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Electronic Supplementary Information

Establishing the Correlation between Catalytic Performance and N→Sb Donor-Acceptor Interaction: Systematic Assessment of Azastibocine Halide Derivatives as Water Tolerant Lewis Acids

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X-ray crystallographic structure determination

Given in Fig. S1 and Table S1 are the results of the crystal structure determination and refinement for azastibocine halide derivatives. In all cases, the diffraction data were collected using graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). The collected frames were processed with SAINT+ software and the collected reflections were subject to absorption correction (SADABS).[1] The structure was solved by the direct method (SHELXTL) in conjunction with standard difference Fourier techniques and subsequently refined by full-matrix least-squares analyses on F^2.[2] The hydrogen atoms were generated in their idealized positions and all non-hydrogen atoms were refined anisotropically.

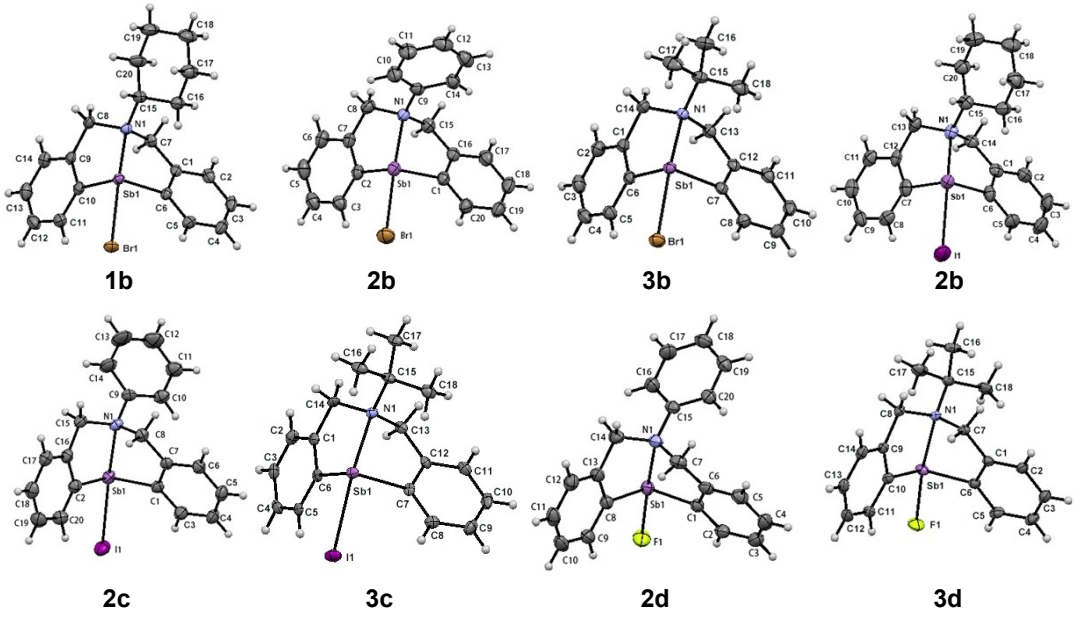


Fig. S1 Crystal structures of azastibocine halide derivatives.

Table S1 Crystallographic data for azastibocine halide derivatives

Complex	1b	2b	3b	1c	2c	3c	1d	2d	3d
Empirical formula	$C_{20}H_{23}BrNSb$	$C_{20}H_{17}BrNSb$	$C_{18}H_{21}BrNSb$	$C_{20}H_{23}INSb$	$C_{20}H_{17}INSb$	$C_{18}H_{21}INSb$	$C_{20}H_{23}FNSb$	$C_{20}H_{17}FNSb$	$C_{18}H_{21}FNSb$
Formula weight	479.05	473.01	453.02	526.04	520.00	500.01	418.14	412.10	392.11
Temperature/K	273	298	273	100	298	100	100	293	273
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*P2(1)/n*	*P2(1)/n*	*P2(1)/n*	*P2(1)/n*	*P2(1)/c*	*P2(1)/c*	*P2(1)/n*	*P2(1)/n*	*Cc*
a/Å	10.2338(5)	9.5744(3)	9.8178(4)	11.3664(3)	9.1637(3)	12.3974(4)	9.3503(3)	10.2974(8)	17.7432(9)
b/Å	16.5885(7)	10.2962(3)	16.1278(5)	12.5996(3)	10.9833(4)	9.4136(3)	15.9263(5)	10.3031(8)	10.6409(6)
c/Å	12.0033(5)	18.1939(6)	11.4078(5)	13.0792(4)	18.0957(7)	14.8803(5)	11.7239(4)	15.7161(11)	17.8551(10)
α/°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
β/°	113.346(2)	100.795(1)	109.895(1)	94.703(2)	95.784(1)	92.218(3)	104.044(3)	101.559 (1)	96.996(2)
γ/°	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
V/Å^3	1870.89(15)	1761.81(10)	1698.50(11)	1866.79(9)	1812.02(11)	1735.29(10)	1693.69(10)	1633.6(2)	3346.0(3)
Z	4	4	4	4	4	4	4	4	8
No. of reflections collected	30234	10613	49645	12759	9043	11089	10827	9422	31989
No. of unique reflections	4636	3417	2978	3284	3510	3058	2982	3560	8232
R_{int}	0.0363	0.038	0.0437	0.0390	0.055	0.0353	0.0376	0.063	0.0229
R_1*(reflections)*	0.0196	0.0294	0.0143	0.0236	0.0354	0.0237	0.0256	0.0323	0.0419
wR_2*(reflections)*	0.0416	0.0709	0.0541	0.0561	0.0912	0.0516	0.0598	0.0840	0.1205
GOF on F^2	1.066	1.041	1.028	1.022	1.070	1.040	1.097	1.065	1.079

Stability experiments

Given in Fig. S2–S5 are the results of stability experiments for selected azastibocine halide derivatives (**1a**, **1b**, **1c** and **1d**). There is no obvious difference between the ^{1}H NMR spectra of freshly prepared samples and ones that were kept in open air for 1 week. Moreover, these organoantimony complexes were found to be stable in the presence of additional H_2O (1 mL), clearly indicating that the compounds are water-tolerant.

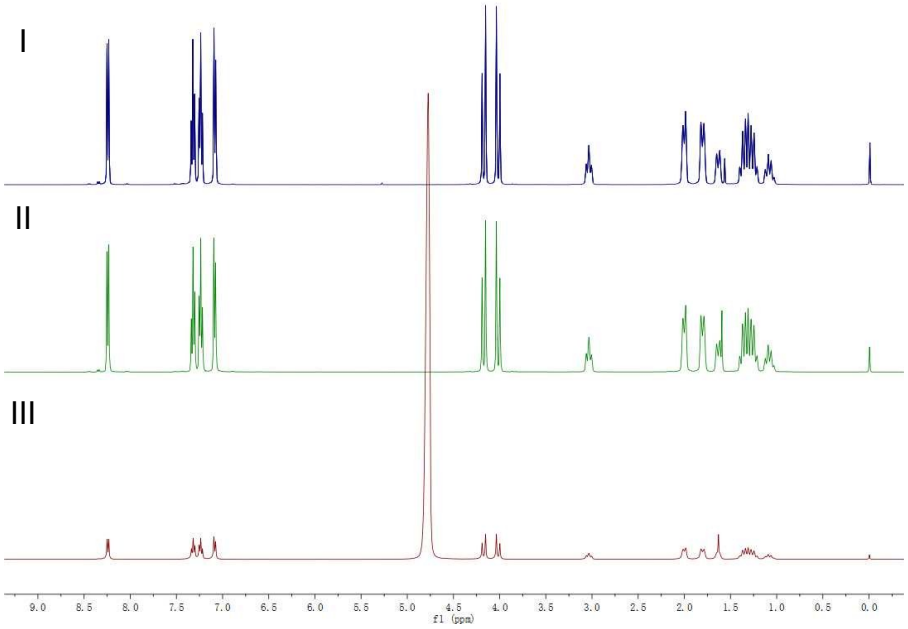


Fig. S2 ^{1}H NMR spectra of **1a** measured in $CDCl_3$: (I) freshly prepared, (II) after being kept in the open air for 1 weeek and (III) in the presence of additional H_2O (1 mL).

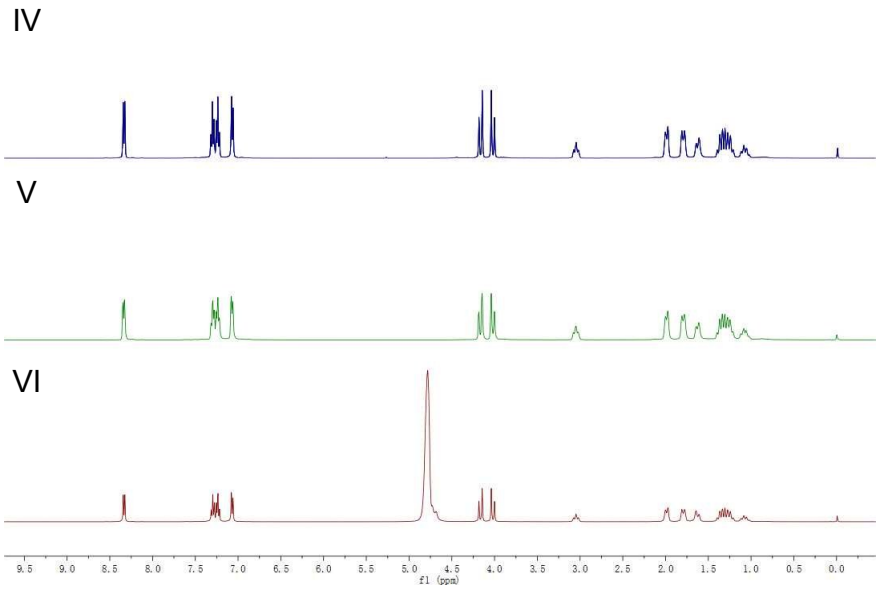


Fig. S3 ^{1}H NMR spectra of **1b** measured in $CDCl_3$: (IV) freshly prepared, (V) after being kept in the open air for 1 weeek and (VI) in the presence of additional H_2O (1 mL).

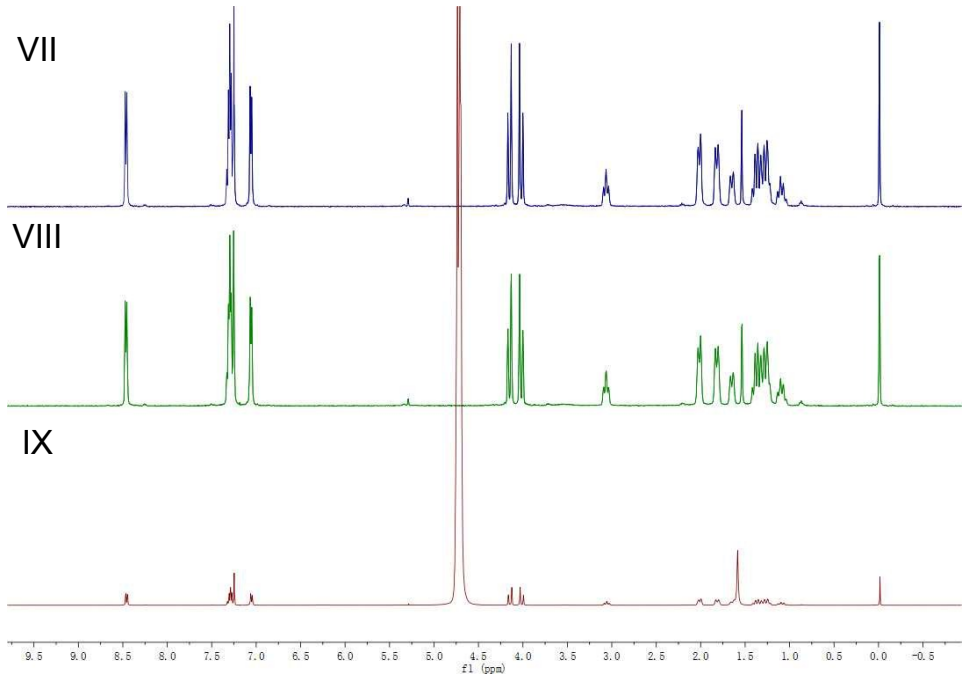


Fig. S4 ^{1}H NMR spectra of **1c** measured in $CDCl_3$: (VII) freshly prepared, (VIII) after being kept in the open air for 1 weeek and (IX) in the presence of additional H_2O (1 mL).

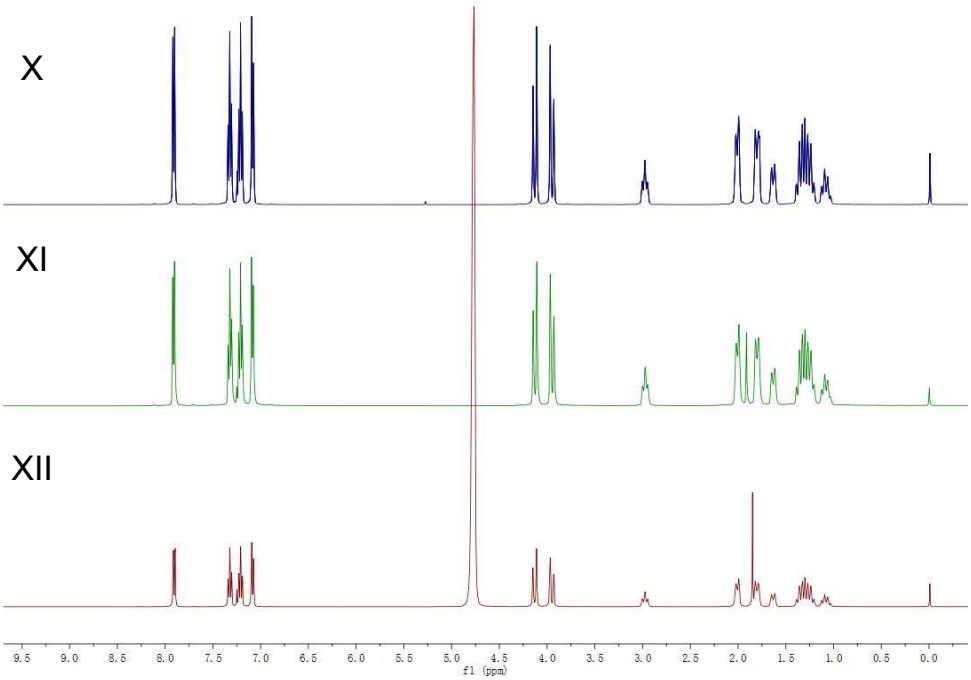


Fig. S5 ^{1}H NMR spectra of **1d** measured in $CDCl_3$: (X) freshly prepared, (XI) after being kept in the open air for 1 weeek and (XII) in the presence of additional H_2O (1 mL).

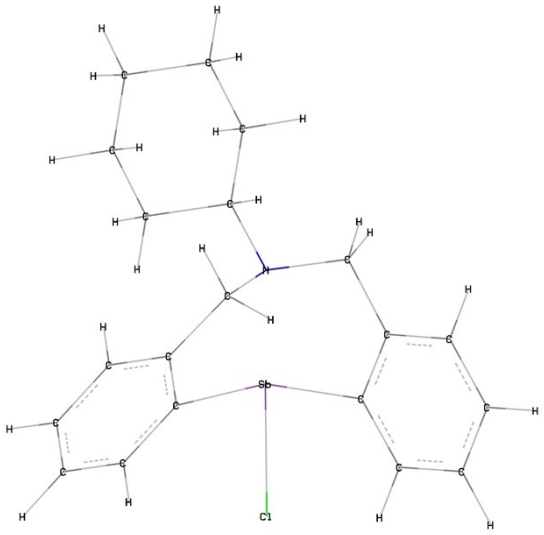
Fluoride ion affinities (FIAs) calculation

Geometry optimizations and single-point energy calculations at M06-2X/Def2TZVPP level were performed on organoantimony compounds **1a–3d**, as well as that of corresponding anion parts of **[1a-F]$^-$–[3d-F]$^-$**. The frequency calculations were carried out for each compound at the same level as in the structure optimization to confirm the absence of any imaginary frequencies, and to obtain the corrected value of enthalpy change. The resulting relative fluoride ion affinities were converted to an absolute scale using the experimentally known value of 209 kJ/mol for the FIA of COF_2.[3,4]

Table S2. Summary of energetic data

	Enthalpy of CF_3O^- (Hartree)	Enthalpy of **Sb** (Hartree)	Enthalpy of CF_2O (Hartree)	Enthalpy of [**Sb-F**]$^-$ (Hartree)	ΔH (Hartree)	FIA (kJ/mol)
1a	-412.966071	-1530.70547	-313.03054	-1630.658261	-0.01726	254.3161300
2a	-412.966071	-1527.138322	-313.03054	-1627.063598	0.010255	182.0754975
3a	-412.966071	-1453.308045	-313.03054	-1553.230638	0.012938	175.0312810
1b	-412.966071	-3644.719324	-313.03054	-3744.674281	-0.019426	260.0029630
2b	-412.966071	-3641.143455	-313.03054	-3741.060176	0.01881	159.6143450
3b	-412.966071	-3567.325704	-313.03054	-3667.270486	-0.009251	233.2885005
1c	-412.966071	-1368.153367	-313.03054	-1468.102843	-0.013945	245.6125975
2c	-412.966071	-1364.581982	-313.03054	-1464.488905	0.028608	133.8896960
3c	-412.966071	-1290.76144	-313.03054	-1390.691004	0.005967	193.3336415
1d	-412.966071	-1170.349469	-313.03054	-1270.285281	-0.000281	209.7377655
2d	-412.966071	-1166.783765	-313.03054	-1266.688772	0.030524	128.8592380
3d	-412.966071	-1092.9571	-313.03054	-1192.867783	0.024848	143.7615760

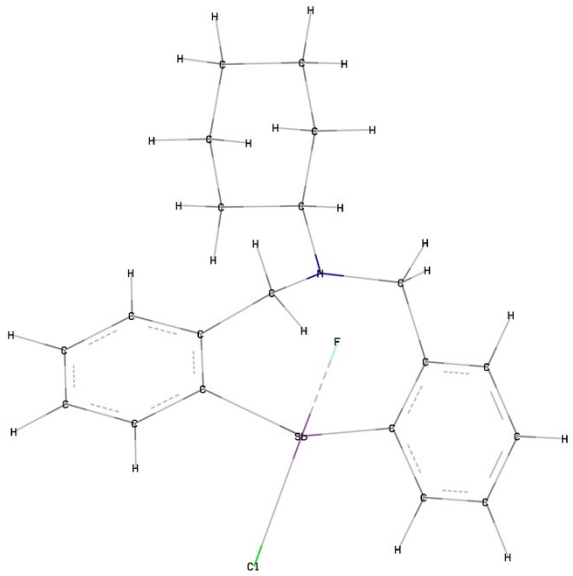
Table S3 Cartesian coordinates for the optimized structure of **1a**



	x	y	z		x	y	z
Sb	0.79654	0.31586	-1.13518	H	3.87273	-0.30578	-0.28053
Cl	2.79717	1.58808	-1.78268	H	5.0218	-2.07842	0.98881

N	-0.88945	-0.92073	0.30255	H	3.72085	-3.93262	1.98585
C	1.91915	-1.14718	-0.01393	H	1.26694	-4.00042	1.70617
C	3.29964	-1.1165	0.14962	H	-0.52506	-2.74356	-0.62175
C	3.94777	-2.11672	0.86433	H	-0.75781	-2.88695	1.1189
C	3.21976	-3.15678	1.42262	H	1.34105	3.37122	-0.33879
C	1.84189	-3.19509	1.26387	H	0.62138	4.90473	1.44841
C	1.19138	-2.20175	0.5417	H	-0.7895	4.06709	3.30407
C	-0.30311	-2.26805	0.3387	H	-1.47306	1.69619	3.35226
C	0.33412	1.66413	0.48145	H	-0.06718	-0.77412	2.20649
C	0.7166	3.00223	0.46462	H	-1.77651	-0.38438	2.15954
C	0.31748	3.86685	1.47557	H	-2.04637	-1.25511	-1.36933
C	-0.47214	3.39806	2.51538	H	-3.42404	-1.56239	1.33332
C	-0.85714	2.06603	2.54021	H	-2.8367	-2.88044	0.32836
C	-0.45887	1.19688	1.53045	H	-4.38443	-2.25603	-1.47771
C	-0.83362	-0.26473	1.61855	H	-5.26639	-2.53925	0.01122
C	-2.22695	-0.90974	-0.34369	H	-6.06334	-0.47191	-1.1543
C	-3.23709	-1.86674	0.29875	H	-5.39543	-0.09797	0.42591
C	-4.5582	-1.86409	-0.47061	H	-4.52932	1.50543	-1.25154
C	-5.13905	-0.45826	-0.57541	H	-3.93699	0.18311	-2.23958
C	-4.12808	0.49262	-1.20743	H	-2.09977	1.17494	-0.90571
C	-2.81189	0.49859	-0.4319	H	-2.99209	0.88718	0.57481

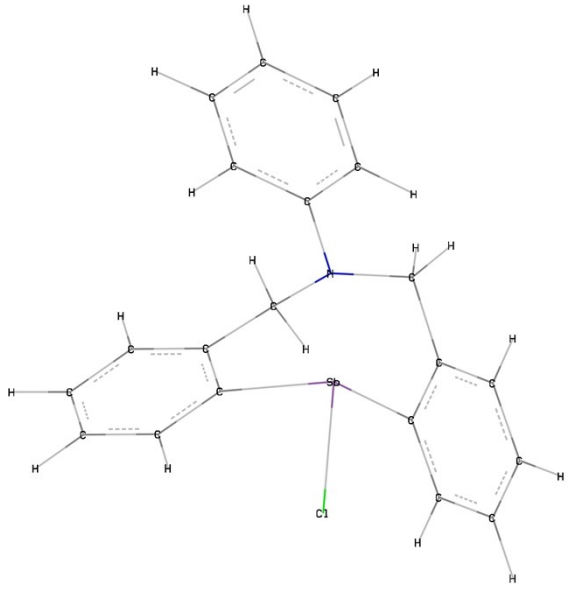
Table S4 Cartesian coordinates for the optimized structure of [**1a-F**]$^-$



	x	y	z		x	y	z
Sb	1.29047	0.51618	-1.17015	H	4.92655	-2.55229	0.87867
Cl	3.35682	1.88958	0.07668	H	3.44892	-4.34708	1.76812
N	-1.06459	-1.01278	0.39761	H	1.00589	-4.13589	1.50818
C	1.90752	-1.23942	-0.0156	H	-0.61917	-2.6545	-0.72518
C	3.28914	-1.37936	0.14573	H	-0.82146	-3.04632	0.98539

C	3.85138	-2.48497	0.76912	H	0.84828	3.4122	-0.70806
C	3.02997	-3.48516	1.26354	H	-0.29724	5.01124	0.75596
C	1.65804	-3.36369	1.11468	H	-1.63233	4.18286	2.68235
C	1.08576	-2.26755	0.46791	H	-1.85301	1.75039	3.04781
C	-0.41523	-2.29454	0.28731	H	0.05372	-0.6624	2.08833
C	0.10941	1.6593	0.28149	H	-1.66402	-0.4075	2.35228
C	0.22349	3.03711	0.09487	H	-2.27803	-1.49698	-1.15998
C	-0.40296	3.94851	0.93415	H	-3.5906	-1.31008	1.59025
C	-1.14468	3.48709	2.0108	H	-3.06516	-2.80458	0.82493
C	-1.26172	2.12094	2.21661	H	-4.63518	-2.43617	-1.04517
C	-0.65698	1.20527	1.35936	H	-5.50771	-2.42785	0.47917
C	-0.8537	-0.27511	1.61833	H	-6.23652	-0.55226	-1.00863
C	-2.39852	-1.00558	-0.1892	H	-5.52084	0.05001	0.47996
C	-3.43836	-1.7986	0.62155	H	-4.63054	1.31382	-1.45464
C	-4.77496	-1.87588	-0.11455	H	-4.09411	-0.17899	-2.20727
C	-5.29918	-0.48239	-0.45137	H	-2.18838	0.93061	-1.07883
C	-4.25981	0.30925	-1.24137	H	-3.08161	0.95113	0.4377
C	-2.93138	0.39324	-0.49139	F	-0.2042	-0.51253	-2.08814
H	3.93943	-0.58596	-0.19938				

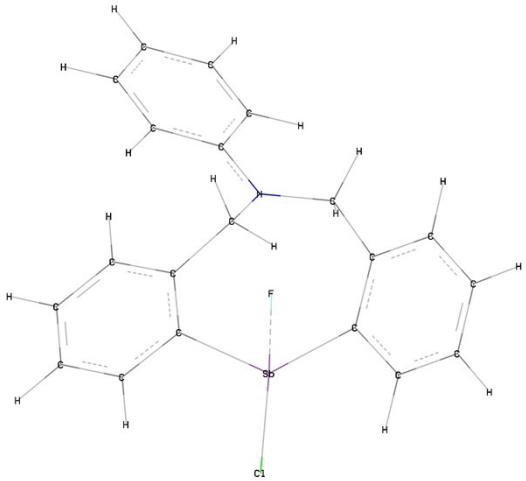
Table S5 Cartesian coordinates for the optimized structure of **2a**



	x	y	z		x	y	z
C	-0.17511	1.70347	0.30878	Cl	2.22267	1.79635	-2.01021
C	-0.16267	3.06755	0.03392	N	-0.8066	-1.06857	0.65979
C	-0.72821	3.97476	0.92083	Sb	0.54899	0.26246	-1.12426
C	-1.31487	3.52353	2.09381	H	0.30318	3.42958	-0.87377
C	-1.33158	2.16571	2.3767	H	-0.7117	5.03214	0.69306
C	-0.76662	1.25549	1.49121	H	-1.75964	4.22539	2.78645
C	-0.71144	-0.20932	1.8446	H	-1.78517	1.80884	3.29467

C	-2.11943	-1.24946	0.11845	H	0.25874	-0.40918	2.30054
C	-3.22949	-0.59174	0.64513	H	-1.47082	-0.47463	2.58606
C	-4.48341	-0.75517	0.06863	H	-3.1342	0.06931	1.49202
C	-4.65627	-1.56652	-1.03821	H	-5.32829	-0.23354	0.49756
C	-3.54908	-2.20426	-1.58229	H	-5.63406	-1.69137	-1.48161
C	-2.29593	-2.04297	-1.01982	H	-3.656	-2.8244	-2.46193
C	0.01598	-2.27855	0.8139	H	-1.44805	-2.51952	-1.49065
C	1.48667	-1.92435	0.83285	H	-0.1864	-2.95101	-0.01594
C	2.36433	-2.69903	1.58139	H	-0.25968	-2.8111	1.731
C	3.72141	-2.41018	1.59534	H	1.98185	-3.53091	2.16144
C	4.20134	-1.33336	0.86627	H	4.39733	-3.01904	2.18061
C	3.32575	-0.55025	0.12356	H	5.25682	-1.09627	0.87756
C	1.96356	-0.83153	0.101	H	3.70865	0.28958	-0.44108

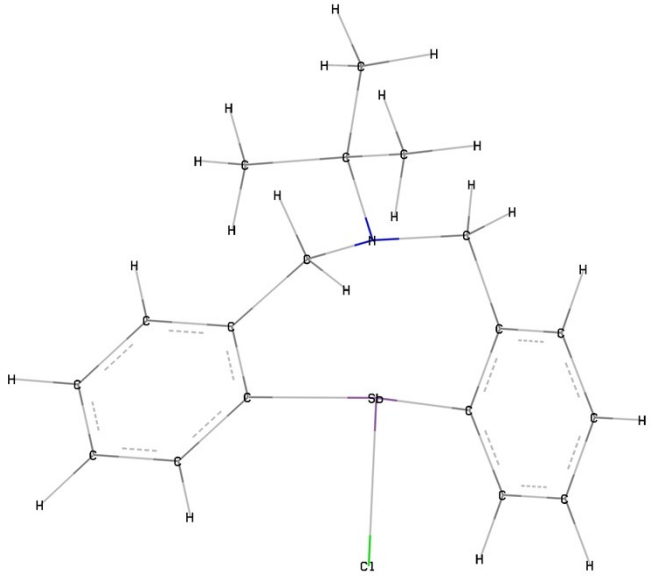
Table S6 Cartesian coordinates for the optimized structure of [**2a-F**]$^-$



	x	y	z		x	y	z
C	-0.13666	1.675	-0.08504	N	1.39814	-0.97377	-0.55659
C	-0.29458	3.03214	0.20237	Sb	-1.33999	0.41567	1.22409
C	0.28927	4.02459	-0.57012	H	-0.92818	3.32687	1.03156
C	1.03422	3.66955	-1.68354	H	0.14449	5.06668	-0.31514
C	1.20152	2.32772	-1.98347	H	1.48363	4.42788	-2.3122
C	0.64483	1.32444	-1.19091	H	1.7894	2.04424	-2.85092
C	0.88443	-0.11803	-1.60505	H	-0.05725	-0.53957	-1.95027
C	2.70912	-0.84766	-0.15603	H	1.56662	-0.12464	-2.46439
C	3.54377	0.16982	-0.66	H	3.15253	0.90558	-1.34165
C	4.86841	0.27107	-0.27128	H	5.46791	1.07504	-0.68054
C	5.42962	-0.6247	0.62739	H	6.46428	-0.5373	0.92943
C	4.61933	-1.63124	1.13345	H	5.02189	-2.34406	1.84275
C	3.29342	-1.7511	0.75544	H	2.70747	-2.54478	1.18824
C	0.69165	-2.18313	-0.15121	H	0.75908	-2.2484	0.93324
C	-0.77107	-2.2526	-0.50879	H	1.19559	-3.06095	-0.57758
C	-1.18161	-3.34407	-1.27374	H	-0.43374	-4.0445	-1.6272

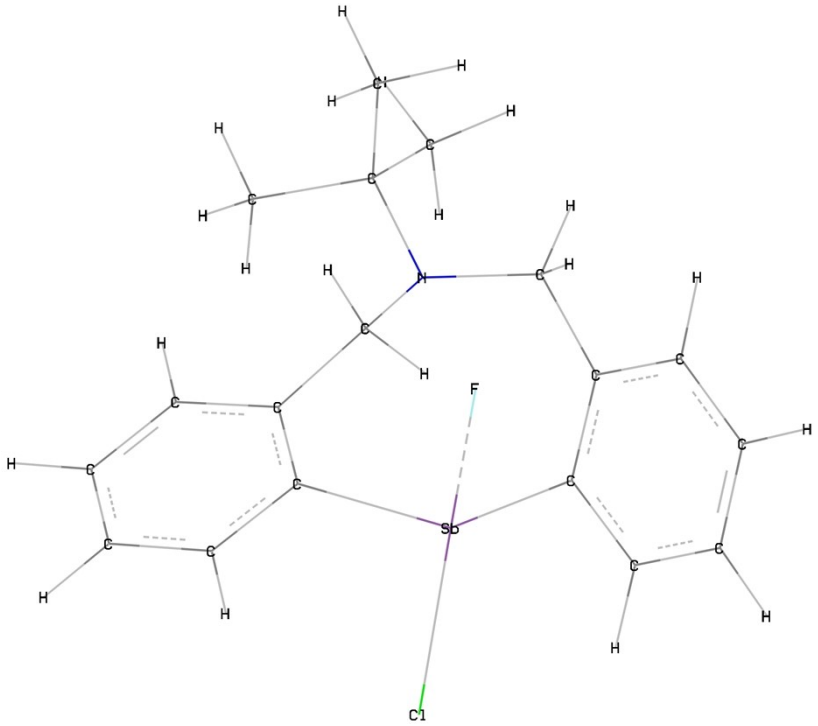
C	-2.5166	-3.55168	-1.58623	H	-2.80904	-4.40898	-2.17957
C	-3.46175	-2.64726	-1.13389	H	-4.51015	-2.78585	-1.36637
C	-3.06037	-1.54533	-0.38894	H	-3.80544	-0.82608	-0.07485
C	-1.72157	-1.31771	-0.06473	F	0.27237	-0.50769	2.01693
Cl	-3.38236	1.68978	-0.07669				

Table S7 Cartesian coordinates for the optimized structure of **3a**



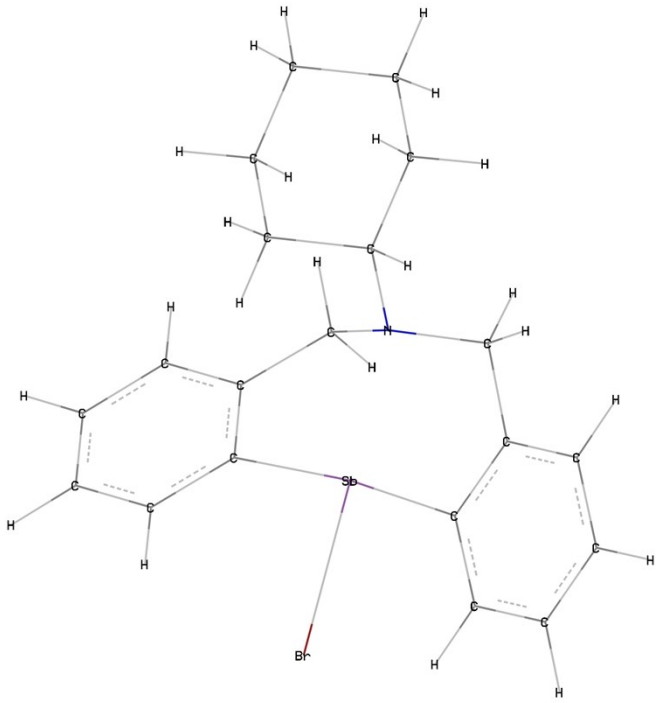
	x	y	z		x	y	z
C	-0.95894	-1.37713	0.39341	H	-0.853	-3.40926	-0.28787
C	-1.31273	-2.72321	0.41186	H	-2.50603	-4.24821	1.33206
C	-2.23936	-3.1998	1.33004	H	-3.54667	-2.69366	2.95595
C	-2.82198	-2.32974	2.2399	H	-2.9284	-0.30475	2.93732
C	-2.47471	-0.98714	2.22725	H	-1.92312	1.54715	1.81591
C	-1.54783	-0.5058	1.3092	H	-0.27189	1.01323	2.0325
C	-1.13184	0.94416	1.36402	H	-3.47487	1.03524	0.24167
C	-1.84289	2.15563	-0.69967	H	-2.77772	0.24842	-1.17494
C	-3.04661	1.21298	-0.74362	H	-3.81941	1.66179	-1.36691
C	-1.42246	2.43389	-2.14587	H	-1.14722	1.51732	-2.6641
C	-2.25652	3.48216	-0.05033	H	-0.59515	3.13731	-2.22094
C	0.44834	2.37357	0.23853	H	-2.26775	2.87807	-2.6714
C	1.67238	1.58767	0.64652	H	-2.52384	3.36449	0.99969
C	1.85885	0.27741	0.19876	H	-3.12993	3.87729	-0.56867
C	3.01557	-0.40376	0.56604	H	-1.46509	4.22797	-0.12343
C	3.97038	0.20308	1.37206	H	0.24783	3.15006	0.985
C	3.77671	1.50062	1.8212	H	0.65125	2.87953	-0.70465
C	2.62639	2.18687	1.46161	H	3.17182	-1.41783	0.22318
Cl	1.54456	-2.69797	-1.37403	H	4.86183	-0.34201	1.65245
N	-0.71895	1.49548	0.0567	H	4.51346	1.97523	2.45538
Sb	0.35722	-0.56639	-1.10494	H	2.4646	3.19699	1.81985

Table S8 Cartesian coordinates for the optimized structure of [**3a-F**]$^-$



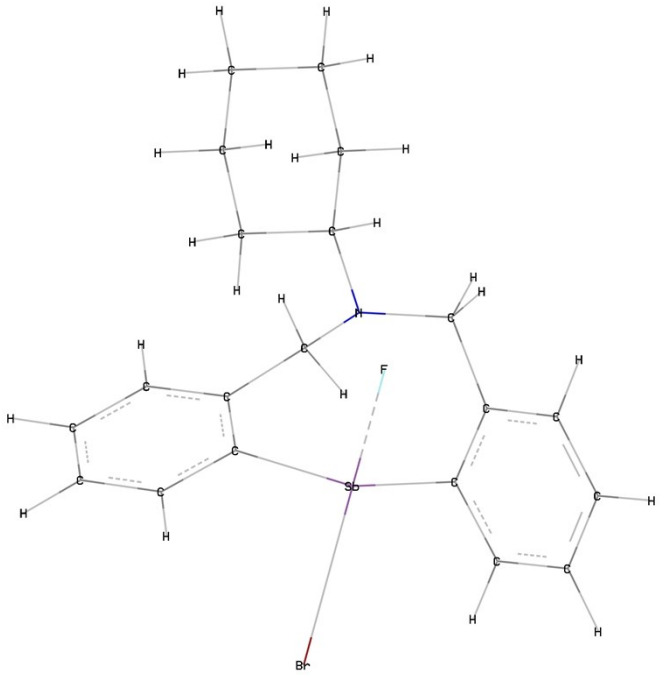
	x	y	z		x	y	z
C	0.46974	1.6196	0.12111	H	1.31993	4.89835	0.52264
C	0.50959	3.00159	-0.06979	H	2.69712	3.91263	2.34385
C	1.31149	3.83064	0.7019	H	2.65685	1.47337	2.70789
C	2.077	3.28187	1.719	H	2.11714	-0.62206	2.1208
C	2.04605	1.91159	1.92478	H	0.38958	-0.71446	1.86904
C	1.27067	1.07161	1.12855	H	3.74118	0.38223	0.573
C	1.32338	-0.42308	1.38694	H	3.0387	0.59957	-1.0319
C	2.8585	-1.42418	-0.28902	H	4.58343	-0.25951	-0.8356
C	3.59807	-0.08878	-0.39819	H	2.16807	-1.50582	-2.33399
C	2.85025	-2.05593	-1.6864	H	2.54694	-3.10319	-1.6595
C	3.64449	-2.34648	0.66275	H	3.86066	-2.02004	-2.09684
C	0.60138	-2.34329	-0.00296	H	3.74601	-1.90772	1.65627
C	-0.83417	-2.16122	0.43424	H	4.64955	-2.51647	0.27127
C	-1.62571	-1.05233	0.09369	H	3.15761	-3.31746	0.76307
C	-2.96697	-1.06107	0.48445	H	0.98457	-3.24411	0.50383
C	-3.52298	-2.11579	1.19639	H	0.57082	-2.55895	-1.07081
C	-2.73114	-3.1953	1.54872	H	-3.58575	-0.20431	0.25114
C	-1.39755	-3.20439	1.17083	H	-4.56648	-2.08107	1.48342
Cl	-2.7173	2.19816	0.42467	H	-3.14028	-4.02072	2.11817
N	1.475	-1.19776	0.17228	H	-0.76971	-4.04261	1.45123
Sb	-1.03707	0.6585	-1.13576	F	0.20401	-0.51532	-2.22813
H	-0.13467	3.4519	-0.81701				

Table S9 Cartesian coordinates for the optimized structure of **1b**



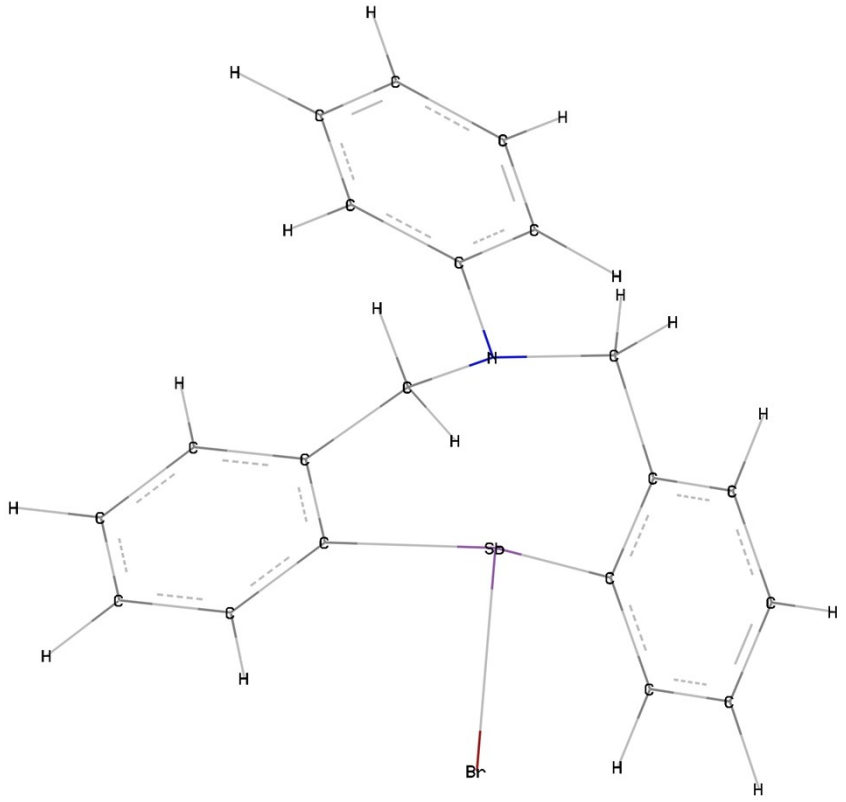
	x	y	z		x	y	z
Sb	0.68662	-0.201	-0.89538	H	-1.54048	2.95826	0.75853
Br	3.05099	-1.29769	-1.28401	H	-1.0972	2.64502	-0.91793
N	-1.29552	0.91245	0.2082	H	-2.28836	0.47318	2.03622
C	0.53881	2.52276	0.46203	H	-0.66512	1.12249	2.17864
C	1.46892	1.53625	0.12455	H	1.55646	-3.04528	0.3354
C	0.25296	-1.41611	0.83466	H	3.54227	0.98958	0.16127
C	-0.91722	2.32977	0.11453	H	0.22148	4.43649	1.37446
C	-1.28618	0.43529	1.60034	H	-3.13537	-1.15646	0.53397
C	-0.704	-0.95216	1.73909	H	-2.05815	-1.47575	-0.81092
C	0.80811	-2.67805	1.02556	H	-2.30428	0.86153	-1.58769
C	2.8113	1.74357	0.42177	H	-1.83113	-1.37928	3.51188
C	0.9532	3.6849	1.10161	H	0.863	-4.4473	2.23427
C	-2.90604	-0.86681	-0.49579	H	-0.8338	-3.61348	3.83541
C	-2.54179	0.61586	-0.54506	H	-3.49659	2.53299	-0.19614
C	-1.08731	-1.74678	2.81391	H	-3.99136	1.2674	0.91998
C	0.42257	-3.46831	2.10061	H	4.2703	3.05613	1.28287
C	-0.52711	-3.00187	2.99744	H	2.6113	4.78972	1.89235
C	-3.74115	1.47287	-0.12555	H	-5.80382	1.78171	-0.6752
C	3.22308	2.91097	1.05332	H	-4.73767	1.46591	-2.0311
C	2.29479	3.88315	1.39419	H	-3.86535	-0.94504	-2.42102
C	-4.95902	1.17315	-0.9999	H	-4.36305	-2.21864	-1.32292
C	-4.11895	-1.15749	-1.37785	H	-6.16757	-0.50733	-1.62155
C	-5.31748	-0.30849	-0.96775	H	-5.62428	-0.58397	0.04627

Table S10 Cartesian coordinates for the optimized structure of [**1b-F**]$^-$



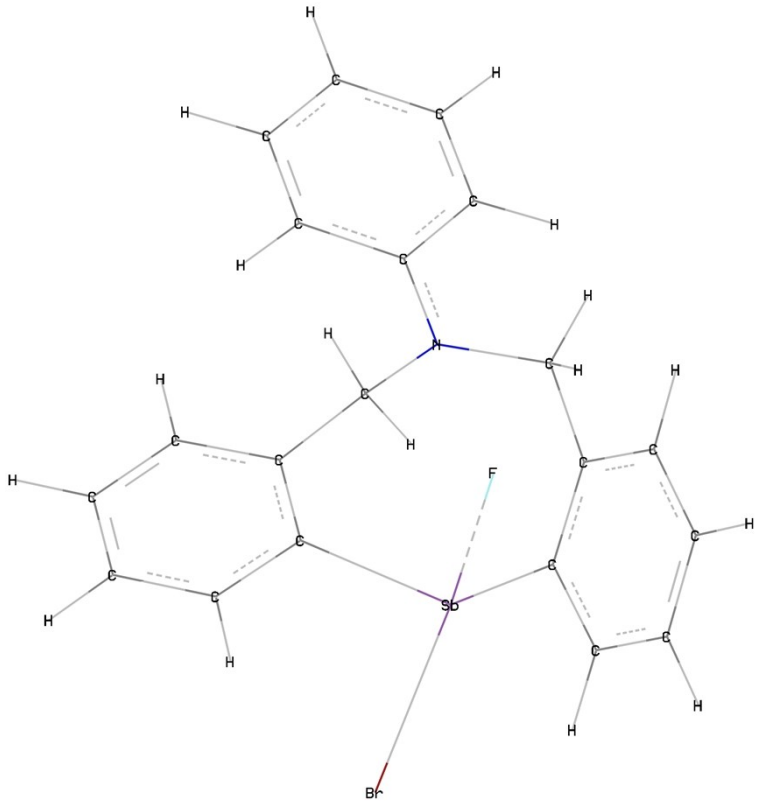
	x	y	z		x	y	z
Sb	1.04142	-0.15845	-1.1927	H	-1.39134	2.65024	-0.65776
Br	3.5503	-1.29291	0.09871	H	-1.97505	0.19393	2.36106
N	-1.50585	0.91521	0.40932	H	-0.32685	0.73593	2.0865
C	0.38826	2.52971	0.48295	H	1.11662	-3.09814	-0.78304
C	1.36489	1.66652	-0.03239	H	3.47653	1.38713	-0.28348
C	0.10131	-1.51386	0.24639	H	0.00905	4.3479	1.54565
C	-1.09826	2.29563	0.33474	H	-3.16826	-1.36143	0.44066
C	-1.16161	0.20752	1.61922	H	-2.30524	-1.17448	-1.08157
C	-0.72166	-1.21406	1.33607	H	-2.80382	1.20682	-1.12893
C	0.44444	-2.84835	0.03024	H	-1.79461	-1.98344	3.01975
C	2.70447	2.0471	0.09124	H	0.26996	-4.89283	0.65722
C	0.77592	3.70476	1.1277	H	-1.16854	-4.33615	2.60583
C	-3.12145	-0.77501	-0.48159	H	-3.77745	2.33704	0.8826
C	-2.82799	0.68964	-0.16435	H	-4.03618	0.76501	1.62884
C	-1.15637	-2.23332	2.17844	H	4.12907	3.48355	0.79724
C	-0.01286	-3.86688	0.8555	H	2.38343	4.98164	1.74838
C	-0.81172	-3.55604	1.9449	H	-6.12393	1.56037	0.54908
C	-3.97752	1.28546	0.6667	H	-5.2805	1.73555	-0.9815
C	3.08003	3.22899	0.71461	H	-4.38006	-0.38438	-2.181
C	2.10888	4.06372	1.24345	H	-4.65087	-1.9553	-1.44539
C	-5.31523	1.14709	-0.05848	H	-6.54282	-0.39098	-0.96116
C	-4.45219	-0.90553	-1.22081	H	-5.72205	-0.88406	0.51325
C	-5.60181	-0.30994	-0.41184	F	-0.60155	0.57834	-2.10112
H	-1.61218	2.93818	1.06953				

Table S11 Cartesian coordinates for the optimized structure of **2b**



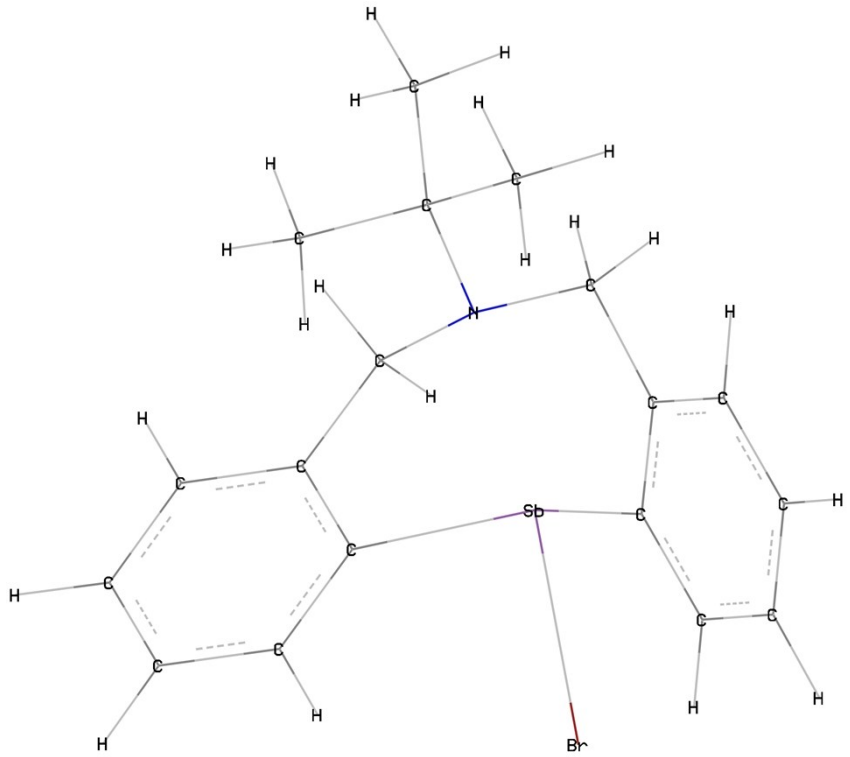
	x	y	z		x	y	z
Sb	-0.50573	0.18665	-0.86591	C	1.14799	3.17453	2.71674
Br	-2.68054	1.54549	-1.3566	C	0.33481	3.68997	1.71861
N	1.31004	-1.09994	0.46911	C	-0.17393	2.85163	0.73484
C	0.12099	1.49175	0.73723	H	-3.49484	-0.59217	0.14603
C	-1.5035	-1.37927	0.25945	H	-4.53362	-2.49416	1.30594
C	-2.87604	-1.41322	0.48271	H	-3.13683	-4.38386	2.08972
C	-3.46516	-2.48881	1.13659	H	-0.69638	-4.34019	1.71491
C	-2.68465	-3.54685	1.57492	H	1.27372	-3.08145	1.21419
C	-1.31407	-3.52304	1.36073	H	0.9799	-2.92187	-0.50816
C	-0.72223	-2.45397	0.6994	H	1.91866	-1.96451	-1.98389
C	0.77074	-2.46886	0.45777	H	3.99493	-1.6171	-3.2011
C	2.55028	-0.89742	-0.2189	H	5.83936	-0.29395	-2.19888
C	2.71779	-1.41483	-1.5074	H	5.53444	0.68014	0.05781
C	3.89242	-1.20466	-2.20657	H	3.47486	0.32997	1.29561
C	4.92357	-0.45986	-1.64926	H	2.09762	-0.72823	2.40487
C	4.75207	0.08076	-0.38772	H	0.36463	-0.97939	2.30078
C	3.57797	-0.12997	0.32553	H	2.08309	1.41223	3.50608
C	1.21094	-0.50272	1.80533	H	1.54857	3.8234	3.48394
C	0.94269	0.97936	1.74354	H	0.09638	4.74498	1.70212
C	1.44944	1.82076	2.72675	H	-0.81633	3.26276	-0.03325

Table S12 Cartesian coordinates for the optimized structure of [**2b-F**]$^-$



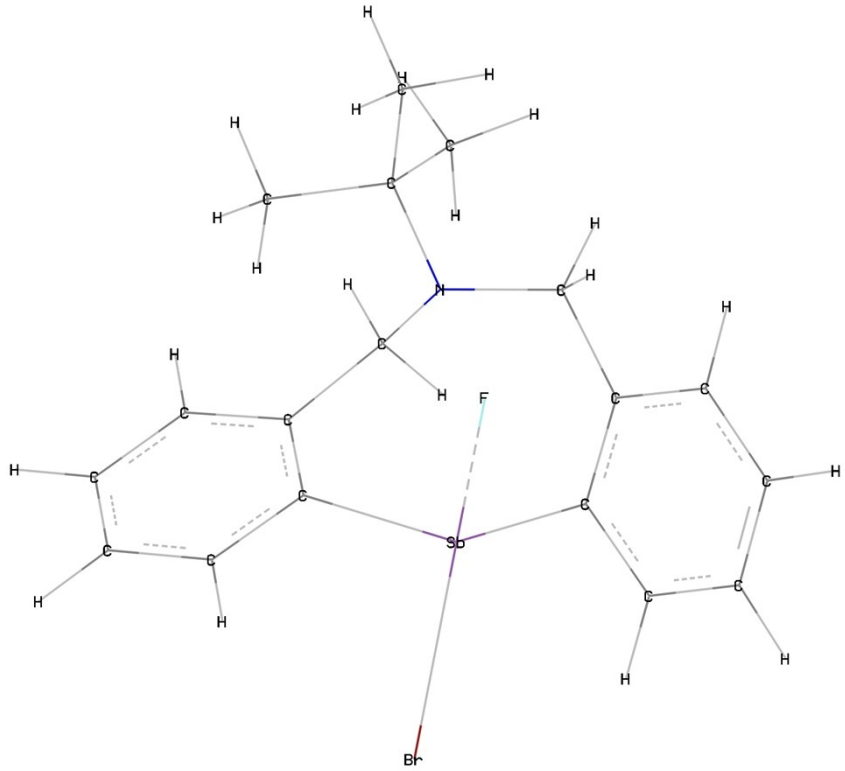
	x	y	z		x	y	z
Sb	1.06125	-0.06964	-1.24854	C	0.09426	-3.9192	0.51852
Br	3.52528	-1.11716	0.07716	C	0.49204	-2.83492	-0.24852
N	-1.83282	0.81498	0.5679	H	3.31153	1.5648	0.0148
C	0.11342	-1.52724	0.06088	H	3.69453	3.59936	1.32079
C	1.17249	1.6894	0.05211	H	1.75746	4.90108	2.18299
C	2.45912	2.13959	0.35294	H	-0.53134	4.14604	1.6624
C	2.6808	3.28684	1.1047	H	-1.9897	2.90652	0.6264
C	1.60402	4.01226	1.58394	H	-1.44244	2.20673	-0.90311
C	0.31784	3.58462	1.29032	H	-3.41013	2.16083	-1.14528
C	0.08492	2.44564	0.52063	H	-5.66159	1.57446	-1.78562
C	-1.34969	2.13413	0.17914	H	-6.76572	-0.46169	-0.88359
C	-3.10913	0.47312	0.17722	H	-5.49497	-1.89614	0.70097
C	-3.84713	1.27349	-0.71839	H	-3.2365	-1.34047	1.34768
C	-5.13675	0.93314	-1.08818	H	-1.84553	-0.0621	2.47151
C	-5.75837	-0.20219	-0.58828	H	-0.31812	0.62612	1.95438
C	-5.04482	-0.99805	0.29608	H	-1.68183	-2.24324	2.84562
C	-3.75332	-0.67618	0.67632	H	-0.98595	-4.53522	2.27226
C	-1.17645	0.05309	1.60972	H	0.40859	-4.91909	0.24842
C	-0.69943	-1.32393	1.18076	H	1.15416	-3.01039	-1.08908
C	-1.06723	-2.41448	1.96743	F	-0.66832	0.57647	-2.03209
C	-0.68099	-3.70557	1.64712				

Table S13 Cartesian coordinates for the optimized structure of **3b**



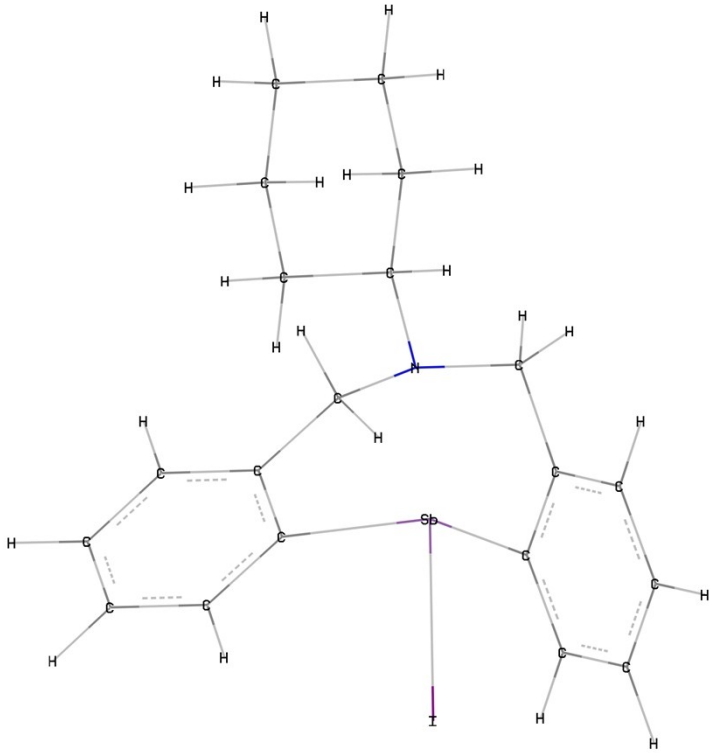
	x	y	z		x	y	z
Sb	0.52654	-0.10293	-0.90348	H	1.6575	-2.88302	0.24059
Br	3.08624	-0.71511	-0.85839	H	2.83743	1.47734	0.73948
N	-1.85505	0.5395	-0.13075	H	-1.2405	4.13218	1.5529
C	0.73181	1.63893	0.36242	H	-2.55622	2.41447	0.59367
C	-0.41526	2.40397	0.59096	H	-1.82609	2.43905	-1.00559
C	0.74737	-2.71887	0.80266	H	-2.46795	-2.14097	2.84236
C	1.94079	2.05815	0.90939	H	-2.96609	-0.21741	1.52416
C	0.01723	-1.54943	0.61127	H	-1.50313	0.6561	1.9187
C	-1.14796	-1.3472	1.35114	H	0.90727	-4.57826	1.85684
C	-0.34179	3.5556	1.36672	H	2.95812	3.52242	2.09756
C	-1.74108	2.00252	-0.01112	H	-1.15954	-4.20738	3.17177
C	-1.562	-2.3055	2.26981	H	0.9159	4.86369	2.50718
C	-1.9291	-0.06289	1.2169	H	-2.60459	1.59869	-2.61933
C	0.32945	-3.67401	1.7202	H	-3.49058	0.17411	-3.12283
C	2.01058	3.21444	1.67605	H	-1.75248	0.0673	-2.85049
C	-0.82738	-3.46674	2.45662	H	-2.14716	-1.89264	-1.28017
C	-2.97357	0.10762	-1.04534	H	-3.84103	-1.72143	-1.74914
C	0.86835	3.96614	1.90522	H	-3.40375	-1.79543	-0.04566
C	-2.67381	0.5202	-2.4895	H	-4.56202	0.52029	0.41016
C	-3.09257	-1.41704	-1.01817	H	-5.10673	0.31734	-1.24882
C	-4.31151	0.73138	-0.62933	H	-4.31201	1.81188	-0.77202

Table S14 Cartesian coordinates for the optimized structure of [**3b-F**]$^-$



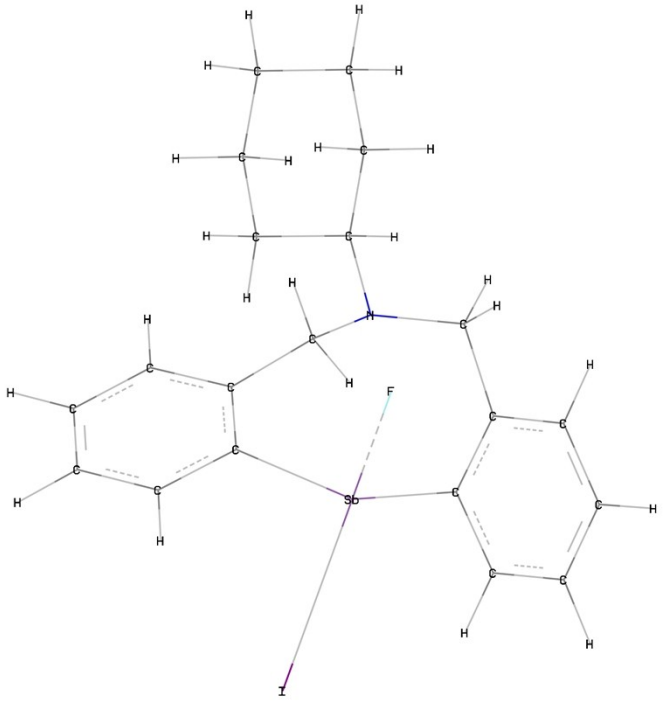
	x	y	z		x	y	z
Sb	0.85511	0.00152	-1.22222	H	2.75203	1.97343	0.06457
Br	3.37385	-0.64975	0.32076	H	-1.48699	3.96156	1.54502
N	-2.15195	0.39813	0.23175	H	-2.69424	2.41348	0.66216
C	0.61861	1.7678	0.03989	H	-2.10167	2.06725	-0.964
C	-0.58688	2.35397	0.45741	H	-1.79151	-2.55503	2.71098
C	0.68361	-2.81612	-0.20075	H	-2.35265	-0.44266	2.1811
C	1.81158	2.41914	0.36247	H	-0.89242	0.46906	1.87547
C	0.06816	-1.58853	0.04699	H	0.90761	-4.87948	0.34264
C	-0.84632	-1.50904	1.10195	H	2.78006	4.0726	1.32298
C	-0.55162	3.53186	1.20478	H	-0.67837	-4.70742	2.24981
C	-1.95591	1.82885	0.08954	H	0.63789	5.07571	2.10004
C	-1.08554	-2.63201	1.8901	H	-4.10049	1.58497	-1.4844
C	-1.59452	-0.22726	1.41535	H	-4.7442	0.01001	-1.925
C	0.41354	-3.9421	0.56401	H	-3.02889	0.38623	-2.23623
C	1.83336	3.6032	1.08746	H	-2.7121	-1.90708	-0.99376
C	-0.46809	-3.84528	1.62916	H	-4.46828	-1.9039	-0.71635
C	-3.49516	-0.06312	-0.17526	H	-3.35793	-2.08878	0.639
C	0.64254	4.16194	1.51878	H	-4.41404	-0.10962	1.815
C	-3.85957	0.52305	-1.54468	H	-5.56125	0.01286	0.48366
C	-3.50363	-1.58692	-0.31609	H	-4.62275	1.4265	0.96182
C	-4.58268	0.34361	0.83735	F	-0.81971	0.44077	-2.24599
H	1.42718	-2.88832	-0.98688				

Table S15 Cartesian coordinates for the optimized structure of **1c**



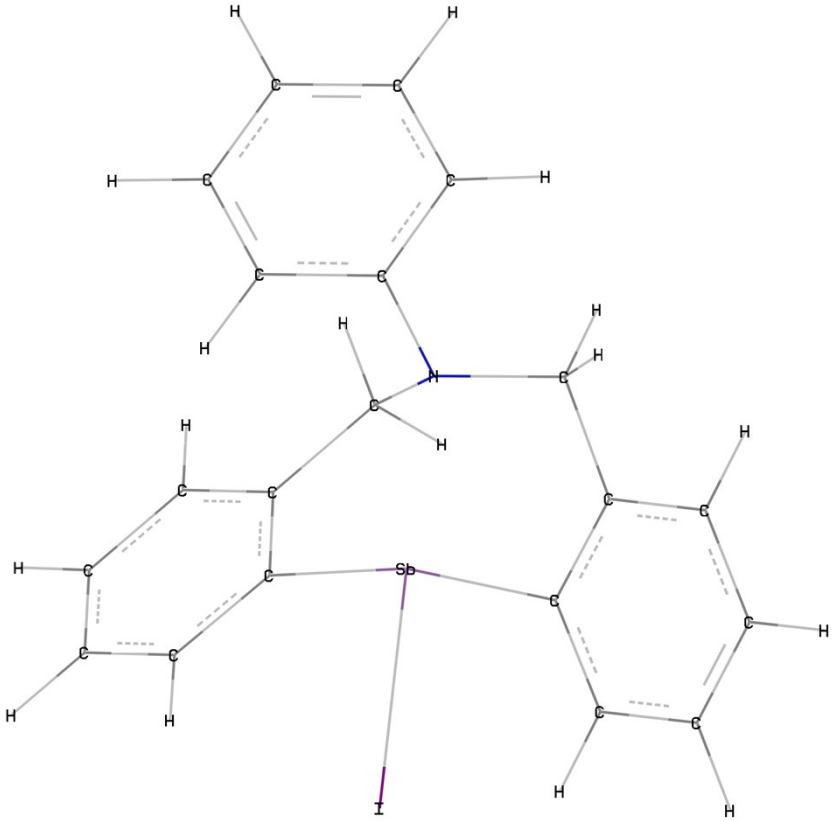
	x	y	z		x	y	z
Sb	0.50752	-0.09971	-0.73087	H	-0.68287	4.62233	1.03727
I	3.19944	-1.01755	-0.94765	H	3.11218	1.52137	0.44918
N	-1.67167	0.85386	0.10861	H	-2.51349	0.52482	-1.7429
C	-0.06317	2.69068	0.34547	H	-2.23302	-1.18736	3.56072
C	1.00138	1.79964	0.18281	H	1.5729	-2.72871	0.8278
C	0.07019	-1.21452	1.06861	H	3.48773	3.74781	1.41832
C	0.15318	3.9463	0.90053	H	-3.28428	-1.38851	0.49554
C	2.27612	2.19707	0.57089	H	-2.06856	-1.68948	-0.73028
C	-2.80822	0.34325	-0.70179	H	-2.19565	2.89483	0.43272
C	-1.39608	-1.52661	2.9608	H	-1.5719	2.48982	-1.16505
C	0.73375	-2.38675	1.41953	H	-6.17874	-1.29998	-1.9282
C	-1.00645	-0.78749	1.84938	H	-5.77222	-1.16673	-0.22542
C	2.49019	3.45668	1.1174	H	-2.75621	0.46262	1.89439
C	-3.00371	-1.16281	-0.53753	H	-1.23182	1.30825	2.08948
C	-1.45015	2.2923	-0.09551	H	-1.03823	-3.25941	4.1701
C	-5.41487	-0.94404	-1.23584	H	1.59124	5.31238	1.71404
C	-1.72366	0.50507	1.53702	H	-6.15982	1.08885	-1.17923
C	-0.7258	-2.6906	3.30459	H	-4.95558	0.78998	-2.41823
C	1.4292	4.33374	1.28257	H	0.86835	-4.03076	2.78737
C	-5.22688	0.5619	-1.38266	H	-3.78248	-1.52183	-2.51171
C	0.34103	-3.12181	2.53058	H	-4.22191	-2.74742	-1.33692
C	-4.09702	-1.67314	-1.4745	H	-4.44016	0.93894	0.58455
C	-4.12838	1.08162	-0.45486	H	-4.0015	2.15343	-0.60905

Table S16 Cartesian coordinates for the optimized structure of [**1c-F**]$^-$



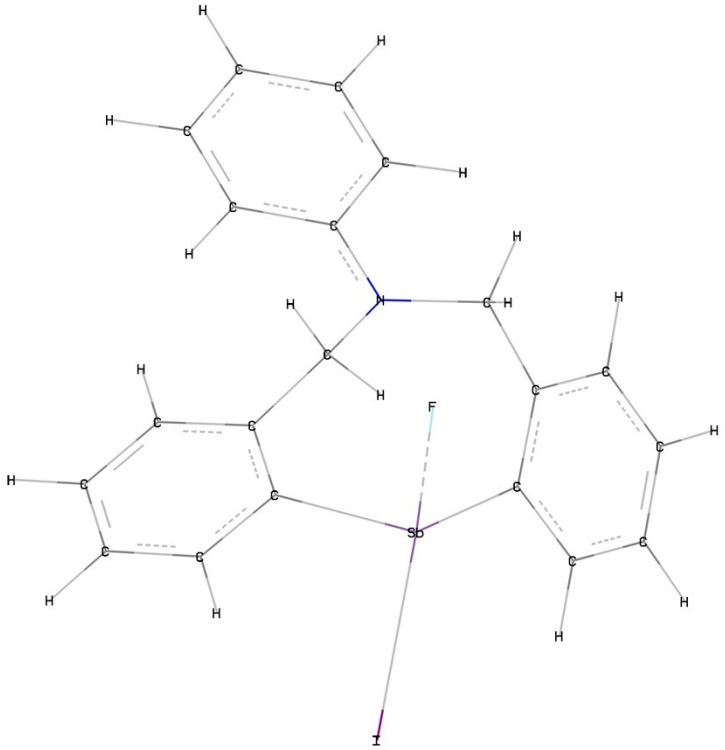
	x	y	z		x	y	z
Sb	0.70146	0.06758	-1.21727	H	2.94967	1.87913	-0.3378
I	3.69572	-0.89525	0.07666	H	-3.25269	0.93923	-1.1159
N	-1.9168	0.80521	0.41446	H	-1.80569	-2.12429	3.01854
C	-0.23974	2.63869	0.49731	H	1.17853	-2.83818	-0.82532
C	0.82291	1.90392	-0.04539	H	3.37033	4.01564	0.77371
C	-0.023	-1.40348	0.22539	H	-3.29445	-1.64743	0.46695
C	0.01825	3.84257	1.15218	H	-2.47362	-1.3695	-1.06376
C	2.11105	2.43562	0.06199	H	-2.26386	2.78323	1.12696
C	-3.20861	0.42507	-0.15035	H	-2.04516	2.56736	-0.61022
C	-1.1506	-2.28519	2.16865	H	-6.77276	-1.10018	-0.90874
C	0.49059	-2.68001	-0.00237	H	-5.88616	-1.48257	0.56022
C	-0.86525	-1.21577	1.3253	H	-2.2915	0.00961	2.35727
C	2.35662	3.64335	0.70048	H	-0.72624	0.76132	2.09443
C	-3.32672	-1.06566	-0.45909	H	-0.87469	-4.37073	2.59008
C	-1.68893	2.22826	0.36708	H	1.47691	5.28792	1.77011
C	-5.84381	-0.90337	-0.36848	H	-6.5787	0.8966	0.58761
C	-1.48487	0.13437	1.61911	H	-5.77573	1.16221	-0.95143
C	-0.6348	-3.54963	1.92615	H	0.59977	-4.72912	0.62235
C	1.30295	4.35138	1.25502	H	-4.6379	-0.84043	-2.14876
C	-5.73159	0.57954	-0.02516	H	-4.70965	-2.42797	-1.40287
C	0.1836	-3.75104	0.82599	H	-4.40223	0.36637	1.65335
C	-4.63801	-1.36062	-1.18538	H	-4.3423	1.95262	0.89524
C	-4.41455	0.88309	0.68757	F	-1.00815	0.57558	-2.12011
H	-0.81135	4.38744	1.58944				

Table S17 Cartesian coordinates for the optimized structure of **2c**



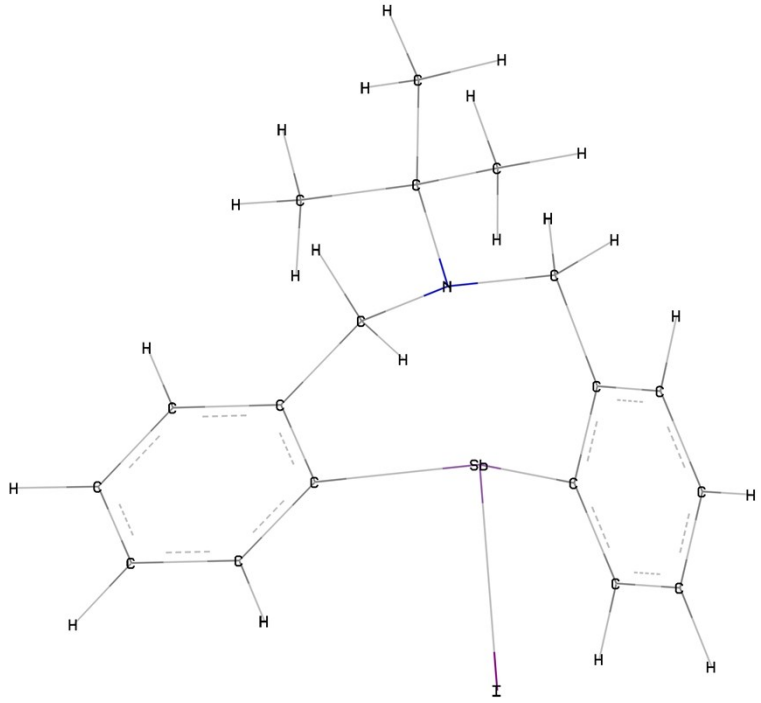
	x	y	z		x	y	z
Sb	-0.35086	-0.1136	-0.74293	C	-1.18624	4.29369	1.38112
I	-3.0353	-0.93526	-1.07089	C	-2.26643	3.4526	1.16593
N	1.88064	0.80336	0.2272	C	-2.07579	2.20737	0.57795
C	-0.02489	-1.20683	1.09546	H	-1.54465	-2.6892	0.77647
C	-0.80622	1.78885	0.19691	H	-1.02994	-3.95853	2.81238
C	-0.74455	-2.35284	1.42271	H	0.78599	-3.20096	4.32097
C	-0.45962	-3.06999	2.57718	H	2.08764	-1.18393	3.75042
C	0.55587	-2.64683	3.42094	H	1.33049	1.29614	2.17531
C	1.28519	-1.5123	3.10007	H	2.81553	0.35459	2.06769
C	1.00313	-0.79021	1.94526	H	2.51606	-1.77129	0.22416
C	1.80601	0.45847	1.66262	H	4.39056	-2.83713	-0.92546
C	2.99874	0.21513	-0.44973	H	5.96548	-1.48725	-2.28509
C	3.19777	-1.16497	-0.35519	H	5.62976	0.9604	-2.44787
C	4.25931	-1.76676	-1.00846	H	3.78678	2.04116	-1.28597
C	5.14102	-1.01284	-1.77161	H	1.73905	2.37782	-1.11279
C	4.94954	0.35445	-1.86466	H	2.42322	2.85223	0.44455
C	3.89144	0.97019	-1.20691	H	0.93704	4.53383	1.18015
C	1.65859	2.22994	-0.03392	H	-1.32981	5.26053	1.84438
C	0.27874	2.64552	0.41095	H	-3.26135	3.75983	1.45934
C	0.08614	3.8856	1.00655	H	-2.92842	1.56074	0.41837

Table S18 Cartesian coordinates for the optimized structure of [**2c-F**]$^-$



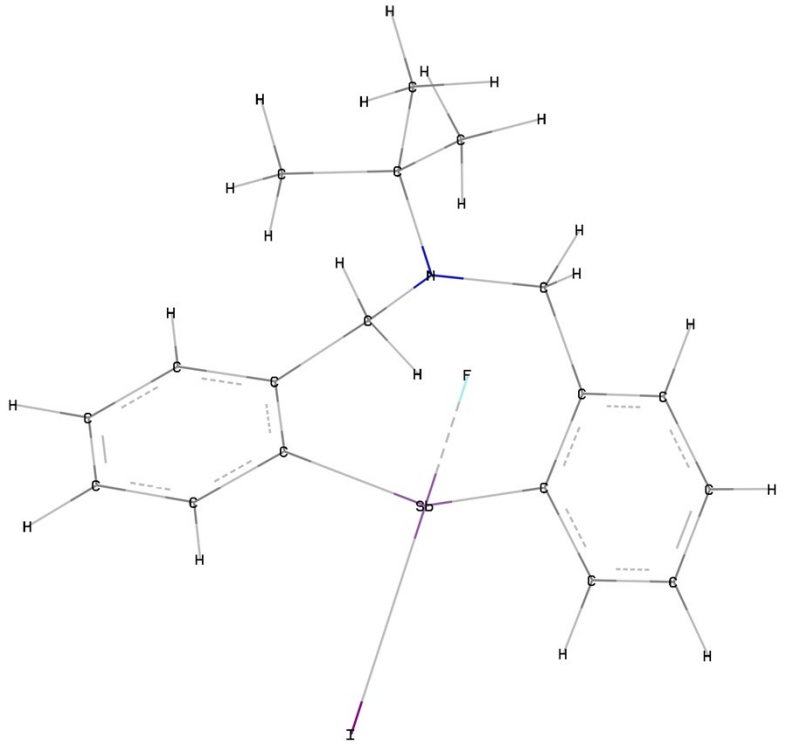
	x	y	z		x	y	z
Sb	-0.70506	0.13352	-1.26847	C	-2.01774	3.61638	1.08285
I	-3.61131	-0.77456	0.05219	C	-1.90151	2.46124	0.31933
N	2.21182	0.68138	0.58333	H	-1.14297	-2.77648	-1.12679
C	0.03878	-1.42528	0.05094	H	-0.65023	-4.75923	0.21825
C	-0.66273	1.88092	0.04344	H	0.74014	-4.54246	2.269
C	-0.48139	-2.6795	-0.27323	H	1.68934	-2.34848	2.86325
C	-0.22605	-3.8036	0.49727	H	0.68841	0.65643	1.97399
C	0.54625	-3.68216	1.64109	H	2.13025	-0.20213	2.48357
C	1.07398	-2.44532	1.97444	H	3.35427	-1.63465	1.33019
C	0.84848	-1.31838	1.18633	H	5.53925	-2.43395	0.68548
C	1.47695	-0.00704	1.62416	H	6.97896	-1.12481	-0.86236
C	3.44653	0.20363	0.19554	H	6.12493	1.04267	-1.72807
C	3.94967	-1.02114	0.67564	H	3.95207	1.8728	-1.08788
C	5.19866	-1.48236	0.29633	H	2.00834	2.14022	-0.85884
C	6.00576	-0.75693	-0.56777	H	2.59925	2.74299	0.69454
C	5.52354	0.45218	-1.0479	H	1.25494	4.12763	1.71643
C	4.27874	0.93141	-0.67845	H	-0.95387	5.11074	2.20221
C	1.88716	2.05444	0.21988	H	-2.99758	4.03101	1.28178
C	0.48826	2.51274	0.54287	H	-2.8031	1.98867	-0.04869
C	0.35985	3.66158	1.32114	F	1.07234	0.59536	-2.03923
C	-0.88133	4.21772	1.59436				

Table S19 Cartesian coordinates for the optimized structure of **3c**



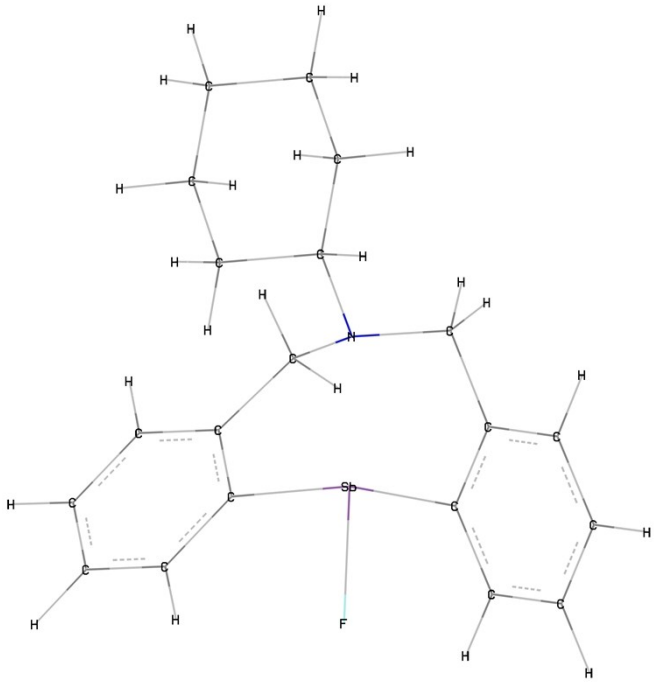
	x	y	z		x	y	z
Sb	0.32507	-0.0185	-0.79208	H	-2.2071	3.9911	1.34439
I	3.153	-0.30545	-0.58451	H	-2.69971	-2.34819	2.7487
N	-2.17583	0.31211	-0.25107	H	-3.1824	2.09552	0.3296
C	0.18584	1.75931	0.43833	H	-2.30822	2.17358	-1.19438
C	-0.11986	-1.49555	0.71776	H	2.24429	1.89097	1.03139
C	-1.0691	2.36916	0.52873	H	-2.84935	1.19926	-2.83061
C	-1.22608	3.53681	1.26721	H	-3.47781	-0.34932	-3.35424
C	-1.73365	-2.41021	2.26037	H	-1.77271	-0.19921	-2.93397
C	-2.26553	1.77971	-0.17958	H	-0.27353	5.02667	2.47845
C	1.26582	2.34829	1.08882	H	1.69285	-2.62982	0.52299
C	-3.14174	-0.29095	-1.24008	H	-2.03672	-2.16422	-1.33651
C	-2.77675	0.12549	-2.66794	H	-3.69157	-2.23728	-1.94833
C	-1.36191	-1.42641	1.35062	H	-3.39642	-2.21102	-0.21324
C	-0.14164	4.11778	1.9069	H	-4.89311	-0.06777	0.0626
C	0.72522	-2.56418	1.00313	H	-5.2573	-0.38002	-1.62834
C	-3.05642	-1.81643	-1.16951	H	-4.71649	1.21947	-1.13747
C	-4.5827	0.15276	-0.95857	H	1.95738	3.95899	2.3201
C	1.10571	3.51965	1.81818	H	-3.31794	-0.54295	1.33253
C	-2.28727	-0.25949	1.1071	H	-2.02127	0.52713	1.81501
C	-0.88273	-3.46767	2.54349	H	-1.18278	-4.22895	3.25108
C	0.34869	-3.54581	1.91051	H	1.01781	-4.36959	2.11976

Table S20 Cartesian coordinates for the optimized structure of [**3c-F**]$^-$



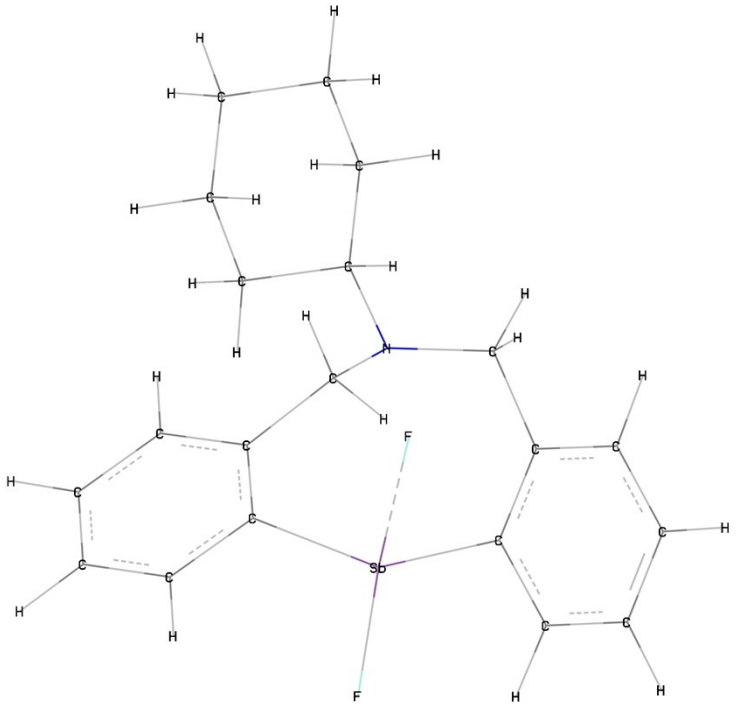
	x	y	z		x	y	z
Sb	0.46452	0.14194	-1.27129	H	-1.71528	-2.71727	2.7318
I	3.4681	-0.29075	0.21585	H	-3.26103	2.10749	0.76384
N	-2.49701	0.1796	0.26809	H	-2.69501	1.86529	-0.88963
C	0.07876	1.85492	0.01961	H	2.17873	2.29421	-0.02338
C	-0.06453	-1.52835	0.02141	H	-4.62456	1.14568	-1.37546
C	-1.16916	2.29924	0.48458	H	-5.08565	-0.4886	-1.8269
C	-1.23759	3.46441	1.24802	H	-3.44064	0.09688	-2.18143
C	-1.02705	-2.70465	1.89273	H	-0.19211	5.11442	2.13323
C	-2.48102	1.62602	0.15206	H	1.42415	-2.64474	-1.04896
C	1.20502	2.6264	0.31442	H	-2.803	-2.15367	-0.99059
C	-3.78561	-0.43665	-0.11505	H	-4.53616	-2.37719	-0.66369
C	-4.25837	0.12217	-1.46247	H	-3.37027	-2.44084	0.65604
C	-0.95364	-1.56223	1.10054	H	-4.64432	-0.63224	1.89408
C	-0.10774	4.21449	1.53685	H	-5.8282	-0.62046	0.59046
C	0.69779	-2.66638	-0.24421	H	-5.05322	0.88492	1.08043
C	-3.60758	-1.94689	-0.28473	H	2.02032	4.35835	1.27781
C	-4.88773	-0.18282	0.93076	H	-2.56201	-0.69785	2.21058
C	1.12231	3.79422	1.06138	H	-1.22901	0.38764	1.89488
C	-1.848	-0.38488	1.43696	H	-0.34459	-4.70813	2.24113
C	-0.26415	-3.82845	1.61488	H	1.20282	-4.67984	0.29575
C	0.59524	-3.81488	0.52788	F	-1.25561	0.37315	-2.2541
H	-2.20249	3.78692	1.62248				

Table S21 Cartesian coordinates for the optimized structure of **1d**



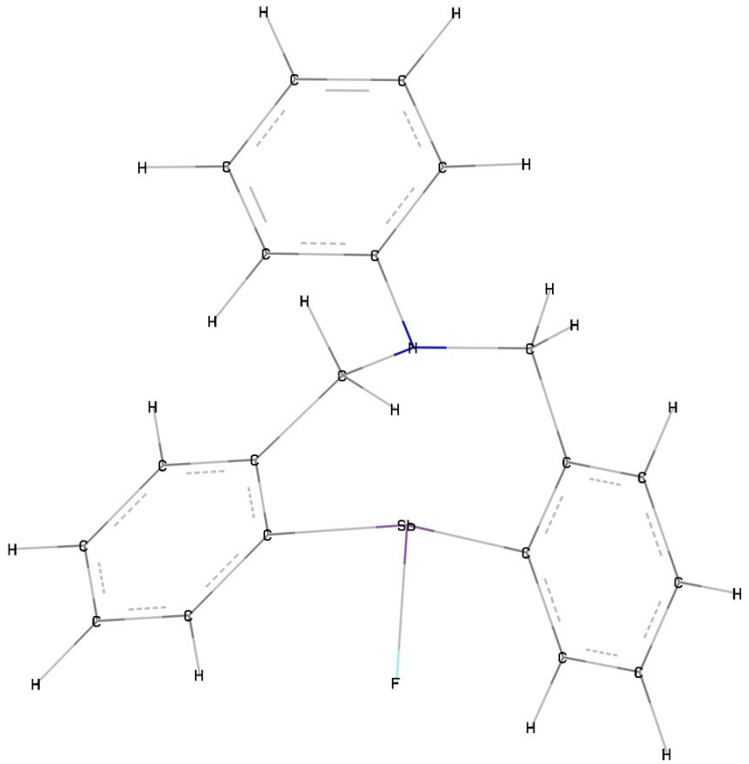
	x	y	z		x	y	z
Sb	0.8103	0.33747	-1.30922	H	-2.91717	0.80712	0.58249
F	2.3668	1.40888	-1.85652	H	-2.12933	0.99263	-0.97177
N	-0.71108	-0.87727	0.36364	H	1.78617	-3.63513	1.91115
C	2.0701	-0.95169	-0.14519	H	-1.26067	2.01361	3.18864
C	0.35797	1.77334	0.21857	H	0.61195	5.09263	0.88073
C	1.47268	-1.98534	0.5754	H	-4.59331	1.12708	-1.19892
C	-2.76576	0.32629	-0.38858	H	-3.96307	-0.2515	-2.081
C	2.25558	-2.84377	1.33809	H	-1.93265	-1.46453	-1.18792
C	-0.34579	1.37825	1.35451	H	-0.2773	-2.76533	-0.38331
C	-0.71188	2.32386	2.30644	H	-0.37718	-2.72698	1.37494
C	0.34058	4.0538	1.01386	H	-2.50837	-2.94641	0.71511
C	-4.11886	0.1531	-1.07611	H	-3.13308	-1.56989	1.61293
C	-2.07863	-1.02408	-0.19354	H	-4.97168	-2.79934	0.51521
C	-0.02485	-2.17045	0.49992	H	-4.19488	-2.6206	-1.04673
C	-2.98187	-1.97027	0.60557	H	-5.97528	-0.92366	-0.80459
C	-4.34005	-2.13544	-0.0763	H	-5.24958	-0.34159	0.68444
C	-5.02369	-0.78902	-0.28874	H	1.27093	3.41601	-0.81174
C	0.70282	3.11244	0.05895	H	-0.66483	4.38776	2.88066
C	-0.37351	3.65851	2.13646	H	5.30692	-1.53839	0.67561
C	4.23275	-1.66518	0.64672	H	3.91131	0.00602	-0.6686
C	3.45174	-0.79868	-0.1086	H	4.23943	-3.35782	1.96607
C	3.63458	-2.68713	1.37048	H	0.18906	-0.48883	2.1972
C	-0.63333	-0.08559	1.60213	H	-1.54013	-0.20056	2.20273

Table S22 Cartesian coordinates for the optimized structure of [**1d-F**]$^-$



	x	y	z		x	y	z
Sb	1.36798	0.73217	-1.208	H	-2.14132	0.8347	-1.03913
F	2.8691	1.80588	-0.22817	H	1.48793	-3.90409	1.52954
N	-0.86789	-1.03746	0.39297	H	-1.78518	1.62821	3.11389
C	2.11541	-0.95113	-0.02496	H	-0.39279	5.04364	0.94741
C	0.11925	1.72894	0.30433	H	-4.61301	1.03519	-1.39238
C	1.39793	-2.05923	0.44801	H	-3.95977	-0.38676	-2.18906
C	-2.83814	0.22818	-0.46226	H	-2.02868	-1.58037	-1.1826
C	2.06241	-3.06659	1.14839	H	-0.23272	-2.54657	-0.81549
C	-0.60205	1.2014	1.38219	H	-0.42441	-3.06898	0.86589
C	-1.22612	2.05667	2.28789	H	-2.70429	-3.00695	0.76062
C	-0.45653	3.97041	1.07915	H	-3.34867	-1.58552	1.57312
C	-4.15991	0.05863	-1.20912	H	-5.17392	-2.82155	0.43102
C	-2.19233	-1.1301	-0.19863	H	-4.30906	-2.71177	-1.09421
C	-0.08639	-2.23758	0.22289	H	-6.0596	-0.96623	-0.99463
C	-3.16122	-2.02982	0.58912	H	-5.38494	-0.353	0.5088
C	-4.49028	-2.19392	-0.1463	H	0.76711	3.55239	-0.61703
C	-5.12714	-0.8377	-0.43928	H	-1.66747	4.0804	2.85289
C	0.18091	3.1185	0.18612	H	5.21405	-1.85601	1.08515
C	-1.16457	3.4345	2.14356	H	4.04482	-0.03724	-0.0945
C	4.14747	-1.9252	0.90847	H	3.92266	-3.81297	1.91545
C	3.4895	-0.9085	0.22807	H	0.2032	-0.6309	2.10053
C	3.42964	-3.01606	1.37209	H	-1.52869	-0.47893	2.33716
C	-0.71669	-0.29547	1.61516	F	-0.07775	-0.48696	-2.08697
H	-3.02629	0.74922	0.48196				

Table S23 Cartesian coordinates for the optimized structure of **2d**

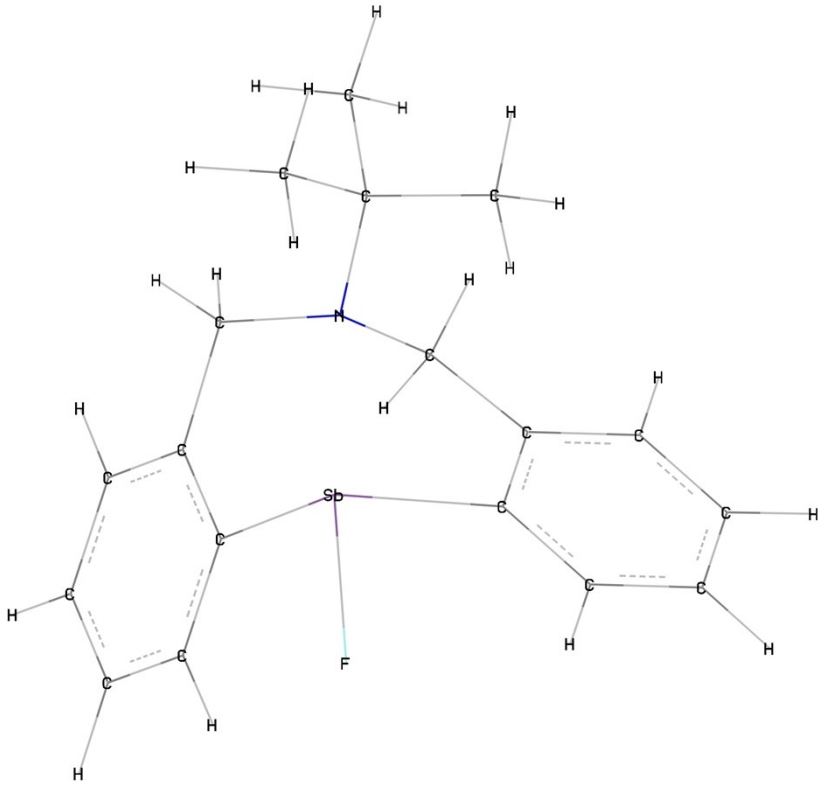


	x	y	z		x	y	z
C	1.89092	-0.30952	0.02112	H	1.05095	2.67688	1.36927
C	-1.24289	2.50531	-0.35331	H	1.34791	2.61696	-0.36212
C	-0.8277	0.85122	1.46664	H	-1.61178	3.55423	1.5373
C	-1.56452	-0.44498	1.22625	H	-2.07168	4.44355	0.09232
C	2.04653	0.90336	0.69254	H	-0.37212	4.30492	0.52386
C	2.84202	-1.31183	0.18794	H	0.18661	3.40658	-1.75922
C	-1.20371	-1.27017	0.16419	H	2.71674	-2.2531	-0.33222
C	-2.79345	-2.92349	0.91958	H	-1.50313	3.60083	-2.1775
C	1.04324	2.01675	0.49439	H	-0.72135	2.03891	-2.4167
C	-1.32226	3.77095	0.50923	H	-3.26712	-3.88874	0.79954
C	-1.81846	-2.51063	0.02051	H	-1.52088	-3.16304	-0.79124
C	-3.16027	-2.09265	1.96893	H	-3.92377	-2.40493	2.66896
C	-2.54427	-0.85893	2.12223	H	-2.82417	-0.21418	2.94793
C	-0.77857	2.90319	-1.75747	H	3.24534	2.03073	2.06848
C	3.13762	1.09433	1.53311	H	4.92971	0.24933	2.34949
C	4.08386	0.09207	1.69358	H	4.66836	-1.89855	1.14811
C	3.93622	-1.11225	1.02028	H	-2.60727	0.97362	-1.07794
C	-2.63679	1.88957	-0.48702	H	-3.28833	2.6014	-0.99305
F	0.75303	-2.44779	-1.63656	H	-3.08495	1.65509	0.47739
H	-1.45388	1.54269	2.03574	N	-0.30639	1.48586	0.23796

Table S24 Cartesian coordinates for the optimized structure of [**2d-F**]$^-$

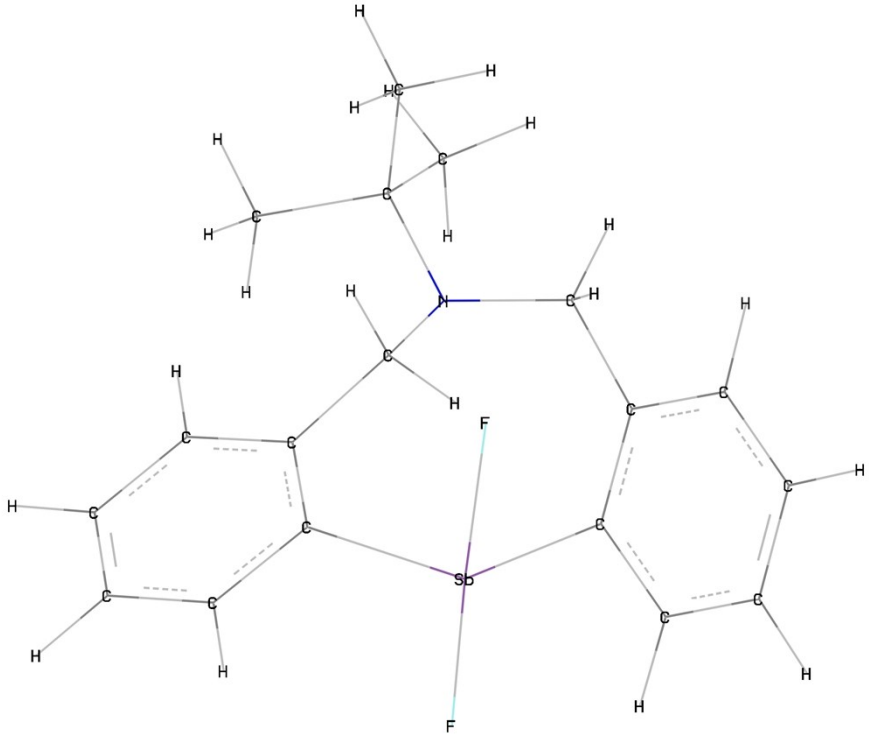
	x	y	z		x	y	z
Sb	-1.45	0.66668	1.22607	C	4.74823	-0.16803	-0.25613
F	-2.91215	1.66079	0.13316	C	3.42087	-0.13418	-0.64715
N	1.17256	-1.05542	-0.54546	H	-0.77363	3.51537	0.94063
C	-0.11693	1.76448	-0.10905	H	0.43333	5.11711	-0.46366
C	-0.16903	3.14099	0.12126	H	1.74642	4.30047	-2.41345
C	0.49647	4.05785	-0.68005	H	1.86112	1.88293	-2.86439
C	1.22721	3.60459	-1.76636	H	-0.22618	-0.48164	-1.94374
C	1.28858	2.24277	-2.01494	H	1.43202	-0.22732	-2.44667
C	0.64161	1.3155	-1.19801	H	-3.94585	-0.24847	-0.17802
C	0.74846	-0.15117	-1.59167	H	-4.85388	-2.09871	-1.52754
C	-1.96281	-1.03209	-0.06243	H	-3.35207	-3.93858	-2.26254
C	-3.30057	-1.06973	-0.46205	H	-0.97304	-3.88904	-1.61173
C	-3.80986	-2.10357	-1.23881	H	0.38103	-2.18772	0.98645
C	-2.97478	-3.12899	-1.65013	H	0.73875	-3.10567	-0.48997
C	-1.63859	-3.10076	-1.27847	H	2.29993	-2.72214	1.2321
C	-1.12359	-2.07546	-0.48541	H	4.6239	-2.7602	1.88823
C	0.33074	-2.16321	-0.10066	H	6.2499	-1.12689	0.95575
C	2.48395	-1.05609	-0.13704	H	5.42887	0.56562	-0.6709
C	2.96902	-2.00352	0.78883	H	3.10793	0.63344	-1.33457
C	4.29944	-2.01865	1.16825	F	0.12777	-0.40664	1.99786
C	5.21208	-1.10888	0.65221				

Table S25 Cartesian coordinates for the optimized structure of **3d**



	x	y	z		x	y	z
C	1.89092	-0.30952	0.02112	H	1.05095	2.67688	1.36927
C	-1.24289	2.50531	-0.35331	H	1.34791	2.61696	-0.36212
C	-0.8277	0.85122	1.46664	H	-1.61178	3.55423	1.5373
C	-1.56452	-0.44498	1.22625	H	-2.07168	4.44355	0.09232
C	2.04653	0.90336	0.69254	H	-0.37212	4.30492	0.52386
C	2.84202	-1.31183	0.18794	H	0.18661	3.40658	-1.75922
C	-1.20371	-1.27017	0.16419	H	2.71674	-2.2531	-0.33222
C	-2.79345	-2.92349	0.91958	H	-1.50313	3.60083	-2.1775
C	1.04324	2.01675	0.49439	H	-0.72135	2.03891	-2.4167
C	-1.32226	3.77095	0.50923	H	-3.26712	-3.88874	0.79954
C	-1.81846	-2.51063	0.02051	H	-1.52088	-3.16304	-0.79124
C	-3.16027	-2.09265	1.96893	H	-3.92377	-2.40493	2.66896
C	-2.54427	-0.85893	2.12223	H	-2.82417	-0.21418	2.94793
C	-0.77857	2.90319	-1.75747	H	3.24534	2.03073	2.06848
C	3.13762	1.09433	1.53311	H	4.92971	0.24933	2.34949
C	4.08386	0.09207	1.69358	H	4.66836	-1.89855	1.14811
C	3.93622	-1.11225	1.02028	H	-2.60727	0.97362	-1.07794
C	-2.63679	1.88957	-0.48702	H	-3.28833	2.6014	-0.99305
F	0.75303	-2.44779	-1.63656	H	-3.08495	1.65509	0.47739
H	-1.45388	1.54269	2.03574	N	-0.30639	1.48586	0.23796
H	0.02985	0.62059	2.10155	Sb	0.21406	-0.5886	-1.29025

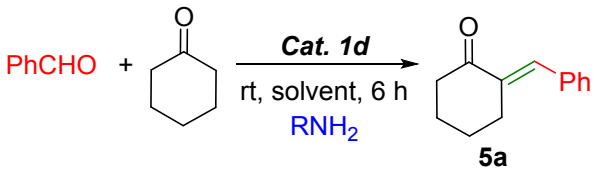
Table S26 Cartesian coordinates for the optimized structure of [**3d-F**]$^-$



	x	y	z		x	y	z
C	1.95402	0.19002	0.12608	H	0.56376	2.34958	-1.18464
C	-1.9981	2.30148	-0.38805	H	-2.64968	3.17084	1.51608
C	-0.99724	0.84505	1.353	H	-3.2201	4.03491	0.08925
C	-1.51571	-0.57042	1.15293	H	-1.53806	4.1964	0.59709
C	1.67151	1.53683	0.40443	H	-1.03355	3.66286	-1.80363
C	3.14151	-0.34595	0.63107	H	3.34605	-1.39489	0.45934
C	-0.98253	-1.43305	0.18656	H	-2.66587	3.17187	-2.2387
C	-2.57699	-3.14137	0.89334	H	-1.31058	2.01886	-2.41375
C	0.4432	2.25385	-0.10594	H	-2.98136	-4.13943	0.77709
C	-2.37008	3.49561	0.51274	H	-1.11427	-3.41025	-0.63297
C	-1.53241	-2.71234	0.08506	H	-3.89163	-2.60069	2.50706
C	-3.08322	-2.28556	1.8587	H	-2.94594	-0.33364	2.72685
C	-2.54522	-1.01358	1.98123	H	2.3286	3.31636	1.39557
C	-1.72761	2.82128	-1.80503	H	4.43332	2.34447	2.23017
C	2.56972	2.28395	1.16785	H	4.95029	-0.04074	1.74625
C	3.75289	1.73904	1.64383	H	-2.94251	0.48398	-1.07613
C	4.03928	0.41133	1.37317	H	-4.03803	1.87861	-0.93284
C	-3.19791	1.35505	-0.47246	H	-3.51785	1.00822	0.50921
F	1.5423	-2.63811	0.2463	N	-0.82136	1.5746	0.11771
H	-1.66728	1.35932	2.05733	Sb	0.79091	-1.21647	-1.08078
H	-0.03256	0.77703	1.85674	F	0.08171	0.36112	-2.22454
H	0.45342	3.26964	0.32382				

Catalytic evaluation

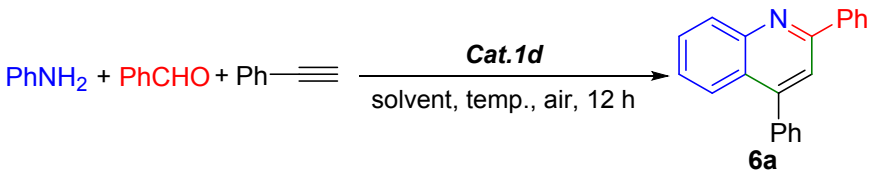
Table S27 Optimization of cross-condensation reactions of benzaldehyde and cyclohexanone catalyzed by compound **1d**.[a]



Entry	RNH_2 (equiv)	**Cat. 1d** (mol%)	Solvent (mL)	Yield of **5a** (%)[b]
1	*n*-propylamine (1)	5	H_2O (2)	85
2	*i*-propylamine (1)	5	H_2O (2)	79
3	*n*-butylamine (1)	5	H_2O (2)	83
4	*tert*-butylamine (1)	5	H_2O (2)	78
5	*n*-hexylamine (1)	5	H_2O (2)	93
6	cyclohexylamine (1)	5	H_2O (2)	76
7	*n*-hexylamine (1)	10	H_2O (2)	93
8	*n*-hexylamine (1)	1	H_2O (2)	46
9	*n*-hexylamine (1)	5	CH_2Cl_2 (2)	92
10	*n*-hexylamine (1)	5	THF (2)	88
11	*n*-hexylamine (1)	5	Et_2O (2)	84
12	*n*-hexylamine (1)	5	MeCN (2)	90
13	*n*-hexylamine (1)	5	MeOH (2)	92
14	*n*-hexylamine (1)	5	EtOH (2)	88

[a] Reaction conditions: benzaldehyde (1 mmol), cyclohexanone (1 mmol), aliphatic amine (1 mmol) and complex **1d** in solvent (1 mL) under air atmosphere for 6 h. [b] Isolated yield.

Table S28 Optimization of cross-condensation reactions of benzaldehyde and cyclohexanone catalyzed by compound **1d**.[a]

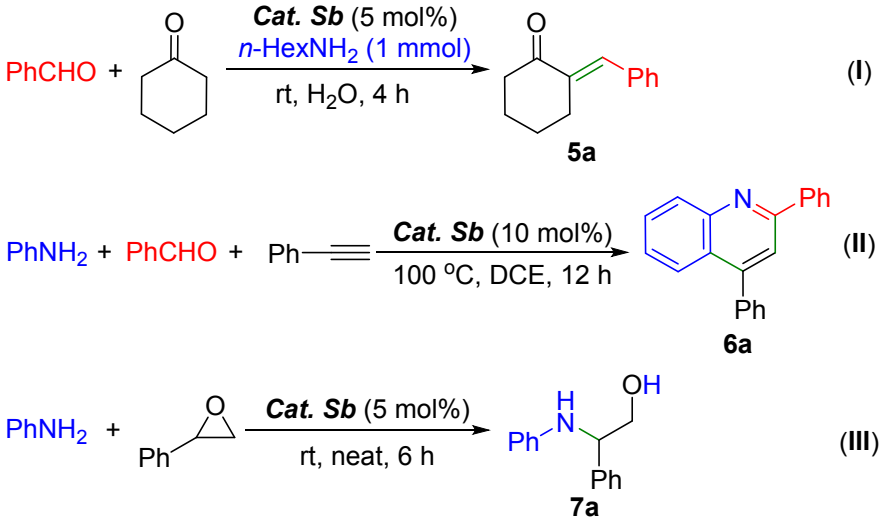


Entry	**Cat. 1d** (mol%)	Temp. (°C)	Solvent (mL)	Yield of **5a** (%)[b]
1	10	110	H_2O (2)	N.R.[c]
2	10	110	$CHCl_3$ (2)	85
3	10	110	MeCN (2)	83
4	10	110	toluene (2)	62
5	10	110	DCE (2)	90
6	10	110	MeOH (2)	76
7	10	110	EtOH (2)	83
8	10	80	DCE (2)	46

9	10	25	DCE (2)	N.R.
10	5	110	DCE (2)	62
11	20	110	DCE (2)	90
12[d]	10	110	DCE (2)	90
13[e]	10	110	DCE (2)	N.R.

[a] Reaction conditions: aniline (1 mmol), benzaldehyde (1 mmol), phenylacetylene (1 mmol), and complex **1d** in solvent (1 mL) under air atmosphere for 6 h. [b] Isolated yield. [c] No reaction. [d] Under O_2 atmosphere. [e] Under N_2 atmosphere.

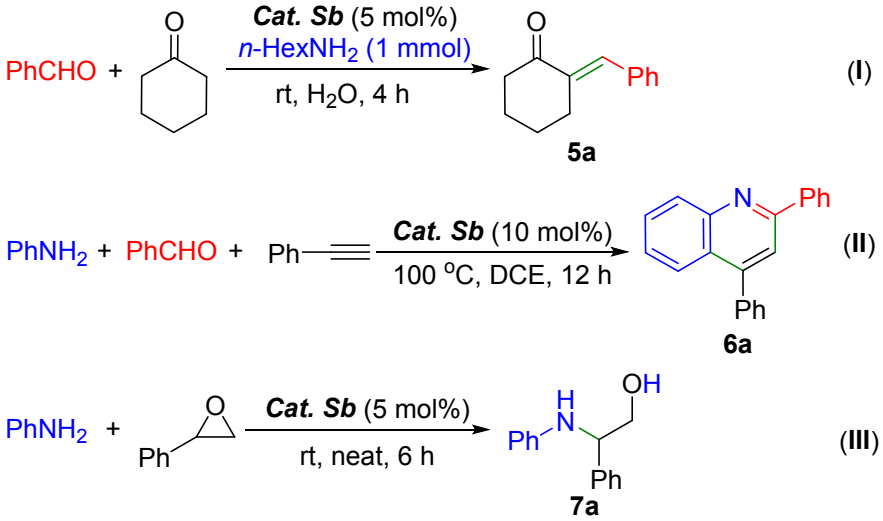
Table S29 Comparison of catalyst performance towards cross-condensation (**I**), cyclization-aromatization (**II**) and aminolysis reactions of epoxides (**III**).[a]



Entry	Compound	Yield of **5a** (%)[b]	Yield of **6a** (%)[b]	Yield of **7a** (%)[b]
1	**1a**	62	59	69
2	**2a**	43	40	52
3	**3a**	41	38	50
4	**1b**	70	68	75
5	**2b**	39	35	47
6	**3b**	53	50	60
7	**1c**	59	54	64
8	**2c**	26	20	30
9	**3c**	45	42	54
10	**1d**	93	90	96
11	**2d**	80	75	81
12	**3d**	84	80	85

[a] Conditions **I**: benzaldehyde (1 mmol), cyclohexanone (1 mmol), *n*-hexylamine (1 mmol) and organoantimony compound (5 mol%) in H_2O (2 mL) under air atmosphere for 4 h. Conditions **II**: aniline (1 mmol), benzaldehyde (1 mmol), phenylacetylene (1 mmol), and organoantimony compound (10 mol%) in DCE (2 mL) under air atmosphere for 12 h. Conditions **III**: aniline (1 mmol), 2-phenyloxirane (1 mmol) and organoantimony compound (5 mol%) under air atmosphere for 4 h. [b] Isolated yield.

Table S30 Comparison of catalyst performance towards cross-condensation (**I**), cyclization-aromatization (**II**) and aminolysis reactions of epoxides (**III**).[a]

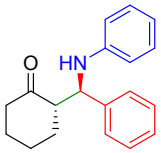


Entry	Cycle number	Yield of **5a** (%)[b]	Yield of **6a** (%)[b]	Yield of **7a** (%)[b]
1	Fresh	91	88	93
2	1st	91	88	93
3	2nd	90	87	91
4	3th	88	87	92
5	4th	90	87	90
6	5th	89	86	90

[a] Conditions **I**: benzaldehyde (5 mmol), cyclohexanone (5 mmol), *n*-hexylamine (5 mmol) and compound **1d** (5 mol%) in H_2O (10 mL) under air atmosphere for 4 h. Conditions **II**: aniline (5 mmol), benzaldehyde (5 mmol), phenylacetylene (5 mmol), and compound **1d** (10 mol%) in DCE (10 mL) under air atmosphere for 12 h. Conditions **III**: aniline (5 mmol), 2-phenyloxirane (5 mmol) and compound **1d** (5 mol%) under air atmosphere for 4 h. [b] Isolated yield.

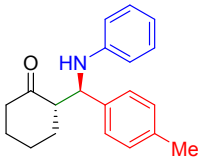
Analytical data

2-(phenyl(phenylamino)methyl)cyclohexan-1-one (4a)



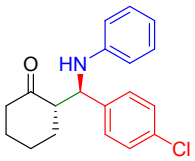
Yellow solid (273.3 mg, 98% yield); mp 138–140 °C; ^{1}H NMR (400 Hz, $CDCl_3$, TMS) δ 7.45 (2H, d, J = 7.4 Hz), 7.37 (2H, t, J = 7.3 Hz), 7.31–7.26 (1H, m), 7.16–7.12 (2H, m), 6.70 (1H, t, J = 7.3 Hz), 6.62 (2H, d, J = 7.4 Hz), 4.83 (1H, s), 4.71 (1H, d, J = 7.1 Hz), 2.85–2.80 (1H, m), 2.53–2.47 (1H, m), 2.43–2.36 (1H, m), 2.02–1.85 (4H, m), 1.83–1.71 (2H, m); ^{13}C NMR (100 MHz, CDCl3, TMS) δ 212.9, 147.1, 141.6, 129.0, 128.4, 127.2, 127.1, 117.4, 113.5, 57.9, 57.4, 41.7, 31.2, 27.8, 23.5. Spectral data obtained for the compound are in good agreement with the reported data.[5]

2-((phenylamino)(*p*-tolyl)methyl)cyclohexan-1-one (4b)



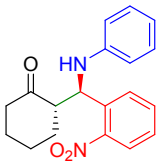
Yellow solid (249.0 mg, 85% yield); mp 115–117 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.26–7.24 (2H, m), 7.11–7.04 (4H, m), 6.62 (1H, t, J = 7.3 Hz), 6.54 (2H, d, J = 8.1 Hz), 4.86 (1H, s), 4.59 (1H, d, J = 7.3 Hz), 2.76–2.71 (1H, m), 2.46–2.40 (1H, m), 2.35–2.32 (1H, m), 2.29 (3H, s), 1.91–1.83 (4H, m, CH_2), 1.72–1.65(2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 213.1, 147.0, 138.4, 136.7, 129.1, 129.0, 127.1, 117.6, 113.7, 57.8, 57.4, 41.7, 31.2, 27.9, 23.5, 21.1. Spectral data obtained for the compound are in good agreement with the reported data.[5]

2-((4-chlorophenyl)(phenylamino)methyl)cyclohexan-1-one (4c)



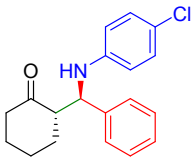
Yellow solid (287.9 mg, 92% yield); mp 266–268 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.32–7.22 (4H, m), 7.06 (2H, t, J = 7.7 H), 6.64 (1H, t, J = 7.2 Hz), 6.50 (2H, d, J = 7.9 Hz), 4.76 (1H, s), 4.59 (1H, d, J = 6.4 Hz), 2.73 (s, 1H), 2.42–2.26 (m, 2H), 1.95–1.66 (m, 6H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 212.4, 146.8, 140.2, 132.6, 129.0, 128.6, 128.5, 117.7, 113.7, 57.4, 57.1, 41.9, 31.4, 27.9, 23.9. Spectral data obtained for the compound are in good agreement with the reported data.[5]

2-((2-nitrophenyl)(phenylamino)methyl)cyclohexan-1-one (4d)



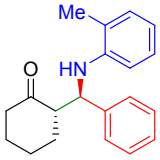
Yellow solid (307.8 mg, 95% yield); mp 155–157 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.92 (1H, d, J = 8.1 Hz), 7.73 (1H, d, J = 7.9 Hz), 7.50 (1H, t, J = 7.6 Hz), 7.35 (1H, t, J = 7.7 Hz), 7.07 (2H, t, J = 7.3 Hz), 6.66 (t, J = 7.3 Hz, 1H), 6.54 (2H, d, J = 7.8 Hz), 5.61 (1H, d, J = 3.9 Hz), 4.41 (1H, s), 2.96–2.93 (1H, m), 2.43 (1H, d, J = 14.0 Hz), 2.36–2.28 (1H, m), 2.07 (2H, d, J = 14.7 Hz), 1.92 (1H, d, J = 8.0 Hz), 1.71–1.54 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 210.0, 149.0, 14.6, 137.2, 133.0, 130.1, 129.1, 127.9, 125.0, 118.2, 113.8, 55.3, 52.0, 42.2, 28.3, 27.2, 24.9. Spectral data obtained for the compound are in good agreement with the reported data.[6]

2-(((4-chlorophenyl)amino)(phenyl)methyl)cyclohexan-1-one (4e)



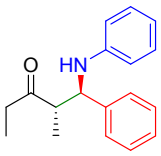
Yellow solid (300.4 mg, 96% yield); mp 135–137 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.35–7.30 (4H, m), 7.25–7.22(1H, m), 6.99 (2H, d, J = 8.7 Hz), 6.45 (2H, d, J = 8.7 Hz, ArH), 4.91 (1H, s), 4.53 (1H, d, J = 6.9 Hz), 2.78–2.73 (1H, m), 2.44 – 2.30 (2H, m), 1.96–1.79 (4H, m), 1.71–1.65 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 212.8, 145.7, 141.1, 128.8, 128.5, 127.3, 127.2, 122.1, 114.8, 58.3, 57.3, 41.9, 31.5, 27.9, 23.8. Spectral data obtained for the compound are in good agreement with the reported data.[6]

2-(phenyl(*o*-tolylamino)methyl)cyclohexan-1-one (4f)



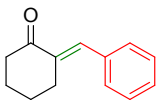
Yellow solid (263.7 mg, 90% yield); mp 136–138 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.36 (2H, d, J = 7.4 Hz), 7.29 (2H, t, J = 7.5 Hz), 7.23–7.18 (1H, m), 7.01 (1H, d, J = 7.3 Hz), 6.91 (1H, t, J = 7.6 Hz), 6.57 (1H, t, J = 7.3 Hz), 6.38 (1H, d, J = 8.0 Hz), 4.72 (1H, s), 4.64 (1H, d, J = 7.0 Hz), 2.79 (1H, s), 2.45–2.38 (1H, m), 2.36–2.29 (1H, m), 2.21 (3H, s), 1.93–1.82 (4H, m), 1.78–1.67 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 213.3, 145.0, 141.7, 129.9, 128.4, 127.1, 126.8, 122.5, 116.9, 110.6, 57.9, 57.5, 41.7, 31.2, 27.8, 23.4, 17.6. Spectral data obtained for the compound are in good agreement with the reported data.[5]

2-methyl-1-phenyl-1-(phenylamino)pentan-3-one (4g)



Yellow oil (251.0 mg, 94% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.37 (4H, d, J = 4.3 Hz), 7.29 (1H, s), 7.13 (2H, t, J = 7.5 Hz), 6.70 (1H, t, J = 7.2 Hz), 6.57 (2H, d, J = 8.0 Hz), 4.74 (1H, d, J = 5.8 Hz), 4.45 (1H, s), 3.10–3.03 (1H, m), 2.48–2.30 (2H, m), 1.17 (3H, d, J = 7.0 Hz), 0.99 (3H, t, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 213.3, 146.9, 141.1, 129.0, 128.5, 127.2, 126.8, 117.5, 113.5, 59.1, 52.2, 35.4, 11.5, 7.4. Spectral data obtained for the compound are in good agreement with the reported data.[7]

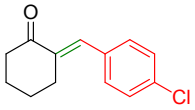
(*E*)-2-benzylidenecyclohexan-1-one (5a)



Yellow oil (173.0 mg, 93% yield); ^{1}H NMR (400 Hz, $CDCl_3$, TMS) δ 7.50 (1H, t, J = 2.2 Hz), 7.41–7.35 (4H, m), 7.34–7.29 (1H, m), 2.85–2.81 (2H, m), 2.53 (2H, t, J = 6.7 Hz), 1.95–1.89

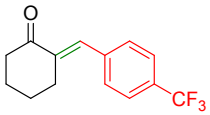
(2H, m), 1.79–1.73 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.6, 136.6, 135.5, 135.5, 130.2, 128.4, 128.2, 40.2, 28.8, 23.8, 23.3. Spectral data obtained for the compound are in good agreement with the reported data.[7]

(*E*)-2-(4-chlorobenzylidene)cyclohexan-1-one (5b)



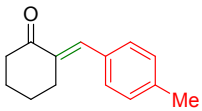
Yellow solid (198.0 mg, 90% yield); mp 52–54 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (1H, t, J = 2.1 Hz), 7.36–7.28 (4H, m), 2.81–2.77 (2H, m), 2.53 (2H, t, J = 6.7 Hz), 1. 96–1.89 (2H, m), 1.80–1.74 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.3, 137.0, 134.3, 134.1, 133.9, 131.4, 128.5, 40.2, 28.8, 23.7, 23.2. Spectral data obtained for the compound are in good agreement with the reported data.[8]

(*E*)-2-(4-(trifluoromethyl)benzylidene)cyclohexan-1-one (5c)



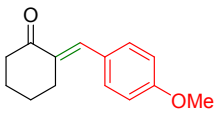
Yellow oil (241.3 mg, 95% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.64 (2H, d, J = 8.2 Hz), 7.48 (3H, d, J = 8.6 Hz), 2.83–2.80 (2H, m), 2.56 (2H, t, J = 6.7 Hz), 1.98–1.92 (2H, m), 1.82–1.75 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.5, 139.1 (d, J = 1.3 Hz), 138.7, 133.5, 130.2, 129.4 (d, J = 100.0 Hz), 125.3 (q, J = 3.8 Hz), 40.4, 28.9, 23.8, 23.4. Spectral data obtained for the compound are in good agreement with the reported data.[7]

(*E*)-2-(4-methylbenzylidene)cyclohexan-1-one (5d)



Yellow solid (170.0 mg, 85% yield); mp 62–64 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.49 (1H, s), 7.31 (2H, d, J = 8.1 Hz), 7.19 (2H, d, J = 8.0 Hz), 2.85–2.82 (2H, m), 2.52 (2H, t, J = 6.7 Hz), 2.37 (3H, s), 1.95–1.89 (2H, m, CH_2), 1.79–1.73 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.7, 138.7, 135.7, 135.7, 132.7, 130.4, 129.0, 40.2, 28.9, 23.8, 23.3, 21.3. Spectral data obtained for the compound are in good agreement with the reported data.[7]

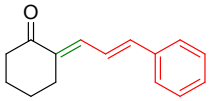
(*E*)-2-(4-methoxybenzylidene)cyclohexan-1-one (5e)



Yellow solid (177.2 mg, 82% yield); mp 64–66 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ= 7.49 (1H, s),7.39 (2H, d, J = 8.8 Hz), 6.91 (2H, d, J = 8.8 Hz), 3.82 (3H, s), 2.84–2.81 (2H, m, CH_2), 2.51 (2H, t, J = 6.7 Hz, CH_2), 1.93–1.87 (2H, m), 1.79–1.73 (2H, m); ^{13}C NMR (100

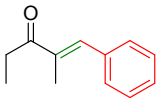
MHz, $CDCl_3$, TMS) δ= 201.3, 159.8, 135.6, 134.2, 132.1, 128.1, 113.7, 55.1, 40.0, 28.8, 23.7, 23.1. Spectral data obtained for the compound are in good agreement with the reported data.[8]

(*E*)-2-((*E*)-3-phenylallylidene)cyclohexan-1-one (5f)



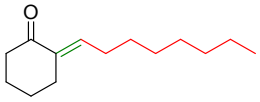
Yellow oil (135.6 mg, 64% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.49–7.47 (2H, m), 7.37–7.24 (4H, m), 7.04–6.91 (2H, m), 2.76–2.73 (2H, m), 2.49 (2H, t, J = 6.7 Hz), 1.92–1.78 (4H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 200.7, 140.9, 136.6, 135.4, 135.0, 128.8, 128.8, 127.1, 123.1, 40.0, 26.9, 23.3, 23.0.

(*E*)-2-methyl-1-phenylpent-1-en-3-one (5g)



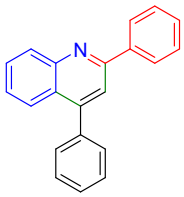
Yellow solid (160.0 mg, 92% yield); mp 34–36 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.39 (1H, s), 7.28–7.25 (4H, m), 7.20–7.19 (1H, m), 2.68 (2H, dd, J = 14.4, 7.1 Hz), 1.95 (3H, s), 1.06 (2H, t, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.7, 137.5, 136.4, 135.4, 129.1, 127.8, 30.0, 12.5, 8.2. Spectral data obtained for the compound are in good agreement with the reported data.[9]

(*E*)-2-octylidenecyclohexan-1-one (5h)



Yellow oil (133.3 mg, 68% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 6.65–6.61 (1H, m), 2.50–2.47 (2H, m), 2.42 (2H , t, J = 6.7 Hz), 2.09 (2H, q, J = 7.3 Hz), 1.88–1.82 (2H, m), 1.79–1.71 (2H, m), 1.45–1.42 (2H, m), 1.32–1.28 (8H, m), 0.90–0.86 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 201.2, 139.8, 136.1, 40.1, 31.7, 29.4, 29.1, 28.4, 27.8, 26.6, 23.6, 23.3, 22.6, 14.0. Spectral data obtained for the compound are in good agreement with the reported data.[10]

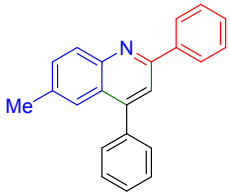
2,4-diphenylquinoline (6a)



Yellow soild (252.9 mg, 90% yield); mp 112–114 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.13 (1H, d, J = 8.4 Hz), 8.06 (2H, d, J = 7.6 Hz), 7.76 (1H, d, J = 8.4 Hz), 7.68 (1H, s), 7.58 (1H, t, J = 7.4 Hz), 7.40–7.29 (9H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.8, 149.1,

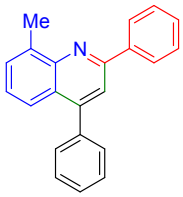
148.7, 139.6, 138.3, 130.0, 129.5, 129.4, 129.3, 128.7, 128.5, 128.3, 127.5, 126.2, 125.7, 126.2, 125.7, 125.5, 119.3. Spectral data obtained for the compound are in good agreement with the reported data.[11]

6-methyl-2,4-diphenylquinoline (6b)



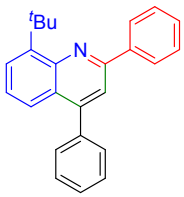
Yellow solid (253.7 mg, 86% yield); mp 92–94 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.33–8.29 (3H, m), 7.89 (1H, s), 7.79 (1H, s), 7.66–7.51 (9H, m), 2.54 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 155.7, 148.2, 147.2, 139.5, 138.4, 136.0, 131.5, 129.7, 129.3, 128.9, 128.6, 128.4, 128.1, 127.3, 125.5, 124.2, 119.1, 21.6. Spectral data obtained for the compound are in good agreement with the reported data.[11]

8-methyl-2,4-diphenylquinoline (6c)



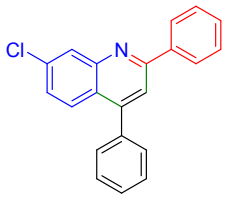
Yellow oil (244.8 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.43 (1H, d, J = 7.6 Hz), 7.96 (1H, s), 7.86 (1H, t, J = 8.4 Hz), 7.69–7.54 (9H, m), 3.12 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 154.8, 149.1, 147.6, 139.7, 138.8, 137.8, 129.5, 129.1, 128.7, 128.4, 128.1, 127.4, 125.8, 125.6, 123.5, 118.5, 18.4. Spectral data obtained for the compound are in good agreement with the reported data.[11]

8-(*tert*-butyl)-2,4-diphenylquinoline (6d)



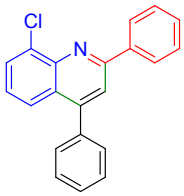
Yellow oil (262.8 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.48 (1H, d, J = 7.8 Hz), 8.00 (1H, s), 7.88 (2H, dd, J = 19.8, 8.3 Hz), 7.70–7.58 (8H, m), 7.51 (1H, t, J = 7.7 Hz), 1.98 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 153.0, 149.6, 148.7, 147.4, 139.9, 139.9, 129.6, 129.1, 128.8, 128.4, 128.1, 127.3, 126.7, 126.3, 125.7, 124.4, 117.7, 36.8, 31.4.

7-chloro-2,4-diphenylquinoline (6e)



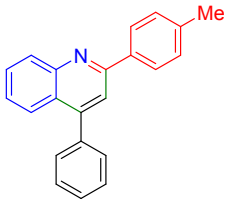
Yellow soild (248.8 mg, 79% yield); mp 107–109 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.19–8.16 (3H, m), 7.75 (1H, s), 7.58 (1H, t, J = 7.9 Hz), 7.51–7.37 (9H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.3, 150.2, 148.8, 141.1, 138.5, 137.8, 130.7, 129.9, 129.7, 129.1, 129.0, 128.8, 127.7, 127.6, 127.5, 123.5, 122.6. Spectral data obtained for the compound are in good agreement with the reported data.[12]

8-chloro-2,4-diphenylquinoline (6f)



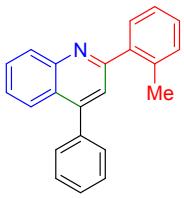
Yellow soild (258.2 mg, 82% yield); mp 107–109 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.28 (1H, d, J = 9.2 Hz), 8.12–8.07 (1H, m), 7.95 (1H, d, J = 8.3 Hz), 7.84–7.76 (2H, m), 7.60–7.45 (8H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 155.2, 149.5, 148.7, 141.4, 138.2, 134.9, 130.1, 130.0, 129.7, 129.5, 129.3, 128.6, 128.5, 127.7, 126.7, 125.9, 125.7, 125.6, 119.0. Spectral data obtained for the compound are in good agreement with the reported data.[12]

4-phenyl-2-(*p*-tolyl)quinoline (6g)



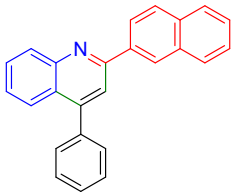
Yellow soild (274.3 mg, 93% yield); mp 112–114 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.40 (1H, d, J = 8.4 Hz), 8.24 (2H, d, J = 8.2 Hz), 7.99 (2H, dd, J = 8.4, 0.7 Hz), 7.90 (1H, s), 7.82–7.78 (1H, m), 7.65–7.57 (5H, m), 7.53–7.49 (1H, m), 7.42 (1H, t, J = 8.0 Hz), 2.51 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 148.7, 148.6, 139.1, 138.3, 136.6, 129.9, 129.3, 129.2, 128.3, 128.1, 127.2, 125.9, 125.5, 125.4, 118.9, 21.1. Spectral data obtained for the compound are in good agreement with the reported data.[11]

4-phenyl-2-(*o*-tolyl)quinoline (6h)



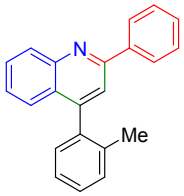
Yellow oil (265.5 mg, 90% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.24 (1H, d, J = 8.4 Hz), 7.95 (1H, d, J = 8.4 Hz), 7.72 (1H, t, J = 7.8 Hz), 7.55–7.45 (8H, m), 7.31–7.27 (3H, m), 2.46 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 159.6, 148.2, 148.2, 140.5, 137.9, 135.8, 130.7, 129.8, 129.5, 129.3, 129.2, 128.3, 128.3, 128.2, 126.2, 125.8, 125.4, 125.0, 122.3, 20.3. Spectral data obtained for the compound are in good agreement with the reported data.[13]

2-(naphthalen-2-yl)-4-phenylquinoline (6i)



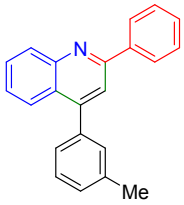
Yellow solid (264.8 mg, 80% yield); mp 98–100 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.72 (1H, s), 8.49 (1H, dd, J = 8.6, 1.8 Hz), 8.38 (1H, dd, J = 8.4, 0.5 Hz), 8.06–8.02 (3H, m), 7.99 (1H, dd, J = 8.4, 0.8 Hz), 7.97–7.93 (1H, m), 7.83–7.79 (1H, m), 7.67–7.52 (8H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.7, 149.3, 149.0, 138.5, 137.0, 134.0, 133.6, 130.2, 129.7, 128.9, 128.7, 128.6, 128.5, 127.8, 127.2, 126.8, 126.5, 126.4, 125.9, 125.7, 125.1, 119.5. Spectral data obtained for the compound are in good agreement with the reported data.[14]

2-phenyl-4-(*o*-tolyl)quinoline (6j)



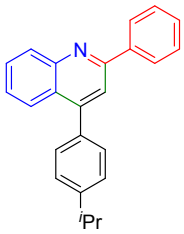
Yellow oil (162.2 mg, 55% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.12 (1H, d, J = 8.4 Hz), 8.06 (2H, d, J = 7.8 Hz), 7.62 (1H, s), 7.54 (1H, t, J = 7.9 Hz), 7.37–7.11 (10H, m), 1.93 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.7, 149.1, 148.4, 139.5, 137.7, 136.0, 130.1, 130.0, 129.5, 129.5, 129.2, 128.7, 128.3, 127.5, 126.2, 126.2, 125.7, 125.6, 119.2, 19.9. Spectral data obtained for the compound are in good agreement with the reported data.[15]

2-phenyl-4-(*m*-tolyl)quinolone (6k)



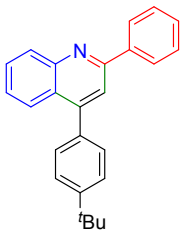
Yellow oil (233.0 mg, 79% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.48 (1H, d, J = 8.4 Hz), 8.39 (1H, d, J = 7.4 Hz), 8.07 (1H, d, J = 8.3 Hz), 7.95 (1H, s), 7.81 (1H, t, J = 8.0 Hz), 7.63 (1H, t, J = 7.3 Hz), 7.57–7.39 (6H, m), 2.55 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.3, 148.9, 148.5, 139.3, 138.0, 137.8, 129.8, 129.1, 129.0, 128.8, 128.4, 128.1, 127.2, 126.3, 125.9, 125.5, 125.3, 118.8, 21.1. Spectral data obtained for the compound are in good agreement with the reported data.[15]

2-phenyl-4-(4-propylphenyl)quinoline (6l)



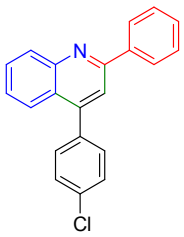
Yellow oil (264.9 mg, 82% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.23 (1H, d, J = 8.4 Hz), 8.16 (2H, d, J = 7.8 Hz), 7.90 (1H, d, J = 8.4 Hz), 7.76 (1H, s), 7.64 (1H, t, J = 7.9 Hz), 7.47–7.35 (6H, m), 7.27 (2H, d, J = 7.5 Hz), 2.63 (2H, t, J = 7.6 Hz), 1.71–1.65 (2H, m), 0.97 (3H, t, J = 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.7, 149.1, 148.7, 142.9, 139.5, 135.5, 130.0, 129.3, 129.3, 129.1, 128.6, 128.5, 127.4, 126.0, 125.7, 125.6, 119.1, 37.7, 24.4, 13.8.

4-(4-(*tert*-butyl)phenyl)-2-phenylquinoline (6m)



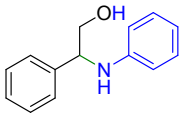
Yellow oil (269.6 mg, 80% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.13 (1H, d, J = 8.4 Hz), 8.06 (2H, d, J = 7.6 Hz), 7.83 (1H, d, J = 8.4 Hz), 7.69 (1H, s), 7.58 (1H, t, J = 8.0 Hz), 7.44–7.30 (8H, m), 1.29 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.8, 151.4, 149.1, 148.8, 139.7, 135.4, 130.0, 129.4, 129.3, 129.2, 128.7, 127.5, 125.7, 125.5, 119.3, 37.7, 31.3. Spectral data obtained for the compound are in good agreement with the reported data.[16]

4-(4-chlorophenyl)-2-phenylquinoline (6n)



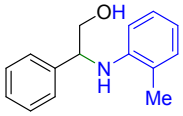
Yellow oil (270.9 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.34 (1H, dd, J = 8.4, 0.5 Hz), 8.27–8.24 (2H, m), 7.88 (1H, dd, J = 8.3, 0.7 Hz), 7.95 (1H, s), 7.81 (1H, m), 7.79–7.74 (1H, m), 7.59–7.48 (8H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 156.5, 148.6, 147.5, 139.2, 136.5, 134.4, 130.7, 130.1, 129.4, 129.2, 128.6, 128.6, 127.3, 126.3, 125.2, 125.0, 118.9. Spectral data obtained for the compound are in good agreement with the reported data.[15]

2-phenyl-2-(phenylamino)ethan-1-ol (7a)



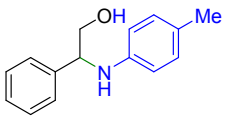
Colorless oil (204.5 mg, 96% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.37–7.31 (4H, m), 7.27–7.23 (1H, m, ArH), 7.11–7.07 (2H,m), 6.68 (1H, t, J = 7.3 Hz), 6.57–6.55 (2H, m), 4.48 (1H, dd, J = 7.0, 4.2 Hz), 3.93–3.89 (1H, m), 3.75–3.71 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 147.1, 140.0, 129.1, 128.8, 127.6, 126.7, 117.9, 113.8, 67.3, 59.8. Spectral data obtained for the compound are in good agreement with the reported data.[17]

2-phenyl-2-(o-tolylamino)ethan-1-ol (7b)



Colourless oil (208.8 mg, 92% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.37–7.31 (4H, m), 7.28–7.24 (1H, m), 7.06 (1H, d, J = 7.0 Hz), 6.96–6.92 (1H, m), 6.65–6.61 (1H, m), 6.37 (1H, d, J = 8.0 Hz), 4.54 (dd, J = 7.0, 4.2 Hz, 1H), 3.99–3.96 (1H, m), 3.82–3.77 (1H, m), 2.27 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 145.0, 140.1, 130.1, 128.8, 127.6, 127.9, 126.6, 122.6, 117.5, 111.5, 67.5, 59.8, 17.6. Spectral data obtained for the compound are in good agreement with the reported data.[17]

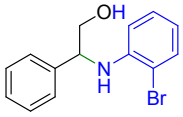
2-(4-Methylphenyl)amino-2-phenylethanol (7c)



Colourless oil (211.1 mg, 93% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.36–7.30 (4H, m), 7.27–7.23 (1H, m), 6.91 (1H, d, J = 8.1 Hz), 6.49 (1H, d, J = 8.4 Hz), 4.47 (1H, dd, J = 7.2, 4.2 Hz), 3.91 (1H, dd, J =11.1, 4.2 Hz, CH_2), 3.93–3.89 (1H, m), 3.74–3.70 (1H, m), 2.19 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 144.8, 140.2, 129.6, 128.8, 127.5, 127.2, 126.7,

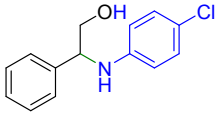
114.1, 67.3, 60.2, 20.3. Spectral data obtained for the compound are in good agreement with the reported data.[17]

2-((2-bromophenyl)amino)-2-phenylethan-1-ol (7d)



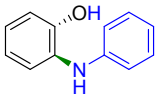
Yellow oil (241.4 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (1H, dd, J = 7.9, 1.4 Hz), 7.34 (4H, d, J = 4.3 Hz), 7.29–7.25 (1H, m, ArH), 7.01–6.97 (1H, m), 6.56–6.52 (1H, m), 6.42 (1H, dd, J = 8.2, 1.1 Hz), 4.55 (1H, dd, J = 6.6, 4.2 Hz), 4.00–3.96 (1H, m), 3.85–3.80 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 143.9, 139.4, 132.3, 128.9, 128.3, 127.7, 126.6, 118.3, 112.9, 110.3, 67.2, 59.7. Spectral data obtained for the compound are in good agreement with the reported data.[18]

2-((4-chlorophenyl)amino)-2-phenylethan-1-ol (7e)



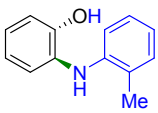
Colourless oil (219.8 mg, 89% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.33–7.22 (5H, m), 7.01 (2H, d, J = 8.8 Hz), 6.46 (2H, d, J = 8.8 Hz), 4.39 (1H, dd, J = 6.9, 4.1 Hz), 3.89–3.85 (1H, m), 3.70–3.66 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 145.7, 139.5, 128.9, 128.8, 127.7, 126.6, 122.3, 114.9, 67.1, 59.8. Spectral data obtained for the compound are in good agreement with the reported data.[17]

2-(phenylamino)cyclohexan-1-ol (7f)



White soild (171.9 mg, 90% yield); mp 52–54 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.20–7.16 (2H, m), 6.77–6.71 (3H, m), 3.38–3.32 (1H, m), 3.17–3.11 (1H, m), 2.98 (2H, s), 2.13–2.09(2H, m), 1.79–1.70 (2H, m), 1.44–1.25 (3H, m), 1.10–1.00 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 147.7, 129.3, 118.3, 114.4, 74.4, 60.1, 33.1, 31.5, 25.0, 24.2. Spectral data obtained for the compound are in good agreement with the reported data.[17]

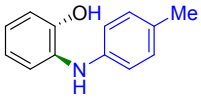
2-(*o*-tolylamino)cyclohexan-1-ol (7g)



Colourless oil (176.3 mg, 86% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.13–7.05 (2H, m), 6.78 (1H, d, J = 8.0 Hz), 6.69 (1H, t, J = 7.3 Hz), 3.44–3.38 (1H, m), 3.22–3.16 (1H, m), 2.95 (2H, s), 2.15 (3H, s), 2.13–2.11 (1H, m), 1.80–1.70 (2H, m), 1.46-1.26 (4H, m), 1.11–1.00 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 145.6, 130.3, 127.0, 123.0, 117.68, 111.4,

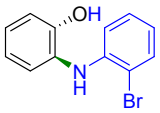
74.3, 59.7, 33.2, 31.7, 24.8, 24.2, 17.6. Spectral data obtained for the compound are in good agreement with the reported data.[17]

2-(*p*-tolylamino)cyclohexan-1-ol (7h)



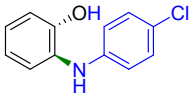
Colourless oil (170.1 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 6.99 (2H, d, J = 8.2 Hz), 6.63 (2H, d, J = 8.4 Hz), 3.35–3.29 (1H, m), 3.10–3.04 (3H, m), 2.24 (3H, s), 2.11–2.06 (2H, m), 1.77–1.68 (2H, m), 1.37-1.26 (3H, m), 1.05 –0.95 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 145.3, 129.7, 127.5, 114.6, 74.2, 60.5, 33.0, 31.4, 24.9, 24.2, 20.3. Spectral data obtained for the compound are in good agreement with the reported data.[17]

2-((2-bromophenyl)amino)cyclohexan-1-ol (7i)



Yellow oil (193.6 mg, 72% yield); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.44–7.41 (1H, m), 7.19–7.15 (1H, m), 6.85–6.83 (1H, m), 6.62–6.58 (1H, m), 4.13 (1H, s), 3.50–3.44 (1H, m), 3.23–3.17 (1H, m), 2.64 (1H, s), 2.15–2.05 (2H, m), 1.81–1.71 (2H, m), 1.47–1.25 (3H, m), 1.20–1.10 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 144.6, 132.6, 128.5, 118.7, 113.2, 111.1, 74.4, 60.1, 33.1, 31.6, 24.9, 24.1. Spectral data obtained for the compound are in good agreement with the reported data.[18]

2-((4-chlorophenyl)amino)cyclohexan-1-ol (7j)



White solid (180.0 mg, 80% yield); mp 105–107 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.11 (2H, d, J = 8.8 Hz), 6.63 (2H, d, J = 8.8 Hz), 3.38–3.32 (1H, m), 3.10–3.04 (1H, m), 2.95 (2H, s), 2.12–2.04 (2H, m), 1.79–1.70 (2H, m), 1.43–1.21 (3H, m), 1.09–0.99 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$, TMS) δ 146.3, 129.1, 122.7, 115.4, 74.4, 60.3, 33.2, 31.4, 24.8, 24.2. Spectral data obtained for the compound are in good agreement with the reported data.[17]

References

1 G. M. Sheldrick, SADABS: Empirical absorption correction program, University of GPttingen, 1995, based upon the method of Blessing.

2 G. Sheldrick, *Acta Crystallogr. Sect. A,* 2008, **64**, 112.

3 K. O. Christe, D. A. Dixon, D. McLemore, W. W. Wilson, J. A. Sheehy, J. A. Boatz, *J. Fluorine Chem.*, 2000, **101**, 151.

4 J. M. Slattery, S. Hussein, *Dalton Trans.*, 2012, **41**, 1808.

5 J. Xia, R.-H. Qiu, S.-F. Yin, X.-W. Zhang, S.-L. Luo, C.-T. Au, K. Xia, W.-Y. Wong, *J. Organometal. Chem.,* 2010, **695**, 1487.

6 A. A. Jafari, F. Moradgholi, F. Tamaddon, *Eur. J. Org. Chem.,* 2009, **2009**, 1249.

7 R. Qiu, Y. Qiu, S. Yin, X. Song, Z. Meng, X. Xin, X. Zhang, S. Luo, C.-T. Au, W.-Y. Wong, *Green Chem.,* 2010, **12**, 1767.

8 M. Barbero, S. Bazzi, S. Cadamuro, S. Dughera, C. Magistris, A. Smarra, P. Venturello, *Org. Biomol. Chem.,* 2011, **9**, 2192.

9 A. Yanagisawa, R. Goudu, T. Arai, *Org. Lett.,* 2004, **6**, 4281.

10 T. Nakano, S. Irifune, S. Umano, A. Inada, Y. Ishii, M. Ogawa, *J. Org. Chem.,* 1987, **52**, 2239.

11 Y. Zhang, P. Li, L. Wang, *J. Heterocyclic Chem.*, 2011, **48**, 153.

12 J. Tang, L. Wang, D. Mao, W. Wang, L. Zhang, S. Wu, Y. Xie, *Tetrahedron,* 2011, **67**, 8465.

13 F. Xiao, Y. Chen, Y. Liu, J. Wang, *Tetrahedron*, 2008, **64**, 2755.

14 R. P. Korivi, C. H. Cheng, *J. Org. Chem.,* 2006, **71**, 7079.

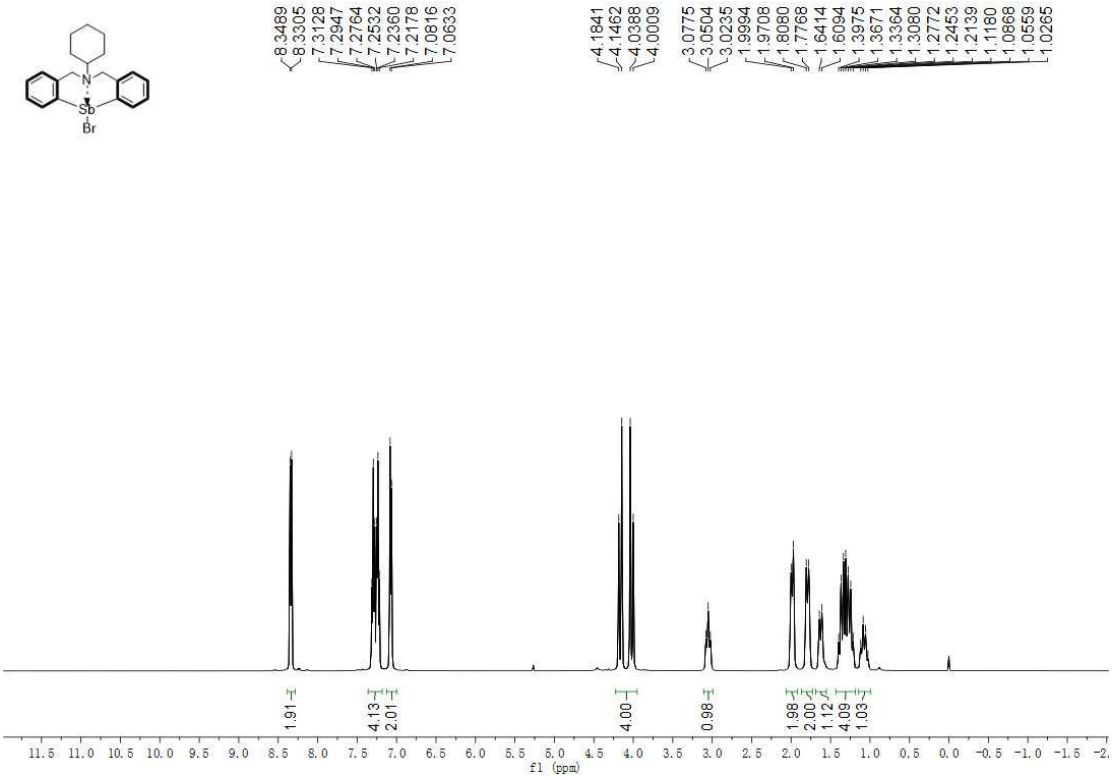
15 J. Yang, X. Meng, K. Lu, Z. Lu, M. Huang, C. Wang, F. Sun, *RSC Adv.,* 2018, **8**, 31603.

16 J. Zhu, W. Hu, S. Sun, J. T. Yu, J. Cheng, *Adv. Synth. Catal.,* 2017, **359**, 3725.

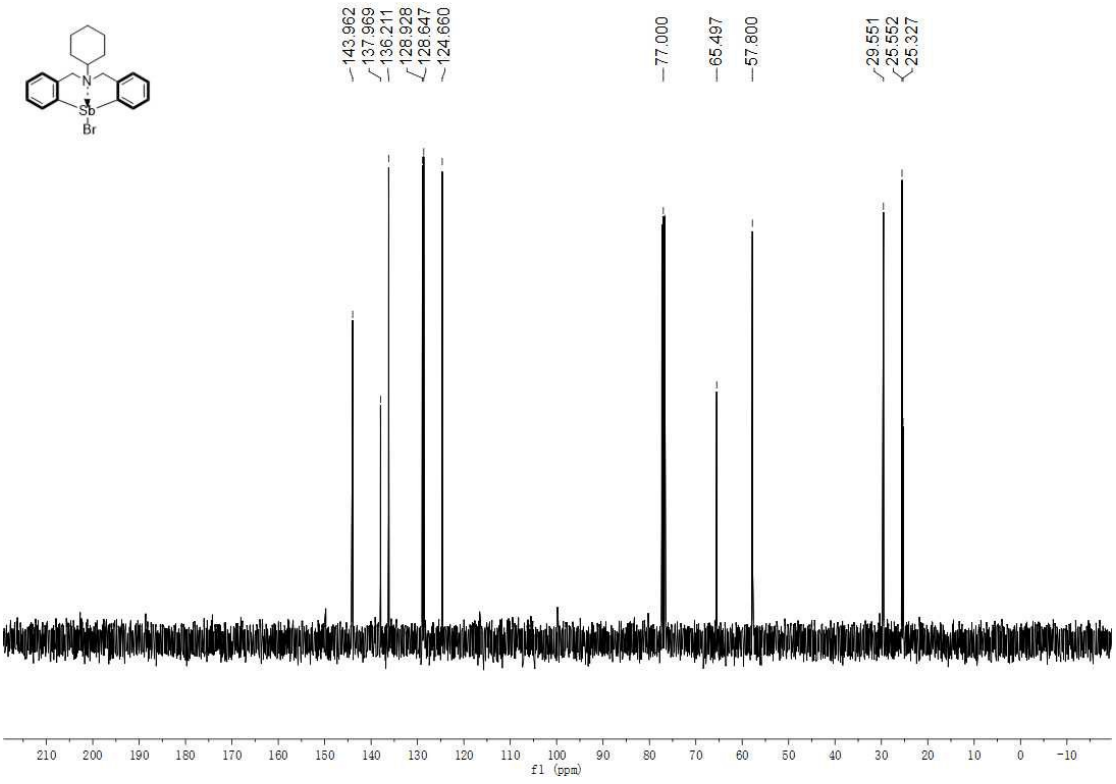
17 N. Li, L. Wang, H. Wang, J. Qiao, W. Zhao, X. Xu, Z. Liang, *Tetrahedron,* 2018, **74**, 1033.

18 N. Tan, S.-F. Yin, Y. Li, R. Qiu, Z. Meng, X. Song, L. Luo, C.-T. Au, W.-Y. Wong, *J. Organometal. Chem.*, 2011, **696**, 1579.

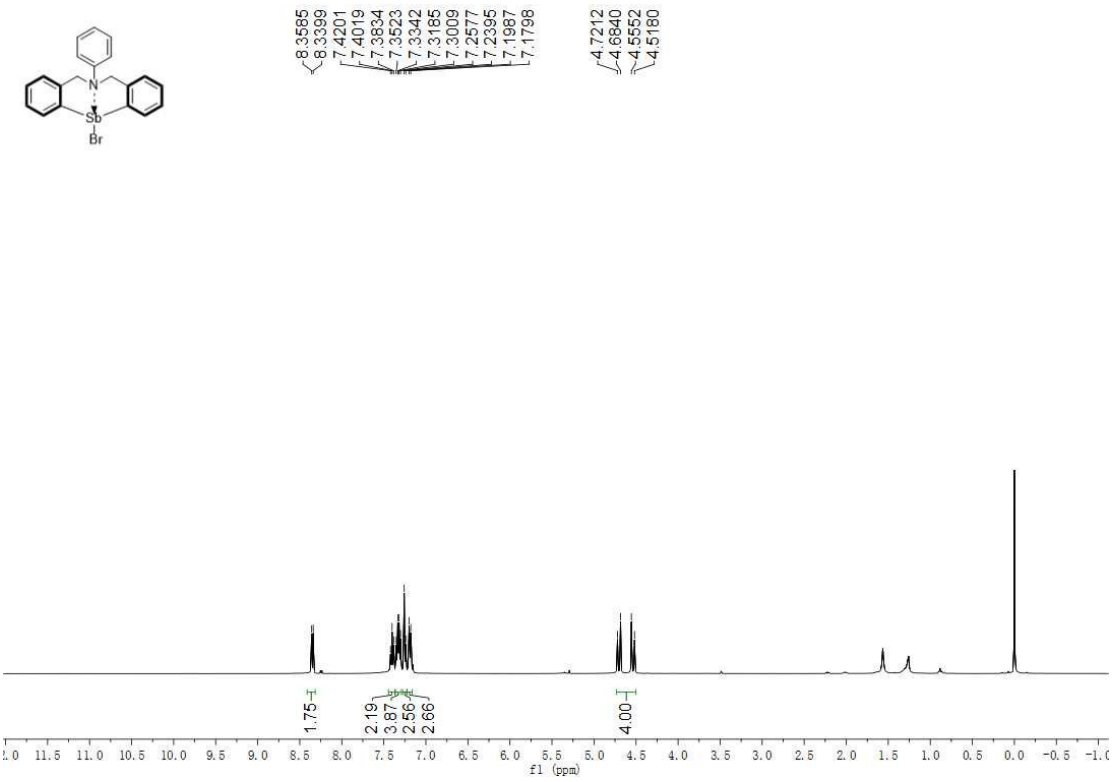
NMR Spectra



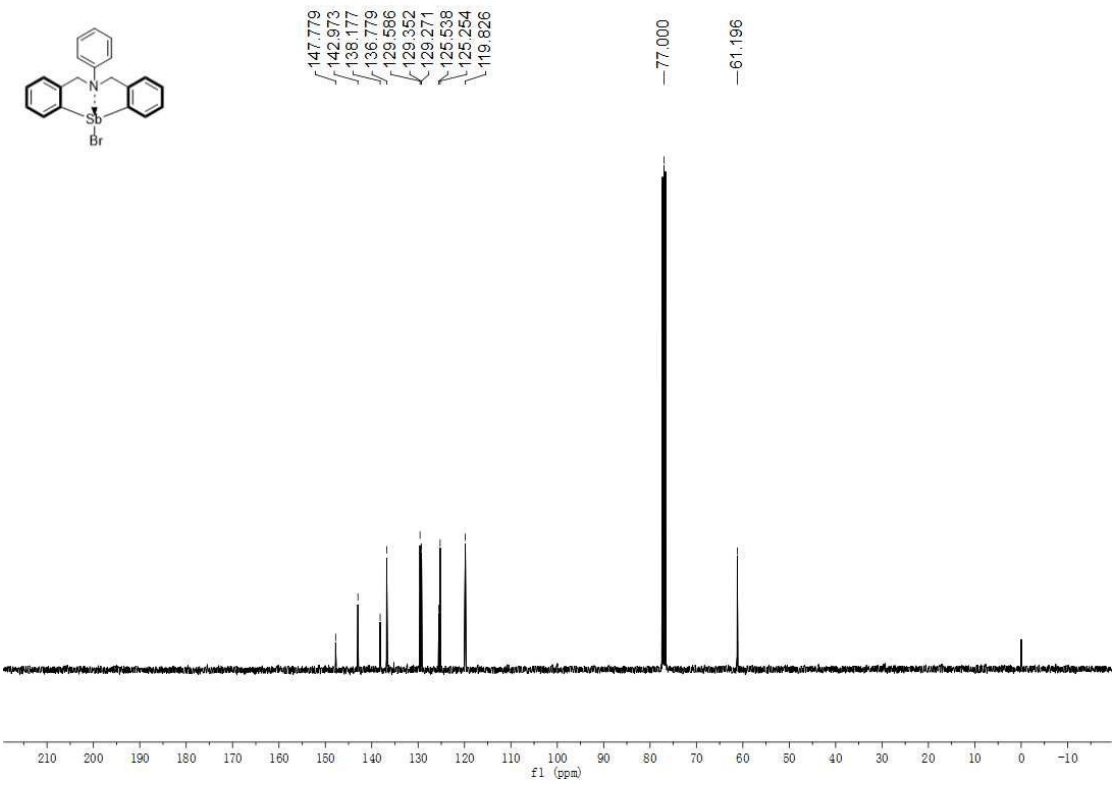
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **1b**



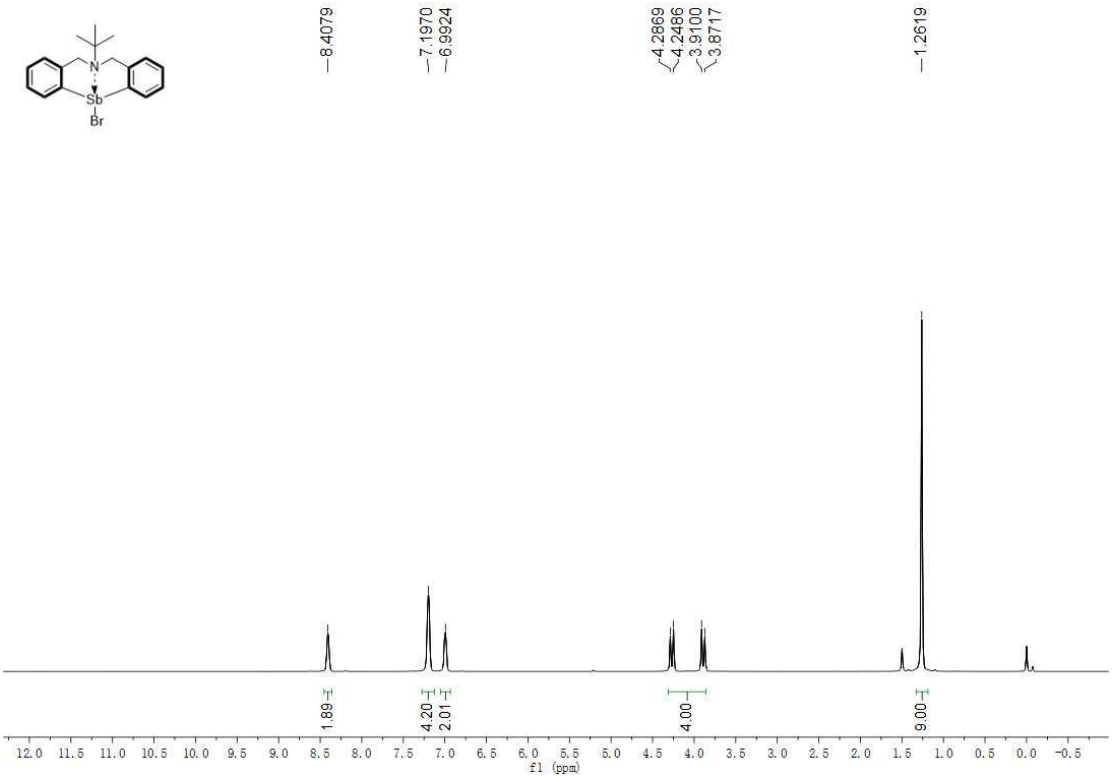
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **1b**



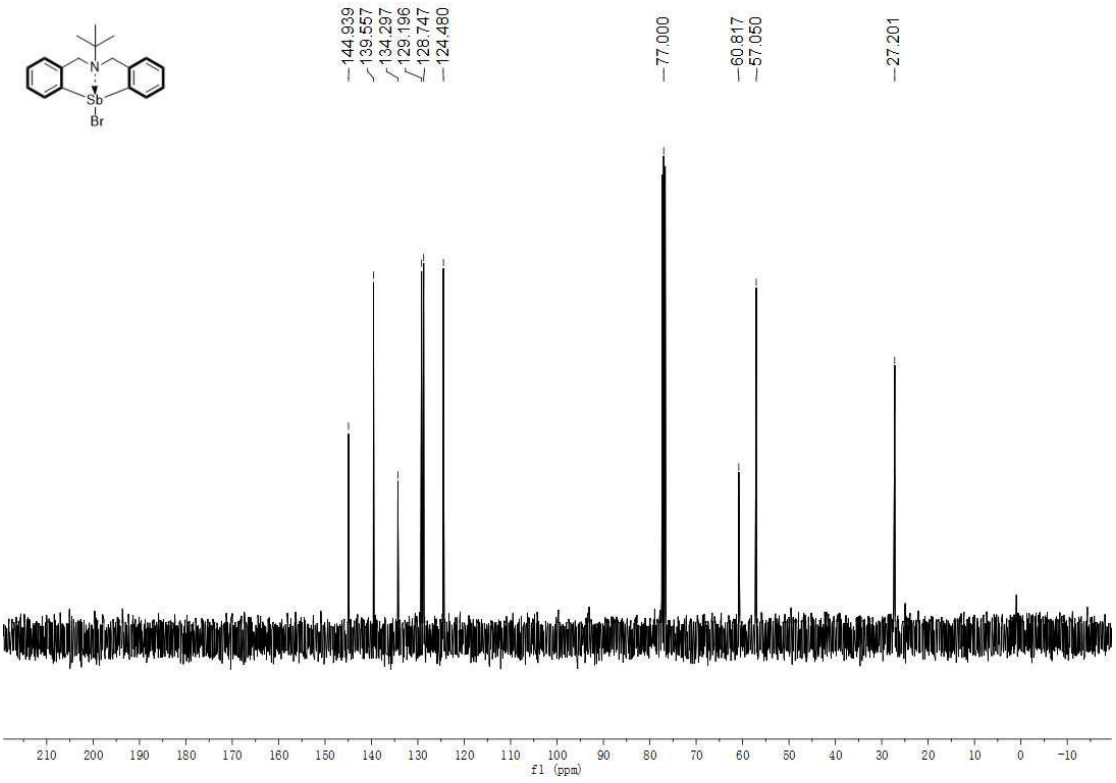
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **2b**



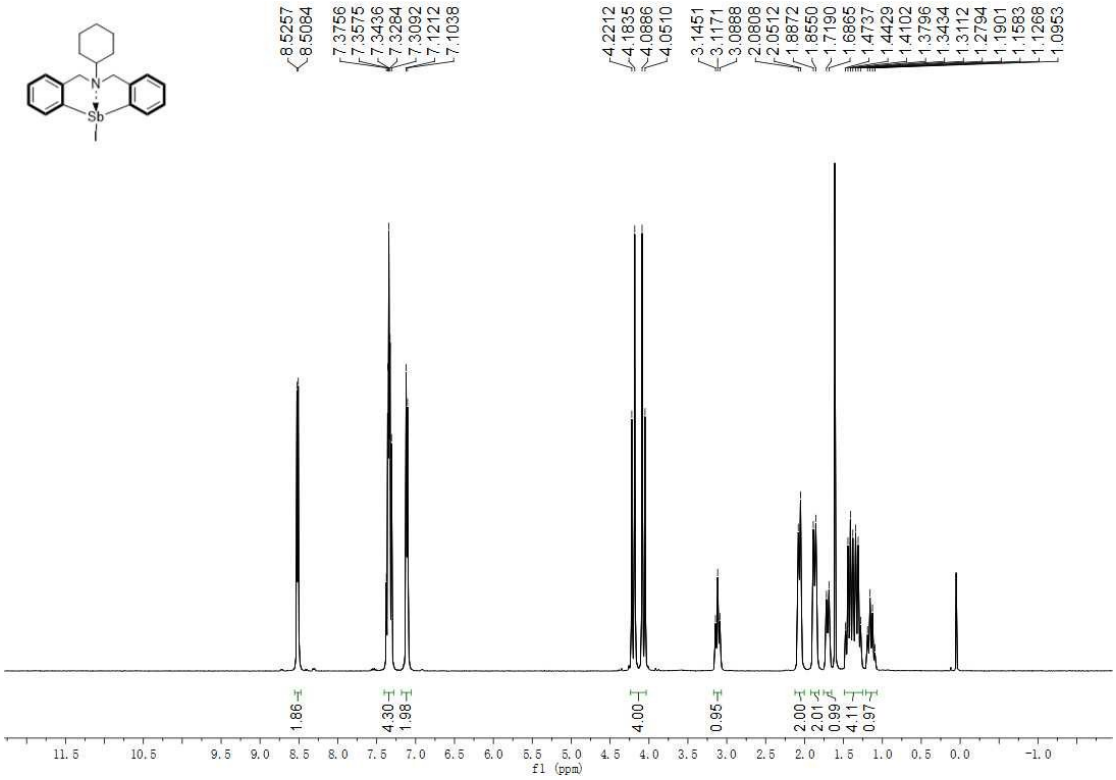
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **2b**



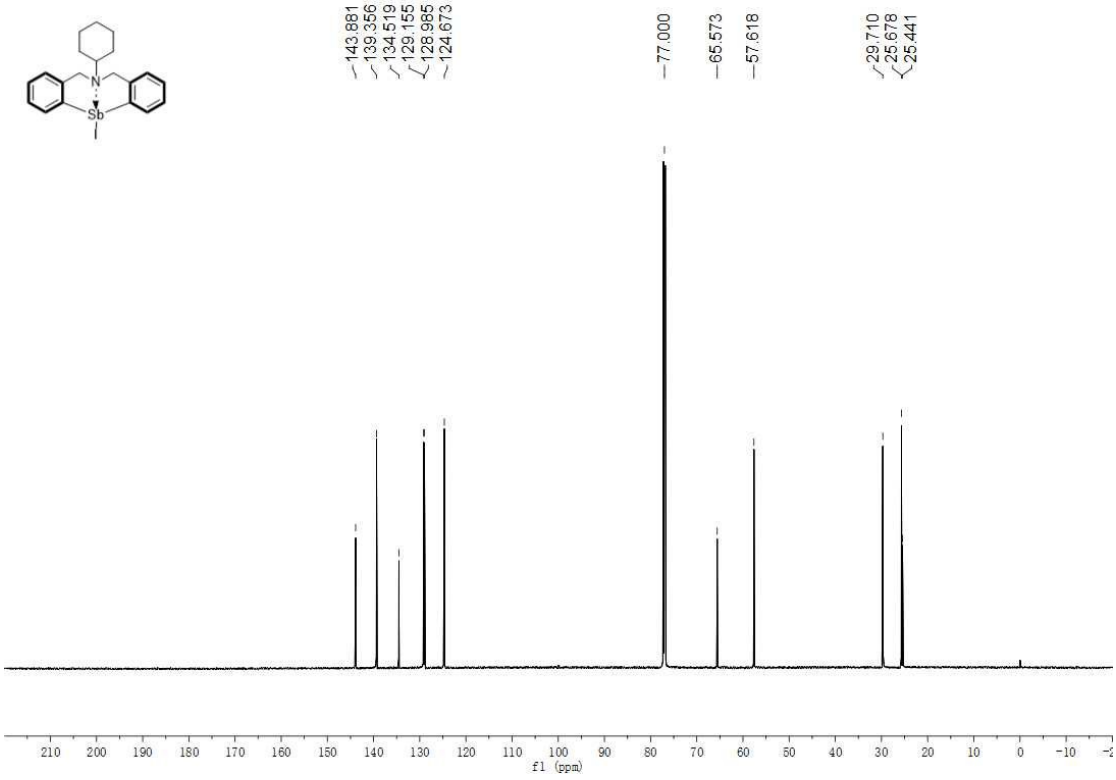
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **3b**



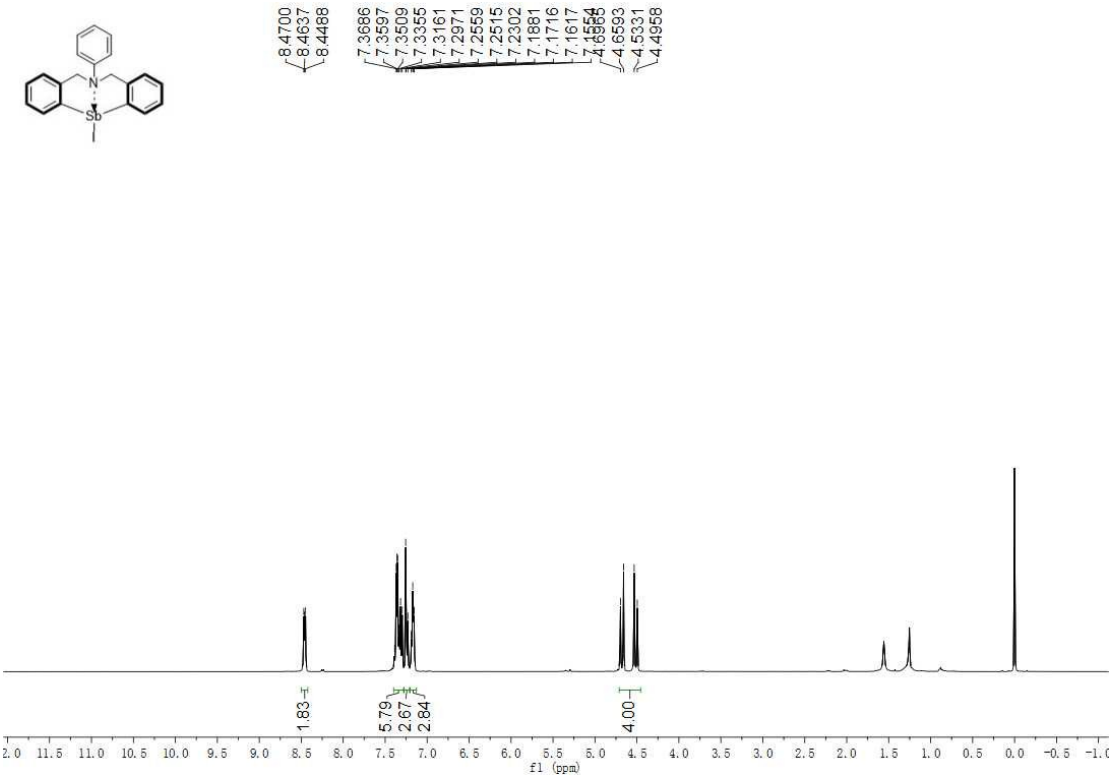
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **3b**



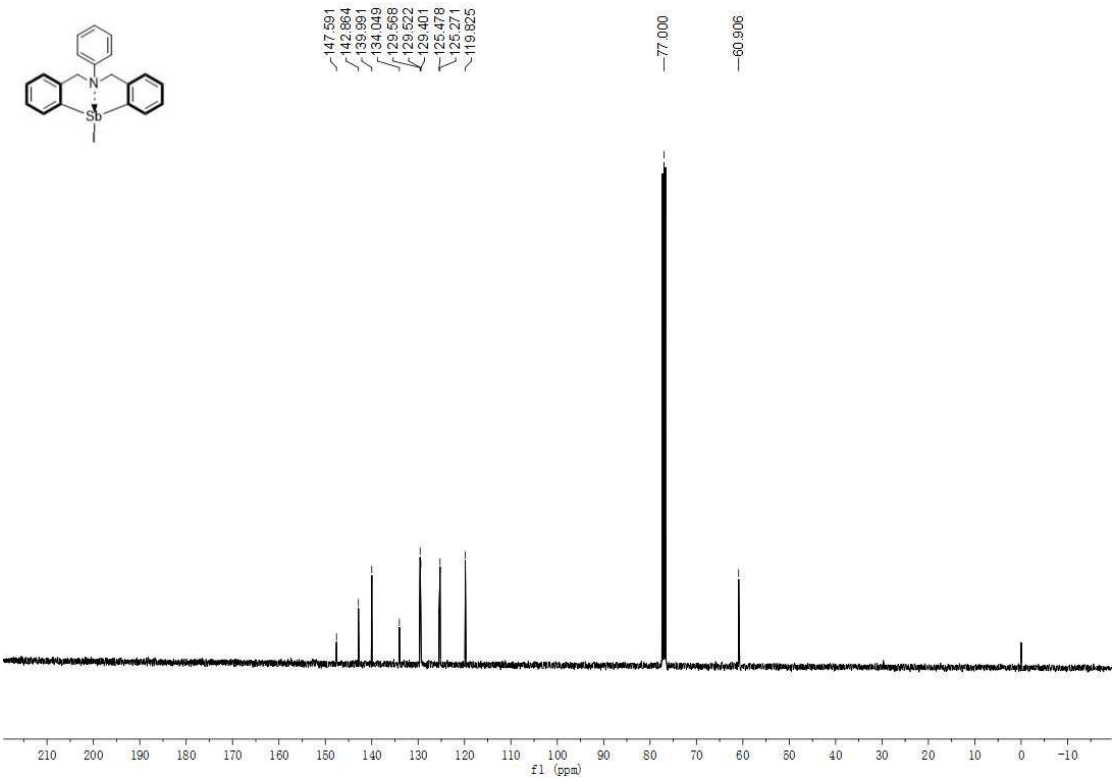
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **1c**



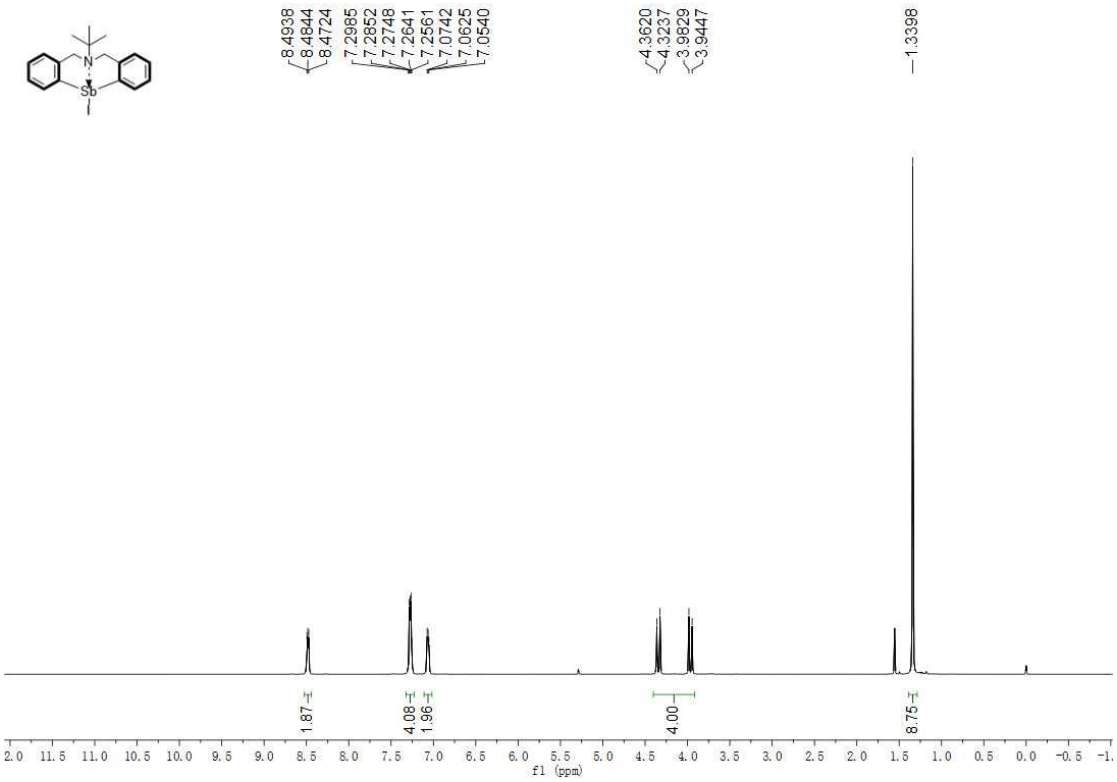
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **1c**



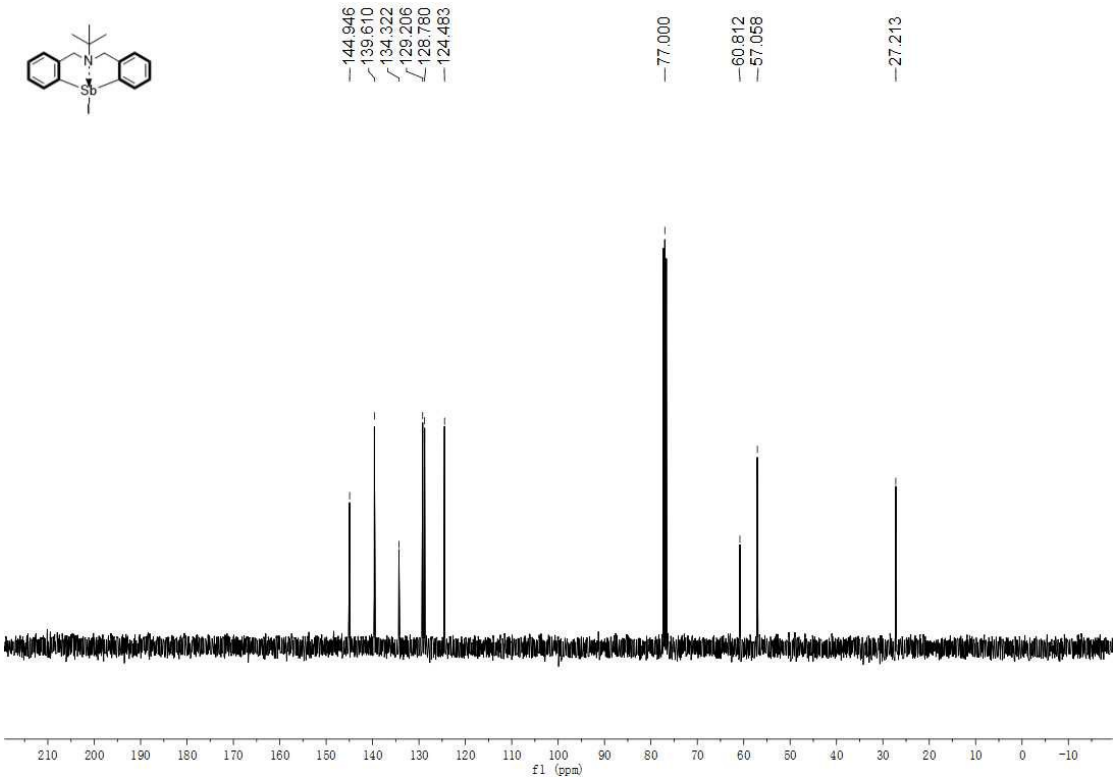
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **2c**



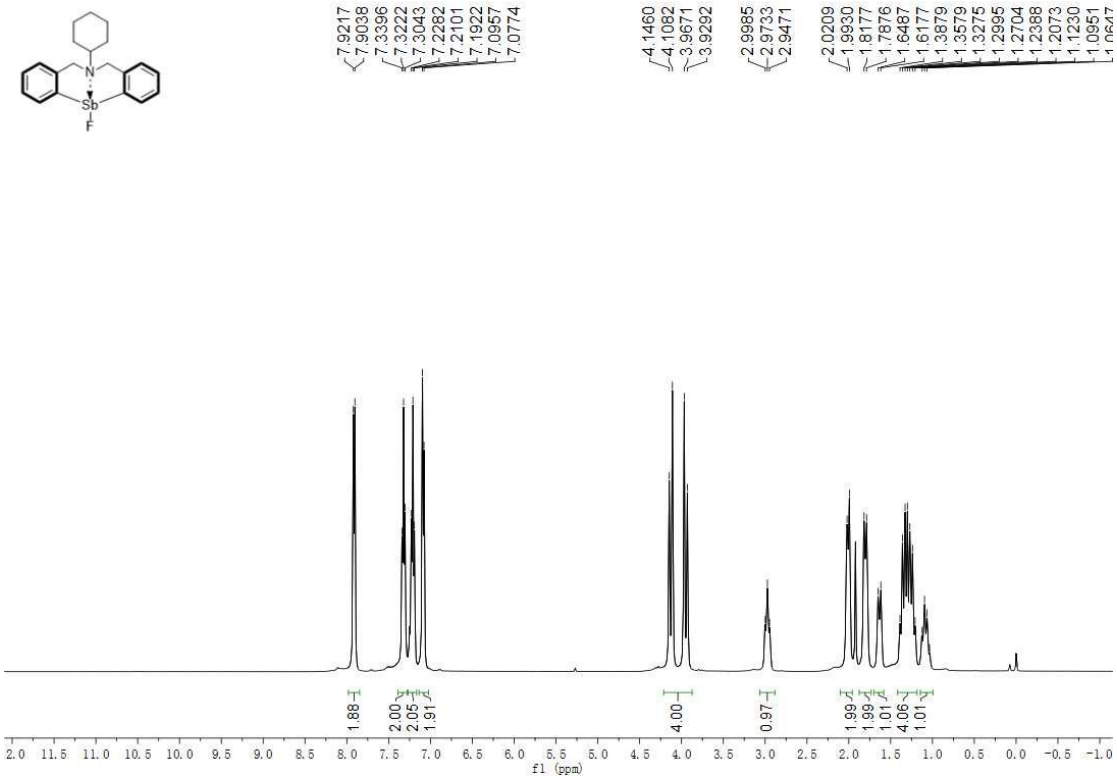
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **2c**



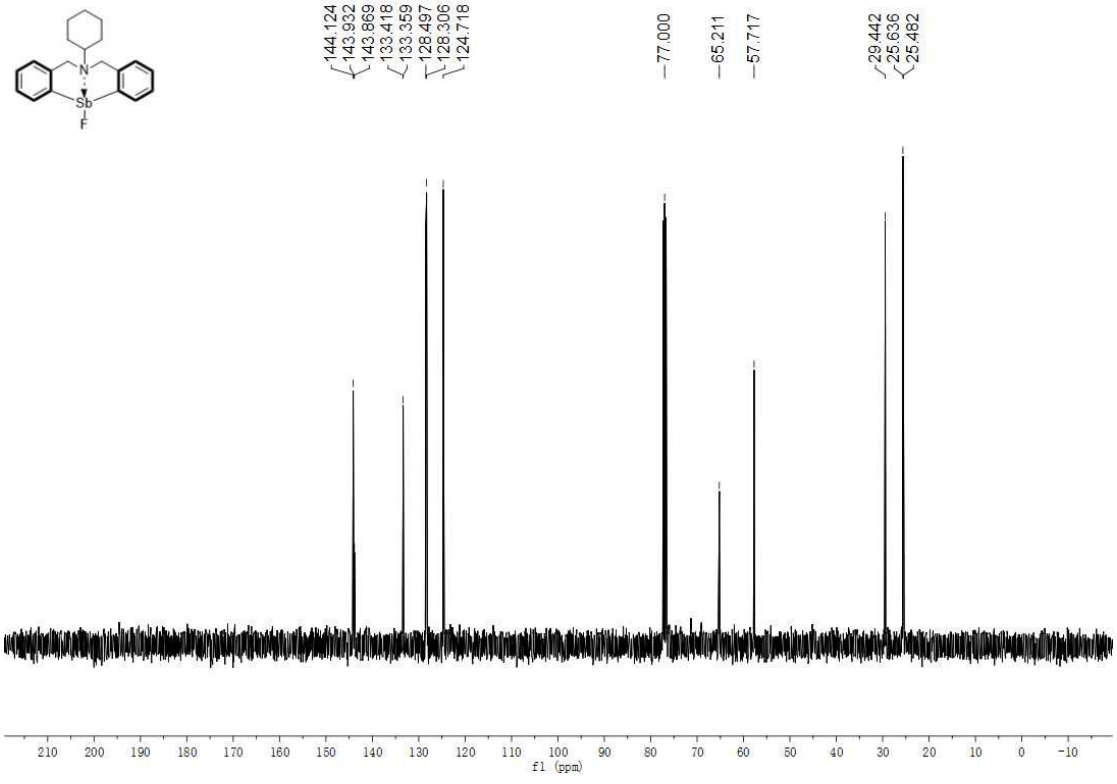
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **3c**



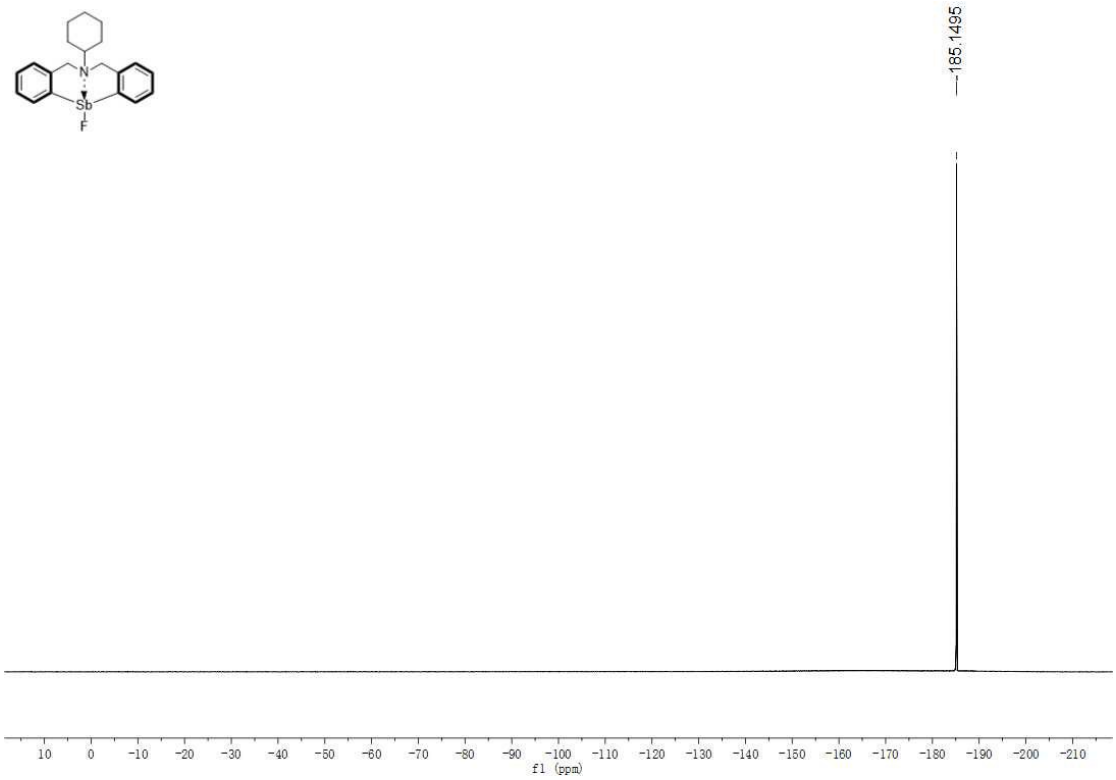
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **3c**



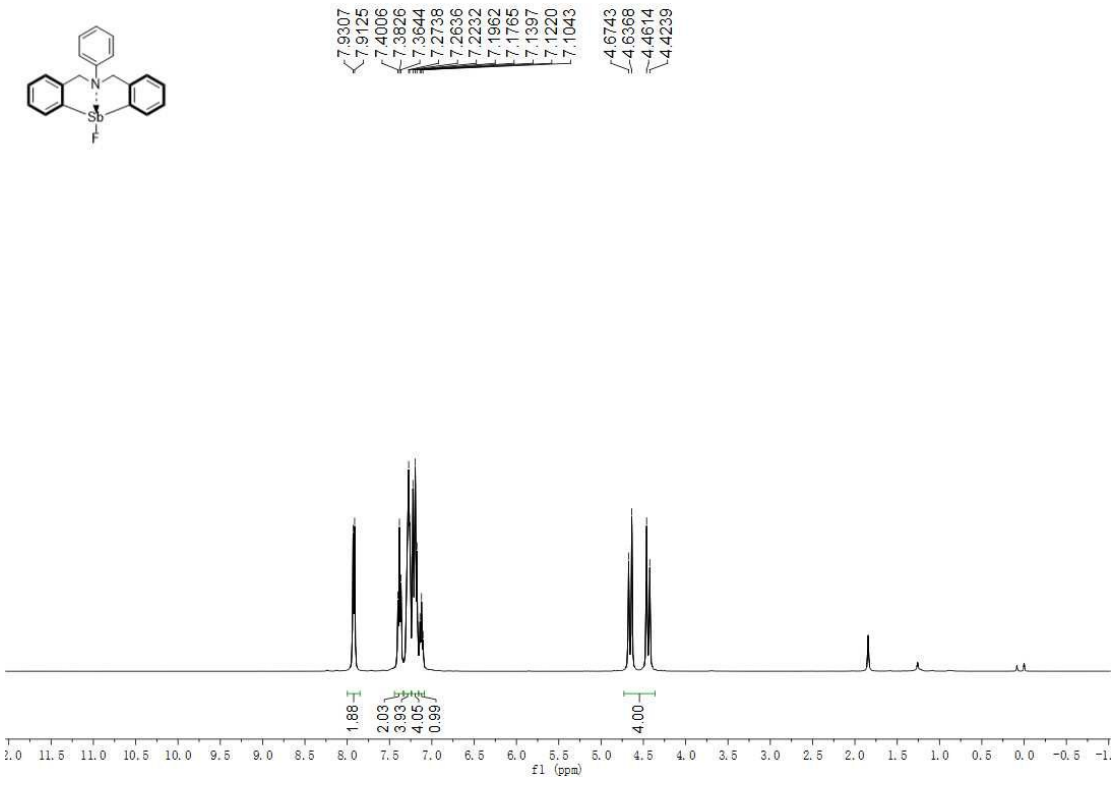
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **1d**



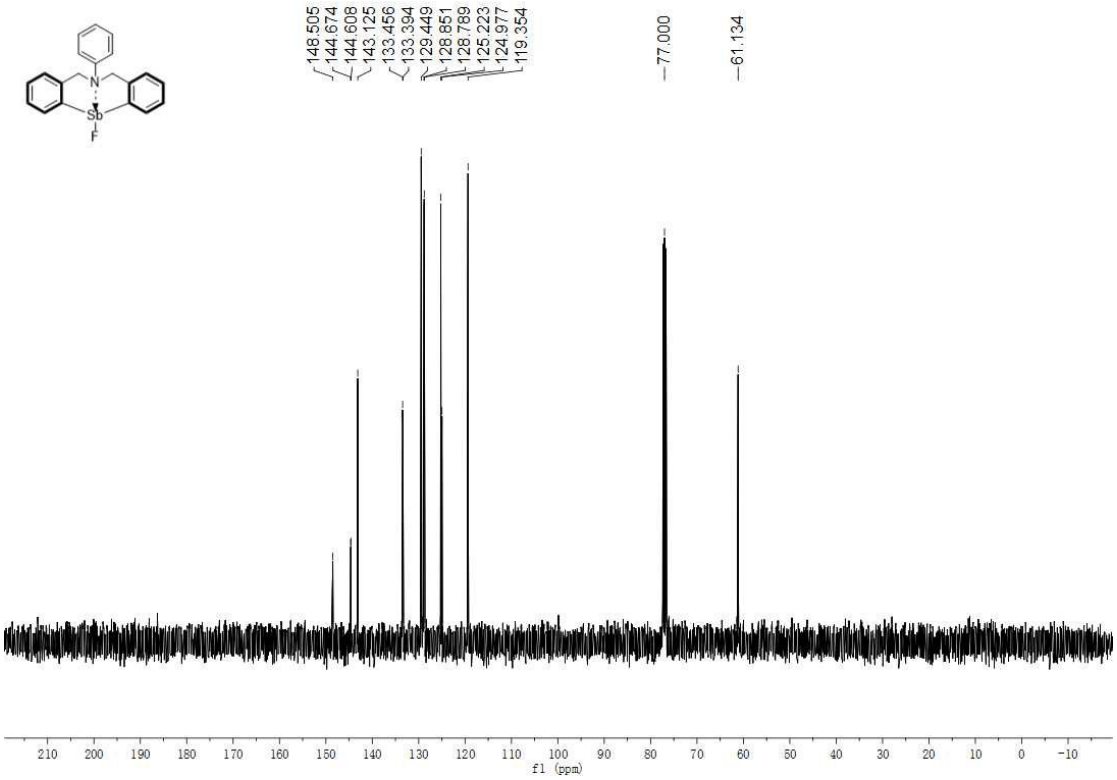
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **1d**



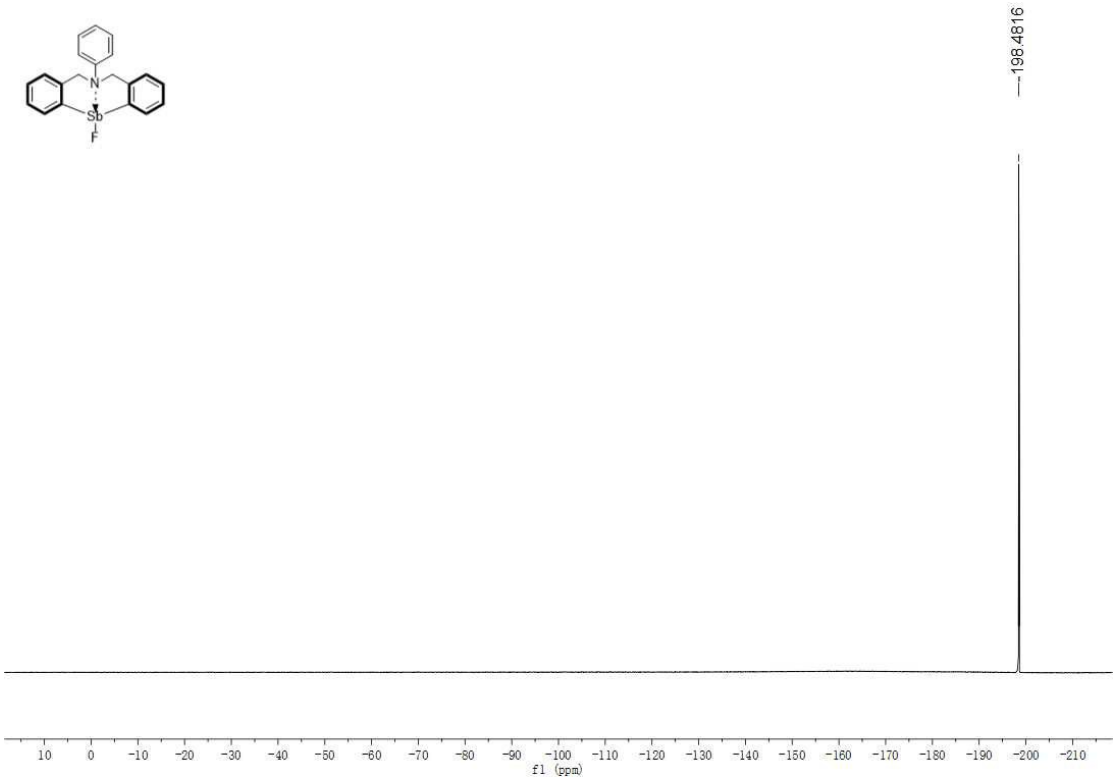
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of catalyst **1d**



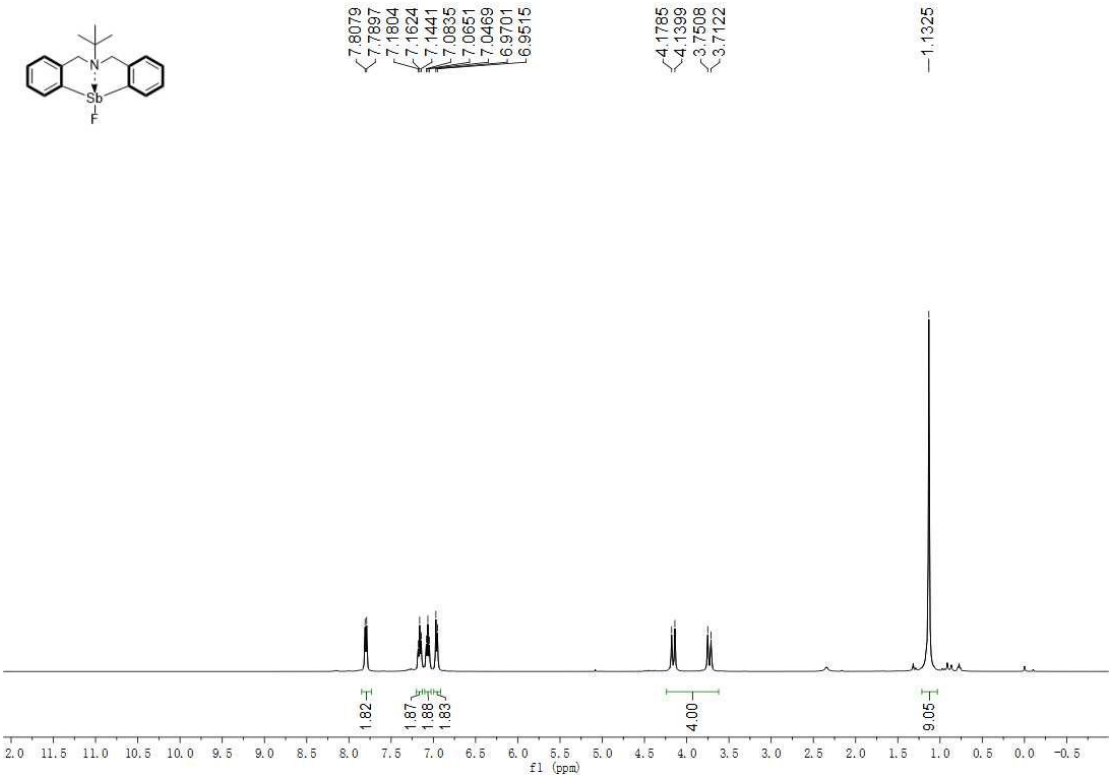
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **2d**



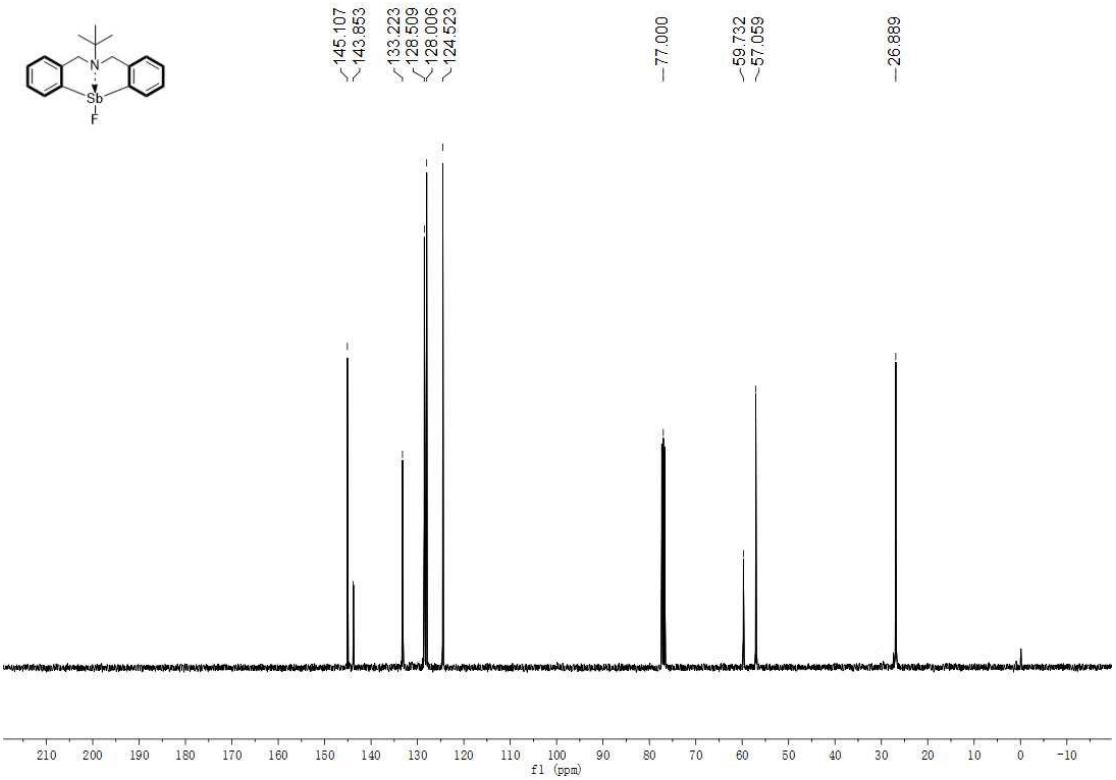
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **2d**



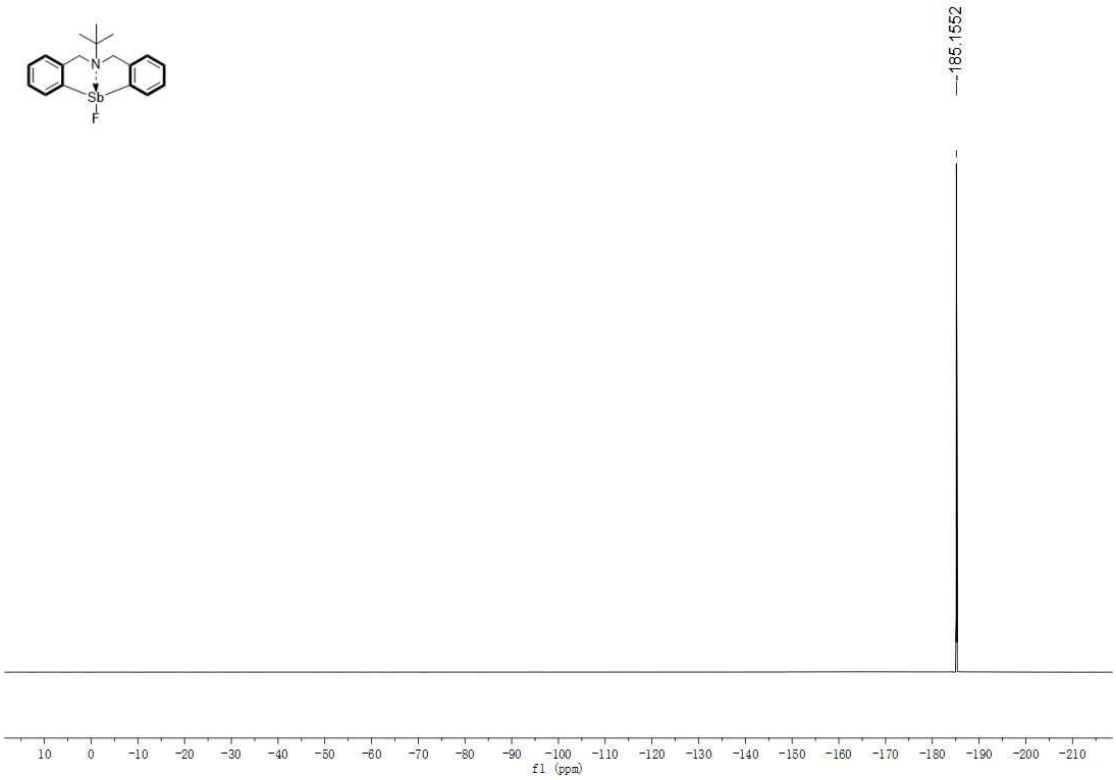
^{19}F NMR (376 MHz, $CDCl_3$) spectrum of catalyst **2d**



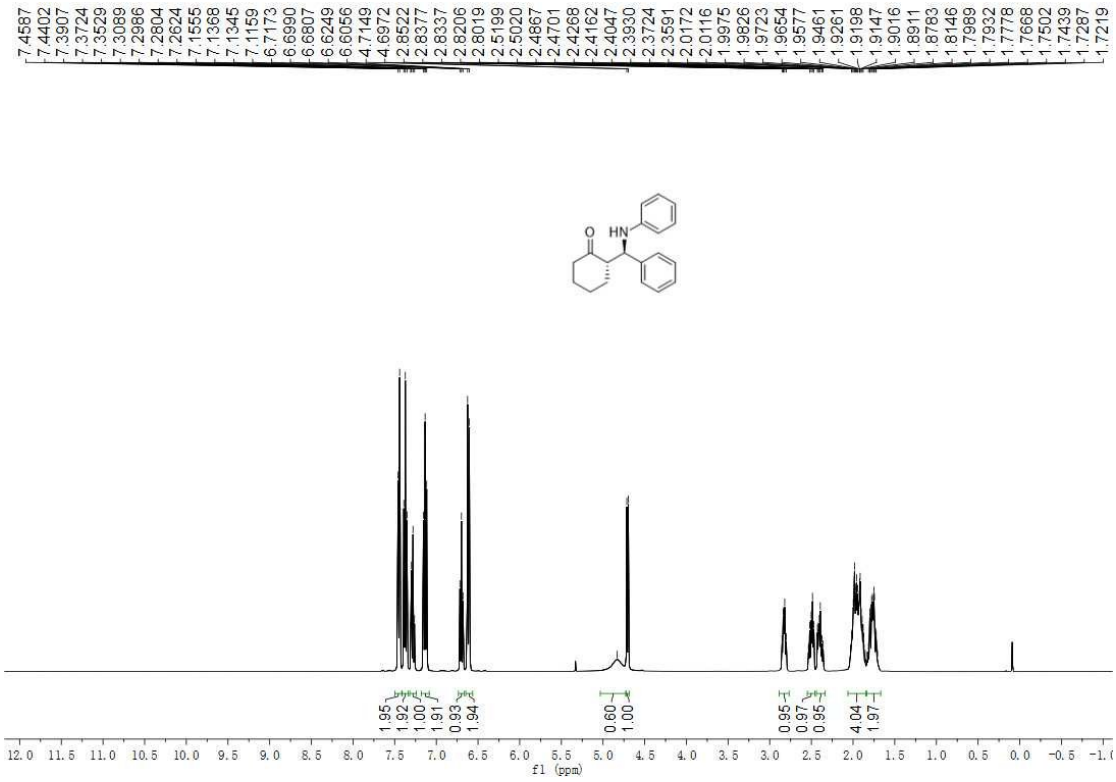
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **3d**



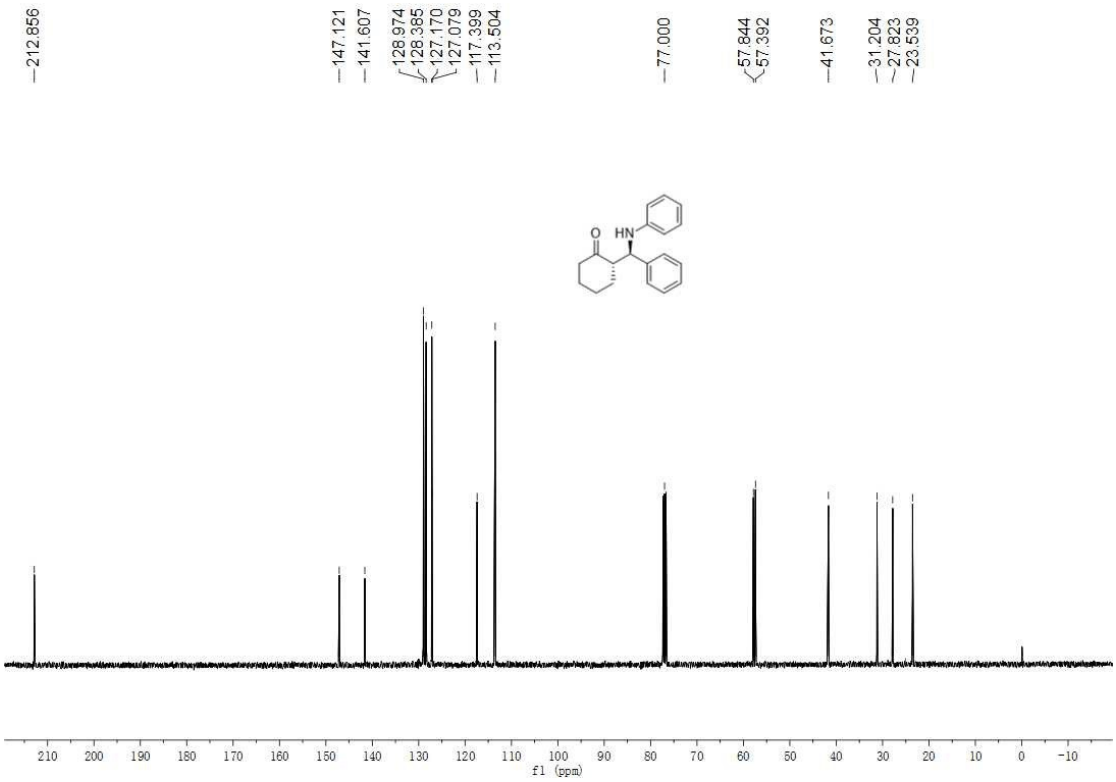
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of catalyst **3d**



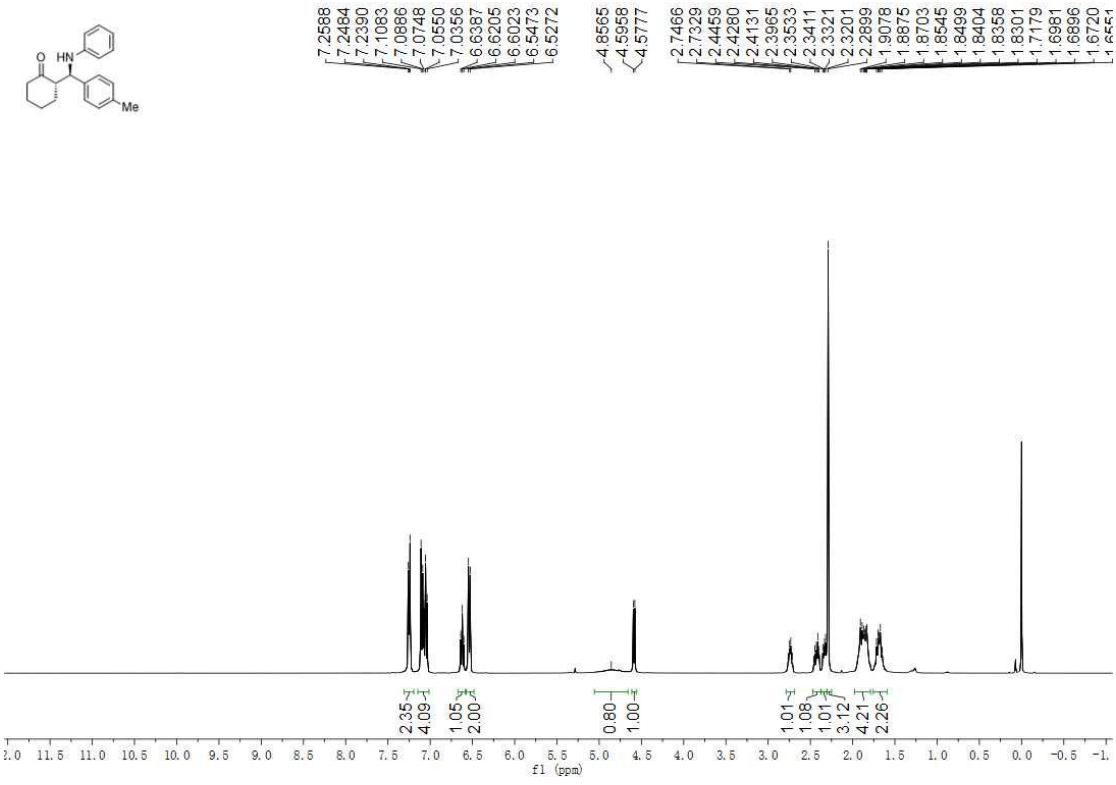
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of catalyst **3d**



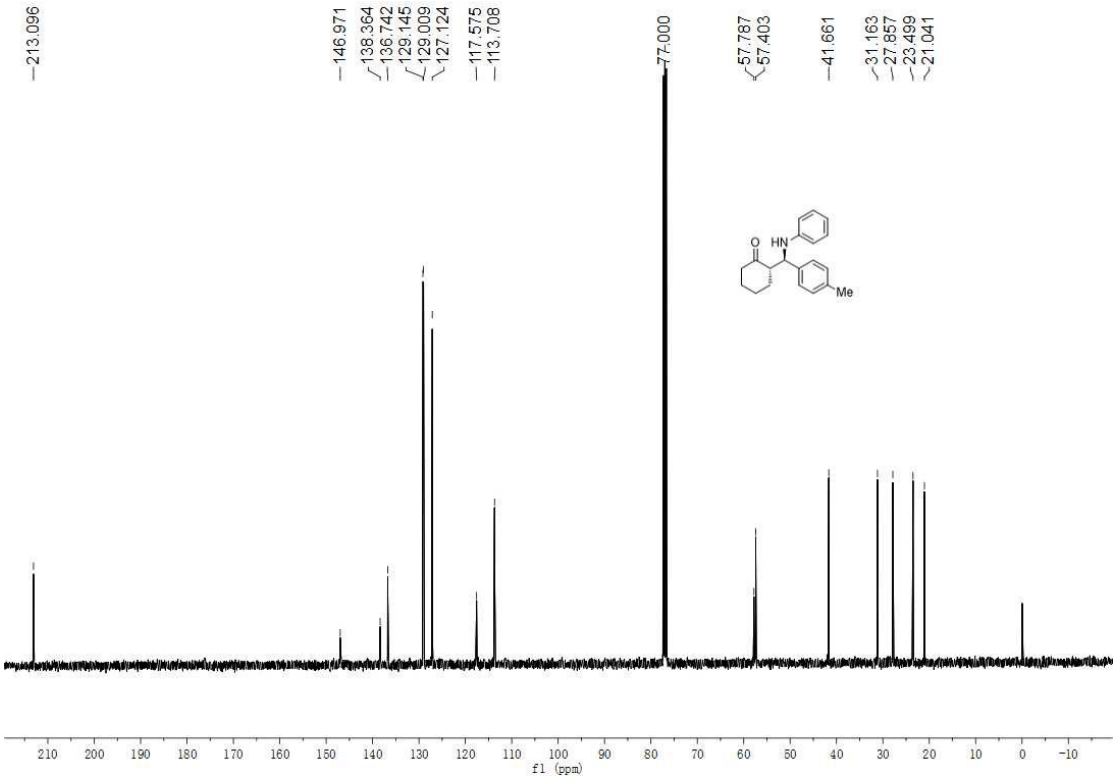
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4a**



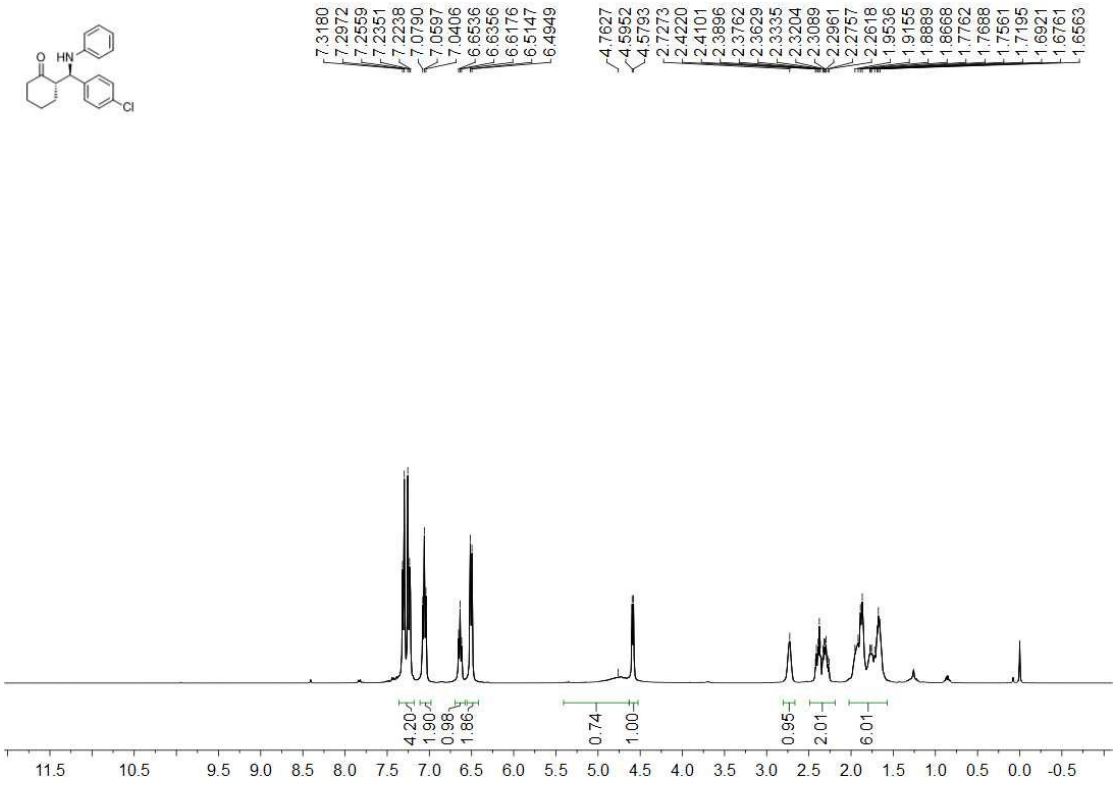
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4a**



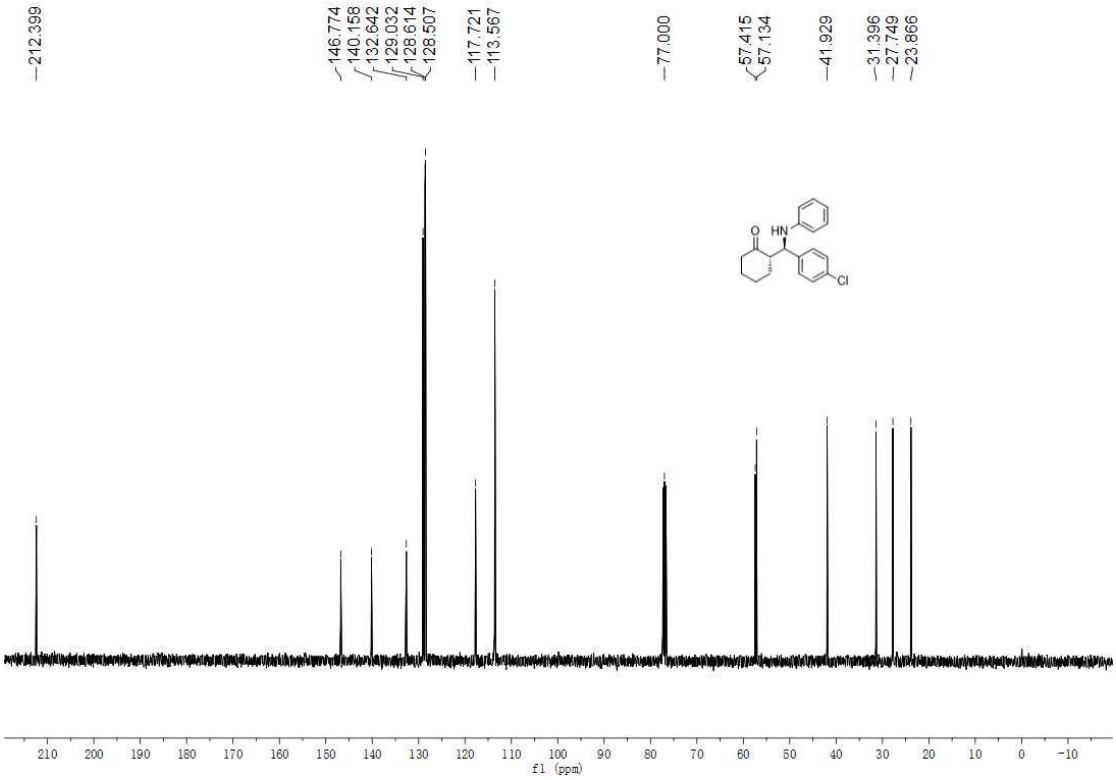
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4b**



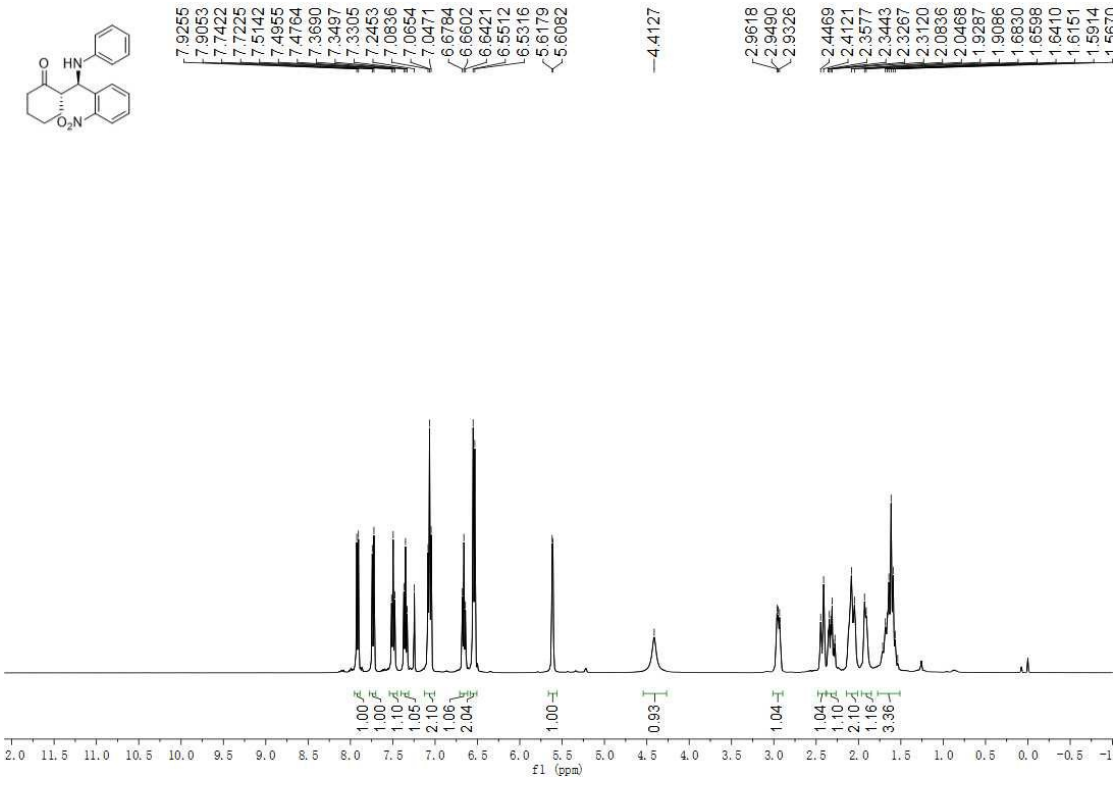
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4b**



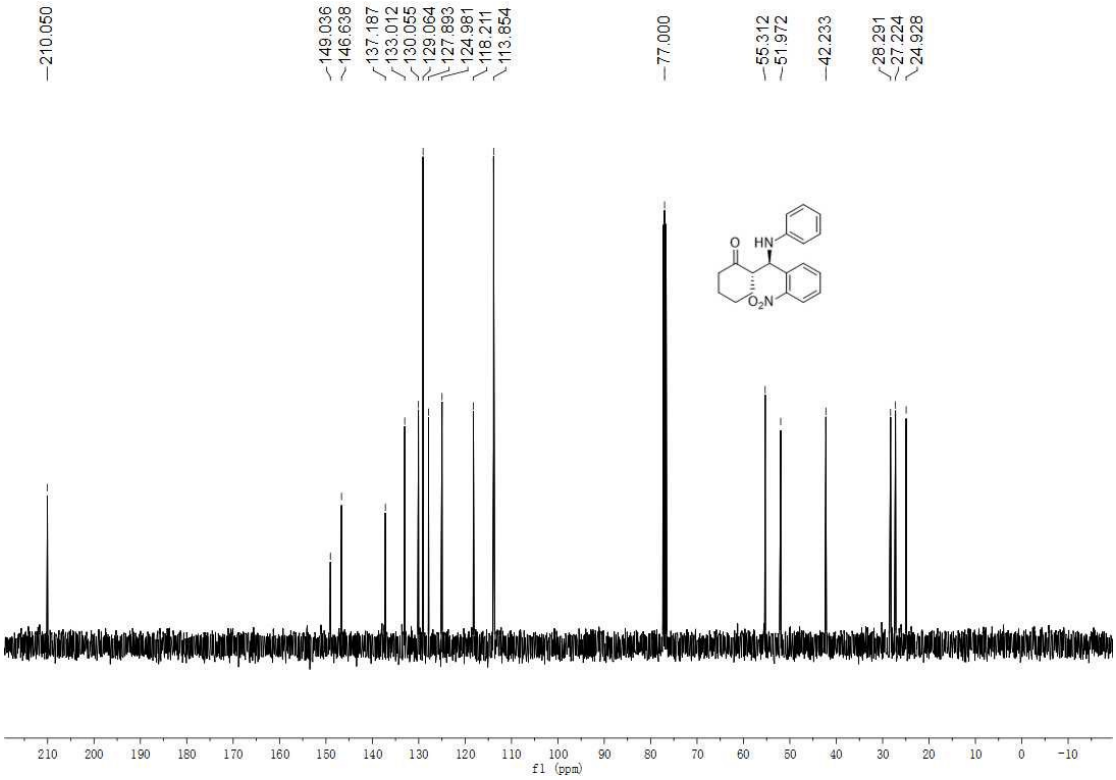
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4c**



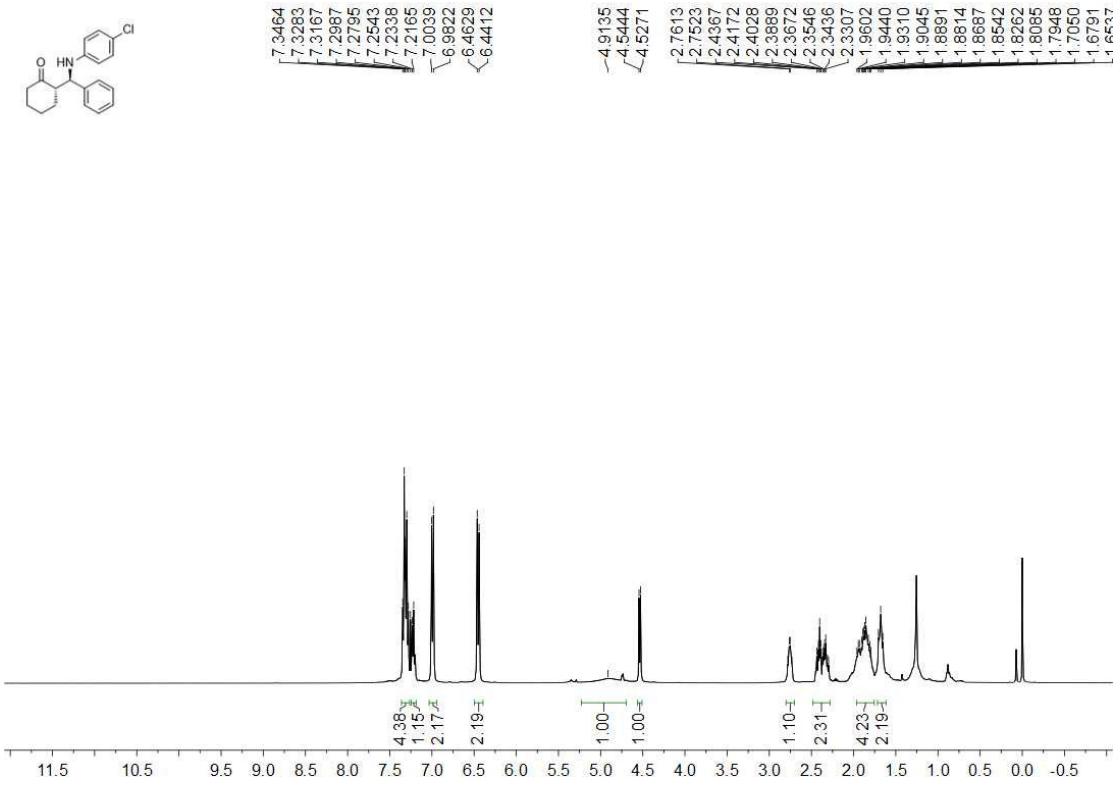
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4c**



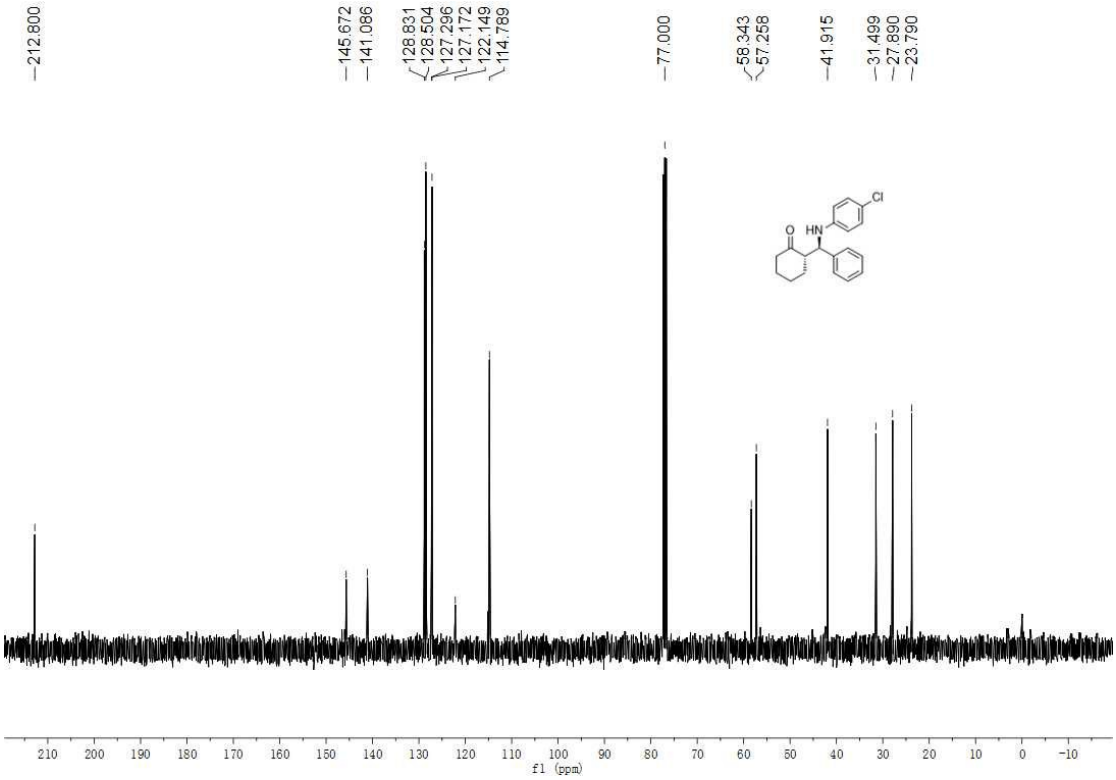
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4d**



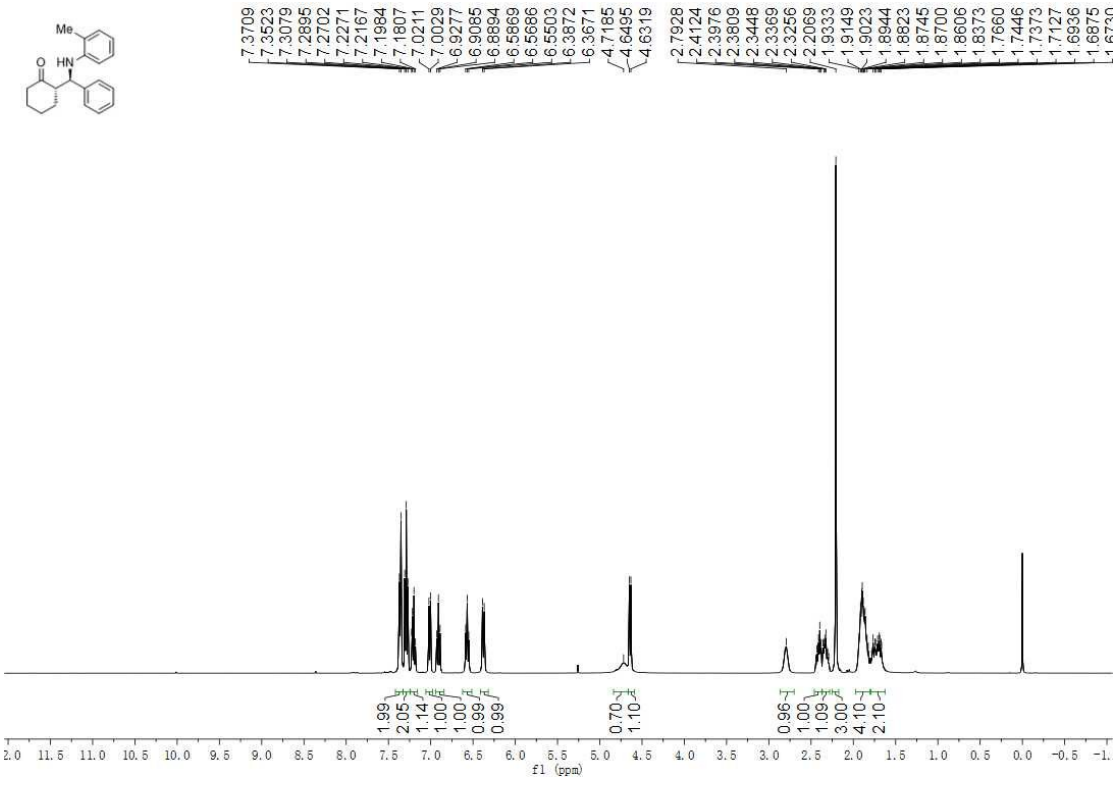
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4d**



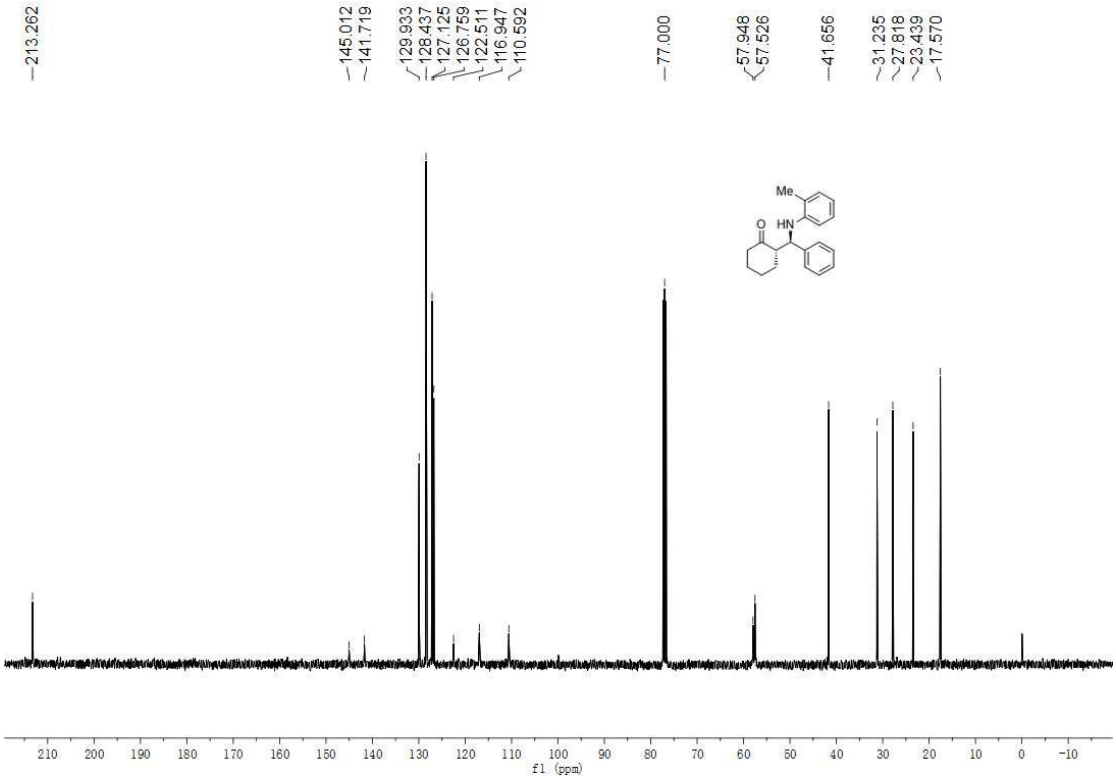
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4e**



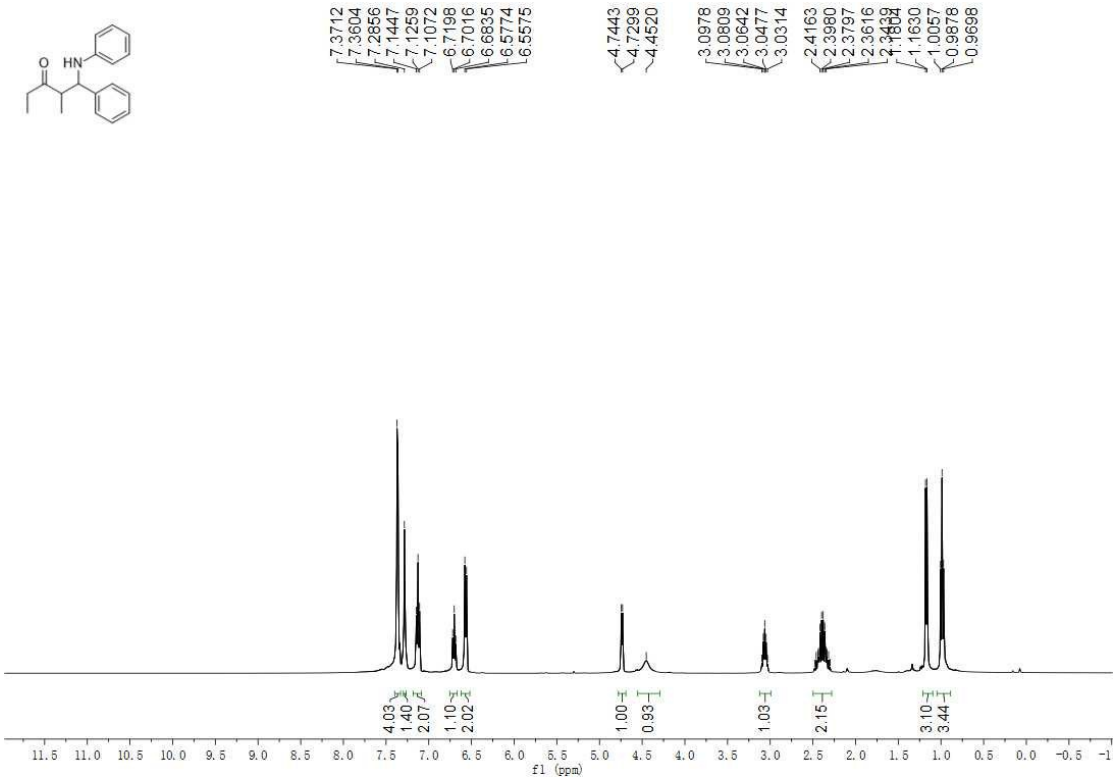
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4e**



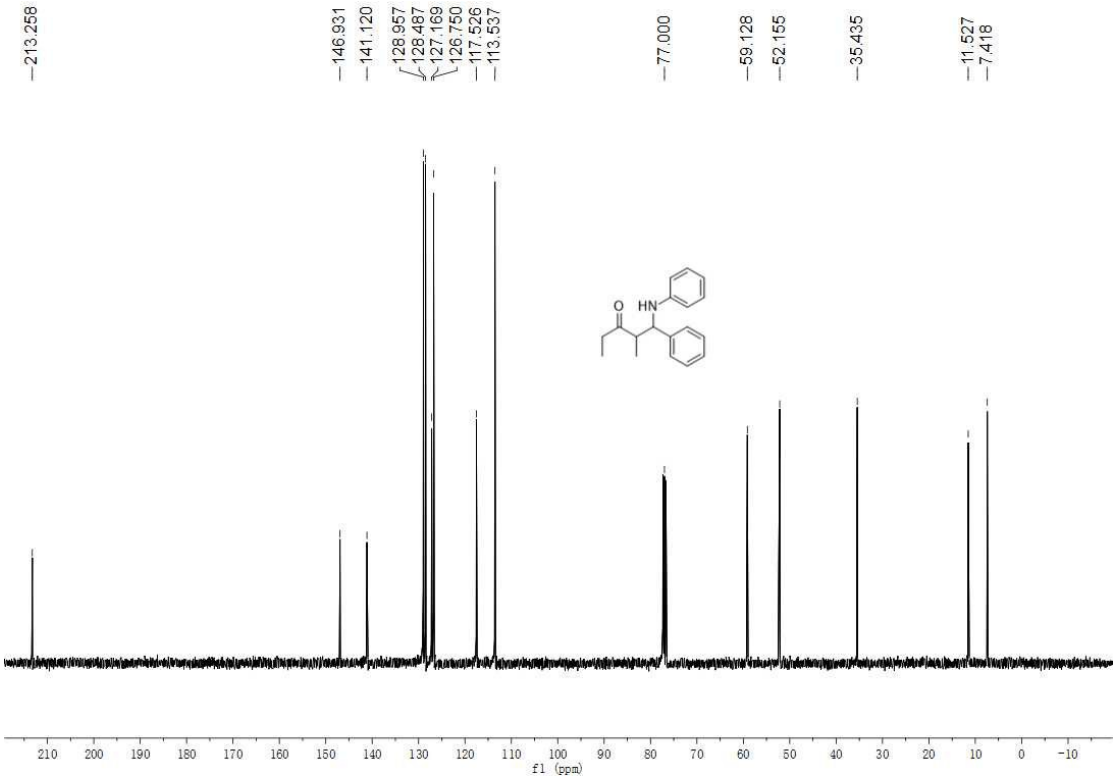
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4f**



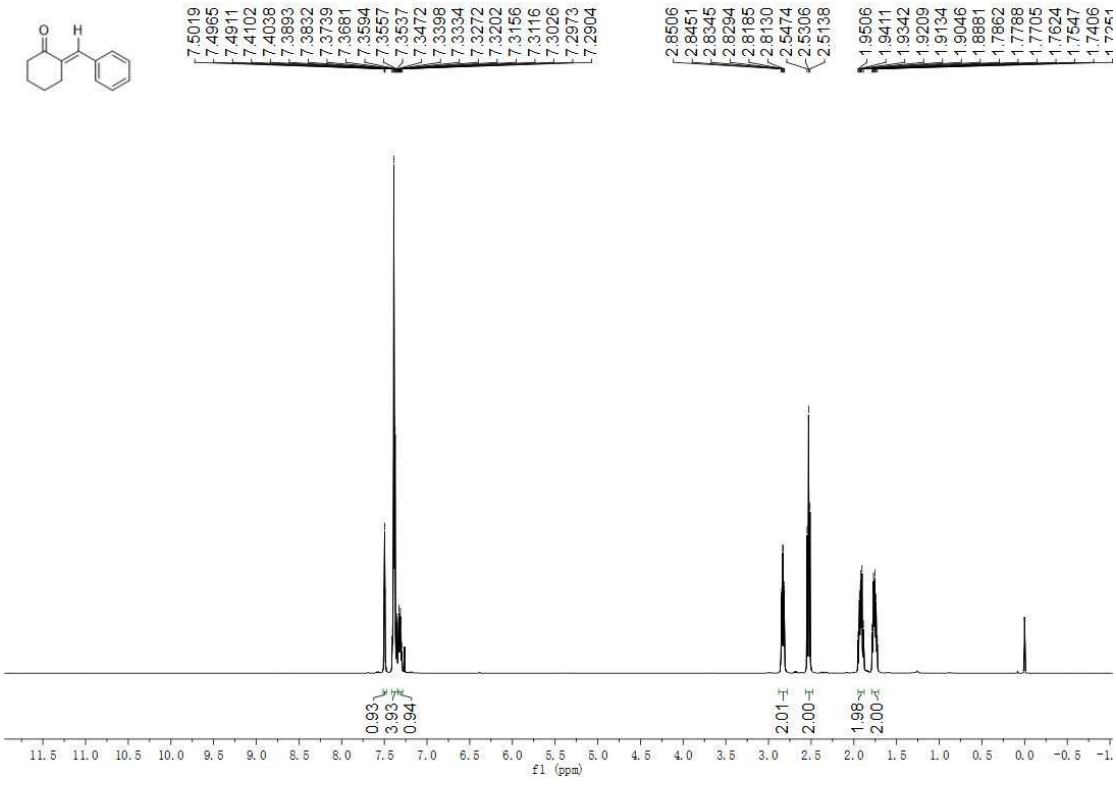
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4f**



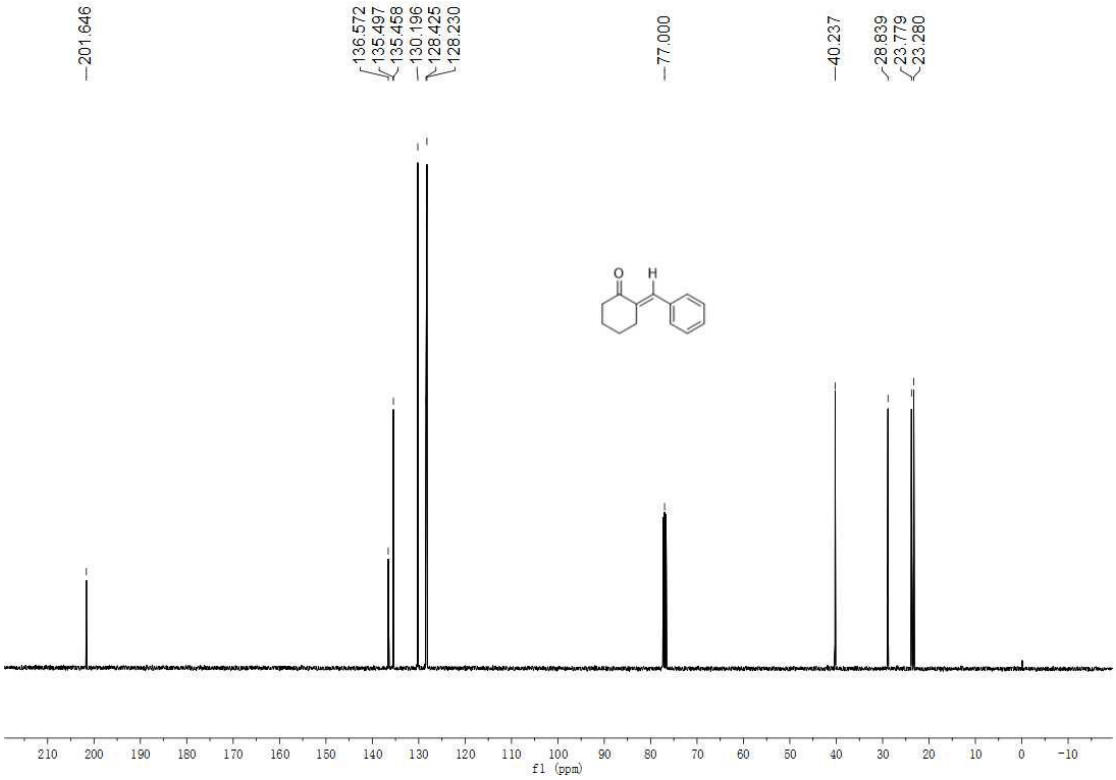
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **4g**



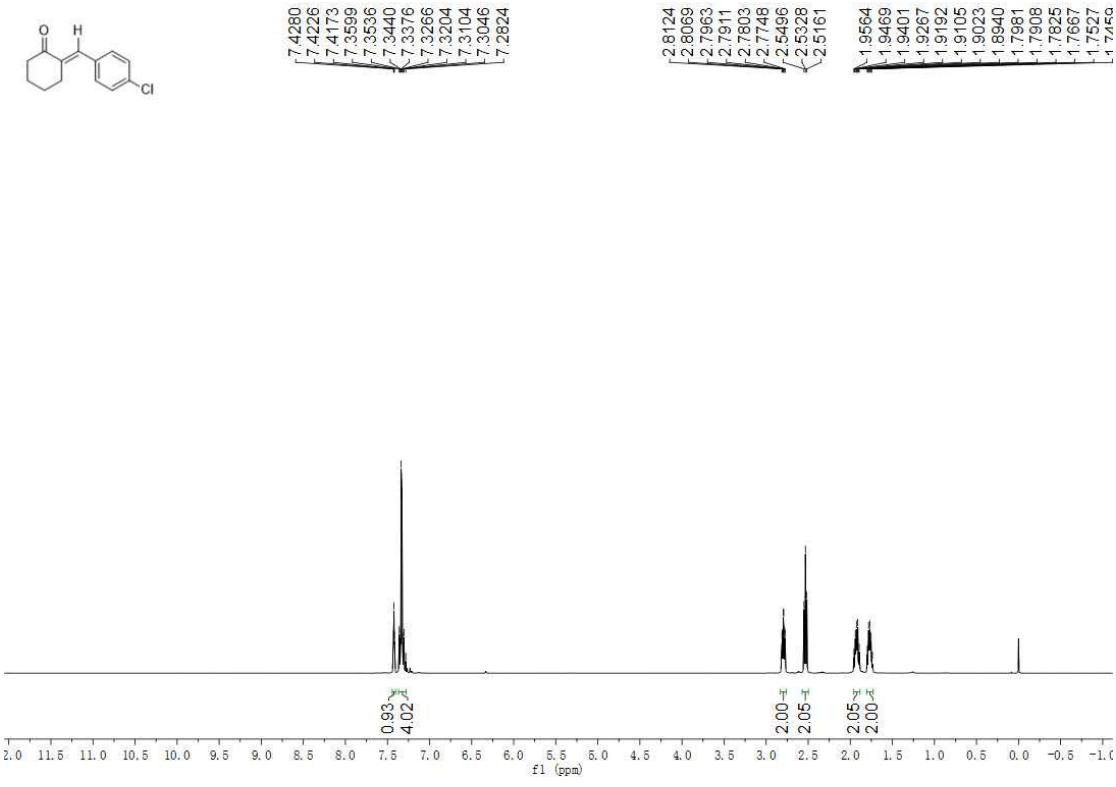
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **4g**



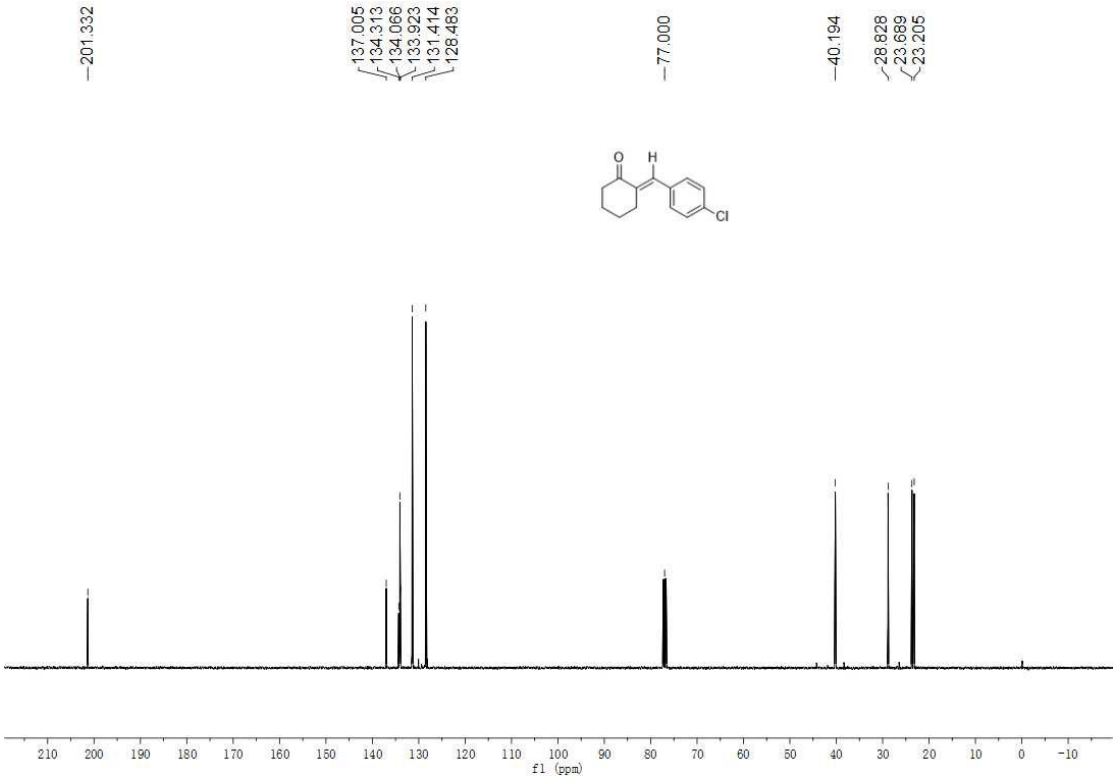
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5a**



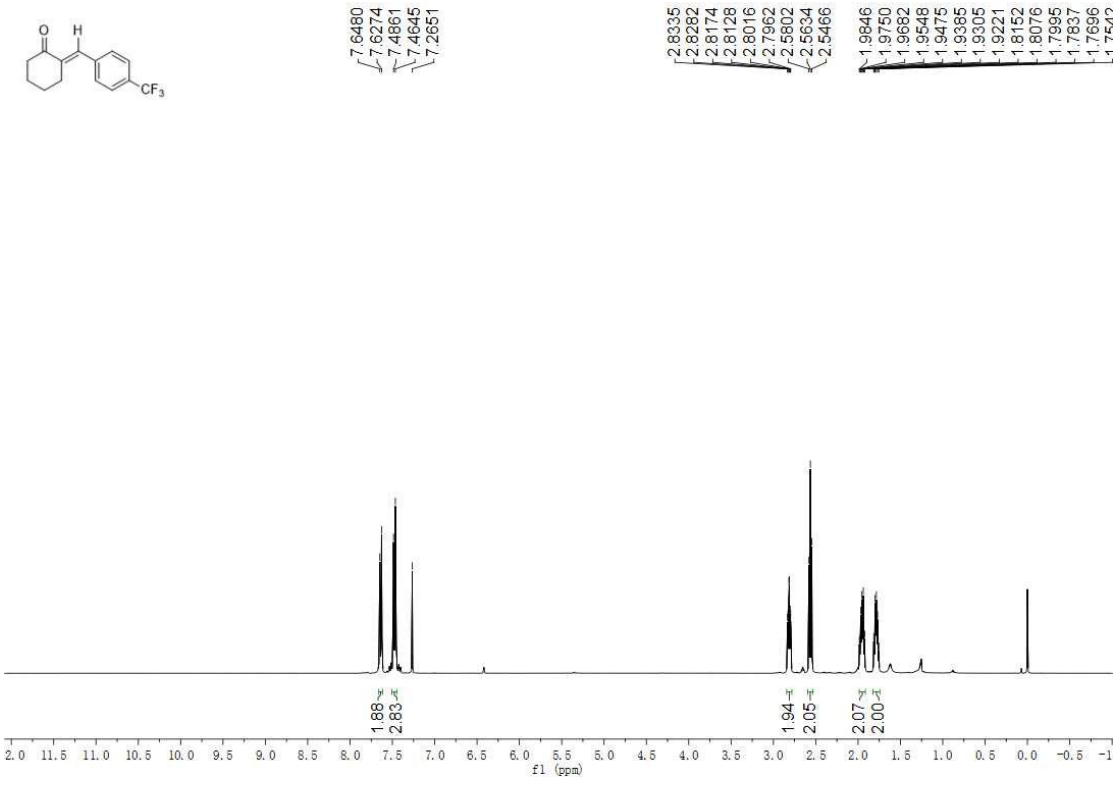
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5a**



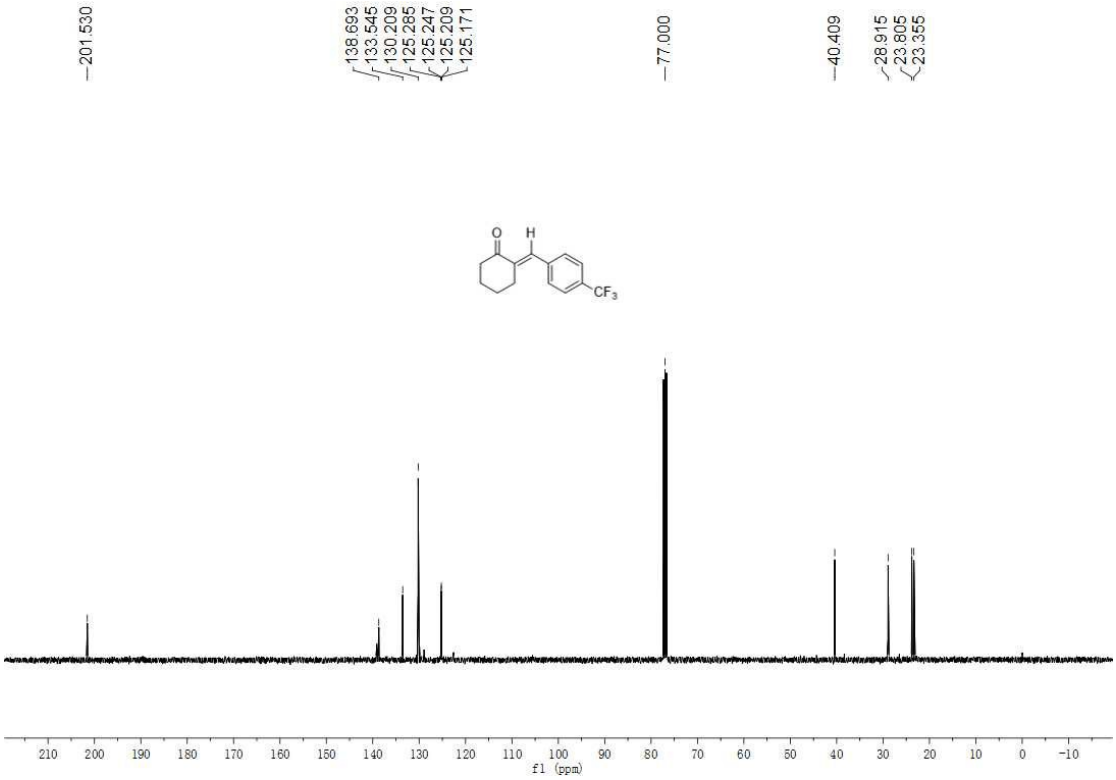
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5b**



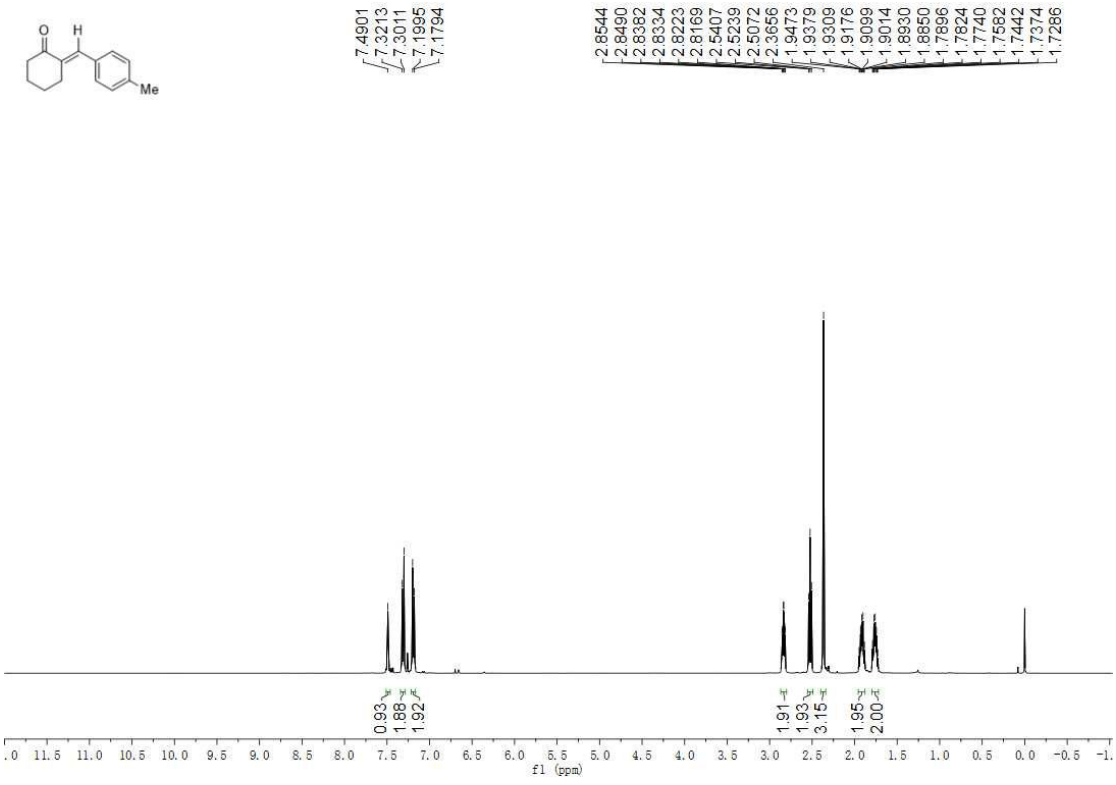
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5b**



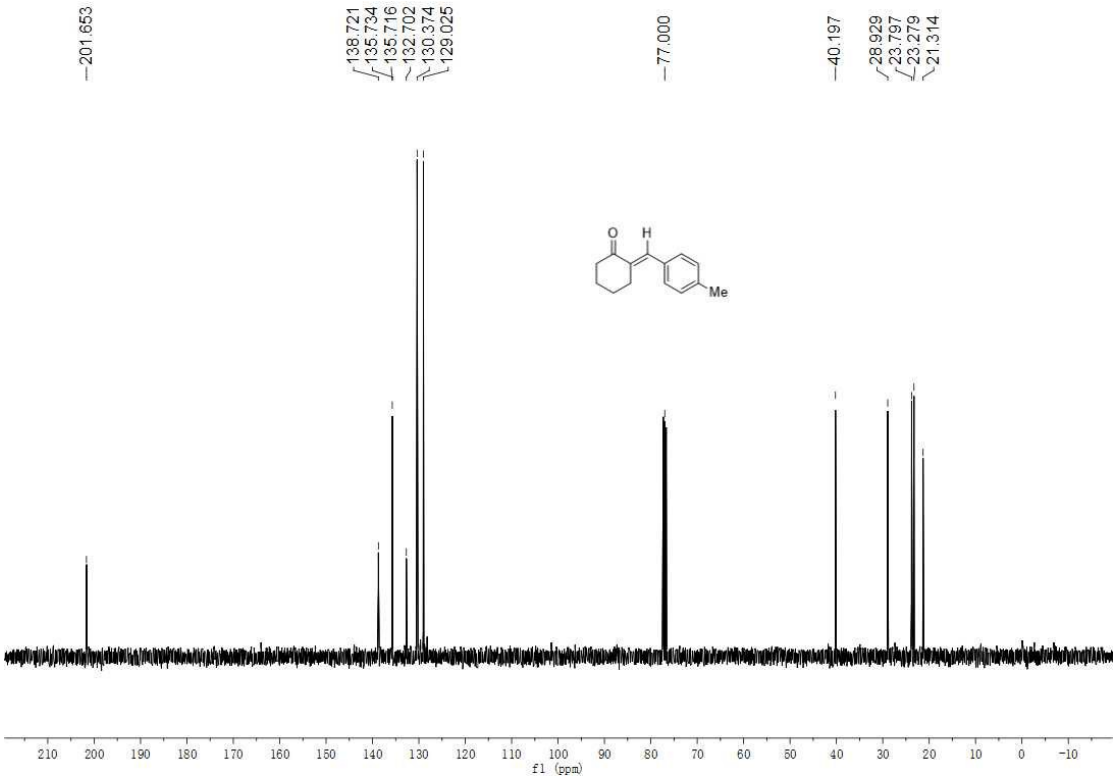
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5c**



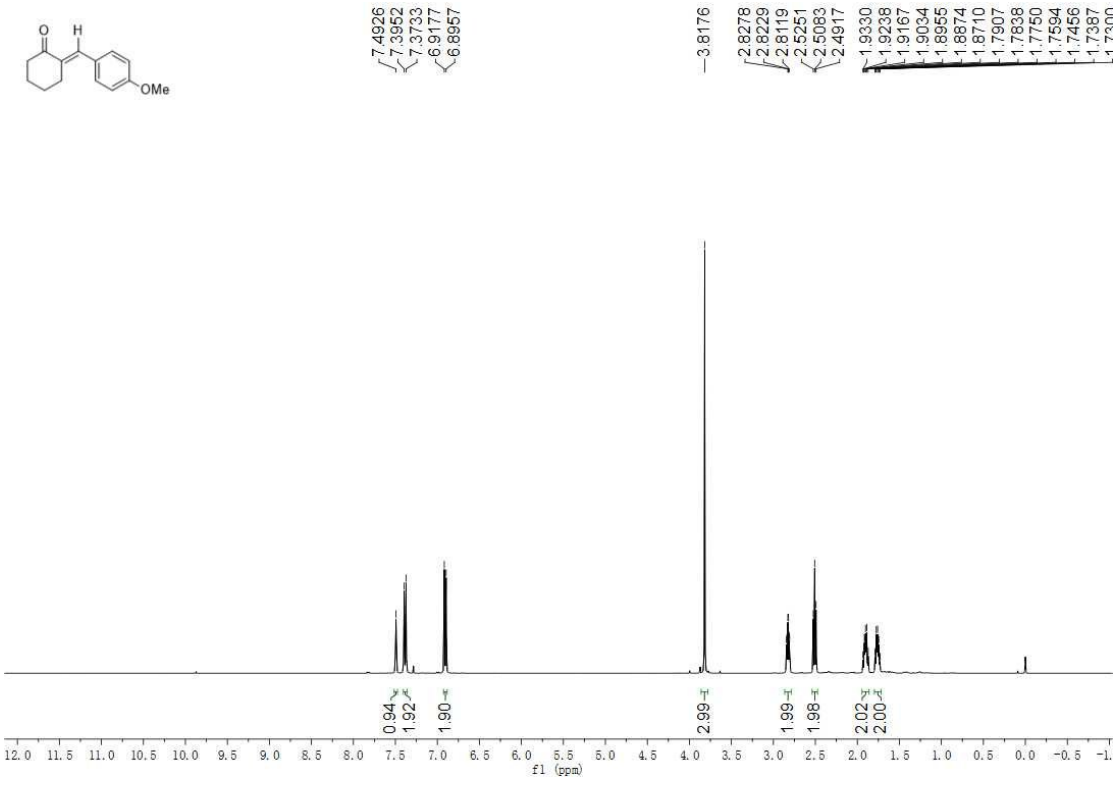
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5c**



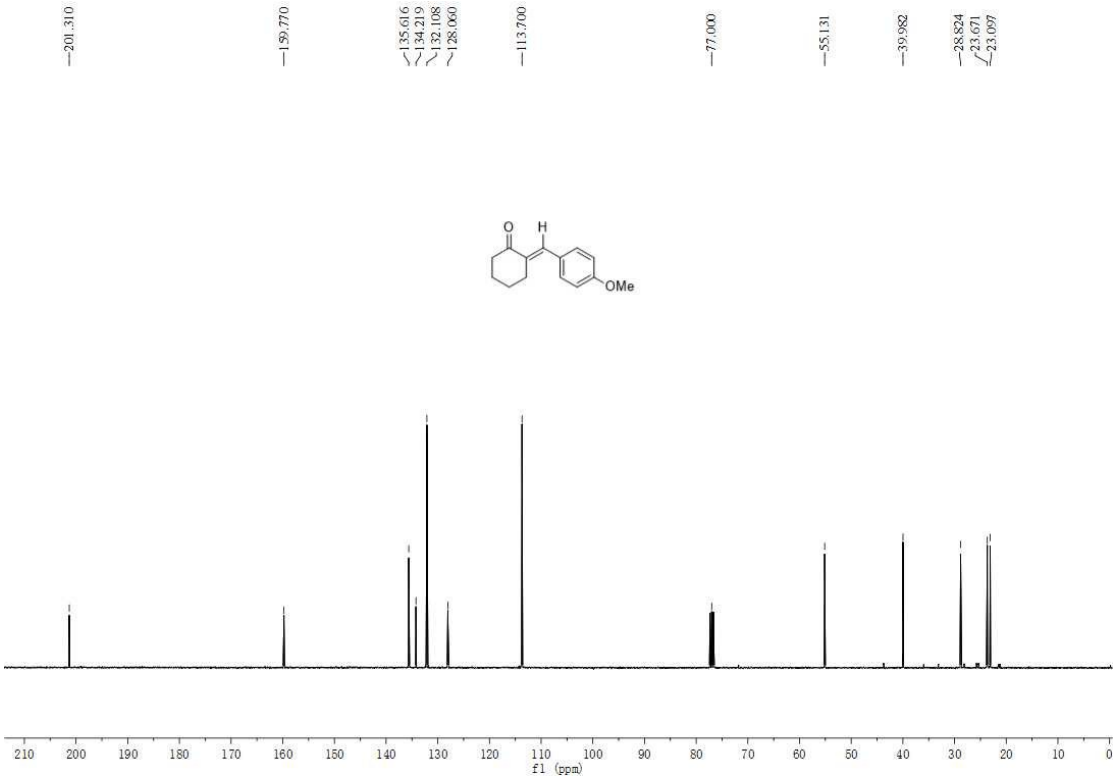
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5d**



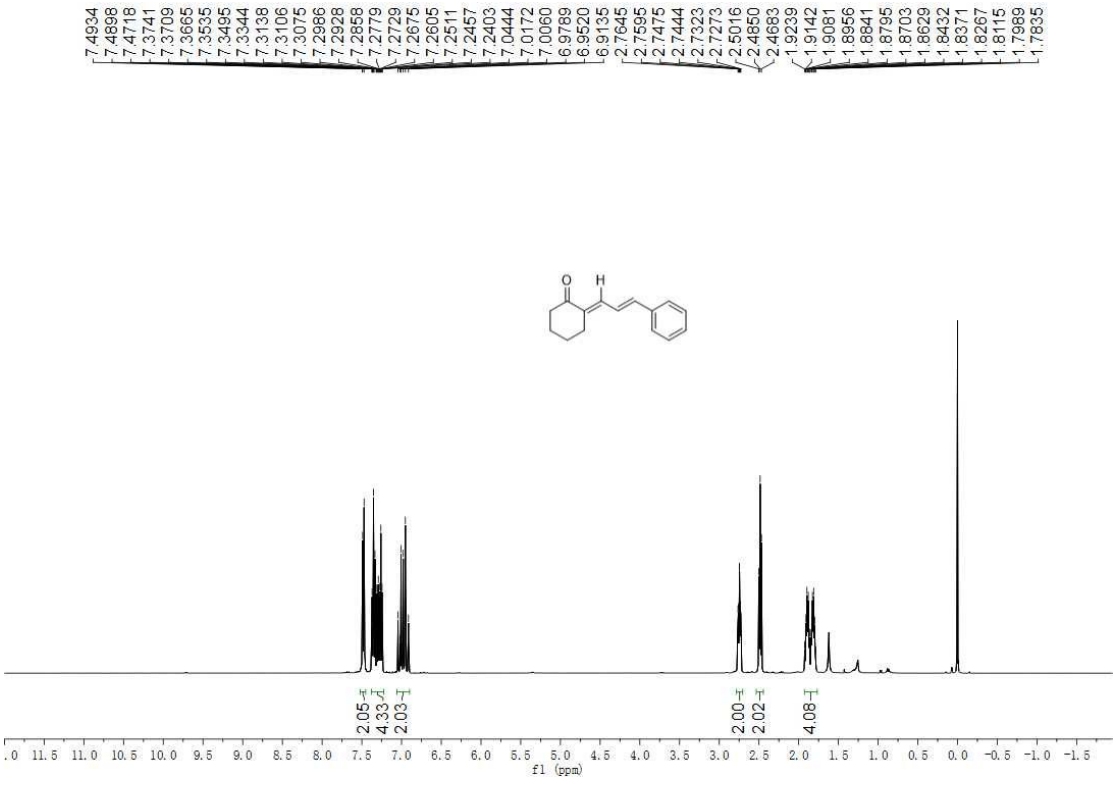
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5d**



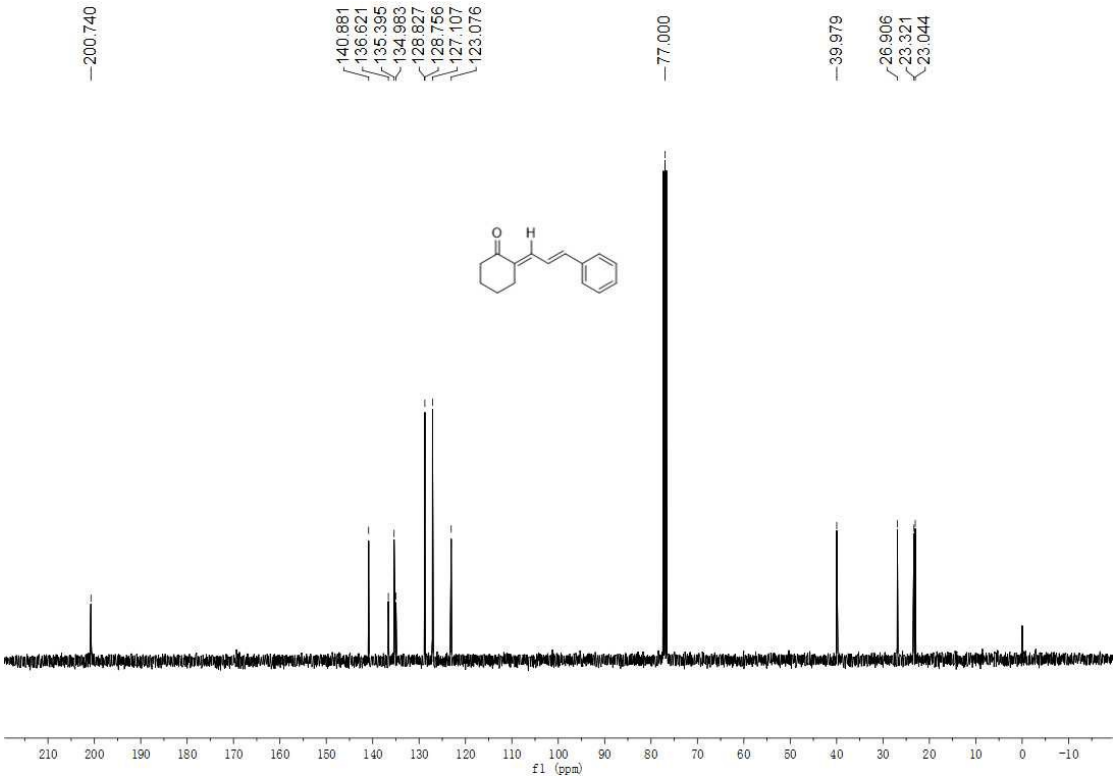
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5e**



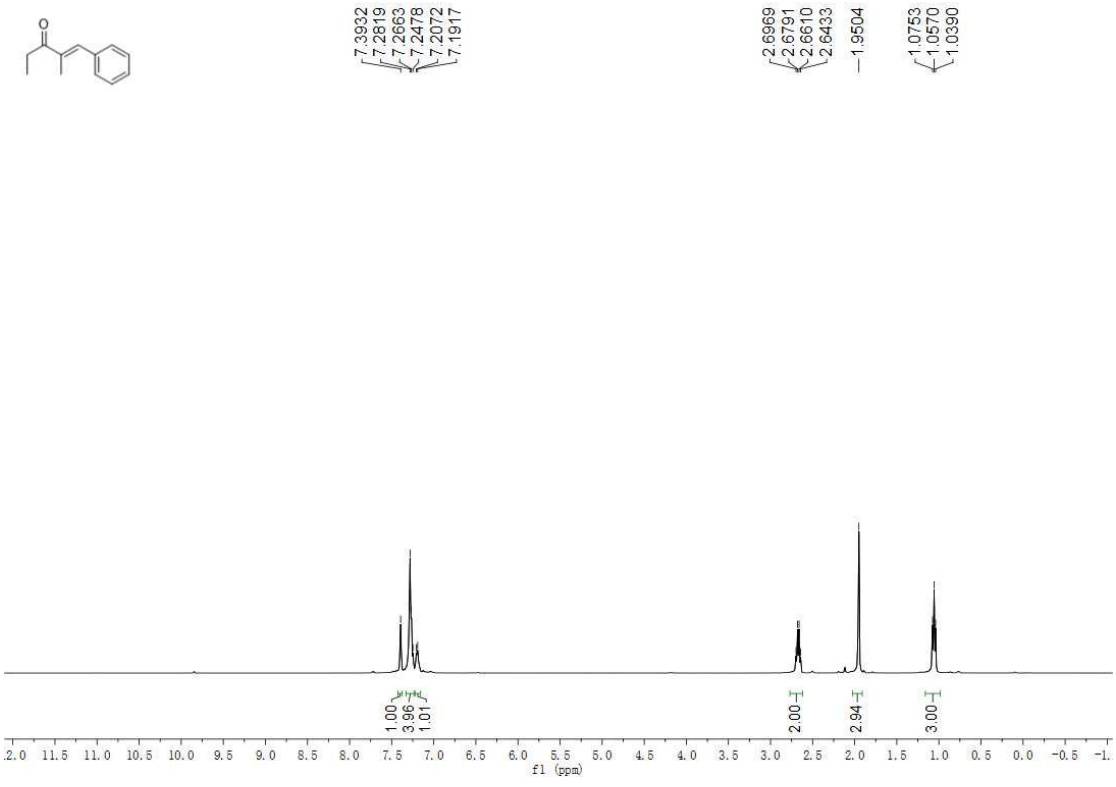
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5e**



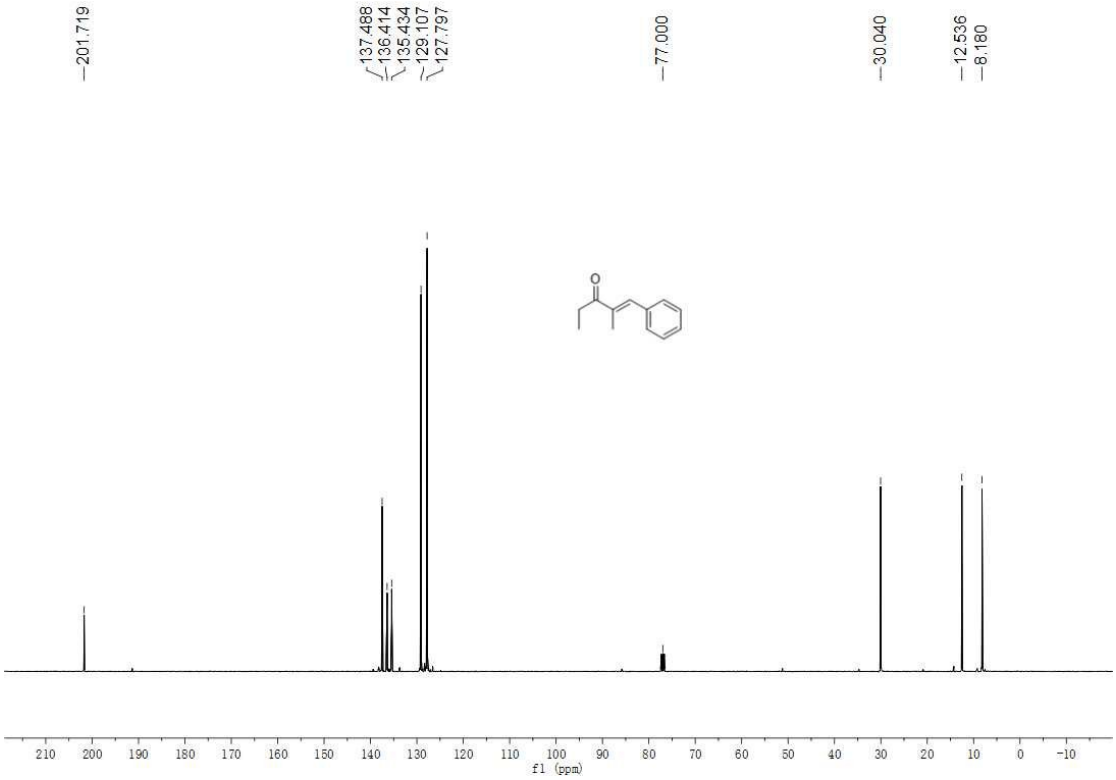
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5f**



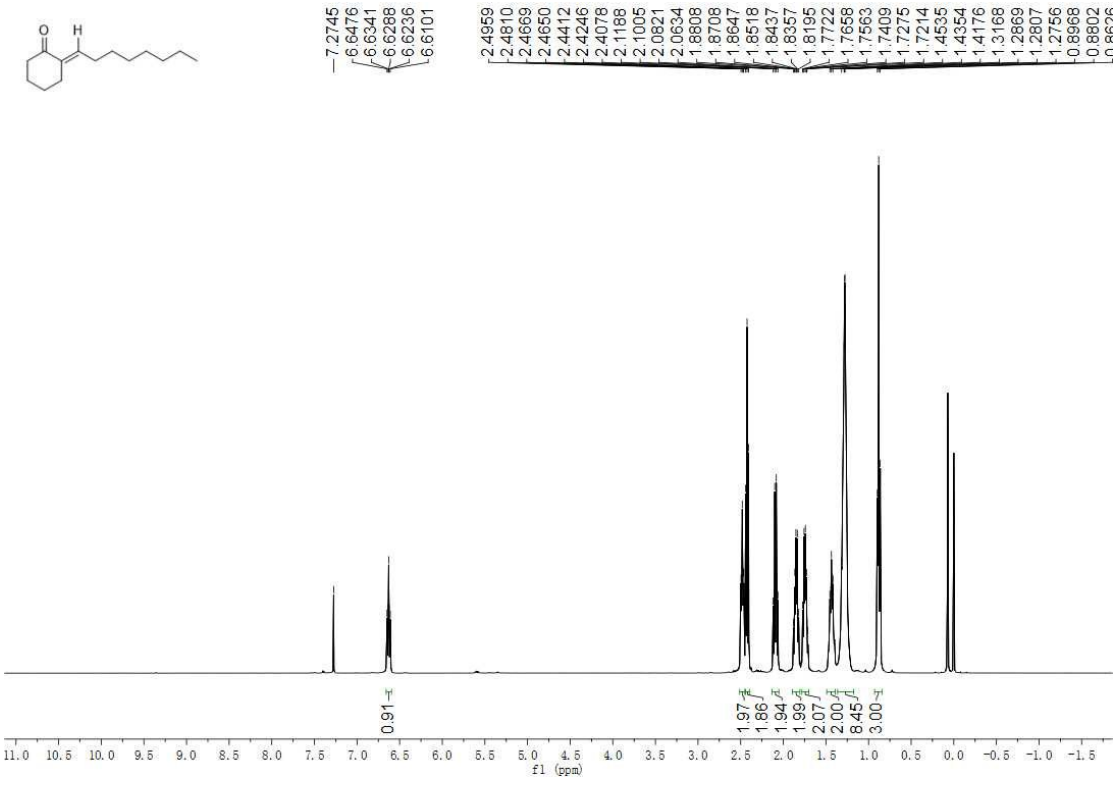
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5f**



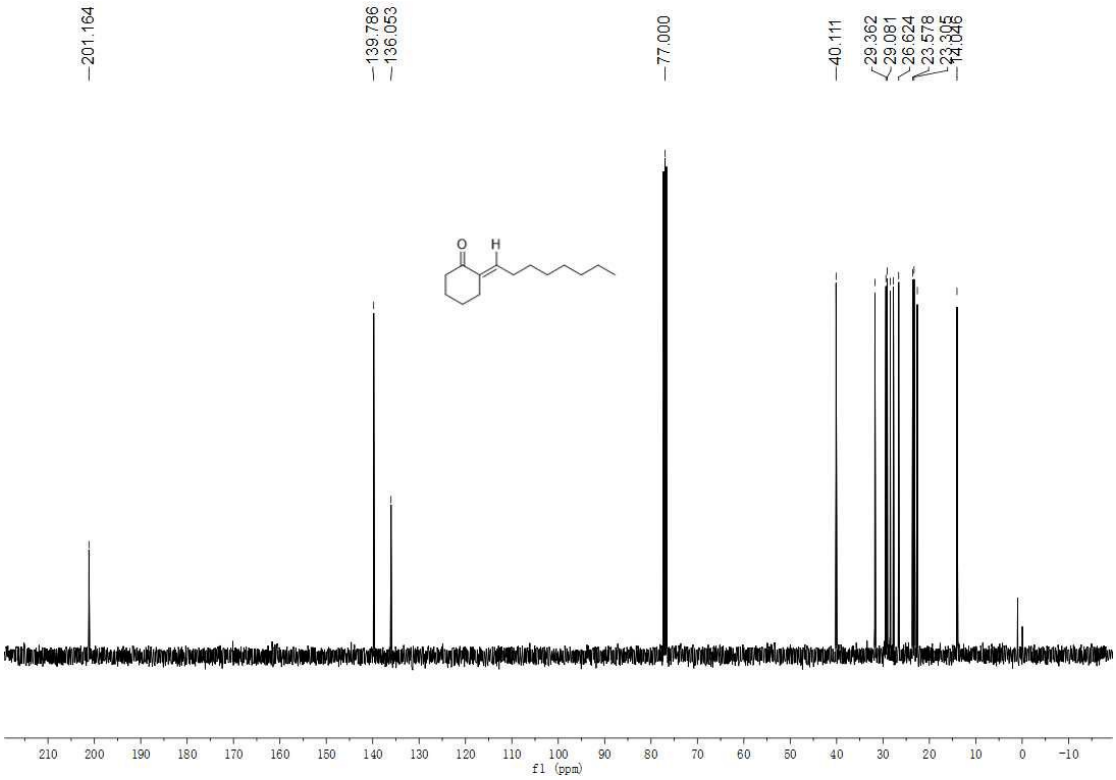
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5g**



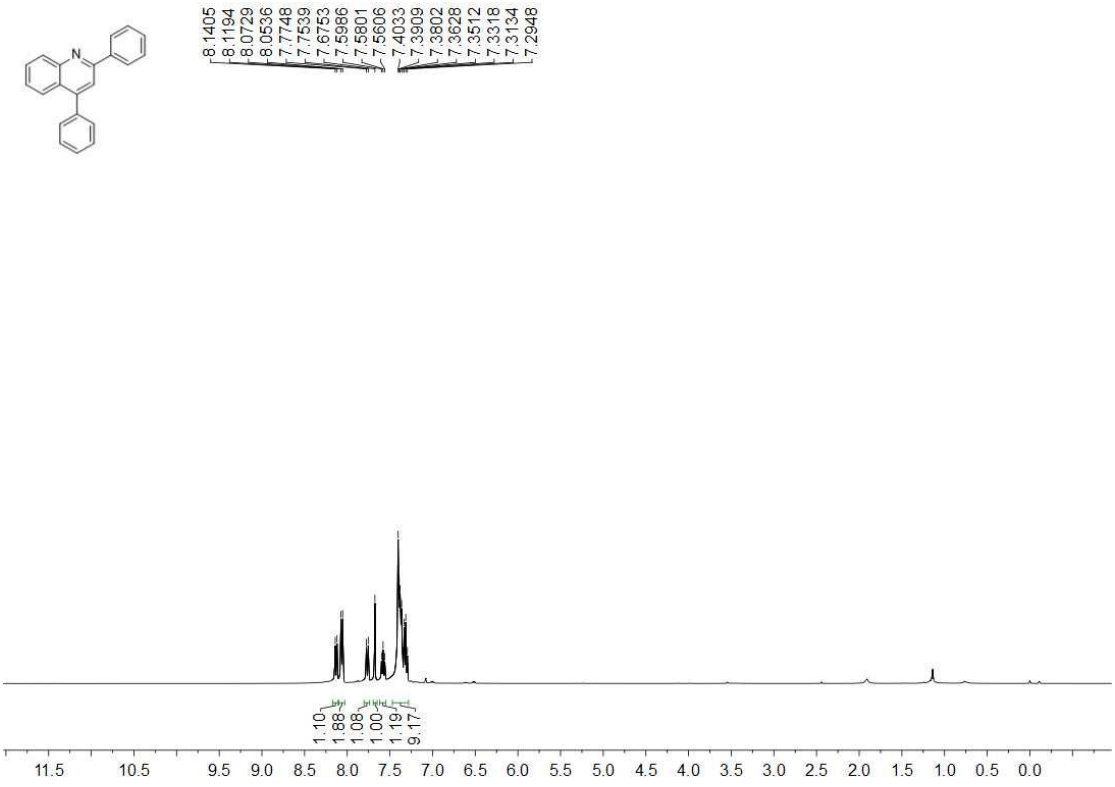
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5g**



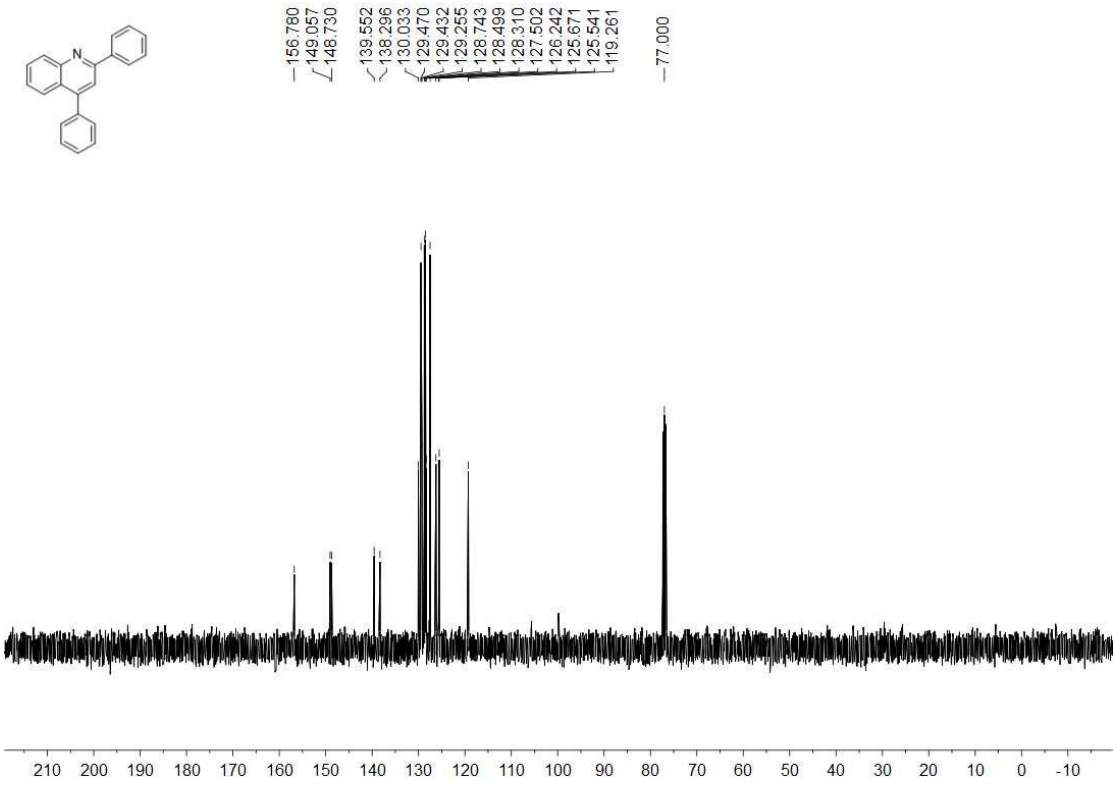
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **5h**



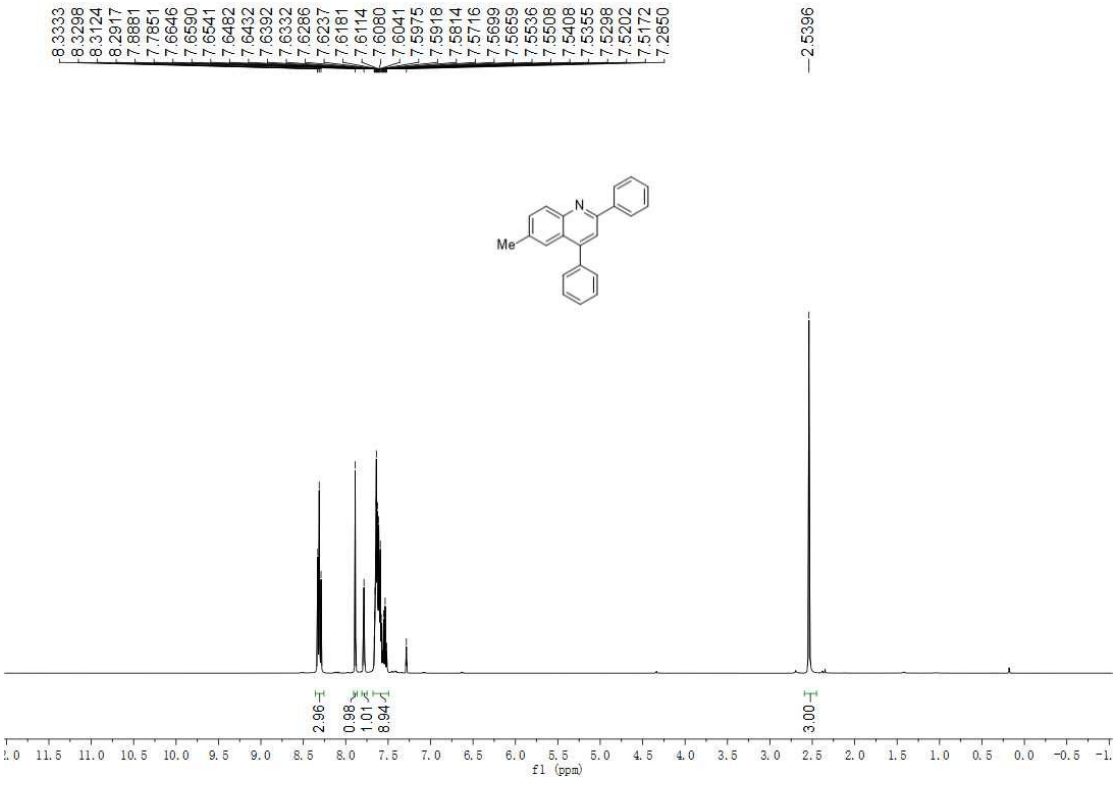
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **5h**



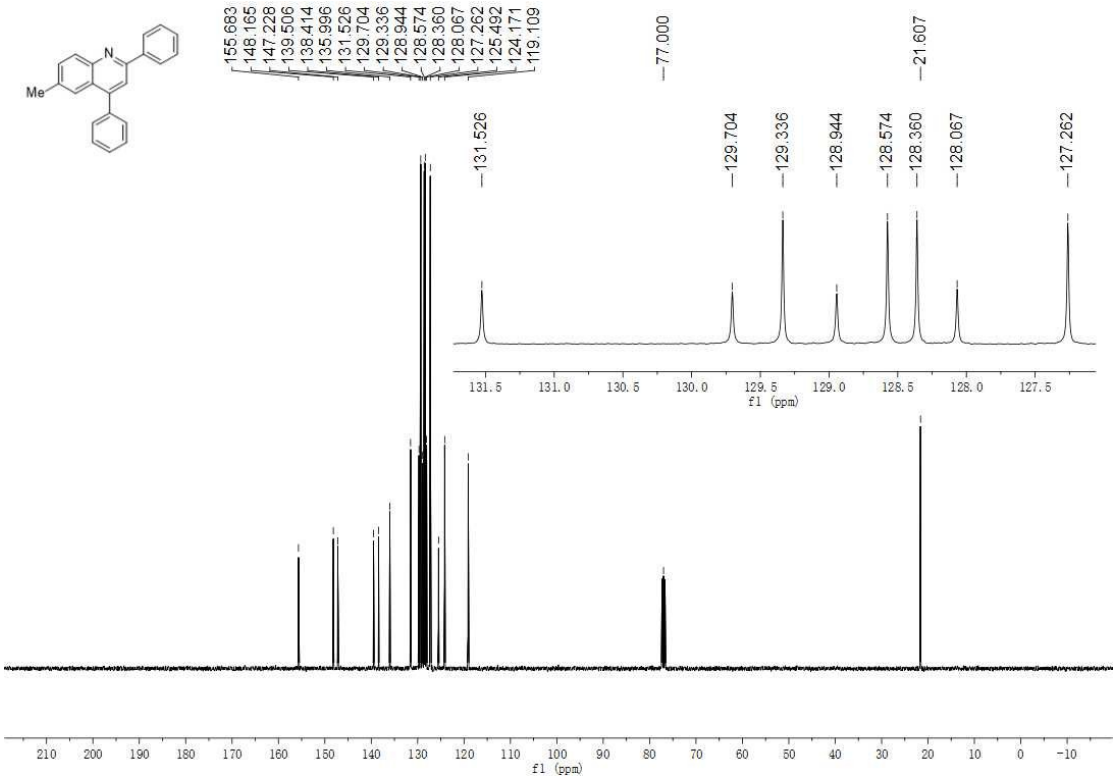
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6a**



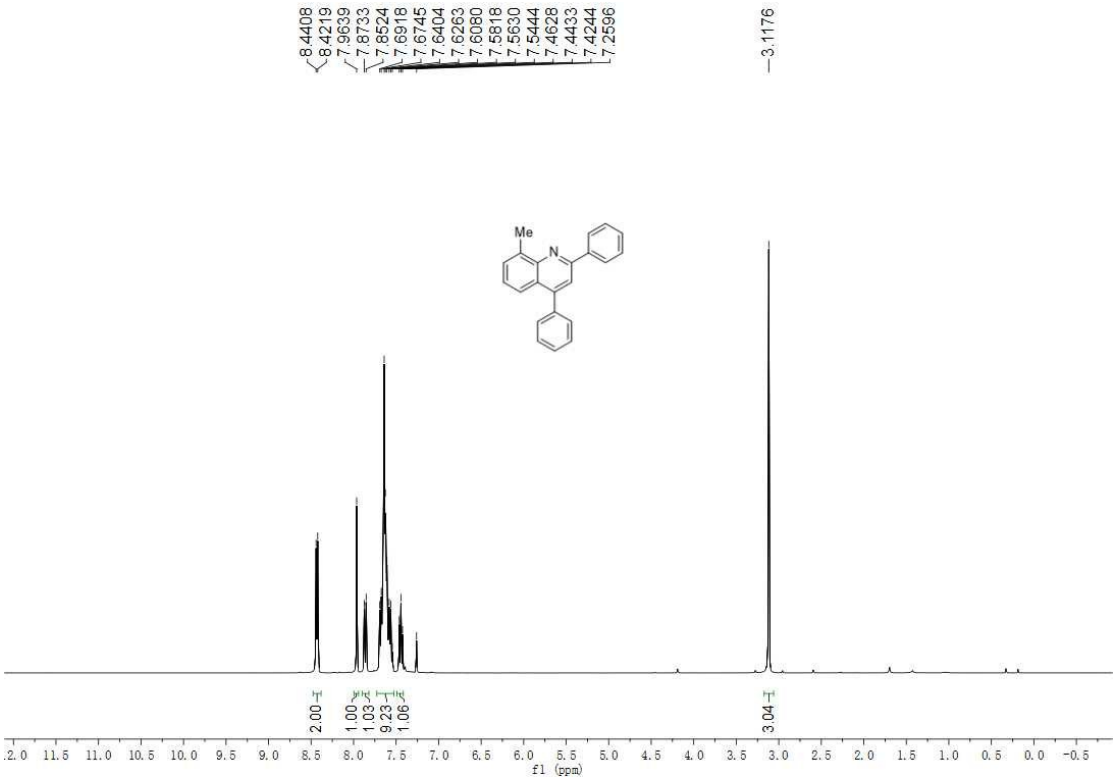
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6a**



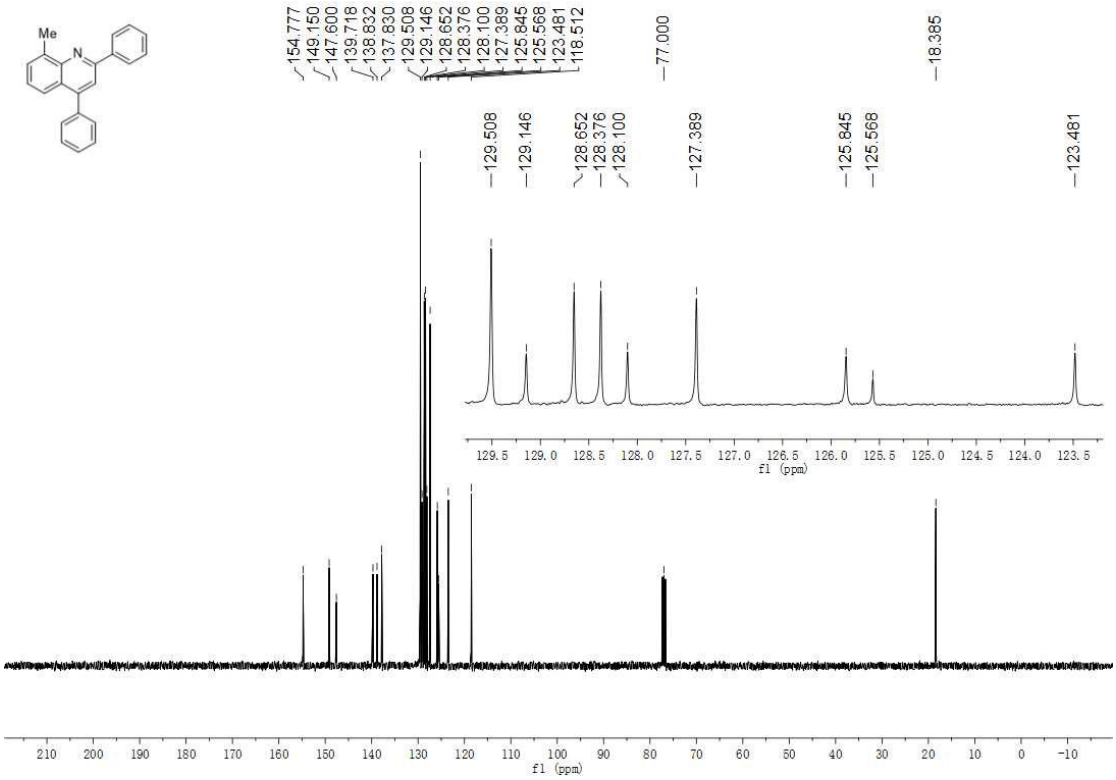
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6b**



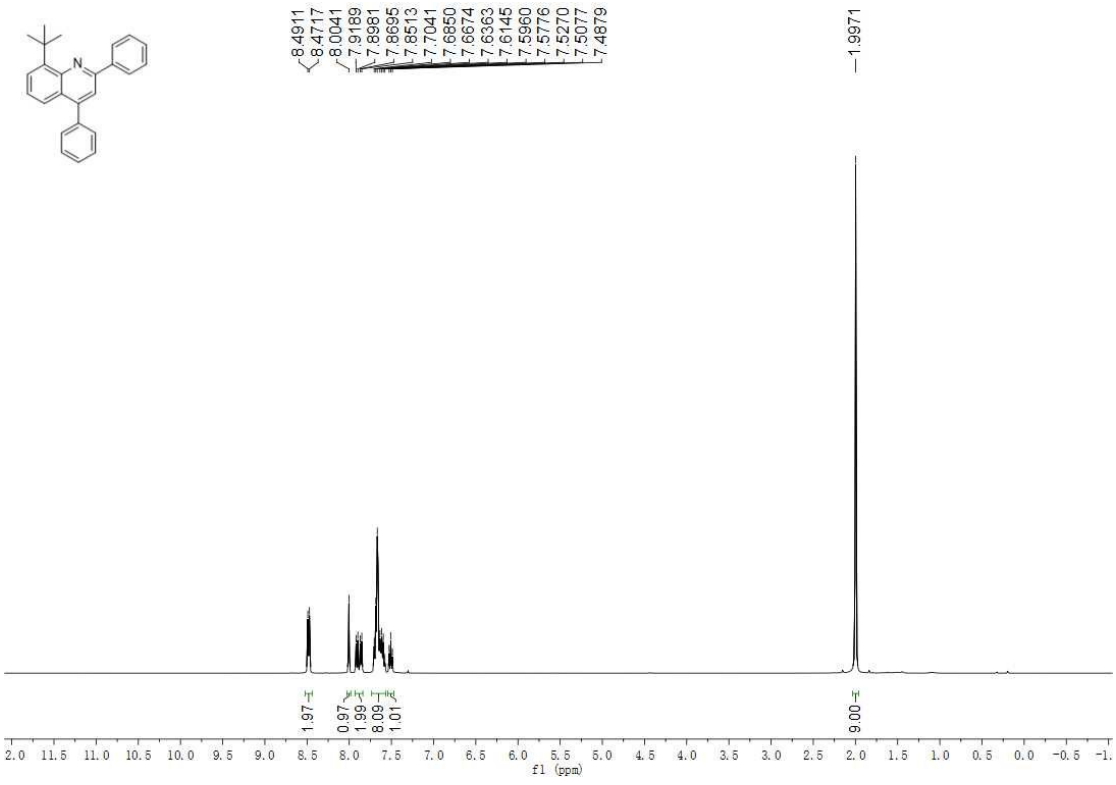
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6b**



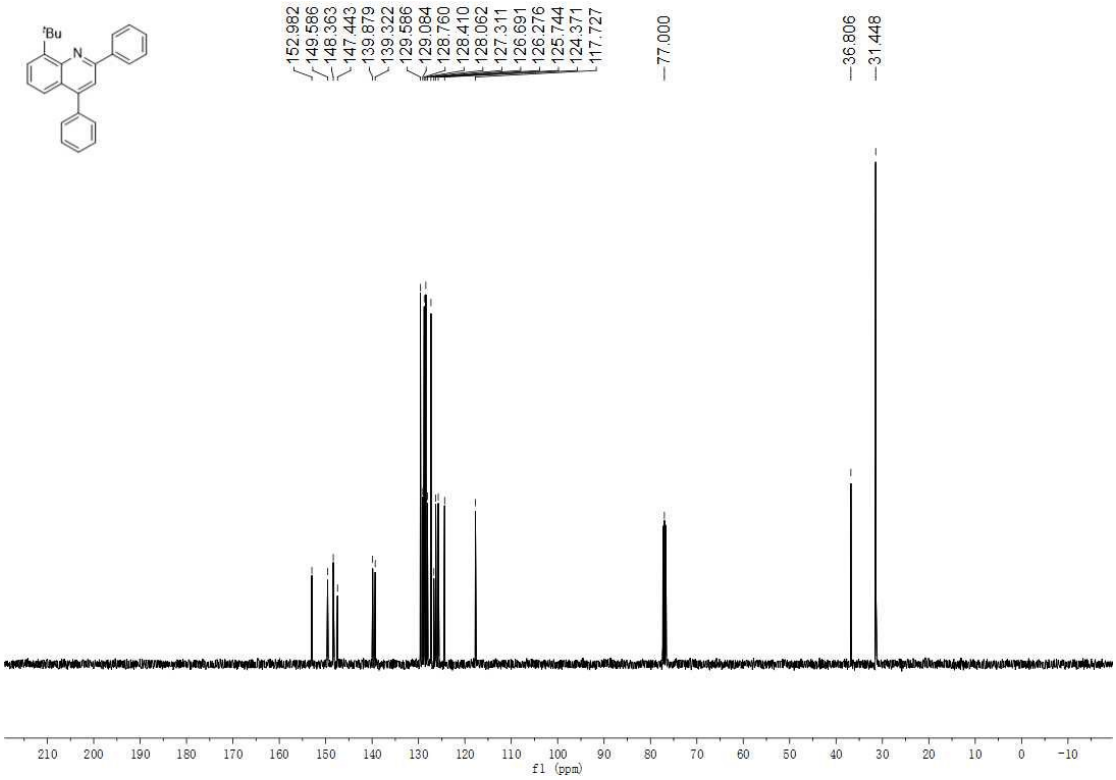
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6c**



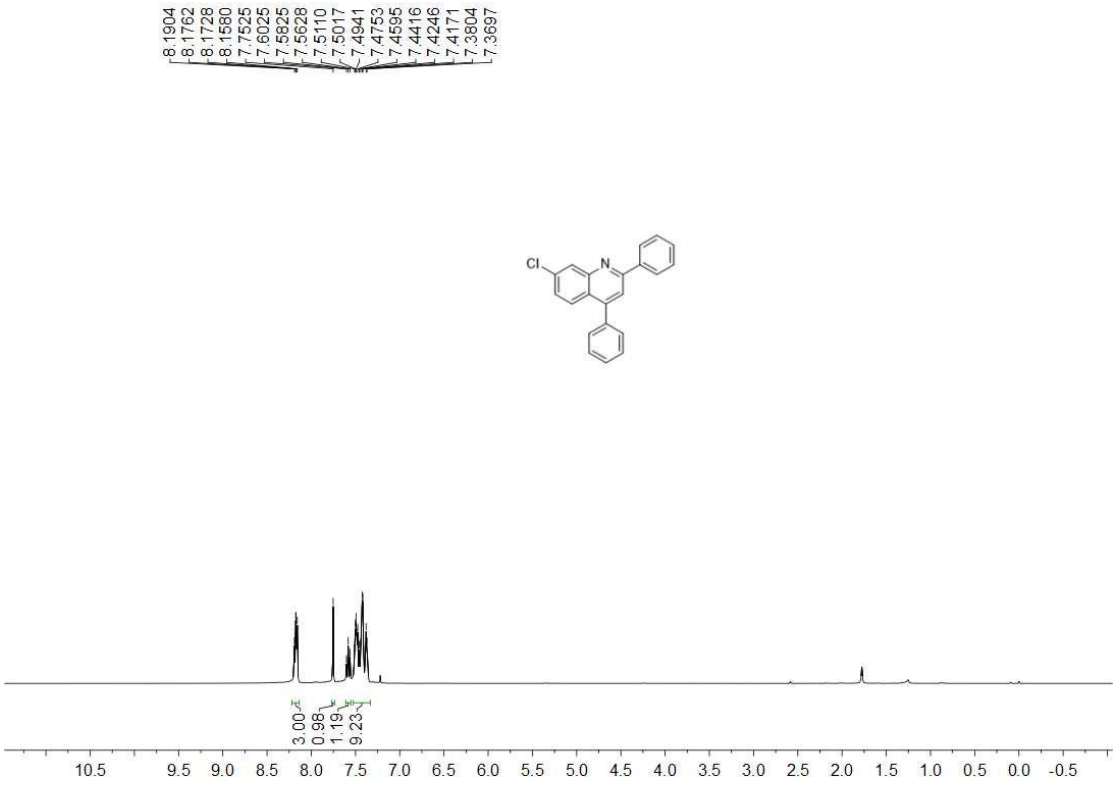
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6c**



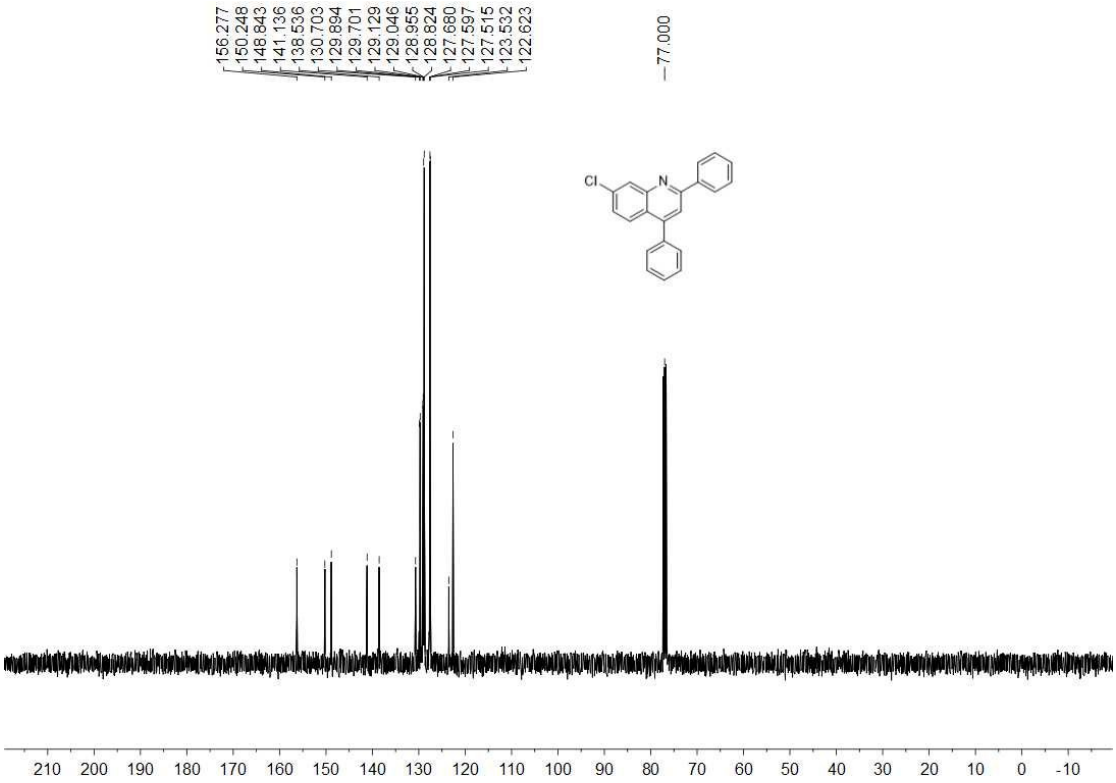
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6d**



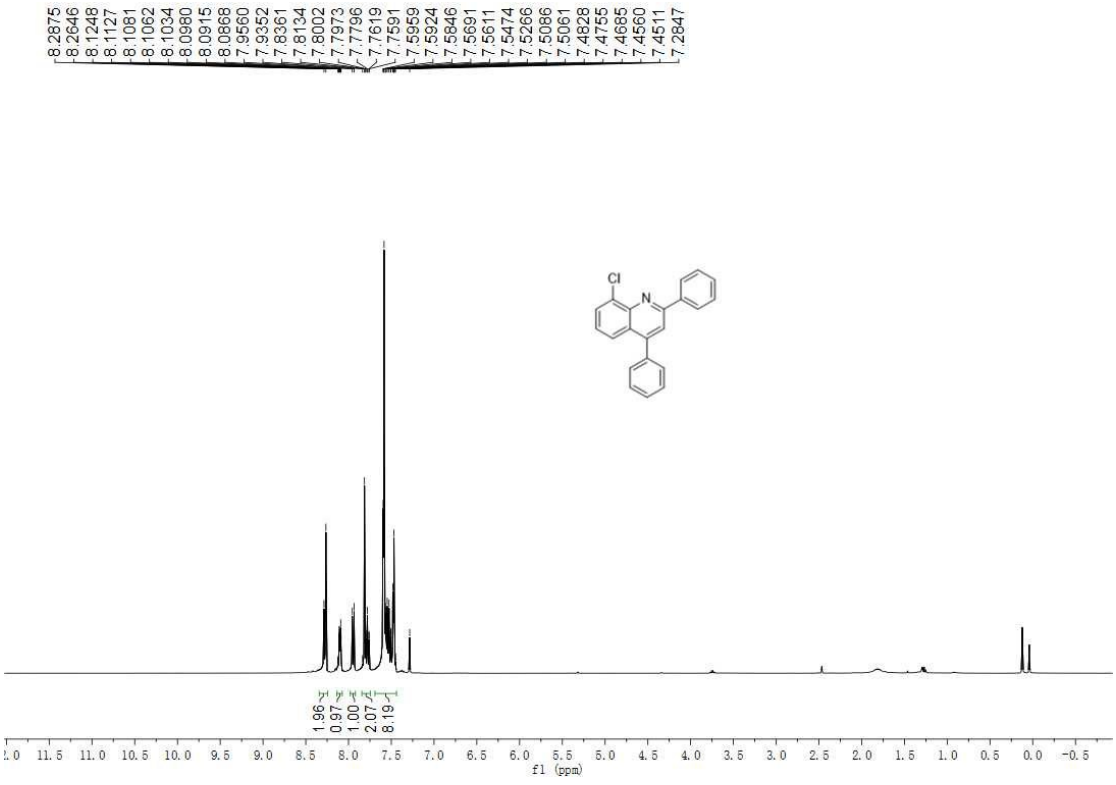
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6d**



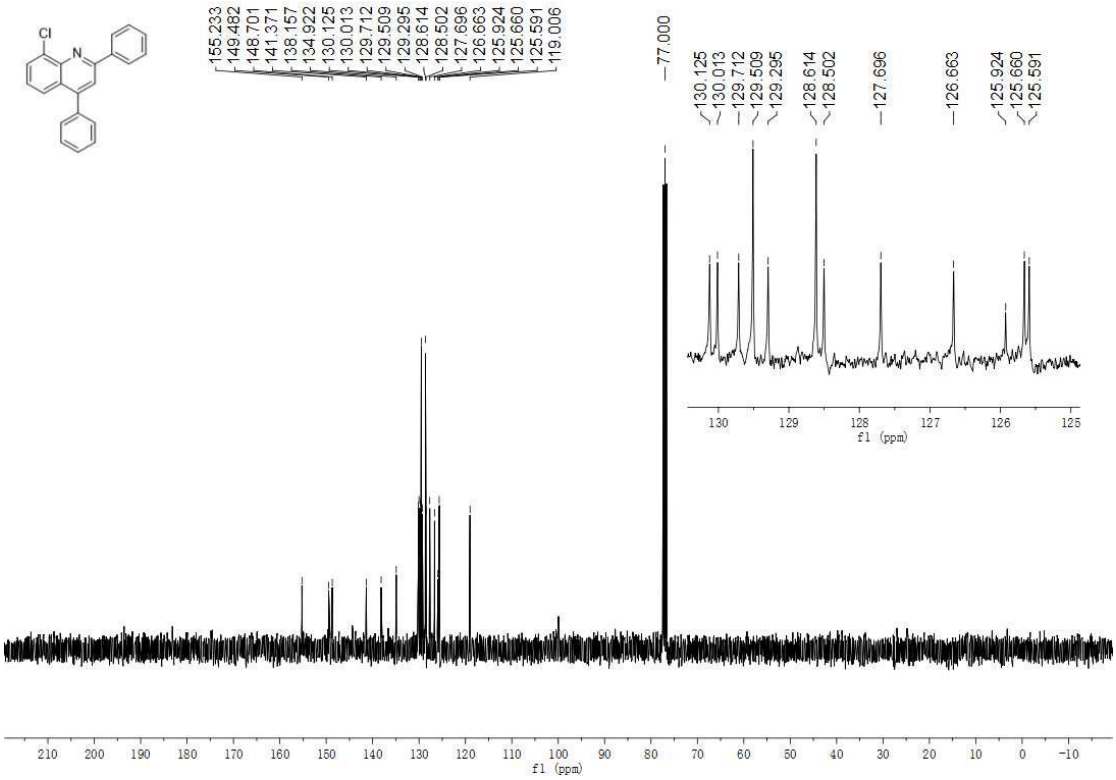
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6e**



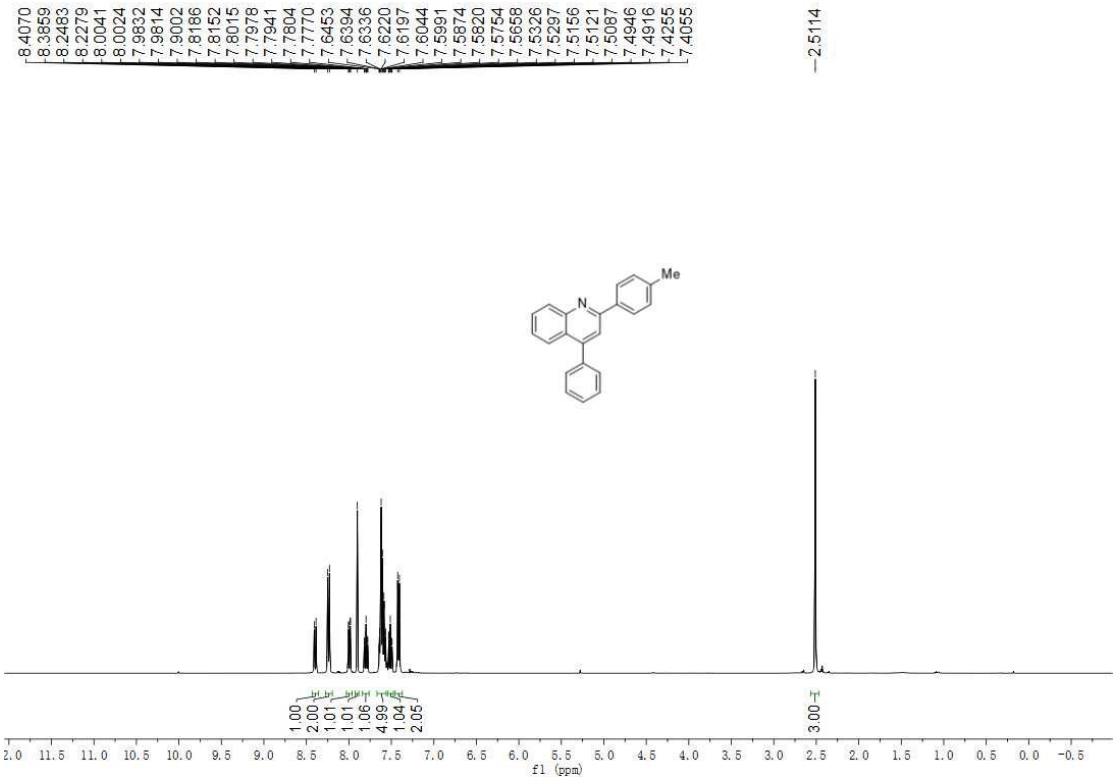
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6e**



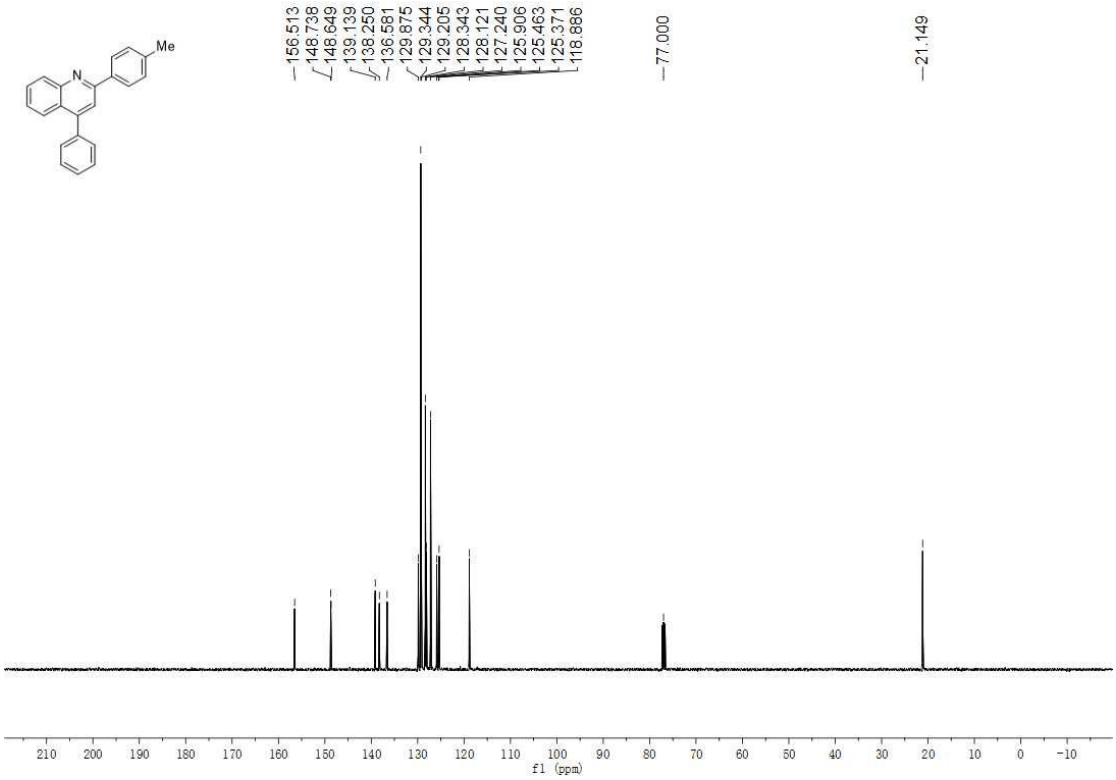
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6f**



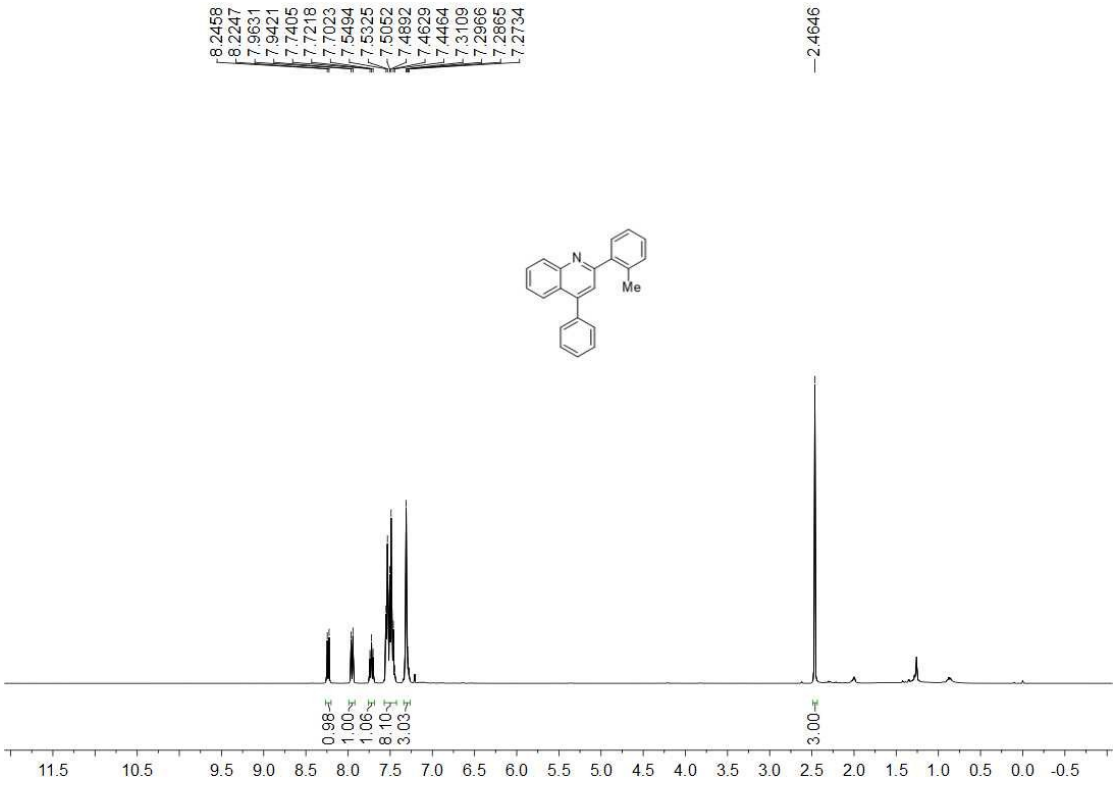
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6f**



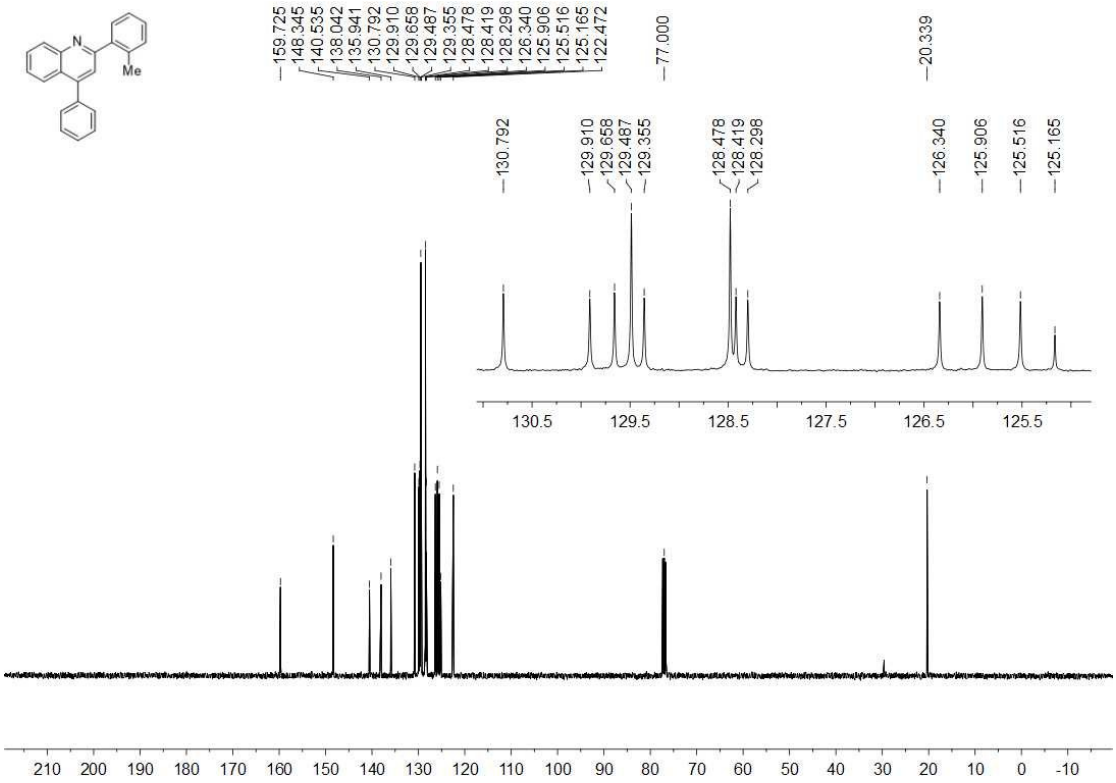
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6g**



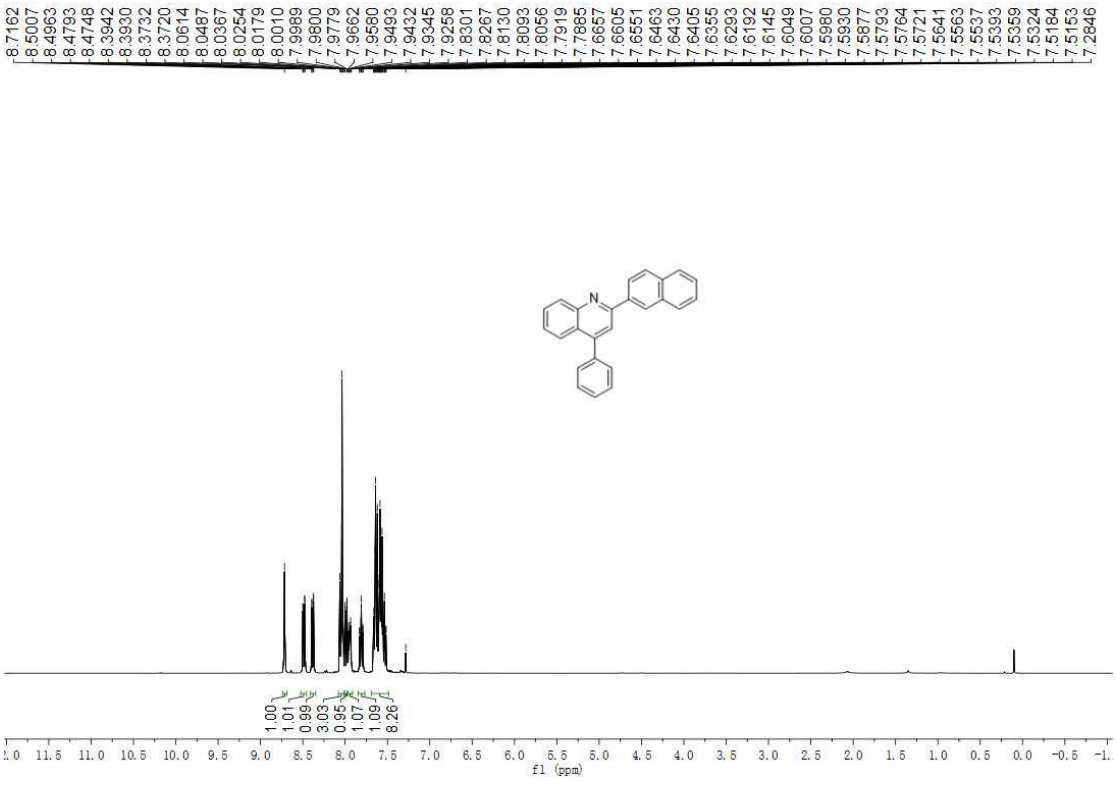
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6g**



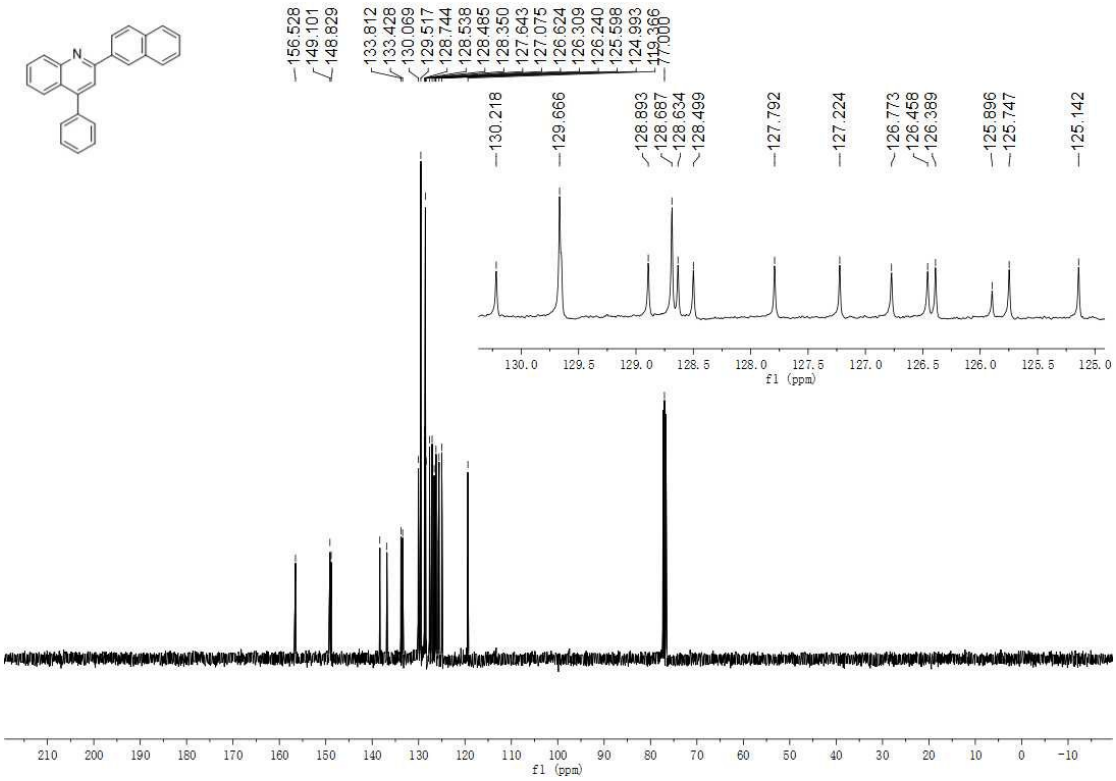
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6h**



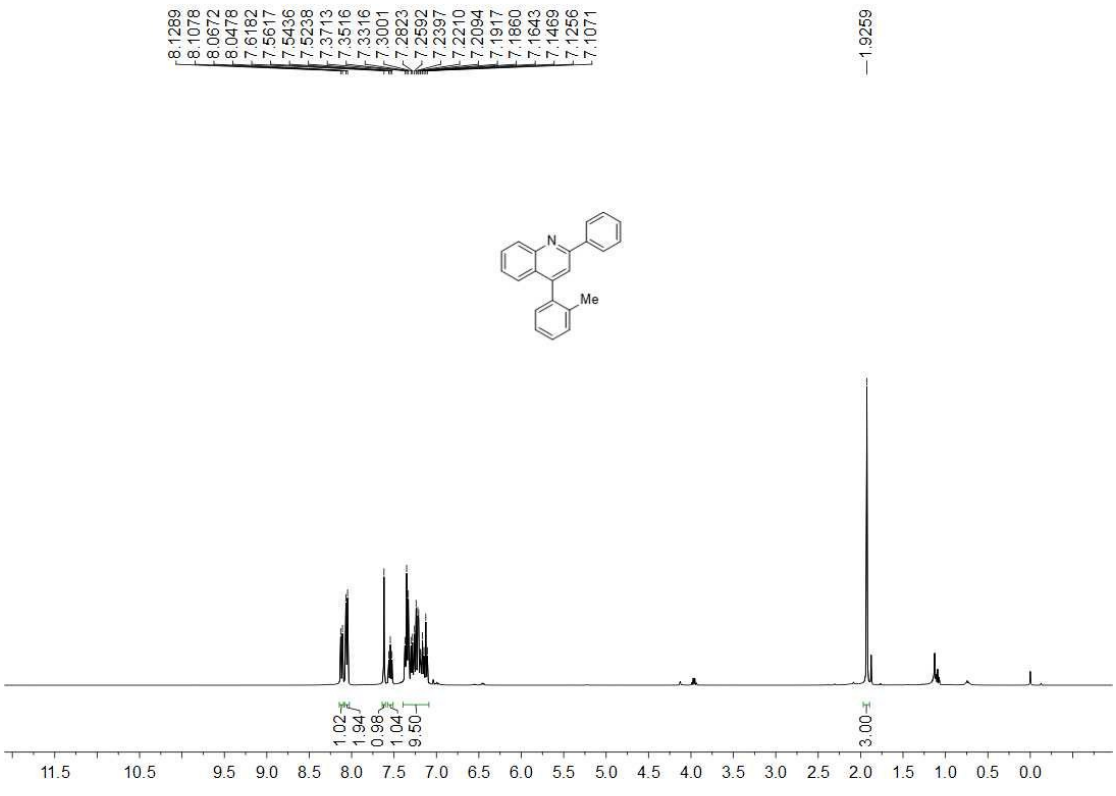
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6h**



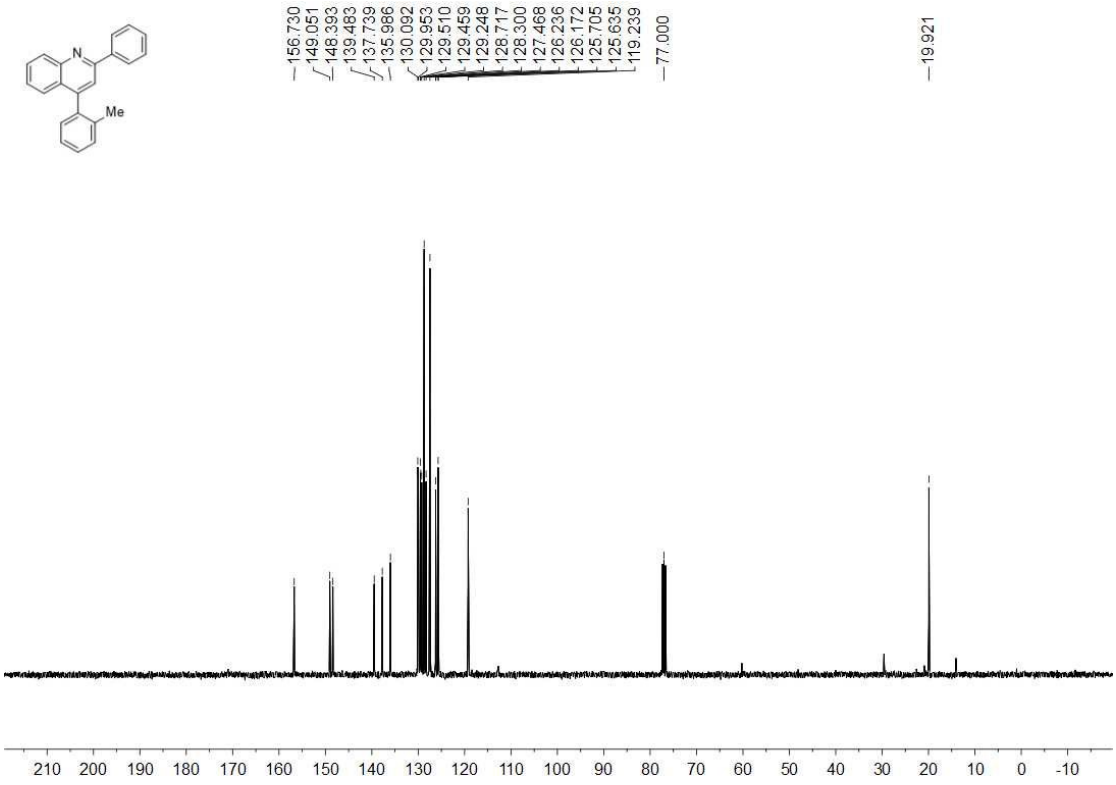
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6i**



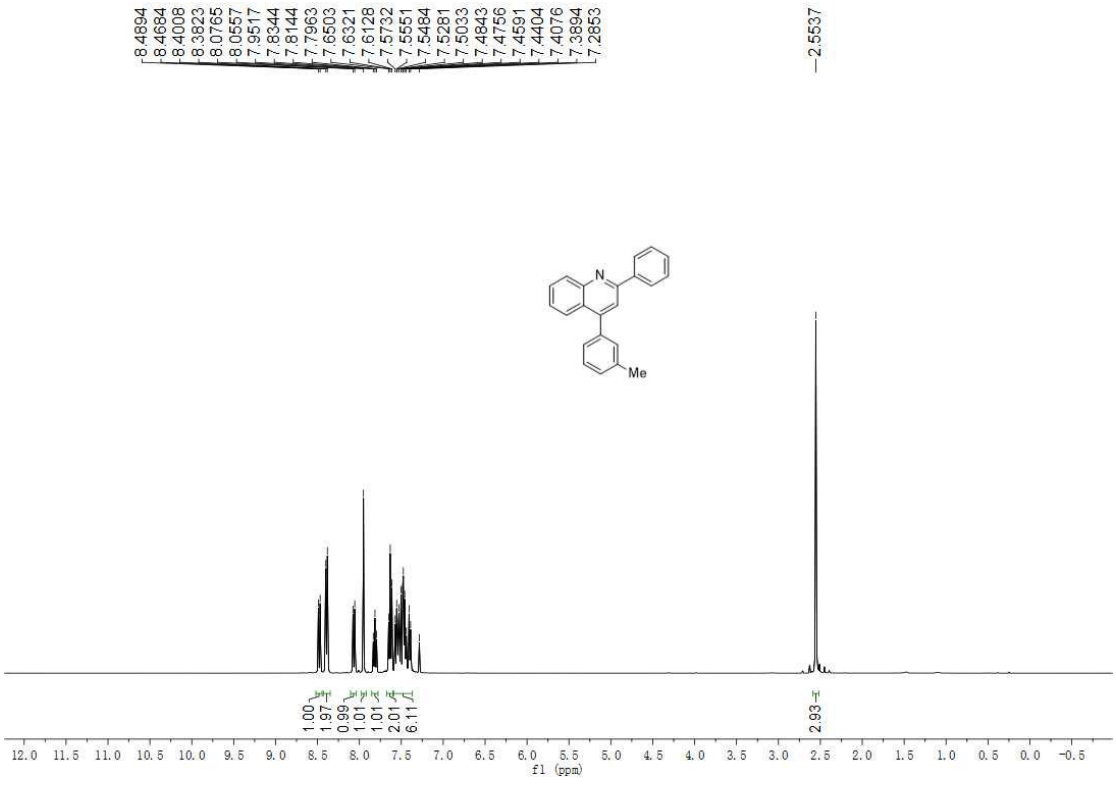
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6i**



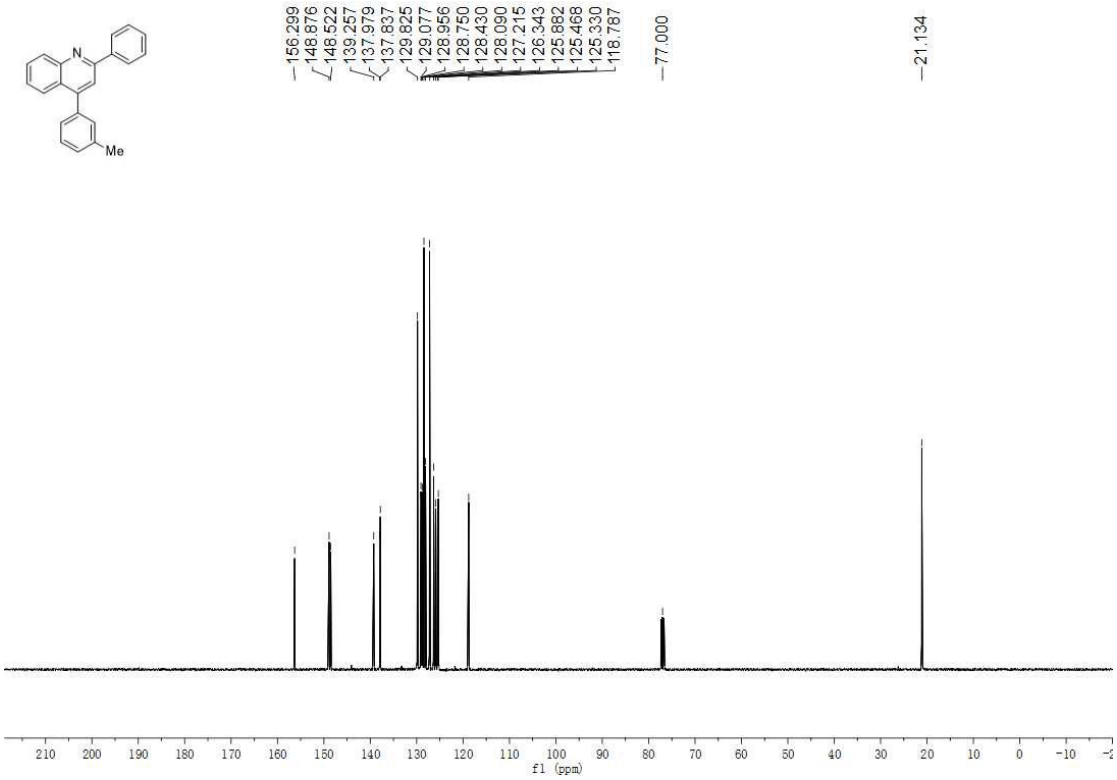
H NMR (400 MHz, $CDCl_3$) spectrum of compound **6j**



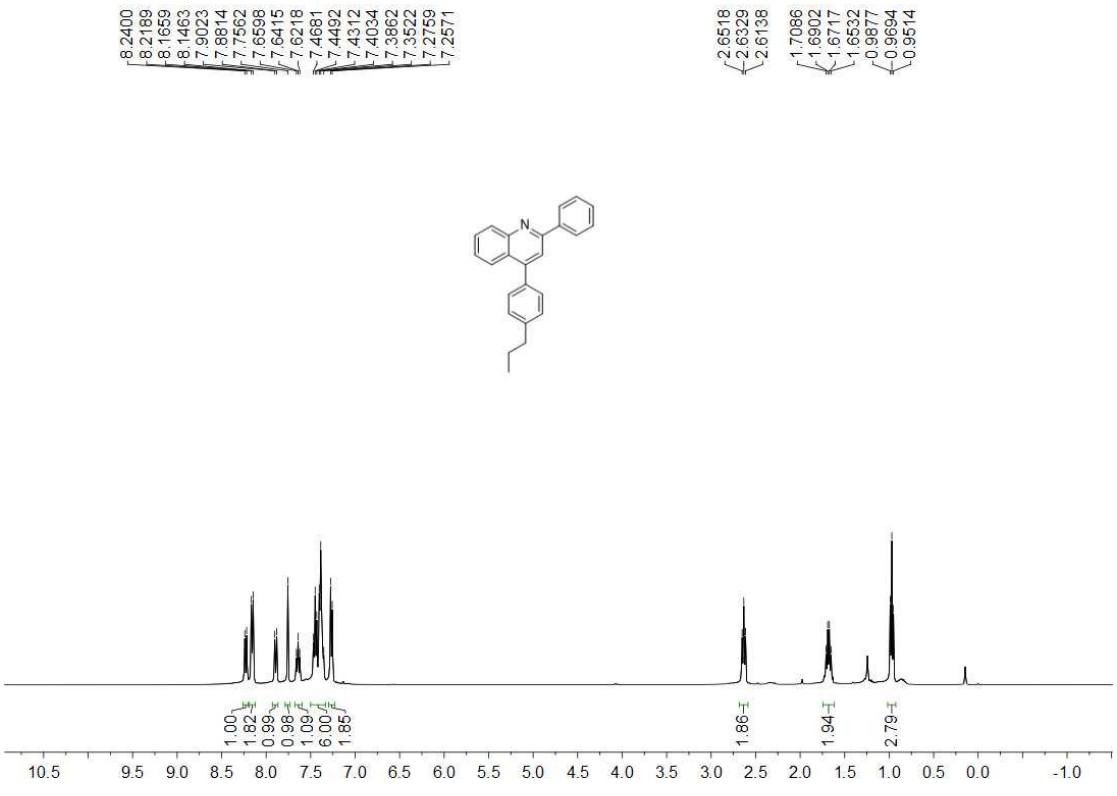
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6j**



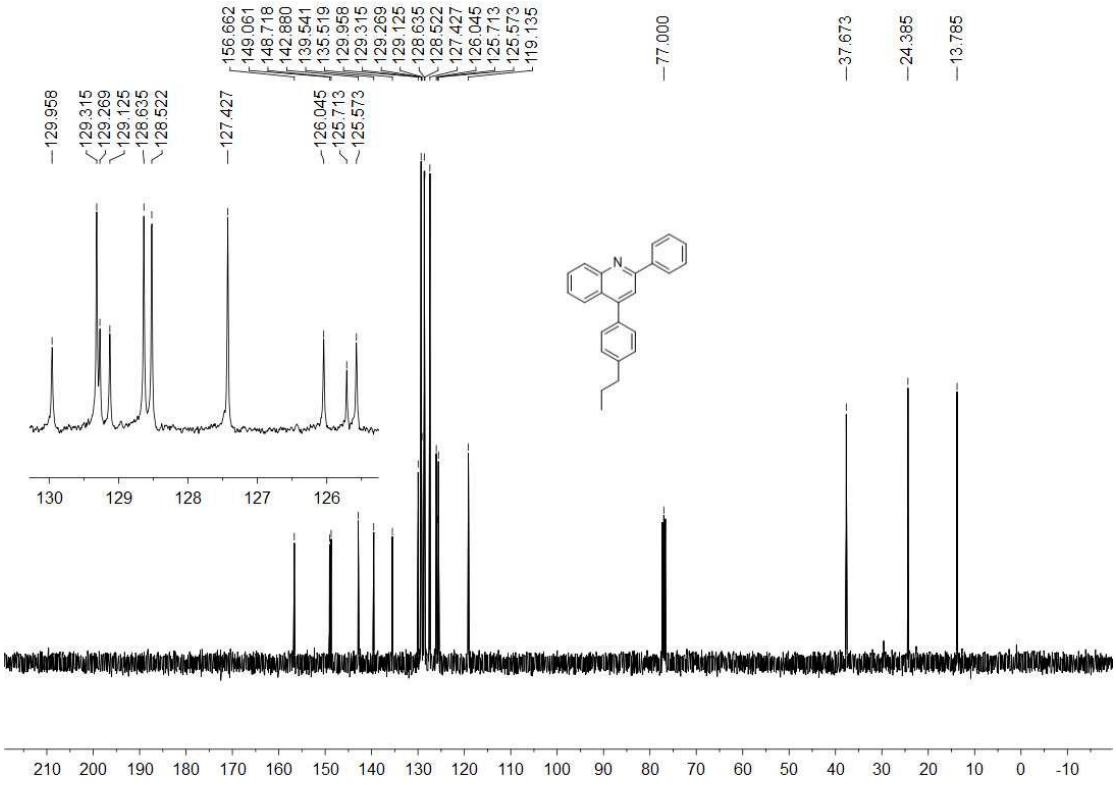
H NMR (400 MHz, $CDCl_3$) spectrum of compound **6k**



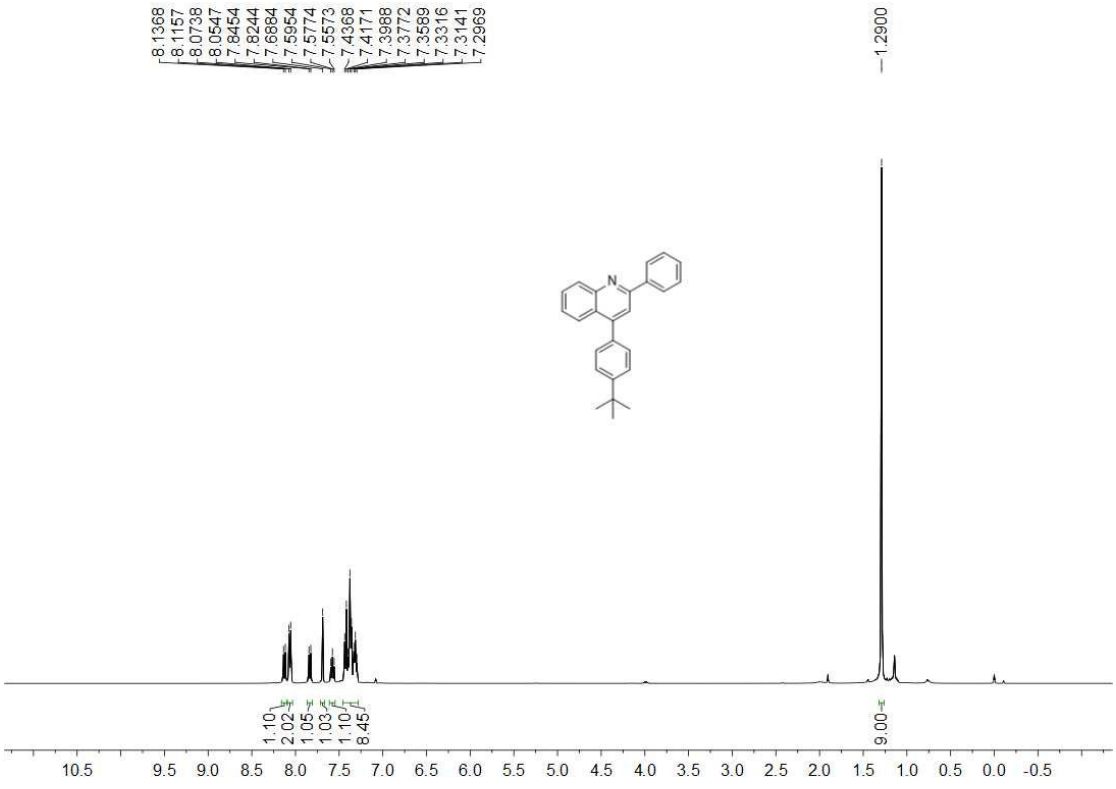
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6k**



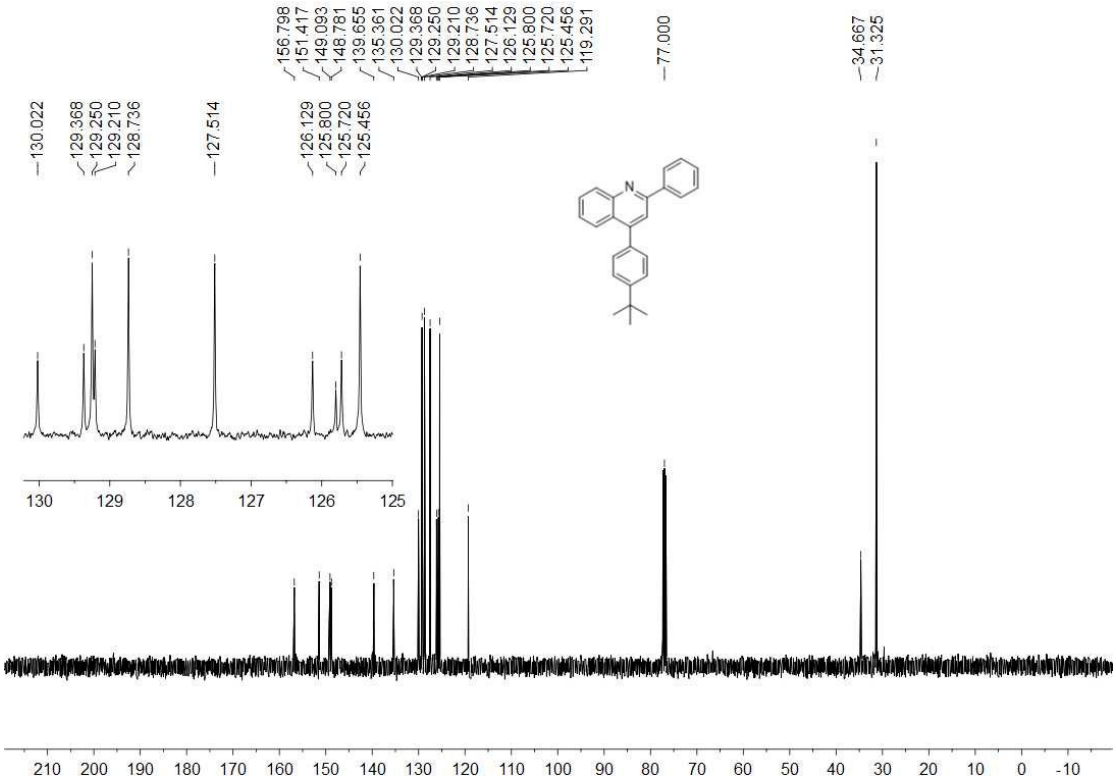
H NMR (400 MHz, $CDCl_3$) spectrum of compound **6l**



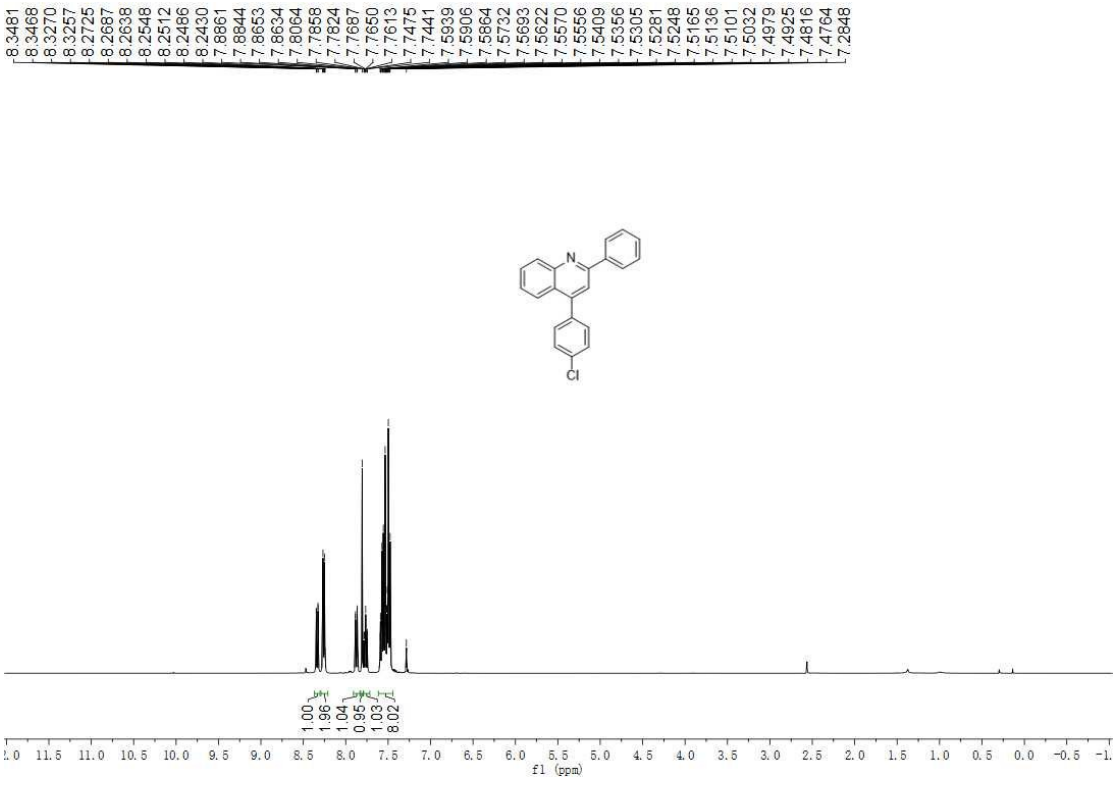
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6l**



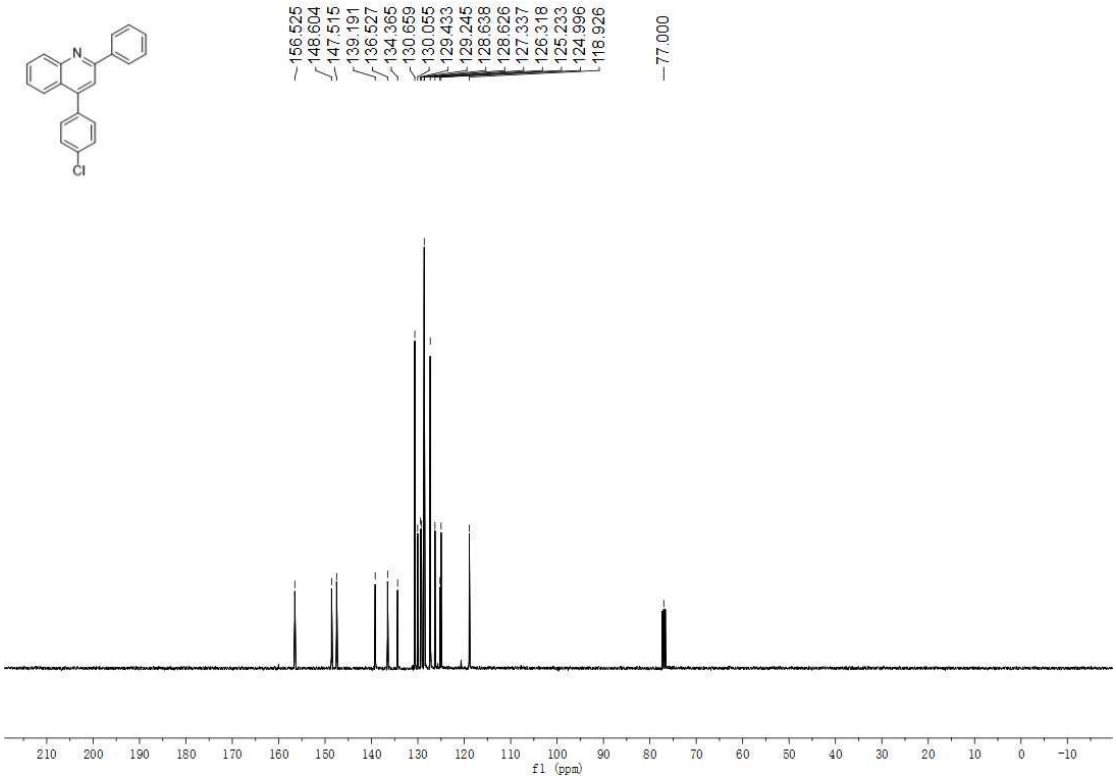
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6m**



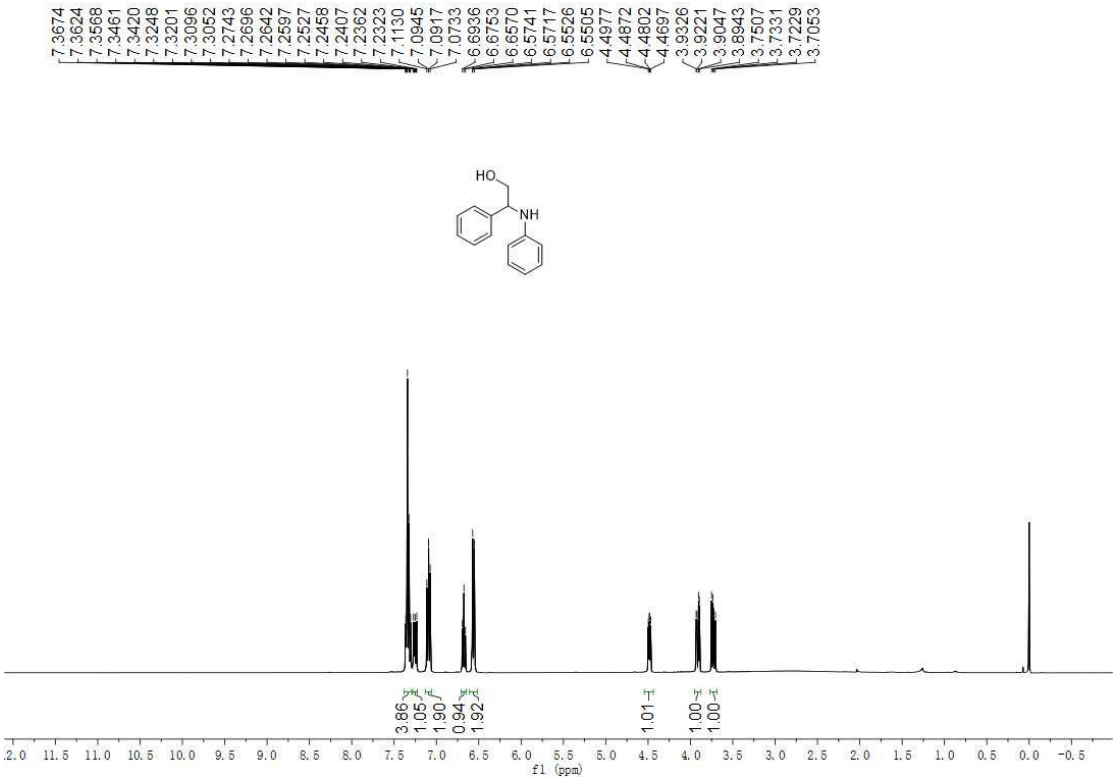
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6m**



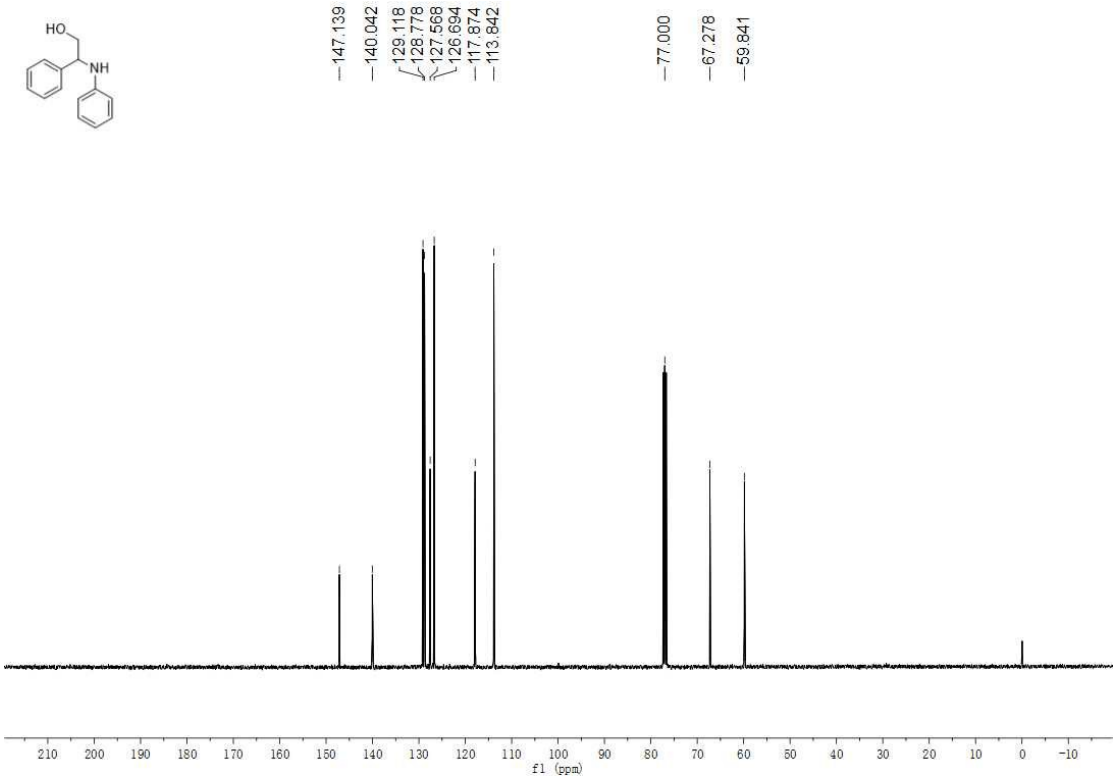
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **6n**



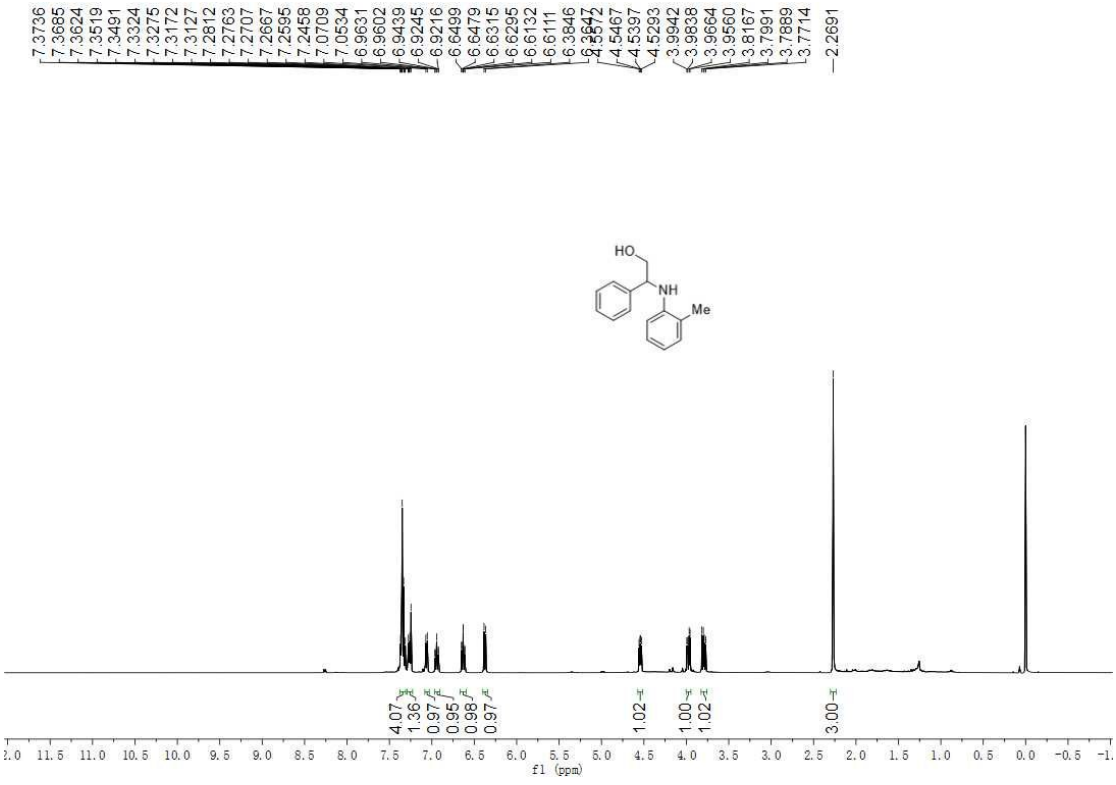
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **6n**



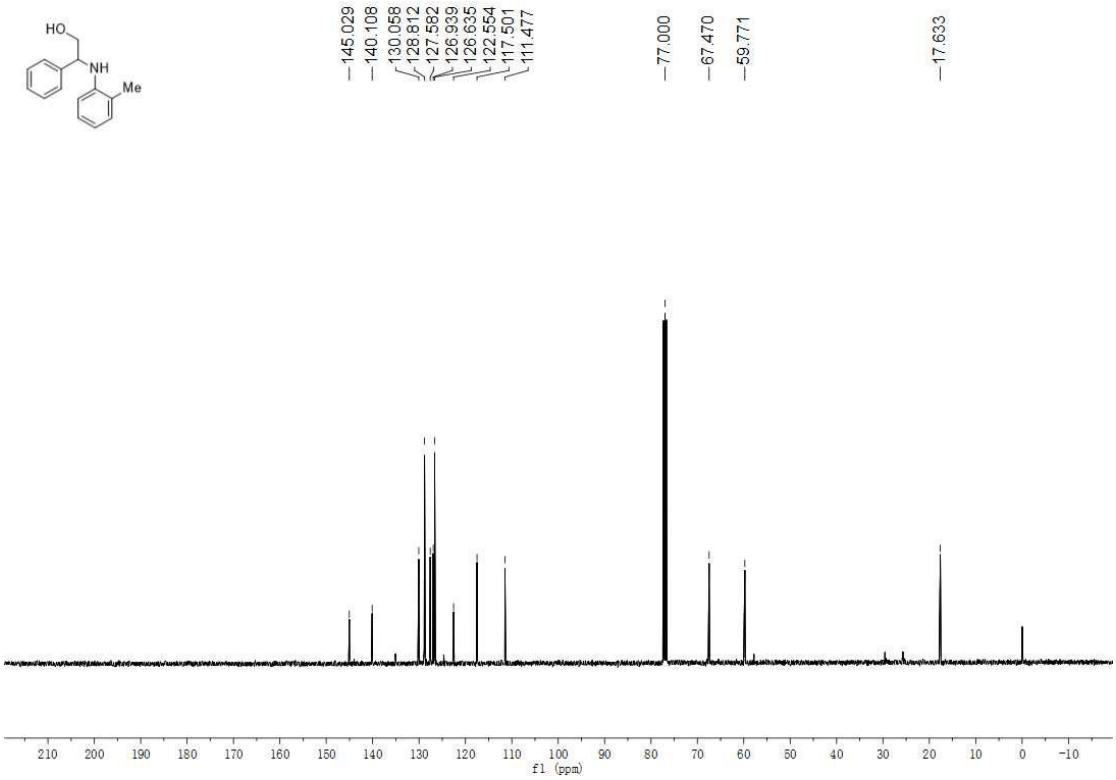
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7a**



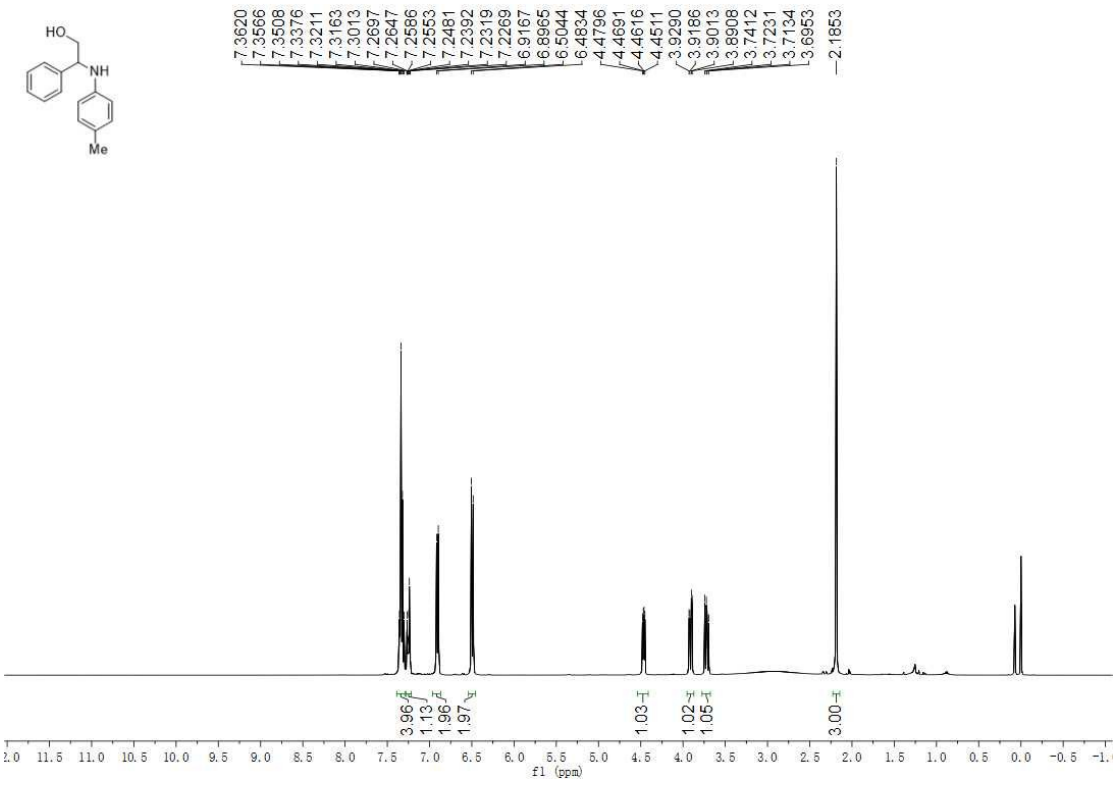
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7a**



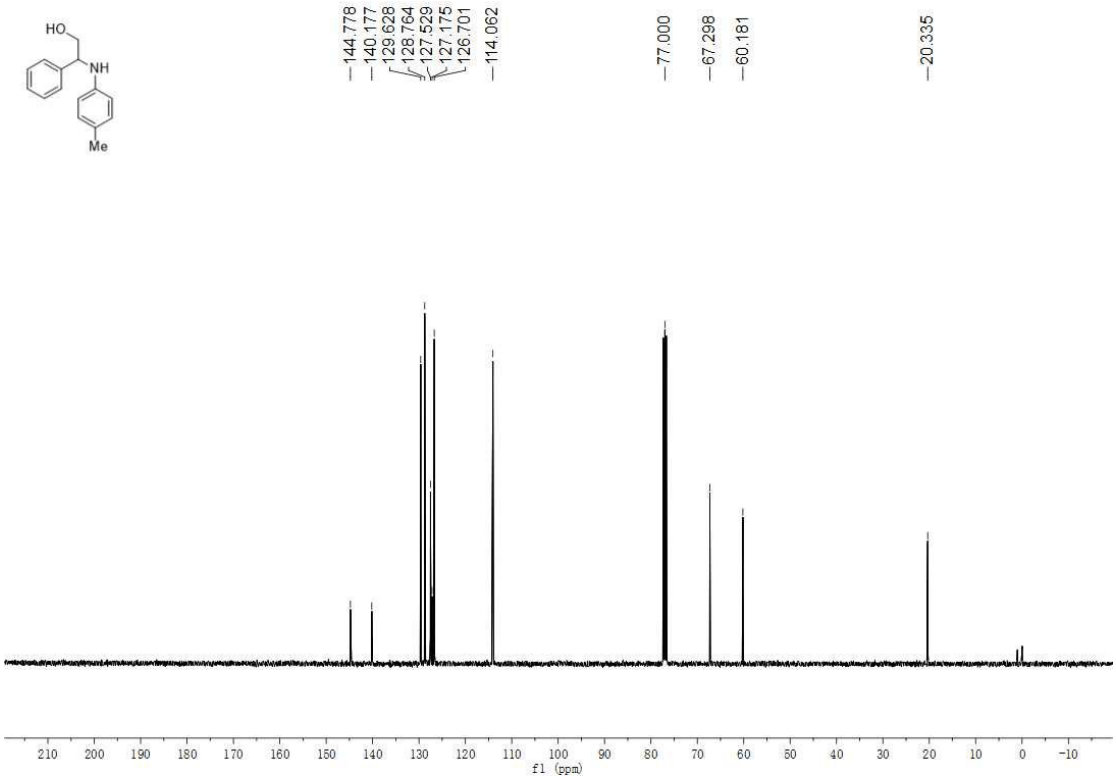
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7b**



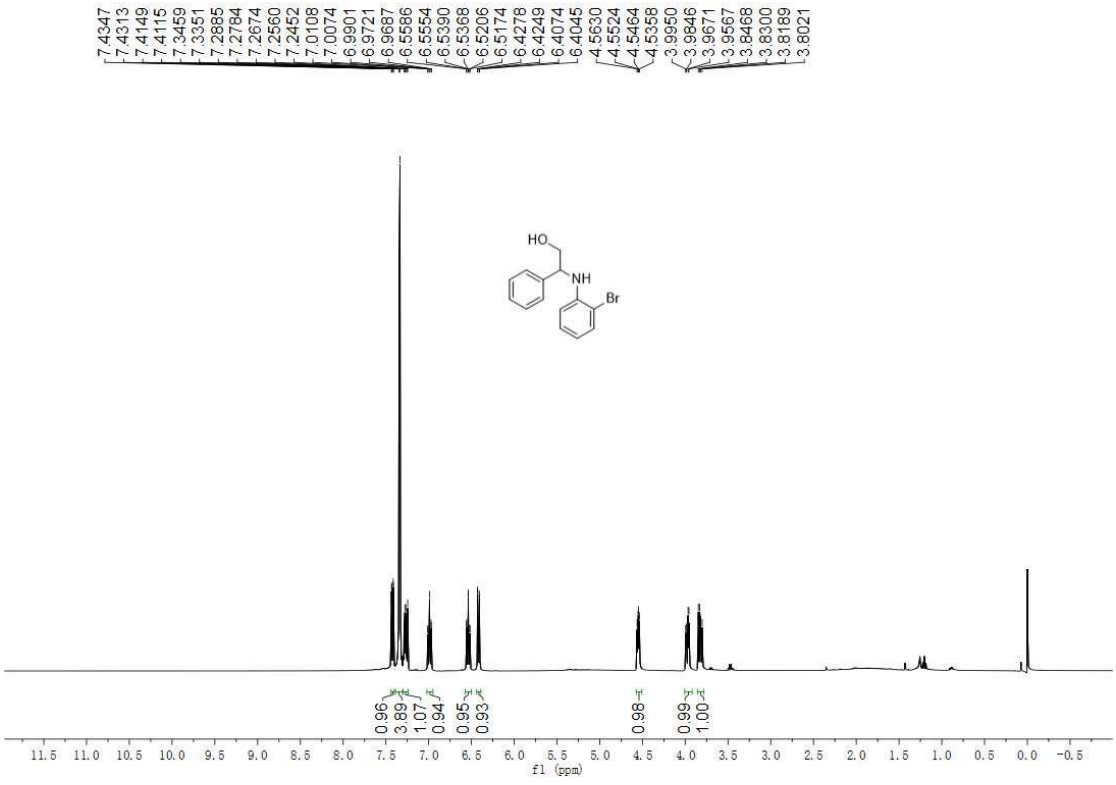
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7b**



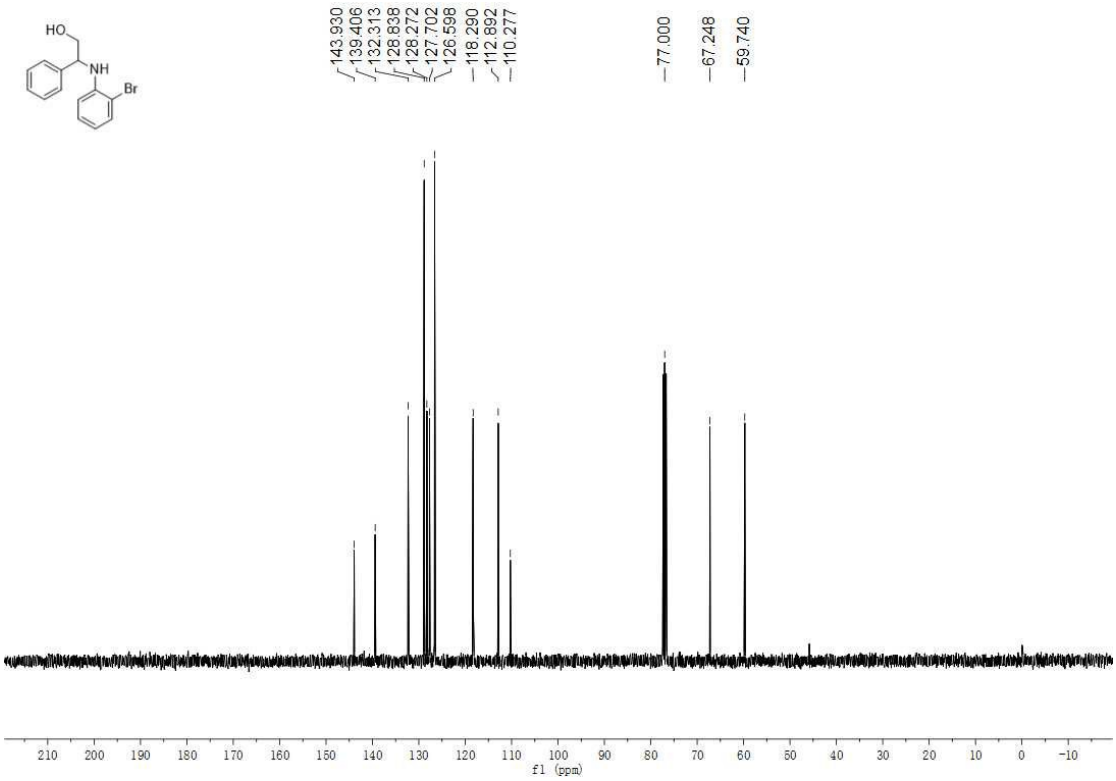
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7c**



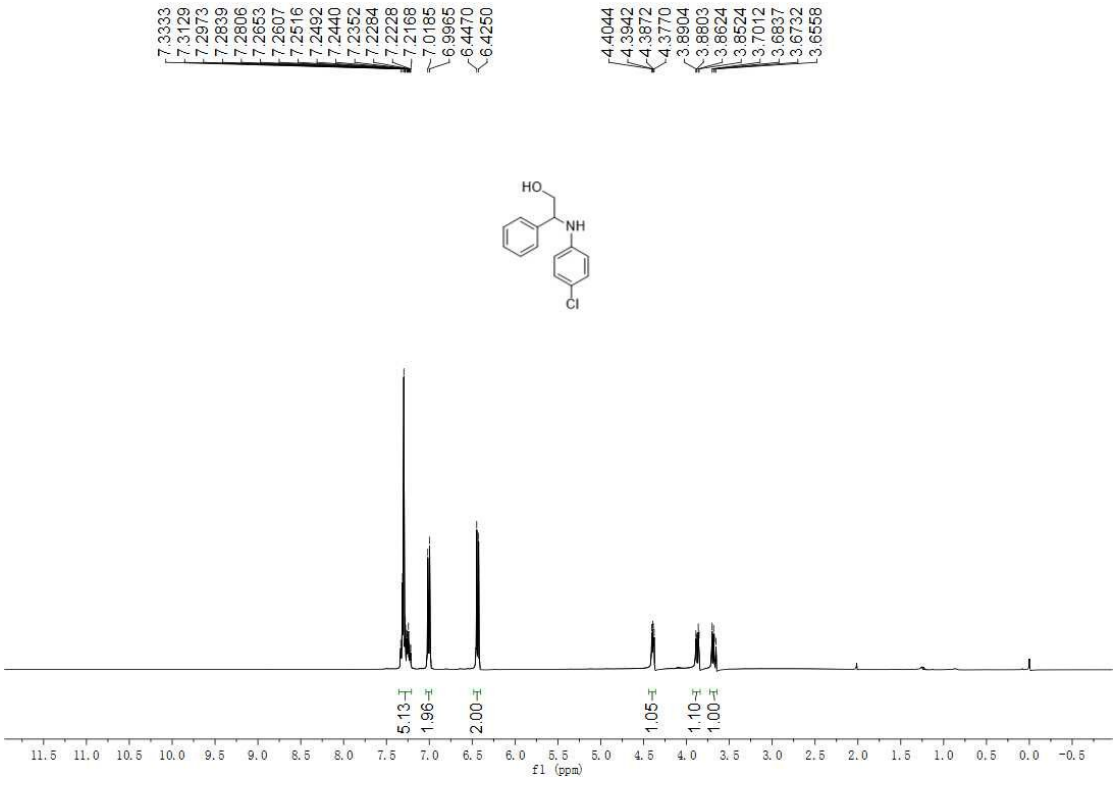
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7c**



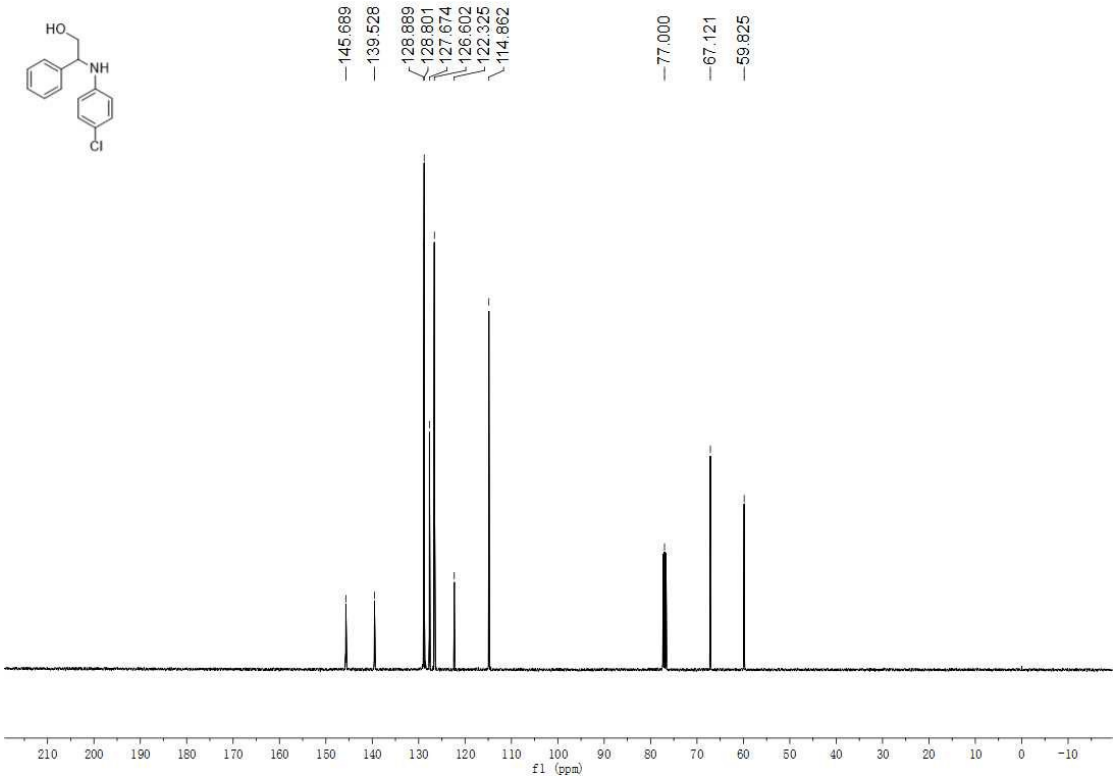
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7d**



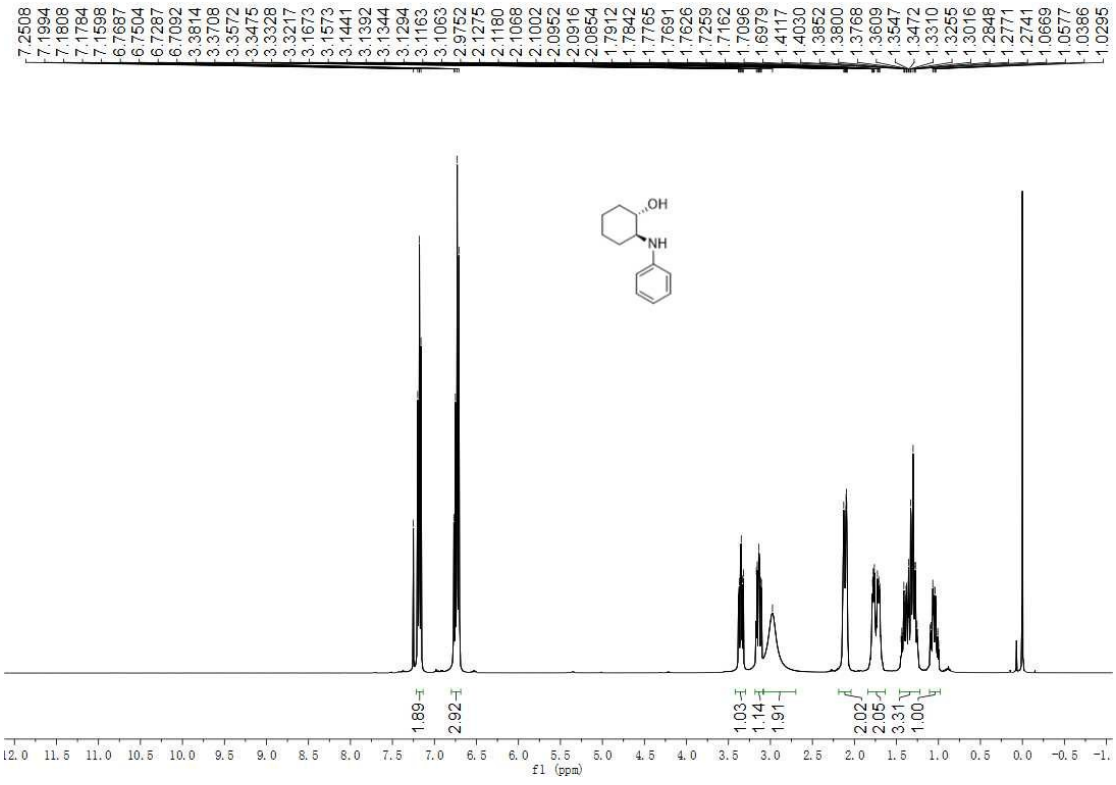
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7d**



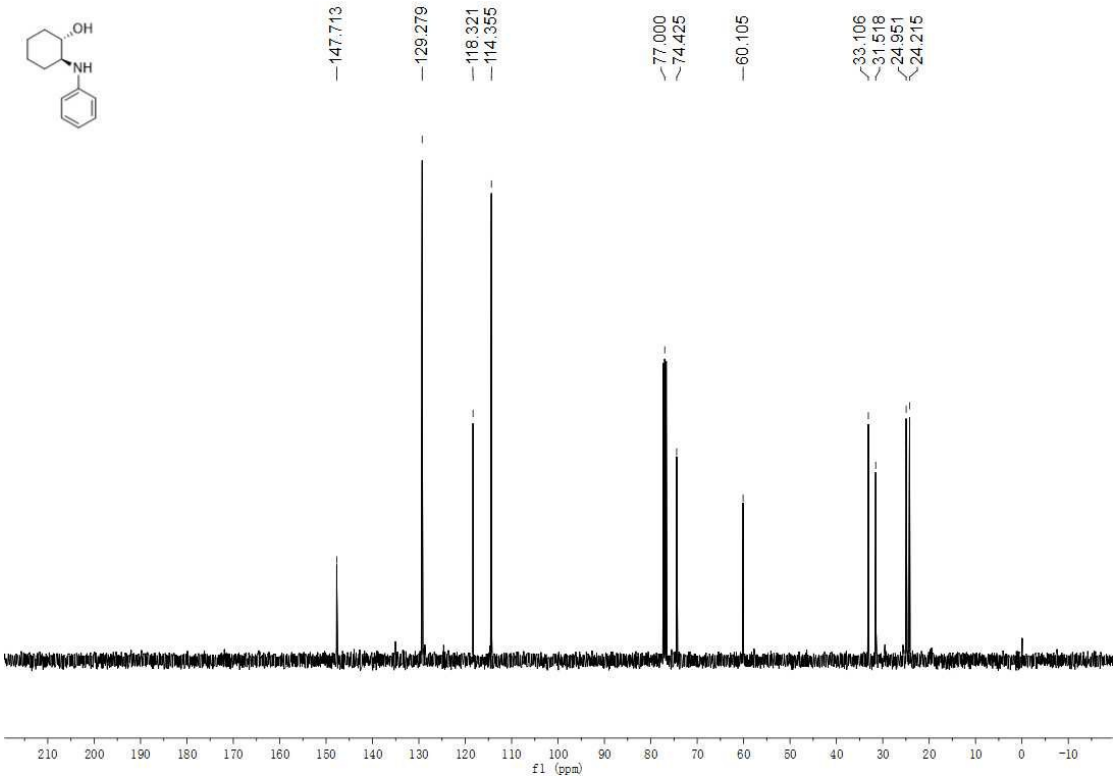
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7e**



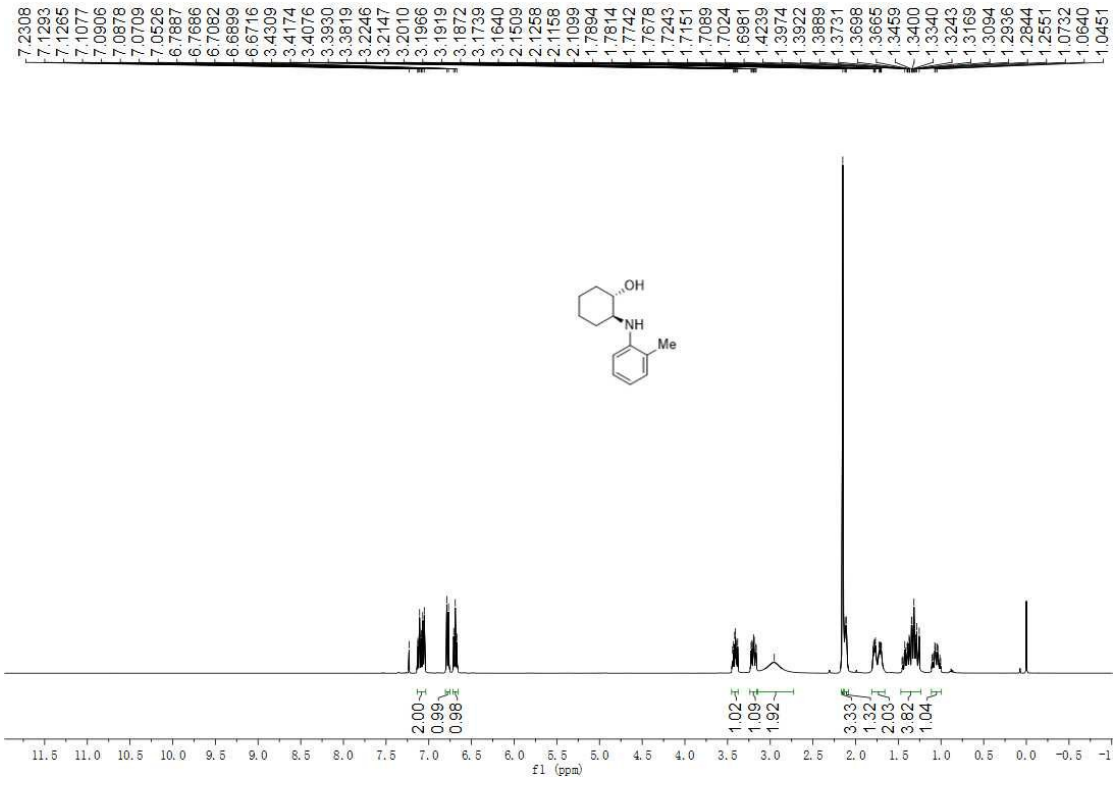
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7e**



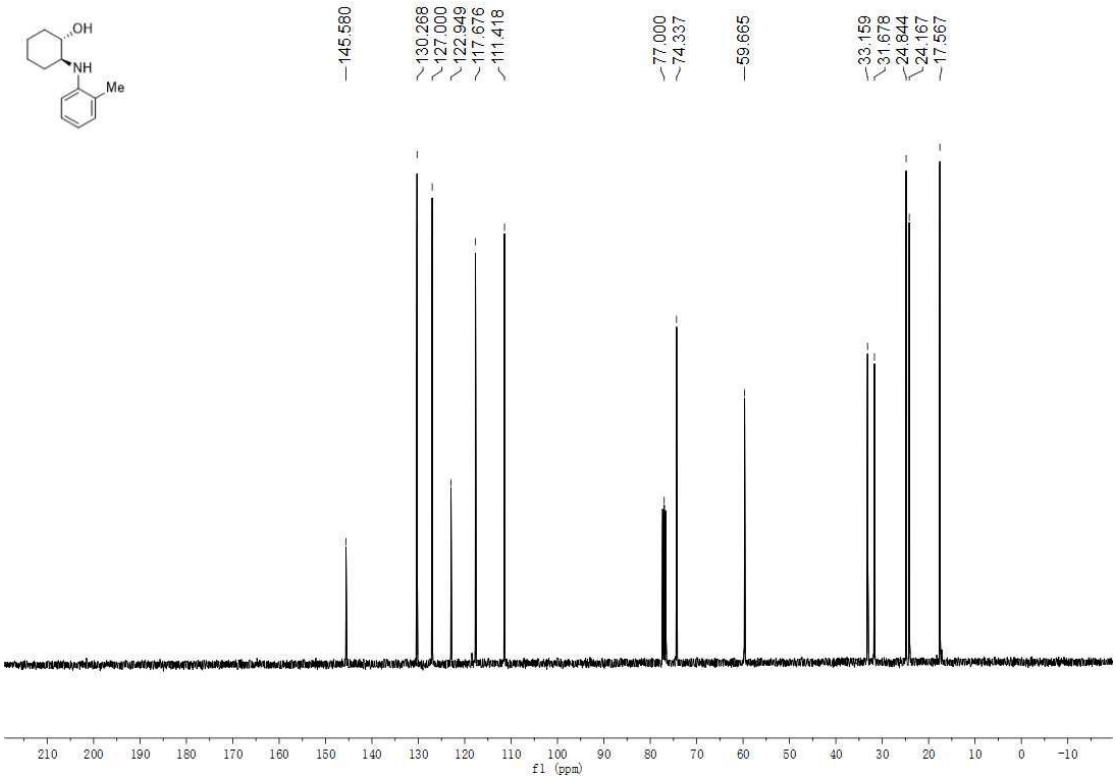
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7f**



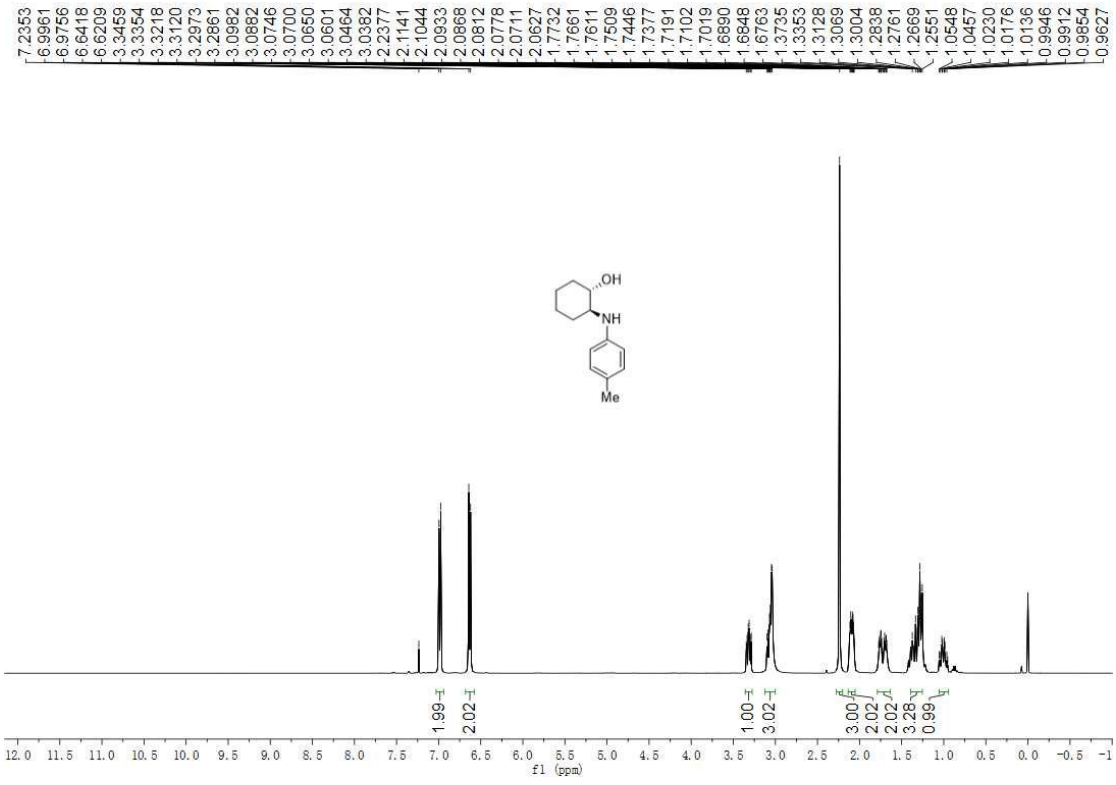
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7f**



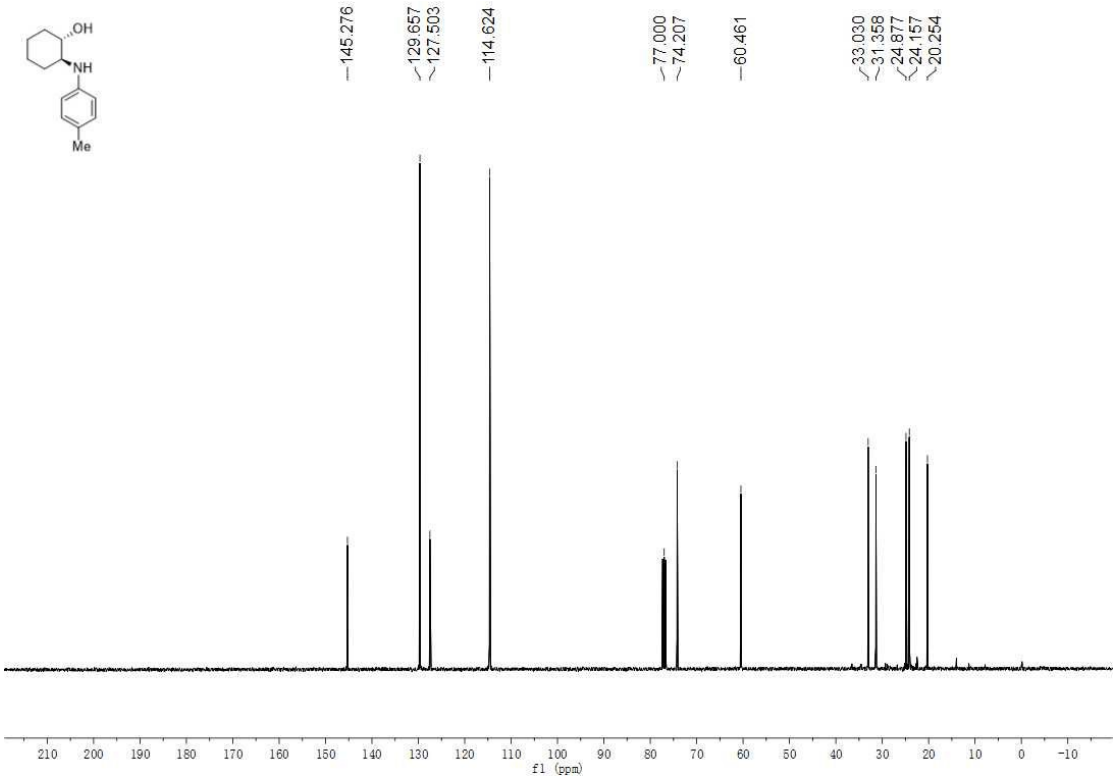
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7g**



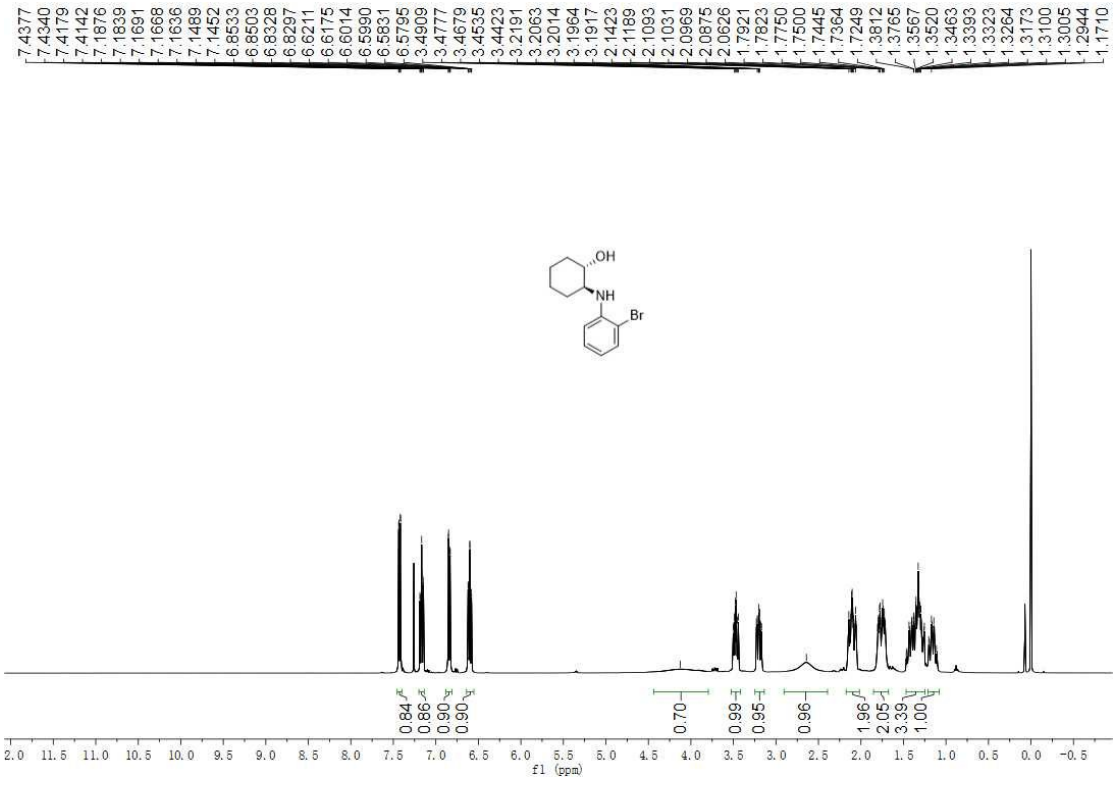
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7g**



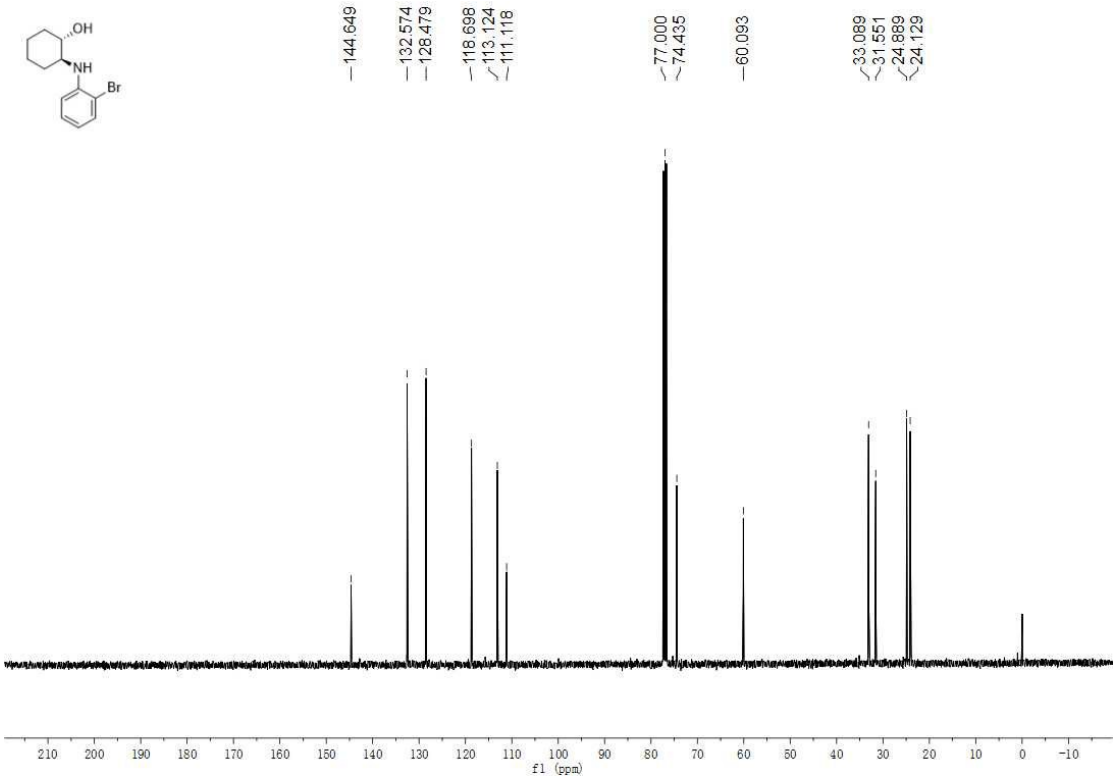
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7h**



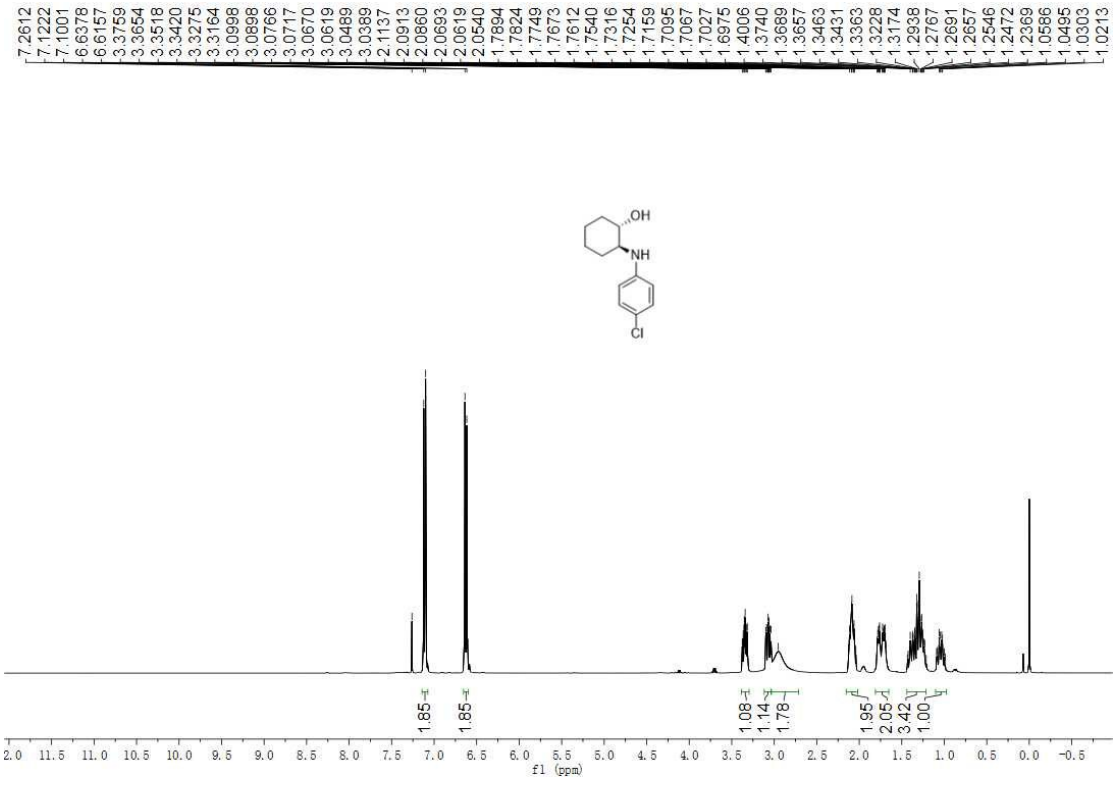
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7h**



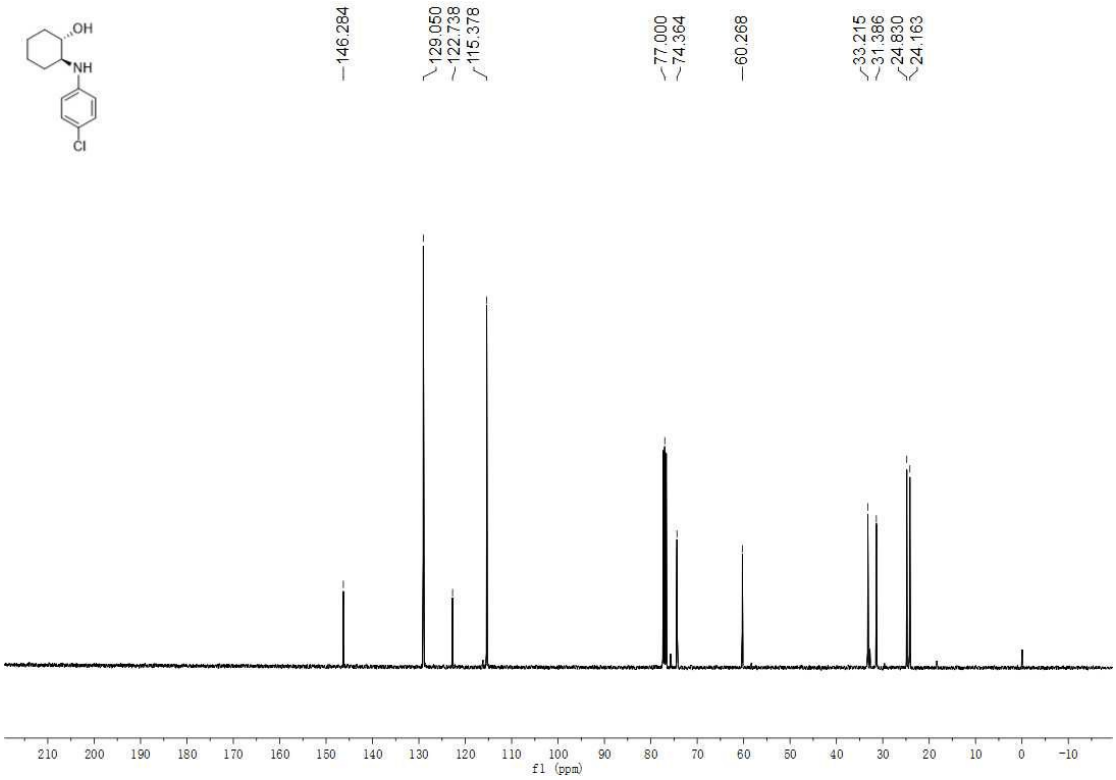
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7i**



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7i**



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7j**



^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7j**