Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

A sugar-derived ligand for room temperature aerial oxidation or non-aqueous Markovnikov hydration of styrenes via a preformed or in situ generated Co complex

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Table of Contents

1. **HRMS, XPS, EPR and Absorption spectra of RibN2, CoRibN2, [CoRibN2]$^+$ and intermediates generated from CoRibN2; TDDFT calculated transitions and relevant molecular orbitals.**

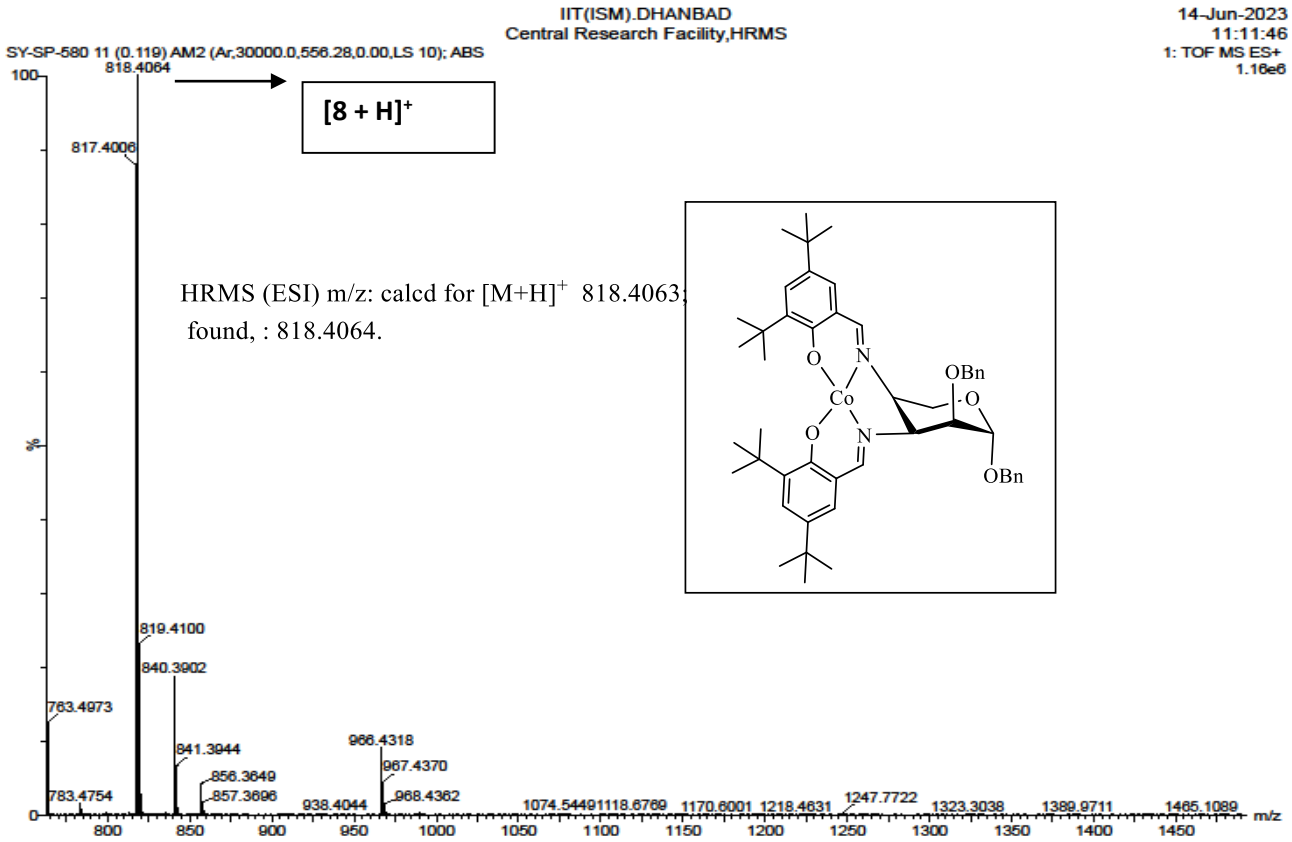


Figure S1. HRMS-ESI spectrum of **8.**

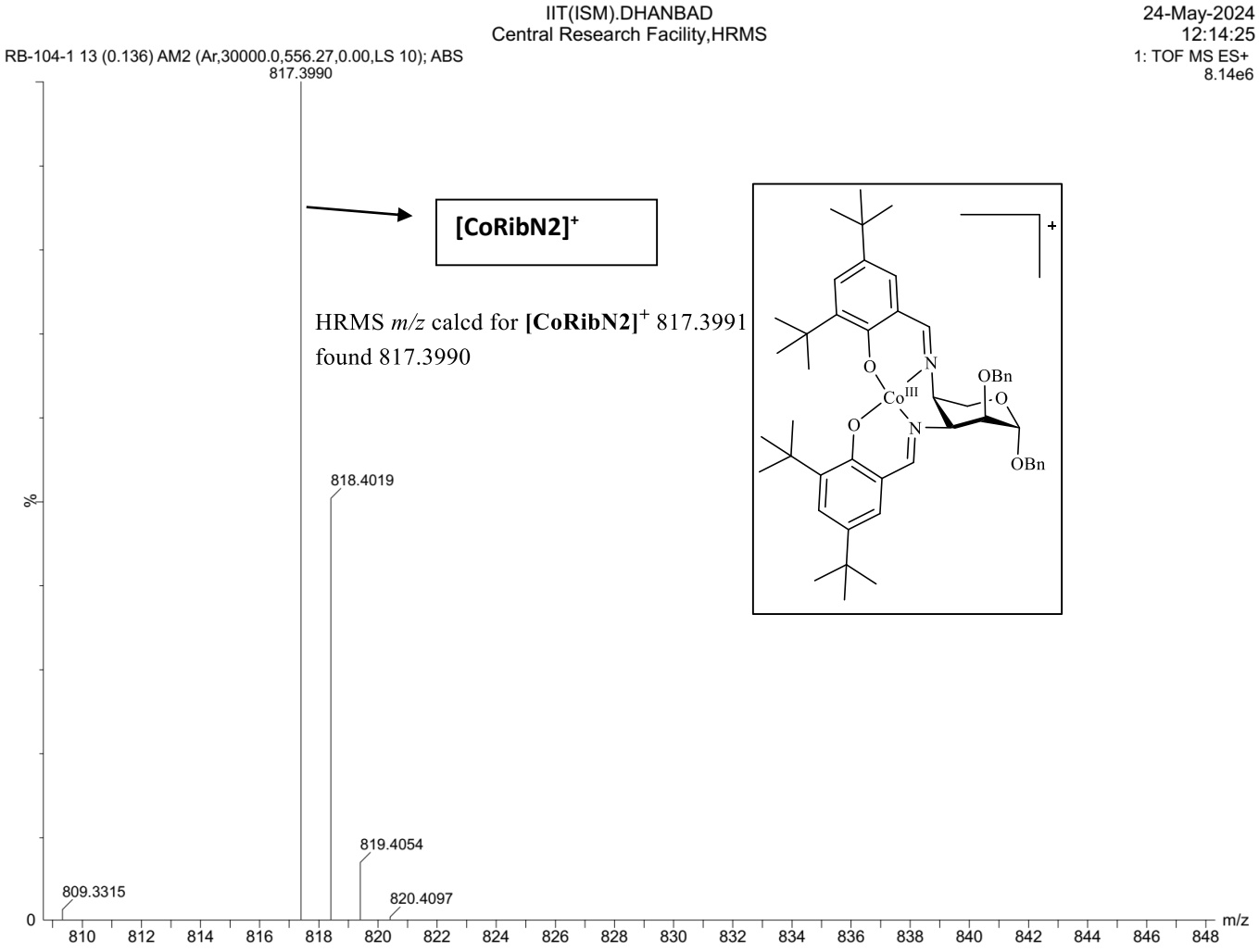


Figure S2. HRMS-ESI spectrum of [**CoRibN2]**$^{+}$**.**

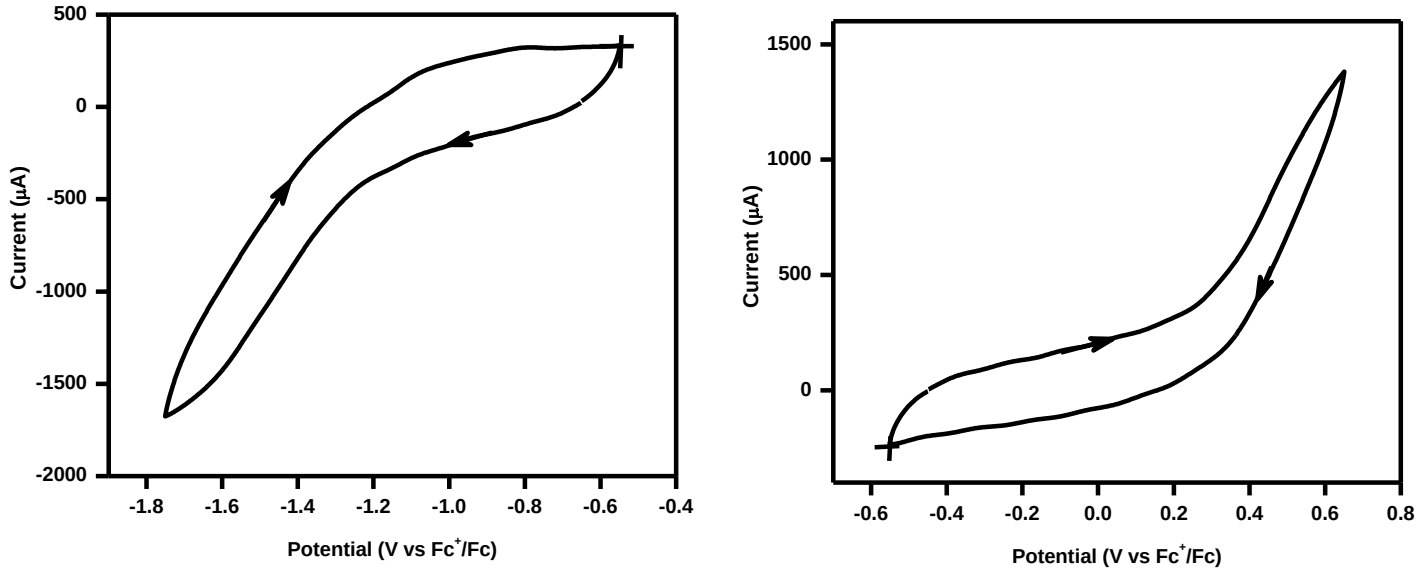


Figure S3. Cyclic voltammograms (100 mV/s) of ~1.0 mM solutions of **RibN2** in CH_2Cl_2 (0.1 M in TBAP) at a glassy carbon working electrode.

1.2 X-ray photoemission spectroscopic data

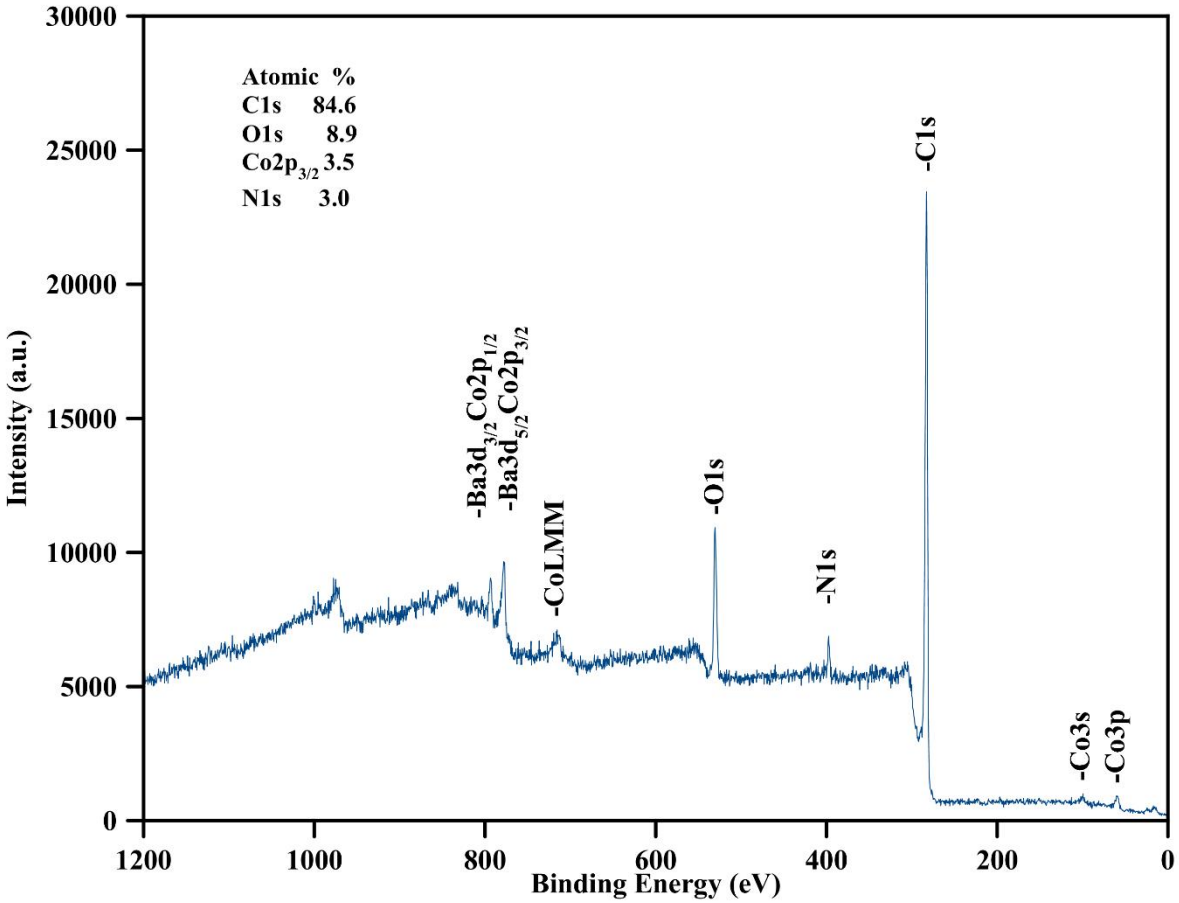


Figure S4. The full spectrum scan of XPS of **8**.

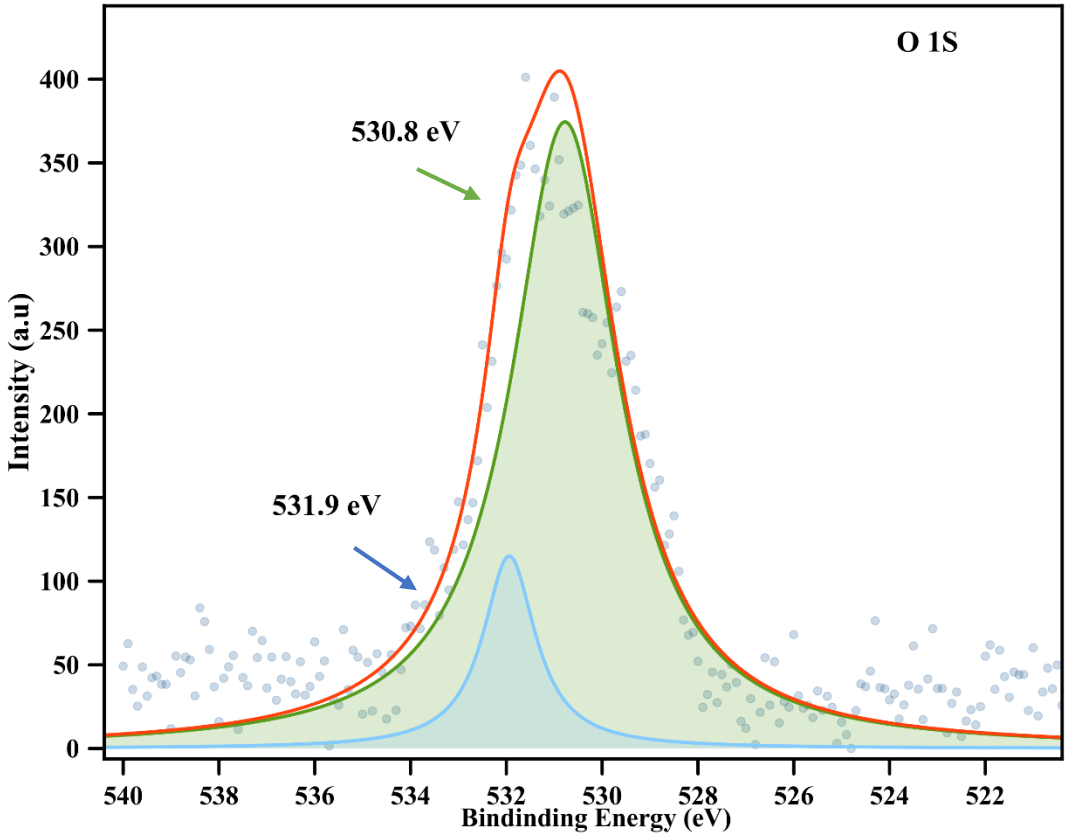


Figure S5. The fine spectrum scan of O1s of **8**.

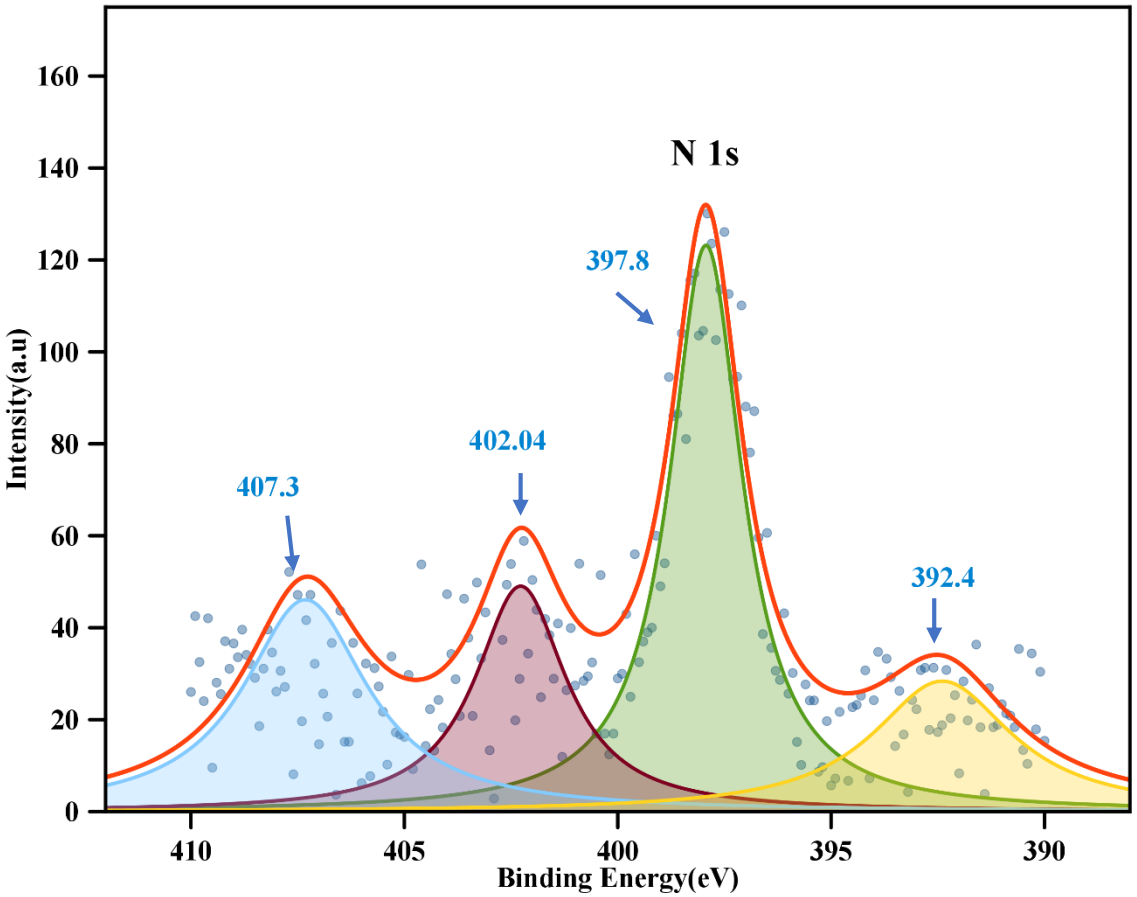


Figure S6. The fine spectrum scan of N1s of **8**.

1.3 EPR spectrum of 8.

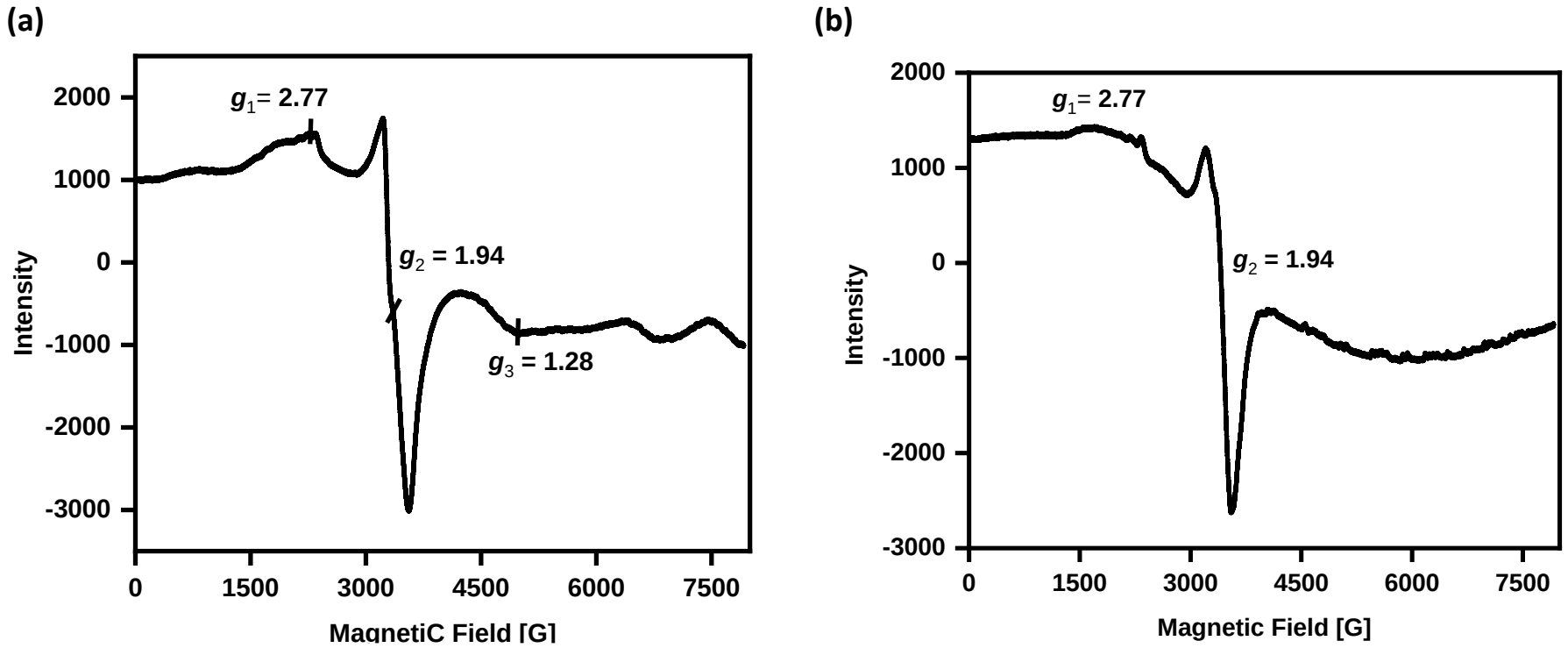


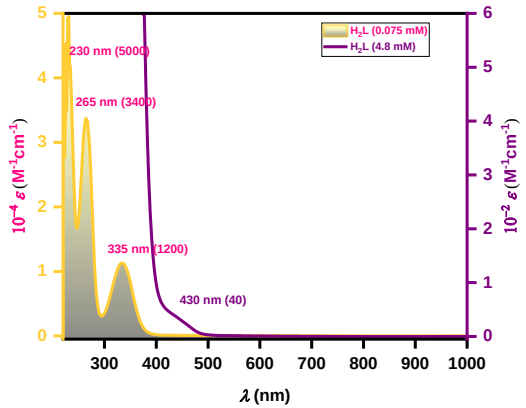
Figure S7. X-band EPR of Co(L) in (a) solid state at 77K. g_1 = 2.77, g_2 = 1.94, g_3 = 1.28 and (b) in CH_2Cl_2 solution at 77K g_1 = 2.77, g_2 = 1.94.

Note: *We have also tried the low temperature EPR experiment under frozen conditions in toluene. However, the hyperfine splitting was is not very prominent. In contrast, the powder sample at low temperature presented the better spectra confirming the low-spin states and the oxidation state of Co(II). This may be due to the formation of a new low-spin Co(II)-complex derived from electron exchange phenomenon. Similar broadening can be observed for low-spin square planar Co(II)-complexes with porphyrins (Zhou et. al, J. Phys. Chem. B, 2015, 119, 14102-14110) where EPR of frozen solution was measured in 130 K. In the specified article, teo Co(II) complexes showed similar much weaker $g_{\perp}$ and $g_{//}$ with broadened signals. Their electronic configurations are converted and they experience a cross-hybrid change [d(x2−y2)sp2↔d(z2)sp2] generating a new low-spin ground state.*

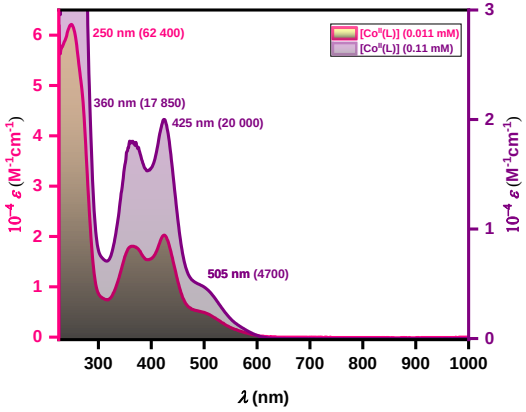
1.4 UV Visible absorption spectra and kinetic experiment for intermediate identification:

Absorption spectra of 7, 8 and [CoRibN2]$^{+}$.

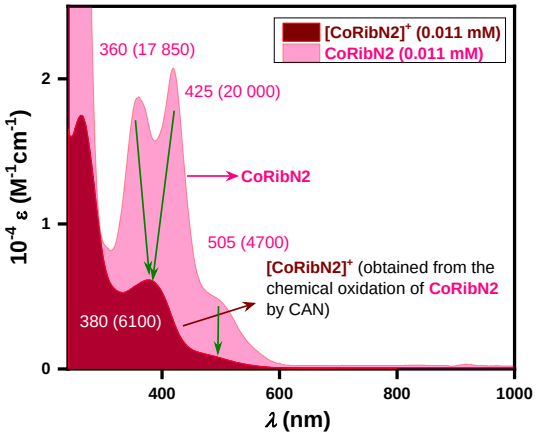
(a)



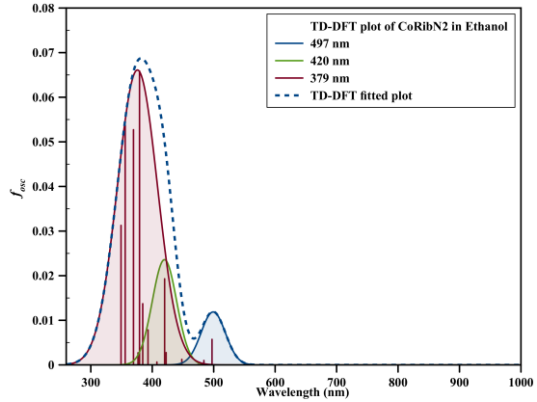
(b)



(c)



(d)



(e)

λ (nm) (ε ($M^{-1}cm^{-1}$)) of RibN2	λ (nm) (ε ($M^{-1}cm^{-1}$)) of CoRibN2	λ (nm) (ε ($M^{-1}cm^{-1}$)) of [CoRibN2]$^{+}$	TD-DFT calculated λ(nm) of CoRibN2
	505 (4700)		497
430 (40)	425 (20 000)	490 (900)	420
335 (1200)	360 (17 850)	380 (6100)	379
265 (3400)	250 (62 400)	260 (17 600)	
230 (5000)			

Figure S8. UV-Vis absorption spectrum of (a) **7**, (b) **8** and (c) [**CoRibN2**]$^{+}$ in CH_2Cl_2 solution, (c) TD-DFT calculated absorption spectrum of **8**.

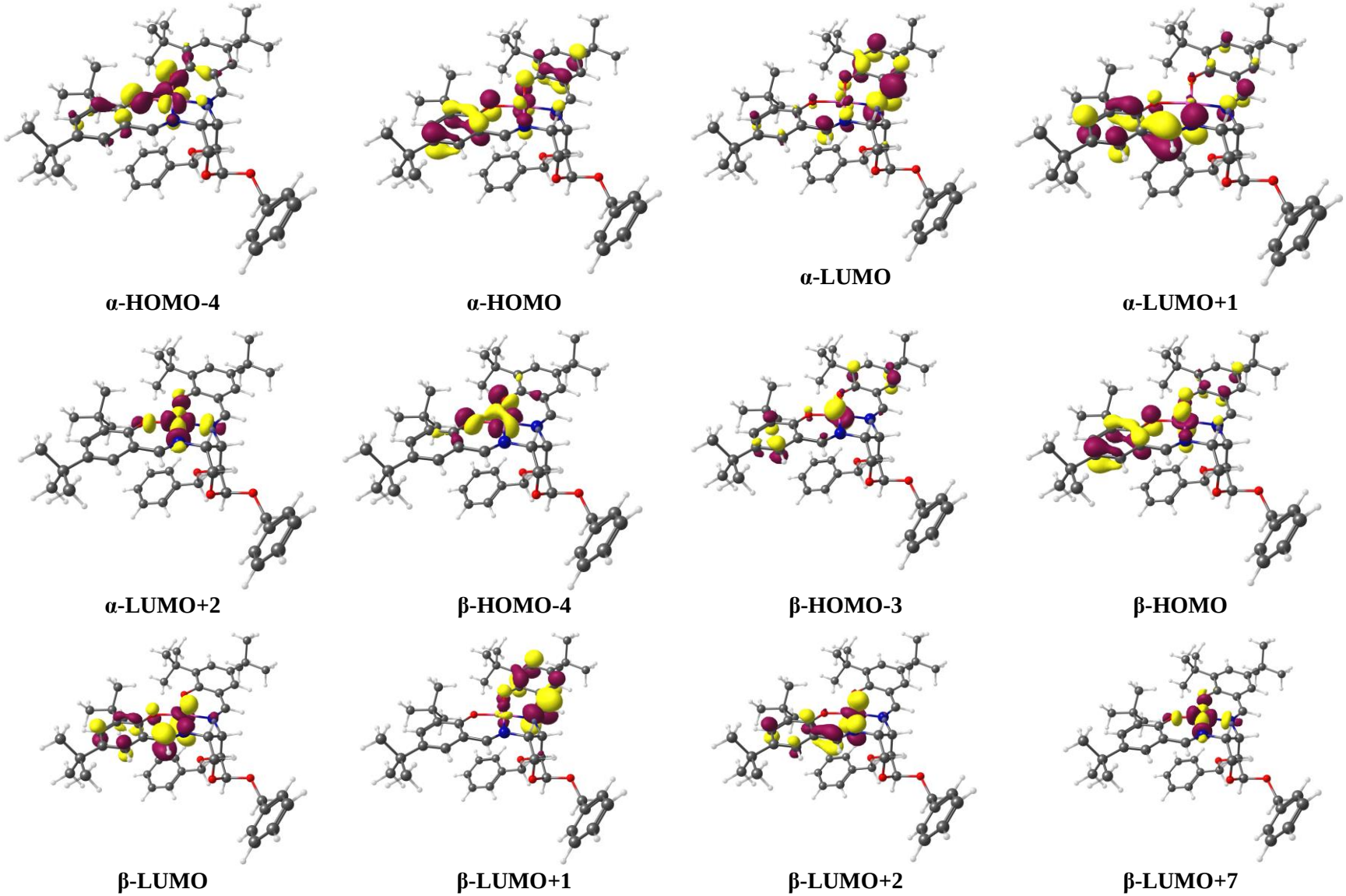


Figure S9. Representative molecular orbitals for TD-DFT calculations on **8**.

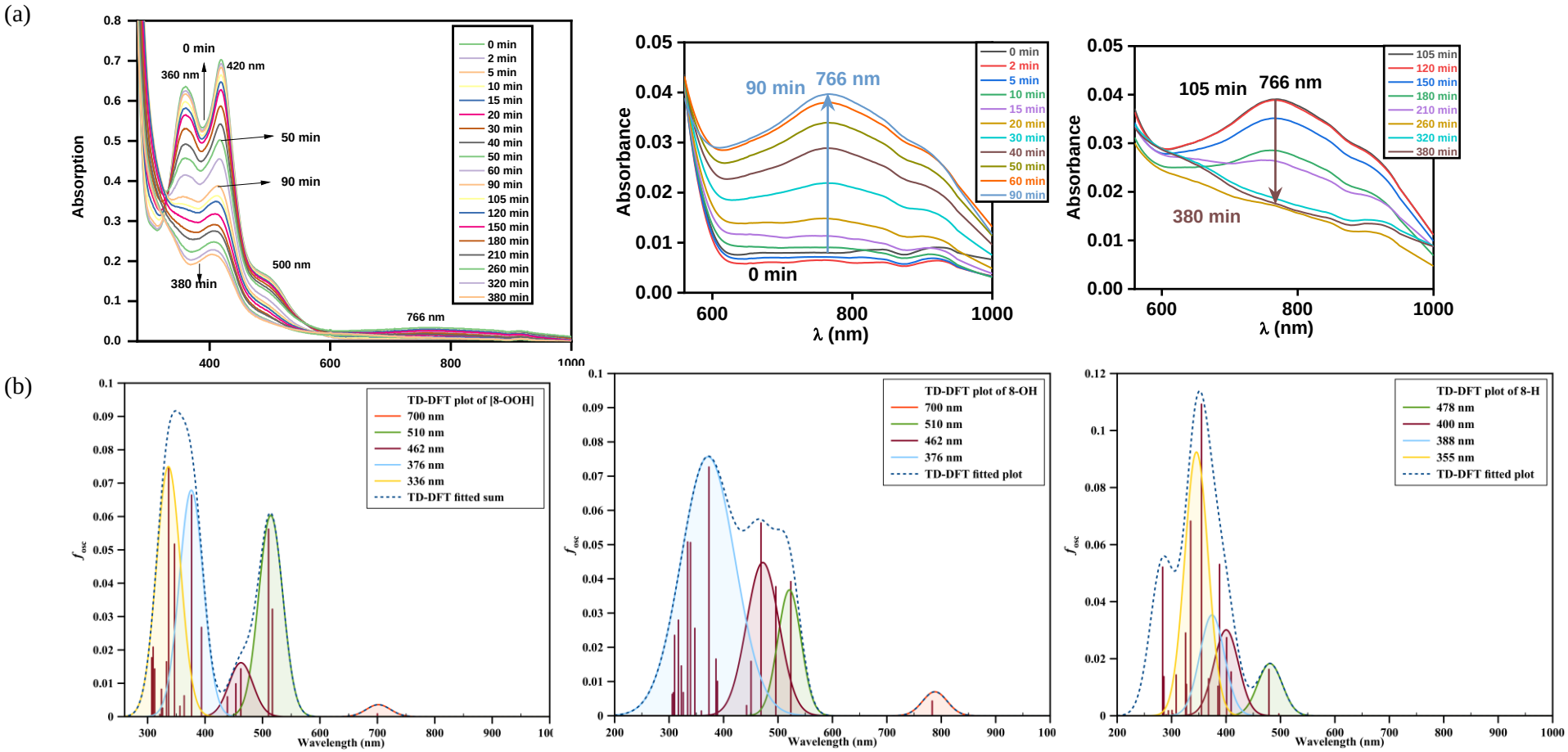


Figure S10. (a) Change in absorption of the catalyst (CoRibN2 **8**) in presence of 1 equiv. Et_3SiH in air in MeCN. Decay in Co(II) spectral features in 500, 420 and 360 nm peaks with generation of a 766 nm peak for first 90 mins and decay of the characteristic 766 nm peak during the rest of the course (90-380 mins). (b) TD-DFT calculated absorption spectra for **8-OOH**, **8-OH** and **8-H**.

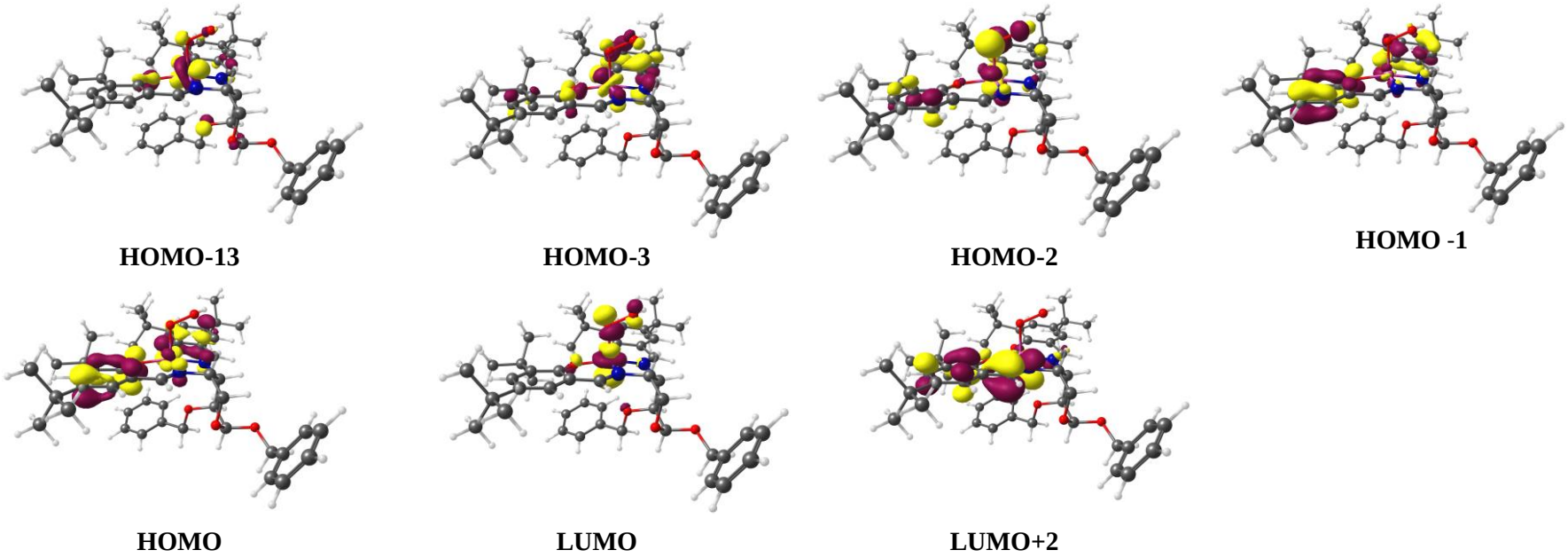


Figure S11. Representative molecular orbitals for TD-DFT calculations on **8-OOH**.

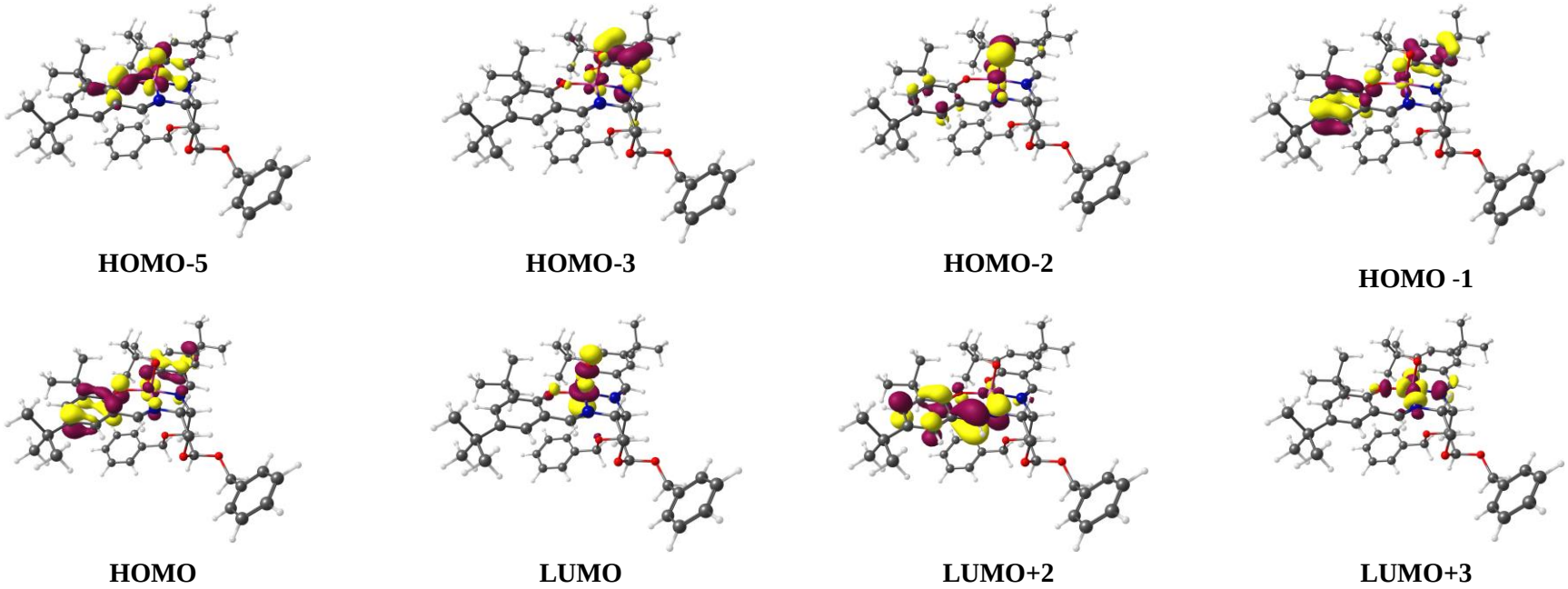


Figure S12. Representative molecular orbitals for TD-DFT calculations on **8-OH**.

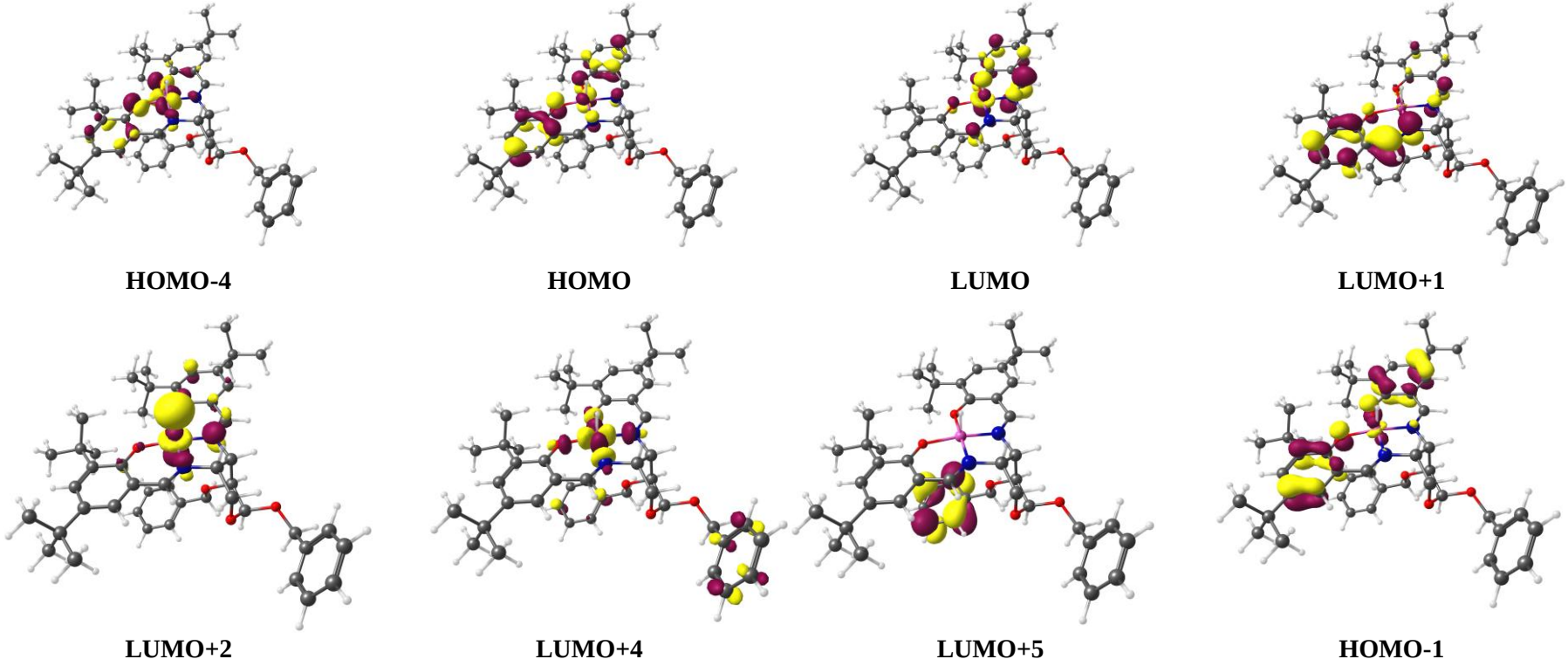


Figure S13. Representative molecular orbitals for TD-DFT calculations on **8-H**.

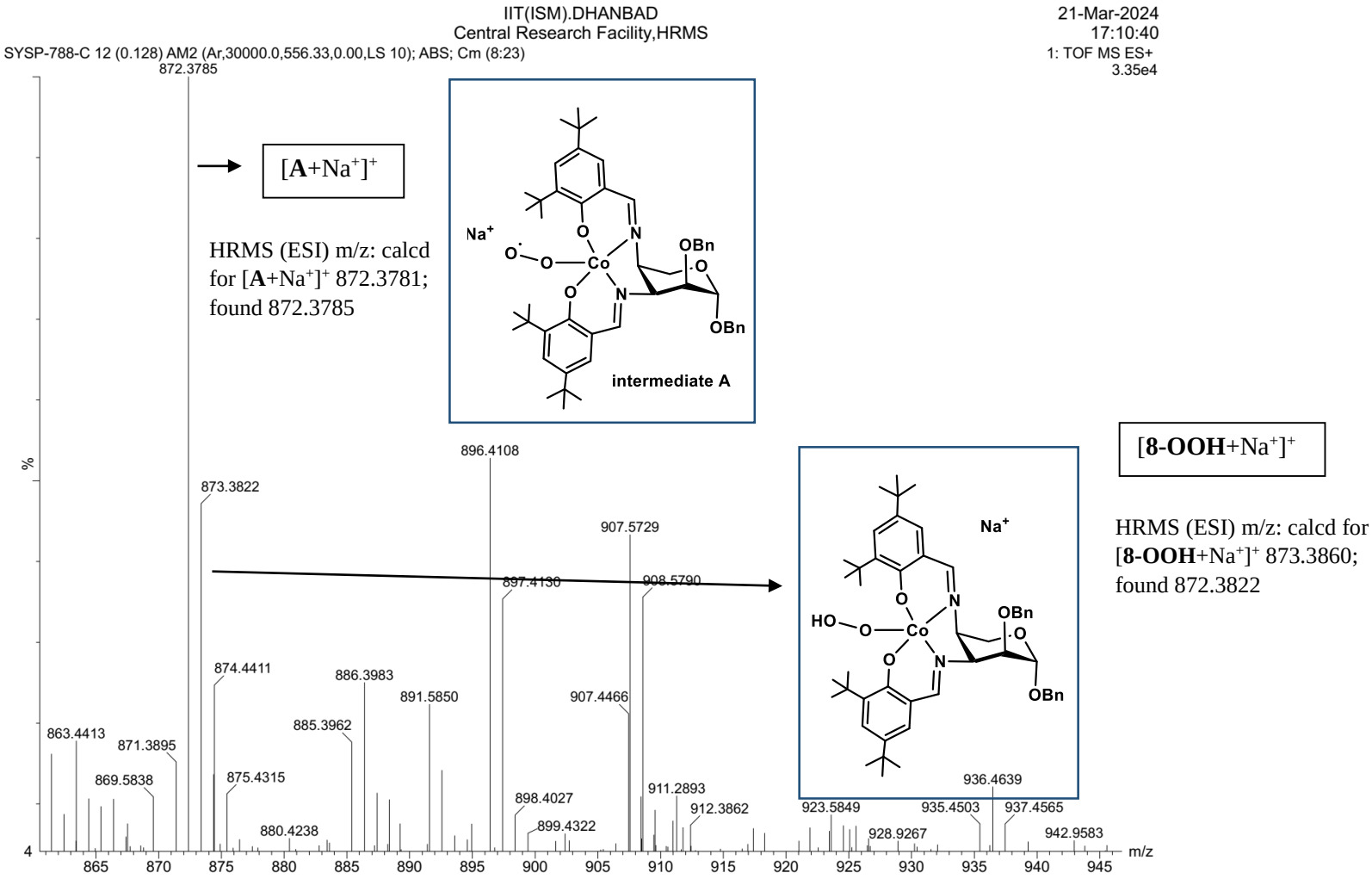


Figure S14. HRSM-ESI spectrum of reaction mixture (1:1 mixture of **8** and Et_3SiH in MeCN) after 30 mins. HRMS (ESI) m/z: calcd for [**A**+Na^+]$^+$ 872.3781; found: 872.3785. and cald for [**8-OOH**+Na^+]$^+$; 873.3860; found 873.3822.

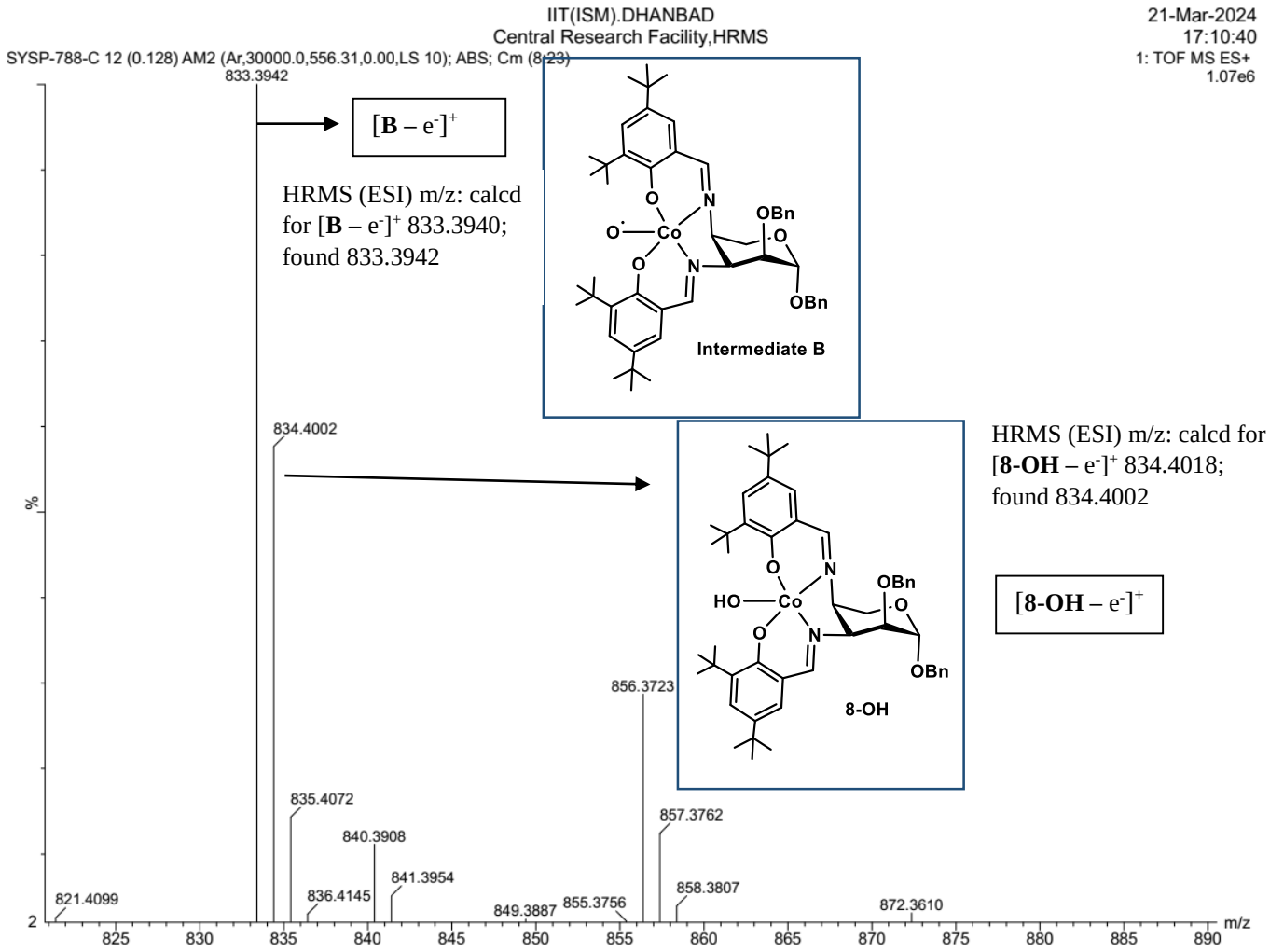
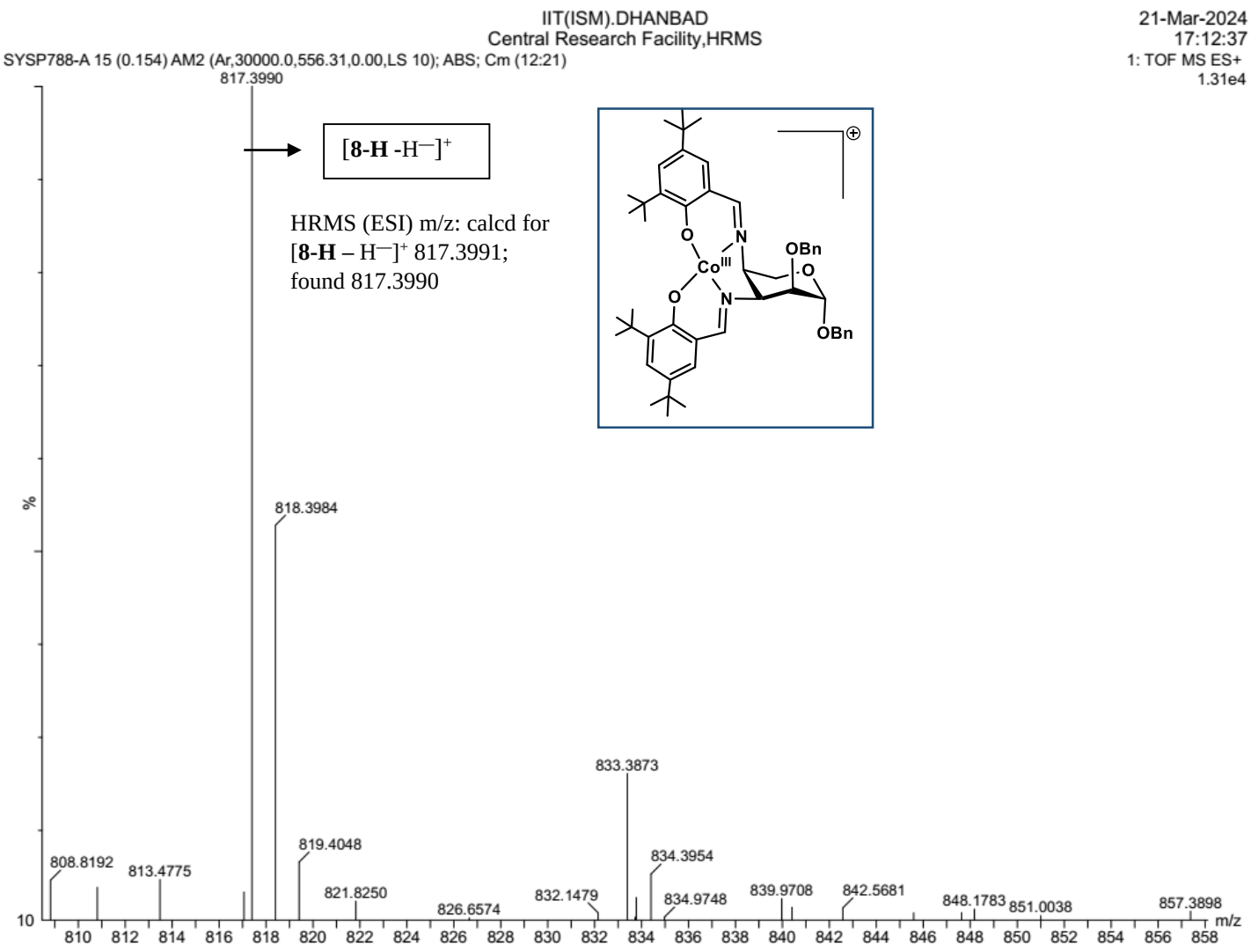


Figure S15. HRSM-ESI spectrum of reaction mixture (1:1 mixture of **8** and Et_3SiH in MeCN) after 90 mins. HRMS (ESI) m/z: calcd for [**B**-e^-]$^+$ 833.3940 found: 833.3942 and cald for [**8-OH**-e^-]$^{+,}$ 834.4018; found 834.4002.

(a)


IIT(ISM).DHANBAD
Central Research Facility,HRMS
21-Mar-2024
17:12:37
SYSP788-A 15 (0.154) AM2 (Ar,30000.0,556.31,0.00,LS 10); ABS; Cm (12:21)
1: TOF MS ES+
1.31e4
817.3990
[8-H -H⁻]⁺
HRMS (ESI) m/z: calcd for [8-H – H⁻]⁺ 817.3991; found 817.3990
OBn
OBn
%
10
818.3984
833.3873
819.4048
834.3954
808.8192
813.4775
821.8250
826.6574
832.1479
834.9748
839.9708
842.5681
848.1783
851.0038
857.3898
m/z
810 812 814 816 818 820 822 824 826 828 830 832 834 836 838 840 842 844 846 848 850 852 854 856 858

(b)

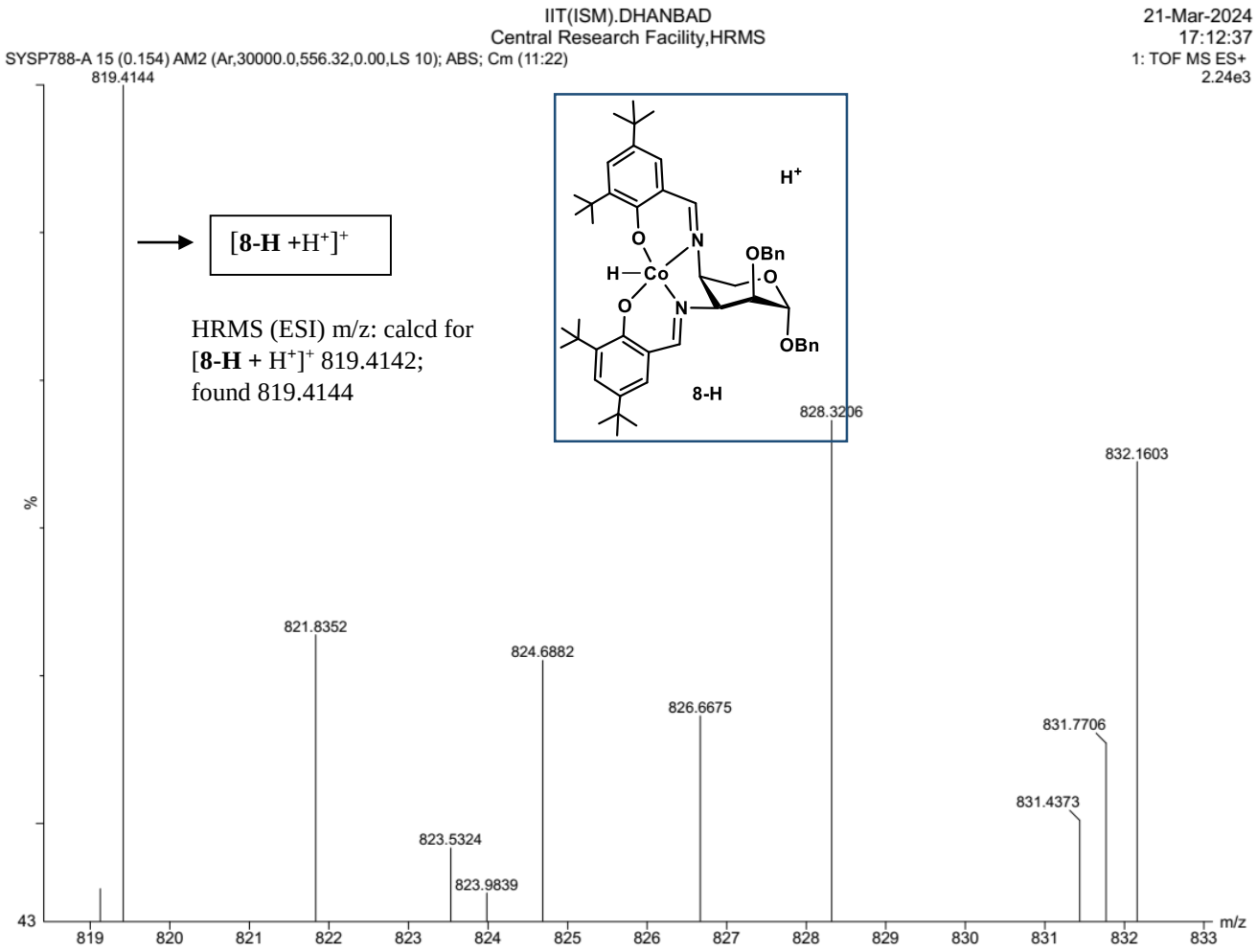


Figure S16. HRSM-ESI spectrum of reaction mixture (1:1 mixture of **8** and Et_3SiH in MeCN) 380 mins. HRMS (ESI) m/z: calcd for [**8-H** - H⁻]⁺, [**8-H**+H⁺]⁺ 817.3991 and 819.4142; found: 817.3990 and 819.4144.

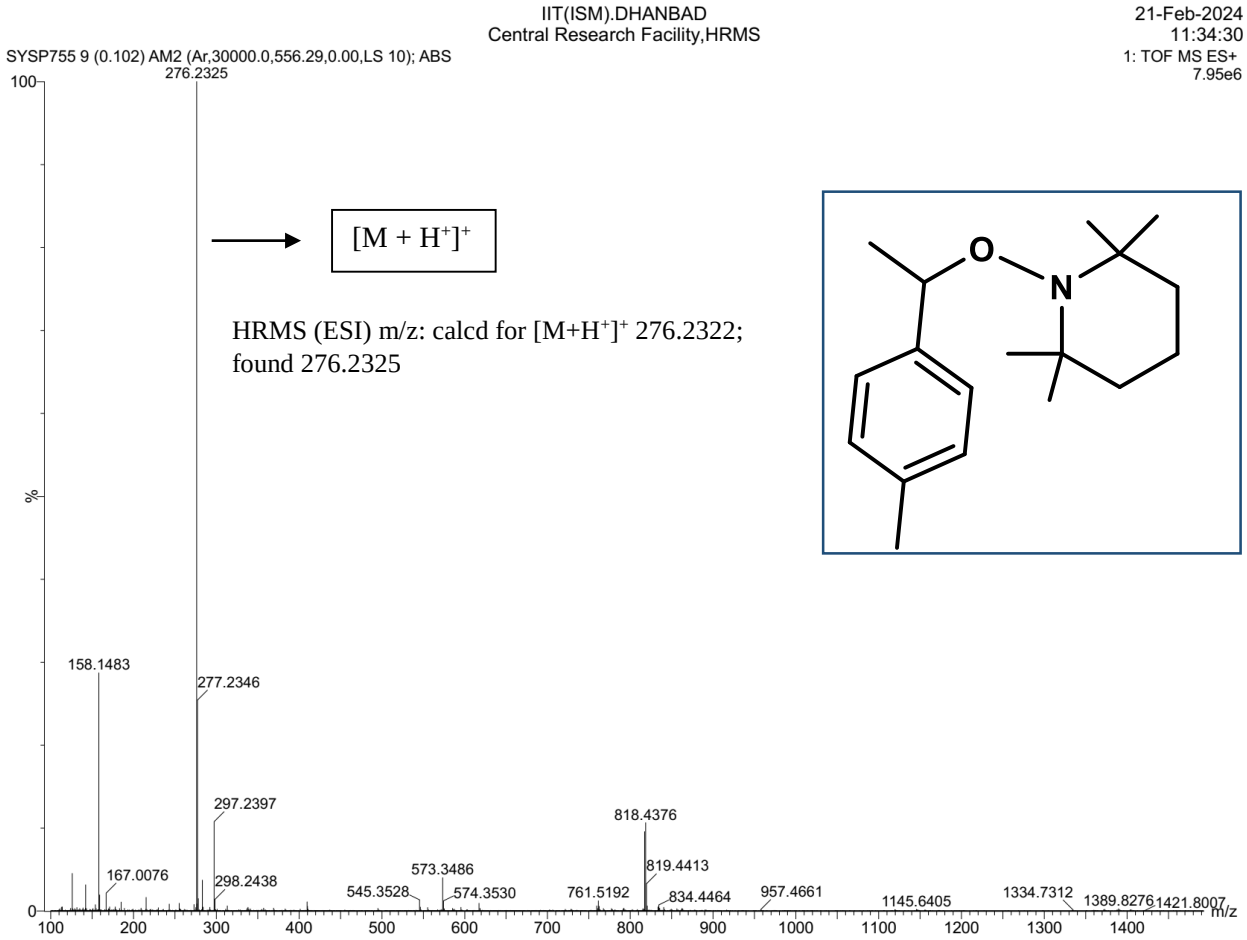
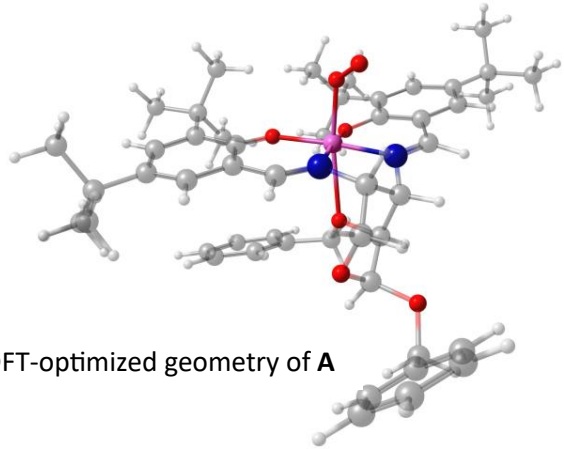
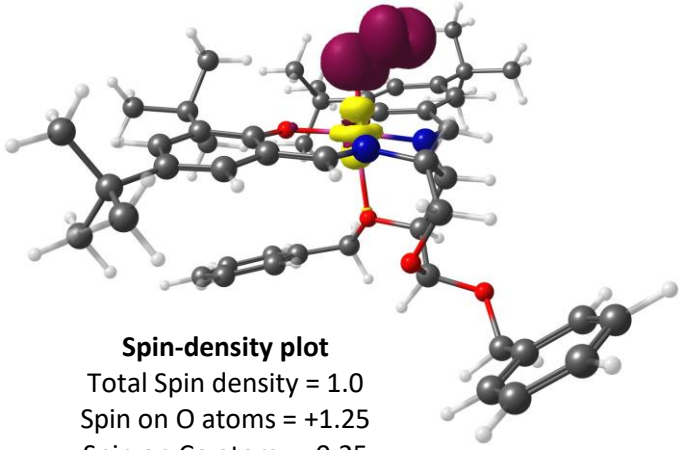


Figure S17. HRSM-ESI spectrum of reaction mixture (TEMPO + reaction mixture under standard condition) after 30 mins. HRMS (ESI) m/z: calcd for $[M+H^+]^+$ 276.2322; found 276.2325.

(a)

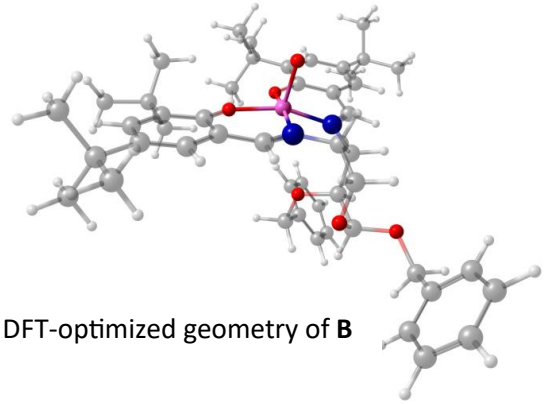


DFT-optimized geometry of **A**

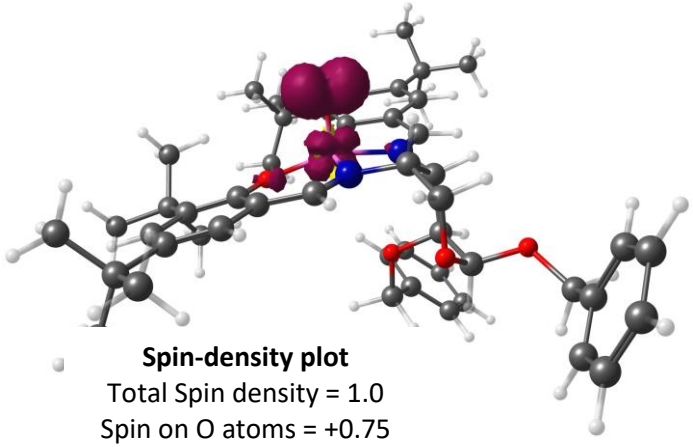


Spin-density plot
Total Spin density = 1.0
Spin on O atoms = +1.25
Spin on Co atom = -0.25

(b)

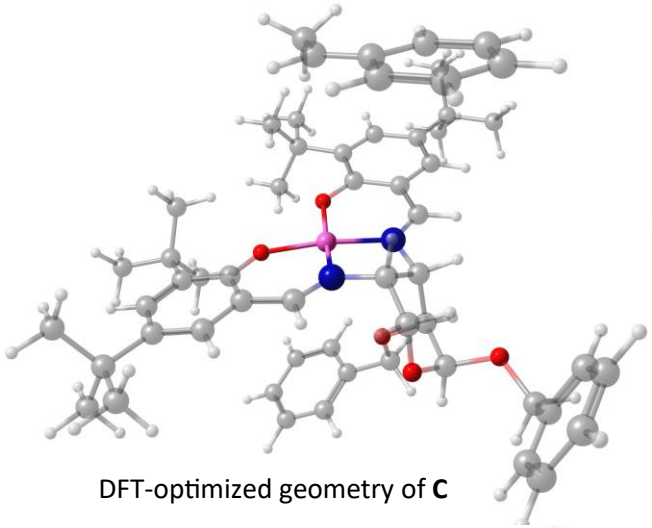


DFT-optimized geometry of **B**

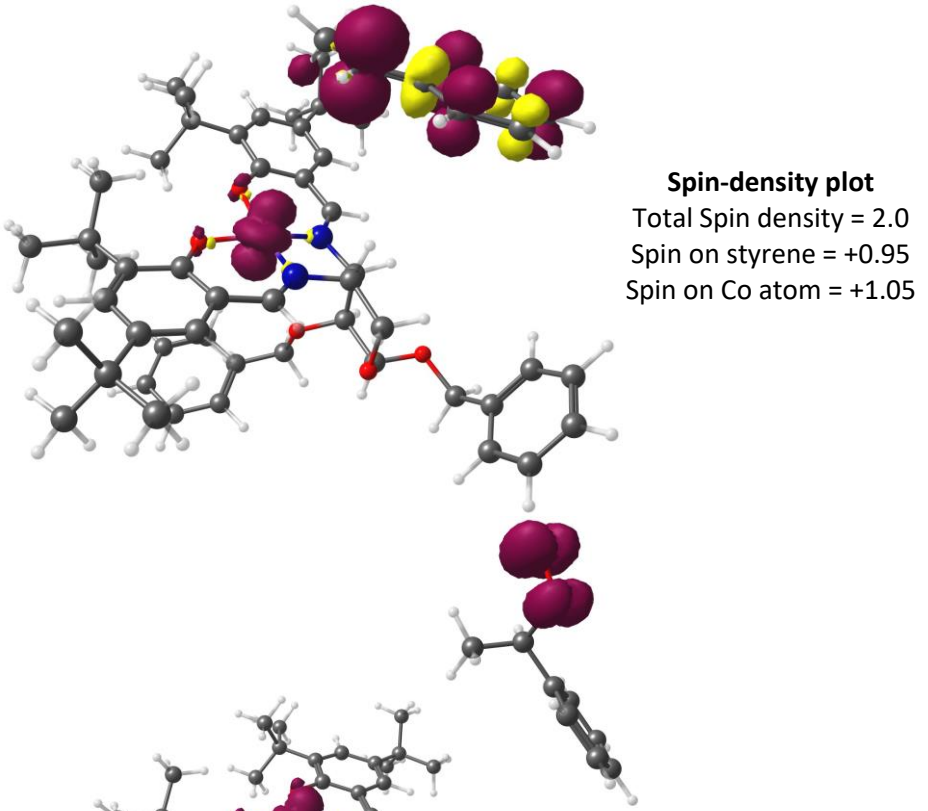


Spin-density plot
Total Spin density = 1.0
Spin on O atoms = +0.75
Spin on Co atom = +0.25

(c)

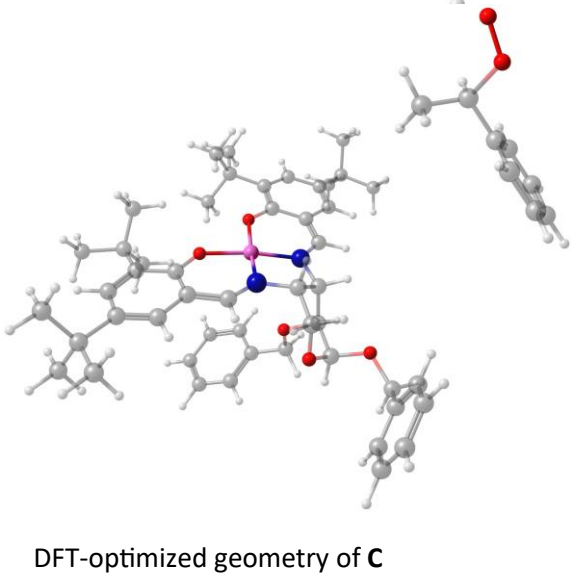


DFT-optimized geometry of **C**



Spin-density plot
Total Spin density = 2.0
Spin on styrene = +0.95
Spin on Co atom = +1.05

(d)



DFT-optimized geometry of **C**

Spin-density plot
Total Spin density = 2.0
Spin on alkylperoxo = +0.95
Spin on Co atom = +1.05

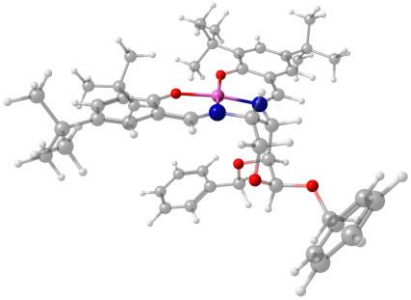
Figure S18. DFT-optimized geometry and spin density plots of intermediates (a) **A**, (b) **B**, (c) **C** and (d) **D**.

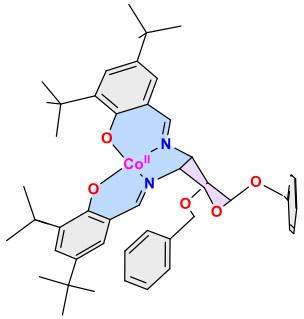
2. Tables

Table S1. TD-DFT calculated electronic transitions of CoRibN2 **8**.

Excitation energy(eV)	λ (nm)	*f*	Transition	Character
2.493	497	0.006	*α*–H-4→ α –L+2 (19%)	LMCT (phenolate → metal)
			β–H-4→ β –L+7 (11%)	LMCT (phenolate → metal)
			β–H-3→ β –L+7 (13%)	LMCT (phenolate → metal) along with minor MLCT (metal to phenolate)
2.950	420	0.019	*α*–H→ α –L (9%)	LMCT (phenolate → metal) along with ILCT (between to phenolate moieties)
			β–H→ β –L (9%)	ILCT (phenolate → Schiff base)
			β–H→ β –L+1 (13%)	MLCT (metal → phenolate) along with minor ILCT (between two phenolates)
3.269	379	0.006	*α*–H→ α –L+1 (33%)	ILCT (phenolate → Schiff base)
			β–H→ β –L (12%)	ILCT (phenolate → Schiff base) along with LMCT (phenolate → metal)
			β–H→ β –L+1 (21%)	ILCT (between two phenolates)
			β–H→ β –L+2 (17%)	ILCT (phenolate → Schiff base)

Table S2. DFT-optimized cartesian coordinates of **8.**





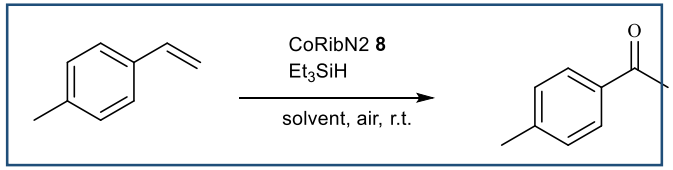
Co	7.11998556044369	4.41999799981854	9.62348915584057
O	7.96841779660384	3.25970719404541	10.86196430342059
N	7.47847851134944	3.27829923457428	8.15224917731605
C	9.83735406012911	-0.42489349014896	10.21330756249114
O	5.55311983003312	2.14466217574244	5.88653359577052
O	7.03470782574288	5.77432283278733	10.95170664284891
O	4.48535996710582	3.07454897558562	8.46337131743849
C	8.64232579769578	1.52255503341375	9.36566834665519
C	8.10095621069732	2.14813246611722	8.19969574842566
H	8.24331089138965	1.59279676318442	7.27579850748505
C	9.72381445102476	0.16249972580818	11.49443949344730
H	10.15218720130096	-0.38134973272475	12.32313457681277
C	4.37689679668367	2.91612412737330	6.05288125514143
H	3.59132612155324	2.17637652005491	6.22735408005385
C	3.38531565685603	0.57203671790469	10.06409532904327
H	3.38713210946358	0.13058460930369	9.07380130810172
C	3.26958858331270	1.95740179569417	10.20004113425412
C	4.71860107177876	11.00066888170482	10.77826836412172
C	6.64795706785284	7.88264804790673	11.99805415795403
C	6.73778905074321	2.92016005176879	5.70171991641113
H	6.64780594432038	3.53439135406521	4.80185170079076
H	7.54283604752594	2.20960147057002	5.52801337092112
C	5.18684266995339	8.70672272461052	9.72655454196260
H	4.64137160971328	8.97957854403689	8.83256284707116
C	9.11198787215061	1.37329471034582	11.76610856551043

C	5.78032881897563	4.69724127182194	7.18203364382259
H	5.62500660648012	5.41107193205814	6.36943330080196
C	6.49935895185516	6.96439801214752	10.89849687007153
C	6.25253782515932	1.48979721079858	0.92062933487961
H	6.95360200196004	1.10745419234363	0.18870184083834
C	5.58275995587502	6.60043191599367	8.60362492235682
H	5.00410349375254	7.03894013141622	7.78996559553552
C	4.43969730805137	2.47983374218499	2.81452684404699
C	7.02356394458061	3.85951447447664	6.86879594159807
H	7.81148841770773	4.54759834800050	6.54359885970953
C	7.57990107457484	2.11578567615787	13.63779331282001
H	7.05946743853189	2.81186442210363	12.98486020696205
H	7.54146825548030	2.50254798091547	14.65962388686316
H	7.04762933123004	1.16126118539864	13.62030380535661
C	9.82426137769758	-2.85013048478250	10.89088466337170
H	8.78895445712434	-2.96748207416803	10.56178931317109
H	9.81451109440919	-2.59460253670940	11.95184570990977
H	10.32673869789934	-3.81501158367749	10.78370476150410
C	6.79869870578273	6.27077290682228	13.94038936813076
H	5.78298458208972	6.50874800525464	14.26738388157481
H	7.37682602276392	5.98729571905049	14.82398281234150
H	6.75372713118740	5.41712735667329	13.26922847592417
C	4.55920172362885	1.10772430565403	2.59471299770134
H	3.94595521198672	0.42028286697183	3.16648371762754
C	8.91122867778183	7.18941669378801	12.88320176254816
H	8.97690343143423	6.38490115143828	12.15497327828675
H	9.47023423760908	6.89508193250471	13.77533625357800
H	9.39152350570813	8.07769008460702	12.46455955003137
O	4.06156363298827	3.70519549832383	4.93544123130045
C	3.25790439118812	2.51073201998264	11.48085923724788
H	3.16324038203171	3.58433385474583	11.59707867442770
C	6.13785323612686	2.86290126334790	1.12943432702441
H	6.74789648161949	3.55130209693003	0.55700429651958
C	9.28358939712198	0.27681555397442	9.17077779254953
H	9.32203057737668	-0.10620616695125	8.15923479913022
C	5.45873772757470	0.61314802903592	1.65324714526829

H	5.54002829455572	-0.45542671385340	1.49444222611952
C	3.49269551973135	-0.24320111197396	11.18562194523452
H	3.58014313197188	-1.31638399278307	11.06660132311753
C	3.95681679155795	11.30920635866721	9.48037322235752
H	4.60765224308084	11.24982938676593	8.60524789200590
H	3.55274017509355	12.32270012113198	9.52670643675311
H	3.11988436428230	10.62346274404539	9.33066394098879
C	5.31744376332983	9.58661026533320	10.77283015580384
C	6.05836733771974	9.12986910924059	11.88738263501270
H	6.17239588715271	9.81450310836755	12.71449155262824
C	7.44468183891757	7.49676853446809	13.25905150955518
C	4.49304817056952	3.85060146088980	7.27285342576936
H	3.63763020704285	4.53342674679497	7.26966358454917
C	3.16674960290160	2.83624072621560	8.98501778935365
H	2.54677517091836	2.35244876020085	8.22273709437018
H	2.70606928127691	3.79616866393131	9.24147062135971
C	9.81688445865893	3.25628344016401	13.29164429160280
H	10.87029632097570	3.10800851524932	13.03944615721347
H	9.76835844861186	3.65089033823288	14.31010951812476
H	9.40259575662065	3.99830740572948	12.61440706798309
C	10.56663851611208	-2.24668287683273	8.58864008613064
H	11.09291086591377	-1.54088649513854	7.94215405648456
H	9.55699847848155	-2.38283119322896	8.19474111786523
H	11.08221582277987	-3.20700517846879	8.52169764316606
C	10.54823805978461	-1.77594159741911	10.05093352009331
N	6.05530672897938	5.40883386462570	8.43167005645202
C	3.47969270964783	0.31902090501403	12.46021866086370
H	3.55798631473606	-0.31561891716396	13.33454433965633
C	3.45343917822365	3.02247014470662	3.82122825936337
H	2.81891882489943	3.77462199257889	3.34933157180099
H	2.81286628730325	2.21910918756196	4.19568037968790
C	12.00913588361581	-1.65672899139658	10.53609239520632
H	12.52082695411375	-2.61730003291350	10.43359120693524
H	12.06393796366915	-1.36011499071923	11.58496180146360
H	12.55477726345429	-0.91626176948444	9.94620953098271
C	9.69286260370037	0.96306889846506	14.22602788371156

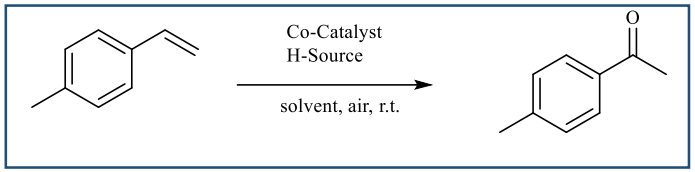
H	9.19198155145367	-0.00721388749656	14.25303816960970
H	9.61143759035941	1.40538345091022	15.22117182243203
H	10.75335656554008	0.79686657017837	14.02492685266094
C	5.84676939416222	12.04307753367257	10.93431313126182
H	6.54993213200540	11.98316320415564	10.10000668699298
H	6.40664671012501	11.89665365334556	11.85959255593018
H	5.42758482293029	13.05243666229407	10.95385625138540
C	9.04989971012271	1.91927244859131	13.20556159144006
C	3.36060599400436	1.69775015110840	12.60636624935328
H	3.34669749520754	2.14043030358785	13.59485048015555
C	5.75963271966105	7.41398879322614	9.76321449274595
C	7.47648577381227	8.62614758356776	14.30428282511230
H	7.95595726252619	9.52920068290740	13.92033411623783
H	8.05194285495778	8.28785721252933	15.16853118483417
H	6.47683281469297	8.89031716229012	14.65636314641797
C	3.73380210845027	11.14604638551148	11.95826433202277
H	3.30939609453078	12.15331083951087	11.97306049507198
H	4.22508377492307	10.97673473007270	12.91798339773585
H	2.91177747884528	10.43203087722298	11.86763854236031
C	5.23417546799463	3.35241039588055	2.06582384487674
H	5.14255954061618	4.42213993799062	2.21708503409852
C	8.54594410992102	2.10764576975923	10.66346448337019

Table S3. Solvent standardization for the oxidation reaction**.**



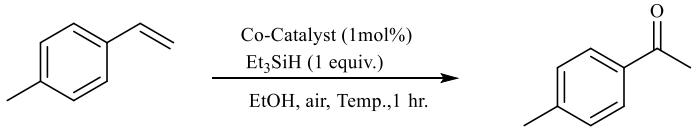
Entry	Solvent	Time	Conversion	C=O	C-OH
1	MeOH	18 h	80 %	85	15
2	DCM	18 h	60 %	90	10
3	DCE	18 h	65 %	90	10
4	Isopropanol	18	60 %	90	10
5	**Anhyd. EtOH**	**30 m**	**99 %**	**90**	**07**
6	Absolute EtOH	30 m	99 %	90	10
6	EtOH/H_2O (96:4)	30 m	99%	85	15
7	H_2O	30 m	90 %	80	20
8	Toluene	18 h	50 %	80	20
9	HFIP	18 h	10 %	n. d.	n. d.
10	Et_2O	18 h	10 %	n. d.	n. d.
11	THF	18 h	90 %	80	20
12	ACN	18h	80%	85	15

Table S4. Influence of hydrogen sources on the oxidation reaction of styrene.



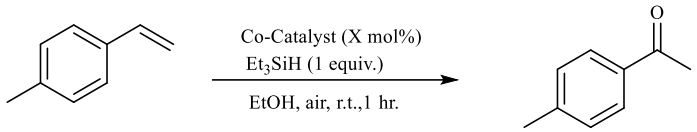
S.N.	H- Source	Time	Conversion	C=O	C-OH
1	**2 equiv. Et_3SiH**	**30 min.**	**99%**	**90%**	**10%**
2	$EtMe_2SiH$	30 min.	99%	88%	12%
3	TMDS	30 min.	99%	90%	10%
4	NaH	18 h	60%	70%	30%

Table S5. Effect of temperature on oxidation reaction



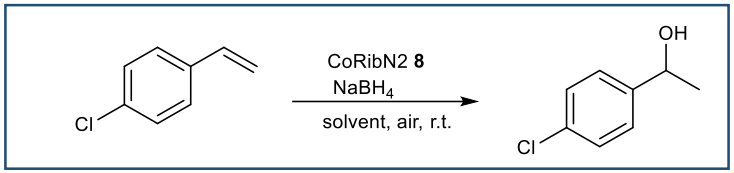
S.N.	Temperature (°C)	Time	Conversion	C=O	C-OH
1	0	6 h	10	100	0
2	15	1.5 h	99%	90	10
3	**27**	**1 h**	**99%**	**90**	**10**
4	40	1 h.	99%	90	10
5	50	30 min.	99 %	90	10

Table S6. Catalyst loading for oxidation reaction.



S.N.	Catalyst Loading	Conversion	Time	C=O	C-OH
1	2 mol%	99%	30 min.	90	10
2	**1 mol%**	**99%**	**30 min.**	**90**	**10**
3	0.5 mol%	70	30 min.	90	10
4	0.1 mol%	50	30 min.	90	10
5	0.01 mol%	10	30 min.	n.d.	n.d.

Table S7. Solvent standardization for the hydration reaction.



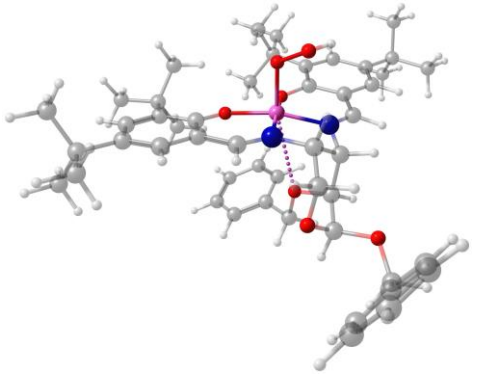
S.N.	Solvent	Time	Conversion	C=O	C-OH
1	MeCN	18 h	90%	0%	100%
2	DCM	18 h	20%	50%	50%
3	DCE	18 h	40%	80%	20%
4	Et_2O	18 h	trace	n.d.	n.d.
5	THF	5 h	>99%	20%	80%
6	MeOH	5 h	>99%	0%	100%
7	**Absolute EtOH**	**30 min**	**>99%**	**0%**	**100%**
8	**Anhyd.EtOH**	**30 min.**	**> 99%**	**0%**	**100%**
9	HFIP	18 h	20%	50%	50%
10	Toluene	18 h	trace	n.d.	n.d.
11	H_2O	18 h	trace	n.d.	n.d.

Table S8. TD-DFT calculated electronic transitions of **8-OOH**.

Excitation energy(eV)	λ (nm)	*f*	Transition	Character
1.771	700	0.001	H-13→ L (25%) H-3→ L (27%)	MLCT (metal → peroxo) LMCT (phenolate → metal)
2.429	510	0.056	H-2→ L (23%) H→ L (36%)	LMCT (peroxo → metal) ILCT (phenolate → peroxo) along with LMCT (phenolate to metal)
2.682	462	0.014	H-1→ L (70%)	ILCT (phenolate → peroxo) along with LMCT (phenolate to metal)
3.292	376	0.066	H→ L+2 (76%)	ILCT (phenolate → Schiff base)

Table S9. DFT-optimized cartesian coordinates of **8-OOH**.

Co	7.15123356053959	4.35548908305912	9.45403395274240
O	7.77708146880347	3.09046485775085	10.70525829058072
N	7.48671418148560	3.22626935310805	7.96836139119075
C	9.77406890595397	-0.50458880769552	10.02988700465344
O	5.55002114139554	2.04986584810316	5.87970222034312
O	6.64546759984073	5.42852780697678	10.93297095604903
O	4.70873155402901	3.12062878823925	8.49995188686096
C	8.60636671131180	1.45081820690910	9.18118430133824
C	8.10427655750194	2.10109900811985	8.01303104458057
H	8.26584410046683	1.56146220188418	7.08357453880039
C	9.57359540801078	0.02914267185281	11.32006931955825
H	9.95924557678156	-0.53813994938749	12.15317835166128
C	4.37536624814498	2.80030743214464	6.10925332561261
H	3.61845485455358	2.05441623498979	6.36525309101530
C	3.65425287237249	1.31692340768592	11.20712346835846
H	3.65391168697125	0.39488930348125	10.63738541262829
C	3.59288830958694	2.53569348963342	10.53665409066205



C	4.53414842424998	10.71427521752907	11.00345202705322
C	6.32347165579225	7.48062605549855	12.07676327362582
C	6.69116226009192	2.85048331352286	5.57558959476083
H	6.51564571690327	3.43566876933786	4.67035026881713
H	7.50118810804528	2.15781311194863	5.36045883210161
C	5.09465202042929	8.54130047363929	9.77108785330690
H	4.64467140566412	8.91078201499849	8.85946809278891
C	8.92463931065938	1.21694605843442	11.59346113710627
C	5.80804368521133	4.66646677525213	7.04086227980558
H	5.59545391020685	5.35853233609375	6.22440851777019
C	6.23038361522644	6.65877753321295	10.90285646726646
C	6.40097409627546	1.22962501560973	1.24187278436025
H	7.15901598370495	0.84199239325989	0.57256185789349
C	5.54598977928768	6.52158735457844	8.51606224964879
H	4.94098539587311	6.96975275646566	7.72752950589956
C	4.44480700331707	2.23076876288799	2.97250573190379
C	7.03183935393592	3.81786269202100	6.69795857120069
H	7.82445262603295	4.48524354324549	6.35175449181950
C	7.26136093298664	1.84931988454134	13.37408488534446
H	6.76059606602515	2.55139856601025	12.71514771227233
H	7.14135424673912	2.19693669108515	14.40347355852199
H	6.76254470584139	0.88163109693025	13.28652867384708
C	9.72553082748501	-2.94053653275326	10.61469498694219
H	8.71858591607194	-3.04738381734440	10.20465804006247
H	9.63538997555465	-2.71781606979073	11.67904403865939
H	10.23907767446130	-3.90001073986024	10.51405795369872
C	6.45123742421629	5.71773987987449	13.89485994532753
H	5.42916898126913	5.91680002360986	14.22562602236509
H	7.02534863125891	5.38026323732031	14.76161356914420
H	6.42759620628844	4.91753587397857	13.16300107047349
C	4.64660453243124	0.85833188639949	2.85167101622941
H	4.04543595222258	0.17741844894580	3.44286342337042
C	8.55297594811294	6.72976919390969	12.91803359102083
H	8.61899994185532	5.99296210990737	12.12216150589482
H	9.11423775953639	6.36167812831942	13.78024750123342
H	9.02496222740290	7.65422368835164	12.57581675341030

O	3.96319246996816	3.54596075063272	4.99598715566446
C	3.59877866457957	3.71982604390792	11.27520636777061
H	3.55946157839375	4.67189315999122	10.75984345214592
C	6.20370215720457	2.60371905651087	1.35405659280462
H	6.80698497088669	3.28780114973975	0.76993247588406
C	9.27878254044614	0.22659895751883	8.97970816102141
H	9.38689654681783	-0.11753613486006	7.95994252893449
C	5.61746156452605	0.35736048299652	1.99011362654468
H	5.76478594601083	-0.71243898009027	1.90659270841132
C	3.70739431321526	1.27714368048273	12.59734038645761
H	3.75713336679009	0.32397821143450	13.10875855843197
C	3.92177352448648	11.17115367376490	9.67430950821262
H	4.66699441675920	11.19878695610916	8.87641421236296
H	3.51560519788800	12.17828432870367	9.78717535111250
H	3.10706897469490	10.51648938399575	9.35739877879337
C	5.12734991050723	9.30832685176667	10.90783444493729
C	5.76333624233793	8.74140078271935	12.03351326508831
H	5.82483898316285	9.35005954675658	12.92248367161728
C	7.08599339793379	6.99584356799456	13.31635945810728
C	4.56005488014927	3.79537590646945	7.26306130585420
H	3.68007259670509	4.44586797906385	7.30198099836395
C	3.49342603286647	2.58574192516654	9.04121228210702
H	3.31382566700321	1.58546878691455	8.63798620977433
H	2.66076960613869	3.23058555300866	8.73971109511640
C	9.46905268910835	3.07032474241357	13.20285479314346
H	10.54123596465775	2.96252278907220	13.01967024839433
H	9.33604120423344	3.43692045058772	14.22374081408807
H	9.07415759942365	3.81321831609455	12.51751452505120
C	10.62857773449768	-2.25108470284015	8.39702607277923
H	11.19195146369123	-1.51559001188238	7.81879784519547
H	9.64994998070025	-2.37706842819593	7.92903752804963
H	11.15601901148866	-3.20462875242050	8.32962678887825
C	10.50317865073015	-1.83866342753788	9.86855137498166
N	6.10783064544790	5.38959771752265	8.27070780287657
C	3.70277767772544	2.46026762851793	13.32561600886010
H	3.74656566132653	2.43237148683103	14.40728865860260

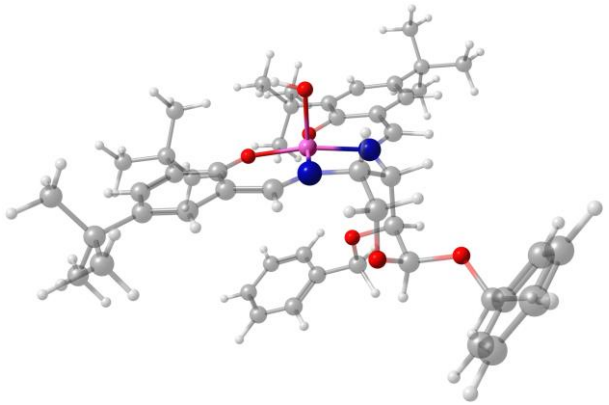
C	3.40505917243404	2.78229001426231	3.91238239290413
H	2.75357212898812	3.48122439984153	3.38631337534835
H	2.79086022701546	1.97410578230093	4.31944838827795
C	11.92035016248706	-1.72788186620765	10.46403576957922
H	12.44776050079532	-2.67974943405045	10.36330012421928
H	11.89166495698355	-1.47132504003800	11.52411866466222
H	12.49842876319331	-0.95978032554624	9.94507921548116
C	9.37105448383989	0.74653570137713	14.05816654855298
H	8.89787531616888	-0.23735584495299	14.02716549449102
H	9.22320899277478	1.15471336837163	15.05999244124337
H	10.44500166177267	0.61611107654014	13.90861491466214
C	5.63508923559206	11.71801215378417	11.39810171954890
H	6.43136562945831	11.73295506331719	10.65030786978562
H	6.08037383841907	11.46934138165629	12.36240686705567
H	5.21713132037894	12.72501279849810	11.47273861910719
C	8.75796505858414	1.71395870696309	13.03501131734230
C	3.65131194249192	3.68304317069058	12.66113165563713
H	3.65291590349189	4.60634296261937	13.22485307958728
C	5.64383292277757	7.24146276654642	9.74097464029595
C	7.09884838169021	8.04409386448251	14.43859577841144
H	7.57385894106497	8.97625117394169	14.12598374287533
H	7.66763228915073	7.64863976832078	15.28251487562287
H	6.09227356026823	8.27402674196949	14.79506783166964
C	3.42958909848591	10.72868525176446	12.07798234316054
H	3.00027303348594	11.72985421941949	12.16625077863621
H	3.81975829763844	10.44286318711209	13.05628051926793
H	2.62759684990411	10.03456076146785	11.81662789606291
C	5.22817821329873	3.09858336084157	2.21073073973107
H	5.07438127368286	4.16839785419182	2.29352393128956
C	8.41287937150937	1.97592153942638	10.48865660400854
O	8.76345214934493	5.21923214120828	9.33938654660958
O	9.03593104352962	5.78762774344952	8.05755944808534
H	8.66070957837740	6.67929503374176	8.13356240878200

Table S10. TD-DFT calculated electronic transitions of **8-OH**.

Excitation energy(eV)	λ (nm)	*f*	Transition	Character
1.583	783	0.004	H-1→ L (22%) H-3→ L (18%) H-2→ L (15%)	LMCT (phenolate → metal) along with MLCT (metal to hydroxo) LMCT (phenolate → metal and metal hydroxo) LMCT (hydroxo → metal)
2.368	534	0.039	H-5→ L (51%) H→ L (16%)	LMCT (phenolate→ metal) LMCT (phenolate → metal and metal hydroxo)
2.500	496	0.038	H-2→ L (15%) H→ L (24%)	LMCT (hydroxo → metal) LMCT (phenolate → metal and metal hydroxo)
2.644	469	0.056	H-5→ L+3 (14%)	LMCT (phenolate → metal and peroxo →metal)
3.324	373	0.073	H→ L+2 (49%) H→ L+3 (13%)	ILCT (phenolate → Schiff base)
3.654	344	0.051	H-3→ L(23%) H-1→ L+2 (41%)	LMCT (phenolate → metal and metal hydroxo) ILCT (phenolate → Schiff base)

Table S11. DFT-optimized cartesian coordinates of **8-OH.**

Co	7.21700046917922	4.42653073533799	9.53367190505858
O	8.03034049072511	3.27411577714453	10.80842759266590
N	7.46918128759962	3.19686193447828	8.10320650020289
C	9.78338458405637	-0.48504426625697	10.24133028749655
O	5.50099445379997	2.02289620206686	5.96167160818746
O	6.68254255948074	5.55358265297367	10.97859934755659
O	4.57210896683043	3.10588792522280	8.54645625909596
C	8.61670918089573	1.46244861460510	9.35915042114557
C	8.05540233786890	2.05535312406139	8.18504168879823
H	8.14914349948772	1.45629473287600	7.28253997602755
C	9.76716748927271	0.17396828032202	11.49049205546475
H	10.22845185995651	-0.33829014003802	12.32131319555780
C	4.33675774024384	2.80698780176219	6.15186892678652



H	3.56027349876943	2.08025259063902	6.40480113108060
C	3.55704530035580	0.69498843373183	10.31773567997694
H	3.52303194730836	0.21311288617359	9.34710413587442
C	3.44195418608049	2.08465495487983	10.40062350031610
C	4.71981729913679	10.91894953541694	10.76368893221512
C	6.19099277474826	7.60393131884755	12.09454186340694
C	6.68009256767987	2.78182862223049	5.69204022449608
H	6.55464342371505	3.36432127631488	4.77564117385365
H	7.47309223980489	2.05981029158150	5.51051650932455
C	5.26735060176978	8.67364817644924	9.64701496319840
H	4.90763268130132	9.03204887217202	8.69151042437726
C	9.21555986856935	1.42100103444054	11.73099444748166
C	5.80487167586366	4.63510873554722	7.11992437611548
H	5.63151675906724	5.31641723048507	6.28421372025243
C	6.24366464459978	6.77965738545754	10.91436862853681
C	6.14893272477695	1.51996374101122	0.91244888913488
H	6.84928788402628	1.20222544677076	0.14962584460606
C	5.64582706829872	6.57333694559192	8.50619742287102
H	5.09064250606218	7.02305017297376	7.68220975818482
C	4.33952745904139	2.34356898774172	2.88686074907113
C	7.01954965244928	3.75754899923836	6.81303072033150
H	7.82564813498423	4.40732063145296	6.45751636159325
C	7.86934371978224	2.33649919645314	13.67196779892887
H	7.31953542662298	3.00673051955202	13.01746739141554
H	7.93259747884659	2.79232531103743	14.66355341454058
H	7.30402317247337	1.40573302504787	13.76747991423407
C	9.73563567116567	-2.86519265653041	11.06378054294604
H	8.67605919926235	-2.96280340393547	10.81535630563272
H	9.81101432592165	-2.54966004237412	12.10573753321206
H	10.19682870428591	-3.85263523995834	10.97975464444627
C	5.81893378990204	5.84403931441529	13.86928985144683
H	4.76580520422883	6.11893864637486	13.97082755971480
H	6.16140093419966	5.46310562429449	14.83497318582897
H	5.89764177028948	5.04531031513388	13.13637286078869
C	4.56662096714963	0.98777604479047	2.65240176916074
H	4.04037702108713	0.24820160127133	3.24535223968196

C	8.15574857060928	6.70187196451798	13.39523392352234
H	8.34806219563929	5.95795655591262	12.62706087576230
H	8.48261465949534	6.29818682428790	14.35700081134873
H	8.75940792528301	7.58755661965129	13.18017880038977
O	3.96566694415432	3.54260199299845	5.01634369756409
C	3.47763888076703	2.69097610151412	11.65658904028511
H	3.38643691084056	3.76848429336641	11.73182204453369
C	5.92617346229082	2.87733104602952	1.13594705600246
H	6.45090290548834	3.61767749841789	0.54412343436638
C	9.20420405721790	0.18778322419615	9.19308308828863
H	9.18052285281976	-0.24211255162620	8.20030292611010
C	5.46446688118310	0.57555663908965	1.67058402557577
H	5.63032718237491	-0.48148763957729	1.50095879715885
C	3.70855257478065	-0.07277318259717	11.46707125997043
H	3.79441330554404	-1.14985312168319	11.38946728504152
C	4.26140285615509	11.36930594747354	9.36855736600972
H	5.07723852675206	11.33509942396366	8.64301025150004
H	3.90386058160616	12.39992567996614	9.41863443489910
H	3.44313679953663	10.75159447017443	8.99199124902942
C	5.23880494688443	9.47457117306804	10.76207039940367
C	5.70570413100871	8.89298832391857	11.96369658360474
H	5.67536325768164	9.50953675824044	12.84954963462827
C	6.65961108181347	7.07418706838948	13.46243276346622
C	4.51616629800387	3.80653636191083	7.30984914998591
H	3.66588402270450	4.49500311090633	7.31055922613590
C	3.28235388009279	2.91029895533256	9.15537868150844
H	2.61764484201842	2.40122533698710	8.44999030341651
H	2.84861207056886	3.88723010171426	9.39204372660043
C	10.11437320991237	3.35441710183894	13.07034744067147
H	11.13818454423421	3.13841678335606	12.75412393142657
H	10.15789596167304	3.81892920955209	14.05882173170142
H	9.68348410524641	4.06941848652162	12.37412878416409
C	10.33076491003635	-2.42438179911366	8.68293035537078
H	10.84018973254270	-1.78218584407394	7.96109787597687
H	9.29147512918742	-2.53660554198097	8.36597719475886
H	10.79985510235787	-3.40949723184282	8.64042289520025

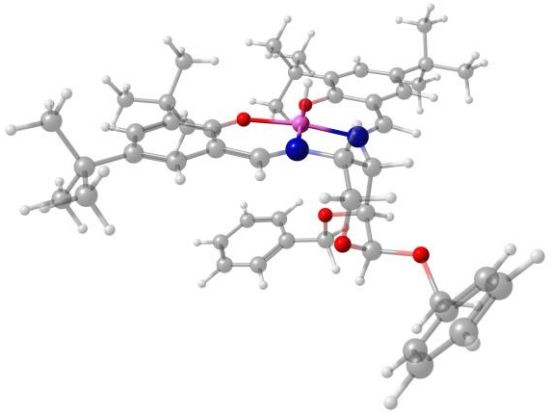
C	10.43328599711586	-1.86993712923722	10.11210052319527
N	6.11371035074092	5.38433147706709	8.33444253672100
C	3.74083829816934	0.54189099699152	12.71699706228161
H	3.85288290714509	-0.05575511464512	13.61343249050404
C	3.35905335144285	2.79594214343414	3.94188489092161
H	2.62924265203848	3.47929082012210	3.50382070284604
H	2.82212250763349	1.93802709065302	4.35518889471314
C	11.92783942273733	-1.77623744907199	10.48716807841065
H	12.40038411907945	-2.75868607297378	10.40632437439245
H	12.06570147395797	-1.42304758815087	11.51060778162460
H	12.45318425348736	-1.08999997288241	9.81865459794543
C	9.97664787850501	1.13196260664705	14.15972188504957
H	9.44349184958725	0.18746418030736	14.28864847922783
H	9.99263437312934	1.63686185338479	15.12784349950520
H	11.01063391808097	0.90955913267609	13.88746591210647
C	5.83865060417935	11.87299375960318	11.23460448464681
H	6.69734967777961	11.82674849691789	10.56056538525614
H	6.18472945015890	11.62642711266214	12.23986562251270
H	5.47380090656761	12.90326487464862	11.25052123545774
C	9.28805102536077	2.05141148135013	13.13475835786232
C	3.62428253263400	1.92531489646801	12.81004118029119
H	3.64710311529261	2.40899837004335	13.77889790681985
C	5.75586508897146	7.34843736221917	9.69820014960069
C	6.50205852373273	8.11627094663106	14.58386643649153
H	7.09863416856890	9.01261217244855	14.40111934624866
H	6.84693173334935	7.67608123471057	15.52184461100864
H	5.46147087064958	8.41748951473010	14.72330123824721
C	3.51712775393076	11.03667065338189	11.72487715022893
H	3.14553436260821	12.06457065197266	11.73913189373296
H	3.78744140245425	10.76538231144187	12.74674307266920
H	2.70076347055413	10.38430255945853	11.40599519232164
C	5.02370714535479	3.28424365575602	2.11202574021620
H	4.84828183517048	4.34162403469439	2.27553895656422
C	8.59617548605009	2.10907569735840	10.62876946353071
O	8.73513603269440	5.37491659728603	9.11480401357006
H	9.36407133955314	5.10778514181565	9.79885217556940

Table S12. TD-DFT calculated electronic transitions of **8-H**.

Excitation energy(eV)	λ (nm)	*f*	Transition	Character
2.590	478	0.016	H-4→ L+4 (11%) H-4→ L+5(31%)	LMCT (phenolate → metal) along with ILCT (phenolate to OBn) ILCT (phenolate to OBn) along with MLCT (metal to OBn)
3.093	400	0.027	H→ L (43%) H→ L+2 (22%)	ILCT (between two phenolates) LMCT (phenolate → metal and metal hydride)
3.194	388	0.053	H→ L+1 (73%) H→ L (24%)	ILCT (between two phenolates) ILCT (between two phenolates)
3.492	355	0.109	H-1→ L (73%)	ILCT (between two phenolates)

Table S13. DFT-optimized cartesian coordinates of **8-H.**

Co	7.23623573867004	4.46331672452663	9.50680567820848
O	8.07247096197546	3.31155607186804	10.76835236889234
N	7.52690310924488	3.26995719127089	8.06531642250025
C	9.89480129344663	-0.40698165045463	10.15712892173378
O	5.54324738350990	2.10630826996916	5.91046126535934
O	6.82154390840112	5.65058907597306	10.94258878329159
O	4.59805657275643	3.17447565865234	8.49033224532861
C	8.69470726541903	1.53188473528844	9.29837003644027
C	8.13067167531287	2.13395968120288	8.13035774330279
H	8.24070015426102	1.55200687565811	7.21864823838540
C	9.85524853016513	0.22968116243742	11.41796351556209
H	10.32070512974800	-0.28778442564400	12.24338924430750
C	4.38393366141711	2.89885416442512	6.09348961614340
H	3.59813444263199	2.17805726588722	6.33414793887663
C	3.60066310658694	0.76986076514625	10.25354229337029
H	3.59757511593624	0.28642032706627	9.28311092482096
C	3.45141712661730	2.15659903396578	10.33244842255328
C	4.73396627452850	10.97272939297073	10.73963771477972
C	6.30074928449855	7.69512784098833	12.05709750003307



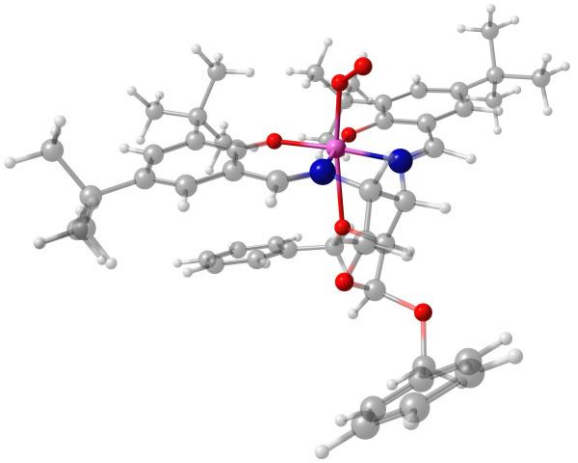
C	6.72850906471009	2.85919108764162	5.65045063090683
H	6.61017194762425	3.44458348276770	4.73484385600091
H	7.51742517537198	2.13260602306118	5.46944148552396
C	5.29524239641822	8.72784481804778	9.62858059057582
H	4.90472788367106	9.07216420642012	8.67978797259712
C	9.27675803678912	1.46065322300941	11.67487824338826
C	5.85820791655381	4.70963148780367	7.08823501048070
H	5.69134130217032	5.39975783725825	6.25804426519561
C	6.34236387968805	6.86141322928636	10.88146825744109
C	6.11459634205086	1.35735925115415	0.93118437413068
H	6.79727721376390	0.96867219741862	0.18535984918573
C	5.69276094045097	6.63343748800613	8.48544172261122
H	5.13118816631243	7.08067574110174	7.66438168890361
C	4.35051173914216	2.36372556770153	2.86198390178340
C	7.07007821234294	3.83037401251343	6.77477933064730
H	7.87270745778868	4.48146326108337	6.41264441161970
C	7.90130779235709	2.32973825773521	13.61755654377025
H	7.34870112255600	2.99929154146436	12.96452790344065
H	7.95020711667310	2.77673432628280	14.61409932488200
H	7.34783729403083	1.39055918641222	13.69939292252297
C	9.89660649493908	-2.80205759830841	10.93888853382395
H	8.84036621351789	-2.91762413294263	10.68395766450180
H	9.96075009297076	-2.50386736560978	11.98669876428450
H	10.37908204509812	-3.77786314131446	10.83922568131521
C	6.00575017535607	5.93653313497231	13.84548468334041
H	4.94963550113556	6.19015015997635	13.96960916078132
H	6.37640104937755	5.56430230069263	14.80428139888016
H	6.08442969545537	5.13823980180034	13.11208202501104
C	4.47325653034795	0.98938885346858	2.65942288667860
H	3.88267758099573	0.30660958069554	3.25989640869613
C	8.31344896039388	6.84556994595587	13.32224061887820
H	8.50773737085275	6.10198092281522	12.55409246242685
H	8.66977615849867	6.45573687004710	14.27938002645162
H	8.89139274224223	7.74406542769764	13.08993917020597
O	4.02976173859295	3.64342253958746	4.95744890653771
C	3.44788553002387	2.76422465076779	11.58821375623038

H	3.32949506677584	3.83934093916569	11.66075451419801
C	5.99629996421419	2.73268795730095	1.12283879016907
H	6.58498233592075	3.41643551778357	0.52311671053086
C	9.30865771257216	0.27151076368981	9.11654211535689
H	9.29987933599043	-0.14283792428593	8.11672066193233
C	5.34847799124782	0.48668348979508	1.69947755712234
H	5.43305679064605	-0.58363215431730	1.55477626730757
C	3.74838382061271	0.00672989752224	11.40636254110498
H	3.86205598565891	-1.06796463041532	11.33140458364648
C	4.25125324780427	11.40975088092678	9.34832291331547
H	5.05840554564949	11.38312596905345	8.61276519349112
H	3.87985839830060	12.43554634343612	9.39788852451708
H	3.43703287857625	10.77915617506135	8.98448745129427
C	5.28065932709329	9.53818526814241	10.73682814441555
C	5.78810777498670	8.97399495192095	11.93045693410674
H	5.76770434792965	9.59558500631827	12.81319691092230
C	6.81049696248787	7.18331088794592	13.41729918411628
C	4.56160321532828	3.88790837766070	7.26089314259361
H	3.71622825687344	4.58264249187779	7.25948880593807
C	3.30195312981279	2.97762774972126	9.08249363731657
H	2.64572317584707	2.46475208101961	8.37153071910903
H	2.86202505189106	3.95359188156709	9.31215318815235
C	10.13678008694239	3.38457703186558	13.05181350320311
H	11.16611971222060	3.18811365374971	12.74052776703755
H	10.16622662396065	3.83469345022461	14.04758517852914
H	9.70071851487383	4.10284584658372	12.36252346408233
C	10.49534446049421	-2.30710041152900	8.56991221466063
H	10.99426959594645	-1.64126633386510	7.86227190243415
H	9.46085598599826	-2.43741358407795	8.24425336026716
H	10.98733223023280	-3.28035435695969	8.51353310895508
C	10.57649535907216	-1.77459811586995	10.00881472161783
N	6.16873308320321	5.44639483641601	8.31125543702125
C	3.74210654895180	0.62275705701699	12.65610304151899
H	3.85184054257327	0.02864938932853	13.55516879300841
C	3.39158831759664	2.91478489241629	3.89014553032805
H	2.72132929723396	3.63807247598271	3.42229347687879

H	2.78584014413043	2.10942169531270	4.31437382243365
C	12.06676634217770	-1.65512436934357	10.39423605883046
H	12.56066316304936	-2.62603566414477	10.30175924165722
H	12.19154125848918	-1.31421942665671	11.42353984995986
H	12.58134796240088	-0.94812510079450	9.73903619294013
C	10.01927531363699	1.14424322161015	14.10676738912155
H	9.49864887034673	0.19016887960294	14.21496117899449
H	10.01828382474227	1.63374138209574	15.08300070058636
H	11.05910012962253	0.94071248068282	13.84205981964115
C	5.83779692053075	11.95176798748610	11.19419405293959
H	6.68985626378429	11.92081901143540	10.51078300727223
H	6.20020100242091	11.71685839728202	12.19637944228157
H	5.45183319060207	12.97437142640744	11.21025392836999
C	9.32812474532070	2.06961831265492	13.08895086083358
C	3.59012140515044	2.00289688369278	12.74529831645248
H	3.58203676679863	2.48748250065820	13.71395414851260
C	5.80850109365112	7.41121246991043	9.67554092371406
C	6.65167312907274	8.22621881643203	14.53789861165745
H	7.22655682824185	9.13391923646322	14.34171783872390
H	7.02177977020302	7.79713004582041	15.47143772228085
H	5.60779646379615	8.50697066862762	14.69433955287485
C	3.54012142552871	11.07059581772455	11.71387617876986
H	3.14847204464036	12.09109563133206	11.73030807230114
H	3.82779837867895	10.80657179665169	12.73299396783055
H	2.73314816668315	10.40155022153542	11.40575406409494
C	5.11659271012891	3.23027487731159	2.07755650022656
H	5.02249461073194	4.30147742109244	2.21616665977143
C	8.65354178497339	2.15907097625585	10.57875439845216
H	8.41213864954928	5.17759924301580	9.13265191072664

Table S14. DFT-optimized Cartesian coordinates of **A**.

Co	7.13294203460924	4.60658330859780	9.35475951152349
O	7.84245644778330	3.41874418637298	10.64704600378476
N	7.64186839477601	3.51135056393658	7.87941140743558
C	9.49626192218845	-0.35806985742462	10.11428691535469
O	5.64495829194234	2.15260783968680	6.14864447188074
O	6.42190568952614	5.62879659489811	10.79217250252979
O	5.17365194218592	3.48012494122958	8.76215033998801
C	8.58079307196773	1.68934366840393	9.17514477755977
C	8.17210621594099	2.34501643780201	7.97545423184930
H	8.31665666908901	1.76600962024735	7.06713617925191
C	9.41805272789131	0.27382878465281	11.37395085684438
H	9.76894056130172	-0.28357535442177	12.22897226145301
C	4.47288401553665	2.84594180065139	6.51846032665876
H	3.84850522333519	2.08623484016252	6.99798347144546
C	5.23207810818197	0.96495447968217	10.04244170424797
H	5.61211228344197	1.01332132572308	9.03188293526941
C	4.48733465643444	2.02802771781079	10.55101211519682
C	4.94156971525082	11.13296377117692	10.77114756261875
C	5.94288595163801	7.62033220443014	11.98235788513412
C	6.67714531520027	2.97507529800226	5.60298373442893
H	6.33329856926606	3.47622591061538	4.69583345070349
H	7.48268812786414	2.30195993971741	5.31980607689131
C	5.46842456667848	8.94981509482981	9.54127105373554
H	5.27565769114095	9.41159923322165	8.58219225400534
C	8.93220827719023	1.54667938400984	11.58939958323090
C	5.91063260877248	4.89070830787799	6.97921649785009
H	5.57230218266298	5.48085556518292	6.12615577263994
C	6.10209498328454	6.88994857362029	10.75683513517815
C	5.92302560623036	1.11964980137582	1.49065368594201
H	6.61611883539467	0.77965199617751	0.73110818907657
C	5.81738005341254	6.89993486185909	8.29162482270911
H	5.32731495645506	7.39517433813774	7.45277709383561
C	4.13815618688717	1.99944001661178	3.45542457260100
C	7.12287266489770	4.03234134202458	6.60209422842430



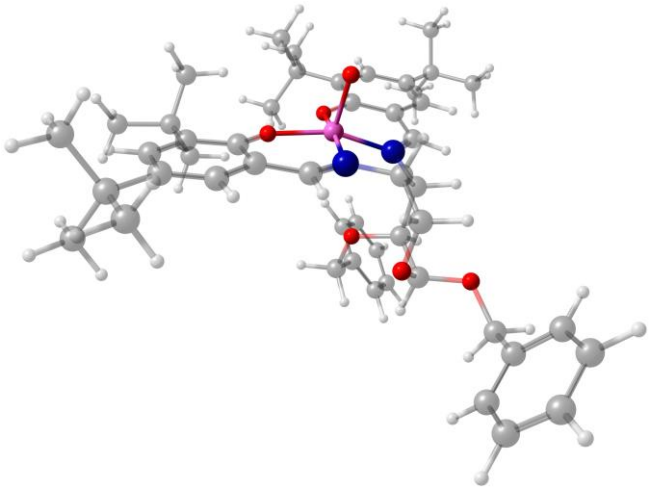
H	7.87986061199577	4.67163672948977	6.14107086778101
C	7.53945608770337	2.53007123454227	13.46853912346057
H	7.03327924723844	3.20321129670916	12.78449304440485
H	7.59113217166261	3.00740660093771	14.45064298980472
H	6.93953794974606	1.62433437781384	13.56556408434467
C	9.10309078162912	-2.71155553174041	10.86628273516109
H	8.07362631427728	-2.67961950702781	10.50180653497723
H	9.09842954275986	-2.41196325498374	11.91546608866171
H	9.45401647981997	-3.74532590596171	10.81331861399225
C	5.21789224751510	5.75206072457653	13.51778622166348
H	4.18219245281792	6.10167901018853	13.50296819921065
H	5.39510650213480	5.27473211722342	14.48505066344372
H	5.34659638374097	5.00590305255404	12.73837851033249
C	4.47825836083679	0.65273879435000	3.36155567032610
H	4.05553049406373	-0.05380046988888	4.06633346512128
C	7.64513904066092	6.45641468262266	13.41371418886250
H	7.86636183365533	5.73712526552381	12.63222976389974
H	7.83295099833812	5.98438971135935	14.38125088043320
H	8.32973623568924	7.30252749795256	13.31266997008675
O	3.79900244334228	3.42119219951837	5.43170953078386
C	4.02785377145640	1.96942399670068	11.86477363647706
H	3.46900250462309	2.80318215948497	12.27386954343017
C	5.58552353476616	2.46809710415432	1.57526071494493
H	6.01376484806662	3.17911796929637	0.87941138147673
C	9.10048624139317	0.38447271259194	9.03157004165915
H	9.15787216063797	-0.01749670252920	8.02885206721553
C	5.36458117487986	0.21158569653802	2.38398184908193
H	5.62301164687422	-0.83852282521990	2.32379326255723
C	5.50170359001803	-0.14500197797801	10.83326479691870
H	6.09281479693914	-0.95903374136020	10.43255550351424
C	4.72792825580956	11.72933902127257	9.37483594102681
H	5.63558041100696	11.67498189254421	8.76999464164023
H	4.44912750565720	12.78101397584848	9.46600711801936
H	3.92756764765126	11.21810128262143	8.83558183931567
C	5.34193473458107	9.65876075242005	10.70876297992905
C	5.58325760658282	8.95095433922102	11.90602602804247

H	5.47278692018352	9.49728663416154	12.83024193867359
C	6.18444982380856	6.93999727303244	13.33570944605381
C	4.76433782834297	3.99678105420399	7.48694627816389
H	3.86573206456951	4.60488998333739	7.60458215008338
C	4.11261926696337	3.19452693266852	9.68192481739103
H	3.20909966515836	2.95640121813592	9.11260769105327
H	3.90622373390649	4.08435769541404	10.28099166306967
C	9.83455477182465	3.45377788161177	12.93579943579542
H	10.86052987384992	3.19468725299257	12.66208477038249
H	9.85616264267576	3.92986813795170	13.91916119882602
H	9.45673033380424	4.17356602987359	12.21514402903865
C	9.99682591697049	-2.31407403231109	8.57608842658876
H	10.64657442513143	-1.72129560220832	7.92860453883203
H	8.99037913995948	-2.30287784833575	8.15219698219088
H	10.35671244464497	-3.34469212382894	8.55618649421223
C	10.00748418167026	-1.79541831442260	10.01876453792138
N	6.27713670161644	5.71413555424128	8.10872211448416
C	5.01997928577607	-0.20966368983254	12.13681079967853
H	5.22721107901629	-1.07727212107057	12.75110171548058
C	3.19181181906029	2.48828249376048	4.52032975868462
H	2.36571304272243	3.03903492477441	4.06857464163287
H	2.77962892997218	1.64652701675776	5.08383931993101
C	11.45099414494123	-1.87190951729737	10.55183721765773
H	11.82104097706125	-2.89891389553187	10.49760429237224
H	11.51330988375858	-1.54859014047200	11.59217626159251
H	12.11481689263399	-1.23754848541661	9.95984657165296
C	9.57863298152248	1.24857034542063	14.03491357944737
H	8.99764209779428	0.33185011189293	14.15675966122584
H	9.59532795725537	1.76116318909789	14.99883383399372
H	10.60599800350478	0.97419056704037	13.78624899833306
C	6.04989374119351	11.93786434778497	11.47702099069974
H	6.99415632206985	11.85233197897806	10.93443296411232
H	6.21306776340013	11.58815179776753	12.49748368330480
H	5.77732598907635	12.99519716139711	11.52418325394744
C	8.96007581104830	2.18377255233191	12.98470759988612
C	4.28378393846616	0.85212673557401	12.65185452308722

H	3.92196759025590	0.81868065190104	13.67206820456879
C	5.84675621616578	7.59052693920259	9.53955717287668
C	5.95266188685779	7.89515233312661	14.51559618338506
H	6.62930583279094	8.75192838157284	14.48957241608594
H	6.13619106319231	7.35598828224766	15.44697350310221
H	4.92671570187243	8.26855479346108	14.54447900775310
C	3.62797748946834	11.27604015007840	11.56422245677352
H	3.33283948005404	12.32687162787426	11.62065645559835
H	3.73000943732427	10.90191095333197	12.58419138275976
H	2.82209493616457	10.72059012857227	11.07888840939374
C	4.69408779202626	2.90240054956424	2.54835094186731
H	4.43256057031299	3.95238944119758	2.61137348915640
C	8.42505902071775	2.27552774882675	10.46164146824869
O	8.72151900621123	5.59672630339078	9.42861504511616
O	9.24307354229721	5.95688346792549	8.31922359054660

Table S15. DFT-optimized Cartesian coordinates of **B**.

Co	7.55833003677205	4.29237046143302	9.64436487238824
O	8.21494327337430	2.97019499581402	10.81380634966941
N	7.79950282996218	3.18966370588733	8.10899117486465
C	10.15658438919749	-0.62841975937540	9.92957351941264
O	5.82227261339929	2.07013930829685	5.94437979701652
O	7.05909297686086	5.29726320727194	11.19813326380681
O	4.98353179501060	2.84882408868207	8.67058704215568
C	8.99411456006898	1.38233081049163	9.20378319676338
C	8.44110378617703	2.07741207260684	8.08139294694884
H	8.56682702658559	1.57707762068774	7.12432599210294
C	9.96641679578666	-0.16456787067521	11.24901000115949
H	10.34586884328606	-0.78449077696119	12.04702661973035
C	4.61931183877884	2.74825576547129	6.25934936858895
H	3.90171598339194	1.94908486418634	6.45737997051325
C	3.14221575448882	4.07875230177473	10.83600735644706
H	4.14314283463444	4.04685133121104	11.24971223258798
C	2.80236429698782	3.22190647665980	9.78541710302208
C	4.81643033127257	10.54909647347710	11.44091111757877
C	6.57264071867491	7.26196426378066	12.46007411336233



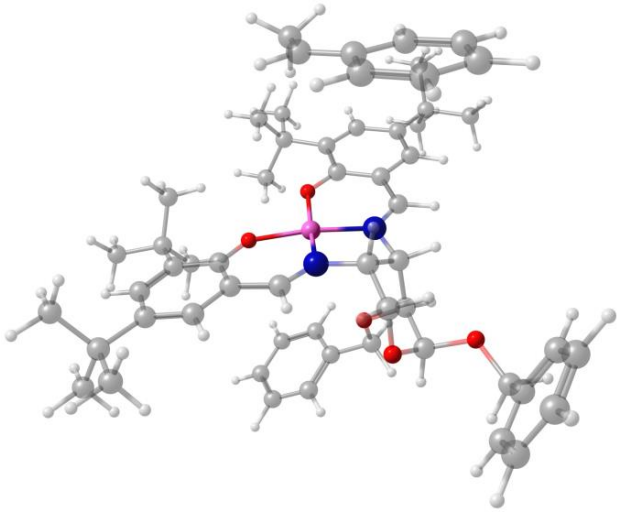
C	6.93586884255631	2.92909614189495	5.70265074819169
H	6.73641615335473	3.57801871716245	4.84566780734700
H	7.76746845851089	2.28202350366534	5.43192875032938
C	5.39219540421792	8.40372741494664	10.15764112941521
H	4.93949593349264	8.79130844957258	9.25460557672946
C	9.33266448377123	1.01652401266341	11.59911670206975
C	5.99823483827999	4.57749570728109	7.33047564441913
H	5.73330755331991	5.31166953180147	6.56724516373278
C	6.56578824787751	6.50182826591462	11.23594727675915
C	5.61207936234232	0.90522981471768	1.13392737049368
H	6.17417824608819	0.39934981398878	0.35833277858390
C	5.80139310289389	6.39712835015157	8.87208706542996
H	5.16410905351463	6.85657234307211	8.11644947081244
C	4.15844403919098	2.21563043551249	3.13811023521451
C	7.25790741413168	3.82732487972646	6.89232284050004
H	7.99675611756515	4.56590512475893	6.56696415688148
C	7.68272346921730	1.56894292931435	13.43473946954436
H	7.20199855834777	2.33226844109005	12.82880563566494
H	7.57871651100061	1.84641843561235	14.48682750438850
H	7.15575926656377	0.62310549046974	13.28410696537768
C	10.09353602223526	-3.10384133778123	10.37177347631187
H	9.08009580613500	-3.17881503488067	9.97037845824365
H	10.01978059592207	-2.95050650089766	11.44971829017372
H	10.59741576333008	-4.05907505245184	10.20367224262563
C	6.48252897301645	5.39739361218326	14.16499733353186
H	5.42662169911344	5.59490031393232	14.36770381921988
H	6.93064080775483	5.00128881427423	15.07999747641006
H	6.54724661265903	4.63651798165061	13.39210942686051
C	4.07855725217869	0.83092588920157	2.99294238170927
H	3.44839025520493	0.25941984188338	3.66510016220411
C	8.70543407030786	6.44036680978362	13.51762246953502
H	8.87246822717884	5.75590635739748	12.69011979968983
H	9.15414576244781	6.01254221013285	14.41769386654428
H	9.22121929466410	7.37892731488740	13.29847575715259
O	4.15431879200797	3.56952128076480	5.22010957556486
C	1.50858689035493	3.27428976756806	9.26684759784018

H	1.23364410436852	2.61334873818685	8.45248194990094
C	5.69569307523608	2.29007671308920	1.26818838797956
H	6.32096836235496	2.86326706880338	0.59426645125282
C	9.65463303833719	0.16560999860061	8.92604655175868
H	9.74266683256158	-0.12471786859975	7.88768149551248
C	4.79939091923971	0.17693615091885	1.99646771559017
H	4.72681781298385	-0.89930314902563	1.89628822081183
C	2.20888411489055	4.96992980462097	11.35201381549431
H	2.48467165205036	5.62729909363185	12.16755050991011
C	4.24239419088594	11.05316437678819	10.10841694141018
H	5.00709115043312	11.09863419935282	9.32983550646433
H	3.84302148775334	12.06058260074122	10.24269519283163
H	3.42839411536787	10.41864542322266	9.75085282406339
C	5.41061137289524	9.13973427536260	11.31536406695886
C	6.00771224579946	8.52382446104902	12.44098597767235
H	6.02085970924359	9.09045146499937	13.35990217586830
C	7.20078437734287	6.69914544992218	13.74807601045677
C	4.78493908336898	3.63806237919109	7.50763866871274
H	3.88567485411714	4.25140229901788	7.61280321119111
C	3.81056216886175	2.23930046275900	9.23709156559196
H	4.20339154999808	1.61108724103644	10.03750650006981
H	3.32787841414721	1.58522833926699	8.50595216136562
C	9.93389803854662	2.73385337556187	13.34496176058091
H	11.00404972003710	2.60148831406813	13.16600798012264
H	9.80221303044299	3.03623717780666	14.38704354747671
H	9.57553988133706	3.53684210440021	12.70654873364468
C	10.98026587909164	-2.29214241331669	8.18647196681881
H	11.54624207641995	-1.53169360093286	7.64380745446272
H	9.99642474294519	-2.38313187960705	7.72096977325334
H	11.49723229211271	-3.24556350481248	8.05971619965683
C	10.87362809252290	-1.96302048473256	9.68310354539773
N	6.32510993790858	5.25209836539455	8.58567572532145
C	0.91796379947713	5.01333390153180	10.82774466515070
H	0.19019726852490	5.70617872585241	11.23239180423514
C	3.36022586717665	2.92690995346329	4.20361131539910
H	2.78282050602782	3.73833648928054	3.75833425390452

H	2.66449425558571	2.23164039629260	4.68149583410422
C	12.30099318733396	-1.90151837836385	10.26810172114429
H	12.81382405020381	-2.85401022217442	10.11164885361828
H	12.28946810989394	-1.70147429105480	11.34082401177562
H	12.88601127524806	-1.11627107728021	9.78342641348822
C	9.75931760141491	0.35930605397862	14.03621125522222
H	9.26052348163084	-0.60718121647321	13.93580337675879
H	9.61430399451444	0.70072379475473	15.06321915234489
H	10.83094757466846	0.21146417669533	13.88657971208433
C	5.90999781111881	11.53776689272636	11.89909058165509
H	6.72423080917602	11.58283740664640	11.17179520994523
H	6.33356495322439	11.25437810575152	12.86393706103702
H	5.48923844190509	12.54130582572676	12.00136373463048
C	9.17776832917027	1.41502416419291	13.07905356994428
C	0.56830280265508	4.16213400131109	9.78524526676426
H	-0.43272928230519	4.18945035964102	9.37201937970439
C	5.95541172872873	7.10746763058217	10.09425989090180
C	7.08587327793369	7.67367183002210	14.93390891910166
H	7.60077200335340	8.61773051143444	14.74351702848416
H	7.55054722327702	7.21573905375037	15.80954075554096
H	6.04637481389201	7.89257608234464	15.18830777678623
C	3.67706230931581	10.53889025958225	12.48300237872564
H	3.25083301239402	11.54023101234204	12.58455069222500
H	4.03134834876018	10.22530841647777	13.46657206096939
H	2.87863548180937	9.85871421756548	12.17735921462667
C	4.97020249953821	2.93927872336987	2.26030967343410
H	5.03125501288959	4.01774000699171	2.35406777135220
C	8.82959175343035	1.84494001503035	10.53881039935067
O	8.92905880896782	5.24570078955458	9.26660621436012

Table S16. DFT-optimized cartesian coordinates of **C**.

Co	7.01483336201098	4.42497208100566	9.86754884326936
O	7.95095099039961	3.31083064398090	11.08514087812810
N	7.35155702983736	3.27421787053059	8.39770924087048
C	9.93972275143458	-0.30425229507882	10.40505617114110
O	5.35282340103011	2.04507780637621	6.24202845248626
O	6.93115564592938	5.79038939918543	11.18504287708414
O	4.37476687654991	2.99807112642198	8.84937060026449
C	8.63580595752082	1.58365058529685	9.58329910488397
C	8.02292974120399	2.17170467327397	8.43320463542811
H	8.15083506689005	1.61077162652912	7.51051650474583
C	9.84972488123399	0.29250467744300	11.68380001063365
H	10.32941883711309	-0.22478060486909	12.50128758306946
C	4.16568135475105	2.78924866359811	6.44843463823337
H	3.40852615709032	2.03212772771369	6.66836715903734
C	3.47268929874613	0.50353246681500	10.54773697005728
H	3.48653191872791	0.04183864775236	9.56683545576407
C	3.26917788177797	1.88122881384313	10.65740858017529
C	4.48544471311406	10.95805288672456	11.02217802398136
C	6.51464425785335	7.89709346076596	12.22353476852047
C	6.50890388809175	2.84574998231070	5.99171421630687
H	6.36588628766810	3.43790765322197	5.08406123992512
H	7.32315653142894	2.15085362389570	5.79875480598583
C	4.97240426922024	8.66088570767565	9.98484842322791
H	4.39512878402329	8.91027703528612	9.10403881000135
C	9.19988953333491	1.48086426359883	11.96631180730031
C	5.56951657320791	4.62596811030471	7.48059022021069
H	5.35780318004991	5.31938721175250	6.66333785512279
C	6.36104862187791	6.96443380757619	11.13675118372129
C	6.02921040844429	1.88682410431250	1.10733110820335
H	6.73572485890759	1.65394242946701	0.31992432021471
C	5.38071363825165	6.54821730129966	8.87734696859850
H	4.76066654845537	6.95910285947000	8.07985500063128
C	4.20177317794884	2.49035320938495	3.14365872071892
C	6.82055413878078	3.81666242719067	7.12620120096564



H	7.57112009060763	4.52078080147899	6.75091688036233
C	7.70762968464276	2.17329327675352	13.88875428572390
H	7.12960884747423	2.83282693881249	13.24643576189995
H	7.69034707935052	2.57513657605472	14.90529788201460
H	7.22116035696948	1.19463929518929	13.90695513487530
C	10.05115948535867	-2.71992121572841	11.10798307498601
H	9.00897576135867	-2.88120669711107	10.82212160764241
H	10.07391460915356	-2.45330576730276	12.16602826289857
H	10.58685645264357	-3.66542174543073	10.98984144092083
C	6.77312408445802	6.29957817809291	14.16815926858512
H	5.75466168372518	6.49824687754589	14.51240595535683
H	7.37823424345207	6.04728169316172	15.04316051180390
H	6.75132073377078	5.43968619384434	13.50417769879772
C	4.53068515956587	1.16648289916611	2.85404496393782
H	4.07582179086272	0.36611995031321	3.42663822001149
C	8.82220531585830	7.29296107144079	13.05284042467285
H	8.90128382655922	6.48168855656593	12.33341250290518
H	9.41831492362356	7.03505864360768	13.93214805378430
H	9.25256782228712	8.19424493361825	12.60853116544678
O	3.78124743587612	3.55231105442265	5.33522505118042
C	3.24416719474387	2.46011421404683	11.92651853934189
H	3.08232242482747	3.52768976943744	12.02278089933344
C	5.70536398344223	3.21297965080160	1.38677821767122
H	6.15744678041388	4.01392526162217	0.81427101798678
C	9.31960962968250	0.36257135507221	9.37707125145782
H	9.33549445749401	-0.03072716135928	8.36889827777804
C	5.43727441130846	0.86362799471002	1.84093810792446
H	5.68195782905052	-0.16991969803242	1.62747792139517
C	3.65274915628452	-0.27847687013030	11.68328161930243
H	3.80827942955175	-1.34599169764172	11.58450683363165
C	3.70296596007188	11.24496807234805	9.73187827127567
H	4.34452306168231	11.19097668278140	8.84952730817674
H	3.28233379549268	12.25177197970866	9.77684732022406
H	2.87574014601812	10.54471727520114	9.59580841373706
C	5.11303605590225	9.55646301024179	11.01649387107075
C	5.89228845085360	9.12850894244917	12.11618269493645

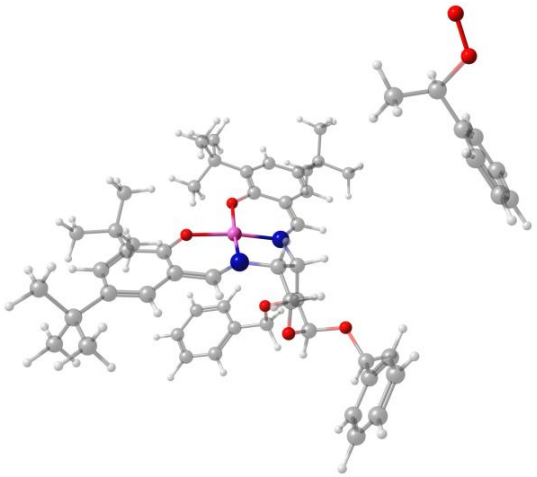
H	6.01074210592560	9.82397106573087	12.93356264379494
C	7.35517467651181	7.54562432517138	13.46603992364348
C	4.31011902672078	3.74864285893023	7.64494522642835
H	3.43832858743109	4.41033573823580	7.66641013128404
C	3.08688508556667	2.72388606667243	9.42605347176540
H	2.45882452742580	2.19669131274832	8.70005951160111
H	2.59839799134982	3.67154951282737	9.67638386162737
C	9.87529725963203	3.40981788253999	13.45007971404219
H	10.92336923299613	3.30848157947397	13.15585473228698
H	9.84995592886117	3.80857536397731	14.46775976988926
H	9.39991457556370	4.12712528414463	12.78677853590399
C	10.68044900276748	-2.11425720015713	8.77240616138586
H	11.15355726555878	-1.39556106386212	8.09953385257337
H	9.66320253788673	-2.29493819035104	8.41786725695980
H	11.23165298921969	-3.05384245757700	8.69578906811734
C	10.69807424524858	-1.62752830598565	10.22951561450095
N	5.87826774212155	5.36693097785468	8.70447481337910
C	3.62542631551851	0.30905723723209	12.94632361535017
H	3.76058279081760	-0.29998581849988	13.83182963492252
C	3.20777597899603	2.82543056356927	4.22923795564369
H	2.43243519588094	3.48310256842966	3.83170787722764
H	2.72970219133150	1.91583971602199	4.60187649159381
C	12.17068933203000	-1.44527693602203	10.65650064279972
H	12.71547631116197	-2.38604805006694	10.54221328660062
H	12.25427170450760	-1.13636758104546	11.69994044601076
H	12.66326599597763	-0.69000131231504	10.03933932139527
C	9.89050393188416	1.12248163376245	14.40636496570807
H	9.43531512575515	0.13110423157110	14.46100325864275
H	9.82615609818615	1.57096613495752	15.40003131160556
H	10.94927297182804	1.00158799103054	14.16715840339381
C	5.59363475647142	12.02430503746785	11.16041189008762
H	6.29003627674259	11.97337416279469	10.31987069225084
H	6.16472381178779	11.89514581683164	12.08126819911616
H	5.15383429021649	13.02485034203866	11.17772429682173
C	9.16765654414795	2.03853087443680	13.40249880795153
C	3.41900977410885	1.67982409342775	13.06636374963614

H	3.39378571771517	2.14204394340049	14.04564378345772
C	5.57610309866988	7.38206453041377	10.01965422477463
C	7.37076236767229	8.68011915070933	14.50632502133847
H	7.81312237314644	9.59679226096915	14.11020444046379
H	7.97387252403167	8.36475750645675	15.36031961764595
H	6.37005385145849	8.91317182808362	14.87689288276092
C	3.51250343569375	11.08903162395263	12.21369167050999
H	3.06693479403810	12.08711723795895	12.22910351812094
H	4.01995347497358	10.93518836323647	13.16766364228761
H	2.70499397760337	10.35704190543020	12.13745616465782
C	4.79439543853324	3.51032332647755	2.39403817143633
H	4.53850619168597	4.54358573107254	2.60019352001407
C	8.56498413255956	2.17979219154813	10.87781339554562
C	11.06724627154597	6.23832380741915	3.46649866254633
C	11.60512853066088	6.02101442225614	4.72002823598284
C	11.32610291869398	6.89319964290792	5.81138909516951
C	10.46188833380643	7.99334107233424	5.54985936379337
C	9.92932998858161	8.20039145513102	4.28931260714884
C	10.22480674386525	7.33136392313188	3.23577888448037
H	11.30098809762804	5.55707044572952	2.65675243952458
H	12.25846914765063	5.17213387779800	4.88819540982750
H	10.21302137988334	8.68066002685939	6.34789327020867
H	9.27460525543926	9.04731765019277	4.11980818706513
H	9.80525952630417	7.50108014225687	2.25216685954591
C	11.90054079957766	6.64280209395567	7.07556146147632
C	11.70353120818604	7.45774550450837	8.30737433608029
H	12.58423389787900	7.40329692411543	8.95096211066852
H	11.50381041229283	8.50871301986759	8.09113045533210
H	10.85864992659504	7.08903506991988	8.90577708383052
H	12.51854354816170	5.75530282609917	7.16339582639848

Table S17. DFT-optimized cartesian coordinates of **D**.

Co	8.60096993525070	1.96617185937245	9.48593902855865
O	9.48028968672000	2.16912750216113	7.81899341255071
N	7.74666957744063	3.65221148828222	9.35785875200526
C	9.15448410386340	5.24440675264363	5.00031409620865

O	4.71267277671273	4.52277794434957	9.79789204232080
O	9.63769329427855	0.41499018218304	9.82897556562616
O	5.38832131104485	1.72667640536657	9.14967780361570
C	8.58448249299532	4.28710082554029	7.16752063850383
C	7.83058466359816	4.47541371032980	8.36702887222316
H	7.28063039911946	5.41189761619232	8.41827493640697
C	9.93255786124185	4.08408244345632	4.78215265765352
H	10.45523990190613	4.01343238163258	3.83984975857017
C	4.12808338518638	3.37942121775749	10.39634568608324
H	3.29870705638053	3.11915648033860	9.73402685171310
C	4.37410162364041	0.96235325175222	6.20122261758564
H	3.73631875239161	1.83023940354827	6.32622028802660
C	4.82490196240313	0.27270422612181	7.32866742455896
C	9.25262690725911	-3.46369012861328	14.01032047091805
C	10.46770085477897	-1.55931652126454	10.87617356054650
C	5.86301161051265	5.01373788933192	10.48663990712842
H	5.59508068113207	5.30386306924685	11.50590934076391
H	6.16813649711141	5.91776650971957	9.96443326967308
C	8.45082719589175	-1.32703539497131	12.83920250549567
H	7.66449672279224	-1.19373476152833	13.57079341295407
C	10.07375510674610	3.03788478990803	5.67715596166624
C	6.44347139965622	2.66578592282820	11.13882072526313
H	6.20872358729517	2.80551463376021	12.19667036101478
C	9.54378902876181	-0.45761337915203	10.79489248732181
C	2.30735773031390	8.51894419921507	11.47698911662983
H	2.29142560177893	9.59928850599662	11.39934496701165
C	7.59249070210371	0.70009460565167	11.83811088298589
H	6.87865251919734	0.68401814979893	12.66234486914388
C	2.34932180016050	5.72491753329636	11.68003643595608
C	6.98506750097840	3.98535733071439	10.58214965881339
H	7.71485815383229	4.37068252955030	11.30261675420700
C	10.07369381982957	0.53746963636337	5.31700204618220
H	9.58815876558824	0.37490722142804	6.27598894415143
H	10.69420872116128	-0.33369497781770	5.09077789862975
H	9.30263826207283	0.60912323015857	4.54553902902415
C	8.51746989212368	5.74179843027563	2.61484132364308



H	7.50624244045759	5.35758130593479	2.76900485875551
H	9.13581499074399	4.92396916343785	2.24096836624948
H	8.47448326614943	6.51005911146994	1.83838889765123
C	10.99348525374367	-1.91968379004930	8.43007808581811
H	10.38181916797166	-2.82508734181778	8.39363657458751
H	11.79570986687118	-2.02823376290357	7.69532504661877
H	10.37505351407066	-1.07359641880329	8.14266279184434
C	1.68496860503608	6.35089965739500	10.62549605841452
H	1.18366044987368	5.74676511100686	9.87764289609676
C	12.52821481943611	-0.50203367765108	9.86366005180877
H	11.99033885802009	0.41411130473913	9.63233883139292
H	13.32863572992564	-0.62847872238620	9.12982736683271
H	12.99086468921107	-0.39366388968846	10.84817060293121
O	3.65551821841744	3.61262822797195	11.69796443766035
C	5.63697217342591	-0.84882115993744	7.15281186466794
H	5.98748796688568	-1.39540367589981	8.02086795871397
C	2.97120232523234	7.90332286146127	12.53667646078057
H	3.46984825792306	8.50542579332456	13.28673889626672
C	8.49192624527498	5.31523756597210	6.20091477950962
H	7.87068620281755	6.16723624452328	6.44462200267694
C	1.66135067532326	7.73978215539410	10.52280799111610
H	1.14127185126100	8.21087806646136	9.69744699389785
C	4.73023421089816	0.54260875804023	4.92368295199540
H	4.37134046301885	1.08508619876775	4.05742225156517
C	8.10392639805607	-3.21218866474084	14.99899465271879
H	8.21685544849429	-2.25750762704995	15.51742984225847
H	8.09533182064906	-4.00155776304263	15.75352065333052
H	7.13221988613415	-3.21720509930531	14.50021805006902
C	9.31718384986436	-2.38933505213420	12.91574557444204
C	10.31230952654917	-2.46213601251715	11.91310556996060
H	11.00328356470088	-3.29027553831576	11.96631597655144
C	11.59437250179565	-1.73224406869780	9.84001878981715
C	5.13266491575727	2.21189994361049	10.45977413512620
H	4.69502398596228	1.41470566294676	11.06951497869064
C	4.44623653469023	0.73402372266336	8.70833943509050
H	3.43576180746898	1.15570373364495	8.69905043790005

H	4.45999869548566	-0.10584969902094	9.41131688217406
C	12.09234223279086	1.67126868080152	6.34853187831361
H	12.74096707298264	2.55093546410026	6.31869347812834
H	12.70206241035184	0.79772648398120	6.10254146139713
H	11.71599775860899	1.55530755209955	7.36131734436977
C	8.18214651431920	7.50622399510980	4.34496637513974
H	8.54880913639412	7.99109414247659	5.25230890325474
H	7.15393742579458	7.18296046307793	4.52214314816261
H	8.16341554524771	8.25587640949521	3.55107966901605
C	9.08344216173769	6.33576856869934	3.92255715457612
N	7.50790937129488	1.67049266970082	10.98678260674072
C	5.54045539239148	-0.57803075303835	4.75900666556427
H	5.81391858084925	-0.90930003031307	3.76460709259531
C	2.35370849352760	4.21994923970827	11.80412675898509
H	1.99656729049974	3.92682542547274	12.79258602160314
H	1.69063201164296	3.77805442897751	11.05485094138661
C	10.49779760183602	6.89287825235020	3.65330684563458
H	10.45906979392700	7.66279523605769	2.87817301482635
H	11.18163415214992	6.11264015400352	3.31493260809478
H	10.91672098561573	7.34144230777672	4.55729064896118
C	11.58967165158542	1.92913390769627	3.93580650243144
H	10.84514384129575	1.99677805333718	3.13960055618551
H	12.18851925045367	1.03454830285427	3.75222461551211
H	12.25394663280775	2.79279577537482	3.85949663369440
C	10.57658519942476	-3.47775023942128	14.80476372855085
H	10.74792211628441	-2.51388465550207	15.28994940669467
H	11.43192706811605	-3.68891413833793	14.16079390801976
H	10.54339260291344	-4.24803408800553	15.57962660616054
C	10.94269337576323	1.81458413466545	5.32781966581110
C	5.99325053030332	-1.27384027313111	5.87641949828657
H	6.62019622294625	-2.14866432148911	5.75414209442577
C	8.54198665634775	-0.36389511537014	11.80749848389240
C	12.46934813369803	-2.96593596317841	10.12447850069203
H	12.96629386523201	-2.90342152657663	11.09510188798976
H	13.24609364397997	-3.03049214705698	9.35951832369503
H	11.89539549788324	-3.89455688199053	10.09114598624520

C	9.03478329731066	-4.85010840015195	13.36710995409994
H	9.00240614213480	-5.62314471330188	14.13930043265019
H	9.83728174674455	-5.10534089998929	12.67309927771091
H	8.09056529387746	-4.87917582157506	12.81795371905354
C	2.98726216562181	6.51694505687283	12.63848413206628
H	3.49855159420484	6.04458102220294	13.46971384081990
C	9.37937673169010	3.12535146379460	6.93660439511561
C	6.39417548777695	7.44369802695860	17.92262383754915
C	7.76641034250771	7.53715406598528	17.72007972387845
C	8.60468459436033	6.46906146773203	18.05188379298458
C	8.04337704565975	5.31031933698286	18.59053500271078
C	6.66871805077483	5.21114098698242	18.78286514862354
C	5.84148517027649	6.27897662574816	18.45010484286353
H	5.75471224355542	8.27921382470512	17.66536361144718
H	8.18282390377383	8.44700185835780	17.30565305653701
H	8.68688694573946	4.47957164542013	18.85606589750207
H	6.24657351059691	4.30297142035174	19.19519334997950
H	4.77144011187464	6.20579742560177	18.60149196878542
C	10.09399337691814	6.54762360980990	17.85196531552604
H	10.56498958224389	5.61332352886118	18.15489510275014
C	10.55956600037972	6.96418948774230	16.46960732481098
H	10.13998457628582	7.92857310630969	16.18209225471536
H	11.64772086033911	7.02539898621485	16.44320654201633
O	11.87243004478845	7.45388674804087	19.06904964322334
O	10.58486362556131	7.55854034792841	18.84528659608706
H	10.23733686114823	6.21525878827710	15.74446764412784

Table S18. DFT-optimized cartesian coordinates of **E**.

Co	8.07252058831673	5.13022486755156	9.16364303493408
O	8.88102721126593	3.93906590480893	10.41140363194516
N	8.32398126187606	3.93268525091425	7.70501197443815
C	10.78232254991968	0.27711271924034	9.72808189499541

O	6.27648603997551	2.73089414807580	5.61178279639387
O	7.47177990918871	6.17552666513361	10.65564757019265
O	5.41469967767065	3.77372407665761	8.22105849672308
C	9.51551888564309	2.19022682613801	8.91324879175739
C	8.90501706744085	2.78548489173854	7.76663575153815
H	8.95920632794361	2.18669372841345	6.86106069092509
C	10.77796125658532	0.91475821866048	10.98906080626930
H	11.28568501005141	0.40864162666678	11.79629390877064
C	5.11371047921901	3.51000061427697	5.83017918709806
H	4.34004774730685	2.78269979479308	6.08870510014091
C	4.52912885175086	1.33757329957748	9.99290379041202
H	4.51336190464479	0.86743369049158	9.01608182567566
C	4.34951372895937	2.71934752067460	10.09529388163755
C	5.29255335843984	11.46277983114148	10.61110810586044
C	6.90632411067511	8.17171044031954	11.83590685355241
C	7.44418575691257	3.49976411353970	5.32096082015376
H	7.29272682274039	4.08404043646372	4.40936427668990
H	8.23792806680078	2.78444350688225	5.11708746117507
C	5.93825094454914	9.28100956385951	9.42399845219162
H	5.56172662745242	9.65403313610171	8.48064332709339
C	10.18321480615007	2.13319421178438	11.26762026990242
C	6.59181606720510	5.33702084187370	6.78497900121532
H	6.38746265193581	6.02825546921025	5.96428647383423
C	6.99101628323146	7.38686765823895	10.63035931864752
C	6.24995941319595	1.36455719958116	0.80837495471660
H	6.82500524273120	0.81374380392717	0.07399934127242
C	6.39478492148781	7.23389822723221	8.21866140664085
H	5.80222046780619	7.67741209882469	7.41765397292649
C	4.76275651194636	2.79101330928991	2.70607706853771
C	7.80732390564458	4.47925778888757	6.43197543357620
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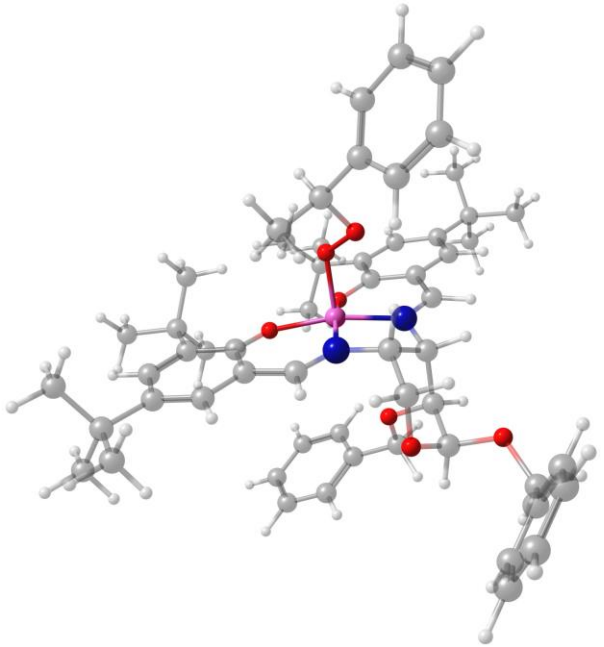
C	8.86420919646402	2.95071600241446	13.26930040390731
H	8.25589601718327	3.59803246577460	12.64392320718746
H	8.93982705926170	3.39803061204329	14.26391418391911
H	8.35291480880042	1.99005584148239	13.37245661327087
C	10.85273468739632	-2.11673952046649	10.50579591525727



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H	11.35011211599576	-3.08312160105920	10.39000202378839
C	6.60016651132670	6.34867617294357	13.55826315060839
H	5.53925665562753	6.58518178878615	13.67449619542184
H	6.96136234465300	5.94810063896060	14.50910780217357
H	6.69985065391468	5.57690053082222	12.79928235351833
C	4.67394192196440	1.40117825721492	2.63276134762462
H	4.02432159750273	0.87128698908613	3.32038118573390
C	8.90428034497984	7.30212398074251	13.10807584195794
H	9.12036992820942	6.58291500350808	12.32318755167075
H	9.24836731311346	6.88972518676384	14.06006932283668
H	9.47550678987781	8.21315473663990	12.91076267425529
O	4.72466960532340	4.25828889265274	4.70765694393909
C	4.36248058908533	3.30937667815332	11.35915933980652
H	4.22199768991898	4.38033949263340	11.44941071721404
C	6.34278811587986	2.75382134579904	0.87088025384393
H	6.98822815372684	3.28567730462100	0.18219895171895
C	10.14543257199260	0.94173511859768	8.70861829152194
H	10.11066932222612	0.52749681018512	7.70960265159146
C	5.41163295436752	0.68956932072112	1.68966741613587
H	5.33195636575598	-0.38991417431841	1.64522765727131
C	4.72274582899466	0.56261213758468	11.13078492863848
H	4.85977432737637	-0.50794946987639	11.03795007139831
C	4.81804216156833	11.93761678654537	9.22935367879435
H	5.63555716587635	11.95610731918629	8.50526568897892
H	4.42126081950577	12.95183241365851	9.30972645105503
H	4.02435624666814	11.30081596078374	8.83242915625279
C	5.87641567788460	10.04383837560719	10.56405739583083
C	6.36871463269111	9.44375892772221	11.74611844294166
H	6.31396440788996	10.02957816854851	12.65144839945397
C	7.39615406650302	7.61896061118530	13.18704055759678
C	5.31694574426669	4.49295417849874	6.99799582518078
H	4.46033476344499	5.17290279228930	7.03313622095590
C	4.14515334420450	3.55327285430887	8.86197222734764
H	3.46927777096120	3.04052717616242	8.16974990510013

H	3.70262049012536	4.52101803667149	9.11925585042418
C	11.02849709801777	4.09347292523069	12.60259049316732
H	12.05180103105999	3.93669801901646	12.25150942095133
H	11.07938888936973	4.54878753204854	13.59494593982003
H	10.53725615031550	4.79063885912392	11.92904887306753
C	11.36700064804803	-1.60867261824255	8.11898489431043
H	11.83022641745356	-0.93232173962785	7.39715223696525
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H	11.87565424976204	-2.57206273917160	8.04484346498413
C	11.48442831323073	-1.07689823825122	9.55562044830352
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C	4.73196007563177	1.16112025922318	12.38912138248897
H	4.87726611127600	0.55749660516910	13.27673316317688
C	3.94640449126802	3.56358156254119	3.71369800679958
H	3.38066027649876	4.35000877752317	3.21169749581720
H	3.23891200135915	2.89741775101802	4.21497780772942
C	12.98365990274890	-0.92995680092859	9.89393647550097
H	13.49111133817228	-1.89205712009768	9.78566543010152
H	13.13430823733997	-0.58687137712807	10.91895856829008
H	13.46477688118411	-0.21403191508411	9.22321657982462
C	11.04892793583811	1.85245197656621	13.66191902851018
H	10.56856621292409	0.88153540052064	13.80212851643118
H	11.08012145122801	2.34809770655414	14.63449653467436
H	12.08046737429247	1.68351060615441	13.34536272433372
C	6.36449053413940	12.45142773363868	11.11769667223675
H	7.22382422533790	12.47227655196391	10.44307517571385
H	6.72318526143254	12.18549477323568	12.11353035146900
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C	10.27512332100692	2.74732027927766	12.67704735460772
C	4.54995229913525	2.53576783738325	12.50163501091293
H	4.55439085078094	3.00683772511633	13.47694105693587
C	6.48247016604261	7.97697712548571	9.43254693300949
C	7.20456554195335	8.62176371479718	14.33874199700857
H	7.76805249467590	9.54373243557737	14.17993530798932
H	7.56795537829789	8.16770362302341	15.26300607742691
H	6.15432352302357	8.88135340126023	14.48901480276863

C	4.08294754951878	11.49349294436581	11.57034090094030
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H	4.36344541745480	11.20475842266980	12.58469041762239
H	3.30008405980067	10.81221513957147	11.22860143100134
C	5.60023538687941	3.46051454504167	1.80974734372419
H	5.66897354045686	4.54194100338323	1.84724742355197
C	9.50173738474598	2.81199088858946	10.19578994778841
O	9.55981396256730	6.19540240023080	8.97431211411248
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C	11.73763263512364	4.99058352961795	7.31878658719345
H	12.82280515302826	4.94084303295222	7.20508841658092
H	11.46266245184732	4.43797221051164	8.21587247366783
C	11.30392262511836	6.44482687610838	7.44119574064627
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C	11.63342439057017	7.29319815755323	6.22985156170867
C	12.37845593506199	8.46335129423488	6.38310093842337
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C	12.25651608078448	8.89568023884835	4.01468409185756
C	11.50509092003755	7.73453107042412	3.85104511978822
C	11.19930159537314	6.93795093264762	4.94966259969776
H	12.71716654026315	8.75290774752974	7.37131223570567
H	13.27918412408267	10.15965124520957	5.42189456034471
H	12.49832739011934	9.51270165112727	3.15781347923324
H	11.15952203007800	7.44697830988950	2.86536196739384
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Table S19. DFT-optimized cartesian coordinates of **E'**.

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C	10.65652359011648	0.00963703245446	9.85651367790186
O	6.39227101264594	2.83959075415742	5.77979801427583

O	7.74220127175739	6.07719596830716	10.92755516974951
O	5.55437385498350	3.84641465791031	8.41966214320723
C	9.53910364459166	2.02900678265762	9.08228360459177
C	8.97868367880325	2.69505704474786	7.94993614175629
H	8.99645457143445	2.11871316327440	7.02865329059065
C	10.67223175171676	0.60724290396964	11.13698260824765
H	11.12460761522489	0.04056205399889	11.93692085609267
C	5.26360506864037	3.66157241352433	6.02015819474877
H	4.46105905112321	2.95860507754057	6.25726241162883
C	4.64975419963382	1.37338429728962	10.02538104515497
H	4.75937804944641	0.98052703711705	9.02100209292540
C	4.39459540556495	2.73522208796537	10.20889741072819
C	5.67586093793887	11.40744568564581	11.06715243463593
C	7.15148946614512	8.01532062826235	12.18872159148385
C	7.59378590092950	3.56390862662466	5.51589352186379
H	7.47215423397769	4.18292003515531	4.62298014863850
H	8.35655243379858	2.82122711571006	5.29252467774457
C	6.28548616426918	9.26009099524448	9.80344149687367
H	5.94039014589405	9.68278579969878	8.86909852306252
C	10.16057634540997	1.85636456388587	11.44359536943997
C	6.81844013584063	5.39140798203009	7.03371053745499
H	6.65116193208894	6.11636431962700	6.23380506913391
C	7.26831761045335	7.29207624806077	10.94810344113734
C	6.49563763183805	1.94487689931038	0.79258722971113
H	7.08234870663273	1.47894119330912	0.01020978491672
C	6.69777545790242	7.24963180504438	8.52607613062903
H	6.12866259368677	7.74281442419474	7.73738611219563
C	4.97741256768626	3.15142844078708	2.81437469623139
C	7.99386285812763	4.48955153566977	6.65894982221987
H	8.80542921705639	5.12796448109243	6.30247669337007
C	8.83445903014104	2.70203331816878	13.42519518247347
H	8.30277023329160	3.41517648941335	12.80199214630759
H	8.90512522173100	3.10863356312457	14.43741026073697
H	8.24776660996878	1.78094798028499	13.47502844775464
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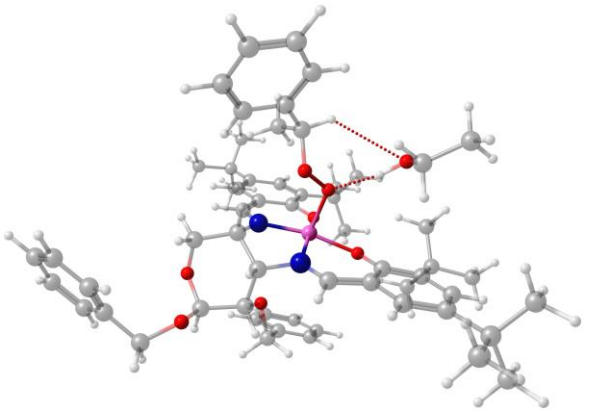
H	9.48298744242003	-2.46845367441343	10.29030335547262



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H	6.98298870673864	5.65178080097848	14.73041909910676
H	6.82950724488532	5.37703081759548	12.98964607653419
C	4.92675432137269	1.77213413306889	2.61558997645618
H	4.29435870079352	1.16394795964184	3.25245587243482
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H	9.29847726299177	6.33712692044233	12.72488529538148
H	9.31548350541883	6.54153414057849	14.48210485341630
H	9.65624983415636	7.91822377344236	13.42758880546120
O	4.90534700601998	4.45692361890689	4.92129654479221
C	4.24751911567517	3.22469848628846	11.50632567059581
H	4.04678235217737	4.27871676810164	11.65959311518417
C	6.55147976310144	3.32463705341526	0.98158617737357
H	7.18000070406884	3.93432112487271	0.34367260144542
C	10.08068044788367	0.74457980967120	8.84914633804950
H	10.02902548520612	0.36171852202880	7.83848005982904
C	5.67936902672483	1.16989266914614	1.60998872363546
H	5.62884725376337	0.09716798046756	1.46748657223411
C	4.75996413151386	0.52092498576151	11.11755150233244
H	4.95639671072359	-0.53295452892354	10.96190630781934
C	5.24631633300353	11.95080206102028	9.69588286653754
H	6.08027485872082	11.97349827393830	8.99092710852927
H	4.87723911488379	12.97238449015753	9.80823634689201
H	4.44390506486712	11.35360373370773	9.25735248780857
C	6.21583842857770	9.97373126853586	10.97385083200504
C	6.65151505717351	9.30487290220195	12.14147081021851
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C	7.54796960551095	7.37545521230330	13.53301066479644
C	5.50378727848853	4.60265240194455	7.21584138842818
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H	3.57777908912708	3.21745988491322	8.28999663818346
H	3.86198966355684	4.62276375366549	9.33238906376164

C	11.10485574503278	3.69592398064121	12.88467397623267
H	12.12622577695880	3.47167441349756	12.56651359794305
H	11.15052880669059	4.10863375107137	13.89580258089212
H	10.69705009816848	4.45501313152879	12.22200940309926
C	11.15579169610973	-1.85547879756948	8.19564377953173
H	11.68093621028445	-1.18603960522792	7.51072558932938
H	10.11466589634958	-1.92569564177156	7.87284703102210
H	11.60154580629260	-2.84756444808002	8.09801318242661
C	11.26943561655609	-1.38312285914196	9.65299912120053
N	7.17612200552480	6.07932474502914	8.27319361633177
C	4.60875466794410	1.01925443873516	12.41045227997536
H	4.68882042839515	0.35401459918027	13.26154476363971
C	4.14120756269689	3.81054280563221	3.88420011965637
H	3.54194123444871	4.61028275714003	3.44577035450635
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C	12.76525828741140	-1.34926916996918	10.03357528393452
H	13.21133518697569	-2.33841780724606	9.90117015371808
H	12.91039310563030	-1.05428100726523	11.07418576356067
H	13.31002500345668	-0.64316347094496	9.40235368194232
C	10.91036641272766	1.42116276648090	13.85261581137446
H	10.35210034988433	0.48568176642015	13.93058296899189
H	10.93772230053698	1.87335943240359	14.84618931199125
H	11.93853281748152	1.18645717754805	13.56899223935410
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H	7.64343447252958	12.35371825415063	10.97723279605954
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H	6.38892405376363	13.35910957100400	11.71697217175019
C	10.24798091023415	2.41110863883357	12.87750441149683
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C	5.79403945374889	3.92224645732813	1.98231877483580
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C	9.55965933778233	2.61764181806887	10.37966149490863
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H	11.55876571884124	4.06189172237971	7.00808327242492
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C	11.65515919574295	6.10040407524610	7.75643488625916
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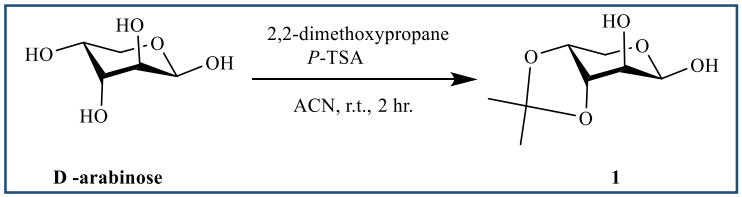
H	10.92144046476672	10.87507830891698	11.49781122215484
H	11.07287241645087	11.71758955081604	9.94776075334135
C	10.57146757756979	9.63034779928345	9.76763143528337
H	9.48969863588983	9.80488512108449	9.74640016489498
H	10.91550153327877	9.55895158434533	8.72870948366960
O	10.86134967483589	8.41849409444765	10.46670848385696
H	10.38403053341877	7.67828857567200	10.04506112721897

3. Experimental details

3.1 General procedure: All chemicals, solvents, and reagents were procured from commercial sources and were used as received. TLC was performed on precoated aluminium plates of silica gel 60-F254. TLC spots were visualized by staining with vanillin solution and subsequent heating on a hot plate. Column chromatography was performed by using silica gel (Merck, 100-200 or 230-400 mesh) under medium pressure. The products were characterised by standard spectroscopic techniques. Absorption spectral data were collected using Shimadzu RF-1600. CV experiments were performed on a three-electrode potential galvanostat (manufacturer:Metrohm Autolab; model: M204) using platinum wire as a counter electrode, a glassy carbon electrode as a working electrode (round shaped, surface area 0.07 cm^2), and a Ag/AgCl as a reference electrode. The glassy carbon electrode was polished using beta-Al_2O_3, following the standard polishing method. CoRibN2 solution was prepared by dissolving CoRibN2 (0.001 M) the presence of tetrabutylammonium perchlorate (TBAP, 0.1 M) as the supporting electrolyte in dry CH_2Cl_2 (40 mL). The voltammograms of the prepared solutions were recorded at room temperature (298 K) after degassing the solutions with nitrogen for 10−15 min to remove oxygen before every experiment. A potential window of −1.8 to 1.8 V was maintained with the following additional parameters: scan rates = 100 mV/s and sample interval = 0.02 V. Under our experimental conditions, the $E_{1/2}$ and peak-to-peak separation (ΔEp) values in CH_2Cl_2 for $[Fe(\eta^5–C_5H_5)_2]^+$/$[Fe(\eta^5–C_5H_5)_2]$ (Fc^+/Fc) couple are 0.55 V vs. Ag/AgCl and 200 mV, respectively, which matches with reported values. All potentials are reported in V vs Fc^+/Fc couple. X-Band EPR spectra were recorded using a JEOL-FA200 ESR Spectrometer (fitted with a quartz Dewar for 100 K measurements), operating at ~ 9.4 GHz. The EPR spectra were calibrated with diphenylpicrylhydrazyl, DPPH (g = 2.0037). X-ray photoemission spectral data were collected using a PHI 5000 versa probe III. ^1H, ^{13}C, and ^{19}F NMR spectra were recorded at room temperature on Bruker AC-400 NMR spectrometer at 400 MHz (1H), 100 MHz (13C), and 376 MHz (19F) in solution of $CDCl_3$ or d_6-DMSO using the peaks of the residual non-deuterated solvent as internal standard. δ values are reported in parts per million (ppm) and coupling constant (J) in Hertz. The chemical shifts were recorded relative to $CDCl_3$ as internal standards. The following calibrations were used: $CDCl_3$ δ = 7.26 ppm and 77.16 ppm. Abbreviations used for signal multiplicity: ^1H - NMR: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, and m = multiplet. High-resolution mass spectra (HRMS) were obtained with Waters XEVO G2-XS QTOF. Single-crystal X-Ray diffraction data were recorded on a Supernova Rigaku Oxford diffractometer. IR spectroscopy was performed on a Perkin Elmer instrument in the solid state.

3.2. Procedure for the synthesis of the monosaccharide-based ligand:

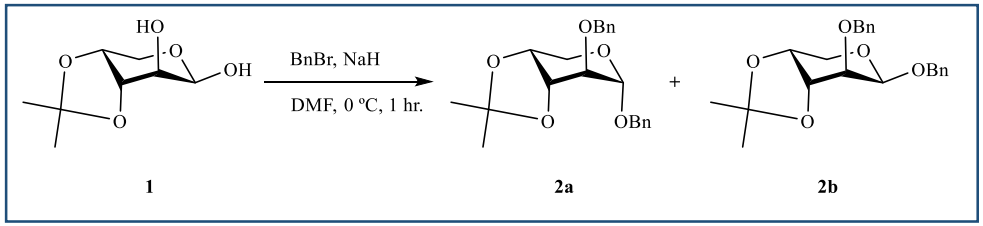
3.2.1 Synthesis of β-3, 4-O-isopropylidene-D-arabinopyranoside (1).[1,2]



D-arabinose (2.0 g, 13.3 mmol) was dissolved in 20 mL DMF and 2,2- dimethoxy propane (4.13g, 39.60 mmol) followed by p-toluene sulphonic acid monohydrate (0.03 g, 0.15 mmol) was added. The reaction mixture was stirred at r.t. for 2h, then it was neutralized by adding triethyl amine, and the solvent was evaporated in vacuo. The crude product was purified by column chromatography using 100-200 mesh silica gel (EA: PE = 3:2) to obtain **1** (1.4 g, 60 % yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.36 (d, *J* = 4.8 Hz 1H), 4.97 (d, *J* = 6.4 Hz, 1H,), 4.84 (d, *J* = 3.6 Hz, 1H), 4.14 - 4.12 (m, 1H), 4.00 - 3.95 (m, 2H), 3.67 (d, *J* = 12.8 Hz, 1H), 3.60 - 3.36 (m, 1H), 1.37 (s, 3H), 1.24 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ. 107.8, 92.3, 75.9, 72.9, 70.2, 58.2, 28.3, 26.4. **HRMS** (ESI) m/z: calcd for $[M+Na]^+$ $C_8H_{14}NaO_5^+$, 213.0733; found, 213.0727. ^{1}H and ^{13}C NMR spectral data matched the previous literature reports.[1,2]

3.2.2. Synthesis of 1, 2-O-benzyl-3, 4-O-isopropylidene-D-arabinopyranoside (2)



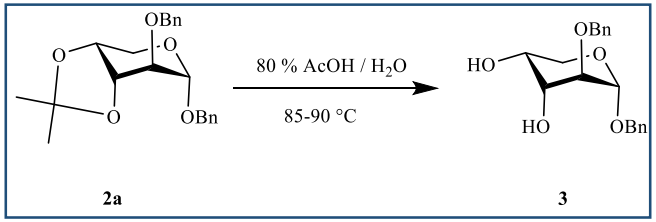
β-3,4-O-isopropylidene-D-arabinopyranoside **1** (1.0 g, 5.3 mmol) was dissolved in a DMF, cooled to 0°C, then benzyl bromide (1.9 mL, 3 equiv.) followed by NaH (0.57 g, 4.5 equiv.) was added portion-wise. After complete addition, the reaction was stirred at room temperature. After 1 h, when the reaction was completed, it was quenched with ethyl acetate (5 mL) and then water (2 mL). The ethyl acetate layer was extracted (2 x 20 mL), and the combined organic layer

was washed with brine (4 x 20 mL), dried in sodium sulfate, and evaporated in a vacuum. The crude product was purified by column chromatography using 230-400 mesh silica gel (EA:PE = 1:19) to get a viscous liquid product.

For α isomer, **2a** (1.078g, 55% yield), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41–7.27 (m, 10H), 4.86 (d, *J* = 3.36 Hz, 1H,), 4.73 (dd, *J* = 12.4, 5.4 Hz, 2H), 4.64 (d, *J* = 12.4 Hz, 1H), 4.53 (d, *J* = 12.4 Hz, 1H), 4.39 (dd, *J* = 7.8, 5.7 Hz, 1H), 4.24 (dd, *J* = 5.6, 1.4 Hz, 1H), 4.01 - 3.92 (m, 2H), 3.54 (dd, *J* = 7.9, 3.4 Hz, 1H), 1.43 (s, 3H), 1.36 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.3, 137.3, 128.5, 128.4, 128.0, 127.9, 127.8, 108.9, 95.8, 76.7, 75.5, 73.6, 72.2, 69.2, 59.0, 28.3, 26.5. **HRMS** (ESI) m/z: calcd for $[M+Na]^+$ $C_{22}H_{26}NaO_5^+$, 393.1672; found, 393.1675.

For β isomer, **2b** (,0.785g, 40% yield),), **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 10H), 4.90 (d, *J* = 12.0 Hz, 1H,), 4.81 (s, 2H), 4.61 (d, *J* = 12.0 Hz, 1H), 4.49 (d, *J* = 6.9 Hz, 1H), 4.29 - 4.26 (m, 1H), 4.17 (t, *J* = 7.9 Hz, 1H), 4.09 (dd, *J* = 12.9, 4.0 Hz, 1H), 3.78 (dd, *J* = 121.9, 4.0 Hz, 1H), 3.57 (t, *J* = 7.0 Hz, 1H), 1.43 (s, 3H); 1.37 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ.138.3, 137.6, 128.5, 128.3, 128.2, 128.0, 127.9, 127.7, 110.1, 101.3, 79.9, 78.1, 73.6, 72.9, 70.3, 62.6, 27.8, 26.1. **HRMS** (ESI) m/z: calcd for M+Na]$^+$ $C_{22}H_{26}NaO_5^+$, 393.1672; found, 393.1692.

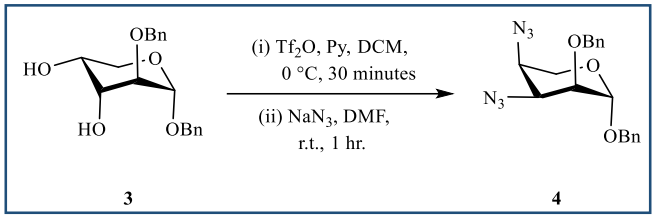
3.2.3. Synthesis of 1, 2-O-benzyl-α-D-arabinopyranoside (3)



1,2-benzyl-3, 4-O-isopropylidene-α-D-arabinopyranoside **2a** (5.0 g. 13.5 mmol) was dissolved in 80% acetic acid. Then the reaction was stirred at 80 ℃ for 4 h. After completion of the reaction, the solvent was removed in vacuo, and the crude product was purified by column chromatography using 100-200 mesh silica gel (EA: PE = 2:3) to afford a white solid product **3** (4.103 g, 92% yield). **M.P.:** 112-115 ℃.

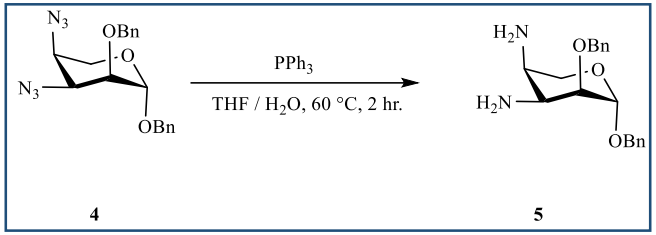
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.28 (m, 10H), 4.94 (d, *J* = 3.4 Hz, 1H,), 4.72 (d, *J* = 12.2 Hz, 1H), 4.52 (dd, *J* = 11.8, 3.3 Hz, 2H), 4.47 (d, *J* = 12.2 Hz, 1H), 4.06 (d, *J* = 9.6 Hz, 1H), 3.97(b, 1H), 3.84 (d, *J* = 12.5 Hz, 1H), 3.76 - 3.69 (m, 2H), 2.89 (d, *J* = 13.0 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ.137.9, 137.3, 128.6, 128.5, 128.2, 128.1, 128.09, 128.0, 95.5, 76.6, 72.4, 69.2, 69.0, 68.6, 62.2. **HRMS** (ESI) m/z: calcd for M+Na]$^+$ $C_{19}H_{22}NaO_5^+$, 353.1359; found, 353.1354.

3.2.4. Synthesis of 3, 4-diazido-1, 2-O-benzyl-3,4-dideoxy -α-D-ribopyranoside (4)



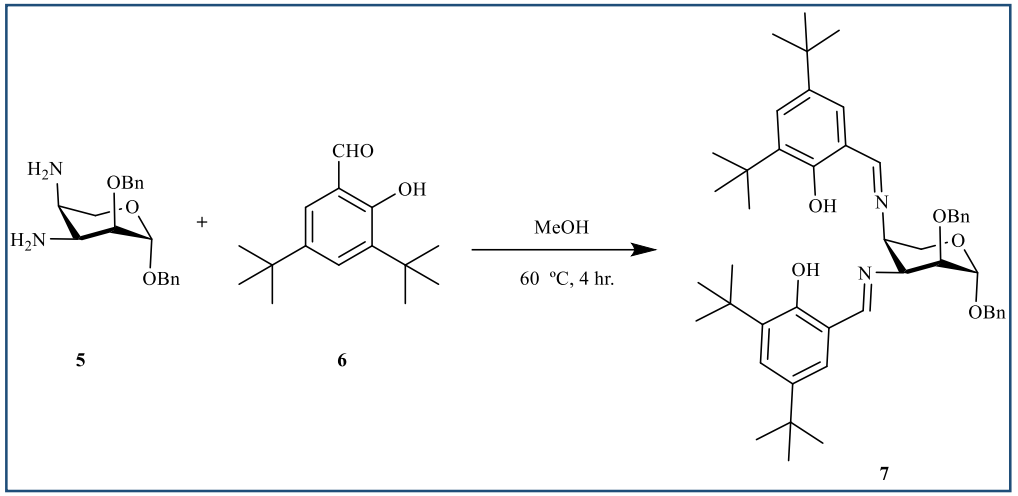
A solution of 1, 2-O-benzyl-α-D-arabinopyranoside **3 (**0.500 g, 1.5 mmol) in DCM at °C, trifluoromethane sulphonic anhydride (0.753 mL, 4.5 mmol, 3 equiv) and pyridine (0.365 mL, 4.5 mmol, 3 equiv.) was added. The reaction mixture was stirred at the same temperature for 30 minutes and then extracted with DCM (3 x 20 mL). Further, it was washed with 2M HCl (20 mL) and saturated sodium bicarbonate (20 mL) solution. DCM layer was collected in sodium sulfate and concentrated in vacuo at ambient temperature. The crude product was dried in a vacuum and dissolved in DMF (5 mL), followed by the addition of sodium azide (0.164 g, 2.52 mmol, 3 equiv.). The reaction mixture was stirred at rt for 4 h, then extracted with ethyl acetate (2 x 20 mL), and the whole ethyl acetate layer was washed with brine solution (4 x 15 mL). The organic layer was dried over sodium sulfate and evaporated in a vacuum to obtain crude product. The crude product was purified by column chromatography using 230-400 mesh silica gel (EA:PE = 1:49) to afford the pure product **4** as liquid (0.434 g, 76 % yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37–7.31 (m, 10H), 4.87 (d, *J* = 1.6 Hz, 1H,), 4.85 (s, 1H), 4.84 (d, *J* = 2.8 Hz, 1H), 4.72 (d, *J* = 12 Hz, 1H), 4.60 (d, *J* = 12 Hz, 1H), 3.96 (t, *J* = 3.2 Hz, 1H), 3.90 (dd, *J* = 12.0, 4.4 Hz, 1H), 3.76 (dd, *J* = 11.6, 8.0 Hz, 1H), 3.53 (ddd, *J* = 10.9, 6.8, 3.8 Hz, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 137.6, 137.2, 128.61 128 .58, 128.07, 128.05, 127.98, 127.94, 99.2, 76.6, 73.5, 71.0, 61.7, 61.1, 57.0. **HRMS** (ESI) m/z: calcd for $[M+Na]^+$ $C_{19}H_{20}N_6NaO_3^+$, 403.1489; found, 403.1487.

3.2.5. Synthesis of, 3, 4-diamino-1, 2-O-benzyl-3,4-dideoxy- α-D-ribopyranoside (5)



3, 4-diazido-1, 2-O-benzyl-3,4-dideoxy-α-D-ribopyranoside **4** (0.500 g, 1.3 mmol), triphenylphosphine (1.03g, 3.9 mmol, 3 equiv.) was dissolved in the mixture of THF/H_2O (3:1, 6 mL). The reaction was stirred at 60 ℃ for 2 h. After the completion of the reaction, the solvents were evaporated in a vacuo, and the crude product was purified by column chromatography using 100-200 mesh silica gel (MeOH: $CHCl_3$ =, 1:19) to obtain pure **5** as liquid (0.390 g, 91% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 10H), 4.95 (d, *J* = 2.3 Hz, 1H,), 4.77 (d, *J* = 12.0 Hz, 1H), 4.68 (d, *J* = 11.7 Hz, 1H), 4.50 (dd, *J* = 11.5, 10.6 Hz, 2H), 3.92 (dd, *J* = 11.6, 2.4 Hz, 1H), 3.64 (dd, *J* = 11.6, 3.1 Hz, 1H), 3.46 (t, *J* = 2.9 Hz, 1H), 3.17 (t, *J* = 3.7 Hz, 1H), 2.79 (d, *J* = 3.2, Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.0, 137.5, 128.5 127.90, 127.85, 127.8, 96.7, 79.4, 73.3, 69.3, 66.0, 51.8, 48.4: **HRMS** (ESI) m/z: calcd for $[M+H]^+$ $C_{19}H_{25}N_2O_3^+$, 329.1860; found, 329.1868.

3.2.6. Synthesis of ligand (7)

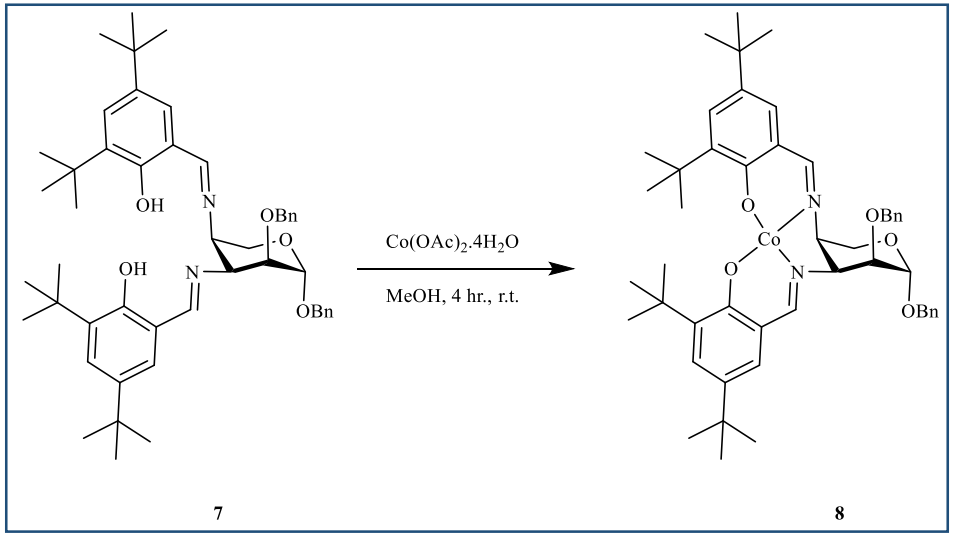


3, 4-diamino 1, 2-O-benzyl-3,4-didoxy-α-D-ribopyranoside **5** (0.500 g, 1.52 mmol, 1 equiv.) and 3, 5-Di-tert-butyl-2-hydroxy benzaldehyde **6** (0.71 g, 3.04 mmol, 2 equiv.) was dissolved in a MeOH. The reaction mixture was stirred at 60 ℃ for 4 h. After completion of the reaction, the solvent was evaporated in a vacuum and dried in a vacuum to obtain an analytically pure product **7** as a yellow solid (1.1g, 95% yield). **M.P.:** 122-125 ℃

^{1}H NMR (400 MHz, $CDCl_3$) δ 13.35 (s,1H), 13.15 (s, 1H) 8.44 (s, 1H), 8.28 (s, 1H), 7.44 – 7.36 (m, 6H), 7.34 - 7.28 (m, 6H), 7.07 (dd, *J* = 9.0, 1.8 Hz, 2H), 5.17 (d, *J* = 7.0 Hz, 1H), 5.02 (d, *J* = 11.6 Hz, 1H), 4.87 (d, *J* = 12.4, 1H), 4.75 (dd, *J* = 11.6, 5.9 Hz, 2H), 4.28 (t, *J* = 10.3 Hz 1H), 3.95 (dd, *J* = 11.5, 4.1 Hz, 1H), 3.82 - 3.79 (m, 2H), 3.70 (dd, *J* = 6.9, 3.4 Hz, 1H) 1.50 (s, 9H), 1.31 (s, 27H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 168.8, 167.2, 158.32, 158.28, 140.10, 140.0, 138.7, 137.7, 137.1, 136.7, 128.5, 128.4, 128.0, 127.9, 127.8, 127.6, 127.5, 127.3, 126.5, 126.1, 118.0, 117.7, 100.6, 77.2, 73.0, 71.4, 67.4, 65.1, 35.2, 35.1, 34.2, 31.61, 31.59, 31.5, 29.6, 29.4. **HRMS** (ESI) m/z: calcd for $[M+H]^+$ $C_{49}H_{65}N_2O_5^+$, 761.4888; found, 761.4899.

3.3. Syntheses of catalyst (8) and [CoRibN2]$^+$

3.3.1 Syntheses of catalyst (8)

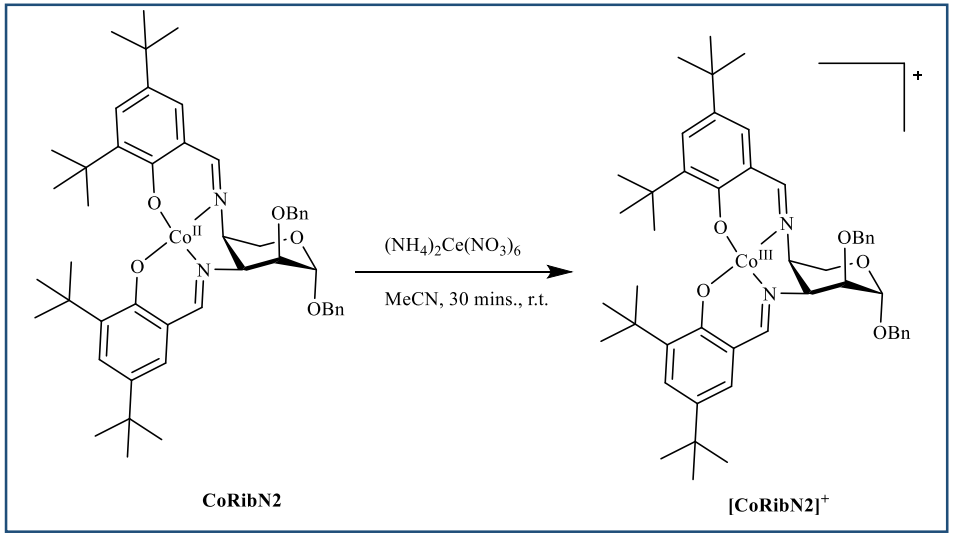


The ligand **7** (0.500g, 0.657 mmol, 1 equiv.) was dissolved in 10 mL of MeOH. The color of the solution turned to yellow. To this solution, $Co(OAc)_2.4H_2O$ (0.164g, 0.657, 1 equiv.) was added pinch-wise. The color of the solution turned to wine-red, and within 1-2 min, the wine-red precipitate started to come. The mixture was kept in stirring condition for another 4 h at room temperature for the completion of the reaction. The mixture was filtered in a cotton-plugged NMR funnel and washed with 10 mL MeOH. The residue was dissolved in 15 mL of CH_2Cl_2. The clear red solution was evaporated to dryness and then washed with 10 mL MeOH and filtered for the second time to isolate pure wine-red solid. The residue was again dissolved in CH_2Cl_2, and the MeOH extract was discarded. The DCM solution was then kept for slow evaporation to isolate the wine-red crystalline solid (0.456 g, 85% yield).

Anal. Calcd. (%) for $C_{49}H_{62}N_2CoO_5$ (fw = 817.9772): C, 71.95; H, 7.64; N, 3.42. Found: C, 71.65; H, 7.18; N, 3.23. **HRMS** (ESI) m/z: calcd for $[M+H]^+$ $C_{49}H_{63}CoN_2O_5^+$, 818.4063; found, : 818.4064.

The single crystals of the composition [Co(RibN2)] (**8**) were obtained for x–ray crystallographic analysis from the CH_2Cl_2-MeOH (3:1, v/v) slow evaporation.

3.3.2 Synthesis of oxidized species of 8, $[CoRibN2]^+$.



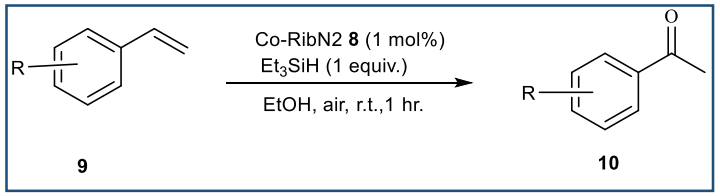
The catalyst **8** (CoRibN2) (10 mg, 0.0122 mmol, 1 equiv.) was dissolved in 1.5 mL CH_3CN solvent. Ammonium ceric nitrate (CAN) (8 mg, 0.0146 mmol, 1.2 equiv.) was added pinch wise to the pinkish red solution. The colour of the pinkish red solution turned to greenish brown immediately. The green solution converted to deep brown solution after 10 mins. The solution was kept for stirring for another 20 mins for completion of the oxidation reaction. The solution was evaporated to dryness and washed with n-pentane (5 mL for 3 times). The brown solid was filtered through a G-4 frit and washed with n-pentane until the washing became colourless and the solid residue was dried *in vacuo*.

HRMS (ESI) m/z: calcd for $[M]^+$ $C_{49}H_{62}CoN_2O_5^+$, 817.3991; found: 818.3990. Absorption Spectra: λ(nm) (ε $M^{-1}cm^{-1}$): 490 (900), 380 (6100), 260 (17 600).

3.4. Substrate scope and product characterization for the oxidation and hydration reaction.

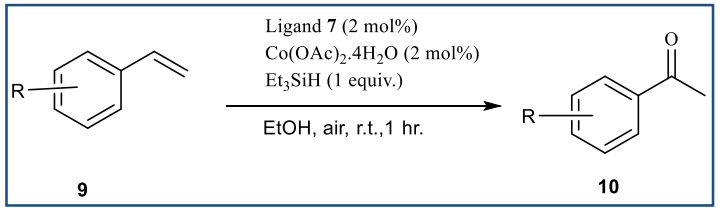
3.4.1. General procedure for the oxidation reaction (Method-A)

A mixture of an alkene derivative **9** (1 mmol, 1 equiv.) and a catalyst **8** (0.008 g, 1 mol%, calculated with respect to the alkene derivative) was stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 1 h. After the complete consumption of the starting material, the solvent was removed at 27 ℃ using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether as an eluent to afford ketone products **10** in an excellent yield.



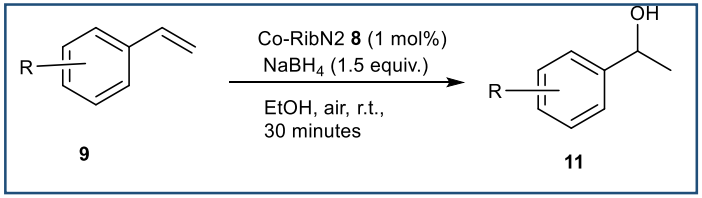
3.4.2. General procedure for the oxidation reaction (Method-B)

A mixture of an alkene derivative **9** (1 mmol, 1 equiv.), ligand **7** (0.011g, 2 mol%) and $Co(OAc)_2.4H_2O$ (0.005g, 2 mol%) were stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask exposed to the ambient atmosphere. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 1 h. After the complete consumption of the starting material, the solvent was removed at 27 ℃ using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether as an eluent to afford ketone products **10** in an excellent yield.



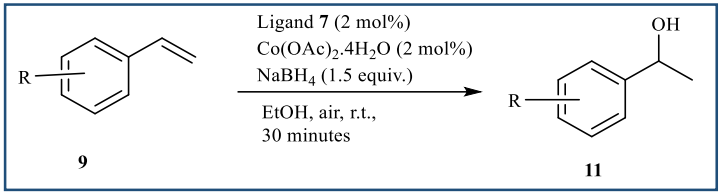
3.4.3. General procedure for the hydration reaction (Method-C)

A mixture of an alkene derivative **9** (1 mmol, 1 equiv.) and a catalyst **8** (0.008 g, 1 mol%, calculated with respect to the alkene derivative) was stirred in anhydrous ethanol (2 mL) at 27 °C in an open flask exposed to the ambient atmosphere. Then $NaBH_4$ (0.056 g, 1.5 mmol, 1.5 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 °C for 30 min. After the complete consumption of the starting material, the solvent was removed at 27 °C using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether as an eluent to afford alcohol products **11** in an excellent yield.



3.4.4. General procedure for the hydration reaction (Method-D)

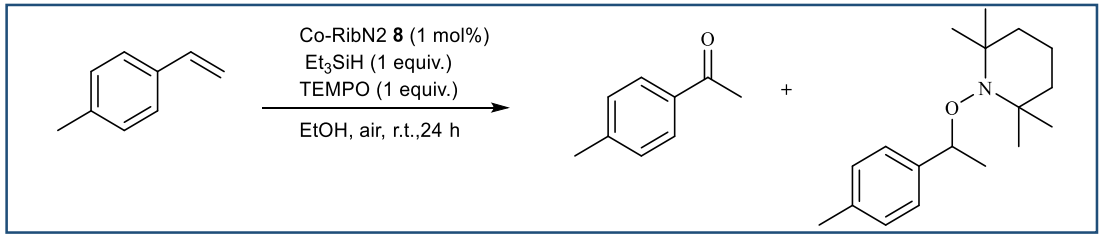
A mixture of an alkene derivative **9** (1 mmol, 1 equiv.), ligand **7** (0.011g, 2 mol%) and $Co(OAc)_2.4H_2O$ (0.005g, 2 mol%) were stirred in anhydrous ethanol (2 mL) at 27 °C in an open flask exposed to the ambient atmosphere. Then $NaBH_4$ (0.056 g, 1.5 mmol, 1.5 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 °C for 30 min. After the complete consumption of the starting material, the solvent was removed at 27 °C using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether as an eluent to afford alcohol products **11** in an excellent yield.



3.5. Control experiments.

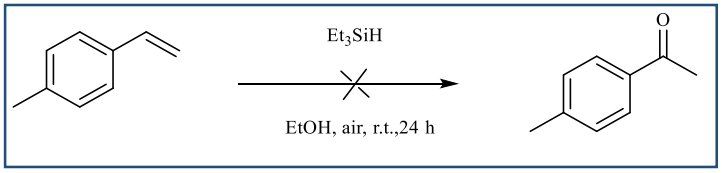
3.5.1 Oxidation reaction using TEMPO as a radical scavenger.

A mixture of a 4-methylstyrene (0.118g, 1 mmol, 1 equiv.), catalyst **8** ((0.008 g, 1 mol%) and TEMPO (0.158 g, 0.001 mmol, 1 equiv.) were stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask exposed to the ambient atmosphere. Then triethylsilane (0.116g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 24 h. The reaction mixture was analyzed by TLC and HRMS, showing that a trace of the desired product along with TEMPO adduct with styrene, was formed. This suggested that the reaction was going through the radical pathway.



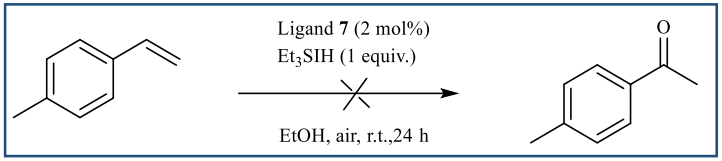
3.5.2. Oxidation reaction without CoRibN2.

4-methylstyrene (0.118g, 1 mmol, 1 equiv.) was stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 24 h. Then, the crude mixture was analyzed by TLC, showing no consumption of starting materials nor formation of product.



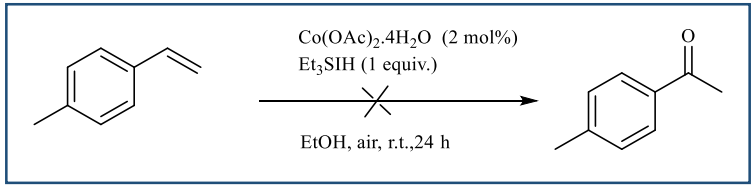
3.5.3. Oxidation reaction with Ligand 7 in absence of Co(II)-salt.

4-methylstyrene (0.118g, 1 mmol, 1 equiv.), ligand **7** (0.011g, 2 mol%) was stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 24 h. Then, the crude mixture was analyzed by TLC, showing no consumption of starting materials nor formation of product.



3.5.4. Oxidation reaction with $Co(OAc)_2.4H_2O$.

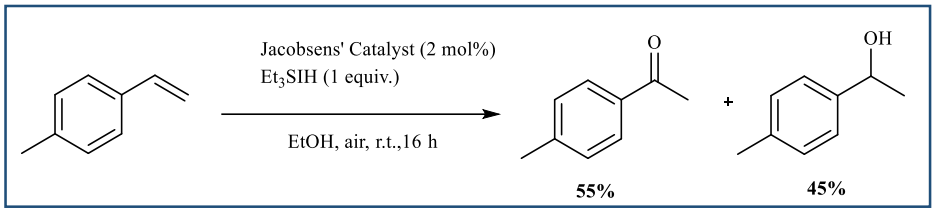
4-methylstyrene (0.118g, 1 mmol, 1 equiv.), $Co(OAc)_2.4H_2O$ (0.005g, 2 mol%) was stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 24 h. Then, the crude mixture was analyzed by TLC, showing no consumption of starting materials nor formation of product.



3.5.5. Oxidation reaction with Jacobsen catalyst.

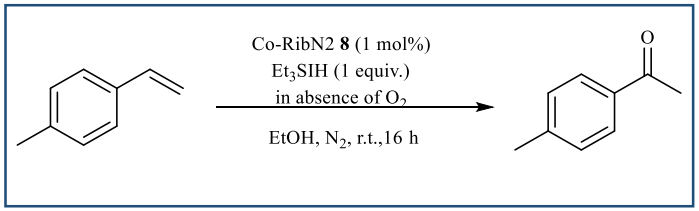
4-methylstyrene (0.118g, 1 mmol, 1 equiv.), Jacobsen's catalyst (0.012g, 2 mol%) was stirred in anhydrous ethanol (2 mL) at 27 ℃ in an open flask. Then triethylsilane (0.116 g, 1 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 16 h. Then, the crude mixture was analyzed

by TLC, showing partial consumption of starting materials, and a mixture of alcohol and ketone products was formed. The products were further separated using column chromatography, isolated, and confirmed with ^{1}H and ^{13}C NMR spectroscopy.



3.5.6. Oxidation reaction with in absence of O_2.

A Schlenk tube was charged with Co-RibN2 (0.008 g, 1mol%) and anhydrous ethanol (1ml) fitted with a septum. The solution was cooled to 0 ℃ and then degassed (consecutively filling with nitrogen gas and applying vacuum by a pump) for 10 mins. The degassing procedure was repeated for three times to eliminate both the aerial and dissolved O_2. To this, a mixture of 4-methylstyrene (0.118 g, 1 mmol, 1 equiv.) and triethylsilane (0.116 g, 1 mmol, 1 equiv.) in 1 ml ethanol (also degassed in a separate Schlenk tube) was transferred using a cannula under nitrogen atmosphere. Resulting mixture was stirred for 27 ℃ for 16 h under nitrogen atmosphere. Then the crude mixture was analyzed by TLC, showing no consumption of starting material and no trace of desired product.



3.6. Gram scale synthesis

3.6.1. **Procedure for gram scale oxidation reaction**: A mixture of a 4-methylstyrene (1.0 g, 8.46 mmol, 1 equiv.) and a catalyst **7** (69.2 mg, 1 mol%, calculated with respect to the 4-methylstyrene) was stirred in ethanol (20 mL) at 27 ℃ in an open flask exposed to the ambient atmosphere. Then triethylsilane (1.4 mL, 8.46 mmol, 1 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 ℃ for 2 h. After the complete consumption of the starting material,

the solvent was removed at 27 °C using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether = 1:99 as an eluent to afford 1-(4-methylphenyl)ethan-1-one **10a** (1.00 g, 88% yield).

3.6.2. Procedure for gram scale hydration reaction.

A mixture of 4-chlorostyrene (1.0 g, 7.22 mmol, 1 equiv.) and a catalyst **7** (59.0 mg, 1 mol%, calculated with respect to the 4-chlorostyrene) was stirred in ethanol (20 mL) at 27 °C in an open flask exposed to the ambient atmosphere. Then $NaBH_4$ (409 mg, 10.8 mmol, 1.5 equiv.) was added to the mixture, and the resulting mixture was stirred at 27 °C for 1h. After the complete consumption of the starting material, the solvent was removed at 27 °C using a rotary evaporator. The crude product was chromatographed over a column of silica gel (100-200 mesh) using EtOAc/Petroleum ether = 1:19 as an eluent to afford 1-(4-chlorophenyl)ethan-1-ol **11a** (1.14 g, 92% yield).

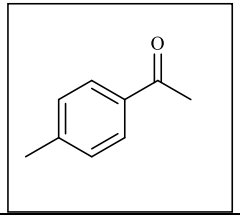
3.7. UV-Vis experiment

The UV-Visible spectroscopic experiments were performed using a quartz cuvette of 1.0 cm path length. Initially, UV spectra of the starting materials **8** in acetonitrile (MeCN) was recorded at concentrations of 3.5×10^{-5} (M) in. Later, the 1:1 (i.e., **8** and **Et_3SiH**) binary mixture was mixed and the UV-Vis spectrum was recorded for 6 hours with regular time interval. The mixture of **8** and **Et_3SiH** showed a gradual decay in 500, 420 and 360 nm transitions. For the first 90 mins a new peak at 766 nm is generated gradually. After 90 mins, slow decay of the 766 nm peak can be observed. After 6 h, complete decay of 766, 500 and 360 nm peaks were observed. The transition at 420 nm in diminished substantially.

3.8. Characterization data for acetophenones

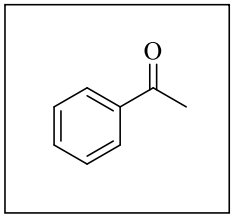
3.8.1 1 4-Methylacetophenone (10a)[3]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.118 g, 1.0 mmol, 4-methylstyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10a** as a light yellow liquid.
Yield: 0.120 g, 90% (**Method A**), 0.115 g 86% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 2.55 (s, 3H), 2.39 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 143.9, 134.7, 129.3, 128.5, 26.6, 21.7.



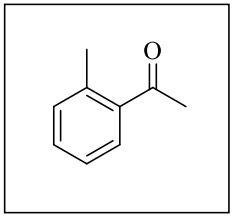
3.8.2 Acetophenone (10b)[4]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.104 g, 1.0 mmol, styrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10b** as a light yellow liquid.
Yield: 0.102 g, 85% (**Method A**), 0.102 g 84% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4, Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 2.60 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 137.1, 133.2, 128.6, 128.4, 26.7.



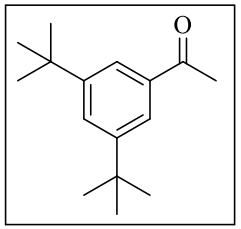
3.8.3 2-Methylacetophenone (10c)[3]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.118 g, 1.0 mmol, 2-Methylstyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10c** as a light yellow liquid.
Yield: 0.115 g, 86% (**Method A**), 0.107 g 80% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.3 Hz, 1H), 7.39 (td, *J* = 7.5, 1.1 Hz, 1H), 7.27 (dd, *J* = 12, 7.9 Hz, 2H), 2.58 (s, 3H), 2.53 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 201.9, 138.6, 137.7, 132.2, 131.6, 129.5, 125.8, 29.7, 21.7.



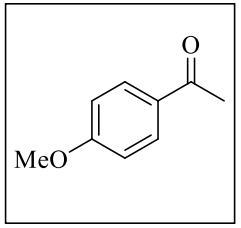
3.8.4 3,5-Di-tert-butylacetophenone (10d)[5]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.216 g, 1.0 mmol, 3, 5-Di-tert-butylstyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10d** as a viscous liquid.
Yield: 0.187 g, 81% (**Method A**), 0.181 g 78% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83(d, *J* = 1.8 Hz, 2H), 7.66 (t, *J* = 1.7 Hz, 1H), 2.63 (s, 3H) 1.37 (s, 18H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 199.0, 151.3, 136.9, 127.5, 122.6, 35.1, 31.5, 26.9.



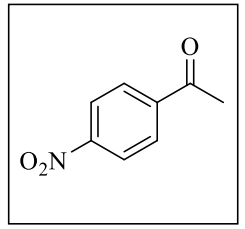
3.8.5 4-Methoxyacetophenone (10e)[3]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.134 g, 1.0 mmol, 4-Methoxystyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10e** as a light yellow liquid.
Yield: 0.124 g, 83% (**Method A**), 0.120 g 80% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.54 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 163.6, 130.7, 130.4, 113.8, 55.6, 26.5.



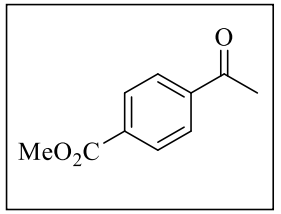
3.8.6 4-Nitroacetophenone (10f)[6]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.150 g, 1.0 mmol, 4-Nitrostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10f** as a yellow solid.
M.P.: 76 - 78 °C
Yield: 0.154 g, 93% (**Method A**), 0.152 g 92% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.4 Hz, 2H), 8.09 (d, *J* = 8.4 Hz, 2H), 2.67 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 150.4, 141.4, 129.4, 123.9, 27.1



3.8.7 4-Methoxycarbonylacetophenone (10g)[7]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.162 g, 1.0 mmol, methyl 4-vinylbenzoate, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **10g** as a white solid.



M.P.: 95 - 98 ℃

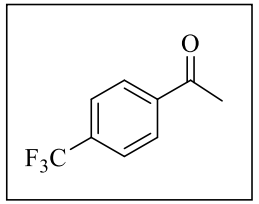
Yield: 0.153 g, 90% (**Method A**), 0.148 g 83% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 2H), 7.95 (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H), 2.59 (s, 3H).

^{13}C NMR (100MHz, $CDCl_3$) δ 197.5, 166.2, 140.2, 133.9, 129.8, 128.2, 52.5, 26.9.

3.8.8 4-Trifluoromethyl-acetophenone (10h)[8]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.172 g, 1.0 mmol, 1-(Trifluoromethyl)-4-vinyl styrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10h** as colorless liquid.



Yield: 0.172g, 92% (**Method A**), 0.169 g 90% (**Method B**).

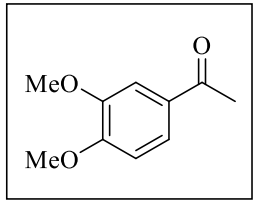
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 2H), 2.60 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 139.7, 134.5, (q, *J* = 32.4 Hz), 128.7, 125.7 (q, *J* = 3.7 Hz), 123.7(q, *J* = 270.8 Hz), 26.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.2.

3.8.9 3,4-Dimethoxyacetophenone (10i)[9]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.164 g, 1.0 mmol, 3,4-Dimethoxystyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10i** as a white sold.



M.P.: 55- 57 ℃

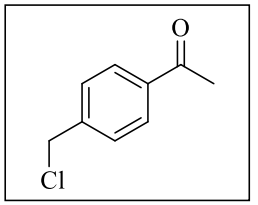
Yield: 0.165 g, 92% (**Method A**), 0.155 g 86% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.51 (d, *J* = 1.9 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H) 3.93 (s, 3H), 3.92 (s, 3H), 2.55 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.0, 153.4, 149.0, 130.5, 123.4, 110.1, 110.0, 56.2, 56.1, 56.1, 26.3.

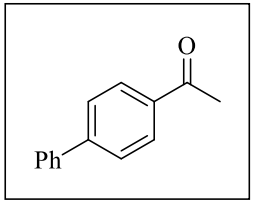
3.8.10 4-Acetylbenzyl chloride (10j)[10]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.115 g, 1.0 mmol, 4-vinylbenzyl chloride and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10j** as colorless liquid.
Yield: 0.156 g, 93% (**Method A**), 0.145 g 86% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 2H), 7.47 (d, *J* = 8.2 Hz, 2H), 4.60 (s, 2H), 2.59 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 142.5, 137.0, 128.9, 128.8, 45.4, 26.8.



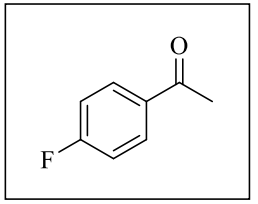
3.8.11 4-Acetylbiphenyl (10k)[11]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.180 g, 1.0 mmol, 4-vinylbiphenyl, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10k** as a white solid.
M.P.: 114 - 116 ℃
Yield: 0.180 g, 92% (**Method A**), 0.173 g 88% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.41, 2H), 7.69 (d, *J* = 8.4Hz, 2H), 7.64 (dd, *J* = 8.6, 1.4 Hz, 2H), 7.49 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.42-7.34 (m, 1H), 2. 64 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) *δ* 197.9, 145.9, 139.9, 135.9, 129.1, 129.0, 128.3, 127.4, 127.3, 26.8.



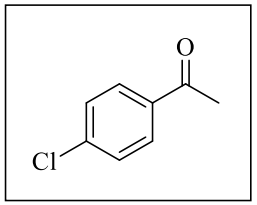
3.8.12 4-Fluoroacetophenone (10l)[3]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.122 g, 1.0 mmol, 4-Fluorostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10l** as a colorless liquid.
Yield: 0.103 g, 75% (**Method A**), 0.102 g 74% (**Method B**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 - 7.93 (m, 2H), 7.13 - 7.07 (m, 2H) 2.56 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) *δ* 196.6, 165.8 (d, J_{C-F} = 253 Hz), 133.6 (d, J_{C-F} = 2.9 Hz), 131.0 (d, J_{C-F} = 9.3 Hz), 115.7 (d, J_{C-F} = 21.8 Hz), 26.6.
^{19}F NMR (376 MHz, $CDCl_3$) δ -105.35.



10.1.13 4-Chloroacetophenone (10m)[3]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.138 g, 1.0 mmol, 4-chlorostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10m** as a colorless liquid.



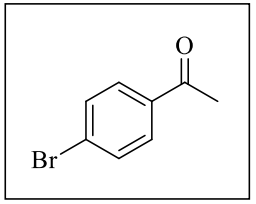
Yield: 0.123 g, 80% (**Method A**), 0.122 g 79% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 8.63, 6.9 Hz, 2H), 7.42 (dd, *J* = 8.4, 6.9 Hz, 2H), 2.58 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) *δ* 197.0, 139.7, 135.5, 129.8, 129.0, 26.7.

3.8.14 4-Bromoacetophenone (10n)[6]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.183 g, 1.0 mmol, 4-bromostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10n** as a white solid.



M.P.: 51 - 53 ℃

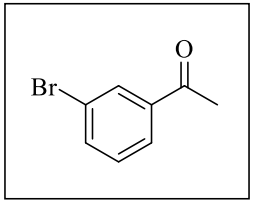
Yield: 0.183 g, 92% (**Method A**), 0.181 g 91% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.5 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 2:57 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.1, 135.9, 132.0, 129.9, 128.4, 26.7.

3.8.15 3-Bromoacetophenone (10o)[12]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.183 g, 1.0 mmol, 3-bromostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10o** as a colorless liquid.



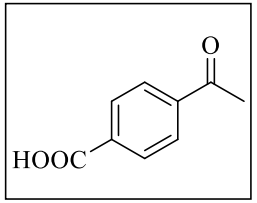
Yield: 0.189 g, 95% (**Method A**), 0.183 g 92% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (t, *J* = 1.6 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.9 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 2.58 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 138.8, 136.1, 131.5, 130.3, 127.0, 123.0, 26.7.

3.8.16 4-Acetylbenzoic acid (10p)[13]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.148 g, 1.0 mmol, 4-vinylbenzoic acid, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 2:23 as eluent, to afford **10p** as a white solid.



M.P.: 200 - 203 ℃

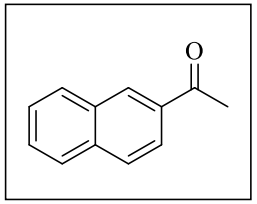
Yield: 0.131 g, 80% (**Method A**), 0.118 g 72% (**Method B**).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.03 (s, 4H), 2.60 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 198.1, 167.0, 140.0, 134.7, 129.8, 128.6, 27.2.

3.8.17 2-Acetylnaphthalene (10q)[11]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.155 g, 1.0 mmol, 2-vinylnaphthalene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10q** as a white solid.



M.P.: 50 - 53 ℃

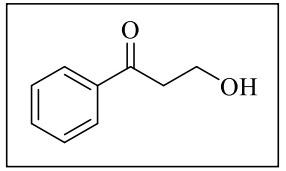
Yield: 0.110 g, 71% (**Method A**), 0.119 g 70% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.05 - 8.02 (dd, 1H, *J* = 8.8, 2.0 Hz), 7.96 (d, *J* = 8.0 Hz 1H), 7.90 - 7.87 (m, 2H), 7.62 - 7.53 (m, 2H), 2.73 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) 198.3, 135.7, 134.6, 132.6, 130.3, 129.7, 128.6, 128.5, 127.9, 126.9, 124.0, 26.8.

3.8.18 3-hydroxy-1-phenylpropan-1-one (10r)[14]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.134 g, 1.0 mmol, cinnamyl alcohol, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:4 as eluent, to afford **10r** as a light yellow liquid.



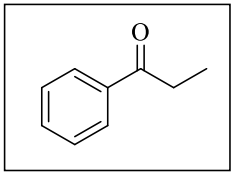
Yield: 0.111 g, 74% (**Method A**), 0.108 g, 72% (**Method B**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 - 7.94 (m, 2H), 7.60 - 7.56 (m, 1H), 7.49 - 7.45 (m, 2H), 4.03 (t, *J* = 5.3 Hz, 2H), 3.23 (t, *J* = 5.4 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 200.6, 136.8, 133.6, 128.8, 128.2, 58.2, 40.5.

3.8.19 Propiophenone (10s)[7]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.118 g, 1.0 mmol, β-methylstyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **10s** as a light yellow liquid.



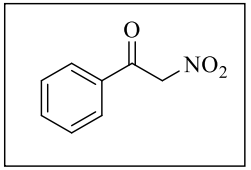
Yield: 0.097 g, 72% (**Method A**), 0.095 g, 71% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 - 7.95 (m, 2H), 7.57 - 7.55 (m, 1H), 7.47 - 7.45 (m, 2H), 3.01 (q, *J* = 7.2 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 201.0, 137.1, 133.0, 128.7, 128.1, 31.9, 8.4.

3.8.20 2-Nitro-1-phenylethan-1-one (10t)[15]

Reaction Condition: It was synthesized following the general procedure **Method A** and **Method B**. The reaction was carried out with 0.149 g, 1.0 mmol, β-nitrostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:9 as eluent, to afford **10t** as a white solid.



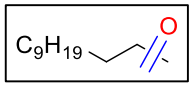
Yield: 0.112 g, 68% (**Method A**), 0.109 g, 66% (**Method B**).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 - 7.78 (m, 2H), 7.71 - 7.67 (m, 1H), 7.56 - 7.51 (m, 2H), 5.90 (s, 2H.)

^{13}C NMR (100 MHz, $CDCl_3$) δ 181.9, 135.2, 133.5, 129.4, 128.4, 81.4

3.8.21 Dodecan-2-one (10u)[16]

Reaction Condition: It was synthesized following the general procedure Method A and Method B. The reaction was carried out with 0.168 g, 1.0 mmol, 1-dodecene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 3:17 as eluent, to afford 10u as a light yellow liquid.



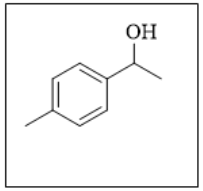
Yield: 0.103 g, 56% (**Method A**), 0.097 g, 53% (**Method B).**

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62- 2.57 (m, 4H), 2.42 (t, *J* = 7.4 Hz, 2H), 2.2 (s, 3H), 1.28 – 1.25 (m, 29H.), 0.87 (t, *J* = 6.0 Hz, 12H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 212.2, 209.9, 43.1, 40.2, 39.2, 37.9, 36.8, 32.8, 31.9, 31.8, 31.0, 30.2, 29.8, 29.7, 29.4, 29.3, 29.2.25.8, 24.1, 23.9, 22.8, 22.7, 14.2.

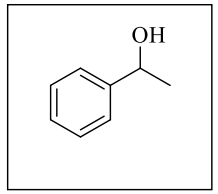
3.9 Characterization data for benzylalcohols

3.9.1 1-(4-methylphenyl)ethan-1-ol. (11a)[17]



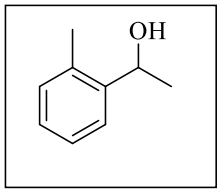
Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.118 g, 1.0 mmol, 4-methylstyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11a** as a colorless liquid.
Yield: 0.125 g, 92% (**Method C**), 0.123 g 90% (**Method D**).
.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8 Hz, 2H), 7.17 (d, *J* = 7.9 Hz, 2H), 4.87 (q, *J* = 6.4 Hz, 1H), 2.36 (s, 3H), 2.22 (d, *J* = 9.4 Hz, 1H) 1.48 (d, *J* = 6.5 Hz, 3H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 143.0, 137.2, 129.2, 125.5, 70.3, 25.1, 21.2.

3.9.2 1-phenylethanol (11b)[17]



Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.104 g, 1.0 mmol, Acetophenone, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11b** as a colorless liquid.
Yield: 0.111g, 91% (**Method C**), 0.109 g 90% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.33 (m, 4H), 7.30 – 7.27 (m, 1H), 4.88 (q, *J* = 6.4 Hz, 1H), 2.27 (s, 1H), 1.49 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) 145.9, 128.6, 127.5, 125.5, 70.4, 25.2.

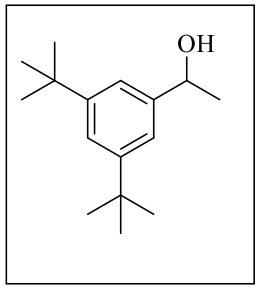
3.9.3 1-(2-methylphenyl)ethan-1-ol (11c)[18]



Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.118 g, 1.0 mmol, 2-Methylacetophenone), and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11c** as a colorless liquid.
Yield: 0.117 g, 86% (**Method C**), 0.113 g 83% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.20 - 7.13 (m, 2H), 5.12 (q, *J* = 6.3 Hz, 1H), 2.34 (s, 3H), 2.12 (s, 1H), 1.45 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) *δ* 143.9, 134.3, 130.4, 127.2, 126.4, 124.6, 66.8, 24.0, 19.0.

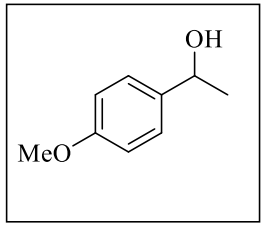
3.9.4 1-(3,5-di-tert-butylphenyl)ethan-1-ol (11d)[19]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.216 g, 1.0 mmol, 3,5-Di-tert-butylacetophenone, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11d** as a white solid.
Yield: 0.225 g, 96% (**Method C**), 0.220 g 94% (**Method D**).
M.P.: 105 - 108 ℃
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (t, *J* = 1.7 Hz, 1H), 7.43 (d, *J* = 1.6 Hz, 2H) 5.08 (q, *J* = 6.1 Hz, 1H), 2.17 (s, 1H), 1.70 (d, *J* = 6.5 Hz, 3H) 1.53 (s, 18H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 145.1, 121.8, 119.7, 71.2, 35.0, 31.6, 25.3.



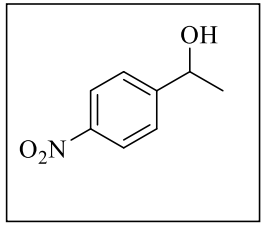
3.9.5 1-(4-methoxyphenyl)ethan-1-ol (11e)[19]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.134 g, 1.0 mmol, 4-Methoxyacetophenone, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11e** as a colorless liquid.
Yield: 0.147 g, 97% (**Method C**), 0.146 g 96% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.6 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 4.83 (q, J = 6.4 Hz, 1H), 3.80 (s, 3H), 2.10 (s, 1H), 1.46 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 138.1, 126.8, 113.9, 70.0, 55.4, 25.1.

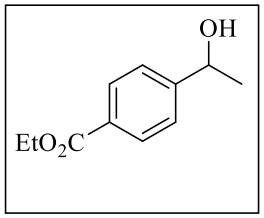


3.9.6 1-(4-nitrophenyl)ethan-1-ol (11f)[20]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.150 g, 1.0 mmol, 4-Nitrostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11f** as a yellow solid.
Yield: 0.142 g, 85% (**Method C**), 0.139 g 83% (**Method D**).
M.P.: 42 - 44 ℃
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.7 Hz, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 5.04 – 4.98 (m, 1H), 2.24 (d, *J* = 3.3 Hz, 1H), 1.50 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 147.2, 126.2, 123.9, 69.6, 25.6.

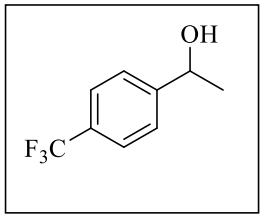


3.9.7. ethyl 4-(1-hydroxyethyl)benzoate (11g)[21]



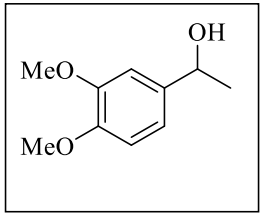
Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.162 g, 1.0 mmol, methyl 4-vinylbenzoate, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11g** (ethyl 4-(1-hydroxyethyl)benzoate was formed instead of methyl 4-(1-hydroxyethyl)benzoate from the unclear mechanism). as a colorless liquid.
Yield: 0.157 g, 81% (**Method C**), 0.155 g 80% (**Method D**).
^{1}H NMR (400 MHz $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 4.93(q, *J* = 6.4 Hz, 1H), 4.34 (q, *J* = 6.4 Hz, 2H), 2.37 (s, 1H), 1.47 (d, *J* = 6.4 Hz, 3H), 1.37 (t, *J* = 7.2, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 151.0, 129.9, 129.5, 125.3, 70.0, 61.1, 25.4, 14.4.

3.9.8 1-(4-trifluoromethylphenyl)ethan-1-ol (11h)[17]



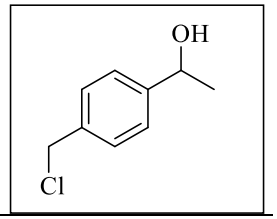
Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.172 g, 1.0 mmol, 1-(Trifluoromethyl)-4-vinyl styrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11h** colorless liquid.
Yield: 0.160g, 84% (**Method C**), 0.158 g 83% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.2 Hz, 2H), 7.45 (d, *J* = 8.1 Hz, 2H), 4.95 (q, J = 6.3 Hz, 1H), 2.11 (s, 1H), 1.49 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 129.7 (d, *J* = 32.1 Hz), 125.8, 125.6 (q, *J* = 3.9 Hz), 121.6 (d, *J* = 270.0 Hz), 70.0, 25.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4.

3.9.9 1-(3,4-dimethoxyphenyl)ethan-1-ol (11i)[22]



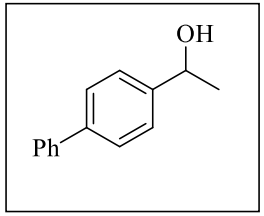
Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.164 g, 1.0 mmol, 3,4-Dimethoxystyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11i** as a colorless liquid.
Yield: 0.174 g, 95% (**Method C**), 0.168 g 92% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$): δ 6. 92 (d, *J* = 1.8 Hz, 1H), 6.87 (dd, *J* = 8.2, 1.8 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 1H), 4.84 (q, *J* = 6.4 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 2.1 (s, 1H), 1.46 (d, *J* = 6:4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 149.0, 148.3, 138.6, 117.6, 111.0, 108.6, 70.3, 56.0, 55.9, 25.2.

3.9.10 1-(4-chloromethylphenyl)ethan-1-ol (11j)[23]



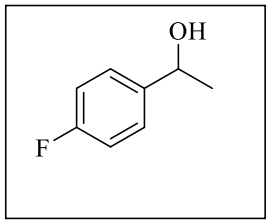
Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.115 g, 1.0 mmol, 4-vinylbenzyl chloride and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11j** colorless liquid.
Yield: 0.140 g, 82% (**Method C**), 0.137 g 80% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 - 7.30 (m, 4H), 4.87 (q, J = 6.5 Hz, 1H), 4.58 (s, 2H), 2.33 (s, 1H), 1.46 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 136.8, 128.9, 125.9, 70.0, 46.1, 25.3.

3.9.11 1-([1,1'-biphenyl]-4-yl)ethan-1-ol (11k)[23]



Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.180 g, 1.0 mmol, 4-vinylbiphenyl, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11k** as a white solid.
Yield: 0.161 g, 81% (**Method C**), 0.159 g 80% (**Method D**).
M.P.: 96 - 98 °C
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.1 Hz, 4H), 7.46 (t, *J* = 8.6 Hz, 4H), 7.36 (t, *J* = 7.3 Hz, 1H), 4.99 – 4.94 (m, 1H), 1.86 (d, *J* = 3.4 Hz, 1H), 1.5 (d, *J* = 6.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 144.9, 141.0, 140.6, 128.9, 127.4, 127.2, 126.0, 70.3 25.3.

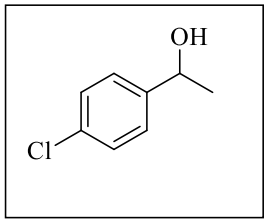
3.9.12 1-(4-fluorophenyl)ethan-1-ol (11l)[17]



Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.122 g, 1.0 mmol, 4-Fluorostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11l** as a colorless liquid.
Yield: 0.123 g, 88% (**Method C**), 0.119 g 85% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 - 7.31 (m, 2H), 7.05 – 7.00 (m, 2H), 4.88 (q, *J* = 6.3 Hz, 1H), 1.99 (s, 1H), 1.47 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$): *δ* 162.2 (d, *J* = 243.6 Hz), 141.6 (d, *J* = 3.0 Hz), 127.1 (d, *J* = 8.0 Hz), 115.5 (d, *J* = 21.2 Hz), 69.8, 25.4.
^{19}F NMR (376 MHz, $CDCl_3$) δ -115.4.

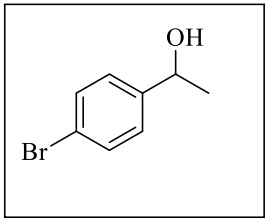
3.9.13 1-(4-chlorophenyl)ethan-1-ol (11m)[23]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.138 g, 1.0 mmol, 4-chlorostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11m**as a colorless liquid.
Yield: 0.153 g, 96% (**Method C**), 0.144 g 92% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 – 7.22 (m, 4H), 4.81 (q, *J* = 6.4, 1H), 2.76 (s, 1H), 1.41 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100MHz, $CDCl_3$): *δ* 144.3, 133.0, 128.6, 126.9, 69.7, 25.3.



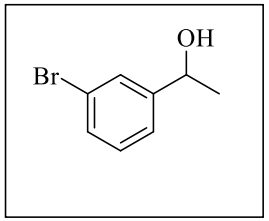
3.9.14 1-(4-bromophenyl)ethan-1-ol (11n)[20]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.183 g, 1.0 mmol, 4-bromostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11n** as a colorless liquid.
Yield: 0.166 g, 83% (**Method C**), 0.165 g 82% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 4.82 (q, *J* = 6.4, 1H), 2.29 (s, 1H), 1.44 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100MHz, $CDCl_3$) δ 144.8, 131.6, 127.2, 121.2, 69.8, 25.3.

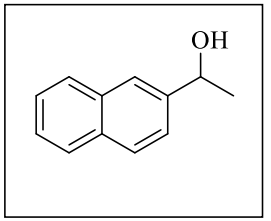


3.9.15 1-(3-bromophenyl)ethan-1-ol (11o)[20]

Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.183 g, 1.0 mmol, 3-bromostyrene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:19 as eluent, to afford **11o** as a colorless liquid.
Yield: 0.160 g, 80% (**Method C**), 0.159 g 79% (**Method D**).
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (s, 1H), 7.39 (d, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 8.0, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 4.86 (q, *J* = 6.4 Hz, 1H), 2.17 (s, 1H), 1.46 (d, *J* = 6.5 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$**)**: *δ* 148.2, 130.6, 130.2, 128.7, 124.1, 122.7, 69.7, 25.4.



3.9.16 1-(naphthalen-2-yl)ethan-1-ol (11p)[20]



Reaction Condition: It was synthesized following the general procedure **Method C** and **Method D**. The reaction was carried out with 0.155 g, 1.0 mmol, 2-vinylnaphthalene, and the crude product was purified by column chromatography on a silica gel column using EtOAc-Petroleum ether = 1:99 as eluent, to afford **11p** as a white solid.
Yield: 0.129 g, 75% (**Method C**), 0.124 g 72% (**Method D**).
M.P.: 63 - 65 °C
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 -7.79 (m, 4H), 7.51-7.46 (m, 3H), 5.05 (q, *J* = 6.0 Hz, 1H,), 2.25 (s, 1H), 1.58 (d, *J* = 7.2 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) 143.3, 133.3, 133.0, 128.4, 128.0, 127.8, 126.2, 125.9, 124.0, 123.9, 70.6, 25.2.

3.10 References for NMR data:

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3.11. Computational studies

ORCA 5.0.4 program[24] with B3LYP functional[25] performed all DFT calculations. Initial geometry of **8** was taken from the xyz coordinates of the crystal structures and the all other interemediates (**A**, **8-OOH**, **B**, **8-OH**, **8-H**, **C**, **D**, **E** and **E'**) were modelled from the cartesian coordinates of the optimized geometries of **8** using Avagadro[26] molecular builder and visualization program. The natures of stationary point for all the modelled geometries were confirmed by the frequency calculations at the same level. All the molecules were optimized to their energy minima geometries. The absence of negative frequencies of the corresponding minima confirmed the localizations of the stable state of molecules on the potential energy surface (PES). def2-TZVP basis set[27] was used for all atoms. TD-DFT calculations[28] for **8**, **8-OOH**, **8-OH** and **8-H** employed the B3LYP functional and the polarizable continuum model, CPCM[29] (ethanol). In TD-DFT calculations, 20 states have been included. TD-DFT derived electronic spectra were plotted using Avagadro and Magicplot 3.0.1. All the optimized geometries were represented with the help of Chemcraft[30] visualization program.

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3.12. Crystallographic details

Single crystals suitable for data collection were obtained by slow evaporation of dichloromethane-methanol (3:1 v/v) solution of **8** at 298 K. Diffraction intensities were collected on a single crystal with a SuperNova, Single source at offset/far, EosS2 diffractometer, with mirror-monochromated Mo-*K*α (λ = 0.71073 Å) radiation at 293(2) K. The 'CrysAlisPro 1.171.40.69a' program was used for data reduction. Data were corrected for Lorentz and polarization effects; empirical absorption correction using spherical harmonics and frame scaling, implemented in SCALE3 ABSPACK scaling algorithm. The structures were solved with SHELXT and refined with the SHELXL–2018/3 package[31,32], incorporated into the Olex2 1.5–alpha crystallographic collective package[33]. The position of the hydrogen atoms was calculated by assuming ideal geometries and included in the last cycle of the refinement. All non–hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least-squares minimization procedures on F^2. Each unit cell contains two symmetric units of cobalt monomer. Only one of the monomers was represented in the manuscript Scheme 2. The packing unit of the crystal is represented in **Figure S17**. The perspective view (20% probability) of **8**, and their data collection and structure refinement details are in **Figures S17** and **Table S20** respectively. CCDC-number 2346304 (**8**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

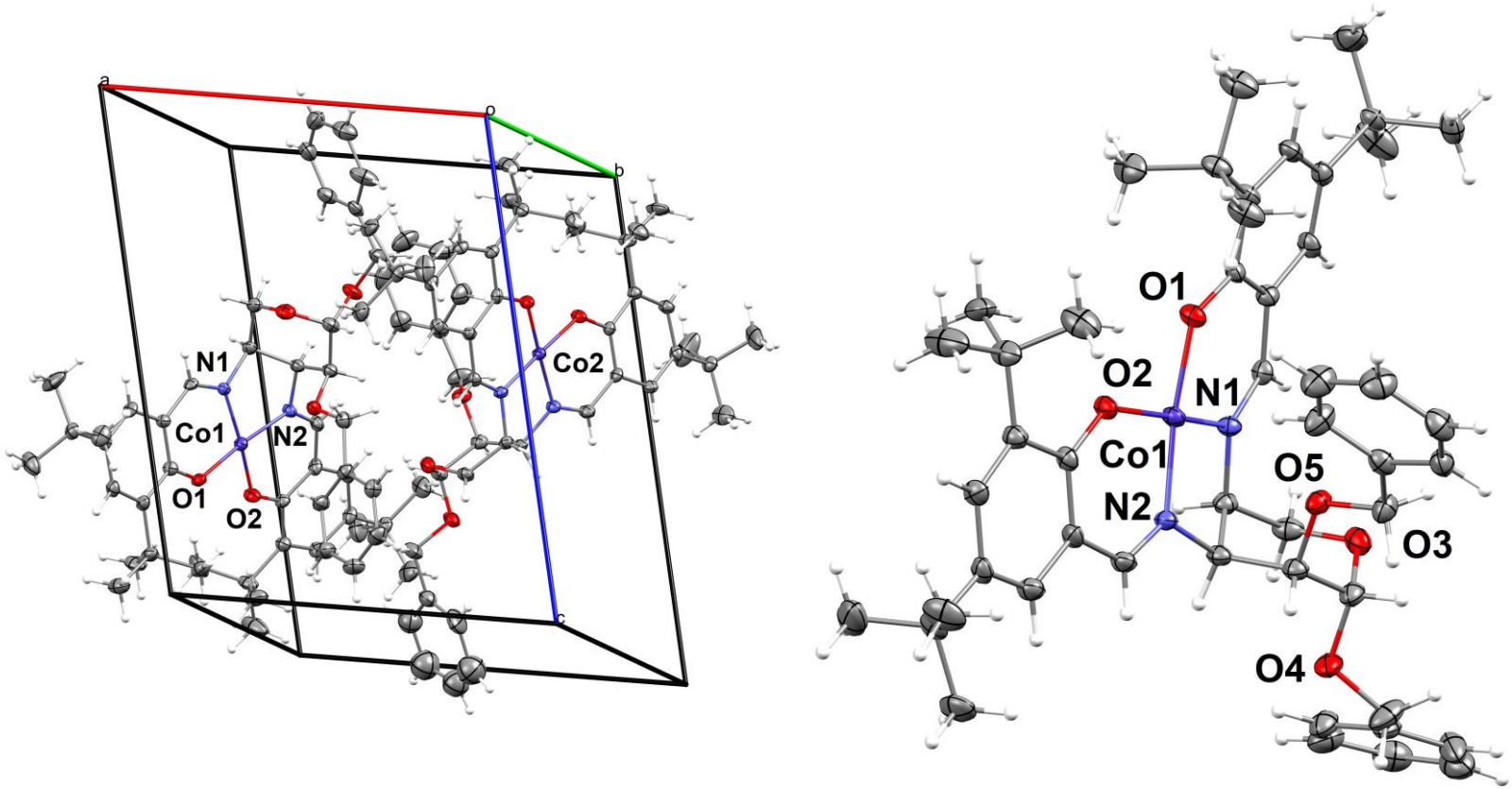

Figure S19. Perspective view (contour probability of 20%) of **8** in the packing unit and also as monomer. Only, O1, O2, O3, O4, O5 N1, N2 and Co1 atoms are labelled. H atoms are omitted for clarity.

Table S20.. Data collection and structure refinement parameters for **8.**

	8
Empirical formula	$C_{98}H_{123}Co_2N_4O_{10}$
Formula weight	1634.86
Crystal color, habit	Red, block
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P1
Crystal size (mm^3)	0.20 x 0.15 x 0.12
a (Å)	11.4614(6)
b (Å)	12.9693(5)
c (Å)	15.9143(6)
α (º)	101.429(3)
β (º)	106.498(4)
γ (º)	92.924(4)
V ($Å^3$)	2208.70(17)
Z	1
D_{calc} ($g\ cm^{-3}$)	1.229
μ (mm^{-1})	0.436
no. reflections collected	17333

no. unique reflection	11148 (R_{int} = 0.0232)
no. reflections used [$I > 2\sigma(I)$]	9626
R_1[a], wR_2[b] [$I > 2\sigma(I)$]	R_1 = 0.0395[a] wR_2= 0.0893[b]
R_1[a], wR_2[b] (All data)	R_1 = 0.0499[a] wR_2= 0.0953[b]
Goodness-of-fit on F^2	1.033

([a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w\,(|F_o|^2 - |F_c|^2)^2]/\Sigma[w(|F_o|^2)^2]\}^{1/2}$)

References for crystallographic details

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4. NMR spectra

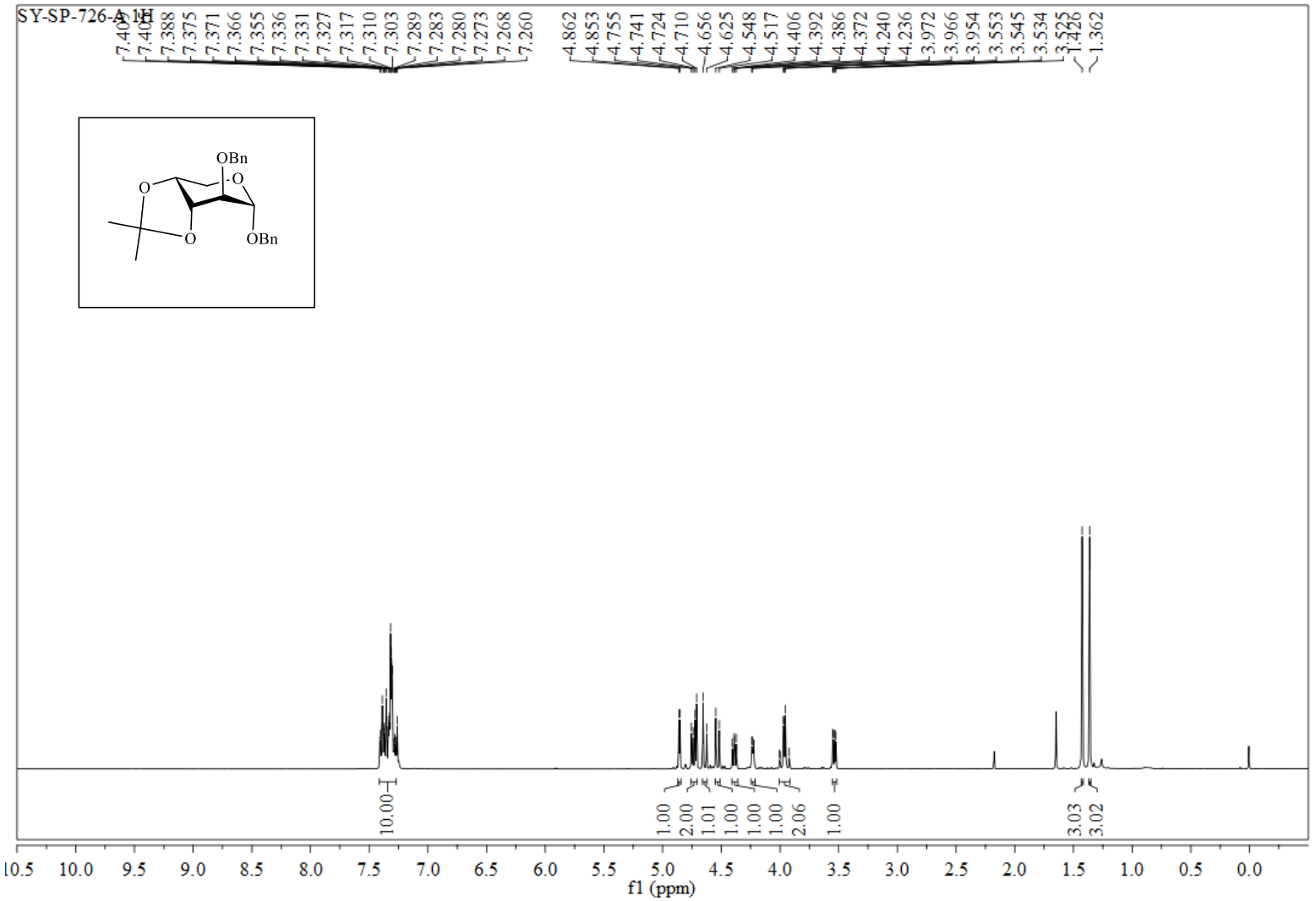

Figure S20. ^{1}H NMR (400 Mz, $CDCl_3$) of **2a**.

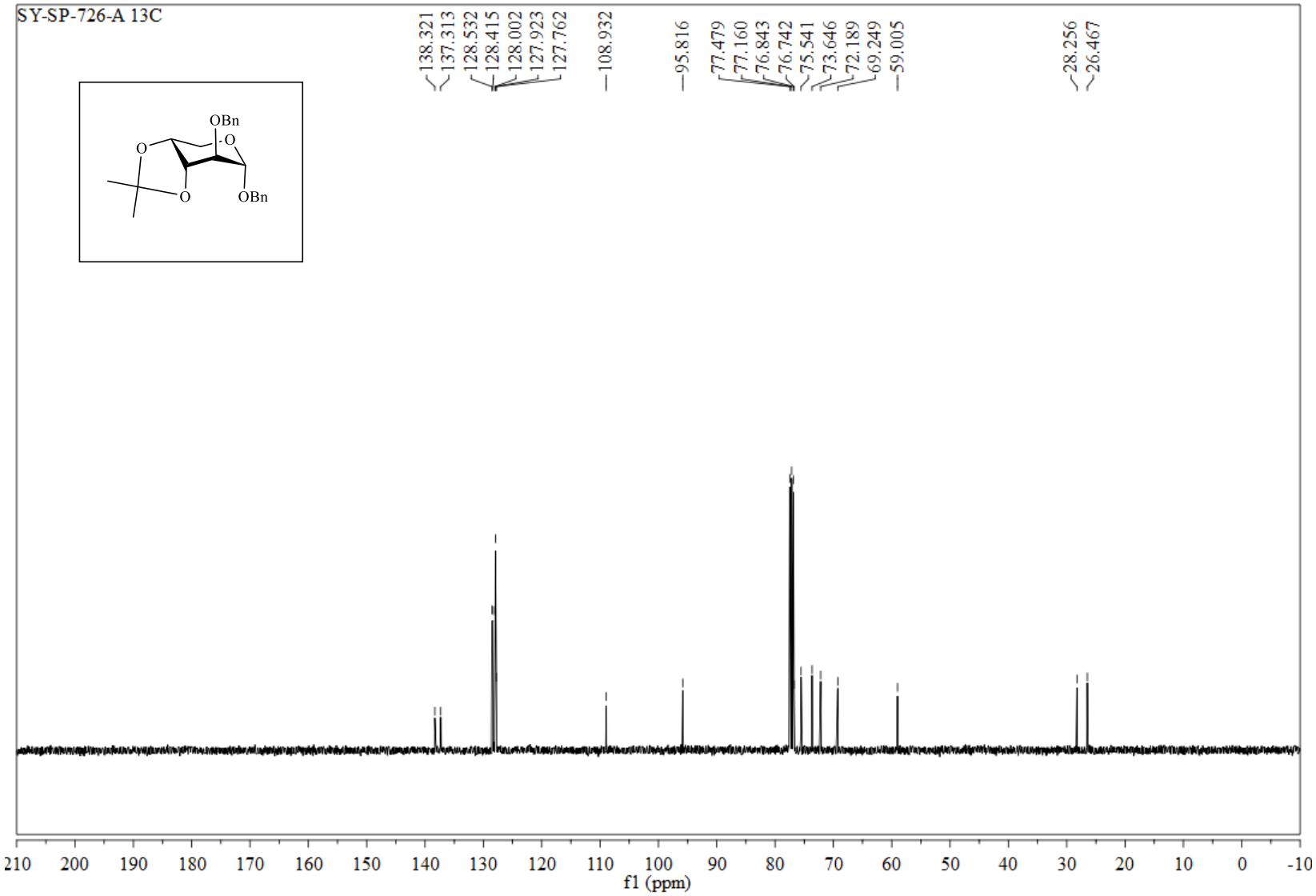

Figure S21. ^{13}C NMR (100 Mz, $CDCl_3$) of **2a**.

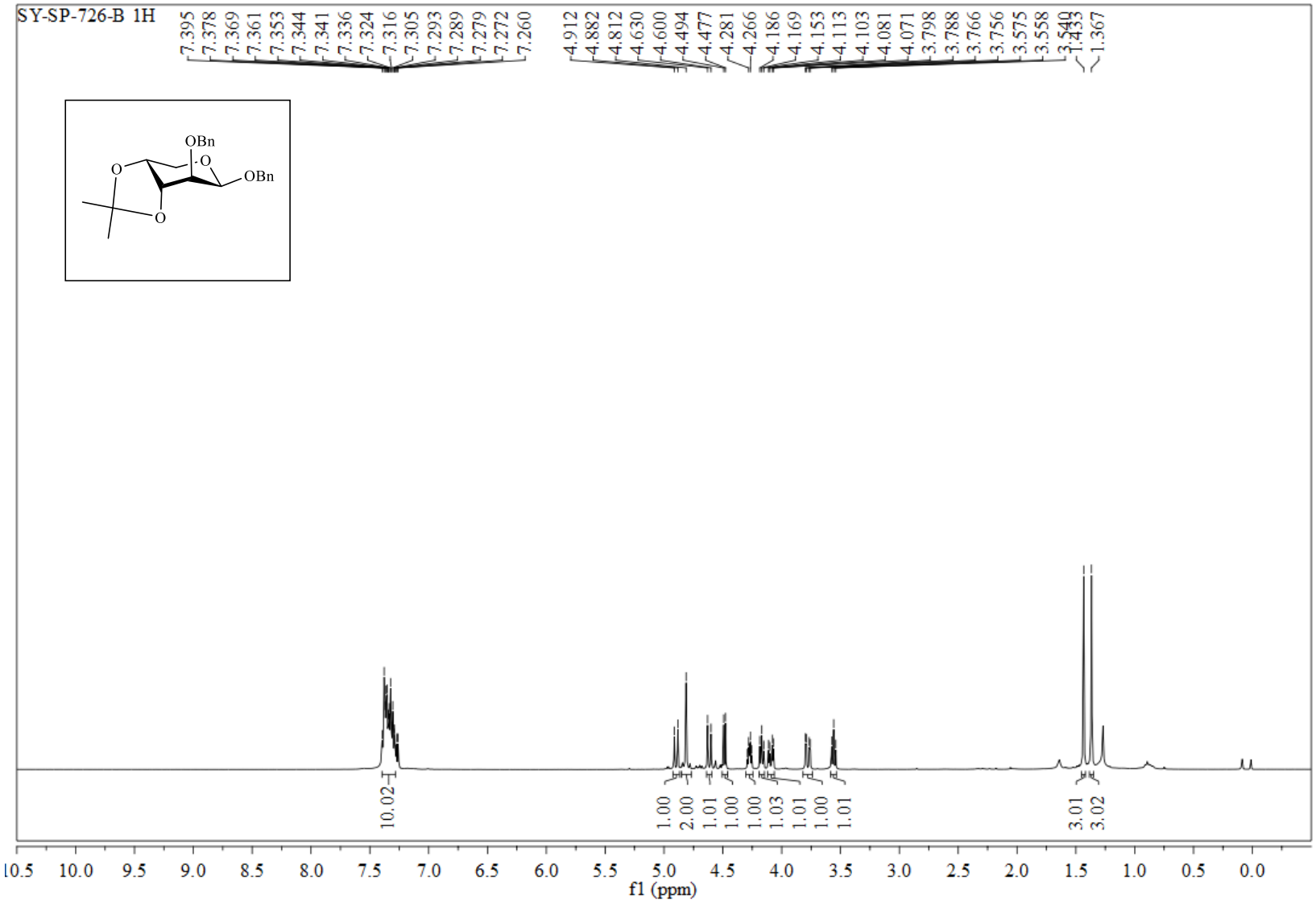

Figure S22. ^{1}H NMR (400 Mz, $CDCl_3$) of **2b**.

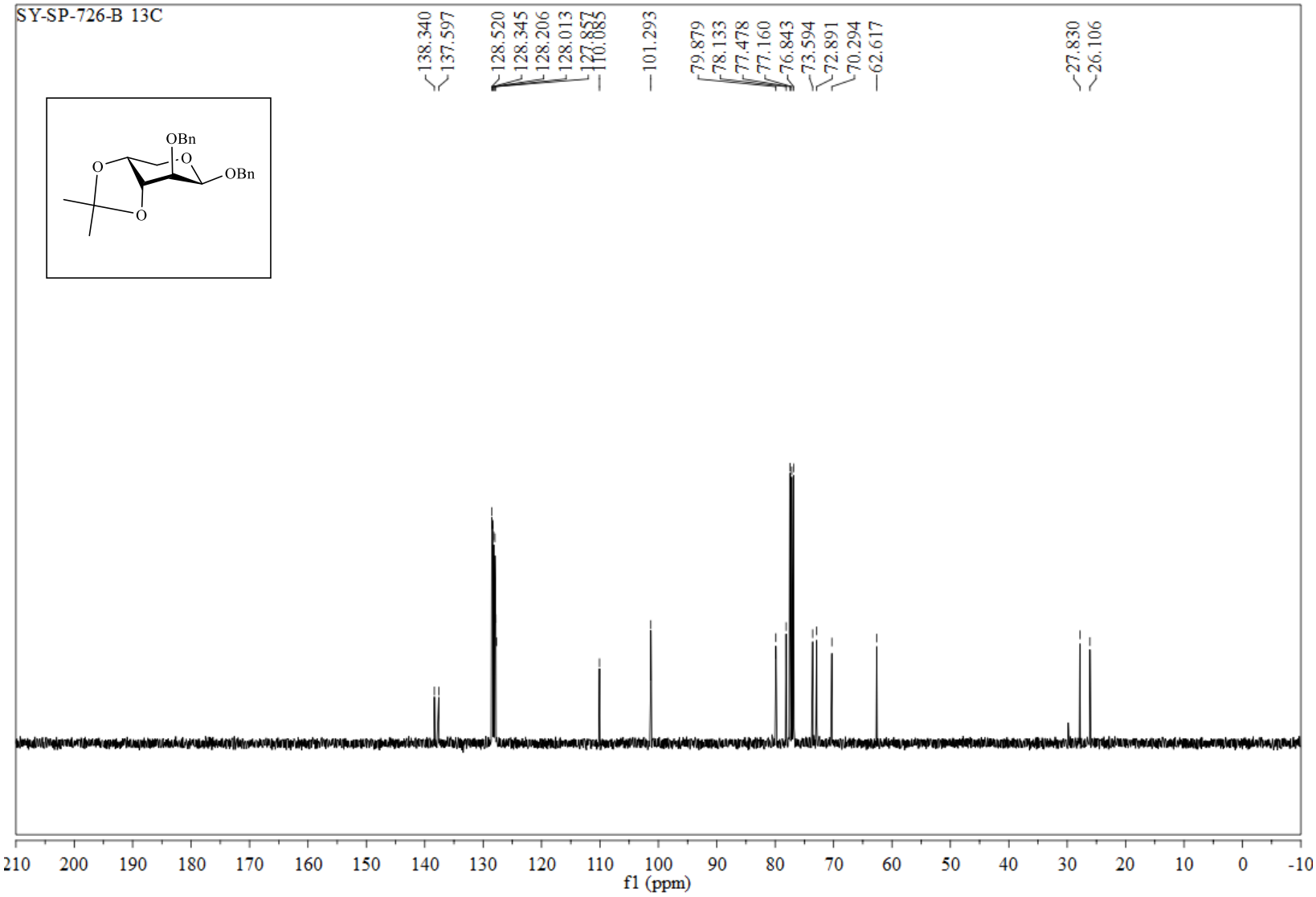

Figure S23. ^{13}C NMR (100 Mz, $CDCl_3$) of **2b**.

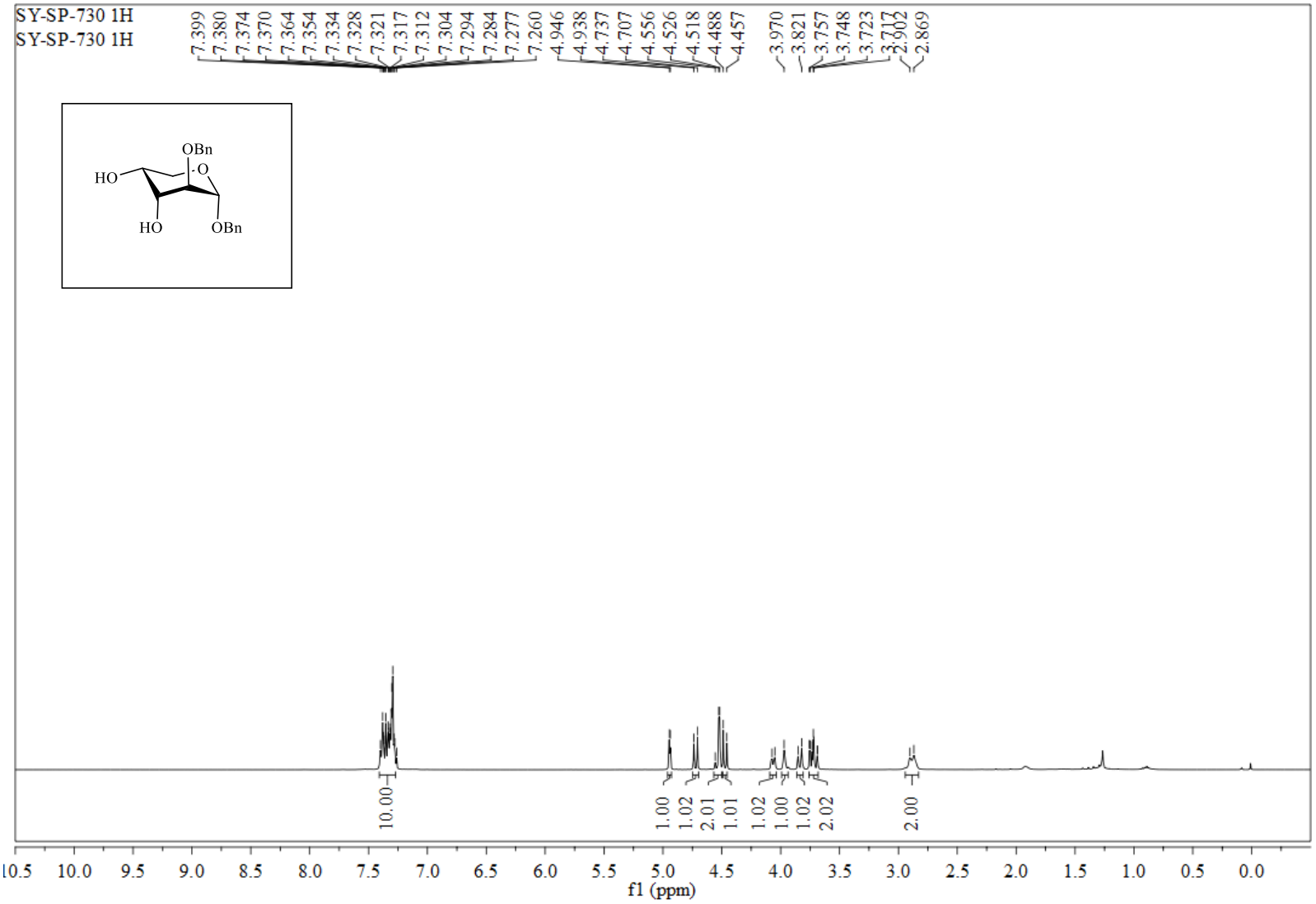

Figure S24. ^{1}H NMR (400 Mz, $CDCl_3$) of **3**.

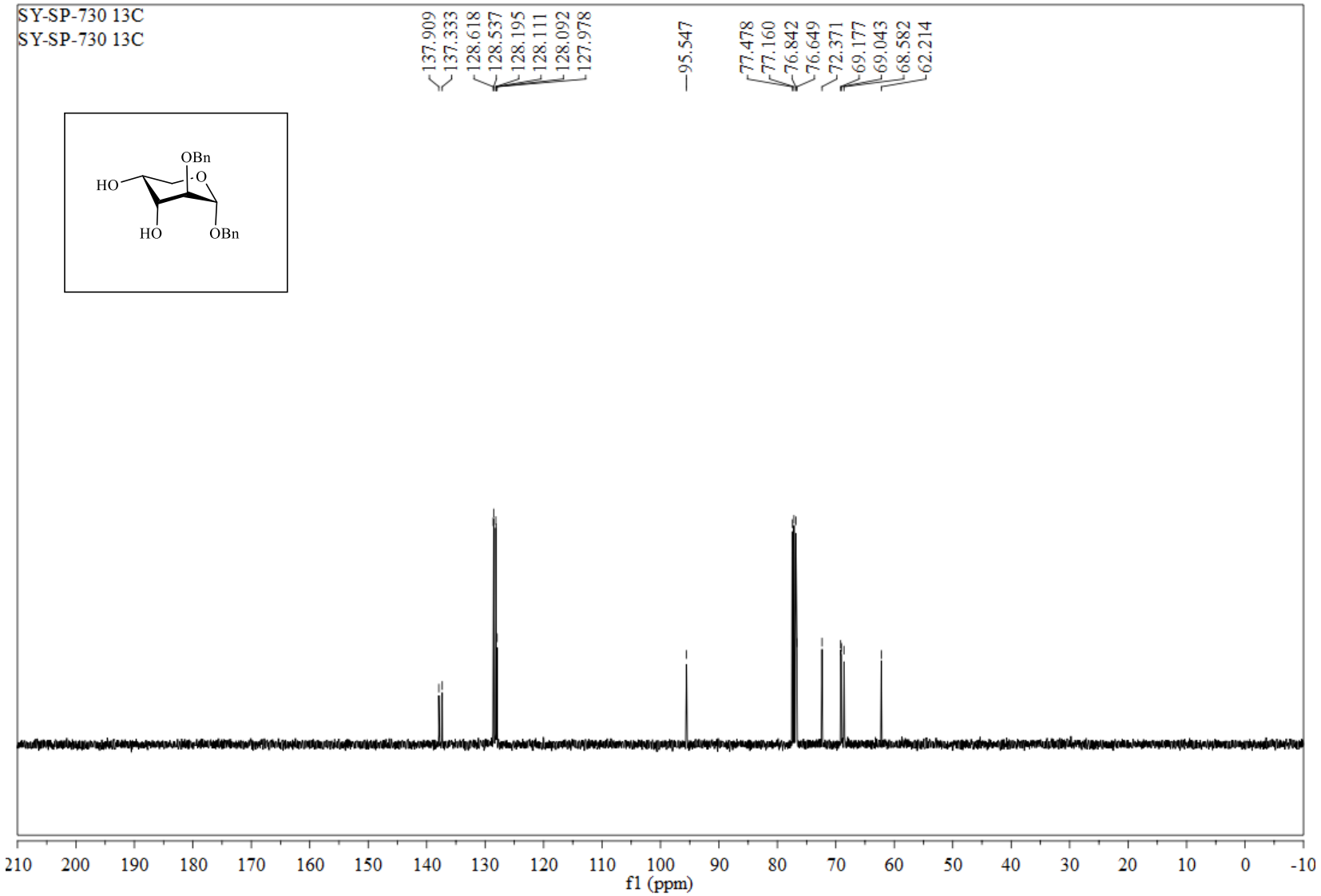

Figure S25. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **3**.

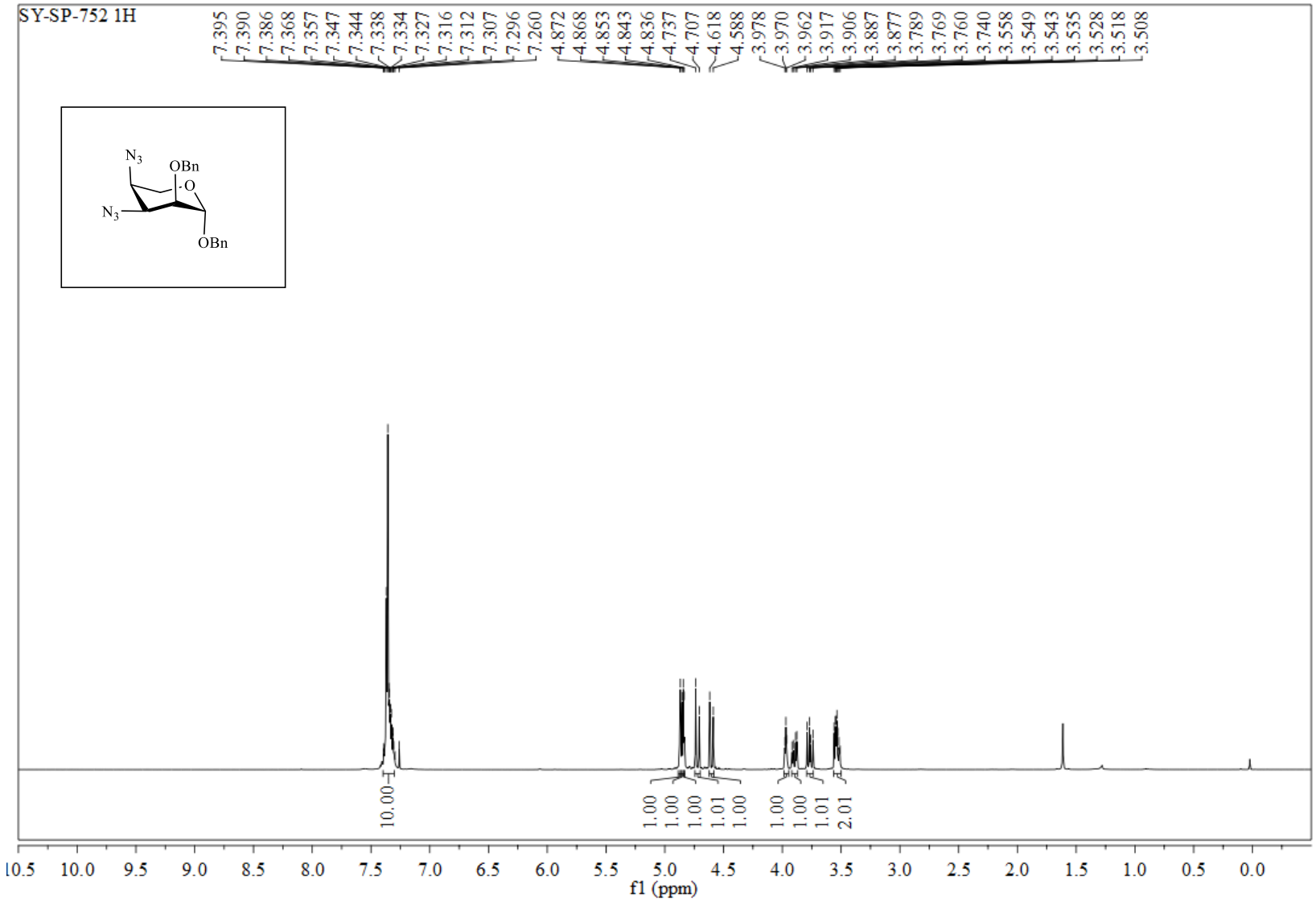

Figure S26. ^{1}H NMR (400 Mz, $CDCl_3$) of **4**.

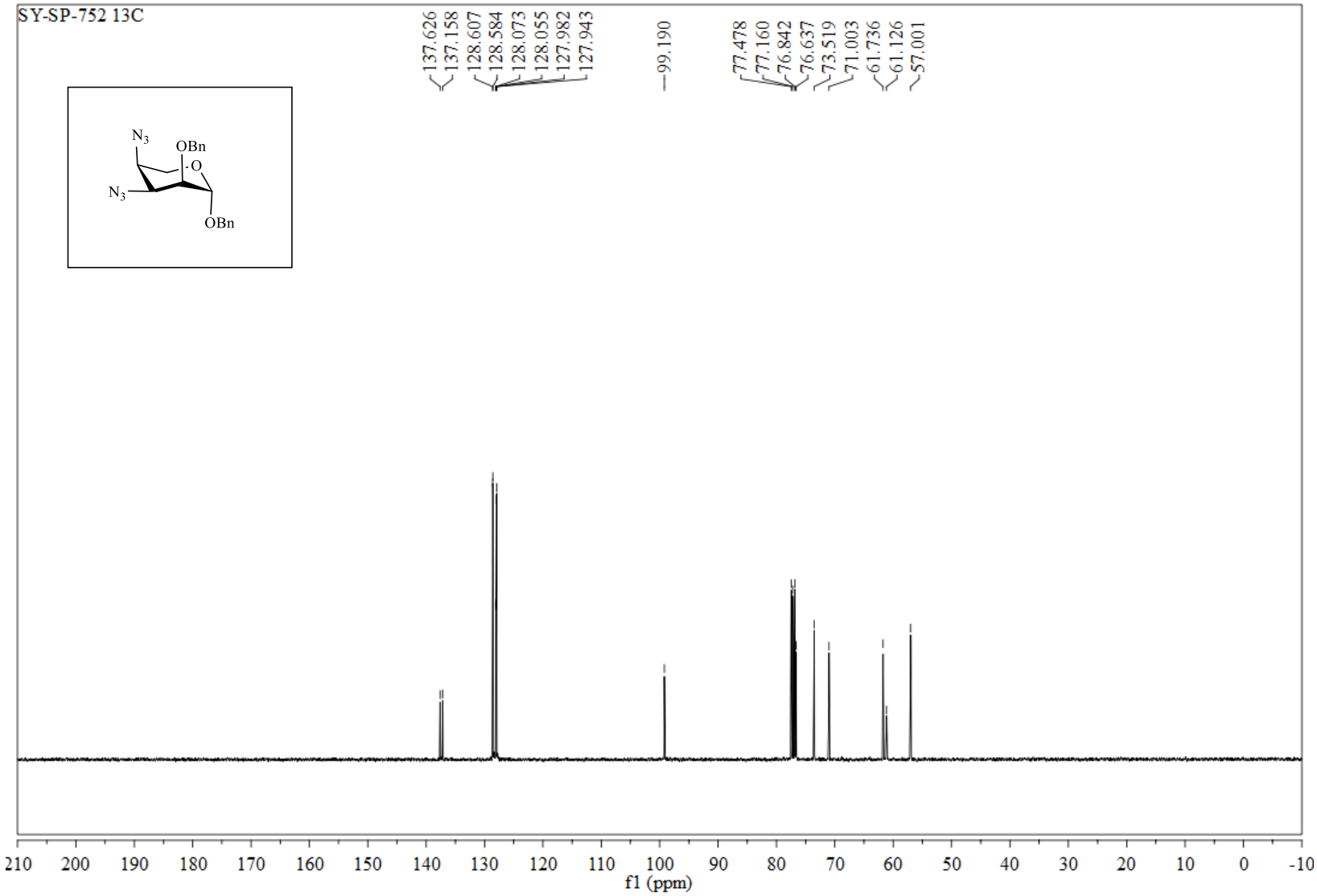

Figure S27. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **4**.

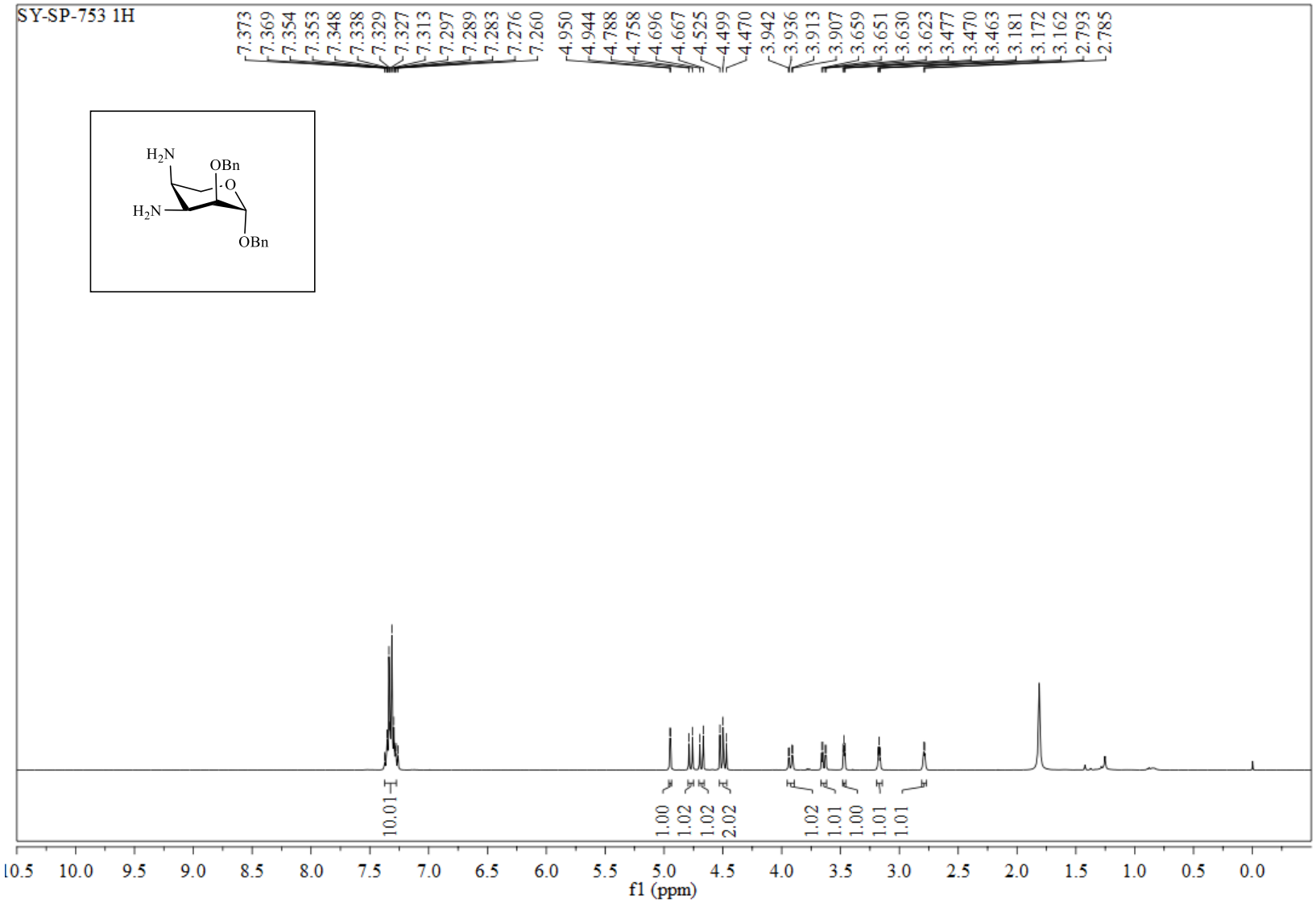

Figure S28. ^{1}H NMR (400 Mz, $CDCl_3$) of **5**.

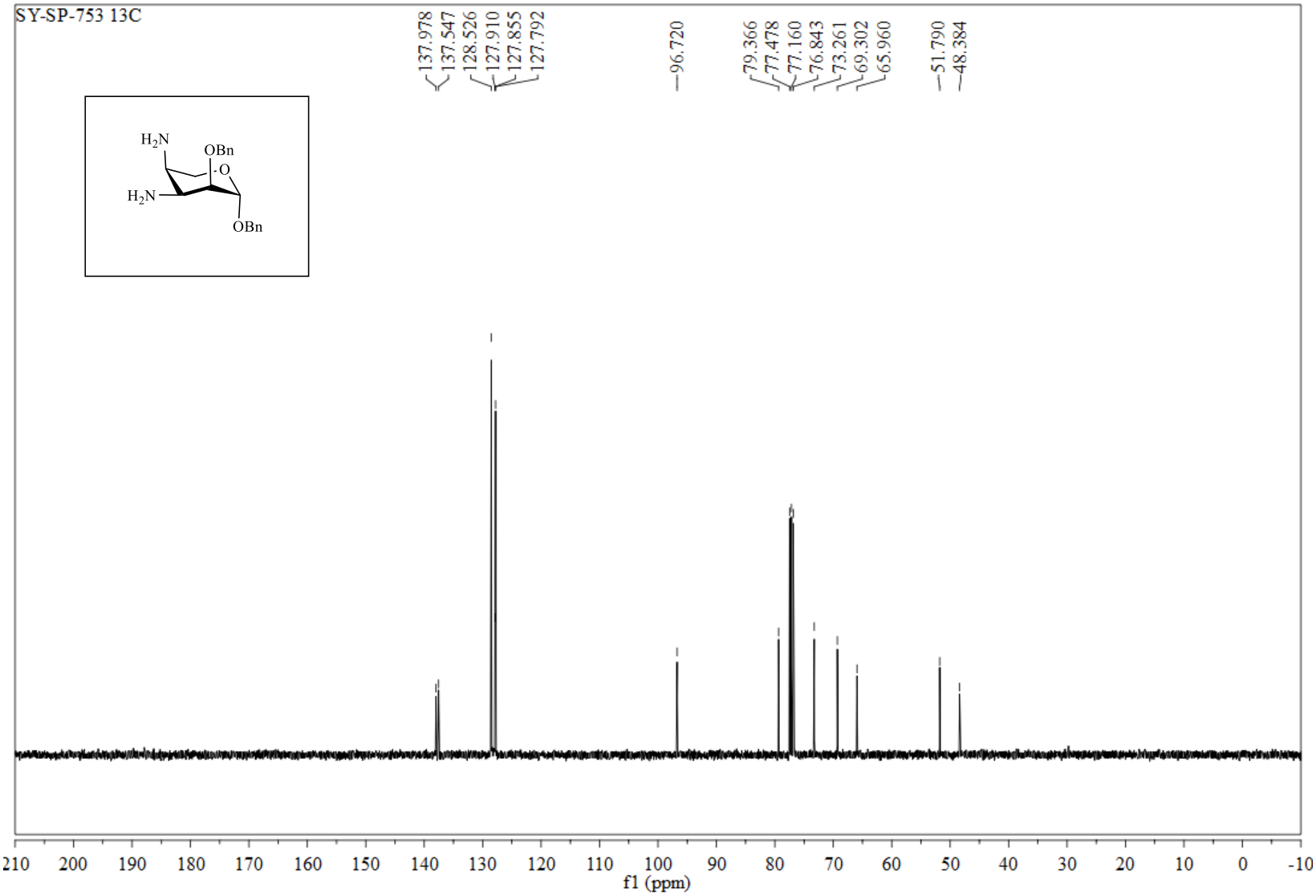

Figure S29. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **5**.

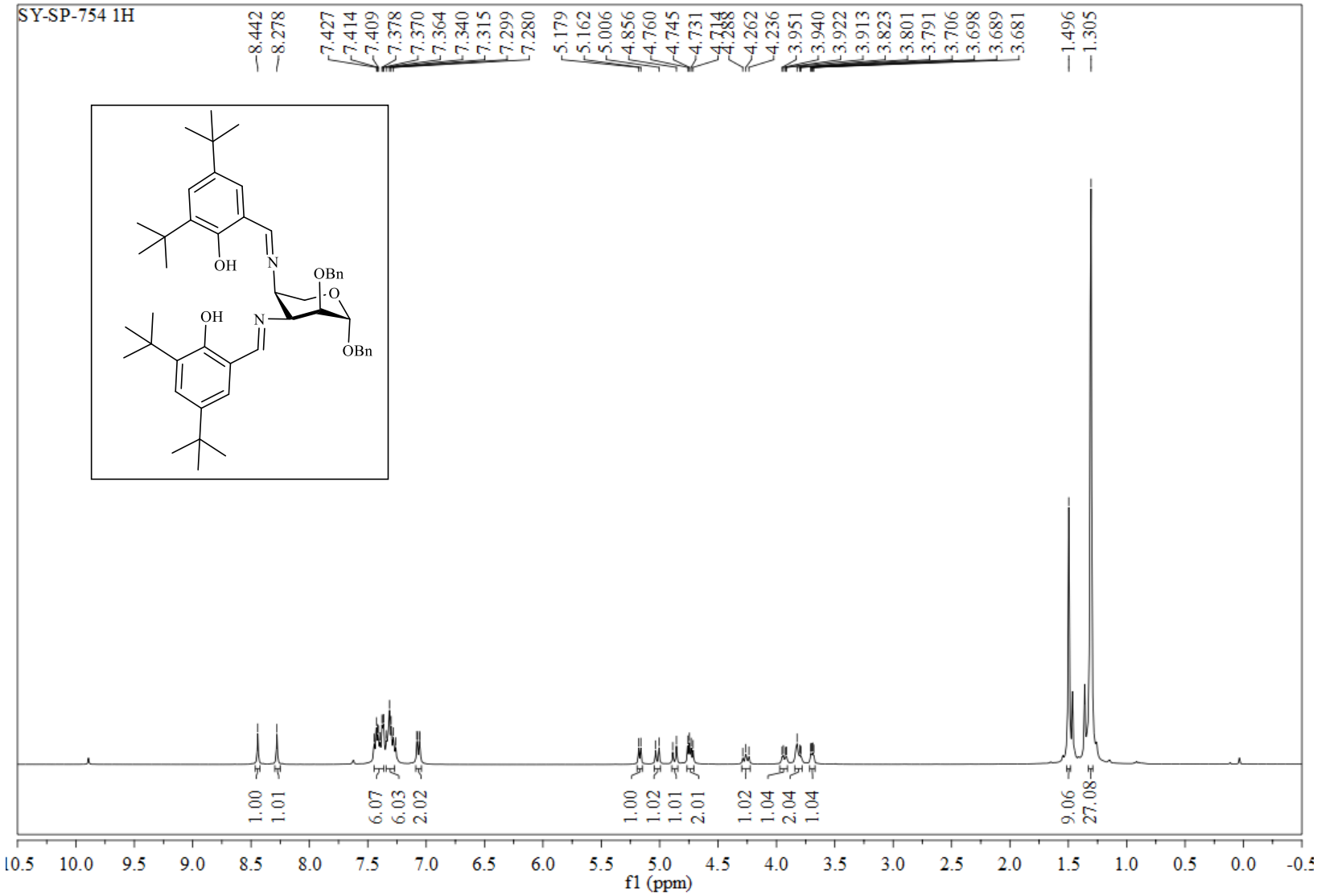

Figure S30. ^{1}H NMR (400 Mz, $CDCl_3$) of **7**.

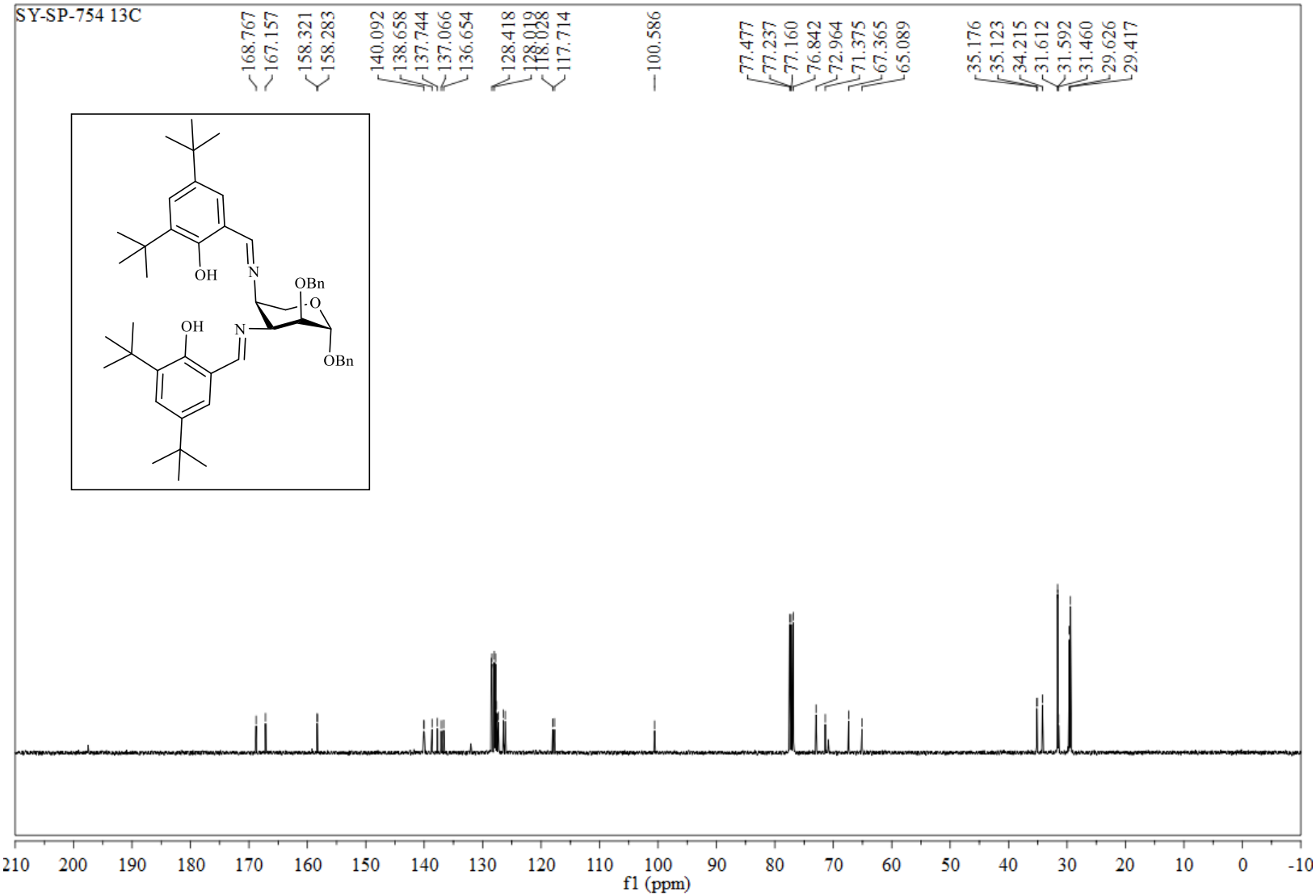

Figure S31. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **7**.

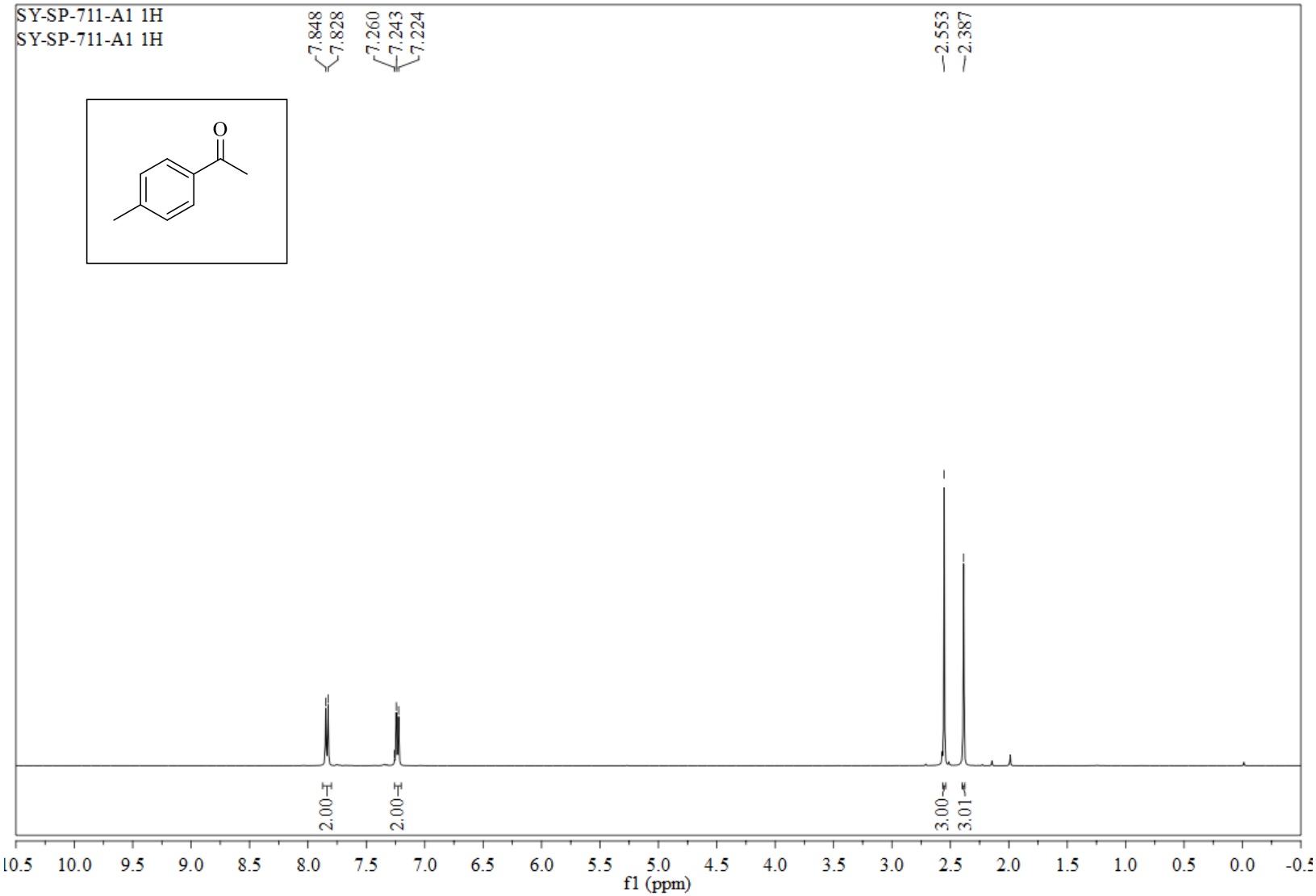

Figure S32. ^{1}H NMR (400 Mz, $CDCl_3$) of **10a.**

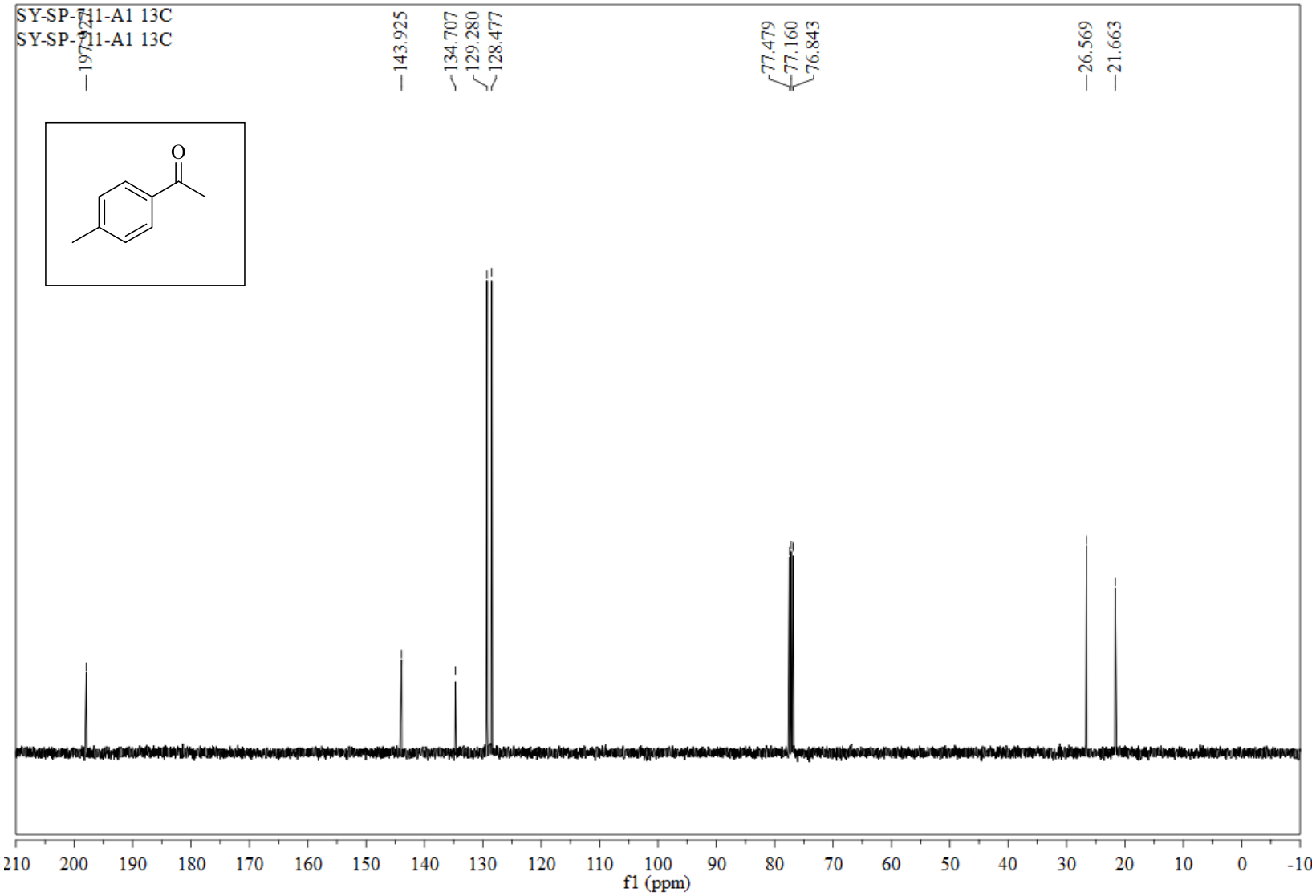

Figure S33. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10a**.

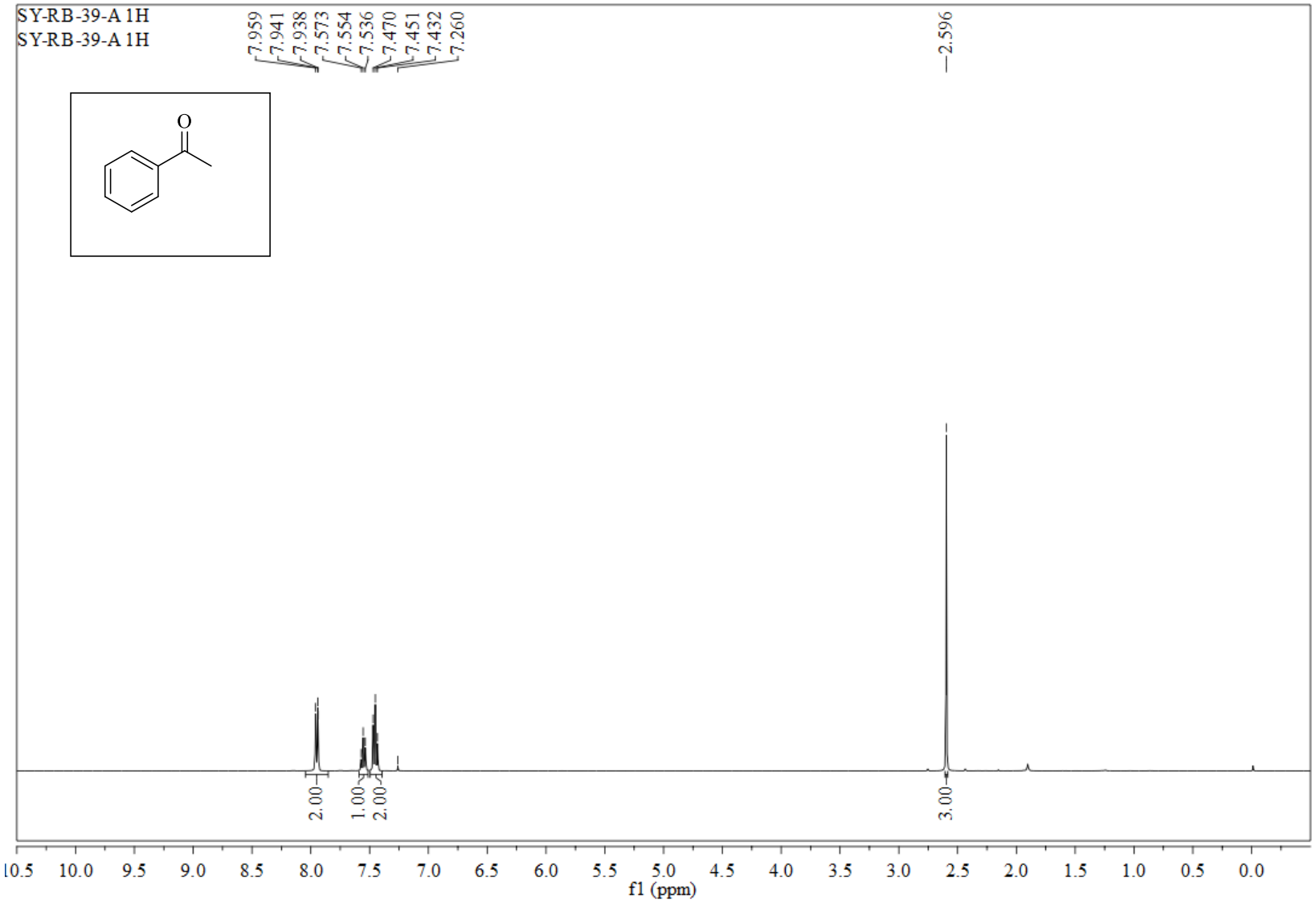

Figure S34. ^{1}H NMR (400 Mz, $CDCl_3$) of **10b**

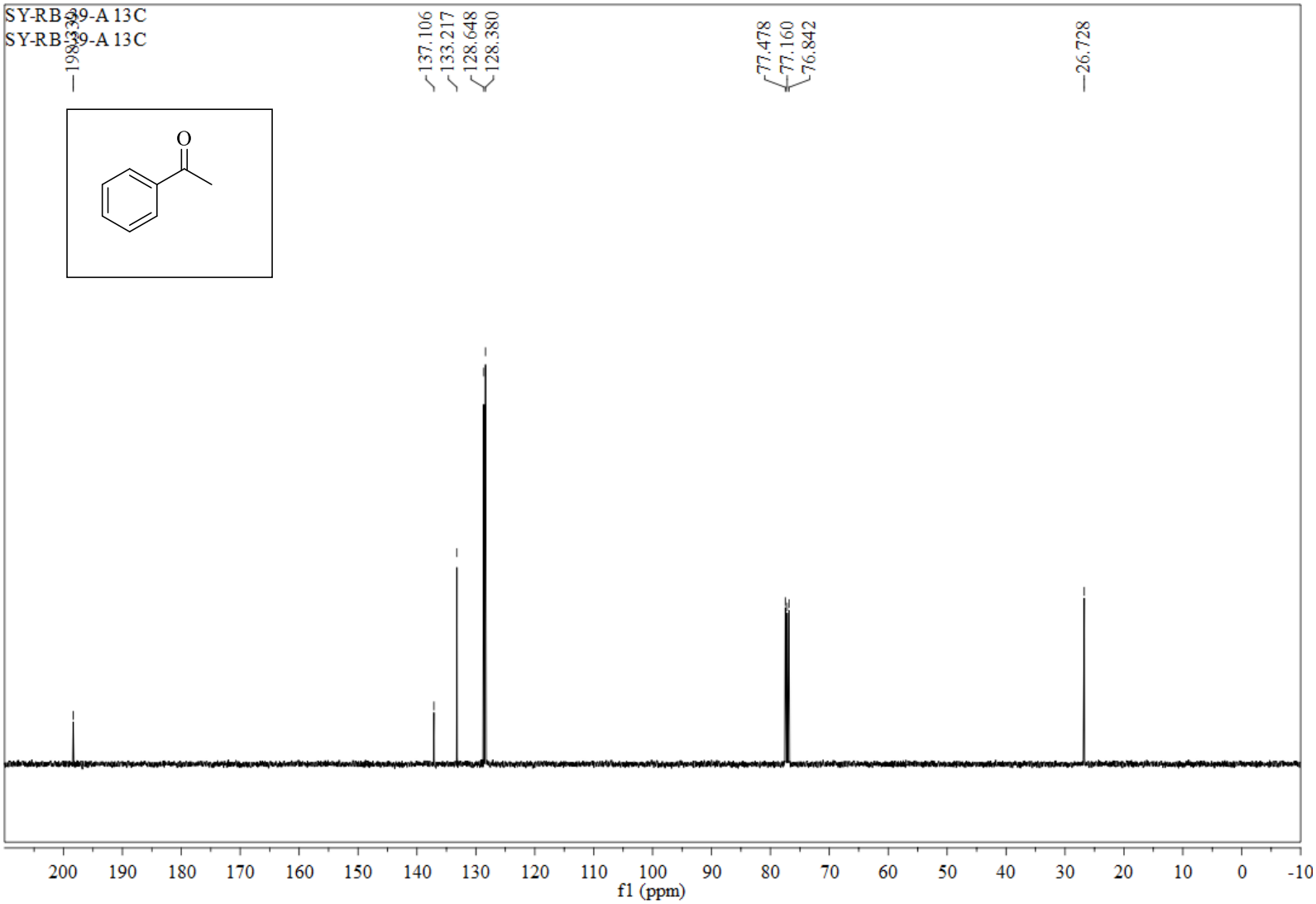

Figure S35. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10b**.

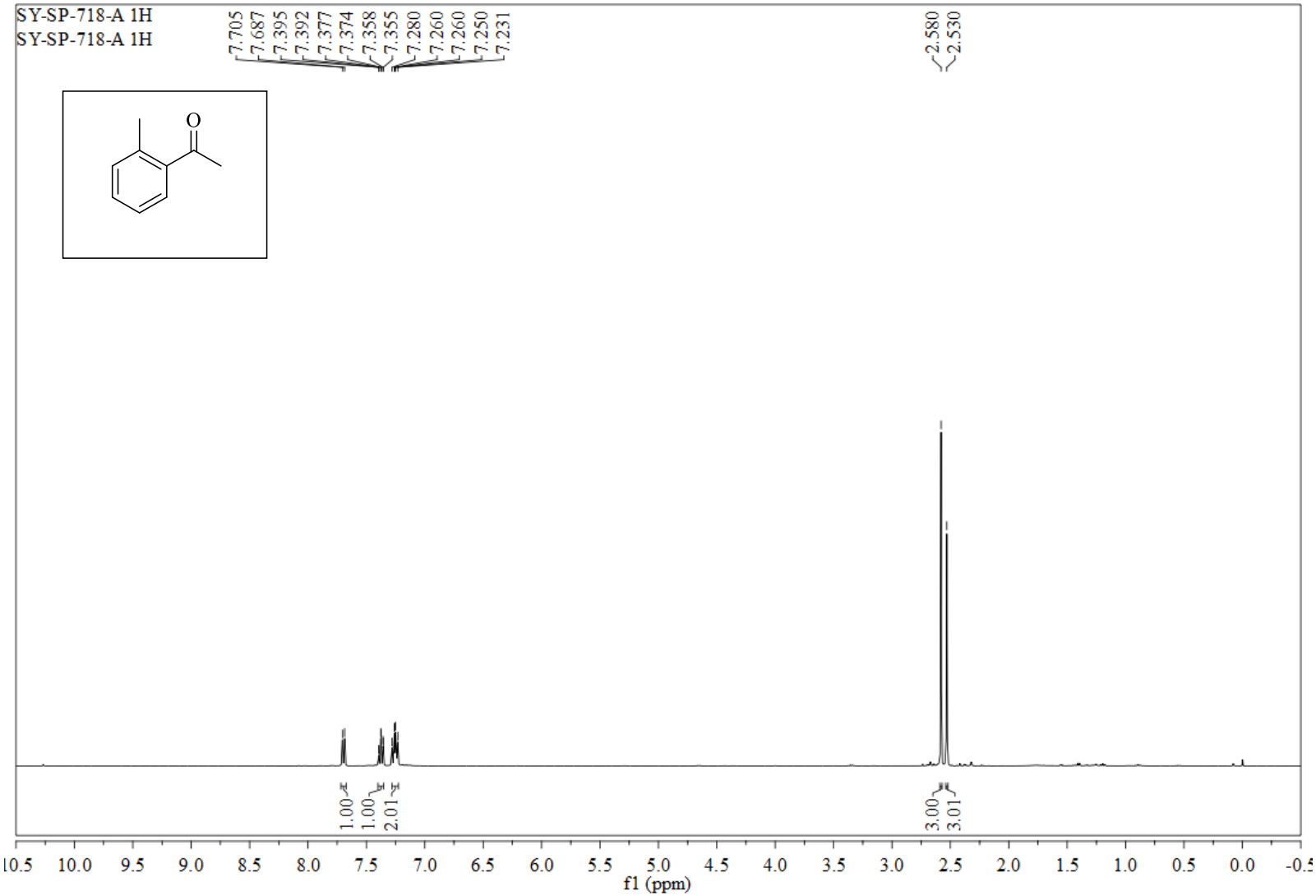

Figure S36. ^{1}H NMR (400 Mz, $CDCl_3$) of **10c**

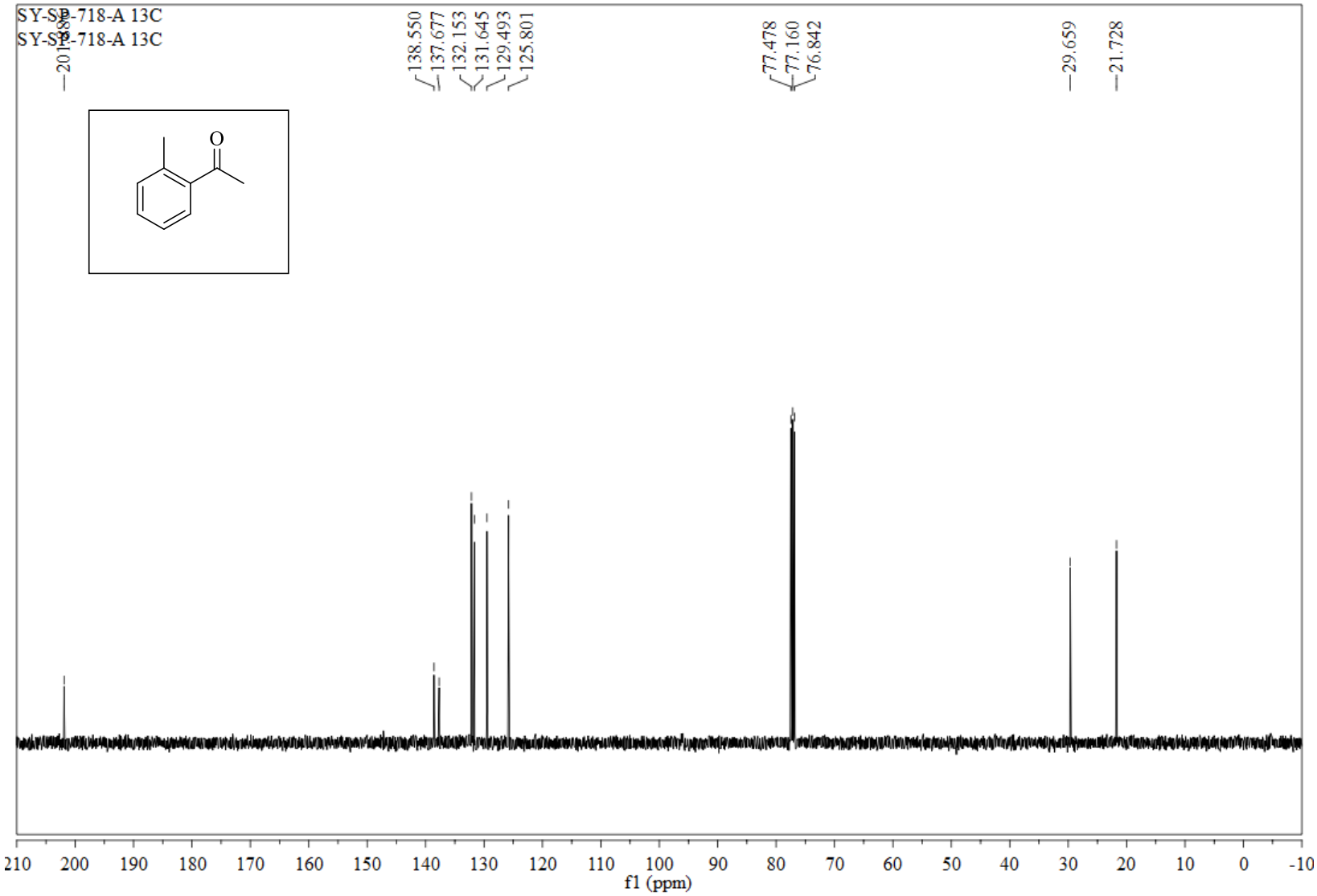

Figure S37. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10c**.

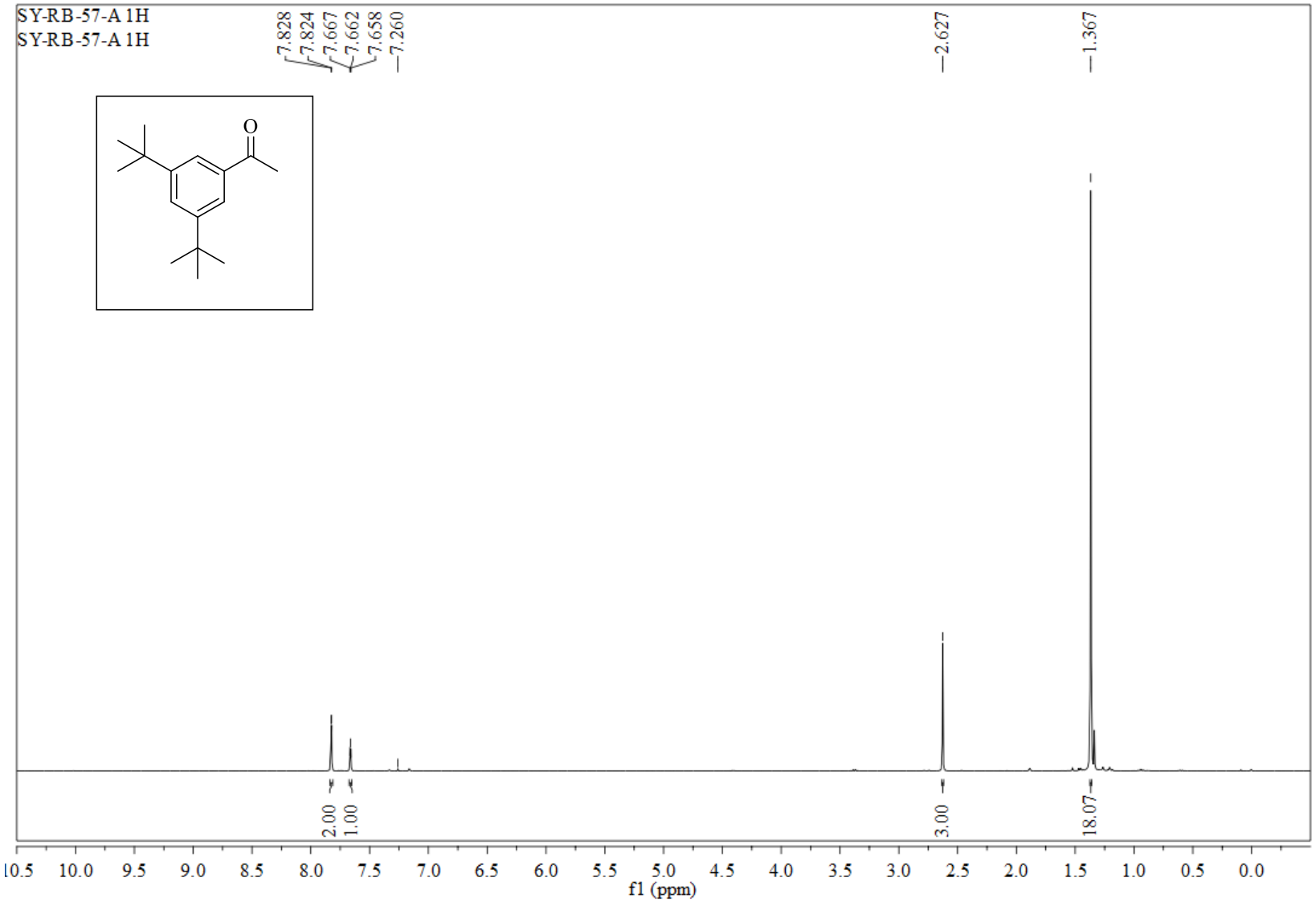

Figure S38. ^{1}H NMR (400 Mz, $CDCl_3$) of **10d**

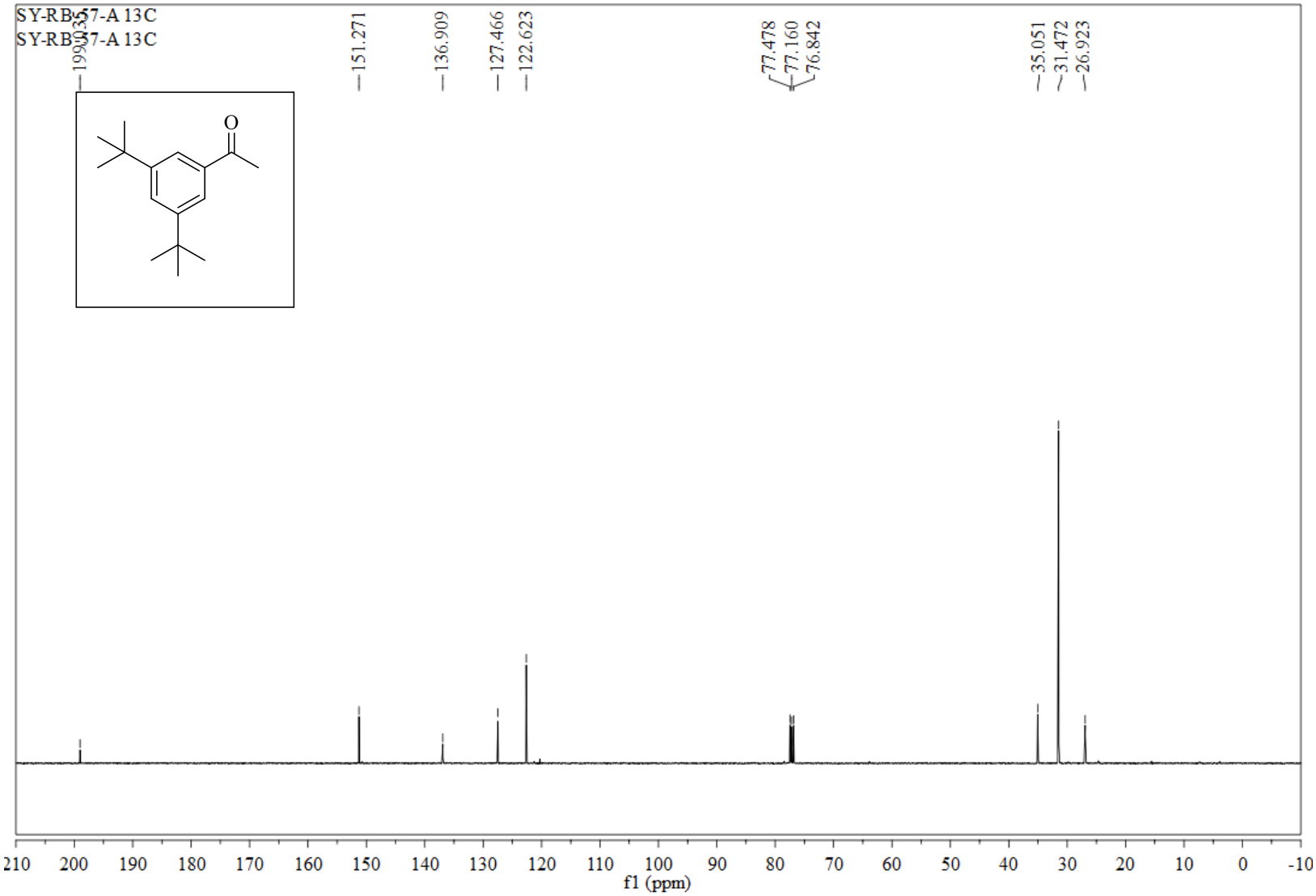

Figure S39. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10d**.

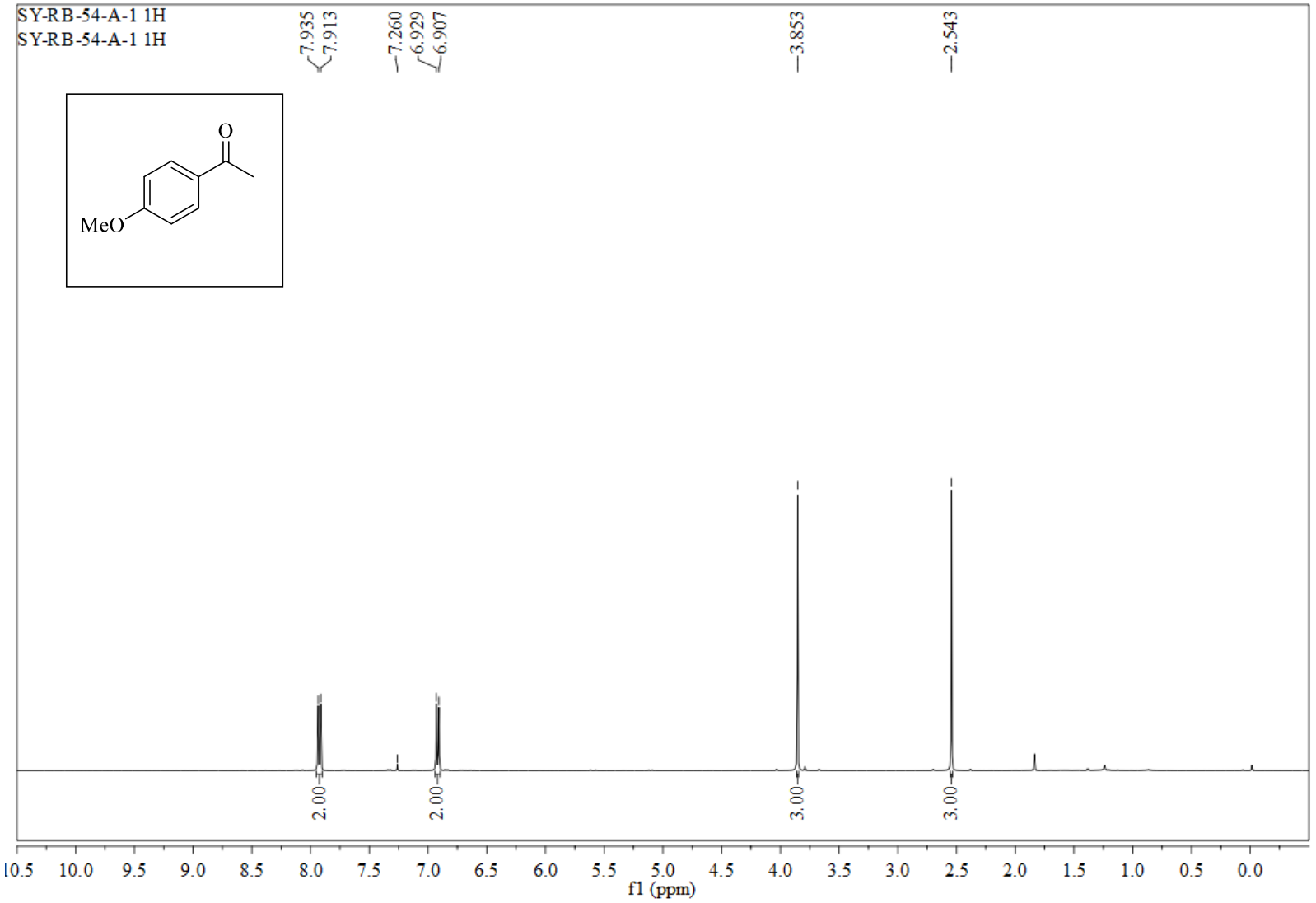

Figure S40. ^{1}H NMR (400 Mz, $CDCl_3$) of **10e**

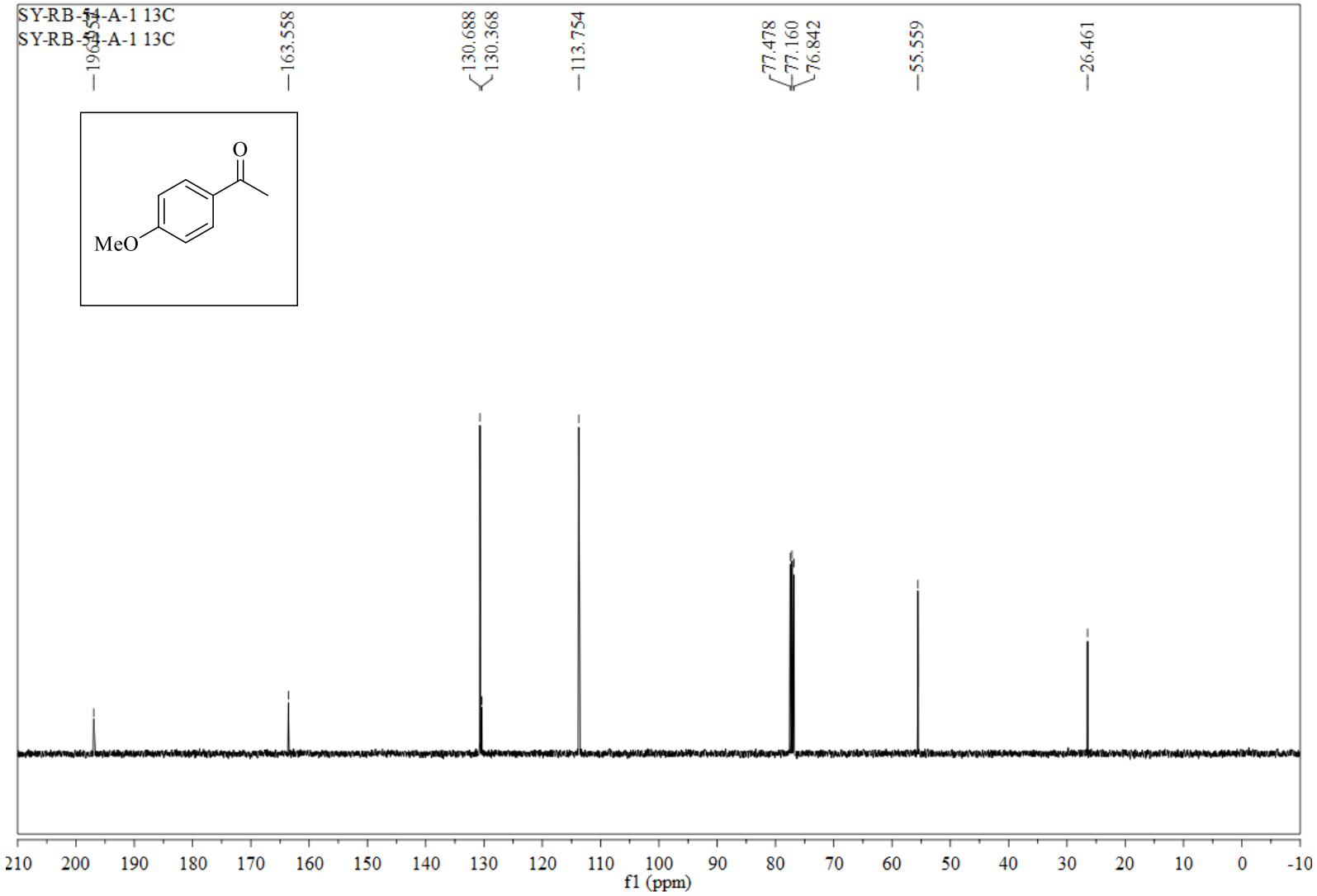

Figure S41. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10e**.

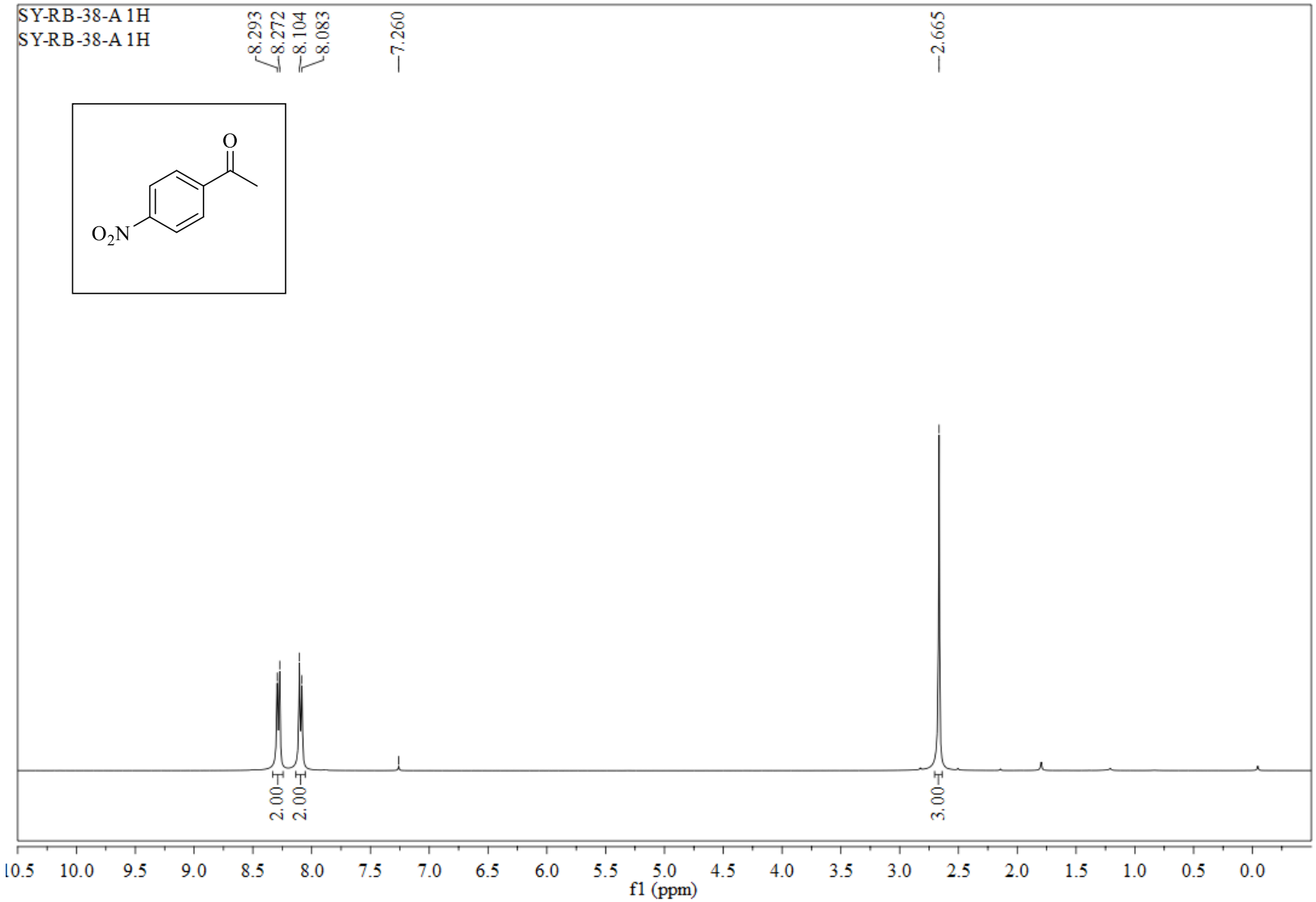

Figure S42. ^{1}H NMR (400 Mz, $CDCl_3$) of **10f.**

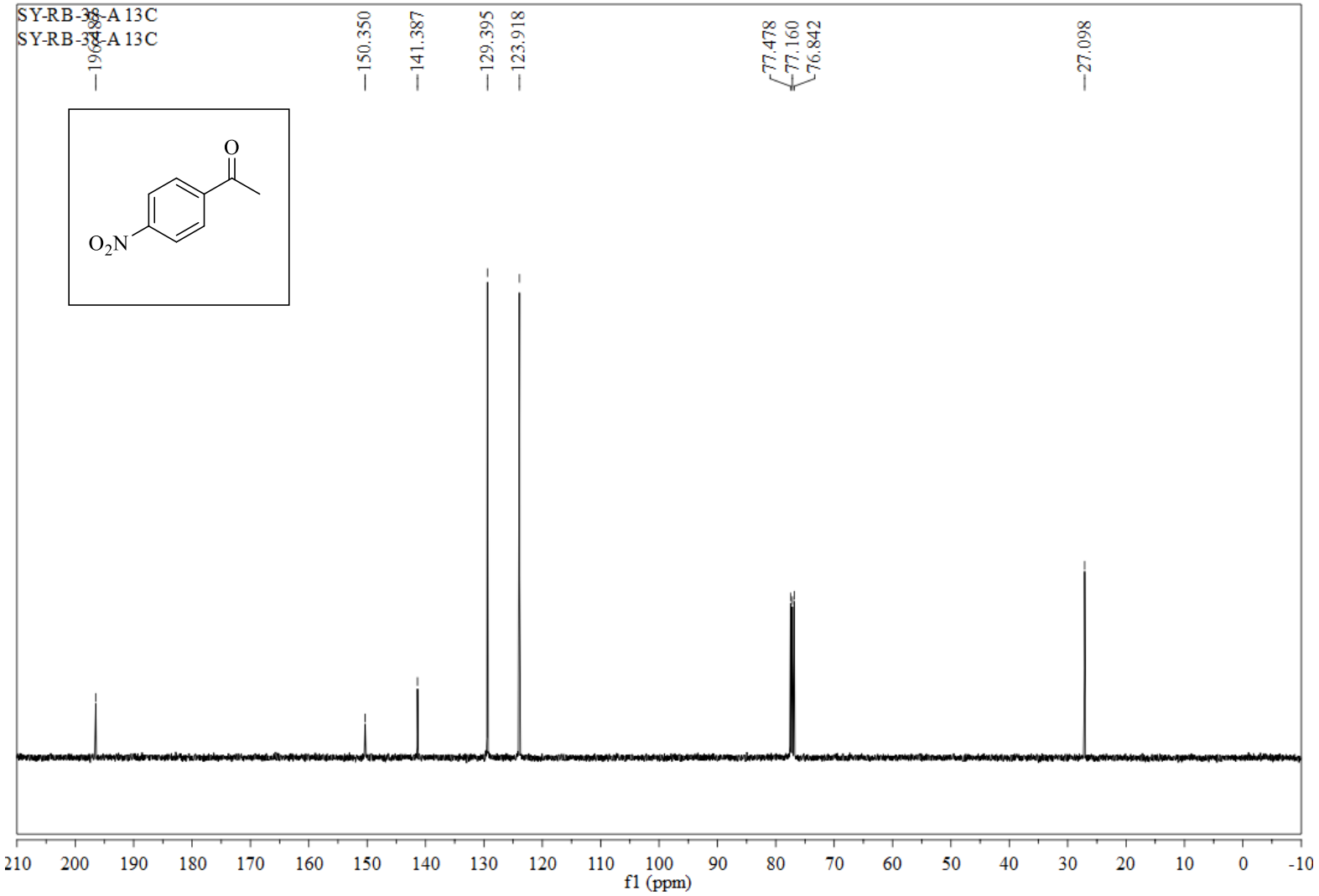

Figure S43. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10f**.

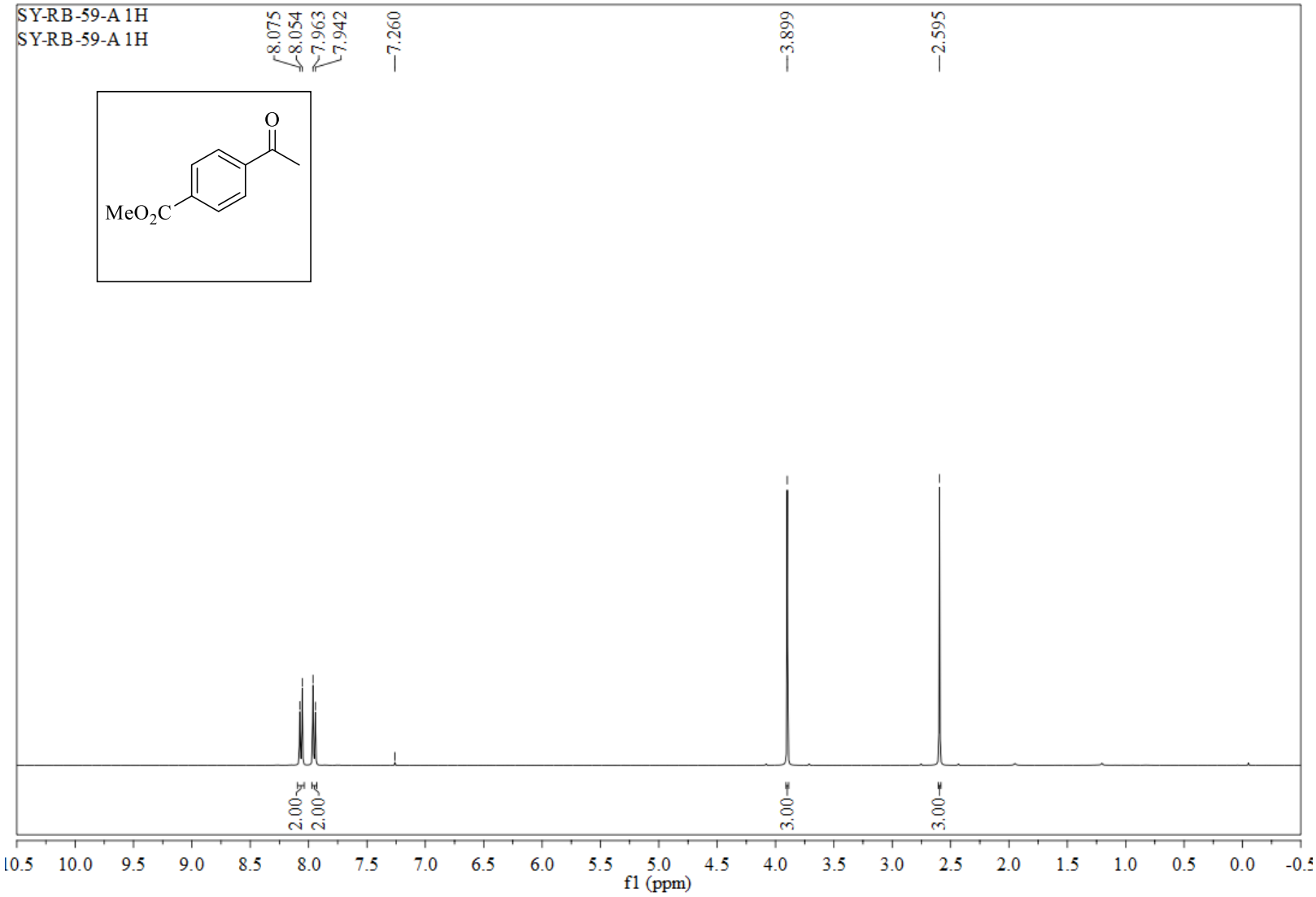

Figure S44. ^{1}H NMR (400 Mz, $CDCl_3$) of **10g**

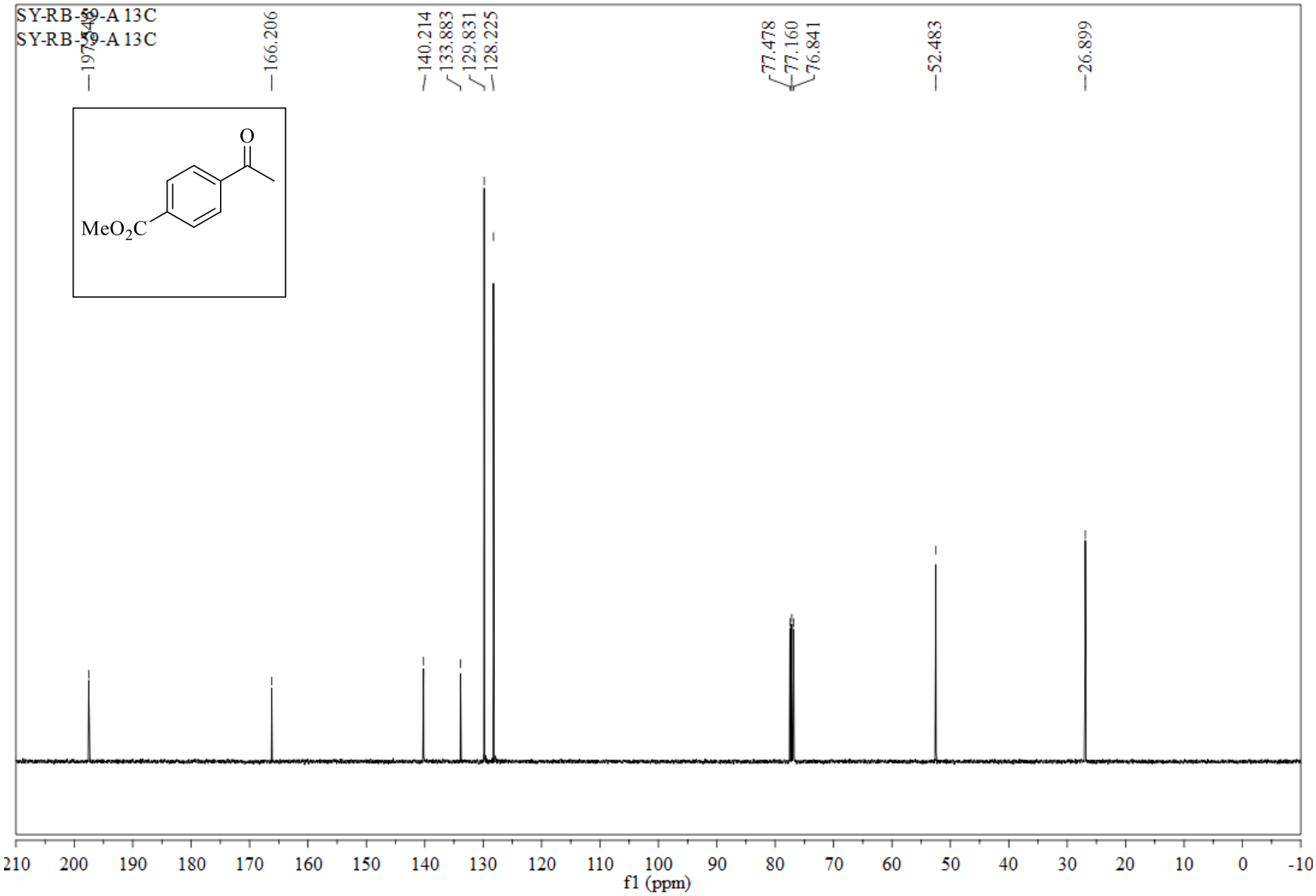

Figure S45. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10g**.

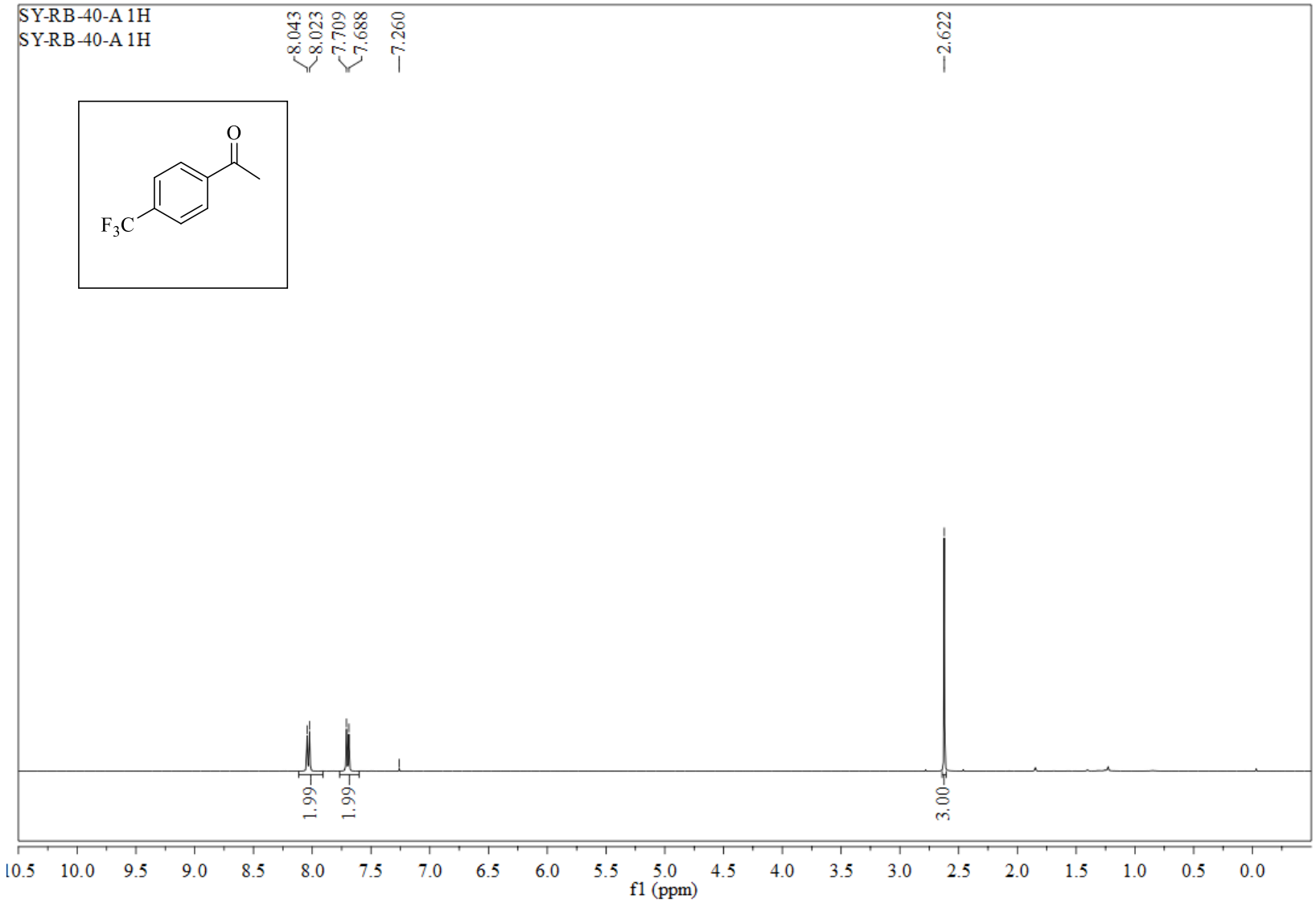

Figure S46. ^{1}H NMR (400 Mz, $CDCl_3$) of **10h**

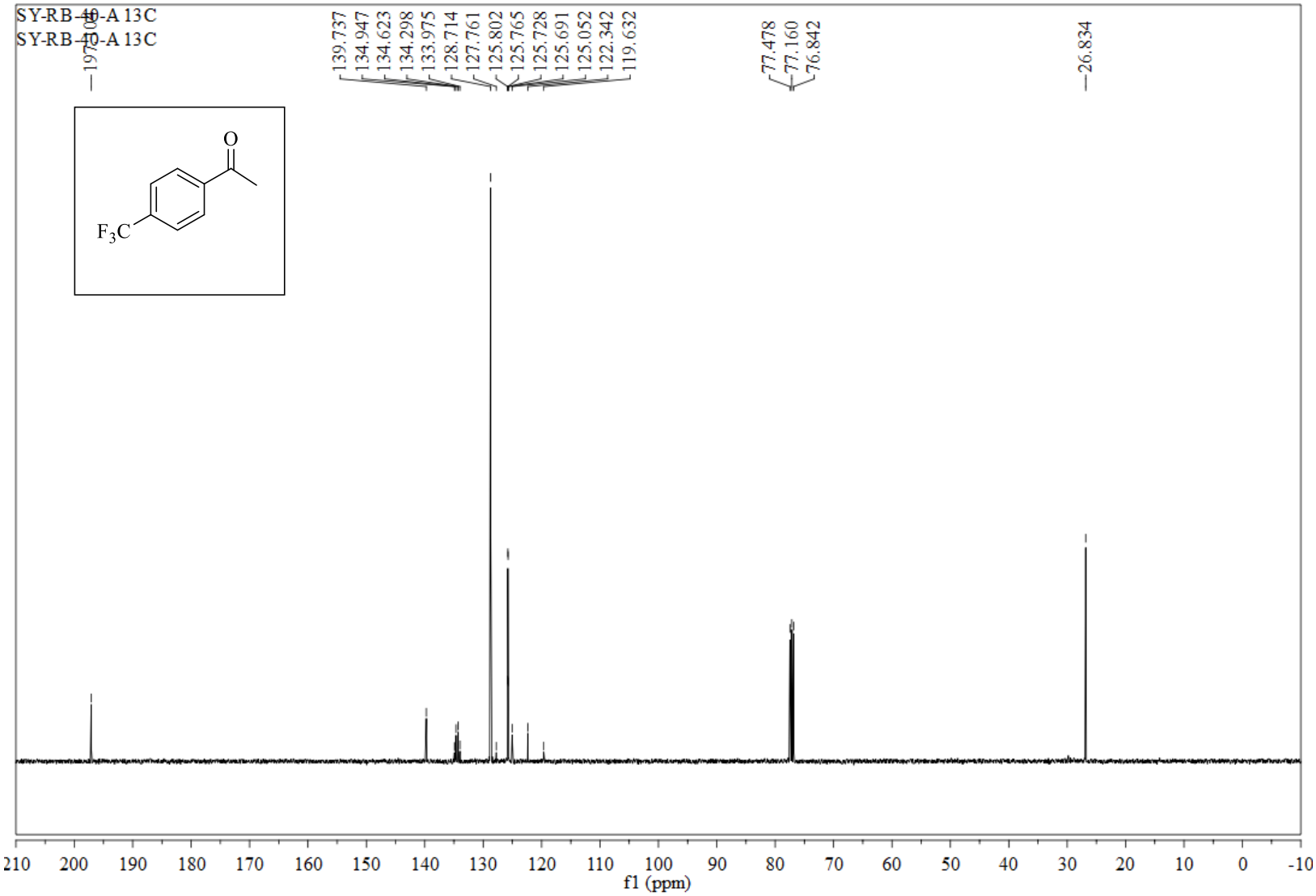

Figure S47. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10h**.

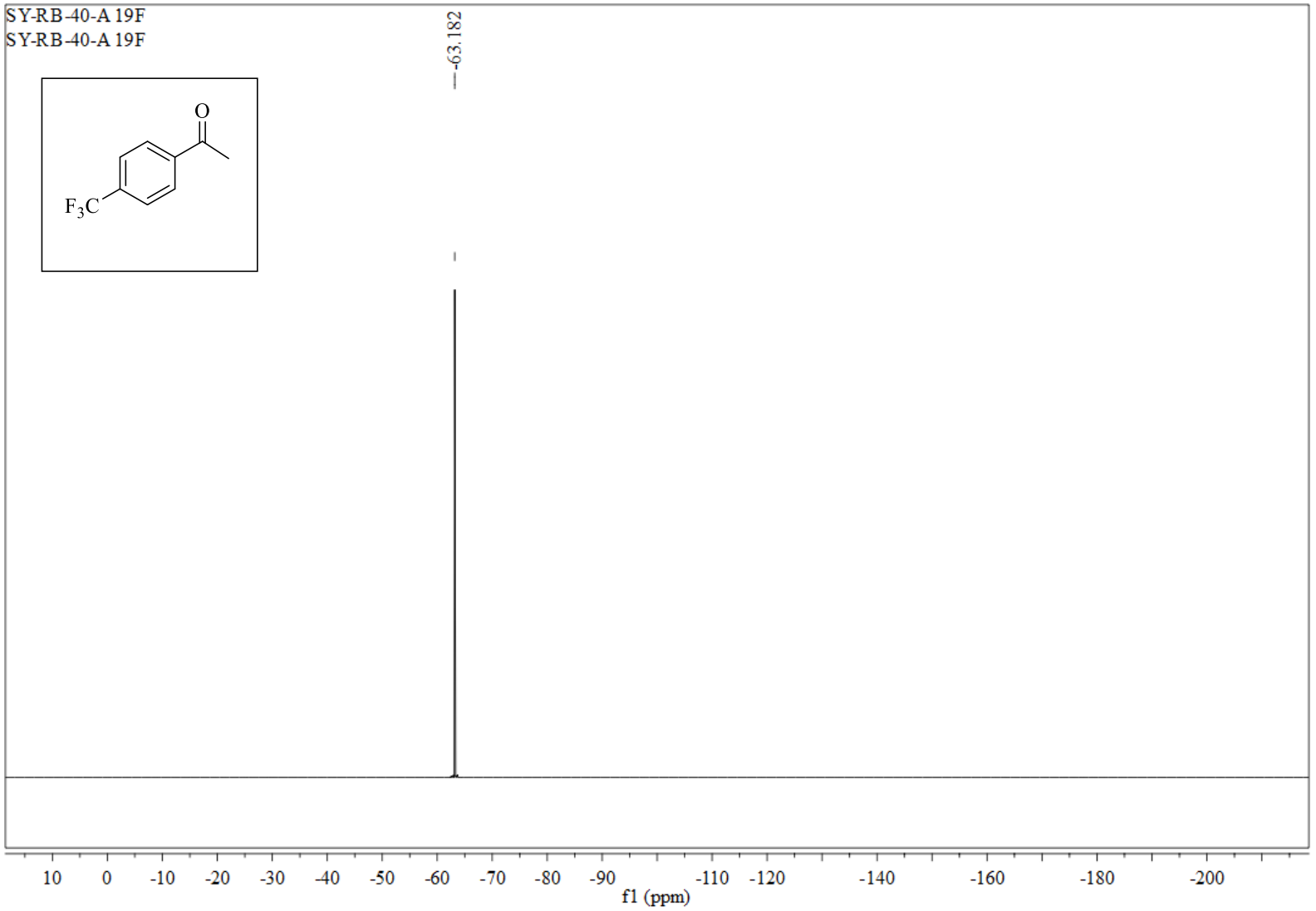

Figure S48. ^{19}F NMR (376 Mz, $CDCl_3$) of **10h**.

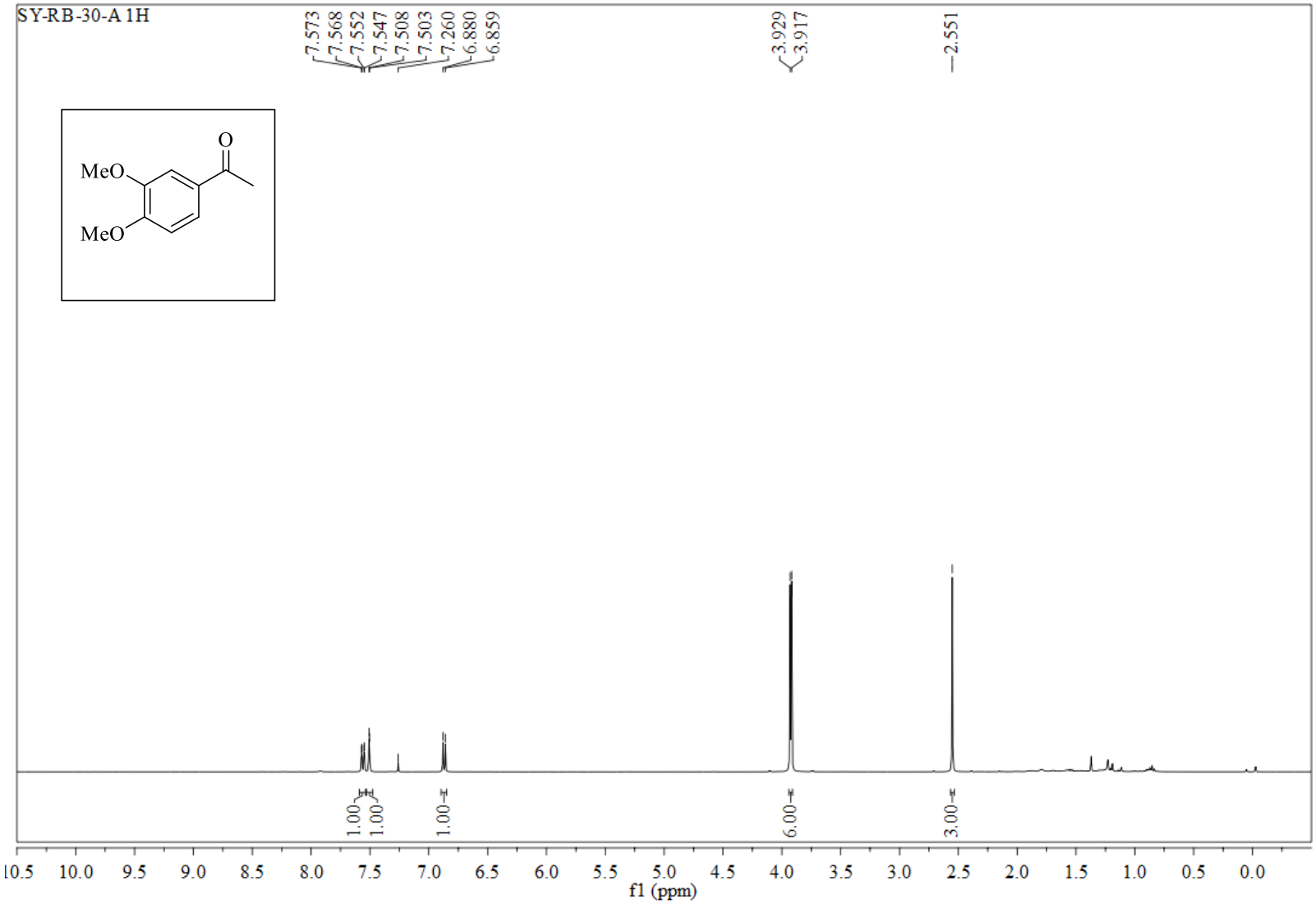

Figure S49. ^{1}H NMR (400 Mz, $CDCl_3$) of **10i**

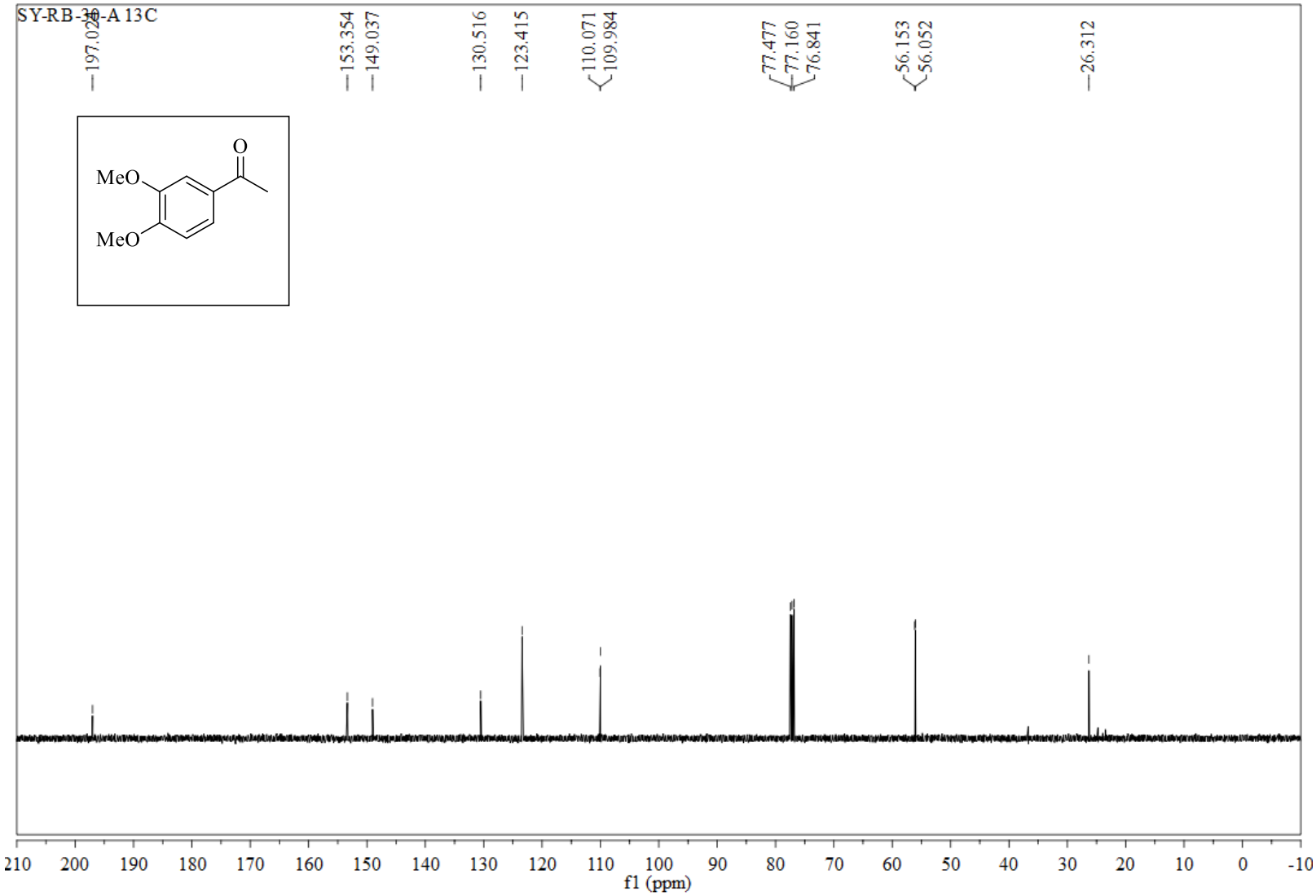

Figure S50. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10i**.

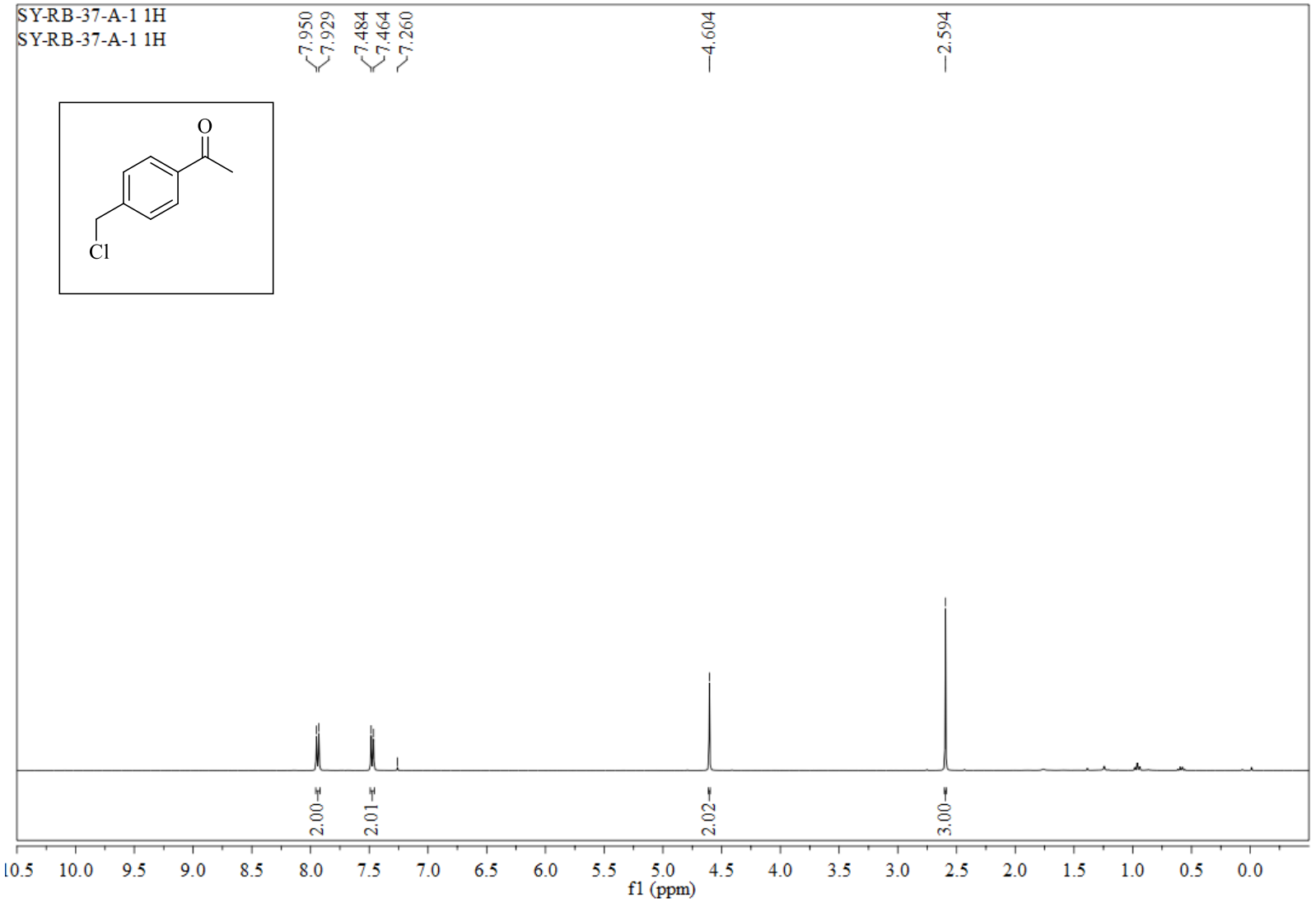

Figure S51. ^{1}H NMR (400 Mz, $CDCl_3$) of **10j**

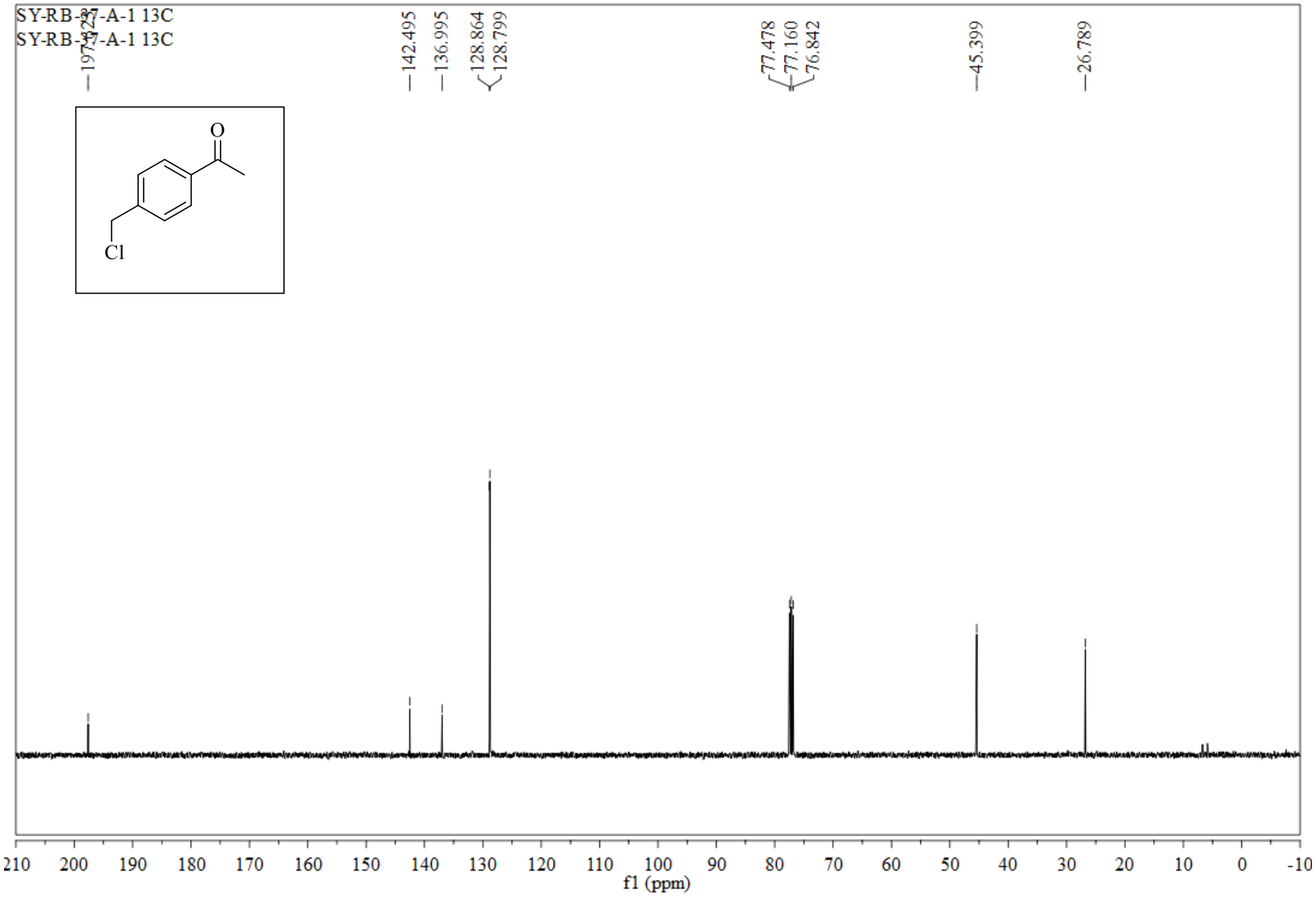

Figure S52. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10j**.

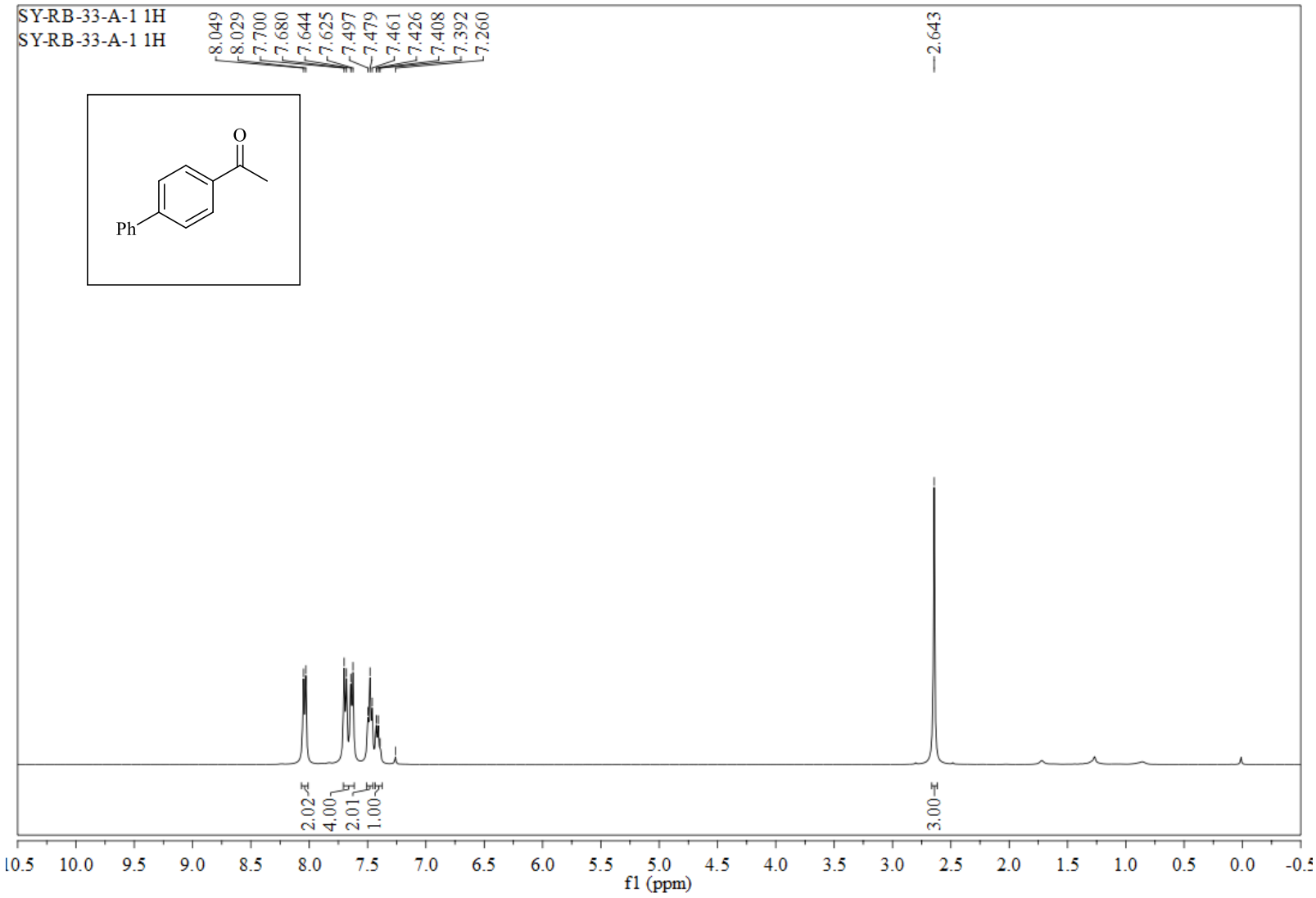

Figure S53. ^{1}H NMR (400 Mz, $CDCl_3$) of **10k**

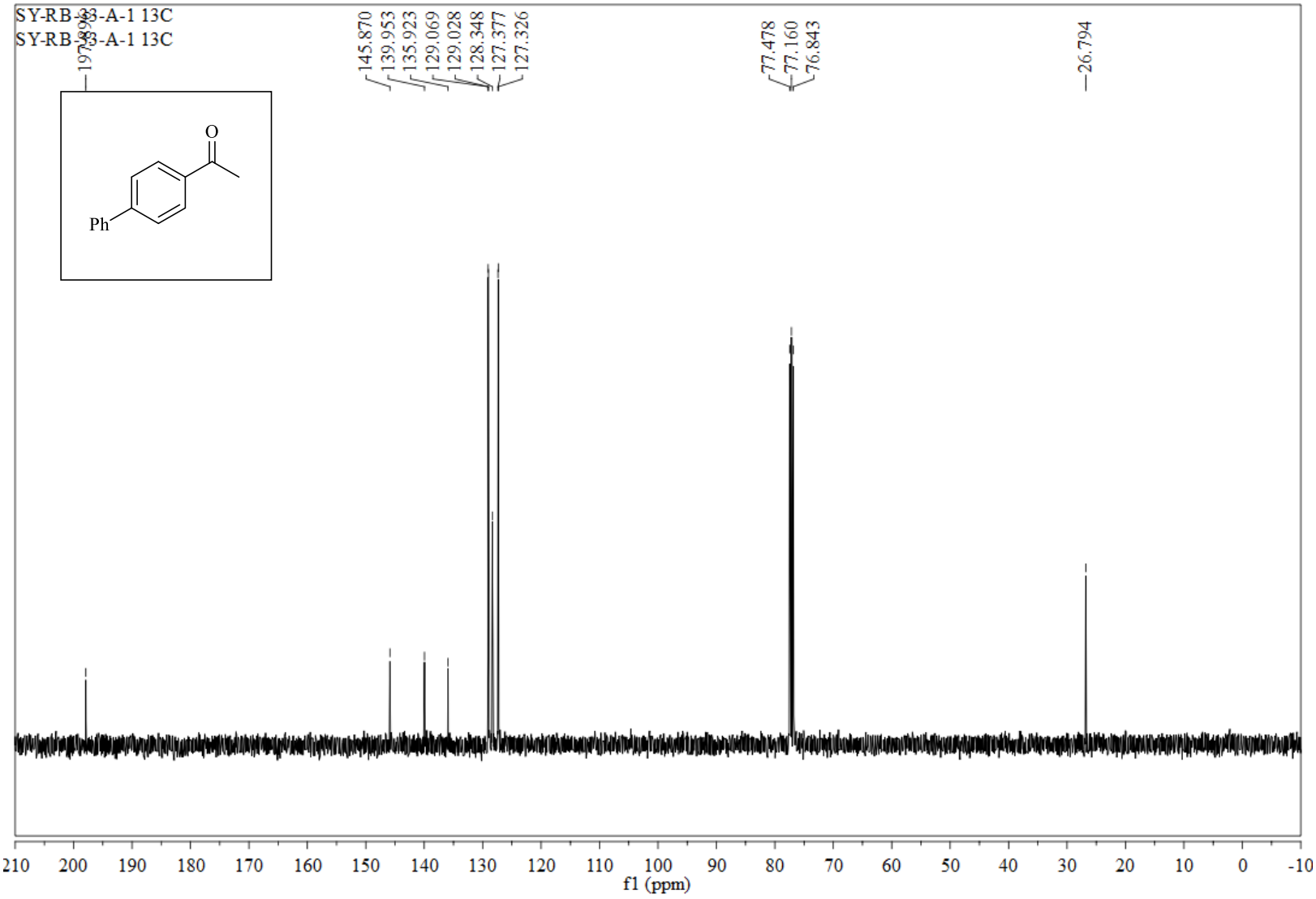

Figure S54. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10k**.

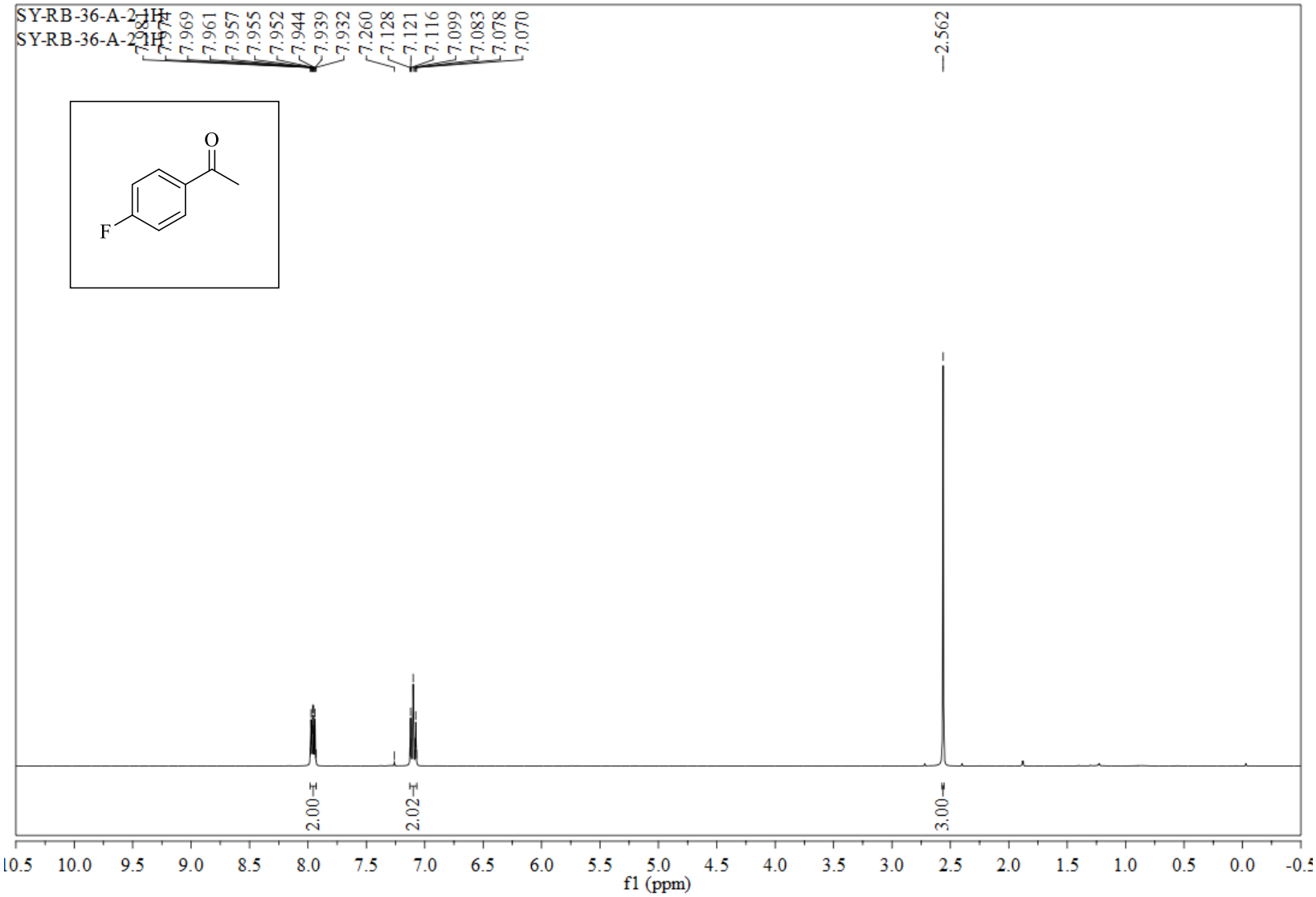

Figure S55. ^{1}H NMR (400 Mz, $CDCl_3$) of **10l**

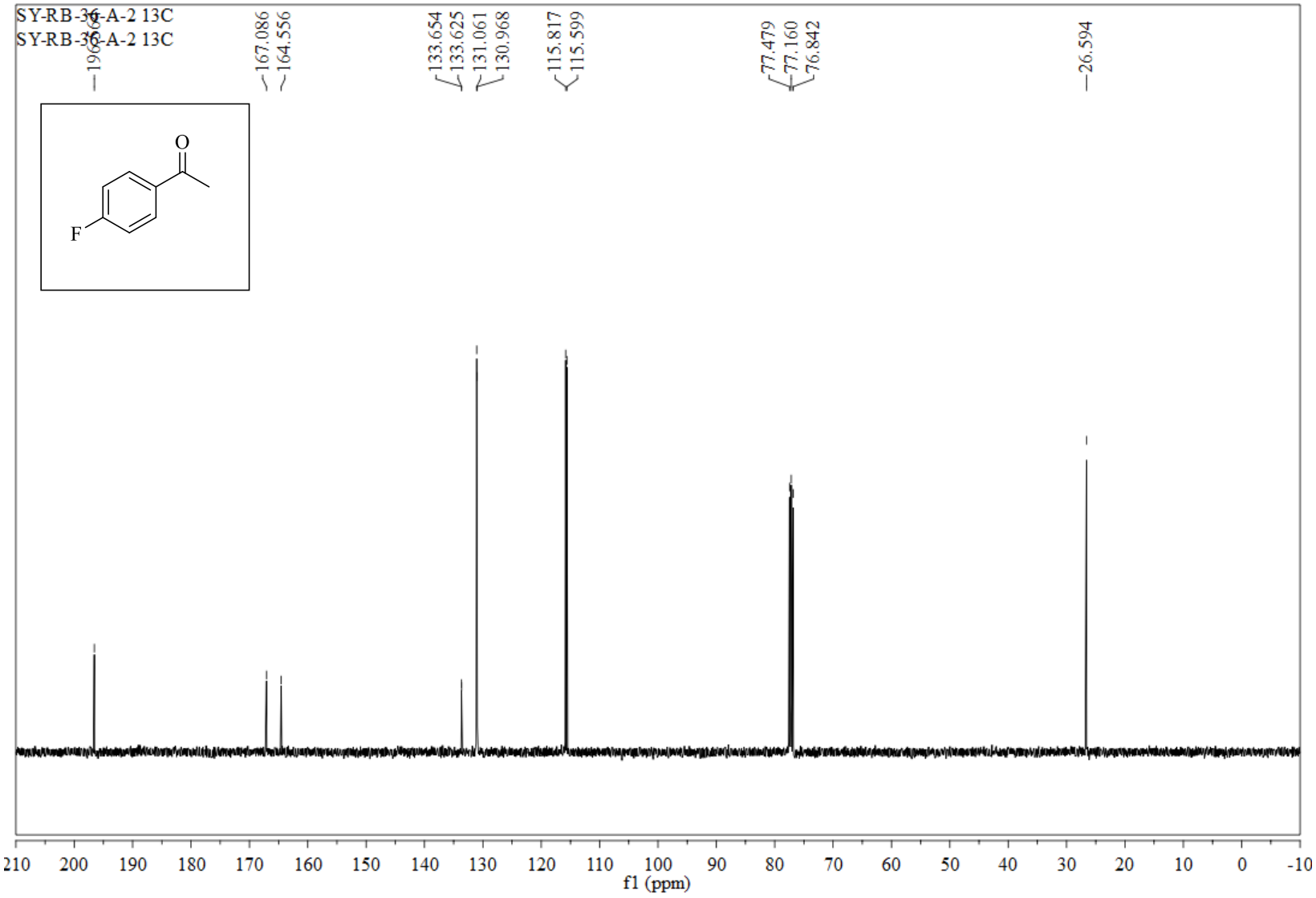

Figure S56. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10l**

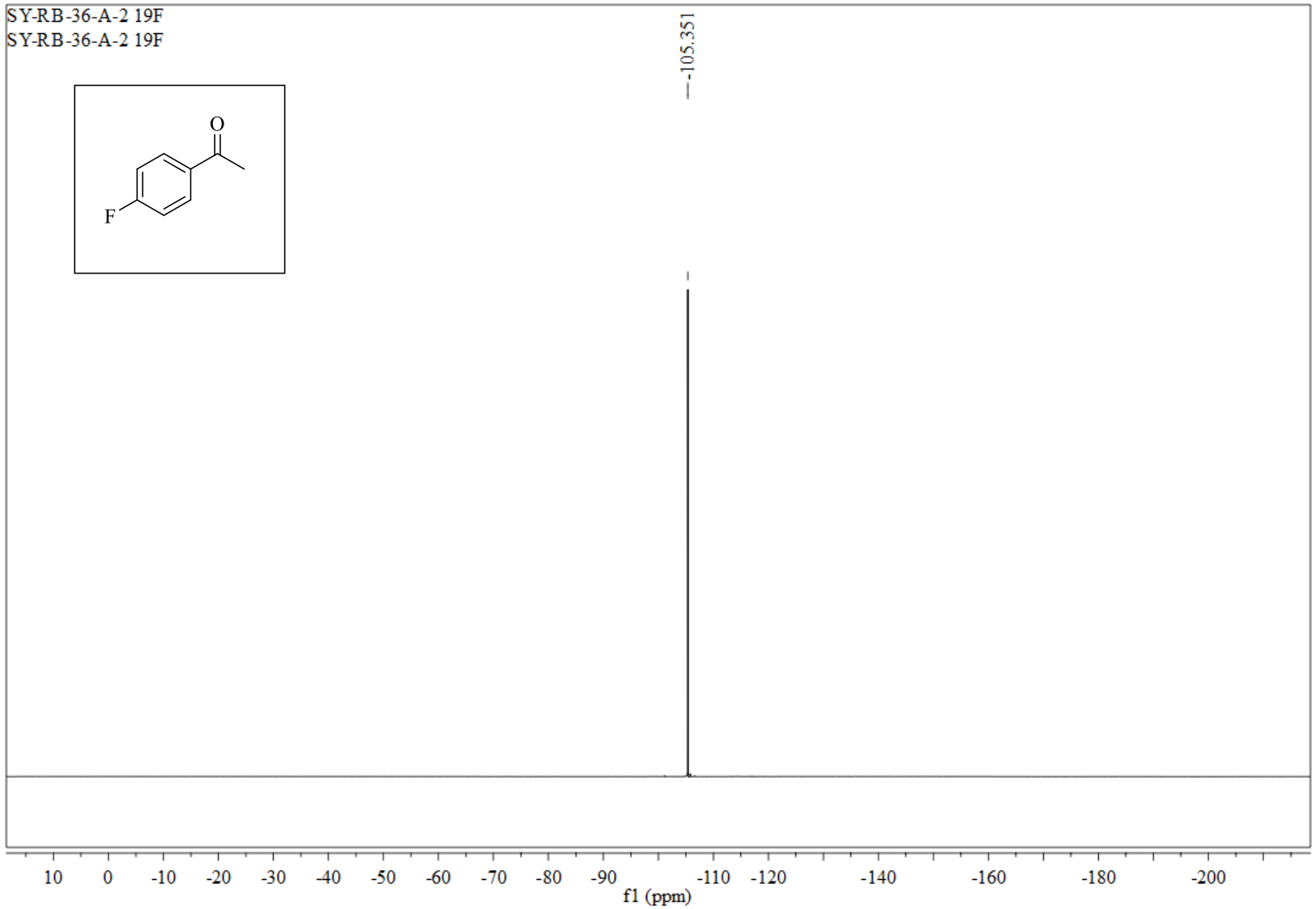

Figure S57. ^{19}F NMR (376 Mz, $CDCl_3$) of **10l**.

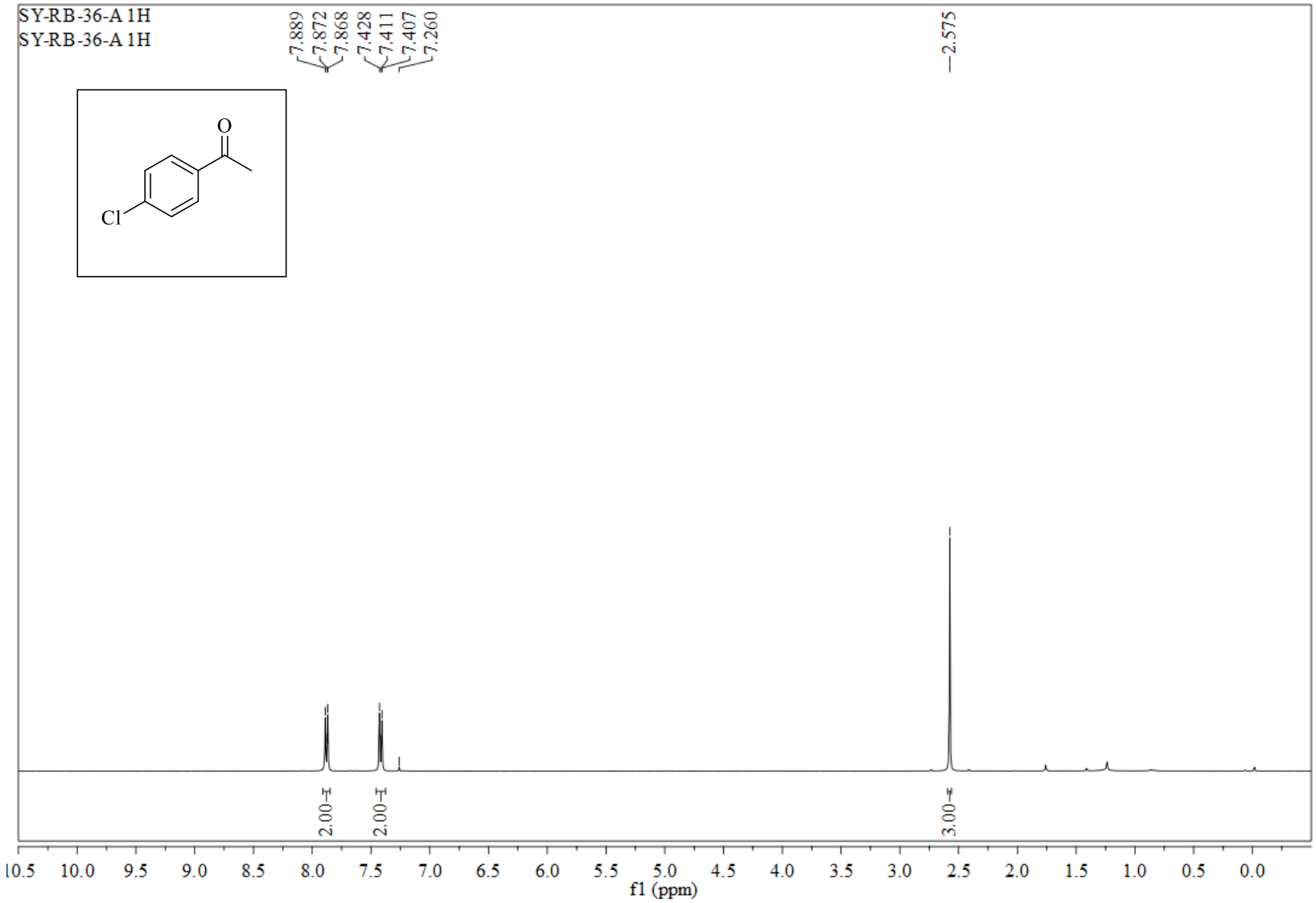

Figure S58. ^{1}H NMR (400 Mz, $CDCl_3$) of **10m**

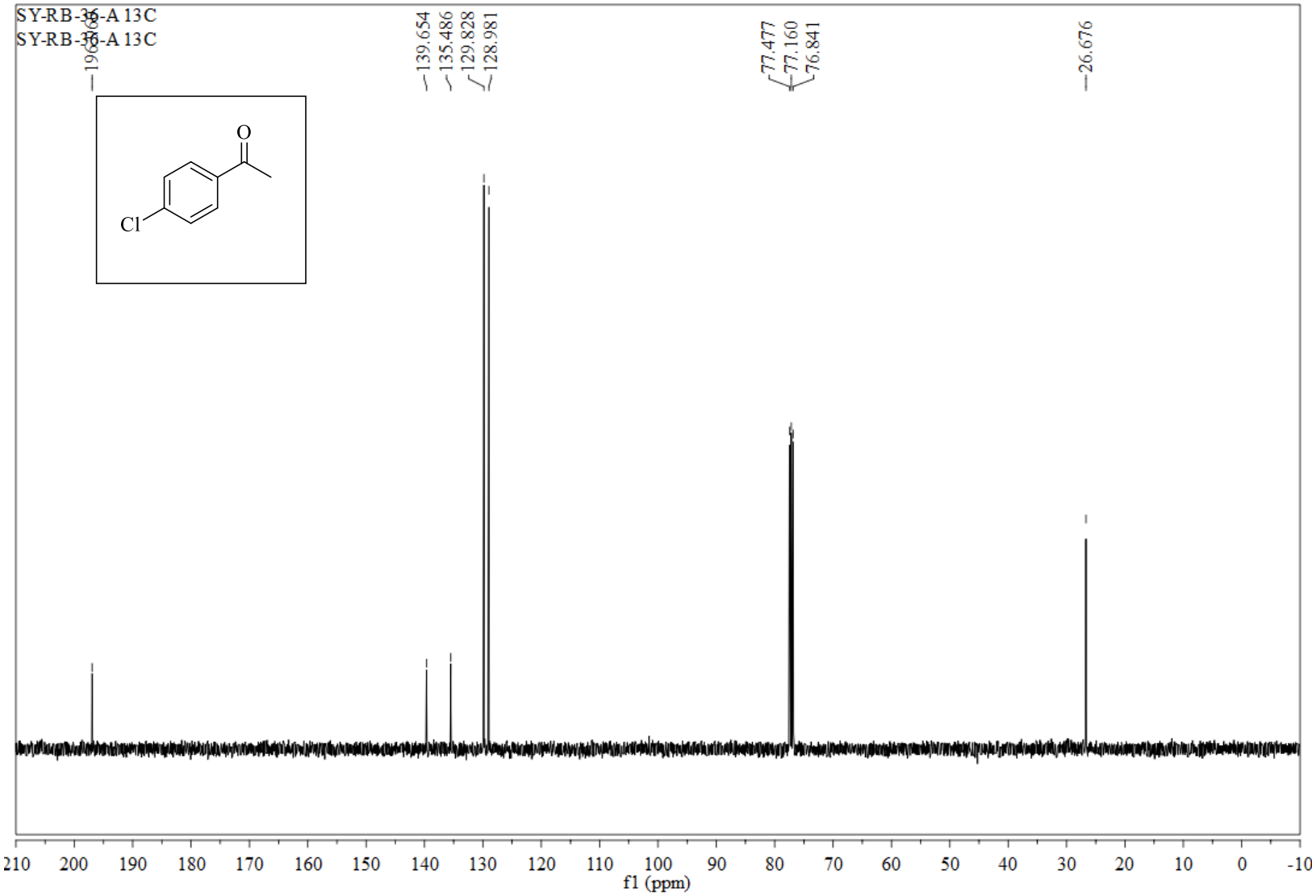

Figure S59. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10m**

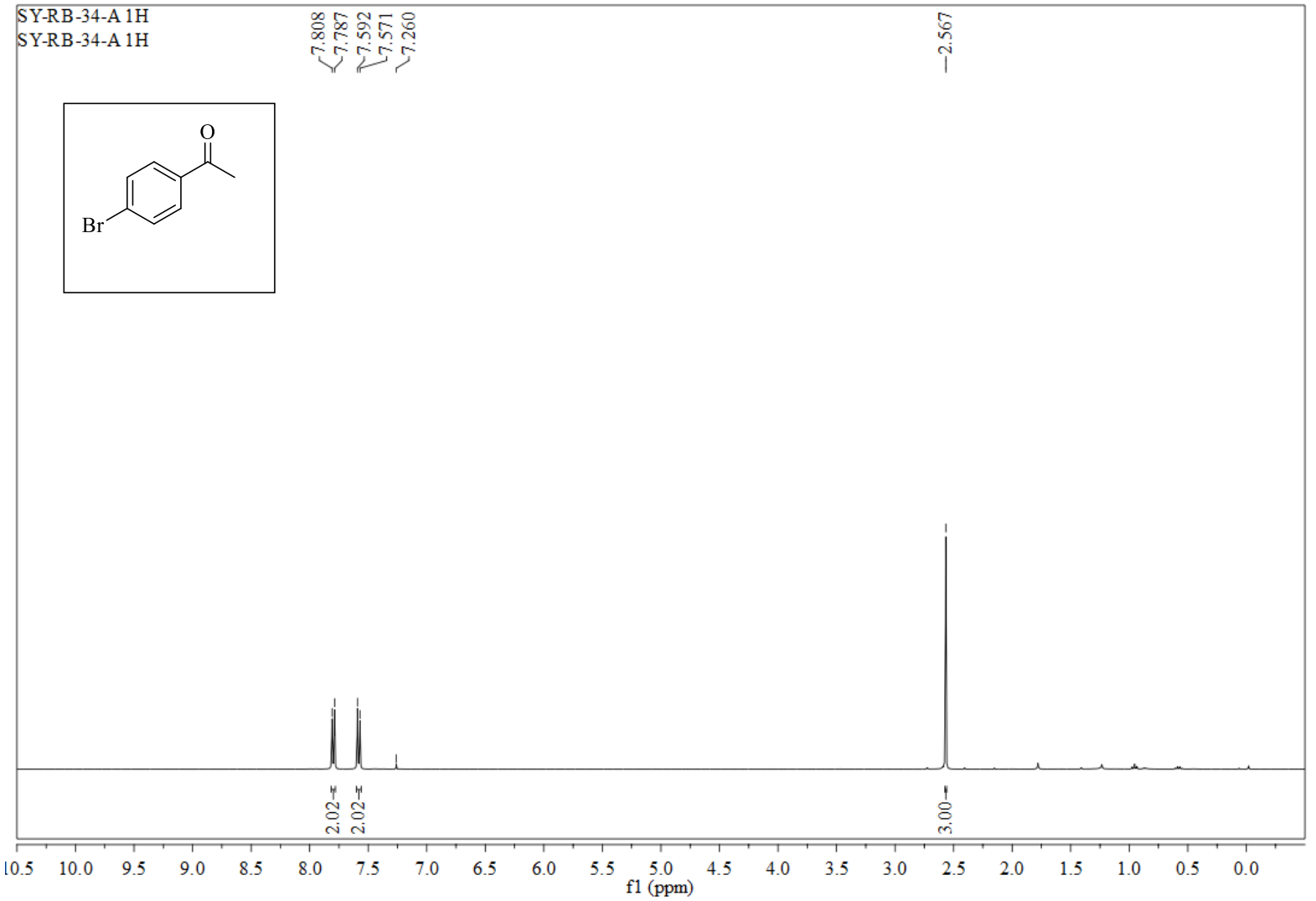

Figure S60. ^{1}H NMR (400 Mz, $CDCl_3$) of **10n**

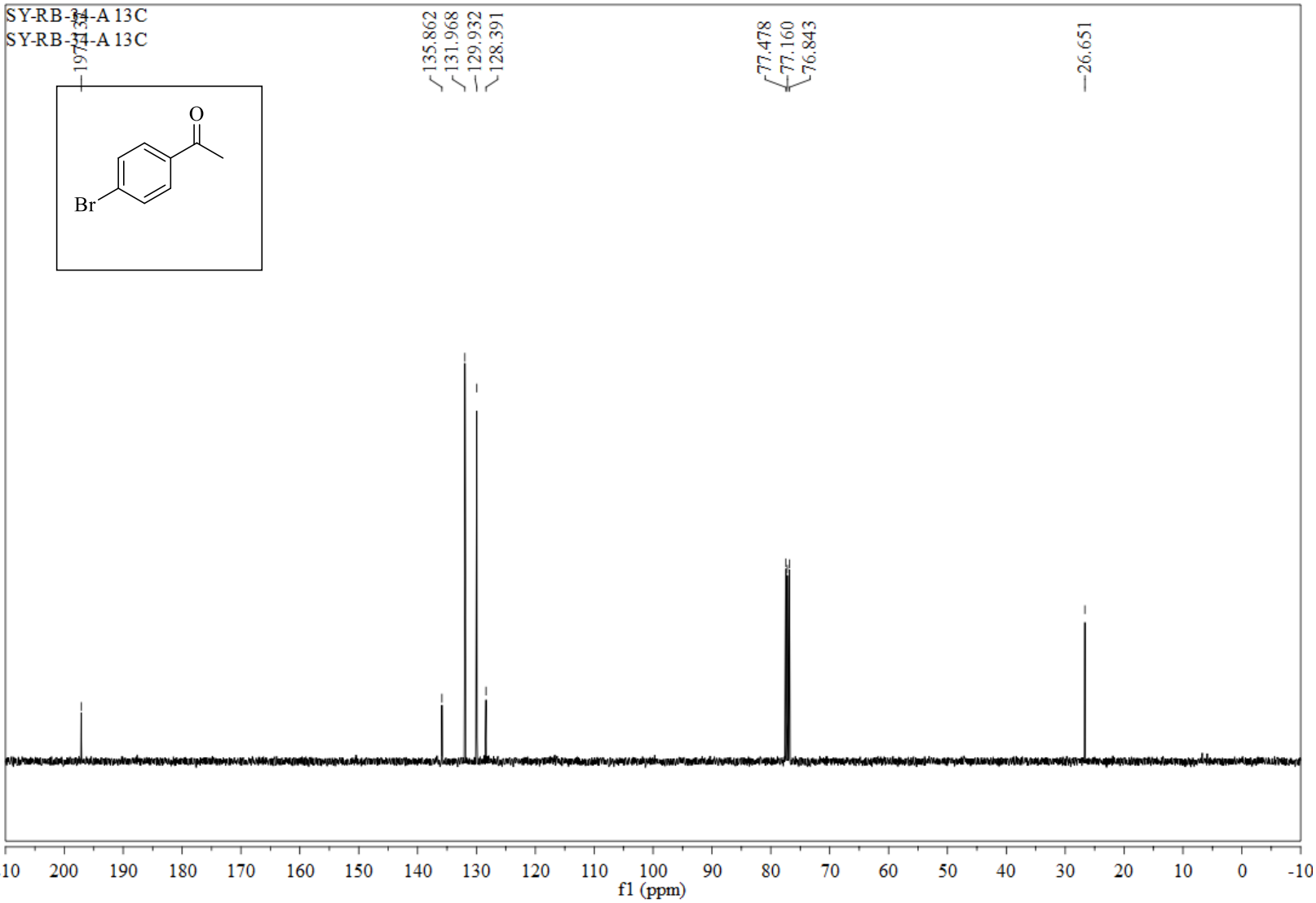

Figure S61. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10n**

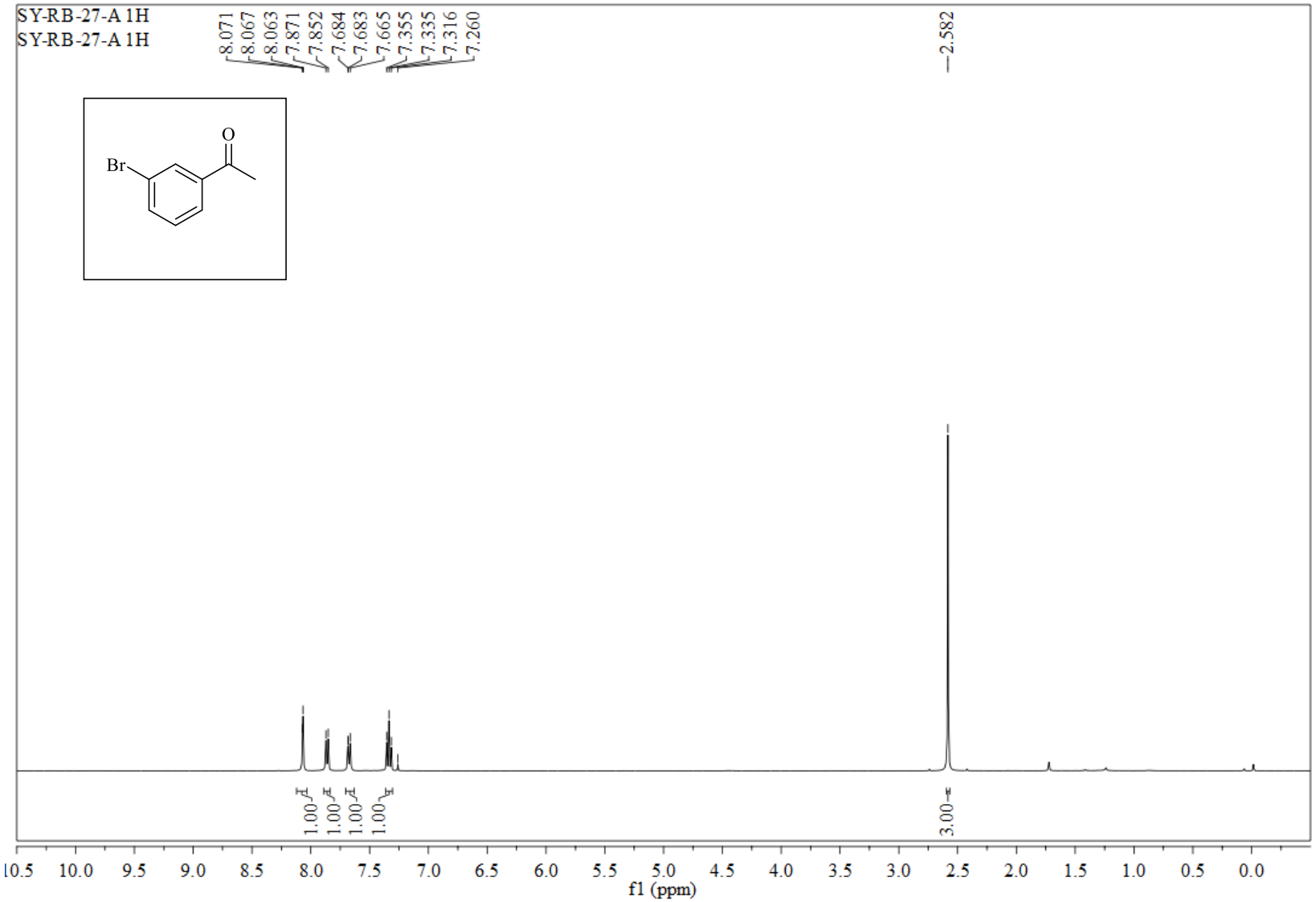

Figure S62. ^{1}H NMR (400 Mz, $CDCl_3$) of **10o**

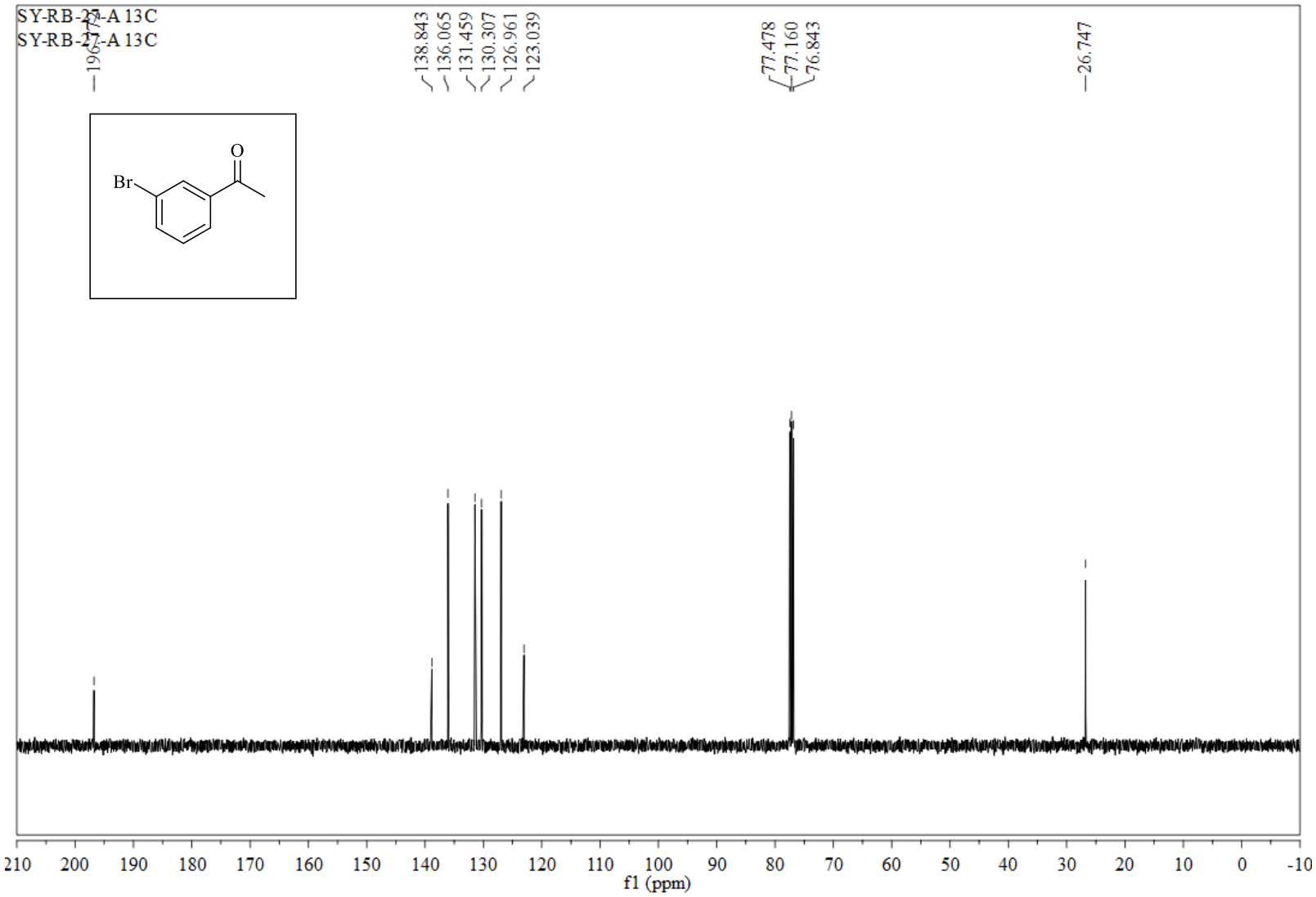

Figure S63. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10o**

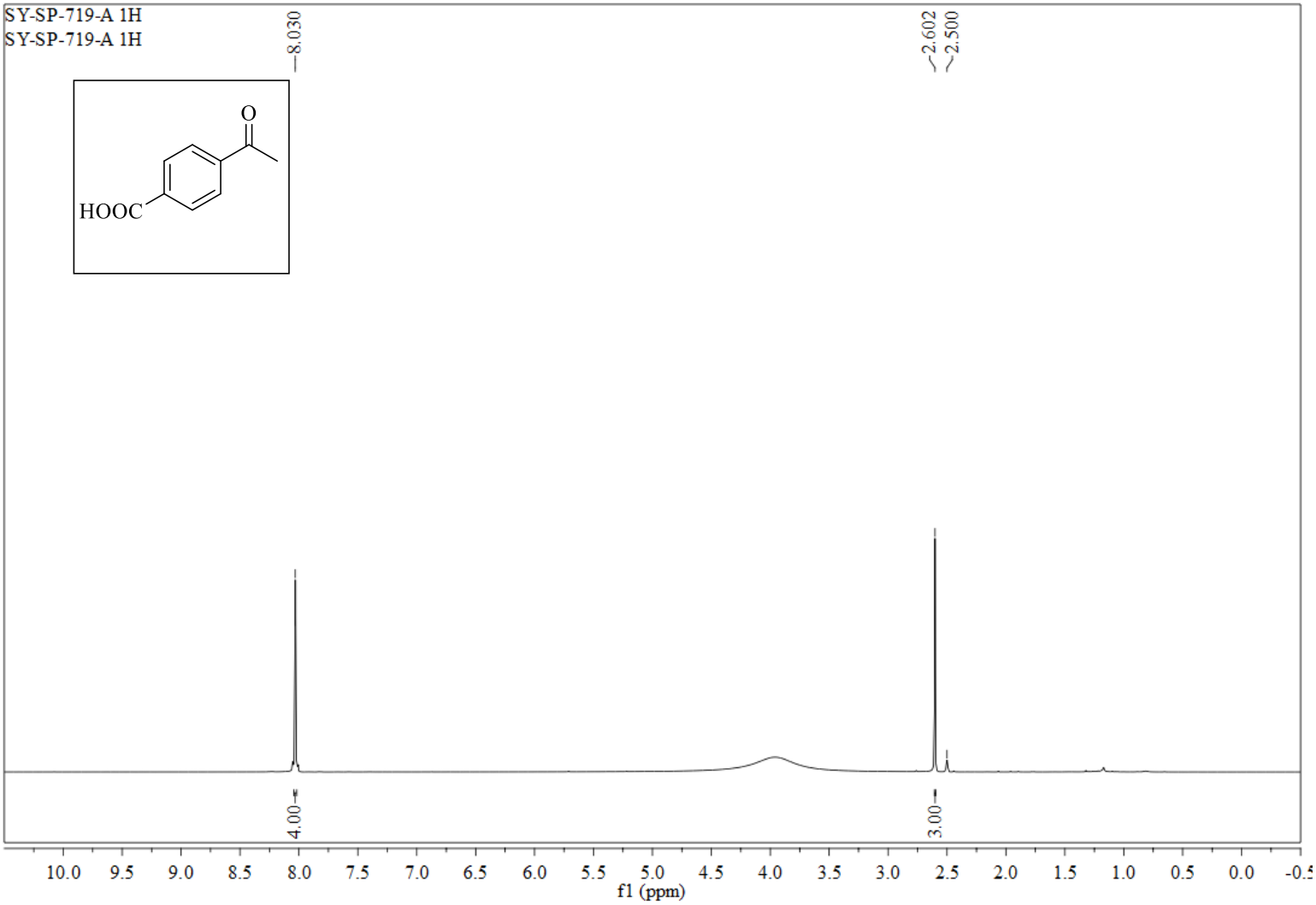

Figure S64. ^{1}H NMR (400 Mz, DMSO-d_6) of **10p**

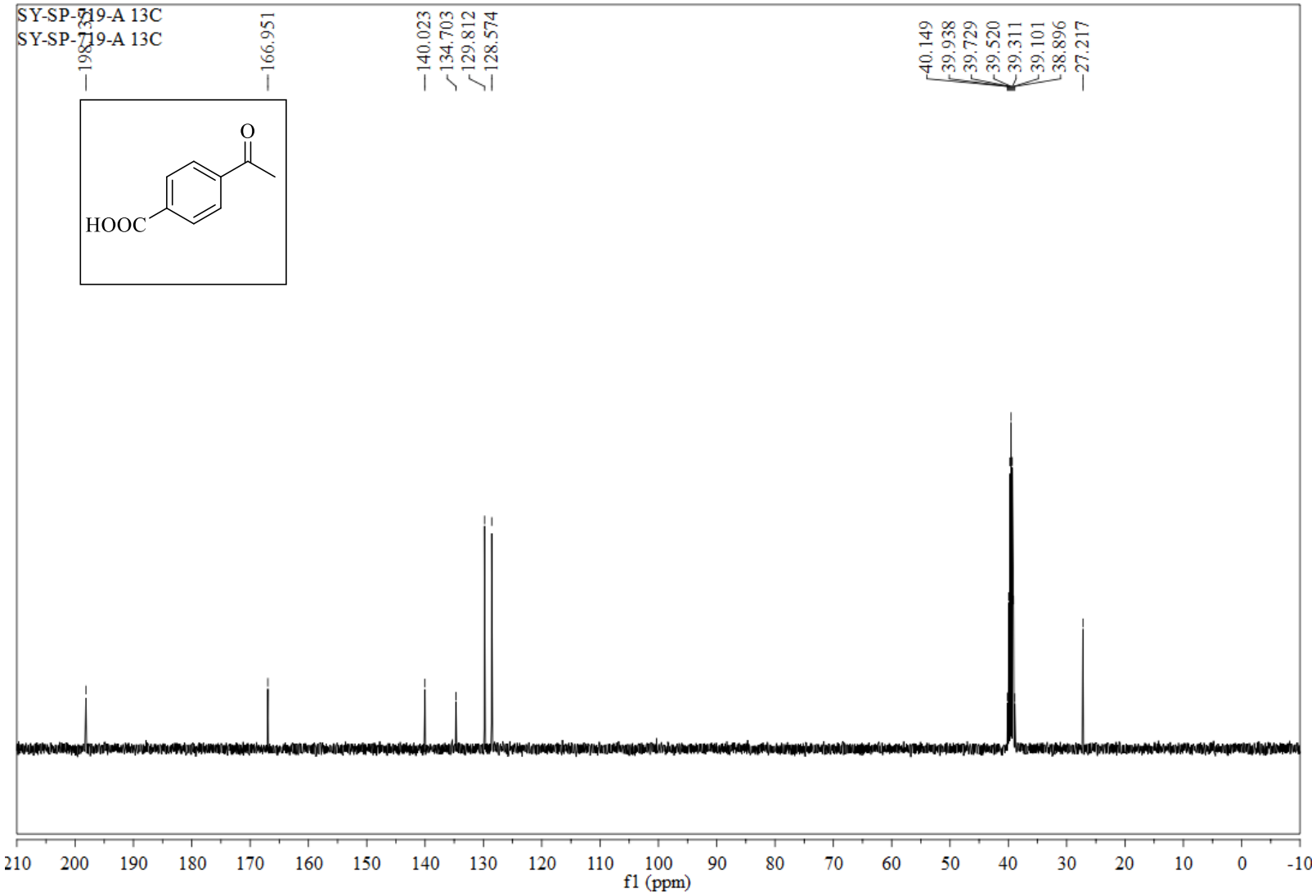

Figure S65. ^{13}C {^{1}H} NMR (100 Mz, DMSO-d_6) of **10p**.

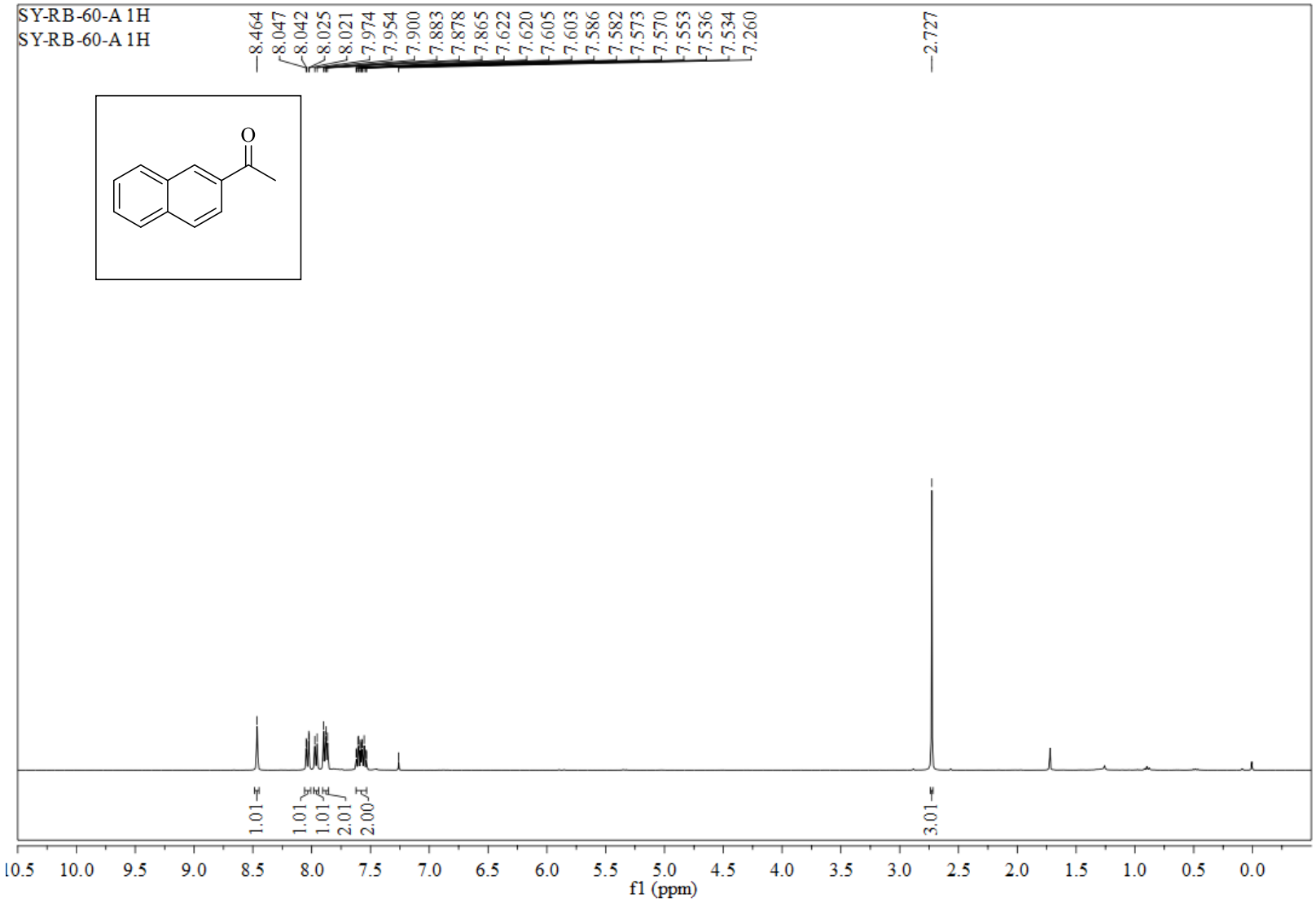

Figure S66. ^{1}H NMR (400 Mz, $CDCl_3$) of **10q**

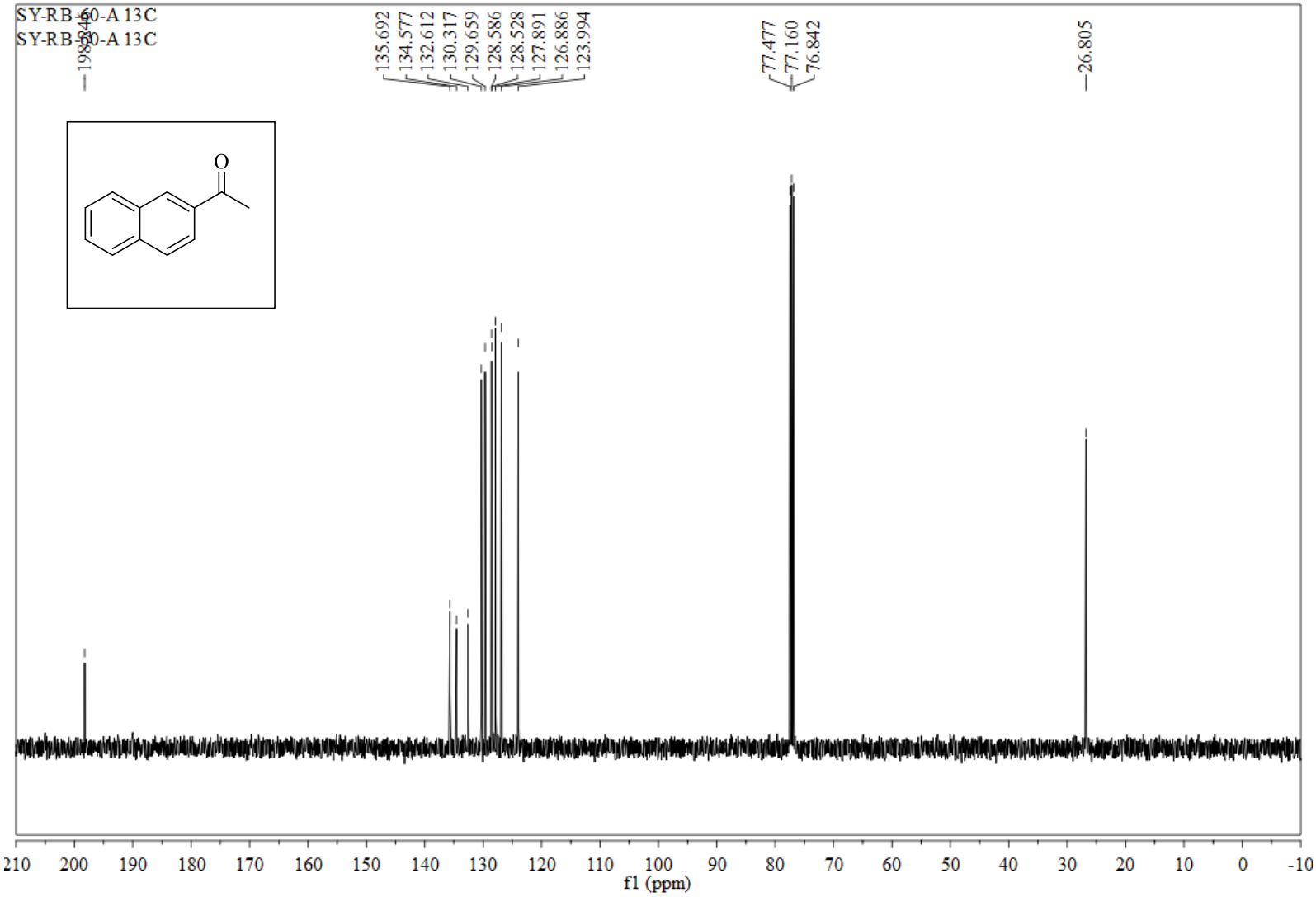

Figure S67. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10q.**

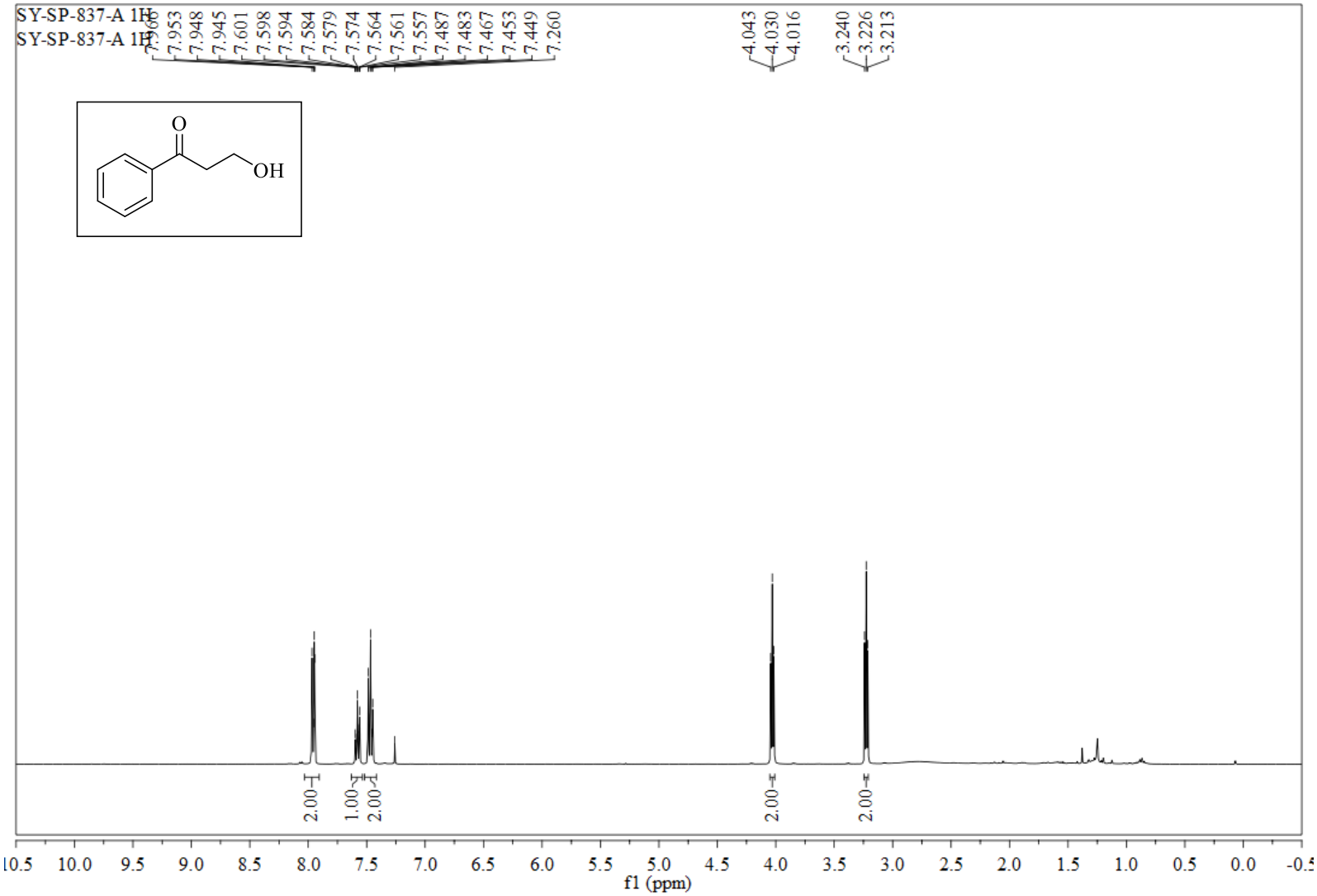

Figure S68. ^{1}H NMR (400 Mz, $CDCl_3$) of **10r.**

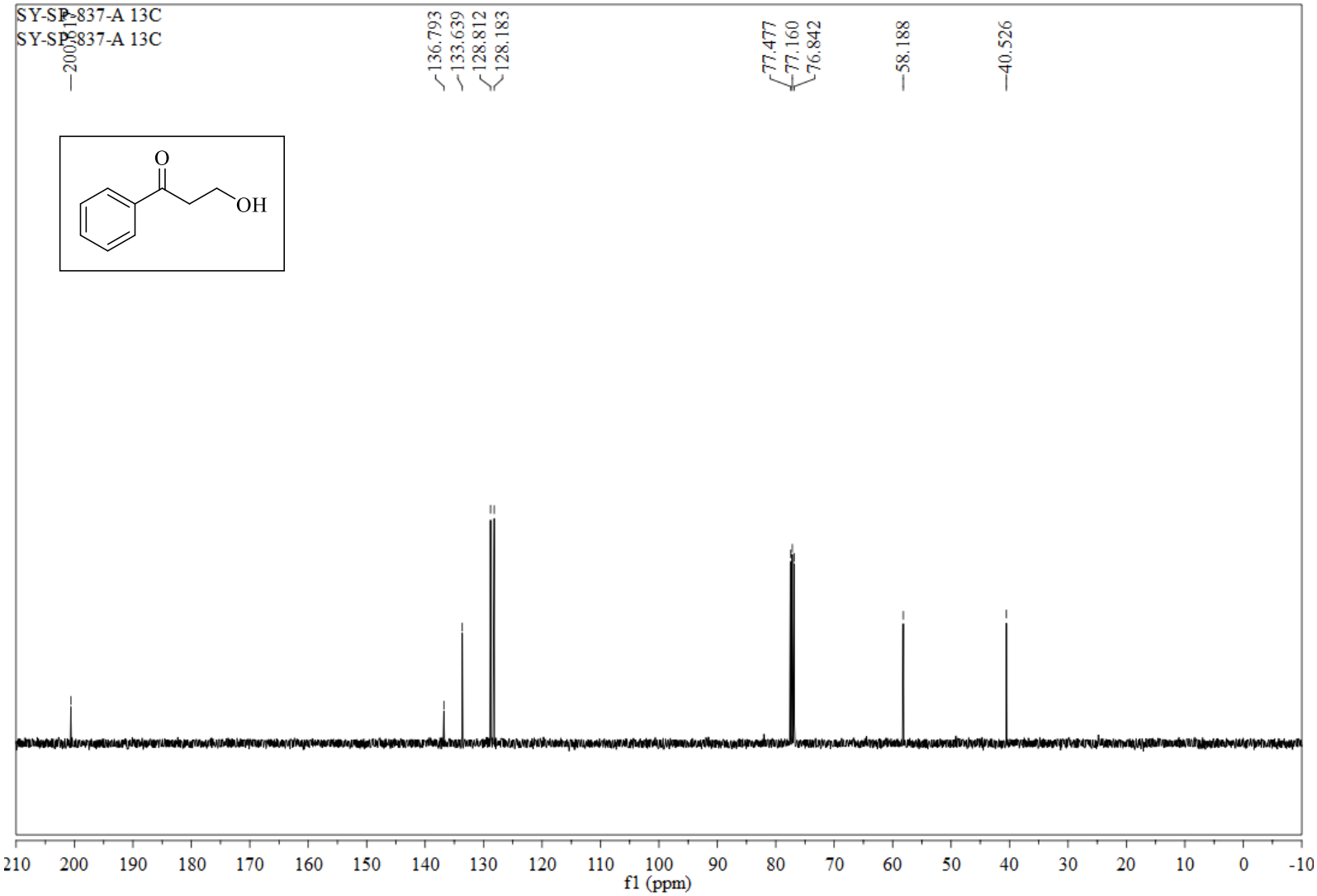

Figure S69. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10r.**

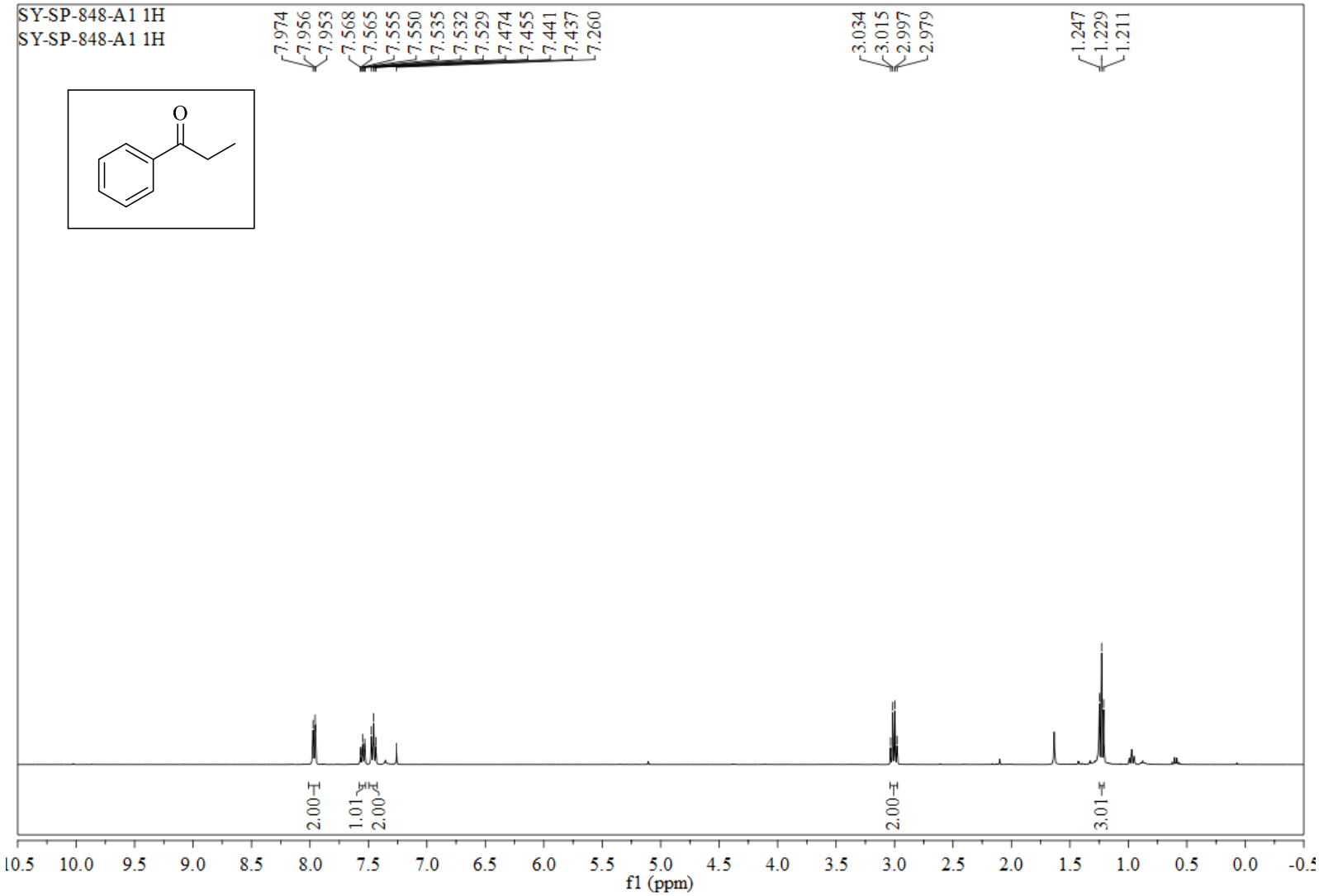

Figure S70. ^{1}H NMR (400 Mz, $CDCl_3$) of **10s.**

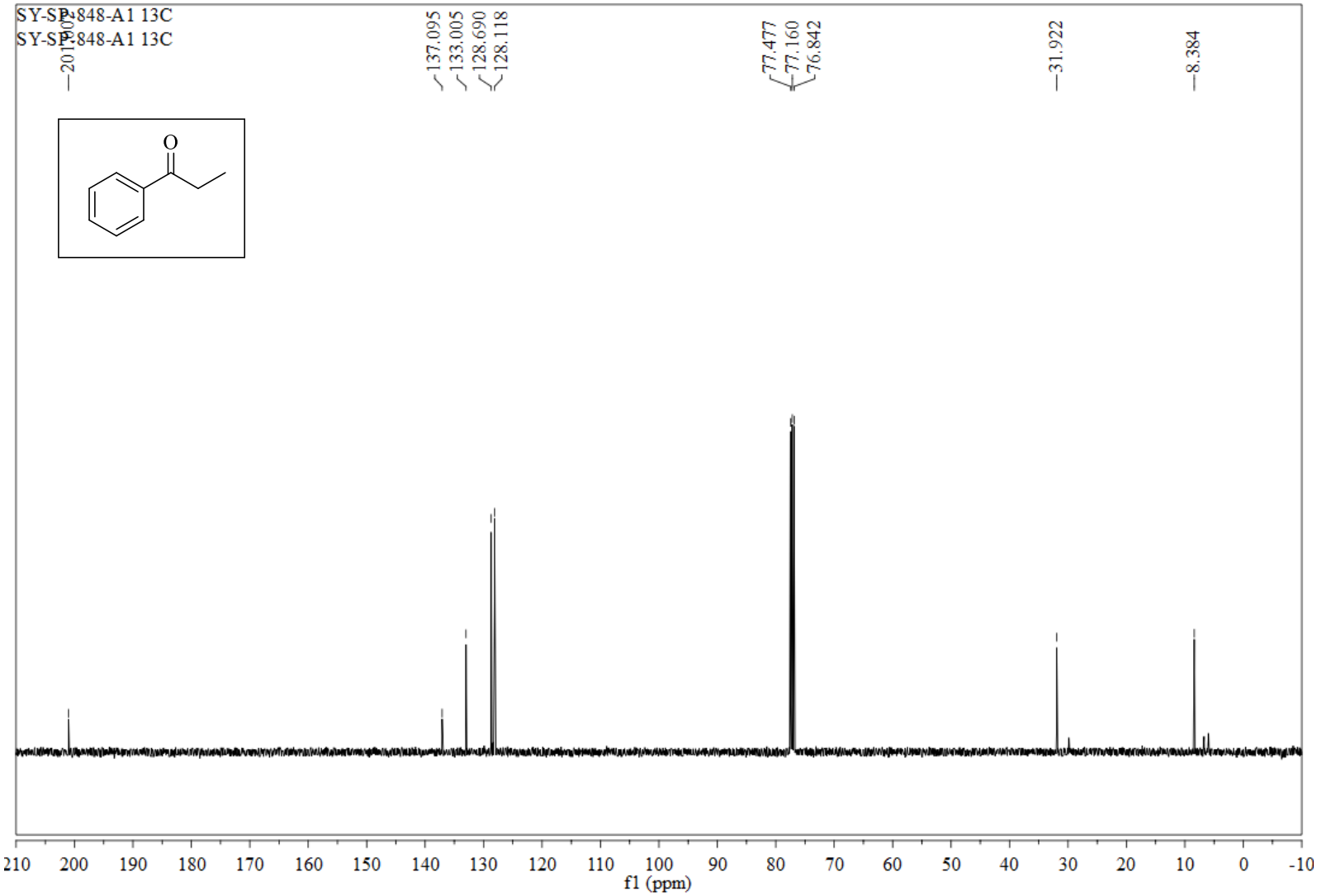

Figure S71. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10s.**

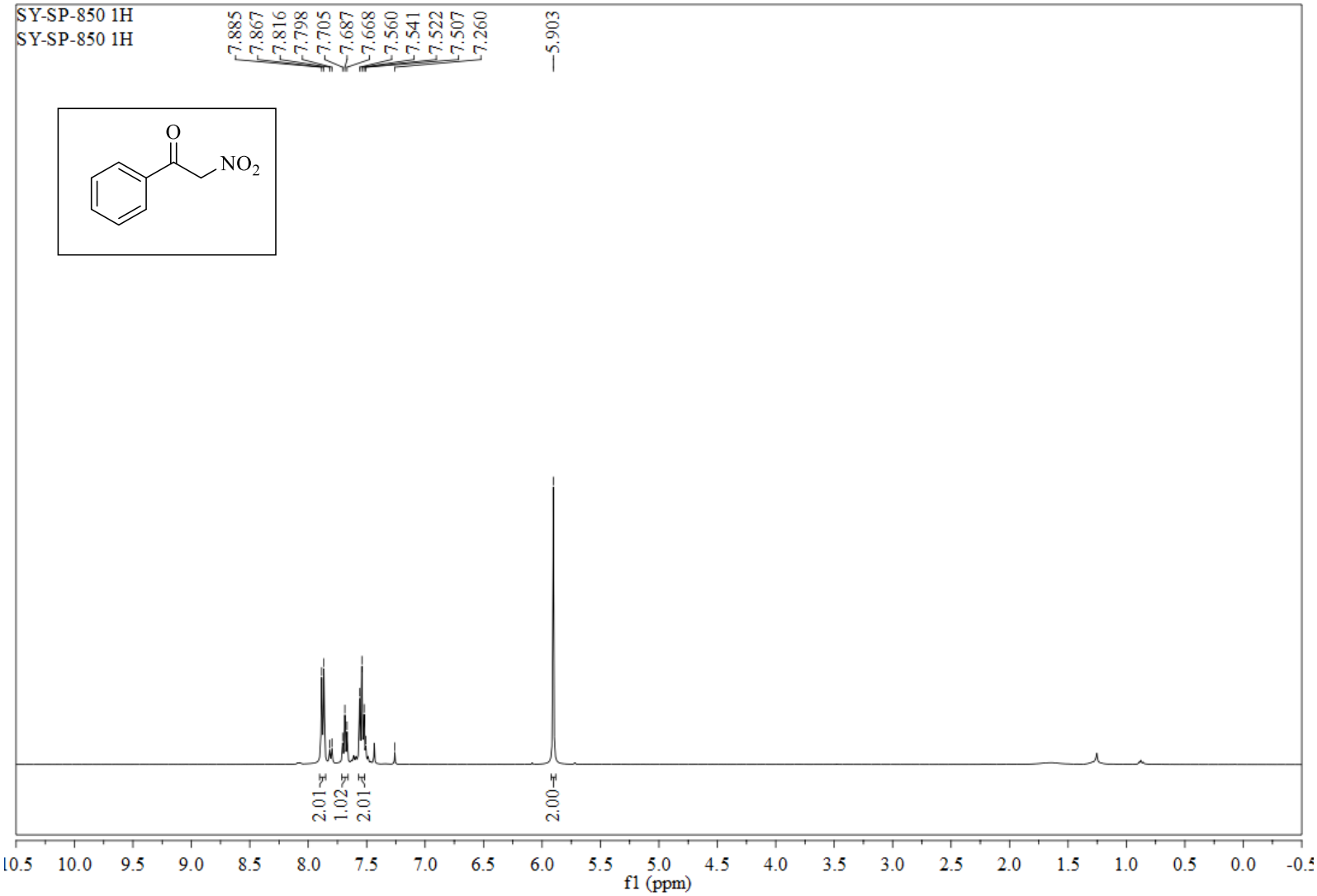

Figure S72. ^{1}H NMR (400 Mz, $CDCl_3$) of **10t.**

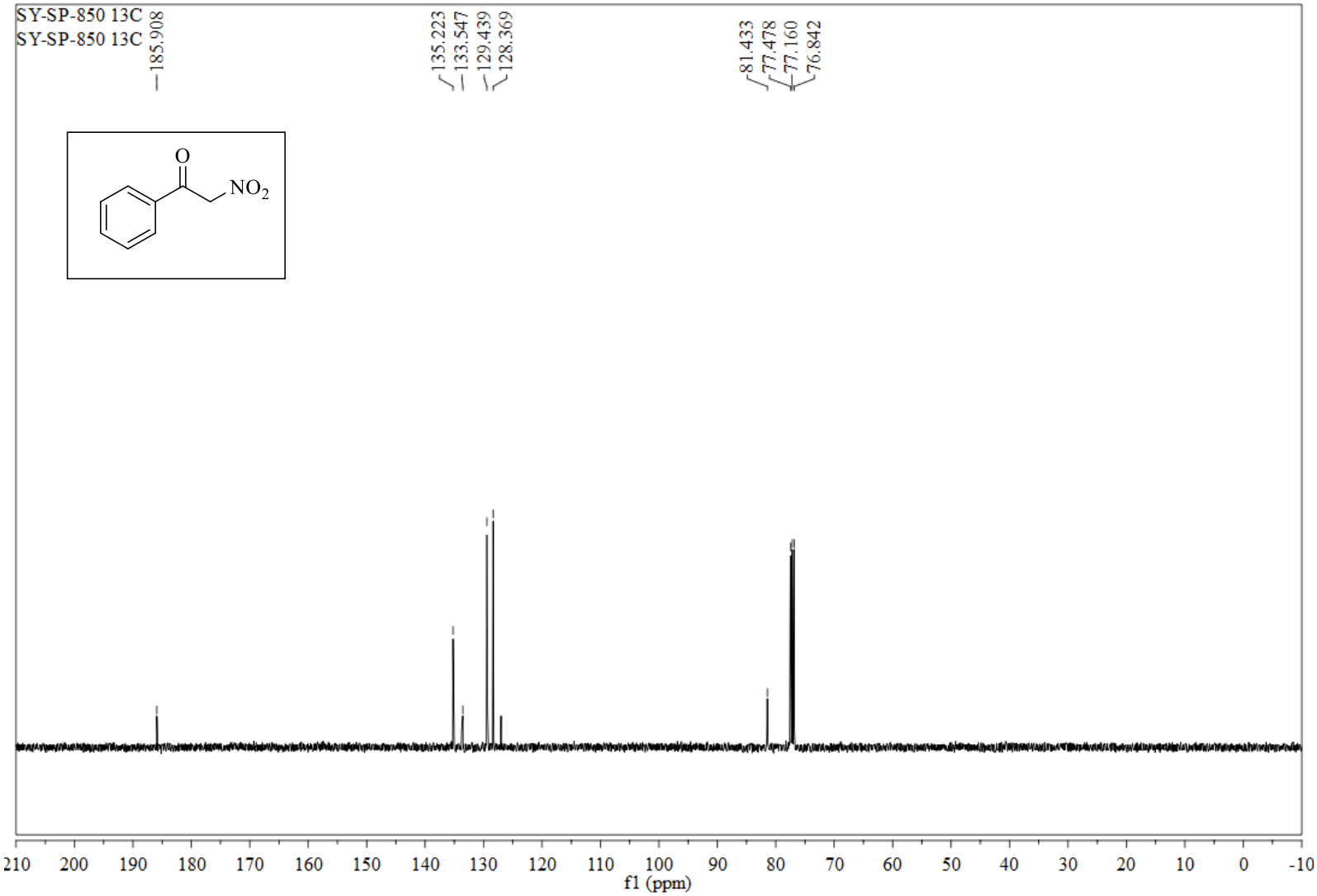

Figure S73. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10t.**

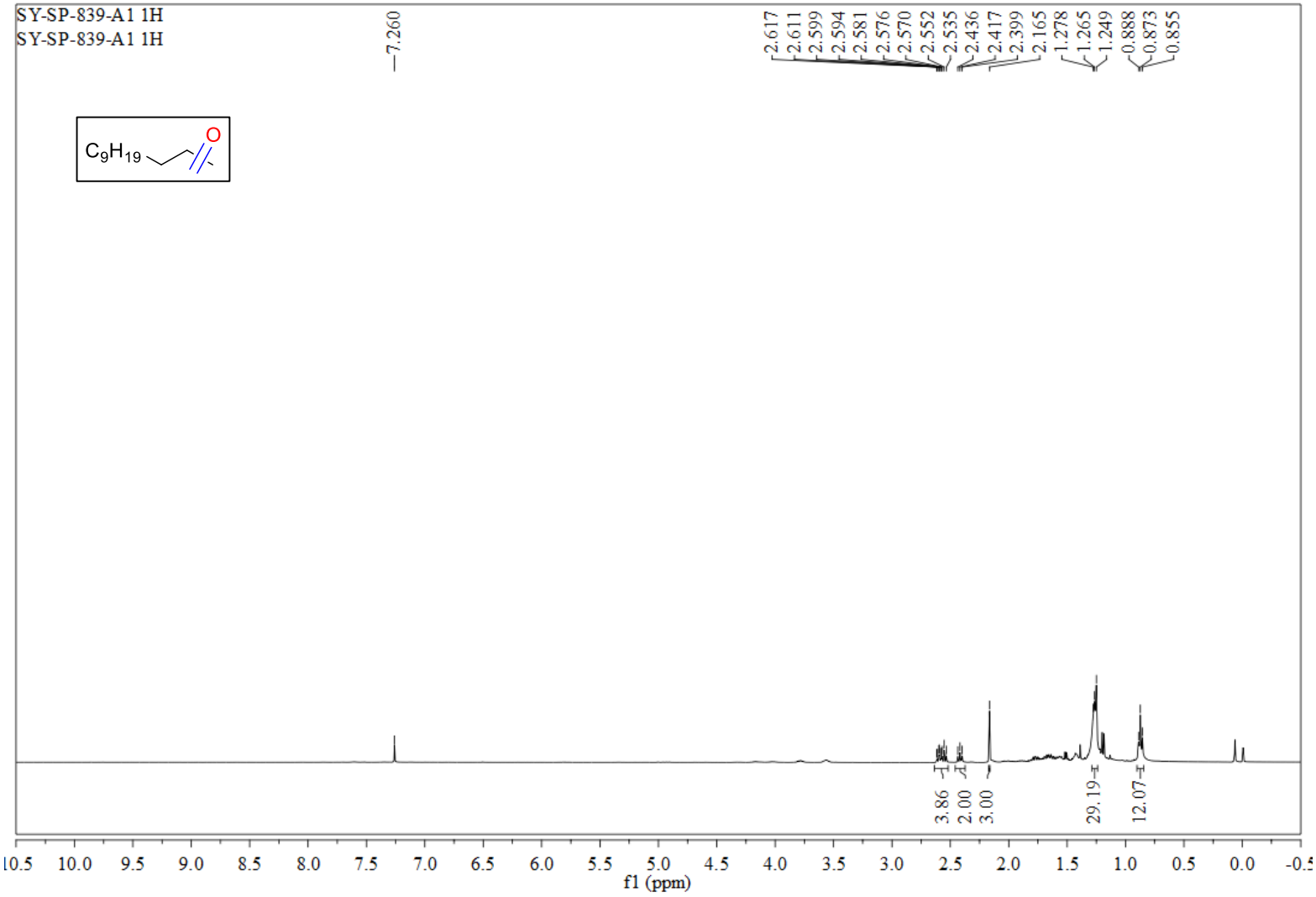

Figure S74. ^{1}H NMR (400 Mz, $CDCl_3$) of **10u.**

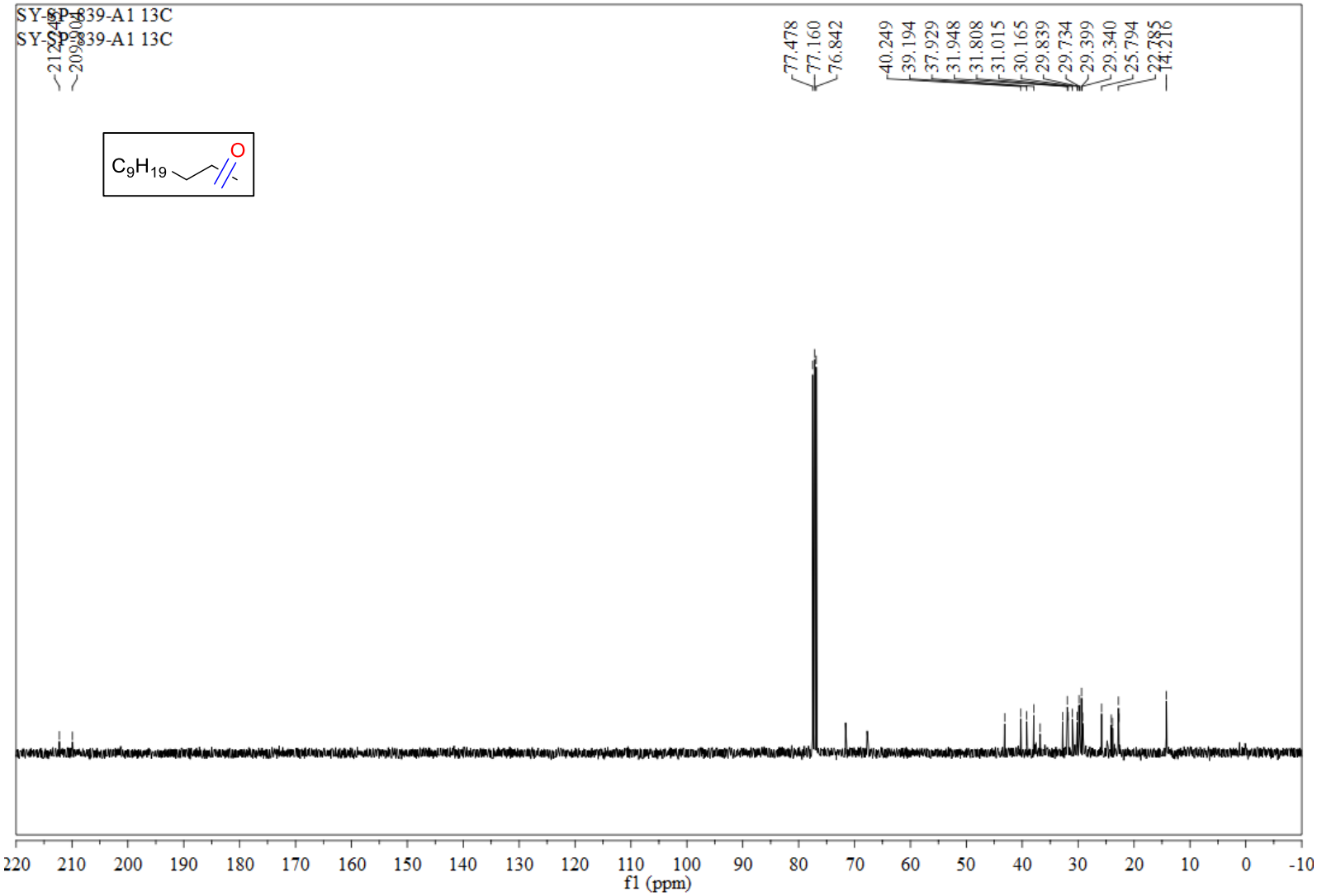

Figure S75. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **10u.**

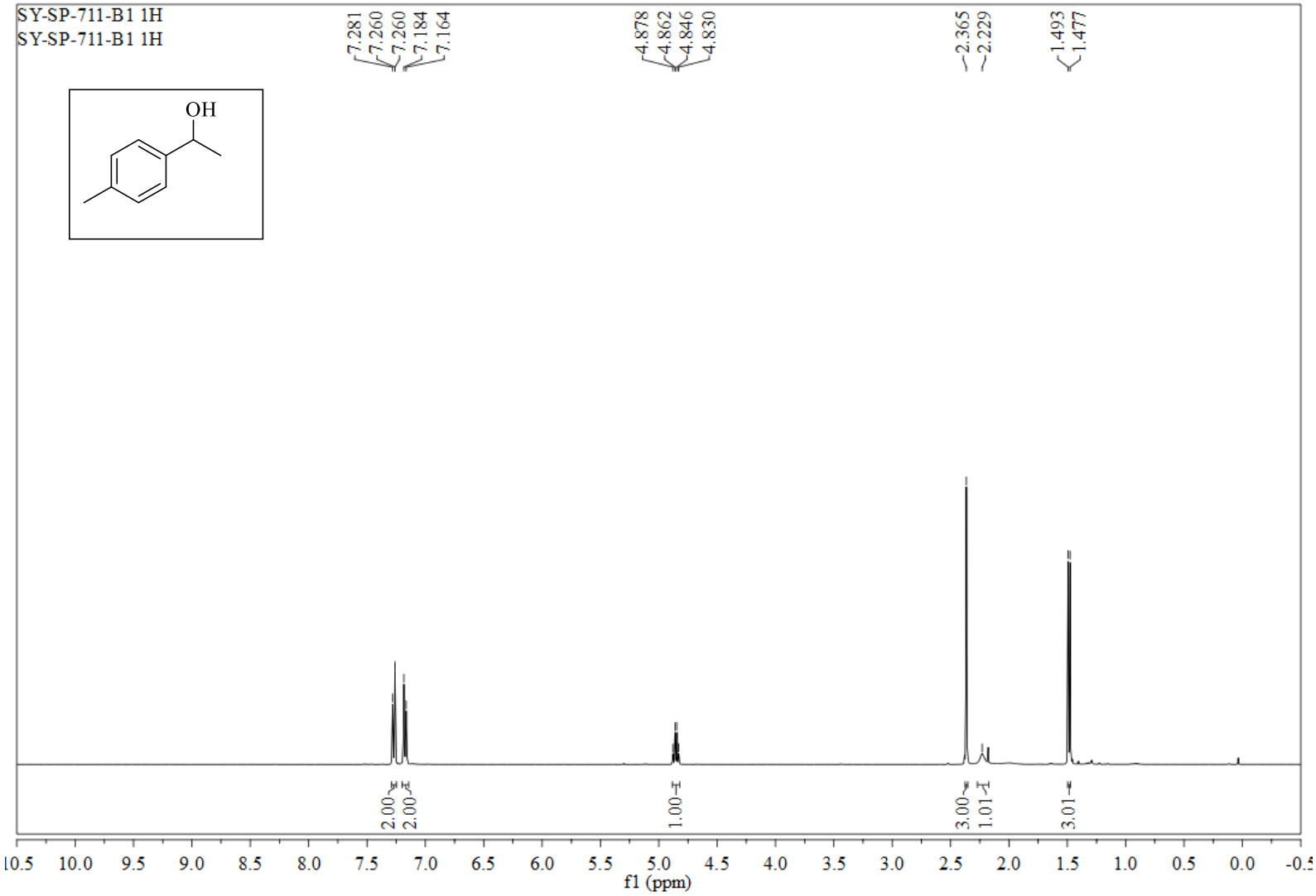

Figure S76. ^{1}H NMR (400 Mz, $CDCl_3$) of **11a**

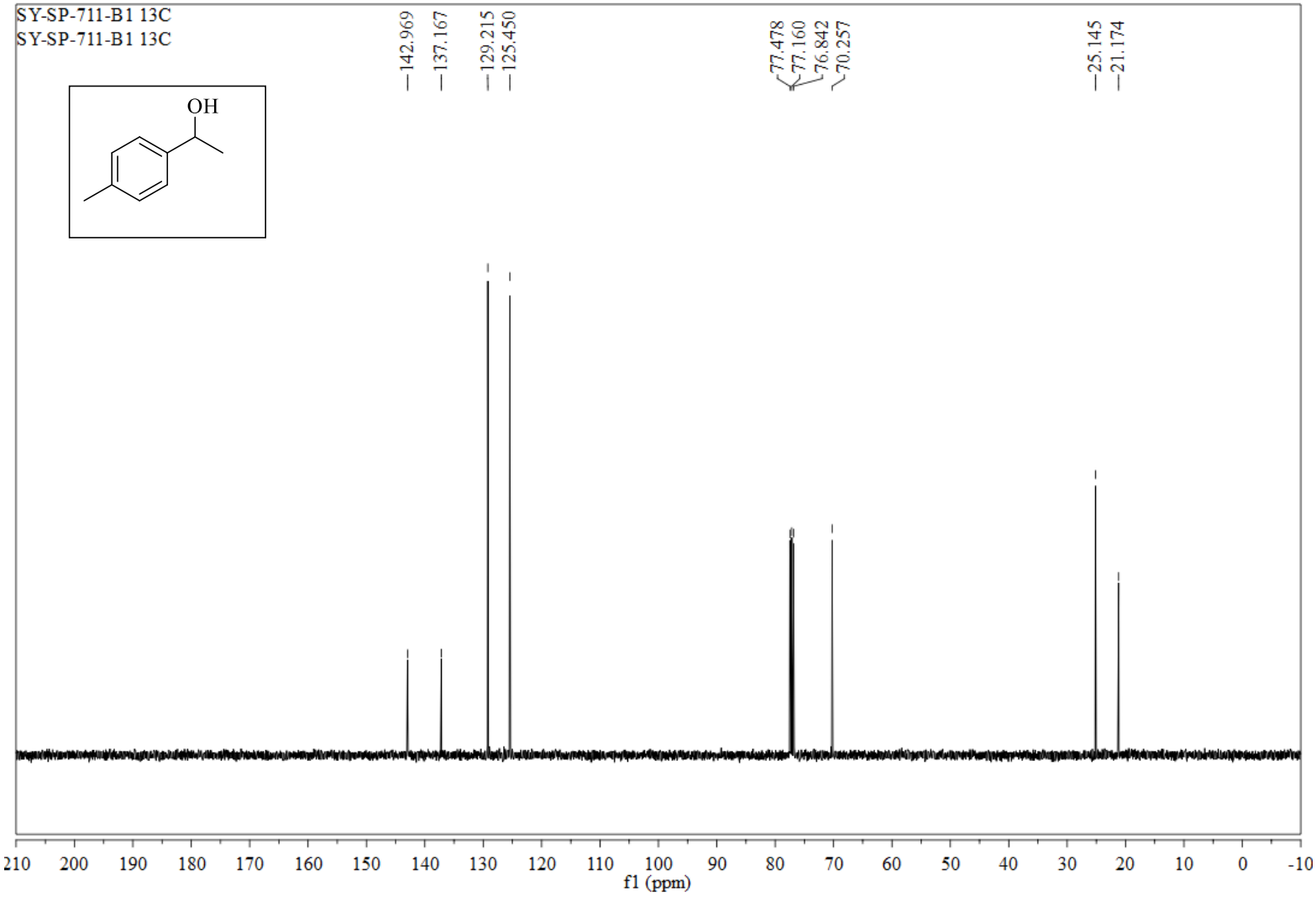

Figure S77. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11a**

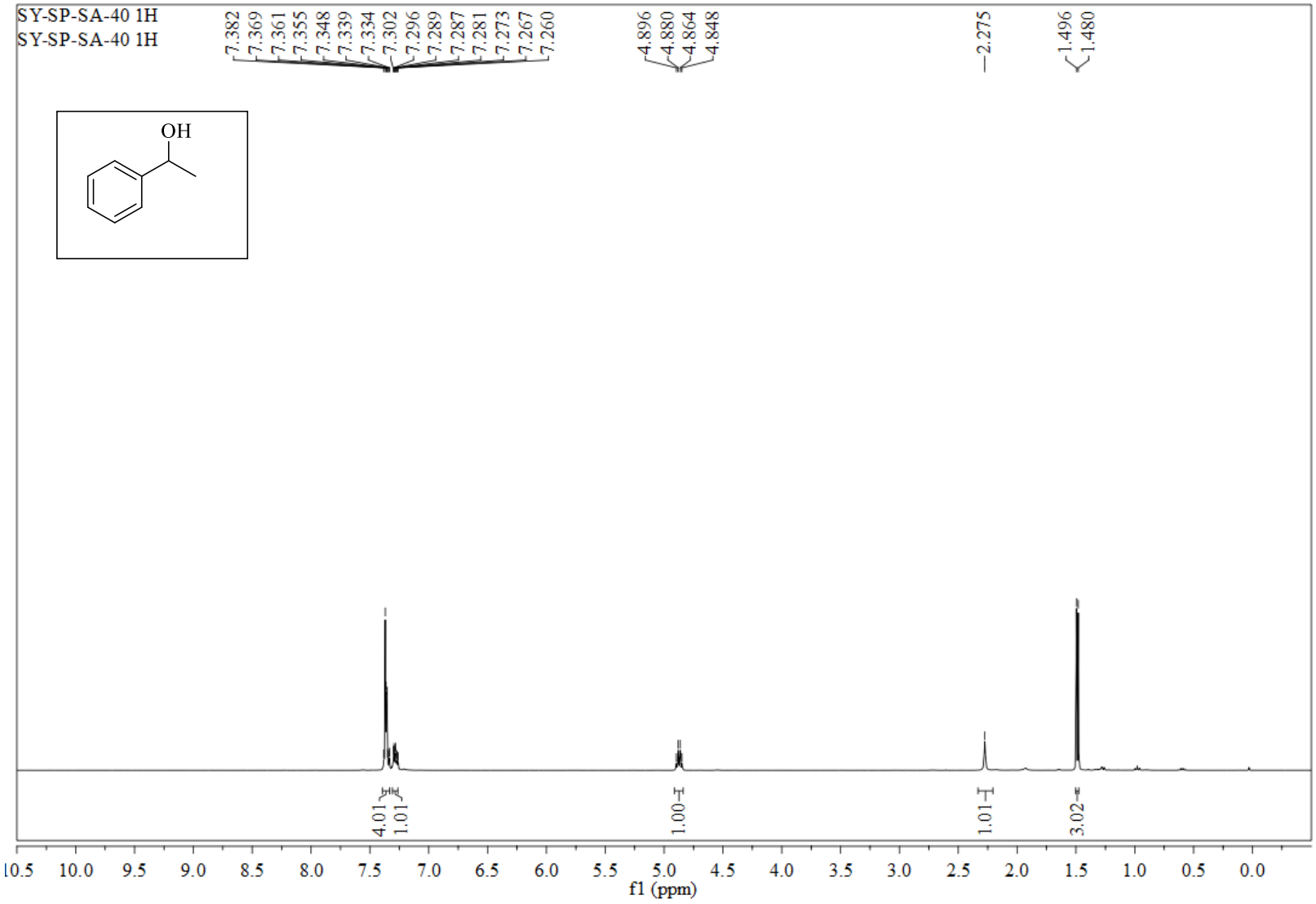

Figure S78. ^{1}H NMR (400 Mz, $CDCl_3$) of **11b**

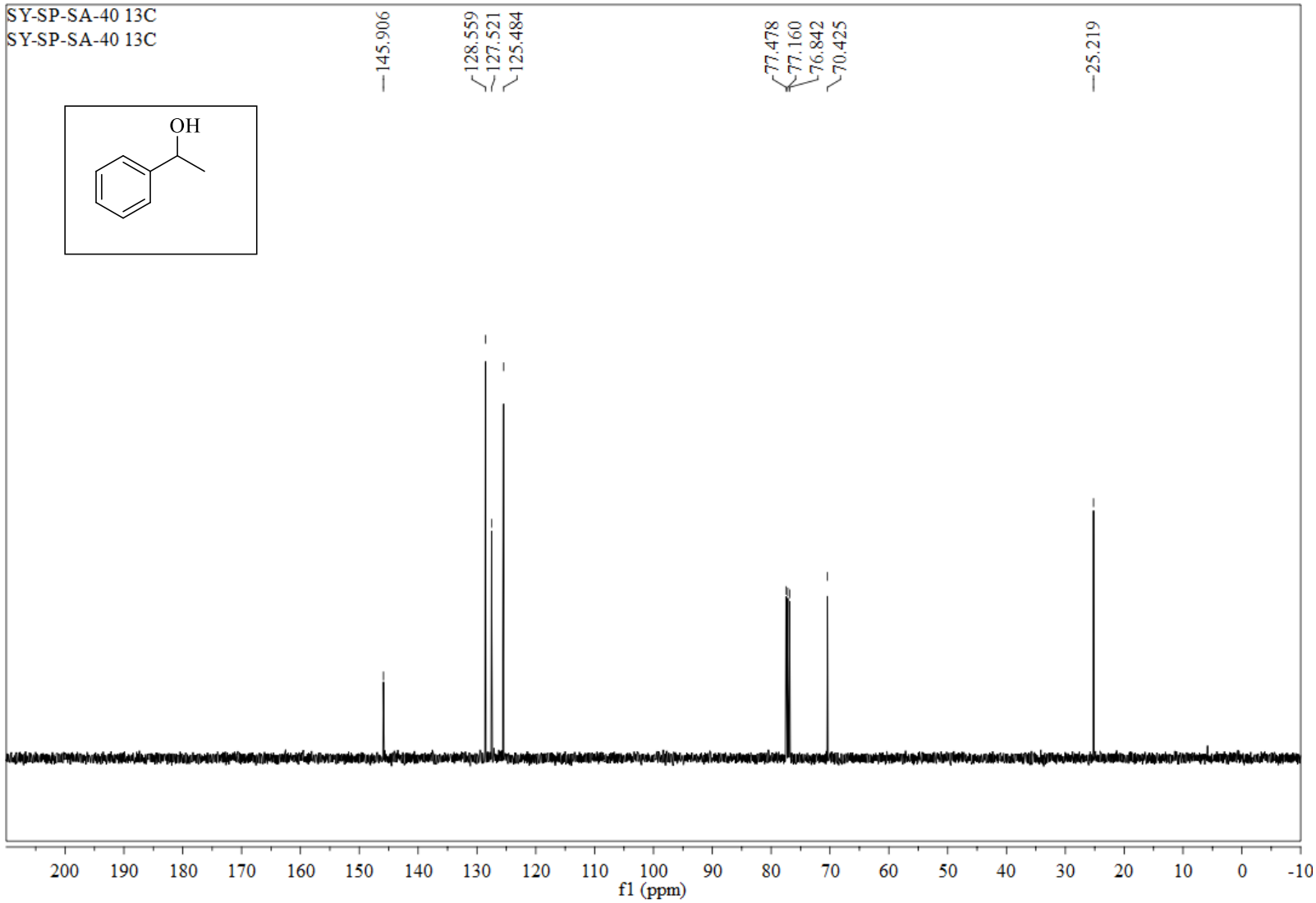

Figure S79. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11b**

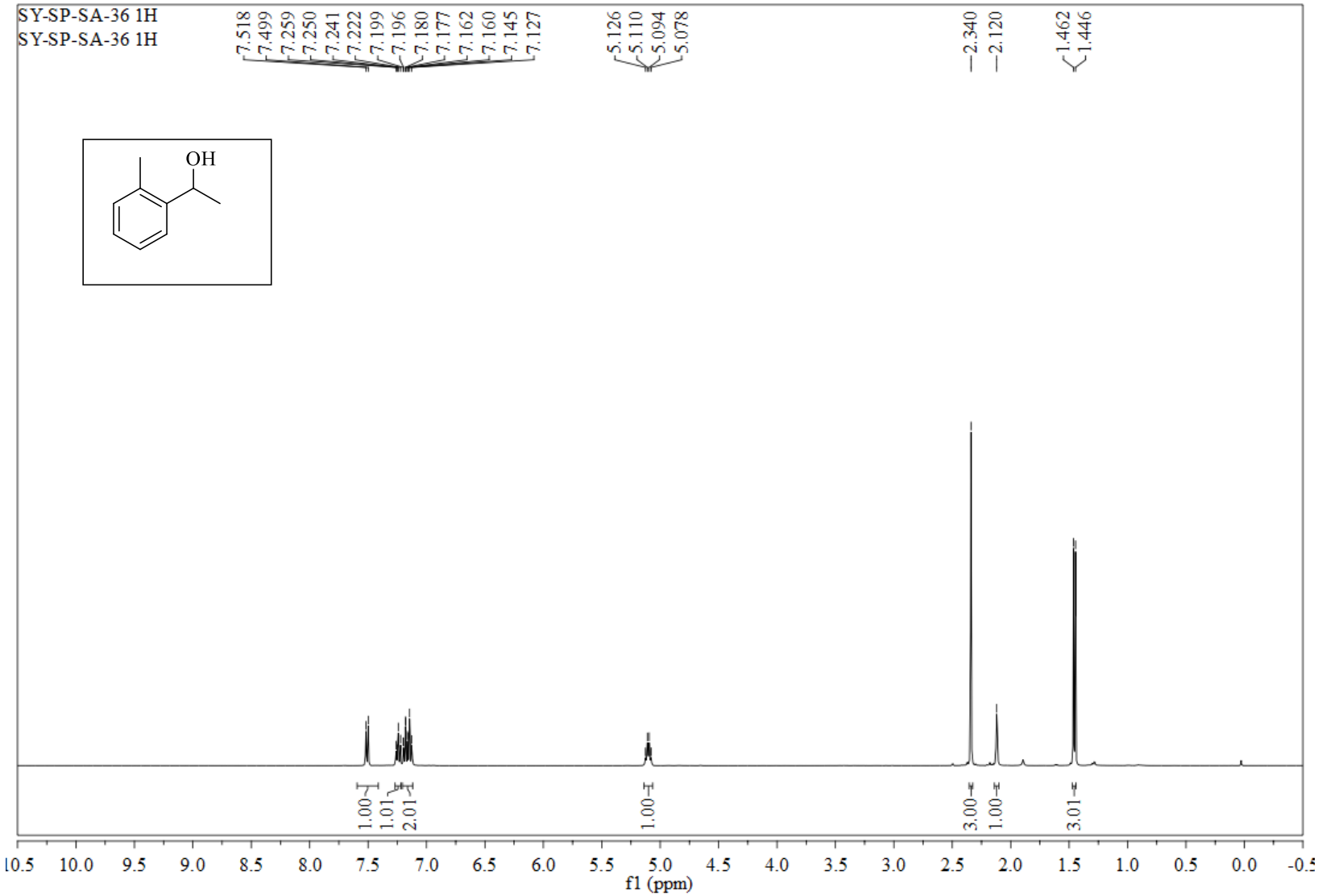

Figure S80. ^{1}H NMR (400 Mz, $CDCl_3$) of **11c.**

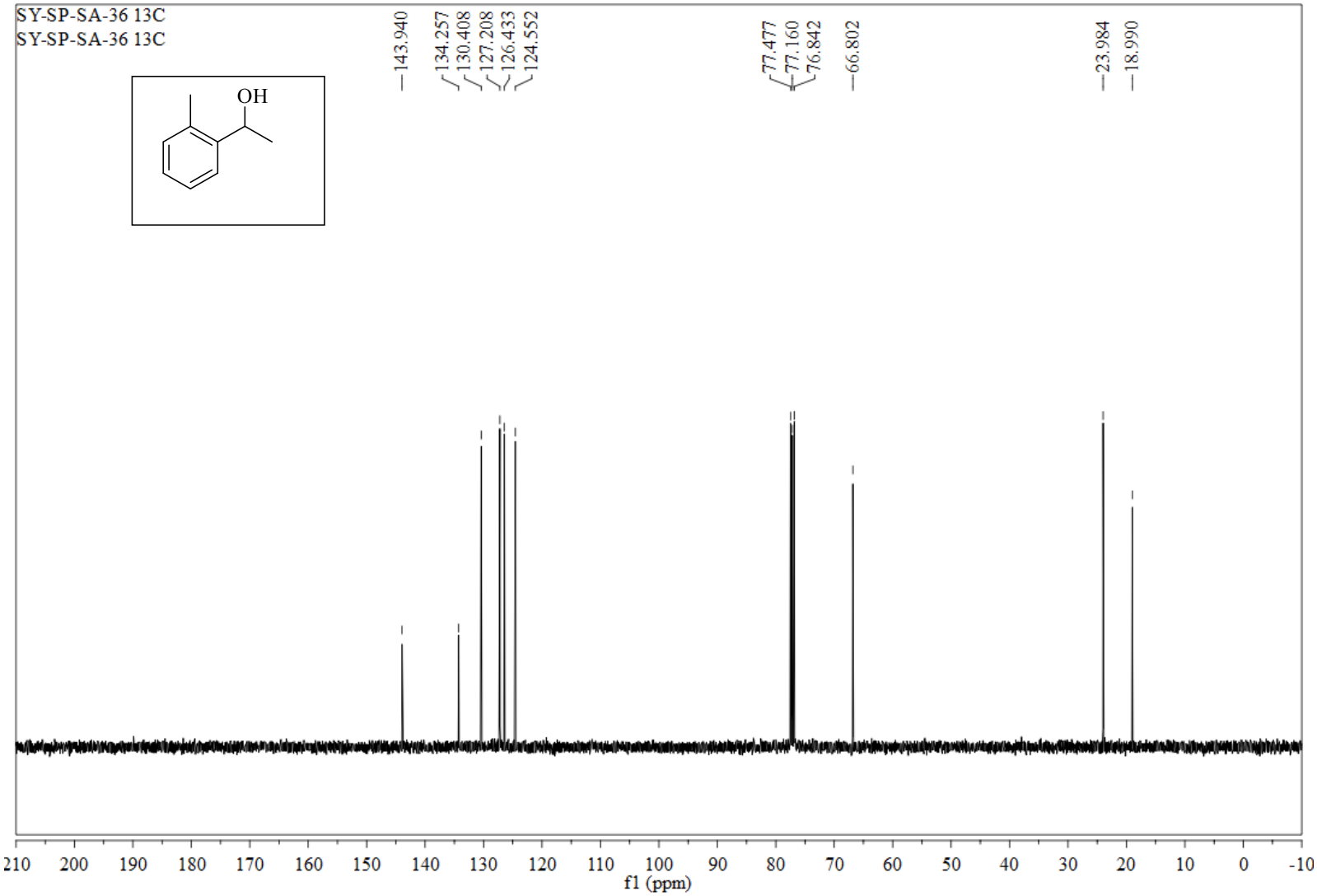

Figure S81. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11c**

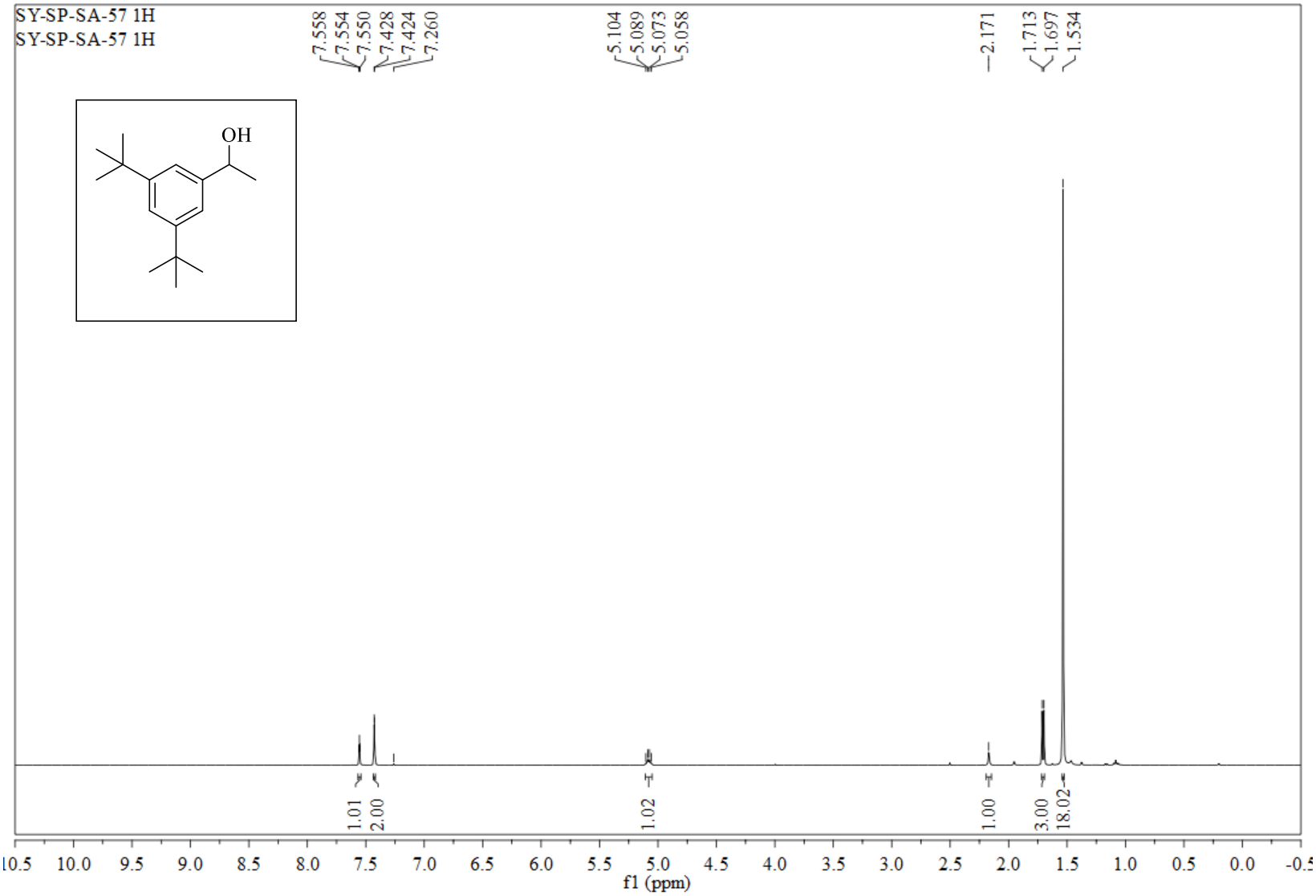

Figure S82. ^{1}H NMR (400 Mz, $CDCl_3$) of **11d**

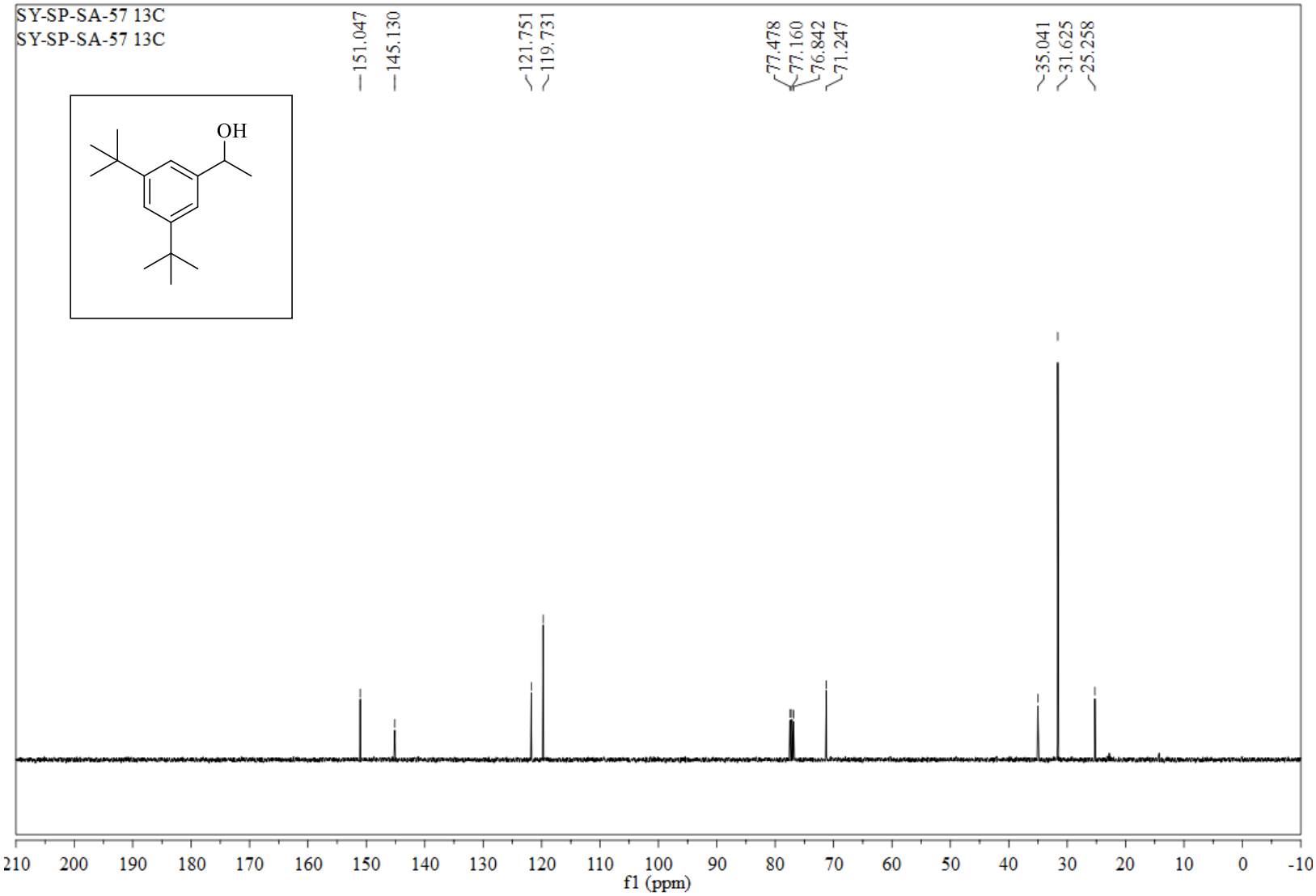

Figure S83. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11d**

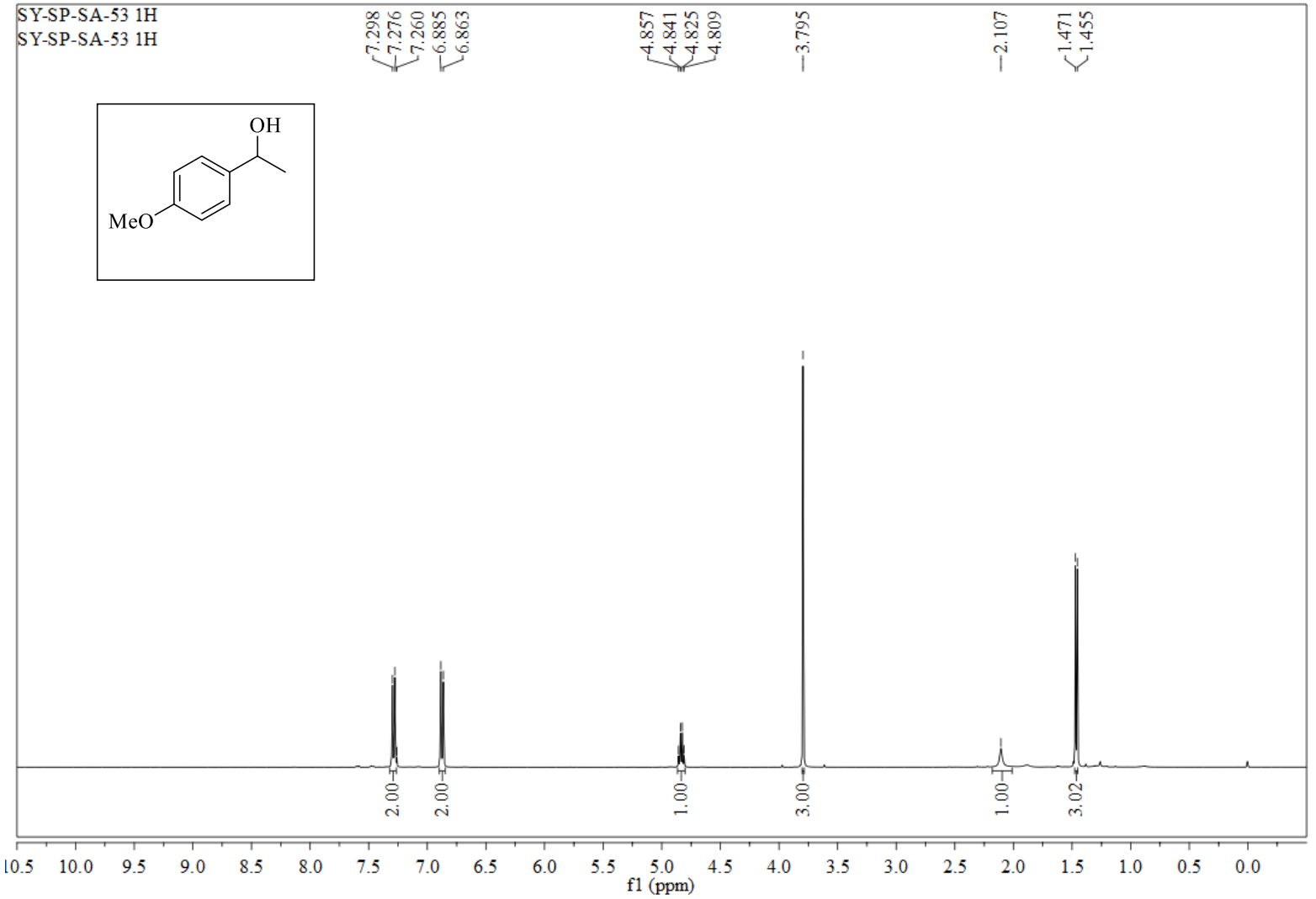

Figure S84. ^{1}H NMR (400 Mz, $CDCl_3$) of **11e**

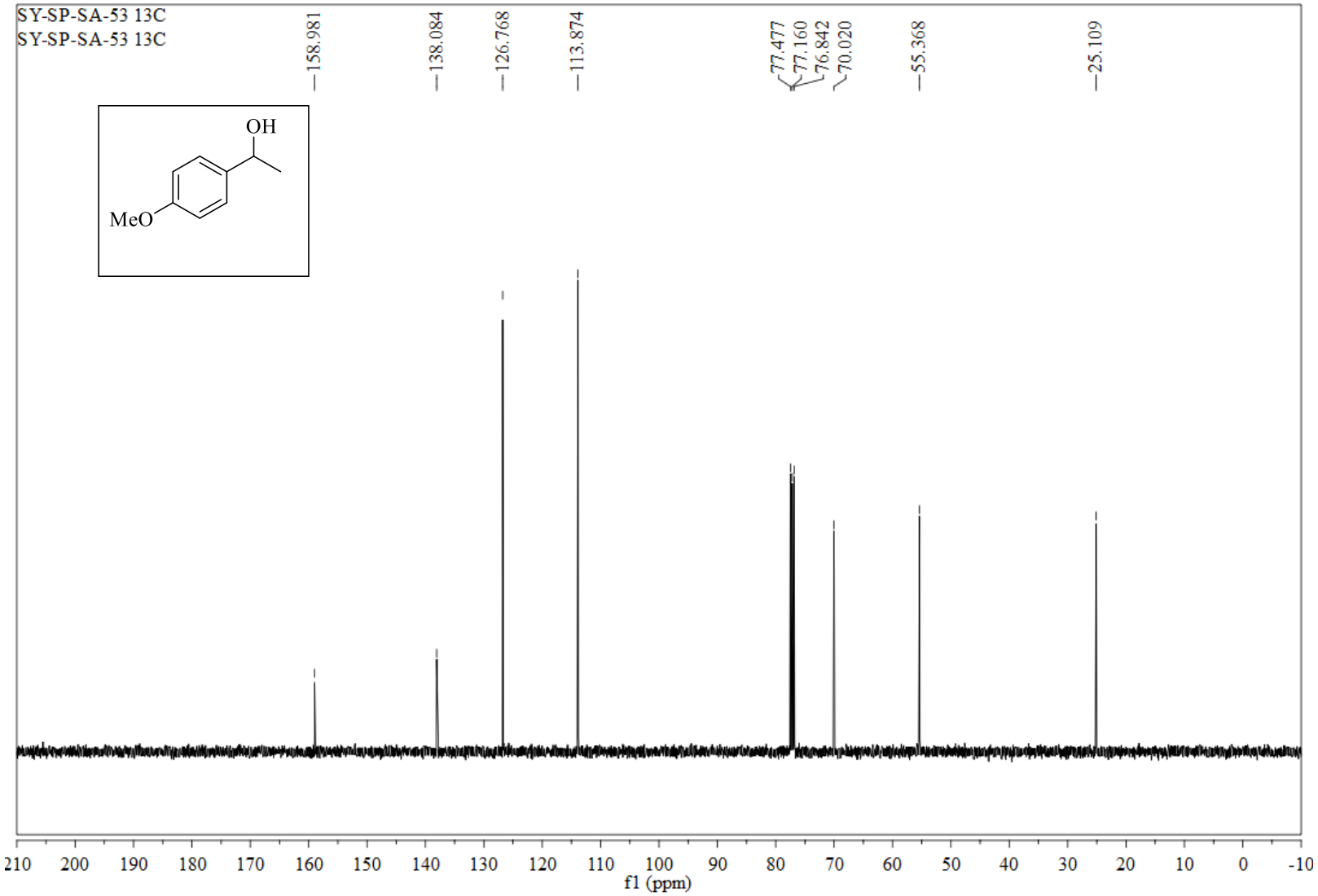

Figure S85. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11e**

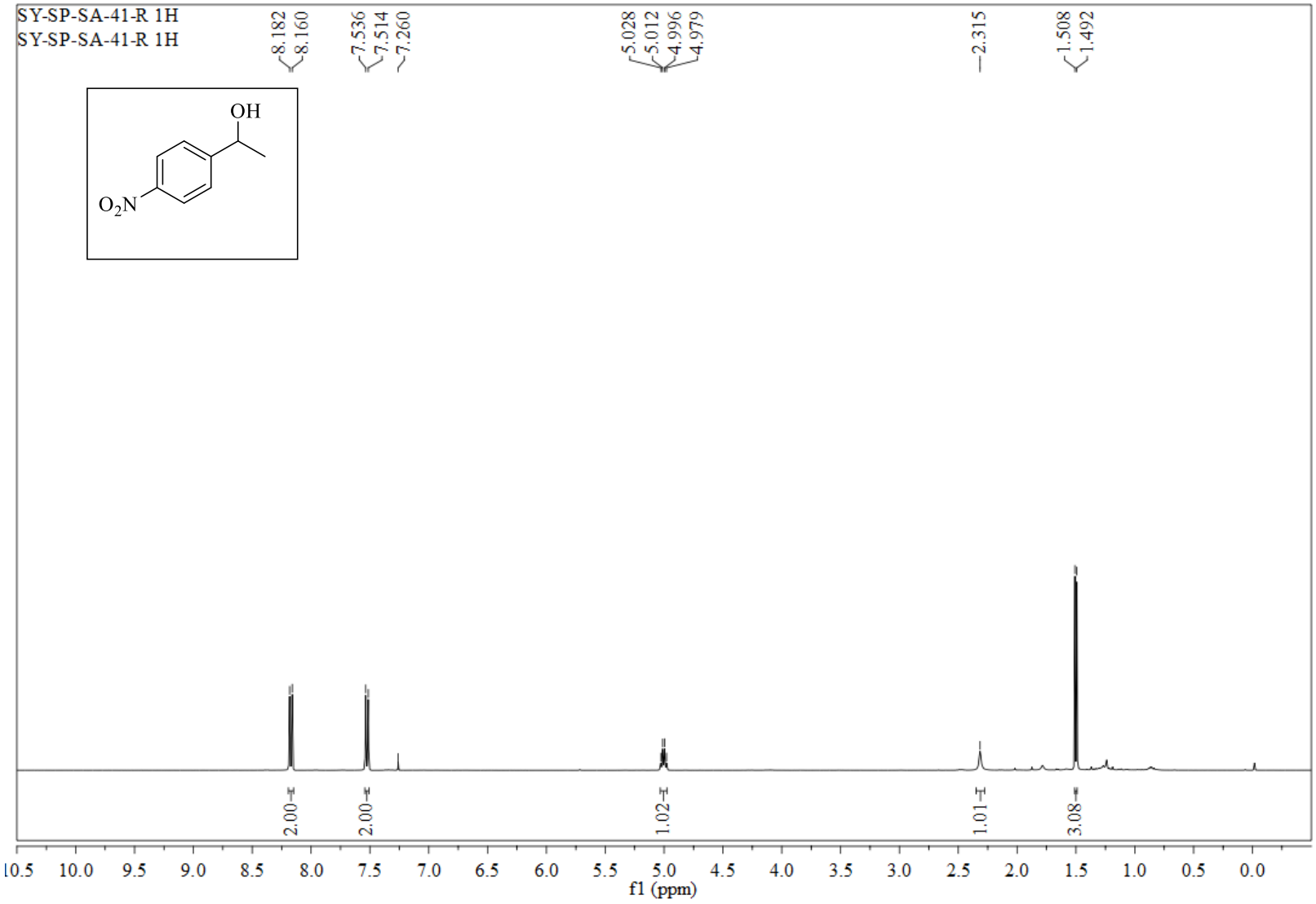

Figure S86. ^{1}H NMR (400 Mz, $CDCl_3$) of **11f**

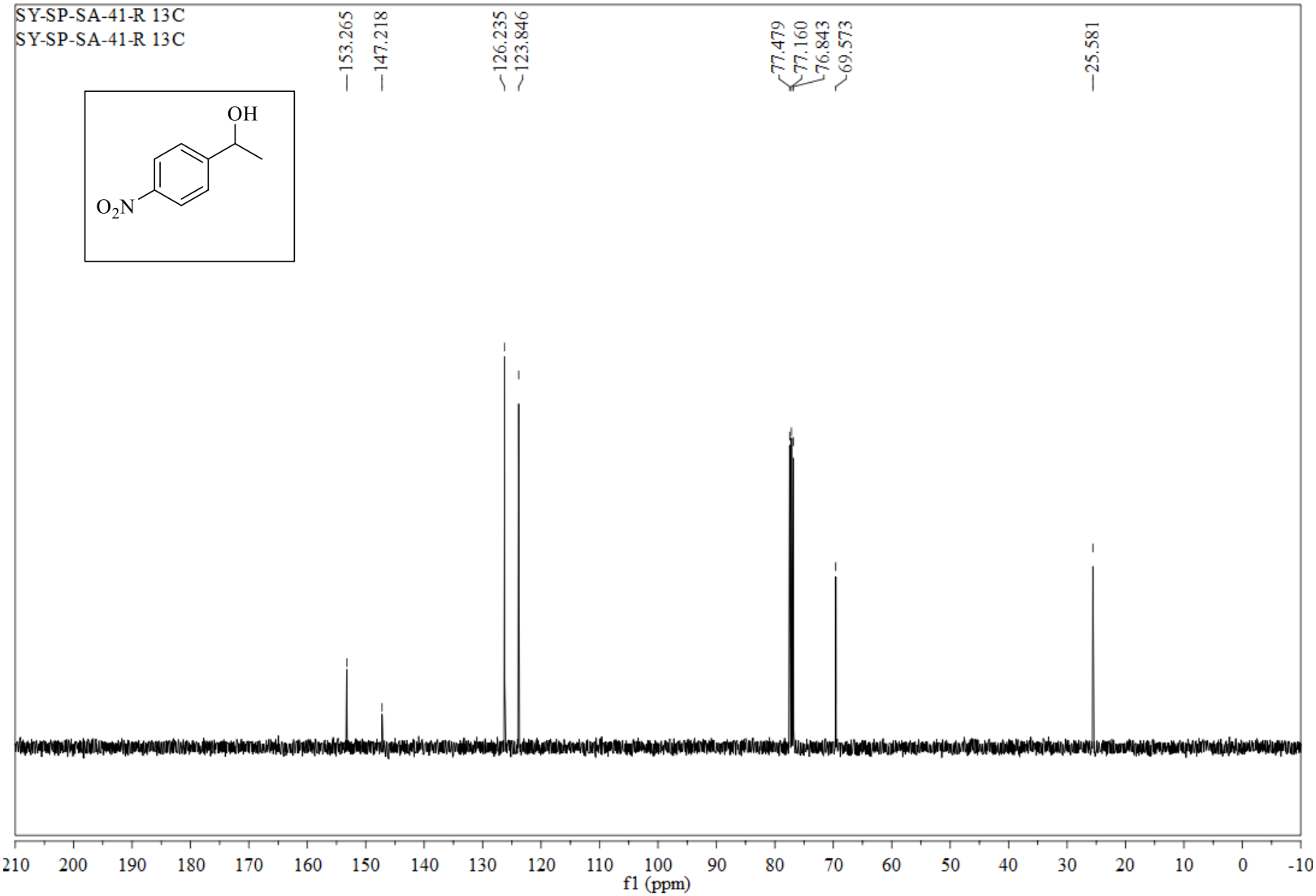

Figure S87.^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11f**

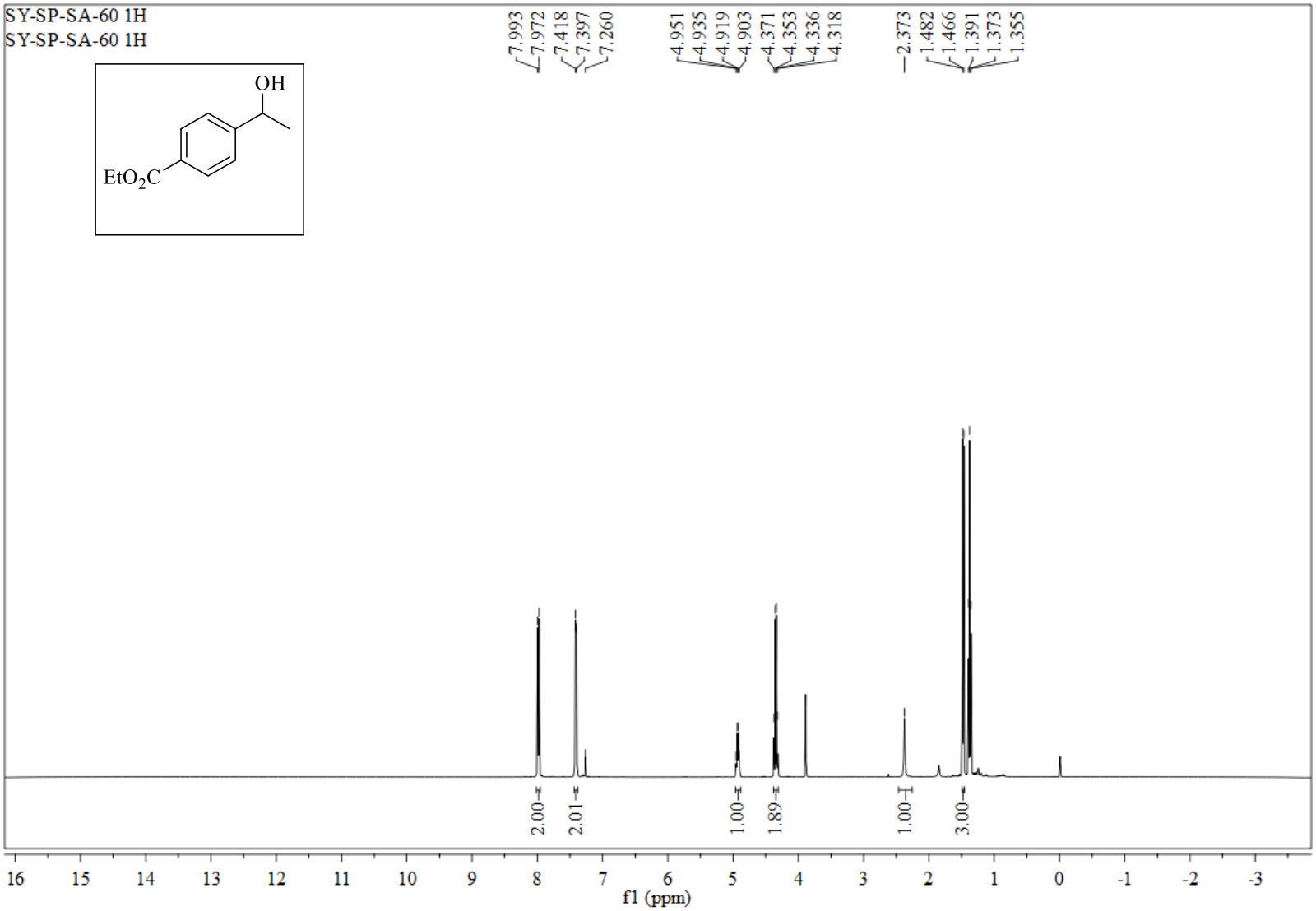

Figure S88. ^{1}H NMR (400 Mz, $CDCl_3$) of **11g**

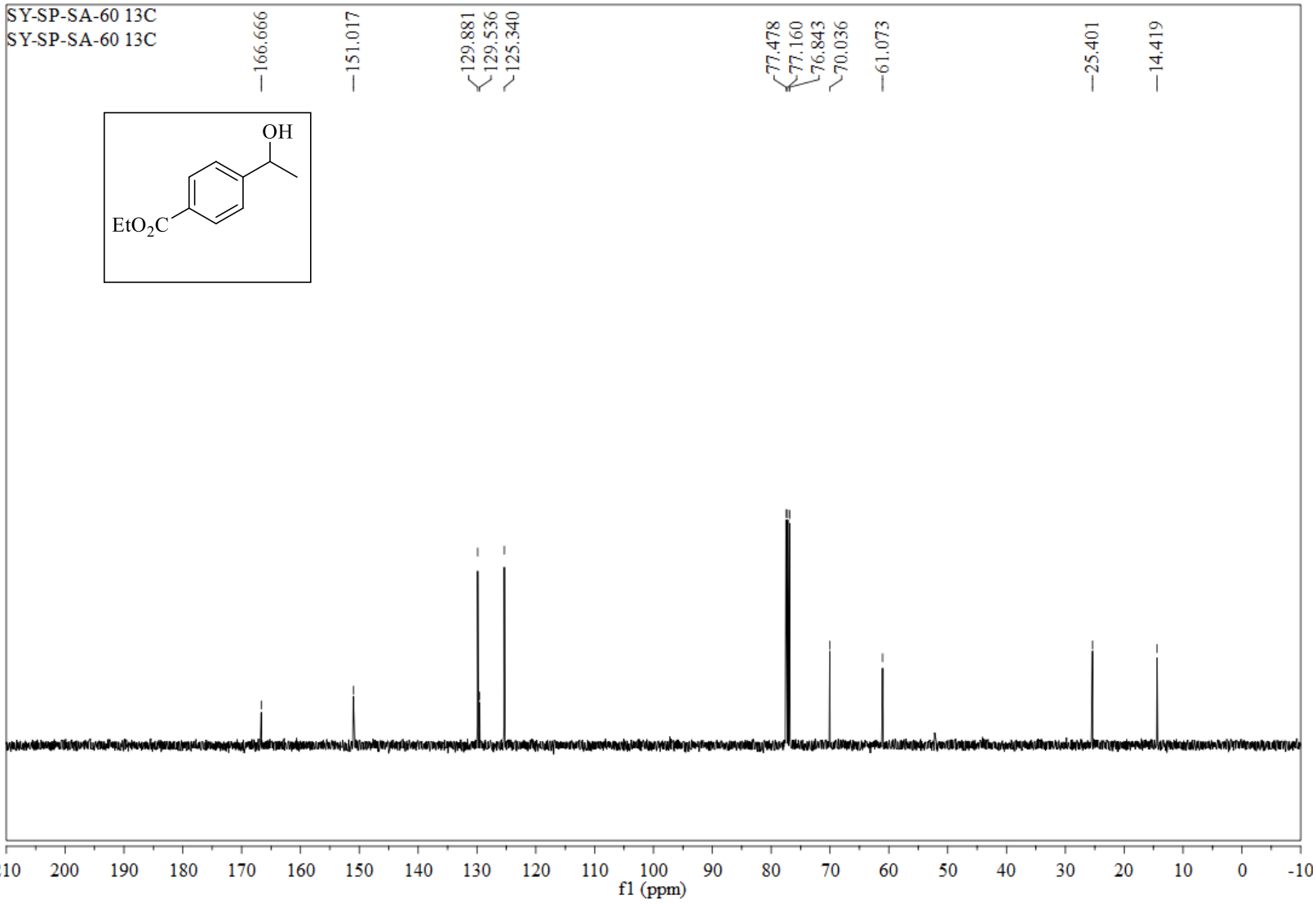

Figure S89. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11g**

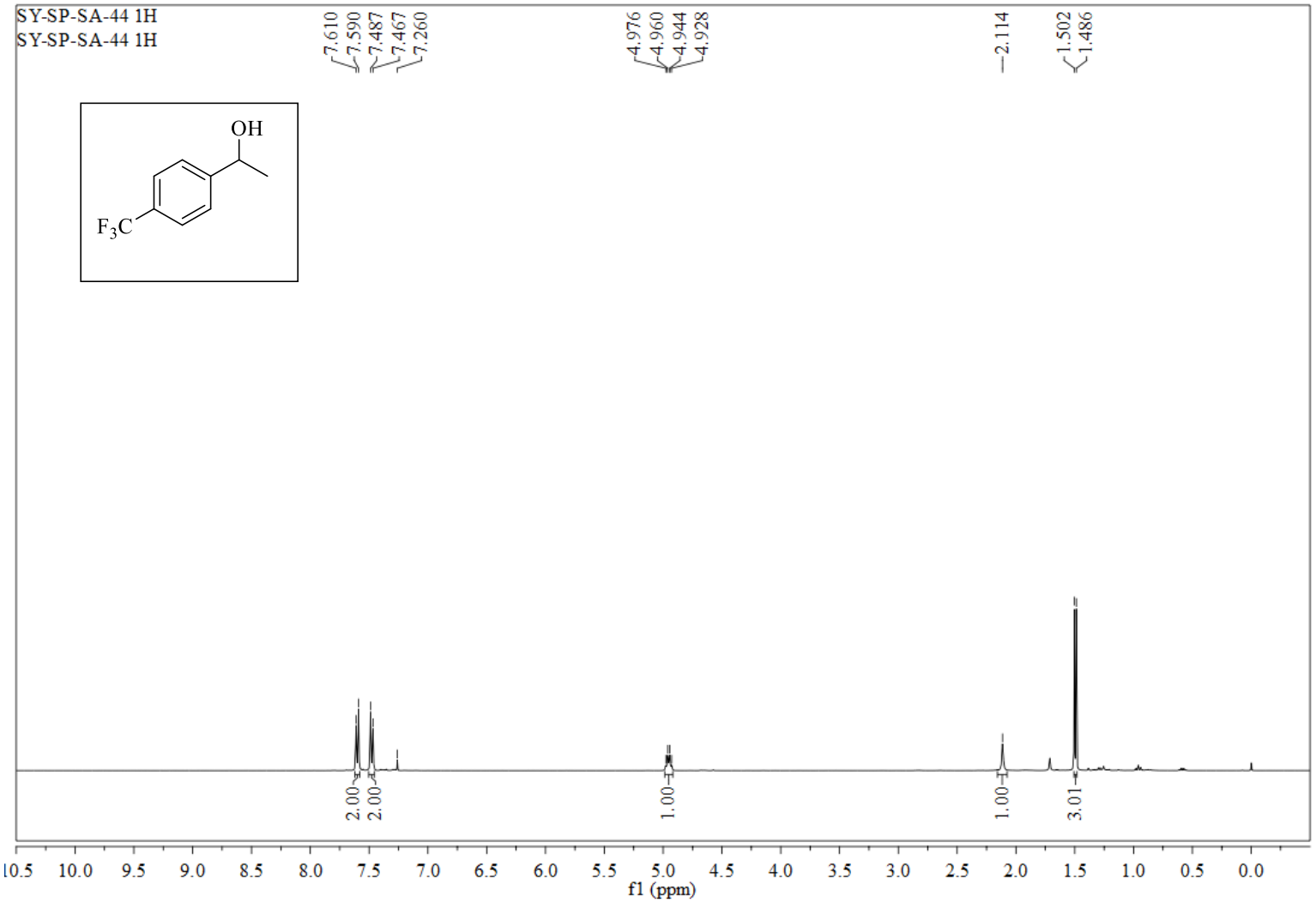

Figure S90. ^{1}H NMR (400 Mz, $CDCl_3$) of **11h**

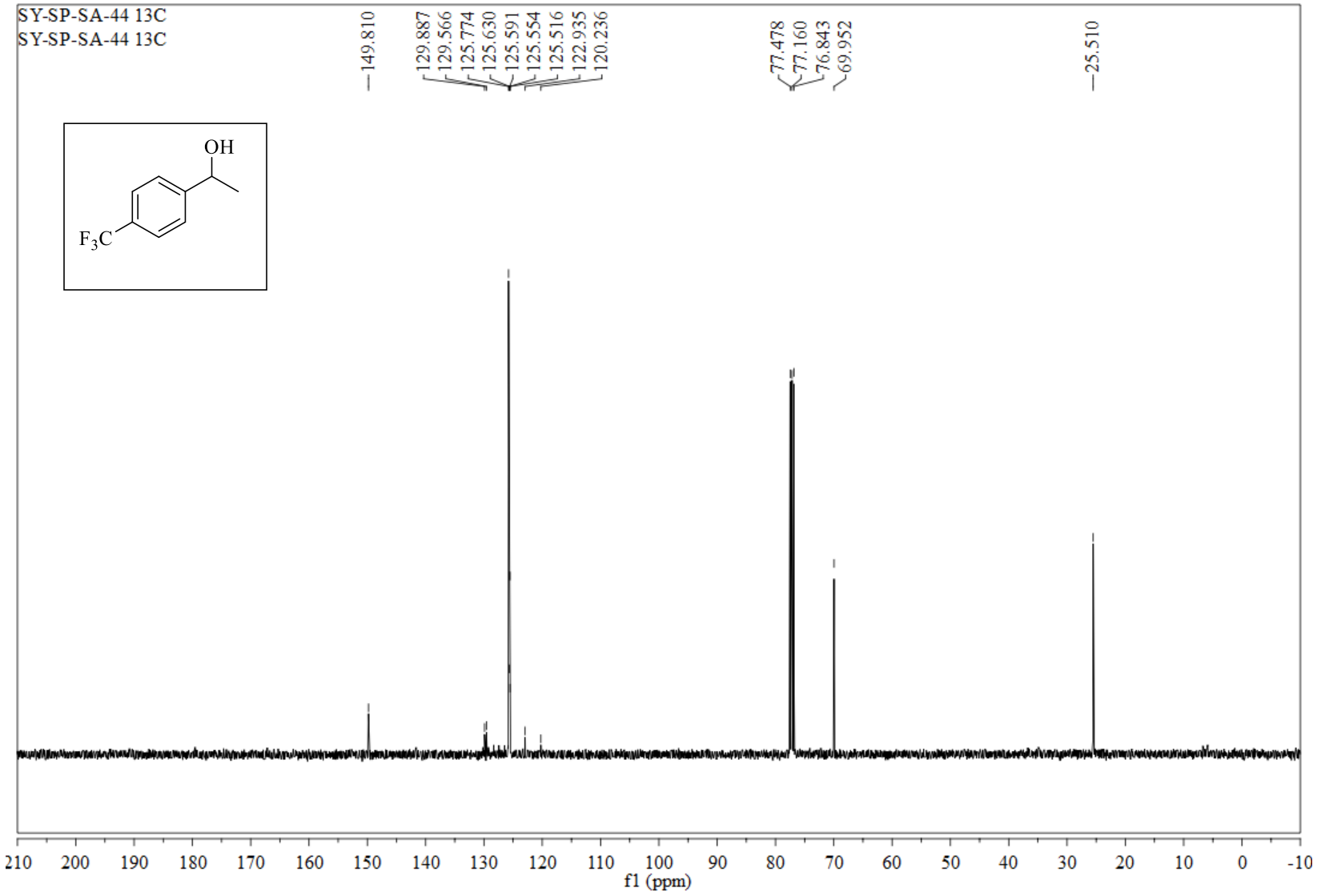

Figure S91. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11h**

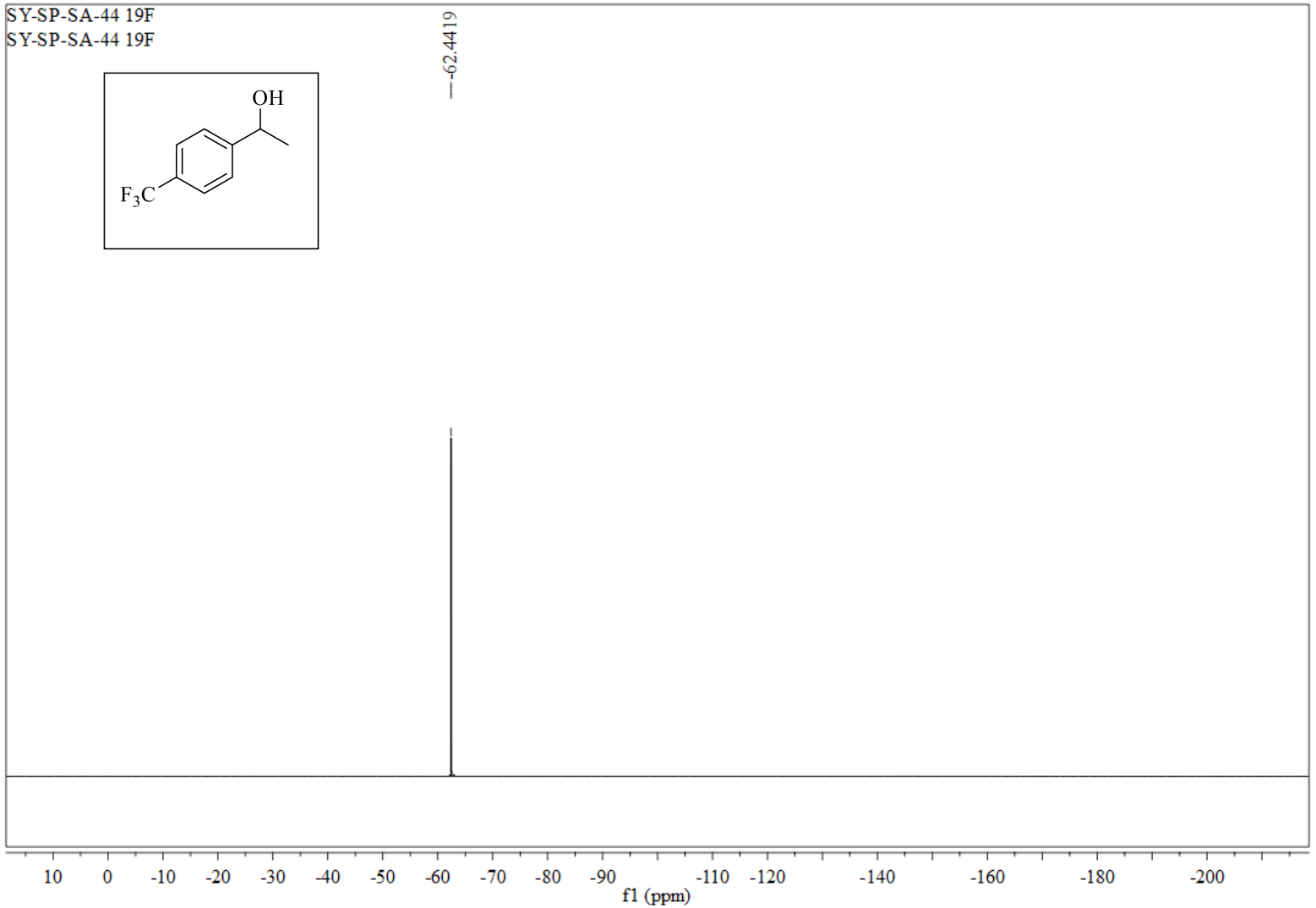

Figure S92. ^{19}F NMR (376 Mz, $CDCl_3$) of **11h**

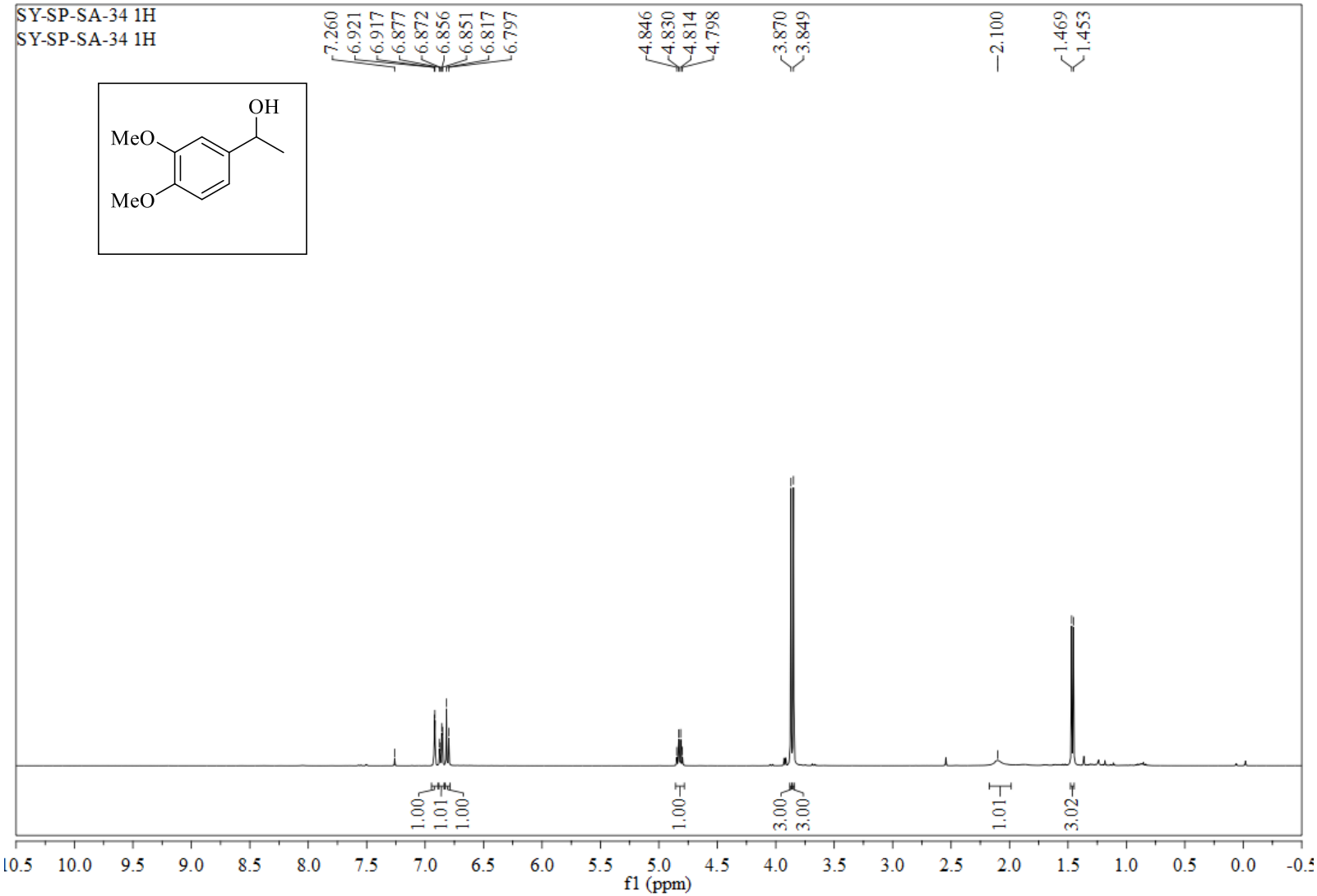

Figure S93. ^{1}H NMR (400 Mz, $CDCl_3$) of **11i**

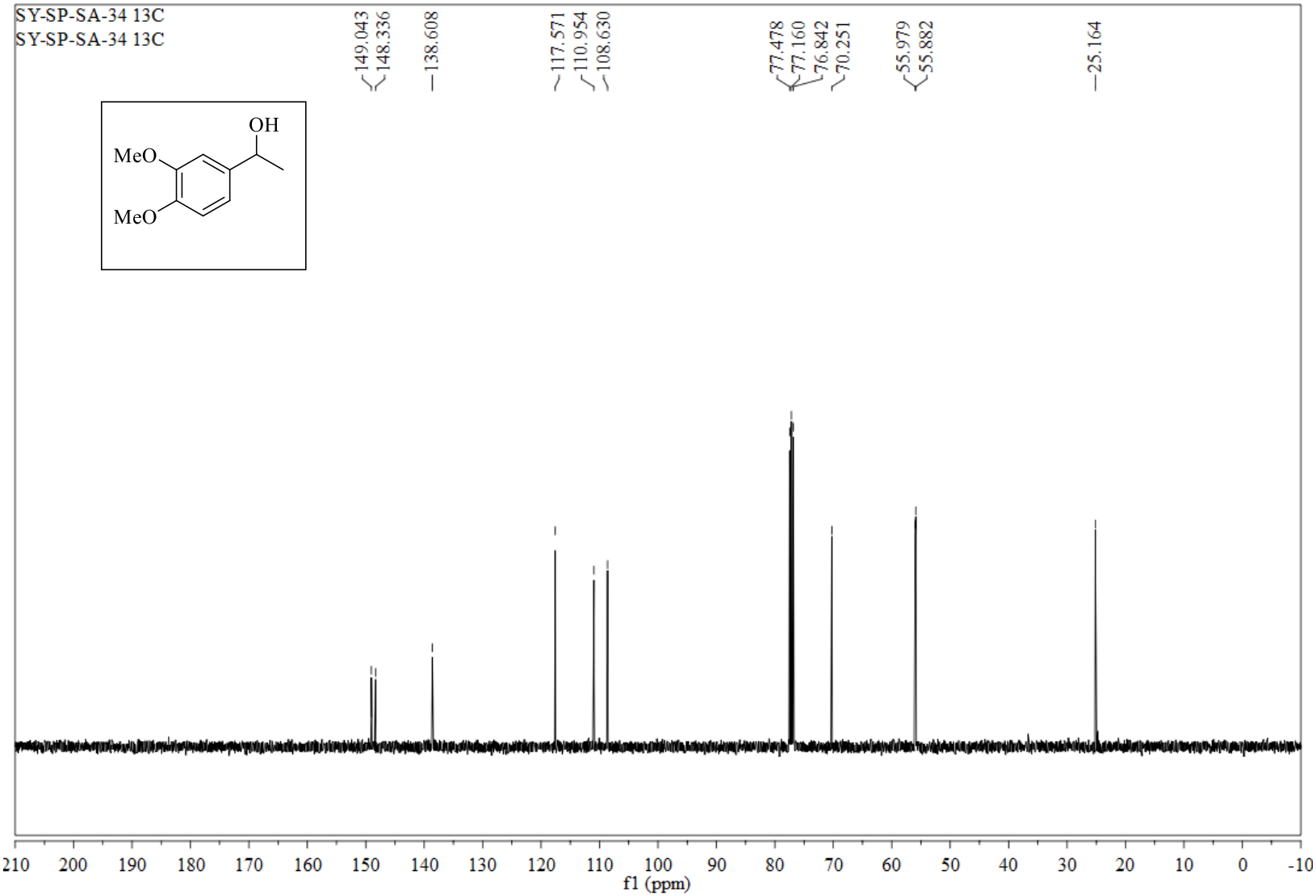

Figure S94. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11i**

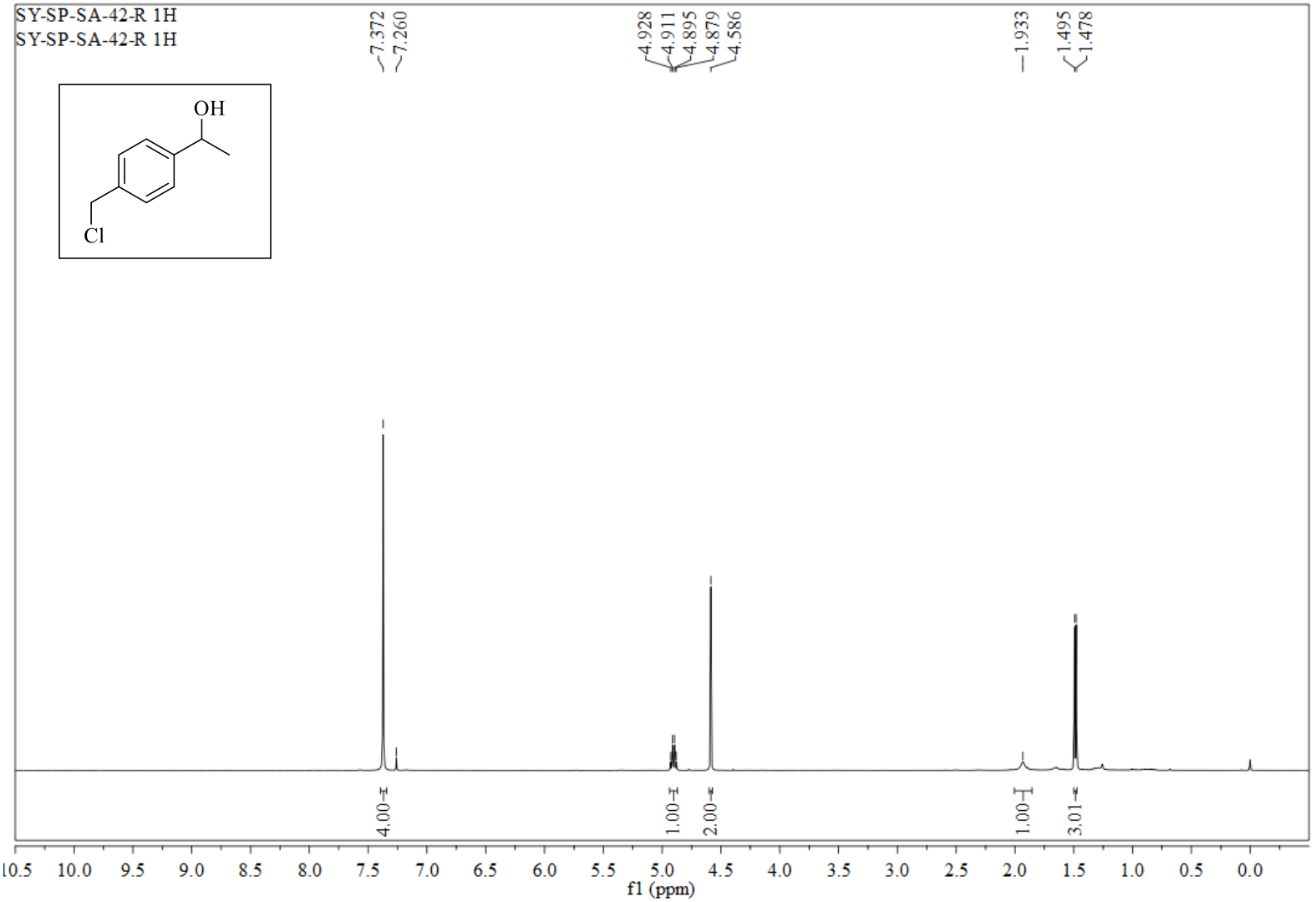

Figure S95. ^{1}H NMR (400 Mz, $CDCl_3$) of **11j**

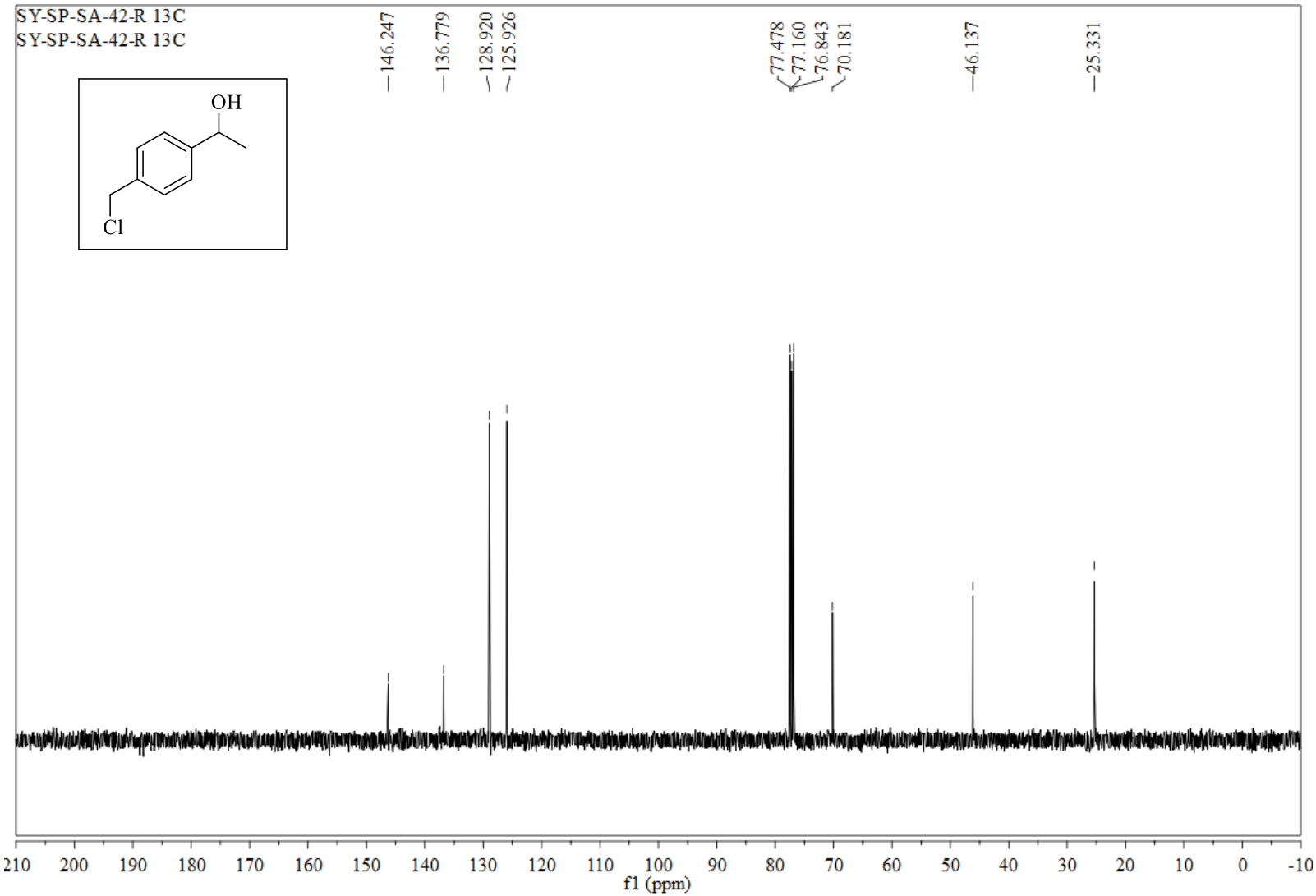

Figure S96. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11j**

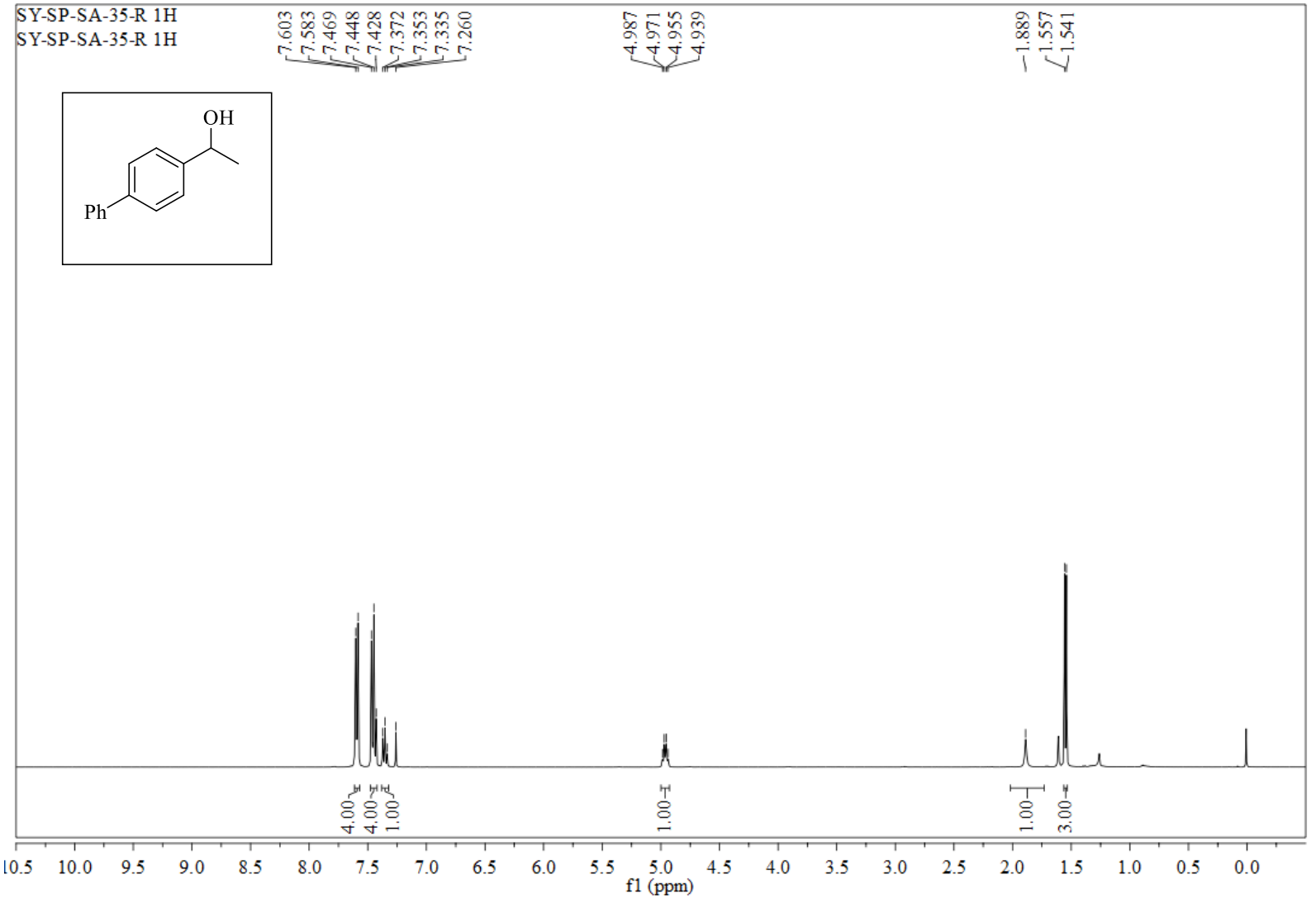

Figure S97. ^{1}H NMR (400 Mz, $CDCl_3$) of **11k**

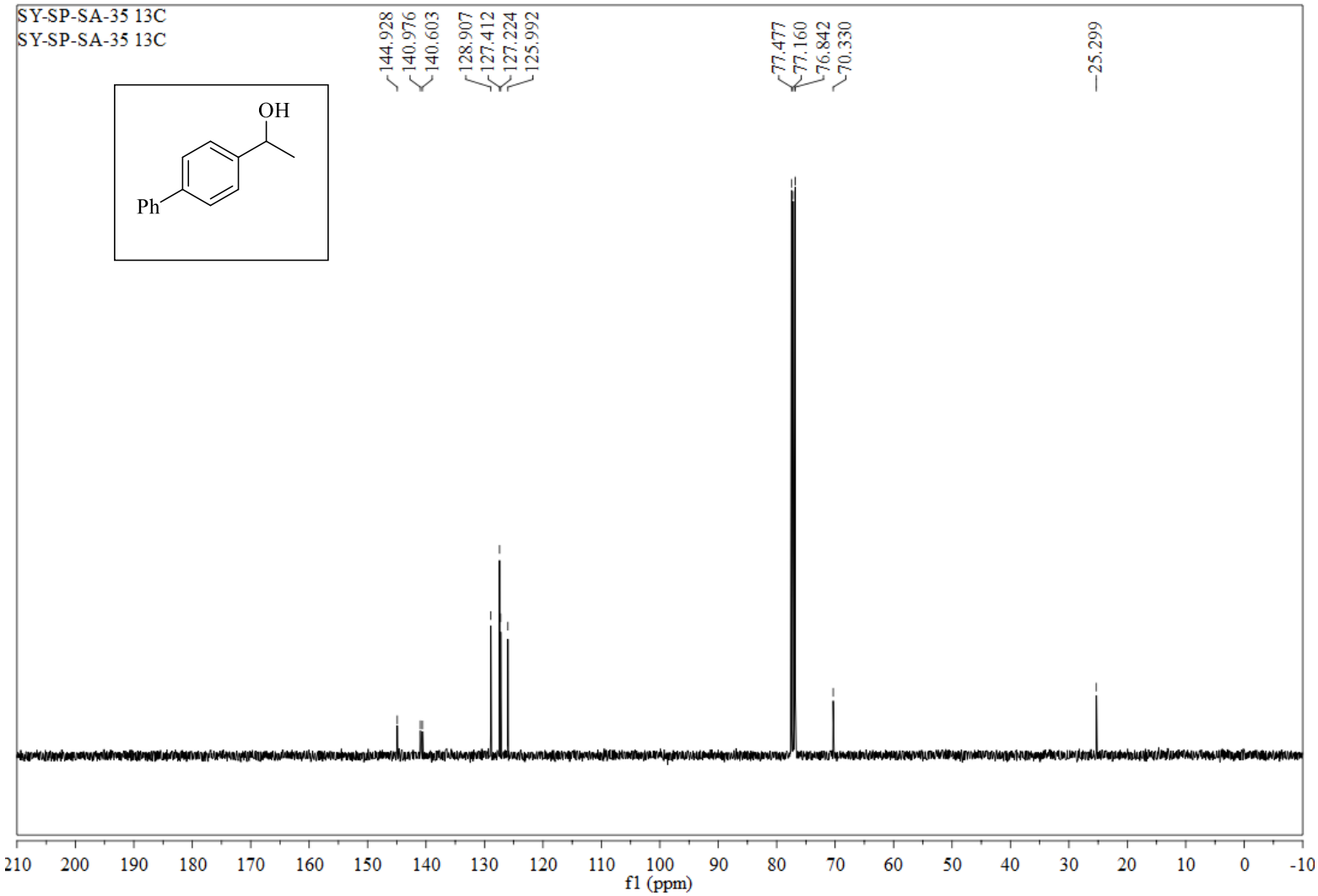

Figure S98. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11k**

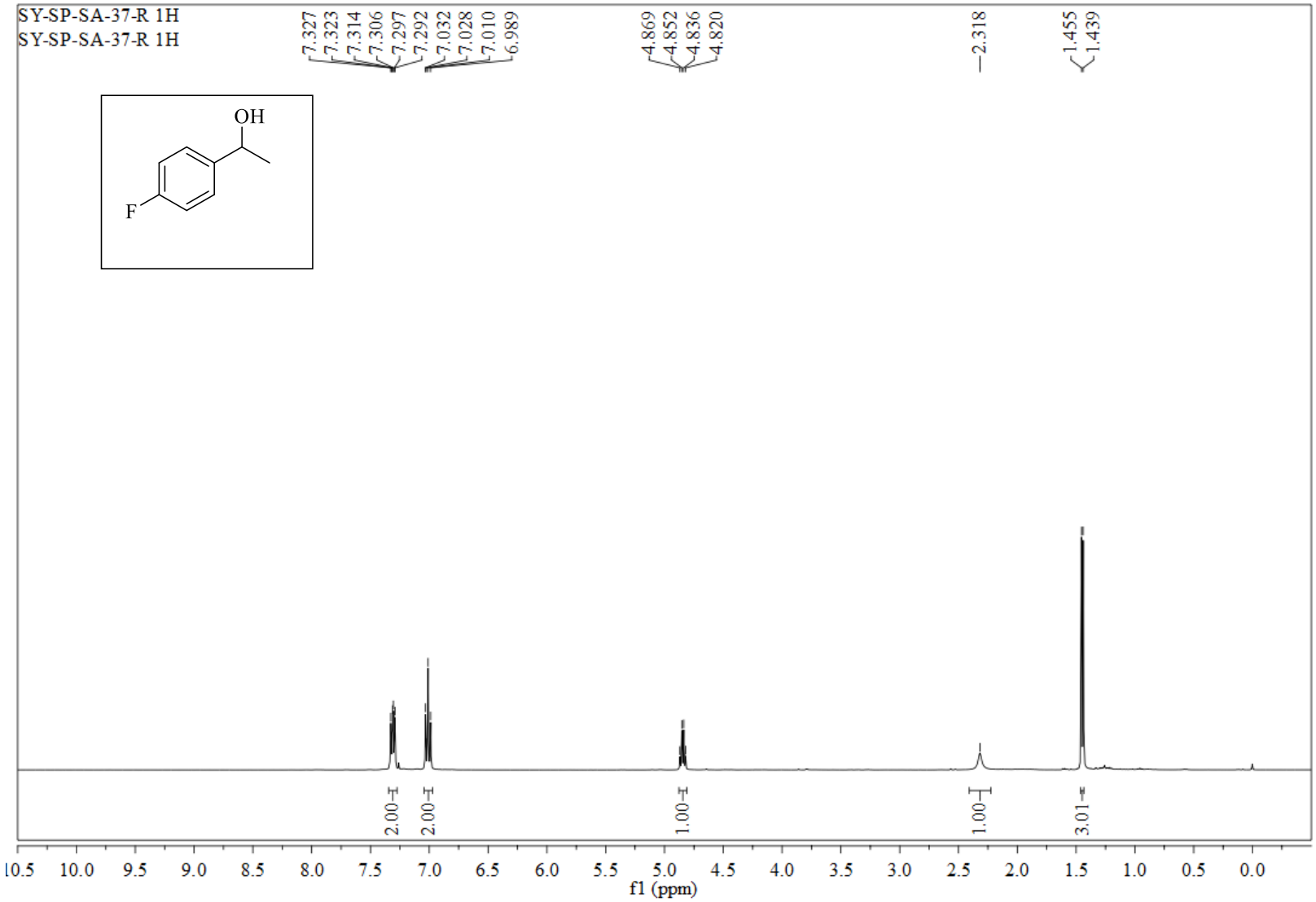

Figure S99. ^{1}H NMR (400 Mz, $CDCl_3$) of **11l**

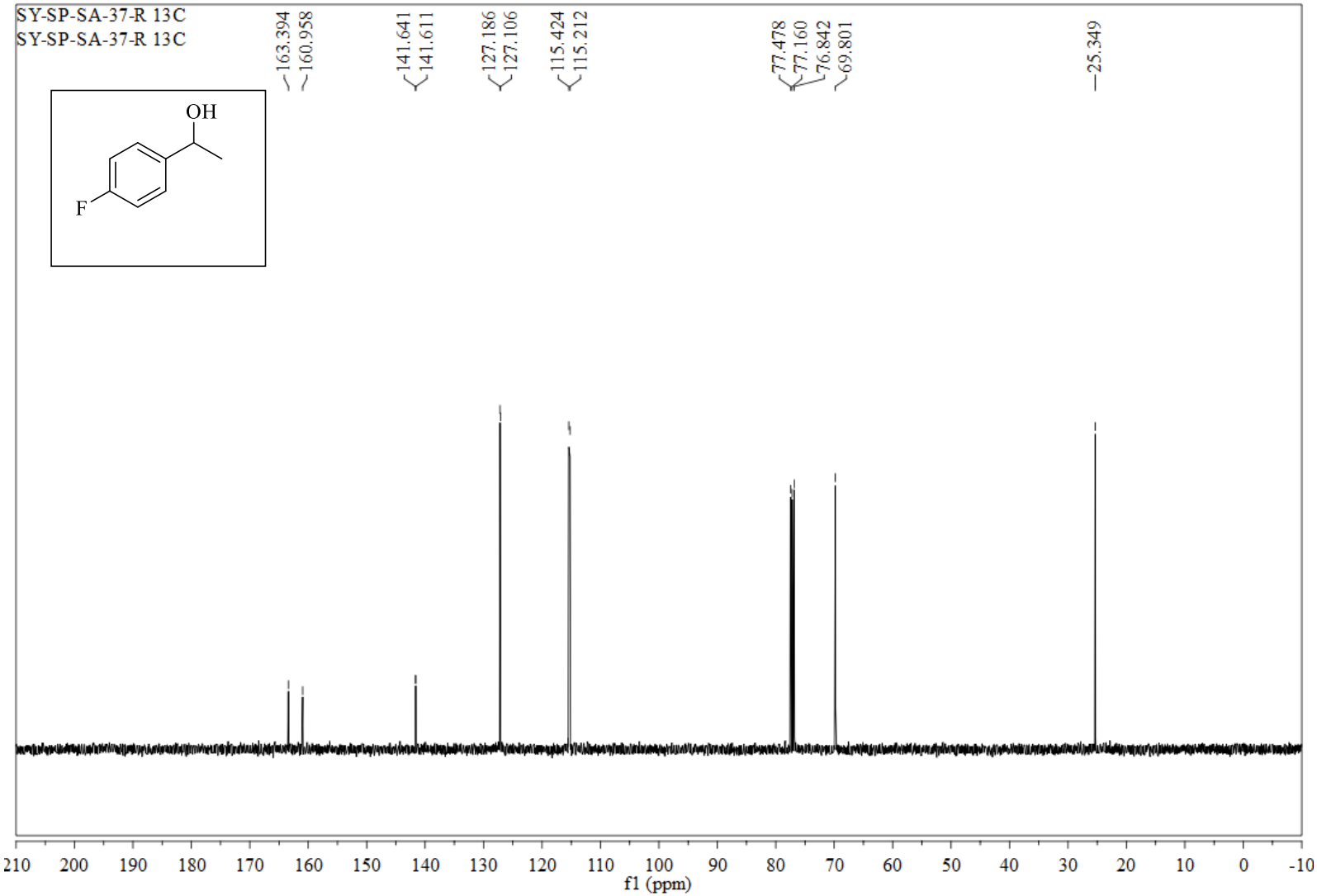

Figure S100. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11l**

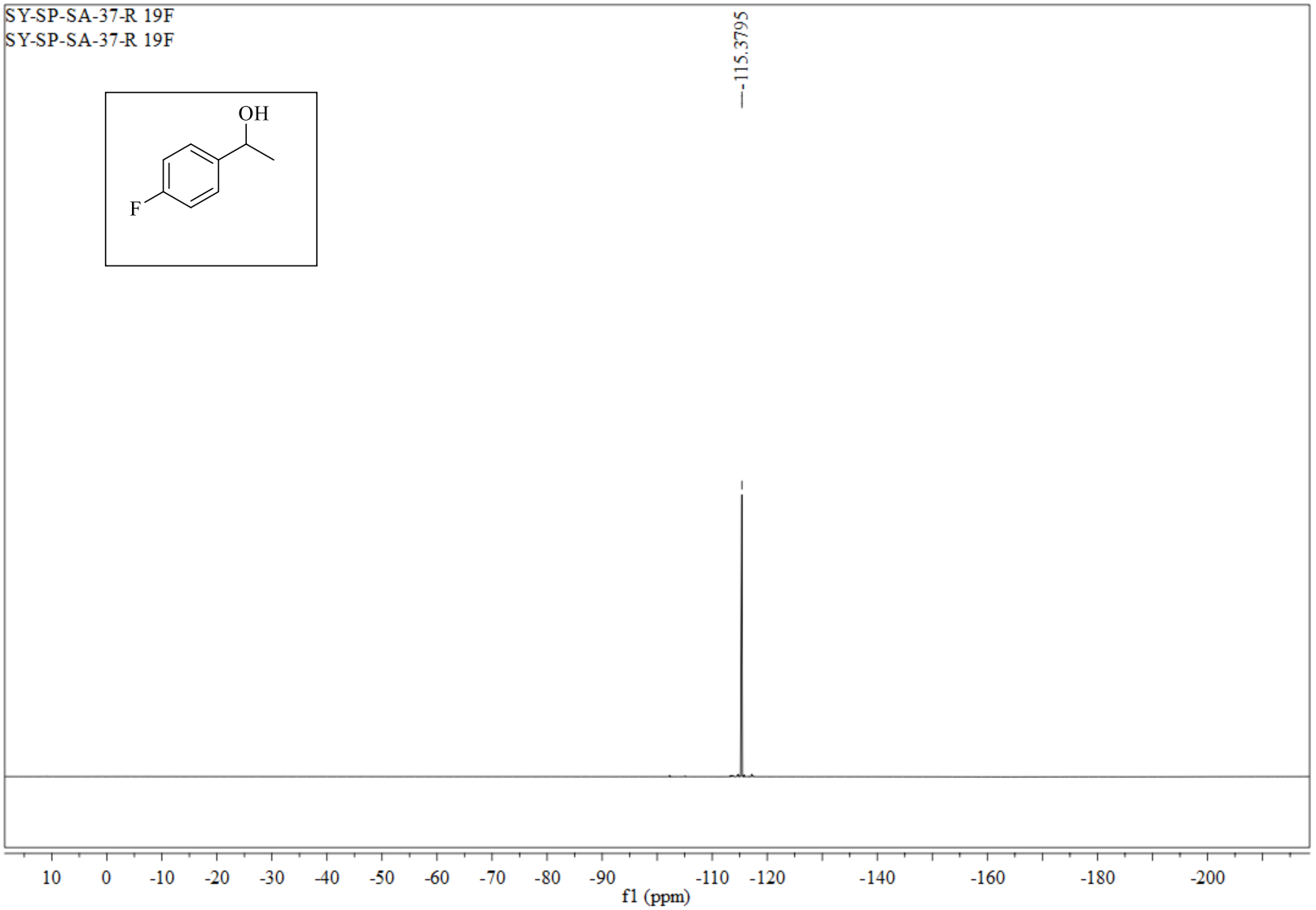

Figure S101. ^{19}F NMR (376 Mz, $CDCl_3$) of **11l**

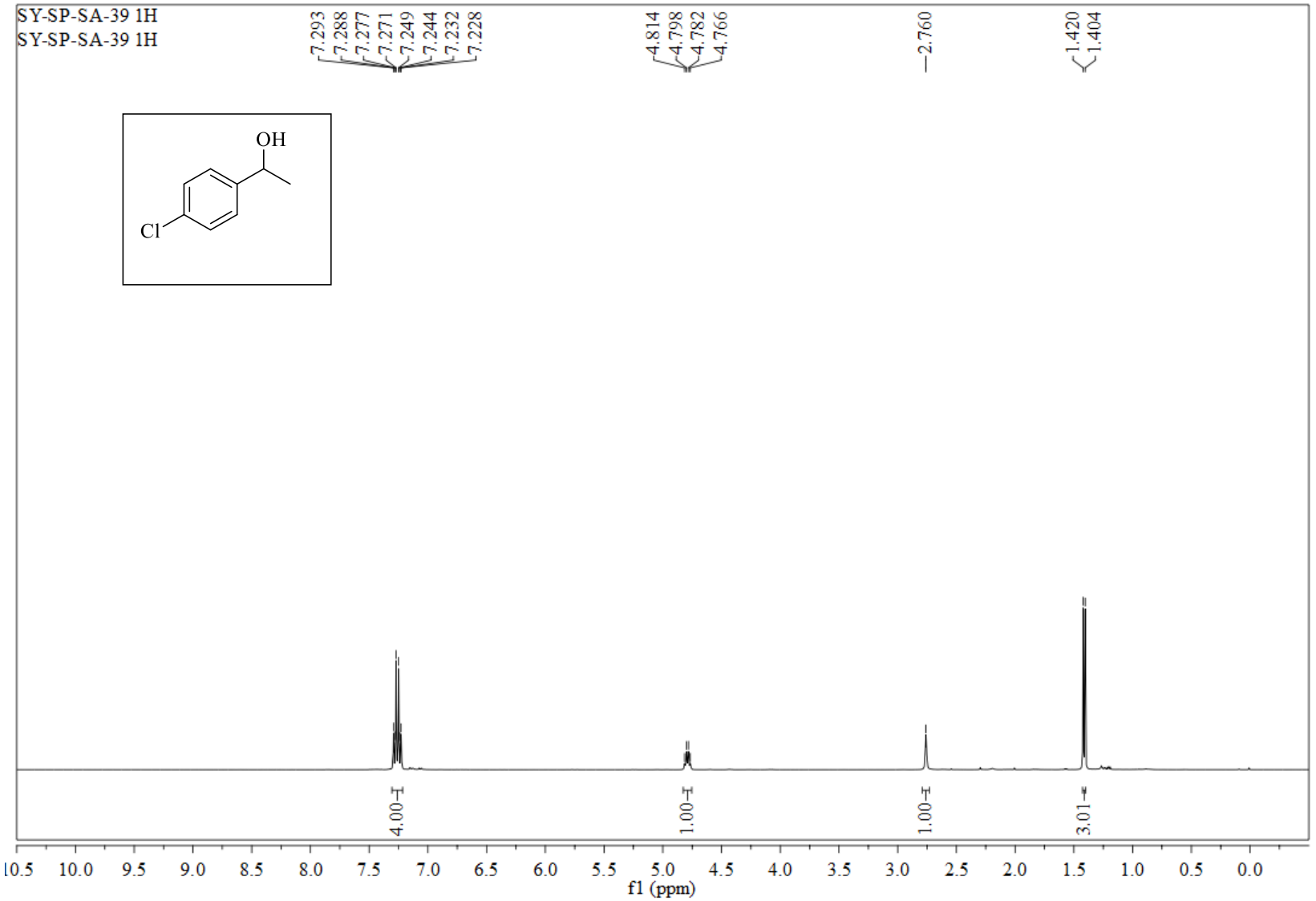

Figure S102. ^{1}H NMR (400 Mz, $CDCl_3$) of **11m**

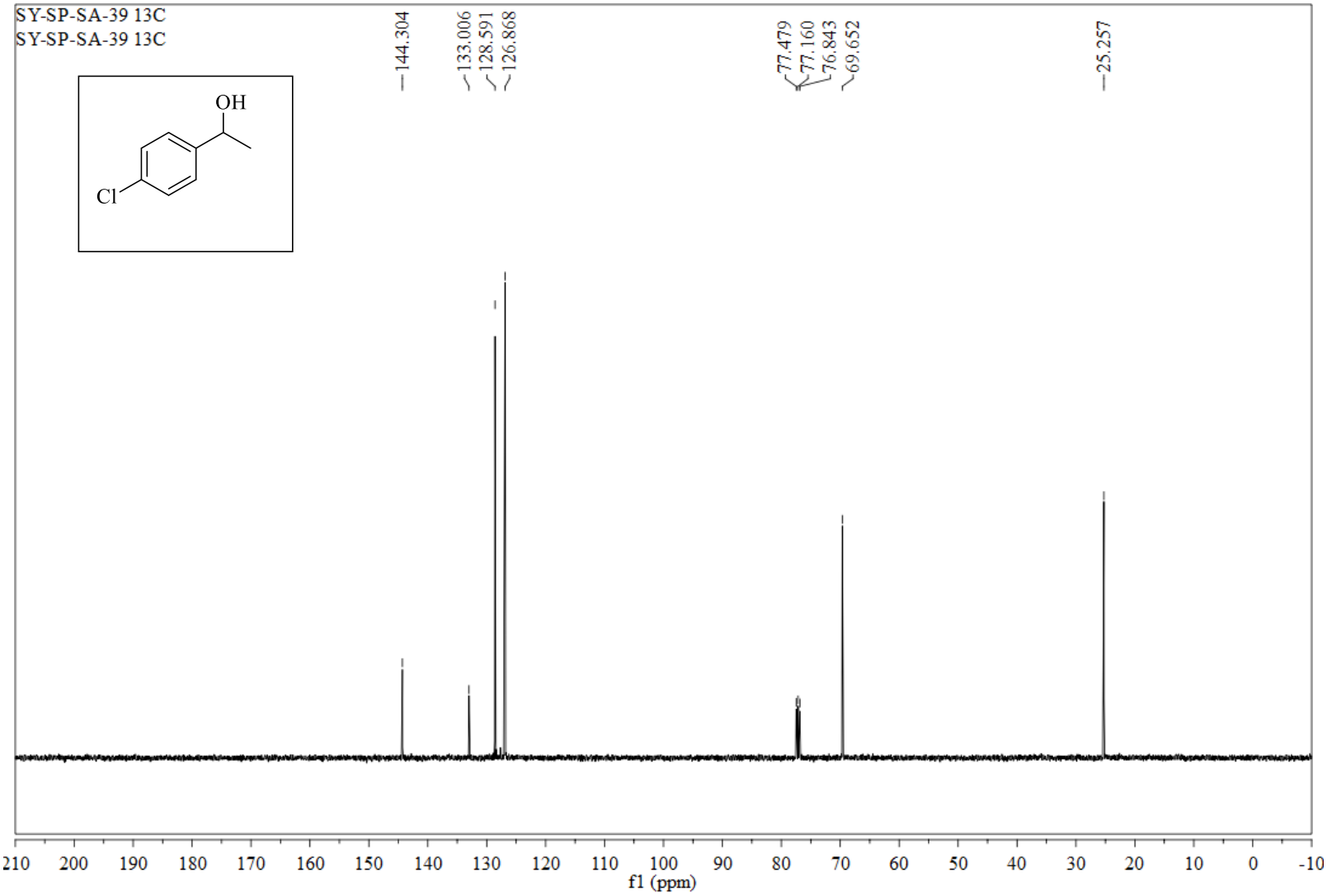

Figure S103. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11m**

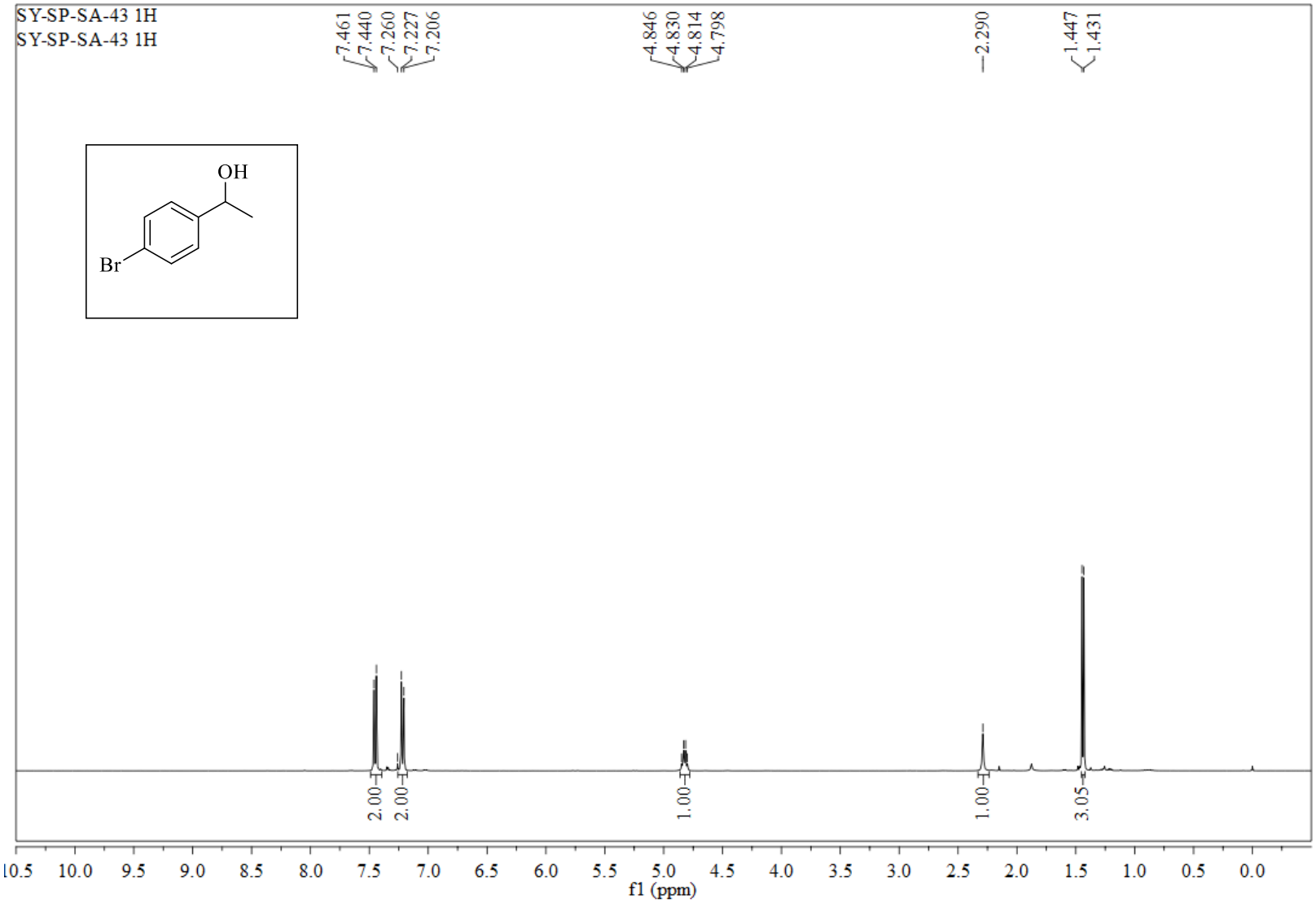

Figure S104. ^{1}H NMR (400 Mz, $CDCl_3$) of **I1n**

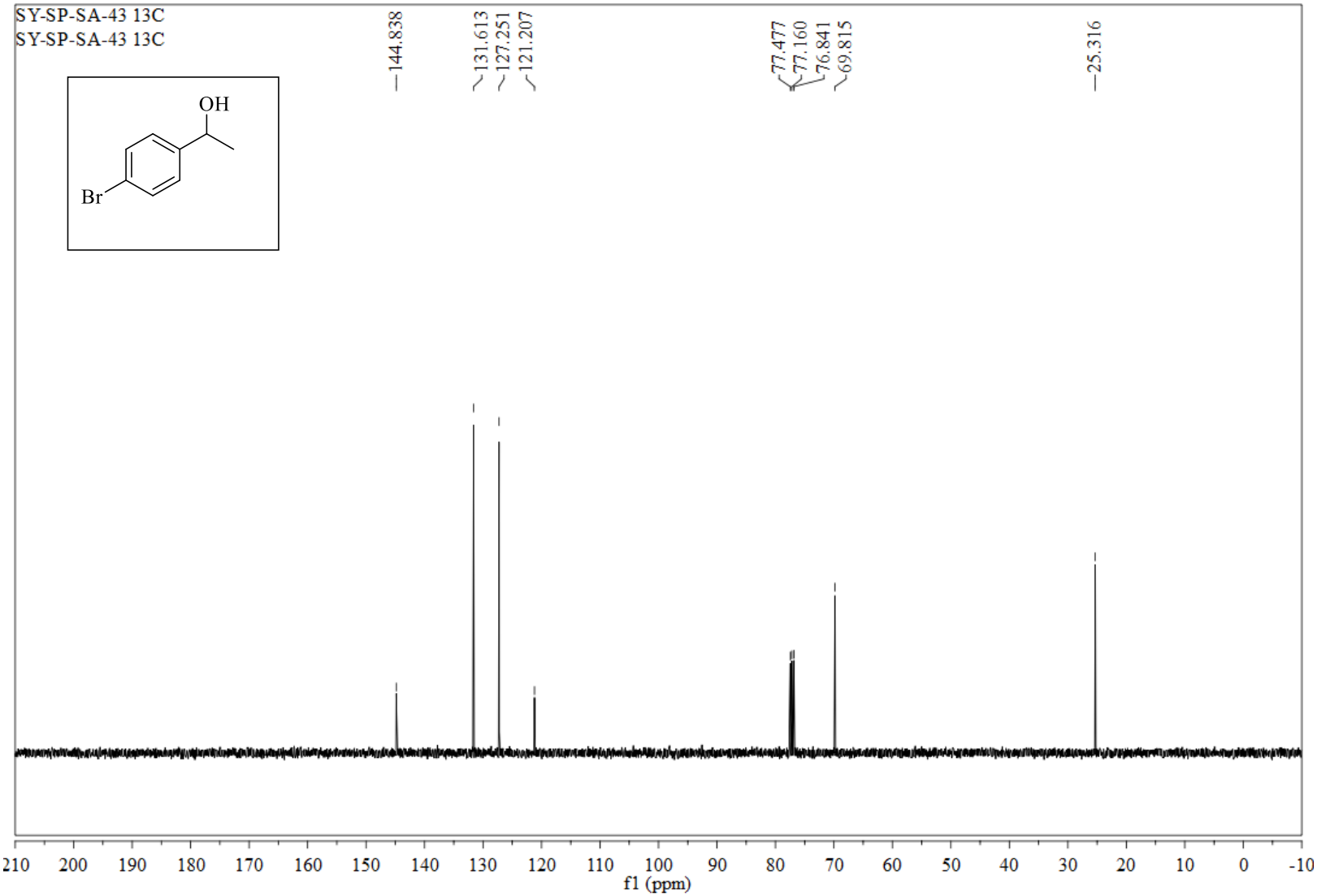

Figure S105. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11n**

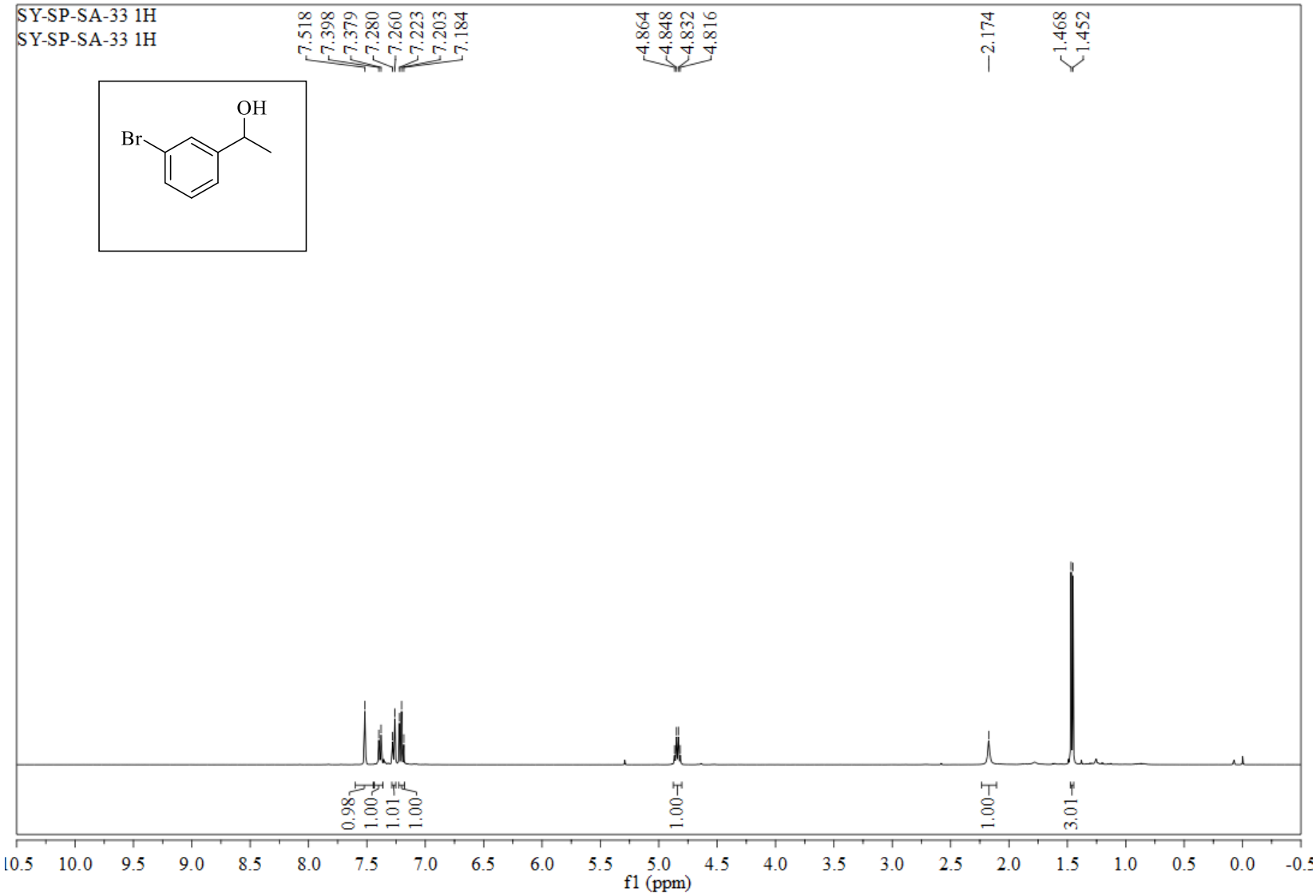

Figure S106. ^{1}H NMR (400 Mz, $CDCl_3$) of **11o**

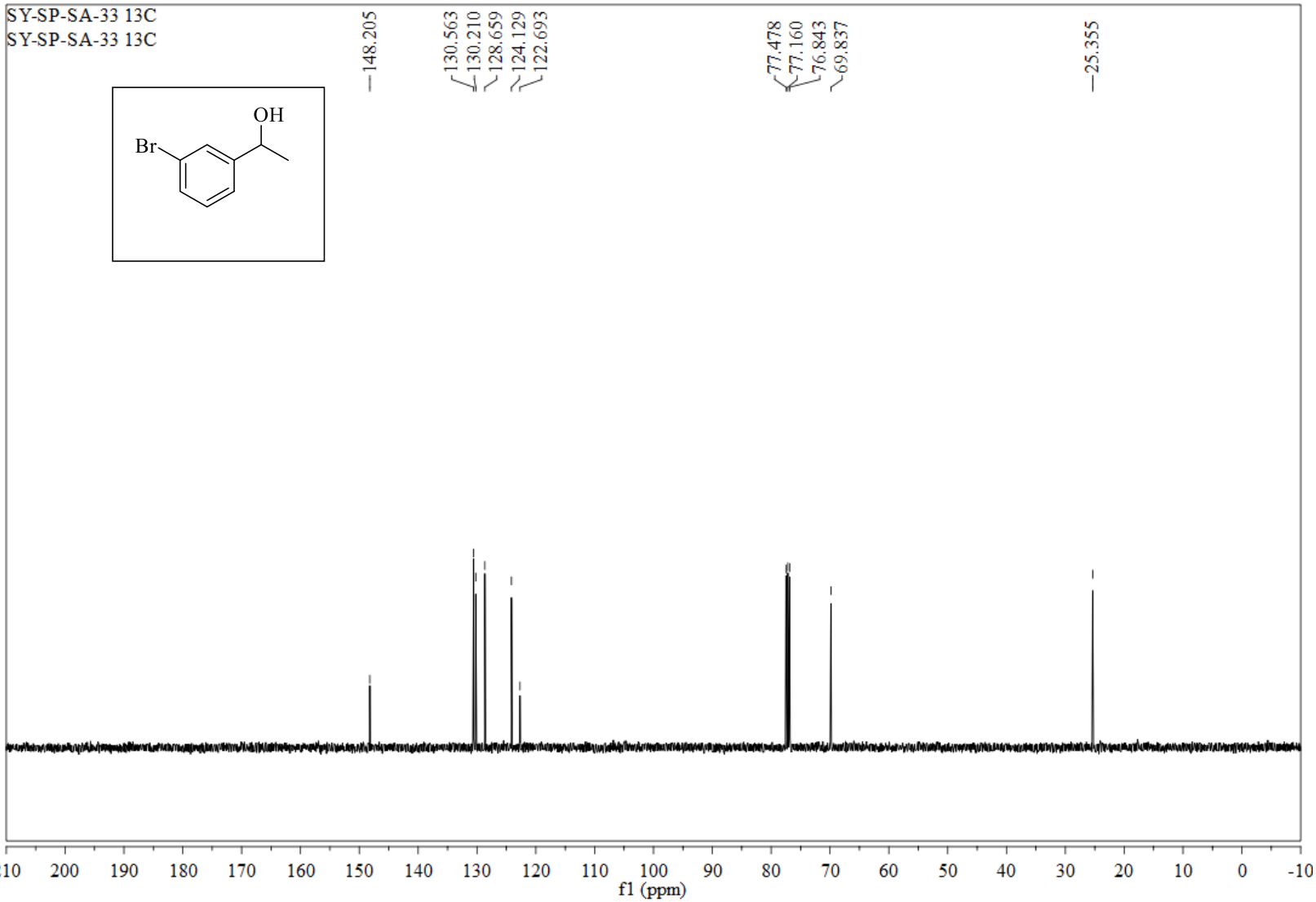

Figure S107. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11o**

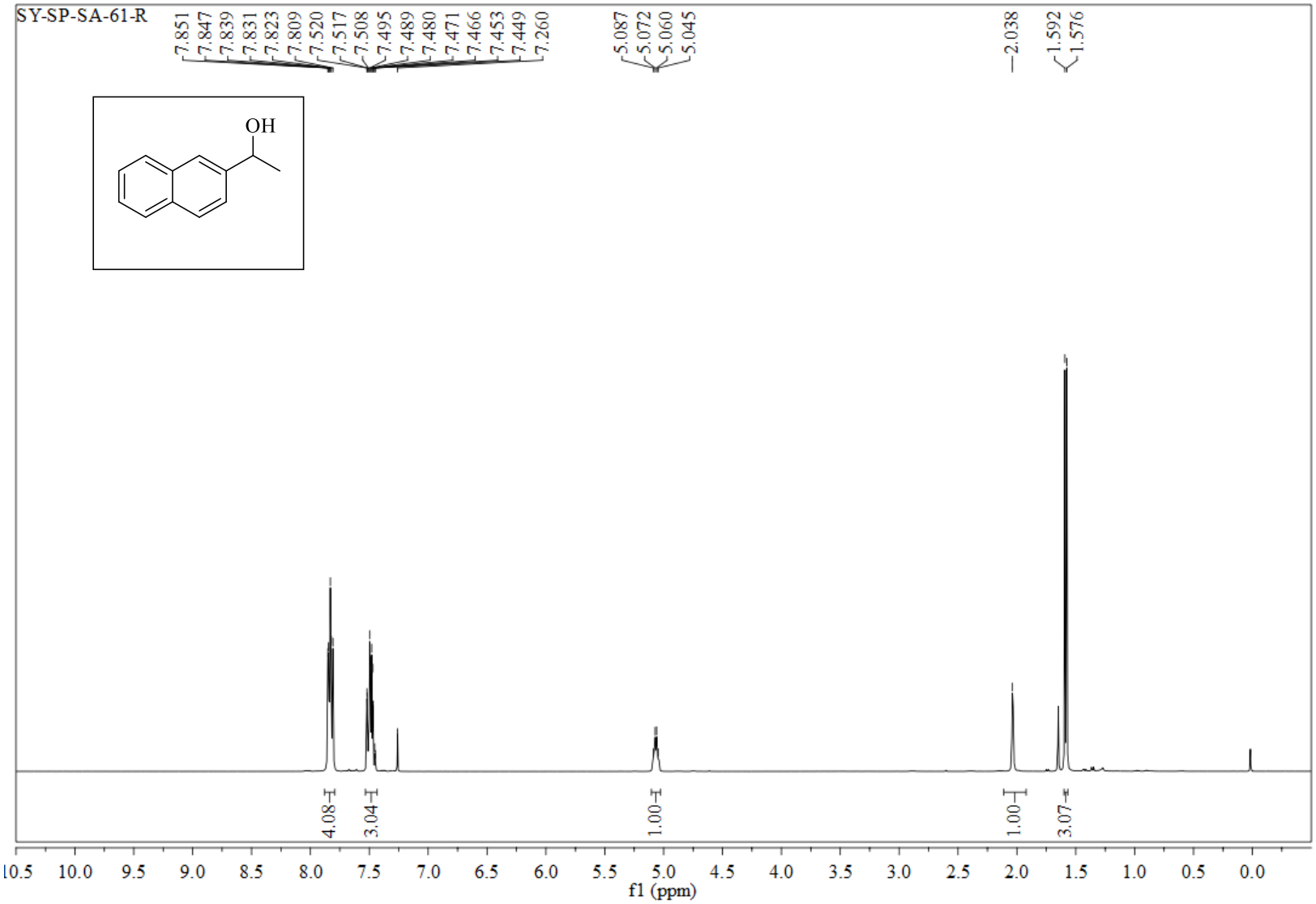

Figure S108. ^{1}H NMR (400 Mz, $CDCl_3$) of **11p**

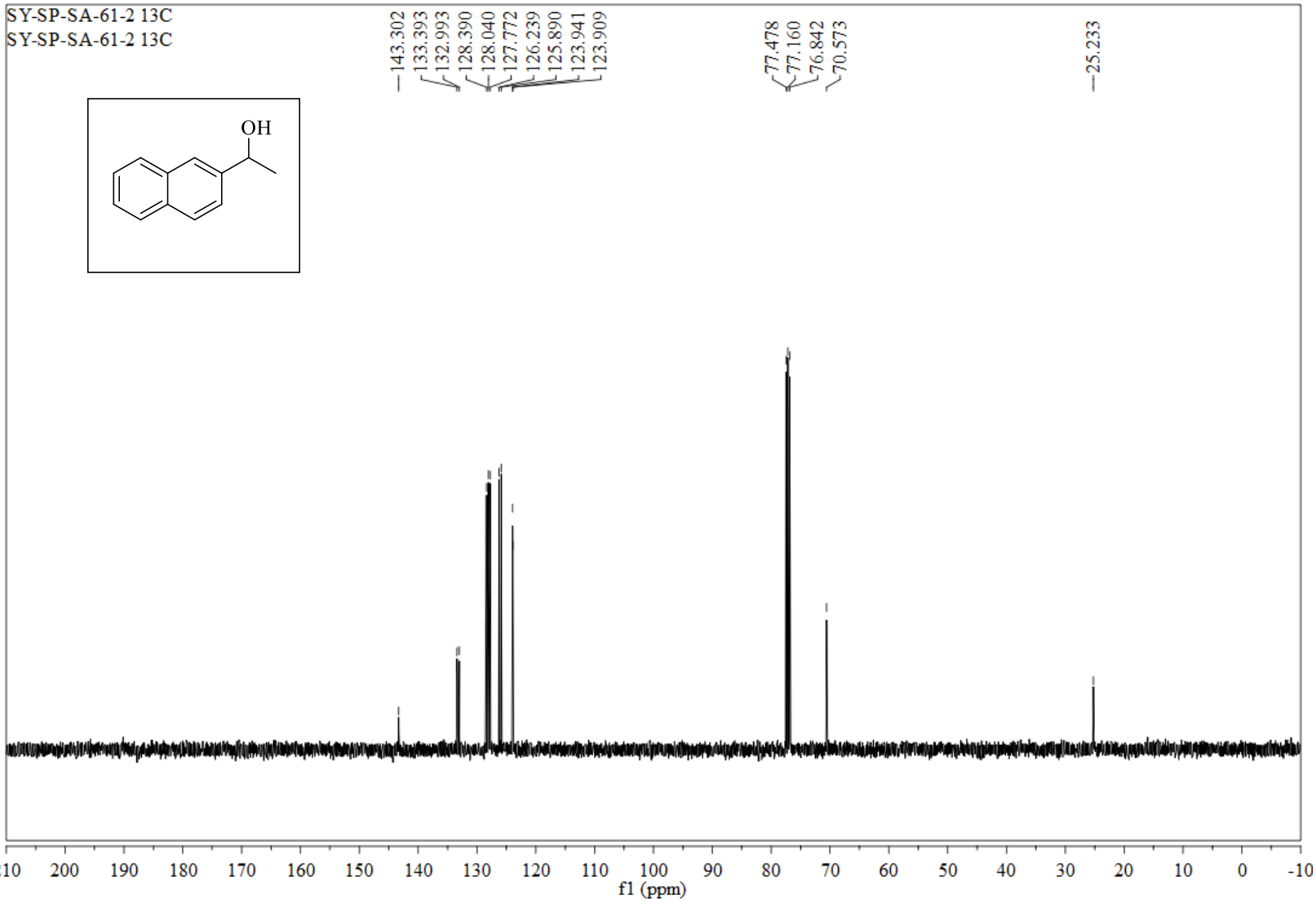

Figure S109. ^{13}C {^{1}H} NMR (100 Mz, $CDCl_3$) of **11o.**