384998202	2.8907028902	1.3556253534
C	1.1083881452	2.0356807214	-0.2079487194

C	1.8223052909	2.4432580598	0.9349259173
C	1.0802023343	2.9201744279	-1.3071871842
C	2.4705337263	3.6797169237	0.9780984878
H	1.8827302608	1.8066374717	1.8095677344
C	1.7232850668	4.1535318465	-1.2557460482
H	0.5675424215	2.6443581011	-2.2220039074
C	2.4249731175	4.5468763668	-0.1121123422
H	3.0107545246	3.9610597604	1.8788500019
H	1.6764173975	4.8104623884	-2.1208285828
H	2.9294816009	5.5080022355	-0.0763924529
C	1.2370496021	0.1716909023	-0.6387619819
N	1.9272302878	-0.5879203281	0.3587140714
C	1.8564468188	-0.1098228617	-1.8428863224
C	1.3834252568	-0.6944797487	1.6022373485
C	2.982638236	-1.3125324574	-0.2291111071
C	2.9384008149	-1.0229198469	-1.6184410419
H	1.6079934611	0.3476017539	-2.79084454
N	0.184151333	-0.0582706643	1.7354018447
N	2.0092899087	-1.3668265698	2.5748942838
C	3.9258379232	-2.173719275	0.3252632017
C	3.8821713131	-1.618654649	-2.4700101058
C	-0.4082306608	-0.117748245	2.9370839864
C	1.3928043791	-1.4195903776	3.7542316783
C	4.8509537514	-2.7534635928	-0.5468701534
H	3.9372853718	-2.3812981999	1.3867560279
C	4.8305378214	-2.4790546093	-1.9246216844
H	3.8668403127	-1.4112798411	-3.536372623
H	-1.3640529039	0.387244663	3.0264587473
C	0.163950436	-0.801600607	4.0009577892
H	1.9058072274	-1.9770409427	4.5354335956
H	5.6019260558	-3.4285765388	-0.1465152333
H	5.5666961676	-2.9466494819	-2.5727234988
H	-0.3243734436	-0.8531361964	4.9663167438
C	-1.1936169284	0.9138001419	-1.6037834083
O	-1.434112649	1.1576970616	-2.707221702
Co	-2.7364044689	-0.9075803977	-0.435036008
C	-3.816131557	0.5353891235	-0.4817596123
C	-3.511513362	-1.7008186142	0.968812523
C	-1.1551006032	-1.7127256028	-0.2112159612
O	-4.5648471246	1.4104446495	-0.5137296477
O	-4.0301754619	-2.2339958684	1.8490224284
O	-0.3298179621	-2.5202381372	-0.0940921165
C	-3.1544185964	-1.6573533087	-2.0188128562
O	-3.4628799001	-2.1718701593	-2.999907405

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D-INT4

Co	-1.1154800327	0.8382570954	-0.0744789803
C	-1.1074377801	2.5701203207	0.2765395464
O	-1.2255053788	3.6846470931	0.540960467
C	2.1505404987	2.2446147479	-0.2154000016
C	2.3469031017	2.7616262217	1.0782281245
C	1.8573358626	3.141941111	-1.2591275614
C	2.2425490483	4.1311548107	1.3184821218
H	2.6246034793	2.0965705718	1.8911861577
C	1.765189542	4.5108911725	-1.0168968424
H	1.6942951391	2.7519845833	-2.2596366947
C	1.9518880193	5.0114656119	0.2737266165
H	2.4058070862	4.51330989	2.3226298473
H	1.5364837349	5.1868647316	-1.836241115
H	1.8738587256	6.0780888697	0.4636930525
C	2.3712619697	0.8252259439	-0.531935072
N	2.0404450574	-0.2571444012	0.3246989518
C	3.1128401013	0.3342139443	-1.5735953791
C	1.2963354621	-0.2163855454	1.5051919892
C	2.6392392778	-1.4269856899	-0.1860313563
C	3.2904827541	-1.0759529071	-1.3924495638
H	3.5559383164	0.9432312007	-2.3495605001
N	0.076249778	0.3782690974	1.5082006987
N	1.8566371229	-0.7965717063	2.570063439
C	2.6136234018	-2.740838135	0.2865522852
C	3.9480176687	-2.0681652225	-2.1368217501
C	-0.5126450843	0.5250306096	2.7156149668
C	1.2142533197	-0.7207220674	3.7342821944
C	3.2726319998	-3.7060131932	-0.4708255816
H	2.1157462039	-3.0042715481	1.2111247045
C	3.9350820003	-3.3757441877	-1.6684069009
H	4.450333441	-1.8135238485	-3.0658827464
H	-1.4636836314	1.0437630537	2.721420322
C	0.0259207121	-0.005949672	3.8765418286
H	1.6806924875	-1.2277172752	4.5763918973
H	3.2763275068	-4.7351367496	-0.1235136906
H	4.4390403163	-4.155957926	-2.2317574936
H	-0.4754209958	0.1063220922	4.8304804727
C	-2.2052533209	1.0491137328	-1.4365981569
O	-2.9044642059	1.2809276971	-2.3229943512
Co	-1.7119547415	-1.6026802293	-0.6647535136
C	-2.5570733558	-0.8797253113	0.7136435531

C	-1.0053975712	-3.0376357099	0.1309601776
C	-0.4596026749	-1.1747110727	-1.8624311676
O	-3.1948859691	-0.5793385543	1.6425368191
O	-0.5999807587	-3.9923660544	0.6361962267
O	0.3016190695	-0.9552754538	-2.7036040658
C	-3.0690502109	-2.1147748833	-1.7224062141
O	-3.9337484928	-2.4976598589	-2.3799187614

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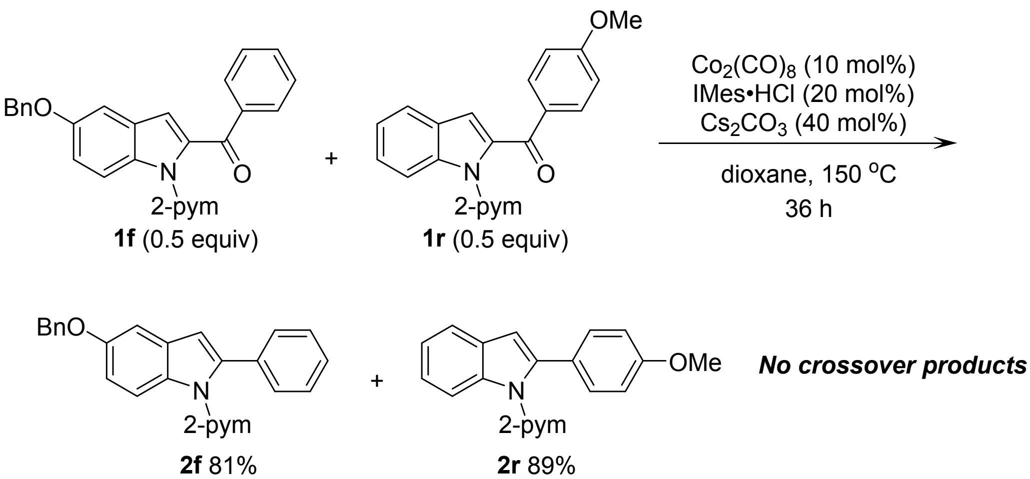
D-INT5

Co	-1.3195933442	-0.9951188157	-1.4132163269
C	-2.0657198493	-1.287824625	-3.0015130561
O	-2.4016401304	-1.5073390771	-4.0824835128
C	-4.4383512082	-0.4705225372	-0.5489175891
C	-5.1666354533	-1.6566995528	-0.753318589
C	-4.5770175111	0.5728343005	-1.4830315622
C	-5.9890772819	-1.8009254113	-1.8700048854
H	-5.1192351277	-2.4547000617	-0.0177724195
C	-5.4082599873	0.4282732248	-2.591563762
H	-4.0078937937	1.4872423894	-1.3467774148
C	-6.1121428739	-0.7613982117	-2.7947077992
H	-6.5489011338	-2.7221071363	-2.0081965443
H	-5.4956485165	1.2426896108	-3.3053002716
H	-6.7545610087	-0.8755858996	-3.6632018933
C	-3.6214177871	-0.2608104839	0.657053679
N	-2.9126899163	-1.2951899893	1.3166668538
C	-3.5762421202	0.8597163964	1.447366963
C	-2.5641072342	-2.5487725355	0.8034640502
C	-2.4419399167	-0.8022886699	2.5468723383
C	-2.8360011032	0.5551497503	2.6364963549
H	-4.0966985625	1.7832255715	1.2334054908
N	-1.9792191247	-2.6095056217	-0.4179650636
N	-2.8056117475	-3.6005447133	1.587168984
C	-1.6838235814	-1.423881742	3.5418939715
C	-2.4778420874	1.3016156108	3.7713939942
C	-1.7289478493	-3.843233814	-0.9031179211
C	-2.4991348753	-4.80923535	1.1119688906
C	-1.3393209024	-0.659483675	4.6536173116
H	-1.3965033234	-2.4660334334	3.467805614
C	-1.7338320208	0.6876247873	4.7704382201
H	-2.7718618404	2.3438686607	3.856801905
H	-1.275856755	-3.8850346463	-1.8860268634
C	-1.985625205	-4.9921956065	-0.1700298386
H	-2.6862304999	-5.6494902537	1.7771288386

H	-0.760010815	-1.117556942	5.4502456858
H	-1.4480622131	1.2518644052	5.653567704
H	-1.7658603769	-5.9742469276	-0.5719649418
C	-0.9054754283	0.7671412205	-1.6713269792
O	-1.1426076592	1.832435317	-2.098810763
Co	0.5889308005	0.2246443236	-0.5080262001
C	2.3274442234	0.5053607901	-0.7405830931
C	0.522084168	-1.5240348696	-1.123295225
O	3.4349368147	0.7397730947	-0.952203759
O	1.0057697119	-2.5757752131	-1.3312845267
C	0.2087161426	1.4894788945	0.6960597788
O	0.0241078339	2.2636394273	1.5268952929

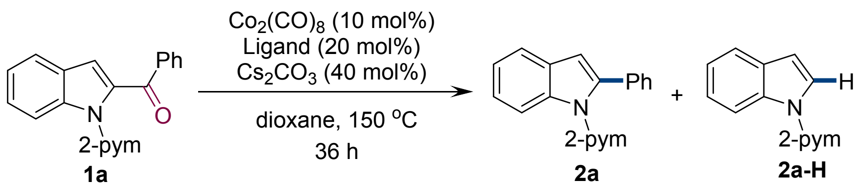
3. Crossover experiment

In a glovebox, substrates **1f** (0.05 mmol) and **1r** (0.05 mmol) were added to a solution of $Co_2(CO)_8$ (0.01 mmol), IMes·HCl (0.02 mmol) and Cs_2CO_3 (0.04 mmol) in 1,4-dioxane (0.5 mL). Then the vessel was sealed and removed from glovebox. The contents of the vial were then stirred at 150 °C for 36 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel.



4. Optimization details

Table S1 Effect of the ligand utilized [a]

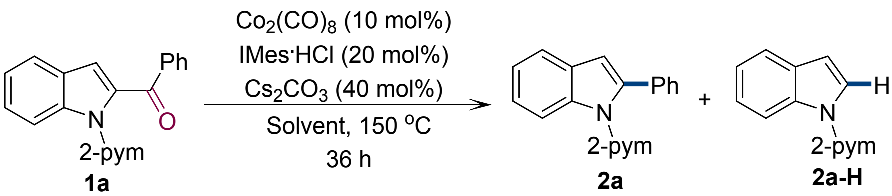


Entry	Ligand (20 mol%)	Yield (**2a**) [b]	Yield (**2a-H**) [b]

1	PPh_3	27%	＜5%
2	IMes·HCl	93%	＜5%
3	SIPr·HCl	14%	17%
4	IPr·HCl	47%	20%
5	ICy·HCl	68%	10%
6	PCy_3	80%	＜5%
7	$P(n\text{-Bu})_3$	72%	＜5%
8	2,2'-bipyridine	15%	＜5%
9	Without ligand	18%	0

[a]Standard conditions: **1a** (0.1 mmol), $Co_2(CO)_8$ (10 mol %), Ligand (20 mol %), Cs_2CO_3 (40 mol %), dioxane (0.5 mL) at 150 °C, 36 h. [b]Isolated yields.

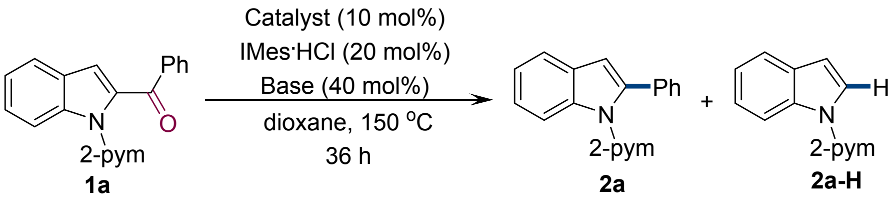
Table S2 Effect of the solvent utilized[a]



Entry	Solvent	Yield (**2a**)[b]	Yield (**2a-H**)[b]
1	toluene	86%	＜5%
2	dioxane	93%	＜5%
3	acetonitrile	0	0
4	^{i}PrOH	0	70%
5	DCE	< 5%	＜5%

[a]Standard conditions: **1a** (0.1 mmol), $Co_2(CO)_8$ (10 mol %), IMes·HCl (20 mol %), Cs_2CO_3 (40 mol %), solvent (0.5 mL) at 150 °C, 36 h. [b] Isolated yields.

Table S3 Screening of cobalt catalysts and bases [a]

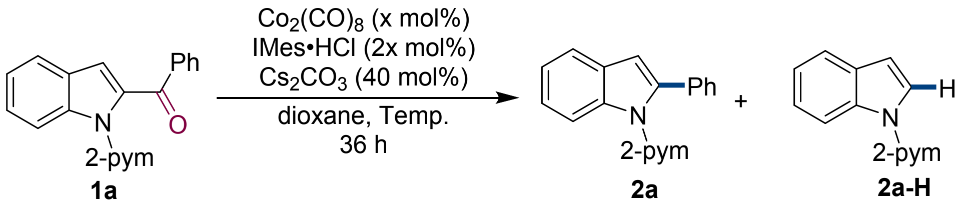


Entry	Catalyst	Base	Yield (**2a**)[b]	Yield (**2a-H**)[b]
1	$Co_2(CO)_8$	Cs_2CO_3	93%	＜5%
2	$CoBr_2$	Cs_2CO_3	0	10%
3	$CoCl_2$	Cs_2CO_3	0	＜5%
4	salenCo(II)	Cs_2CO_3	0	19%
5	$Co(acac)_2$	Cs_2CO_3	0	＜5%
6	$Co_2(CO)_8$	NaO^{t}Bu	77%	8%
7	$Co_2(CO)_8$	KO^{t}Bu	80%	9%

8	$Co_2(CO)_8$	K_2CO_3	<5%	0

[a] Standard conditions: **1a** (0.1 mmol), Catalyst (10 mol %), IMes·HCl (20 mol %), base (40 mol %), dioxane (0.5 mL) at 150 °C, 36 h. [b] Isolated yields.

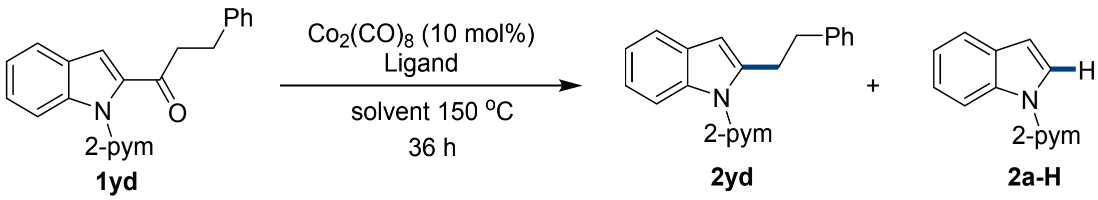
Table S4 Screening of catalyst loadings and temperature [a]



Entry	X (mol%)	Temp. (°C)	Yield (**2a**)[b]	Yield (**2a-H**)[b]
1	10	rt	0	0
2	10	120	0	0
3	10	150	93%	<5%
4[c]	10	150	88%	<5%
5	5	150	10%	<5%
6	15	150	92%	<5%

[a]Standard conditions: **1a** (0.1 mmol), $Co_2(CO)_8$ (x mol %), IMes·HCl (2x mol %), base (40 mol %), dioxane (0.5 mL), 36 h. [b] Isolated yields. [c] IMes (10 mol%).

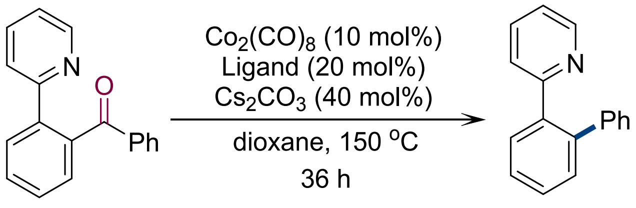
Table S5 Screening of reaction conditions of **1yd**[a]



Entry	Ligand (20 mol%)	Base (40 mol%)	Solvent	Yield(**2yd**) [b]	Yield(**2a-H**) [b]
1	PCy_3	---	1,4-dioxane	40%	30%
2	PCy_3	---	toluene	52%	20%
3	IMes·HCl	Cs_2CO_3	1,4-dioxane	7%	20%
4	IMes·HCl	Cs_2CO_3	toluene	8%	25%
5[c]	PCy_3	---	toluene	trace	<5%

a)Standard conditions: **1yd** (0.1 mmol), $Co_2(CO)_8$ (10 mol %), Ligand (20 mol %), base (40 mol %), solvent (0.5 mL), 36 h, 150 °C. b) Isolated yields. c) 120 °C.

Table S6 Effect of the ligand utilized[a]

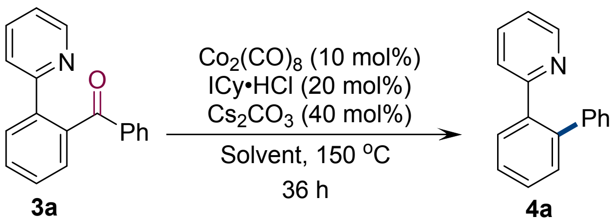


3a 4a

Entry	Ligand (20 mol%)	Yield[b]
1	PPh_3	0%
2	IMes·HCl	35%
3	SIPr·HCl	5%
4	IPr·HCl	54%
5	ICy·HCl	90%
6	PCy_3	0%
7	P(*n*-Bu)$_3$	0%
8	Without ligand	0%

[a] Standard conditions: **3a** (0.1 mmol), $Co_2(CO)_8$ (10 mol %), Ligand (20 mol %), Cs_2CO_3 (40 mol %), dioxane (0.5 mL) at 150 °C, 36 h. [b] Isolated yields.

Table S7 Effect of the solvent utilized[a]

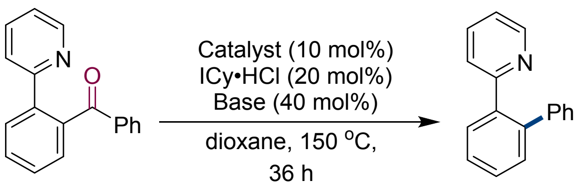


3a 4a

Entry	Solvent	Yield[b]
1	toluene	45%
2	dioxane	90%
3	acetonitrile	0
4	THF	0
5	DCE	0

[a]Standard conditions: **3a** (0.1 mmol), $Co_2(CO)_8$ (10 mol %), ICy·HCl (20 mol %), Cs_2CO_3 (40 mol %), solvent (0.5 mL) at 150 °C, 36 h. *b* Isolated yields.

Table S8 Screening of cobalt catalysts and bases[a]



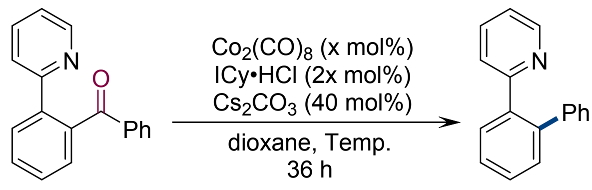
3a 4a

Entry	Catalyst	Base	Yield[b]
1	$Co_2(CO)_8$	Cs_2CO_3	90%

2	$CoBr_2$	Cs_2CO_3	20%
3	$Co(OAc)_2$	Cs_2CO_3	0
4	salenCo(II)	Cs_2CO_3	0
5	$Co(acac)_2$	Cs_2CO_3	0
6	$Co_2(CO)_8$	NaO^tBu	30%
7	$Co_2(CO)_8$	KO^tBu	18%
8	$Co_2(CO)_8$	K_2CO_3	0

^{a}Standard conditions: **3a** (0.1 mmol), Catalyst (10 mol %), ICy·HCl (20 mol %), base (40 mol %), dioxane (0.5 mL) at 150 °C, 36 h. ^{b} Isolated yields.

Table S9 Screening of catalyst loadings and temperature^a



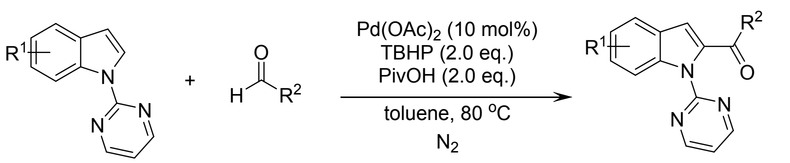
3a **4a**

Entry	X (mol%)	Temp.(°C)	Yield^b
1	10	rt	0
2	10	120	0
3	10	150	90%
4	5	150	51%
5	15	150	90%

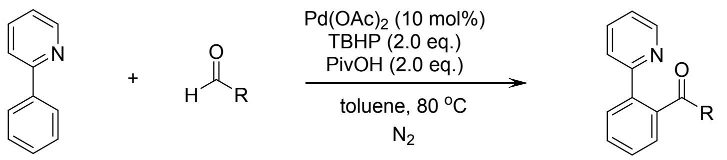
^{a}Standard conditions: **3a** (0.1 mmol), $Co_2(CO)_8$ (x mol %), ICy·HCl (2x mol %), base (40 mol %), dioxane (0.5 mL), 36 h. ^{b} Isolated yields.

5. Experiment procedure

6.1 Preparation of substrates**.**



1



3

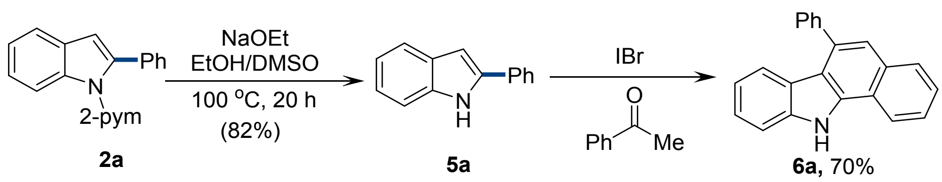
Method 1[16a]. A 100 mL Schlenk flask was charged with indole[17] or 2-phenylpyridine (3 mmol), then, aldehyde (9 mmol), $Pd(OAc)_2$ (0.3 mmol), TBHP (6 mmol, 70% aqueous solution), PivOH (6 mmol) were added to the flask. Then the flask was evacuated and backfilled with N_2 for three times and then toluene (25 mL) was added. The mixture was stirred at 80 °C. After completion of reaction, the mixture was diluted with ethyl acetate (30 mL), and washed with NaOH (40 mL, 10% aq.), H_2O (40 mL) and brine (40 mL). Then, the organic layers was dried over Na_2SO_4, and concentrated to give the crude product. The crude product was purified by column chromatography on silica gel to afford the substrate **1** or **3**.

Method 2[16b]**.** This method is suitable for substrates **3m, 3n** and **3o.** A 25 mL Schlenk flask was charged with pyridine-directed substrates (2 mmol), then, aldehyde (4 mmol), $Pd(OAc)_2$ (0.2 mmol), NHPI (0.4 mmol) were added to the flask. Then the flask was evacuated and backfilled with O_2 for three times and then dioxane (5 mL) was added. The mixture was stirred at 100 °C. After completion of reaction, the mixture was diluted with ethyl acetate (30 mL) and washed with brine (30 mL, 3 times). Then, the organic layers was dried over Na_2SO_4, and concentrated to give the crude product. The crude product was purified by column chromatography on silica gel to afford the corresponding substrate**.**

6.2 Typical Procedure for the Co(0)/NHC-Catalysed decarbonylation.

In a glovebox, ketone substrate **1** or **3** (0.1 mmol) was added to a solution of $Co_2(CO)_8$ (0.01 mmol), IMes·HCl or ICy·HCl (0.02 mmol) and Cs_2CO_3 (0.04 mmol) in 1,4-dioxane (0.5 mL). Then the vessel was sealed and removed from glovebox. The contents of the vial were then stirred at 150 °C for 36 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* to give a residue, which was purified by flash column chromatography over silica gel.

6.3 Typical Procedure for Carbazole Derivative **6a**

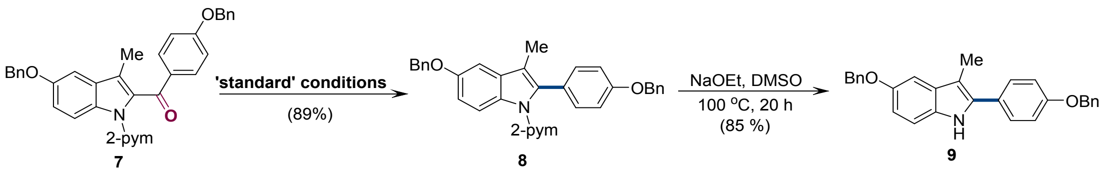


Step 1[18]**.** Indole **2a** (2 mmol) and EtONa (6 mmol) were added to a Schlenk flask (50 mL), then the flask was evacuated and backfilled with N_2 for three times and then DMSO (25 mL) was added. The mixture was heated at 100 °C for 20 h. After completion of reaction, H_2O (30 mL) was employed to quench the reaction. The mixture was extracted with EtOAc (20 mL) for three times, then the combined organic layer was washed with H_2O (40 mL) and brine (40 mL), dried over Na_2SO_4, purified by flash column chromatography (Petroleum ether/EtOAc = 15/1) to afford **5a** (316.9 mg, 82% yield).
2-Phenyl-1H-indole (5a). [21a] Yellow solid. M. p. = 153 – 155 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.66 (d, *J* = 7.2 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.83 (d, *J*=1.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.8, 136.8, 132.3, 129.2, 129.0, 127.7, 125.1, 122.3, 120.6, 120.2, 110.9, 100.0; HRMS (ESI) m/z calculated for $C_{14}H_{11}NNa$ [M+Na] 216.0784, found 216.0779.

Step 2[19]**.** 2-Phenyl-1*H*-indole (58.2 mg, 0.3 mmol) and IBr (42.0 mg, 0.2 mmol) were added to a solution of acetophenone (0.2 mmol) in chlorobenzene (0.5 mL). The reaction vessel was stirred at 130 °C for 4 h under air atmosphere. The mixture was the cool down to room temperature and flushed through a short column of silica gel with ethyl acetate. The solvent was removed and the residue was purified by flash column chromatography (Petroleum ether/EtOAc = 10/1) to afford **6a** in 70% yield.

6-Phenyl-11H-benzo[a]carbazole(6a)[19]. Brown oil (41.1 mg, 70% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 6.6 Hz, 2H), 7.60 – 7.54 (m, 5H), 7.52 – 7.49 (m, 2H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.2, 138.6, 136.5, 135.2, 132.1, 129.3, 128.9, 128.3, 127.6, 125.7, 125.4, 124.6, 123.8, 122.1, 120.9, 120.3, 120.2, 119.6, 116.7, 110.9; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{15}NNa$) requires *m/z* 316.1097, found *m/z* 316.1091. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).

6.4 Typical Procedure for Bazedoxifene



Step 1. In a glovebox, ketone **7** (52.5 mg, 0.1 mmol) was added to a solution of $Co_2(CO)_8$ (0.01 mmol), IMes·HCl (0.02 mmol) and Cs_2CO_3 (0.04 mmol) in 1,4-dioxane (0.5 mL). Then the vessel was sealed and removed from glovebox. The contents of the vial were then stirred at 160 °C for 36 h. The reaction was cooled to room temperature, and the crude mixture was filtered through a pad of silica gel. The filtrate was then concentrated *in vacuo* and the residue was purified by flash column chromatography (Petroleum ether/EtOAc = 3/1) to afford **8** in 89% yield (44.2 mg).

5-(Benzyloxy)-2-(4-(benzyloxy)phenyl)-3-methyl-1-(pyrimidin-2-yl)-1H-indole (8). White solid. M. p. = 140 – 142 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.8 Hz, 2H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 2H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.39 (td, *J* = 7.8, 1.8 Hz, 4H), 7.33 (q, *J* = 7.2 Hz, 2H), 7.17 (d, *J* = 9.0 Hz, 2H), 7.13 (d, *J* = 2.4 Hz, 1H), 7.01 – 6.97 (m, 2H), 6.95 (d, *J* = 9.0 Hz, 2H), 5.16 (s, 2H), 5.08 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.1, 157.9, 157.7, 154.6, 137.5, 136.9, 136.4, 131.9, 131.2, 130.8, 128.6, 128.5, 128.0, 127.8, 127.6, 127.6, 126.5, 116.6, 114.3, 114.3, 113.8, 113.2, 102.8, 70.8, 70.0, 9.6. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{33}H_{27}N_3NaO_2$) requires *m/z* 520.1995, found *m/z* 520.1992.

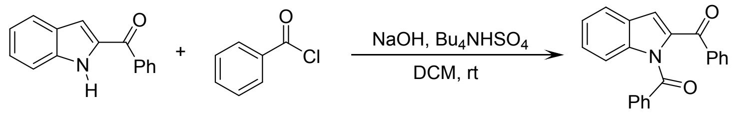
Step 2[20]. **8** (0.2 mmol) and EtONa (0.6 mmol) were added to a Schlenk flask (10 mL), then the flask was evacuated and backfilled with N_2 for three times and then DMSO (4 mL) was added. The mixture was heated at 100 °C for 24 h. After completion of reaction, H_2O (10 mL) was employed to quench the reaction. The mixture was extracted with EtOAc (10 mL) for three times, then the combined organic layer was washed with H_2O (20 mL) and brine (20 mL), dried over Na_2SO_4, purified by flash column chromatography (Petroleum ether/EtOAc = 5/1) to afford **9** in 85% yield (71.3 mg).

5-(Benzyloxy)-2-(4-(benzyloxy)phenyl)-3-methyl-1H-indole (9). Yellow solid. M. p. = 148 – 150 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (s, 1H), 7.51 – 7.46 (m, 6H), 7.42 – 7.32 (m, 6H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 2H), 5.14 (s, 2H), 5.12 (s, 2H), 2.39 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.1, 153.3, 137.8, 136.8, 135.0, 131.0, 130.5, 128.9, 128.6, 128.5, 128.1, 127.7, 127.6, 127.5, 126.2, 115.2, 112.7, 111.2, 107.7, 102.5, 71.0, 70.1, 9.7; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{29}H_{25}NNaO_2$) requires *m/z* 442.1778, found *m/z* 442.1782.

6.5 Preparation of **1a-2**[18], **1a-3**[21a] and **1a-4**[22].

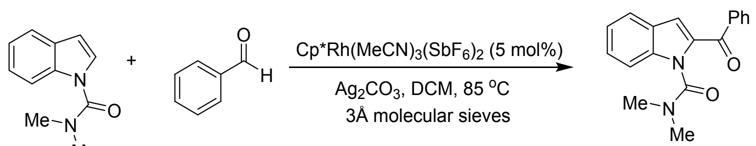
Compound **1a** (2 mmol) and EtONa (6 mmol) were added to a Schlenk flask (50 mL), then the flask was evacuated and backfilled with N_2 for three times and then DMSO (25 mL) was added. The mixture was heated at 100 °C for 24 h. After completion of reaction, HCl (10%, 20 mL) was employed to quench the reaction. The mixture was extracted with EtOAc (20 mL) for three times, then the combined organic layer was washed with H_2O (40 mL) and brine (40 mL), dried over Na_2SO_4, purified by flash column chromatography to afford **1a-2** in 60% yield (265 mg).

(1H-indol-2-yl)(phenyl)methanone (1a-2) [18]. White solid, M. p. = 157 – 158 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.61 (s, 1H), 8.01 (d, *J* = 7.2 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 1H), 7.38 (t, *J*=7.2 Hz, 1H), 7.18 – 7.15 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.3, 138.0, 137.6, 134.3, 132.3, 129.2, 128.5, 127.7, 126.5, 123.2, 121.0, 112.9, 112.2.



(1H-indol-2-yl)(phenyl)methanone (0.4 mmol) was add to a mixture of NaOH (1.0 mmol) and Bu_4NHSO_4 (0.04 mmol) in DCM (3.0 mL). The mixture was stirred at room temperature for 30 min. Then a solution of benzoyl chloride (0.6 mmol) in DCM (1 mL) was added dropwise and the mixture was stirred for another 60 min. Then the reaction was quenched by $NaHCO_3$ (sat.), extracted with DCM and dried with Na_2SO_4. The mixture was filtered and the filtrate was evaporated under reduced pressure. The solvent was removed and the residue was purified by flash column chromatography to afford the **1a-3** in 50% yield.

(1H-indole-1,2-diyl)bis(phenylmethanone) (1a-3) [21a]**.** White solid. M. p. = 124 – 126 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 9.0 Hz, 1H), 7.81 (dd, *J* = 8.4, 1.1 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.68 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.46 – 7.41 (m, 4H), 7.34–7.29 (m, 3H), 7.16 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.0, 169.2, 139.1, 138.1, 137.1, 135.5, 132.9, 132.9, 129.2, 129.2, 128.6, 128.4, 127.6, 127.3, 123.6, 122.9, 118.0, 114.3.



An oven-dried reaction sealed tube (10 mL) was charged with $Cp^*Rh(MeCN)_3(SbF_6)_2$ (8.4 mg, 5 mol%, 0.01 mmol), CH_2Cl_2 (2 mL), indole substrate (0.2 mmol) , aldehyde (0.4 mol), 3Å molecular sieves (50mg) and Ag_2CO_3 (0.4 mol). The vessel was sealed and heated at 85°C for 24 h. The resulting mixture was cooled to room temperature. The solvent was removed and the residue was purified by flash column chromatography to afford **1a-4** in 74% yield.

2-Benzoyl-N,N-dimethyl-1H-indole-1-carboxamide (1a-4) [22]**.** White solid, M. p. = 125 – 127 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.8 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.44 – 7.40 (m, 2H), 7.23 (t, *J* = 6.6 Hz, 1H), 7.15 (s, 1H), 3.23 – 2.96 (m, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.4, 153.6, 137.7, 137.4, 135.4, 132.7, 129.6, 128.4, 127.2, 126.8, 123.3, 122.1, 115.6, 111.5, 37.7

6. X-Ray Crystallographic Data for 2yd.

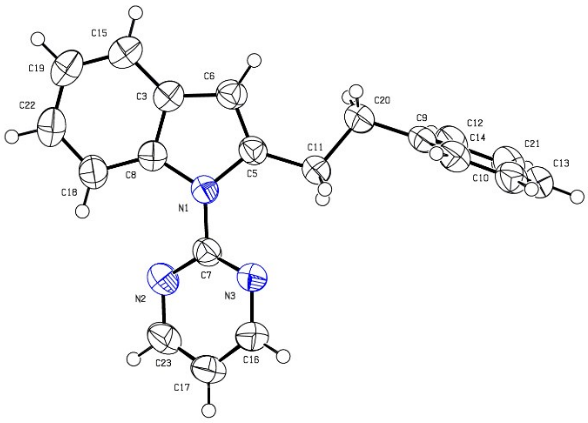
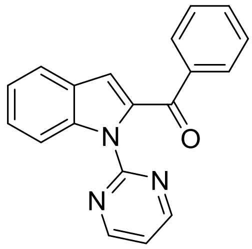


Table S10. Crystal data and structure refinement for **2yd**

CCDC number	**1965066**
Empirical formula	C_{20} H_{17} N_3
Formula weight	299.36
Temperature/K	296K
Crystal system	triclinic
Space group	P -1
a/Å	7.7352(18)
b/Å	10.022(2)
c/Å	10.902(3)
α/°	75.534(4)
β/°	83.910(4)
γ/°	71.785(3)
Volume/Å^3	777.0(3)
Z	2
Density (calculated) g/cm^3	1.279
μ/mm^{-1}	0.077
F(000)	316
Crystal size/mm^3	0.5*0.2*0.1
Radiation	MoK\a（wavelength = 0.71073）
Index ranges	-9 ≤ h ≤ 9, -12 ≤ k ≤ 11, -13 ≤ l ≤ 5
Reflections collected	4220
Independent reflections	3017
Data/restraints/parameters	3017/0/209
Goodness-of-fit on F^2	0.867
Final R indexes [I>=2σ (I)]	R_1= 0.0417, wR_2= 0.1342

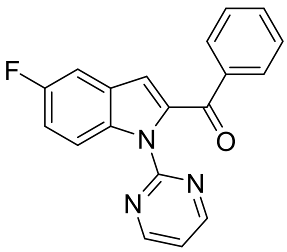
Final R indexes [all data] R_1= 0.0515, wR_2= 0.1450

7. Spectra data



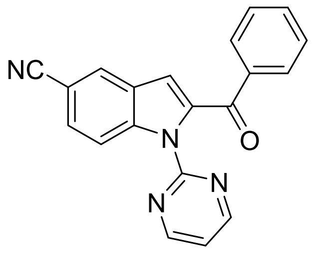
1a

Phenyl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1a).[21a] White solid. M. p. = 128 – 129 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 8.40 (d, *J* = 9.0 Hz, 1H), 7.97 (d, *J* = 7.2 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.29 (t, *J*= 7.0 Hz, 1H), 7.13 (s, 1H), 7.05 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.6, 157.9, 157.3, 138.2, 137.9, 137.1, 132.7, 129.5, 128.3, 128.0, 126.5, 122.8, 122.5, 117.3, 115.4, 114.2; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{13}N_3NaO$) requires *m/z* 322.0951, found *m/z* 322.0962.



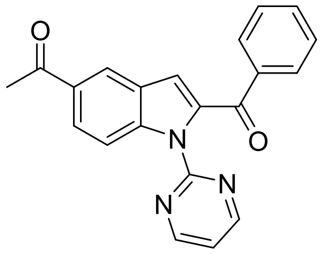
1b

(5-fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (1b).[21a] White solid. M. p. = 142 – 143 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.58 (d, *J* = 4.8 Hz, 2H), 8.41 (dd, *J*=9.0, 4.8 Hz, 1H), 7.94 (d, *J* = 6.6 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 8.4 Hz, 2H), 7.32 (dd, *J* = 8.7, 2.4, 1H), 7.16 (td, *J* = 9.0, 2.4 Hz, 1H), 7.04 (s, 1H), 7.02 (t, *J* = 4.8 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -120.4 (s, 1F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.5, 159.9, 158.3, 157.9, 156.9, 138.5, 137.7, 134.4, 132.8, 129.4, 128.7 (d, *J* = 9.9 Hz), 128.3, 117.4, 115.7 (d, *J* = 8.7 Hz), 114.6, 114.1 (d, *J* = 4.8 Hz) , 107.2, 107.0; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{12}FN_3NaO$) requires *m/z* 340.0857, found *m/z* 340.0867.



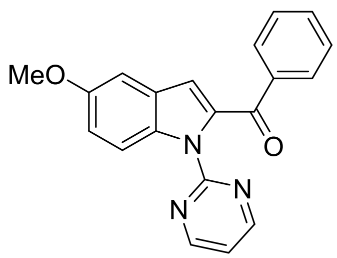
1c

2-Benzoyl-1-(pyrimidin-2-yl)-1H-indole-5-carbonitrile (1c).[21b] White solid. M. p. = 155 – 157 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 5.4 Hz, 2H), 8.51 (d, *J* = 8.4 Hz, 1H), 8.05 (s, 1H), 7.96 (d, *J* = 7.2 Hz, 2H), 7.65 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.59 (t, *J*=7.2 Hz, 1H), 7.47 (t, *J*=7.2 Hz, 2H), 7.14 (t, *J* = 4.8 Hz, 1H), 7.12 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.1, 158.1, 156.6, 139.3, 139.0, 137.2, 133.2, 129.5, 128.7, 128.5, 127.9, 127.5, 119.6, 118.2, 115.4, 113.6, 106.1; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{12}N_4NaO$) requires *m/z* 347.0903, found *m/z* 347.0913.



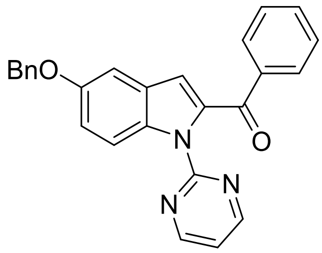
1d

1-(2-benzoyl-1-(pyrimidin-2-yl)-1H-indol-5-yl)ethan-1-one (1d). White solid. M. p. = 178 – 179 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 8.41 (d, *J* = 9.0 Hz, 1H), 8.34 (s, 1H), 8.06 (dd, *J* = 9.0, 1.2 Hz, 1H), 7.96 (d, *J* = 7.2 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.18 (s, 1H), 7.10 (t, *J* = 4.8 Hz, 1H), 2.67 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.5, 187.1, 158.0, 156.7, 140.3, 138.3, 137.4, 132.9, 132.2, 129.4, 128.3, 127.5, 126.1, 124.0, 117.9, 115.3, 114.1, 26.5. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{21}H_{15}N_3NaO_2$) requires *m/z* 364.1056, found *m/z* 364.1046.



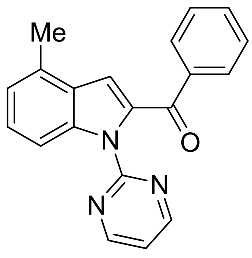
1e

(5-Methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (1e).[18] White solid. M. p. = 134 – 136 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.8 Hz, 2H), 8.34 (d, *J* = 9.6 Hz, 1H), 7.95 (d, *J* = 6.6 Hz, 2H), 7.53 (t, *J*=7.2 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 2H), 7.12 (d, *J* = 2.4 Hz, 1H), 7.08 (dd, *J*=9.6, 2.4 Hz, 1H), 7.05 (s, 1H), 7.01 (t, *J* = 4.8 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.6, 157.8, 157.2, 156.0, 138.1, 137.6, 133.2, 132.6, 129.4, 128.7, 128.3, 117.1, 116.4, 115.4, 114.8, 103.5,55.7; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{13}N_3NaO_2$) requires *m/z* 352.1056, found *m/z* 352.1072.



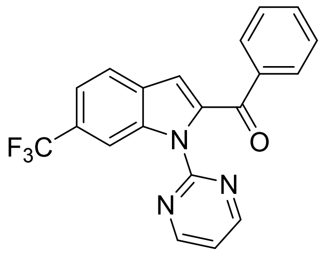
1f

(5-Benzyloxy)-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (1f). White solid. M. p. = 128 – 129 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.8 Hz, 2H), 8.34 (d, *J* = 9.0 Hz, 1H), 7.93 (d, *J* = 7.2 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.42 – 7.37 (m, 4H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.18 (s, 1H), 7.16 (d, *J* = 9.0 Hz, 1H), 7.02 (s, 1H), 6.99 – 6.96 (m, 1H), 5.12 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.5, 157.8, 157.1, 155.1, 138.0, 137.6, 137.1, 133.3, 132.6, 129.4, 128.7, 128.5, 128.2, 127.9, 127.5, 117.1, 115.4, 114.8, 105.1, 70.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{26}H_{19}N_3NaO_2$) requires *m/z* 428.1369, found *m/z* 428.1377.



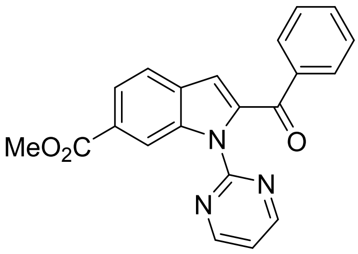
1g

(4-Methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (1g).[21a] White solid. M. p. = 135 – 136 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.8 Hz, 2H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 7.2 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.33 (t, *J* = 8.4 Hz, 1H), 7.17 (s, 1H), 7.08 (d, *J* = 7.2 Hz, 1H), 7.01 (t, *J* = 4.8 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.5, 157.9, 157.3, 138.2, 138.1, 136.6, 132.5, 132.1, 129.4, 128.3, 127.8, 126.7, 123.0, 117.3, 114.0, 111.6, 18.5; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO$) requires *m/z* 336.1107, found *m/z* 336.1131.



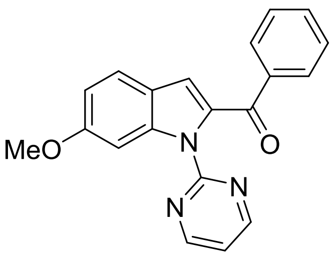
1h

Phenyl(1-(pyrimidin-2-yl)-6-(trifluoromethyl)-1H-indol-2-yl)methanone (1h). Yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.63 (d, *J* = 4.8 Hz, 2H), 7.94 (d, *J* = 7.2 Hz, 2H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.56 – 7.53 (m, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.12 (s, 1H), 7.08 (t, *J* = 4.8 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.0 (s, 3F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.5, 158.1, 156.7, 139.3, 137.5, 136.8, 133.0, 130.5, 129.4, 128.4, 124.7 (d, *J* = 270.8 Hz), 122.7, 119.4, 119.4, 117.7, 113.4, 112.4 (t, *J* = 4.5 Hz); HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{20}H_{13}F_3N_3O$) requires *m/z* 368.1005, found *m/z* 368.0985.



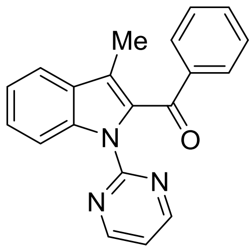
1i

Methyl 2-benzoyl-1-(pyrimidin-2-yl)-1H-indole-6-carboxylate (1i). White solid. M. p. = 130 – 132 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.64 (d, *J* = 4.8 Hz, 2H), 7.98 (dd, *J* = 8.44, 1.2 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.11 (s, 1H), 7.08 (t, *J* = 4.8 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.5, 167.5, 158.1, 156.8, 139.5, 137.5, 137.2, 132.9, 131.5, 129.4, 128.4, 127.7, 123.6, 122.0, 117.7, 116.5, 113.7, 52.1; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{16}N_3O_3$) requires *m/z* 358.1186, found *m/z* 358.1170.



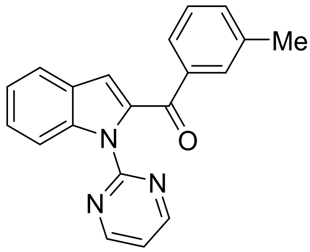
1j

(6-Methoxy-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (**1j**). White solid. M. p. = 109 – 111 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.66 (d, *J* = 4.8 Hz, 2H), 7.97 (d, *J* = 7.2 Hz, 2H), 7.85 (d, *J* = 2.4 Hz, 1H), 7.56 (d, *J* = 9.0 Hz, 1H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.09 (s, 1H), 7.07 (t, *J* = 4.8 Hz, 1H), 6.93 (dd, *J* = 9.0, 2.4 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.7, 159.8, 158.0, 157.5, 140.0, 138.1, 136.4, 132.4, 129.5, 128.2, 123.3, 121.8, 117.4, 116.8, 113.0, 97.0, 55.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO_2$) requires *m/z* 352.1056, found *m/z* 352.1069.



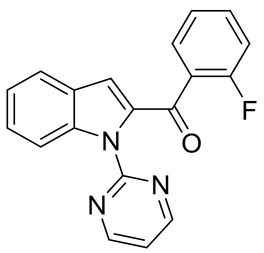
1k

(3-Methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)(phenyl)methanone (1k).[21a] White solid. M. p. = 152 – 153 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.4 Hz, 1H), 8.44 (d, *J* = 4.8 Hz, 2H), 7.78 (d, *J* = 7.2 Hz, 2H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.35 – 7.30 (m, 3H), 6.83 (t, *J* = 4.8 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 189.4, 157.5, 139.2, 136.4, 133.2, 132.2, 130.2, 130.1, 128.5, 128.4, 128.3, 126.1, 122.5, 120.1, 116.1, 115.2, 9.3 HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO$) requires *m/z* 336.1107, found *m/z* 336.1137.



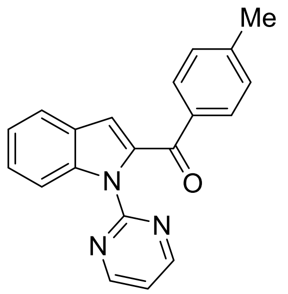
1l

(1-(Pyrimidin-2-yl)-1H-indol-2-yl)(m-tolyl)methanone (1l).[21a] White solid. M. p. = 112 – 114 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.8 Hz, 2H), 8.38 (d, *J* = 8.4 Hz, 1H), 7.80 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.37 – 7.27 (m, 3H), 7.11 (s, 1H), 7.06 (t, *J* = 4.8 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.7, 157.9, 157.3, 138.3, 138.1, 137.9, 137.3, 133.5, 130.0, 128.2, 128.0, 126.9, 126.4, 122.7, 122.4, 117.3, 115.3, 114.2, 21.3. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO$) requires *m/z* 336.1107, found *m/z* 336.1134.



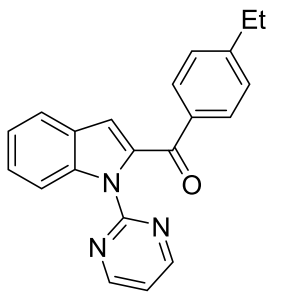
1m

(2-Fluorophenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1m).[21c] Pale yellow oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.8 Hz, 2H), 8.35 (d, *J* = 8.4 Hz, 1H), 7.72 – 7.69 (m, 2H), 7.48 – 7.43 (m, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.11 – 7.07 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.5 (s, 1F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.1, 166.3, 164.6, 157.9, 157.2, 138.2, 136.9, 134.4 (d, *J* = 3.2 Hz), 132.0 (d, *J* = 9.8 Hz), 127.9, 126.5, 122.9, 122.4, 117.3, 115.5 (d, *J* = 22.0 Hz), 115.2, 115.1, 114.3; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{12}FN_3NaO$) requires *m/z* 340.0857, found *m/z* 340.0877.



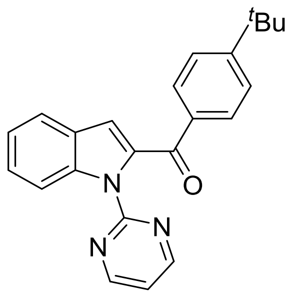
1n

(1-(Pyrimidin-2-yl)-1H-indol-2-yl)(p-tolyl)methanone(1n).[21a] White solid. M. p. = 120 – 121 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.8 Hz, 2H), 8.40 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.09 (s, 1H), 7.03 (t, *J* = 4.8 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.3, 157.9, 157.3, 143.5, 138.2, 137.3, 135.4, 129.7, 129.0, 128.0, 126.3, 122.7, 122.3, 117.3, 114.9, 114.2, 21.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO$) requires *m/z* 336.1107, found *m/z* 336.1124.



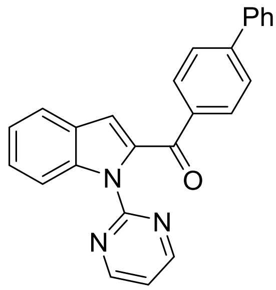
1o

(4-Ethylphenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1o).[21a] White solid. M. p. = 123 – 124 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.38 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.4 Hz, 1H), 7.29 – 7.24 (m, 3H), 7.10 (s, 1H), 7.03 (t, *J* = 4.8 Hz, 1H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H);^{13}C NMR (151 MHz, $CDCl_3$) δ 187.3, 157.9, 157.3, 149.7, 138.2, 137.3, 135.5, 129.8, 128.0, 127.8, 126.3, 122.7, 122.4, 117.3, 115.0, 114.1, 28.9, 15.2. HRMS (ESI) m/z calculated for $C_{21}H_{17}N_3NaO$ [M+Na] *m/z* 350.1264, found *m/z* 350.1263.



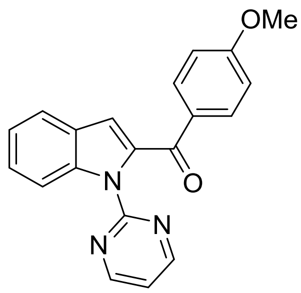
1p

(4-(tert-butyl)phenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1p).[21a] Pale yellow solid. M. p. = 190 – 192 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.8 Hz, 2H), 8.37 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 9.0 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.11 (s, 1H), 7.06 (t, *J* = 4.8 Hz, 1H), 1.35 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.2, 157.9, 157.4, 156.5, 138.3, 137.3, 135.2, 129.7, 128.0, 126.3, 125.3, 122.7, 122.4, 117.3, 115.2, 114.1, 35.1, 31.1; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{23}H_{21}N_3NaO$) requires *m/z* 378.1577, found *m/z* 378.1578.



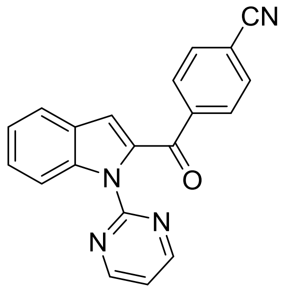
1q

[1,1'-biphenyl]-4-yl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1q).[21a] White solid. M. p. = 167 – 168 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.8 Hz, 2H), 8.42 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 2H), 7.73 – 7.62 (m, 5H), 7.49 – 7.39 (m, 4H), 7.30 – 7.28 (m, 1H), 7.16 (s, 1H), 7.06 (t, *J* = 4.8 Hz, 1H);^{13}C NMR (151 MHz, $CDCl_3$) δ 187.1, 157.9, 157.3, 145.4, 139.9, 138.2, 137.2, 136.7, 130.1, 128.9, 128.1, 128.0, 127.2, 127.0, 126.4, 122.8, 122.4, 117.3, 115.2, 114.3; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{25}H_{17}N_3NaO$) requires *m/z* 398.1264, found *m/z* 398.1271.



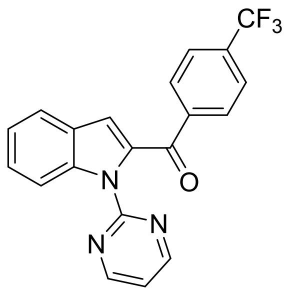
1r

(4-Methoxyphenyl)(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1r).[21a] White solid. M. p. = 116 – 117 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 8.40 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 8.4 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.07 (s, 1H), 7.05 (t, *J* = 4.8 Hz, 1H), 6.93 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.5, 163.3, 157.9, 157.3, 138.1, 137.3, 131.9, 130.8, 128.0, 126.2, 122.7, 122.3, 117.3, 114.5, 114.2, 113.6, 55.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO_2$) requires *m/z* 352.1056, found *m/z* 352.1074.



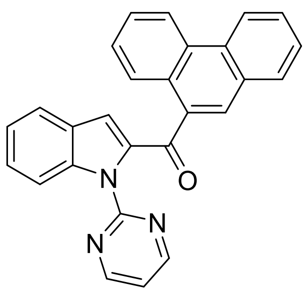
1s

4-(1-(pyrimidin-2-yl)-1H-indole-2-carbonyl)benzonitrile (1s).[21d] Yellow solid. M. p. = 155 – 157 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.45 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.72 –7.71 (m, 3H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.15 (s, 1H), 7.07 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 185.8, 158.0, 157.0, 141.5, 138.3, 136.2, 132.2, 129.5, 127.9, 127.1, 123.2, 122.6, 118.0, 117.4, 115.9, 115.7, 114.6. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{20}H_{13}N_4O$) requires *m/z* 325.1084, found *m/z* 325.1090.



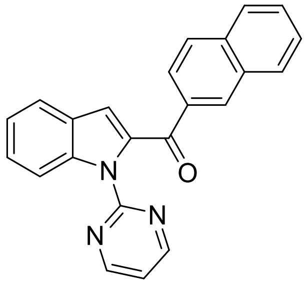
1t

(1-(pyrimidin-2-yl)-1H-indol-2-yl)(4-(trifluoromethyl)phenyl)methanone (1t).[21a] White solid. M. p. = 110 – 112 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.43 (d, *J* = 8.4 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 2H), 7.70 (t, *J* = 8.4 Hz, 3H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.30 (t, *J* = 7.2 Hz, 1H), 7.14 (s, 1H), 7.05 (t, *J* = 4.8 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9 (s, 3F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.3, 157.9, 157.1, 141.0, 138.4, 136.5, 133.9, 133.7, 129.6, 127.9, 126.9, 125.3 (q, *J* = 4.2 Hz), 123.6 (d, *J* = 270.9 Hz), 123.0, 117.4, 115.8, 114.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{12}F_3N_3NaO$) requires *m/z* 390.0825, found *m/z* 390.0835.



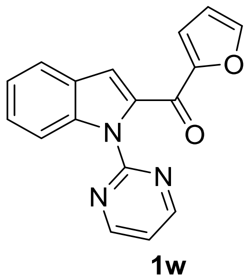
1u

Phenanthren-9-yl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1u).[21a] White solid. M. p. = 161 – 162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 – 8.75 (m, 1H), 8.67 – 8.65 (m, 1H), 8.60 (d, *J* = 8.4 Hz, 1H), 8.44 (d, *J* = 4.8 Hz, 2H), 8.42 (d, *J* = 8.4 Hz, 1H), 7.99 (s, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.63 (m, 4H), 7.52 – 7.48 (m, 1H), 7.47 – 7.43 (m, 1H), 7.31– 7.27 (m, 1H), 7.23 (d, *J* = 0.8 Hz, 1H), 6.84 (t, *J* = 4.8 Hz, 1H);^{13}C NMR (151 MHz, $CDCl_3$) δ 188.7, 157.8, 157.3, 138.8, 138.5, 135.2, 131.7, 130.7, 130.6, 129.9, 129.7, 129.3, 128.6, 128.0, 127.3, 127.1, 127.0, 126.9, 126.7, 126.6, 122.9, 122.6, 122.6, 117.3, 116.1, 114.5; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{27}H_{17}N_3NaO$) requires *m/z* 422.1264, found *m/z* 422.1258.



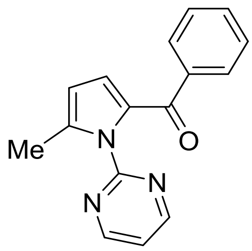
1v

Naphthalen-2-yl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1v).[21e] White solid. M. p. = 129 – 131 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.48 (s, 1H), 8.45 (d, *J* = 8.8 Hz, 1H), 8.07 (dd, *J*=8.8, 2.0 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.87 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.61–7.57 (m, 1H), 7.54–7.50 (m, 1H), 7.49–7.45 (m, 1H), 7.34–7.30 (m, 1H), 7.18 (d, *J* = 0.4 Hz, 1H), 7.07 – 6.97 (t, *J* = 4.8 Hz, 1H);^{13}C NMR (151 MHz, $CDCl_3$) δ 187.7, 157.9, 157.3, 138.2, 137.3, 135.5, 135.4, 132.4, 131.4, 129.5, 129.4, 128.3, 128.1, 127.8, 126.7, 126.4, 125.1, 122.8, 122.4, 117.3, 115.2, 114.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{23}H_{15}N_3NaO$) requires *m/z* 372.1107, found *m/z* 372.1126.



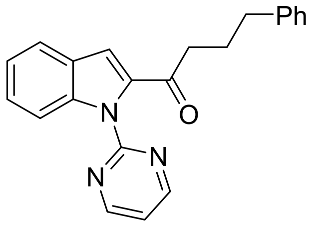
1w

Furan-2-yl(1-(pyrimidin-2-yl)-1H-indol-2-yl)methanone (1w).[21a] White solid. M. p. = 121 – 123 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.8 Hz, 2H), 8.35 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.62 (s, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.36 (s, 1H), 7.30 – 7.28 (m, 2H), 7.12 – 7.10 (m, 1H), 6.56 – 6.54 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.3, 158.0, 157.4, 152.6, 146.9, 138.5, 136.1, 127.9, 126.7, 122.8, 122.6, 119.3, 117.5, 115.2, 114.1, 112.2; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{12}N_3O_2$) requires *m/z* 290.0924, found *m/z* 290.0929.



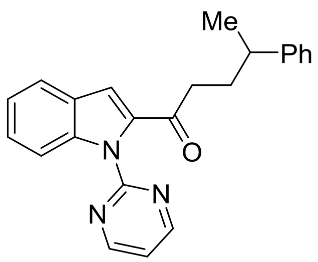
1x

(5-Methyl-1-(pyrimidin-2-yl)-1H-pyrrol-2-yl)(phenyl)methanone (1x).[21a] White solid. M. p. = 151 – 153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.8 Hz, 2H), 7.89 (d, *J* = 7.2 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 4.8 Hz, 1H), 6.81 (d, *J*=3.6 Hz, 1H), 6.11 (d, *J*=3.6 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.9, 158.5, 158.3, 139.4, 138.5, 132.4, 131.8, 129.4, 128.1, 123.0, 119.6, 109.7, 12.9. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{16}H_{13}N_3NaO$) requires *m/z* 286.0951, found *m/z* 286.0970.



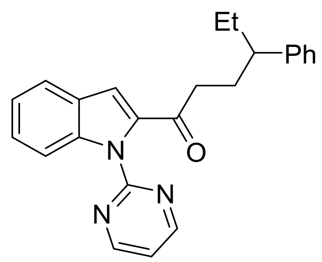
1ya

4-Phenyl-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)butan-1-one (1ya). Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.8 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.23 (q, *J* = 7.6 Hz, 3H), 7.19 – 7.13 (m, 4H), 7.05 (t, *J* = 4.8 Hz, 1H), 2.89 (t, *J* = 7.2 Hz, 2H), 2.69 (t, *J* = 7.2 Hz, 2H), 2.07 (p, *J* = 7.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 158.0, 157.6, 141.6, 138.9, 137.8, 128.3, 128.2, 127.3, 126.5, 125.7, 122.5, 122.4, 118.0, 113.3, 113.1, 39.4, 34.8, 26.0; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{19}N_3NaO$) requires *m/z* 364.1420, found *m/z* 364.1440.



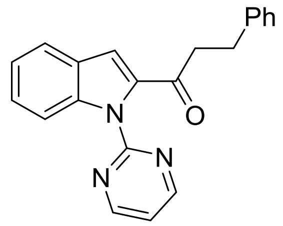
1yb

4-Phenyl-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)pentan-1-one (**1yb**). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.39-7.35 (m, 1H), 7.31 – 7.28 (m, 2H), 7.25 – 7.18 (m, 5H), 7.11 (s, 1H), 2.87 – 2.76 (m, 3H), 2.14 – 1.94 (m, 2H), 1.29 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 158.2, 157.8, 146.5, 139.1, 137.7, 128.4, 127.4, 127.1, 126.7, 126.1, 122.6, 122.5, 118.2, 113.5, 113.1, 39.3, 38.6, 32.8, 22.4. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{23}H_{22}N_3O$) requires *m/z* 356.1757, found *m/z* 356.1750.



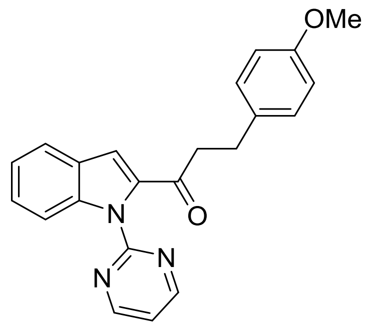
1yc

4-Phenyl-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)hexan-1-one (1yc). Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.8 Hz, 2H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.14 (m, 5H), 7.06 (s, 1H), 2.78 – 2.71 (m, 2H), 2.53 – 2.48 (m, 1H), 2.27 – 2.15 (m, 1H), 1.98 – 1.89 (m, 1H), 1.74 – 1.56 (m, 2H), 0.78 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 158.2, 157.8, 144.7, 139.1, 137.7, 128.3, 127.8, 127.4, 126.7, 126.1, 122.6, 122.5, 118.1, 113.6, 113.1, 47.1, 38.5, 31.0, 29.8, 12.1. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{24}H_{24}N_3O$) requires *m/z* 370.1914, found *m/z* 370.1926.



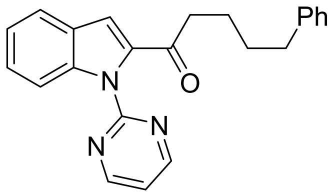
1yd

3-Phenyl-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)propan-1-one (1yd).[21f] White solid. M. p. = 60 – 63 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.8 Hz, 2H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.30 – 7.16 (m, 8H), 3.25 (t, *J*=8.0 Hz, 2H), 3.07 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 158.2, 157.8, 141.1, 139.1, 137.7, 128.4, 127.5, 126.7, 126.1, 122.6, 122.6, 118.1, 113.5, 113.3, 42.2, 30.4; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{21}H_{18}N_3O$) requires *m/z* 328.1444, found *m/z* 328.1425.



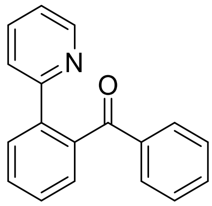
1ye

3-(4-methoxyphenyl)-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)propan-1-one (1ye). Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.8 Hz, 2H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.36 (m, 1H), 7.26 – 7.24 (m, 2H), 7.20 (t, *J* = 4.8 Hz, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.77 (s, 3H), 3.22 (t, *J* = 8.0 Hz, 2H), 3.01 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.7, 158.1, 157.8, 157.6, 139.0, 137.6, 133.0, 129.3, 127.4, 126.7, 122.6, 122.5, 118.1, 113.7, 113.5, 113.2, 55.1, 42.4, 29.4. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{22}H_{20}N_3O2$) requires *m/z* 358.1550, found *m/z* 358.1545.



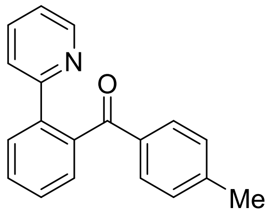
1yf

5-phenyl-1-(1-(pyrimidin-2-yl)-1H-indol-2-yl)pentan-1-one (1yf). Yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 5.2 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.38(t, *J* = 8.4 Hz, 1H), 7.28 – 7.22 (m, 4H), 7.20 – 7.15 (m, 4H), 2.94 (t, *J* = 7.2 Hz, 2H), 2.65 (t, *J* = 7.2 Hz, 2H), 1.83 – 1.65 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 158.2, 157.8, 142.3, 139.1, 137.8, 128.4, 128.2, 127.4, 126.7, 125.7, 122.6, 122.5, 118.2, 113.5, 113.2, 40.3, 35.7, 30.9, 24.3; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{23}H_{21}N_3NaO$) requires m/z 378.1577, found m/z 378.1580.



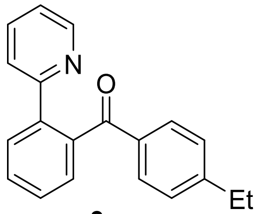
3a

Phenyl(2-(pyridin-2-yl)phenyl)methanone (3a).[21a] Yellow solid. M. p. = 106 – 108 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.36 (d, *J* = 4.2 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.57 – 7.48 (m, 4H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.26 (t, *J* = 7.8 Hz, 2H), 7.01 – 6.99 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.2, 156.8, 149.0, 139.6, 139.5, 137.9, 136.2, 132.3, 130.2, 129.4, 129.1, 128.7, 128.4, 128.0, 122.6, 121.9; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{14}NO$) requires *m/z* 260.1070, found *m/z* 260.1060.



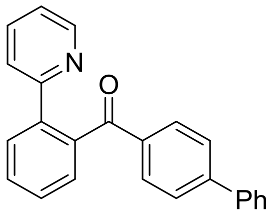
3b

(2-(Pyridin-2-yl)phenyl)(p-tolyl)methanone (3b).[21a] White solid. M. p. = 102 – 103 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.8 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.61 – 7.54 (m, 4H), 7.51 – 7.49 (m, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 7.03-7.01 (m, 1H), 2.30 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.9, 156.9, 149.0, 143.1, 139.6, 139.5, 136.2, 135.2, 130.0, 129.7, 128.9, 128.9, 128.7, 128.3, 122.9, 121.9, 21.5; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}NNaO$) requires *m/z* 296.1046, found *m/z* 296.1045.



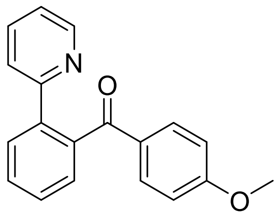
3c

(4-ethylphenyl)(2-(pyridin-2-yl)phenyl)methanone (3c).[21a] Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.4 Hz, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.61 – 7.54 (m, 2H), 7.52 – 7.46 (m, 3H), 7.09 (d, *J* = 8.4 Hz, 2H), 7.01 – 6.98 (m, 1H), 2.60 (q, *J* = 7.6 Hz, 2H), 1.17 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 156.8, 149.2, 149.0, 139.5, 139.5, 136.1, 135.3, 129.9, 129.7, 128.8, 128.8, 128.2, 127.5, 122.7, 121.8, 28.7, 15.0; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{20}H_{18}NO$) requires *m/z* 288.1383, found *m/z* 288.1386.



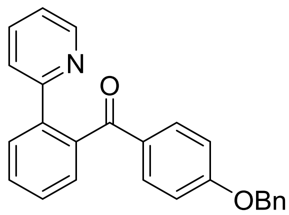
3d

[1,1'-biphenyl]-4-yl(2-(pyridin-2-yl)phenyl)methanone (3d).[21a] White solid. M. p. = 96 – 97 ^{o}C.; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 5.2 Hz, 1H), 7.78 – 7.75 (m, 3H), 7.62 – 7.45 (m, 9H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.35 (d, *J* = 7.2 Hz, 1H), 7.00 – 6.97 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.7, 156.8, 149.0, 144.8, 139.9, 139.6, 139.5, 136.6, 136.3, 130.1, 130.0, 129.0, 128.8, 128.8, 128.4, 128.0, 127.1, 126.7, 122.7, 121.9; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{24}H_{18}NO$) requires *m/z* 336.1383, found *m/z* 336.1378.



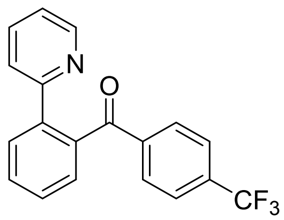
3e

(4-Methoxyphenyl)(2-(pyridin-2-yl)phenyl)methanone (3e).[21g] White solid. M. p. = 94 – 96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 4.4 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.60 – 7.55 (m, 2H), 7.50 – 7.45 (m, 3H), 7.05 – 7.01 (m, 1H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H) ; ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 163.0, 157.0, 149.1, 139.7, 139.5, 136.2, 131.9, 130.7, 129.9, 129.0, 128.8, 128.3, 122.9, 121.9, 113.3, 55.3; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{16}NO_2$) requires *m/z* 290.1176, found *m/z* 290.1178.



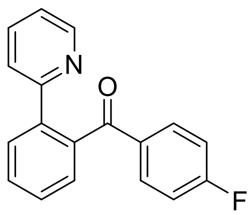
3f

(4-(Benzyloxy)phenyl)(2-(pyridin-2-yl)phenyl)methanone (3f). White solid. M. p. = 97 – 99 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, *J* = 6.0 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 9.0 Hz, 2H), 7.60 – 7.53 (m, 2H), 7.50 – 7.49 (m, 2H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 4.2 Hz, 4H), 7.34 –7.31 (m, 1H), 7.04 – 7.02 (m, 1H), 6.83 (d, *J* = 9.0 Hz, 2H), 5.04 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.0, 162.1, 157.1, 149.1, 139.6, 139.5, 136.2, 131.9, 130.9, 130.0, 129.0, 128.8, 128.6, 128.6, 128.4, 128.1, 127.4, 123.0, 121.9, 114.2, 70.0; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{25}H_{20}NO_2$) requires *m/z* 366.1489, found *m/z* 366.1499.



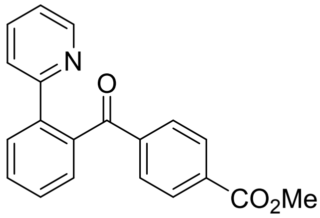
3g

(2-(pyridin-2-yl)phenyl)(4-(trifluoromethyl)phenyl)methanone (3g).[21h] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 4.8 Hz, 1H), 7.78 (t, *J* = 7.2 Hz, 3H), 7.65 – 7.62 (m, 1H), 7.61 – 7.60 (m, 1H), 7.58 – 7.51 (m, 5H), 7.03 – 7.01 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 156.1, 148.8, 141.0, 139.4, 138.8, 136.6, 133.4, 133.1, 130.5, 129.4, 129.1, 128.8, 128.4, 125.0 (q, *J* = 3.8 Hz), 122.3, 122.1; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{13}F_3NO$) requires *m/z* 328.0944, found *m/z* 328.0943.



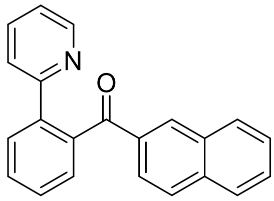
3h

(4-Fluorophenyl)(2-(pyridin-2-yl)phenyl)methanone (3h).[21i] Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 4.8 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.70 (dd, *J* = 8.8, 5.6 Hz, 2H), 7.63 – 7.56 (m, 2H), 7.53 – 7.49 (m, 3H), 7.05 – 7.01 (m, 1H), 6.93 (t, *J* = 8.8 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -106.1 (s, 1F); ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 163.9, 156.6, 149.0, 139.5, 139.2, 136.4, 134.4 (d, *J* = 3.0 Hz), 132.0 (d, *J* = 9.0 Hz), 130.3, 129.8, 129.0, 128.7, 128.6, 122.3 (d, *J* = 57.5 Hz), 115.1 (d, *J* = 21.8 Hz); HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{13}FNO$) requires *m/z* 278.0976, found *m/z* 278.0979.



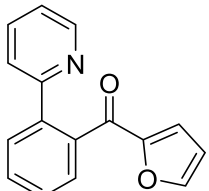
3i

Methyl 4-(2-(pyridin-2-yl)benzoyl)benzoate (3i).[21i] Yellow solid. M. p. = 101 – 103 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 4.8 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 7.7, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.59 – 7.53 (m, 4H), 7.00 – 6.97 (m, 1H), 3.89 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.4, 166.3, 156.2, 148.8, 141.6, 139.4, 139.0, 136.5, 132.8, 130.4, 129.2, 128.9, 128.7, 128.4, 122.2, 122.1, 52.3; ; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{20}H_{16}NO_3$) requires *m/z* 318.1125, found *m/z* 318.1136.



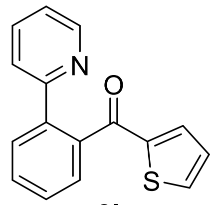
3j

Naphthalen-2-yl(2-(pyridin-2-yl)phenyl)methanone (3j).[21a] White solid. M. p. = 112 – 113 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (d, *J* = 4.8 Hz, 1H), 8.07 (s, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.76-7.73 (m, 3H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.58 (d, *J*=6.6 Hz, 1H), 7.4 – 7.45 (m, 4H), 7.41 (t, *J* = 6.6 Hz, 1H), 6.90–6.87 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.0, 156.7, 148.9, 139.6, 139.6, 136.2, 135.3, 135.1, 132.1, 131.4, 130.1, 129.3, 129.0, 128.7, 128.4, 128.0, 127.9, 127.5, 126.3, 124.9, 122.4, 121.8; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{22}H_{16}NO$) requires *m/z* 310.1226, found *m/z* 310.1219.



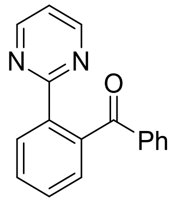
3k

Furan-2-yl(2-(pyridin-2-yl)phenyl)methanone (3k).[21a] White solid. M. p. = 85 – 86 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.47 (d, *J* = 4.8 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.66 – 7.59 (m, 3H), 7.54 – 7.50 (m, 2H), 7.42 – 7.41 (m, 1H), 7.09 (dd, *J* = 7.2, 4.4 Hz, 1H), 6.80 (d, *J* = 3.6 Hz, 1H), 6.33 (dd, *J* = 3.6, 1.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 185.3, 157.0, 152.8, 149.2, 146.5, 139.7, 138.3, 136.4, 130.6, 129.1, 129.0, 128.4, 122.7, 121.9, 119.3, 111.9; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{16}H_{11}NNaO_2$) requires *m/z* 272.0682, found *m/z* 272.0695.



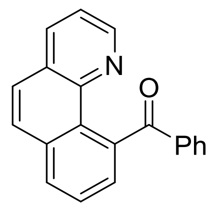
3l

(2-(pyridin-2-yl)phenyl)(thiophen-2-yl)methanone(3l).[21h] White solid. M. p. = 100 – 102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.8 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.62 – 7.58 (m, 3H), 7.53 – 7.50 (m, 3H), 7.19 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.08 – 7.05 (m, 1H), 6.88 (dd, *J* = 4.8, 4.0 Hz, 1H);^{13}C NMR (101 MHz, $CDCl_3$) δ 190.4, 156.9, 149.2, 145.0, 139.3, 139.1, 136.3, 134.5, 133.8, 130.4, 129.2, 128.7, 128.4, 127.7, 122.9, 122.0; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{16}H_{11}NOS$) requires *m/z* 266.0634, found *m/z* 266.0634.



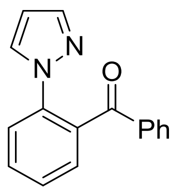
3m

Phenyl(6-(pyrimidin-2-yl)cyclohexa-1,3-dien-1-yl)methanone (3m).[21j] White solid. M. p. = 125 – 127 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.8 Hz, 2H), 8.36 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.2 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.60 – 7.57 (m, 1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 2H), 6.96 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.8, 163.9, 156.5, 140.5, 138.1, 136.9, 132.1, 130.2, 129.9, 129.3, 129.0, 128.5, 128.1, 118.7; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{16}NO_3$) requires *m/z* 283.0842, found *m/z* 283.0856.



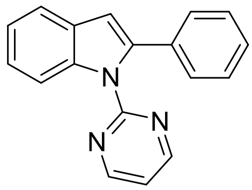
3n

Benzo[*h*]quinolin-10-yl(phenyl)methanone (3n).[21j] White solid. M. p. = 149 – 151 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 9.0 Hz, 1H), 7.76 (t, *J* = 7.8 Hz, 3H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.5, 147.0, 144.6, 139.2, 138.9, 135.2, 133.7, 131.6, 129.1, 128.9, 128.6, 128.0, 127.7, 127.6, 126.9, 126.3, 126.0, 121.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{13}NNaO$) requires *m/z* 306.0889, found *m/z* 306.0908.



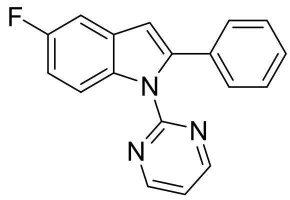
3o

(6-(1H-Pyrazol-1-yl)cyclohexa-1,3-dien-1-yl)(phenyl)methanone (3o).[21j] White solid. M. p. = 85 – 87 °C. NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.55 (m, 6H), 7.49 – 7.38 (m, 3H), 7.28 (t, J = 4.0 Hz, 2H), 6.16 (t, J = 2.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 141.1, 138.5, 136.7, 133.8, 132.8, 131.2, 129.7, 129.5, 129.0, 128.1, 127.4, 123.2, 107.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{16}H_{12}N_2NaO$) requires *m/z* 271.0842, found *m/z* 271.0861.



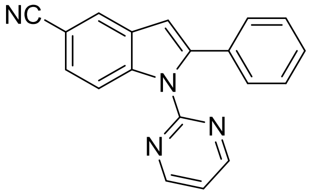
2a

2-Phenyl-1-(pyrimidin-2-yl)-1H-indole (2a).[21a] Pale yellow solid (25.2 mg, 93% yield). M. p. = 122 – 124 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.65 (d, J = 4.8 Hz, 2H), 8.13 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.37 – 7.19 (m, 7H), 7.09 (t, J = 4.8 Hz, 1H), 6.80 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 158.1, 140.5, 138.1, 134.0, 129.3, 128.1, 128.1, 127.1, 123.5, 122.1, 120.7, 117.6, 112.8, 108.2. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{18}H_{13}N_3Na$) requires *m/z* 294.1002, found *m/z* 294.0997. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 7/1).



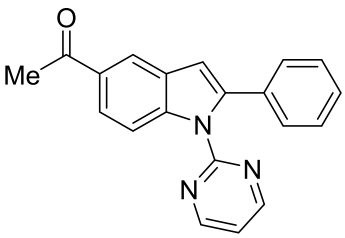
2b

5-Fluoro-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2b). Yellow solid (25.9 mg, 90% yield). M. p. = 128 – 129 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, J = 4.8 Hz, 2H), 8.09 (dd, J = 9.0, 4.8 Hz, 1H), 7.36 – 7.25 (m, 6H), 7.10 (t, J = 4.8 Hz, 1H), 7.00 (td, J = 9.0, 2.4 Hz, 1H), 6.74 (s, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -121.9 (s, 1F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.9, 158.3, 158.2, 157.9, 142.1, 134.5, 133.7, 129.9 (d, J = 9.9 Hz), 128.1 (d, J=3.3 Hz), 127.4, 117.7, 113.9 (d, J = 9.6 Hz), 111.3 (d, J = 25.1 Hz), 107.9 (d, J = 3.6 Hz), 105.8 (d, J = 23.8 Hz). HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{18}H_{13}FN_3Na$) requires *m/z* 312.0907, found *m/z* 312.0887. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



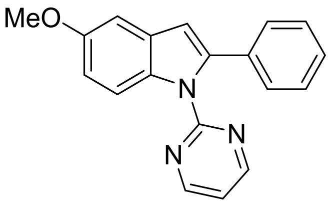
2c

2-Phenyl-1-(pyrimidin-2-yl)-1H-indole-5-carbonitrile (2c).[21j] Yellow solid (24.6 mg, 83% yield). M. p. = 166 – 168 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.8 Hz, 2H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.98 (s, 1H), 7.51 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.34 – 7.30 (m, 3H), 7.28 – 7.25 (m, 2H), 7.21 (t, *J* = 4.8 Hz, 1H), 6.83 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.5, 157.4, 142.9, 139.5, 132.8, 129.1, 128.3, 128.2, 127.9, 126.4, 125.7, 120.2, 118.6, 113.7, 107.3, 105.2, HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{12}N_4Na$) requires *m/z* 319.0954, found *m/z* 319.0952. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 4/1).



2d

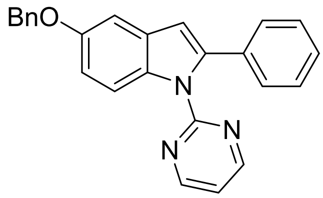
1-(2-Phenyl-1-(pyrimidin-2-yl)-1H-indol-5-yl)ethan-1-one (2d). White solid (25.3 mg, 81% yield). M. p. = 137– 139 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.8 Hz, 2H), 8.31 (s, 1H), 8.12 (d, *J* = 9.0 Hz, 1H), 7.94 (dd, *J* = 9.0, 1.7 Hz, 1H), 7.32 – 7.26 (m, 5H), 7.19 (t, *J* = 4.8 Hz, 1H), 6.88 (s, 1H), 2.69 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 198.0, 158.4, 157.7, 142.1, 140.5, 133.3, 131.8, 128.9, 128.2, 127.5, 123.7, 122.3, 118.2, 112.6, 108.5, 26.7. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO$) requires *m/z* 336.1107, found *m/z* 336.1101. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 2/1).



2e

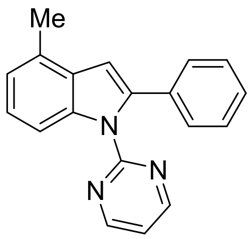
5-Methoxy-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2e).[21f] Yellow solid (25.6 mg, 85% yield). M. p. = 125 – 126 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.30 – 7.26 (m, 5H), 7.10 (d, *J* = 2.4 Hz, 1H), 7.06 (t, *J* = 4.8 Hz, 1H), 6.92 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.73 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.1, 158.0, 155.6, 141.0, 134.1, 133.1, 130.0, 128.1, 128.0, 127.1, 117.3, 113.9, 112.9, 108.2, 102.7, 55.7. HRMS (ESI+) exact mass calculated for

$[M+Na]^+$ ($C_{19}H_{15}N_3NaO$) requires *m/z* 324.1107, found *m/z* 324.1092. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 7/1).



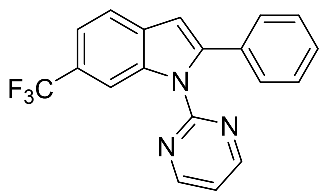
2f

5-(Benzyloxy)-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2f).[21f] Pale yellow solid (32.8, 87% yield). M. p. = 155 – 156 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.08 (d, *J* = 9.0 Hz, 1H), 7.47 (d, *J* = 7.2 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 2H), 7.32 – 7.25 (m, 6H), 7.18 (d, *J* = 2.4 Hz, 1H), 7.04 (t, *J* = 4.8 Hz, 1H), 6.99 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.71 (s, 1H), 5.13 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2 158.1, 154.8, 141.1, 137.5, 134.0, 133.2, 130.0, 128.5, 128.1, 128.0, 127.8, 127.5, 127.1, 117.3, 113.9, 113.6, 108.2, 104.3, 70.7. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{25}H_{19}N_3NaO$) requires *m/z* 400.1420, found *m/z* 400.1411. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 6/1).



2g

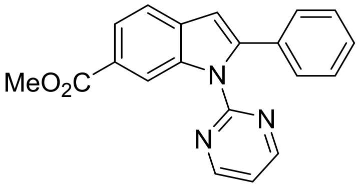
4-Methyl-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2g).[21a] Yellow solid (21.7 mg, 76% yield). M. p. = 165 – 166 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.30 – 7.24 (m, 5H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 4.8 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.83 (s, 1H), 2.59 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3, 158.2, 139.9, 137.9, 134.1, 130.1, 129.0, 128.1, 128.1, 127.0, 123.6, 122.4, 117.5, 110.4, 106.7, 18.6. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}N_3Na$) requires *m/z* 308.1158, found *m/z* 308.1149. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



2h

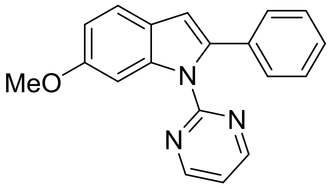
2-Phenyl-1-(pyrimidin-2-yl)-6-(trifluoromethyl)-1H-indole (2h). Yellow oil (28.8 mg, 85% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.8 Hz, 2H), 8.42 (s, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.33 – 7.28 (m, 5H), 7.16 (t, *J* = 4.8 Hz, 1H), 6.83 (s, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.5 (s, 3F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.4, 157.7, 143.2, 137.0, 133.3, 131.7, 128.3

(d, J = 8.7 Hz), 127.7, 125.4, 125.2, 125.1 (d, J = 270.1 Hz), 120.9, 118.8 (d, J = 3.5 Hz), 118.2, 110.6 (d, J = 4.7 Hz), 107.6; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{12}F_3N_3Na$) requires m/z 362.0876, found m/z 362.0865. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



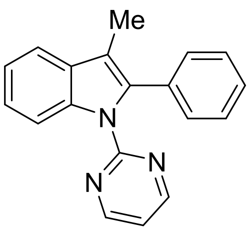
2i

Methyl 2-phenyl-1-(pyrimidin-2-yl)-1H-indole-6-carboxylate (2i). White solid (26.8 mg, 82% yield). M. p. = 207 – 209 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.72 (d, J = 4.8 Hz, 2H), 7.94 (dd, J = 8.4, 1.2 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.32 – 7.28 (m, 5H), 7.18 (t, J = 4.8 Hz, 1H), 6.83 (s, 1H), 3.94 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.9, 158.5, 157.7, 143.6, 137.4, 133.2, 132.9, 128.3, 128.2, 127.7, 125.0, 123.2, 120.2, 118.2, 114.9, 107.7, 52.0. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{15}N_3NaO_2$) requires m/z 352.1056, found m/z 352.1046. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 4/1).



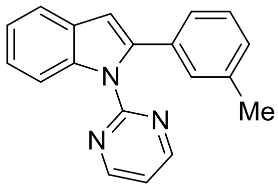
2j

6-Methoxy-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2j). White solid (24.9 mg, 83% yield). M. p. = 154 – 156 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, J = 5.4 Hz, 2H), 7.74 (d, J = 2.4 Hz, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.29 – 7.23 (m, 5H), 7.09 (t, J = 4.8 Hz, 1H), 6.89 (dd, J=8.4, 2.4 Hz, 1H), 6.73 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 158.2, 158.1, 139.5, 139.1, 134.1, 128.1, 127.8, 126.7, 123.5, 121.1, 117.4, 111.2, 108.2, 97.2, 55.7. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}N_3NaO$) requires m/z 324.1107, found m/z 324.1109. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 7/1).



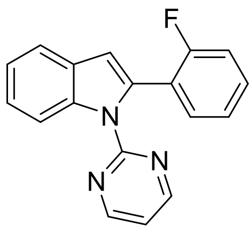
2k

3-Methyl-2-phenyl-1-(pyrimidin-2-yl)-1H-indole (2k).[21a] Yellow solid (24.8 mg, 87% yield). M. p. = 139 – 140 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.56 (d, J = 4.8 Hz, 2H), 8.19 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 7.8 Hz, 1H), 7.34 – 7.29 (m, 3H), 7.28 – 7.23 (m, 4H), 6.98 (t, J = 4.8 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.1, 157.9, 136.9, 135.9, 133.8, 130.5, 129.6, 127.8, 126.7, 123.7, 121.7, 118.9, 116.9, 115.0, 112.9, 9.4. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}N_3Na$) requires *m/z* 308.1158, found *m/z* 308.1149. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



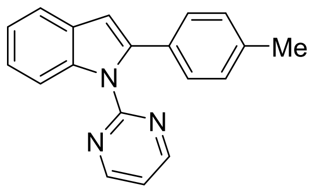
2l

1-(Pyrimidin-2-yl)-2-(m-tolyl)-1H-indole (2l). Yellow solid (25.4 mg, 89% yield). M. p. = 115 – 117 ^oC. ^1H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.20 (m, 3H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.10 – 7.06 (m, 2H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.79 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2,1 158.1, 140.6, 138.1, 137.8, 133.7, 129.3, 128.7, 127.9, 127.9, 125.3, 123.4, 122.0, 120.6, 117.5, 112.7, 108.0, 21.4. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{16}N_3$) requires *m/z* 286.1339, found *m/z* 286.1329. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



2m

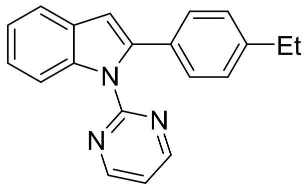
2-(2-fluorophenyl)-1-(pyrimidin-2-yl)-1H-indole (2m). Yellow oil (13.8 mg, 48% yield). ^1H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.8 Hz, 2H), 8.33 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.53 (td, *J* = 7.8, 1.8 Hz, 1H), 7.34 – 7.28 (m, 2H), 7.26 – 7.23 (m, 1H), 7.20 (t, *J* = 7.2 Hz, 1H), 7.09 (t, *J* = 4.8 Hz, 1H), 6.96 – 6.93 (m, 1H), 6.82 (s, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.5 (s, 1F); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 158.1, 158.0, 137.5, 134.6, 130.5(d, *J* = 3.6 Hz), 129.3 (d, *J* = 8.0 Hz), 129.1, 124.1 (d, *J* = 3.6 Hz), 123.9, 123.0, 122.1, 120.7, 117.3, 115.2 (d, *J* = 22.0 Hz), 113.6, 109.6. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{18}H_{12}FN_3Na$) requires *m/z* 312.0907, found *m/z* 312.0912. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



2n

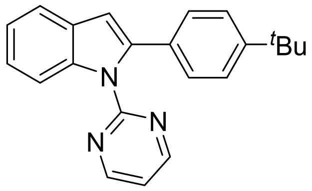
1-(Pyrimidin-2-yl)-2-(p-tolyl)-1H-indole (2n).Yellow solid (25.8 mg, 91% yield). M. p. = 119 – 121 ^oC. ^1H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.21 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.10 – 7.07 (m, 3H), 6.77 (s, 1H), 2.34 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 140.5, 138.0, 136.9, 131.0, 129.4, 128.8, 128.0, 123.3, 122.0, 120.5, 117.6, 112.7, 107.7, 21.2. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}N_3Na$) requires *m/z* 308.1158, found *m/z* 308.1160. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



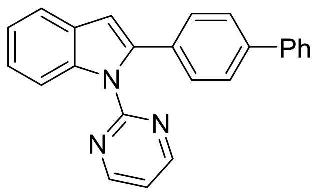
2o

2-(4-Ethylphenyl)-1-(pyrimidin-2-yl)-1H-indole (2o).[21a] Pale Yellow solid (24.4 mg, 82% yield). M. p. = 120 – 122 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, J = 4.8 Hz, 2H), 8.10 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 7.2 Hz, 1H), 7.28 – 7.24 (m, 4H), 7.13 – 7.08 (m, 3H), 6.77 (s, 1H), 2.65 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 152.4, 143.2, 140.6, 138.0, 131.2, 129.4, 128.1, 127.6, 123.3, 122.0, 120.5, 117.6, 112.7, 107.7, 28.5, 15.3. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{17}N_3Na$) requires *m/z* 322.1315, found *m/z* 322.1306. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



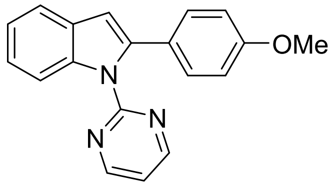
2p

2-(4-(tert-Butyl)phenyl)-1-(pyrimidin-2-yl)-1H-indole (2p). Yellow solid (27.2 mg, 83% yield). M. p. = 117 – 118 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, J = 4.8 Hz, 2H), 8.10 (d, J = 8.4 Hz, 1H) 7.63 (d, J = 7.2 Hz, 1H), 7.31 (d, J = 8.4 Hz, 2H), 7.28 – 7.20 (m, 4H), 7.10 (t, J = 4.8 Hz, 1H), 6.78 (s, 1H), 1.32 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3,158.2, 150.1, 140.5, 138.1, 130.8, 129.4, 127.7, 125.1, 123.3, 122.0, 120.5, 117.6, 112.6, 107.8, 34.5, 31.3. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{21}N_3Na$) requires *m/z* 350.1628, found *m/z* 350.1618. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



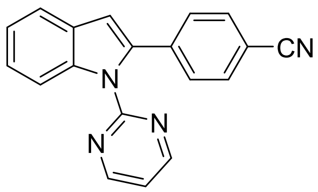
2q

2-([1,1'-Biphenyl]-4-yl)-1-(pyrimidin-2-yl)-1H-indole (2q).[21a] White solid (30.2 mg, 87% yield). M. p. = 100 – 102 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.68 (d, J = 4.8 Hz, 2H), 8.15 (d, J = 8.4 Hz, 1H), 7.65 (d, J = 7.8 Hz, 1H), 7.60 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.36 – 7.23 (m, 5H), 7.10 (t, J = 4.8 Hz, 1H), 6.86 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 158.2, 140.6, 140.1, 139.8, 138.2, 132.9, 129.4, 128.8, 128.5, 127.3, 126.9, 126.8, 123.6, 122.2, 120.7, 117.6, 112.8, 108.3. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{24}H_{17}N_3Na$) requires *m/z* 370.1315, found *m/z* 370.1320. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



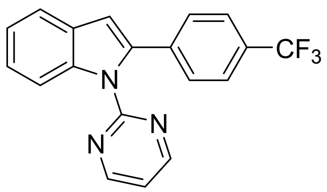
2r

2-(4-Methoxyphenyl)-1-(pyrimidin-2-yl)-1H-indole (2r).[21a] White solid (26.6 mg, 88% yield). M. p. = 134 – 135 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.27 – 7.19 (m, 4H), 7.09 (t, *J* = 4.8 Hz, 1H), 6.83 (d, *J* = 9.0 Hz, 2H), 6.73 (s, 1H), 3.80 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.9, 158.2, 158.1, 140.3, 137.9, 137.1, 129.4, 126.5, 123.2, 122.0, 120.4, 117.5, 113.6, 112.6, 107.2, 55.2. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{15}N_3NaO$) requires *m/z* 324.1107, found *m/z* 324.1106. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 7/1).



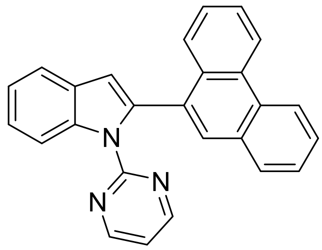
2s

4-(1-(Pyrimidin-2-yl)-1H-indol-2-yl)benzonitrile (2s).[21m] Yellow solid (20.1 mg, 68% yield). M. p. = 155– 157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 8.24 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.32 – 7.25 (m, 2H), 7.14 (t, *J* = 4.8 Hz, 1H), 6.88 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 158.0, 157.8, 138.8, 138.5, 138.3, 131.8, 129.0, 128.5, 124.6, 122.6, 121.1, 118.9, 117.7, 113.3, 110.4. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{12}N_4Na$) requires *m/z* 319.0954, found *m/z* 319.0945. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 5/1).



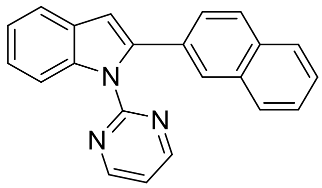
2t

1-(Pyrimidin-2-yl)-2-(4-(trifluoromethyl)phenyl)-1H-indole (2t).[21a] Yellow solid (23.7 mg, 70% yield). M. p. = 77 – 78 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 2H), 8.21 (d, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.13 (t, *J* = 4.8 Hz, 1H), 6.86 (s, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.3 (s, 3F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3, 157.9, 138.9, 138.3, 137.7, 129.1, 129.0, 128.2, 125.1, 125.0 (d, *J* = 4.2 Hz), 123.4 (d, *J* = 268.0 Hz), 123.3, 121.0, 117.7, 113.2, 109.6. HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{13}F_3N_3$) requires *m/z* 340.1056, found *m/z* 340.1069. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



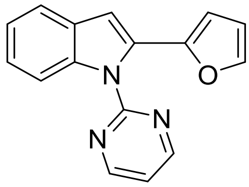
2u

2-(Phenanthren-9-yl)-1-(pyrimidin-2-yl)-1H-indole (2u).[21a] White solid (34.5 mg, 93% yield). M. p. = 110 – 112 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (t, *J* = 8.4 Hz, 2H), 8.41 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 4.8 Hz, 2H), 7.87 (d, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.65 (t, *J* = 8.4 Hz, 1H), 7.59 (t, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 6.91 (s, 1H), 6.76 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.8, 157.7, 138.9, 137.1, 131.6, 131.6, 130.2, 130.0, 129.4, 128.9, 128.9, 128.2, 126.7, 126.7, 126.5, 126.2, 126.1, 123.6, 122.6, 122.5, 122.2, 120.6, 116.8, 113.9, 109.8; HRMS (ESI) m/z calculated for $[M+Na]^+$($C_{26}H_{17}N_3Na$) equires *m/z* 394.1315, found *m/z* 394.1309. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 12/1).



2v

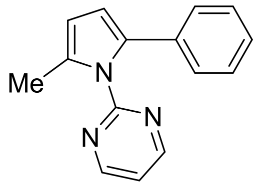
2-(Naphthalen-2-yl)-1-(pyrimidin-2-yl)-1H-indole (2v).[21m] White solid (28.7 mg, 90% yield). M. p. = 141– 142 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.8 Hz, 2H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.88 (s, 1H), 7.80 – 7.77 (m, 2H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.47 – 7.43 (m, 2H), 7.32 – 7.23 (m, 3H), 7.04 (t, *J* = 4.8 Hz, 1H), 6.91 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.2, 158.2, 140.5, 138.2, 133.3, 132.4, 131.6, 129.4, 128.1, 127.6, 127.4, 126.6, 126.5, 126.2, 126.0, 123.6, 122.2, 120.7, 117.5, 113.0, 108.8; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{15}N_3Na$) requires *m/z* 344.1158, found *m/z* 344.1151. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



2w

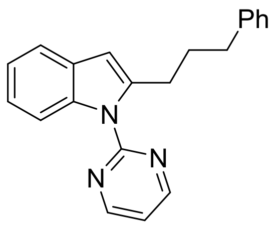
2-(Furan-2-yl)-1-(pyrimidin-2-yl)-1H-indole (2w).[21a] Yellow oil (23.4 mg, 90% yield). M. p. = 123 – 124 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.8 Hz, 2H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.63 (d, *J* =

7.6 Hz, 1H), 7.34 – 7.21 (m, 3H), 7.15 (t, J = 4.8 Hz, 1H), 6.92 (s, 1H), 6.46 – 6.42 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 157.9, 147.5, 142.1, 137.7, 130.2, 128.9, 124.0, 122.2, 120.8, 117.8, 113.0, 111.1, 108.3, 108.0; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{16}H_{11}N_3NaO$) requires m/z 284.0794, found m/z 284.0785. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 7/1).



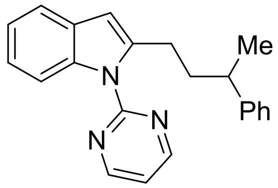
2x

2-(2-Methyl-5-phenyl-1H-pyrrol-1-yl)pyrimidine (2x).[21a] Yellow oil (11.9 mg, 51% yield). M. p. = 56 – 57 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (d, J = 4.8 Hz, 2H), 7.18 – 7.15 (m, 3H), 7.11 (t, J = 7.2 Hz, 1H), 7.02 (d, J = 7.2 Hz, 2H), 6.32 (d, J = 3.0 Hz, 1H), 6.08 (d, J = 3.0 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.5, 158.3, 134.3, 134.1, 132.3, 128.0, 127.3, 125.8, 118.6, 110.8, 109.3, 13.7; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{15}H_{13}N_3Na$) requires m/z 258.1002, found m/z 258.1001. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



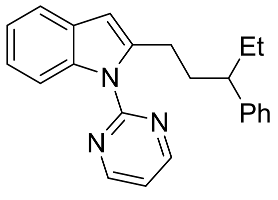
2ya

2-(3-Phenylpropyl)-1-(pyrimidin-2-yl)-1H-indole (2ya). Colorless oil (16.3 mg, 52% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (d, J = 4.8 Hz, 2H), 8.23 (d, J = 8.4 Hz, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.28 – 7.25 (m, 2H), 7.22 – 7.15 (m, 5H), 7.11 (t, J = 4.8 Hz, 1H), 6.48 (s, 1H), 3.21 (t, J = 7.2 Hz, 2H), 2.69 (t, J = 7.2 Hz, 2H), 1.96 (p, J =7.2 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3, 158.1, 142.3, 141.8, 137.0, 129.3, 128.5, 128.3, 125.7, 122.5, 121.7, 119.6, 117.0, 113.7, 105.8, 35.6, 30.9, 28.9; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{21}H_{19}N_3Na$) requires m/z 336.1471, found m/z 336.1464. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 20/1).



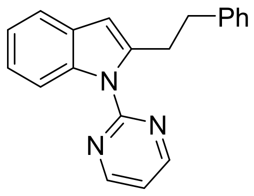
2yb

2-(3-phenylbutyl)-1-(pyrimidin-2-yl)-1H-indole (2yb). Colorless oil (18.6 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, J = 4.8 Hz, 2H), 8.21 (d, J = 7.6 Hz, 1H), 7.52 – 7.50 (m, 1H), 7.28 (t, J = 7.6 Hz, 2H), 7.20 – 7.16 (m, 5H), 7.09 (t, J = 4.8 Hz, 1H), 6.43 (s, 1H), 3.08 (t, J = 8.0 Hz, 2H), 2.79 – 2.72 (m, 1H), 1.95 – 1.85 (m, 2H), 1.25 (d, J = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 158.0, 147.2, 142.0, 136.9, 129.3, 128.3, 127.1, 125.9, 122.4, 121.7, 119.6, 117.0, 113.6, 105.7, 39.7, 38.0, 27.5, 22.3. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{21}N_3Na$) requires *m/z* 350.1628, found *m/z* 350.1627. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 30/1).



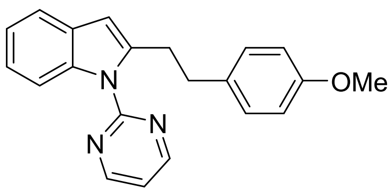
2yc

2-(3-phenylpentyl)-1-(pyrimidin-2-yl)-1H-indole (2yc). Colorless oil (20.6 mg, 61% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.8 Hz, 2H), 8.20 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.50 (m, 1H), 7.27 (t, *J* = 7.2 Hz, 2H), 7.22 – 7.16 (m, 3H), 7.13-7.11 (m, 2H), 7.08 (t, *J* = 4.8 Hz, 1H), 6.42 (s, 1H), 3.05 – 2.96 (m, 1H), 2.51-2.44 (m, 1H), 2.28 – 2.19 (m, 1H), 1.98 – 1.83 (m, 2H), 1.69 – 1.54 (m, 2H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 158.0, 145.4, 142.2, 136.9, 129.3, 128.2, 127.8, 125.9, 125.8, 122.3, 121.7, 119.6, 116.9, 113.6, 47.6, 36.2, 29.6, 27.4, 12.1. HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{23}H_{23}N_3Na$) requires *m/z* 346.1784, found *m/z* 364.1791. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 30/1).



2yd

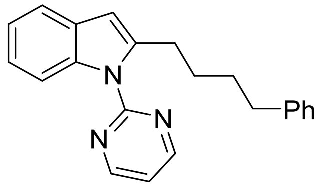
2-Phenethyl-1-(pyrimidin-2-yl)-1H-indole (2yd). White solid (15.6 mg, 52% yield). M. p. = 91 – 93 ^oC. ^1H NMR (600 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.8 Hz, 2H), 8.28 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.24 – 7.17 (m, 5H), 7.13 (t, *J* = 4.8 Hz, 1H), 6.50 (s, 1H), 3.80 (t, *J* = 7.8 Hz, 2H), 2.98 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.3, 158.1, 141.8, 141.4, 136.9, 129.3, 128.4, 128.3, 125.9, 122.6, 121.8, 119.7, 117.0, 113.9, 106.0, 35.8, 31.5; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{20}H_{17}N_3Na$) requires *m/z* 322.1315, found *m/z* 322.1302. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 20/1).



2ye

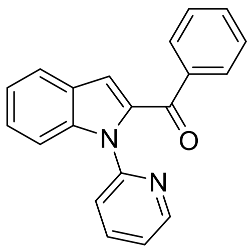
2-(4-methoxyphenethyl)-1-(pyrimidin-2-yl)-1H-indole (2ye). Colorless oil (13.8 mg, 42% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.8 Hz, 2H), 8.27 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 6.8 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.19 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.16 (t, *J* = 4.8 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 6.49 (s, 1H), 3.79 (s, 3H), 3.44 (t, *J* = 7.6 Hz, 2H), 2.92 (t, *J* = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 158.2, 157.8, 141.4, 136.9, 133.9, 129.3, 129.3, 122.6, 121.8, 119.7, 117.0, 113.8, 113.7, 105.9, 55.2, 34.8, 31.8. HRMS (ESI+) exact mass calculated for

[M+Na]$^+$ ($C_{21}H_{19}N_3NaO$) requires *m/z* 352.1420, found *m/z* 352.1420. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 15/1).



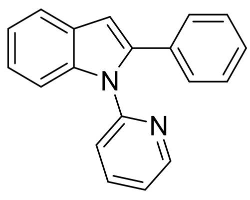
2yf

2-(4-phenylbutyl)-1-(pyrimidin-2-yl)-1H-indole (2yf). Colorless oil (19.5 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2H), 8.21 (d, *J* = 8.0 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.20 – 7.10 (m, 6H), 6.44 (s, 1H), 3.18 (t, *J* = 7.2 Hz, 2H), 2.62 (t, *J* = 7.2 Hz, 2H), 1.73 – 1.64 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 158.1, 142.5, 142.0, 136.9, 129.3, 128.4, 128.2, 125.6, 122.4, 121.7, 119.6, 117.0, 113.6, 105.5, 35.7, 31.2, 29.2, 28.6; HRMS (ESI+) exact mass calculated for [M+Na]$^+$ ($C_{22}H_{21}N_3Na$) requires *m/z* 350.1628, found *m/z* 350.1610. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 20/1).



1a-1

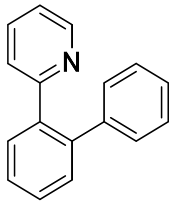
Phenyl(1-(pyridin-2-yl)-1H-indol-2-yl)methanone (1a-1) [21a]**.** White solid. M. p. = 95 – 96 ^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (d, *J* = 3.6 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 2H), 7.83 (t, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 2H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.23 – 7.19 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.8, 151.4, 149.2, 139.6, 138.1, 138.0, 135.9, 132.5, 129.8, 128.2, 126.8, 126.5, 122.9, 122.2, 121.9, 121.0, 116.0, 111.5. HRMS (ESI+) exact mass calculated for [M+Na]$^+$ ($C_{20}H_{14}N_2NaO$) requires *m/z* 321.0998, found *m/z* 321.1002.



2a-1

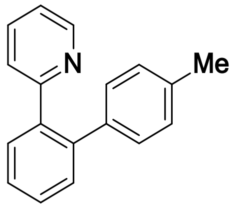
2-Phenyl-1-(pyridin-2-yl)-1H-indole (2a-1). Yellow solid (19.9 mg, 74%). M. p. = 122 – 124 ^{o}C. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.63 (d, *J* = 3.6 Hz, 1H), 7.67 (t, *J* = 7.8 Hz, 2H), 7.61 (td, *J* = 7.8, 1.8 Hz, 1H), 7.28 – 7.22 (m, 5H), 7.21 – 7.18 (m, 3H), 6.89 (d, *J* = 8.4 Hz, 1H), 6.80 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 152.1, 149.2, 140.0, 138.5, 137.7, 132.7, 128.7, 128.7, 128.3, 127.4, 123.0, 122.0, 121.6, 121.3, 120.6, 111.5, 105.6; HRMS (ESI+) exact mass calculated for [M+Na]$^+$ ($C_{19}H_{14}N_2Na$)

requires *m/z* 293.1049, found *m/z* 293.1037. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



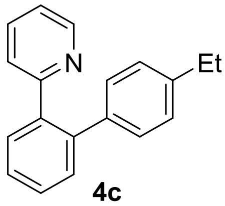
4a

2-([1,1'-biphenyl]-2-yl)pyridine (4a). White solid (20.8 mg, 90% yield). M. p. = 87 – 89 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 1H), 7.71 – 7.68 (m, 1H), 7.49 – 7.42 (m, 3H), 7.37 (td, *J* = 8.0, 1.6 Hz, 1H), 7.24 – 7.21 (m, 3H), 7.17 – 7.14 (m, 2H), 7.11 – 7.07 (m, 1H), 6.88 (d, *J*=8.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 149.4, 142.6, 141.3, 140.6, 139.5, 135.1, 130.5, 129.7, 128.5, 128.0, 127.6, 126.7, 125.4, 121.3; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{14}N$) requires *m/z* 232.1121, found *m/z* 232.1123. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



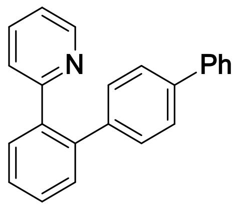
4b

2-(4'-Methyl-[1,1'-biphenyl]-2-yl)pyridine (4b). White solid (22.1 mg, 90% yield). M. p. = 54 – 56 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.2 Hz, 1H), 7.69 – 7.67 (m, 1H), 7.45 – 7.10 (m, 3H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.26 (s, 1H), 7.11 – 7.09 (m, 1H), 7.04 (s, 3H), 6.90 (d, *J* = 7.9 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.4, 149.4, 140.5, 139.4, 138.4, 136.3, 135.2, 130.5, 130.5, 129.5, 128.8, 128.5, 127.4, 125.4, 121.2, 21.1; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{16}N$) requires *m/z* 246.1277, found *m/z* 246.1279. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



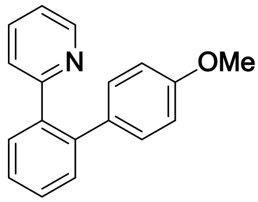
4c

2-(4'-ethyl-[1,1'-biphenyl]-2-yl)pyridine (4c). Colorless oil (20.6 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.0 Hz, 1H), 7.70 – 7.68 (m, 1H), 7.46 – 7.42 (m, 3H), 7.38 (td, J = 8.0, 2.0 Hz, 1H), 7.11 – 7.08 (m, 1H), 7.07 – 7.04(m, 4H), 6.89 (dt, *J* = 7.6, 1.2 Hz, 1H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 149.4, 142.7, 140.5, 139.3, 138.5, 135.1, 130.5, 130.4, 129.6, 128.5, 127.5, 127.4, 125.4, 121.2, 28.4, 15.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{17}NNa$) requires m/z 282.1253, found m/z 282.1256. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



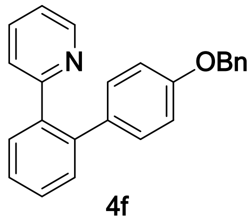
4d

2-([1,1':4',1''-terphenyl]-2-yl)pyridine (4d). White solid (25.1 mg, 82% yield). M. p. = 149 – 150 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, J = 4.8 Hz, 1H), 7.72 – 7.70 (m, 1H), 7.59 (d, J = 7.8 Hz, 2H), 7.53 – 7.46 (m, 5H), 7.44 – 7.39 (m, 3H), 7.34 – 7.32 (m, 1H), 7.25 – 7.22 (m, 2H), 7.12 – 7.10 (m, 1H), 6.96 (d, J = 7.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.3, 149.5, 140.6, 140.3, 140.2, 139.5, 139.4, 135.3, 130.6, 130.4, 130.1, 128.7, 128.6, 127.7, 127.3, 126.9, 126.7, 125.4, 121.4; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{23}H_{18}N$) requires *m/z* 308.1434, found *m/z* 308.1431. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



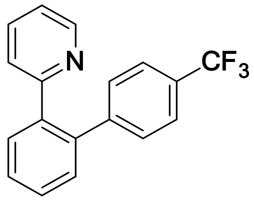
4e

2-(4'-Methoxy-[1,1'-biphenyl]-2-yl)pyridine (4e). Yellow solid. (23.8 mg, 91% yield). M. p. = 69 – 71 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, J = 5.4 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.46 – 7.38 (m, 4H), 7.11 – 7.09 (m, 1H), 7.07 (d, J = 8.4 Hz, 2H), 6.90 (d, J=7.8 Hz, 1H), 6.77 (d, J = 9.0 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.5, 158.5, 149.4, 140.2, 139.4, 135.2, 133.7, 130.7, 130.5, 130.4, 128.5, 127.3, 125.4, 121.2, 113.5, 55.2; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{16}NO$) requires *m/z* 262.1226, found *m/z* 262.1235. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 6/1).



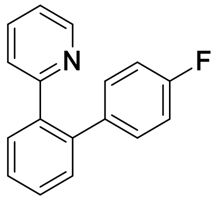
4f

2-(4'-(Benzyloxy)-[1,1'-biphenyl]-2-yl)pyridine (4f). Yellow oil (30.3 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, J = 4.4 Hz, 1H), 7.68 – 7.66 (m, 1H), 7.46 – 7.32 (m, 9H), 7.11 – 7.09 (m, 1H), 7.07 (d, J = 8.4 Hz, 2H), 6.90 (d, J = 7.6 Hz, 1H), 6.85 (d, J = 8.8 Hz, 2H), 5.02 (s, 2H);^{13}C NMR (151 MHz, $CDCl_3$) δ 159.4, 157.8, 149.4, 140.1, 139.4, 136.9, 135.2, 134.0, 130.8, 130.5, 130.4, 128.5, 128.5, 127.9, 127.5, 127.3, 125.4, 121.2, 114.5, 70.0; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{24}H_{20}NO$) requires *m/z* 338.1539, found *m/z* 338.1538. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 6/1).



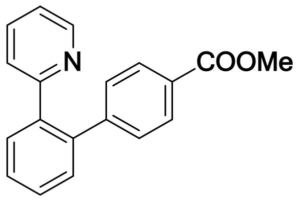
4g

2-(4'-(Trifluoromethyl)-[1,1'-biphenyl]-2-yl)pyridine (4g).[21p] Colorless oil (13.9 mg, 47% yield). ^1H NMR (600 MHz, $CDCl_3$) δ 8.61 (s, 1H), 7.70 (d, *J* = 6.0 Hz, 1H), 7.52 – 7.42 (m, 6H), 7.28 – 7.26 (m, 2H), 7.14 (t, *J* = 6.6 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9 (s, 3F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.8, 149.6, 145.1, 139.7, 139.2, 135.6, 130.6, 130.4, 129.9, 128.9, 128.7, 128.3, 125.2, 125.0 (d, *J* = 3.5 Hz), 125.0, 121.6; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{18}H_{13}F_3N$) requires *m/z* 300.0995, found *m/z* 300.0998. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



4h

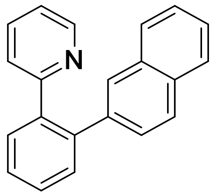
2-(4'-Fluoro-[1,1'-biphenyl]-2-yl)pyridine (4h).[21p] White solid (14.8 mg, 60% yield). M. p. = 78– 79 ^oC. ^1H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.2 Hz, 1H), 7.68 – 7.67 (m, 1H), 7.47 – 7.45 (m, 2H), 7.44 – 7.40 (m, 2H), 7.13 – 7.09 (m, 3H), 6.94 – 6.89 (m, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.9 (s, 1F); ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.7, 161.1, 159.2, 149.5, 139.6, 137.3 (d, *J* = 3.6 Hz), 135.3, 131.2 (d, *J* = 8.3 Hz), 130.5, 130.4, 128.6, 127.7, 125.3, 121.4, 115.0 (d, *J* = 21.6 Hz); HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{17}H_{13}FN$) requires *m/z* 250.1027, found *m/z* 250.1022. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



4i

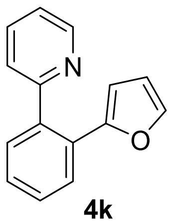
Methyl 2'-(pyridin-2-yl)-[1,1'-biphenyl]-4-carboxylate (4i).[21q] Colorless oil (14.6 mg, 51% yield). ^1H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 6.6 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.70 – 7.69 (m, 1H), 7.51 – 7.48 (m, 2H), 7.45 – 7.43 (m, 1H), 7.41 (td, *J* = 7.8, 1.8 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.12 – 7.10 (m, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.0, 158.8, 149.5, 146.2, 139.6, 139.6, 135.5, 130.6, 130.3, 129.7, 129.3, 128.6, 128.4, 128.2, 125.2, 121.5, 52.1; HRMS

(ESI+) exact mass calculated for $[M+H]^+$ ($C_{19}H_{16}NO_2$) requires *m/z* 290.1176, found *m/z* 290.1167. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 6/1).



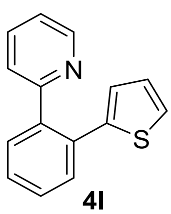
4j

2-(2-(Naphthalen-2-yl)phenyl)pyridine (4j).[21a] White solid (23.9 mg, 85% yield). M. p. = 92 – 93 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.4 Hz, 1H), 7.79 – 7.73 (m, 4H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.54 (m, 1H), 7.52 – 7.50 (m, 2H), 7.47 – 7.43 (m, 2H), 7.30 (t, *J* = 7.8 Hz, 1H), 7.16 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.08 – 7.06 (m, 1H), 6.91 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.2, 149.5, 140.5, 139.6, 139.0, 135.3, 133.4, 132.1, 130.8, 130.6, 128.6, 128.3, 128.2, 128.0, 127.8, 127.6, 127.3, 126.0, 125.9, 125.4, 121.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{21}H_{15}NNa$) requires *m/z* 304.1097, found *m/z* 304.1098. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).



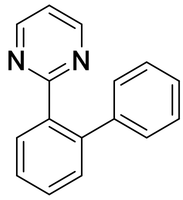
4k

2-(2-(furan-2-yl)phenyl)pyridine (4k).[21a] Yellow oil (17.9 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.8 Hz, 1H), 7.74 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.64 (td, *J* = 8.0, 2.0 Hz, 1H), 7.51 – 7.37 (m, 3H), 7.30 (d, *J* = 2.0 Hz, 1H), 7.26 – 7.20 (m, 2H), 6.28 (dd, J = 3.6, 2.0 Hz, 1H), 5.81 (dd, J = 3.2, 0.4 Hz, 1H); 13C NMR (101 MHz, $CDCl_3$) δ 159.8, 152.9, 149.4, 141.8, 138.3, 135.9, 135.9, 130.4, 128.4, 127.7, 124.2, 121.9, 111.3, 108.6.; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{12}NO$) requires m/z 222.0913, found m/z 222.0926. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).



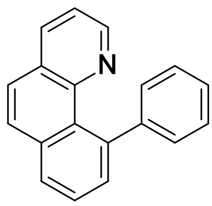
4l

2-(2-(thiophen-2-yl)phenyl)pyridine (4l).[21p] Yellow oil (14.1 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.0 Hz, 1H), 7.61 – 7.59 (m, 1H), 7.56 – 7.49 (m, 2H), 7.45 – 7.43 (m, 2H), 7.21 – 7.16 (m, 2H), 7.12 (dt, *J* = 7.6, 1.2 Hz, 1H), 6.89 – 6.87 (m, 1H), 6.69 (dd, J = 3.6, 1.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.2, 149.4, 142.8, 139.8, 135.5, 133.0, 130.7, 130.5, 128.5, 128.0, 127.1, 127.0, 124.9, 124.9, 121.8; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{12}NS$) requires m/z 238.0685, found m/z 238.0691. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).



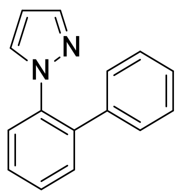
4m

2-([1,1'-Biphenyl]-2-yl)pyrimidine (4m). White solid (19.6 mg, 85% yield). M. p. = 94 – 96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 7.81 – 7.78 (m, 1H), 7.54 – 7.45 (m, 3H), 7.25 – 7.20 (m, 3H), 7.15 – 7.13 (m, 2H), 7.09 (t, *J* = 4.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 156.7, 141.6, 141.4, 138.2, 130.7, 130.5, 129.4, 129.1, 127.9, 127.4, 126.4, 118.4; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{16}H_{12}N_2Na$) requires *m/z* 255.0893, found *m/z* 255.0885. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).



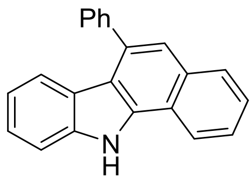
4n

10-Phenylbenzo[h]quinolone (4n).[21r] Colorless oil (23.3 mg, 92% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (dd, *J* = 4.2, 2.0 Hz, 1H), 8.06 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.91 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.54 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.42 – 7.33 (m, 5H), 7.30 (dd, *J* = 8.0, 4.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.8, 146.8, 146.4, 141.7, 135.1, 135.0, 131.5, 129.0, 128.7, 128.3, 127.9, 127.3, 127.2, 127.0, 125.9, 125.6, 121.0; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{19}H_{13}NNa$) requires *m/z* 278.0940, found *m/z* 278.0929. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).



4o

1-([1,1'-Biphenyl]-2-yl)-1H-pyrazole (4o).[21s] Yellow solid (15.8 mg, 72% yield). M. p. =45 – 47 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 1.8 Hz, 1H), 7.62 – 7.61 (m, 1H), 7.48 – 7.45 (m, 3H), 7.30 – 7.27 (m, 3H), 7.12 – 7.10 (m, 2H), 7.07 (d, *J* = 2.4 Hz, 1H), 6.18 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 140.2, 138.5, 136.6, 131.3, 131.0, 128.5, 128.4, 128.4, 128.3, 128.2, 127.4, 126.5, 106.3; HRMS (ESI+) exact mass calculated for $[M+H]^+$ ($C_{15}H_{13}N_2$) requires *m/z* 221.1073, found *m/z* 221.1066. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 8/1).

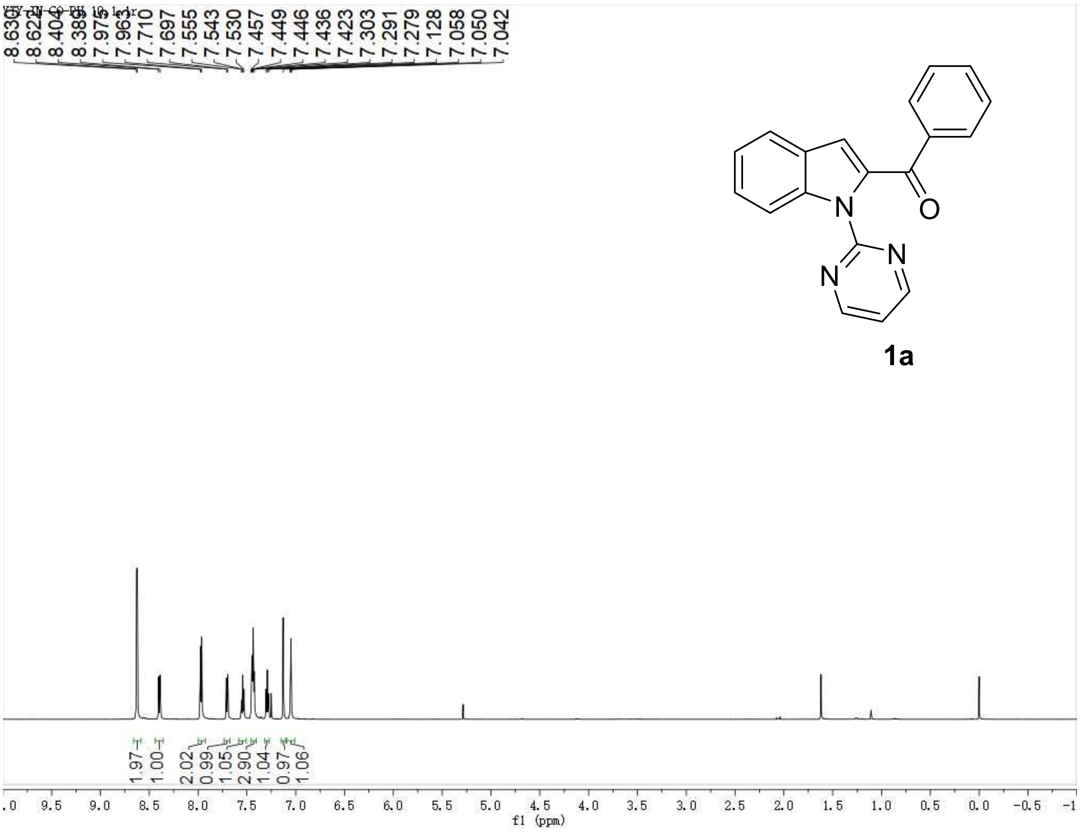


6a

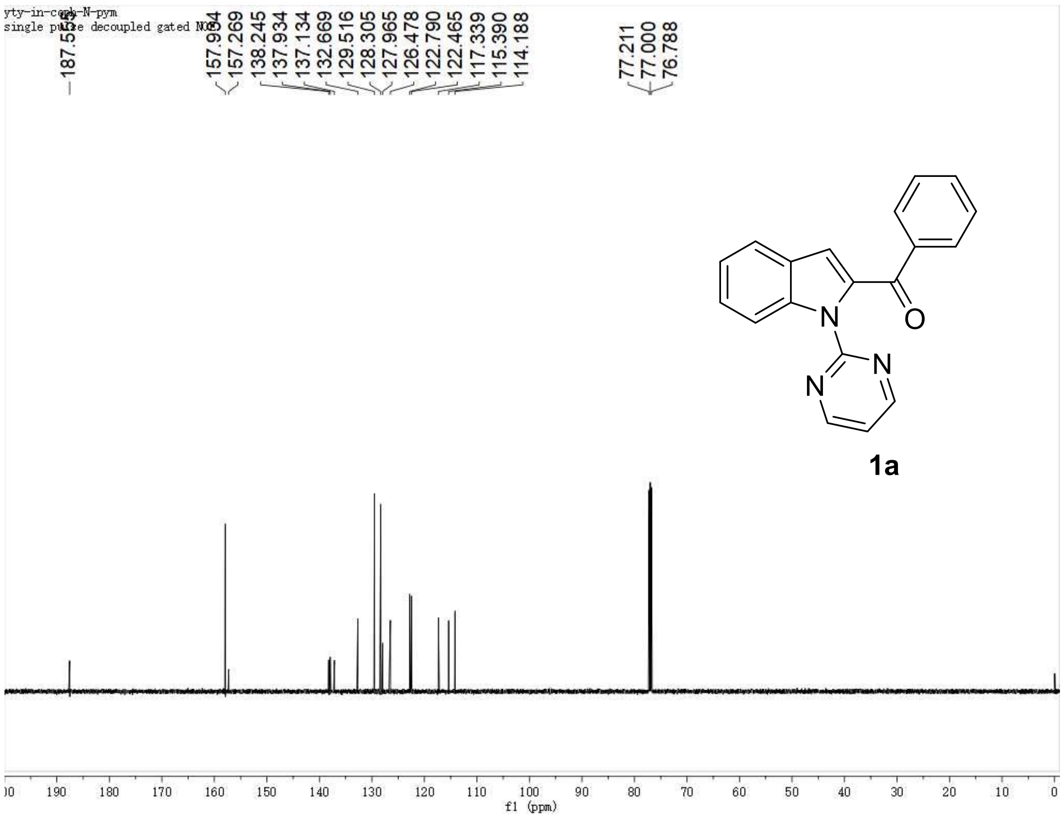
6-Phenyl-11H-benzo[*a*]carbazole(6a)[19]. Brown oil (41.1 mg, 70% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 6.6 Hz, 2H), 7.60 – 7.54 (m, 5H), 7.52 – 7.49 (m, 2H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.2, 138.6, 136.5, 135.2, 132.1, 129.3, 128.9, 128.3, 127.6, 125.7, 125.4, 124.6, 123.8, 122.1, 120.9, 120.3, 120.2, 119.6, 116.7, 110.9; HRMS (ESI+) exact mass calculated for $[M+Na]^+$ ($C_{22}H_{15}NNa$) requires *m/z* 316.1097, found *m/z* 316.1091. This product was purified by silica gel column chromatography (Petroleum ether/EtOAc = 10/1).

8. NMR spectra

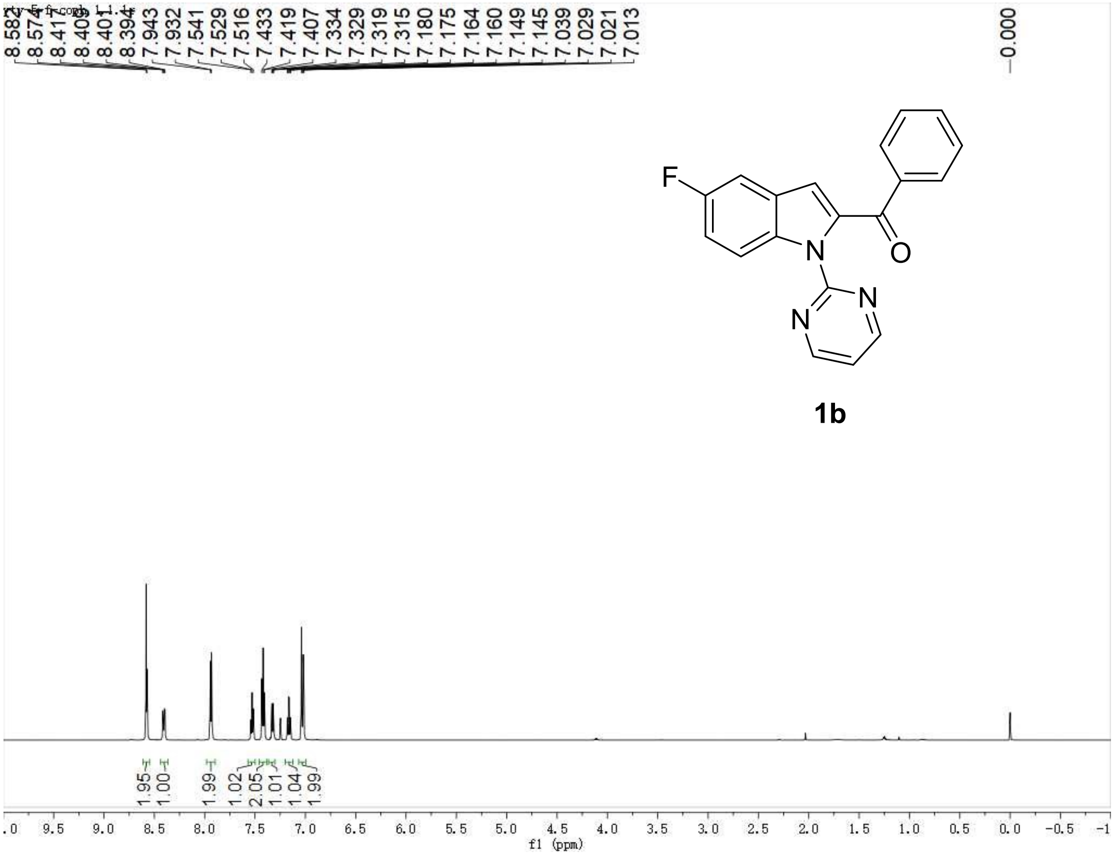
^{1}H NMR spectrum of compound **1a** ($CDCl_3$, 600 MHz)



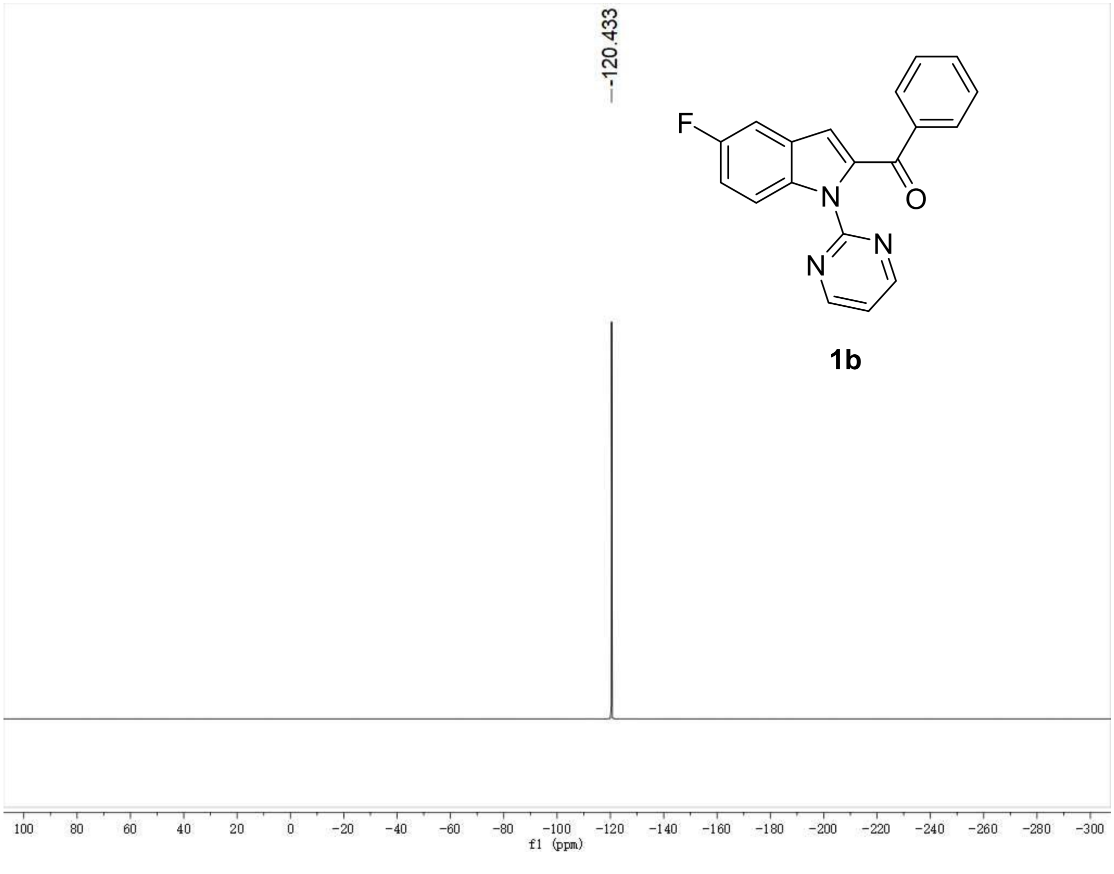
^{13}C NMR spectrum of compound **1a** ($CDCl_3$, 151 MHz)



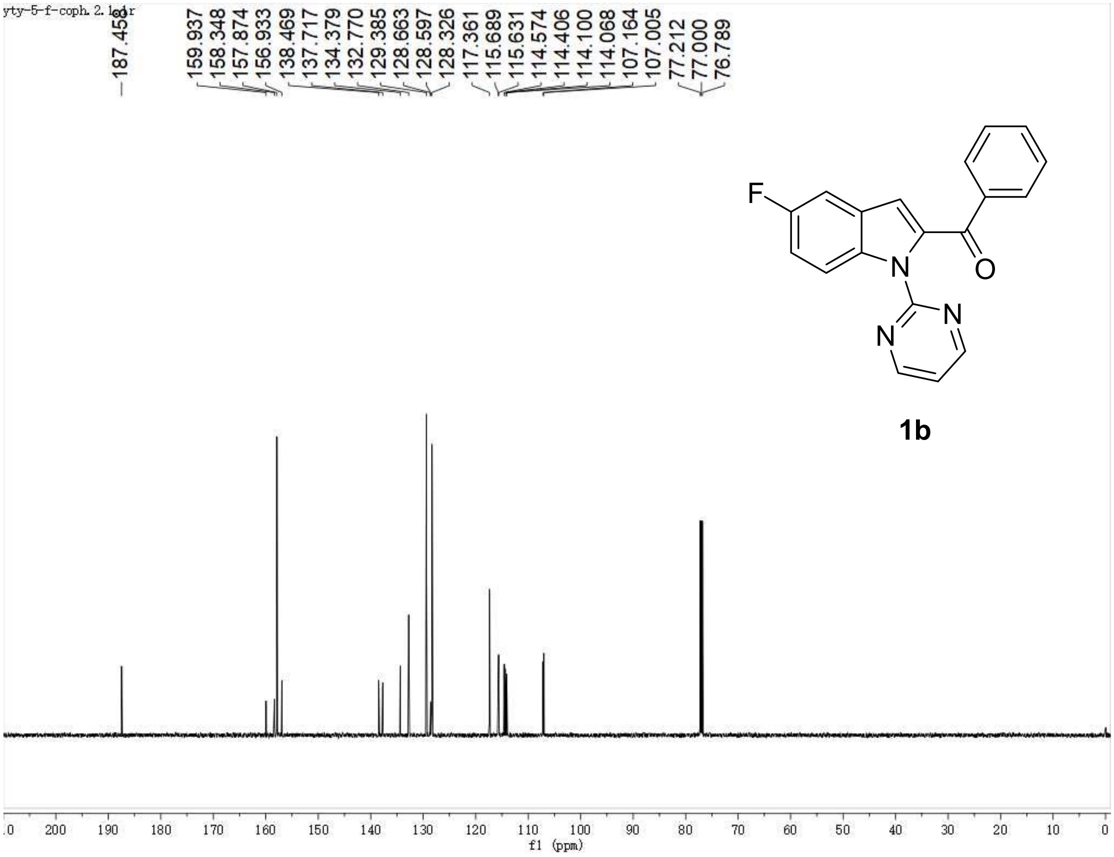
^{1}H NMR spectrum of compound **1b** ($CDCl_3$, 600 MHz)



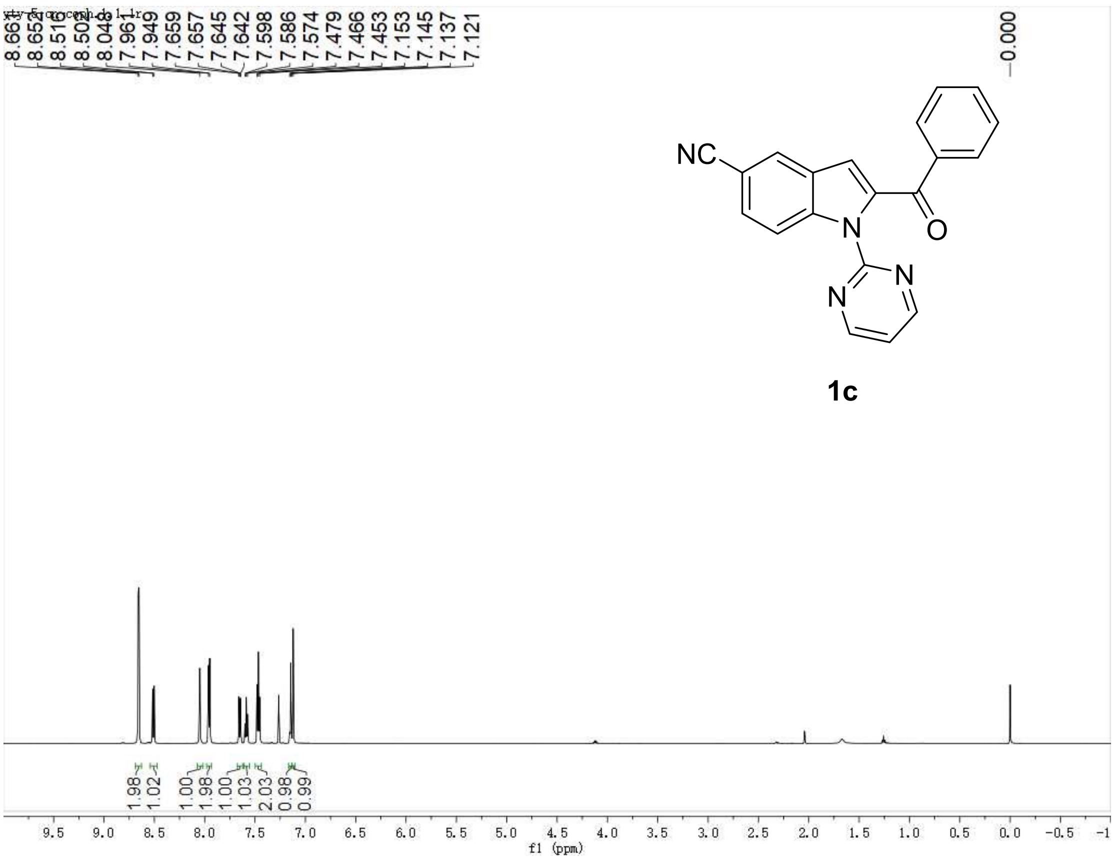
^{19}F NMR spectrum of compound **1b** ($CDCl_3$, 376 MHz)



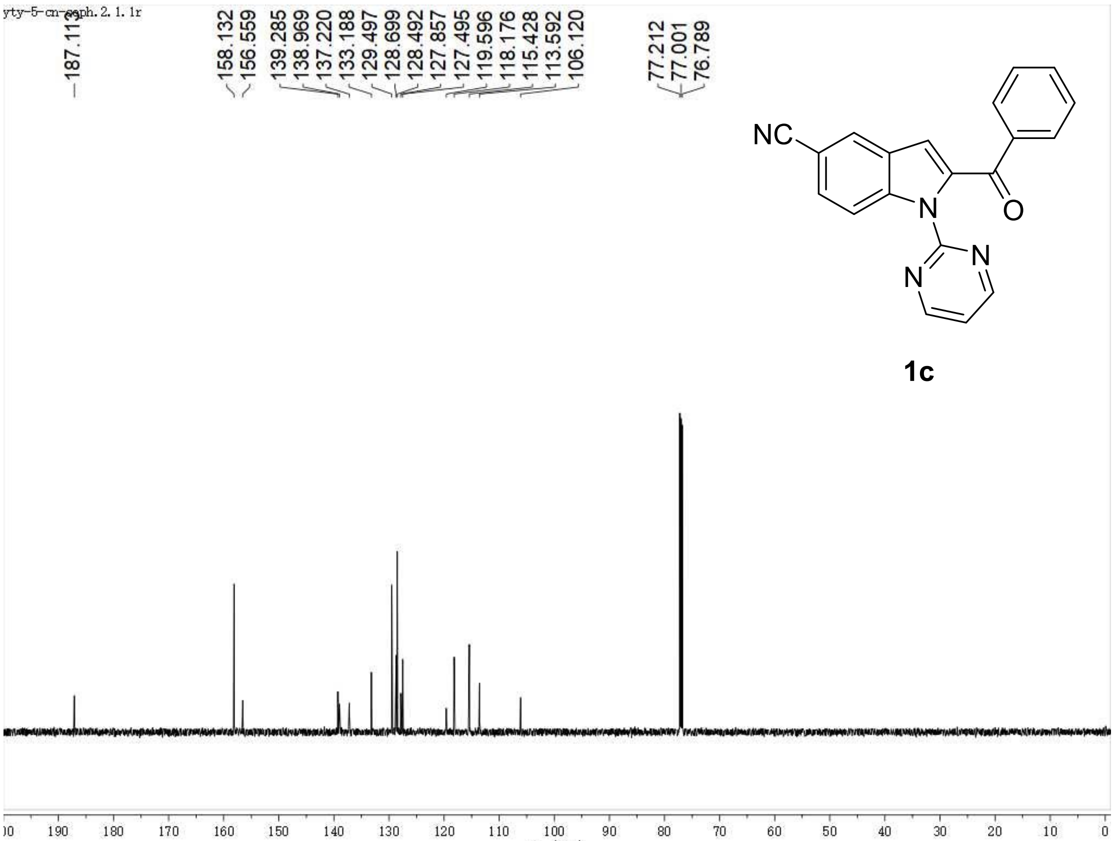
^{13}C NMR spectrum of compound **1b** ($CDCl_3$, 151 MHz)



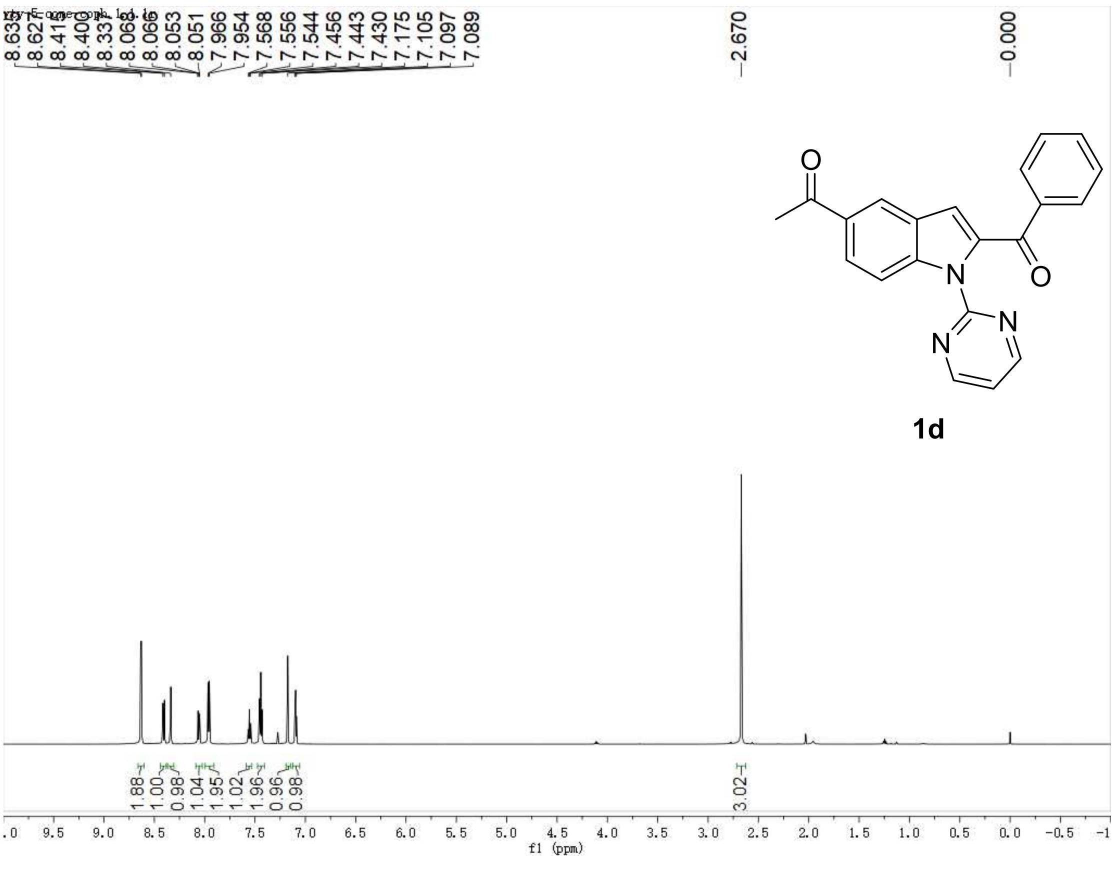
^{1}H NMR spectrum of compound **1c** ($CDCl_3$, 600 MHz)



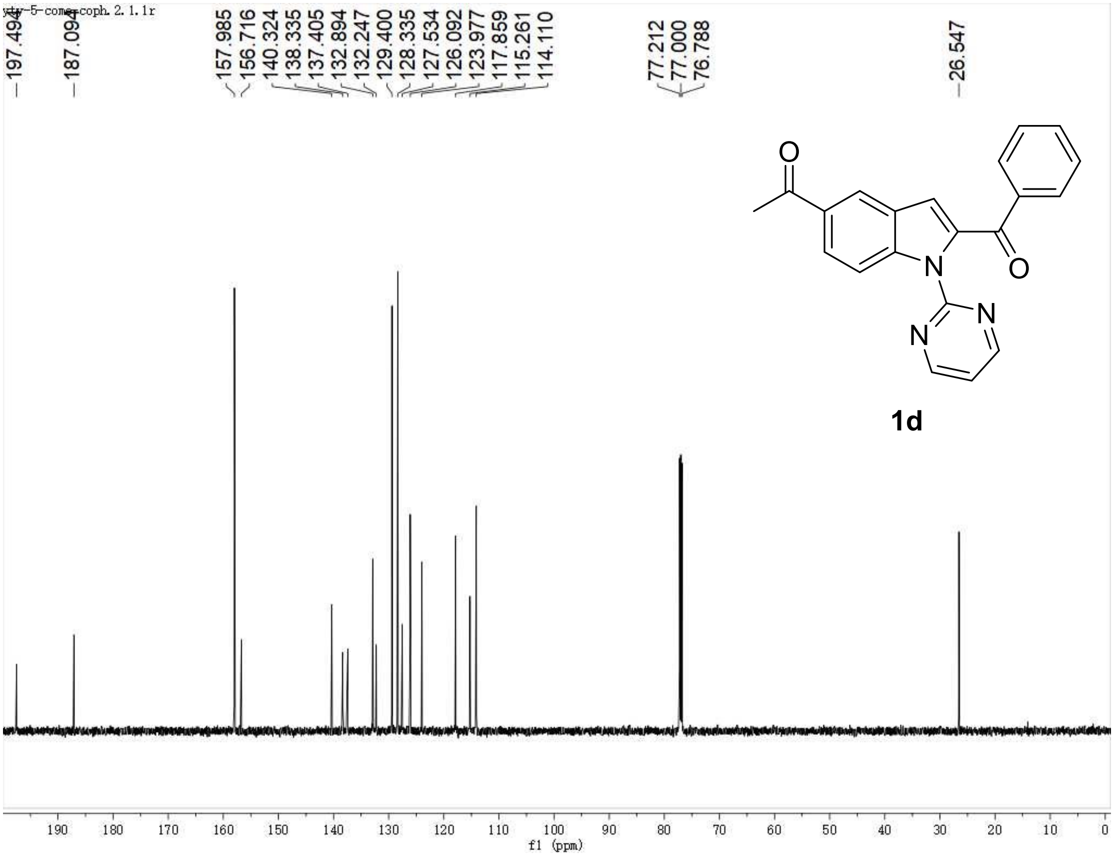
[13]C NMR spectrum of compound **1c** ($CDCl_3$, 151 MHz)



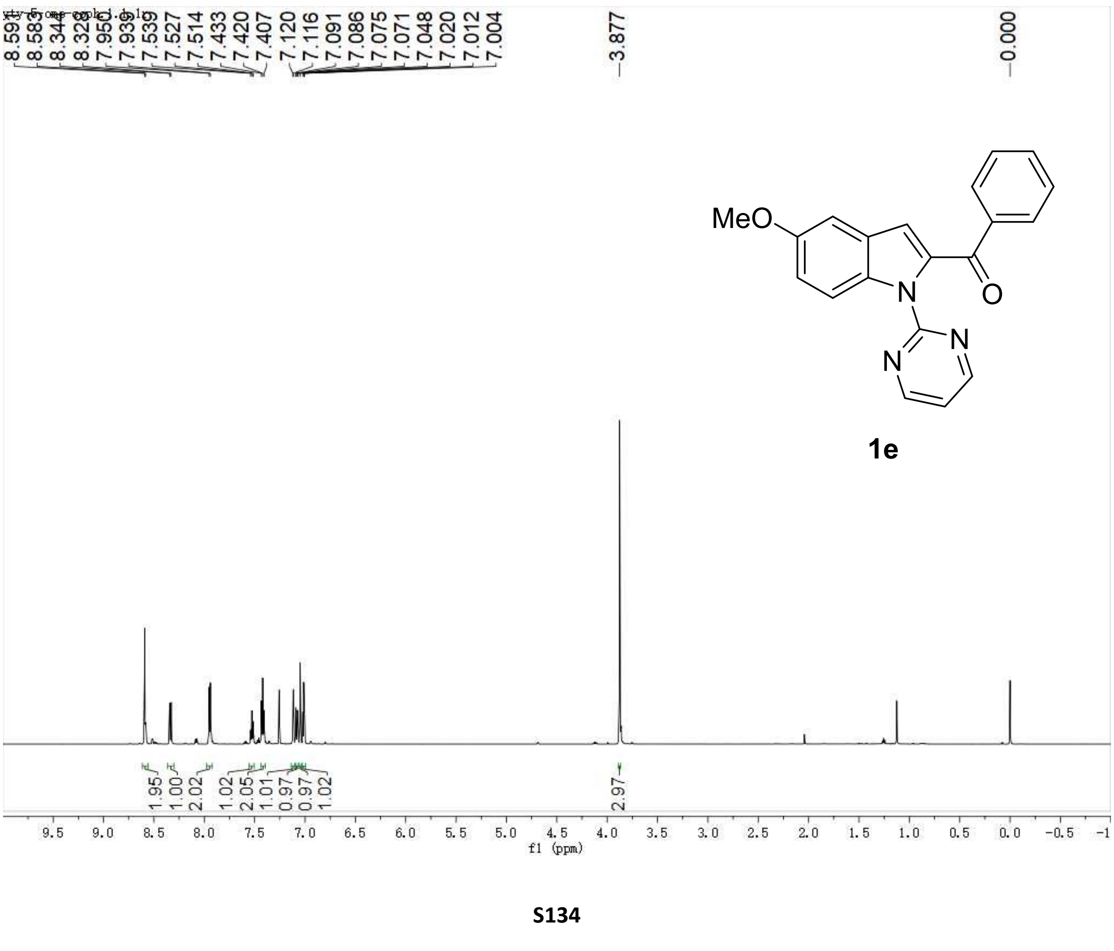
[1]H NMR spectrum of compound **1d** ($CDCl_3$, 600 MHz)



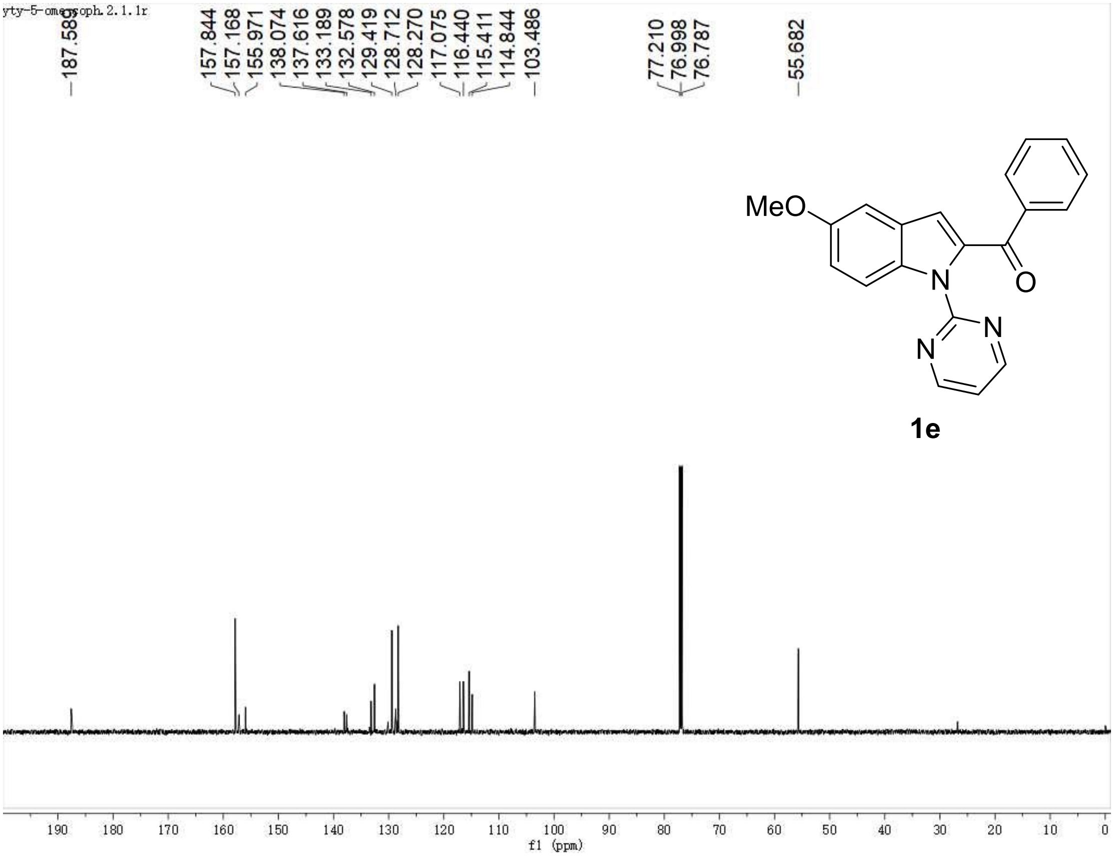
^{13}C NMR spectrum of compound **1d** ($CDCl_3$, 151 MHz)



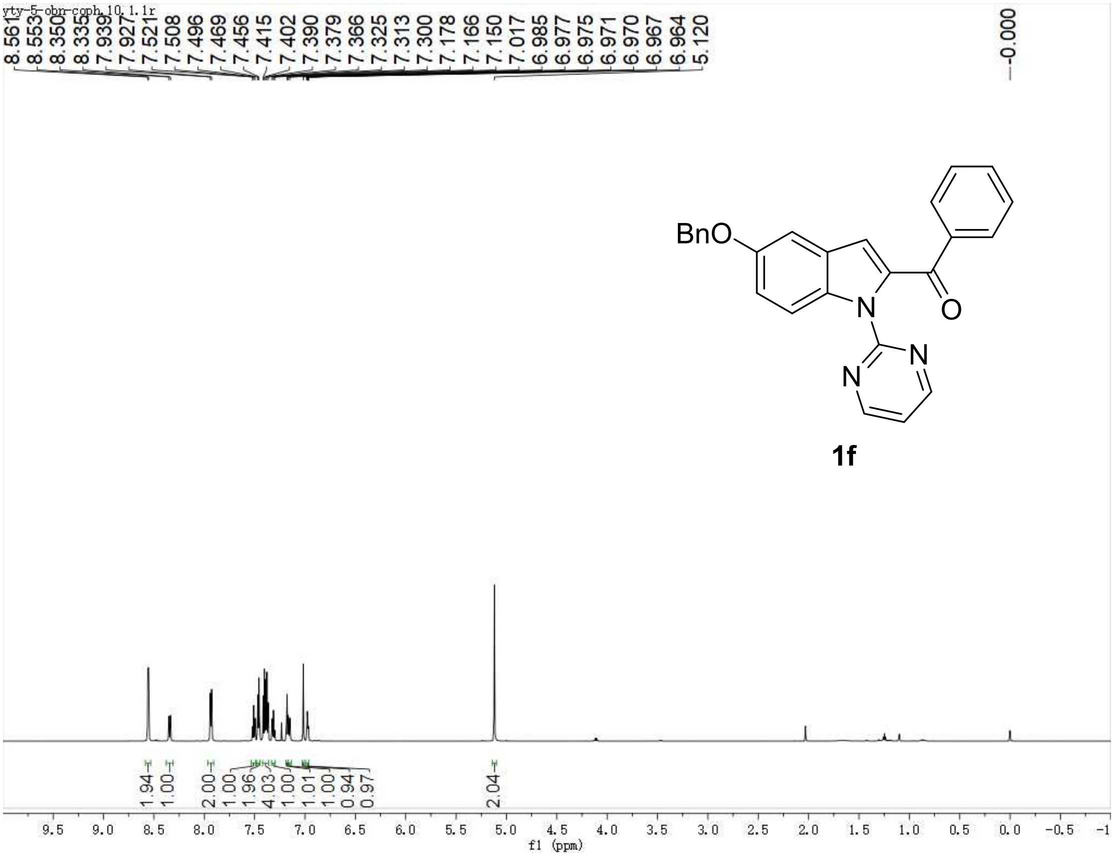
^{1}H NMR spectrum of compound **1e** ($CDCl_3$, 600 MHz)



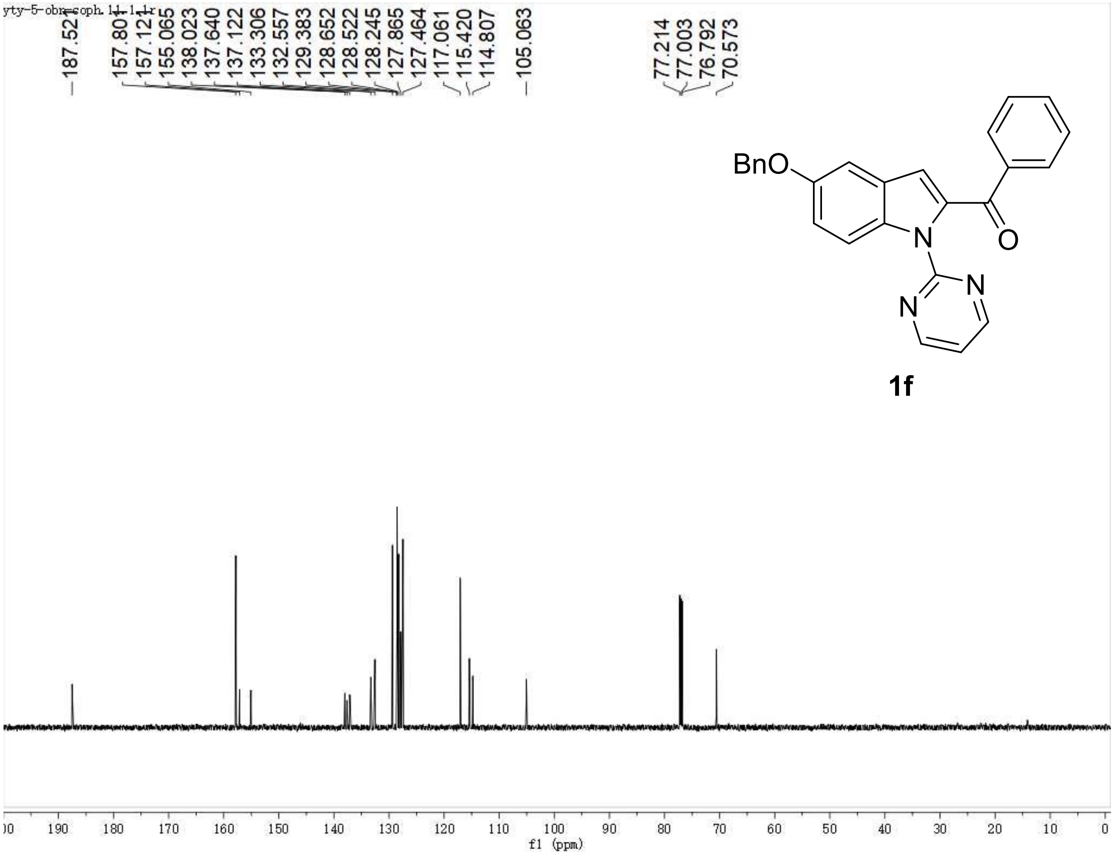
^{13}C NMR spectrum of compound **1e** ($CDCl_3$, 151 MHz)



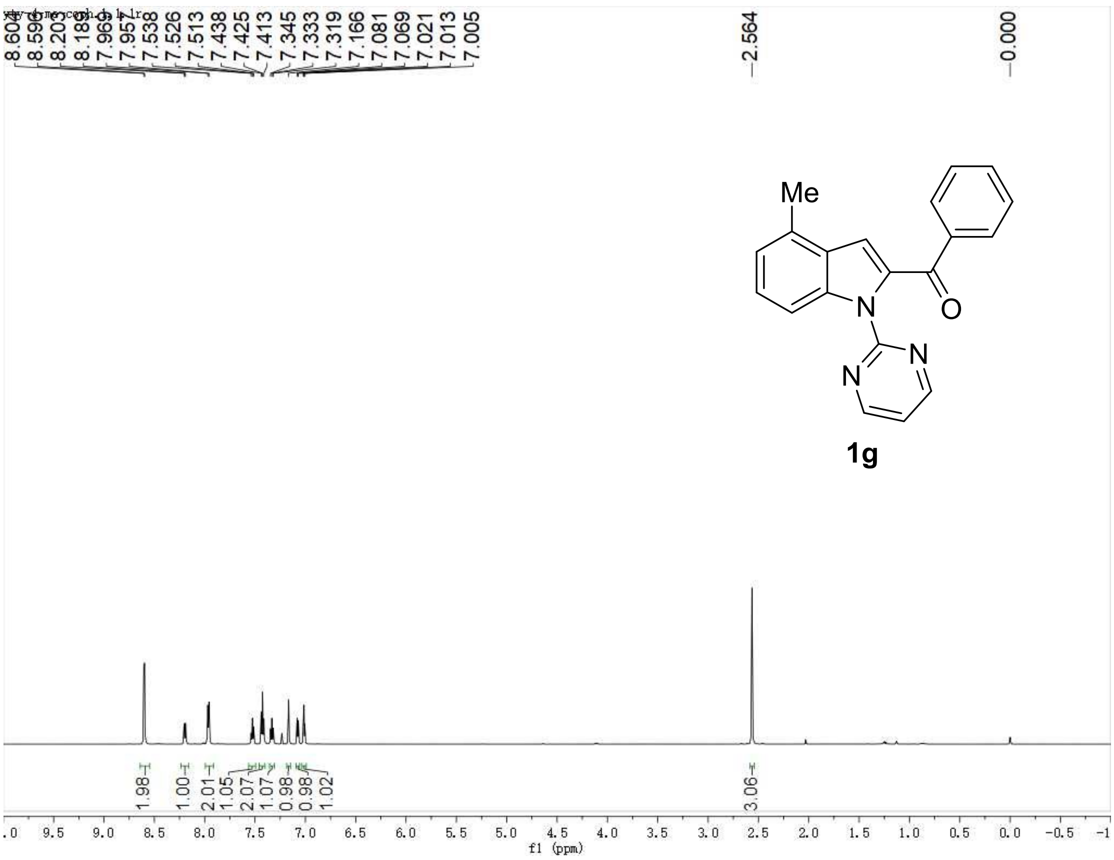
^1H NMR spectrum of compound **1f** ($CDCl_3$, 600 MHz)



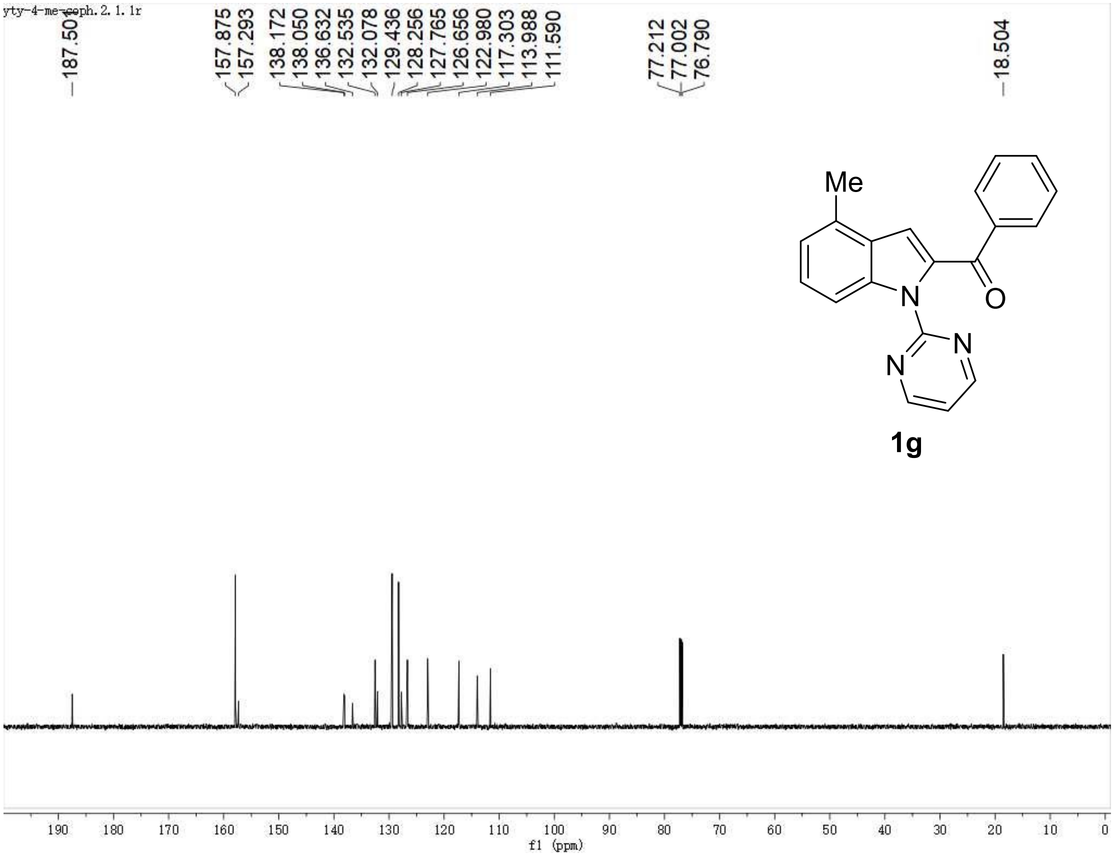
^{13}C NMR spectrum of compound **1f** ($CDCl_3$, 151 MHz)



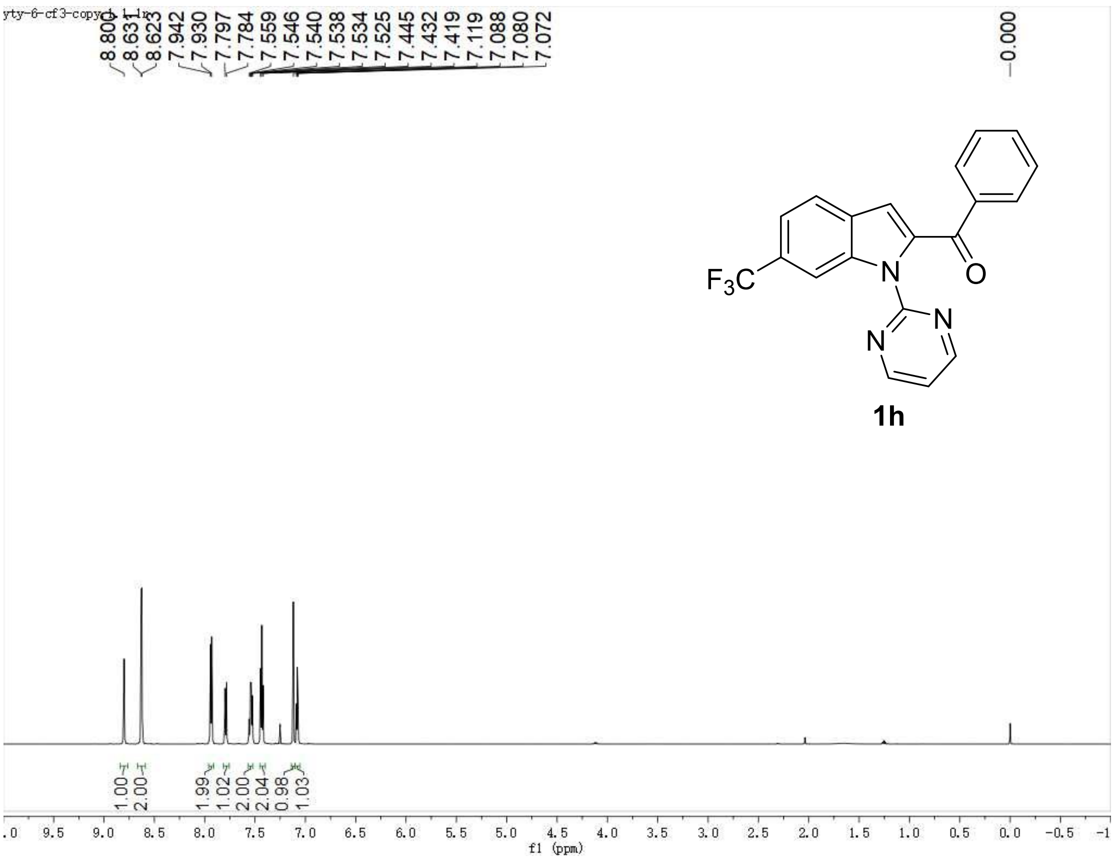
^{1}H NMR spectrum of compound **1g** ($CDCl_3$, 600 MHz)



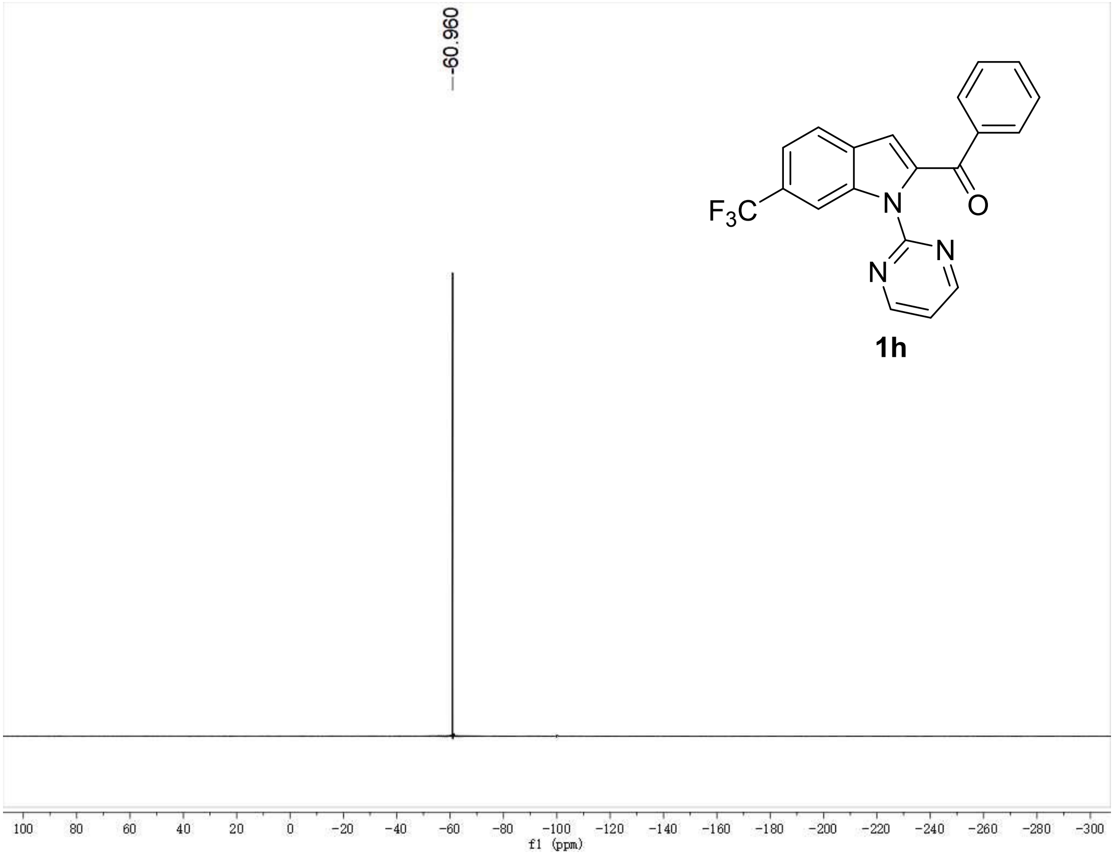
^{13}C NMR spectrum of compound **1g** ($CDCl_3$, 151 MHz)



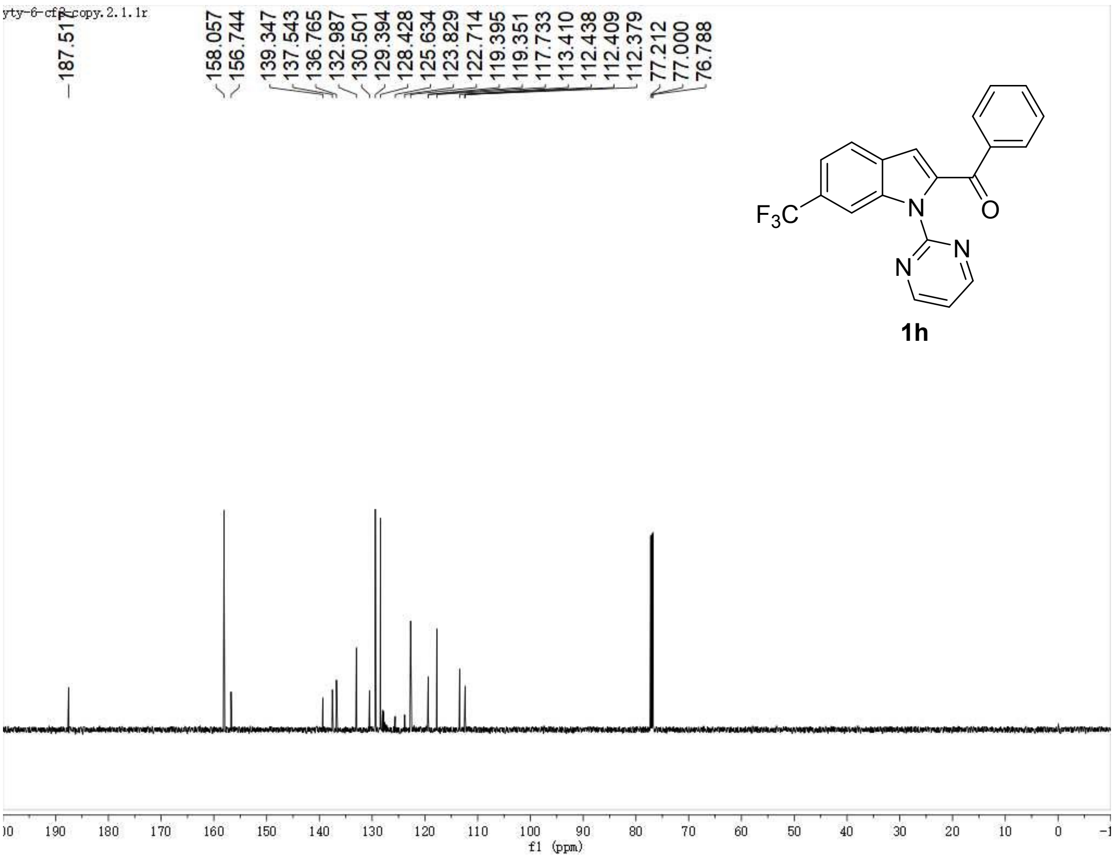
^{1}H NMR spectrum of compound **1h** ($CDCl_3$, 600 MHz)



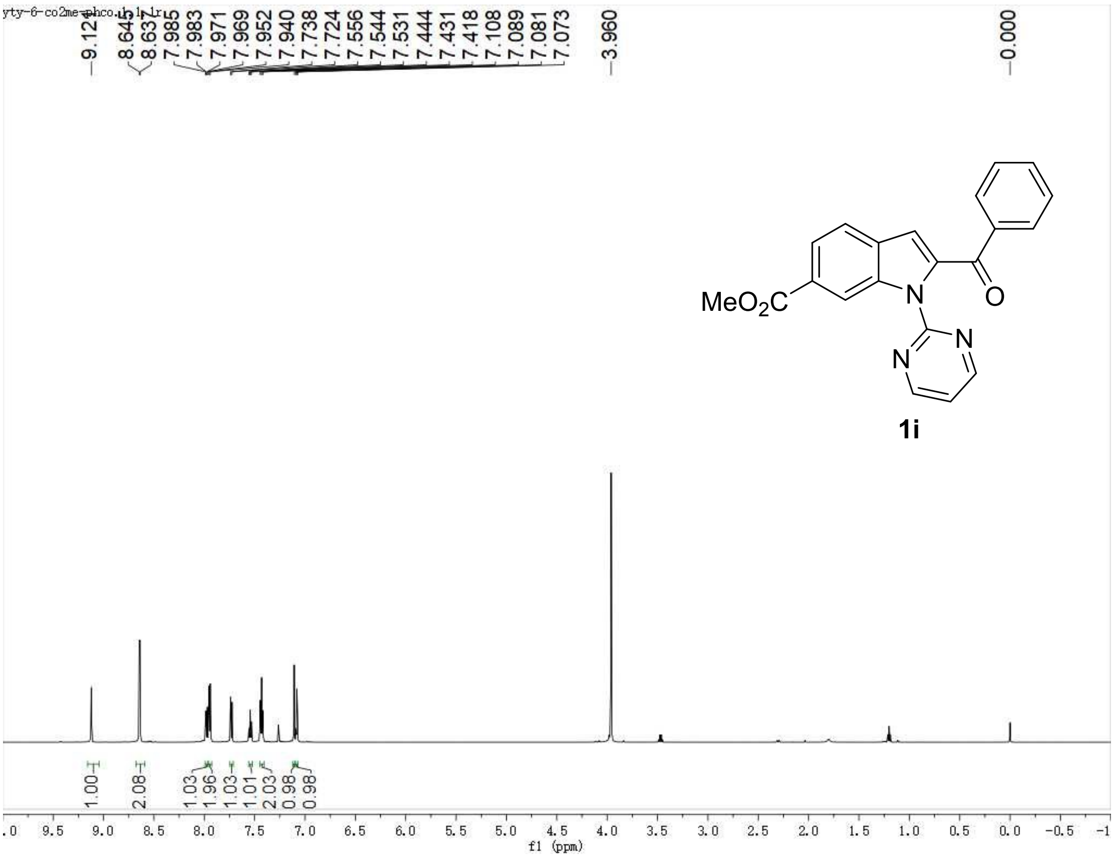
^{19}F NMR spectrum of compound **1h** ($CDCl_3$, 376 MHz)



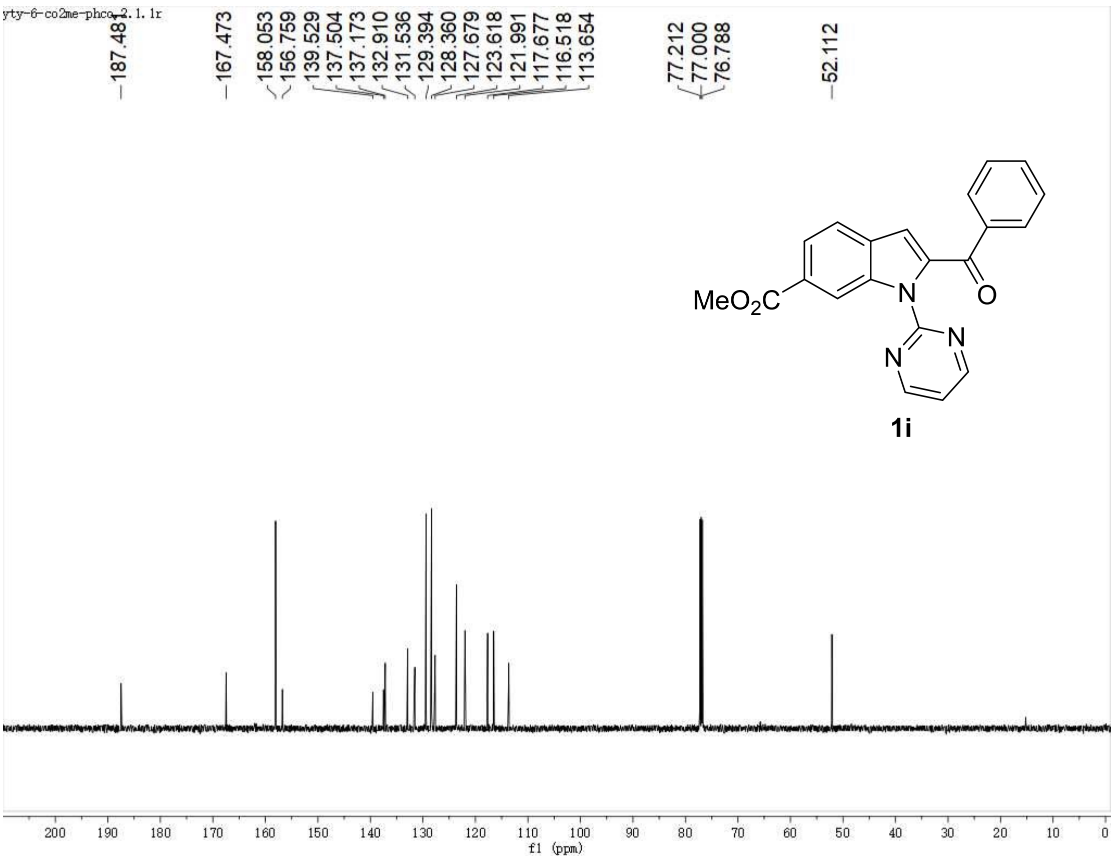
^{13}C NMR spectrum of compound **1h** ($CDCl_3$, 151 MHz)



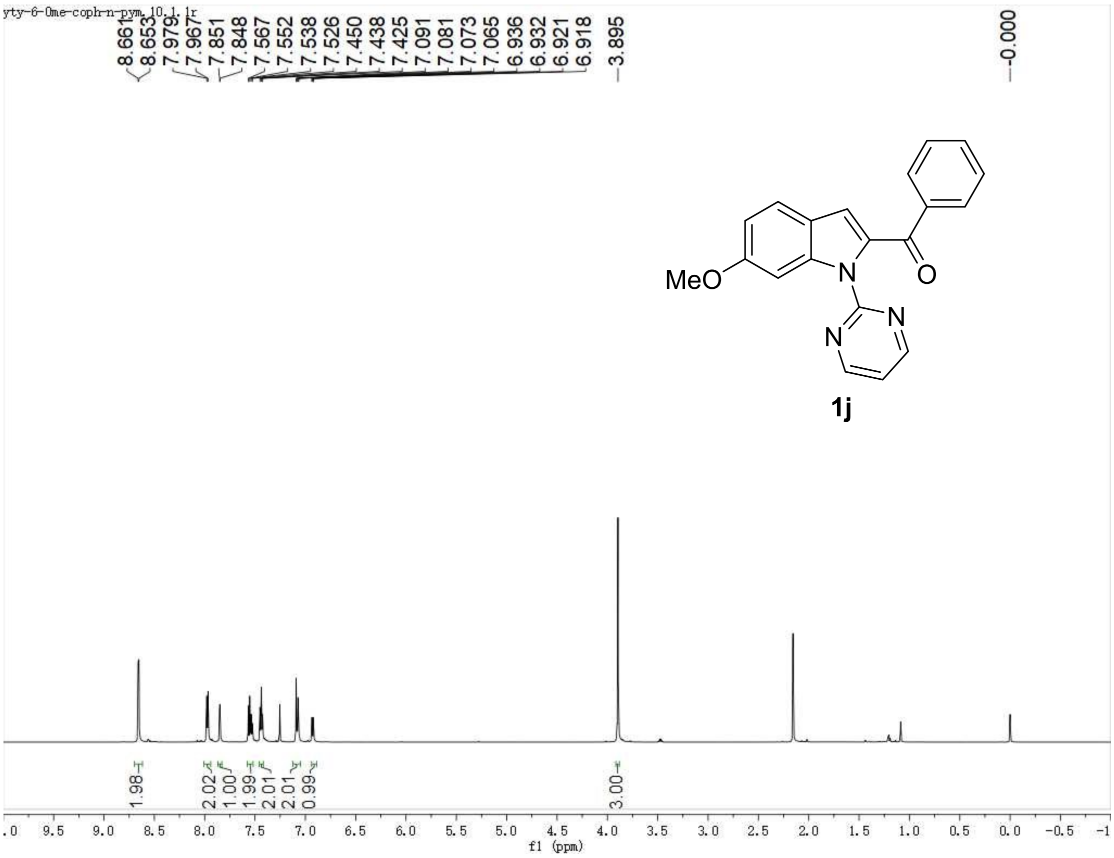
^{1}H NMR spectrum of compound **1i** ($CDCl_3$, 600 MHz)



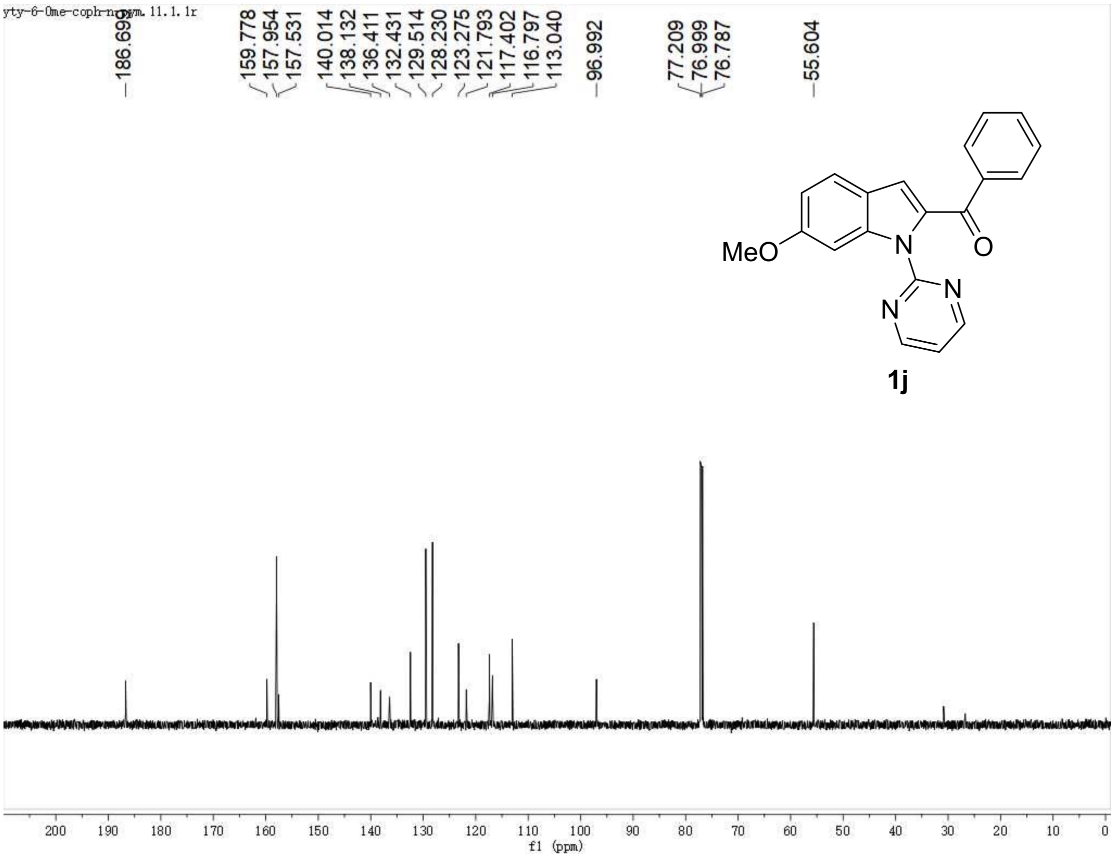
^{13}C NMR spectrum of compound **1i** ($CDCl_3$, 151 MHz)



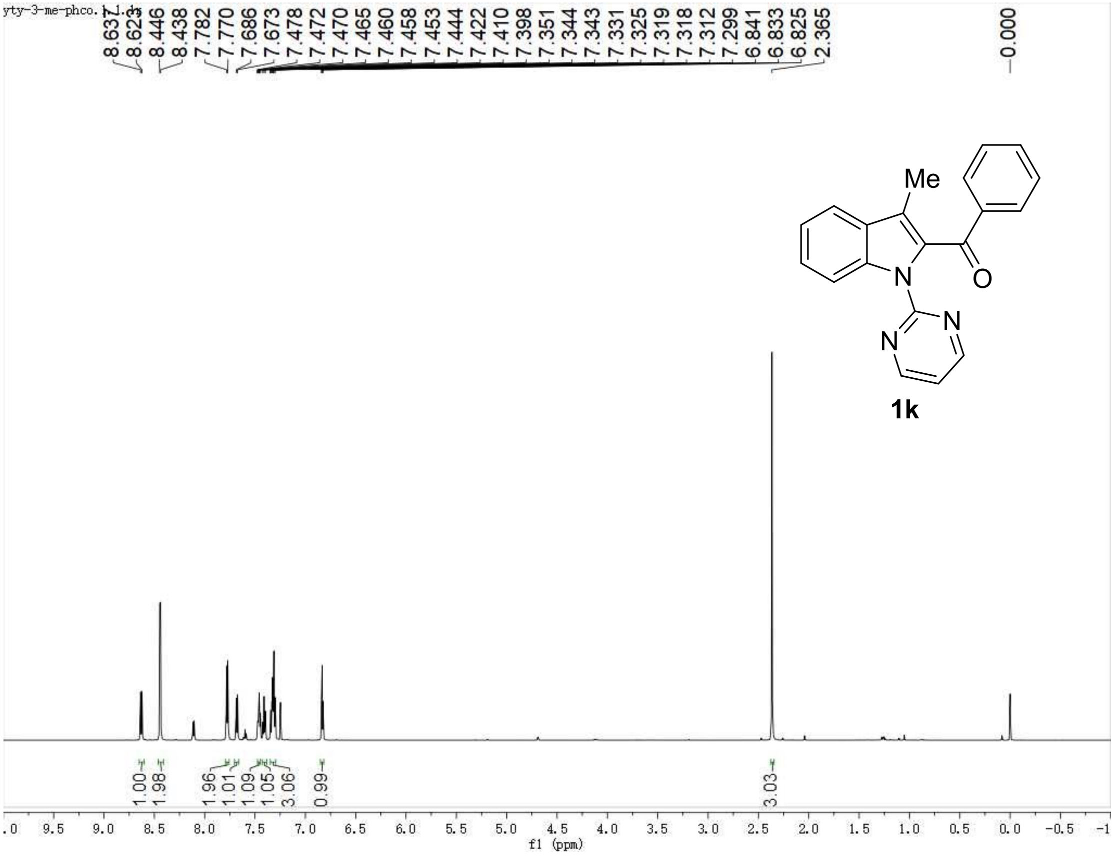
^{1}H NMR spectrum of compound **1j** ($CDCl_3$, 600 MHz)



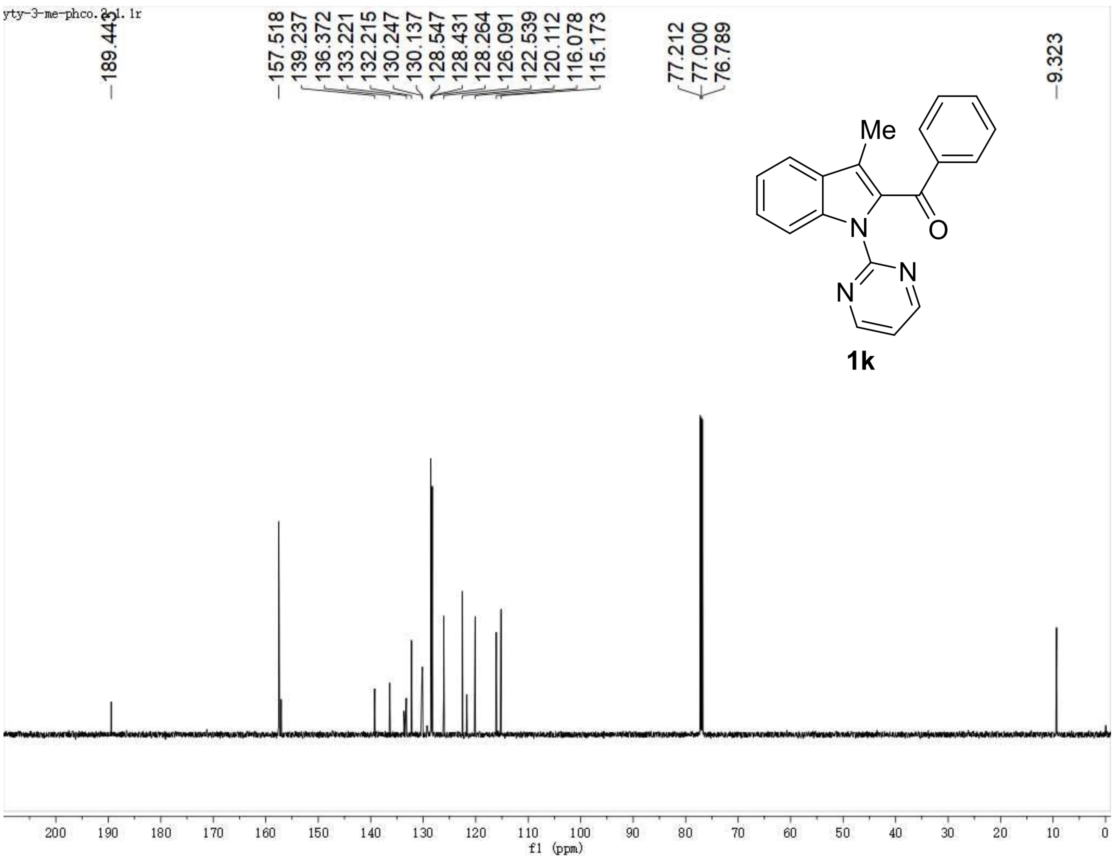
^{13}C NMR spectrum of compound **1j** ($CDCl_3$, 151 MHz)



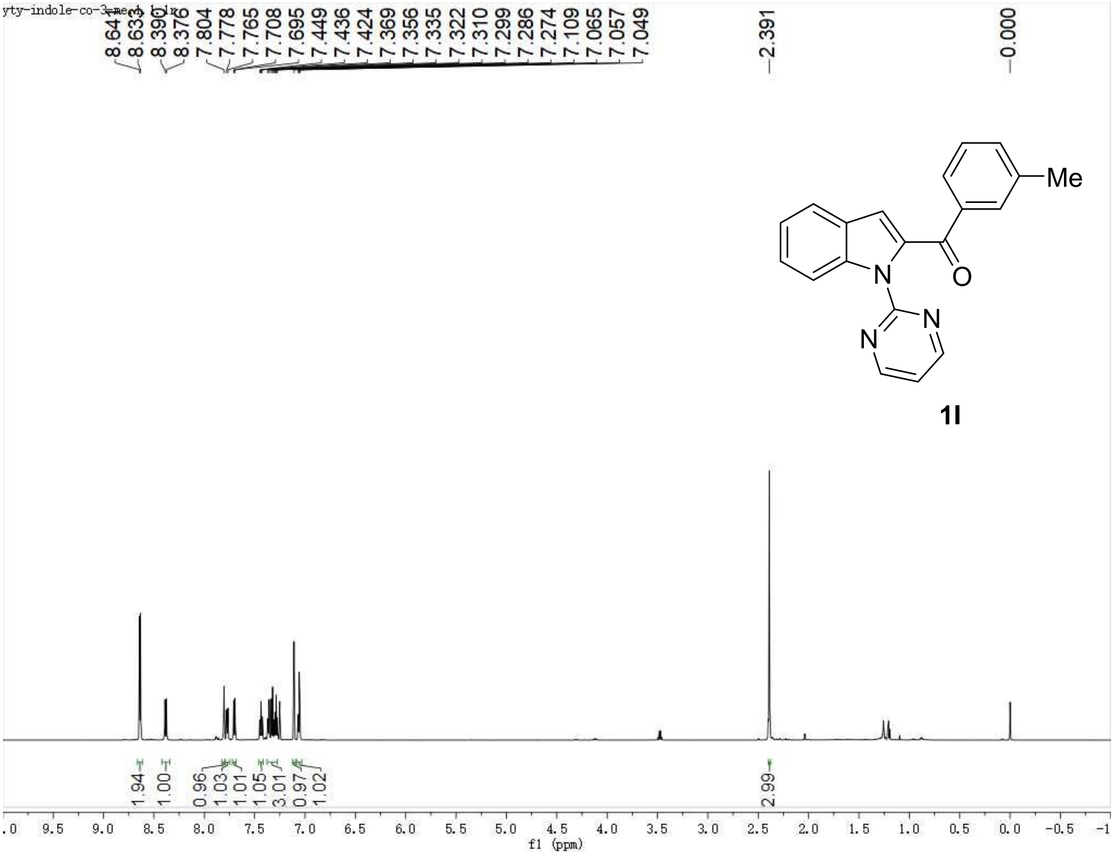
[1]H NMR spectrum of compound **1k** ($CDCl_3$, 600 MHz)



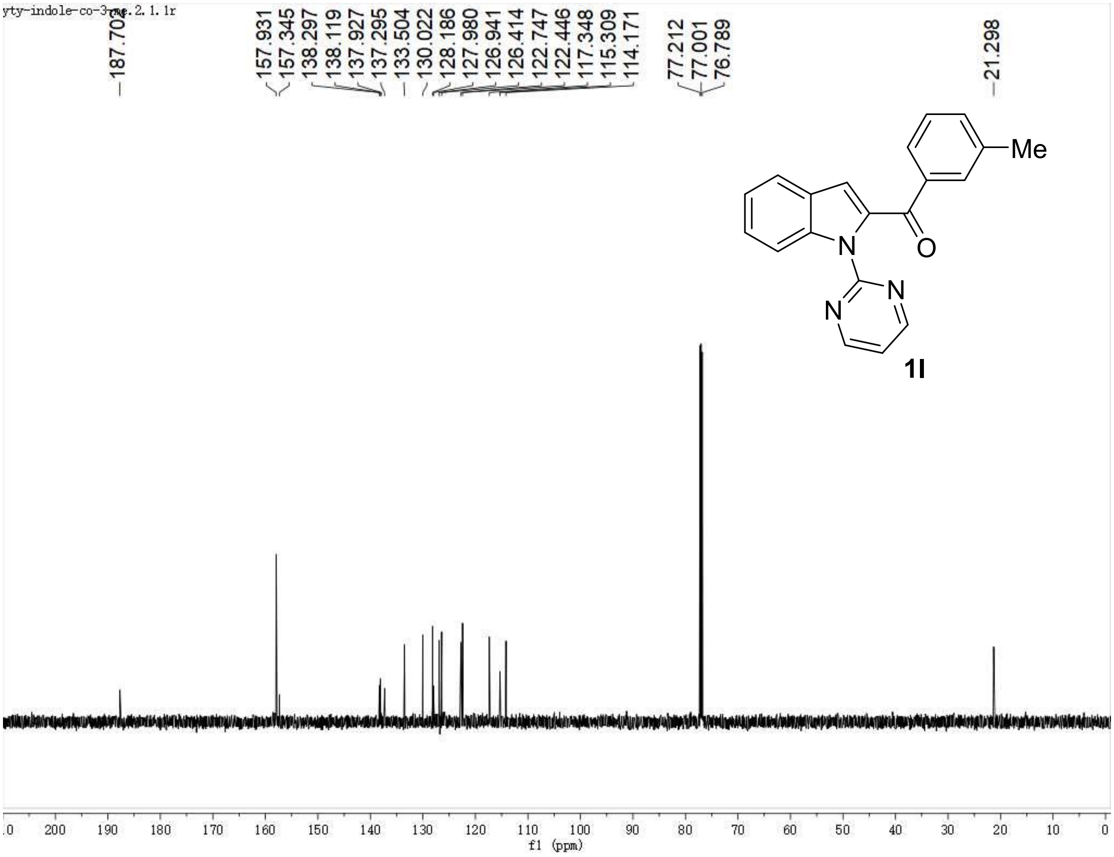
[13]C NMR spectrum of compound **1k** ($CDCl_3$, 151 MHz)



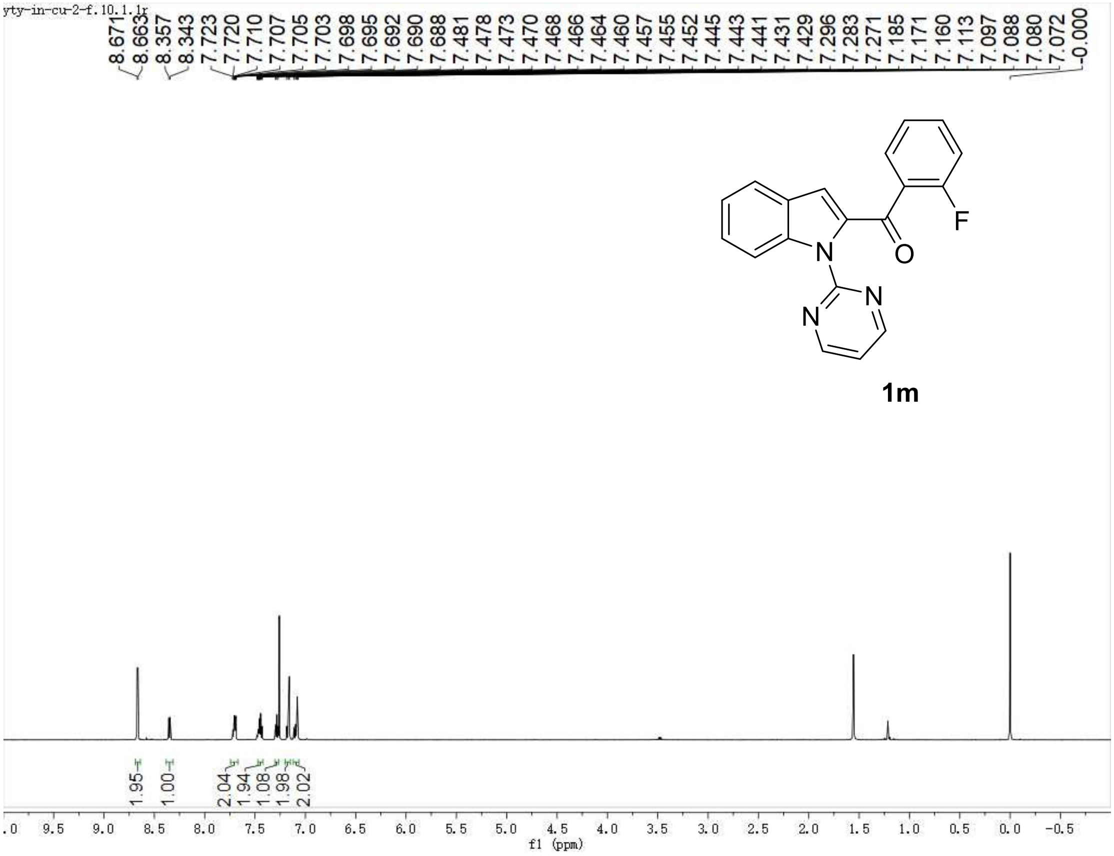
^{1}H NMR spectrum of compound **1l** ($CDCl_3$, 600 MHz)



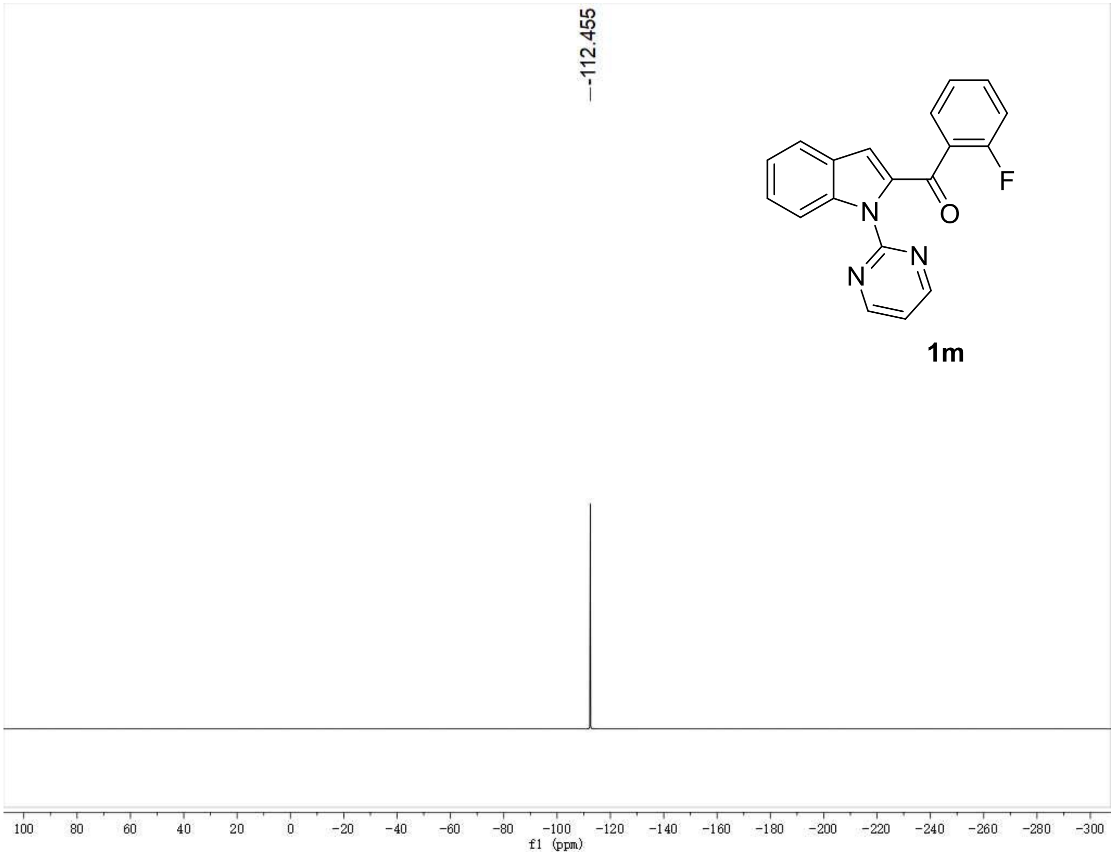
^{13}C NMR spectrum of compound **1l** ($CDCl_3$, 151 MHz)



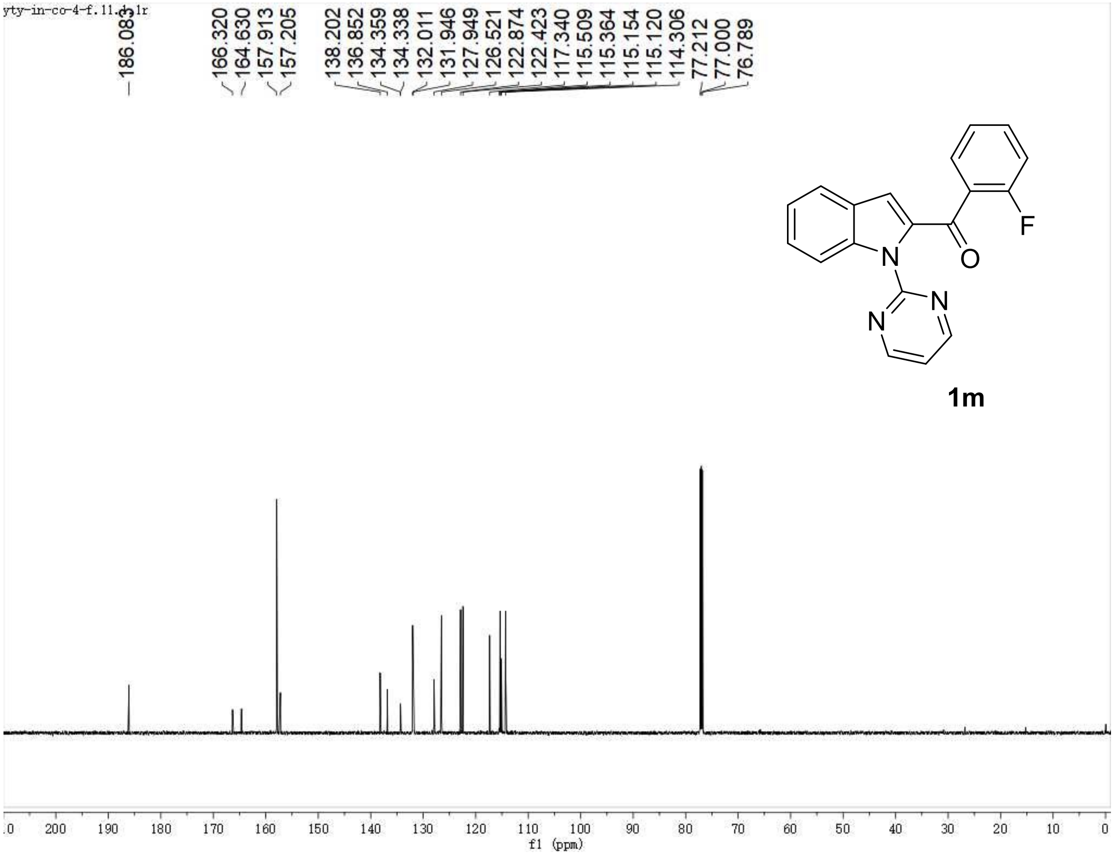
^1H NMR spectrum of compound **1m** ($CDCl_3$, 600 MHz)



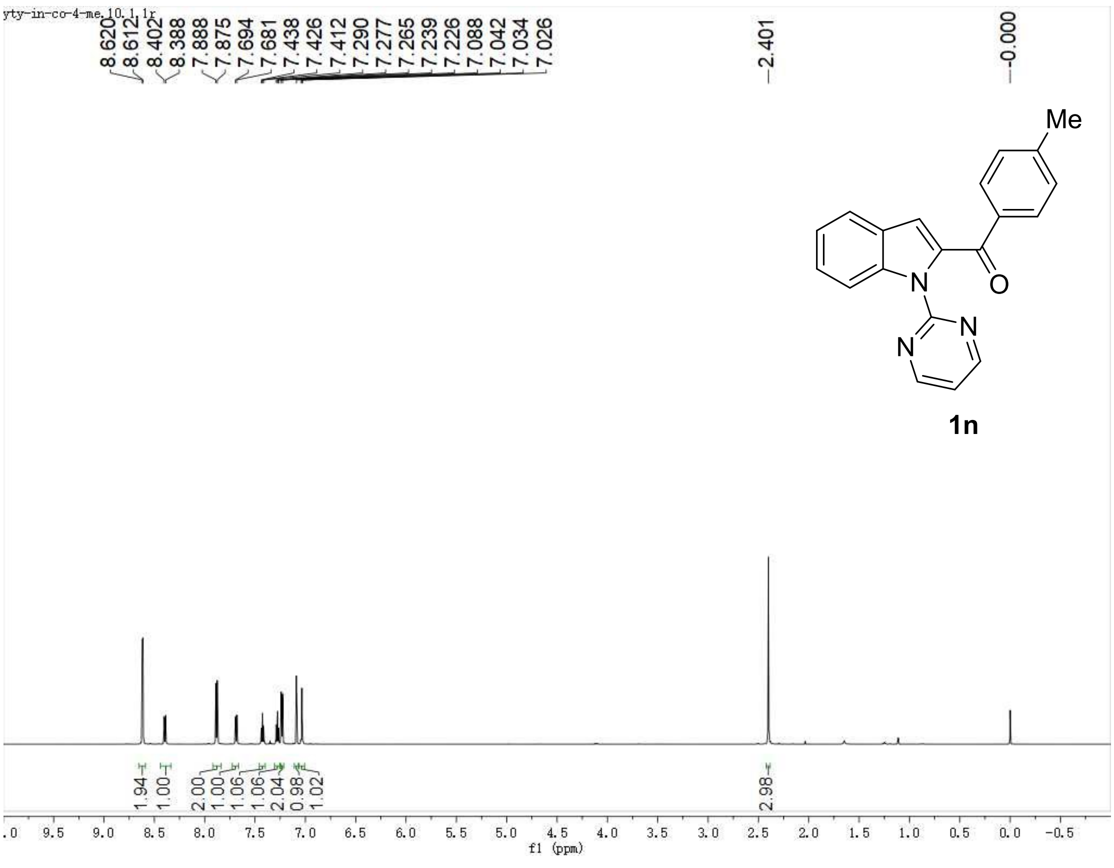
^{19}F NMR spectrum of compound **1m** ($CDCl_3$, 376 MHz)



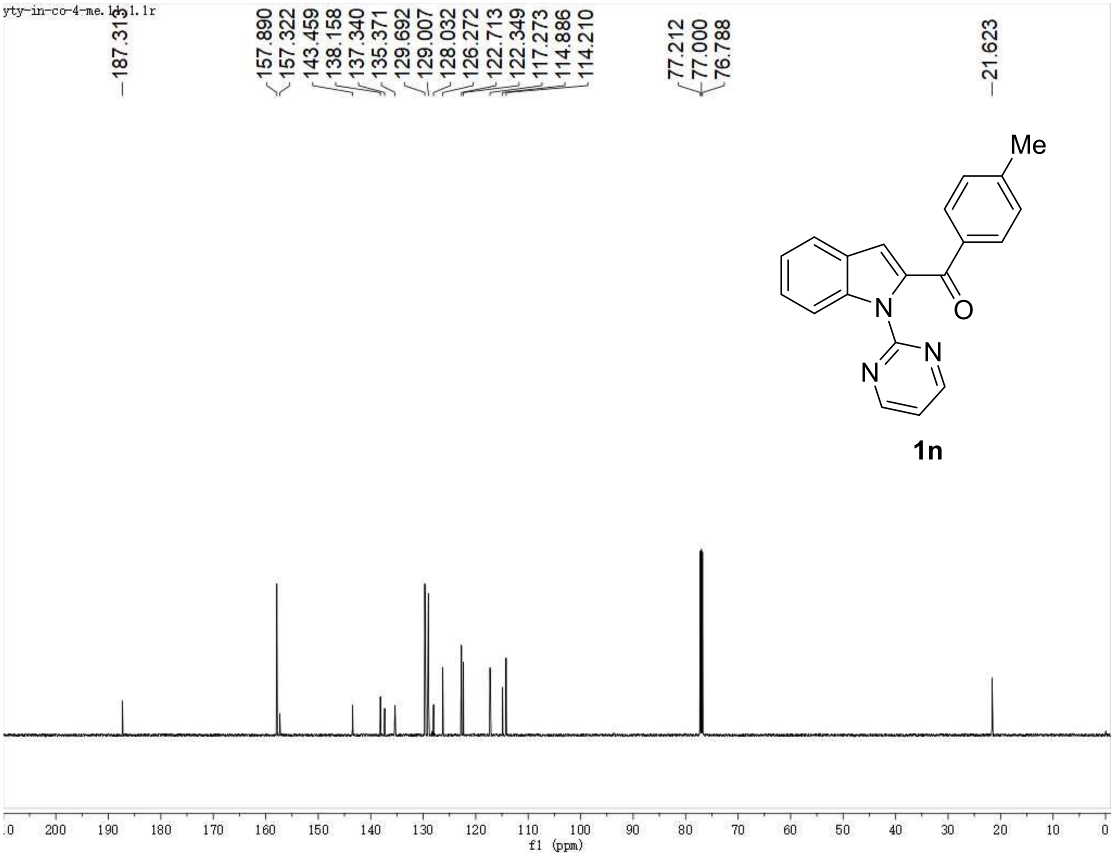
^{13}C NMR spectrum of compound **1m** ($CDCl_3$, 151 MHz)



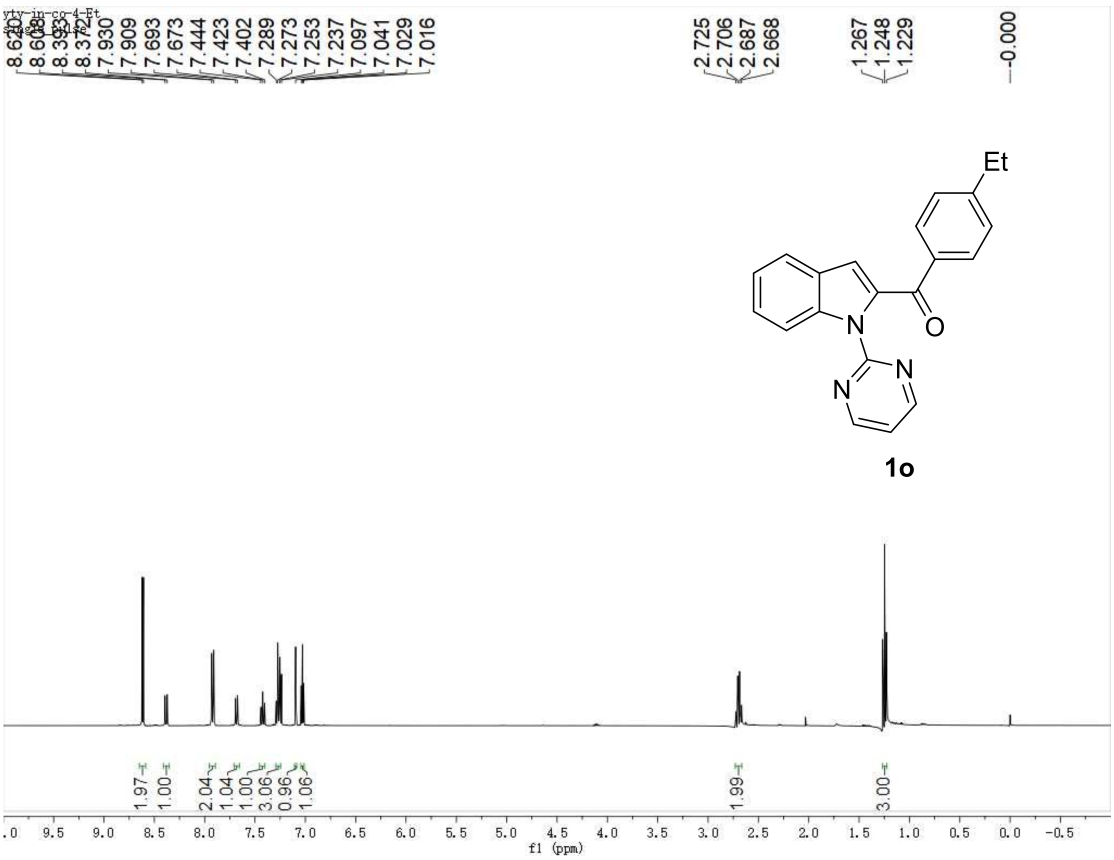
^{1}H NMR spectrum of compound **1n** ($CDCl_3$, 600 MHz)



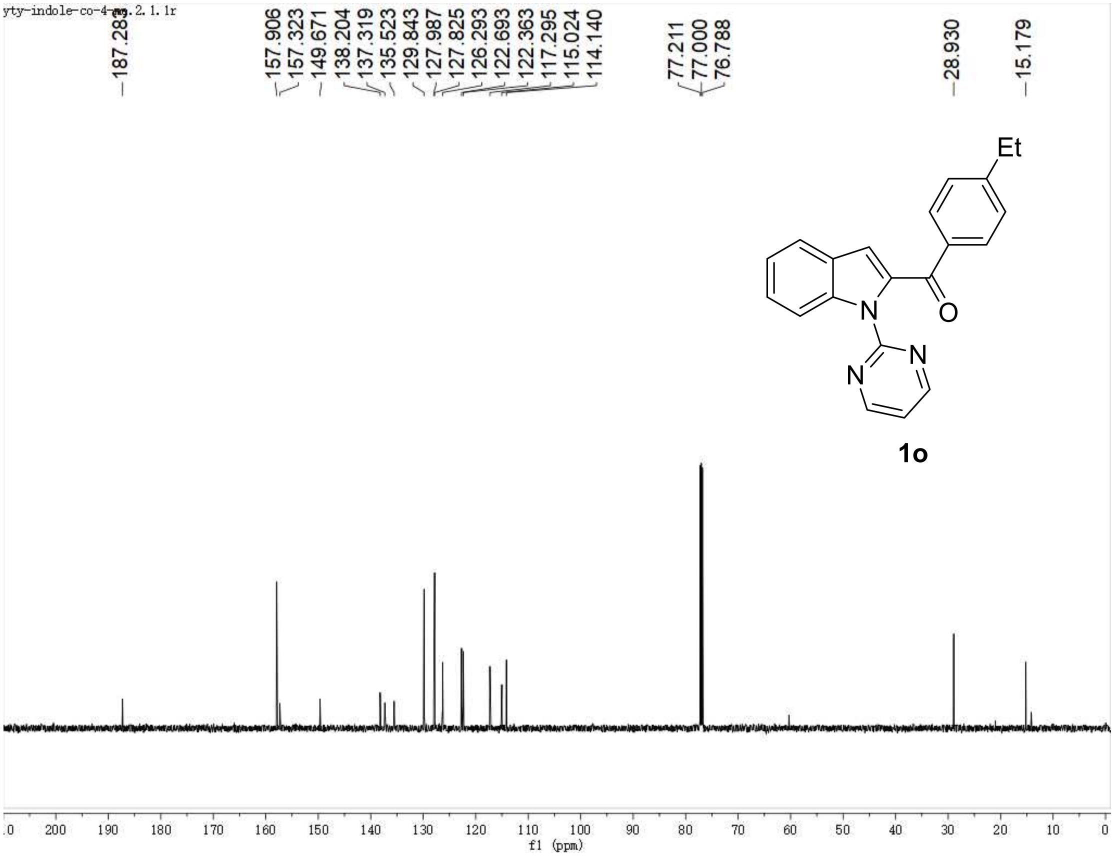
^{13}C NMR spectrum of compound **1n** ($CDCl_3$, 151 MHz)



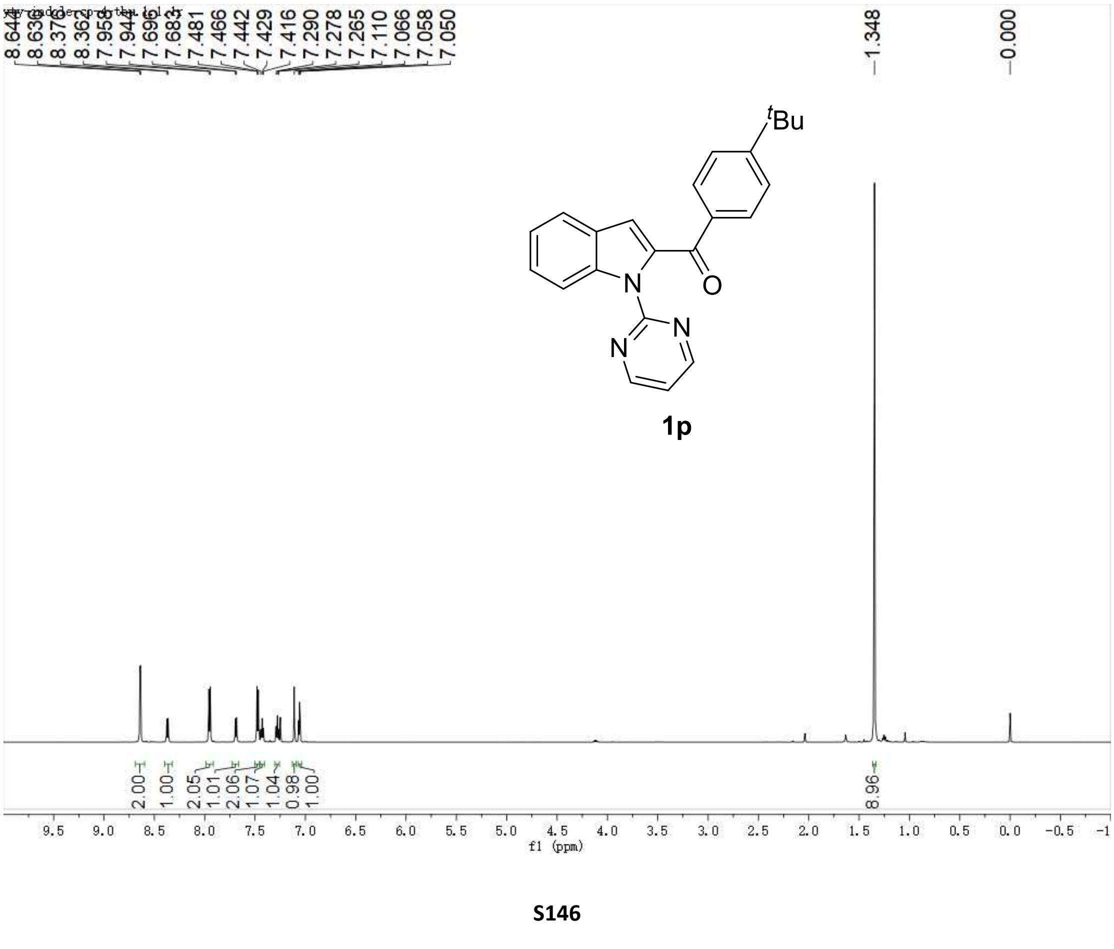
^{1}H NMR spectrum of compound **1o** ($CDCl_3$, 400 MHz)



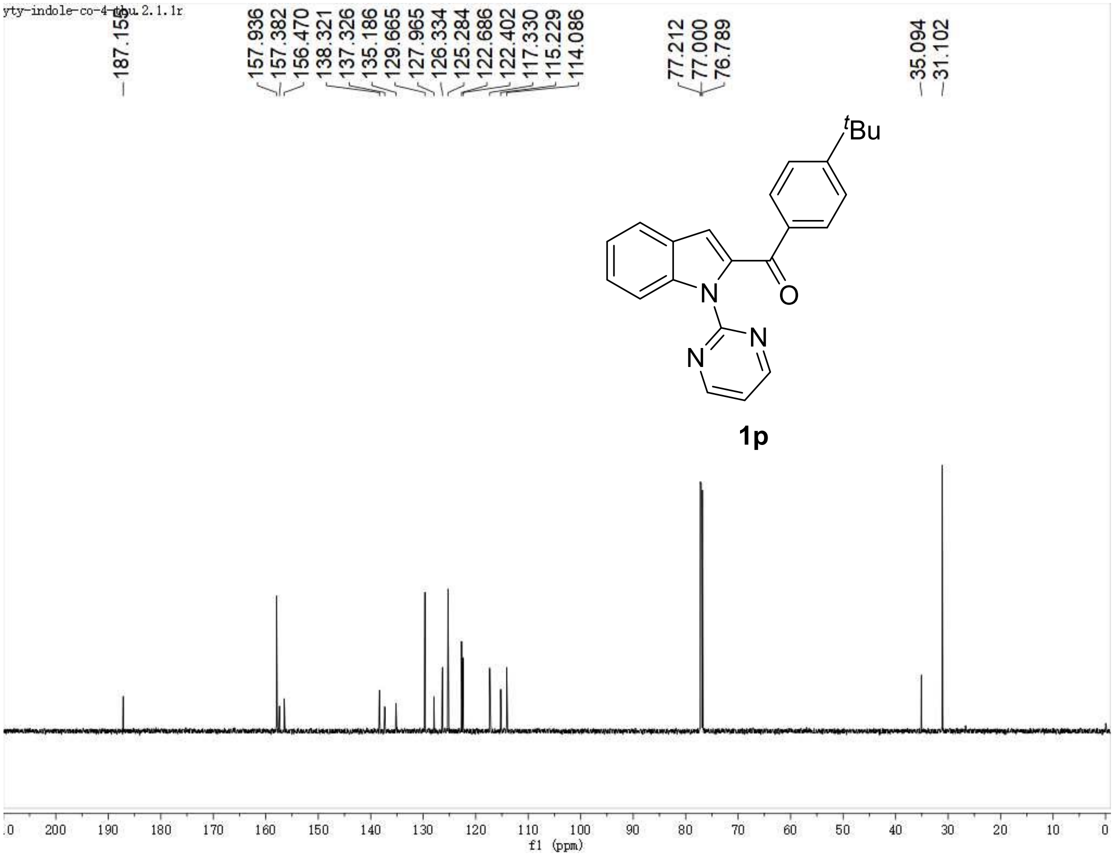
^{13}C NMR spectrum of compound **1o** ($CDCl_3$, 151 MHz)



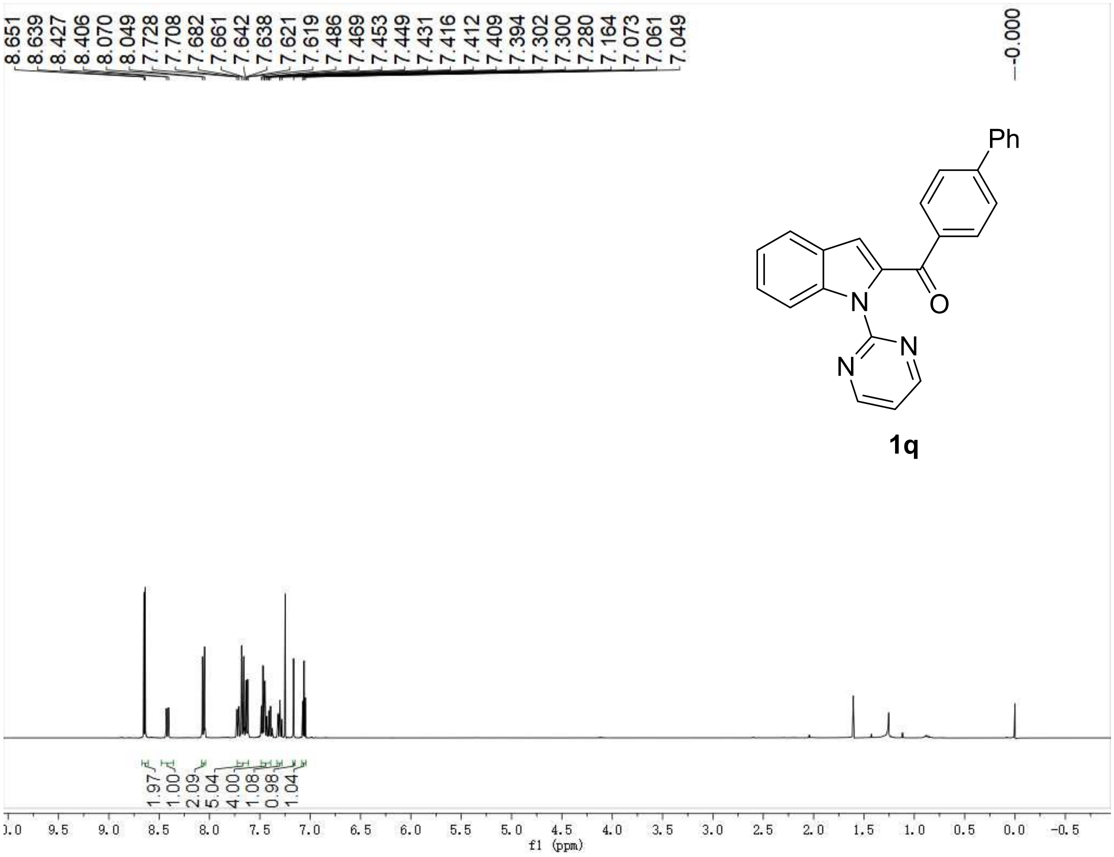
^{1}H NMR spectrum of compound **1p** ($CDCl_3$, 600 MHz)



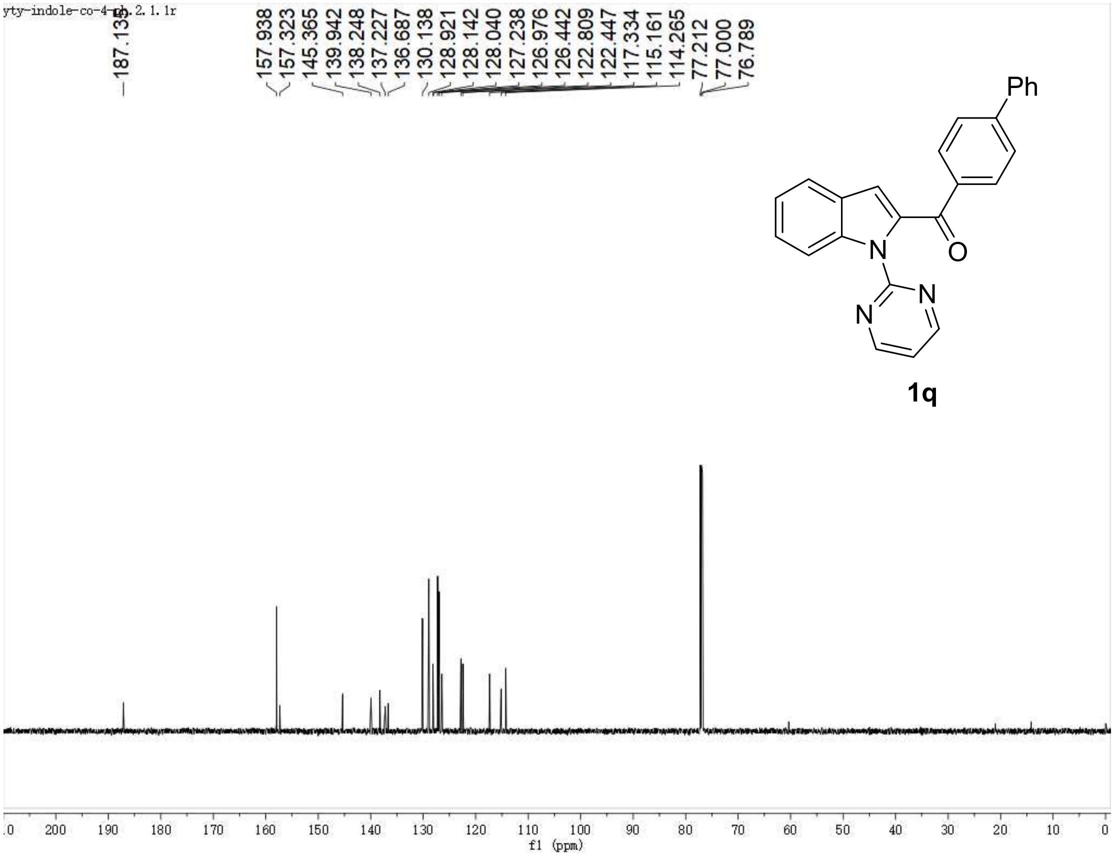
^{13}C NMR spectrum of compound **1p** ($CDCl_3$, 151 MHz)



^{1}H NMR spectrum of compound **1q** ($CDCl_3$, 400 MHz)

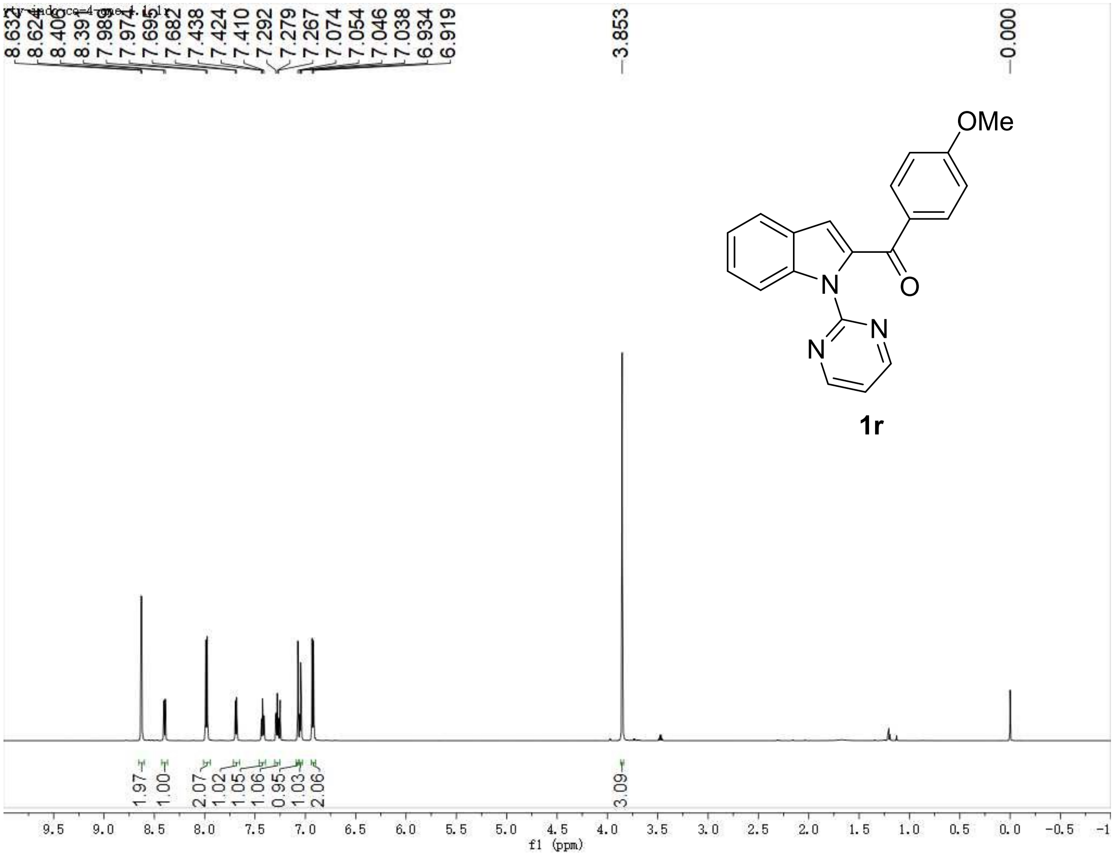


^{13}C NMR spectrum of compound **1q** ($CDCl_3$, 151 MHz)



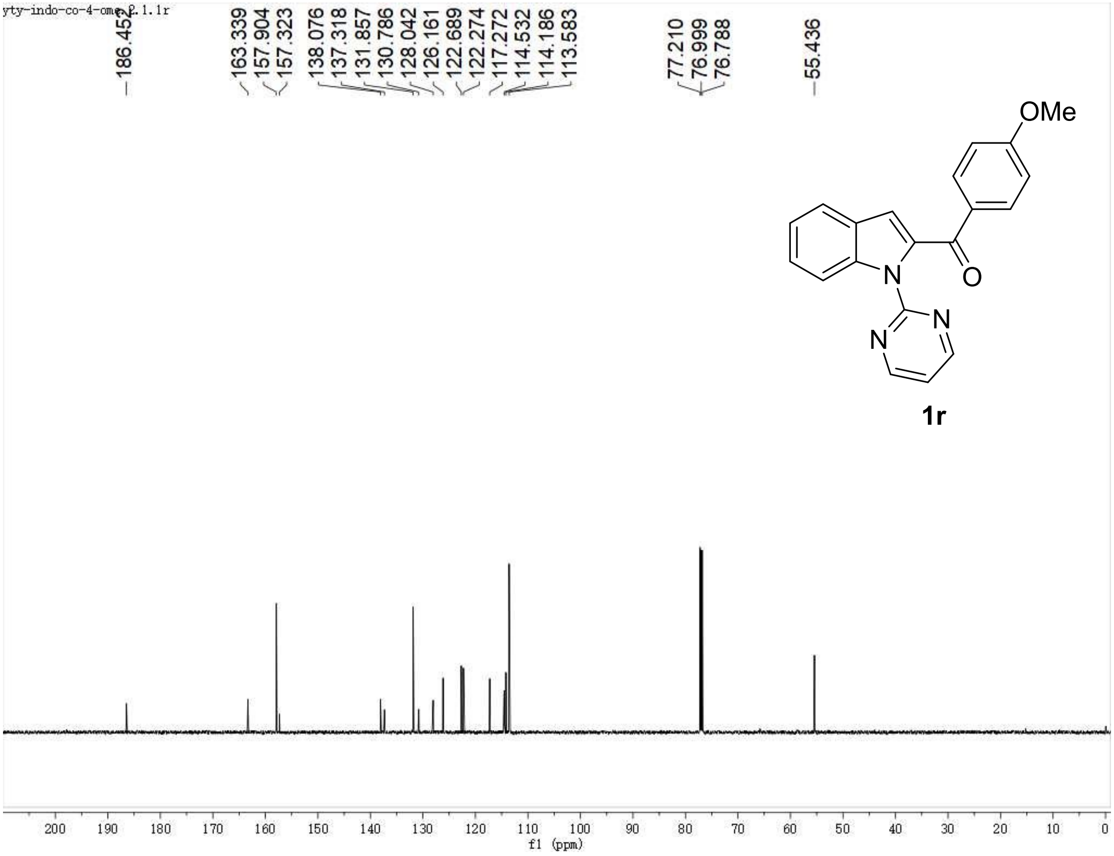
1q

^{1}H NMR spectrum of compound **1r** ($CDCl_3$, 600 MHz)

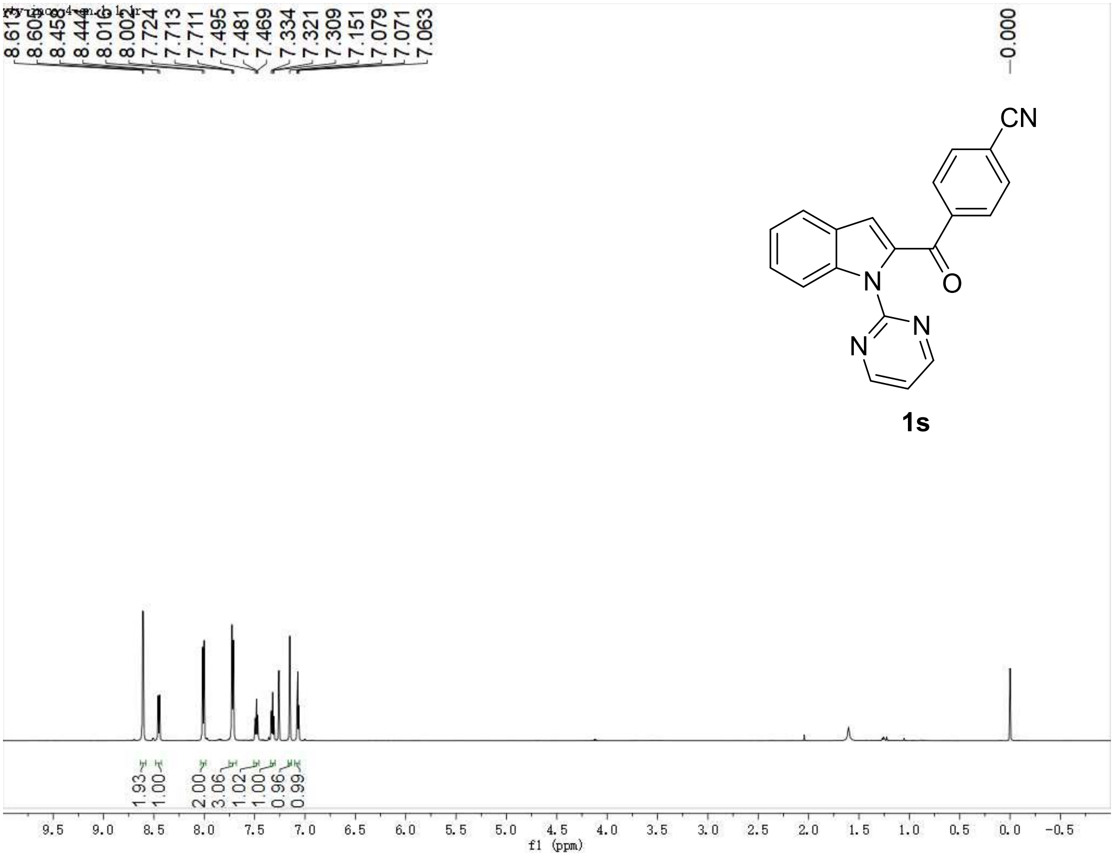


1r

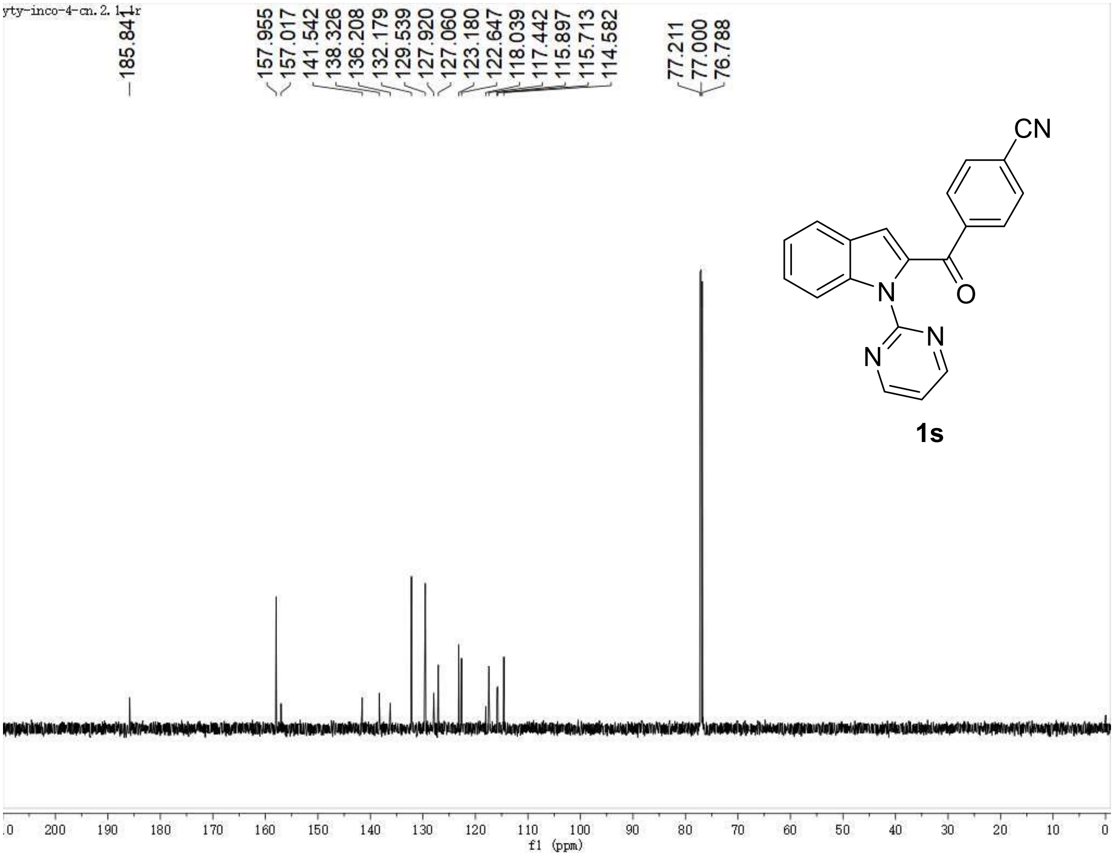
^{13}C NMR spectrum of compound **1r** ($CDCl_3$, 151 MHz)



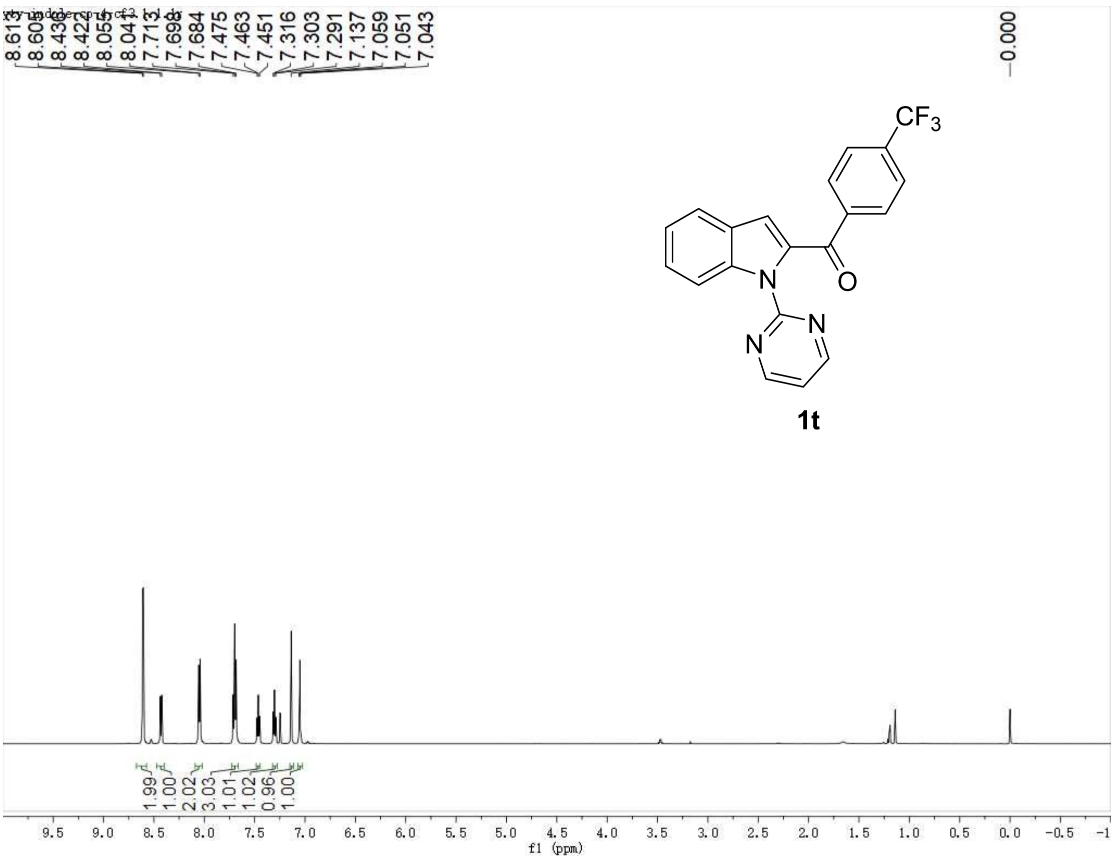
^{1}H NMR spectrum of compound **1s** ($CDCl_3$, 600 MHz)



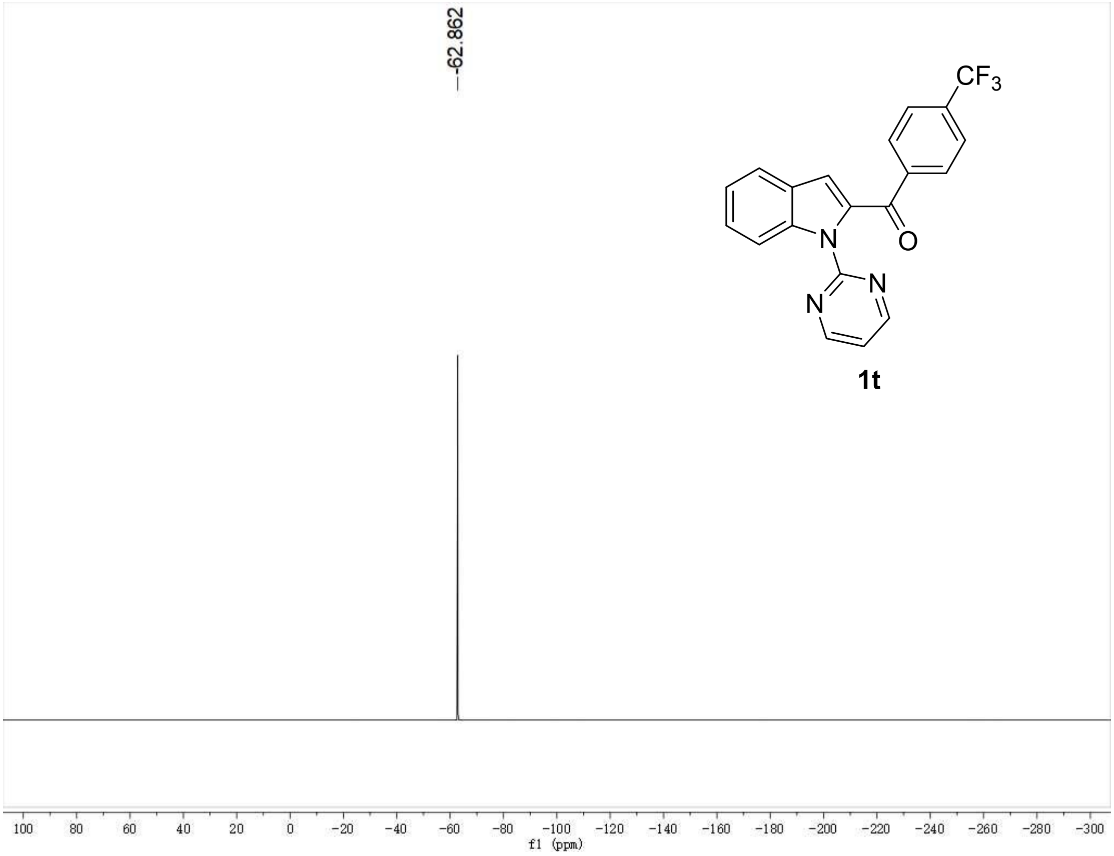
[13]C NMR spectrum of compound **1s** ($CDCl_3$, 151 MHz)



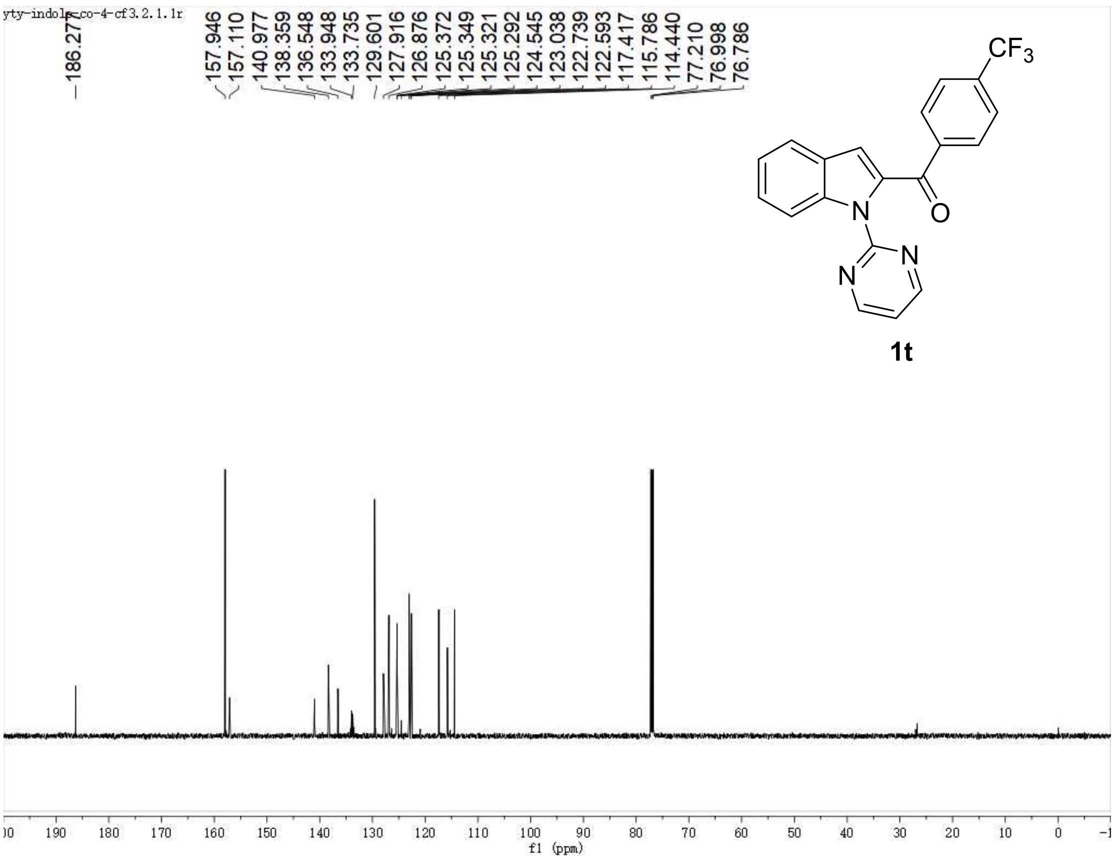
[1]H NMR spectrum of compound **1t** ($CDCl_3$, 600 MHz)



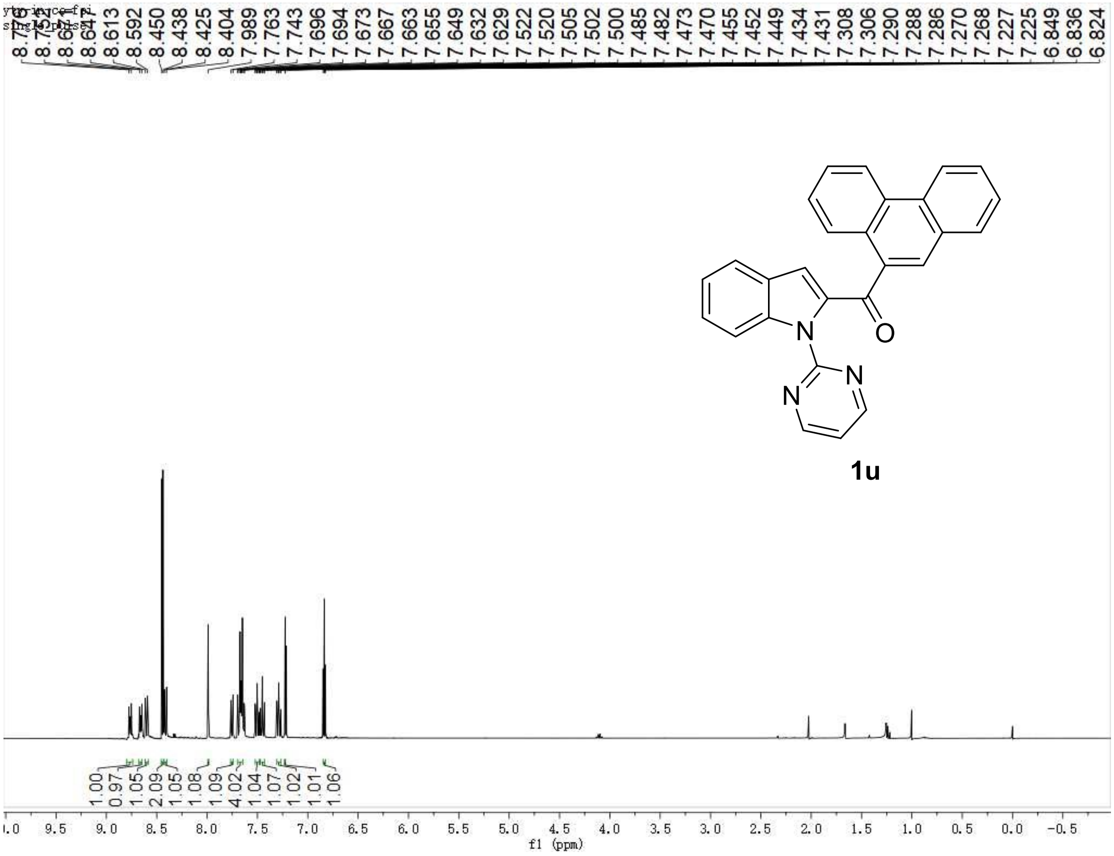
^{19}F NMR spectrum of compound **1t** ($CDCl_3$, 376 MHz)



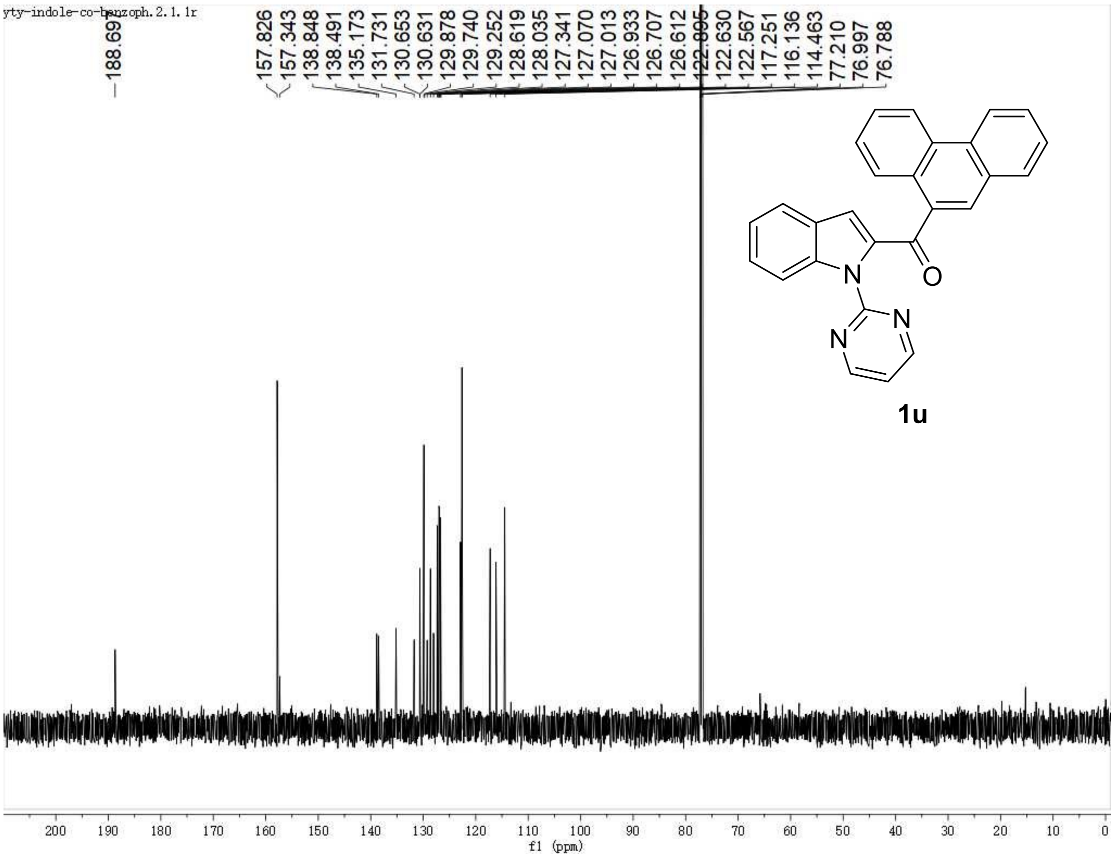
^{13}C NMR spectrum of compound **1t** ($CDCl_3$, 151 MHz)



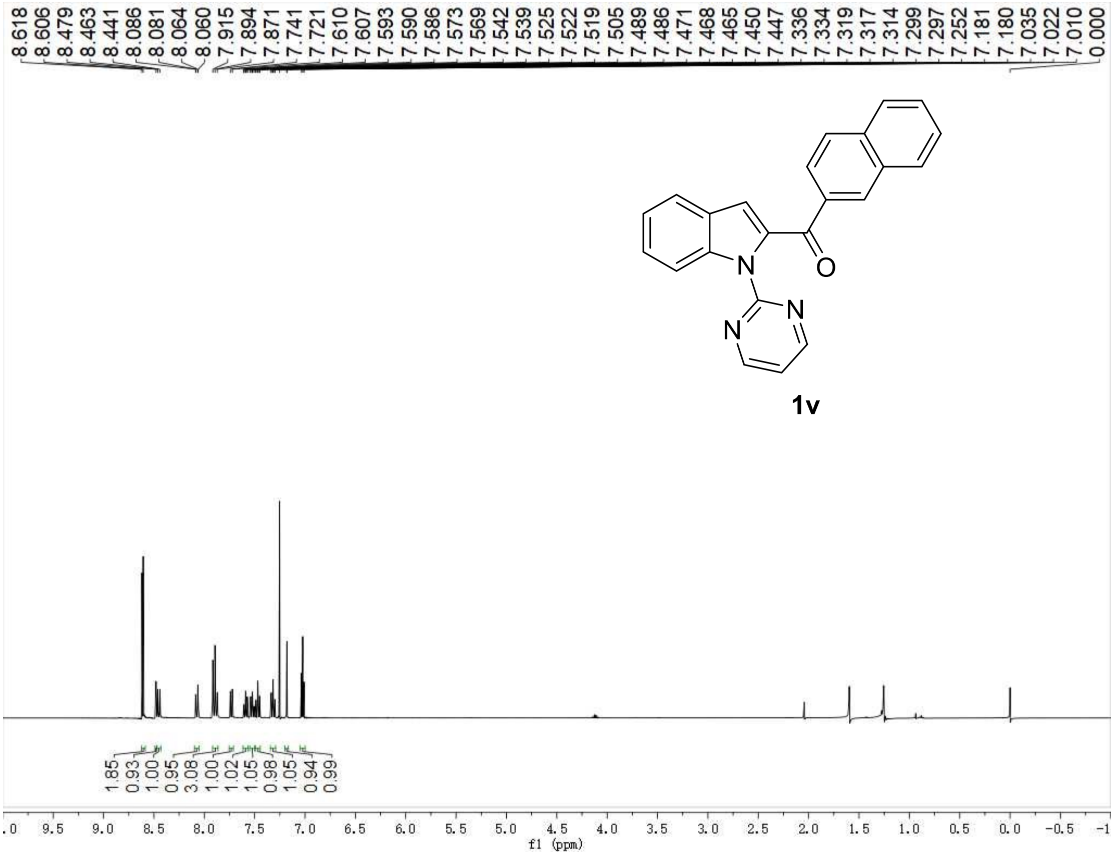
^1H NMR spectrum of compound **1u** ($CDCl_3$, 400 MHz)



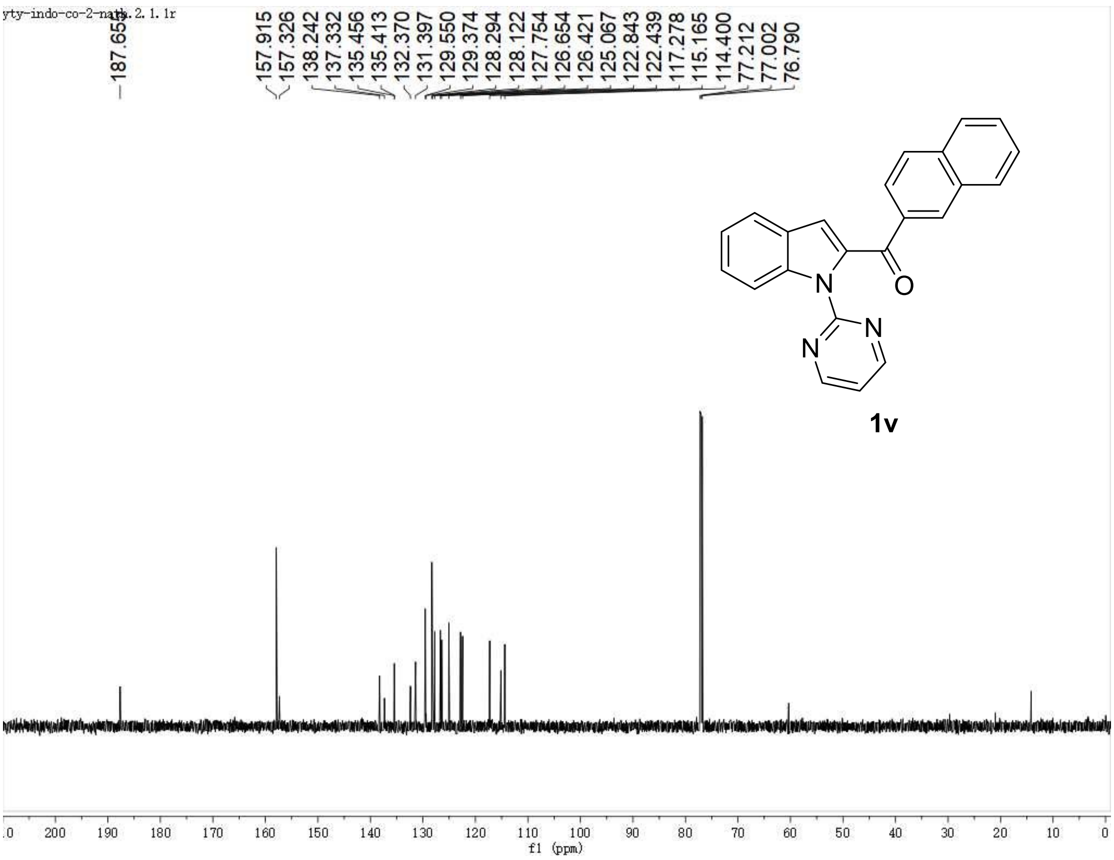
^{13}C NMR spectrum of compound **1u** ($CDCl_3$, 151 MHz)



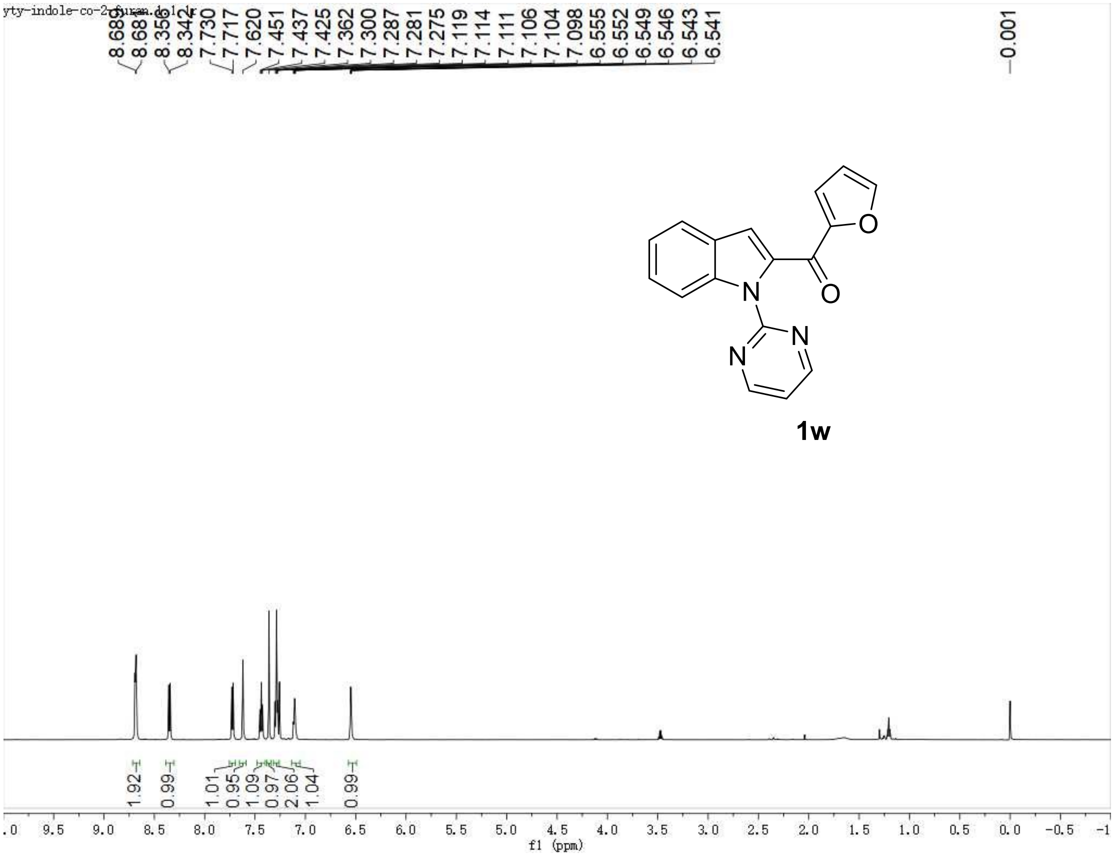
[1]H NMR spectrum of compound **1v** ($CDCl_3$, 400 MHz)



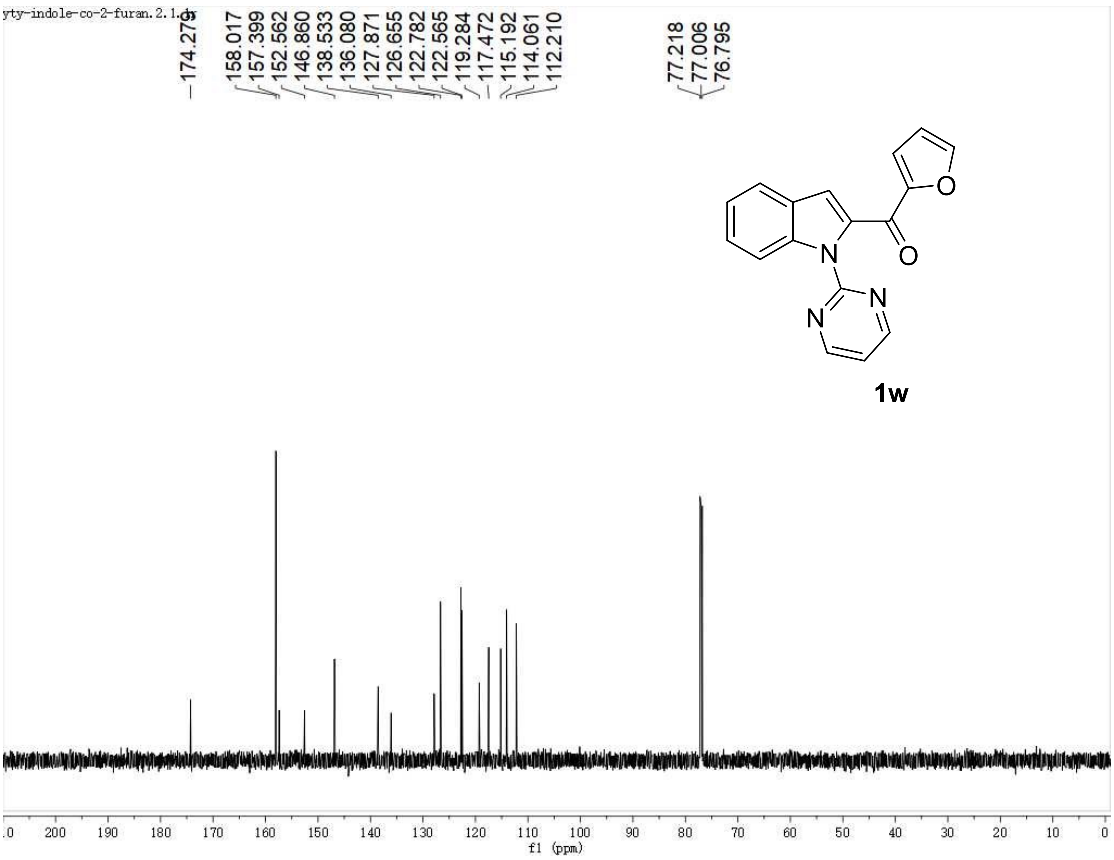
[13]C NMR spectrum of compound **1v** ($CDCl_3$, 151 MHz)



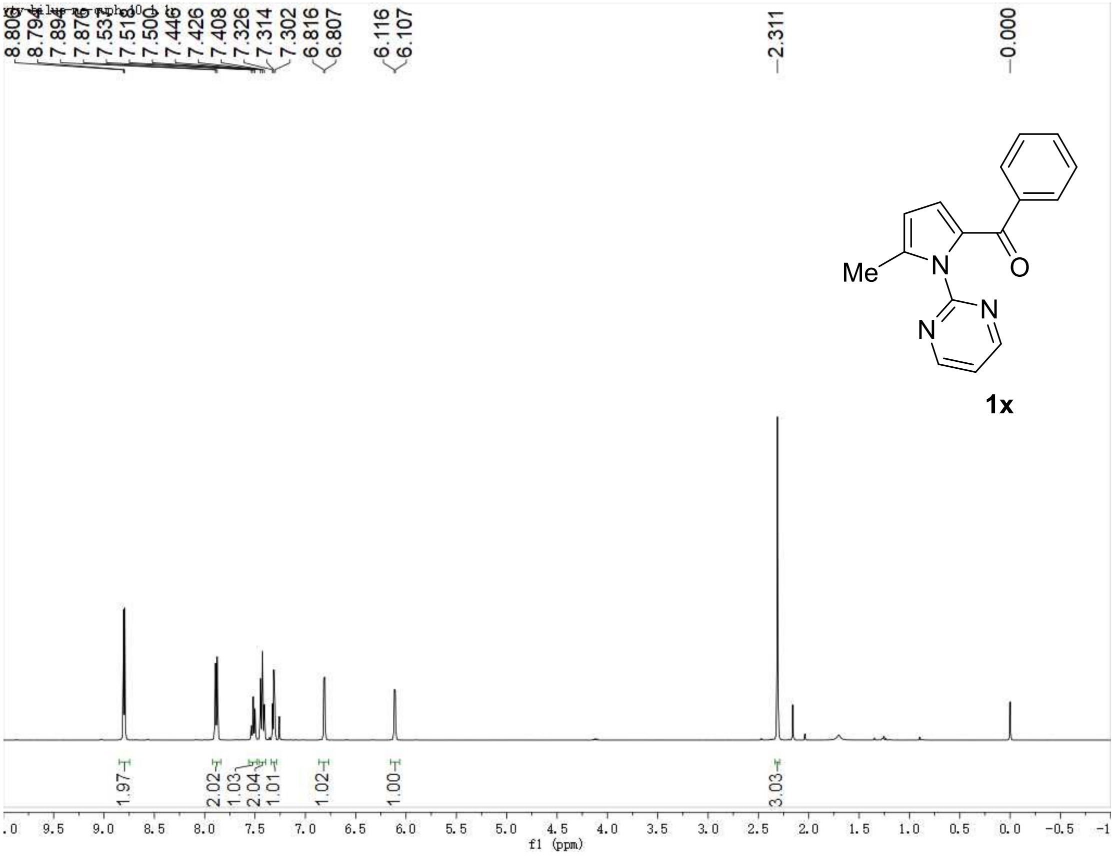
^1H NMR spectrum of compound **1w** ($CDCl_3$, 600 MHz)



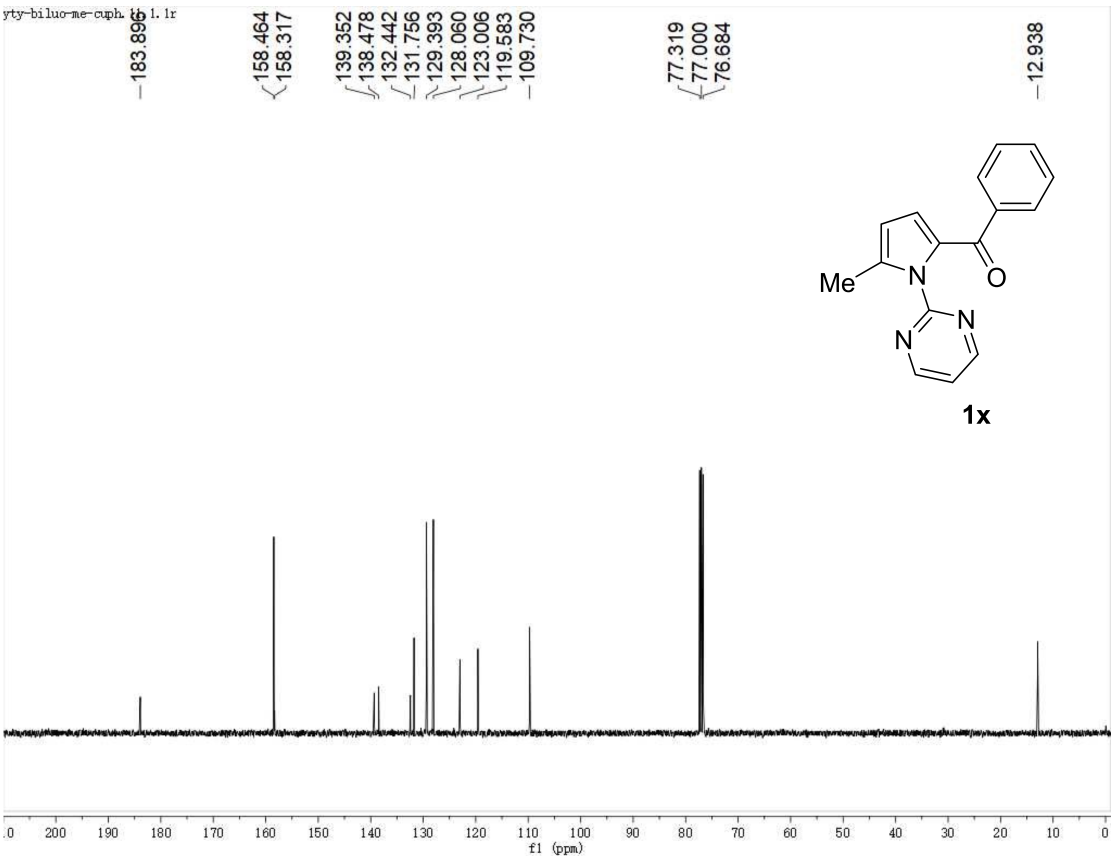
^{13}C NMR spectrum of compound **1w** ($CDCl_3$, 151 MHz)



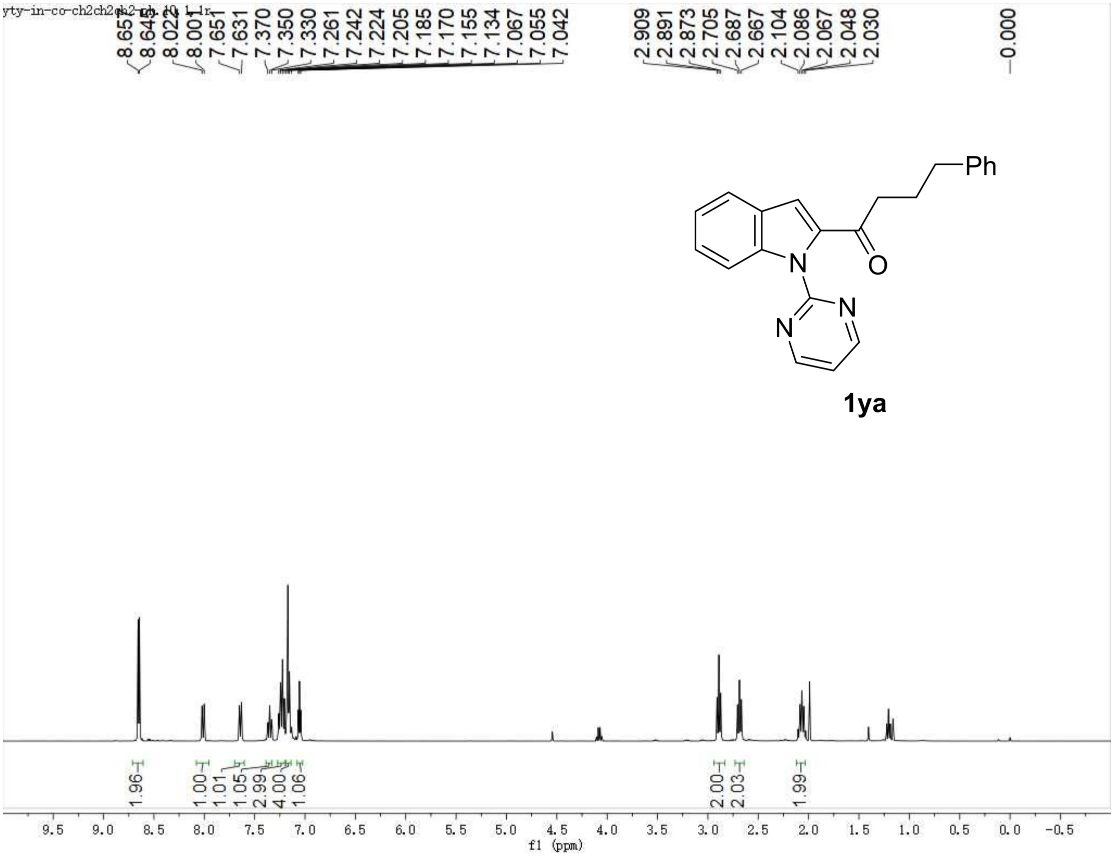
^{1}H NMR spectrum of compound **1x** ($CDCl_3$, 400 MHz)



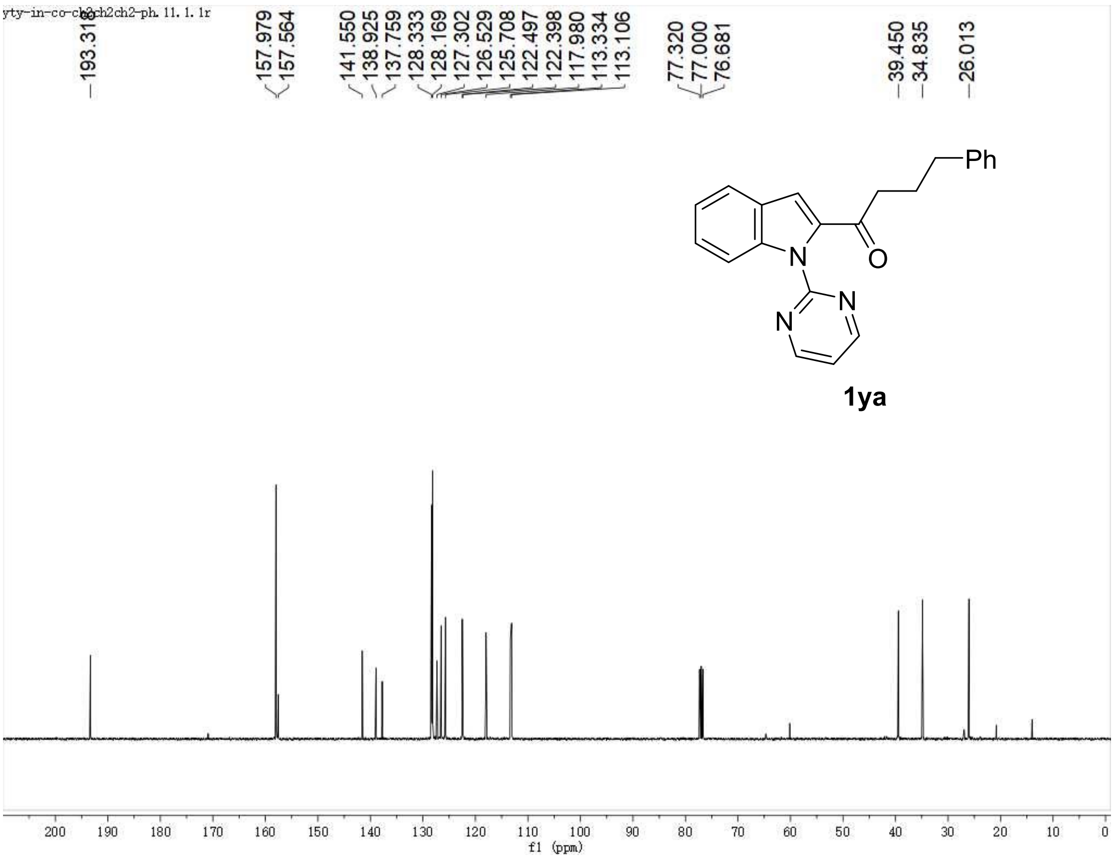
^{13}C NMR spectrum of compound **1x** ($CDCl_3$, 101 MHz)



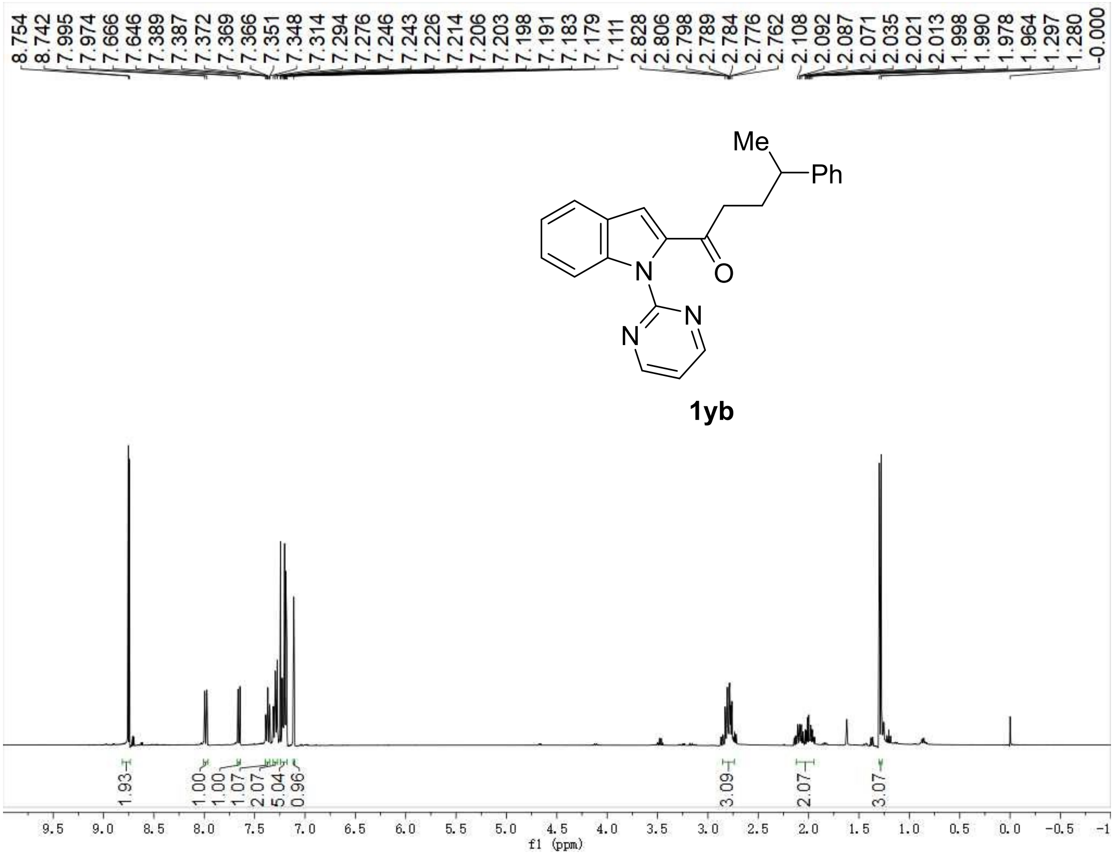
^{1}H NMR spectrum of compound **1ya** ($CDCl_3$, 400 MHz)



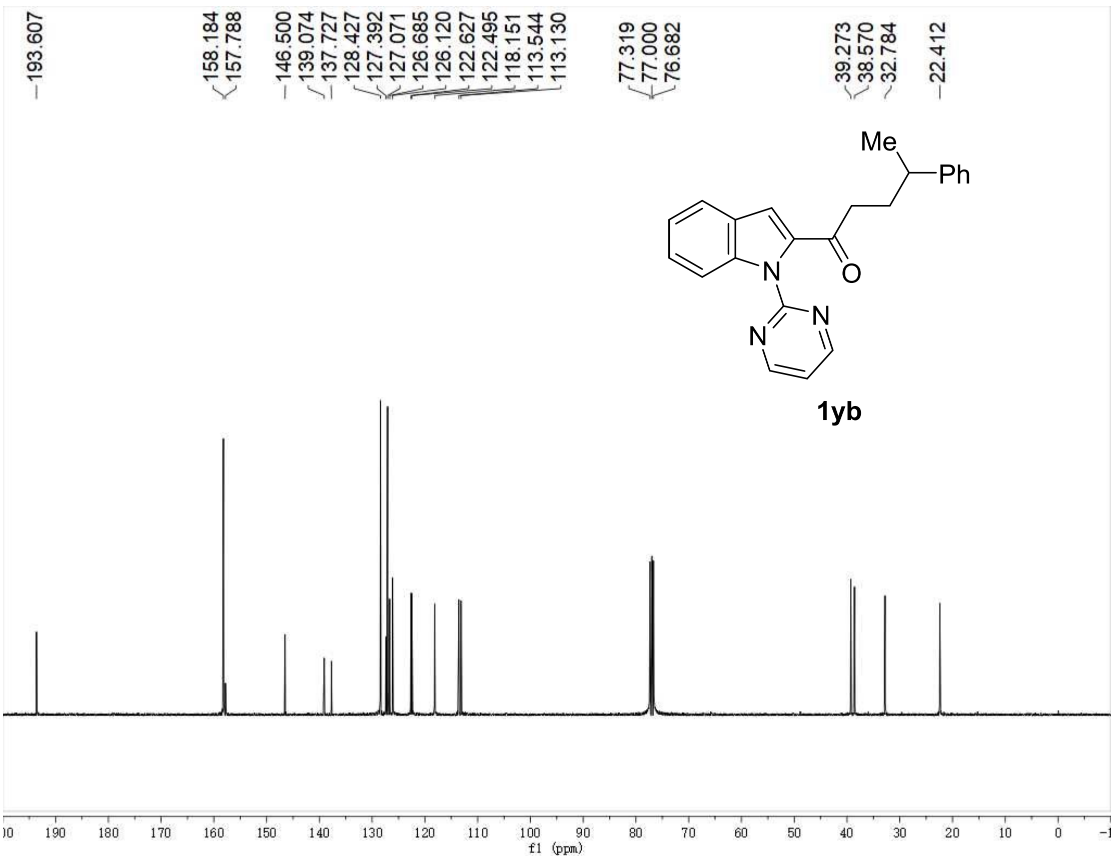
^{13}C NMR spectrum of compound **1ya** ($CDCl_3$, 101 MHz)



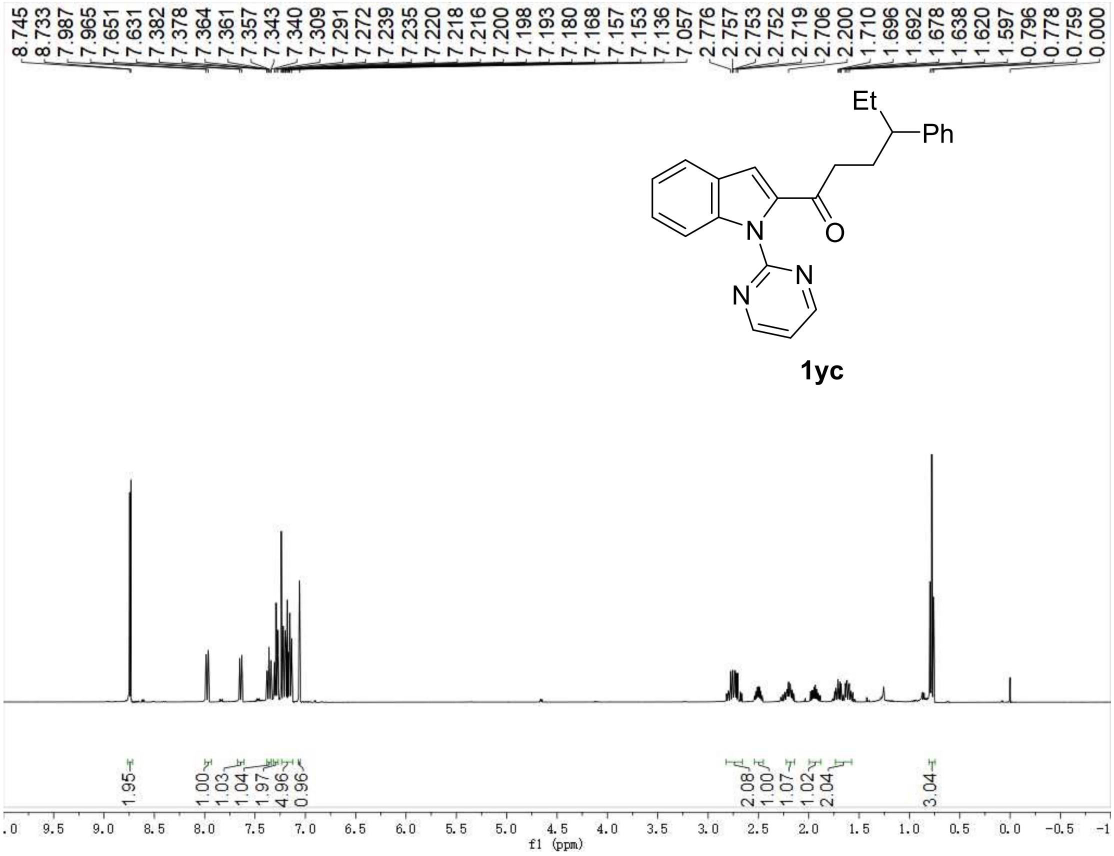
[1]H NMR spectrum of compound **1yb** ($CDCl_3$, 400 MHz)



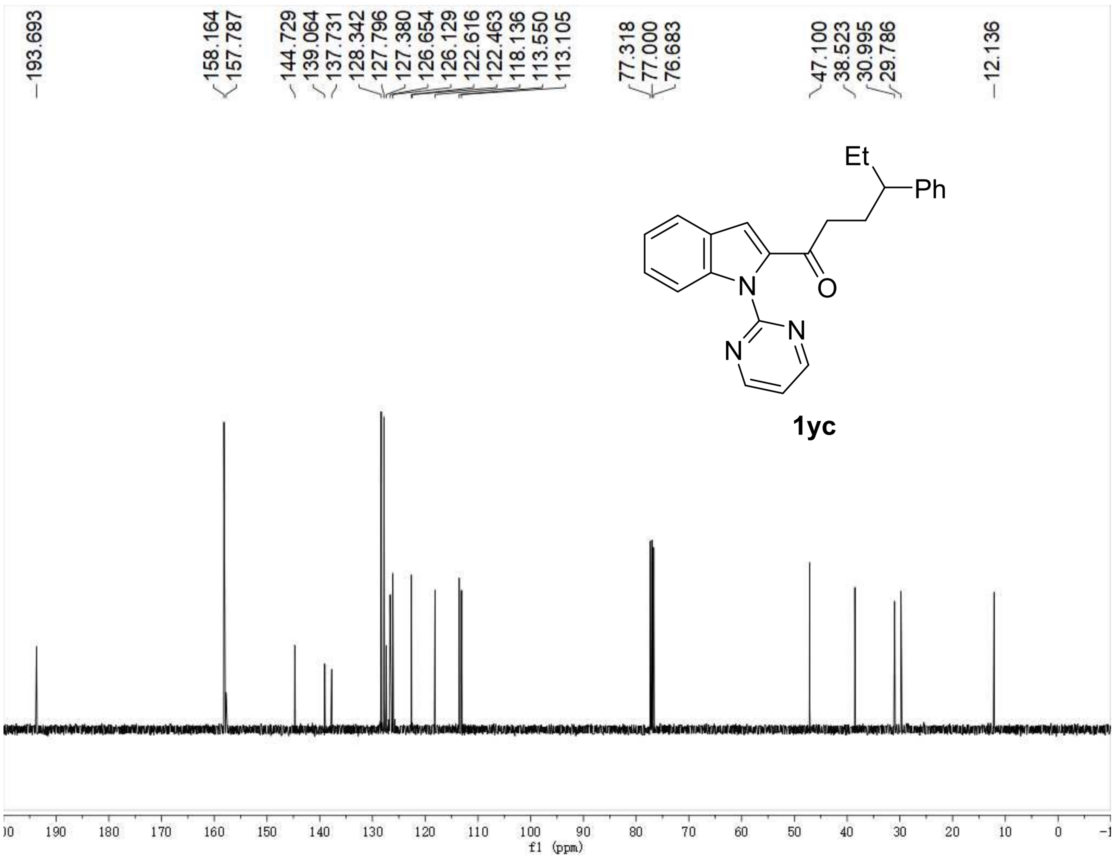
[13]C NMR spectrum of compound **1yb** ($CDCl_3$, 101 MHz)



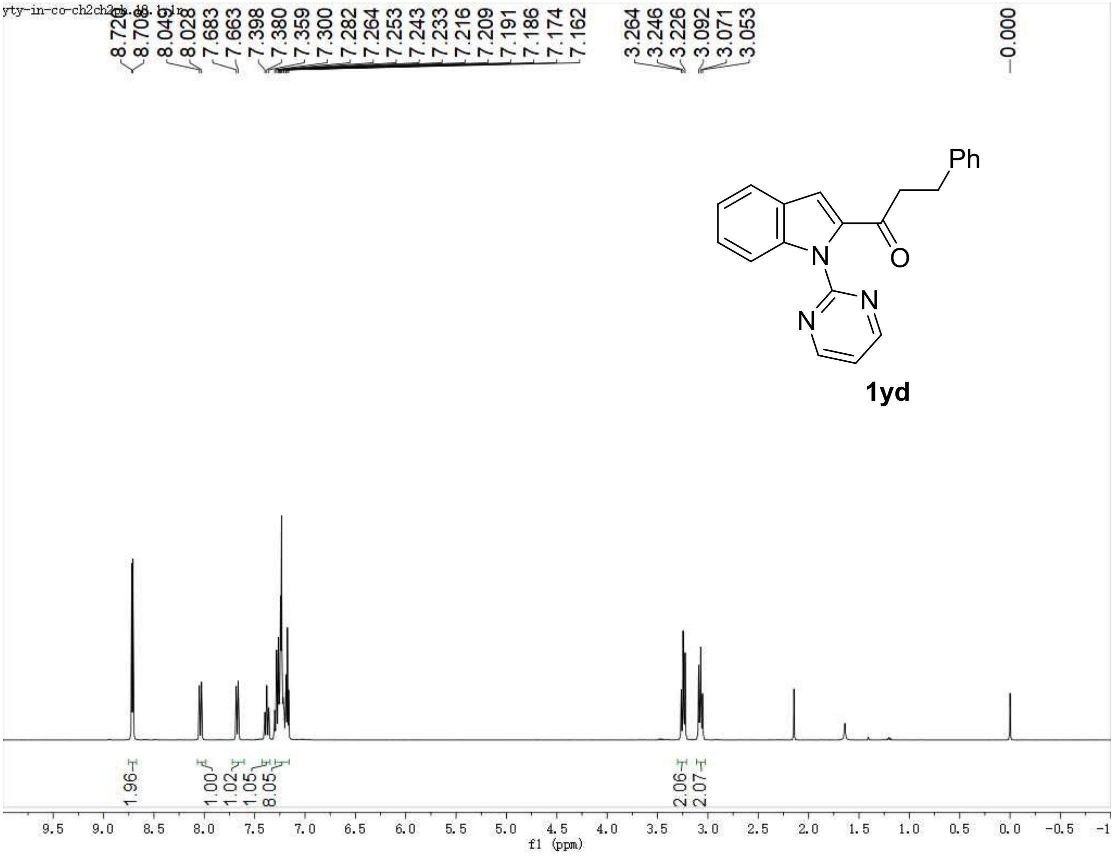
[1]H NMR spectrum of compound **1yc** ($CDCl_3$, 400 MHz)



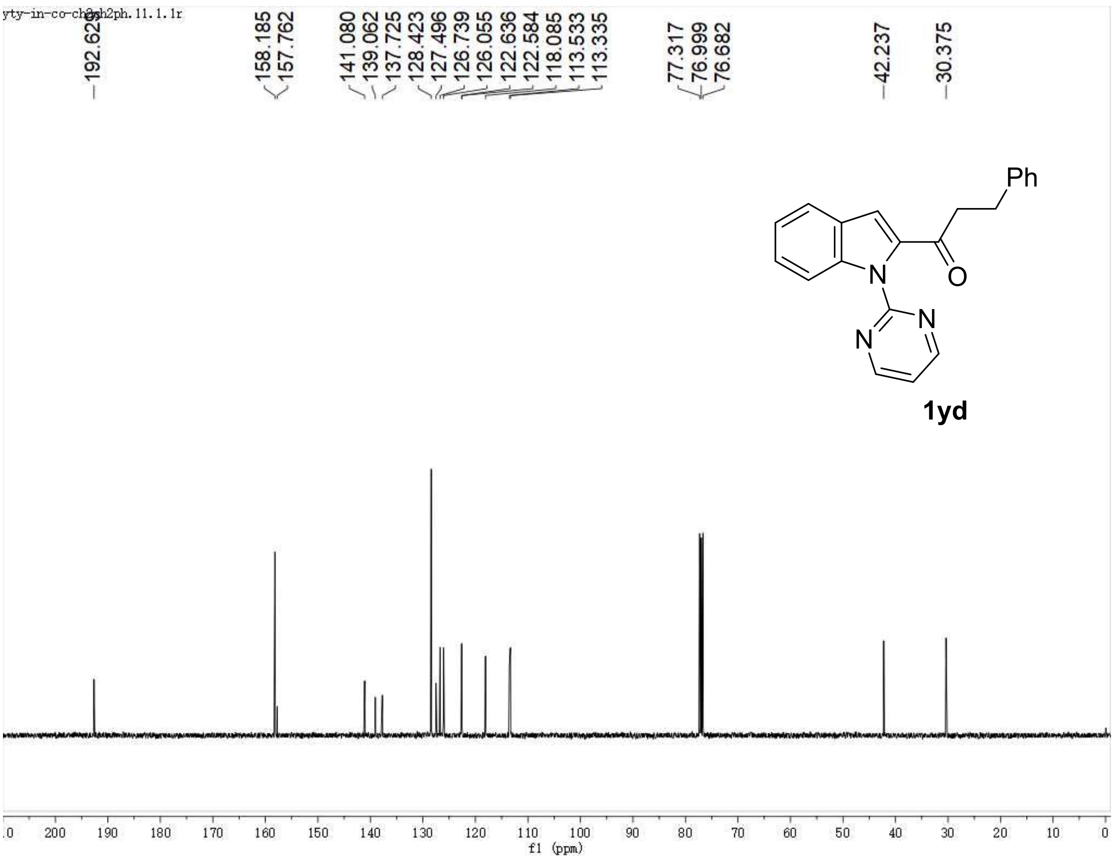
[13]C NMR spectrum of compound **1yc** ($CDCl_3$, 101 MHz)



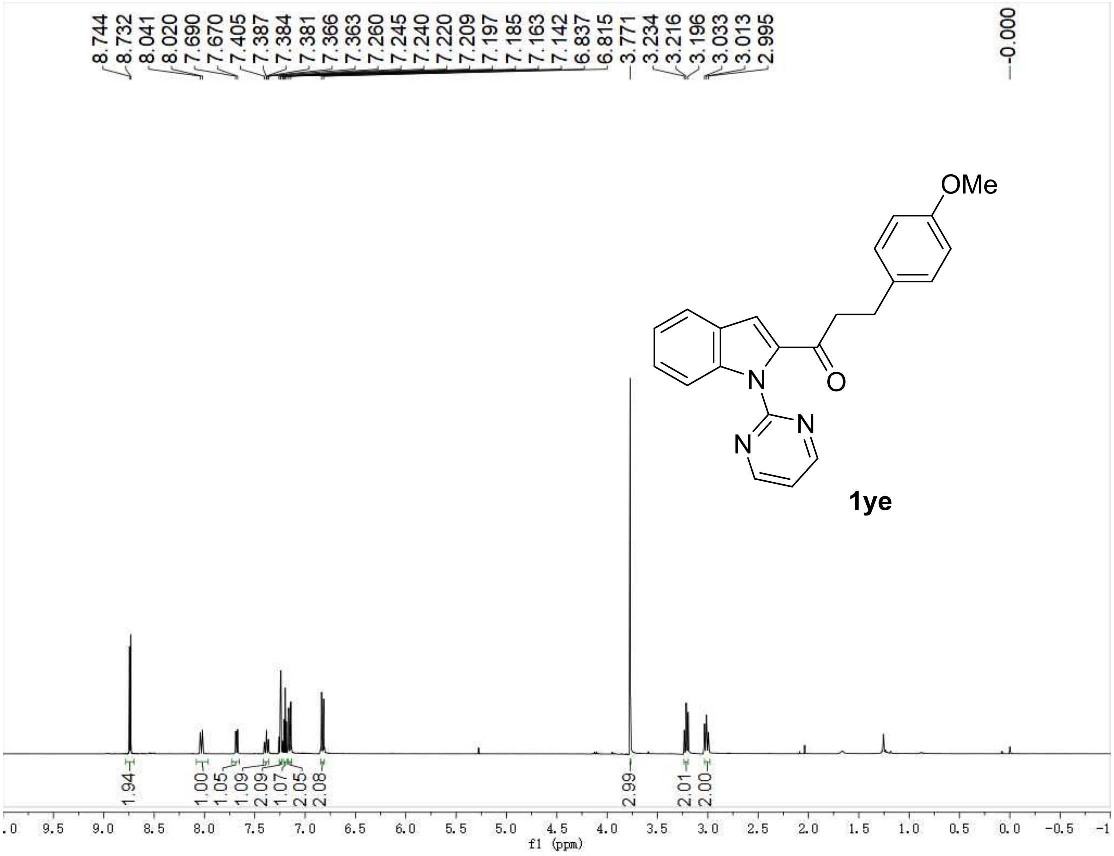
^{1}H NMR spectrum of compound **1yd** ($CDCl_3$, 400 MHz)



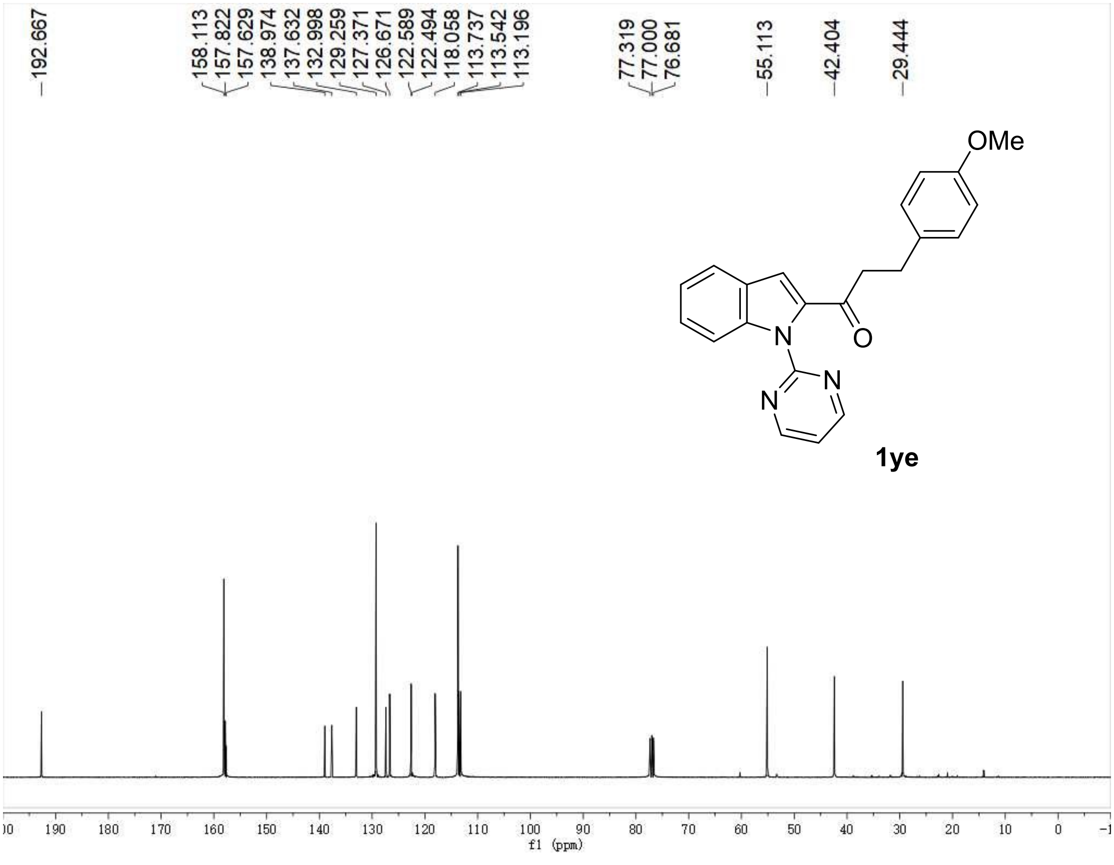
^{13}C NMR spectrum of compound **1yd** ($CDCl_3$, 101 MHz)



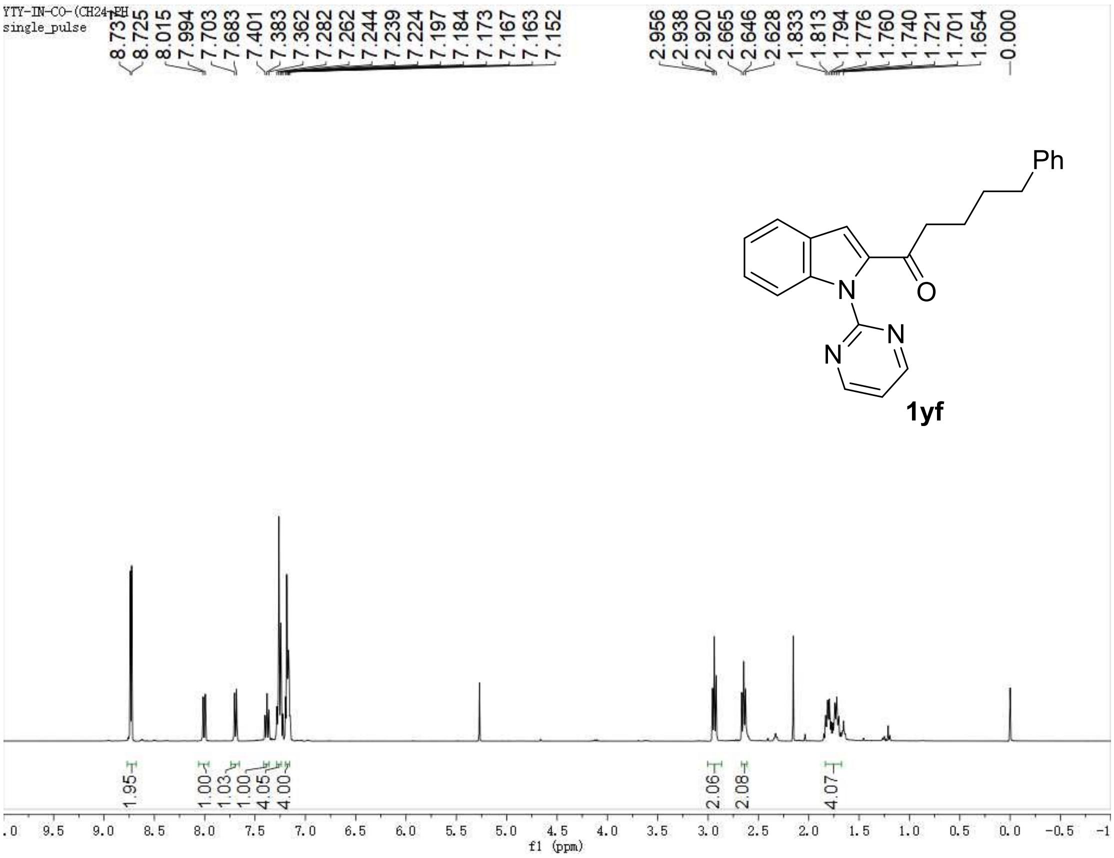
^{1}H NMR spectrum of compound **1ye** ($CDCl_3$, 400 MHz)



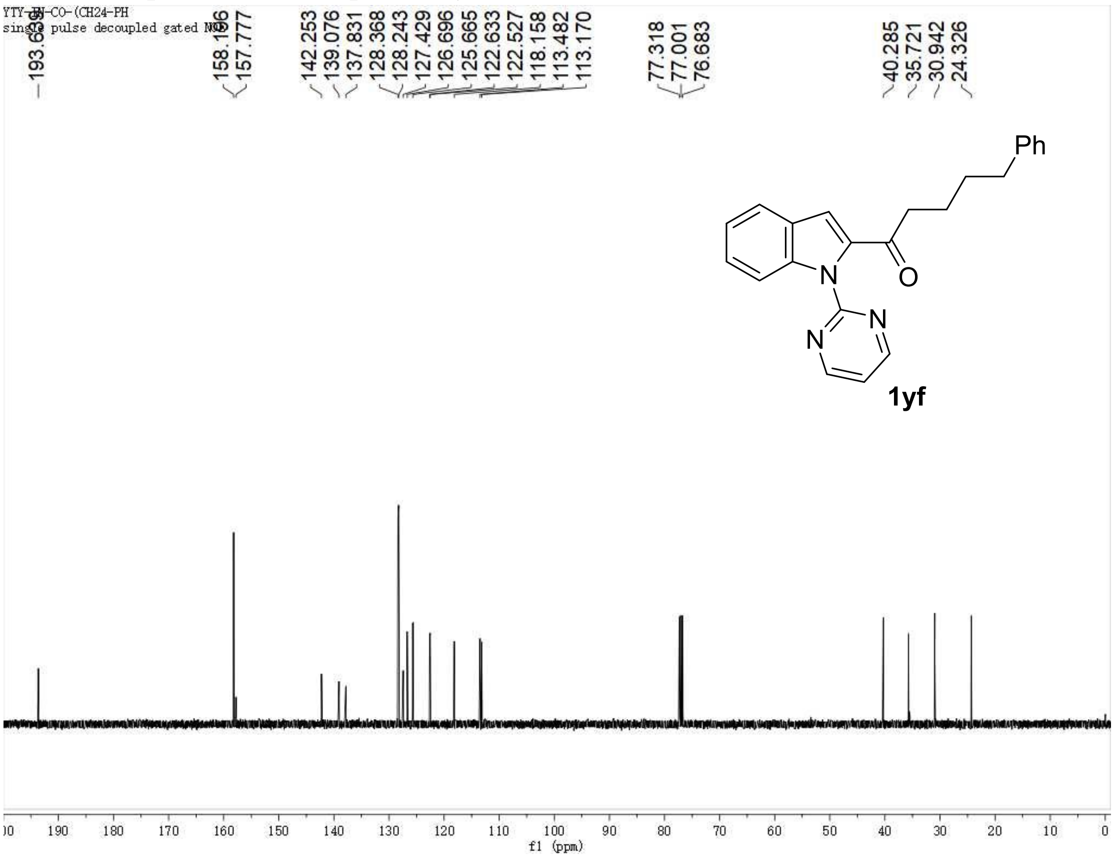
^{13}C NMR spectrum of compound **1ye** ($CDCl_3$, 101 MHz)



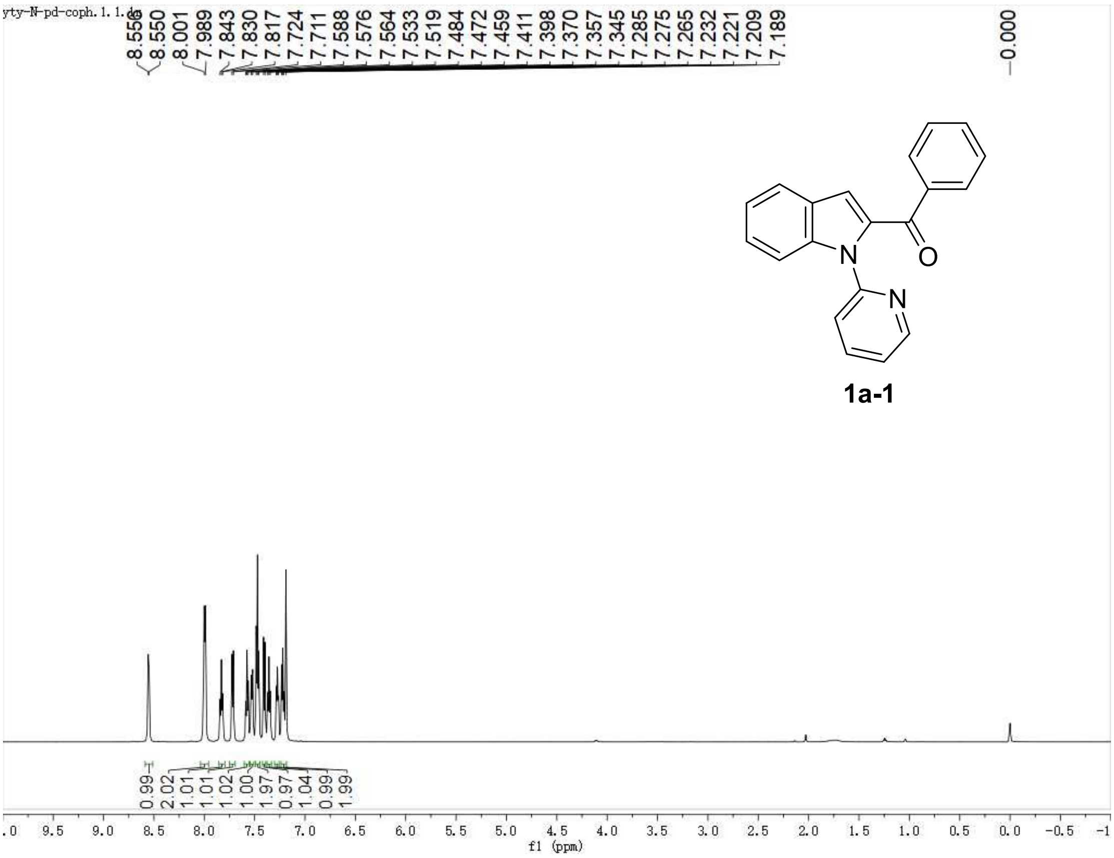
^{1}H NMR spectrum of compound **1yf** ($CDCl_3$, 400 MHz)



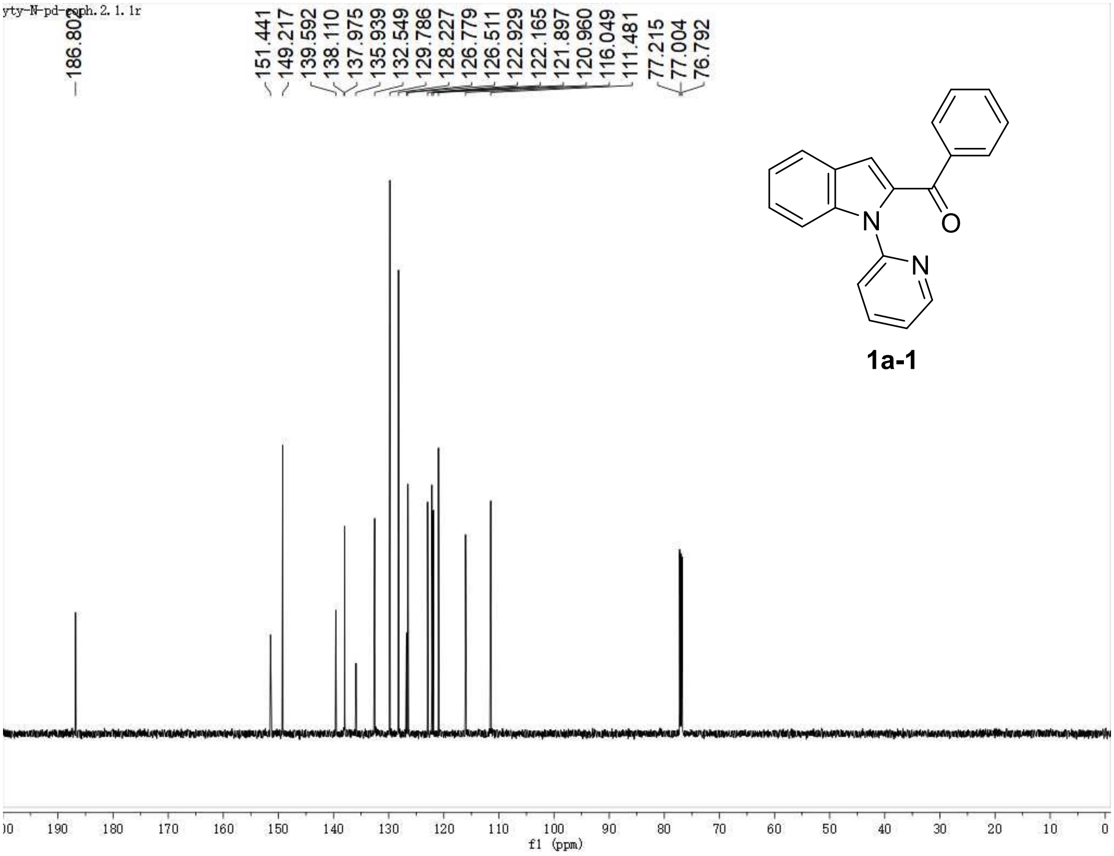
^{13}C NMR spectrum of compound **1yf** ($CDCl_3$, 101 MHz)



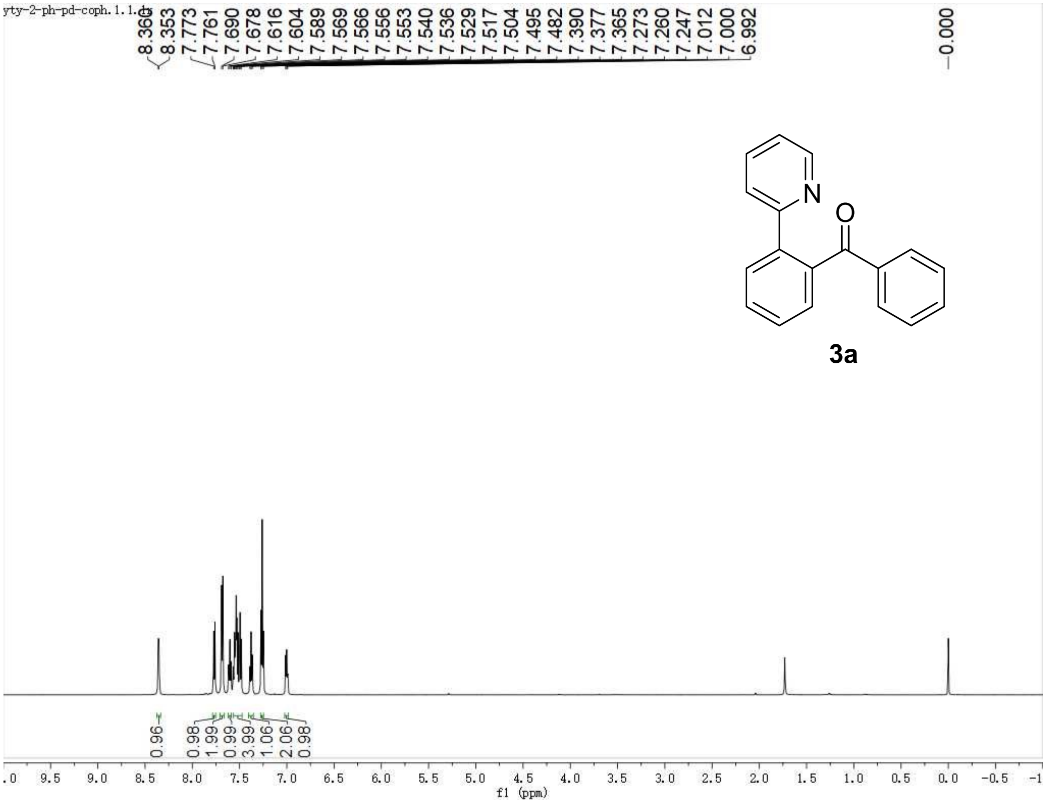
^{1}H NMR spectrum of compound **1a-1** ($CDCl_3$, 600 MHz)



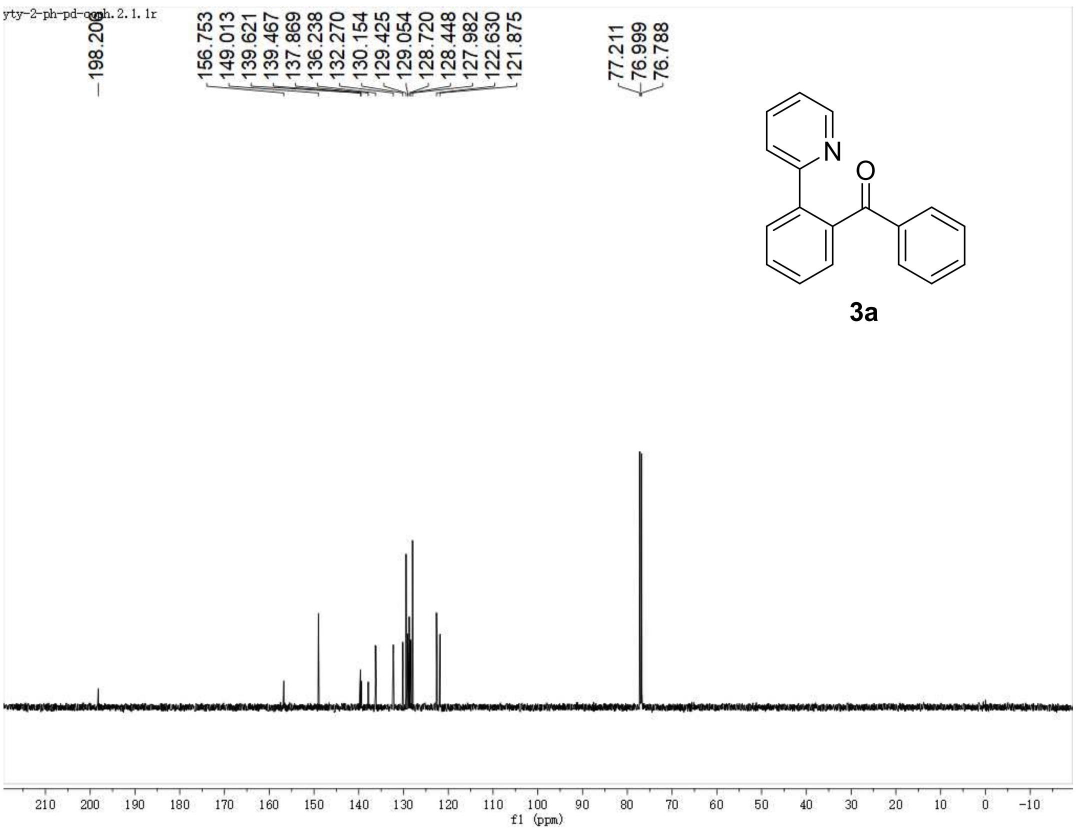
^{13}C NMR spectrum of compound **1a-1** ($CDCl_3$, 151 MHz)



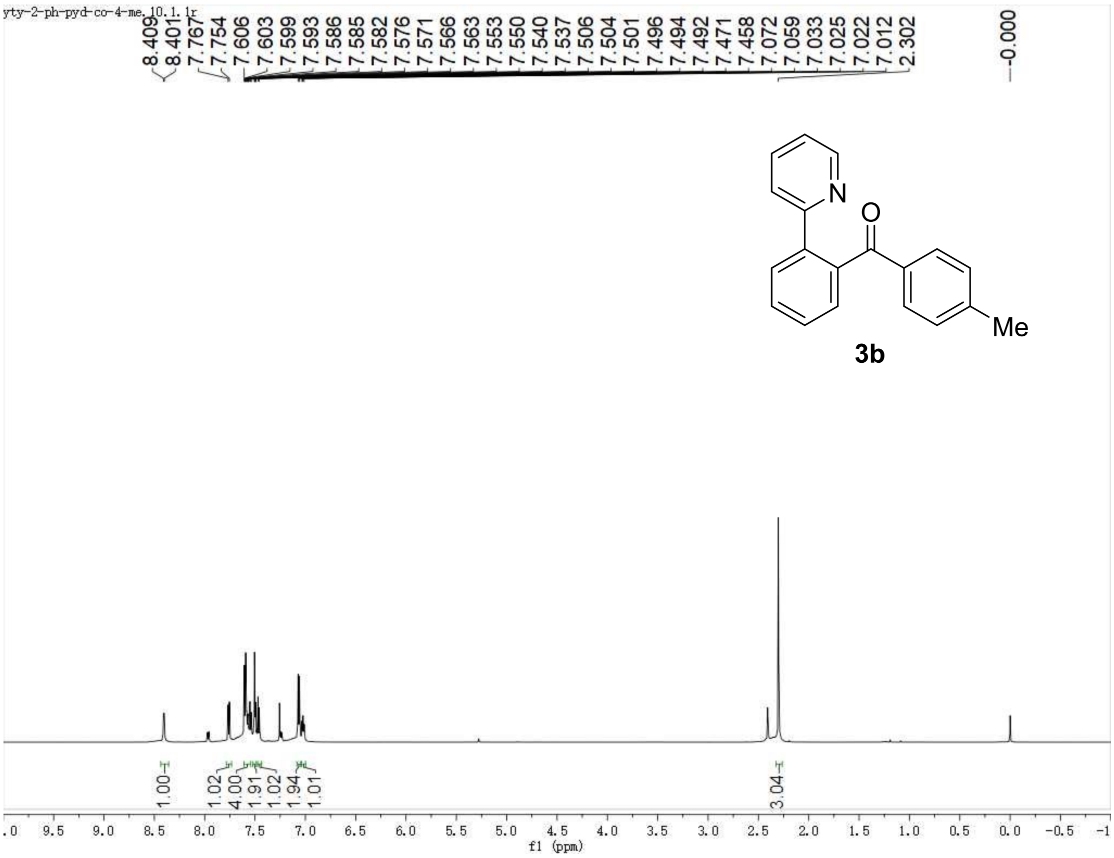
^{1}H NMR spectrum of compound **3a** ($CDCl_3$, 600 MHz)



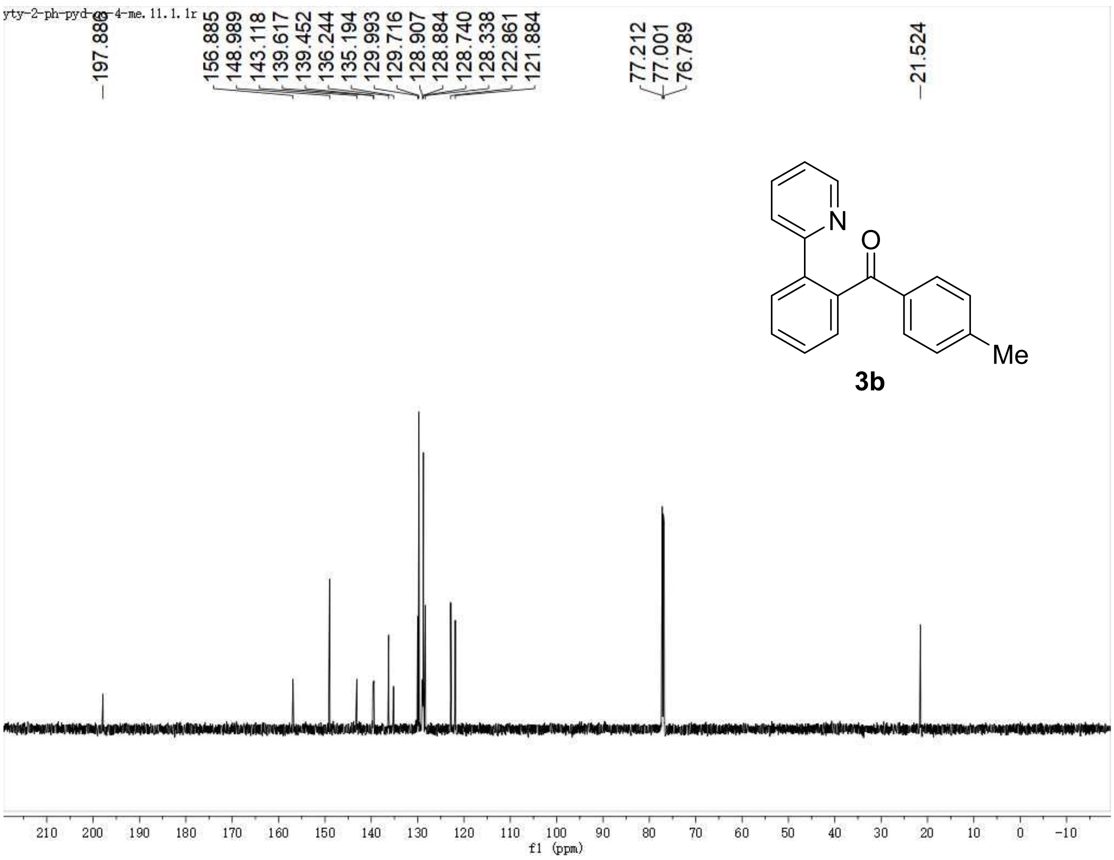
^{13}C NMR spectrum of compound **3a** ($CDCl_3$, 151 MHz)



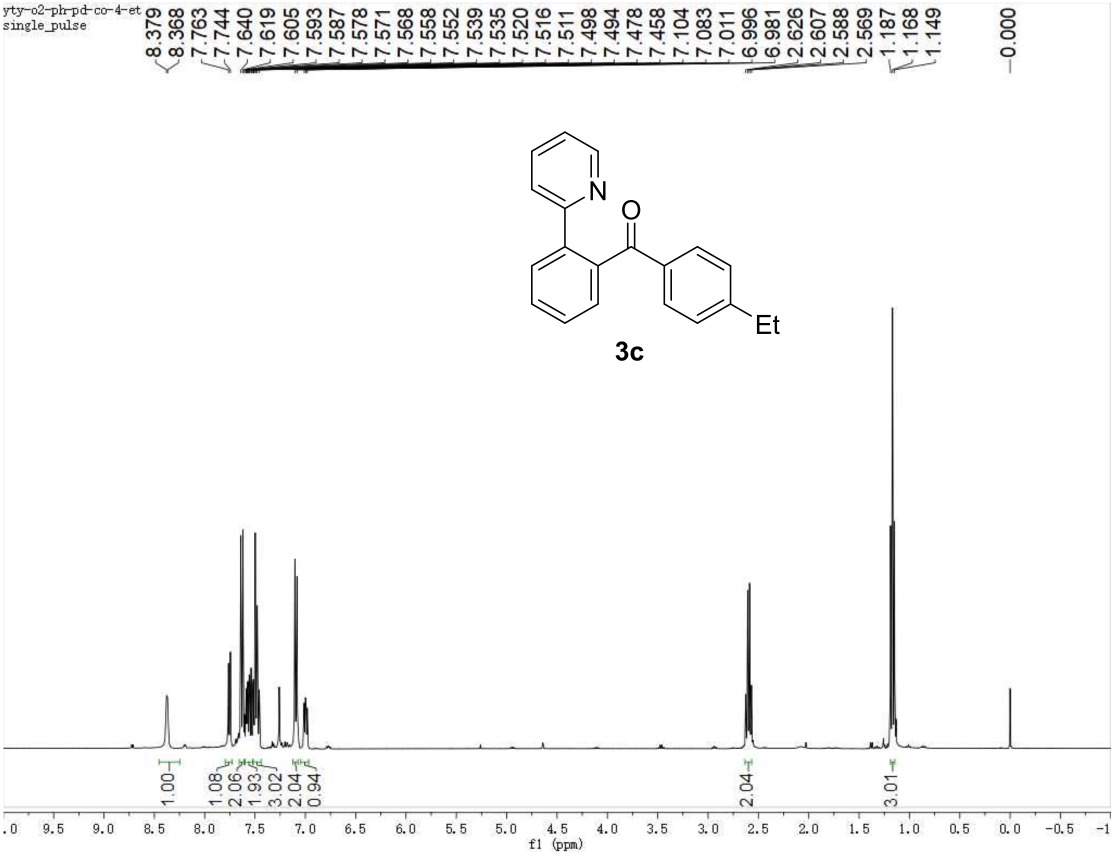
^{1}H NMR spectrum of compound **3b** ($CDCl_3$, 600 MHz)



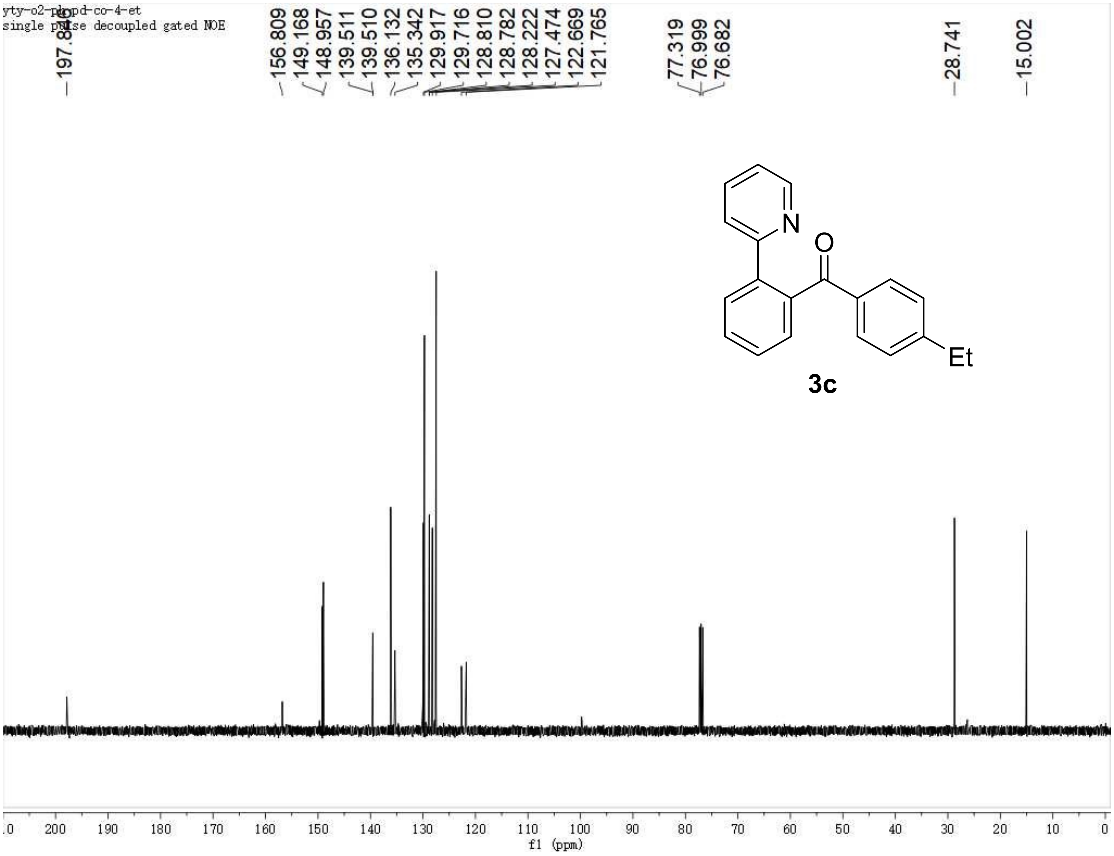
^{13}C NMR spectrum of compound **3b** ($CDCl_3$, 151 MHz)



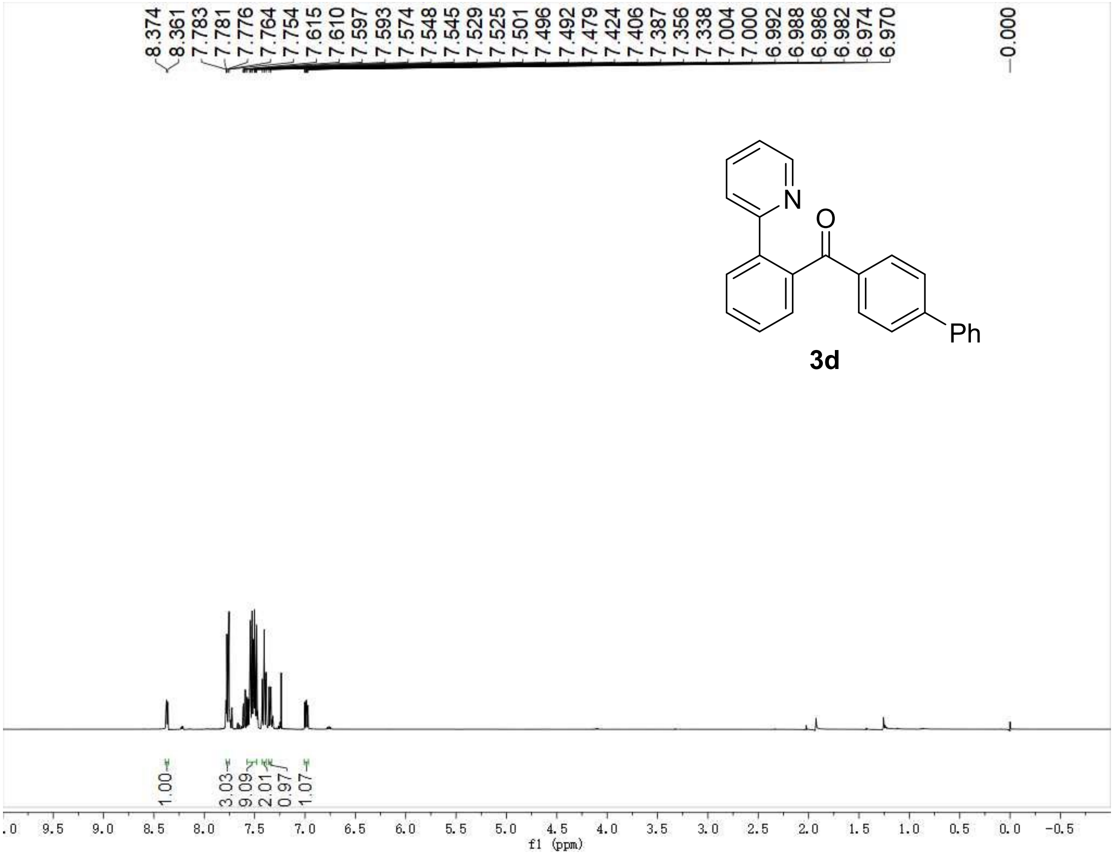
^{1}H NMR spectrum of compound **3c** ($CDCl_3$, 400 MHz)



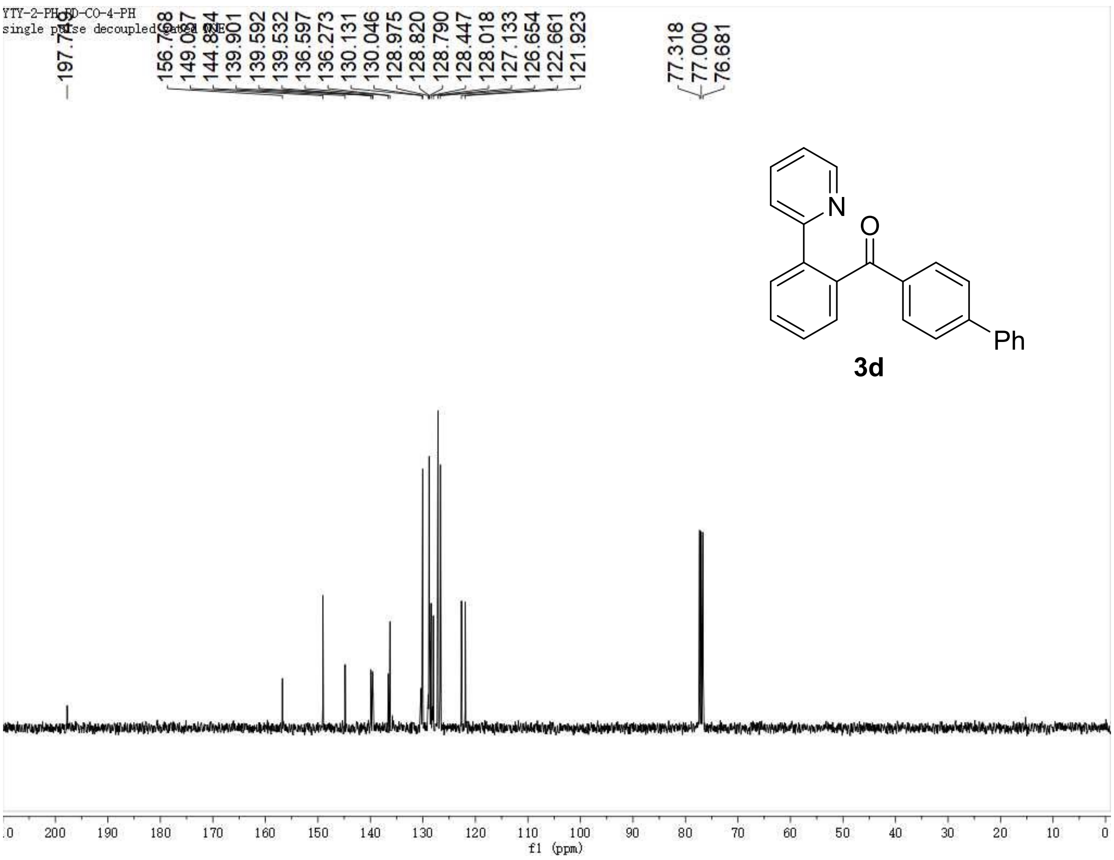
^{13}C NMR spectrum of compound **3c** ($CDCl_3$, 101 MHz)



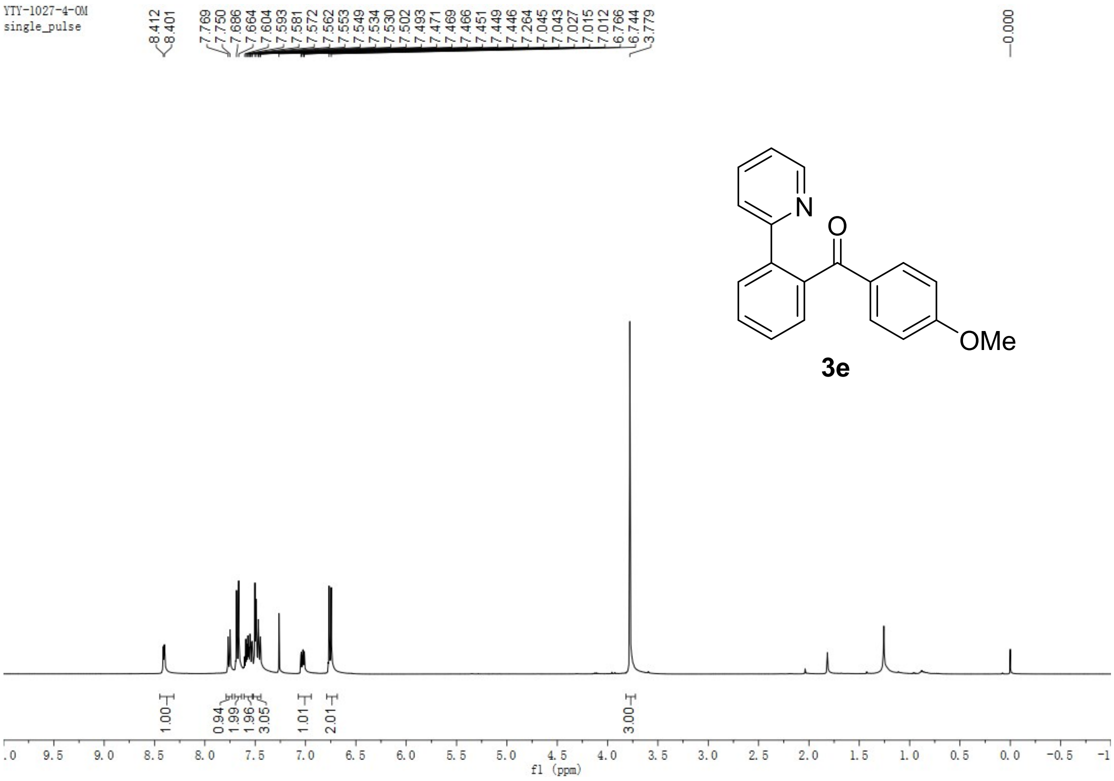
^{1}H NMR spectrum of compound **3d** ($CDCl_3$, 400 MHz)



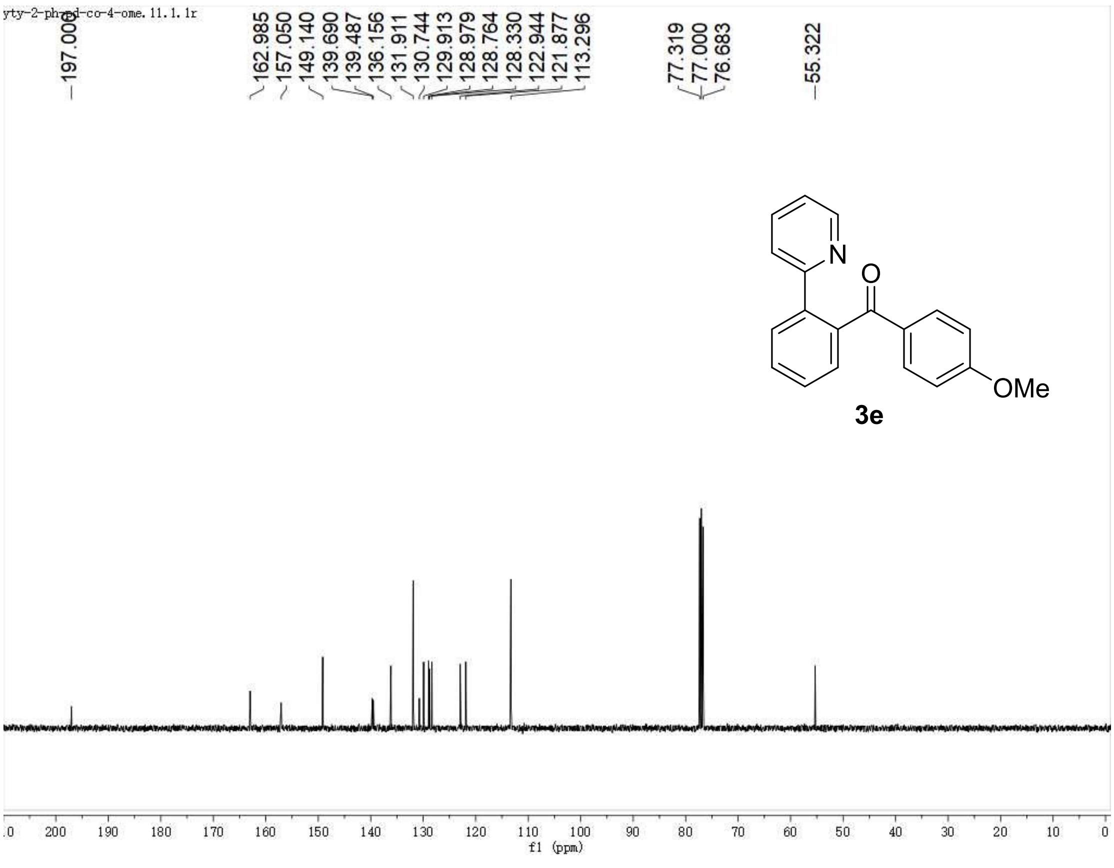
^{13}C NMR spectrum of compound **3d** ($CDCl_3$, 101 MHz)



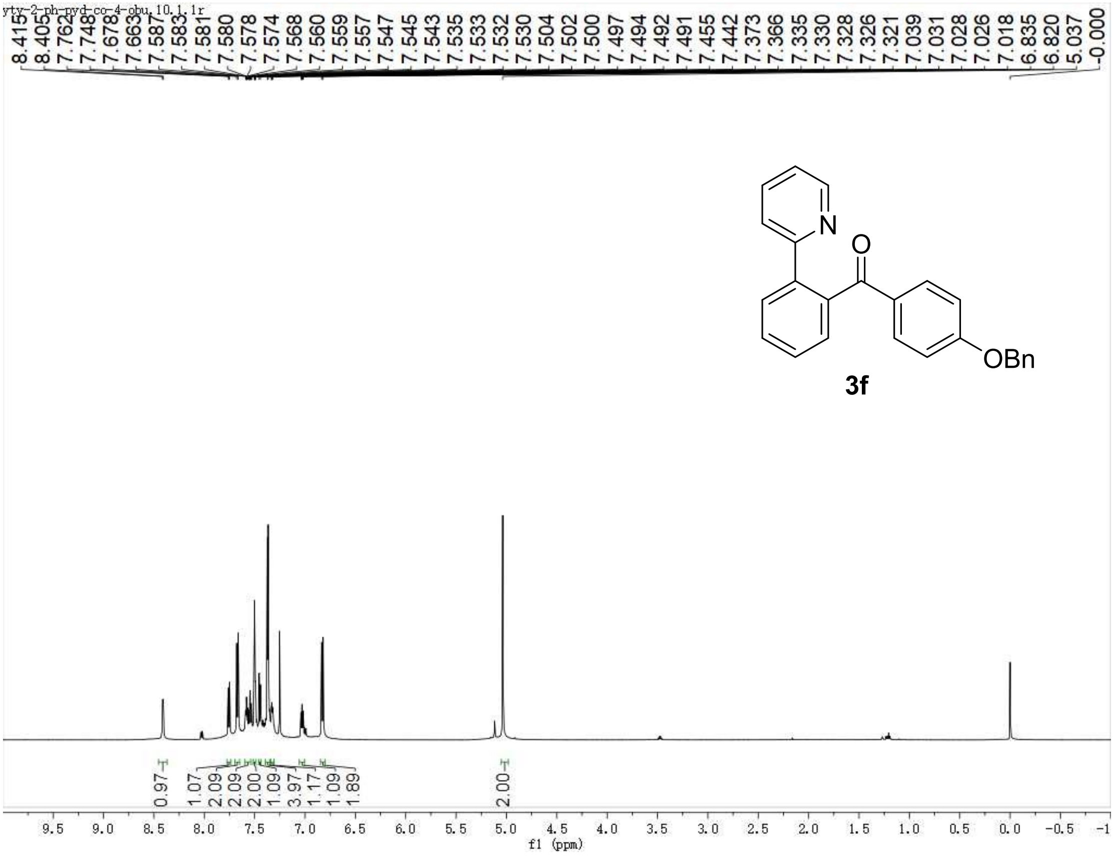
^{1}H NMR spectrum of compound **3e** ($CDCl_3$, 400 MHz)



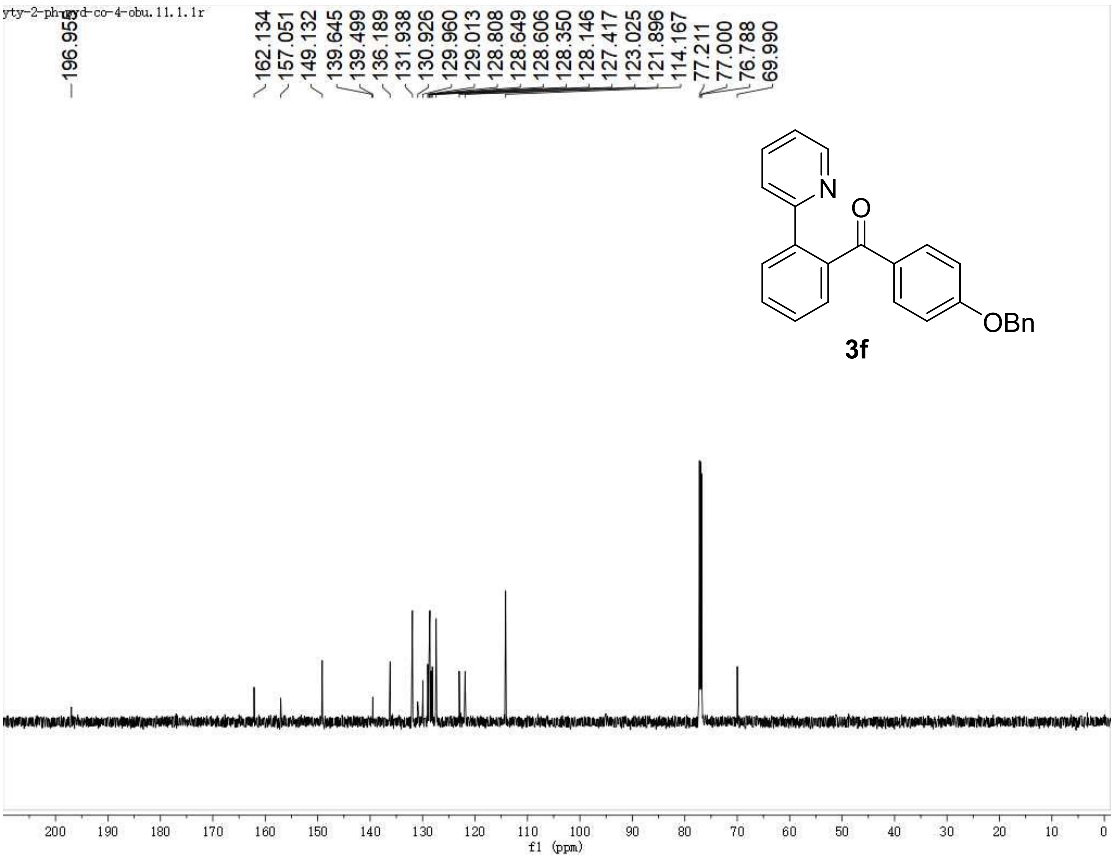
^{13}C NMR spectrum of compound **3e** ($CDCl_3$, 101 MHz)



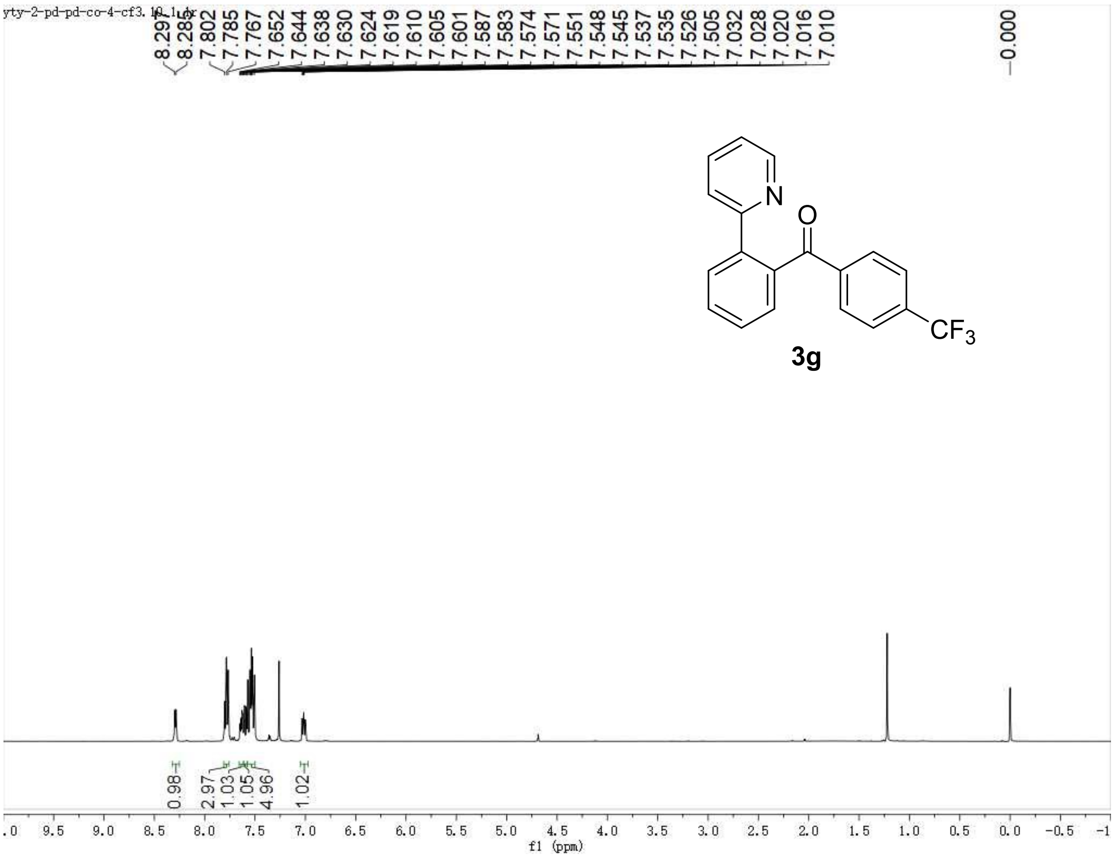
^{1}H NMR spectrum of compound **3f** ($CDCl_3$, 600 MHz)



^{13}C NMR spectrum of compound **3f** ($CDCl_3$, 151 MHz)

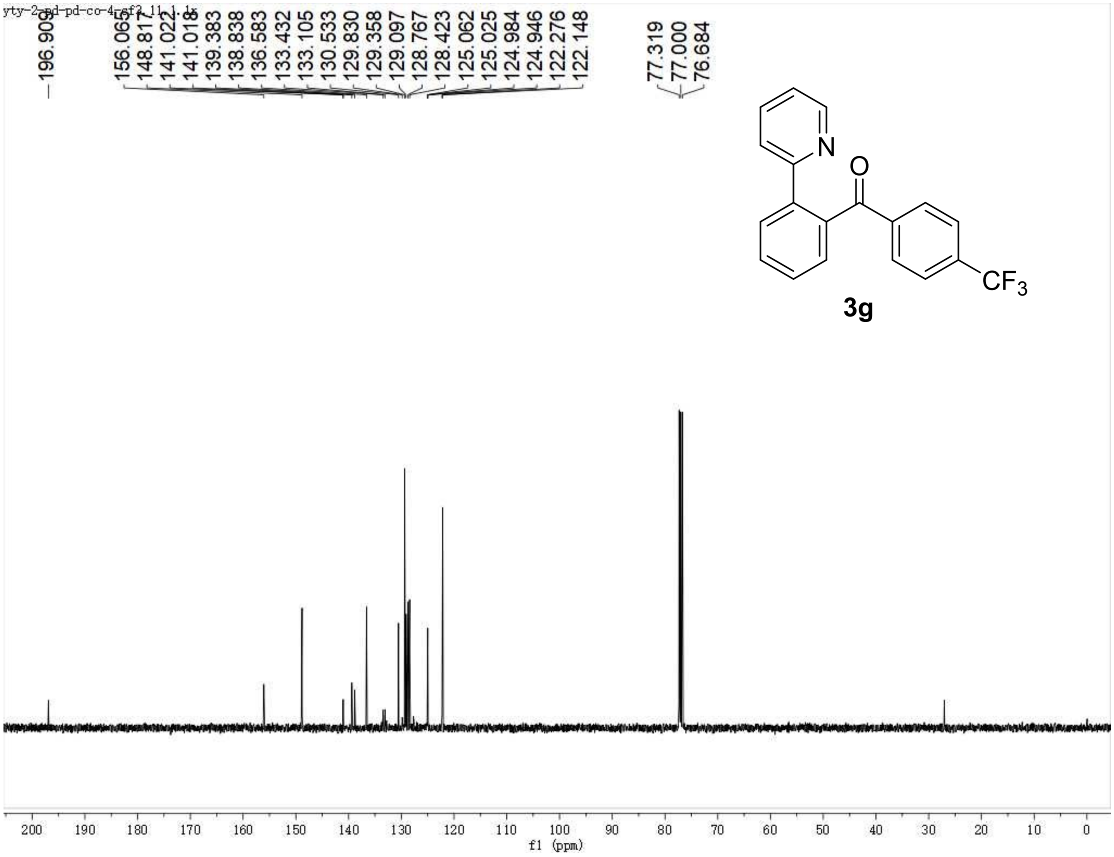


^{1}H NMR spectrum of compound **3g** ($CDCl_3$, 400 MHz)

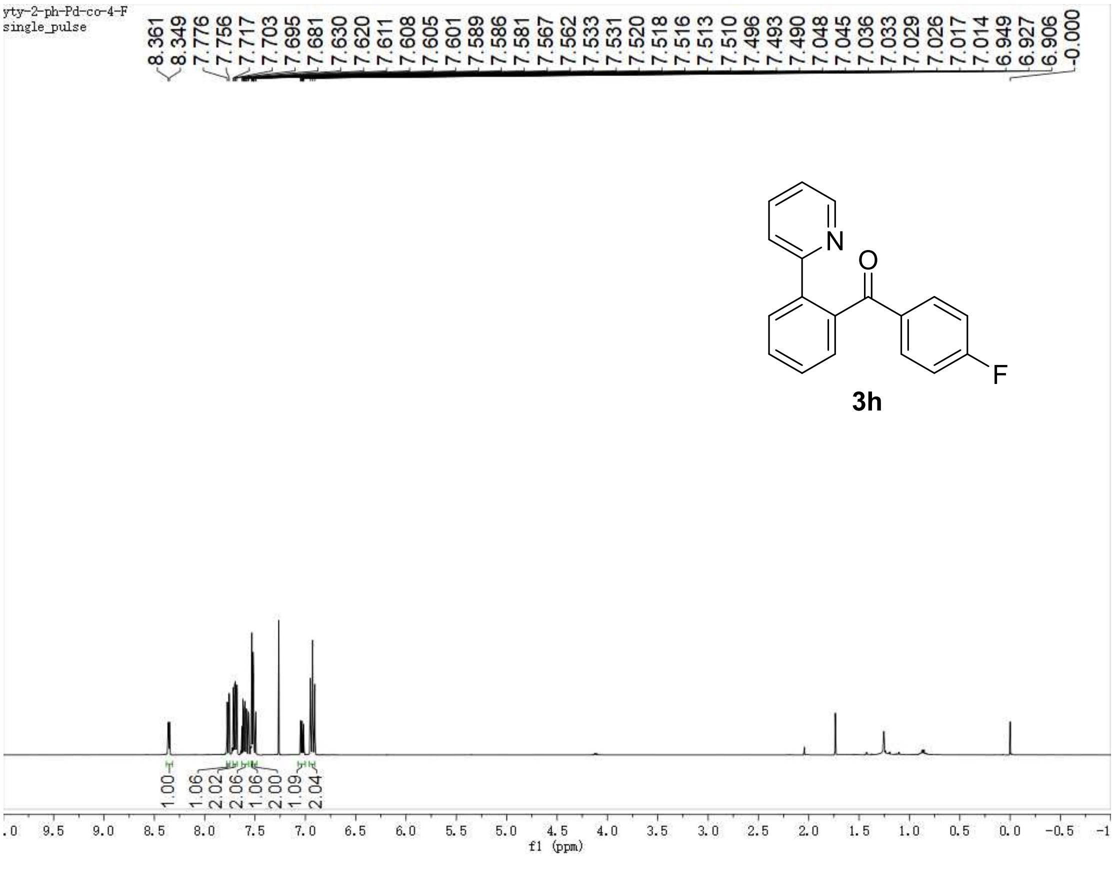


^{19}F NMR spectrum of compound **3g** ($CDCl_3$, 376 MHz)

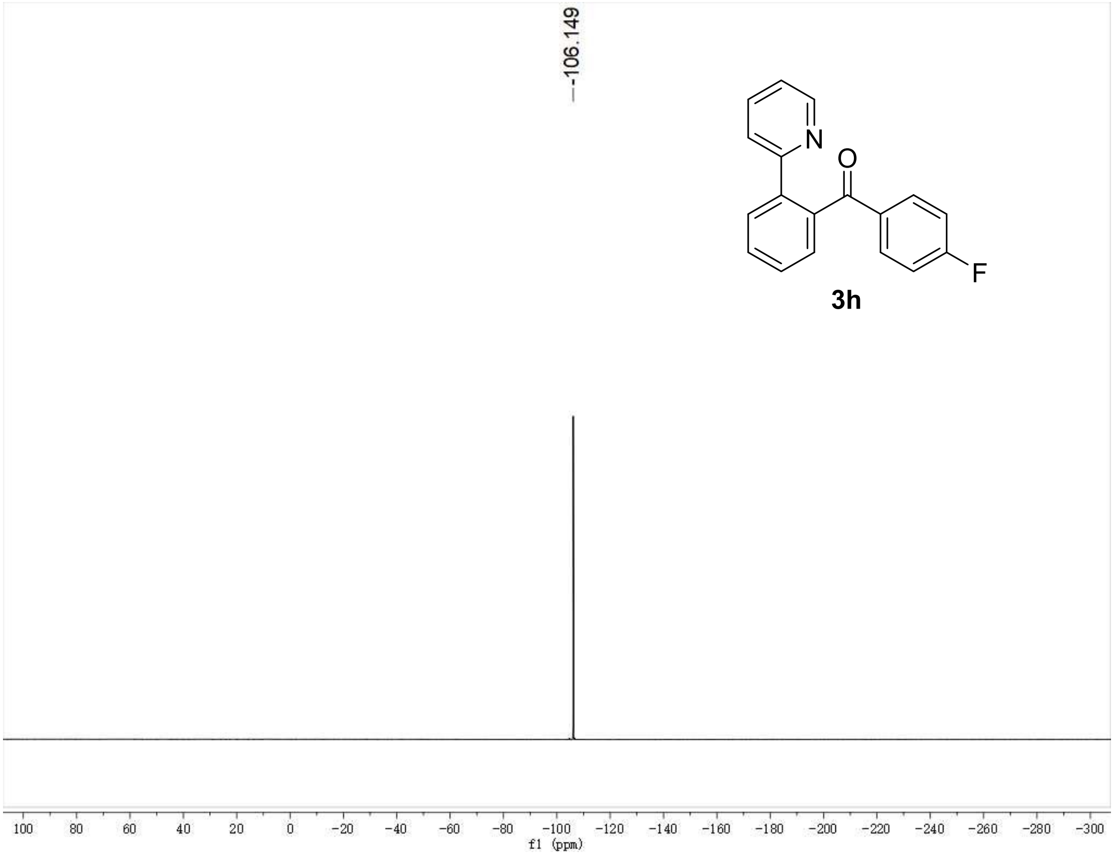
^{13}C NMR spectrum of compound **3g** ($CDCl_3$, 101 MHz)



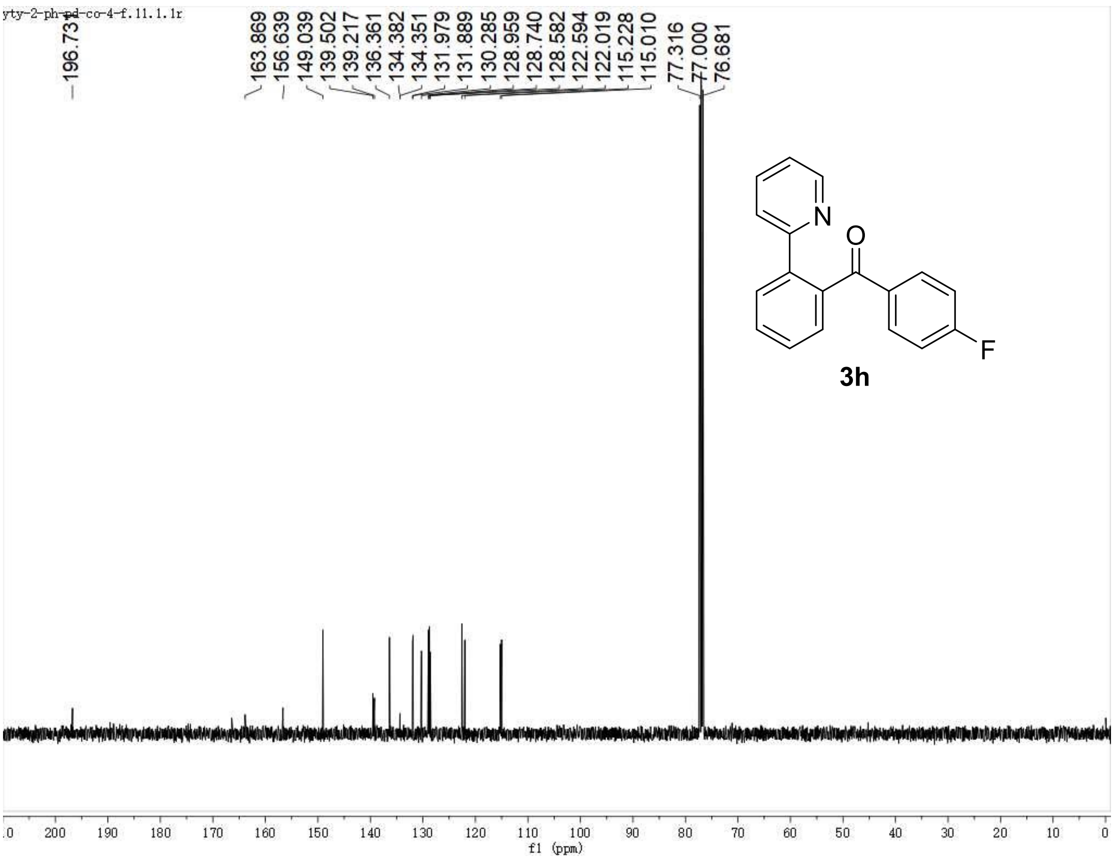
^{1}H NMR spectrum of compound **3h** ($CDCl_3$, 400 MHz)



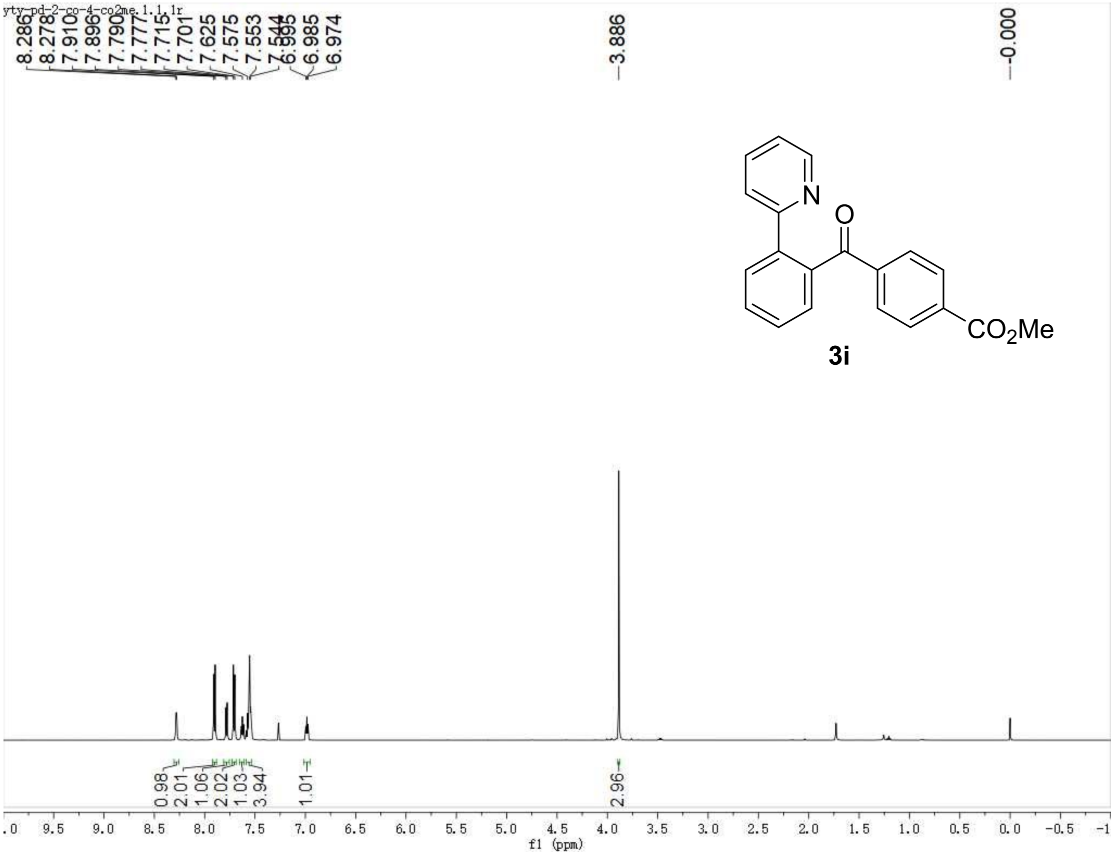
^{19}F NMR spectrum of compound **3h** ($CDCl_3$, 376 MHz)



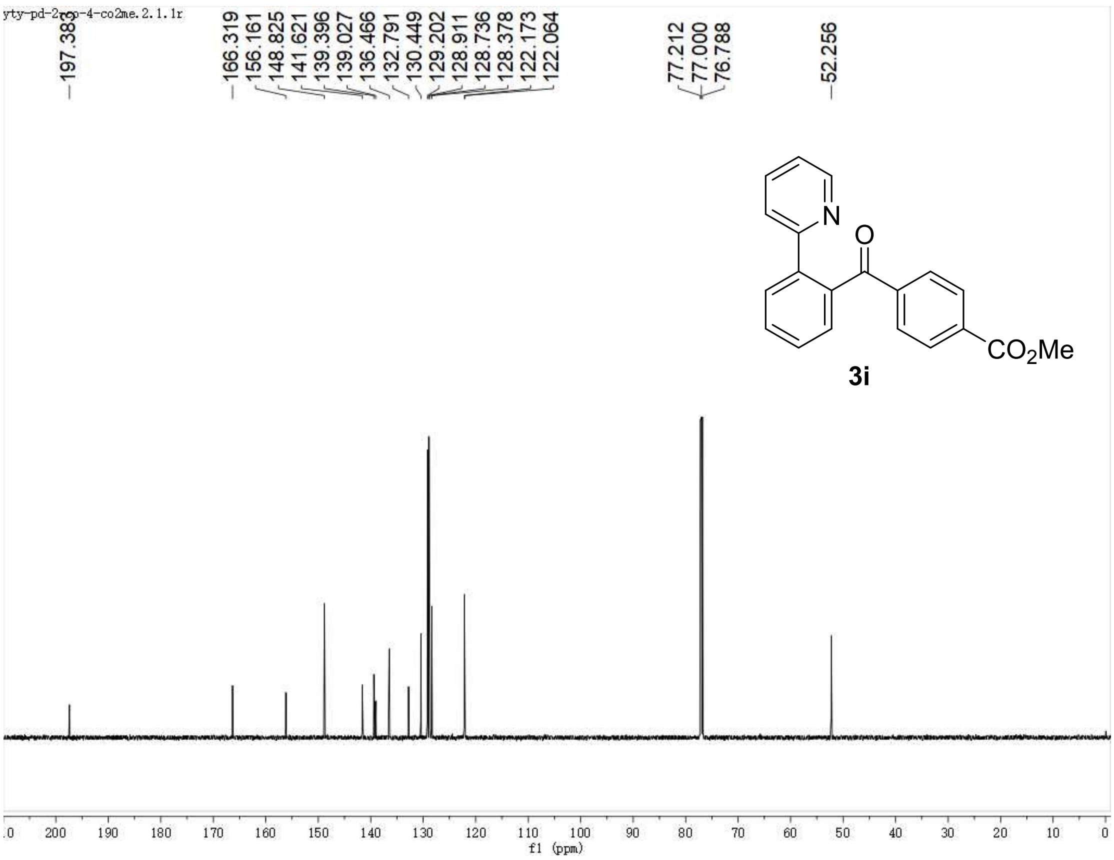
^{13}C NMR spectrum of compound **3h** ($CDCl_3$, 101 MHz)



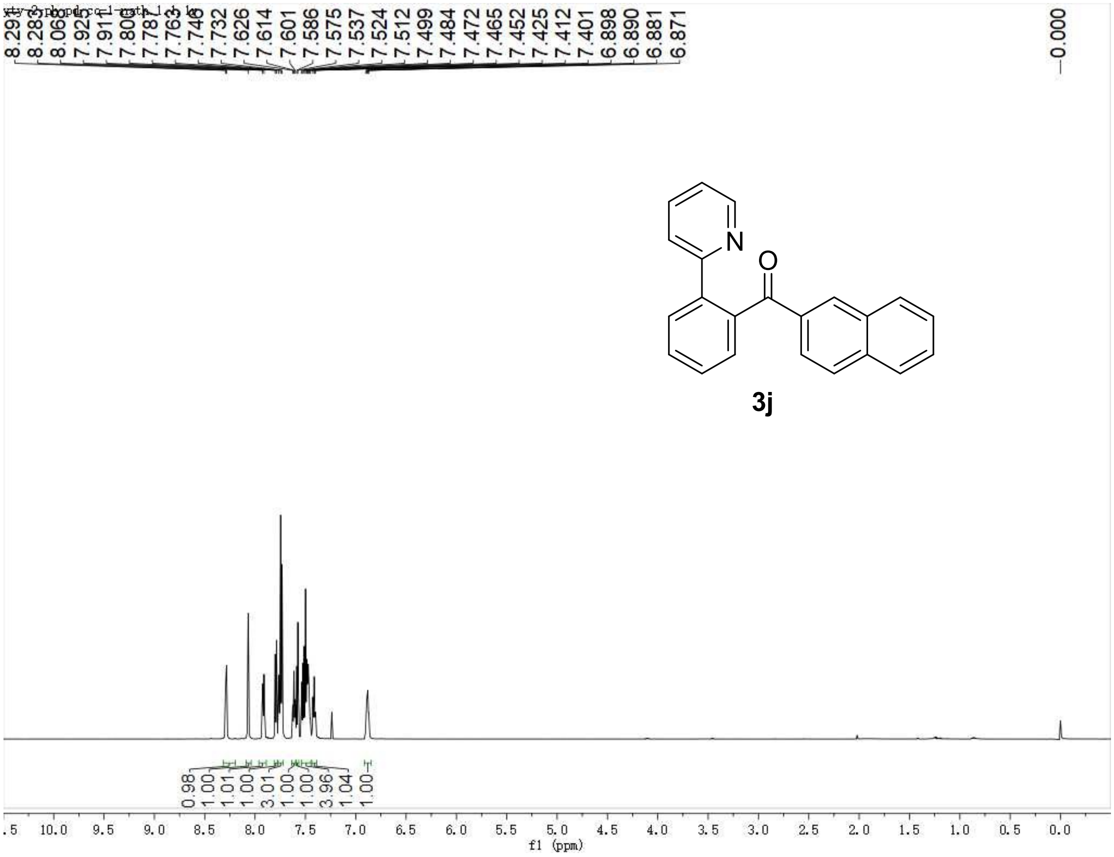
[1]H NMR spectrum of compound **3i** ($CDCl_3$, 600 MHz)



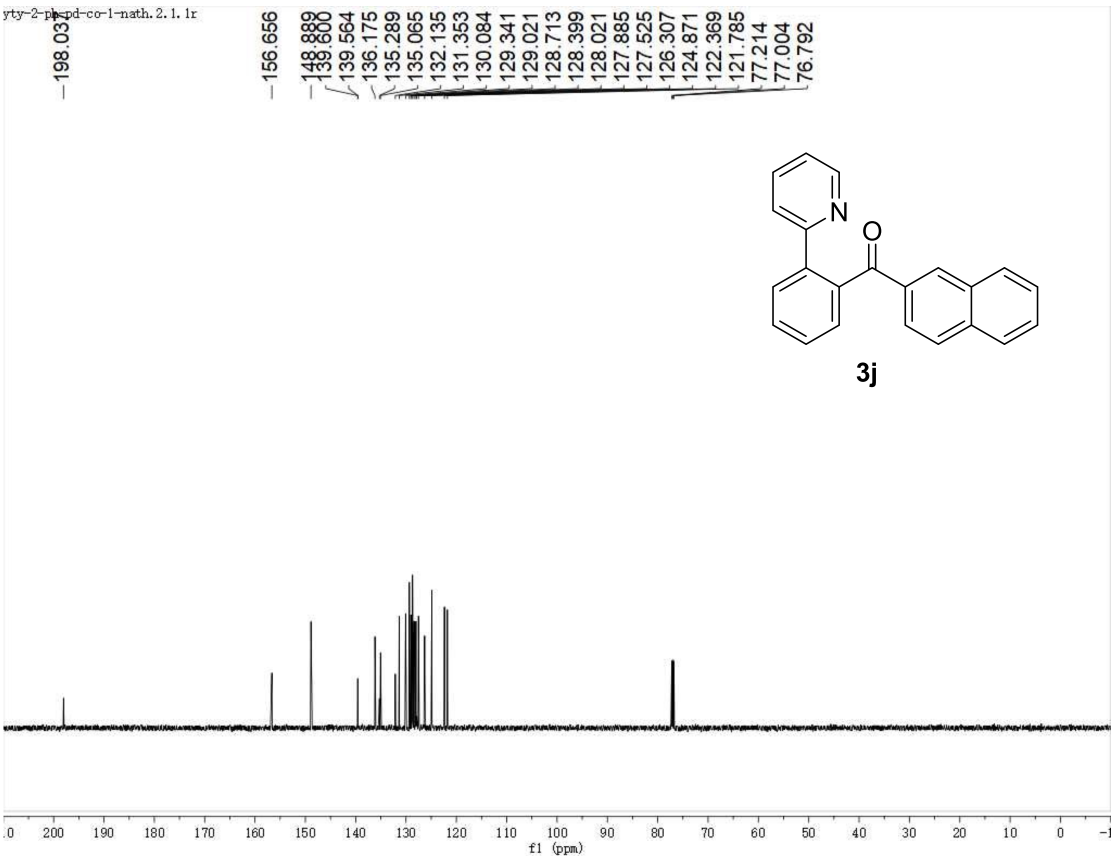
[13]C NMR spectrum of compound **3i** ($CDCl_3$, 151 MHz)



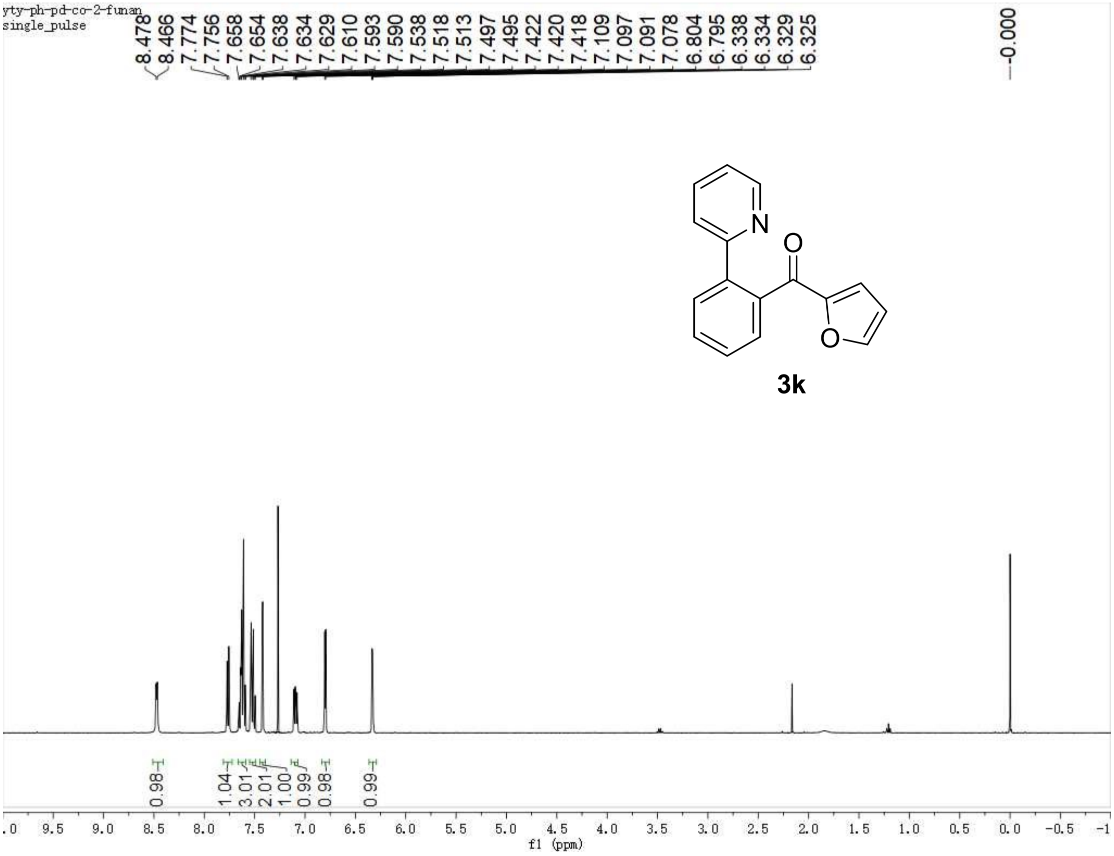
^{1}H NMR spectrum of compound **3j** ($CDCl_3$, 600 MHz)



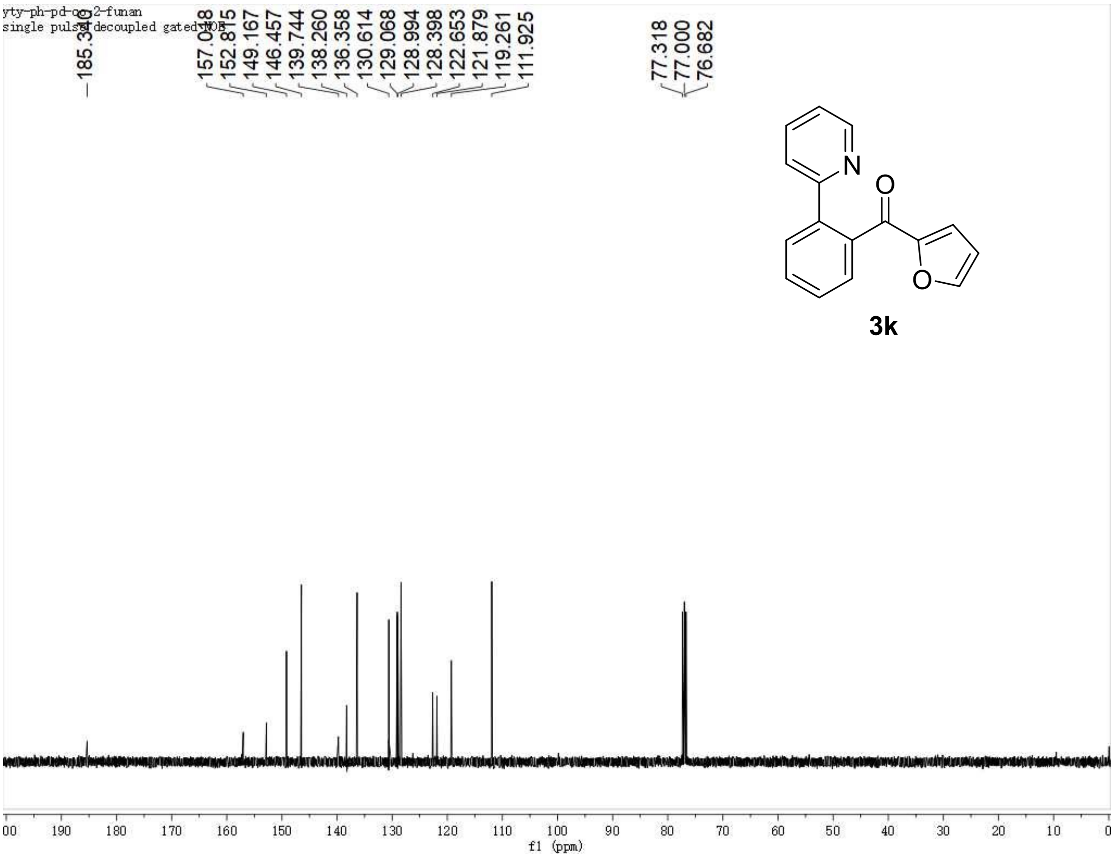
^{13}C NMR spectrum of compound **3j** ($CDCl_3$, 151 MHz)



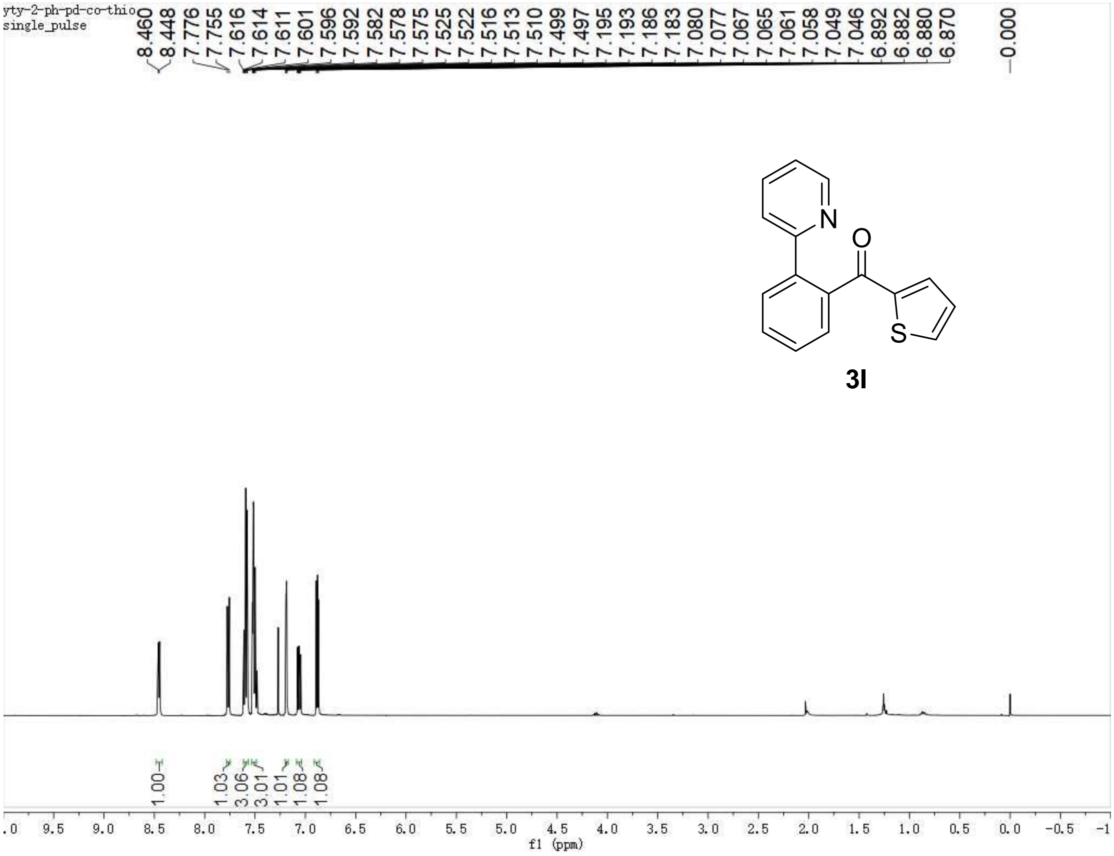
^{1}H NMR spectrum of compound **3k** ($CDCl_3$, 400 MHz)



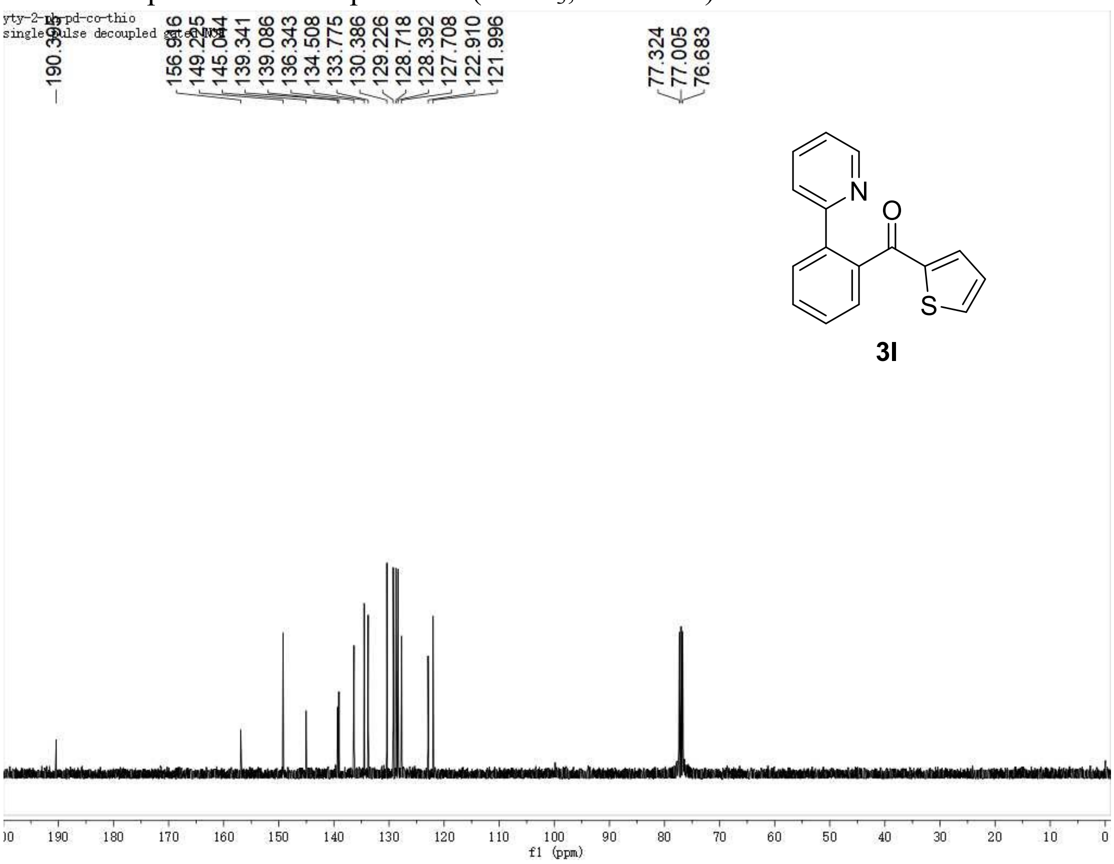
^{13}C NMR spectrum of compound **3k** ($CDCl_3$, 101 MHz)



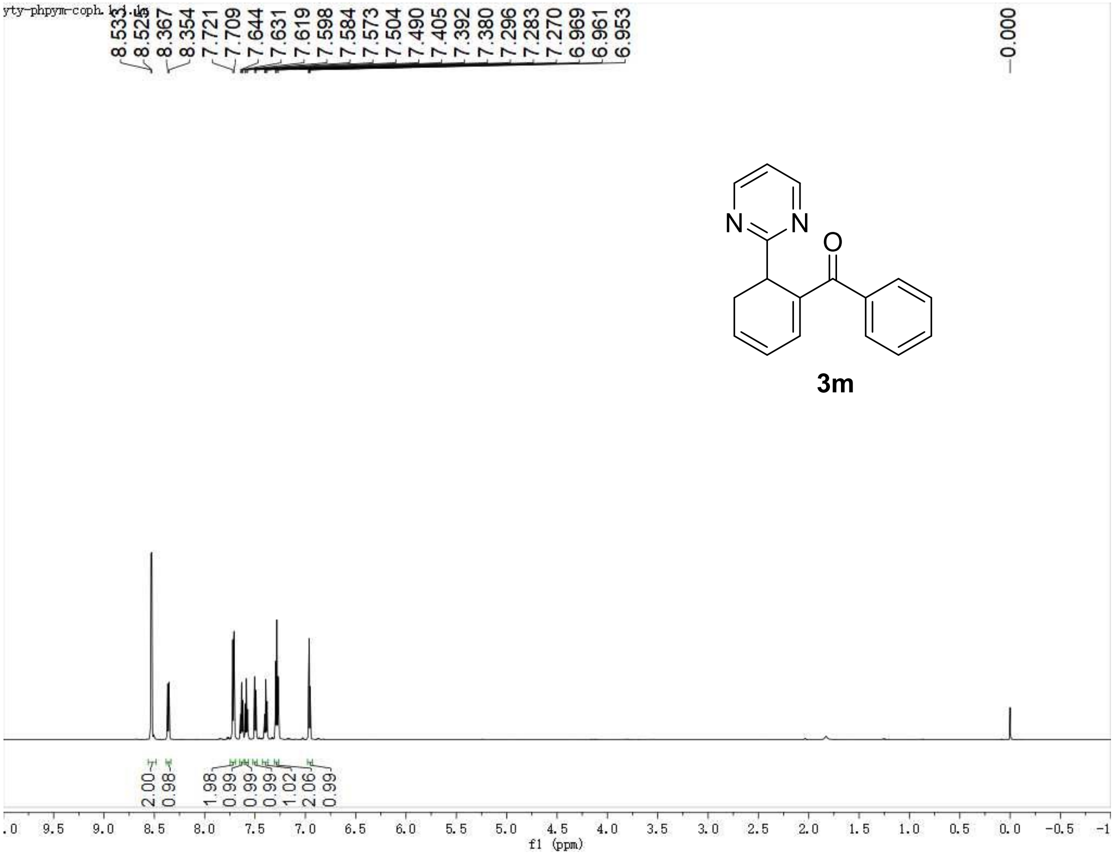
^{1}H NMR spectrum of compound **3l** ($CDCl_3$, 400 MHz)



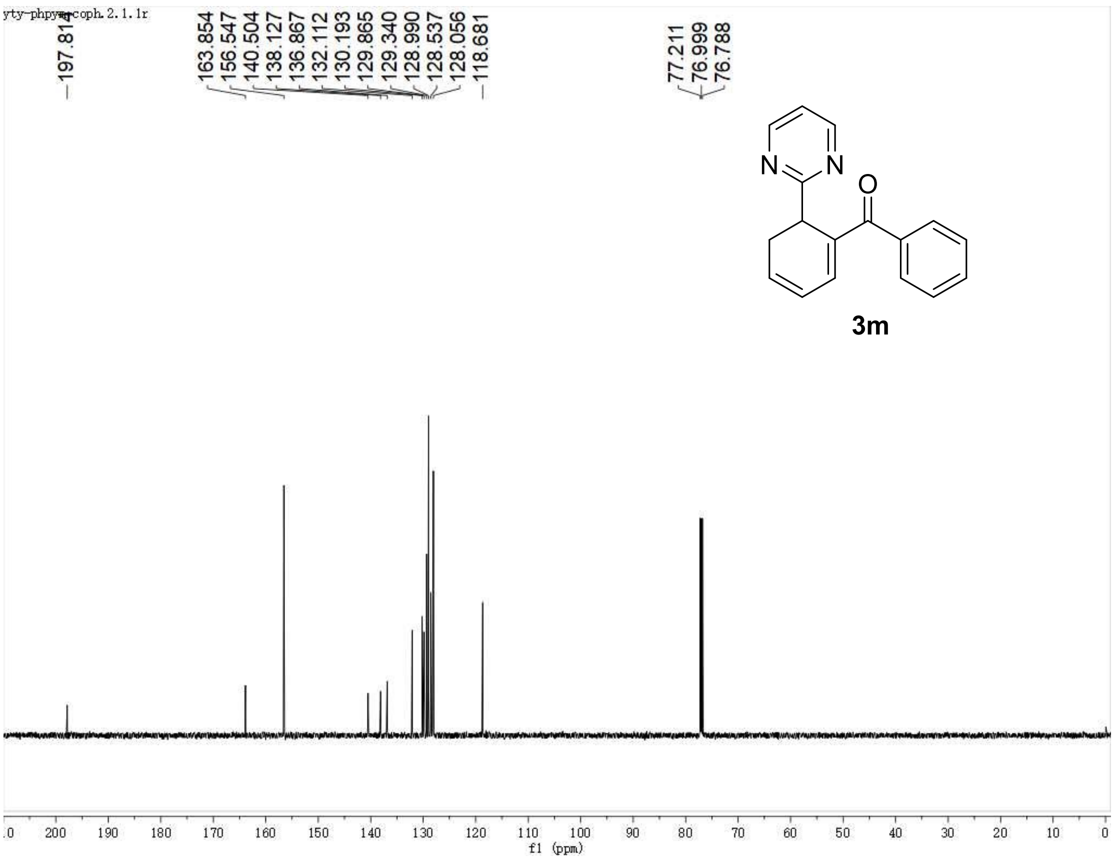
^{13}C NMR spectrum of compound **3l** ($CDCl_3$, 101 MHz)



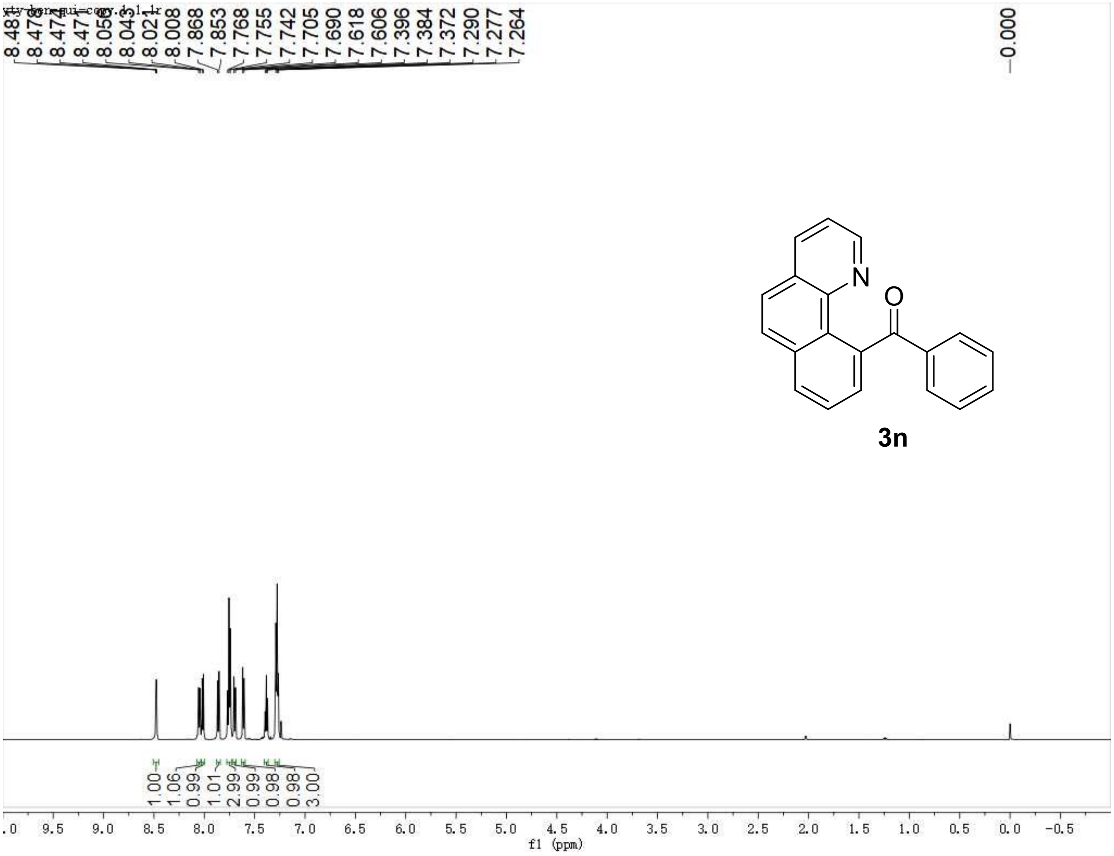
^{1}H NMR spectrum of compound **3m** ($CDCl_3$, 600 MHz)



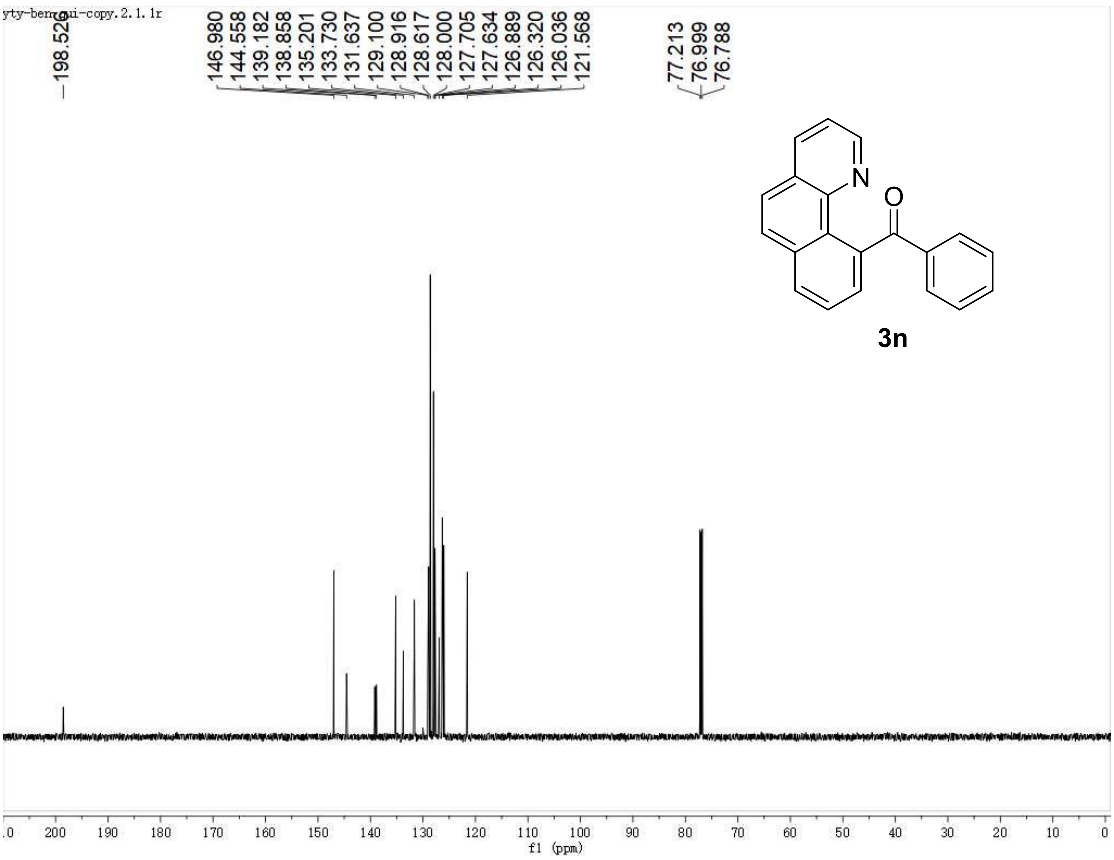
^{13}C NMR spectrum of compound **3m** ($CDCl_3$, 151 MHz)



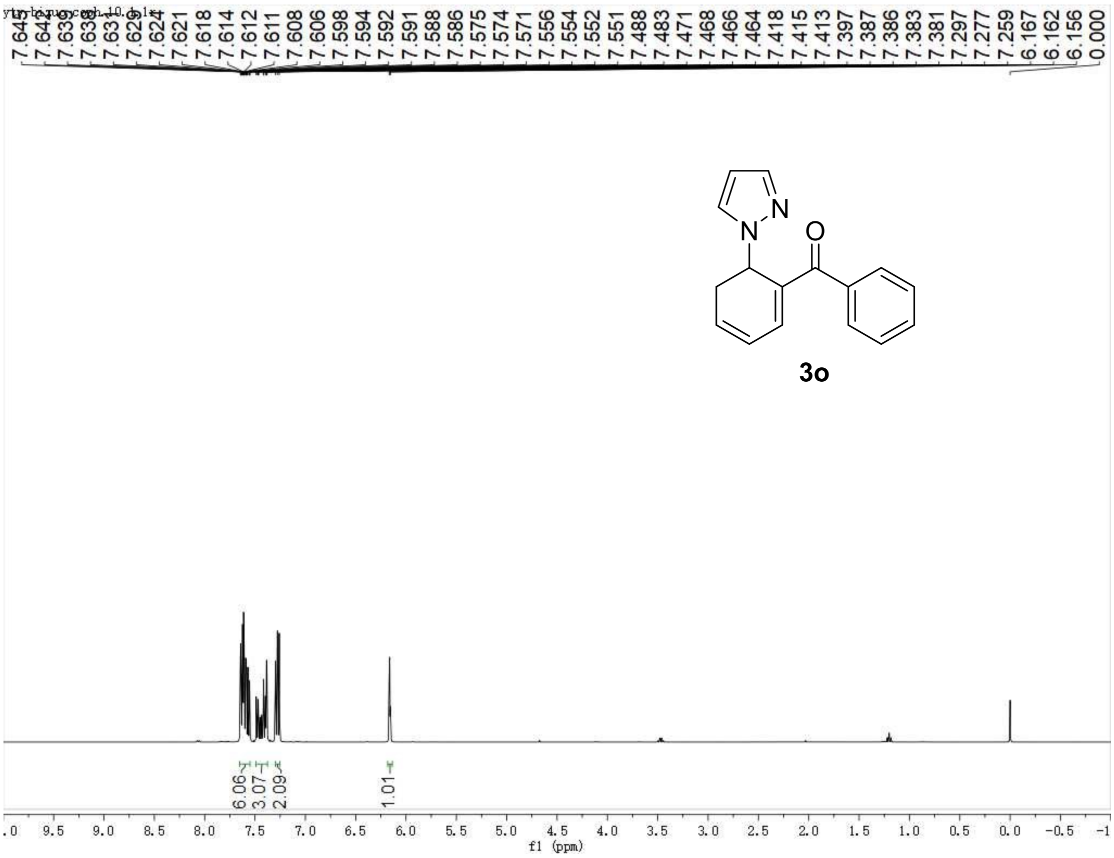
[1]H NMR spectrum of compound **3n** ($CDCl_3$, 600 MHz)



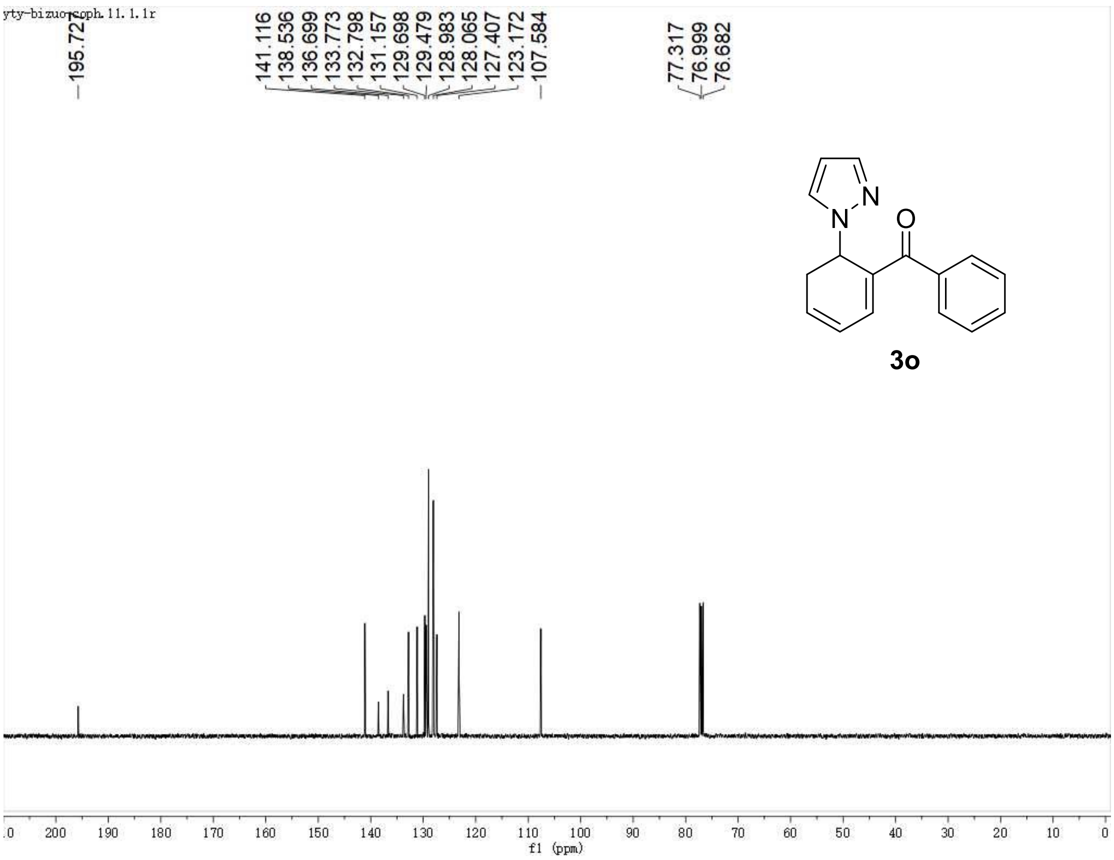
[13]C NMR spectrum of compound **3n** ($CDCl_3$, 151 MHz)



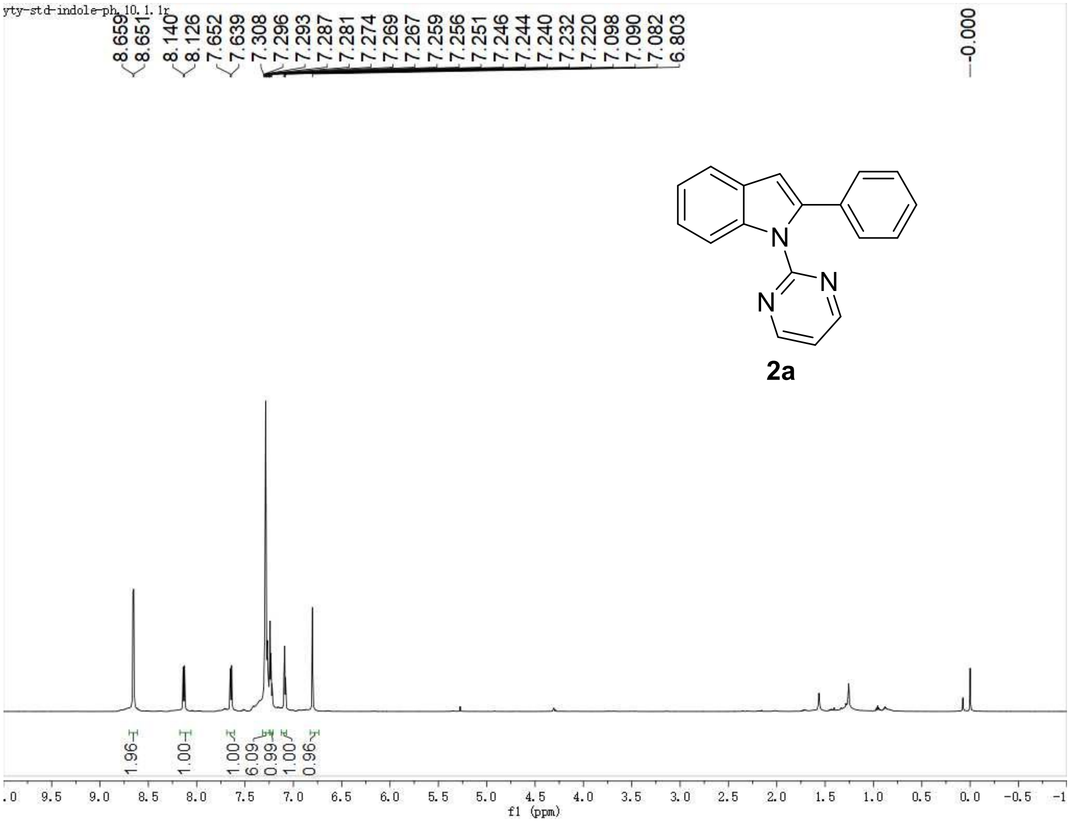
^{1}H NMR spectrum of compound **3o** ($CDCl_3$, 600 MHz)



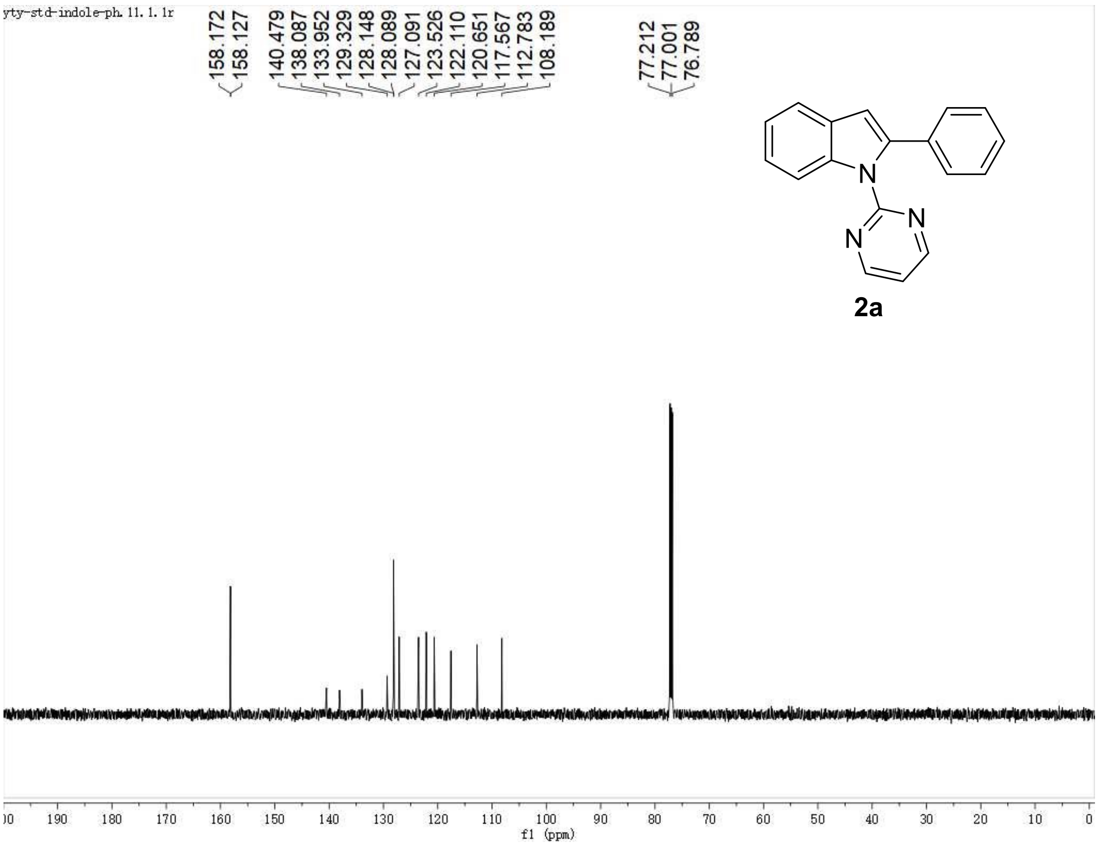
^{13}C NMR spectrum of compound **3o** ($CDCl_3$, 151 MHz)



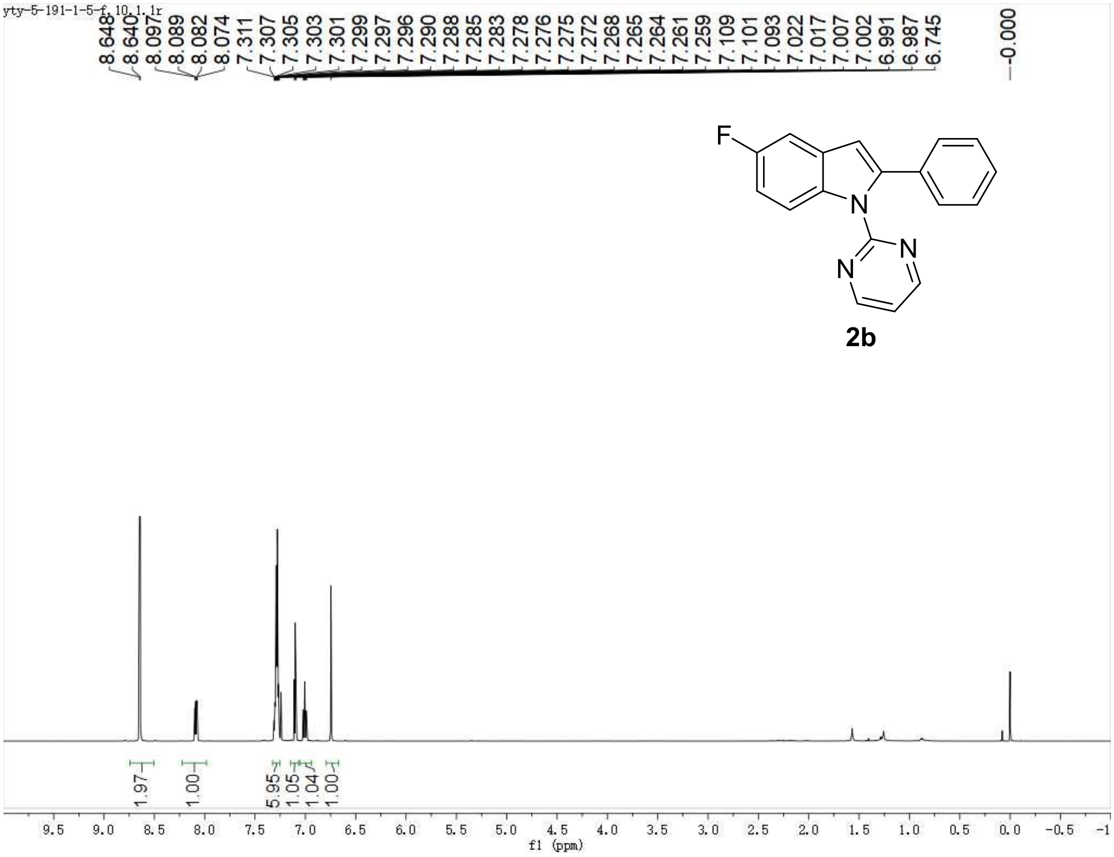
^{1}H NMR spectrum of compound **2a** ($CDCl_3$, 600 MHz)



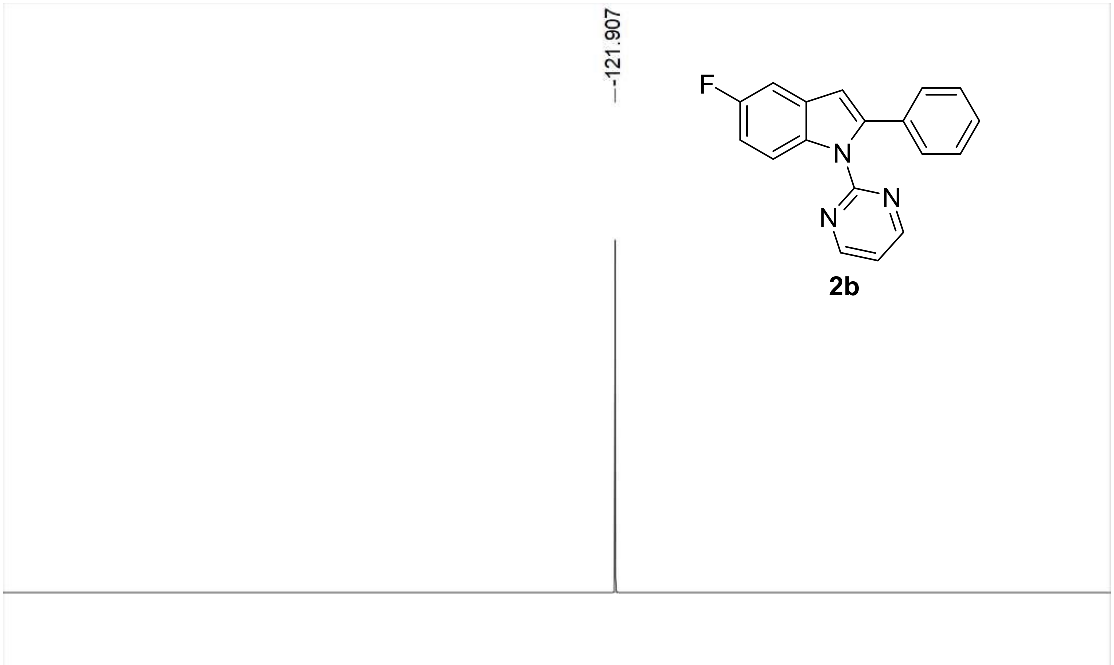
^{13}C NMR spectrum of compound **2a** ($CDCl_3$, 151 MHz)



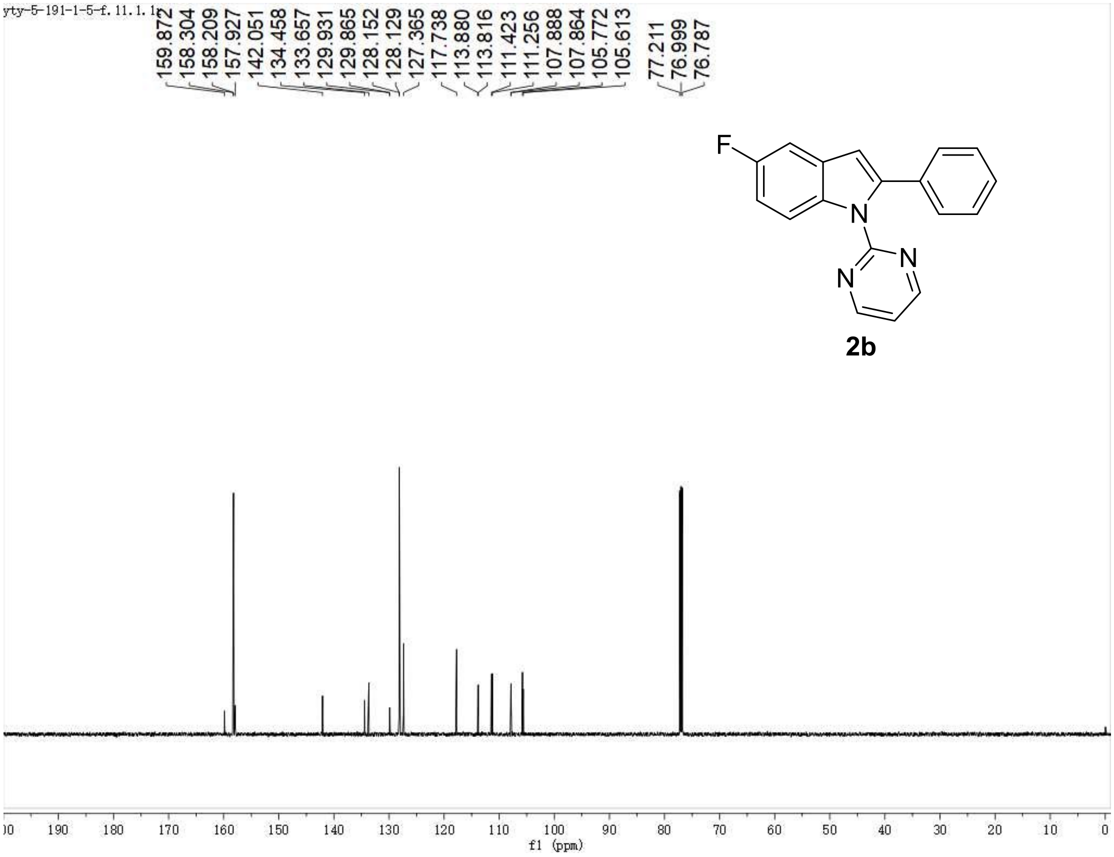
^{1}H NMR spectrum of compound **2b** ($CDCl_3$, 600 MHz)



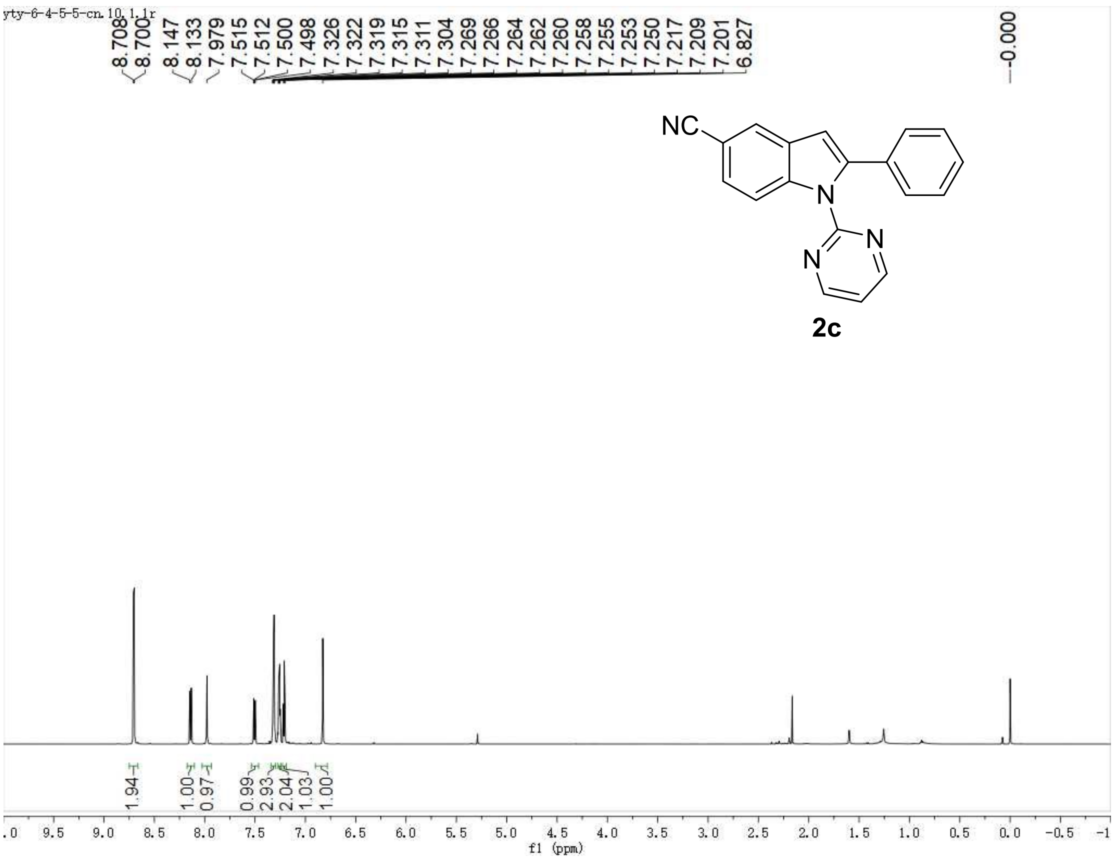
^{19}F NMR spectrum of compound **2b** ($CDCl_3$, 376 MHz)



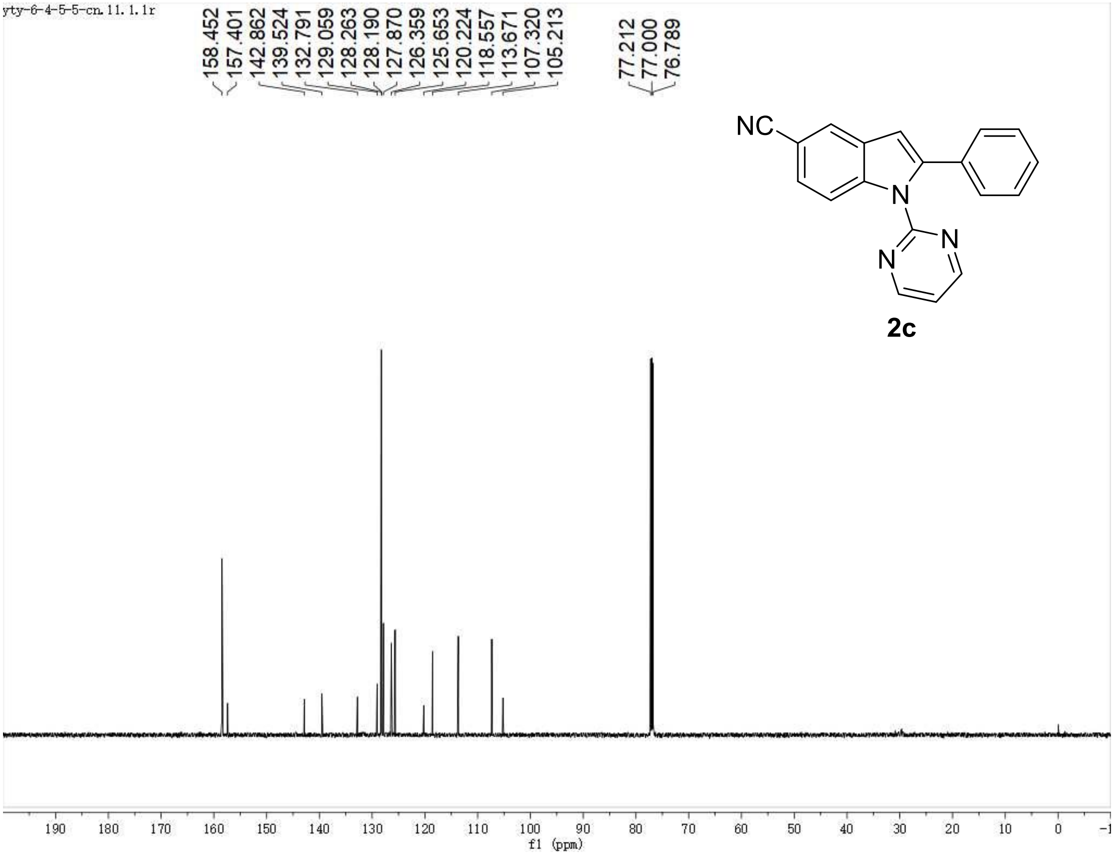
^{13}C NMR spectrum of compound **2b** ($CDCl_3$, 151 MHz)



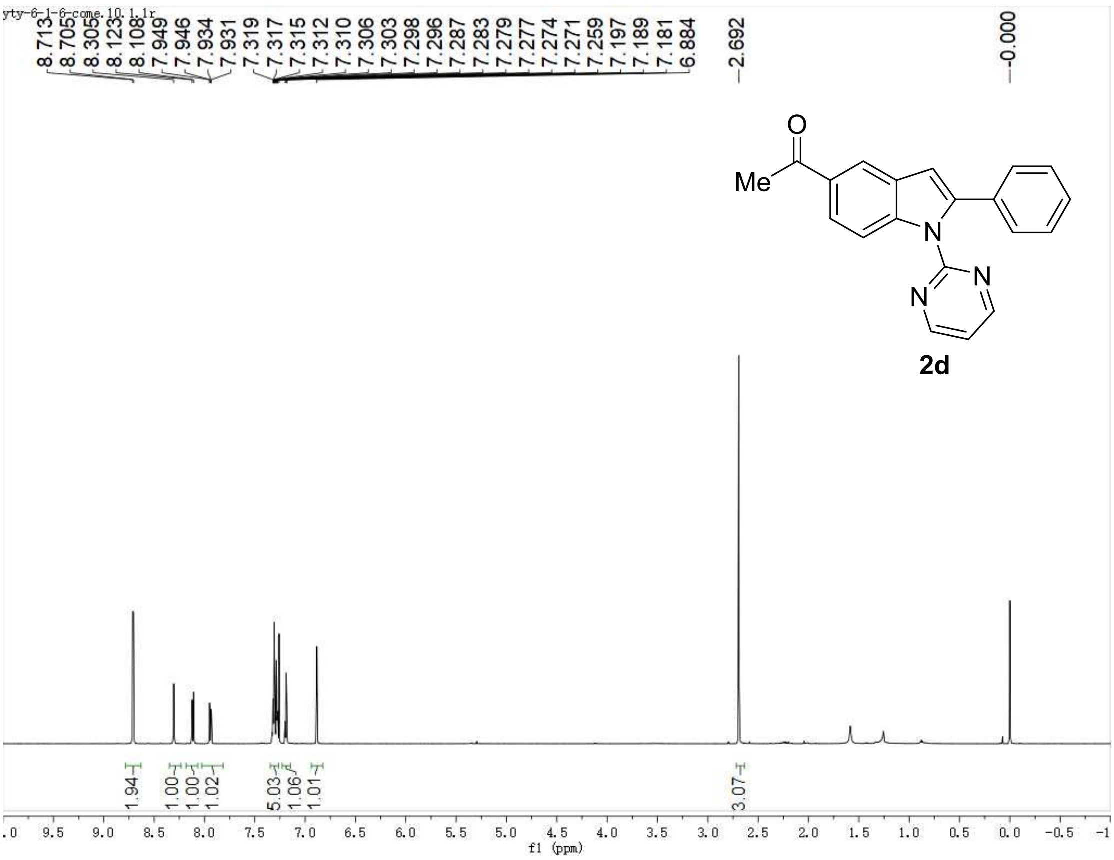
^{1}H NMR spectrum of compound **2c** ($CDCl_3$, 600 MHz)



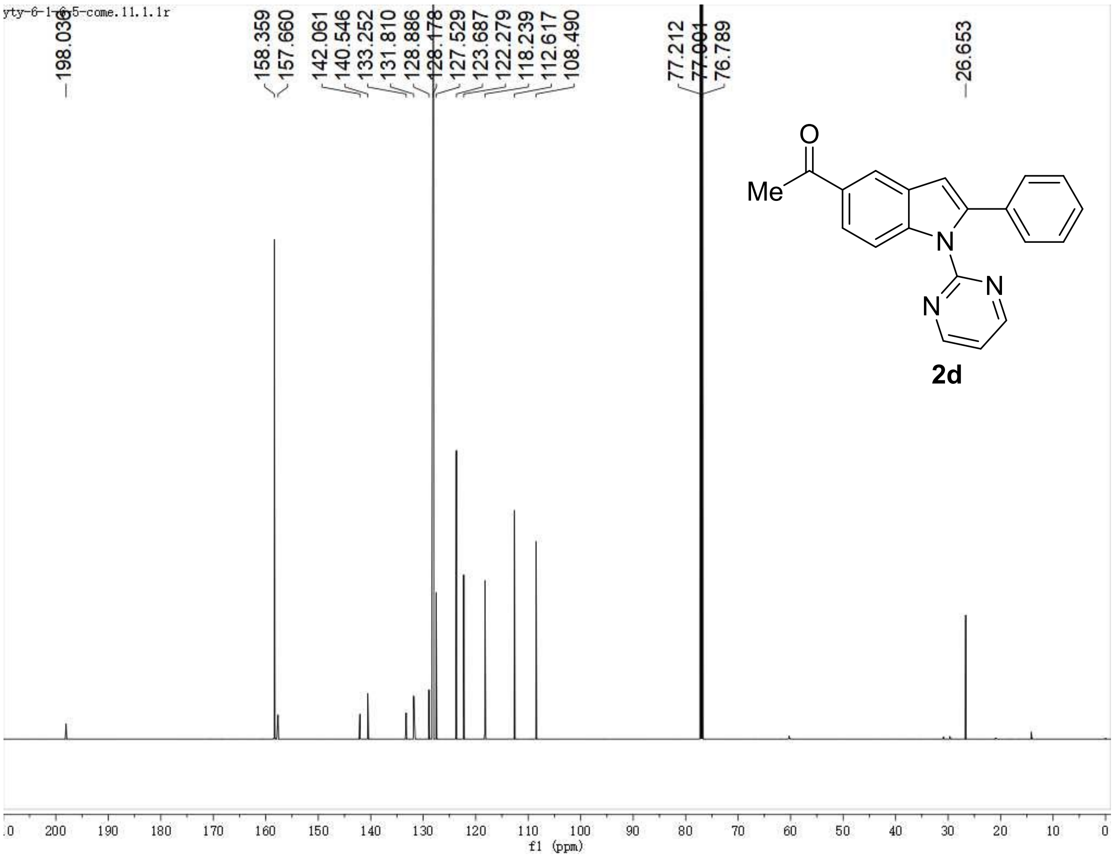
^{13}C NMR spectrum of compound **2c** ($CDCl_3$, 151 MHz)



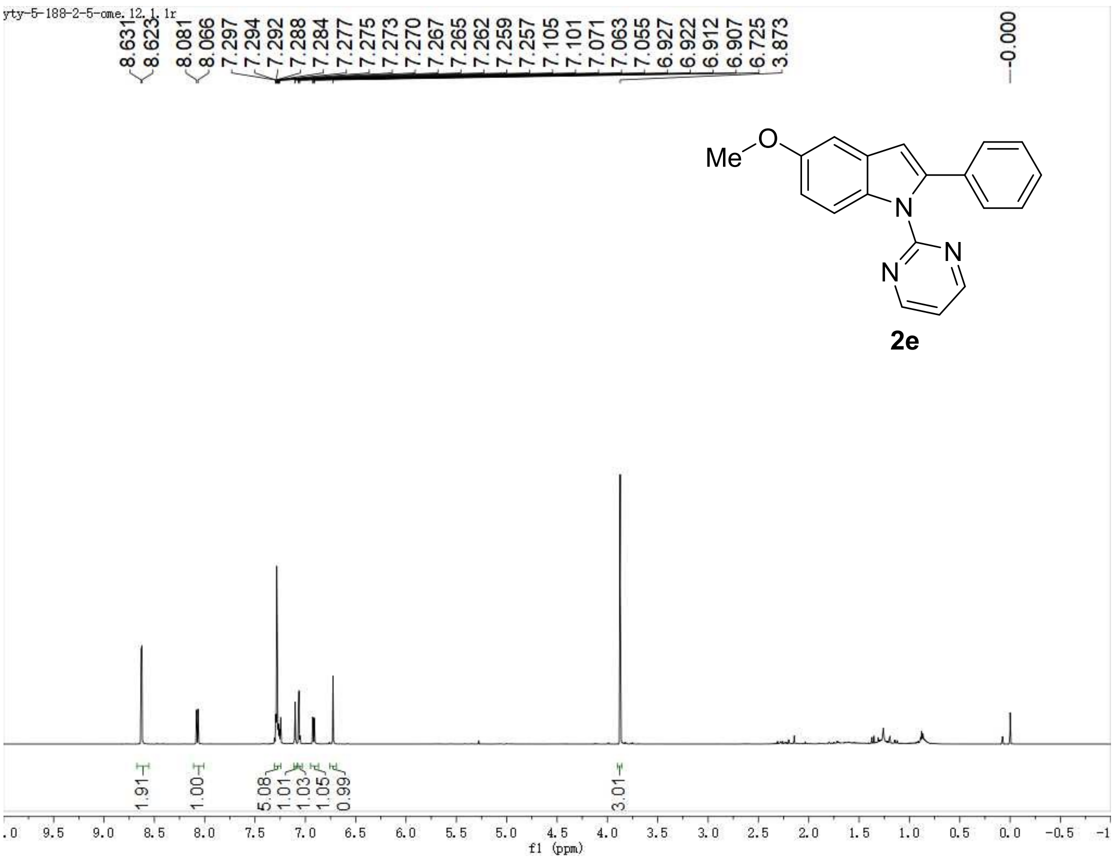
^{1}H NMR spectrum of compound **2d** ($CDCl_3$, 600 MHz)



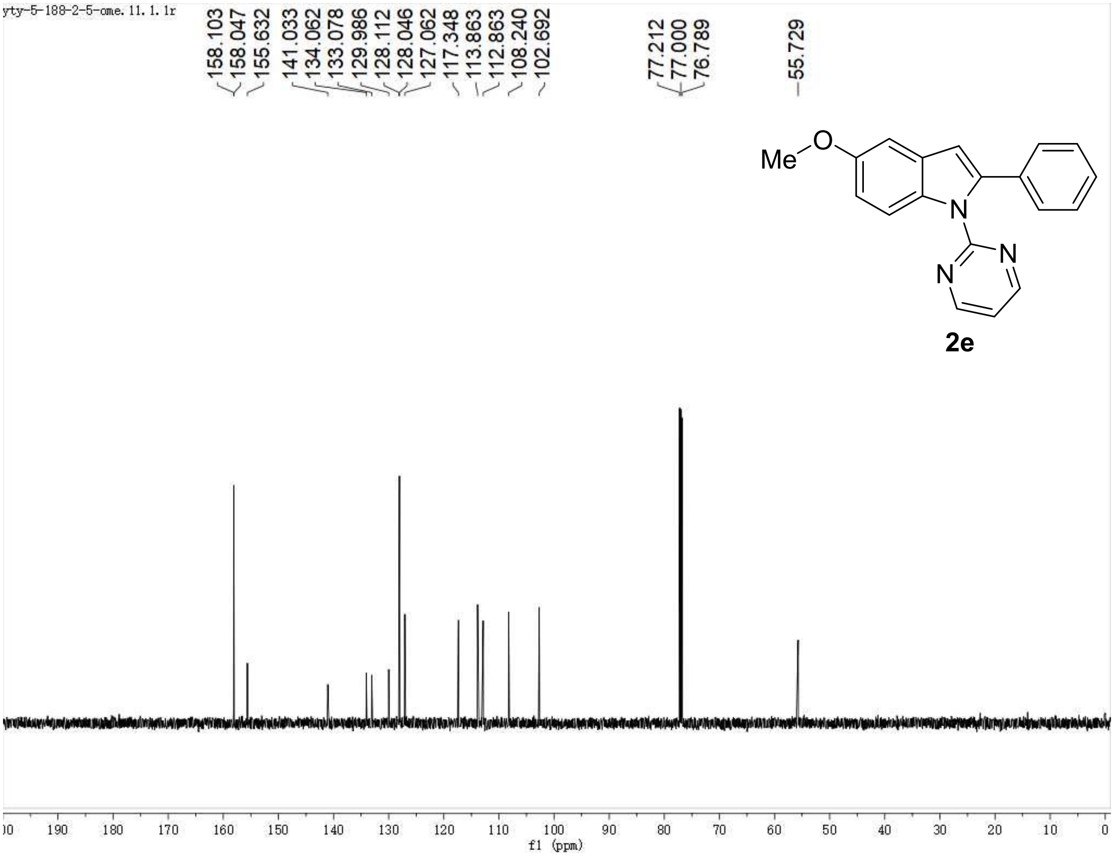
^{13}C NMR spectrum of compound **2d** ($CDCl_3$, 151 MHz)



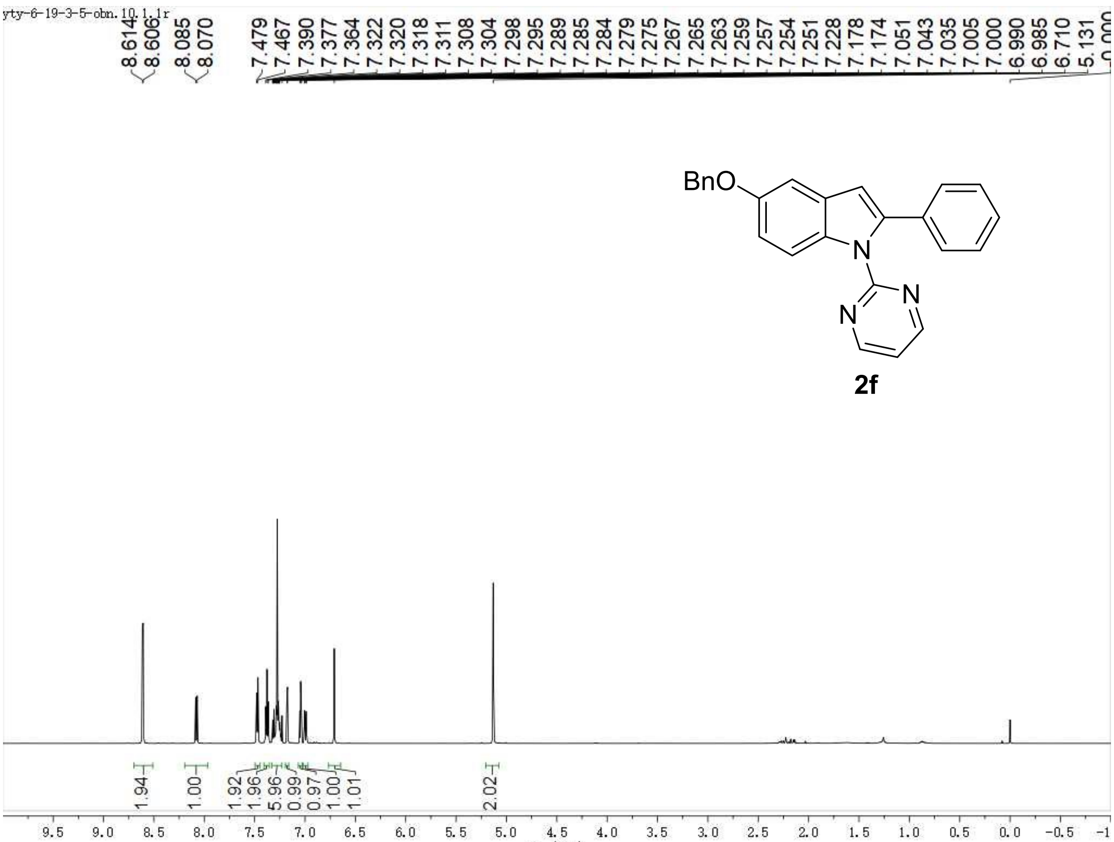
^{1}H NMR spectrum of compound **2e** ($CDCl_3$, 600 MHz)



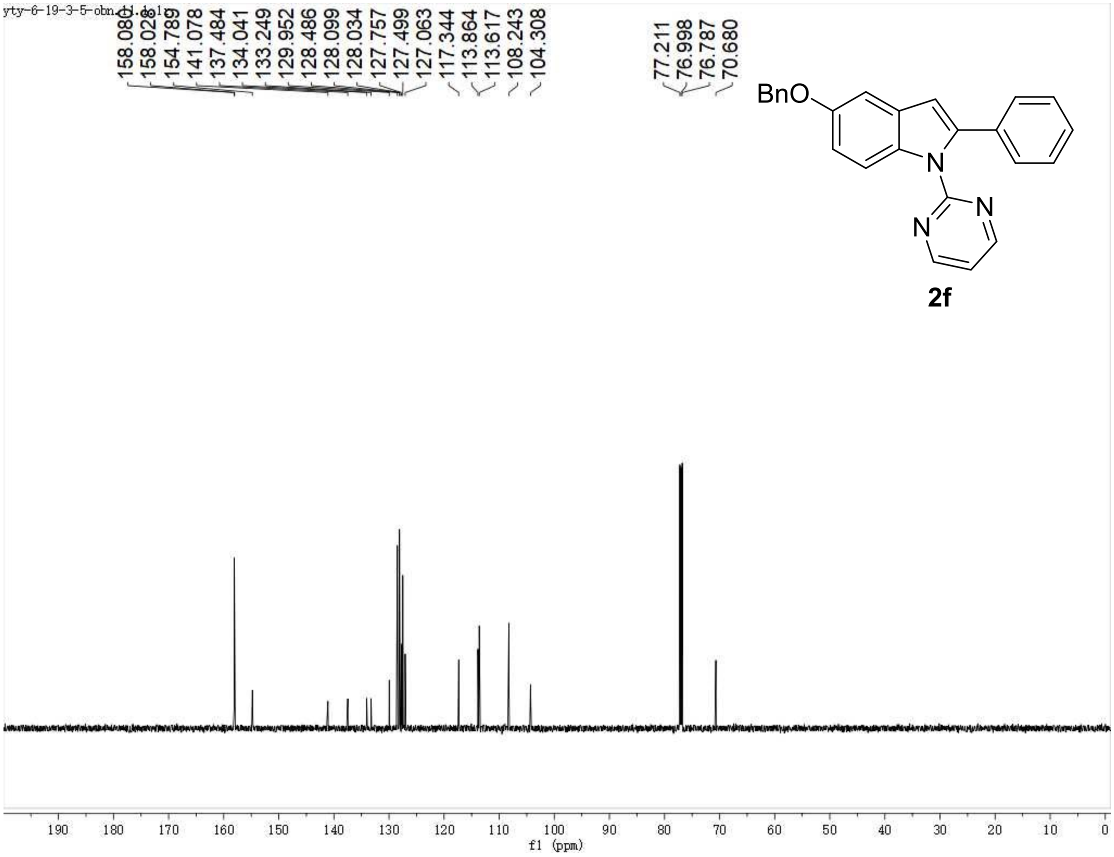
^{13}C NMR spectrum of compound **2e** ($CDCl_3$, 151 MHz)



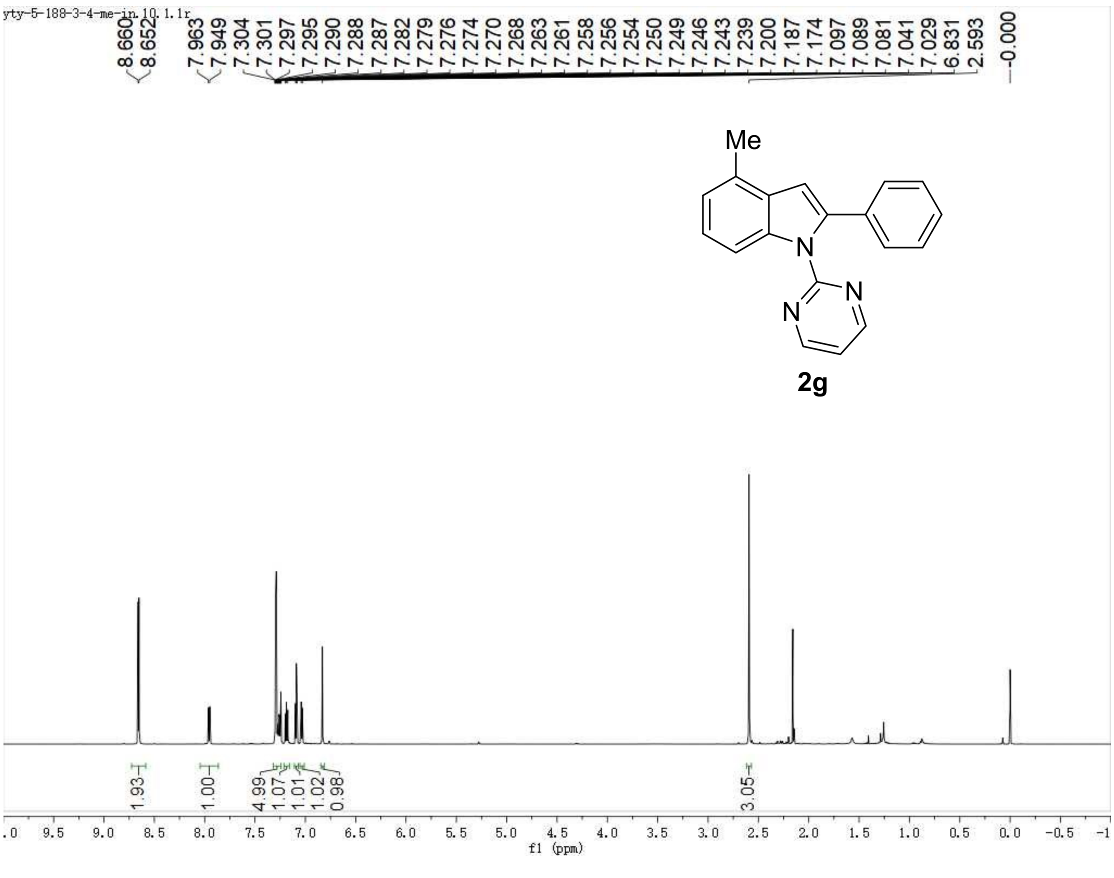
^{1}H NMR spectrum of compound **2f** ($CDCl_3$, 600 MHz)



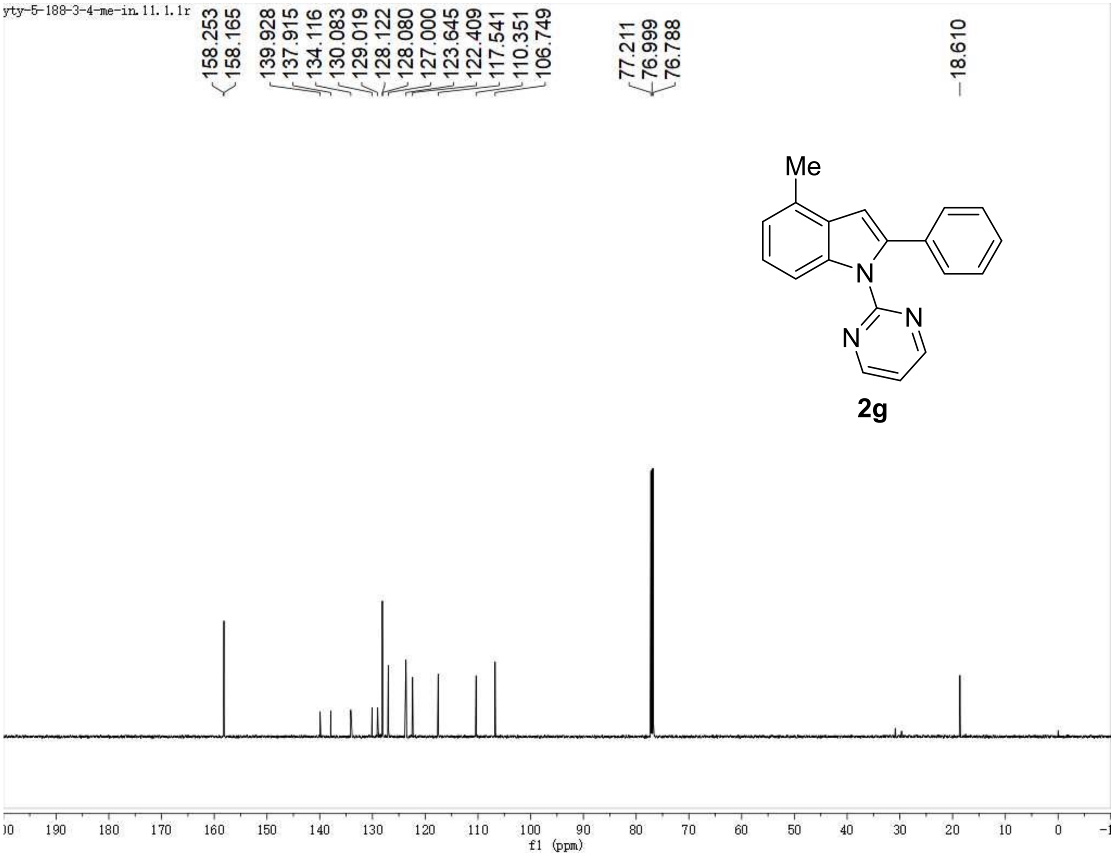
^{13}C NMR spectrum of compound **2f** ($CDCl_3$, 151 MHz)



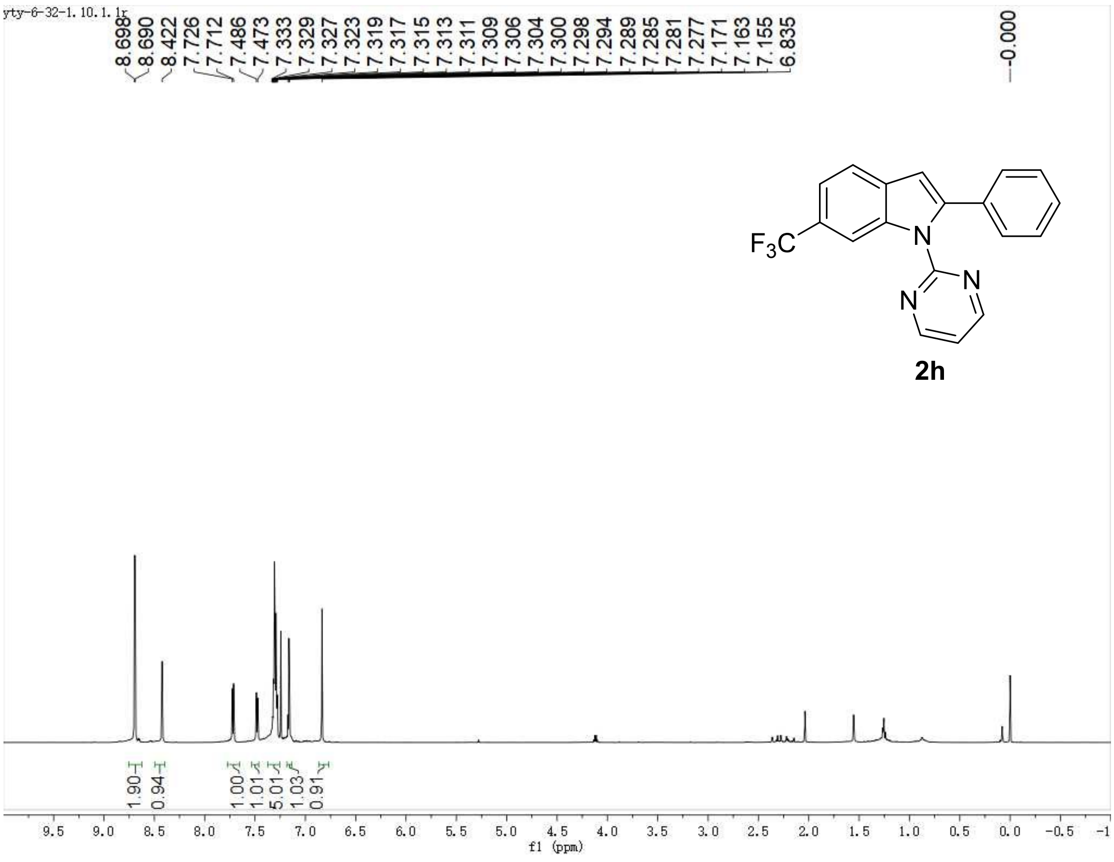
^{1}H NMR spectrum of compound **2g** ($CDCl_3$, 600 MHz)



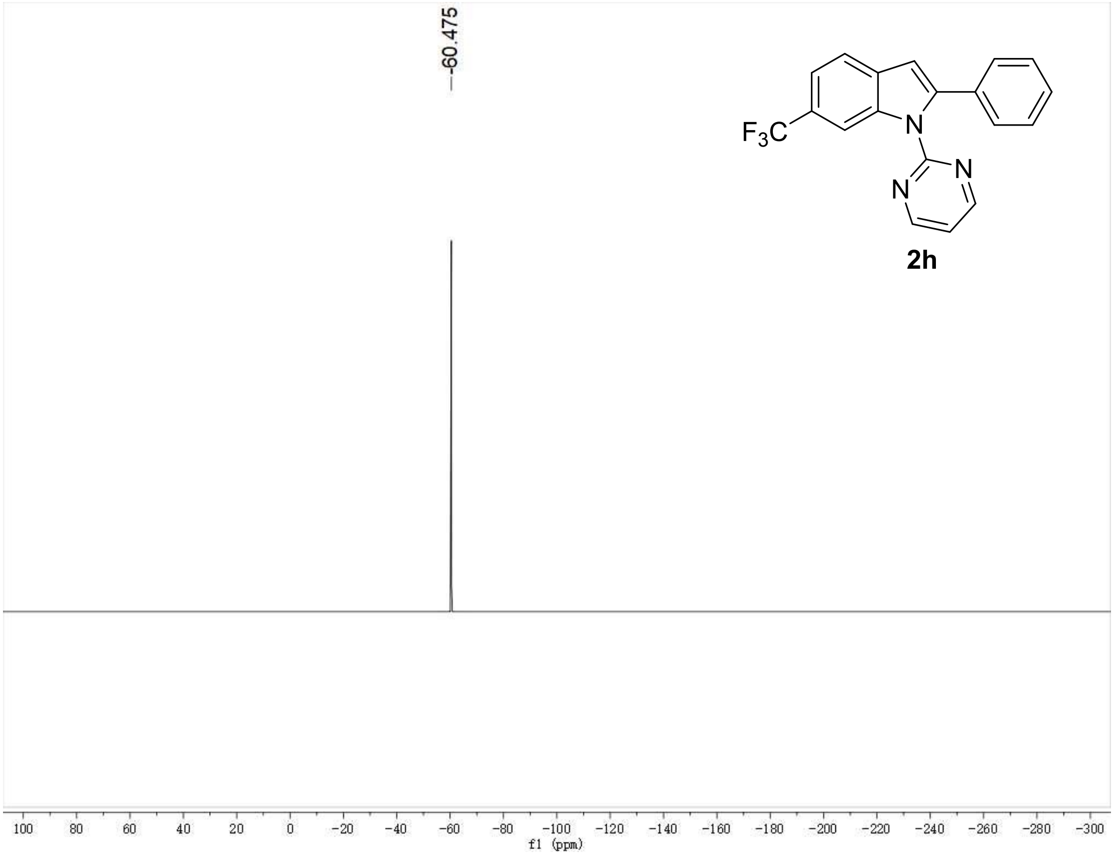
^{13}C NMR spectrum of compound **2g** (CDCl$_3$, 151 MHz)



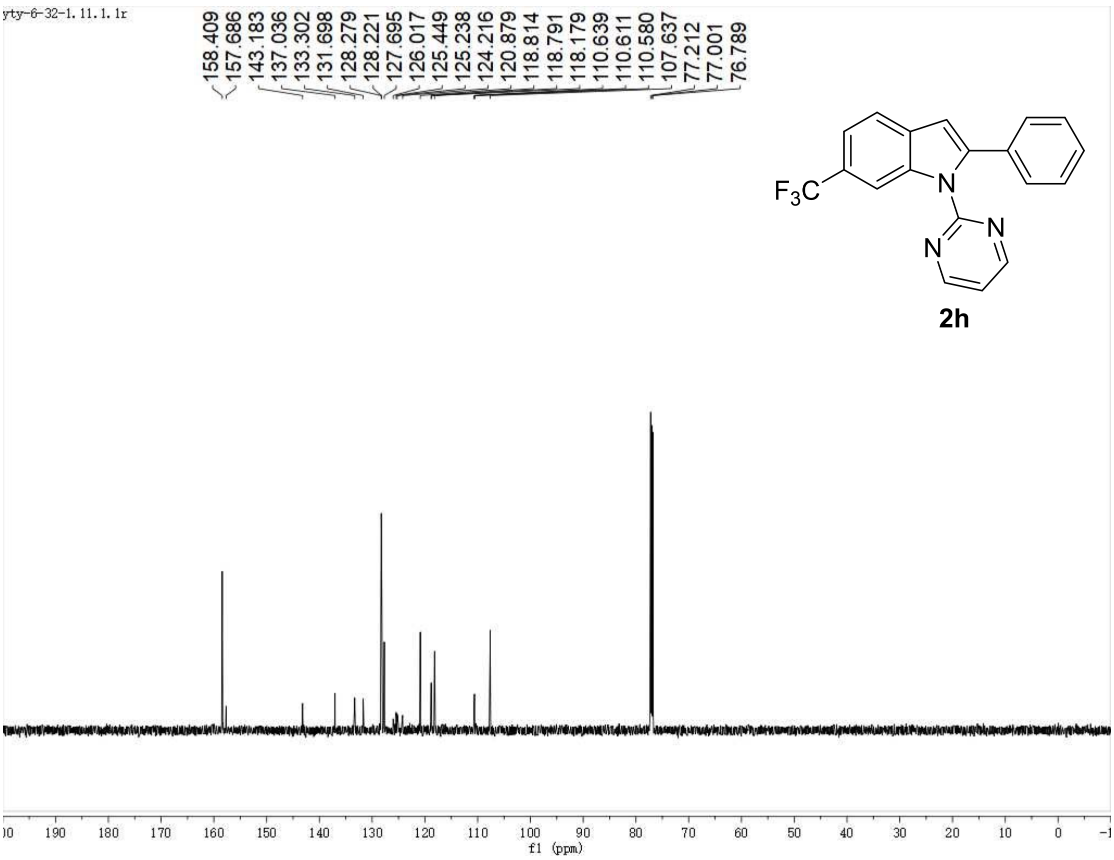
^{1}H NMR spectrum of compound **2h** (CDCl$_3$, 600 MHz)



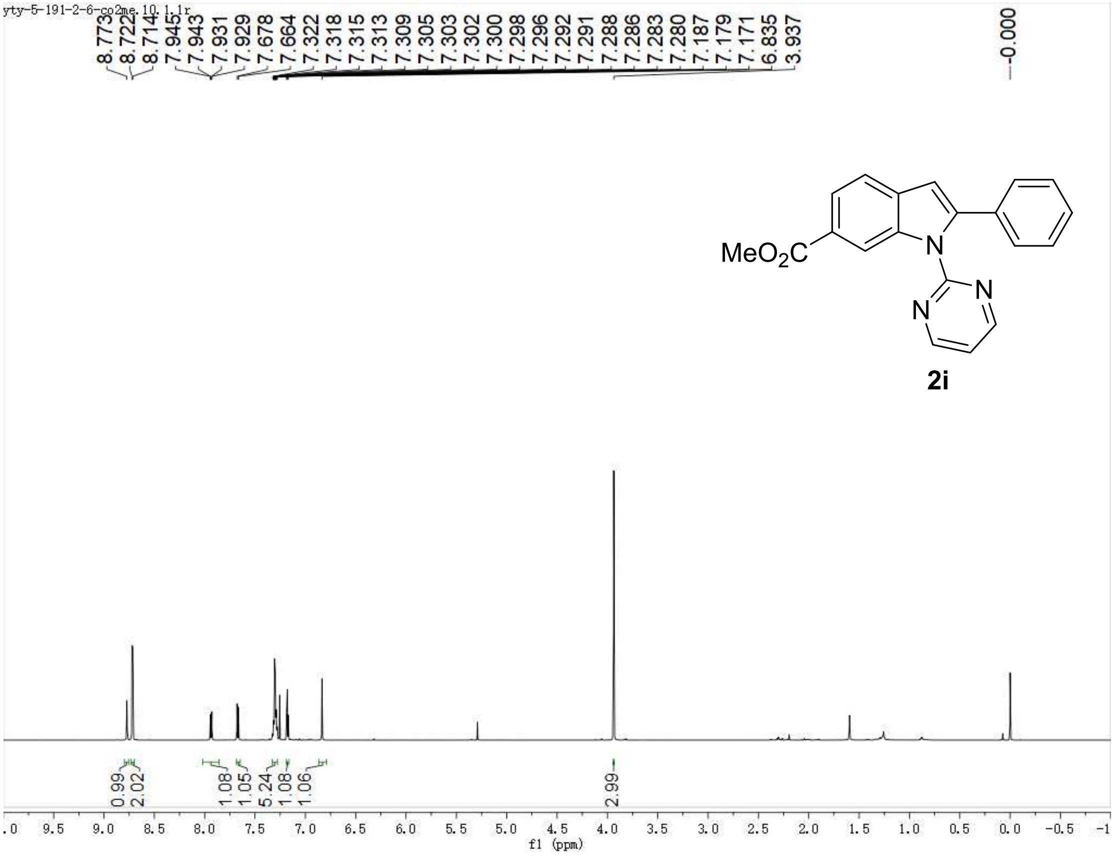
^{19}F NMR spectrum of compound **2h** ($CDCl_3$, 376 MHz)



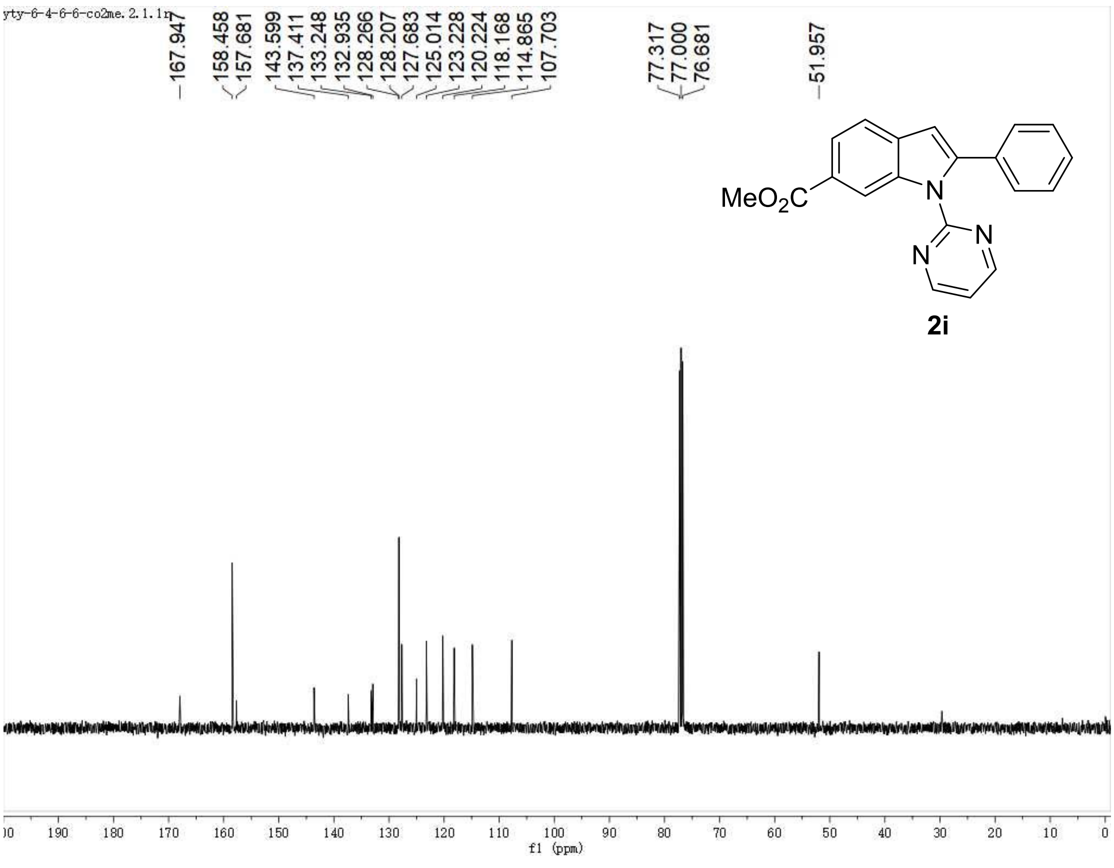
^{13}C NMR spectrum of compound **2h** ($CDCl_3$, 151 MHz)



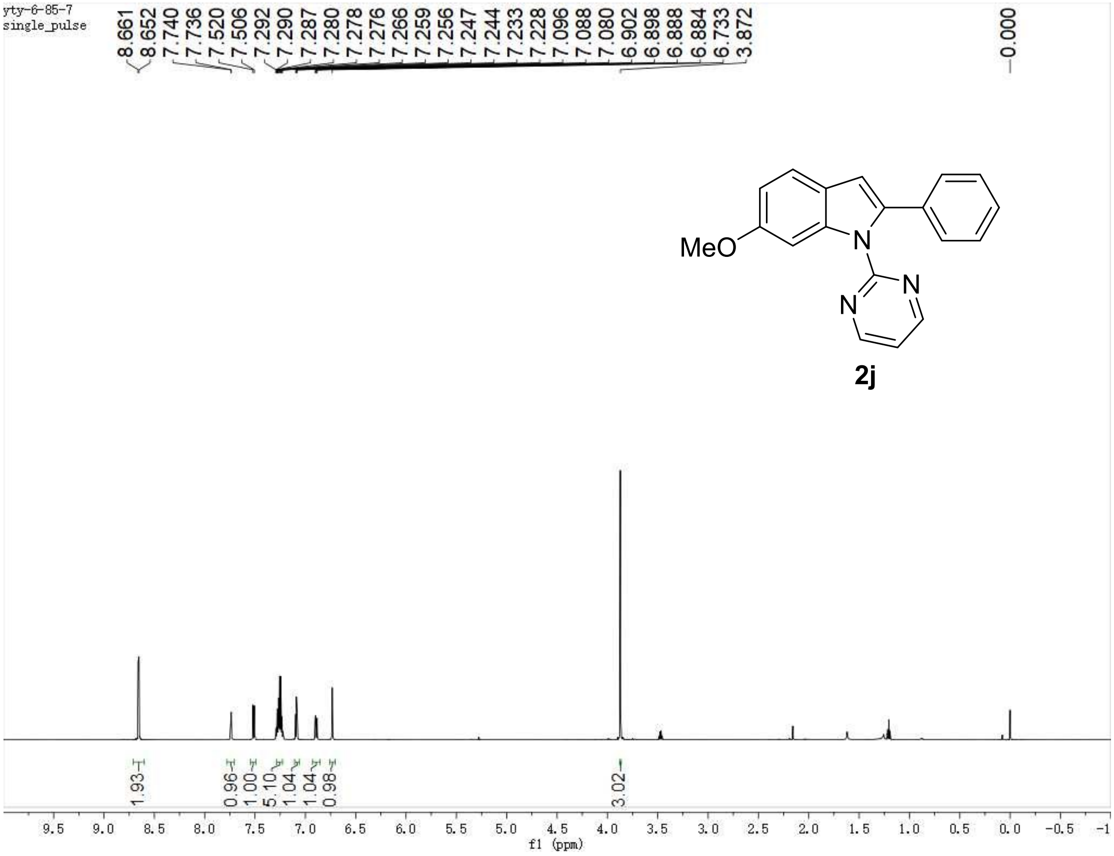
^1H NMR spectrum of compound **2i** ($CDCl_3$, 600 MHz)



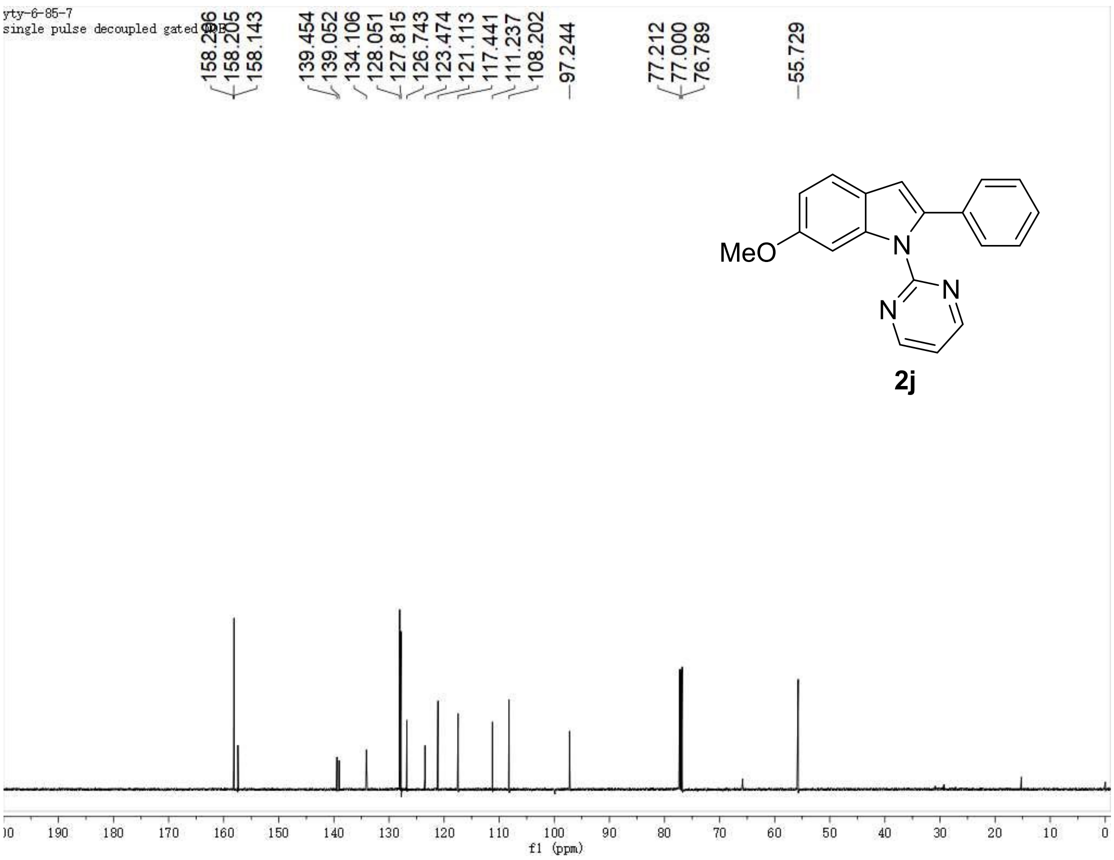
^{13}C NMR spectrum of compound **2i** ($CDCl_3$, 151 MHz)



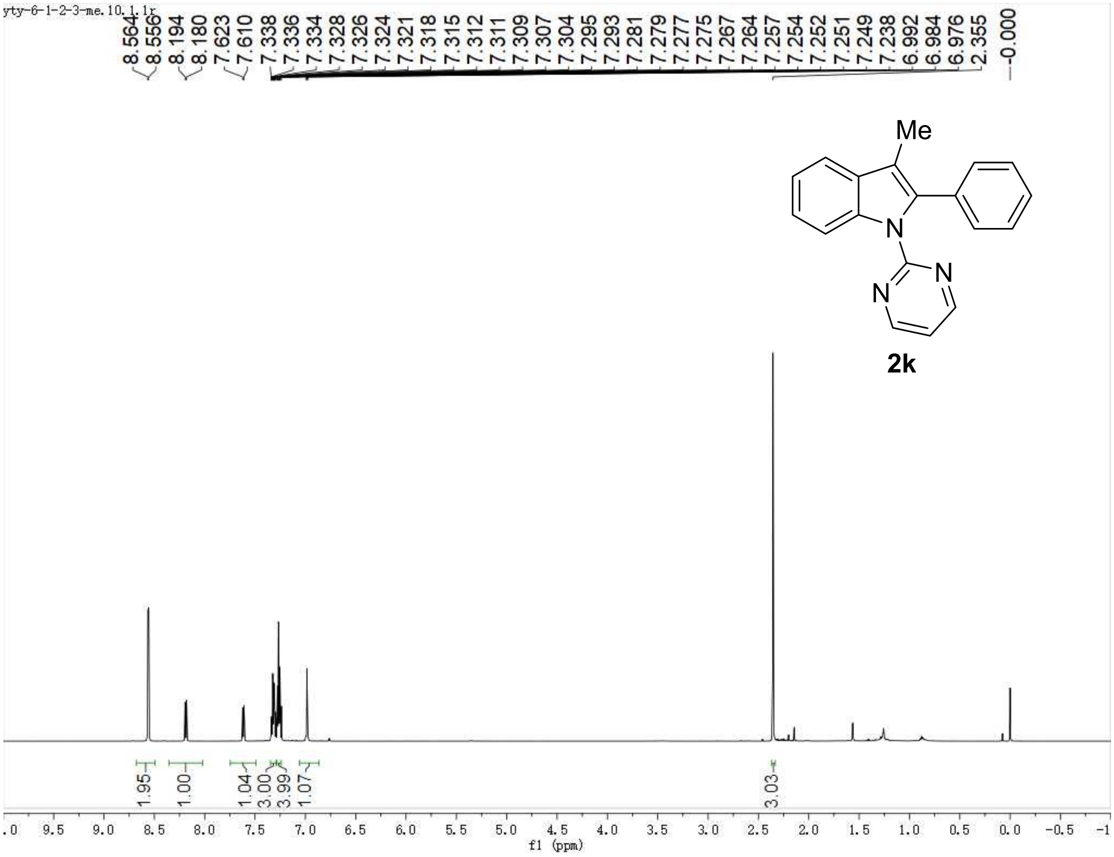
^{1}H NMR spectrum of compound **2j** ($CDCl_3$, 600 MHz)



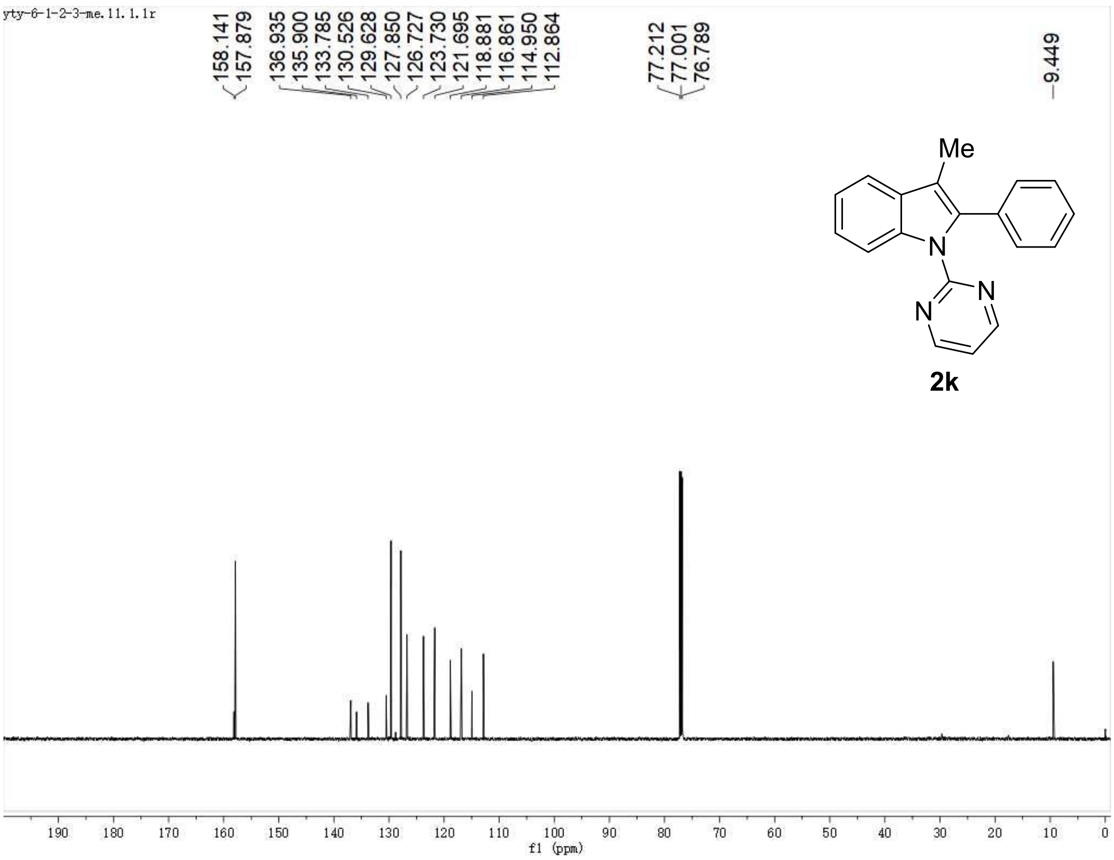
^{13}C NMR spectrum of compound **2j** ($CDCl_3$, 151 MHz)



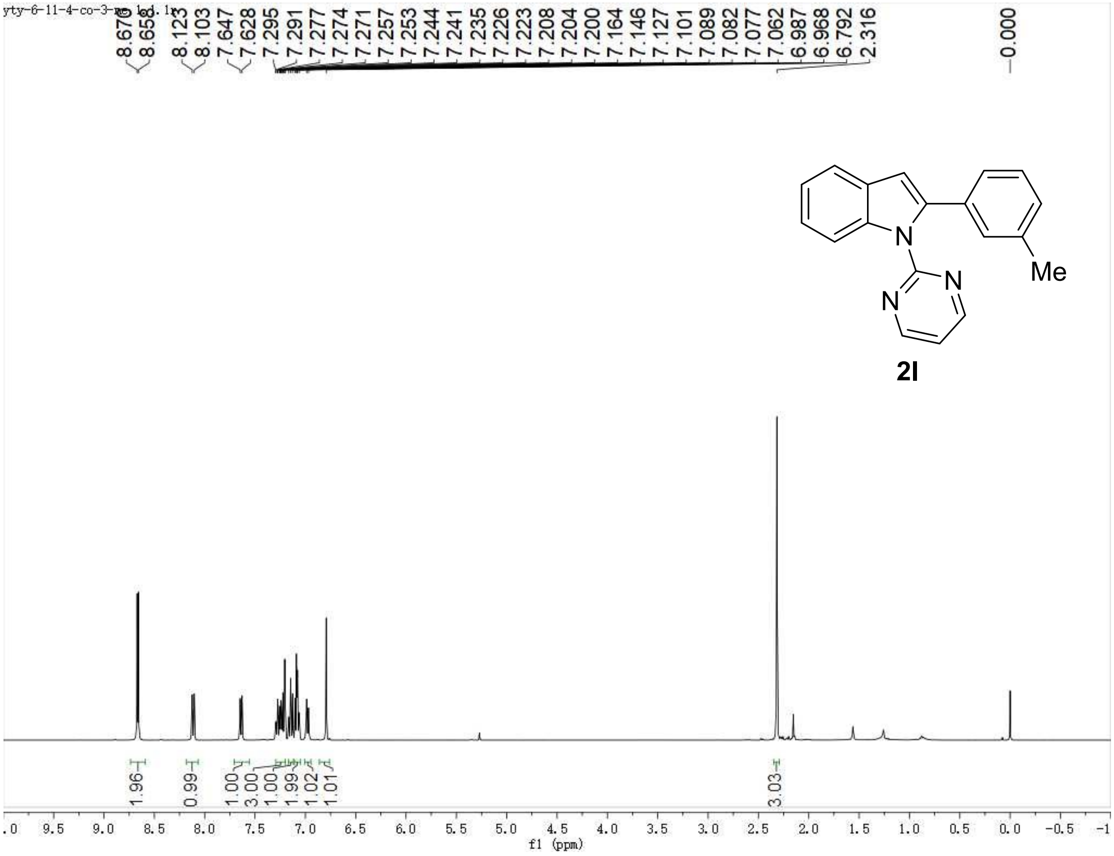
^{1}H NMR spectrum of compound **2k** ($CDCl_3$, 600 MHz)



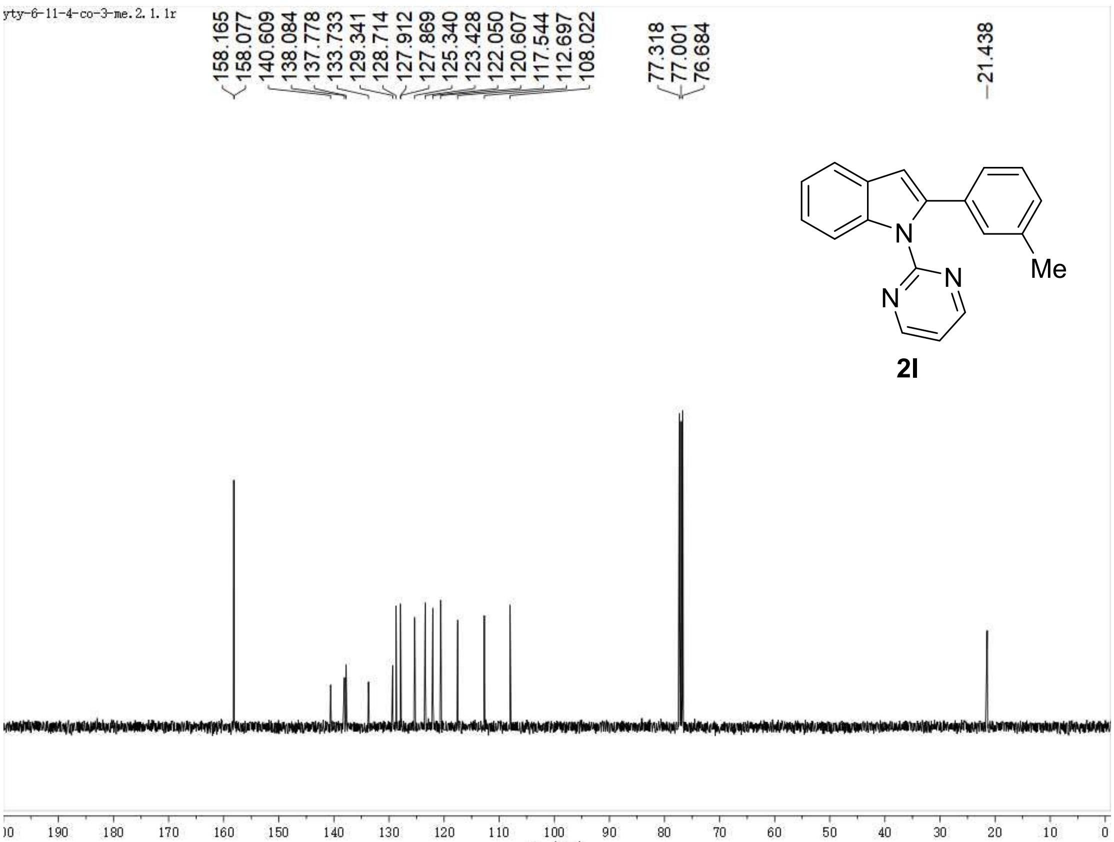
^{13}C NMR spectrum of compound **2k** ($CDCl_3$, 151 MHz)



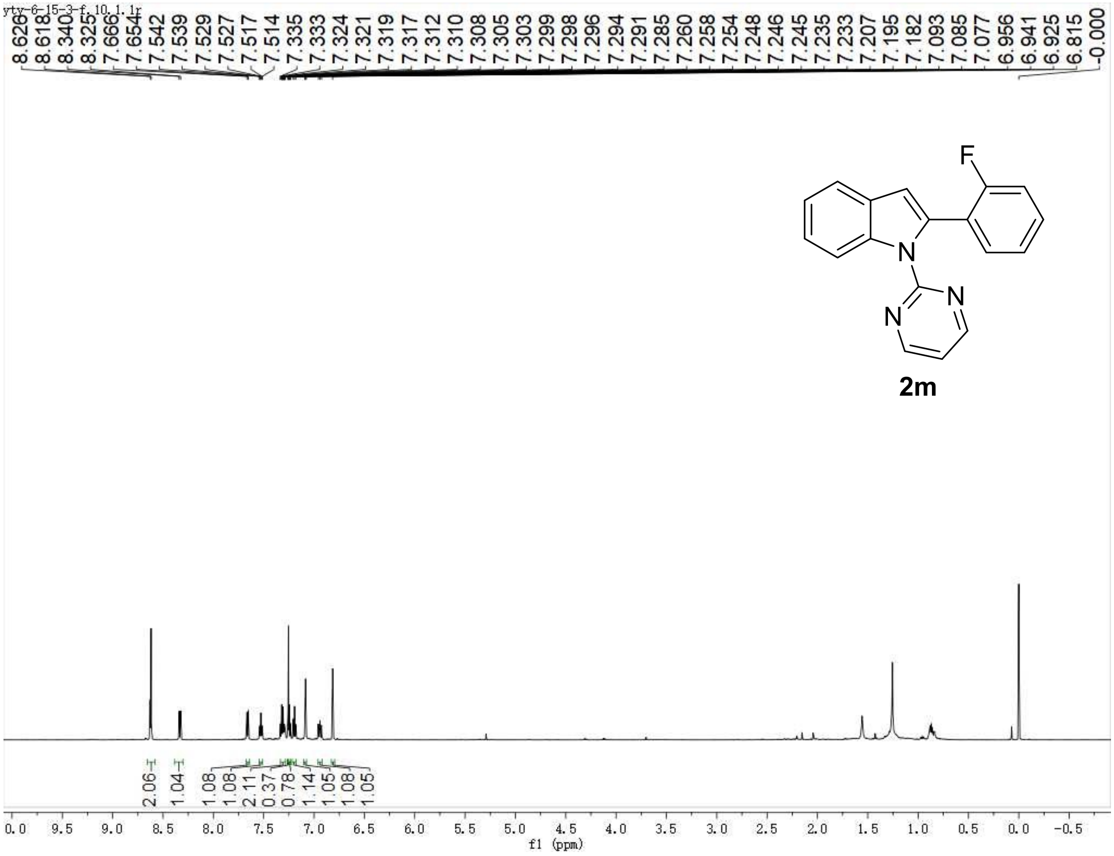
^{1}H NMR spectrum of compound **2l** ($CDCl_3$, 400 MHz)



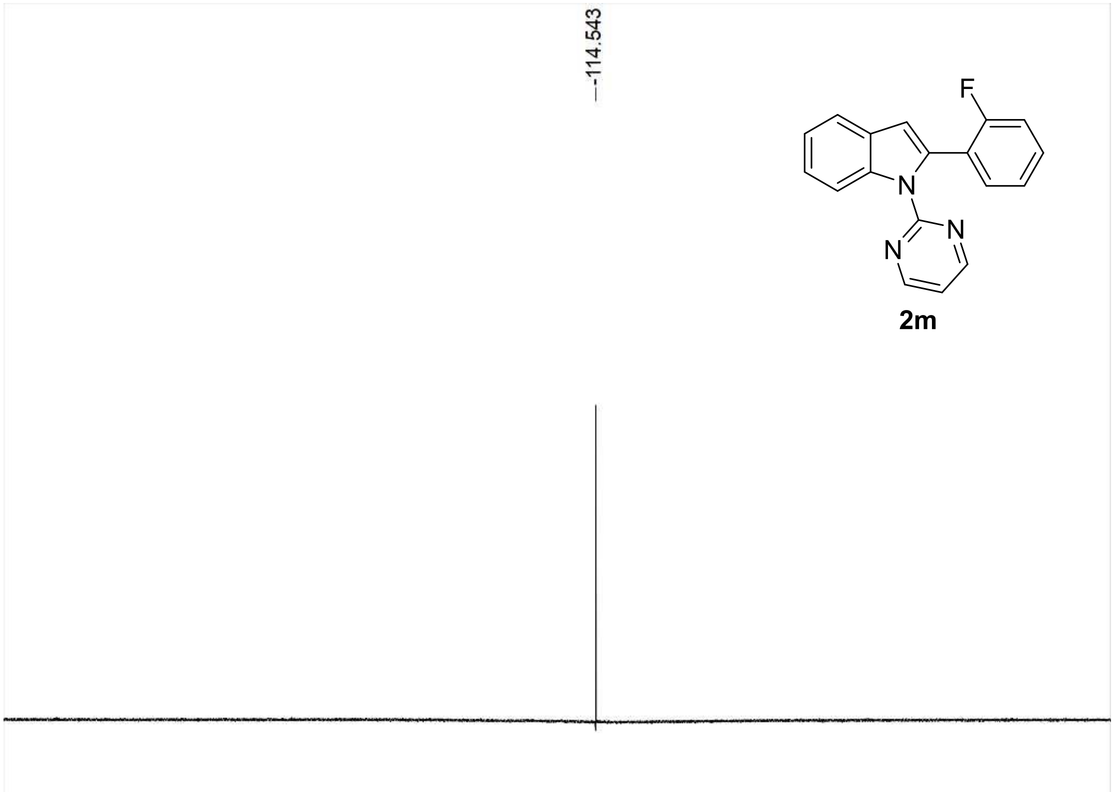
^{13}C NMR spectrum of compound **2l** ($CDCl_3$, 101 MHz)



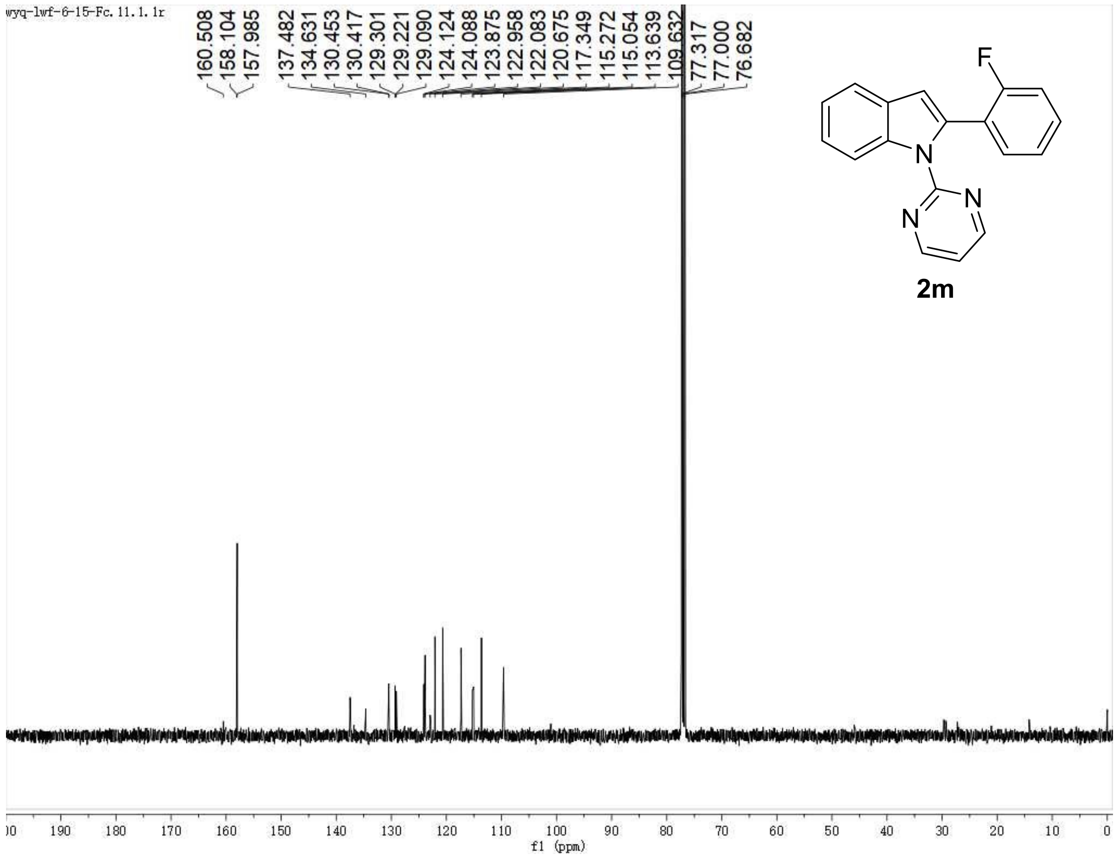
[1]H NMR spectrum of compound **2m** ($CDCl_3$, 600 MHz)



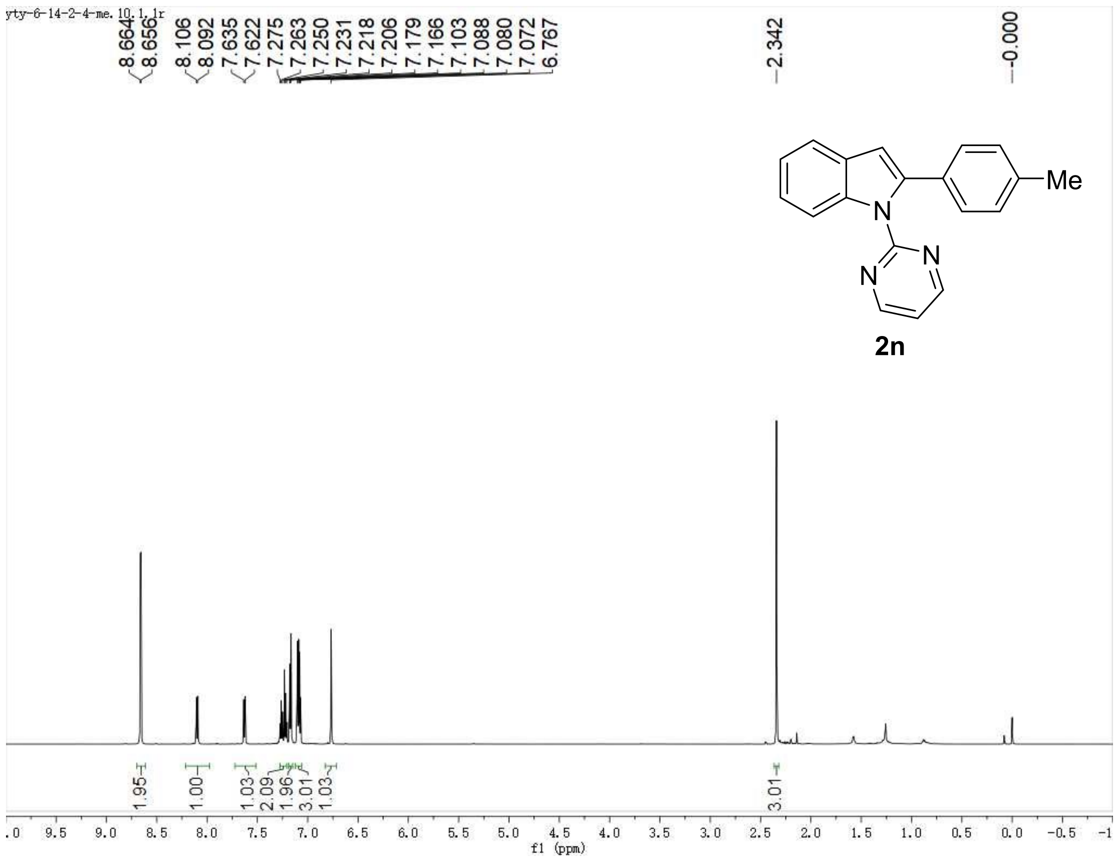
[19]F NMR spectrum of compound **2m** ($CDCl_3$, 376 MHz)



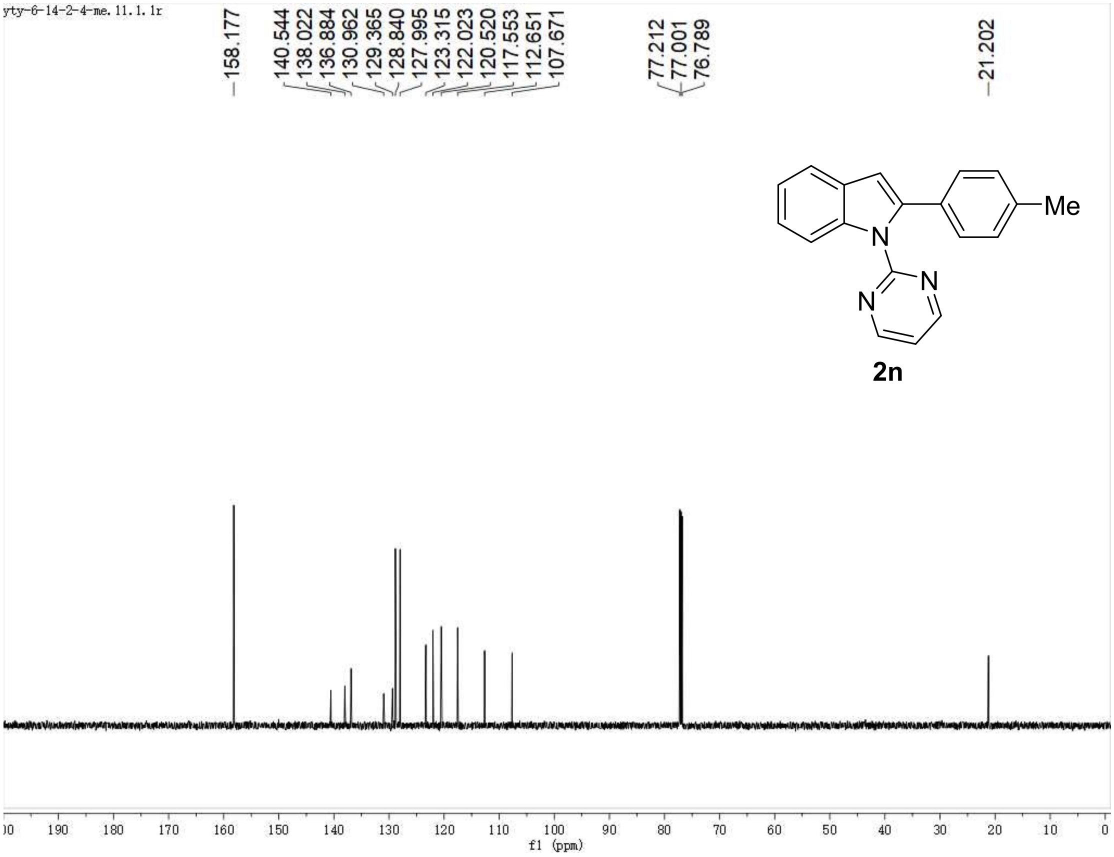
^{13}C NMR spectrum of compound **2m** ($CDCl_3$, 151 MHz)



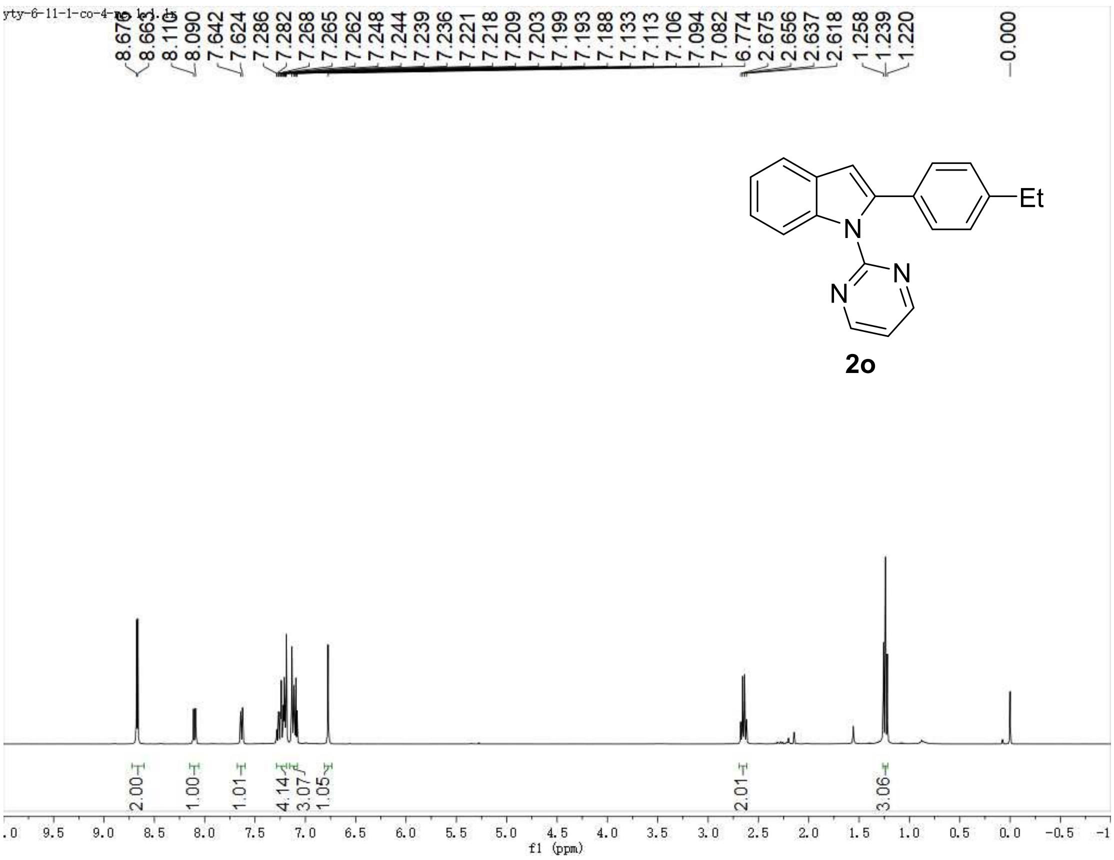
^{1}H NMR spectrum of compound **2n** ($CDCl_3$, 600 MHz)



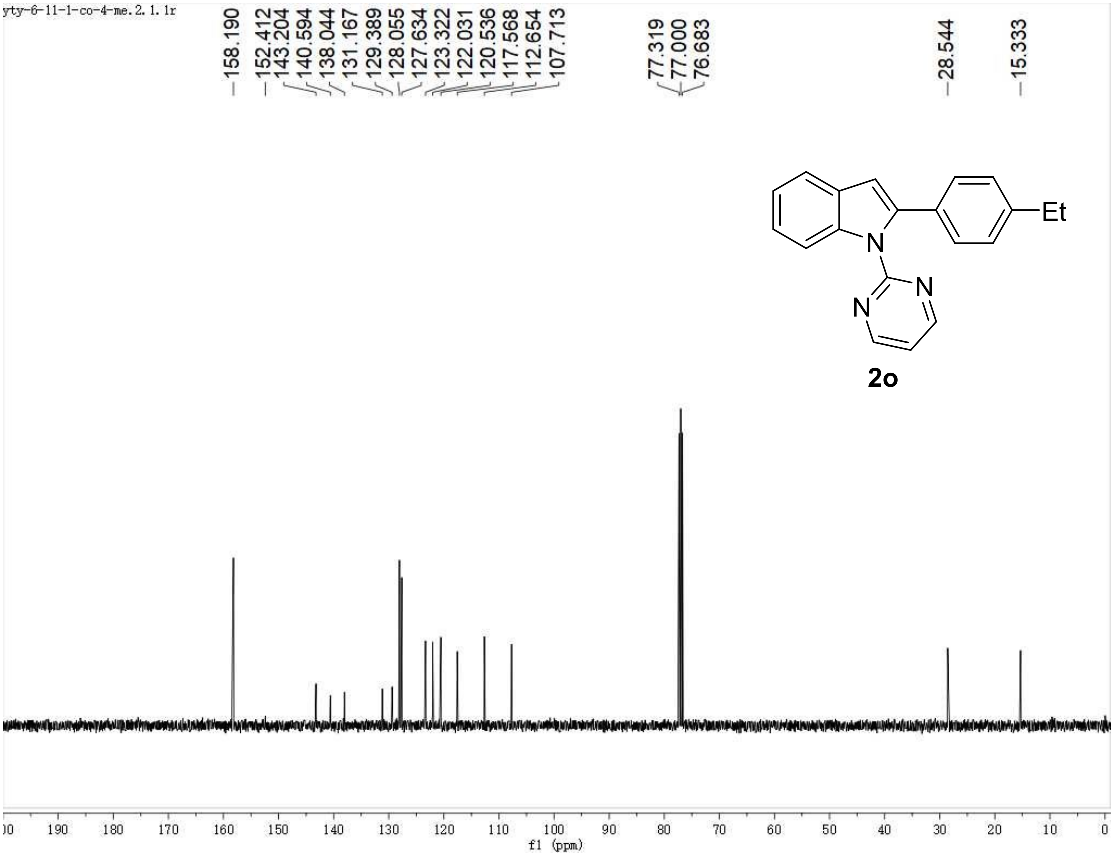
^{13}C NMR spectrum of compound **2n** ($CDCl_3$, 151 MHz)



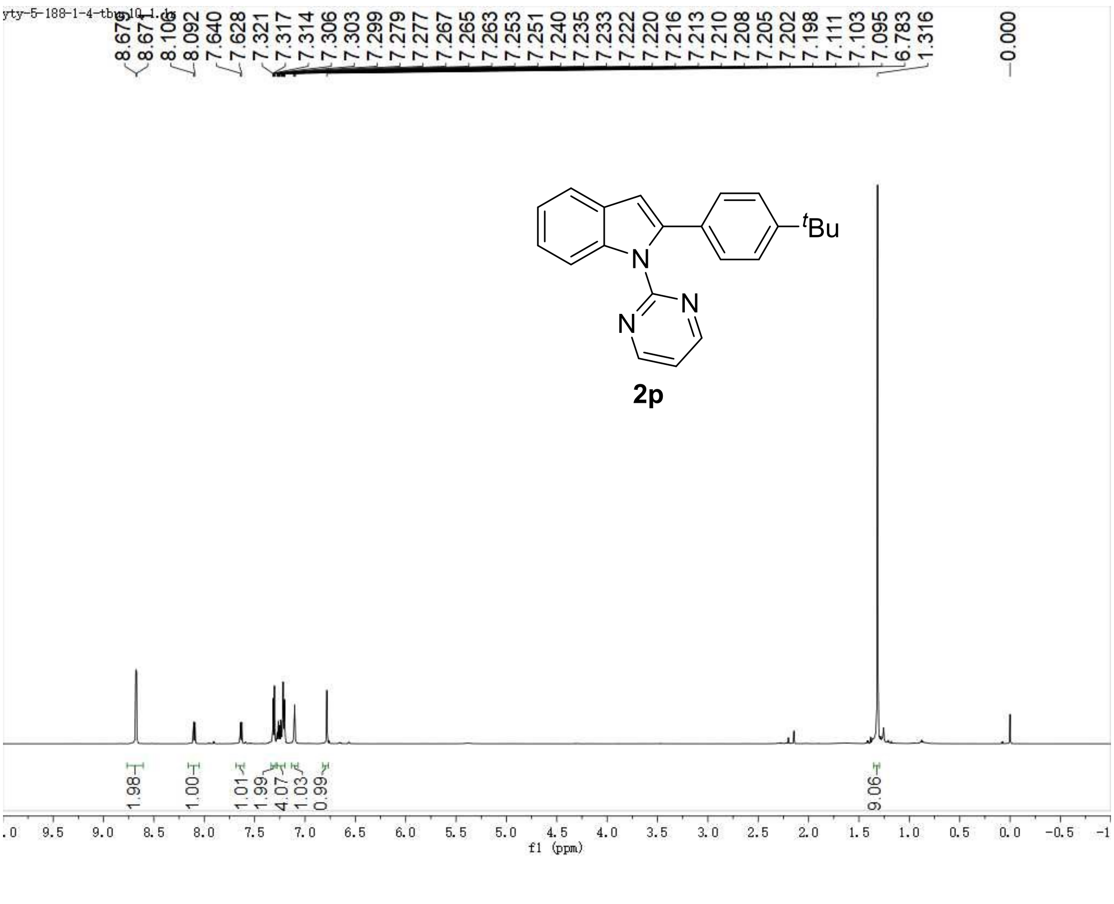
^1H NMR spectrum of compound **2o** ($CDCl_3$, 400 MHz)



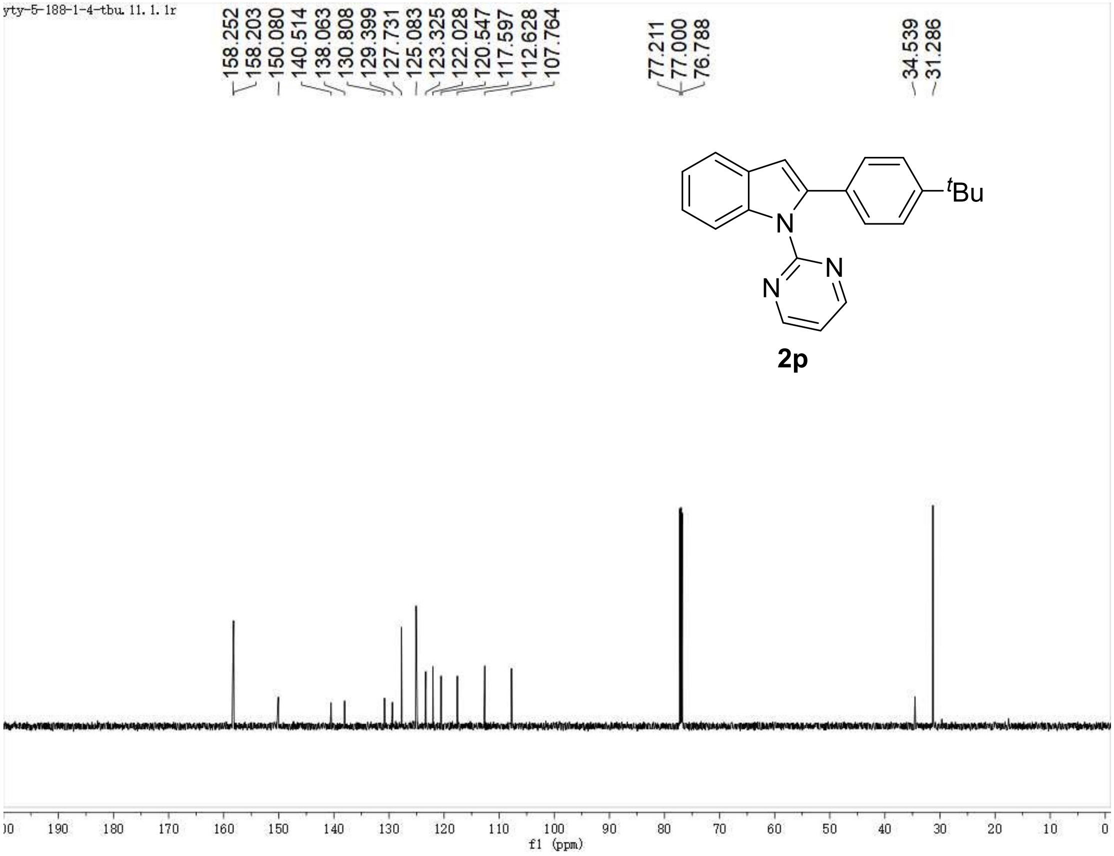
^{13}C NMR spectrum of compound **2o** ($CDCl_3$, 101 MHz)



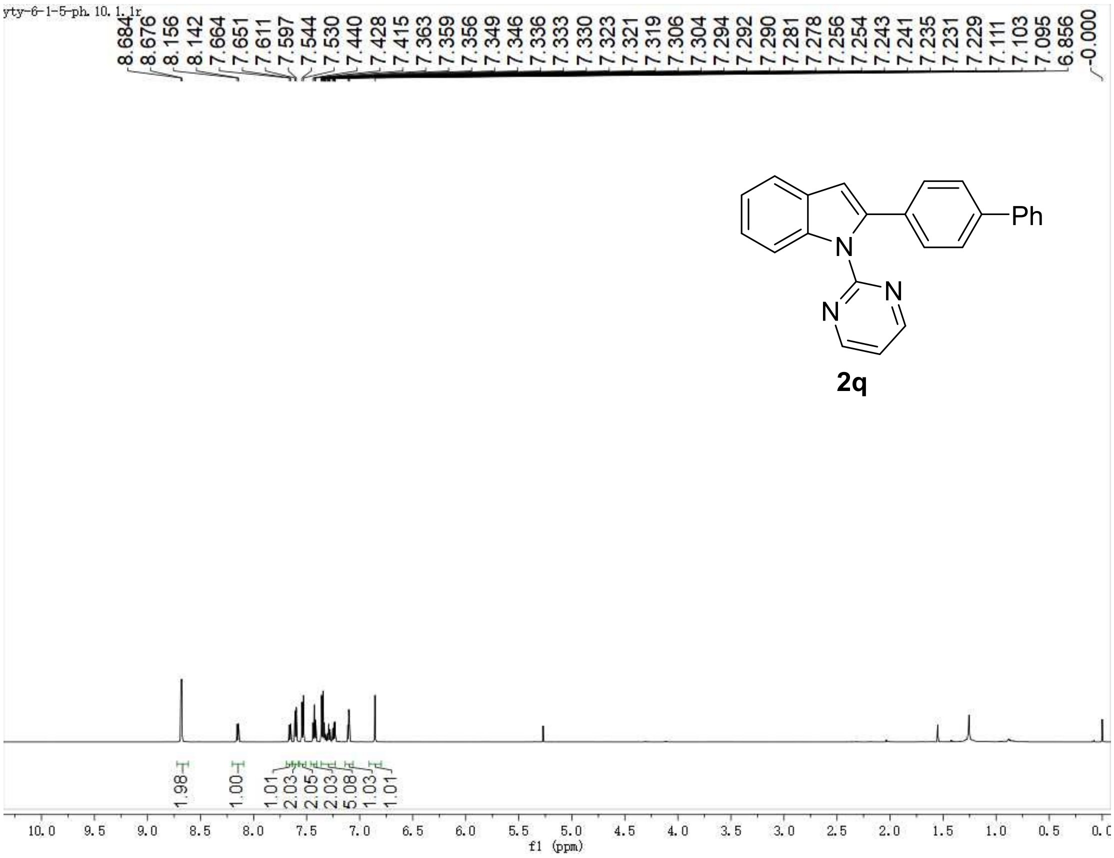
^{1}H NMR spectrum of compound 2**p** ($CDCl_3$, 600 MHz)



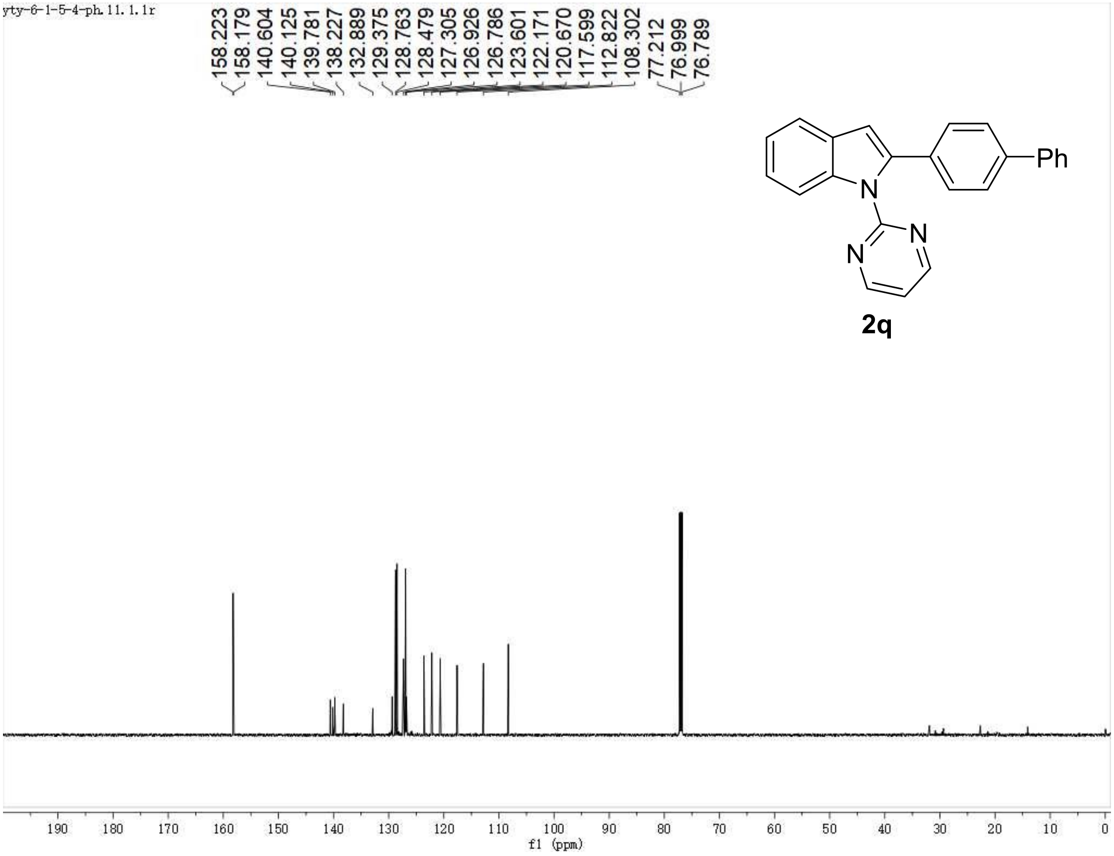
^{13}C NMR spectrum of compound **2p** ($CDCl_3$, 151 MHz)



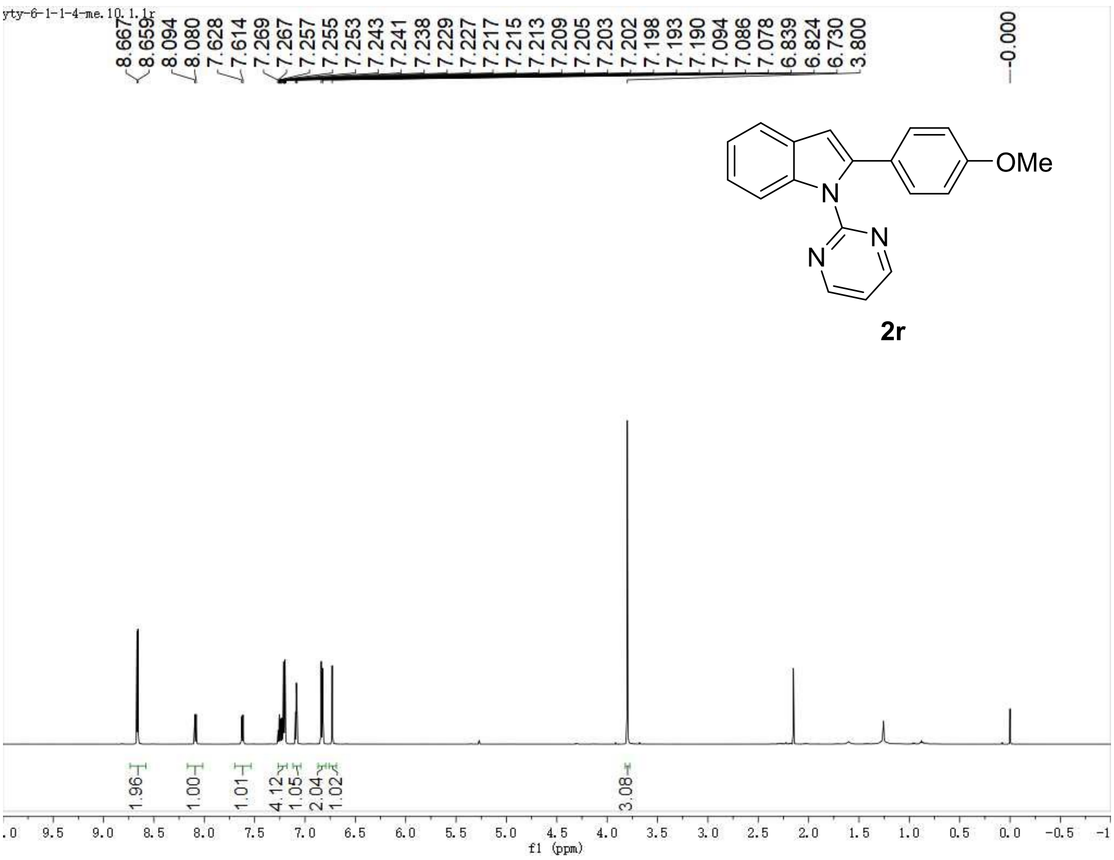
^{1}H NMR spectrum of compound **2q** ($CDCl_3$, 600 MHz)



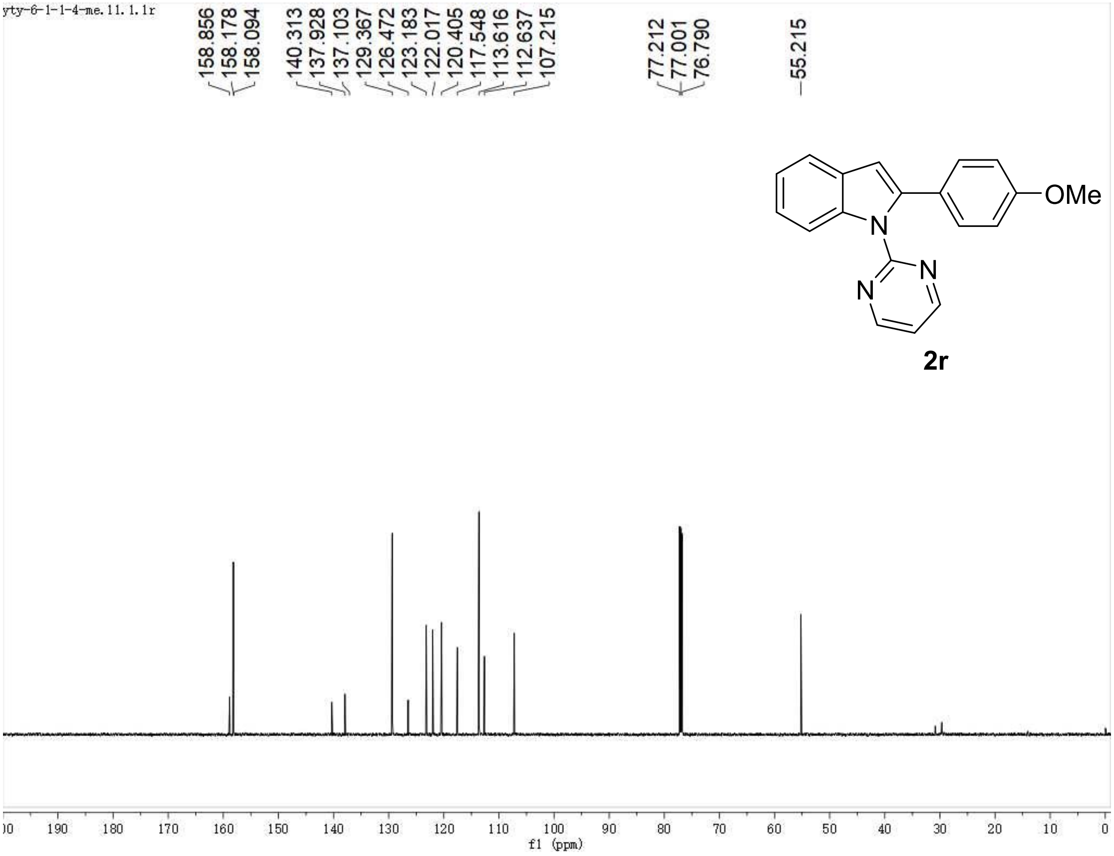
^{13}C NMR spectrum of compound **2q** ($CDCl_3$, 151 MHz)



^{1}H NMR spectrum of compound **2r** ($CDCl_3$, 600 MHz)

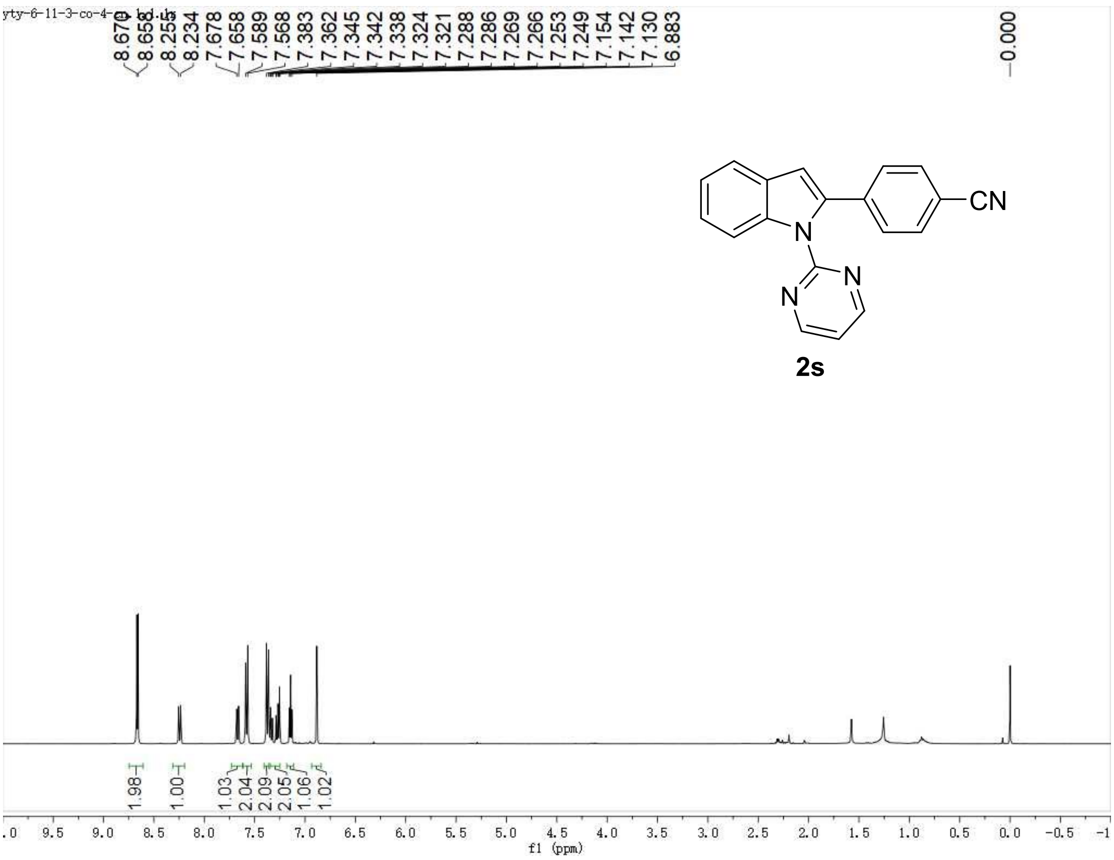


^{13}C NMR spectrum of compound **2r** ($CDCl_3$, 151 MHz)



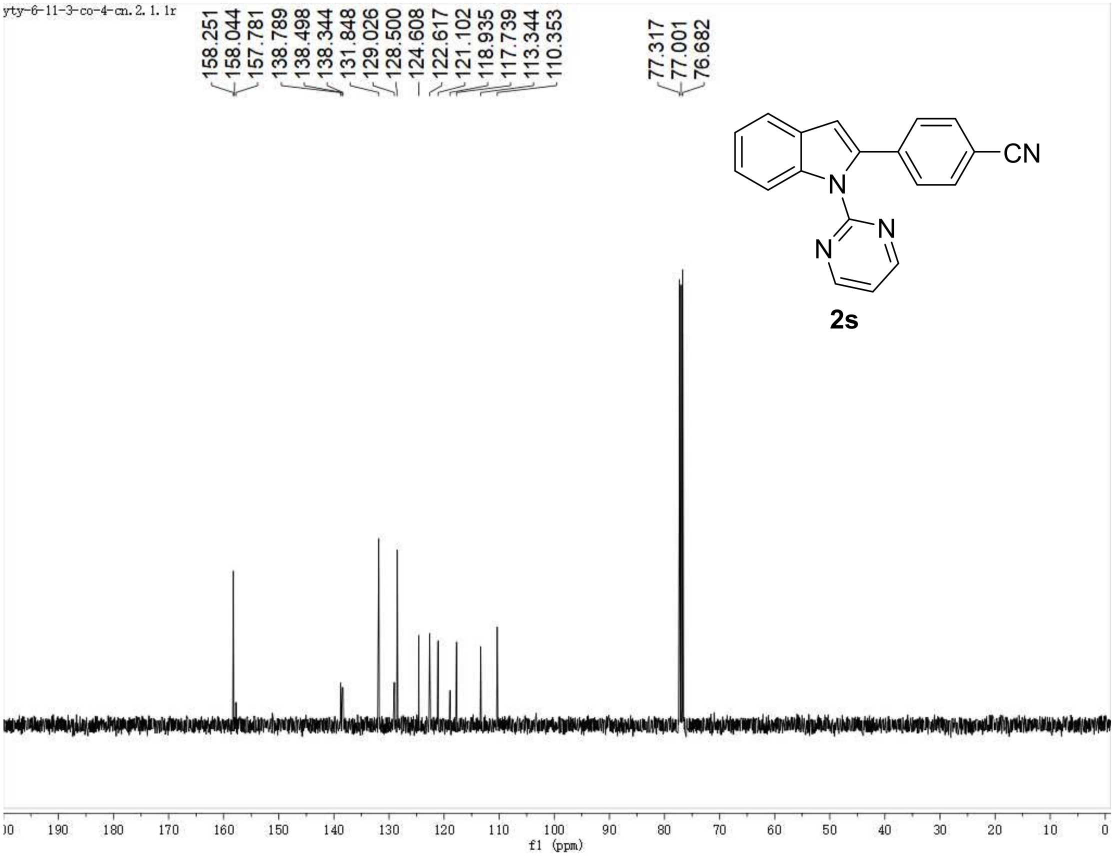
2r

^{1}H NMR spectrum of compound **2s** ($CDCl_3$, 400 MHz)

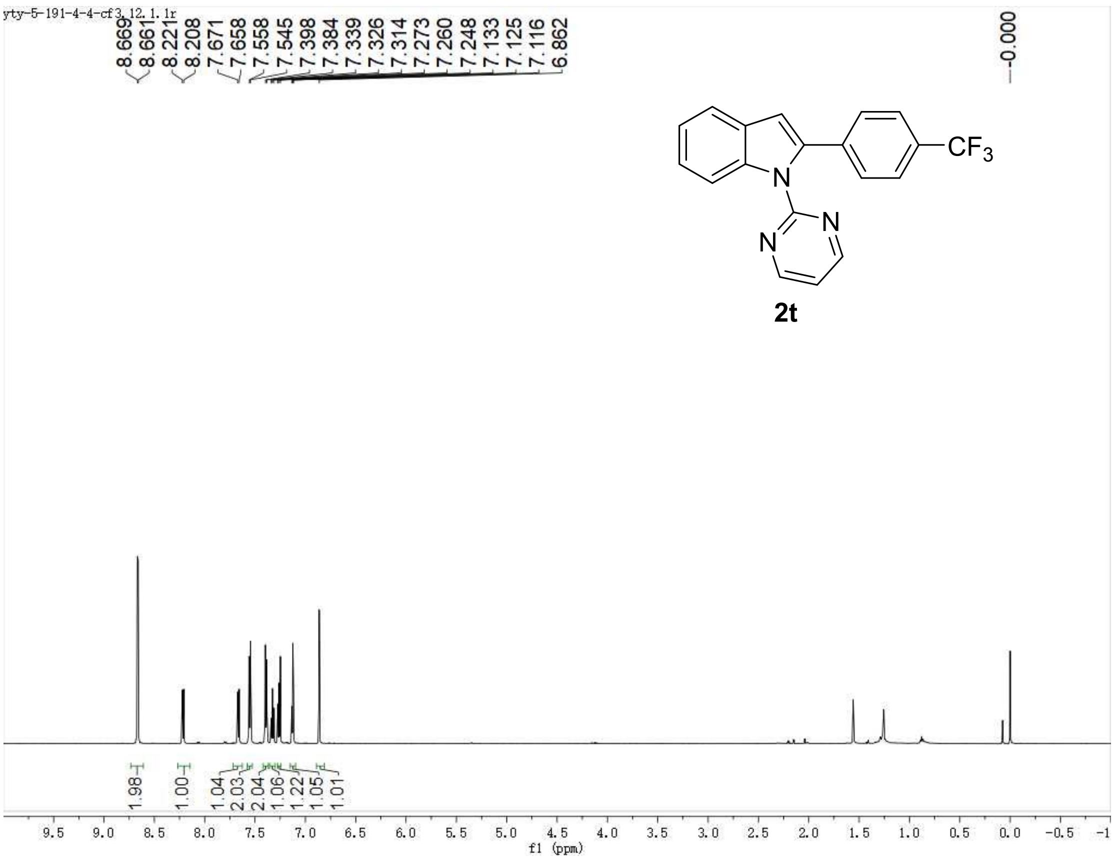


2s

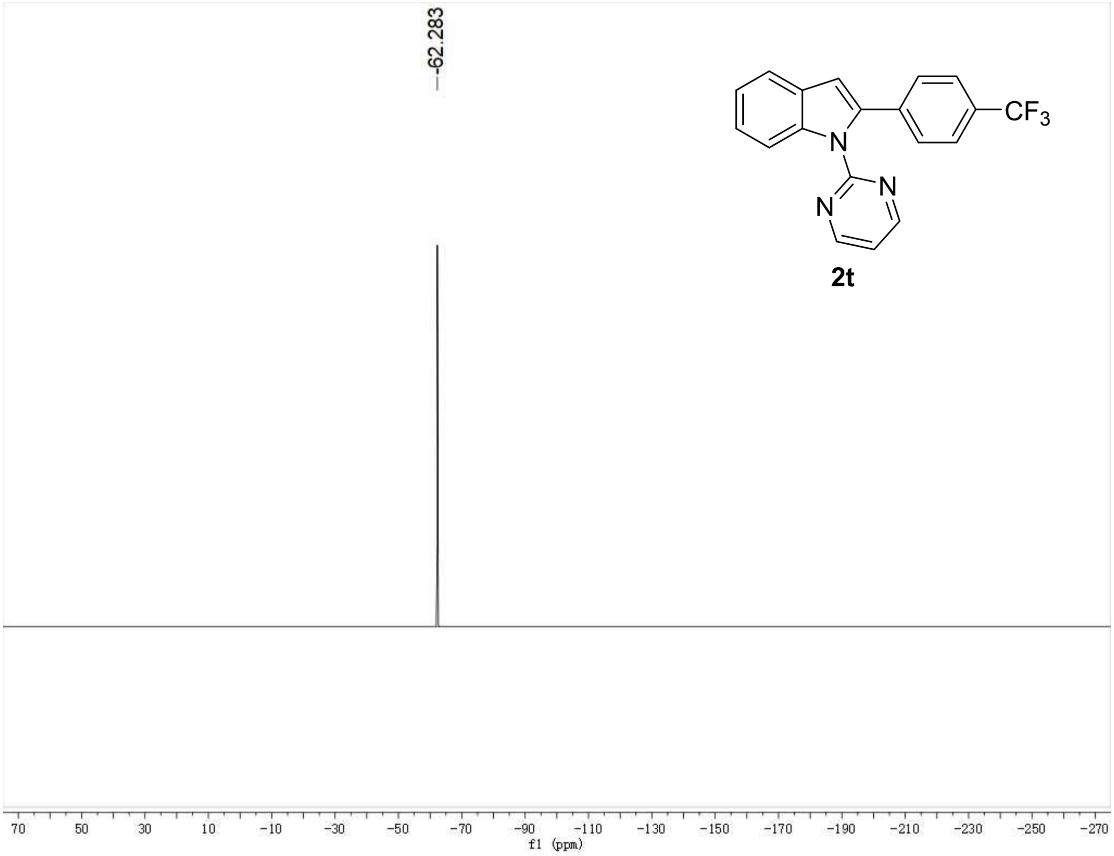
^{13}C NMR spectrum of compound **2s** ($CDCl_3$, 101 MHz)



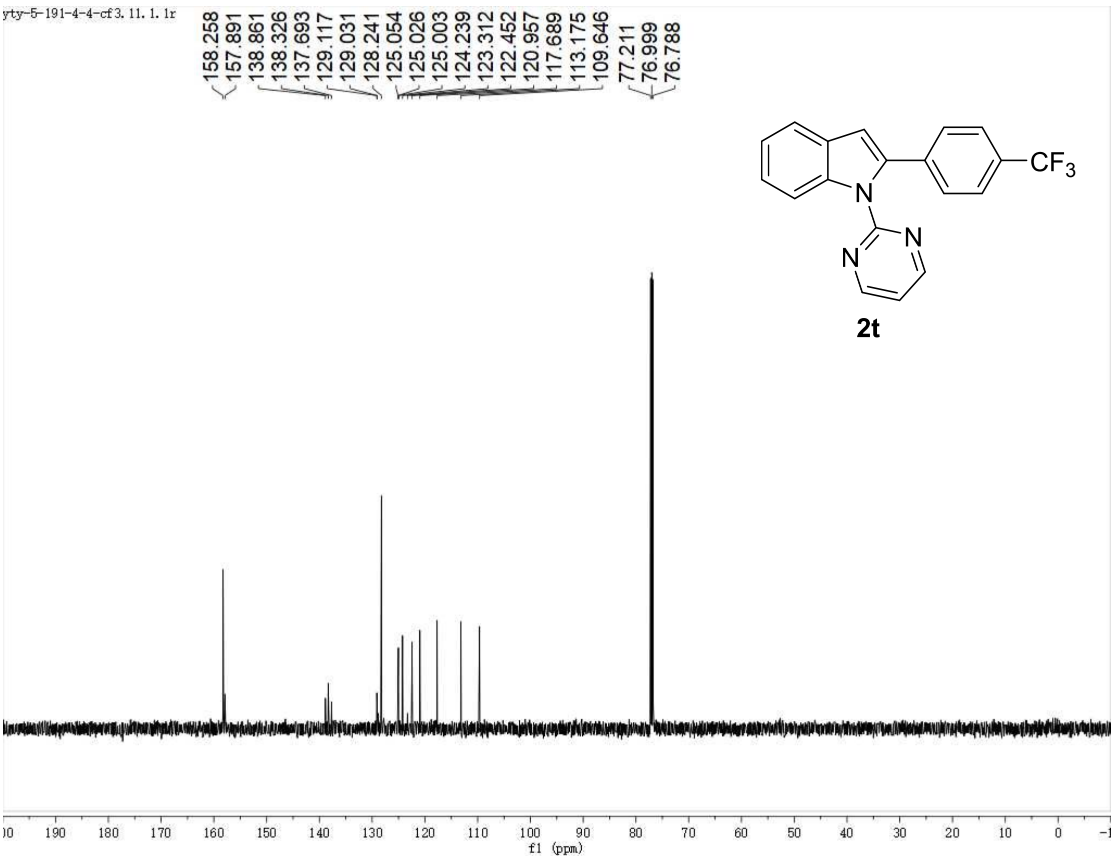
^{1}H NMR spectrum of compound **2t** ($CDCl_3$, 600 MHz)



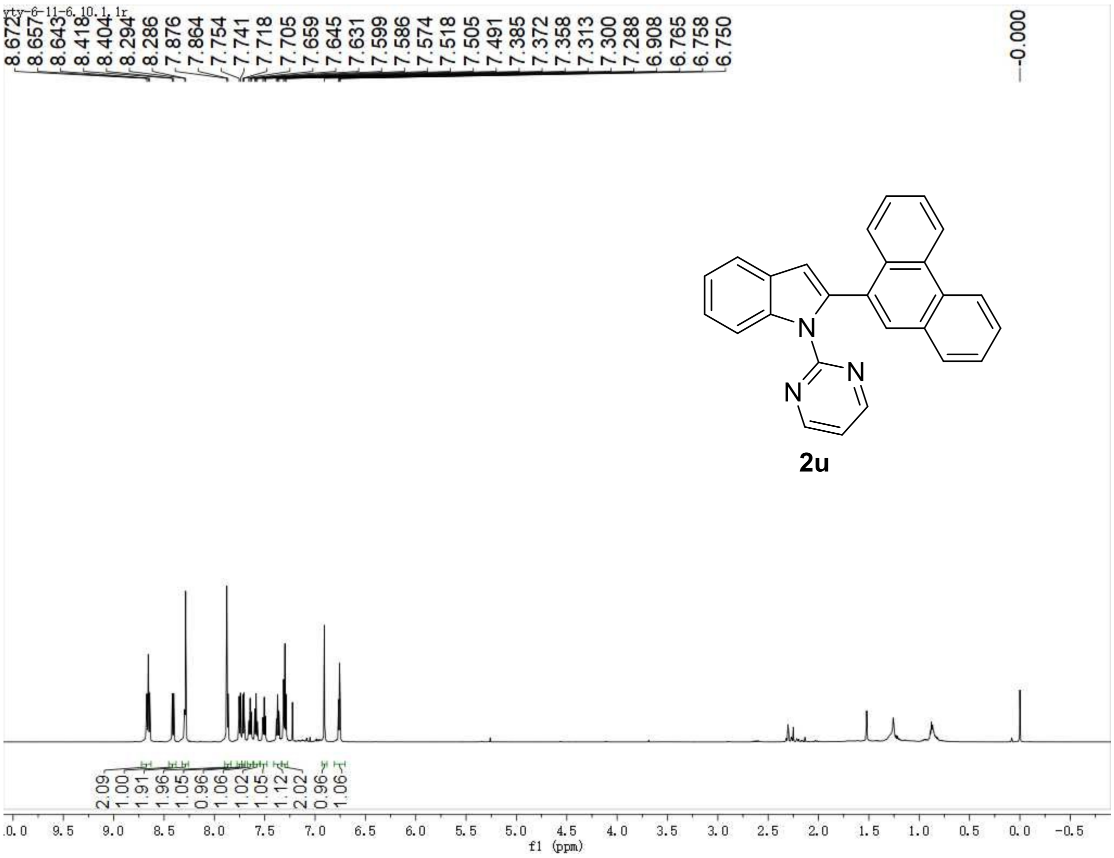
^{19}F NMR spectrum of compound **2t** ($CDCl_3$, 376 MHz)



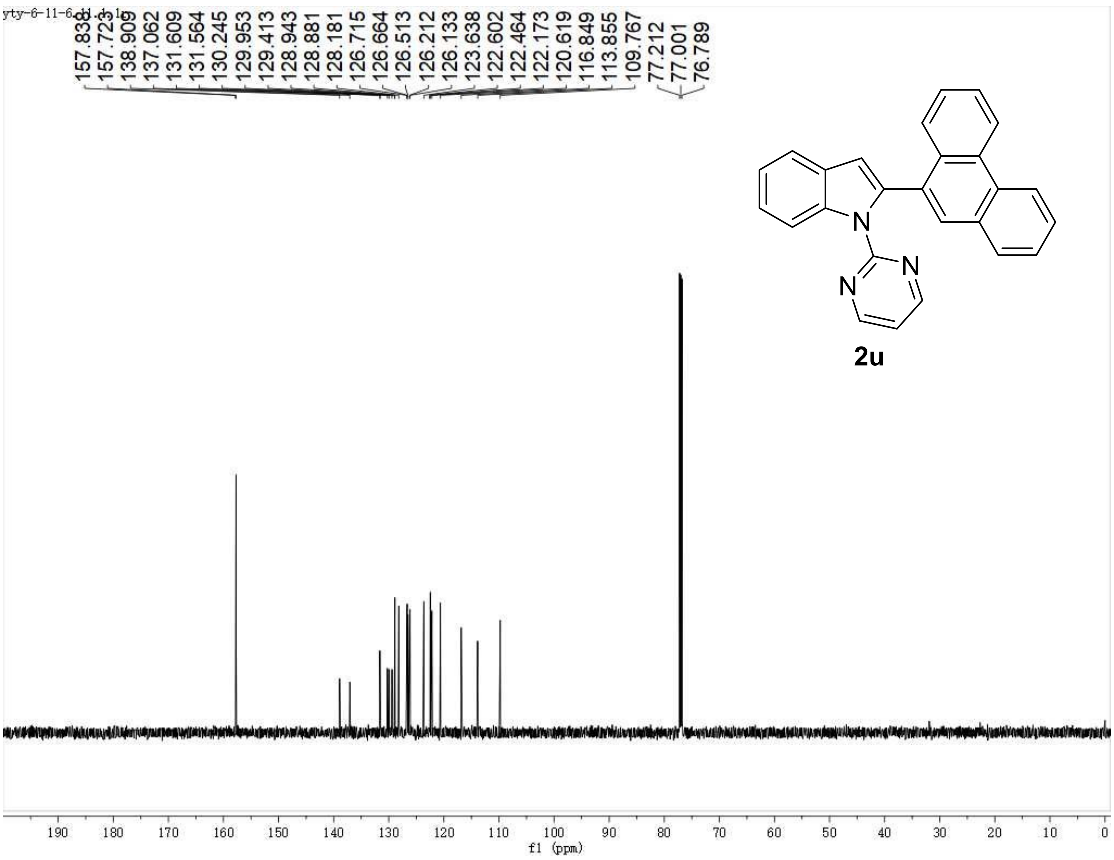
^{13}C NMR spectrum of compound **2t** ($CDCl_3$, 151 MHz)



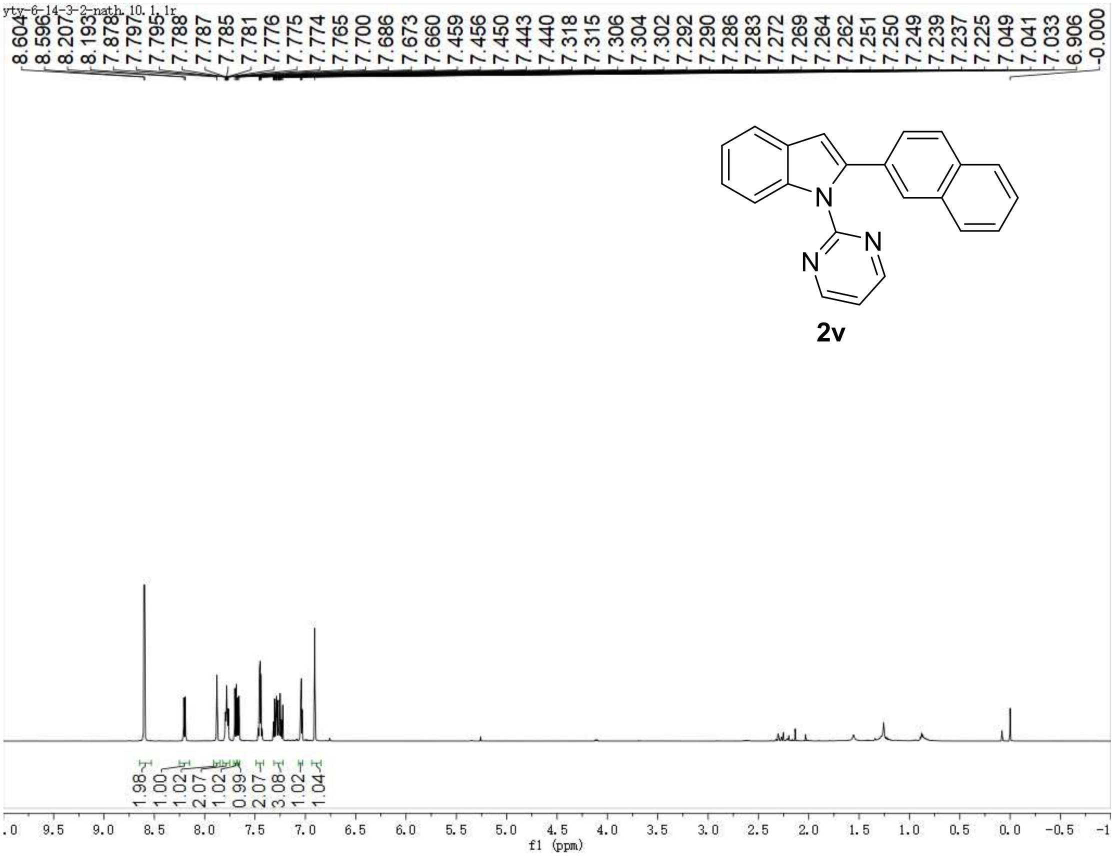
[1]H NMR spectrum of compound **2u** ($CDCl_3$, 600 MHz)



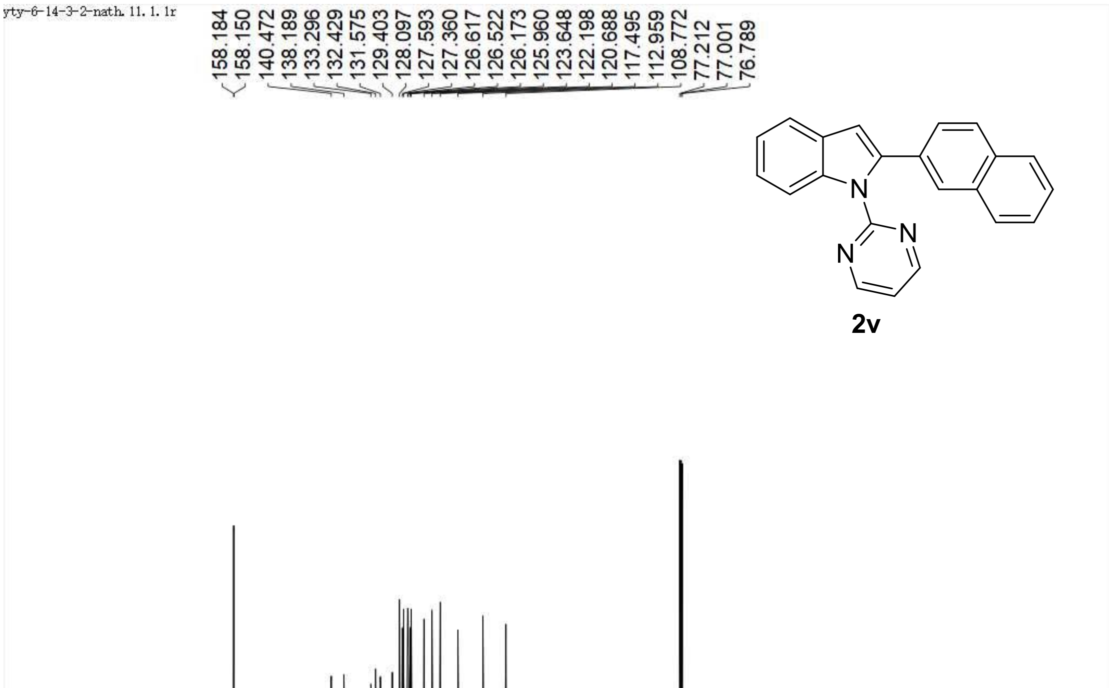
[13]C NMR spectrum of compound **2u** ($CDCl_3$, 151 MHz)



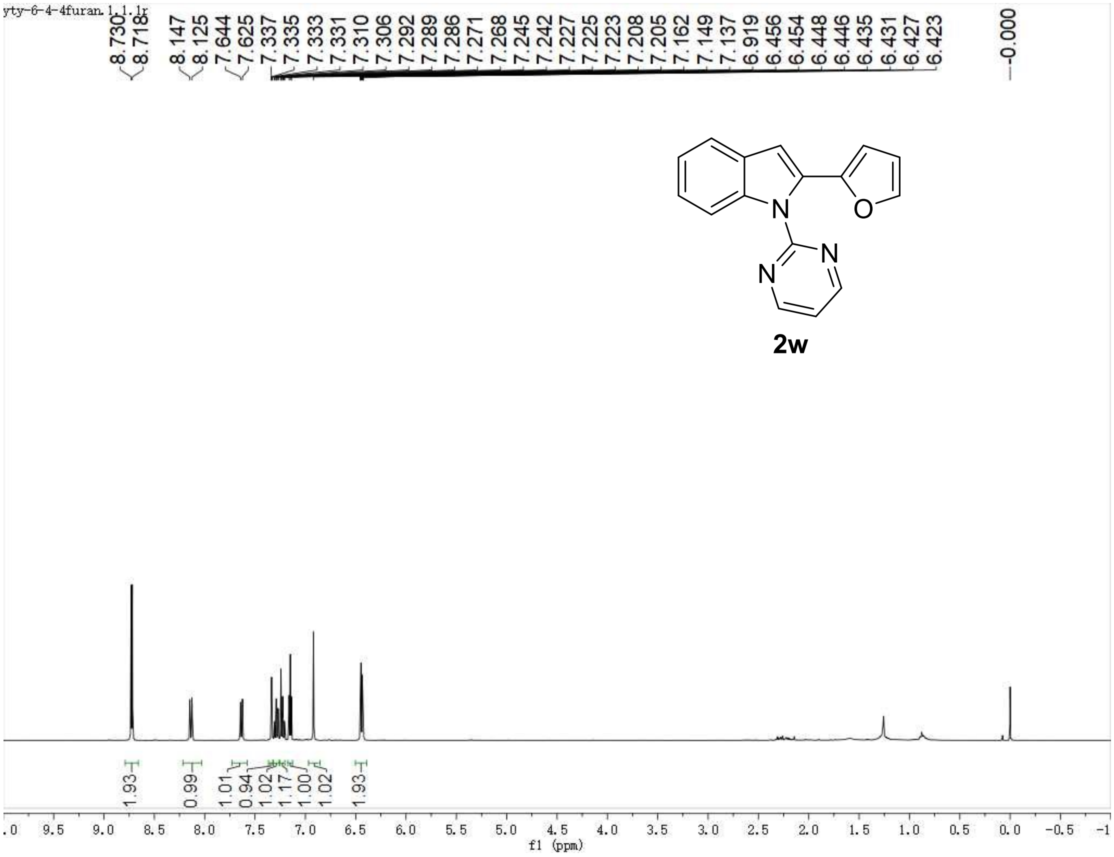
^{1}H NMR spectrum of compound **2v** ($CDCl_3$, 600 MHz)



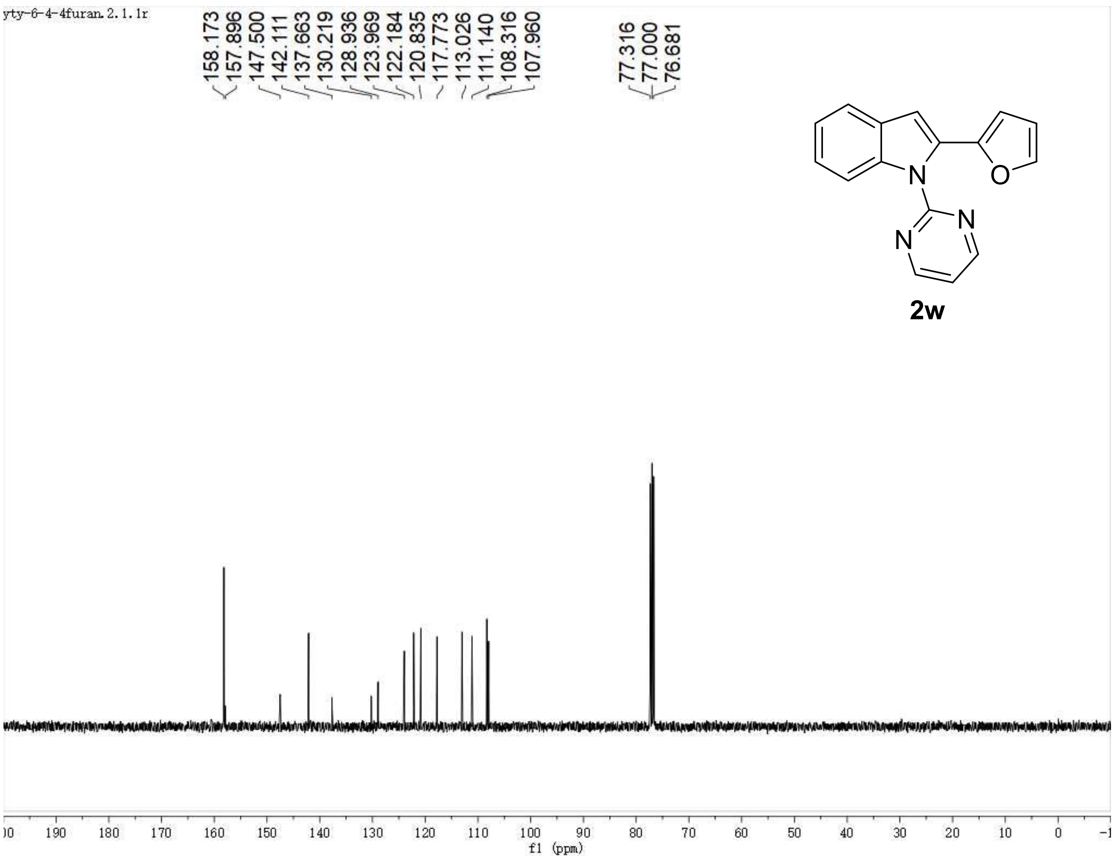
^{13}C NMR spectrum of compound **2v** ($CDCl_3$, 151 MHz)



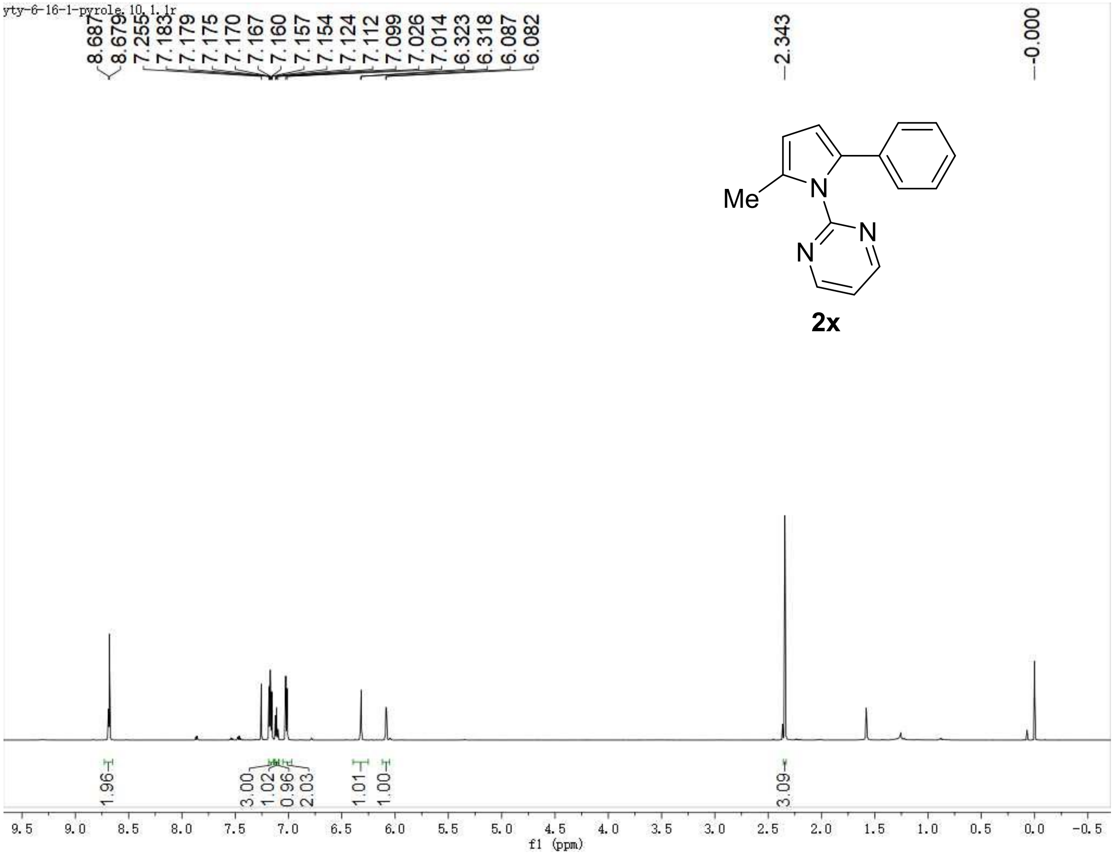
[1]H NMR spectrum of compound **2w** ($CDCl_3$, 400 MHz)



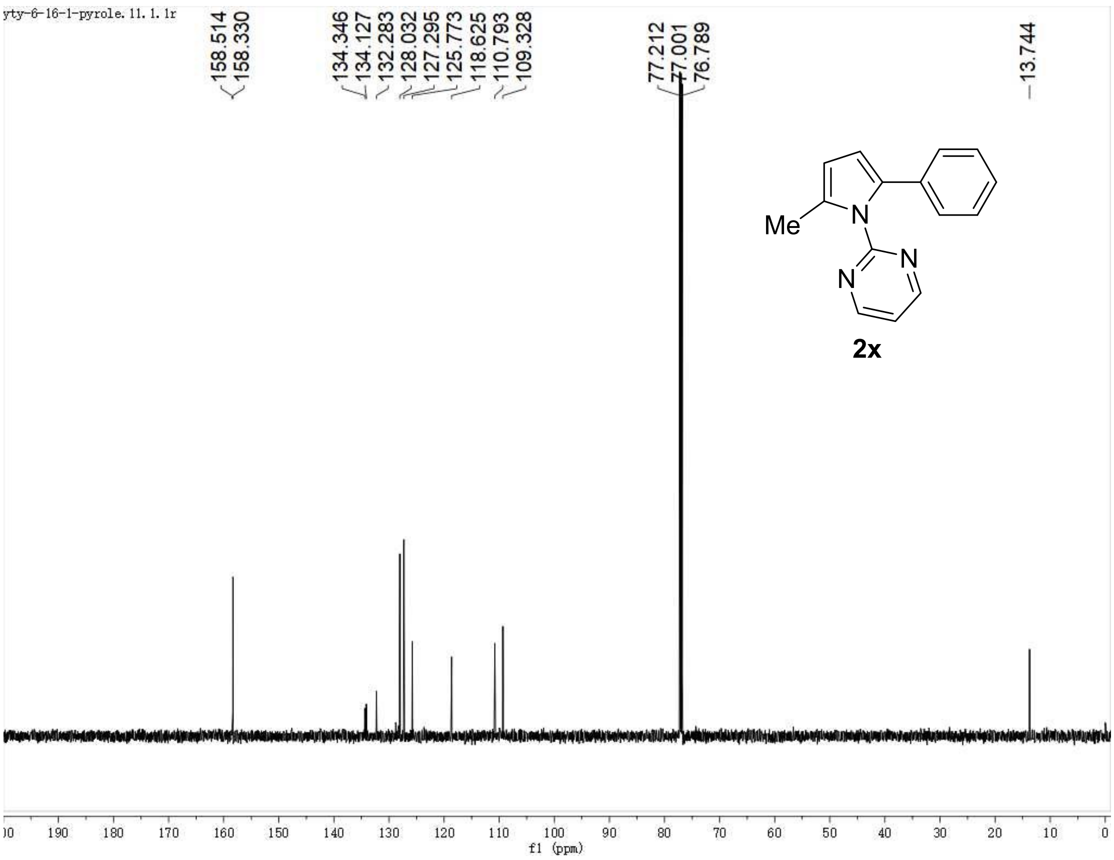
[13]C NMR spectrum of compound **2w** ($CDCl_3$, 101 MHz)



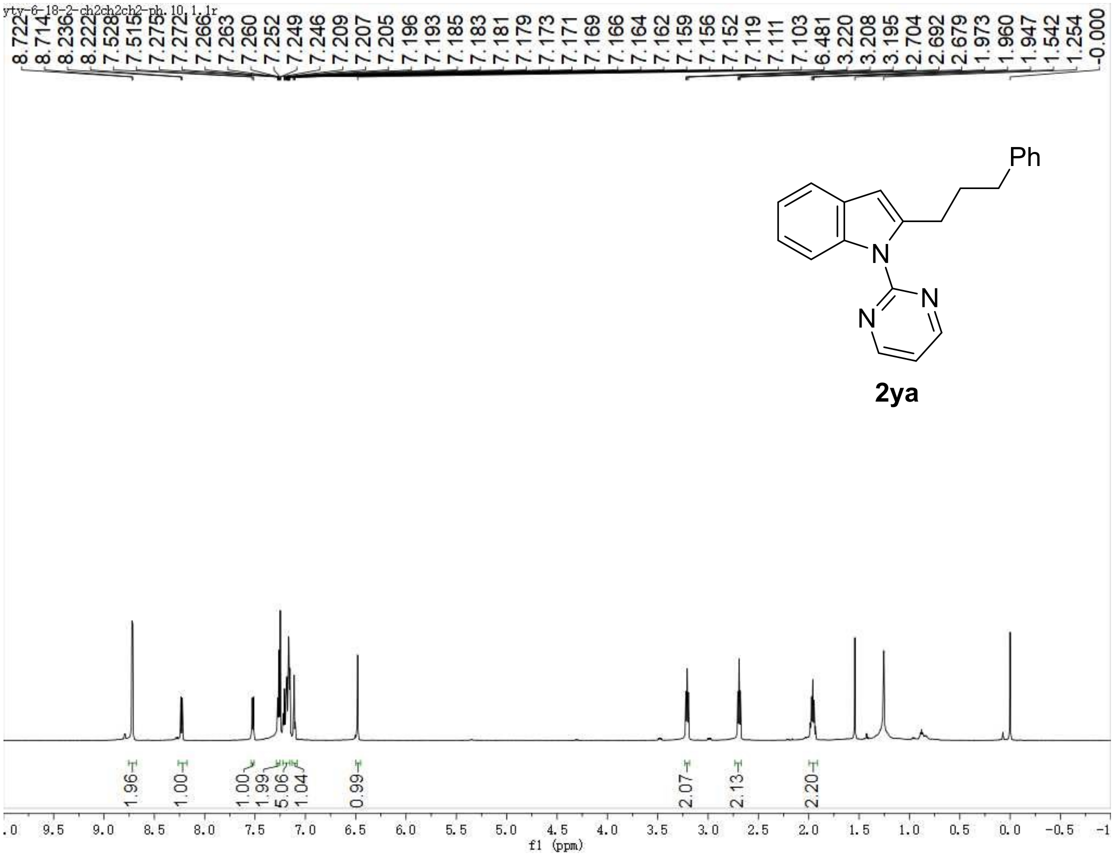
^{1}H NMR spectrum of compound **2x** ($CDCl_3$, 600 MHz)



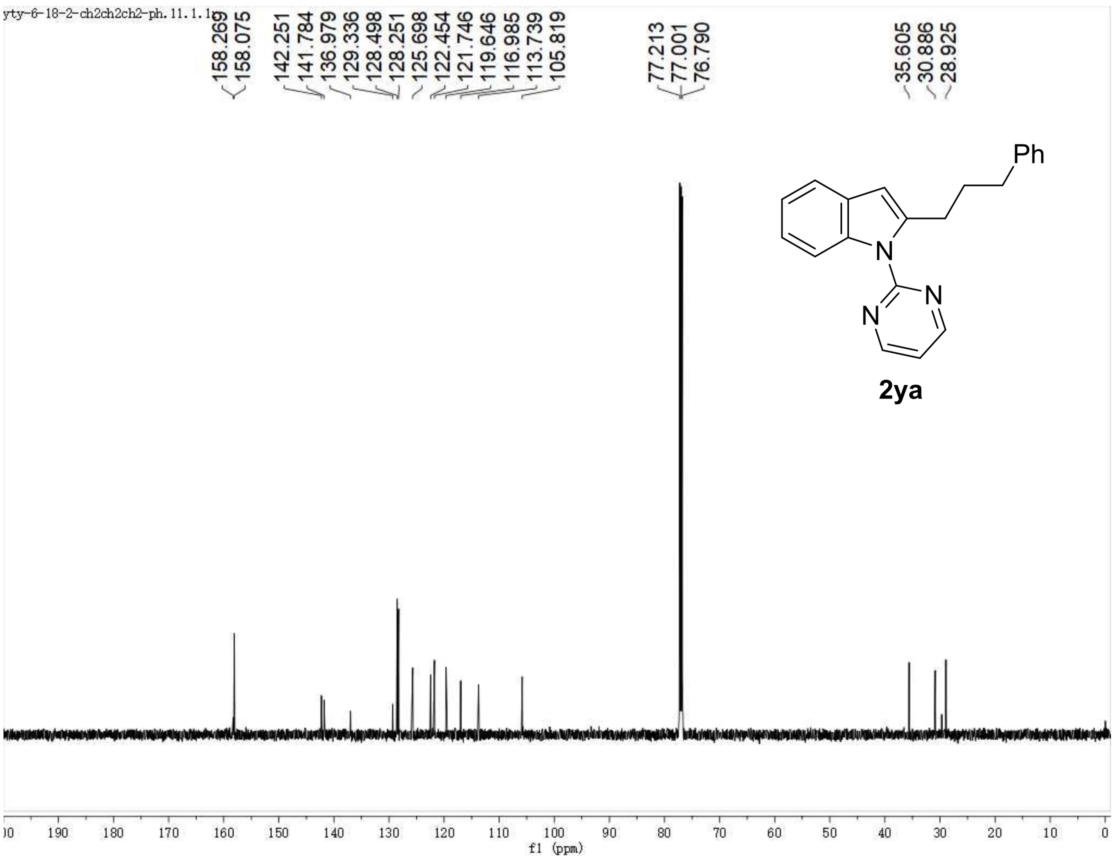
^{13}C NMR spectrum of compound **2x** ($CDCl_3$, 151 MHz)



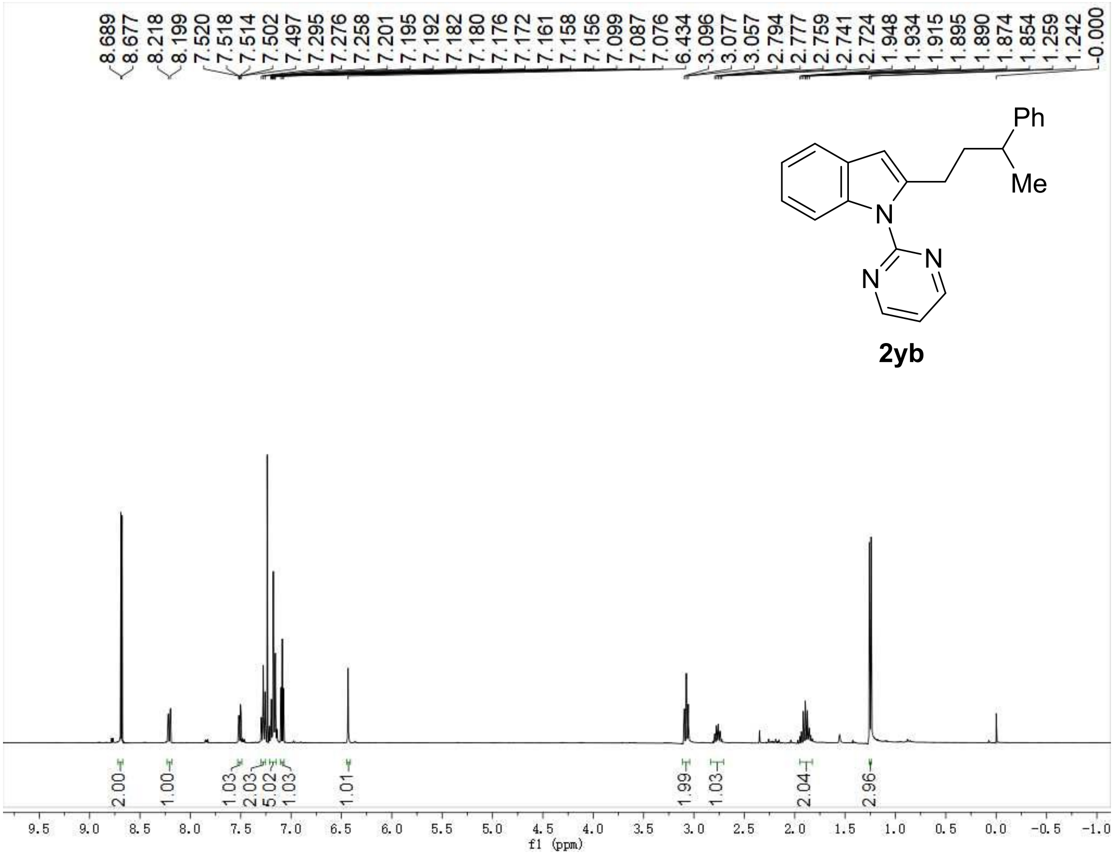
^{1}H NMR spectrum of compound **2ya** ($CDCl_3$, 600 MHz)



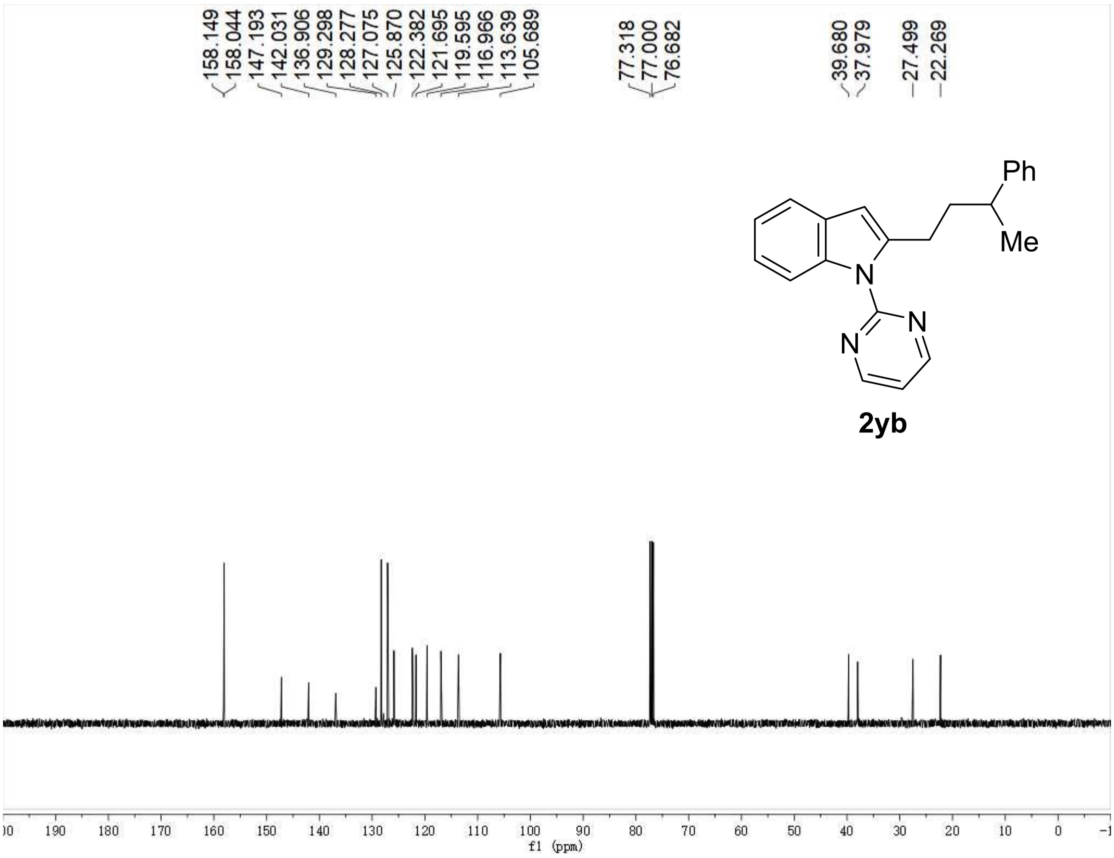
^{13}C NMR spectrum of compound **2ya** ($CDCl_3$, 151 MHz)



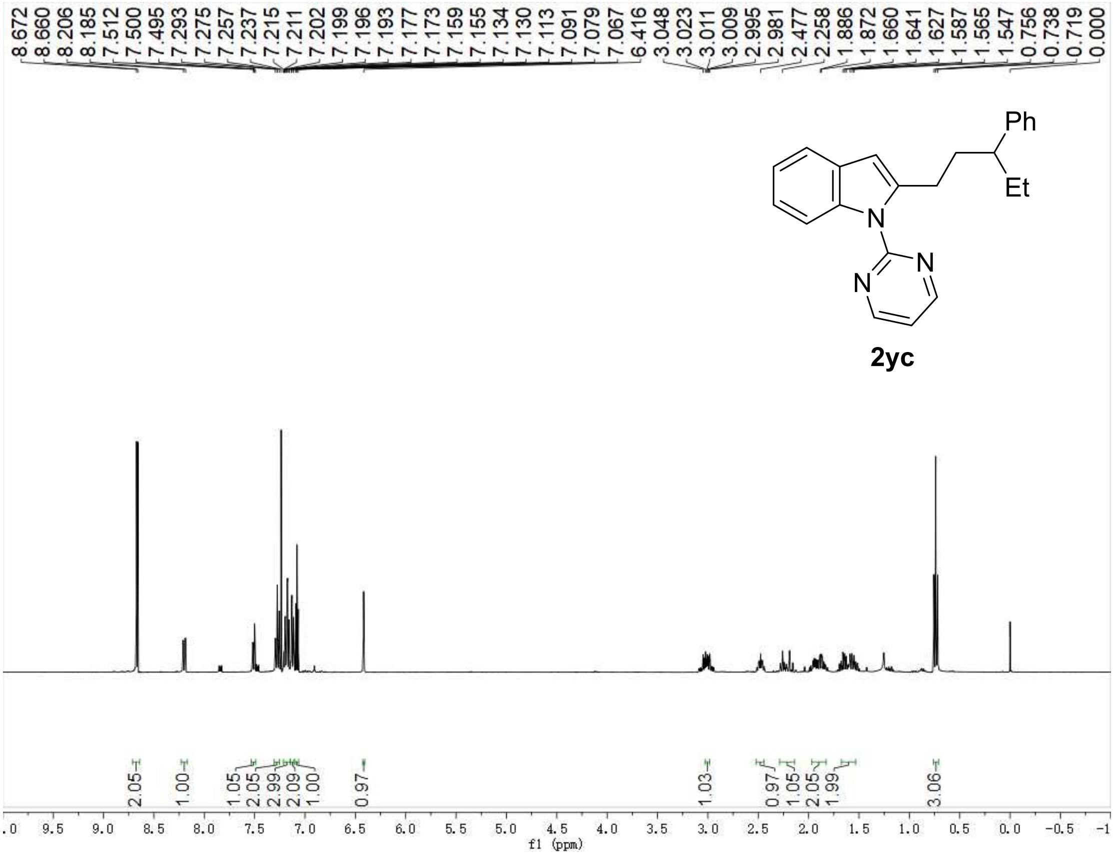
^{1}H NMR spectrum of compound **2yb** ($CDCl_3$, 400 MHz)



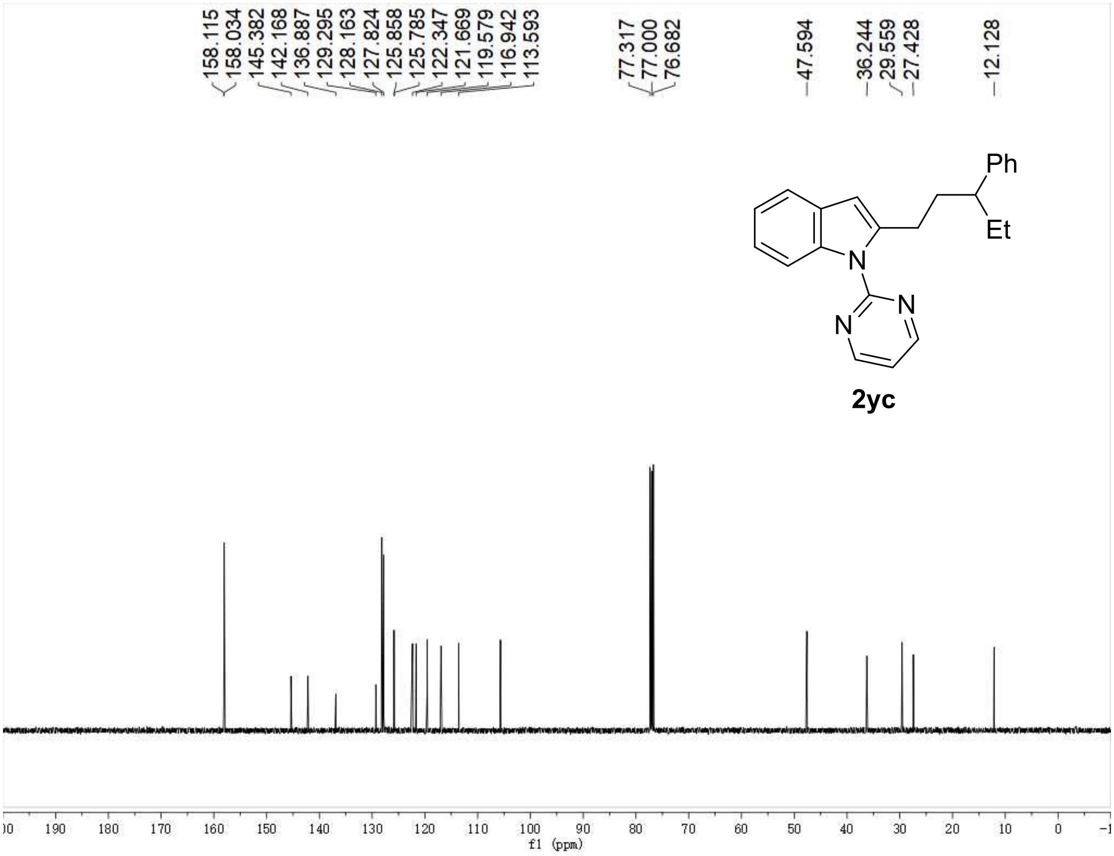
^{13}C NMR spectrum of compound **2yb** ($CDCl_3$, 101 MHz)



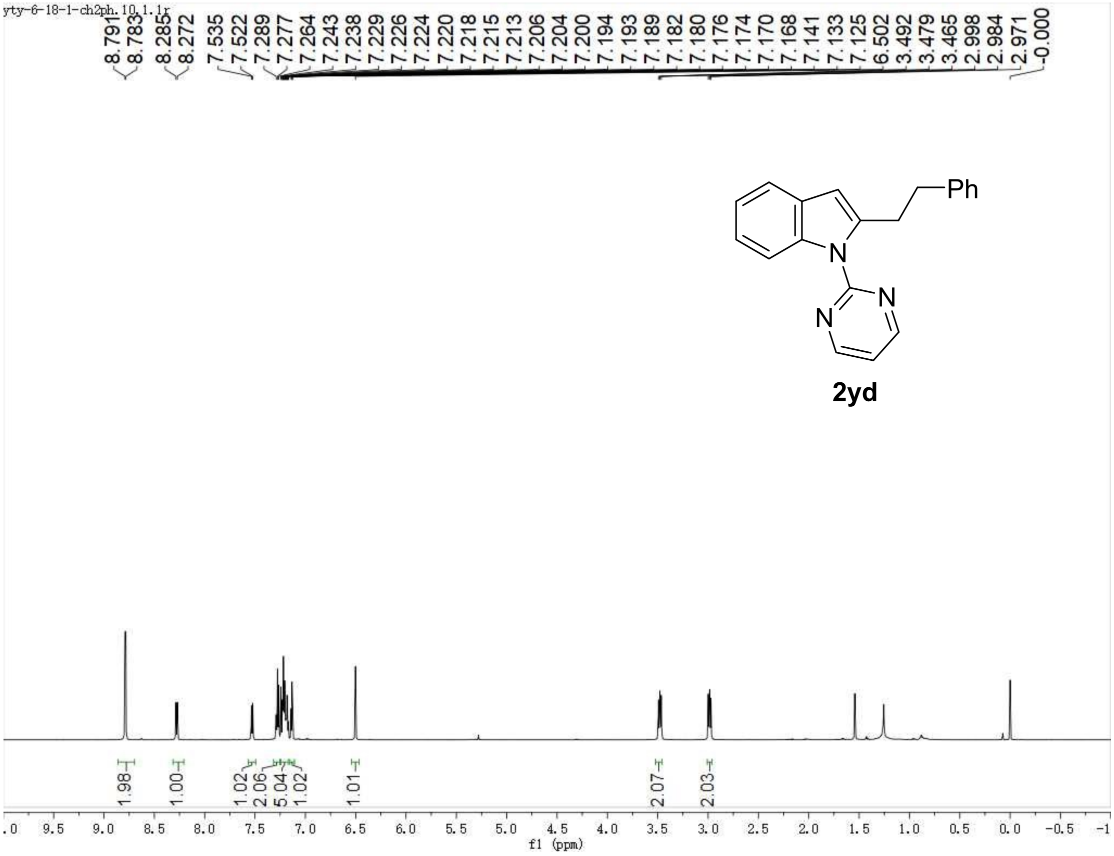
^1H NMR spectrum of compound **2yc** ($CDCl_3$, 400 MHz)



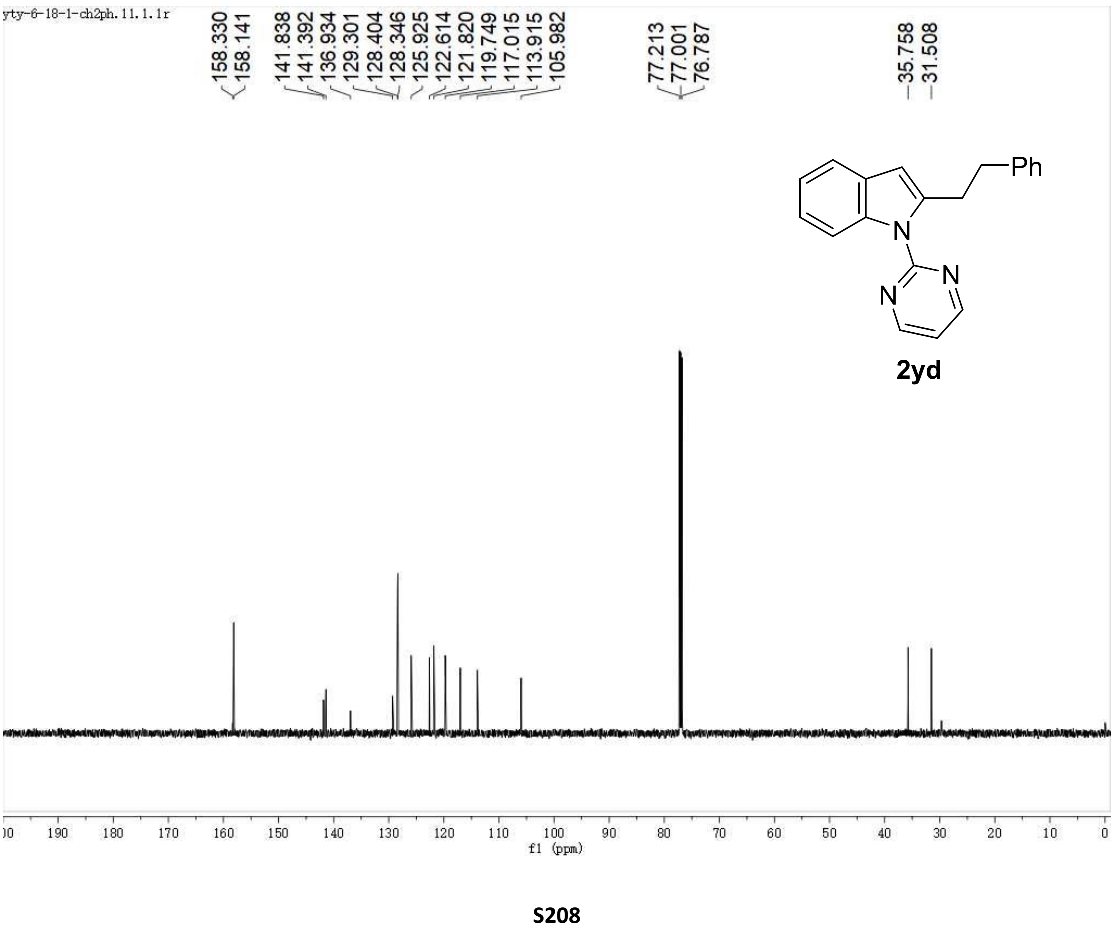
^{13}C NMR spectrum of compound **2yc** ($CDCl_3$, 101 MHz)



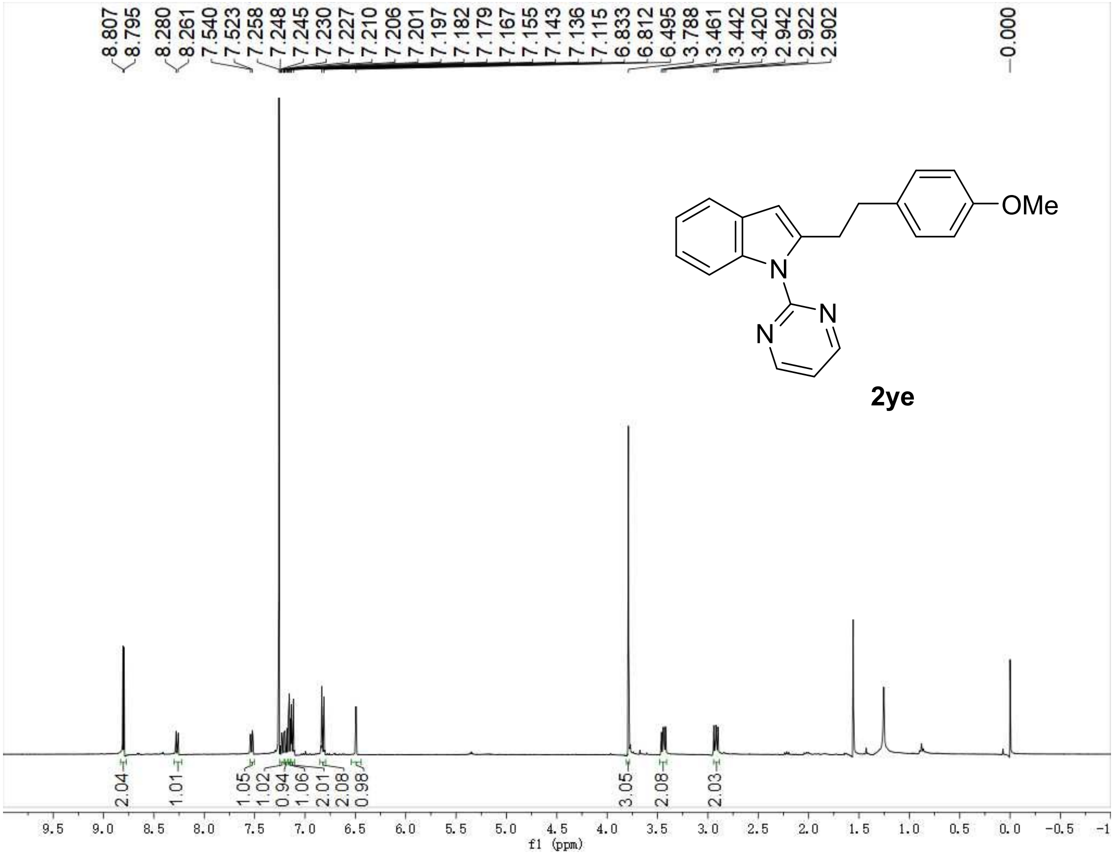
[1]H NMR spectrum of compound **2yd** ($CDCl_3$, 600 MHz)



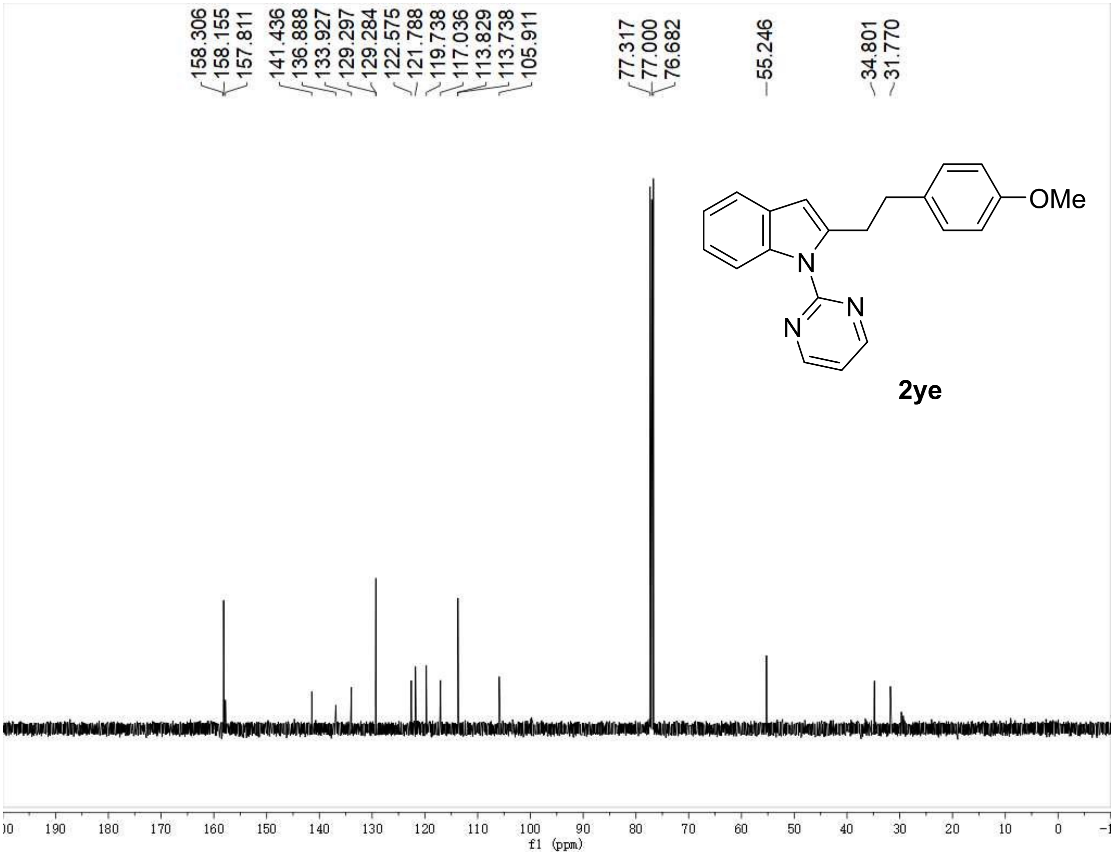
[13]C NMR spectrum of compound **2yd** ($CDCl_3$, 151 MHz)



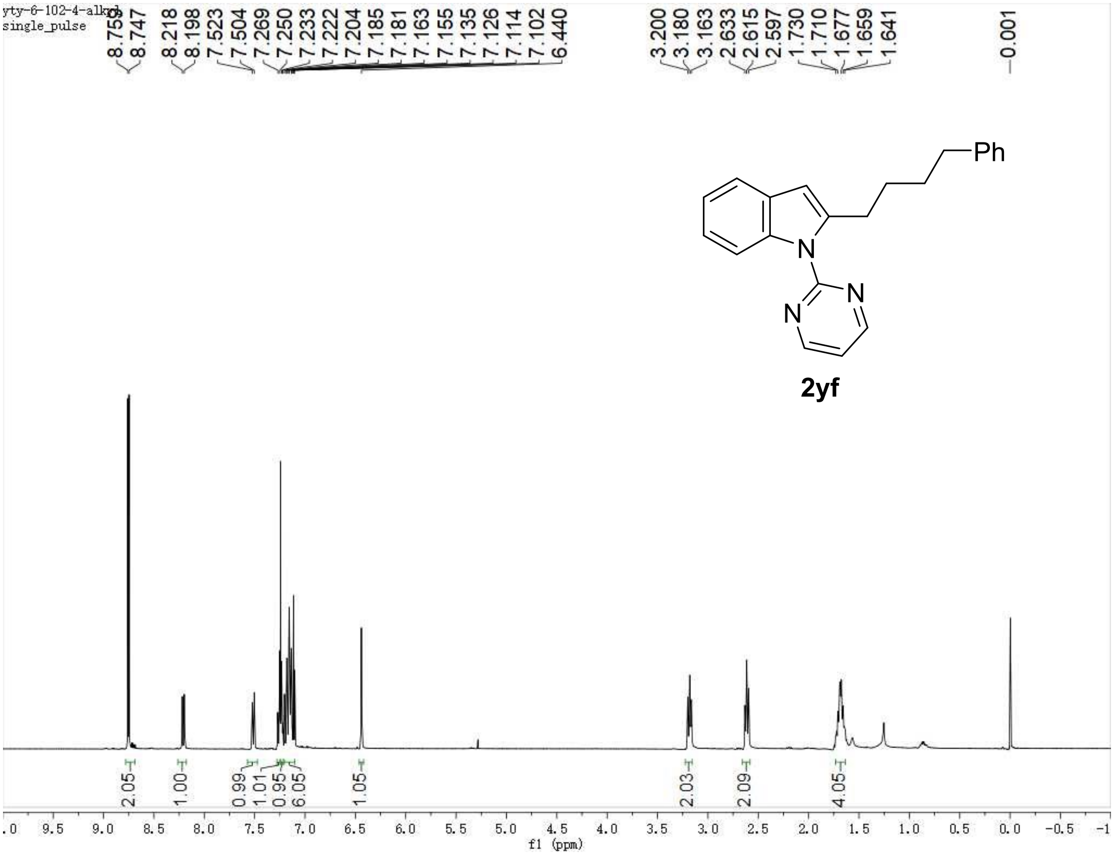
^{1}H NMR spectrum of compound **2ye** ($CDCl_3$, 400 MHz)



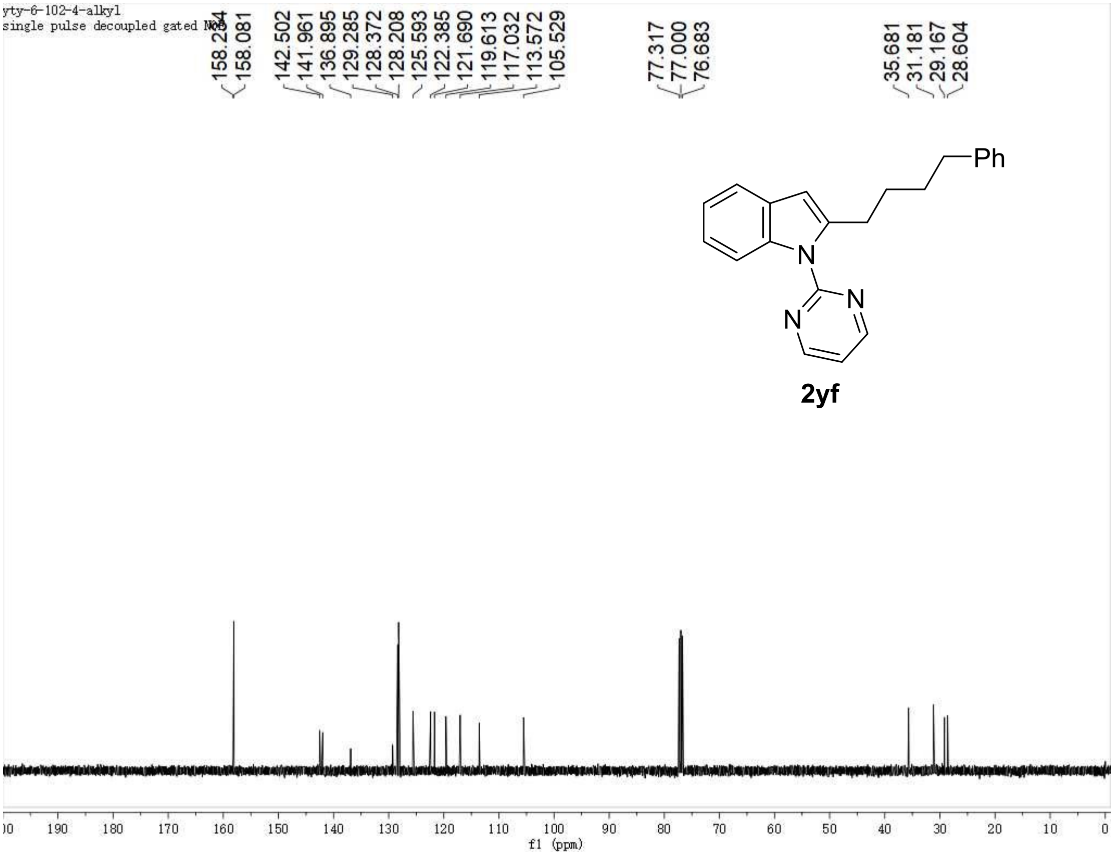
^{13}C NMR spectrum of compound **2ye** ($CDCl_3$, 101 MHz)



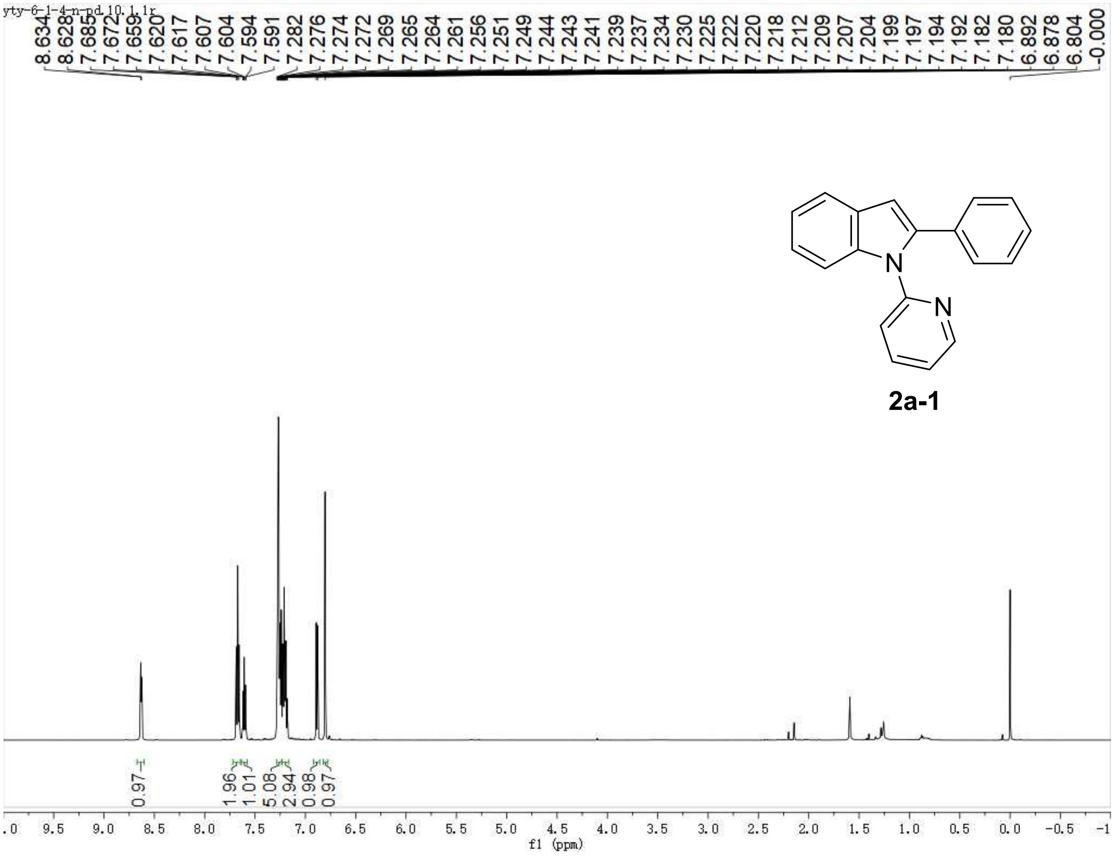
[1]H NMR spectrum of compound **2yf** ($CDCl_3$, 400 MHz)



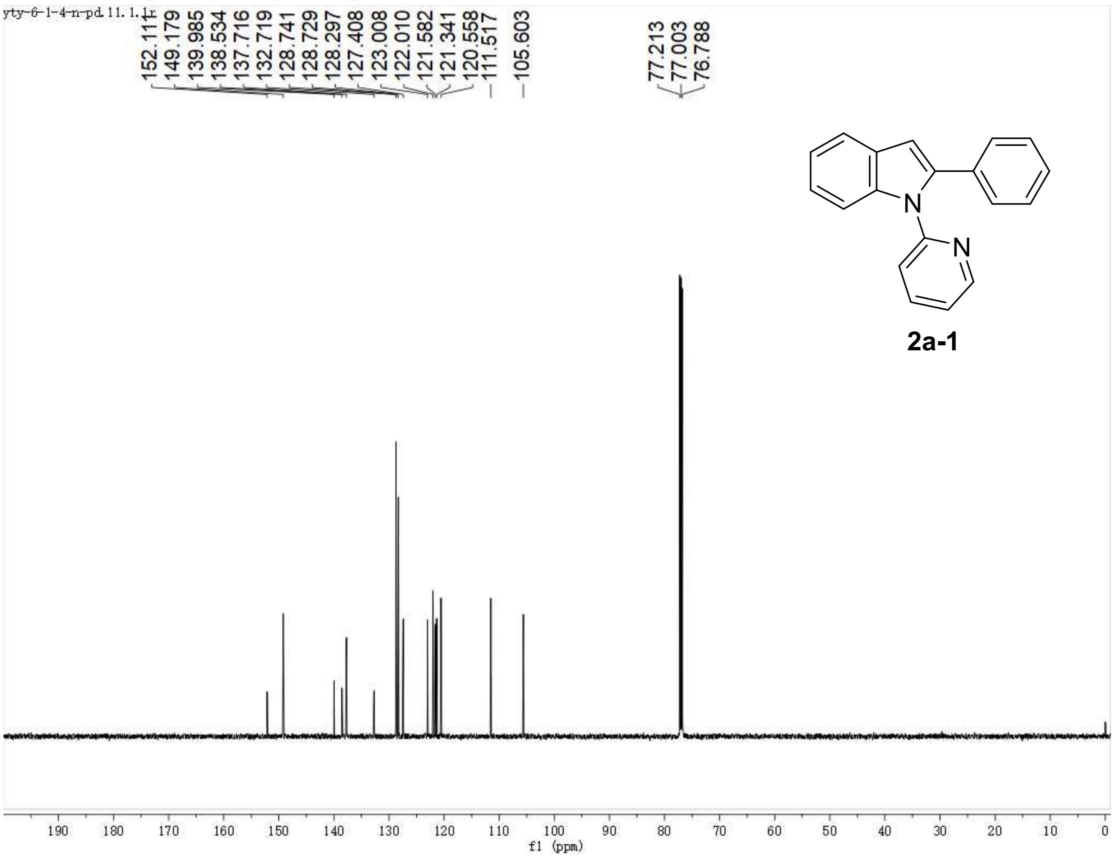
[13]C NMR spectrum of compound **2yf** ($CDCl_3$, 101 MHz)



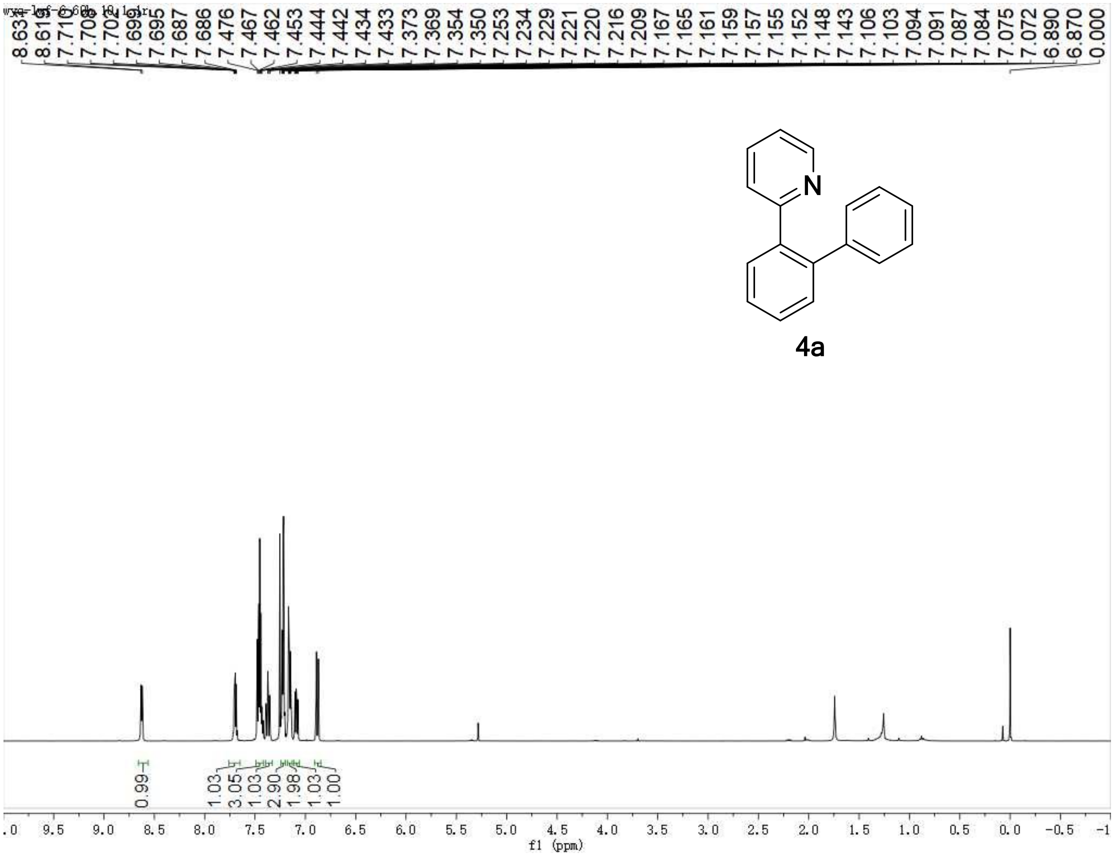
^{1}H NMR spectrum of compound **2a-1** ($CDCl_3$, 600 MHz)



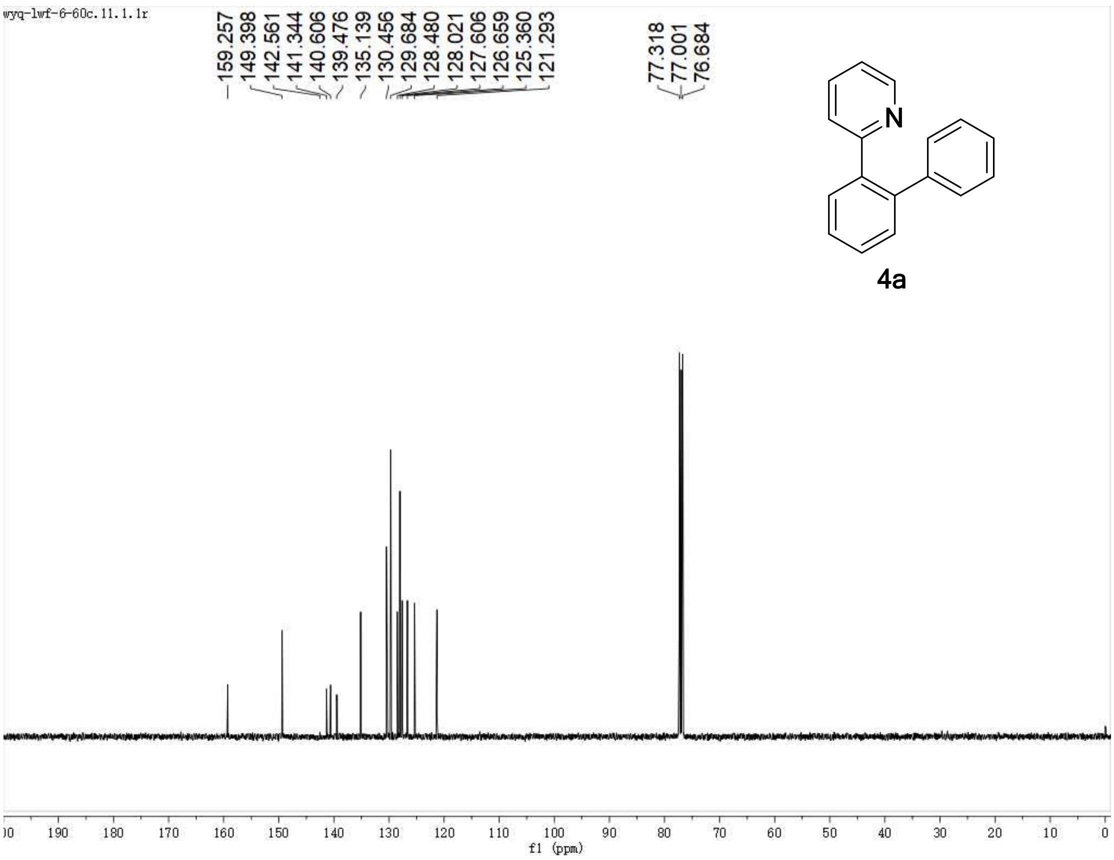
^{13}C NMR spectrum of compound **2a-1** ($CDCl_3$, 151 MHz)



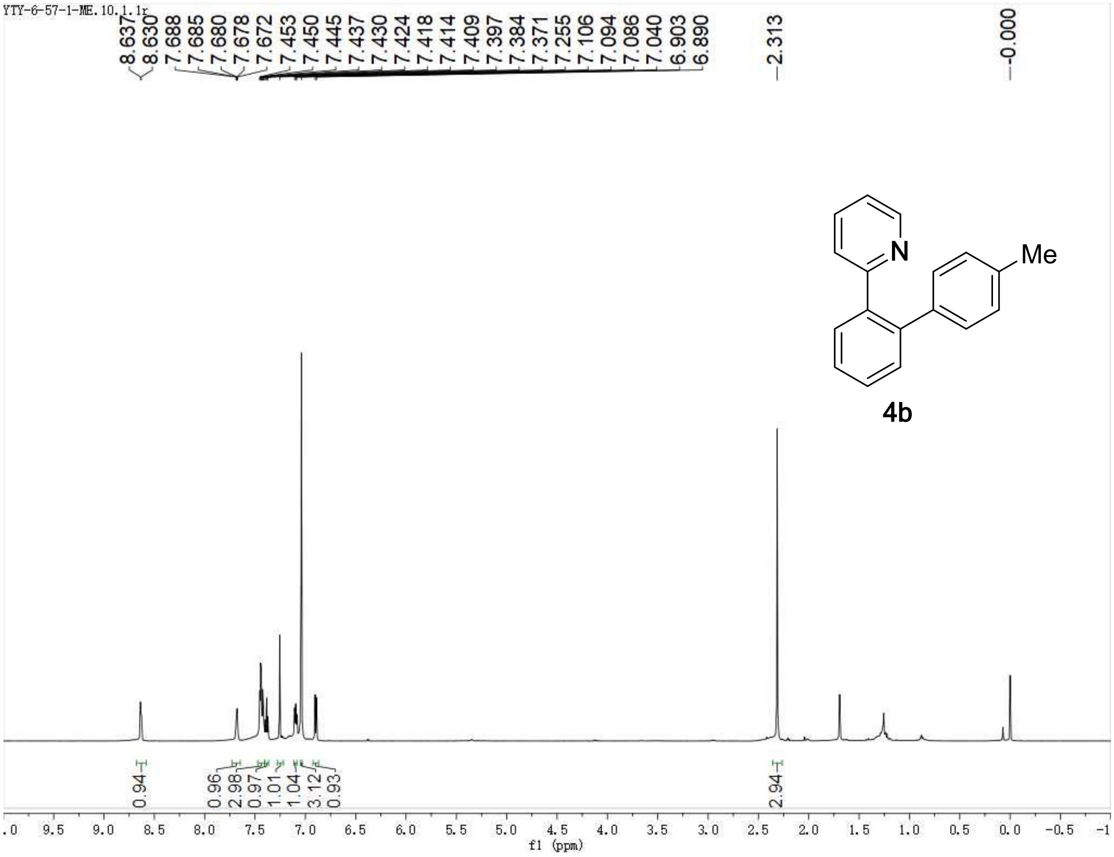
^{1}H NMR spectrum of compound **4a** ($CDCl_3$, 400 MHz)



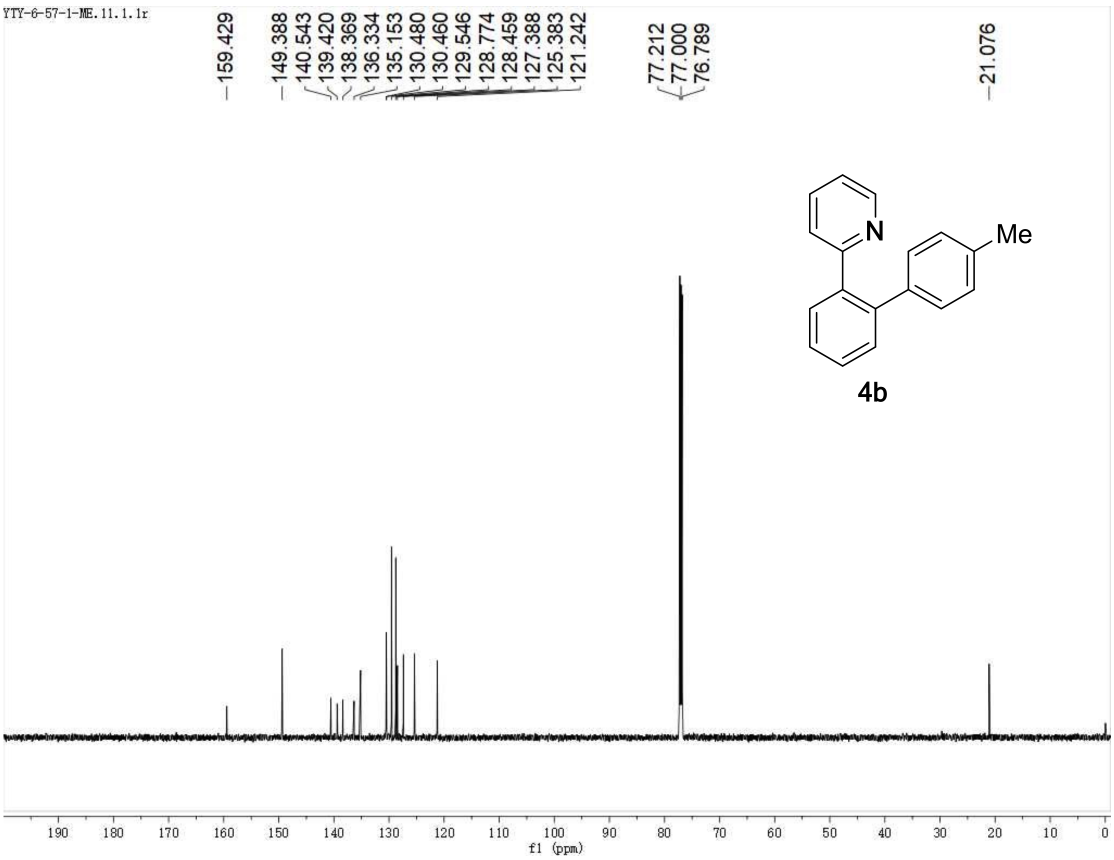
^{13}C NMR spectrum of compound **4a** ($CDCl_3$, 101 MHz)



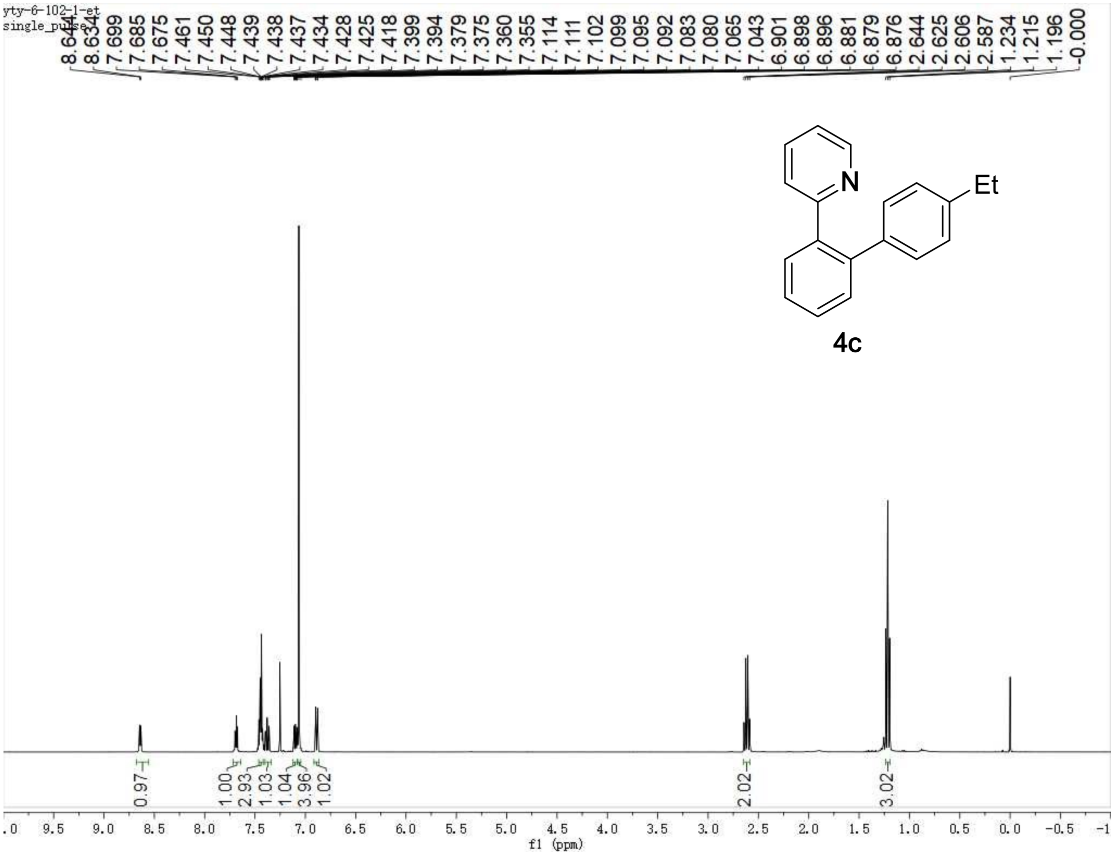
^{1}H NMR spectrum of compound **4b** ($CDCl_3$, 600 MHz)



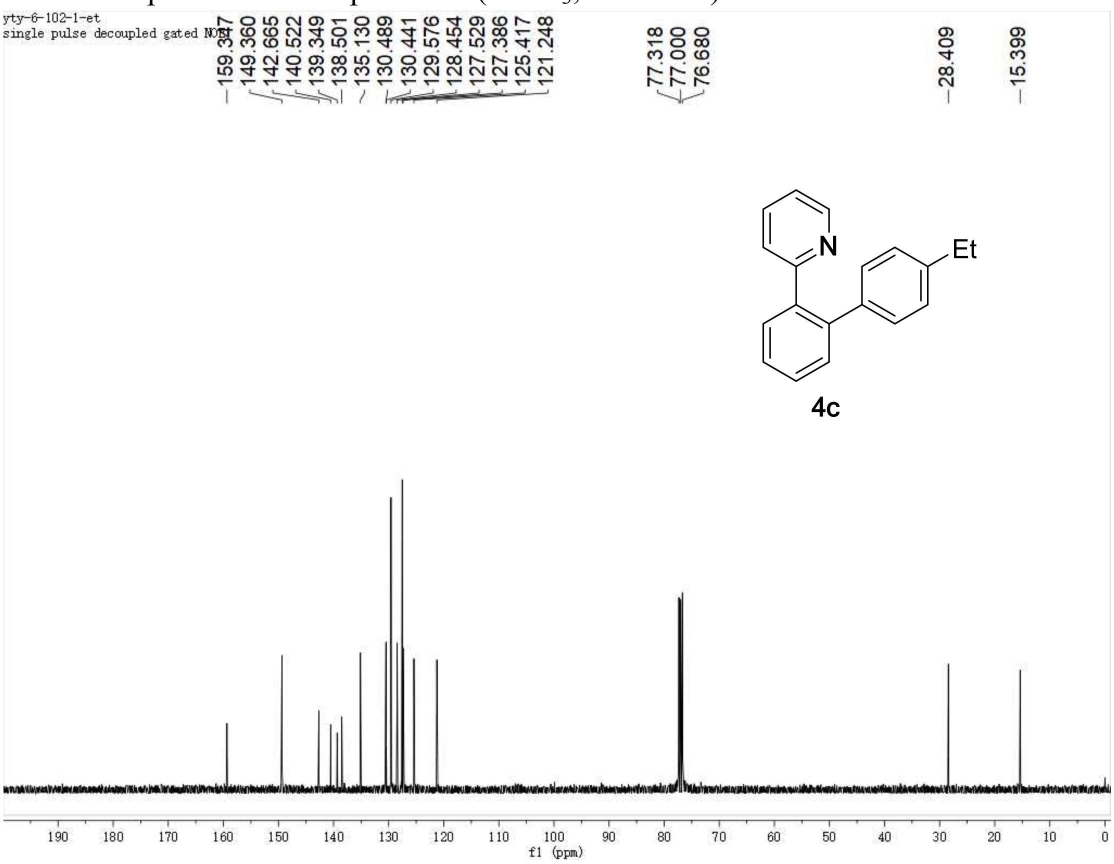
^{13}C NMR spectrum of compound **4b** ($CDCl_3$, 151 MHz)



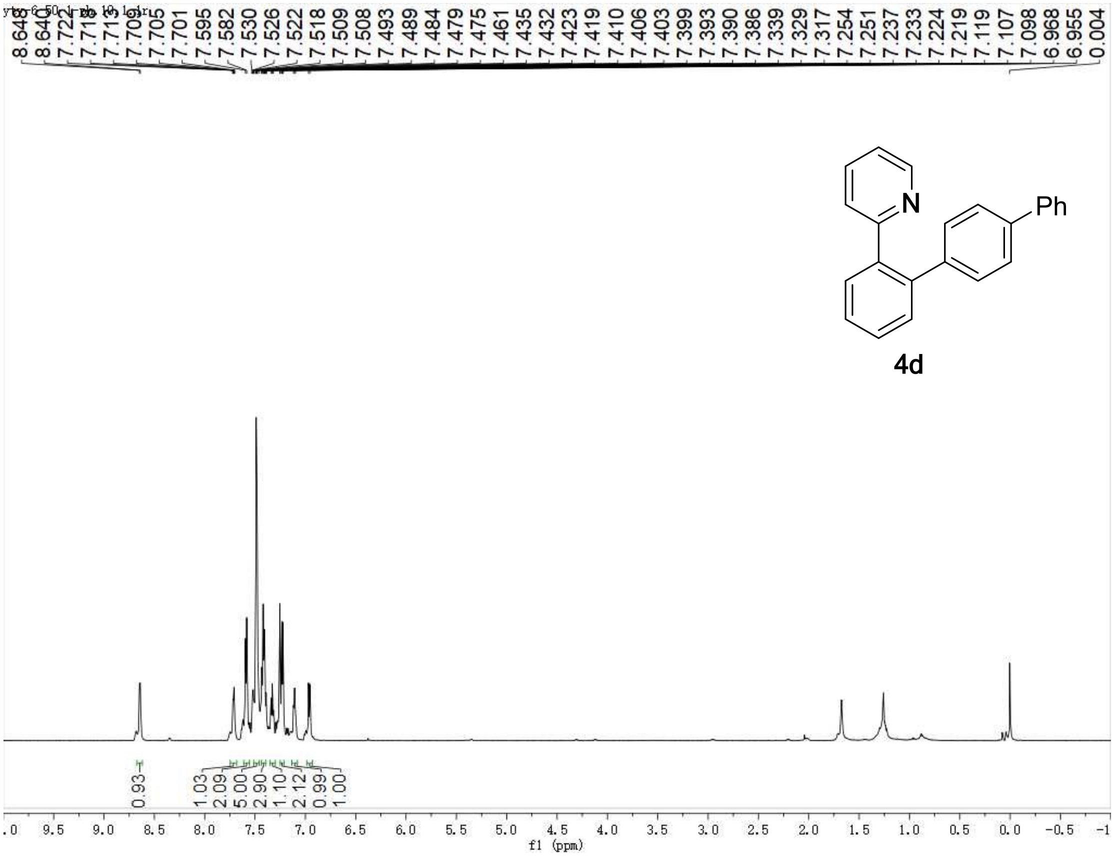
[1]H NMR spectrum of compound **4c** ($CDCl_3$, 400 MHz)



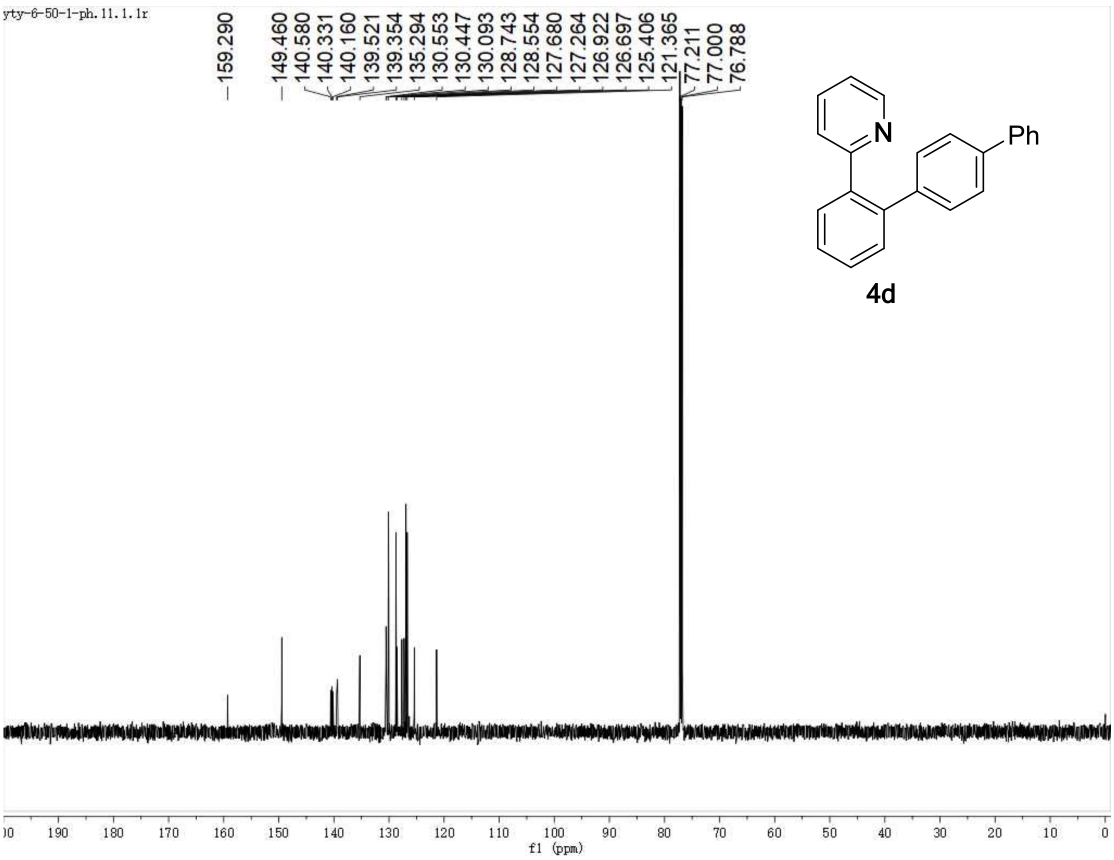
[13]C NMR spectrum of compound **4c** ($CDCl_3$, 101 MHz)



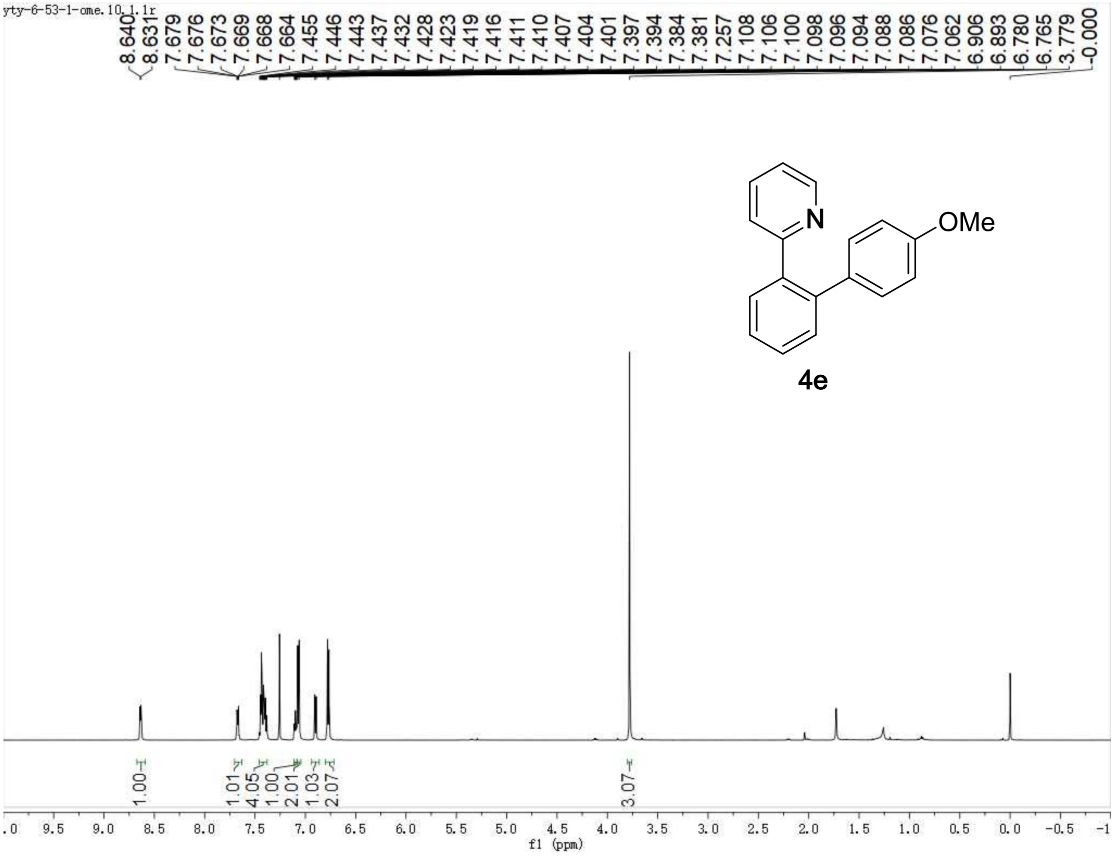
[1]H NMR spectrum of compound **4d** ($CDCl_3$, 600 MHz)



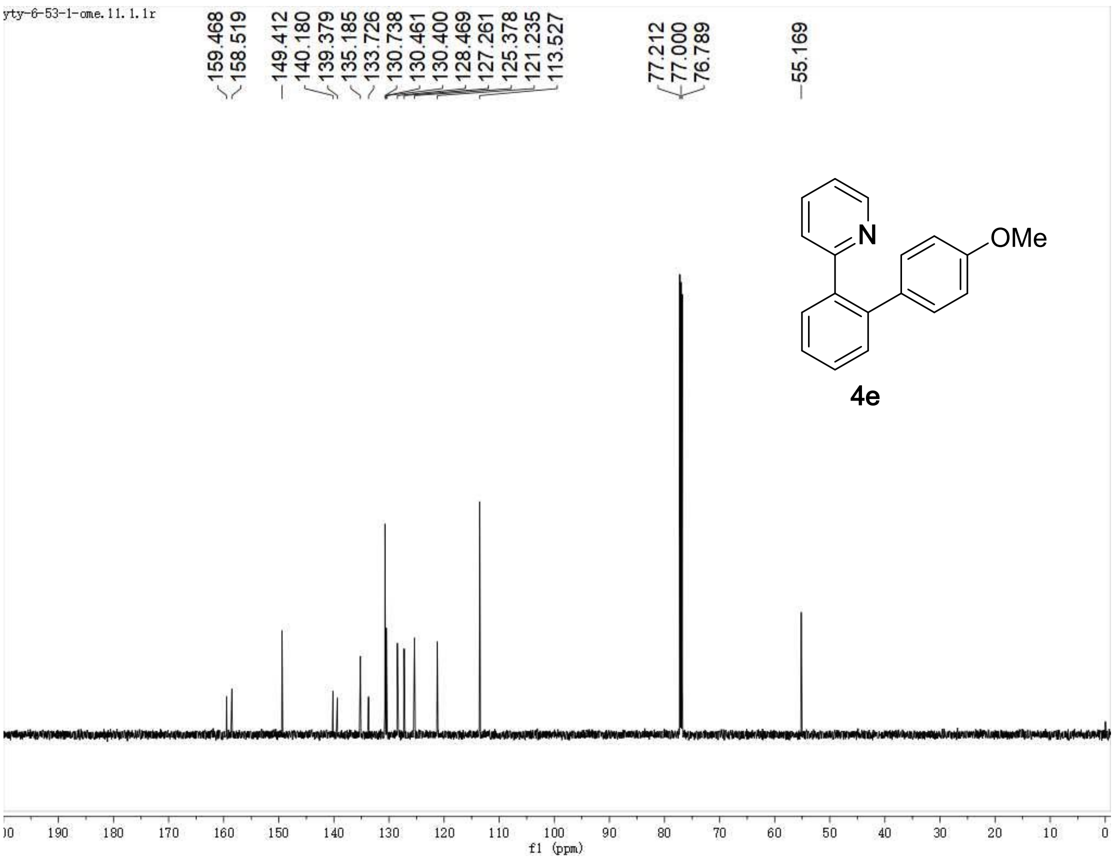
[13]C NMR spectrum of compound **4d** ($CDCl_3$, 151 MHz)



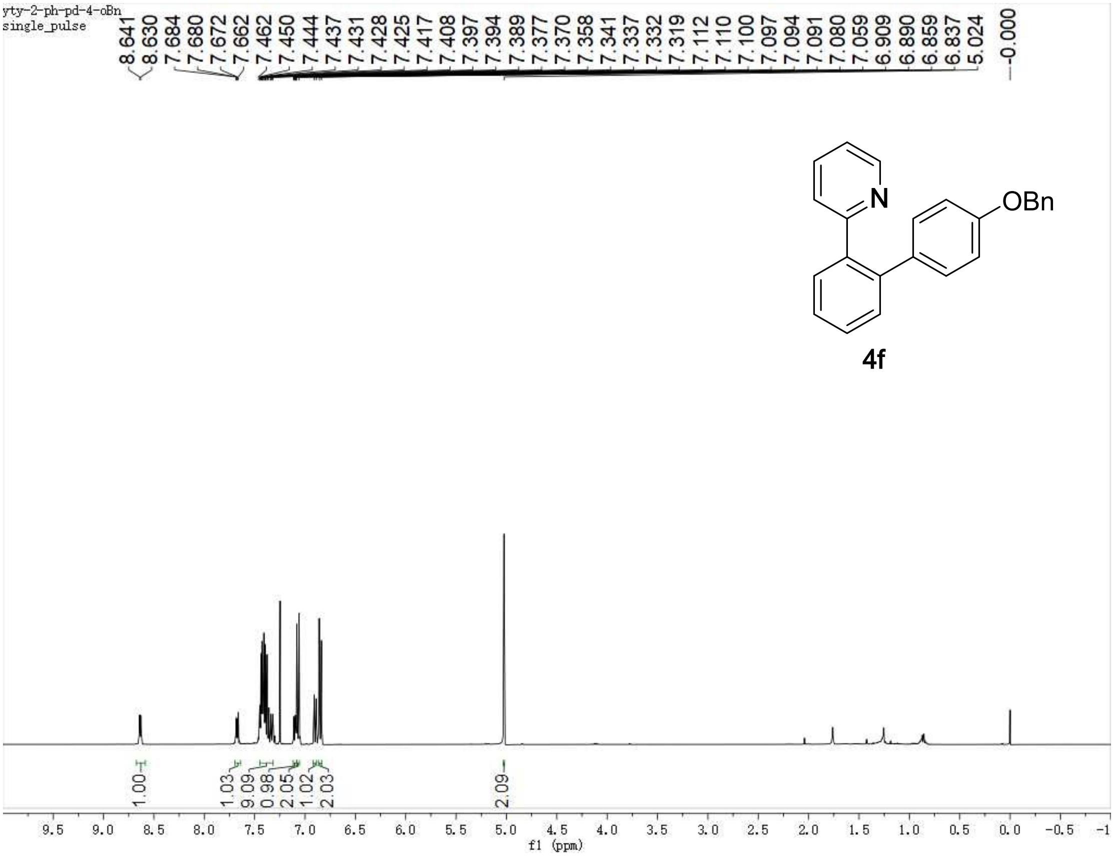
^{1}H NMR spectrum of compound **4e** ($CDCl_3$, 600 MHz)



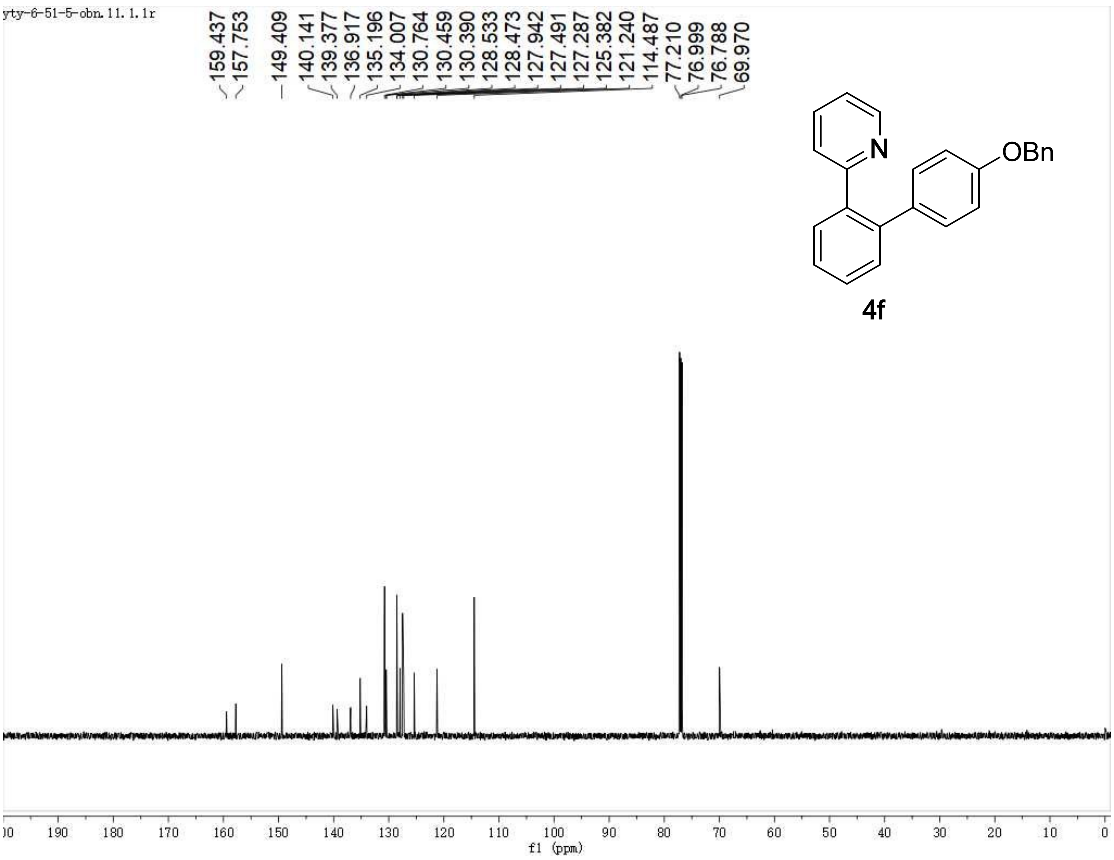
^{13}C NMR spectrum of compound **4e** ($CDCl_3$, 151 MHz)



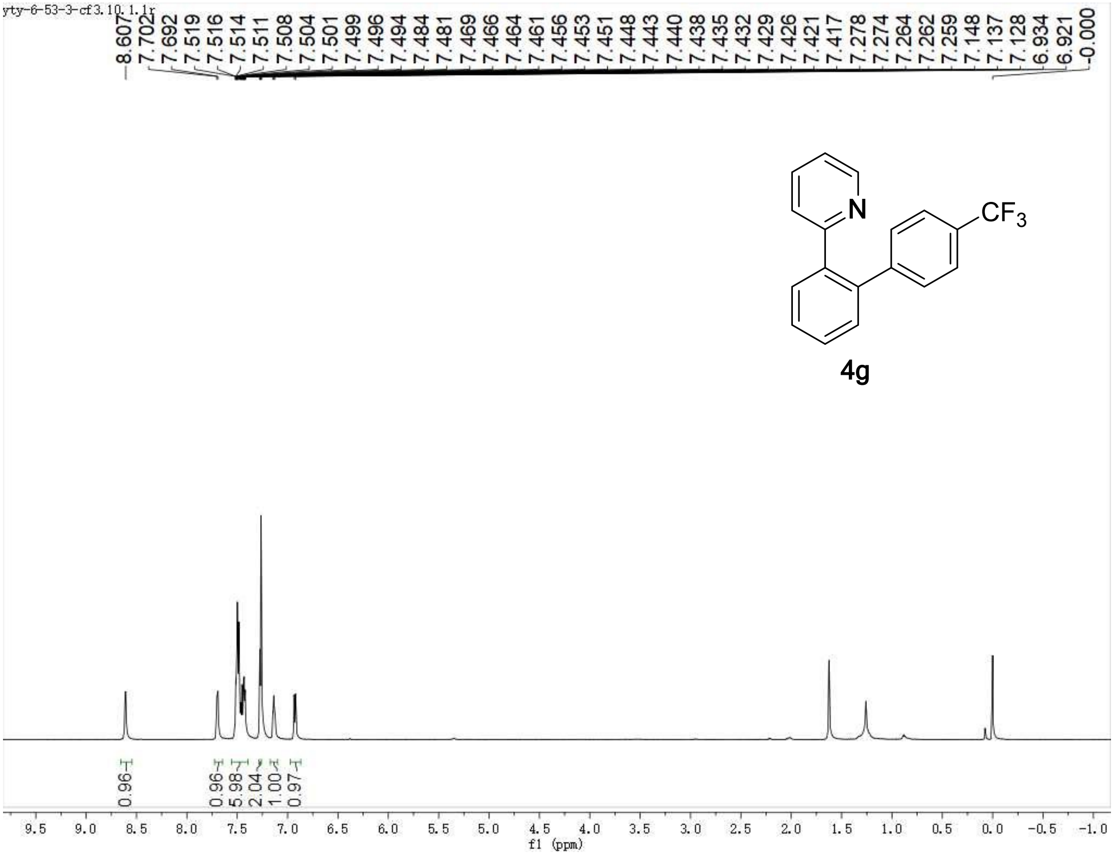
^{1}H NMR spectrum of compound **4f** ($CDCl_3$, 400 MHz)



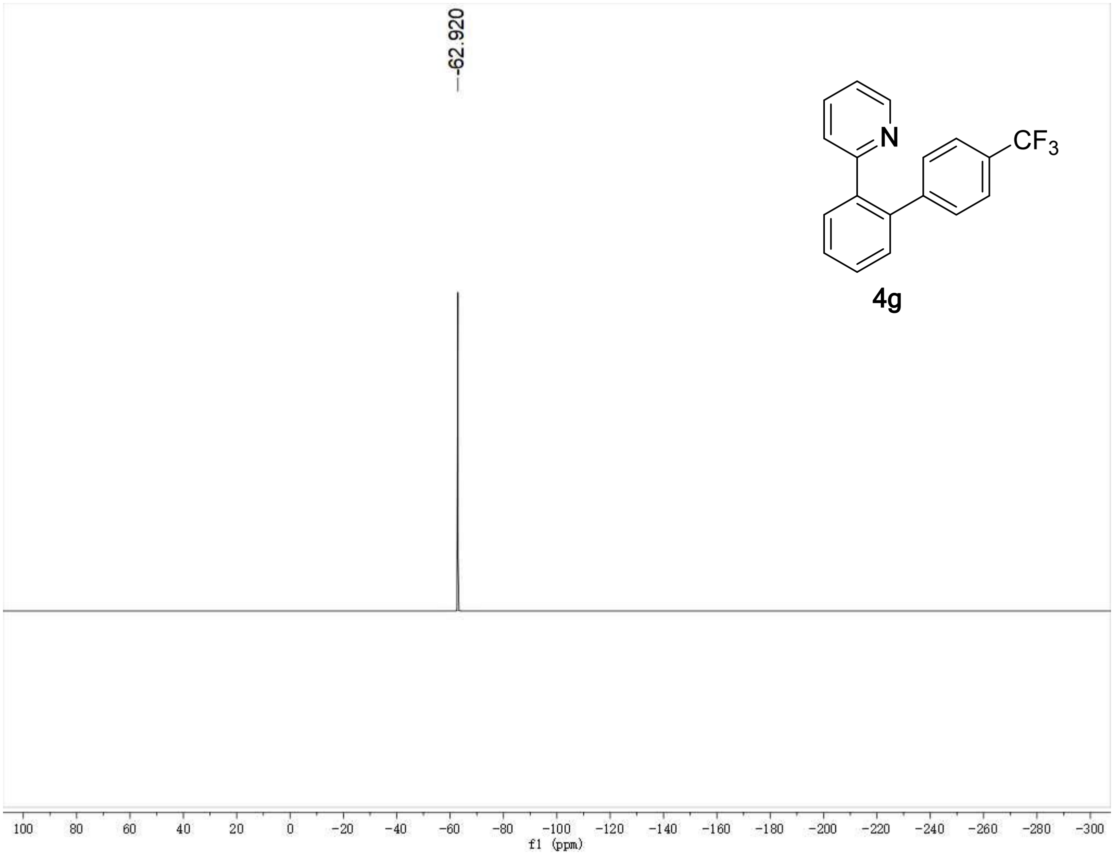
^{13}C NMR spectrum of compound **4f** ($CDCl_3$, 151 MHz)



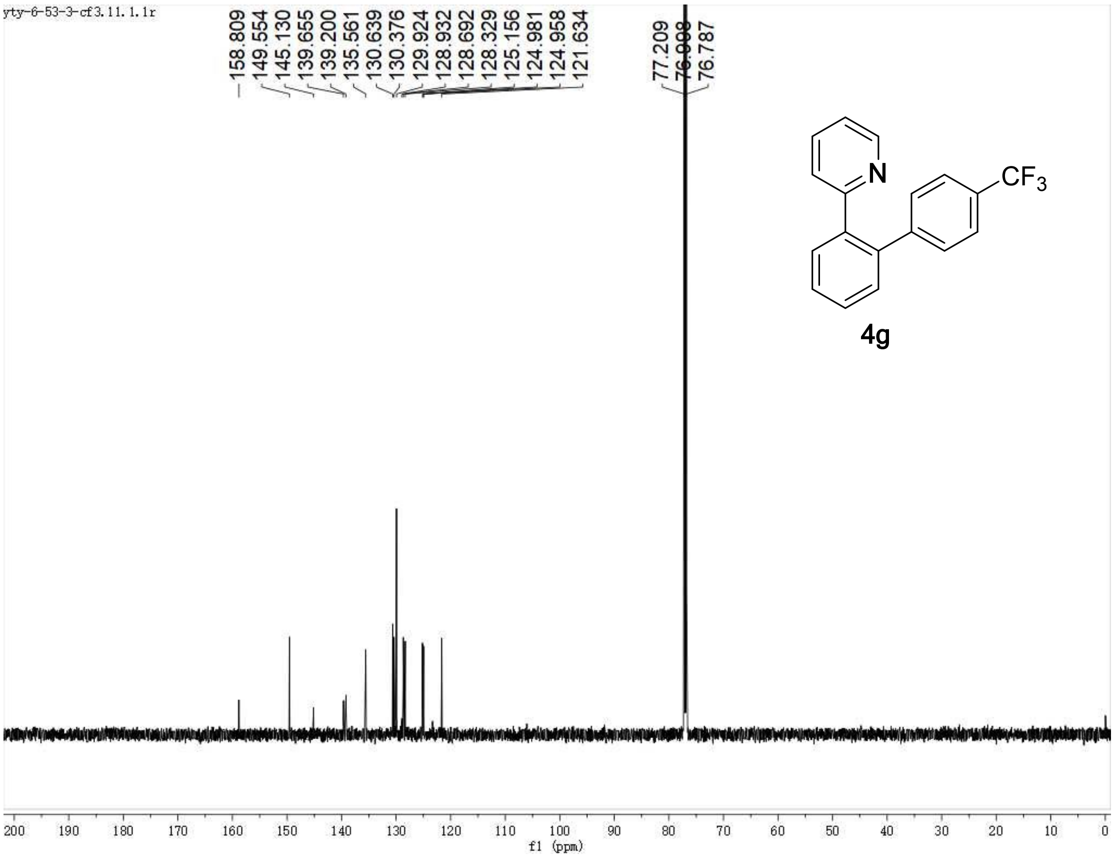
^{1}H NMR spectrum of compound **4g** ($CDCl_3$, 600 MHz)



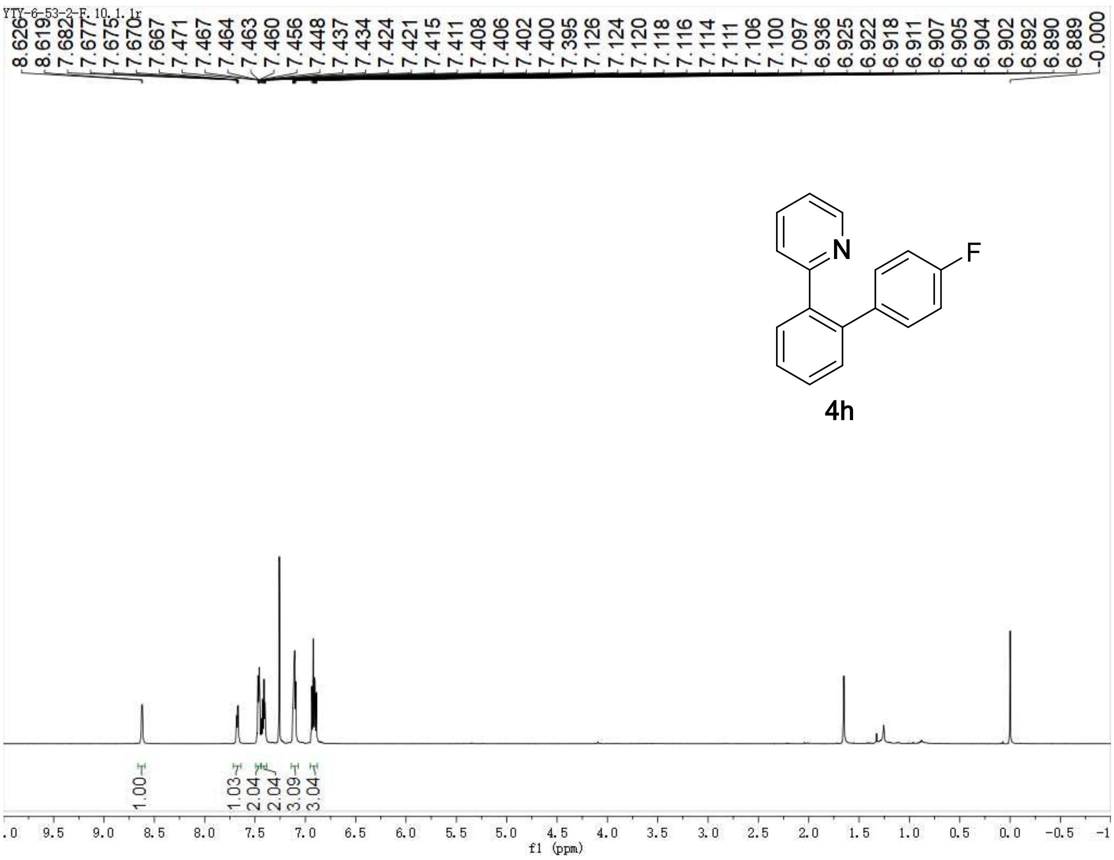
^{19}F NMR spectrum of compound **4g** ($CDCl_3$, 376 MHz)



^{13}C NMR spectrum of compound **4g** ($CDCl_3$, 151 MHz)

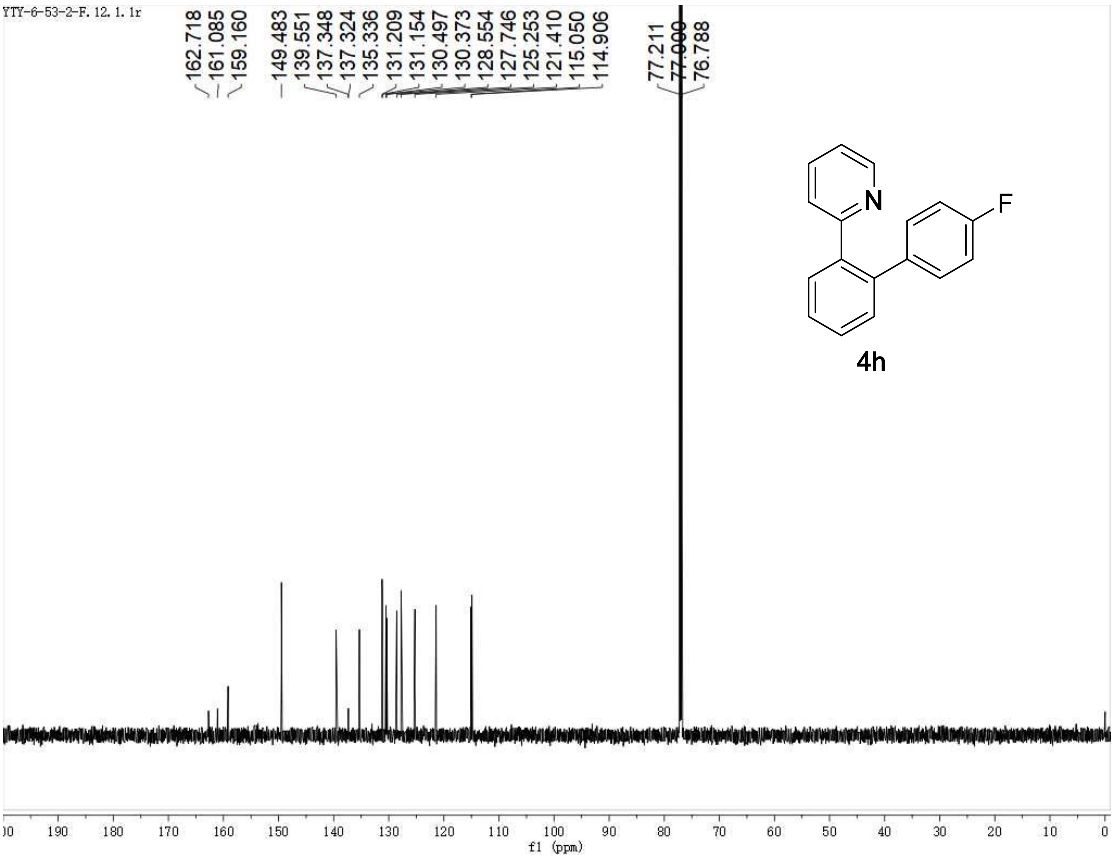


^{1}H NMR spectrum of compound **4h** ($CDCl_3$, 600 MHz)

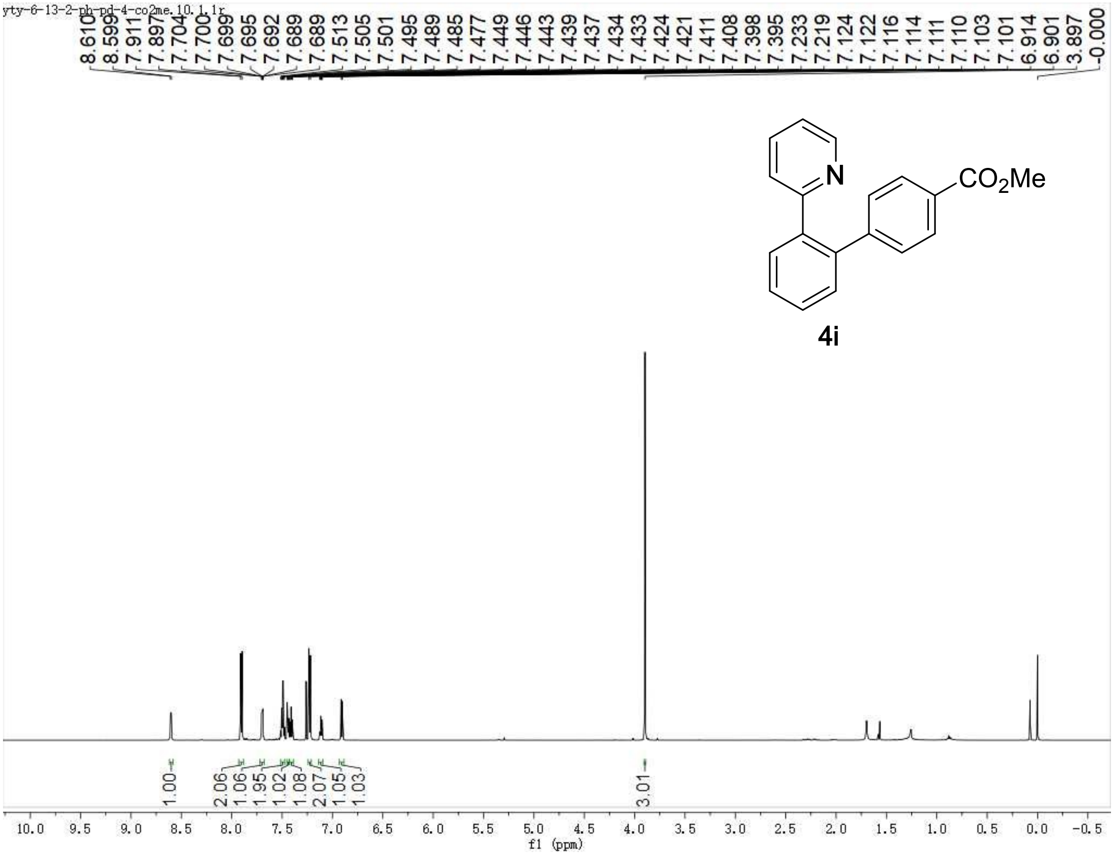


^{19}F NMR spectrum of compound **4h** ($CDCl_3$, 376 MHz)

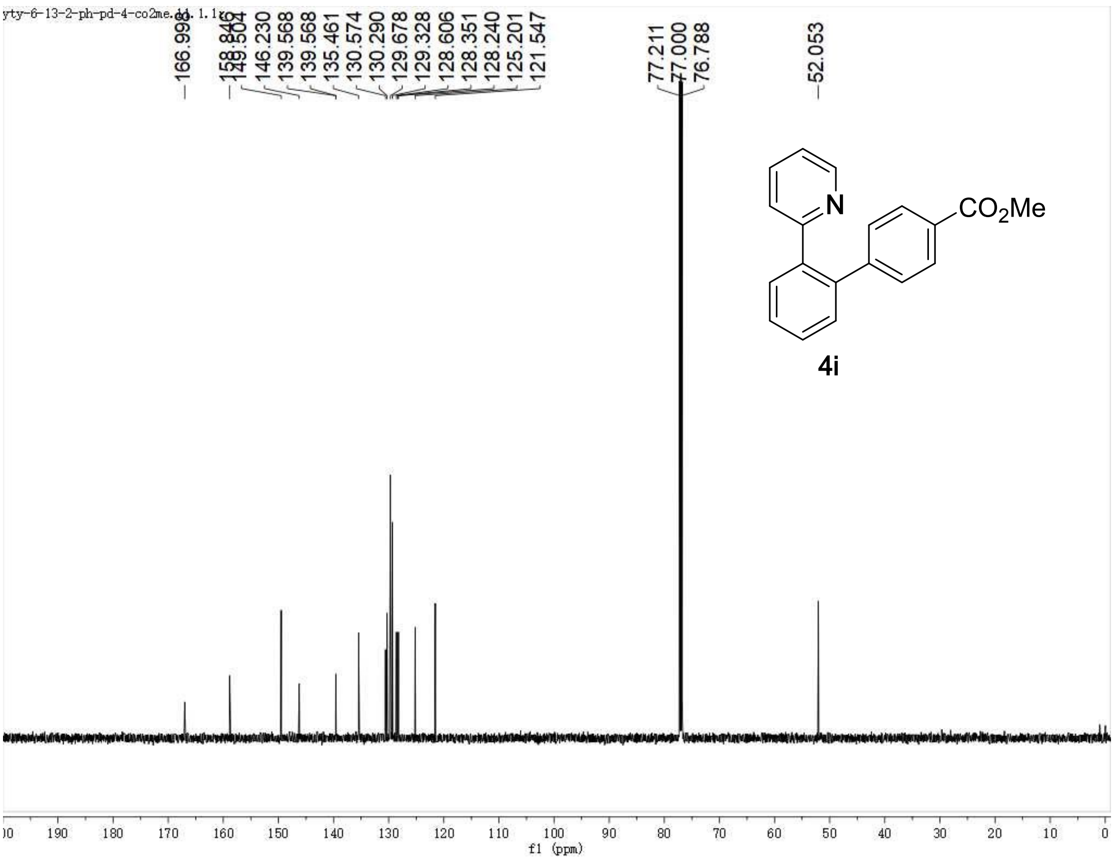
^{13}C NMR spectrum of compound **4h** ($CDCl_3$, 151 MHz)



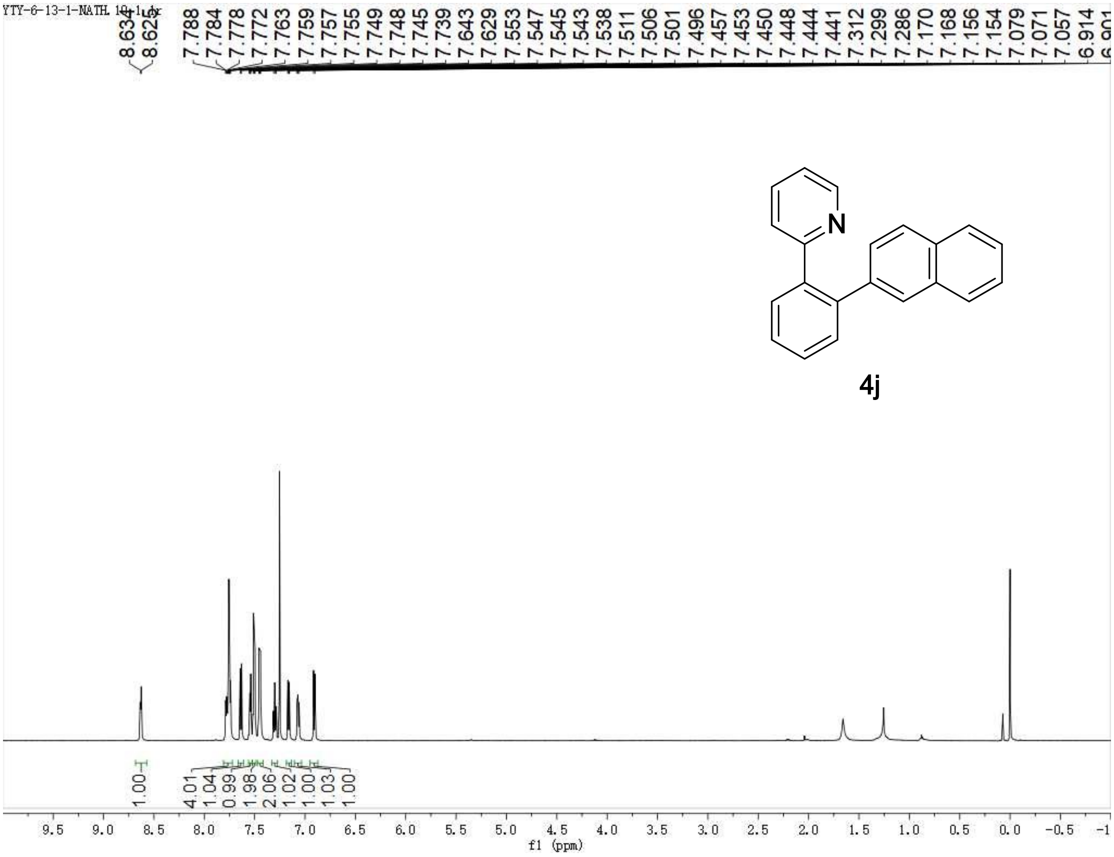
[1]H NMR spectrum of compound **4i** ($CDCl_3$, 600 MHz)



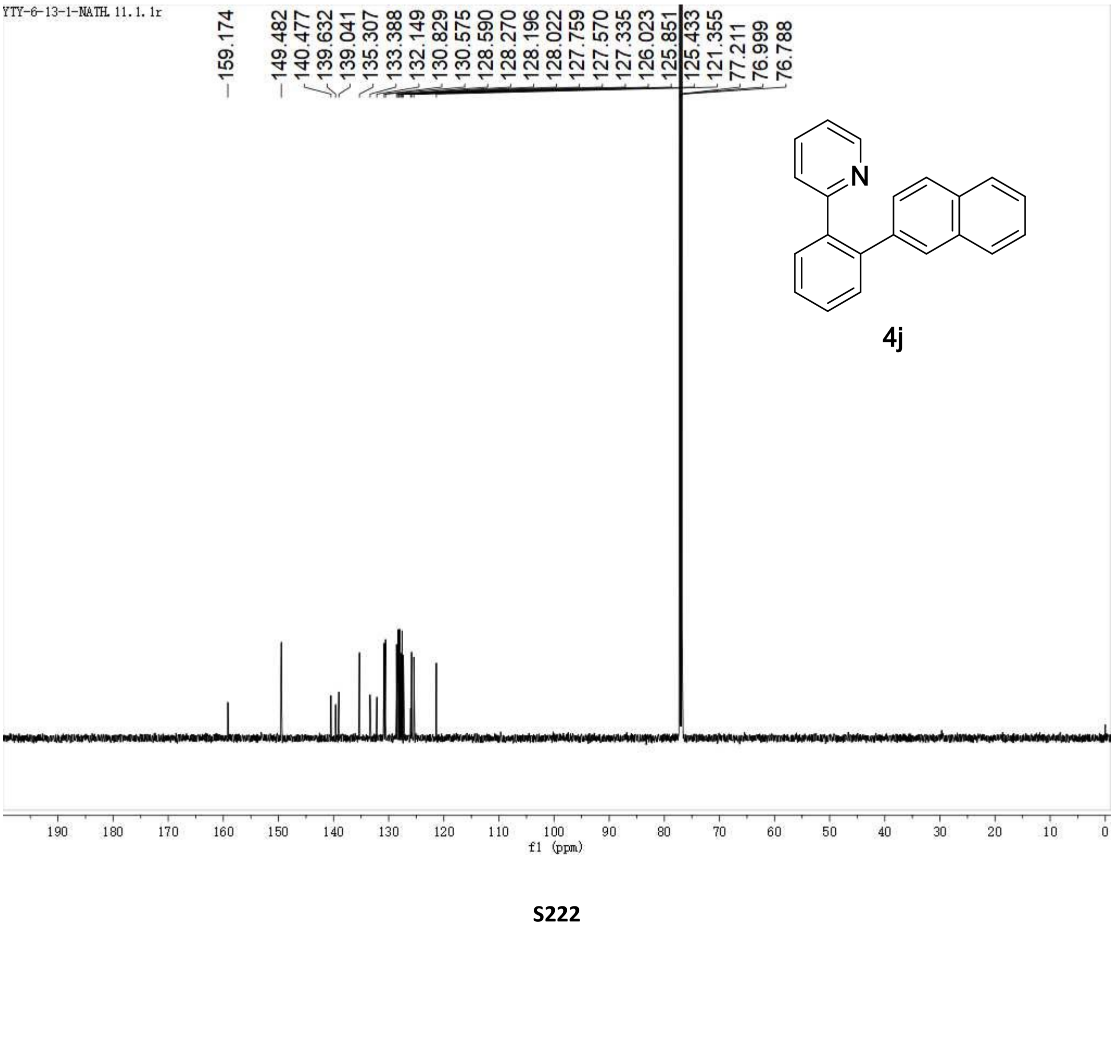
[13]C NMR spectrum of compound **4i** ($CDCl_3$, 151 MHz)



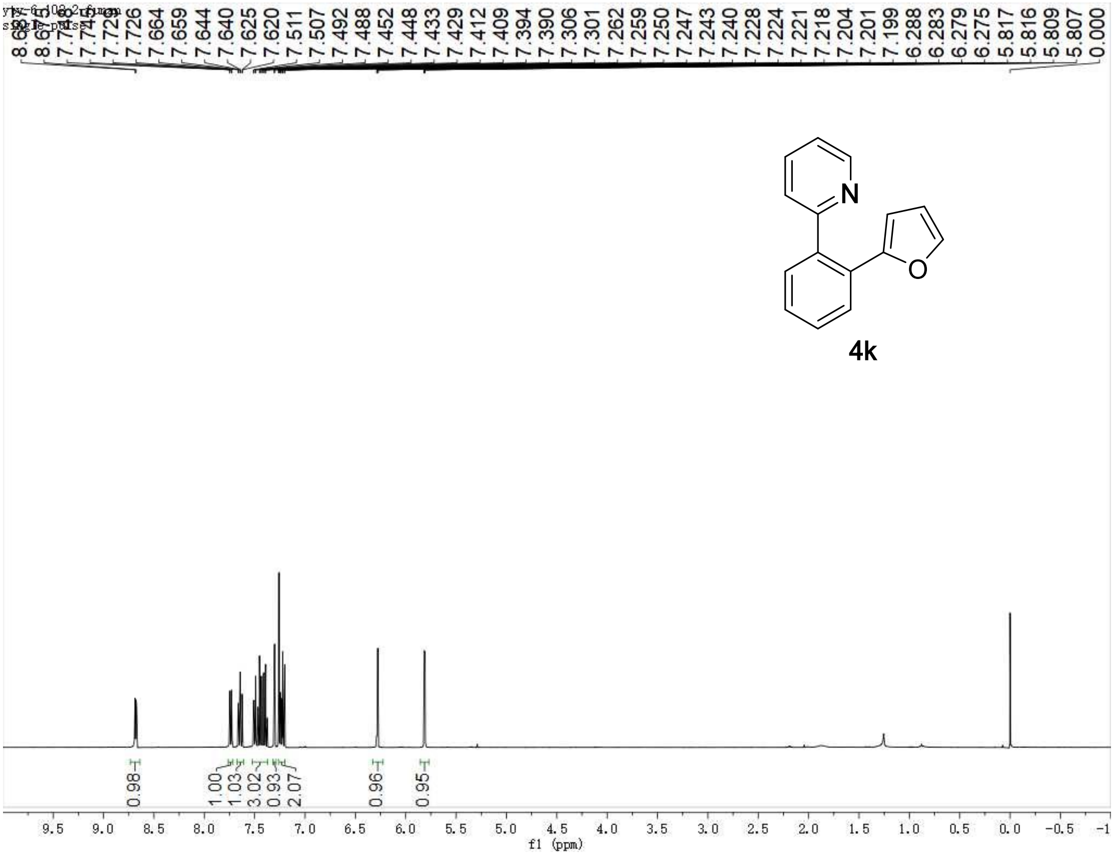
^{1}H NMR spectrum of compound **4j** ($CDCl_3$, 600 MHz)



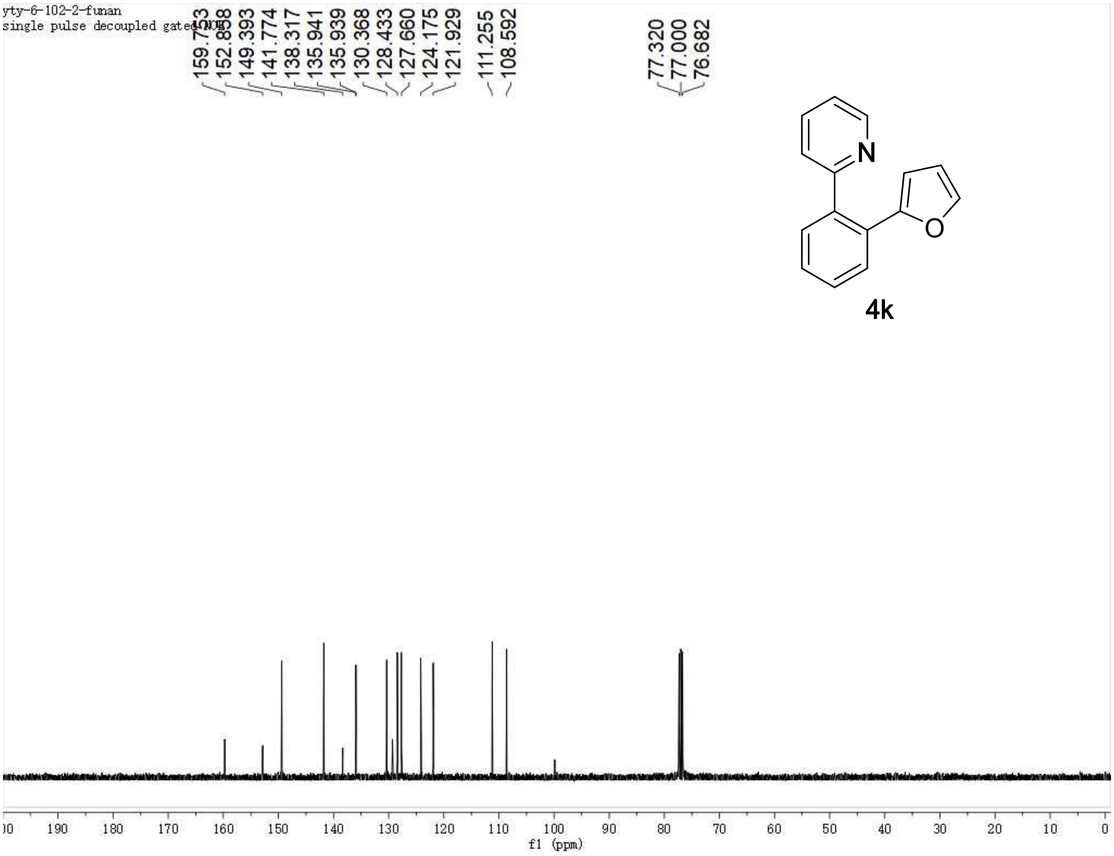
^{13}C NMR spectrum of compound **4j** ($CDCl_3$, 151 MHz)



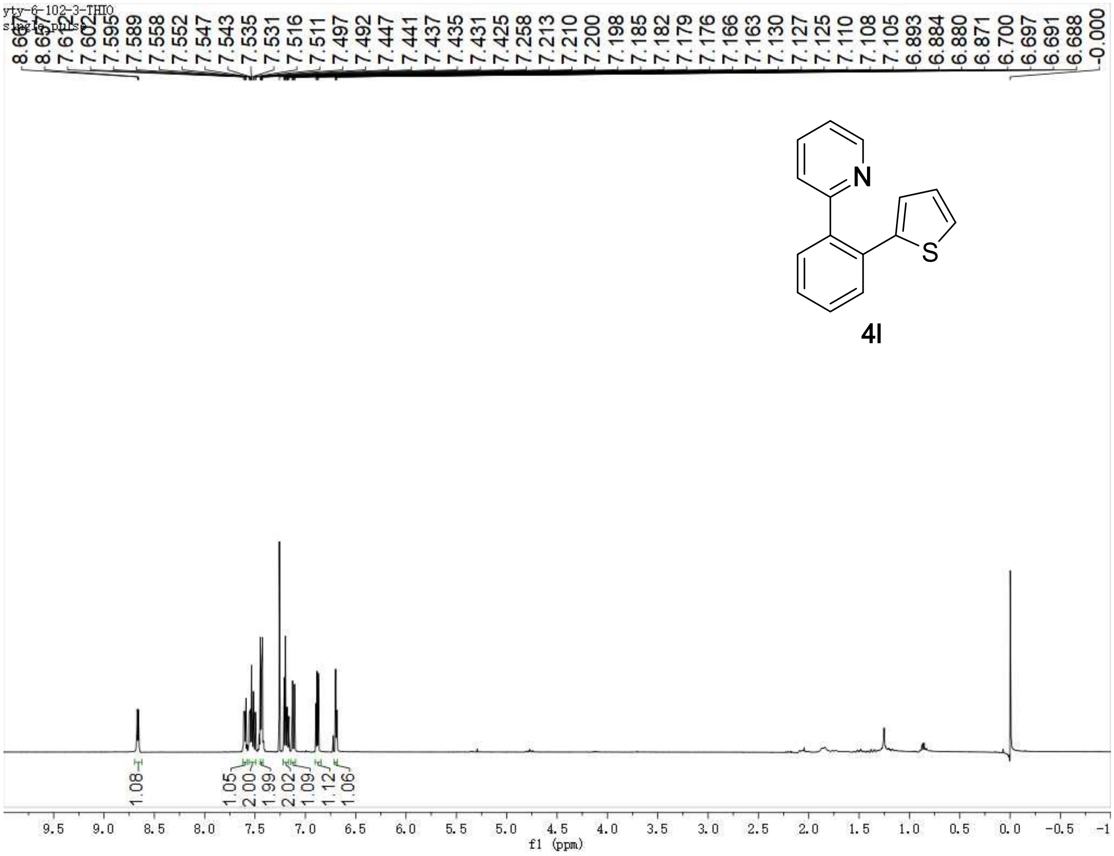
^{1}H NMR spectrum of compound **4k** ($CDCl_3$, 400 MHz)



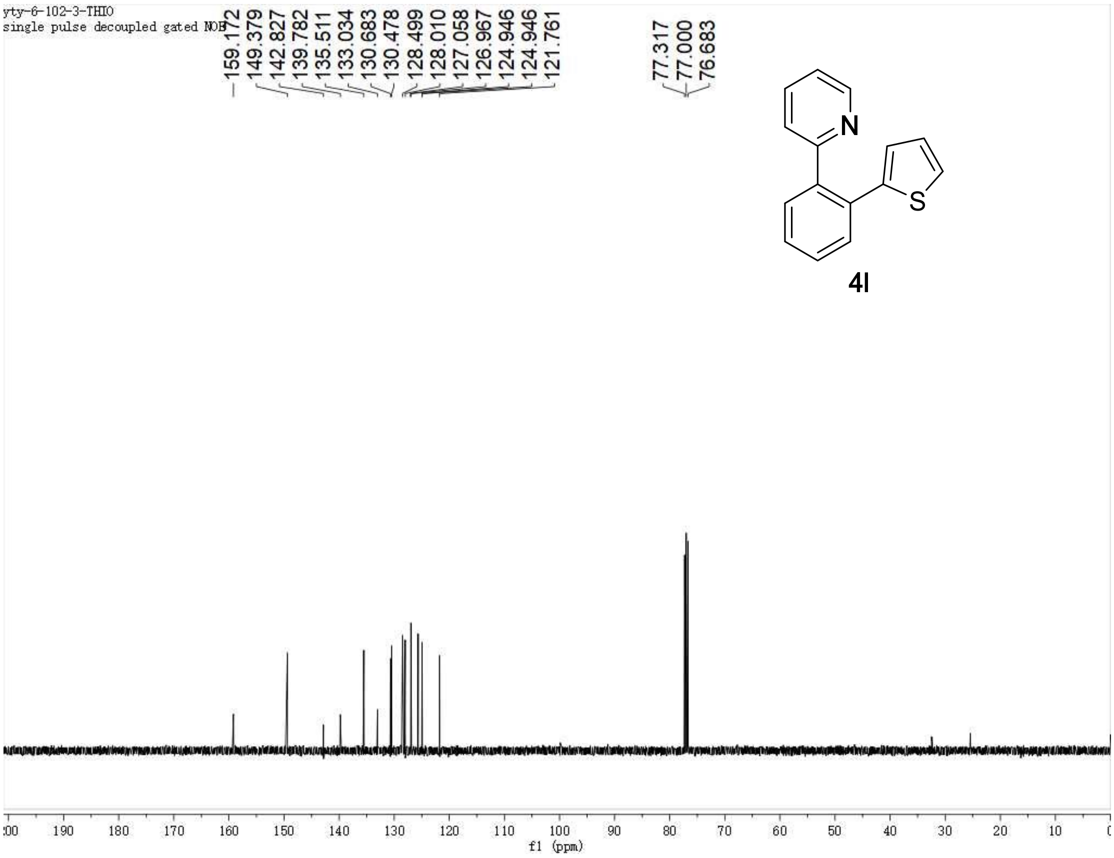
^{13}C NMR spectrum of compound **4k** ($CDCl_3$, 101 MHz)



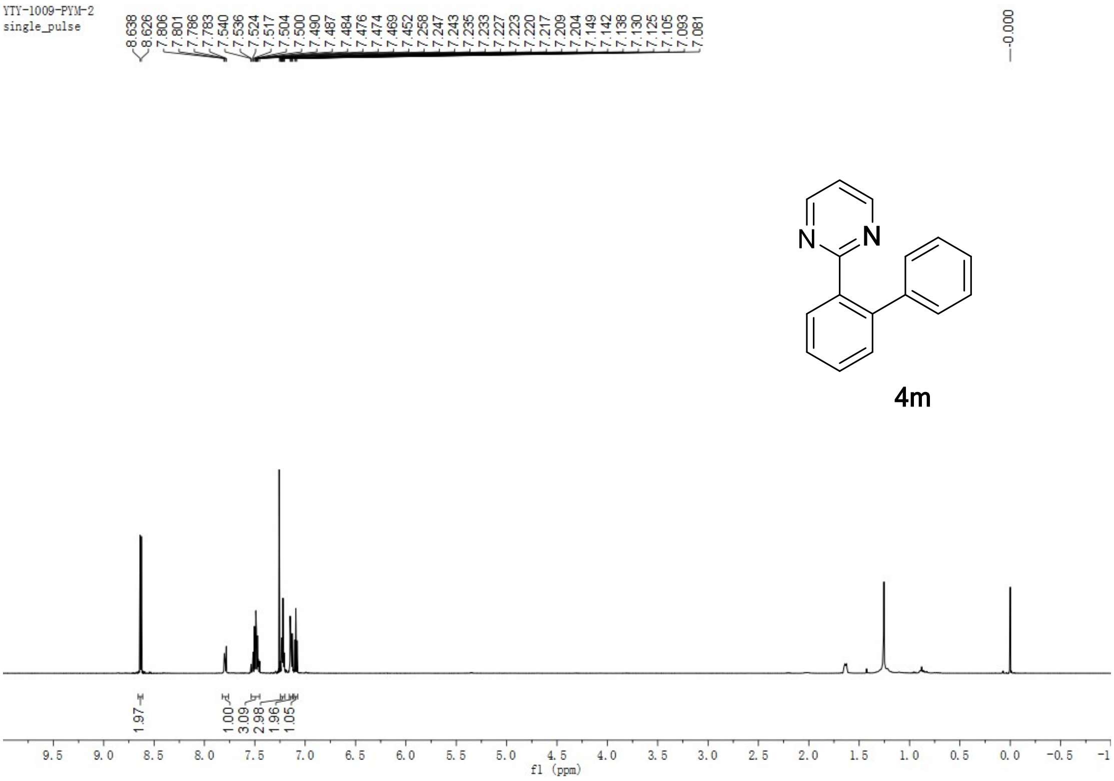
^{1}H NMR spectrum of compound **4l** ($CDCl_3$, 400 MHz)



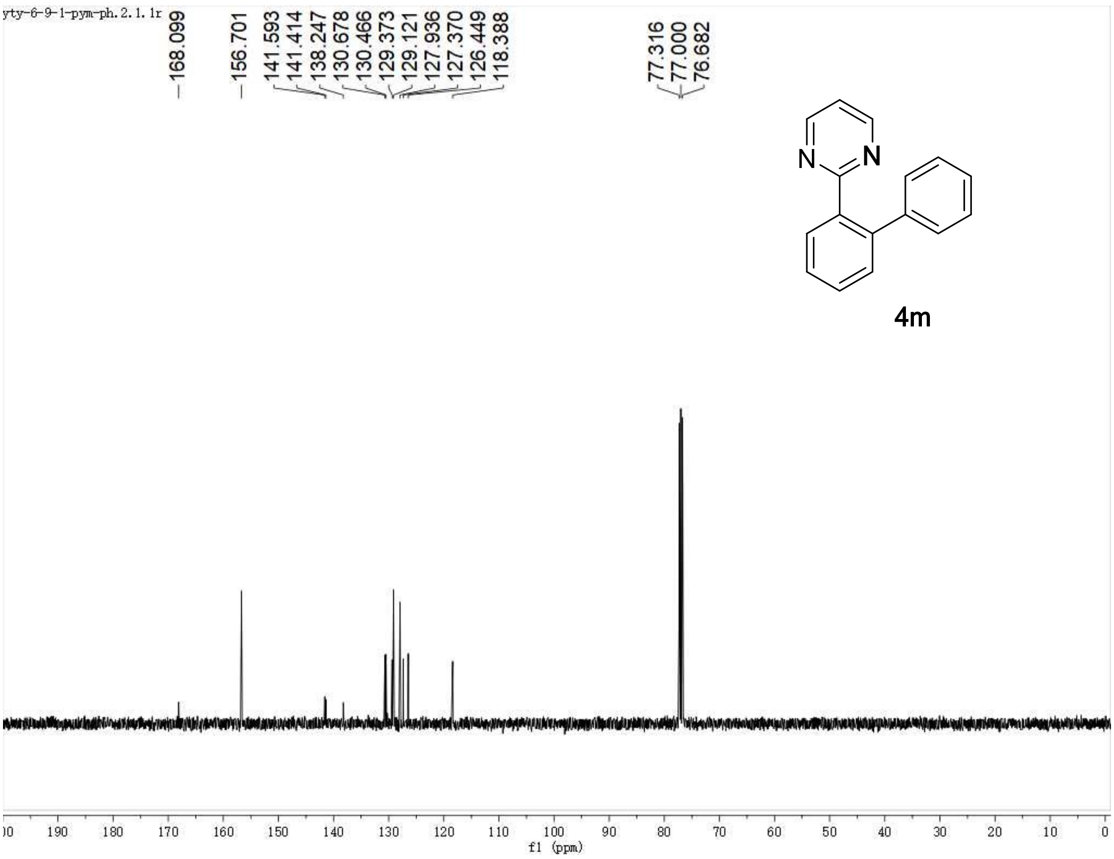
^{13}C NMR spectrum of compound **4l** ($CDCl_3$, 101 MHz)



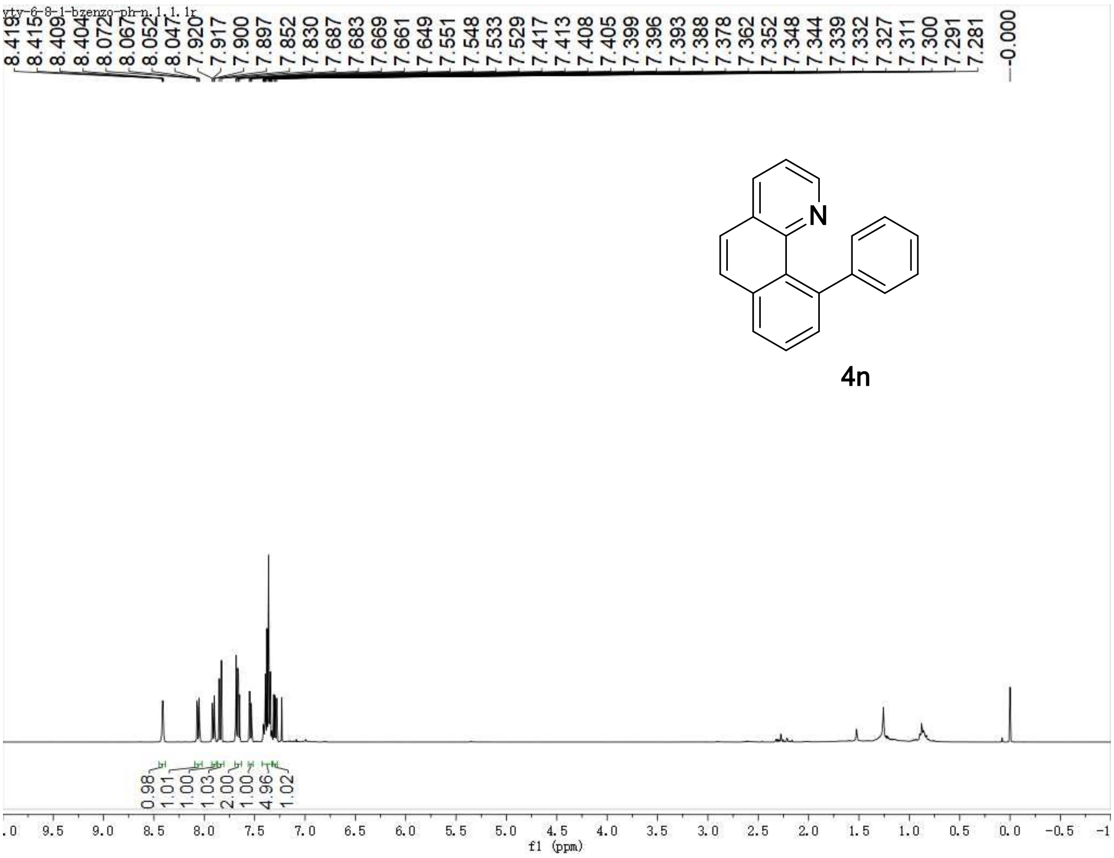
^{1}H NMR spectrum of compound **4m** ($CDCl_3$, 400 MHz)



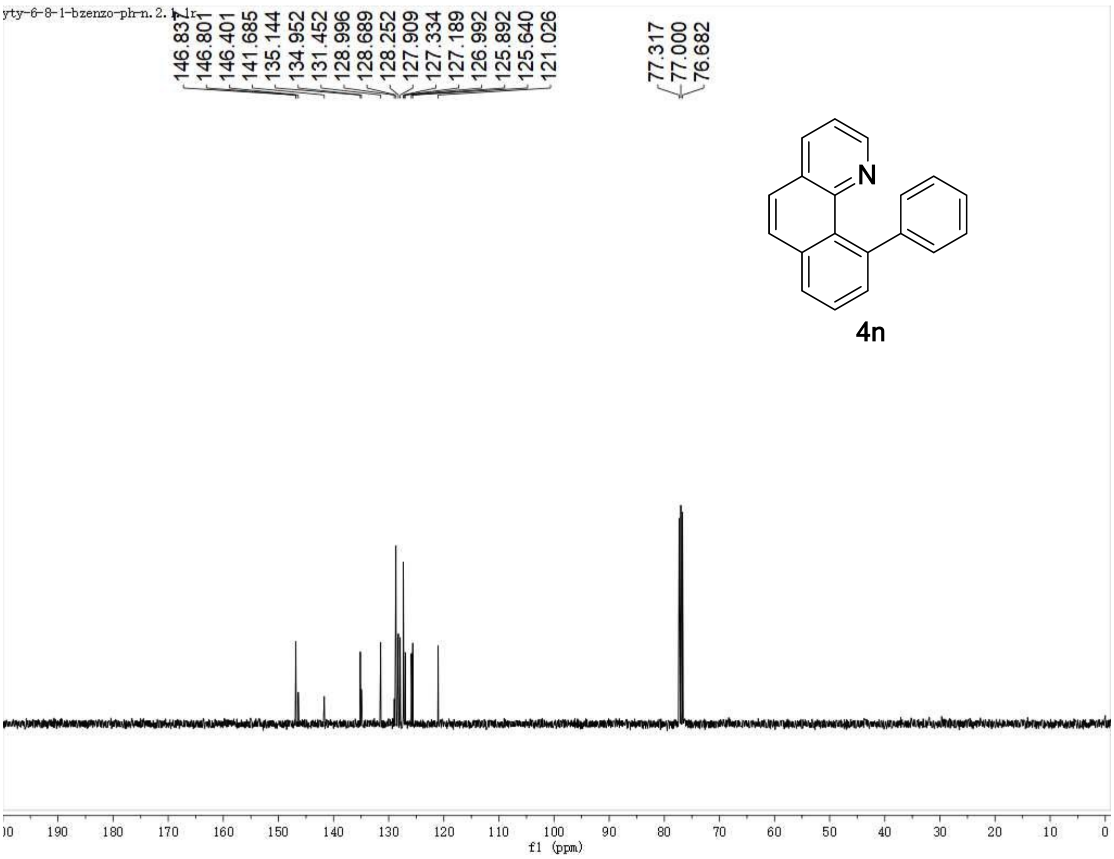
^{13}C NMR spectrum of compound **4m** ($CDCl_3$, 101 MHz)



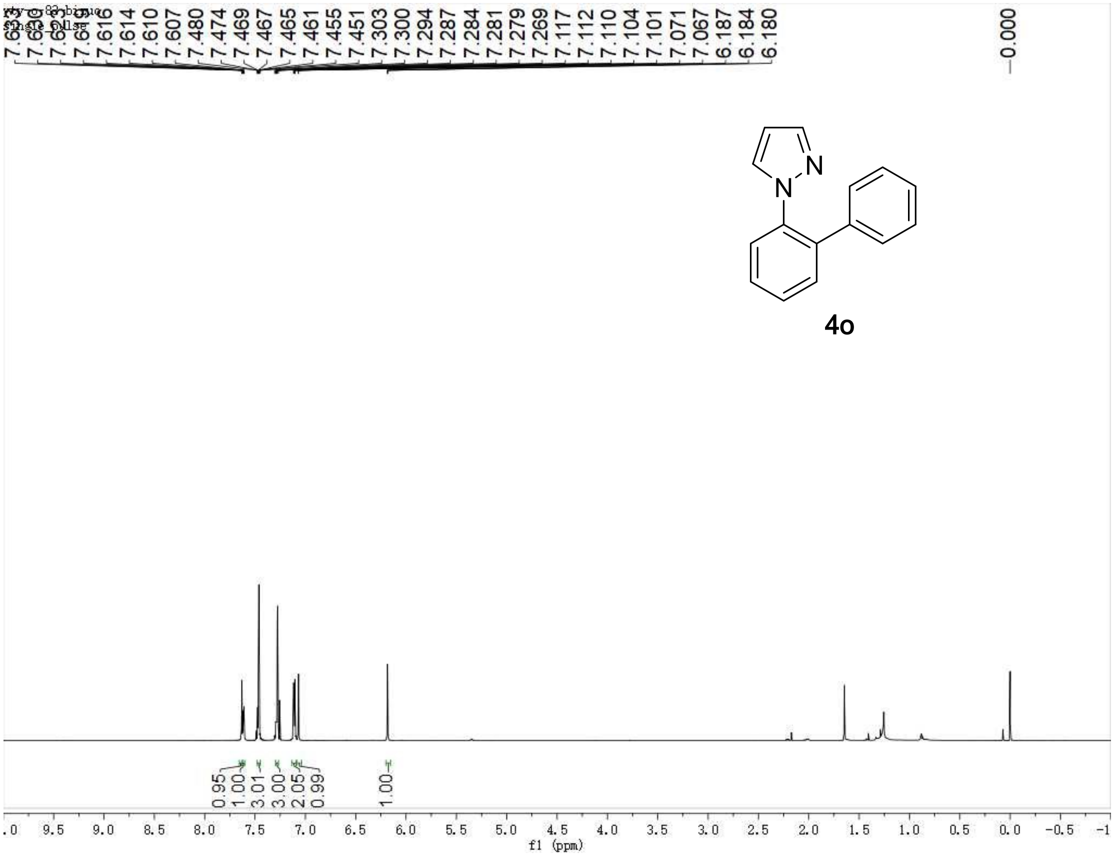
^{1}H NMR spectrum of compound **4n** ($CDCl_3$, 400 MHz)



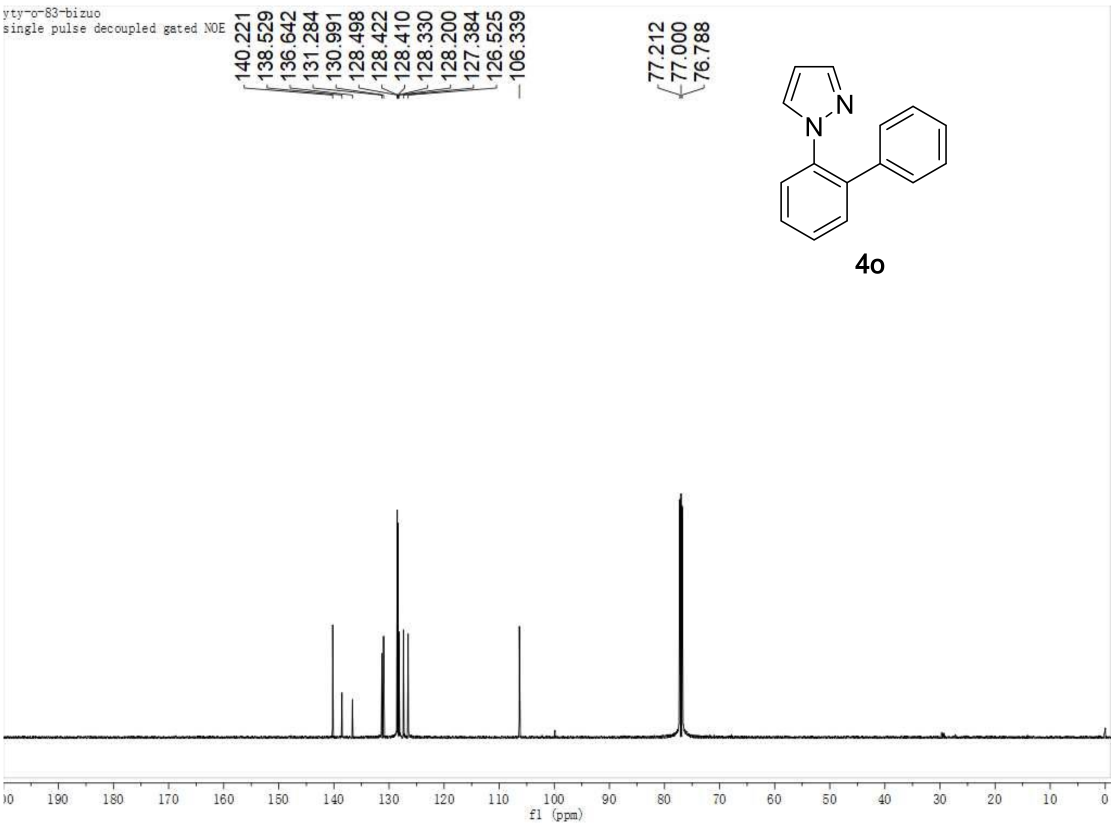
^{13}C NMR spectrum of compound **4n** ($CDCl_3$, 101 MHz)



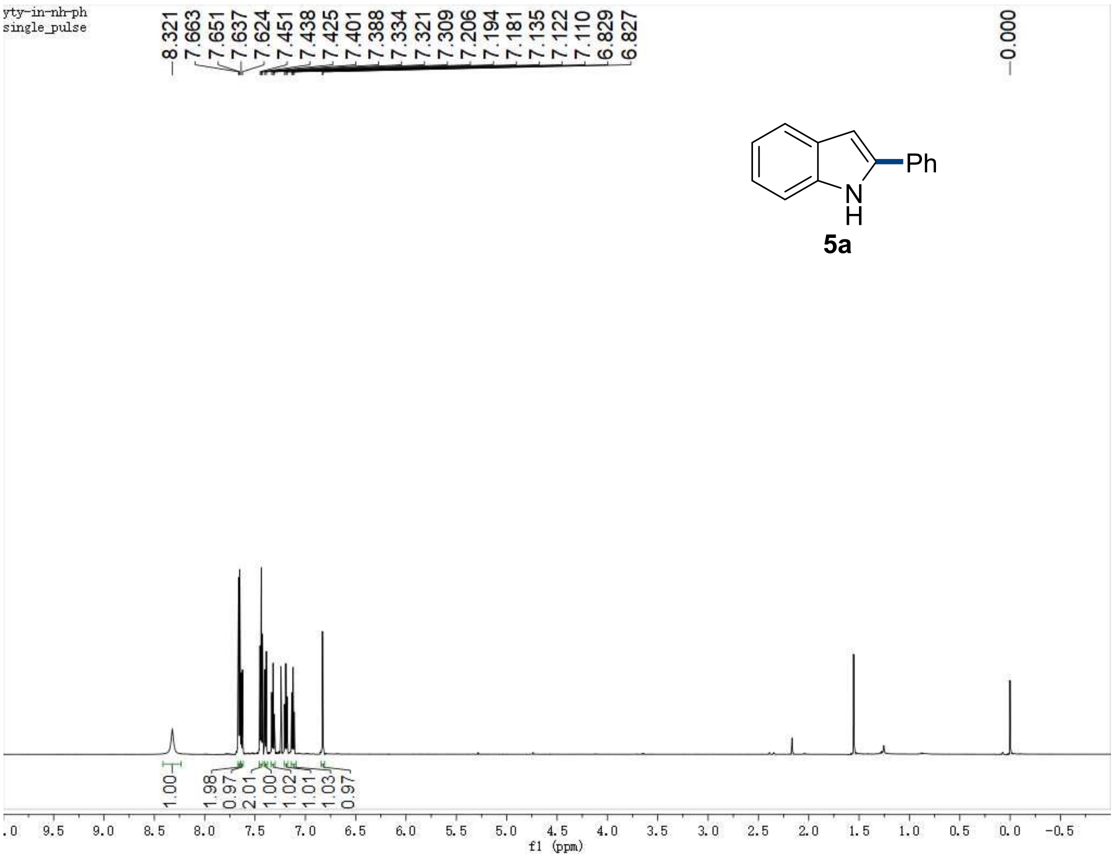
^{1}H NMR spectrum of compound **4o** ($CDCl_3$, 600 MHz)



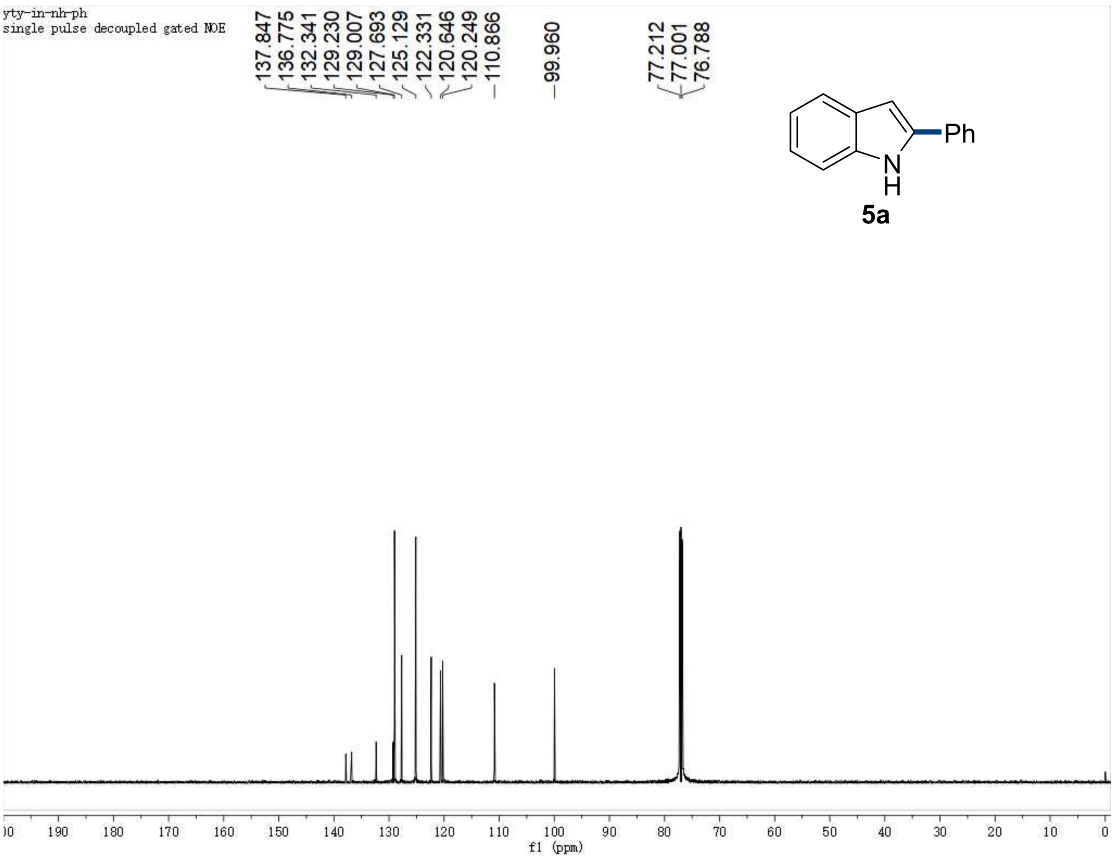
^{13}C NMR spectrum of compound **4o** ($CDCl_3$, 151 MHz)



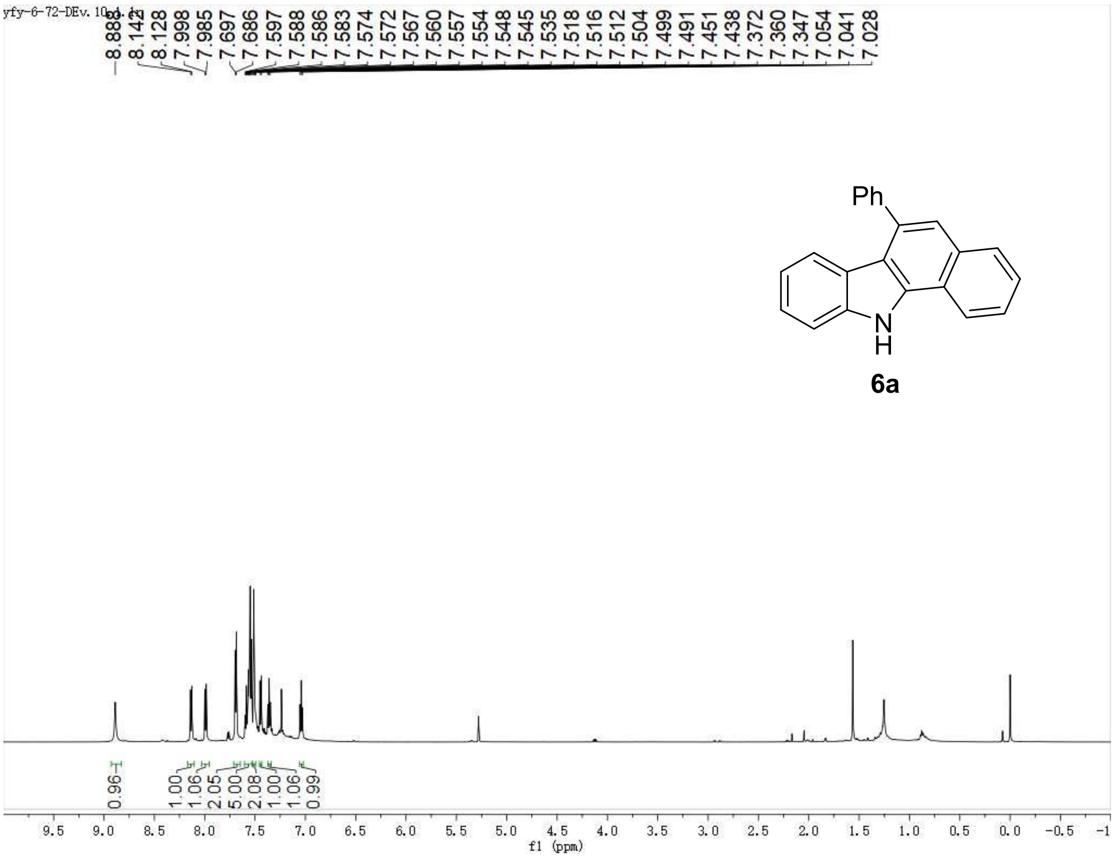
^{1}H NMR spectrum of compound **5a** ($CDCl_3$, 600 MHz)



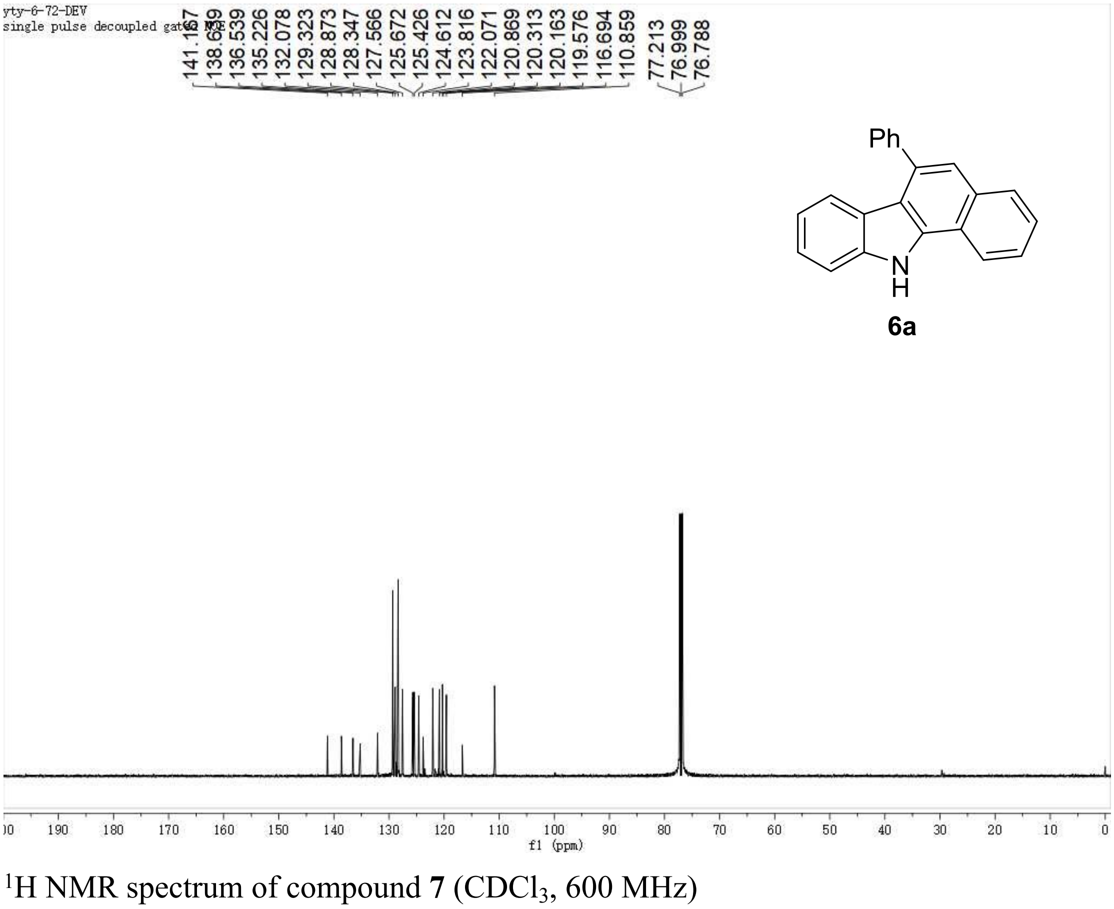
^{13}C NMR spectrum of compound **5a** ($CDCl_3$, 151 MHz)



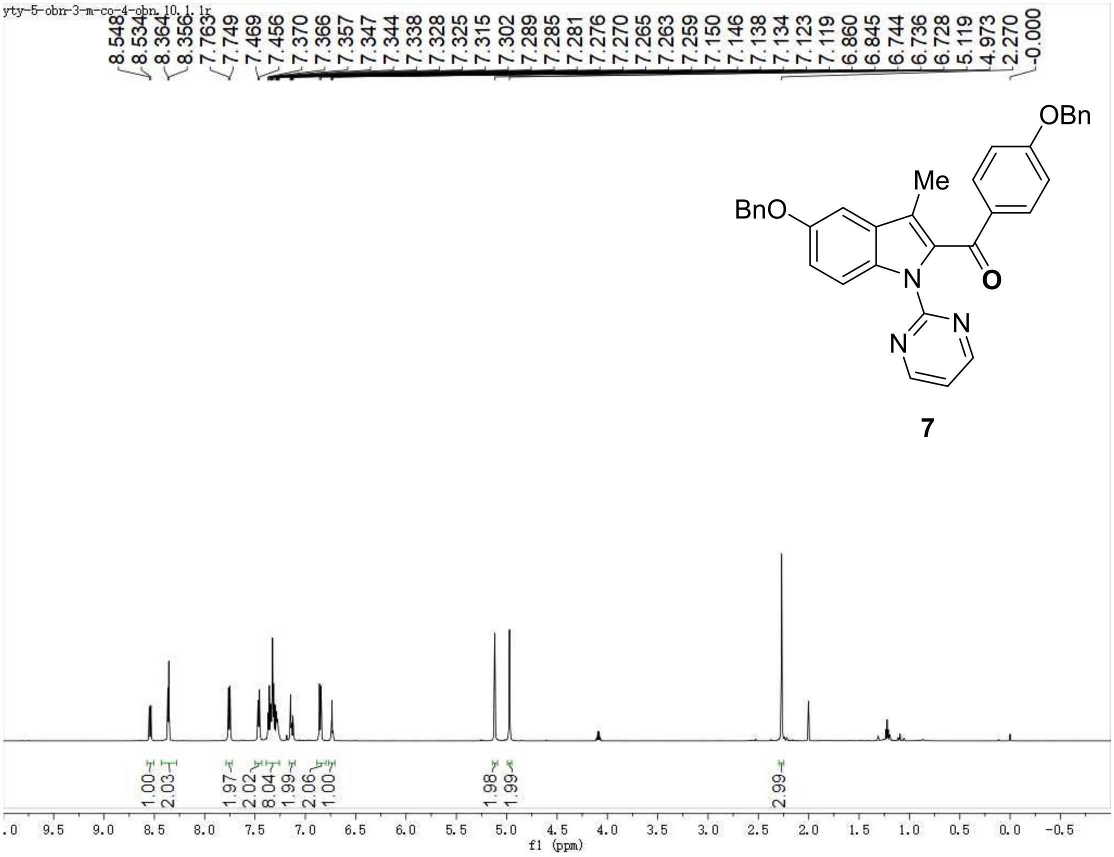
^{1}H NMR spectrum of compound **6a** ($CDCl_3$, 600 MHz)



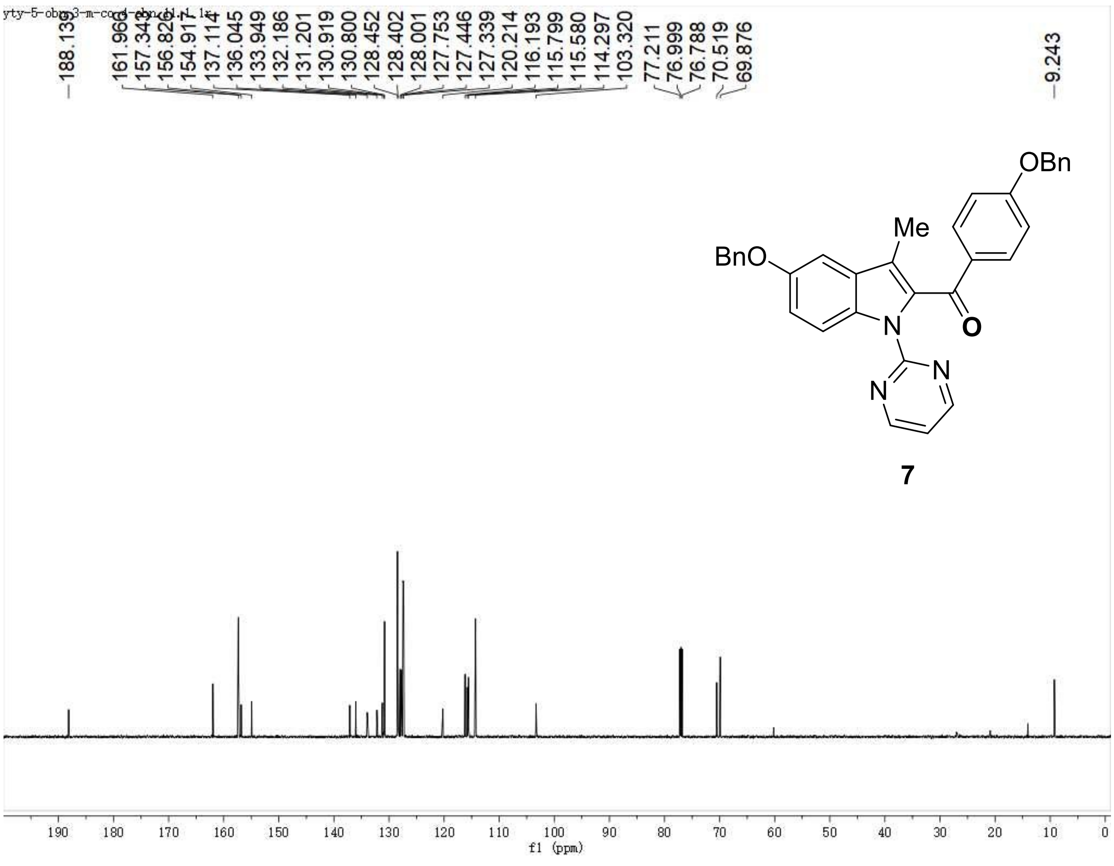
^{13}C NMR spectrum of compound **6a** ($CDCl_3$, 151 MHz)



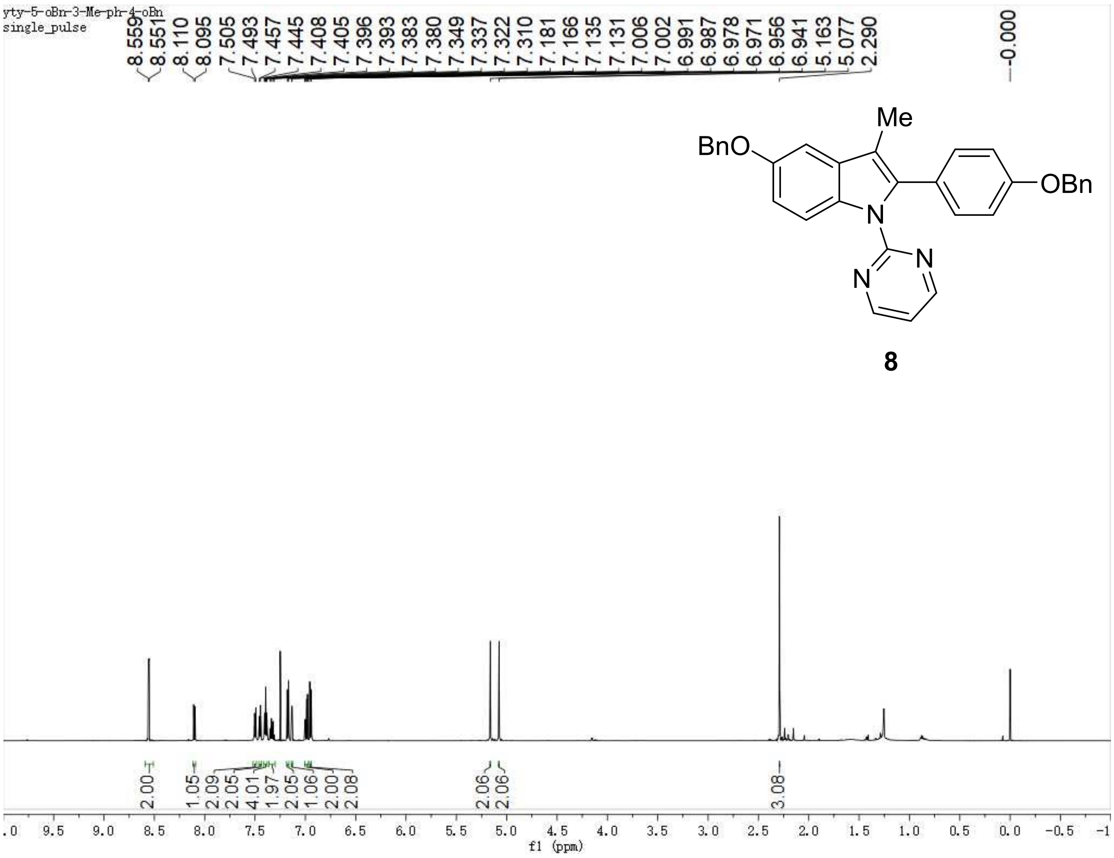
^{1}H NMR spectrum of compound **7** ($CDCl_3$, 600 MHz)



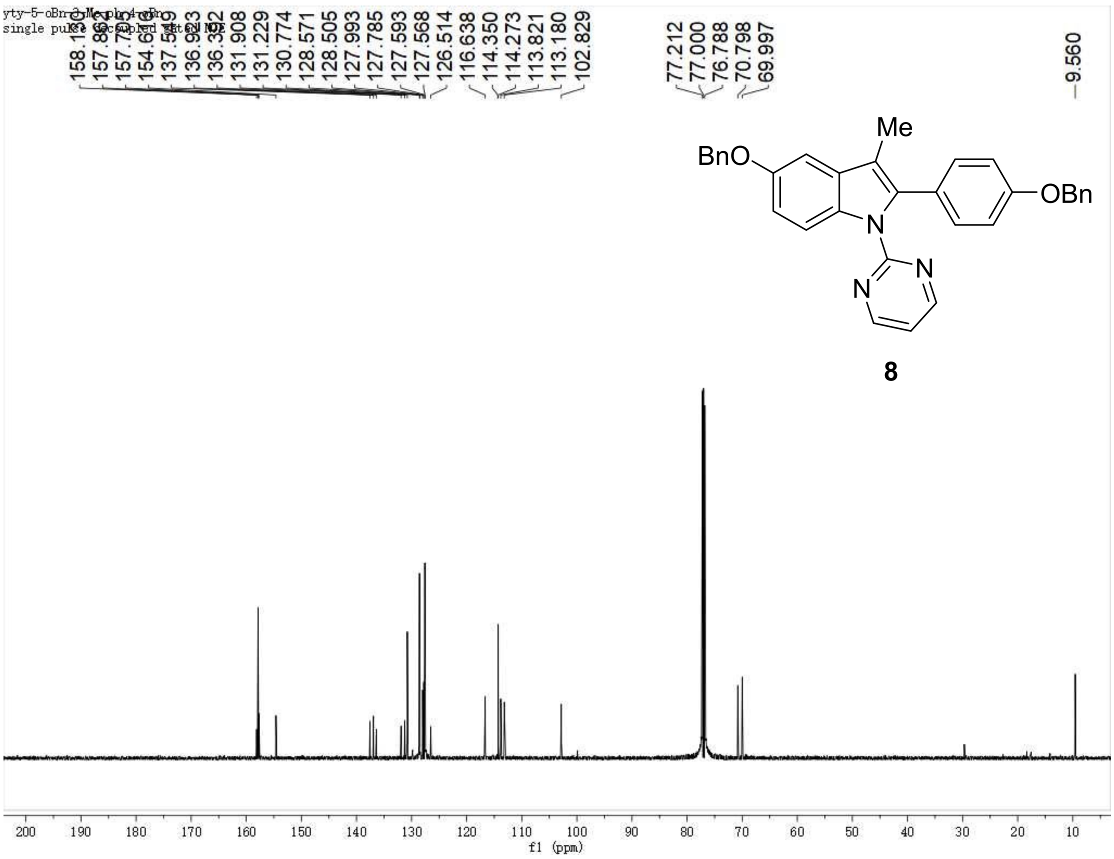
^{13}C NMR spectrum of compound **7** ($CDCl_3$, 151 MHz)



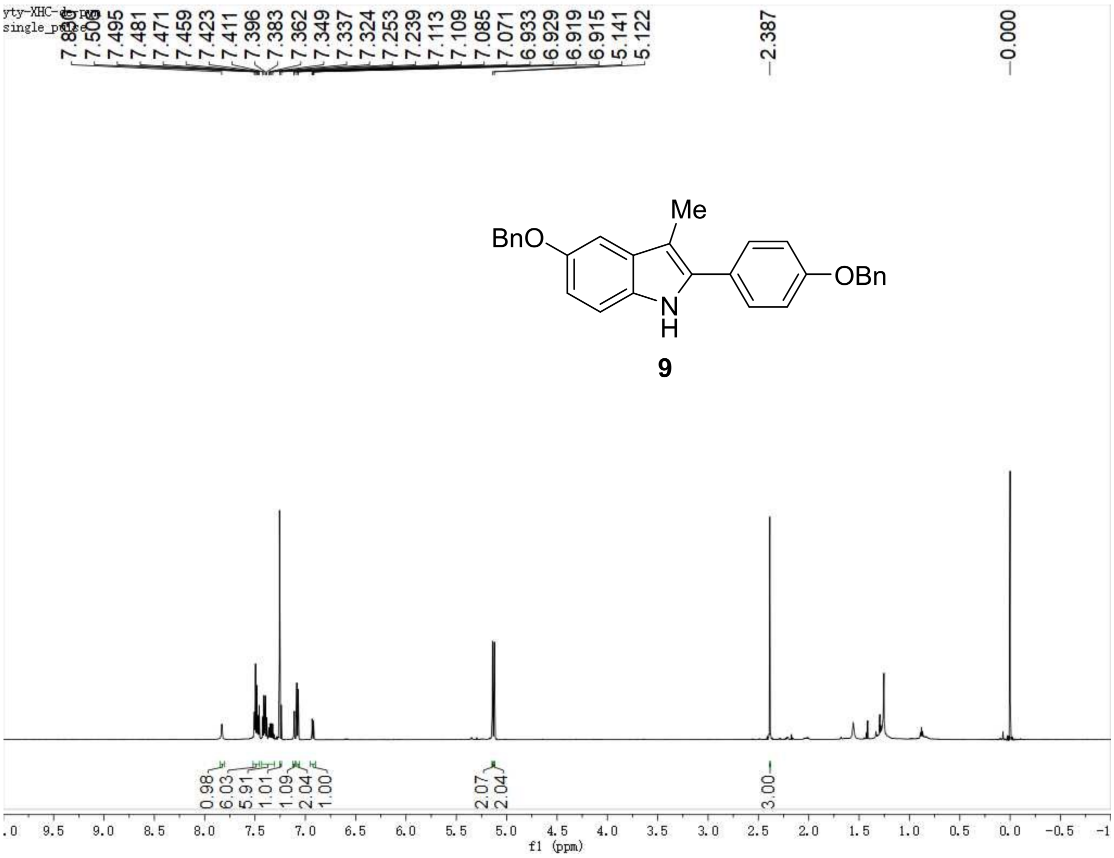
^{1}H NMR spectrum of compound **8** ($CDCl_3$, 600 MHz)



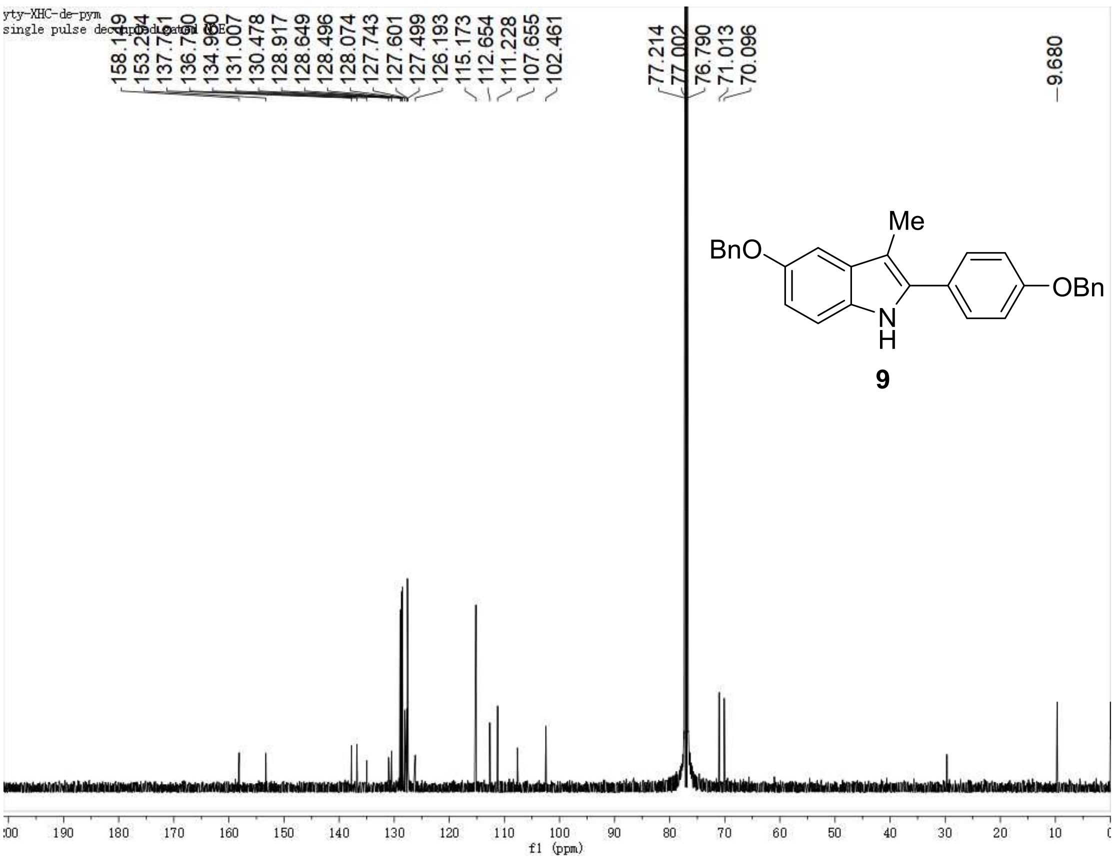
^{13}C NMR spectrum of compound **8** ($CDCl_3$, 151 MHz)



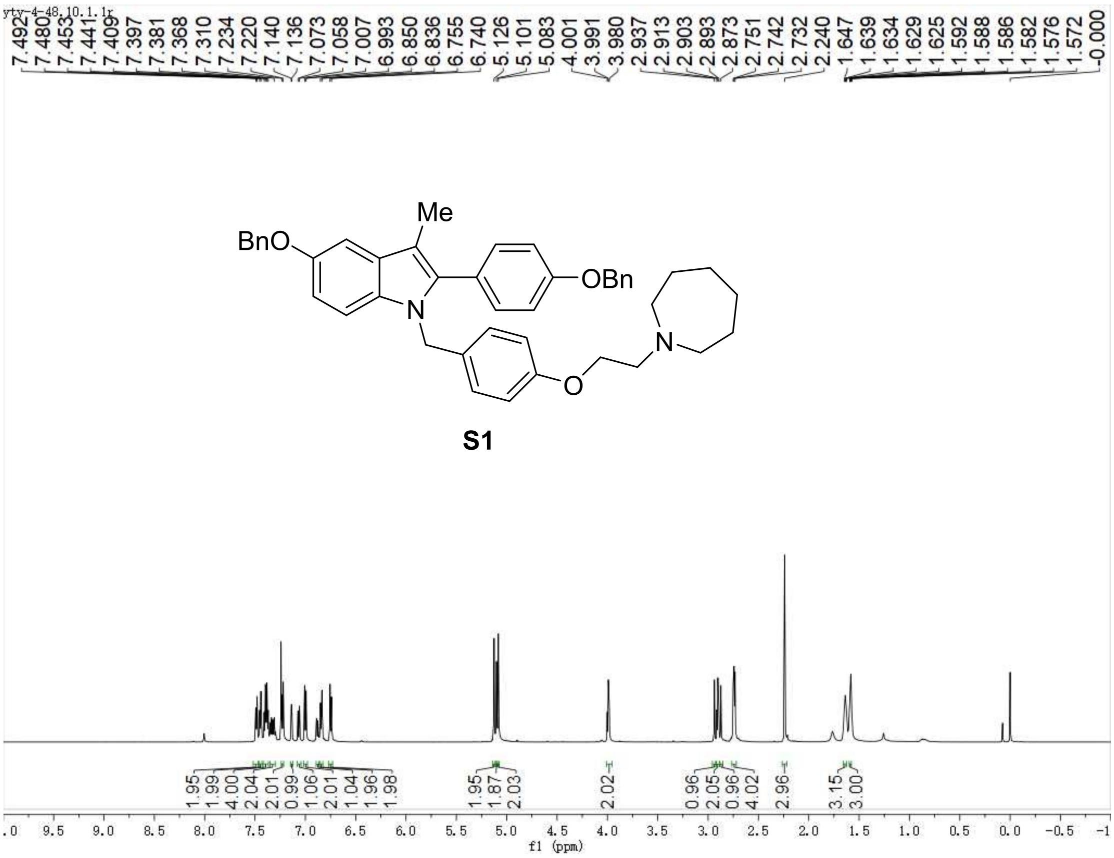
^{1}H NMR spectrum of compound **9** ($CDCl_3$, 600 MHz)



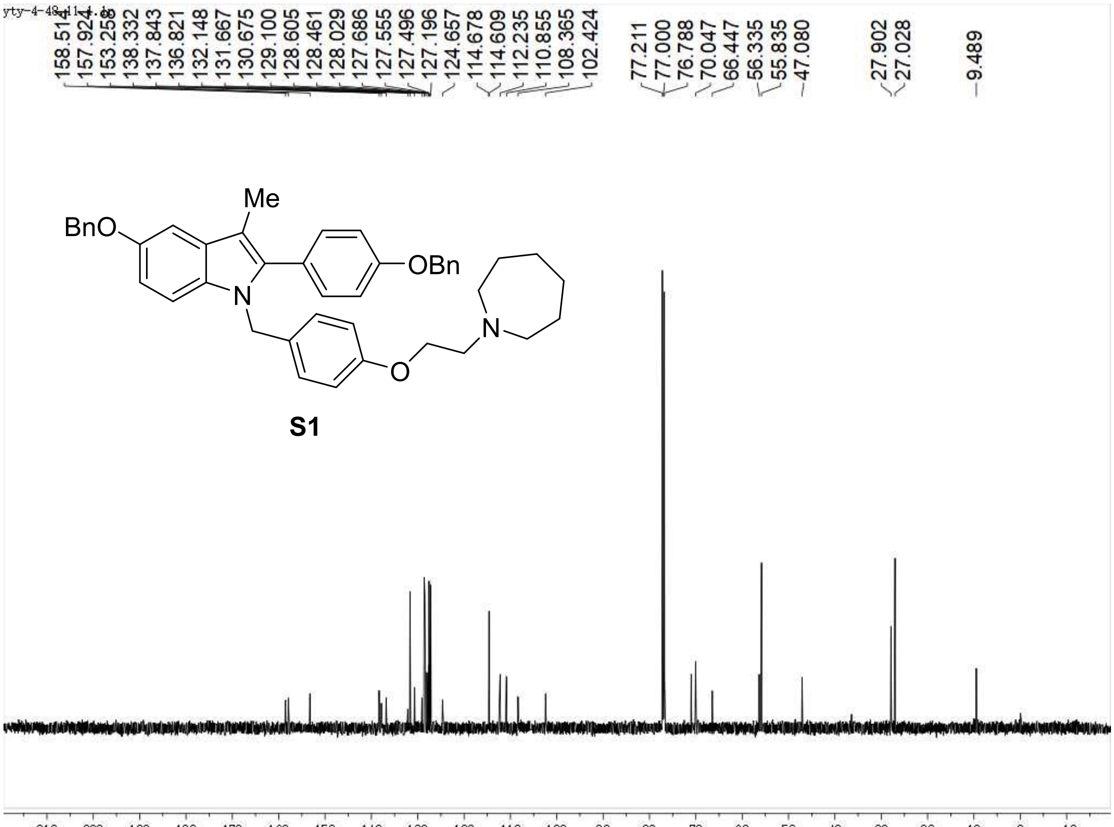
^{13}C NMR spectrum of compound **9** ($CDCl_3$, 151 MHz)



^{1}H NMR spectrum of compound **S1** ($CDCl_3$, 600 MHz)



^{13}C NMR spectrum of compound **S1** ($CDCl_3$, 151 MHz)



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