Supporting Information

Dynamic Kinetic Resolution for Construction of Three Transannular Stereocenters of Dihydrobenzofuranols

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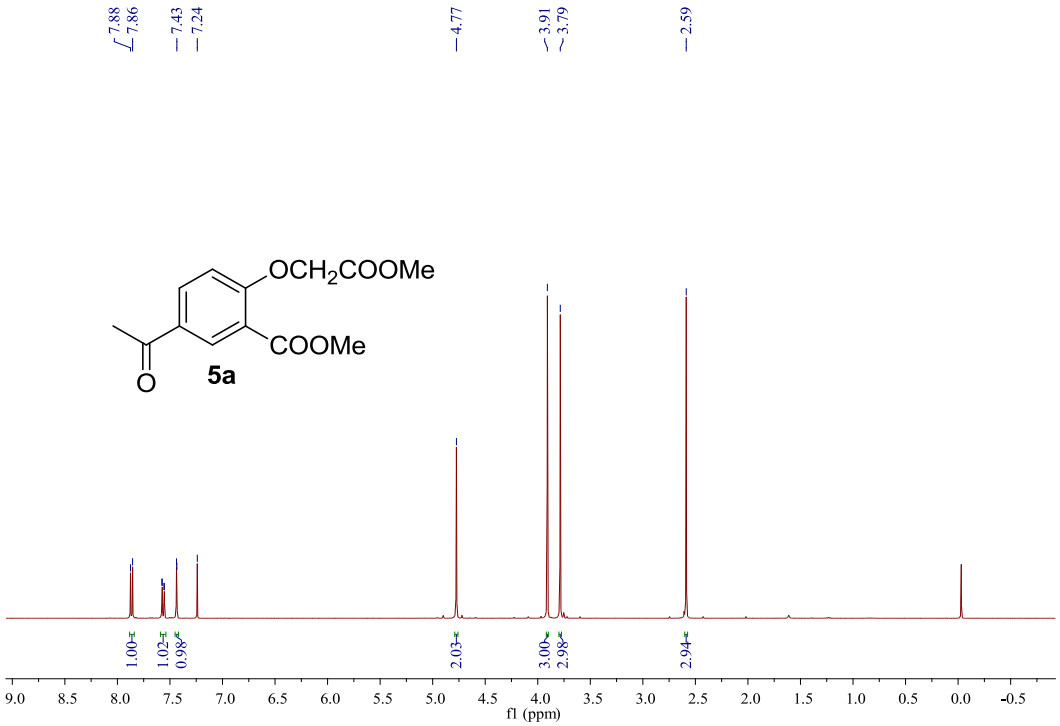
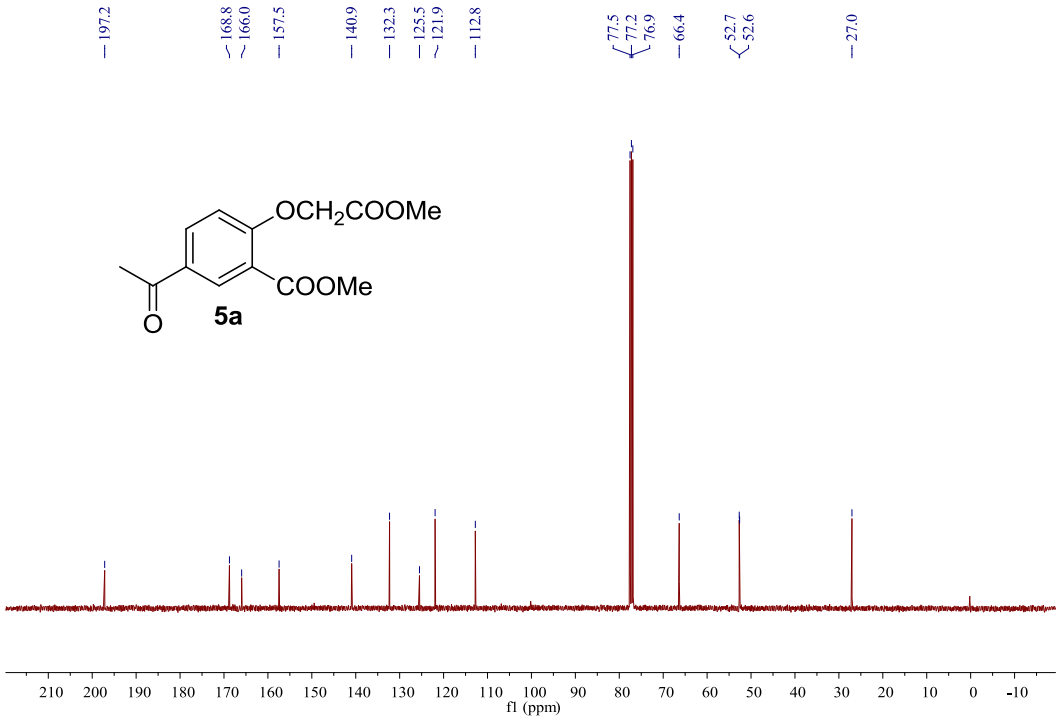
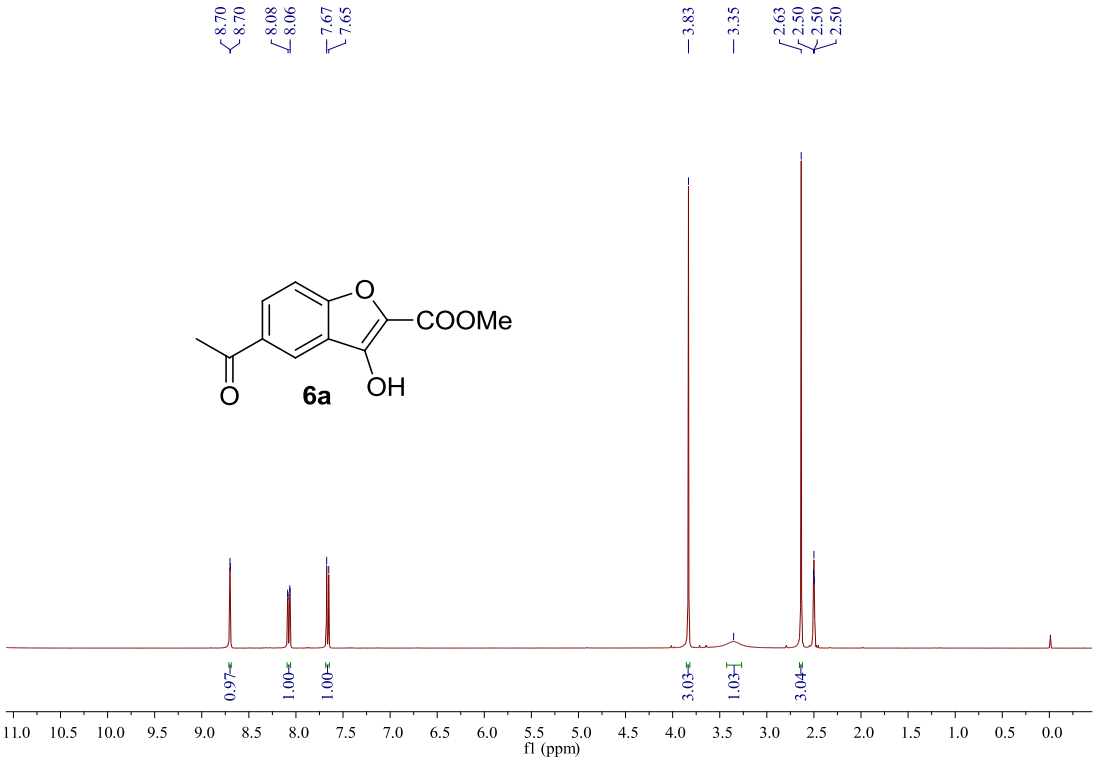
^{1}H-NMR spectrum for 5a (in $CDCl_3$)



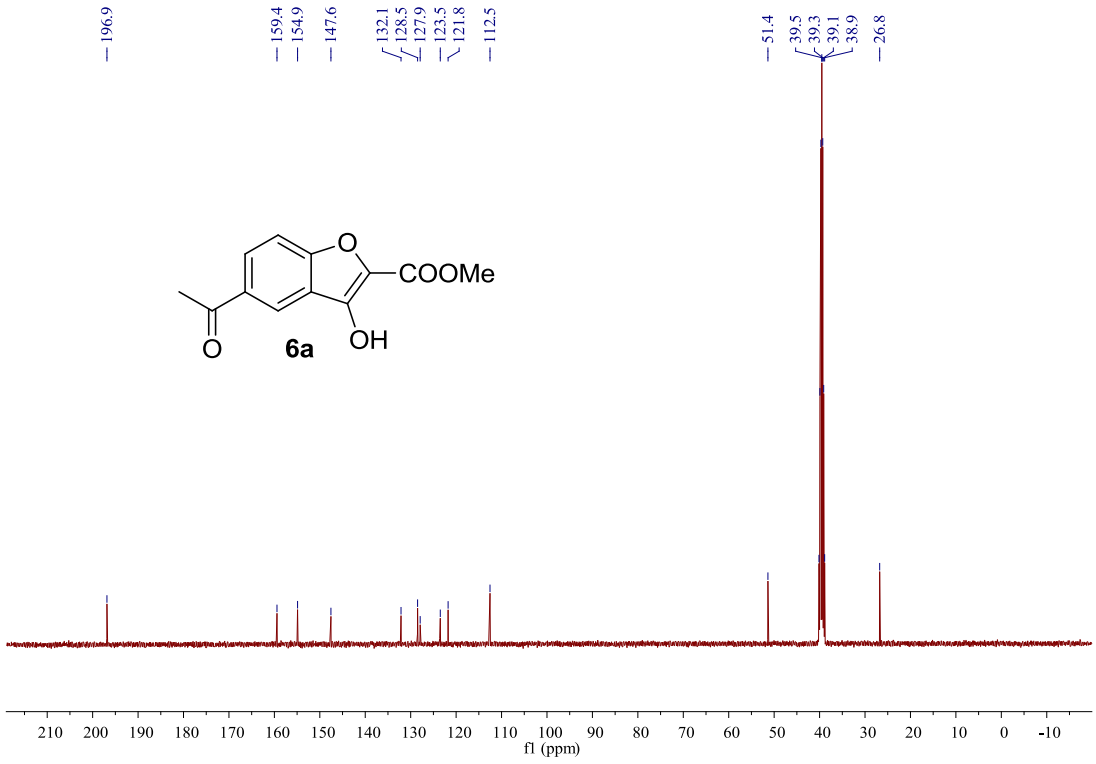
^{13}C-NMR spectrum for 5a (in $CDCl_3$)



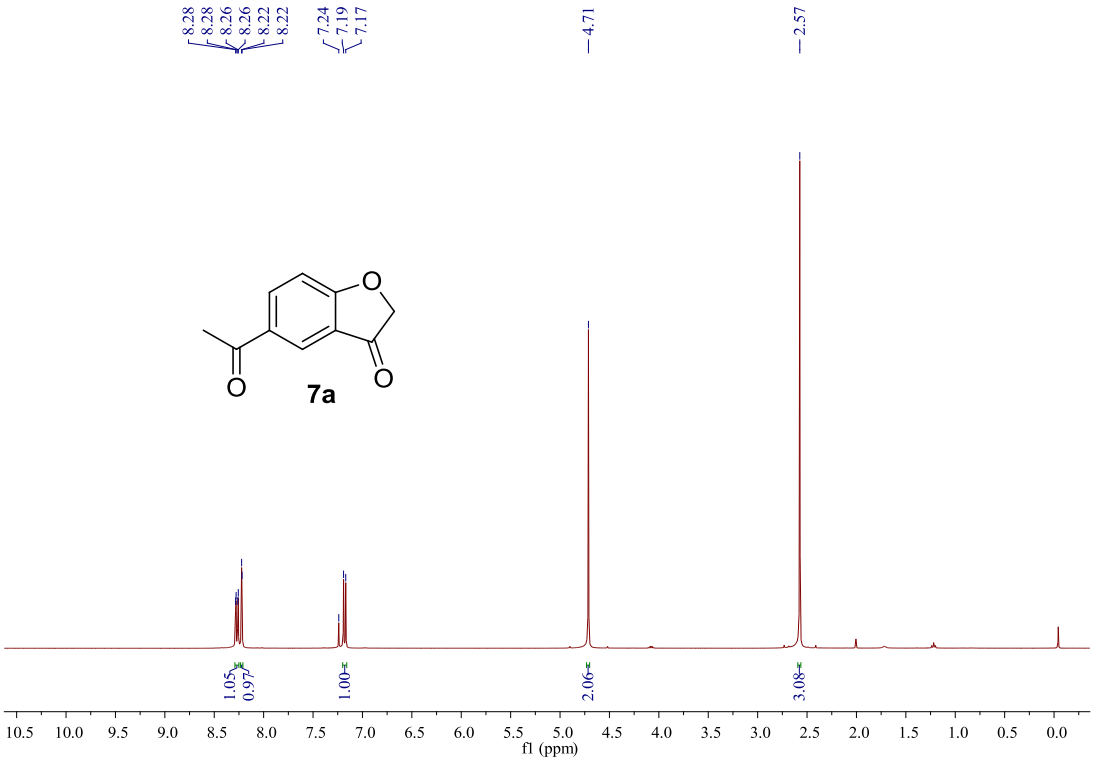
^{1}H-NMR spectrum for 6a (in CD_3SOCD_3)



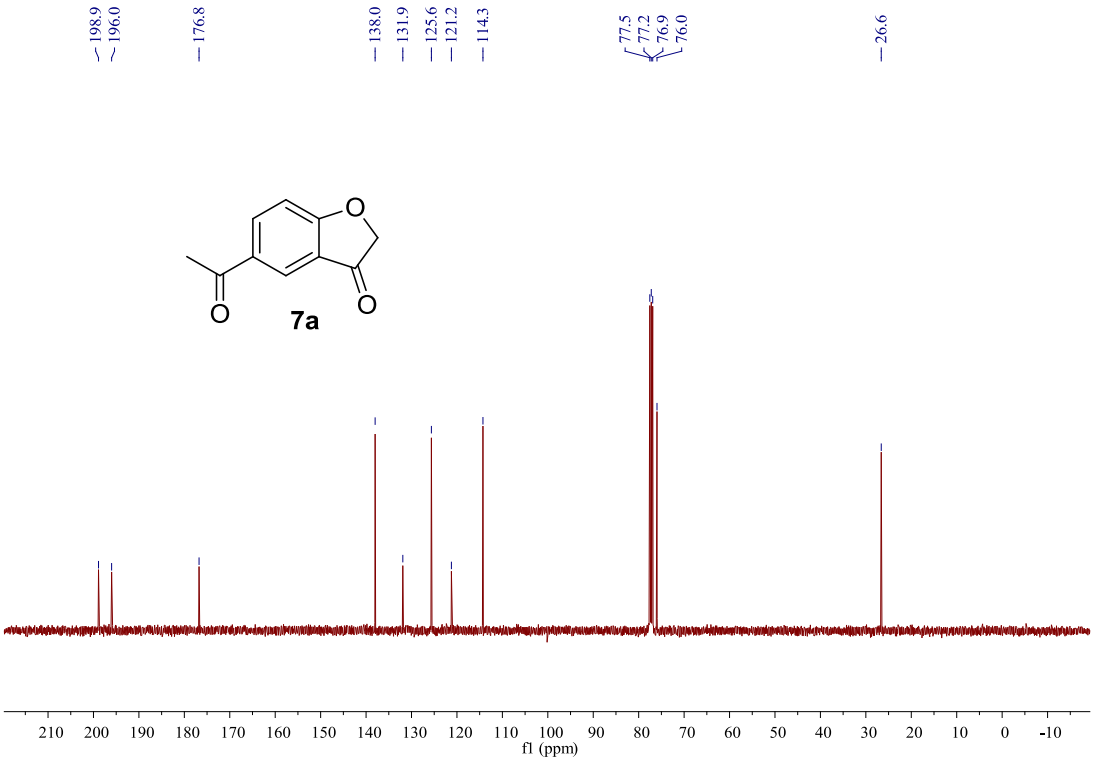
^{13}C-NMR spectrum for 6a (in CD_3SOCD_3)



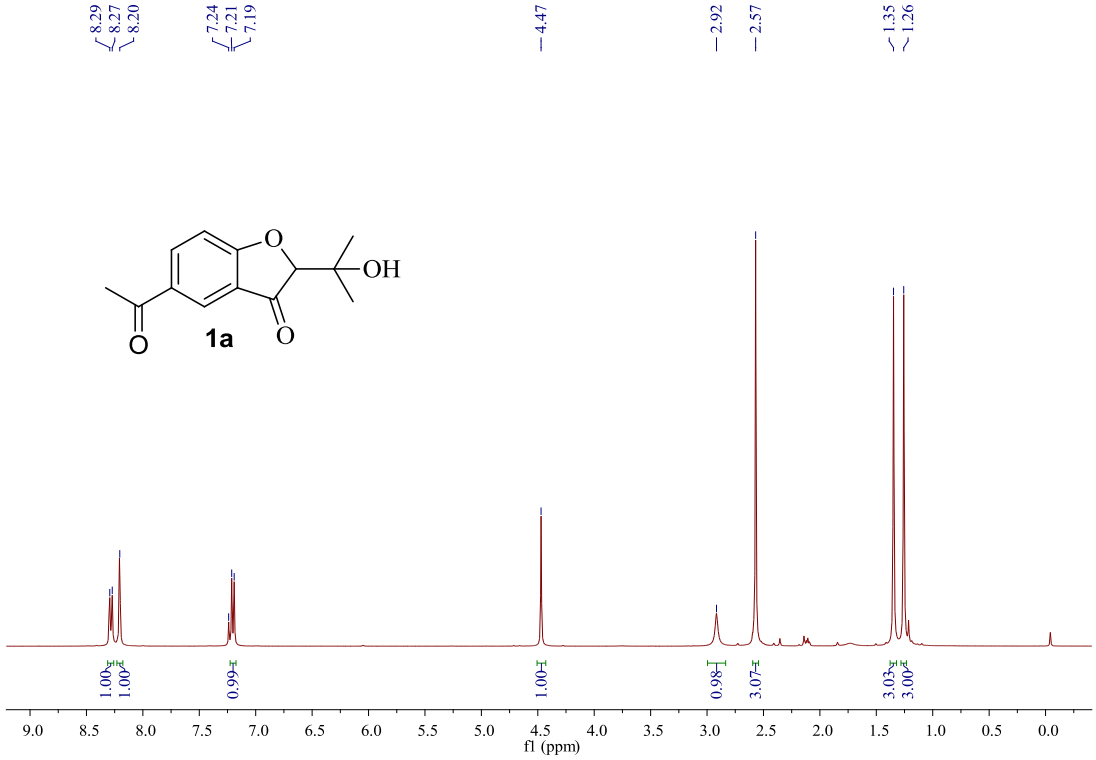
^{1}H-NMR spectrum for 7a (in $CDCl_3$)



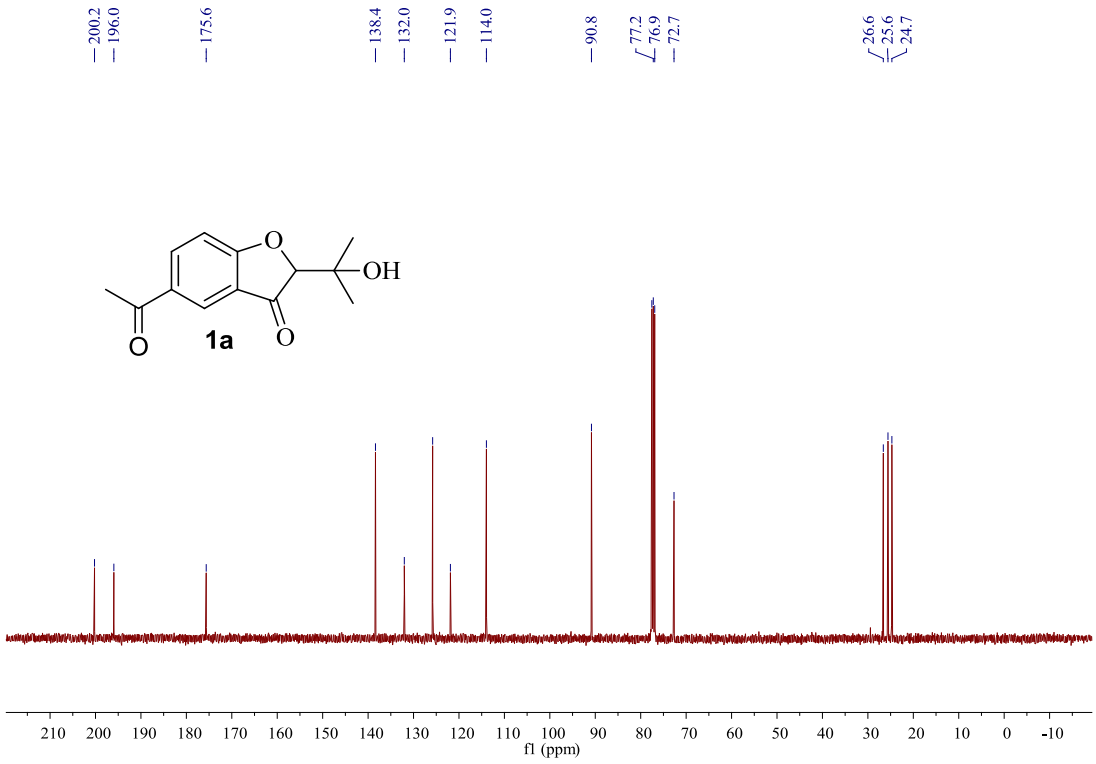
^{13}C-NMR spectrum for 7a (in $CDCl_3$)



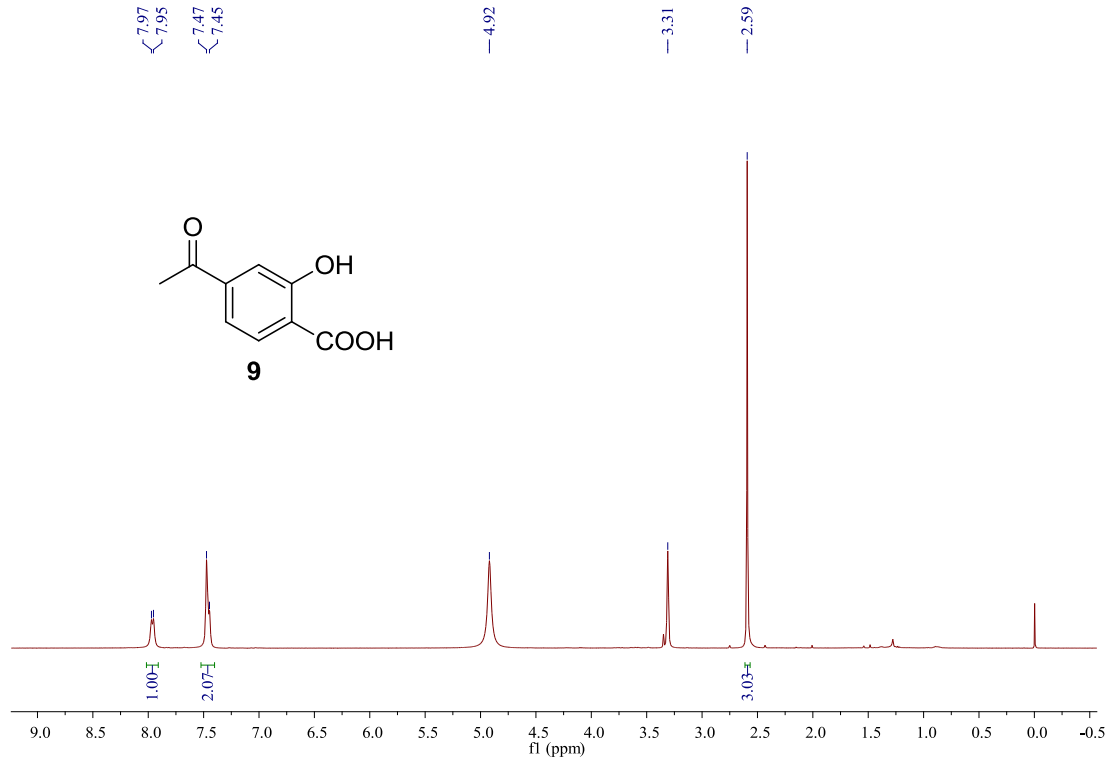
^{1}H-NMR spectrum for 1a (in $CDCl_3$)



^{13}C-NMR spectrum for 1a (in $CDCl_3$)



^{1}H-NMR spectrum for 9 (in CD_3OD)



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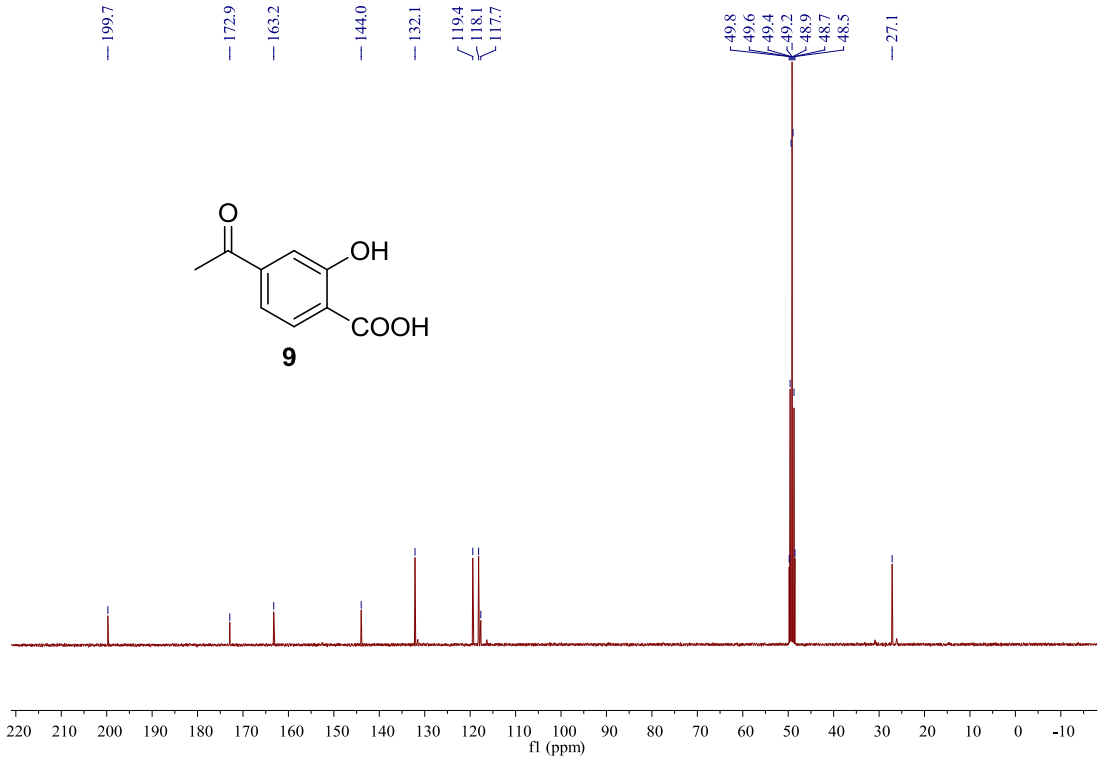
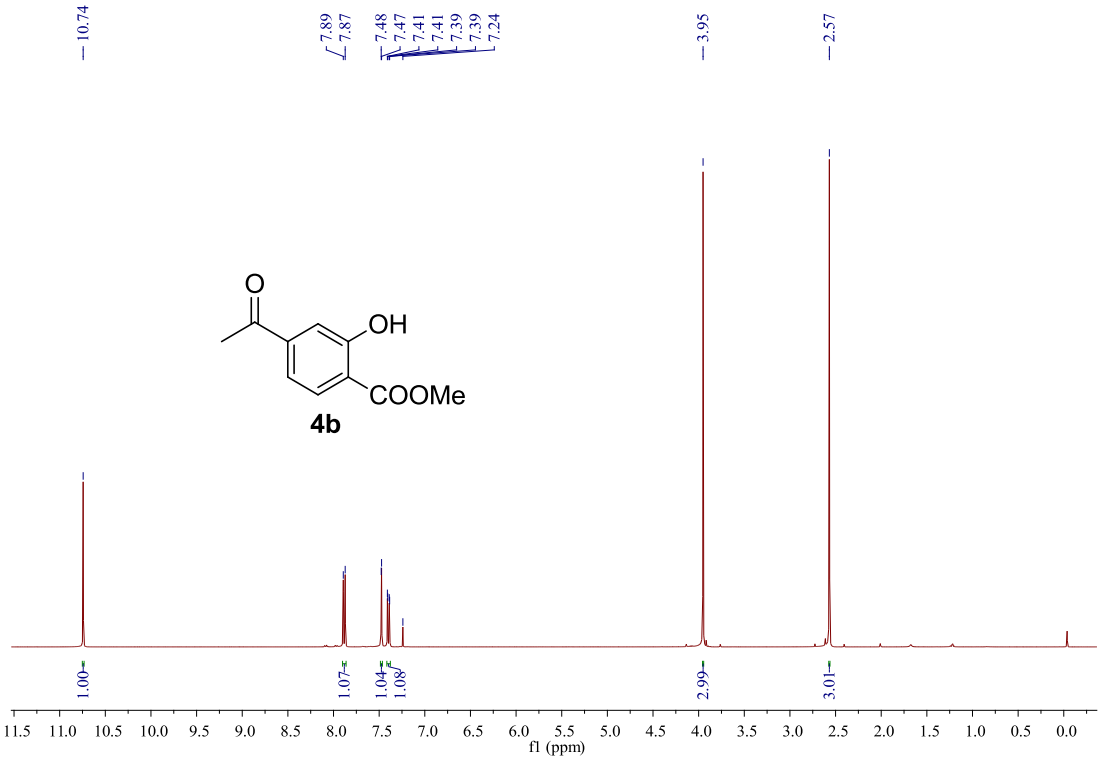


^{1}H-NMR spectrum for 4b (in $CDCl_3$)



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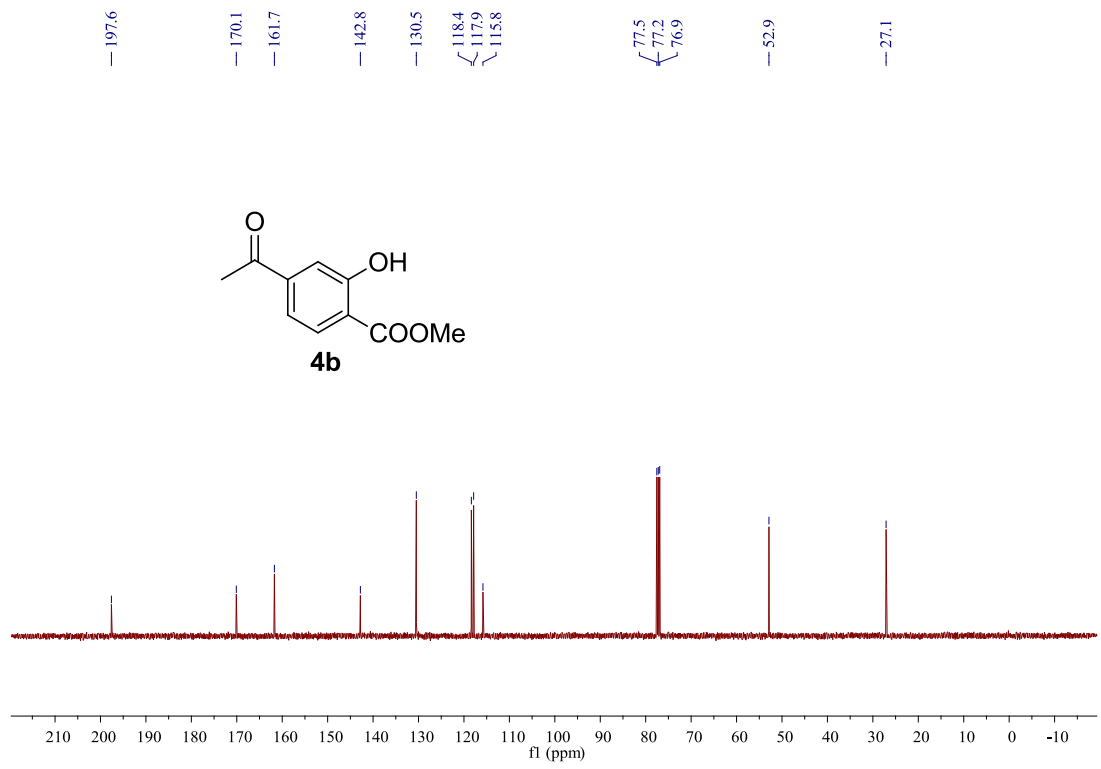
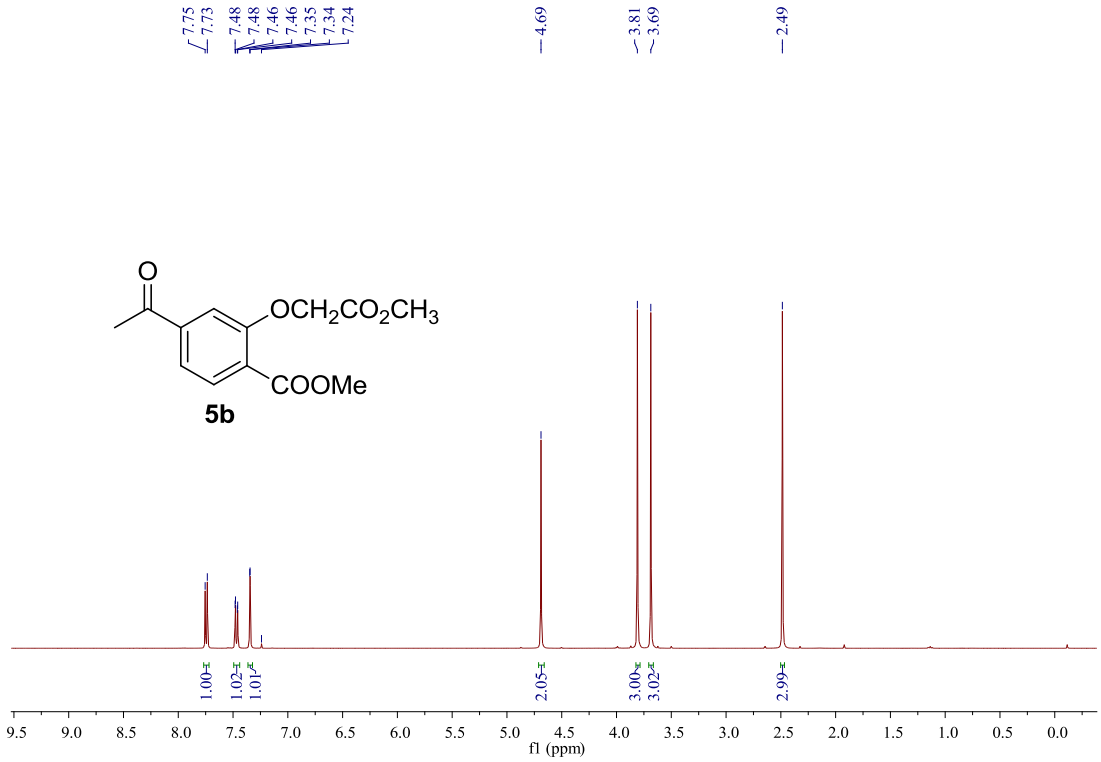
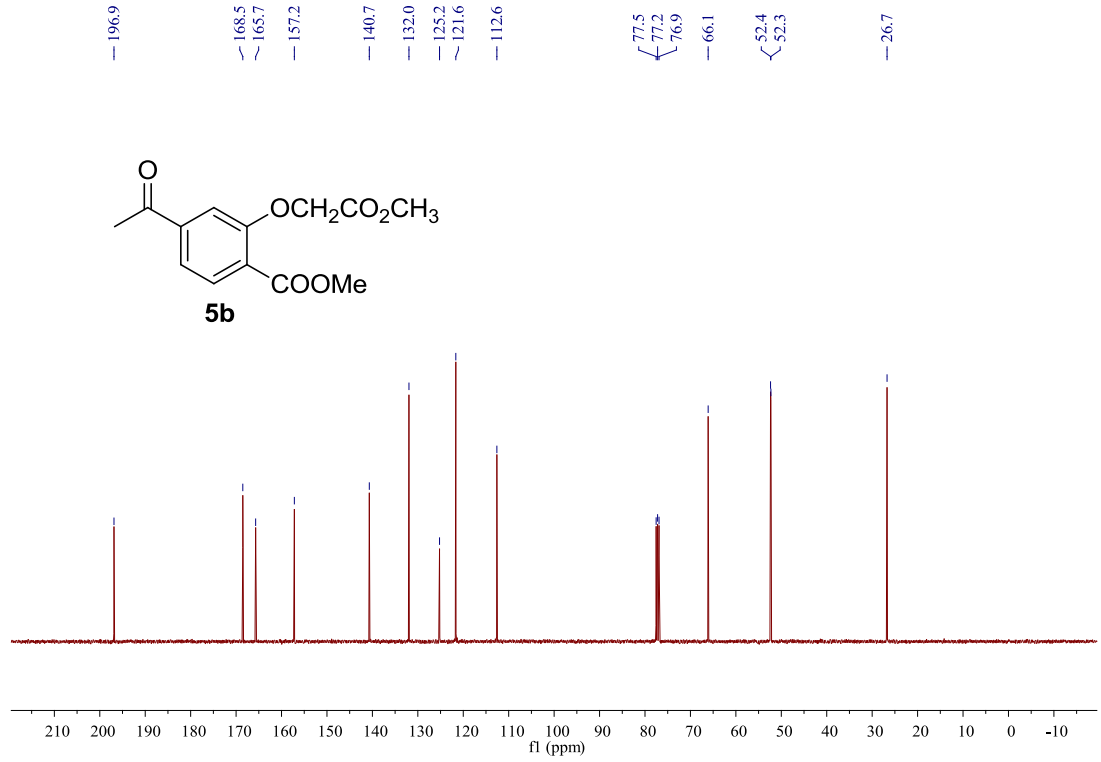


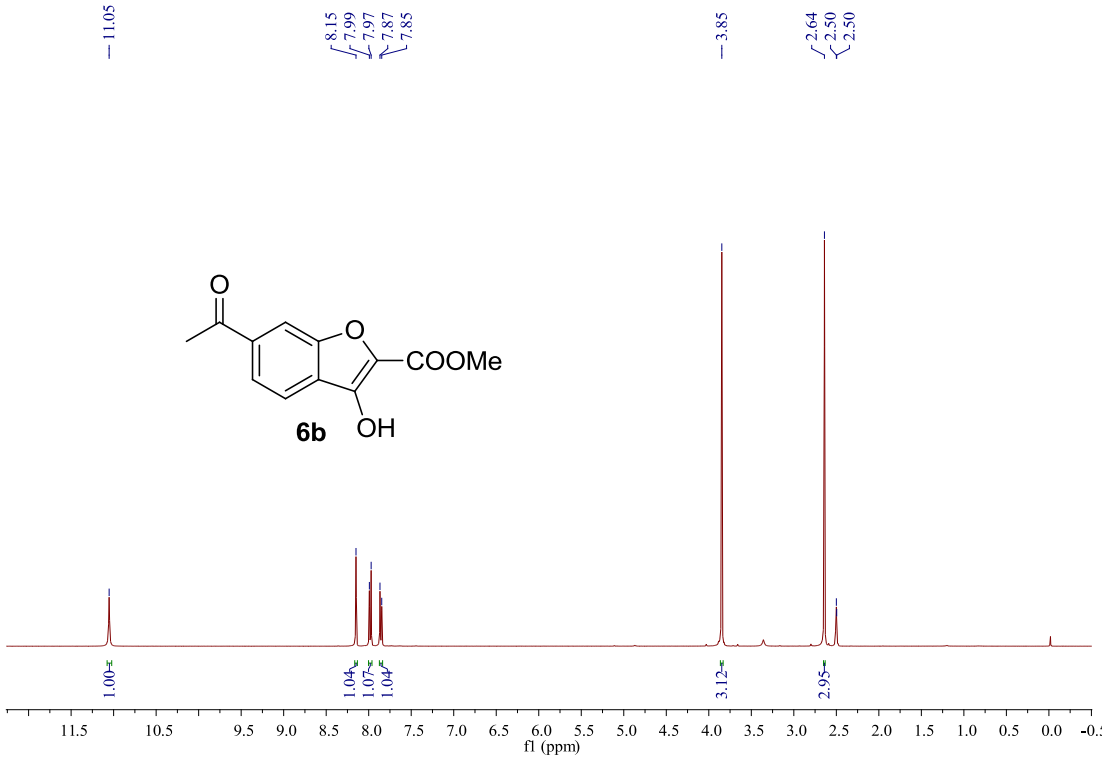
^{1}H-NMR spectrum for 5b (in $CDCl_3$)



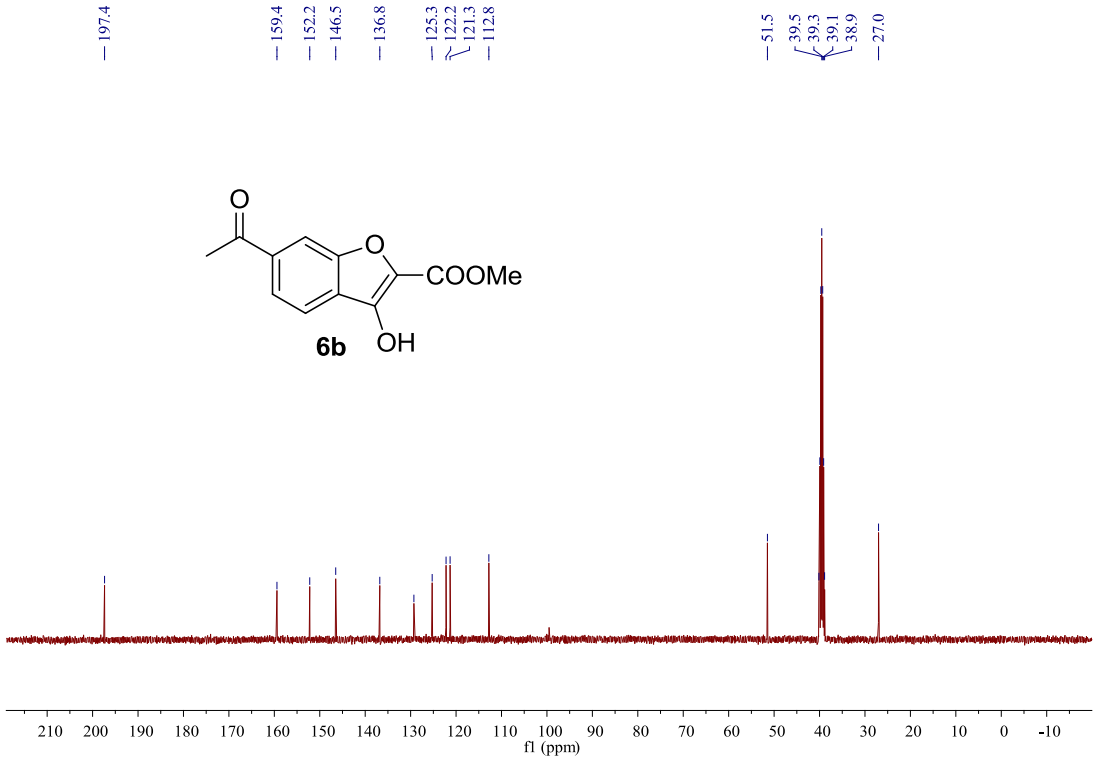
^{13}C-NMR spectrum for 5b (in $CDCl_3$)



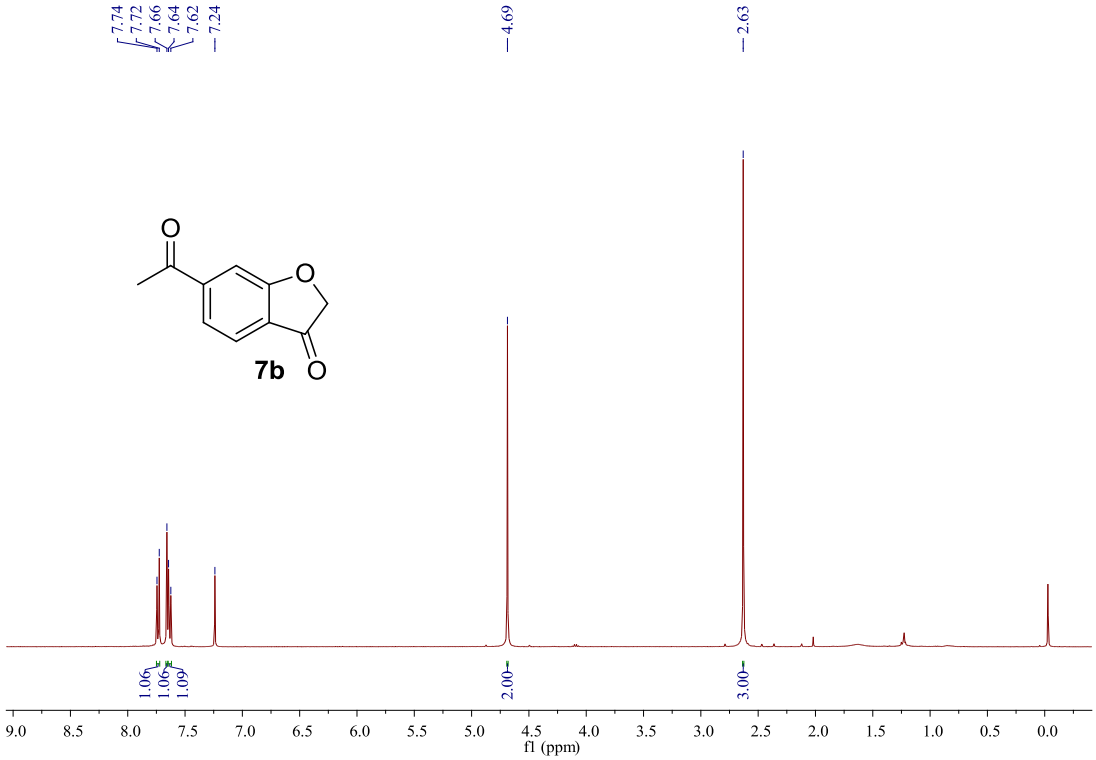
^{1}H-NMR spectrum for 6b (in CD_3SOCD_3)



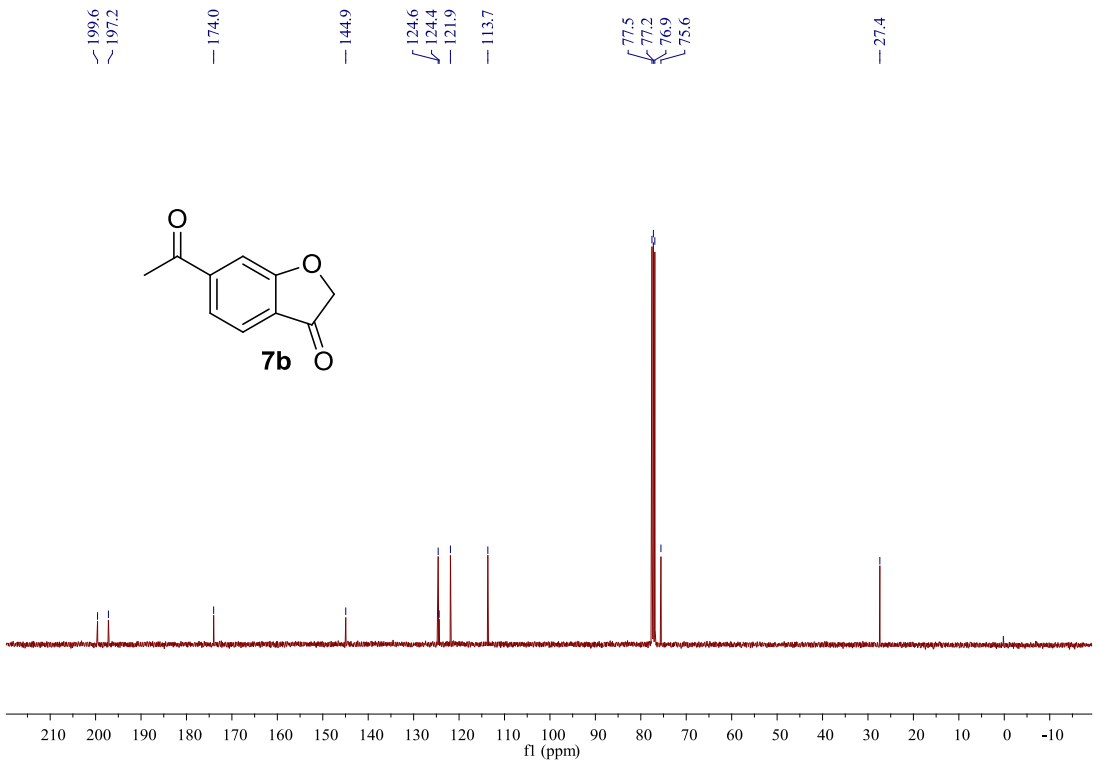
^{13}C-NMR spectrum for 6b (in CD_3SOCD_3)



^{1}H-NMR spectrum for 7b (in $CDCl_3$)



^{13}C-NMR spectrum for 7b (in $CDCl_3$)



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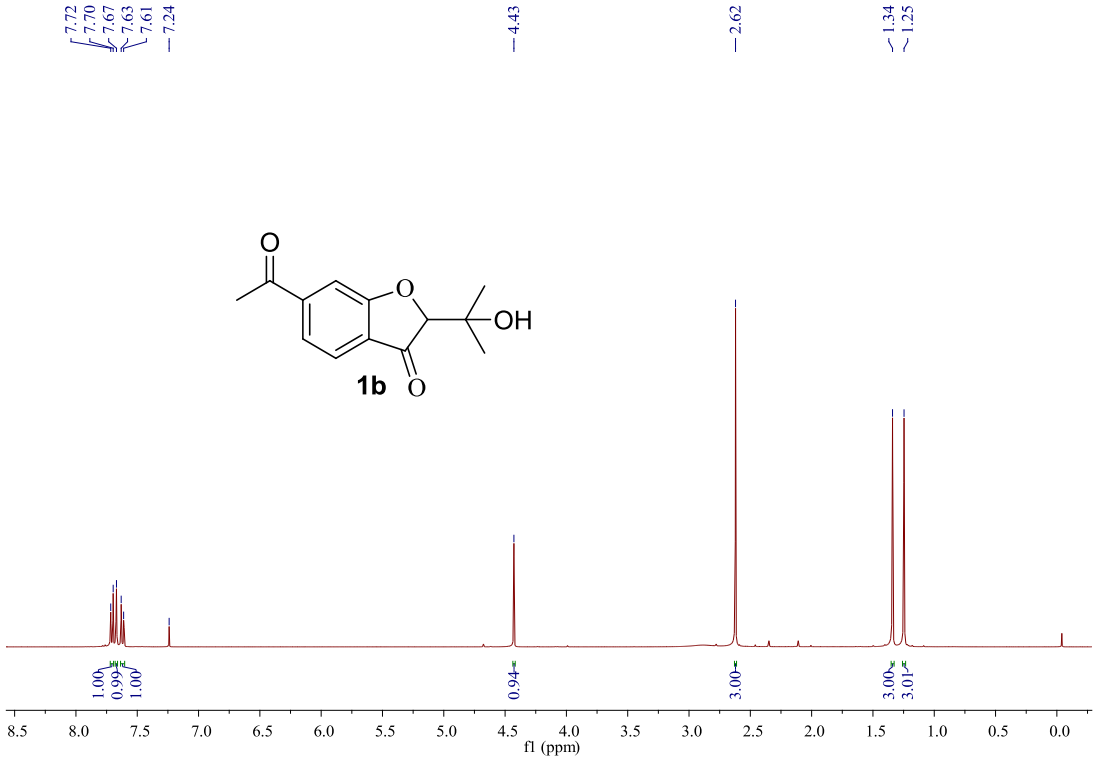
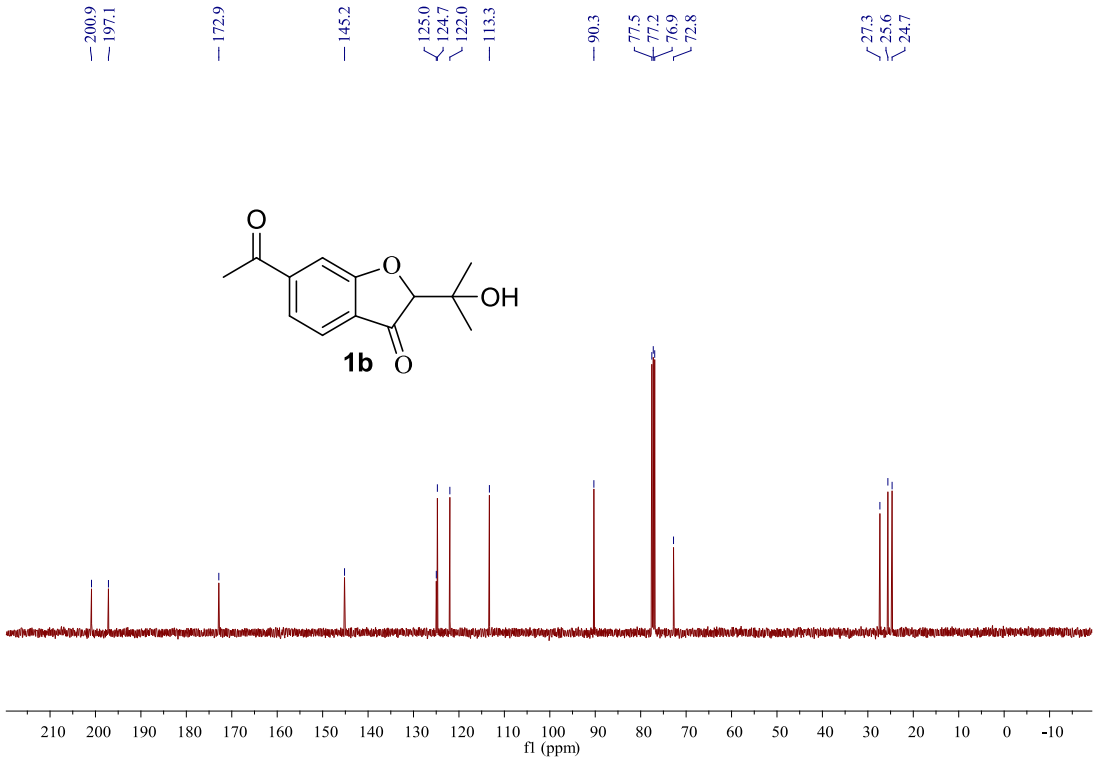
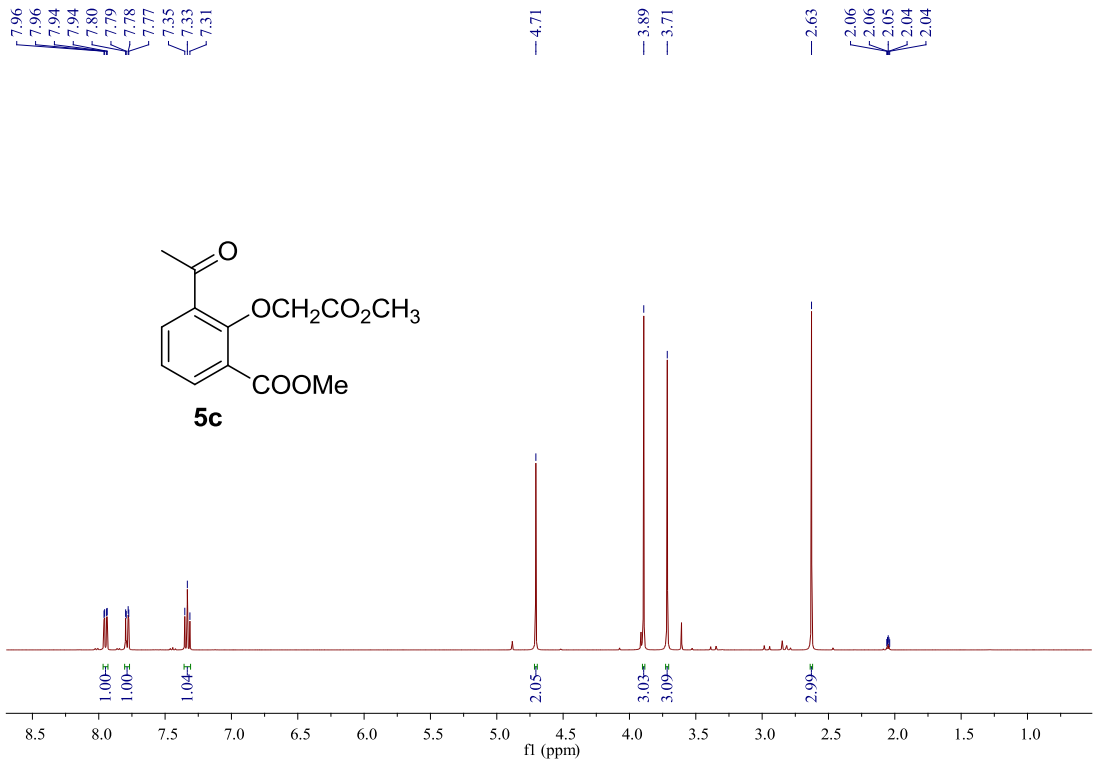


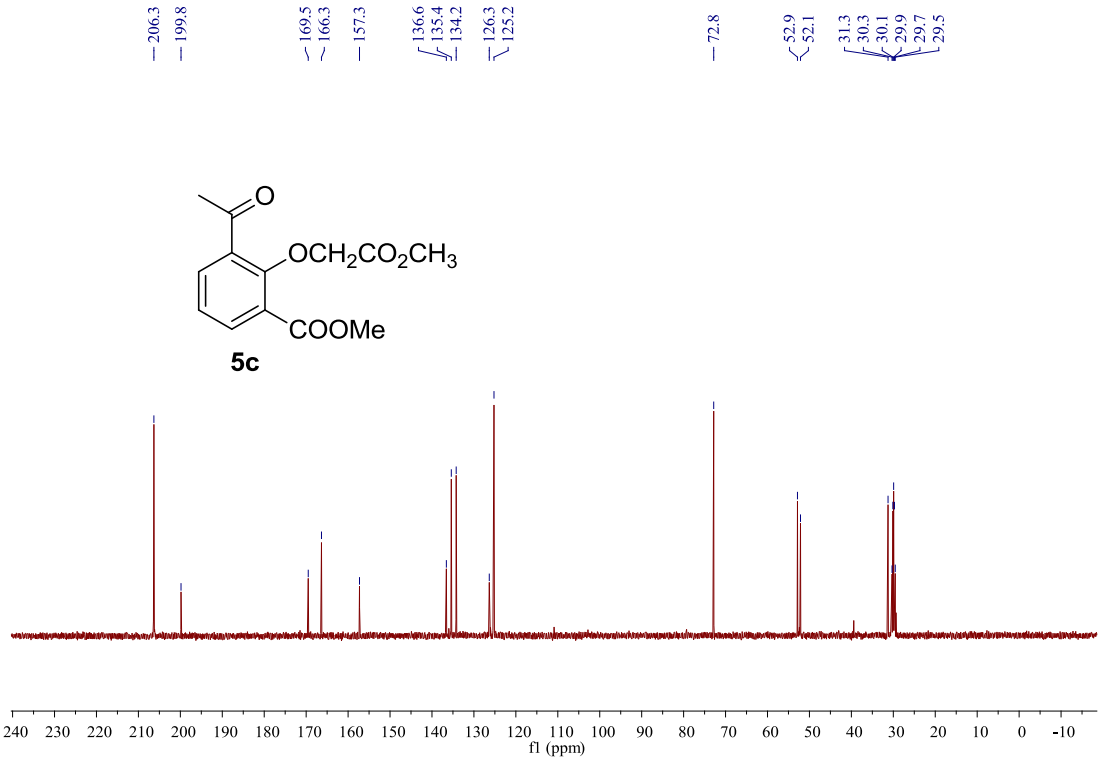
^{13}C-NMR spectrum for 1b (in $CDCl_3$)



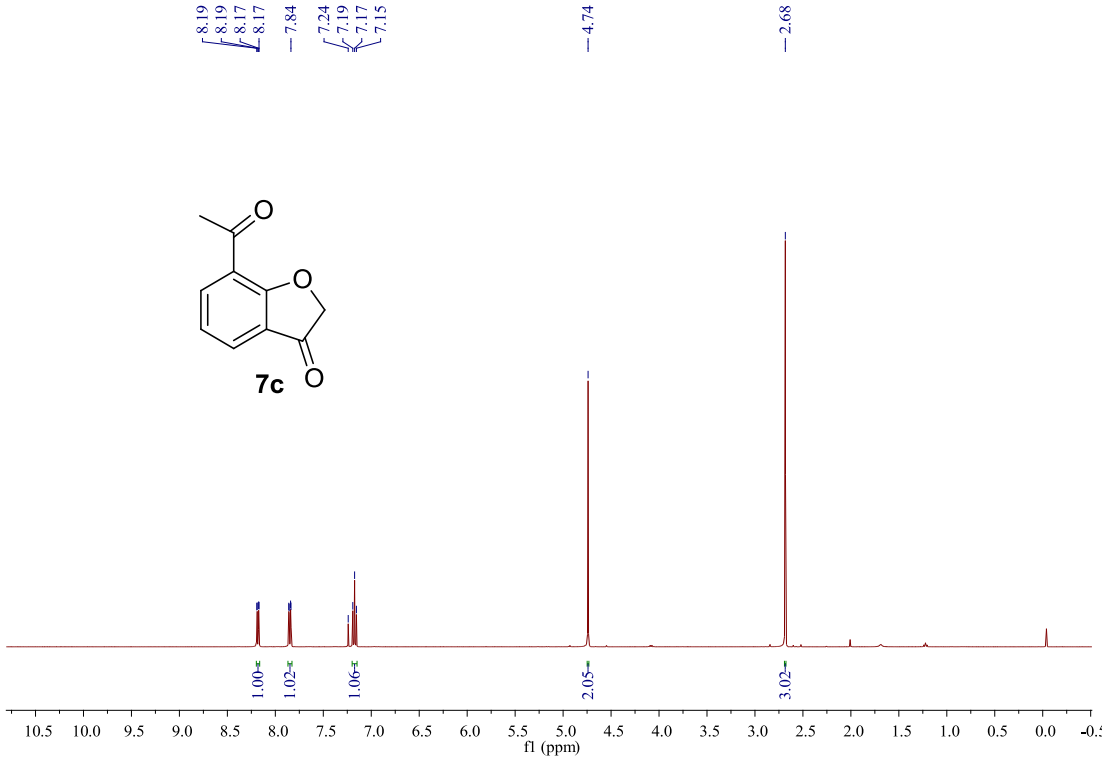
^{1}H-NMR spectrum for 5c (in CD_3COCD_3)



^{13}C-NMR spectrum for 5c (in CD_3COCD_3)



^{1}H-NMR spectrum for 7c (in $CDCl_3$)



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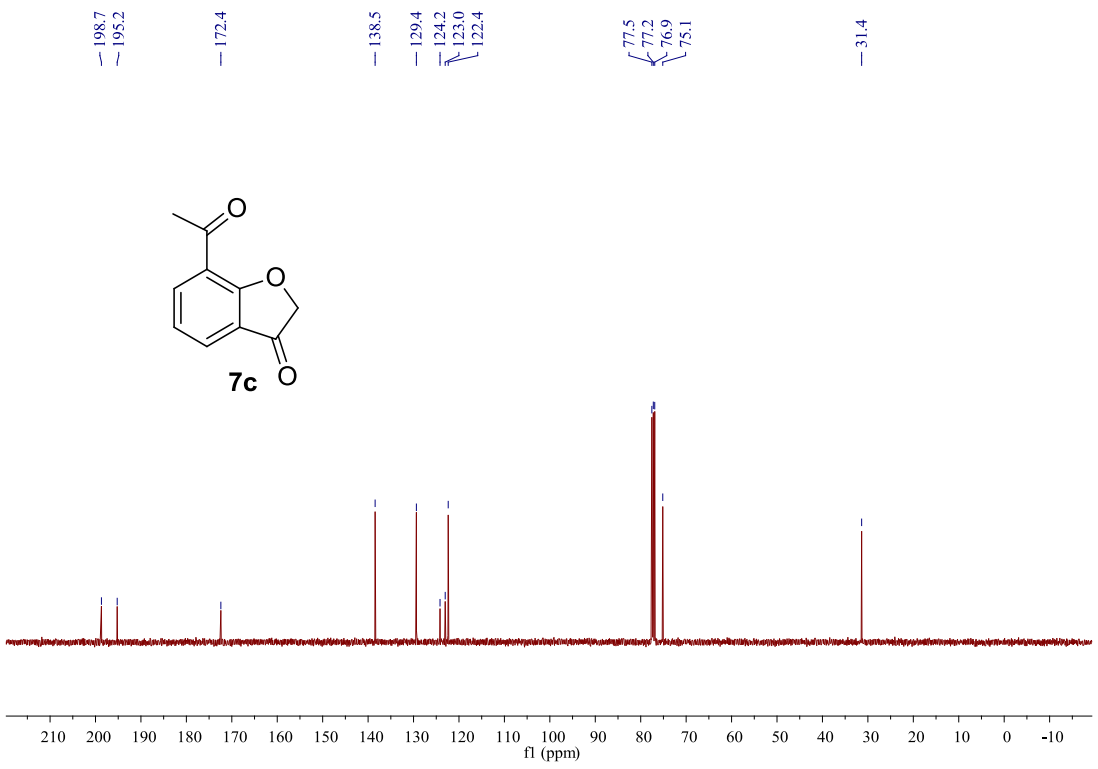

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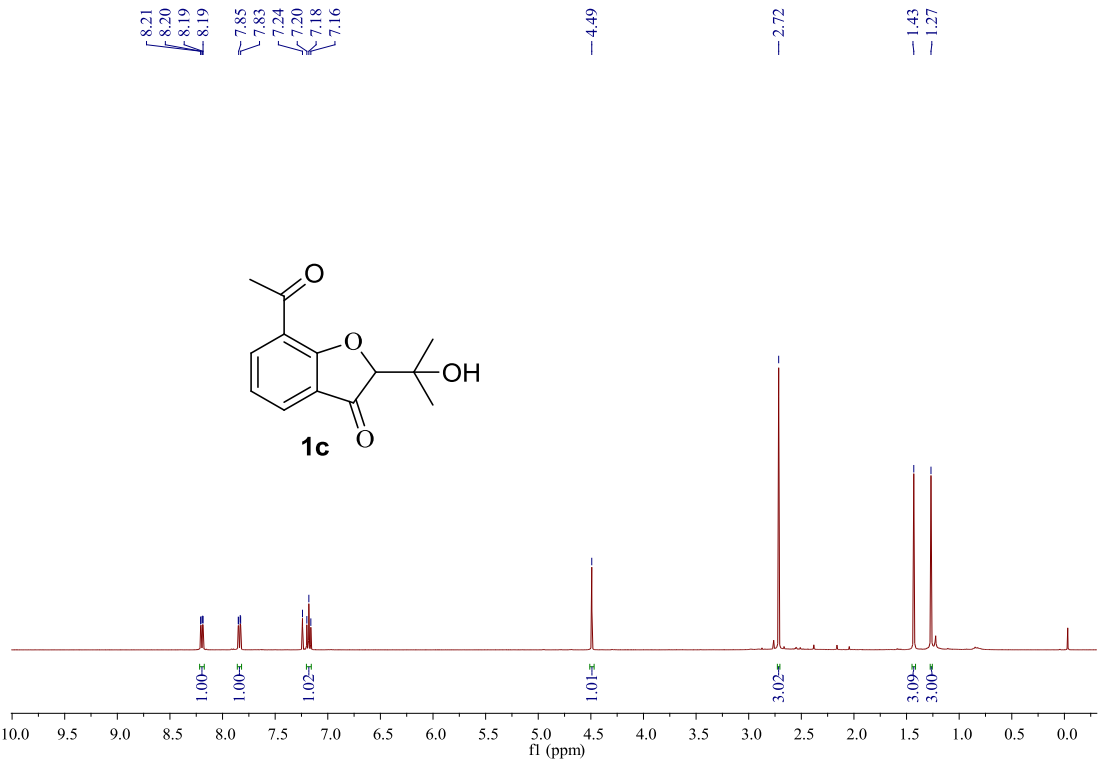

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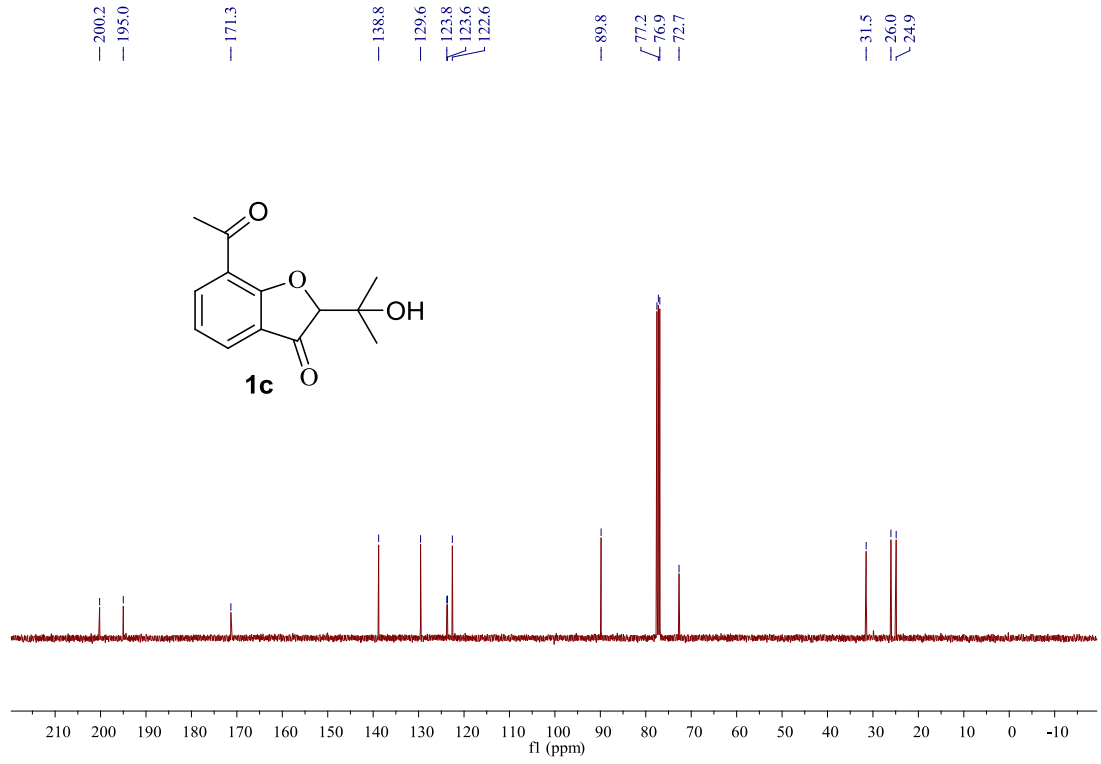

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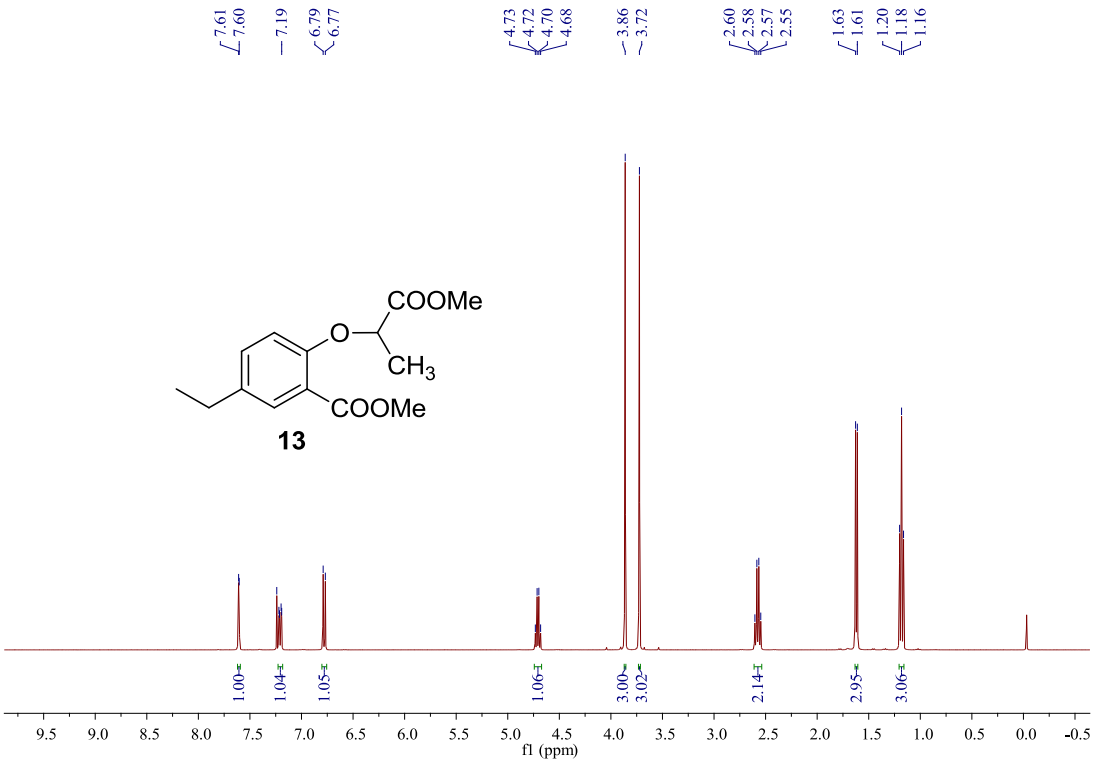
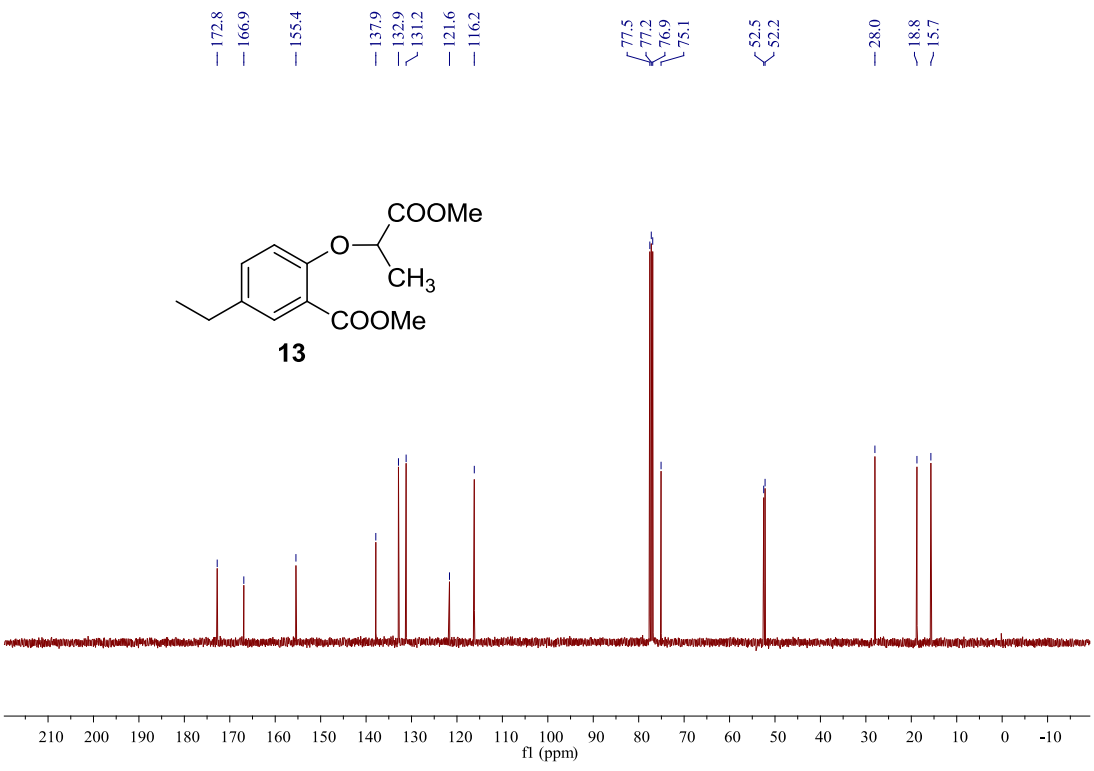
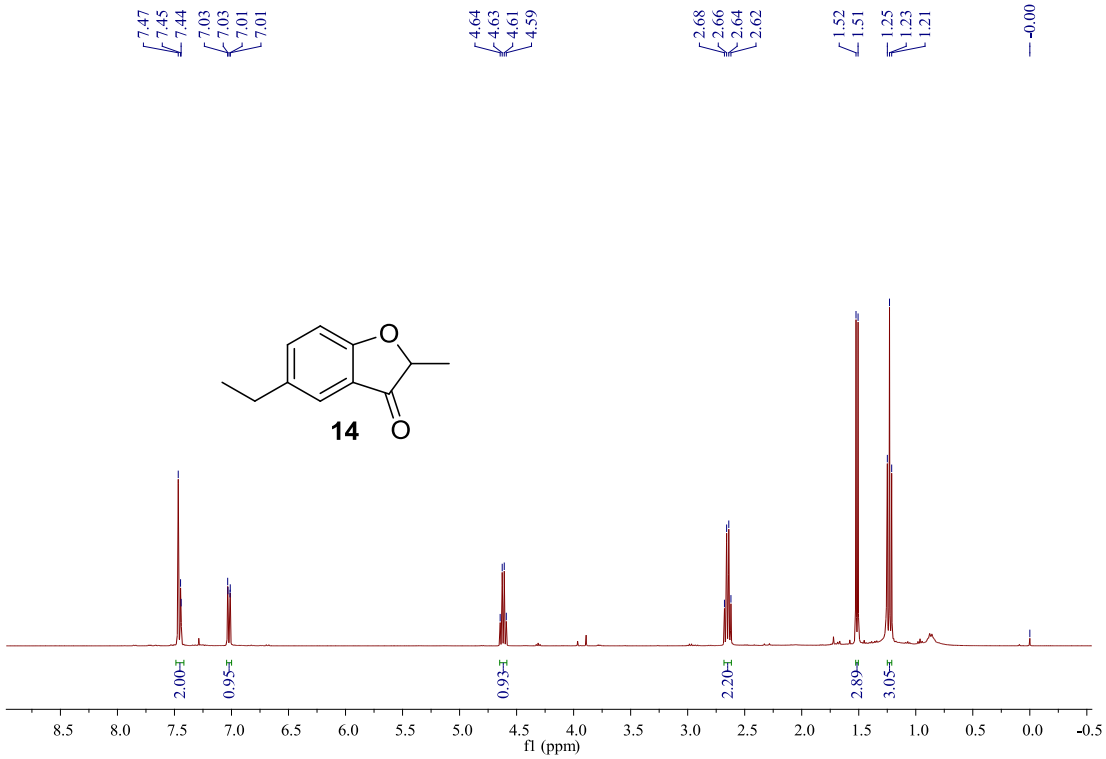


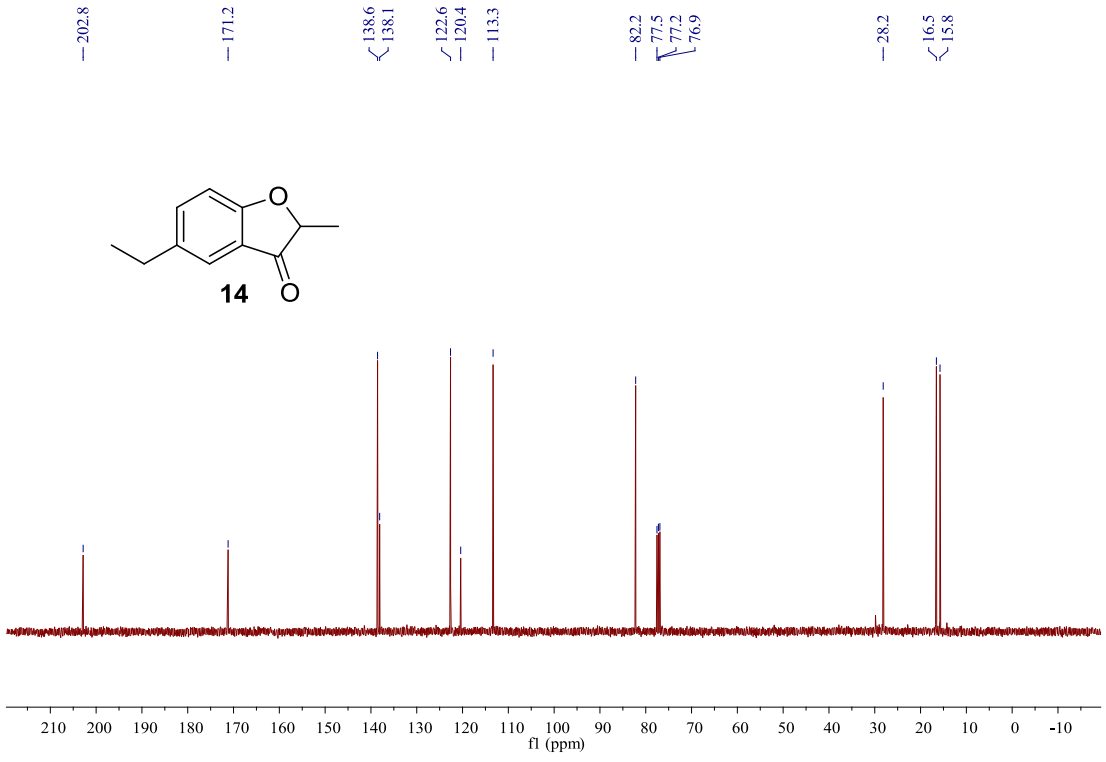
^{13}C-NMR spectrum for 13 (in $CDCl_3$)



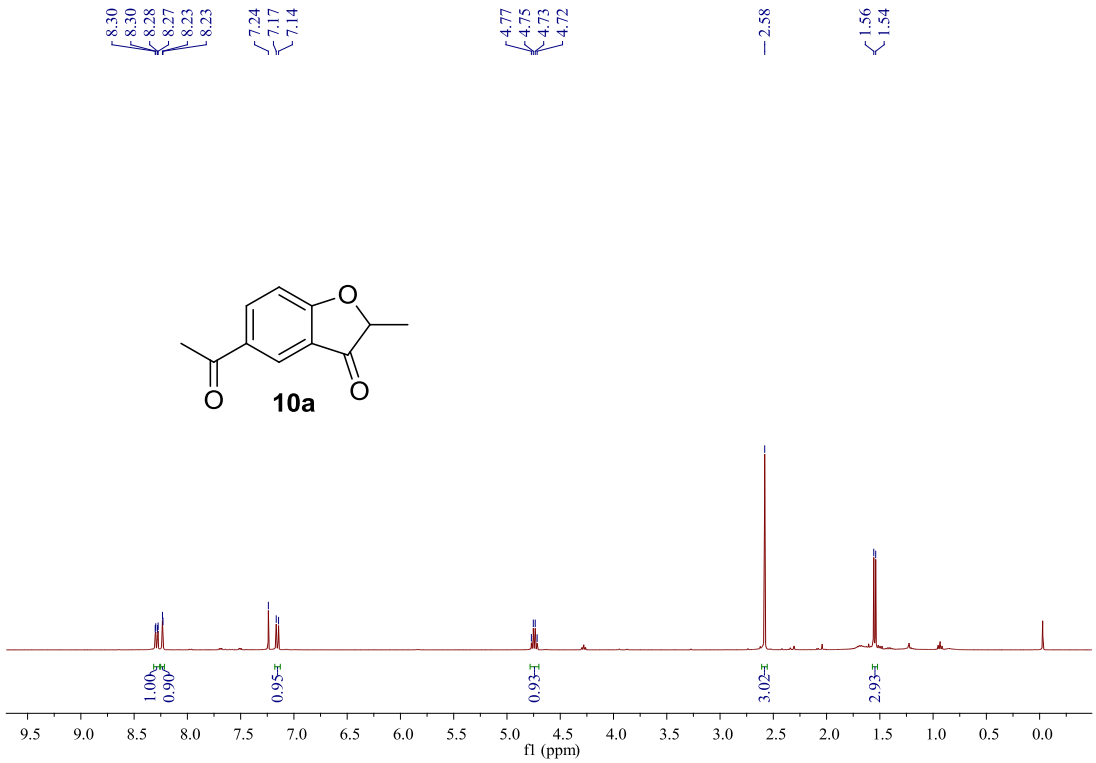
^{1}H-NMR spectrum for 14 (in $CDCl_3$)



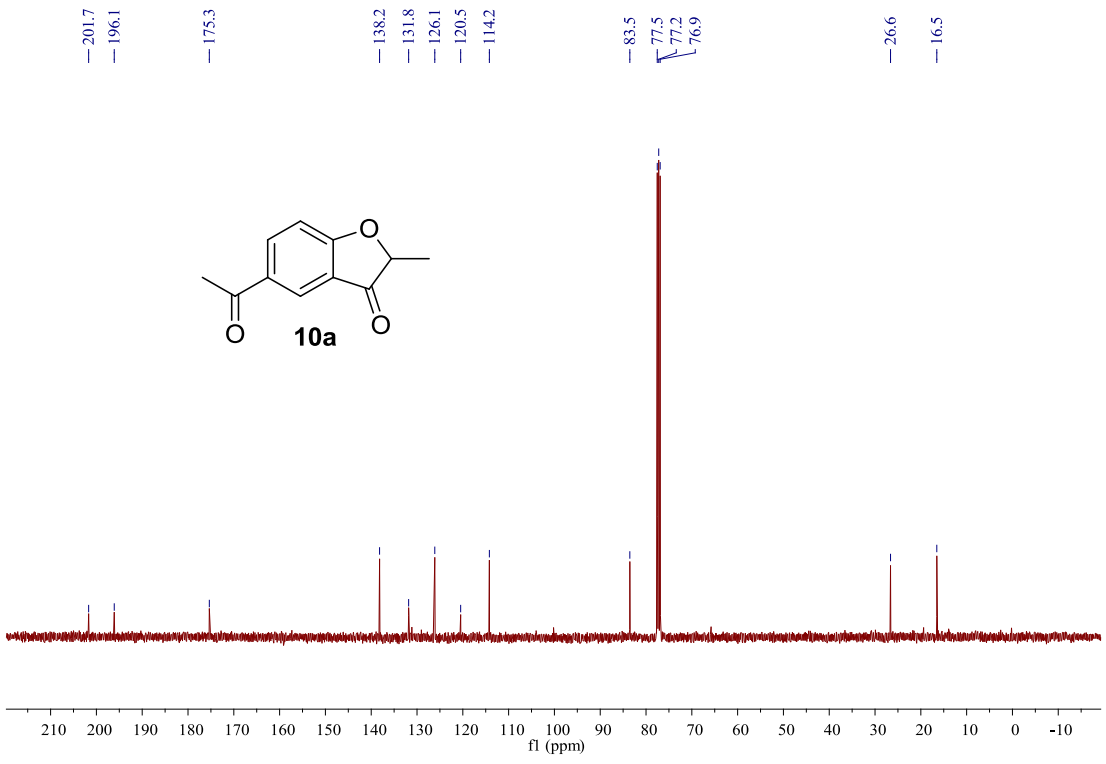
^{13}C-NMR spectrum for 14 (in $CDCl_3$)



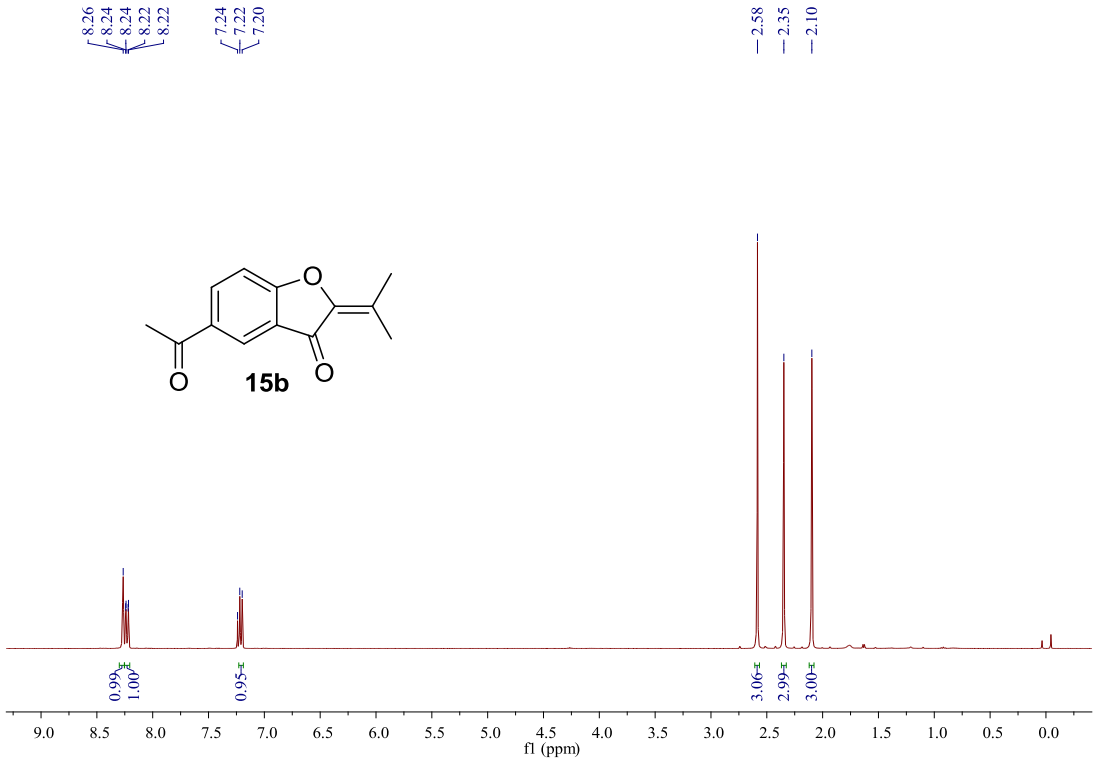
^{1}H-NMR spectrum for 10a (in $CDCl_3$)



^{13}C-NMR spectrum for 10a (in $CDCl_3$)



^{1}H-NMR spectrum for 15b (in $CDCl_3$)



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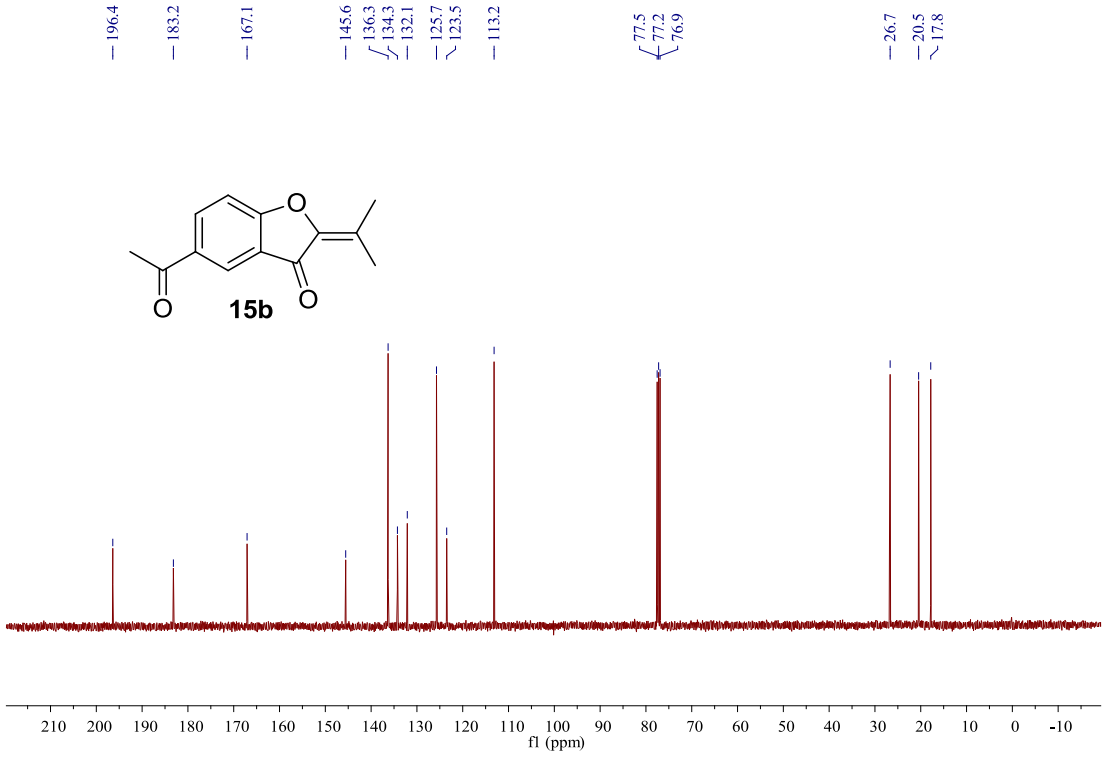

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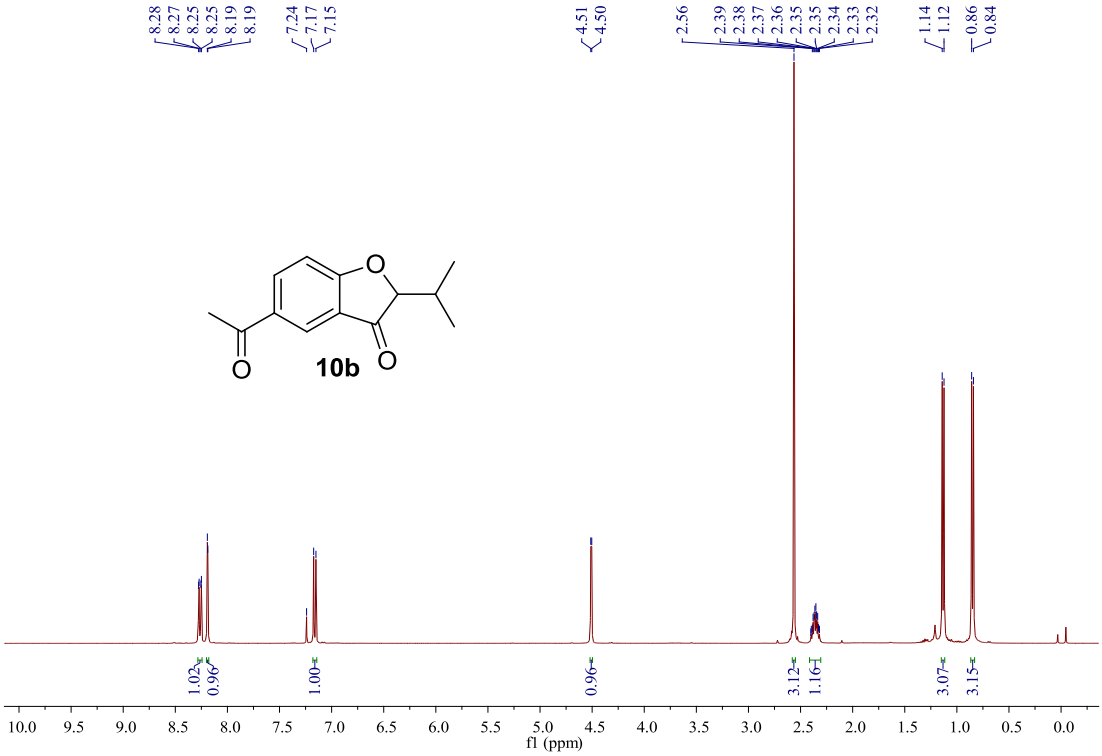
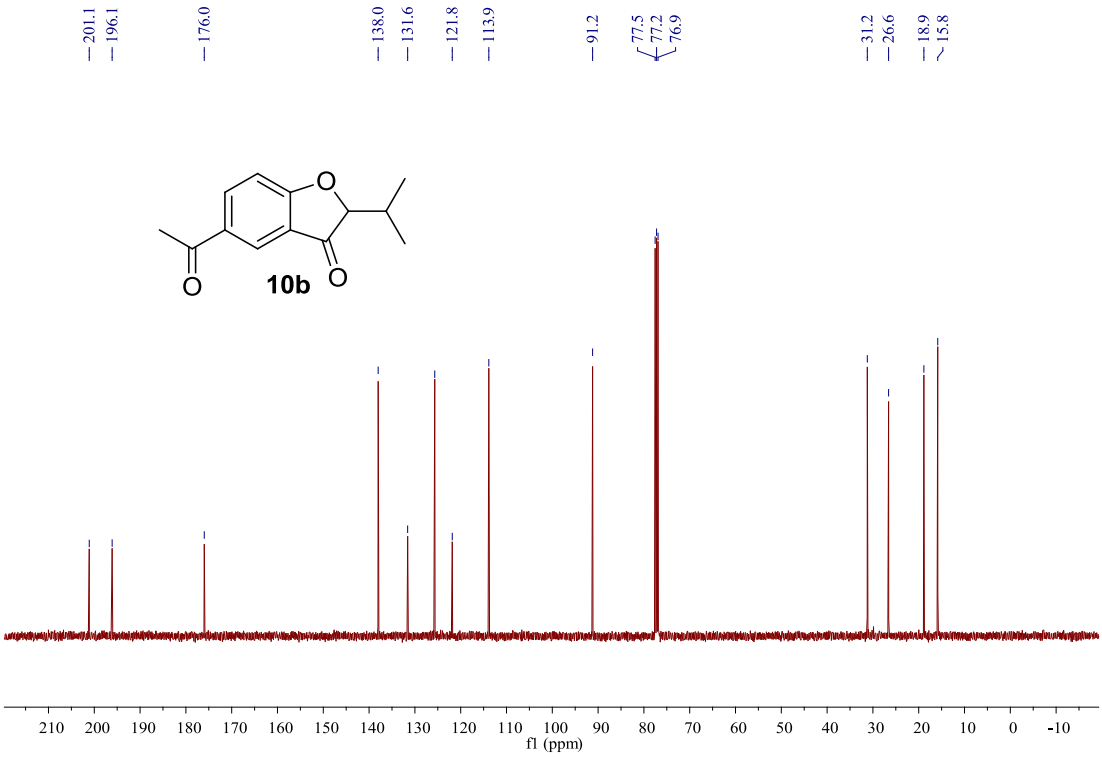
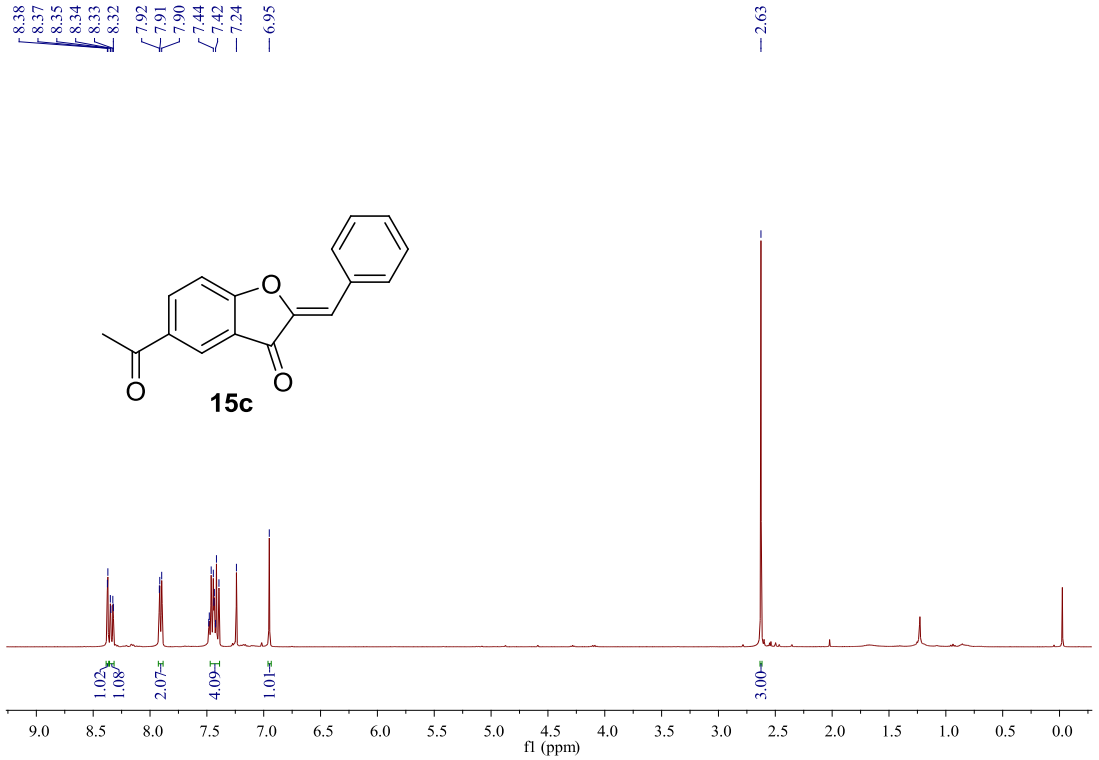


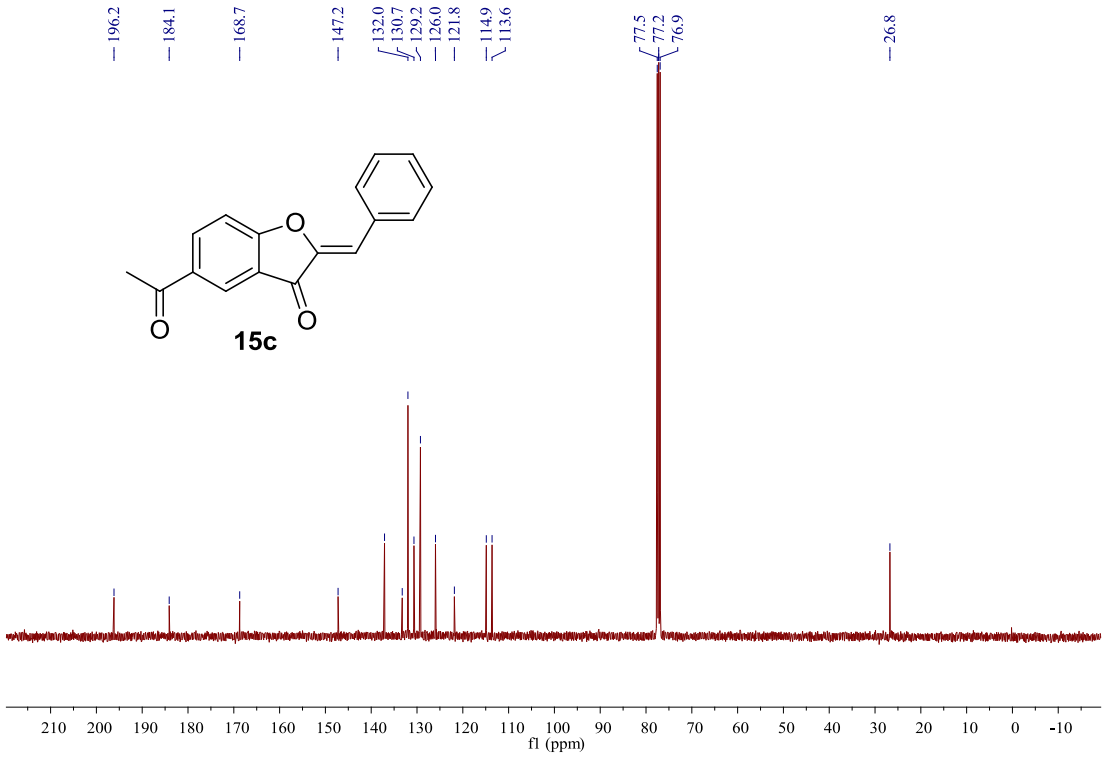
^{13}C-NMR spectrum for 10b (in $CDCl_3$)



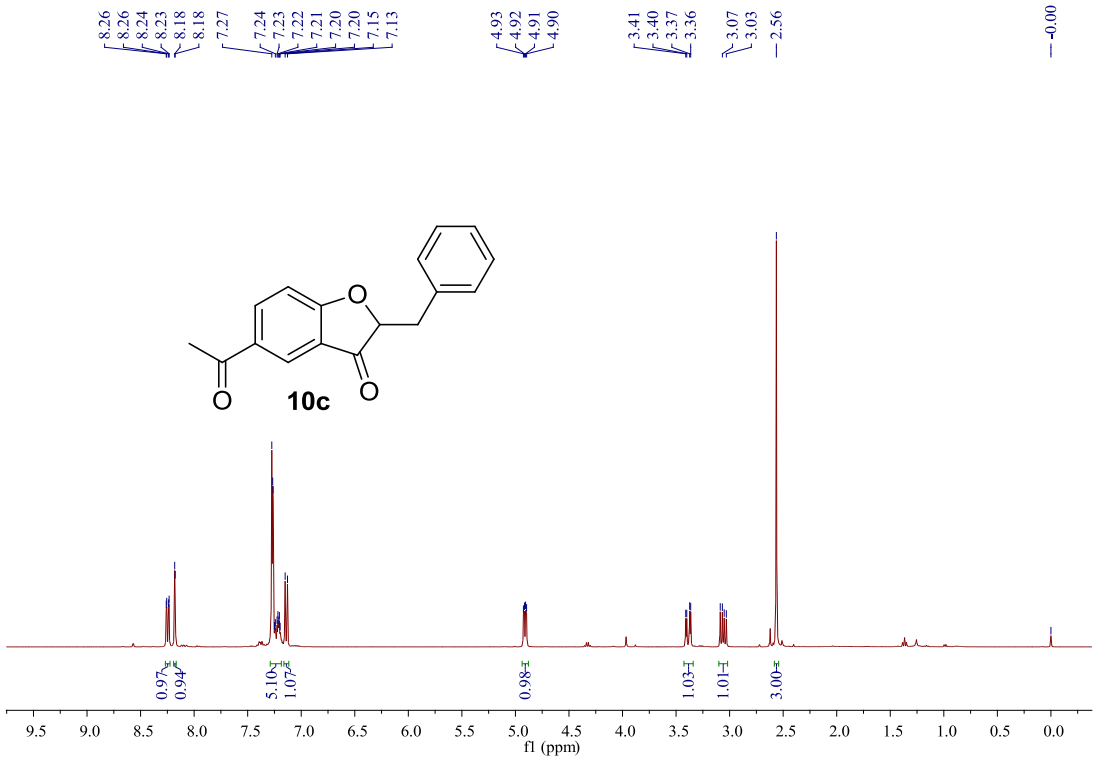
^{1}H-NMR spectrum for 15c (in $CDCl_3$)



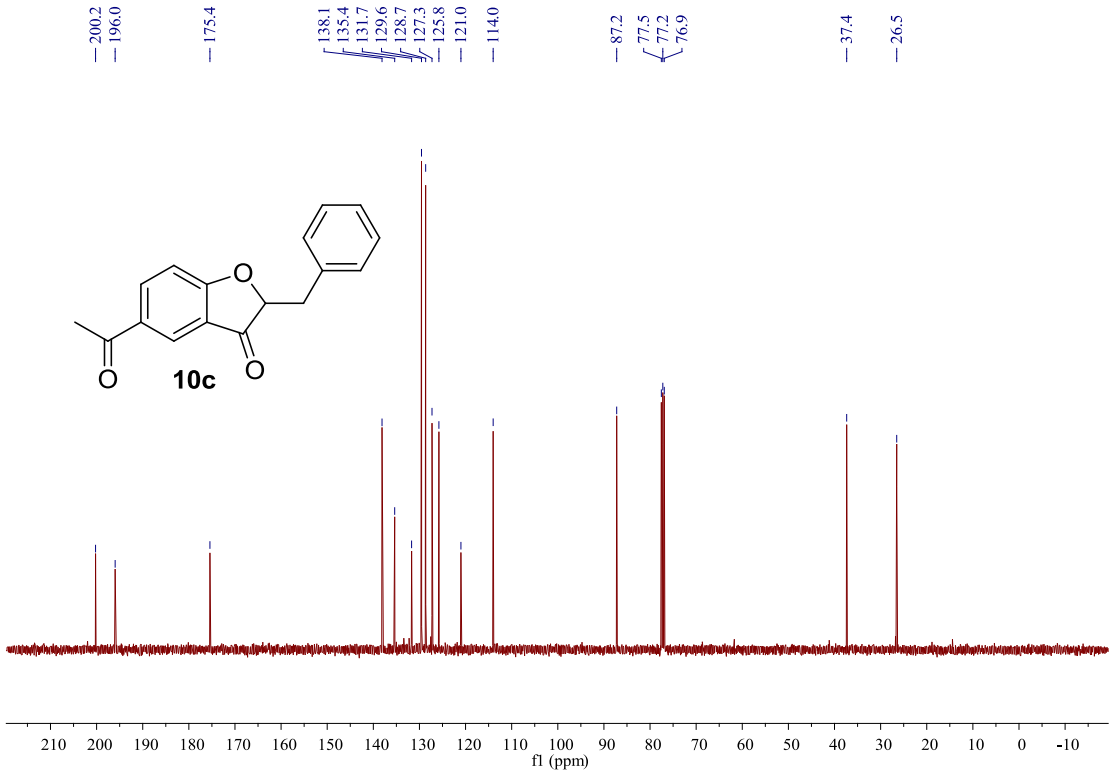
^{13}C-NMR spectrum for 15c (in $CDCl_3$)



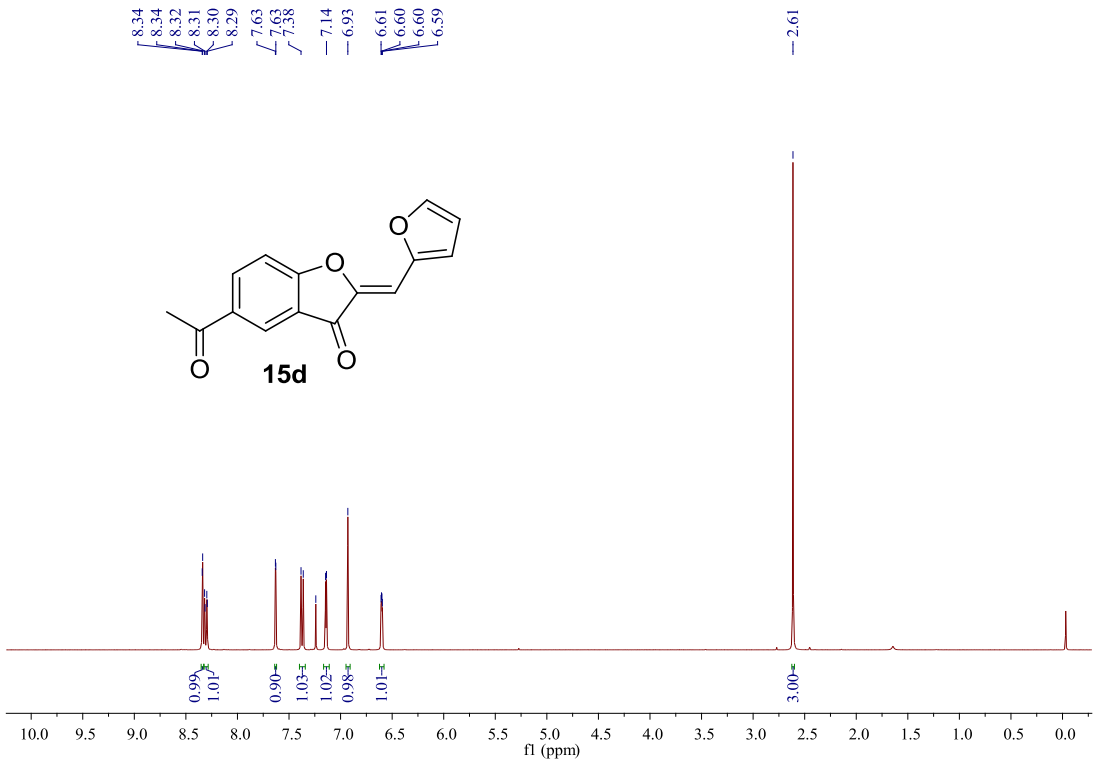
^{1}H-NMR spectrum for 10c (in $CDCl_3$)



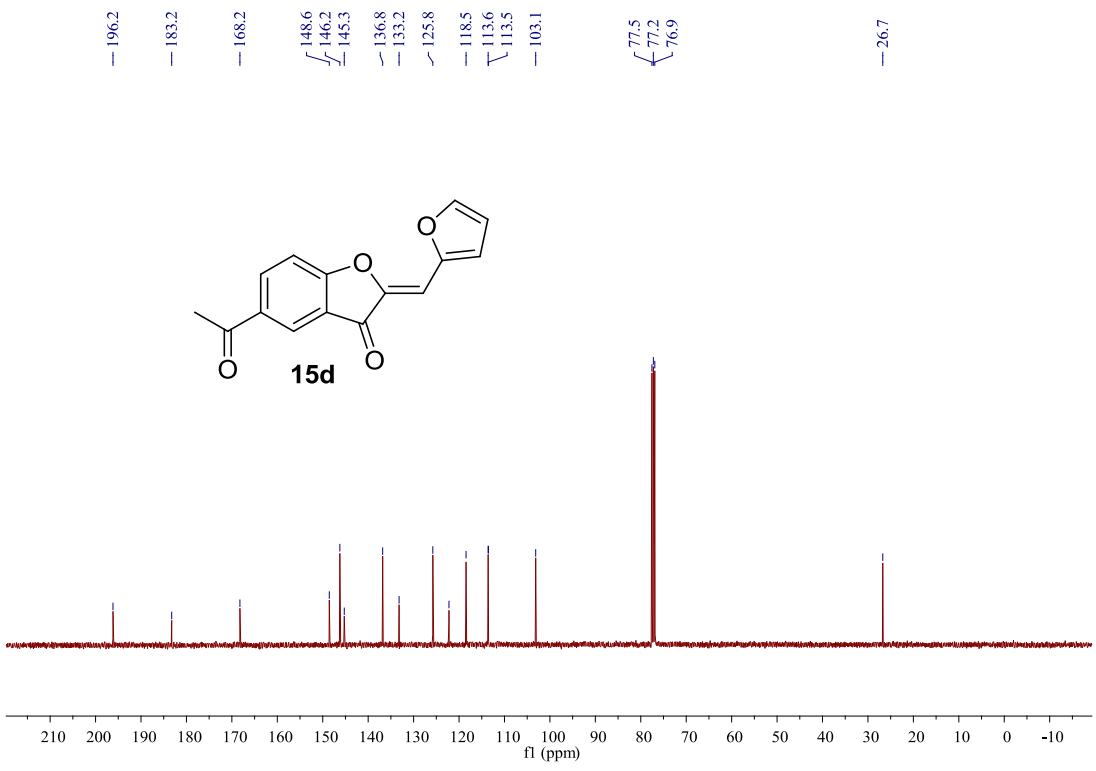
^{13}C-NMR spectrum for 10c (in $CDCl_3$)



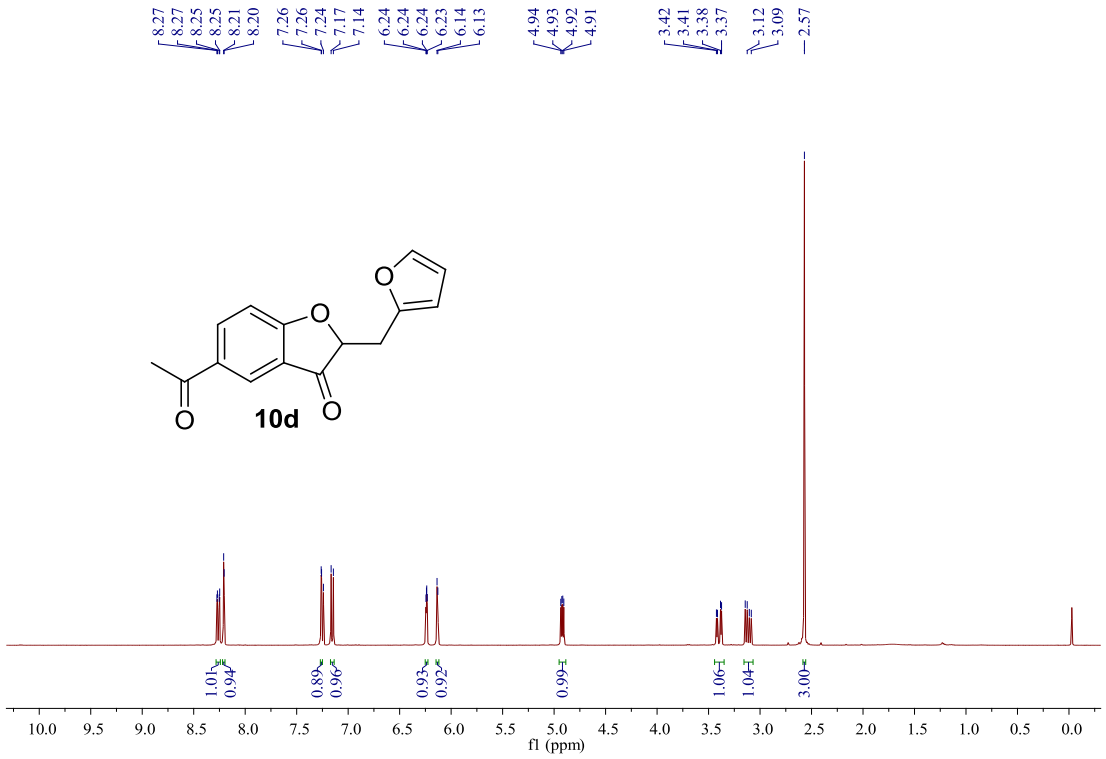
^{1}H-NMR spectrum for 15d (in $CDCl_3$)



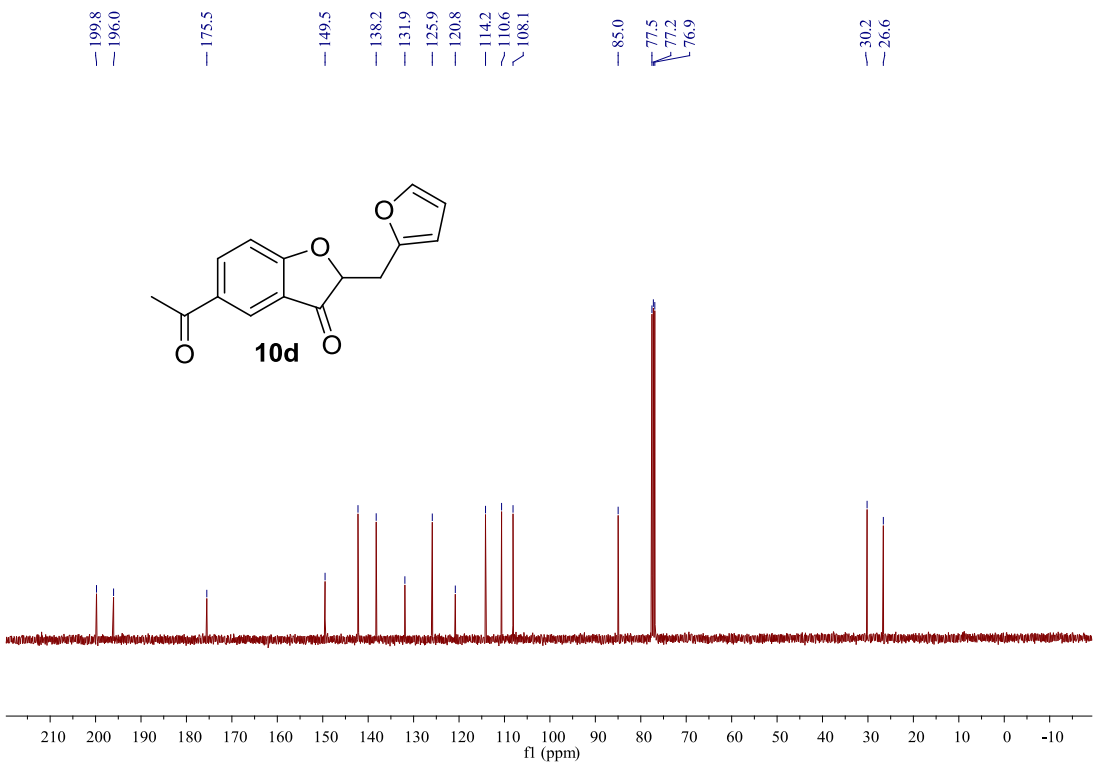
^{13}C-NMR spectrum for 15d (in $CDCl_3$)



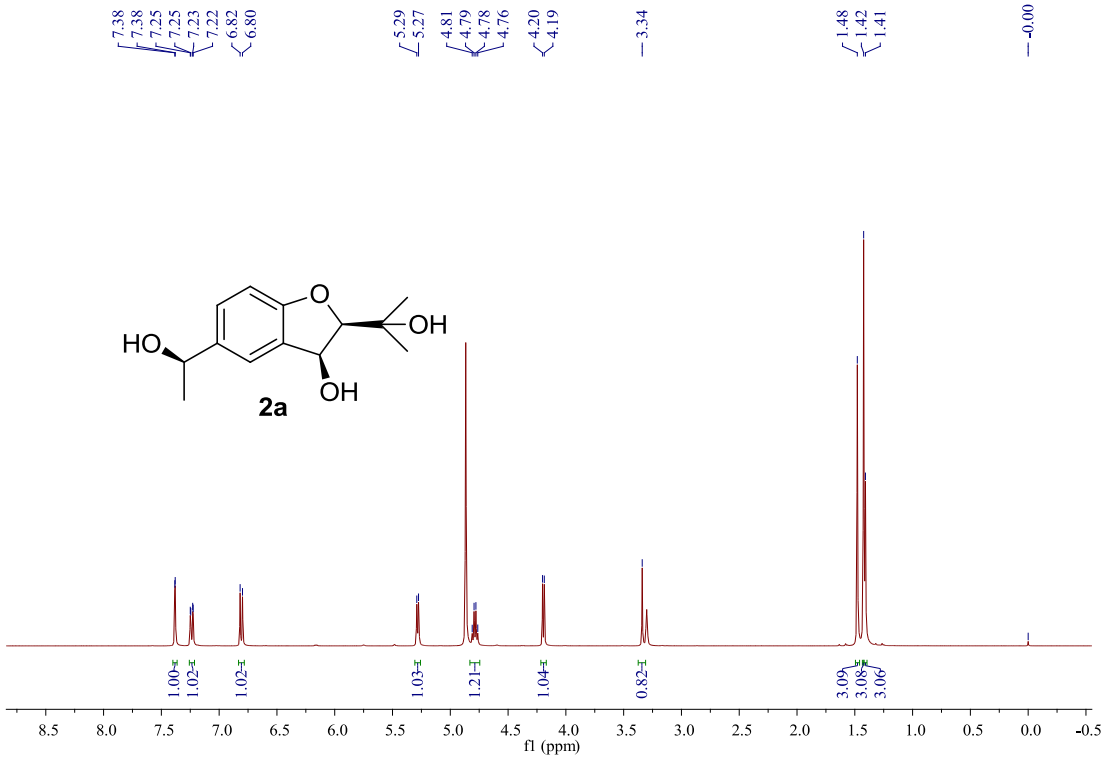
^{1}H-NMR spectrum for 10d (in $CDCl_3$)



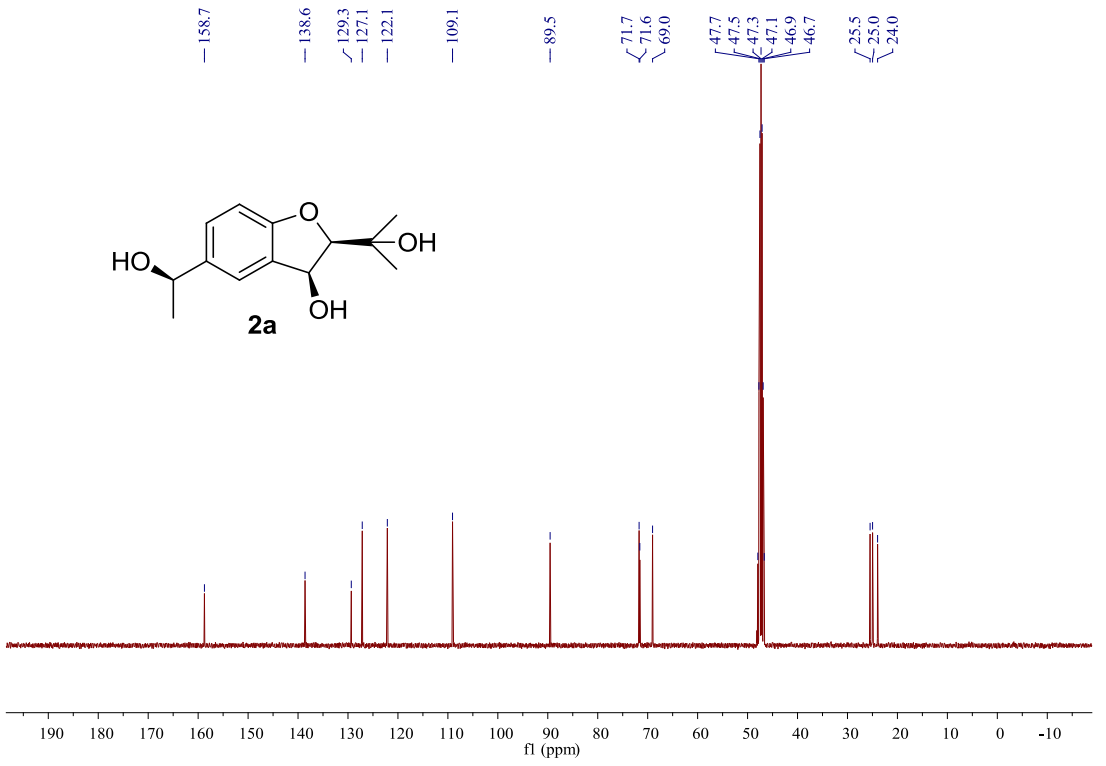
^{13}C-NMR spectrum for 10d (in $CDCl_3$)



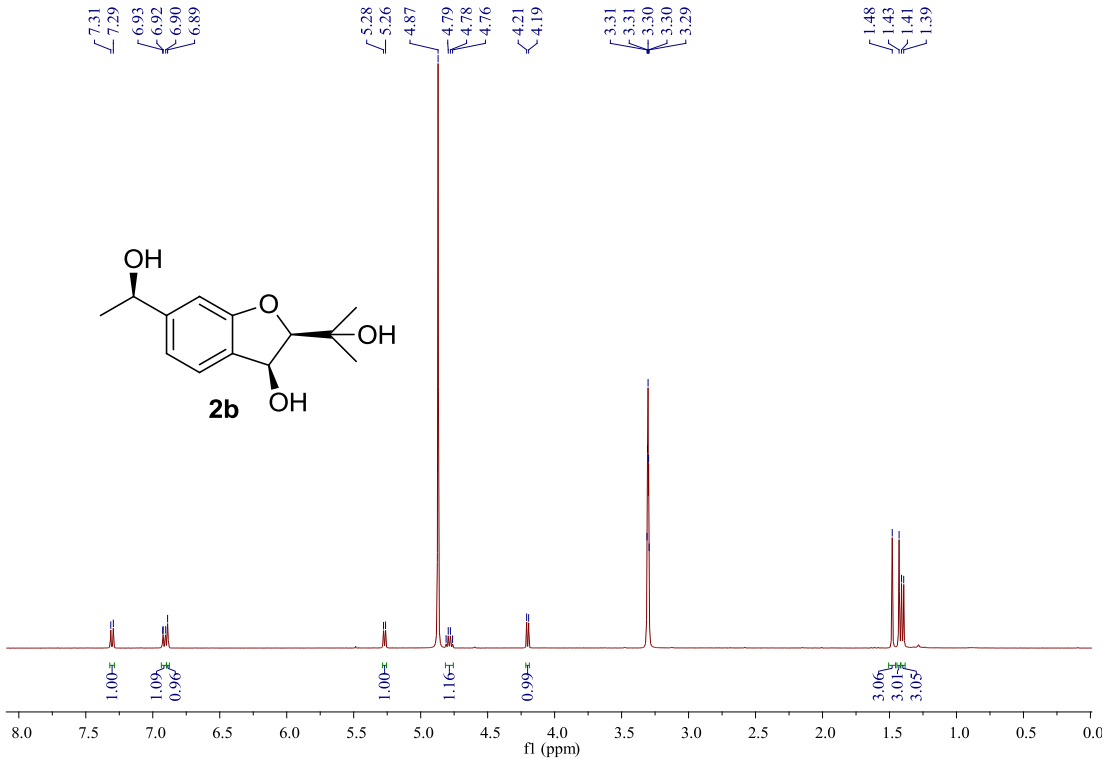
^{1}H-NMR spectrum for 2a (in CD_3OD)



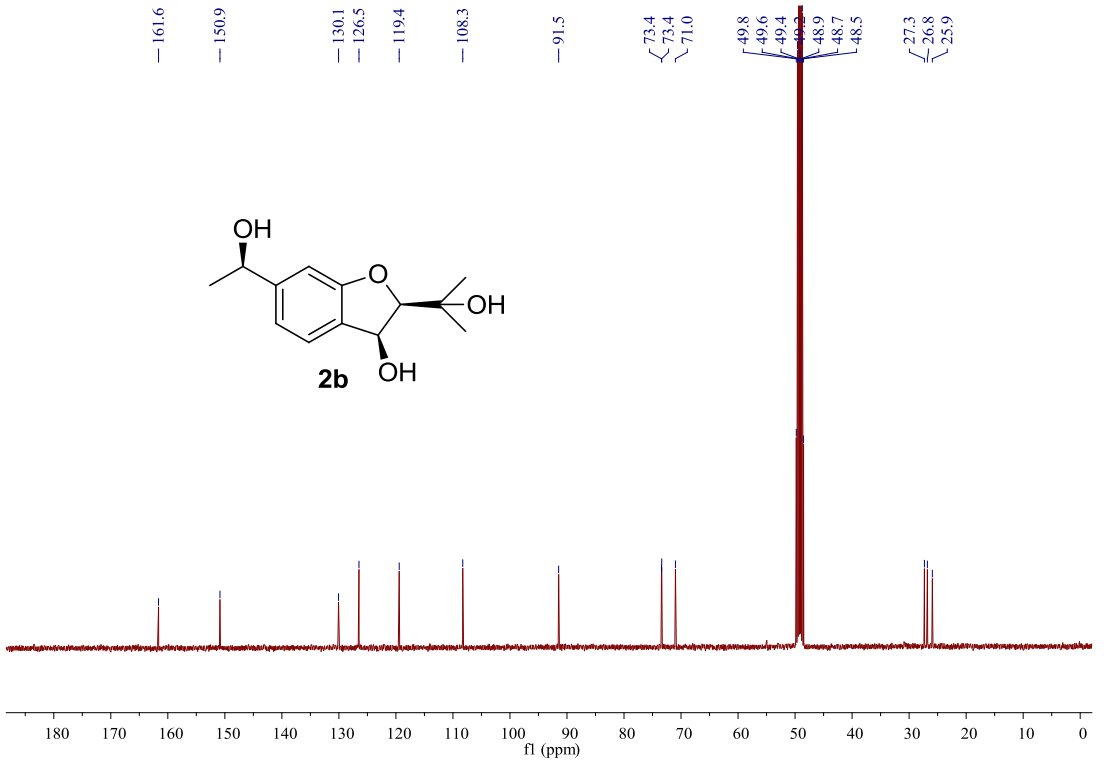
^{13}C-NMR spectrum for 2a (in CD_3OD)



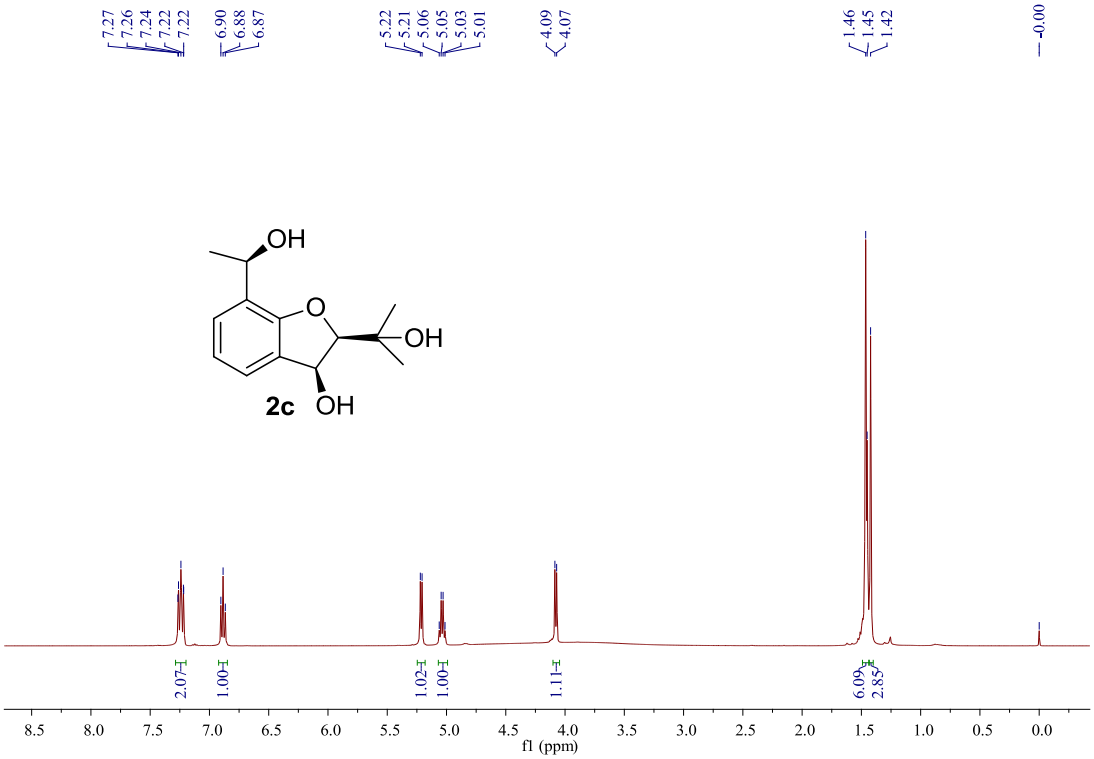
^{1}H-NMR spectrum for 2b (in CD_3OD)



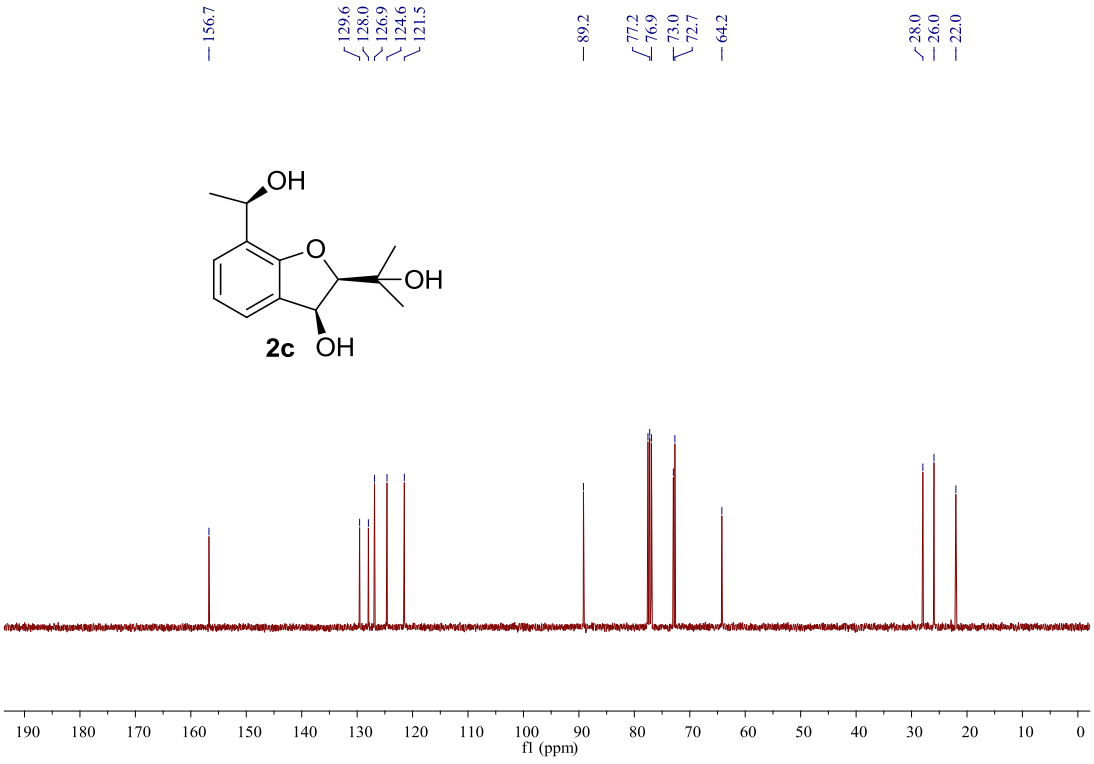
^{13}C-NMR spectrum for 2b (in CD_3OD)



^{1}H-NMR spectrum for 2c (in CD_3OD)



^{13}C-NMR spectrum for 2c (in CD_3OD)



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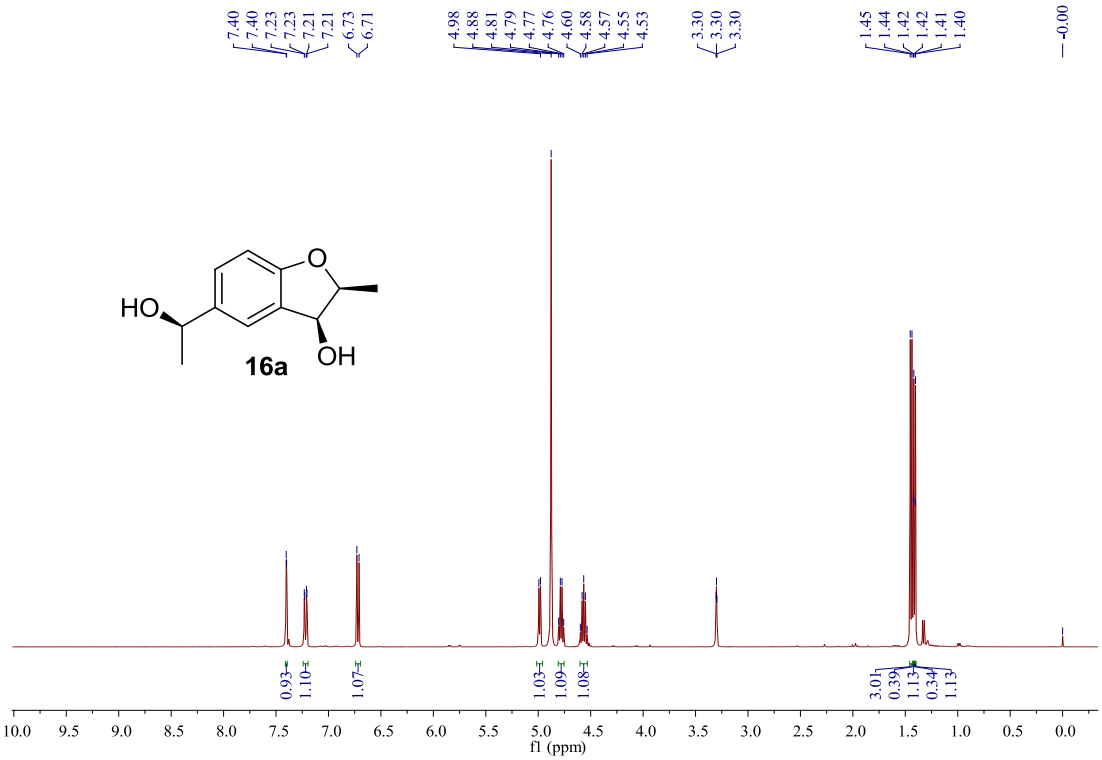
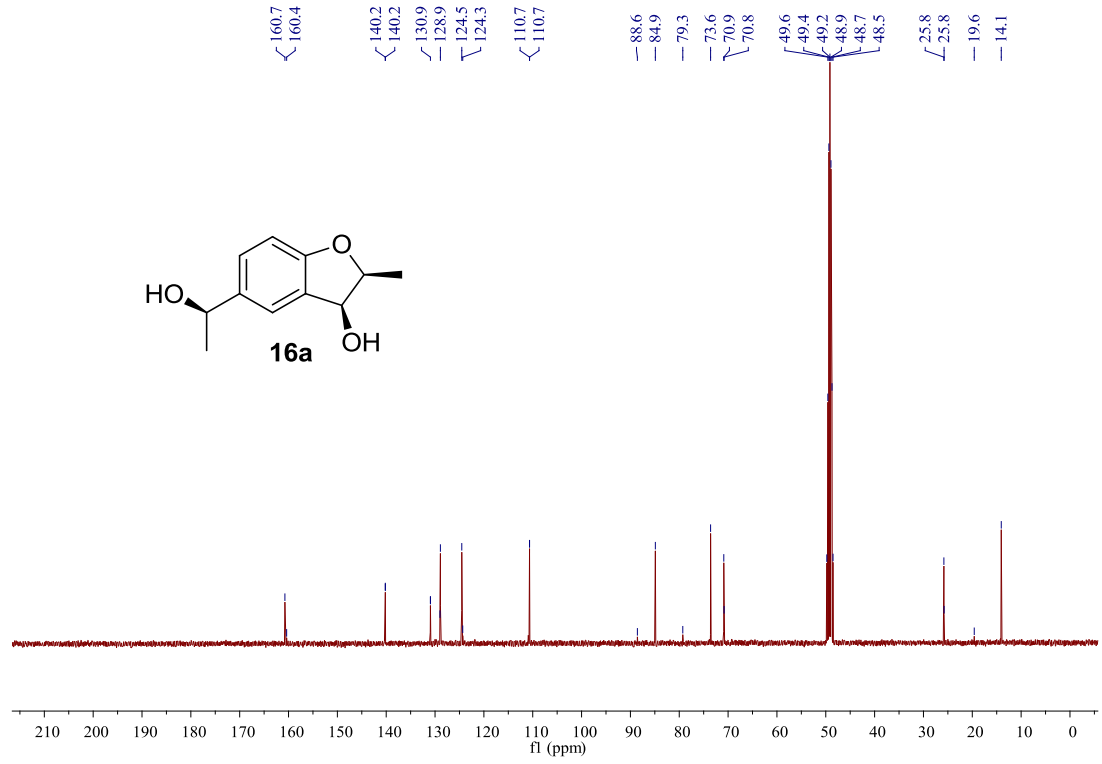
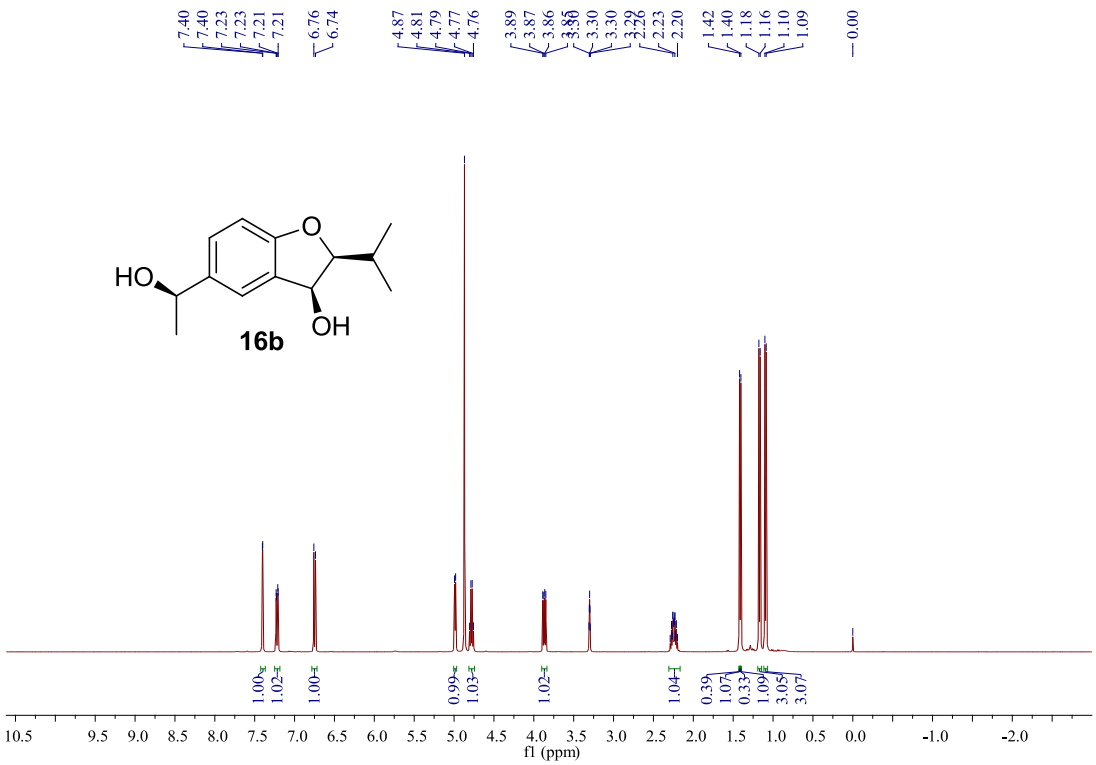


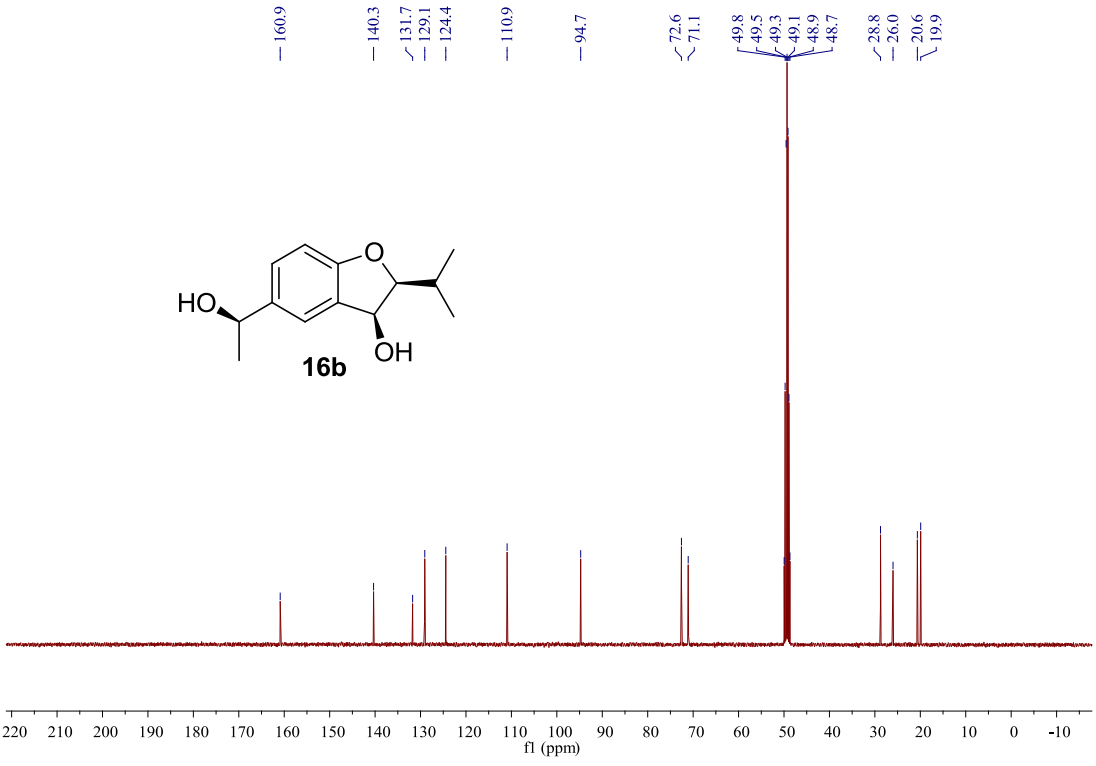
^{13}C-NMR spectrum for 16a (in CD_3OD)



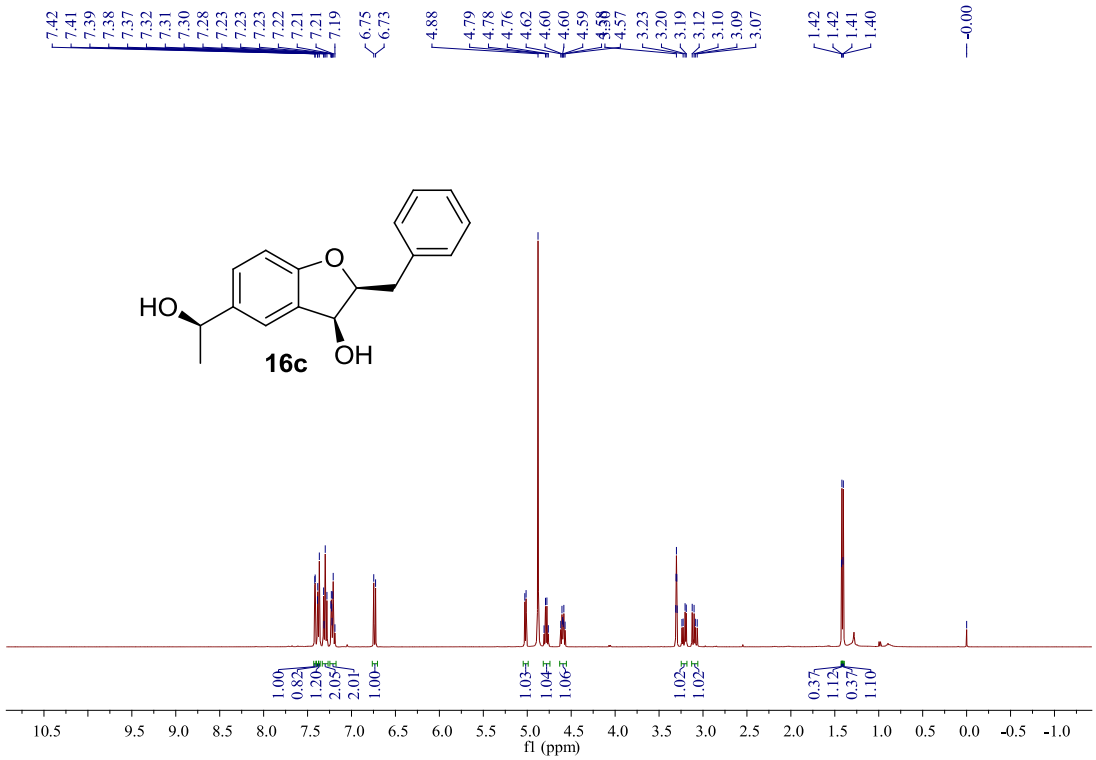
^{1}H-NMR spectrum for 16b (in CD_3OD)



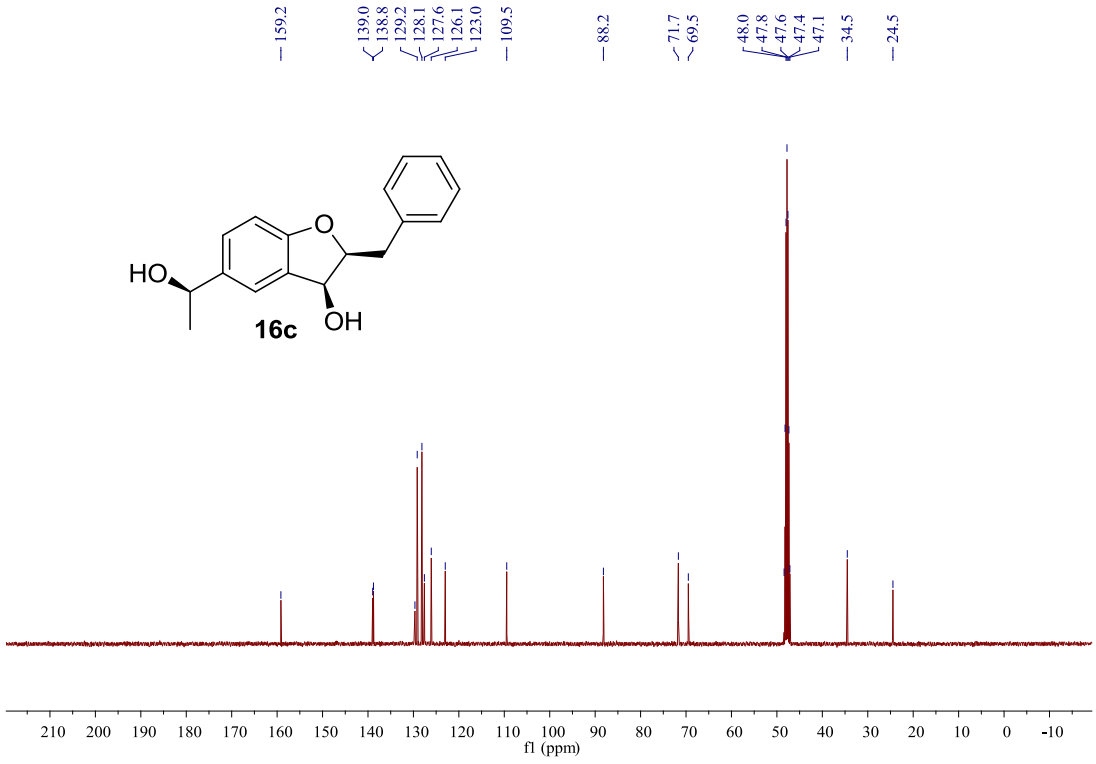
^{13}C-NMR spectrum for 16b (in CD_3OD)



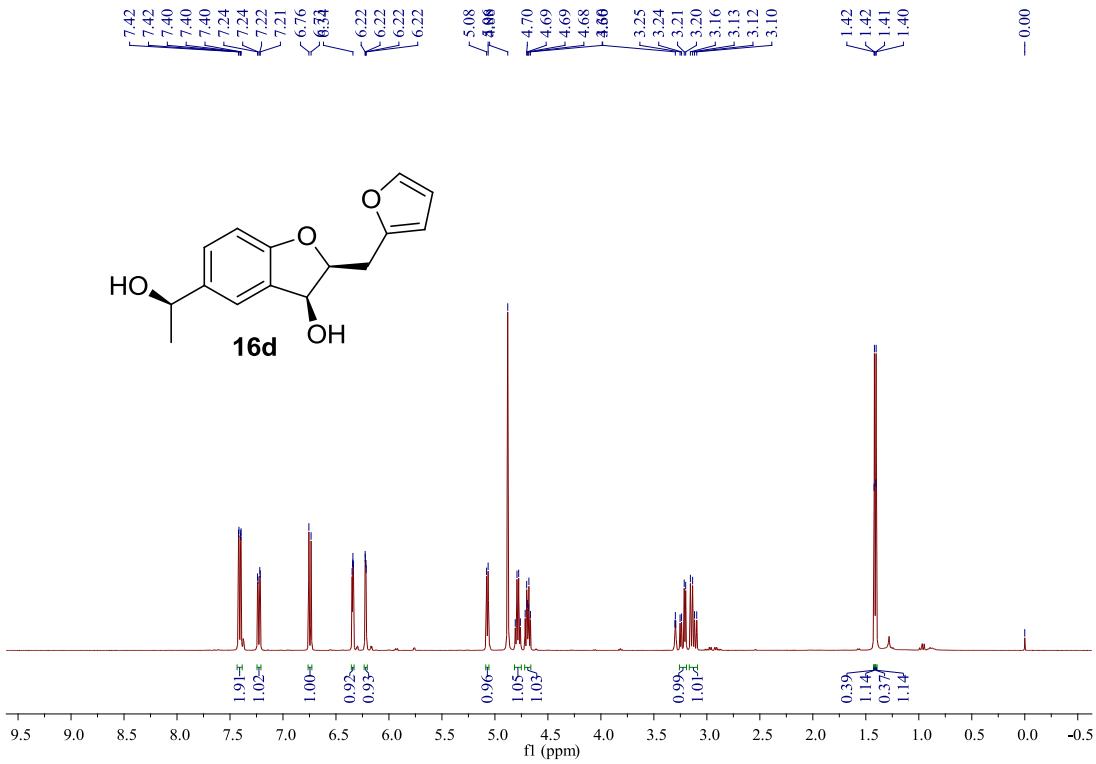
^{1}H-NMR spectrum for 16c (in CD_3OD)



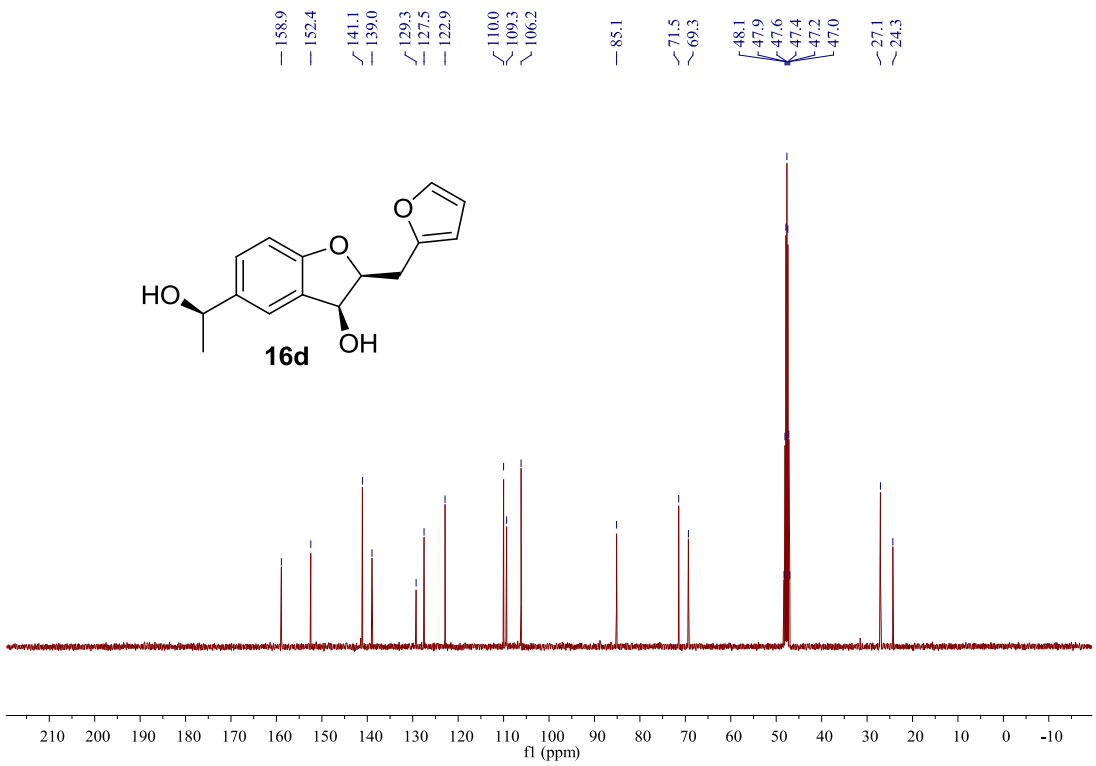
^{13}C-NMR spectrum for 16c (in CD_3OD)



^{1}H-NMR spectrum for 16d (in CD_3OD)



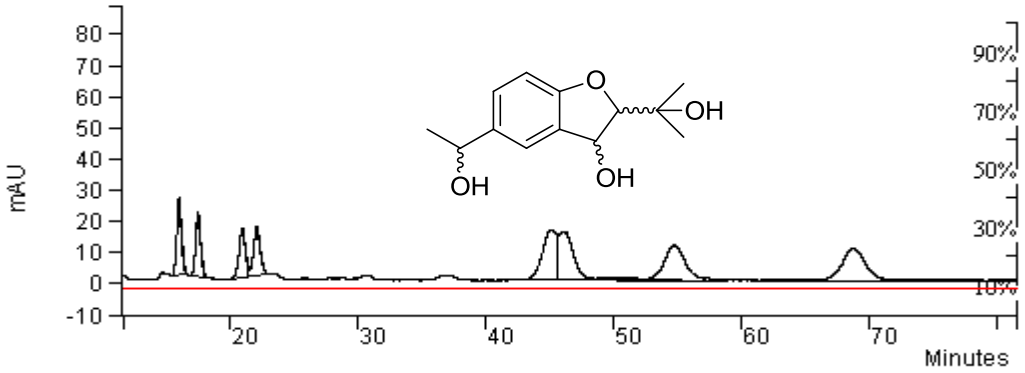
^{13}C-NMR spectrum for 16d (in CD_3OD)



2. HPLC Analysis Spectra

(±)-5-(1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

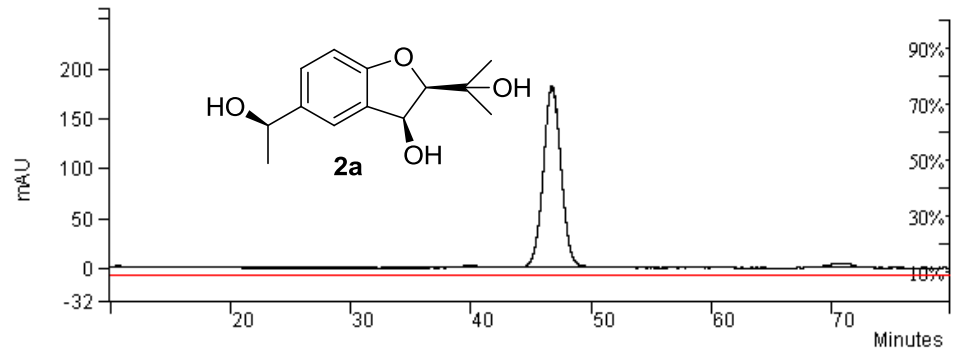
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		8.2261	15.882	0.000	23.2	6172810
2		7.4864	17.365	0.000	24.5	5617700
3		7.3912	20.830	0.000	32.5	5546308
4		7.5832	21.968	0.000	35.7	5690388
5		17.1987	44.951	0.000	82.4	12905719
6		17.2564	46.015	0.000	124.5	12949000
7		16.7471	54.627	0.000	0.0	12566850
8		18.1109	68.586	0.000	111.0	13590208
	Totals	**100.0000**		**0.000**		**75038984**

(2*R*,3*S*)-5-((*R*)-1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

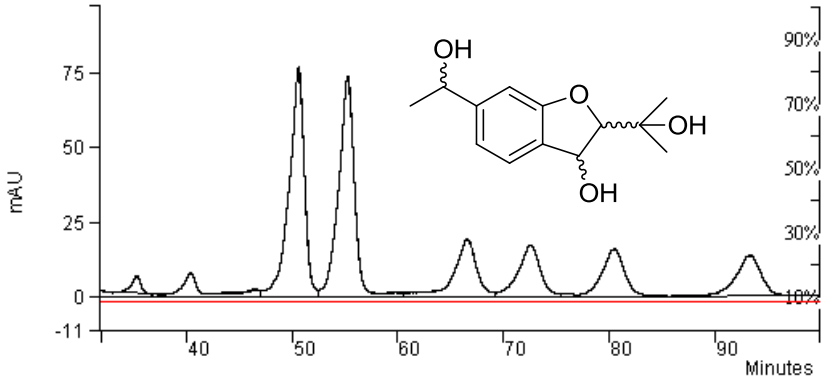
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		98.0277	46.693	0.000	94.8	188381504
2		1.9723	70.744	0.000	116.0	3790177
	Totals	**100.0000**		**0.000**		**192171680**

(±)-6-(1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

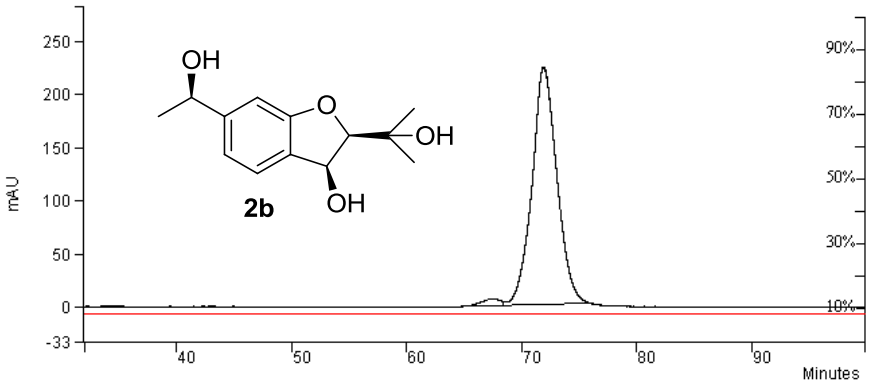
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		1.4322	35.192	0.000	0.0	3846354
2		4.0368	40.305	0.000	73.8	10841409
3		28.5422	50.490	0.000	89.2	76653792
4		28.8126	55.151	0.000	0.0	77379920
5		10.6371	66.469	0.000	117.2	28567396
6		9.4622	72.459	0.000	124.3	25411870
7		8.7356	80.350	0.000	129.5	23460666
8		8.3413	93.189	0.000	146.8	22401560
	Totals	**100.0000**		**0.000**		**268562976**

(2*R*,3*S*)-6-((*R*)-1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

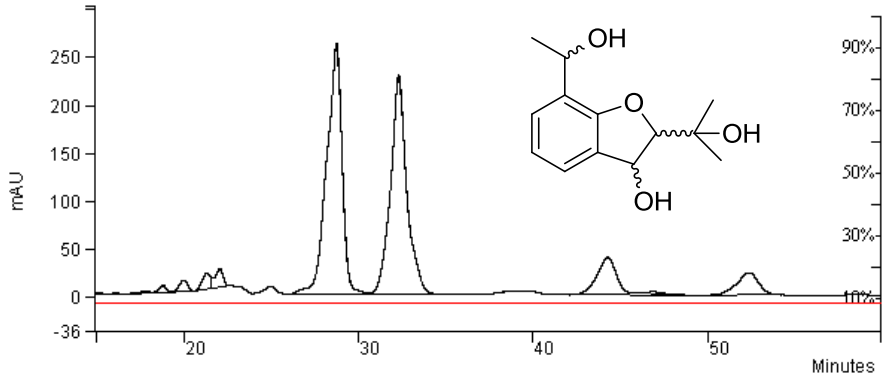
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		2.1445	67.444	0.000	134.3	7417418
2		97.8555	71.917	0.000	137.1	338464032
	Totals	**100.0000**		**0.000**		**345881440**

(±)-7-(1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

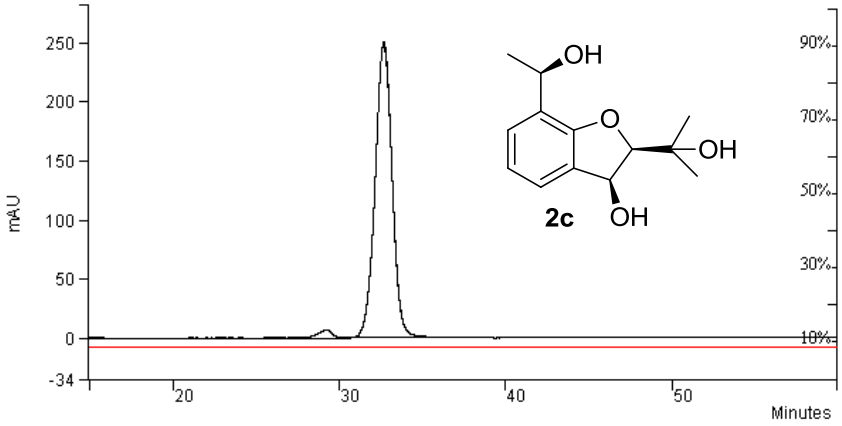
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C), ee =95%.



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		0.5794	18.743	0.000	39.6	2178767
2		1.0629	19.945	0.000	41.7	3997237
3		1.5914	21.360	0.000	54.1	5984797
4		1.7442	21.968	0.000	53.2	6559319
5		42.8573	28.697	0.000	58.0	161170448
6		39.3099	32.267	0.000	53.1	147829824
7		7.5617	44.225	0.000	68.8	28436694
8		5.2932	52.325	0.000	79.1	19905616
	Totals	**100.0000**		**0.000**		**376062720**

(2*R*,3*S*)-7-((*R*)-1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran-3-ol

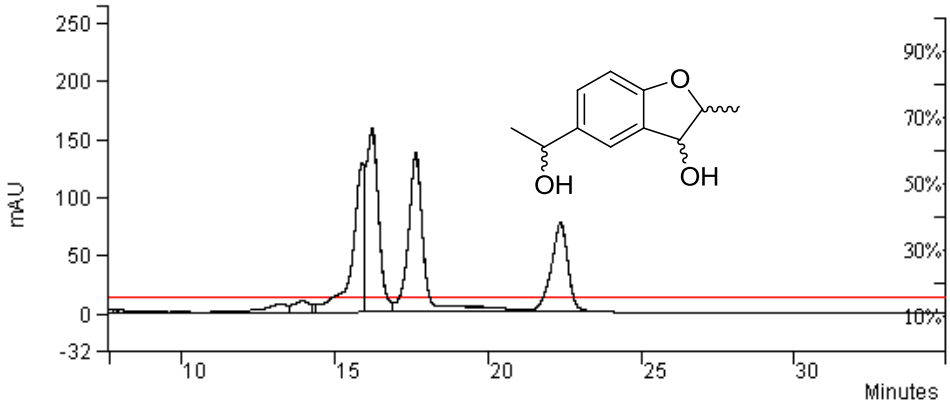
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		2.4327	29.140	0.000	54.1	4431853
2		97.5673	32.640	0.000	65.6	177747408
	Totals	**100.0000**		**0.000**		**182179264**

(±)-5-(1-hydroxyethyl)-2-methyl-2,3-dihydrobenzofuran-3-ol

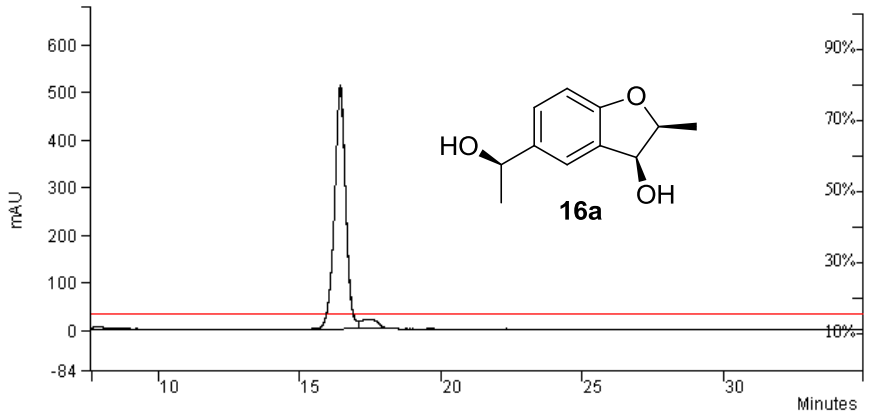
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =85/15, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		22.8547	15.867	0.000	31.4	36535308
2		27.3350	16.197	0.000	37.5	43697568
3		31.1687	17.618	0.000	27.1	49826060
4		18.6416	22.342	0.000	34.1	29800406
	Totals	**100.0000**		**0.000**		**159859344**

(2*S*,3*S*)-5-((*R*)-1-hydroxyethyl)-2-methyl-2,3-dihydrobenzofuran-3-ol

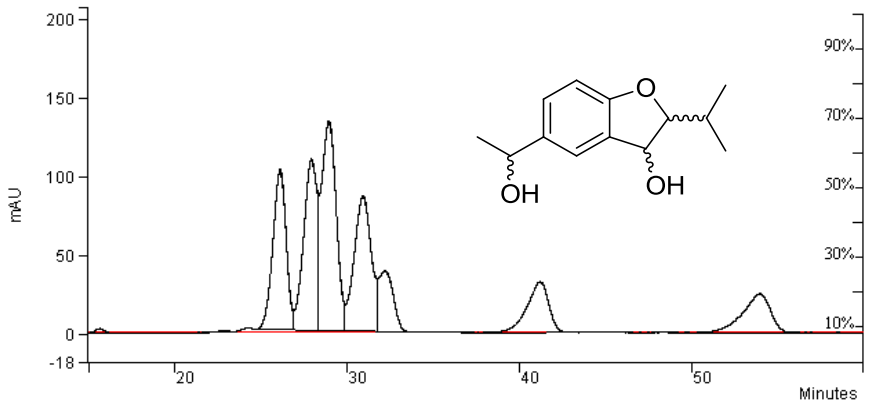
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =85/15, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		95.3563	16.421	0.000	24.9	141000800
2		4.6437	17.479	0.000	54.0	6866449
	Totals	**100.0000**		**0.000**		**147867248**

(±)-5-(1-hydroxyethyl)-2-isopropyl-2,3-dihydrobenzofuran-3-ol

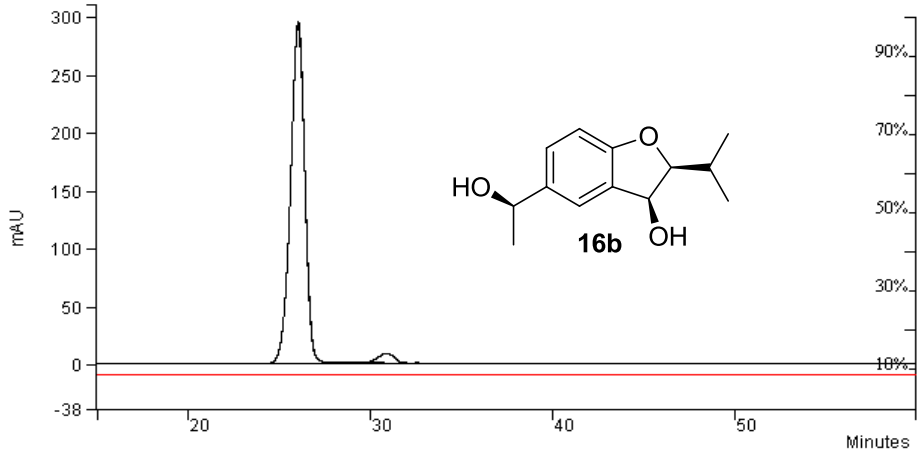
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		16.5036	26.054	0.000	50.1	55007024
2		17.7234	27.872	0.000	58.8	59072572
3		23.9139	28.885	0.000	72.2	79705472
4		17.9277	30.864	0.000	65.8	59753456
5		6.8251	32.134	0.000	80.1	22748310
6		8.5600	41.144	0.000	78.5	28530704
7		8.5463	53.887	0.000	100.6	28484880
	Totals	**100.0000**		**0.000**		**333302400**

(2*S*,3*S*)-5-((*R*)-1-hydroxyethyl)-2-isopropyl-2,3-dihydrobenzofuran-3-ol

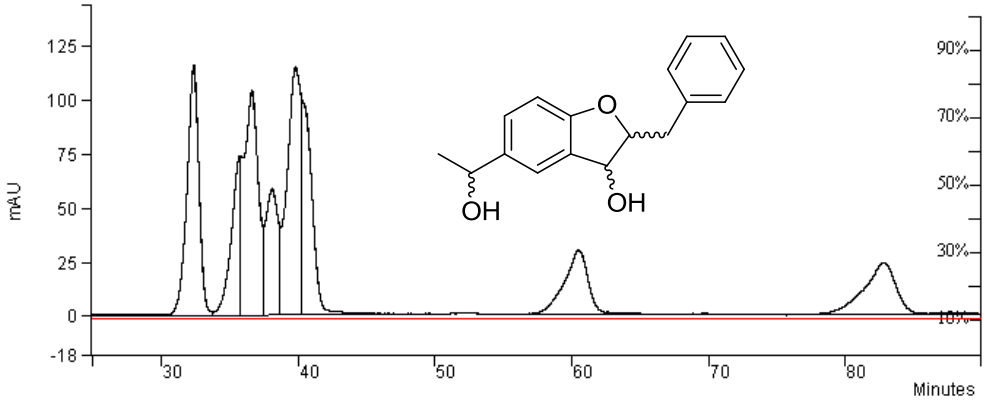
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		96.9757	25.972	0.000	50.1	163027984
2		3.0243	30.824	0.000	0.0	5084254
	Totals	**100.0000**		**0.000**		**168112240**

(±)-2-benzyl-5-(1-hydroxyethyl)-2,3-dihydrobenzofuran-3-ol

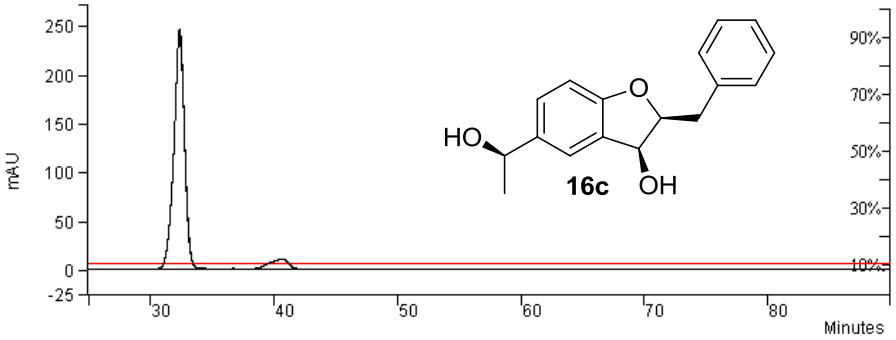
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =90/10, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		16.4574	32.321	0.000	55.0	70497768
2		8.3121	35.703	0.000	0.0	35606260
3		17.6438	36.571	0.000	113.4	75579840
4		8.4985	38.059	0.000	0.0	36404372
5		19.0503	39.826	0.000	0.0	81604568
6		11.7892	40.283	0.000	113.7	50500540
7		8.8674	60.466	0.000	103.8	37984944
8		9.3813	82.737	0.000	136.1	40186224
	Totals	**100.0000**		**0.000**		**428364544**

(2*S*,3*S*)-2-benzyl-5-((*R*)-1-hydroxyethyl)-2,3-dihydrobenzofuran-3-ol

HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =90/10, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)

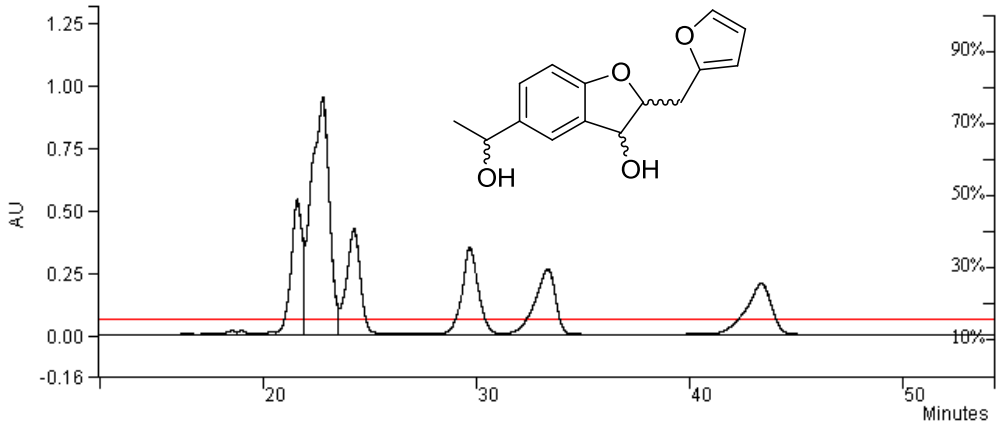


Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		92.5673	32.286	0.000	54.3	149205440
2		7.4327	40.577	0.000	103.7	11980534
	Totals	**100.0000**		**0.000**		**161185968**

(±)-2-(furan-2-ylmethyl)-5-(1-hydroxyethyl)-2,3-dihydrobenzofuran-3-ol

HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =85/15, detector:

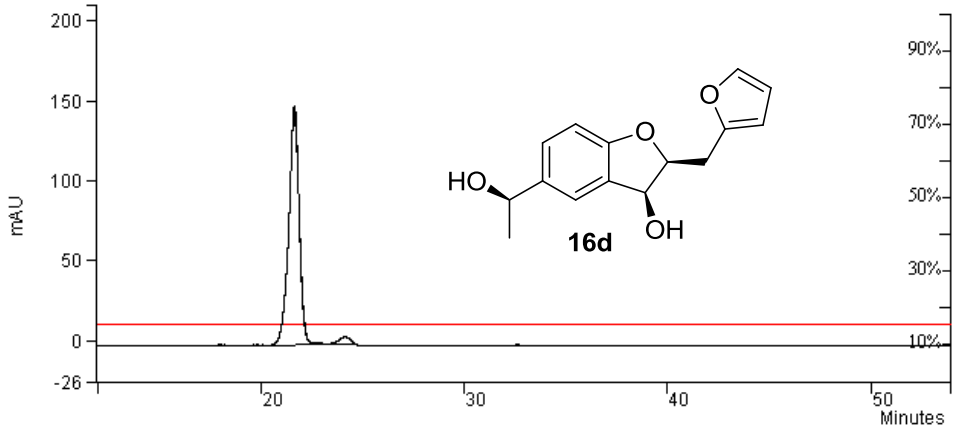
280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		13.3756	21.545	0.000	34.2	201672112
2		37.1583	22.751	0.000	60.6	560257472
3		13.2637	24.212	0.000	41.7	199984064
4		12.4919	29.628	0.000	46.0	188347872
5		12.1911	33.298	0.000	57.0	183812544
6		11.5194	43.301	0.000	67.8	173684304
	Totals	**100.0000**		**0.000**		**507758464**

(2*S*,3*S*)-2-(furan-2-ylmethyl)-5-((*R*)-1-hydroxyethyl)-2,3-dihydrobenzofuran-3-ol

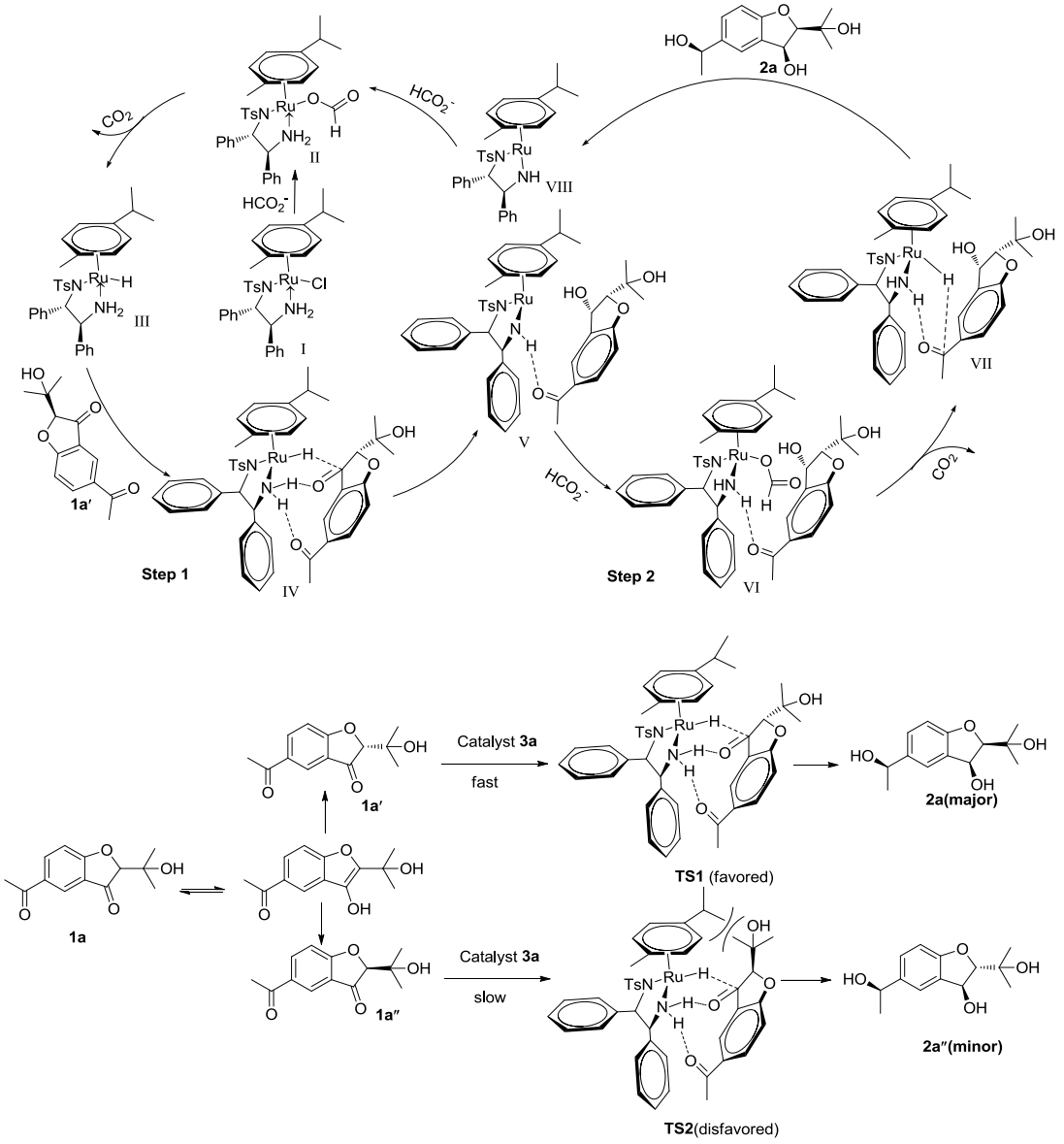
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =85/15, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		96.2490	21.590	0.000	34.5	53571832
2		3.7510	24.028	0.000	41.3	2087787
	Totals	**100.0000**		**0.000**		**55659620**

3. Proposed catalytic mechanism

Scheme S1. Proposed catalytic cycle (**1a** as a model)

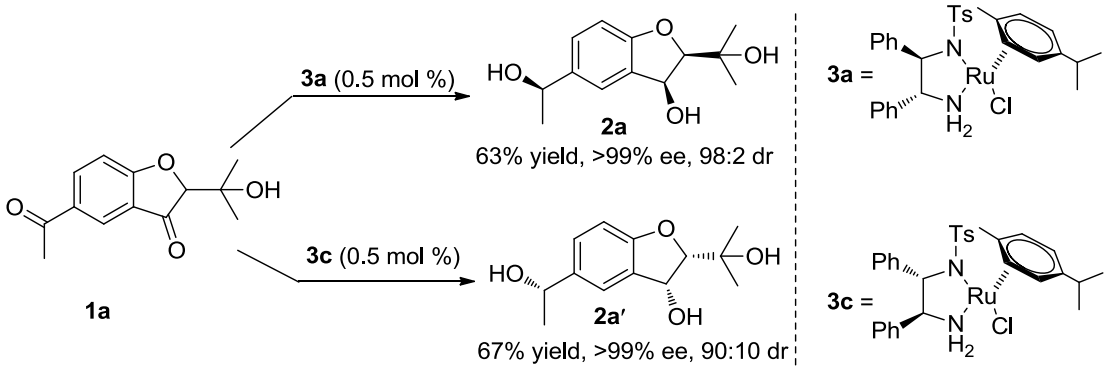


Explanation:

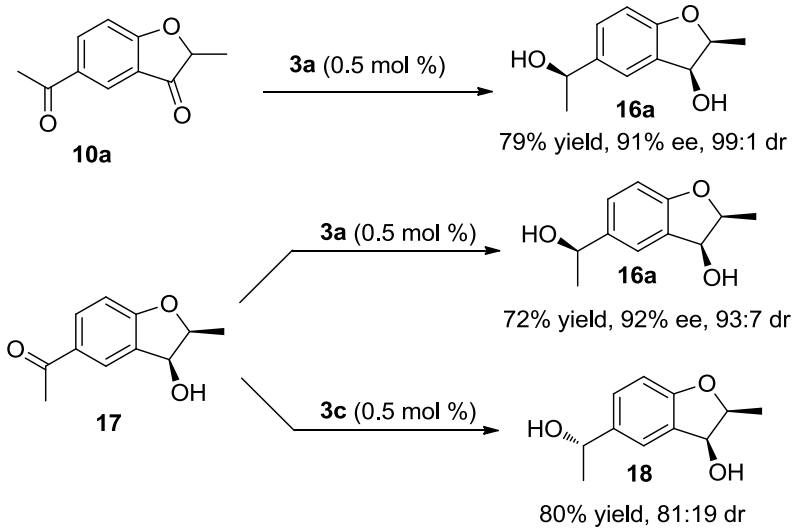
Based on the reported catalytic mechanism,[4] we propose that the process of transfer hydrogenation reaction of **1a** probably includes two different stages: the first stage that the furanone part of **1a** was reduced through DKR-ATH process (from I-V), and the second stage that the acetophenone part of **1a** with the same configuration fixed in the first stage was reduced through a ATH process (from V-VIII). The racemization of **1a** was occurred through keto-enol tautomerism as shown as follows. The catalyst **3a** was bonded with the compound **1a** and formed the energy favoured transition **TS1** and the energy disfavored transition **TS2** respectively due to the steric hindrance between **1a** and the catalyst, and they then generated the corresponding products major **2a** and **2a″**.

Experiments supplied to study the mechanism:

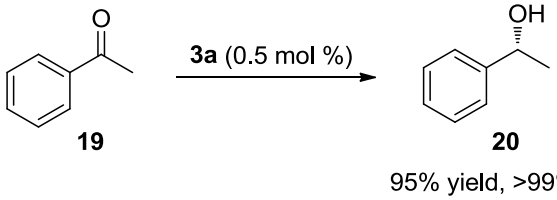
Scheme S2



Scheme S3



Scheme S4



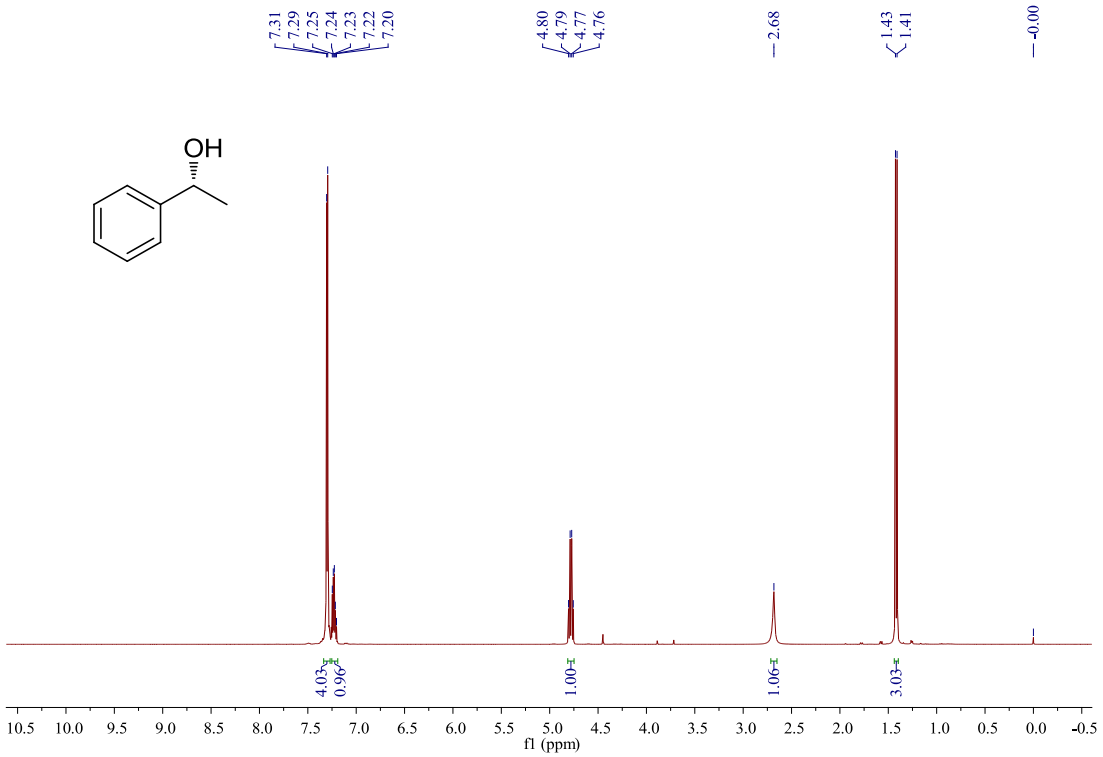
All reactions were run on a 1.0 mmol scale in a 25 mL sealed flask under the protection of argon. 5.0 mmol sodium formate, 5.0 μmol catalyst **3a** or **3c** and 0.2 mmol CTAB were added into 4 mL CH_3OH and the mix-ture was stirred at 65 ˚C for 12 h.

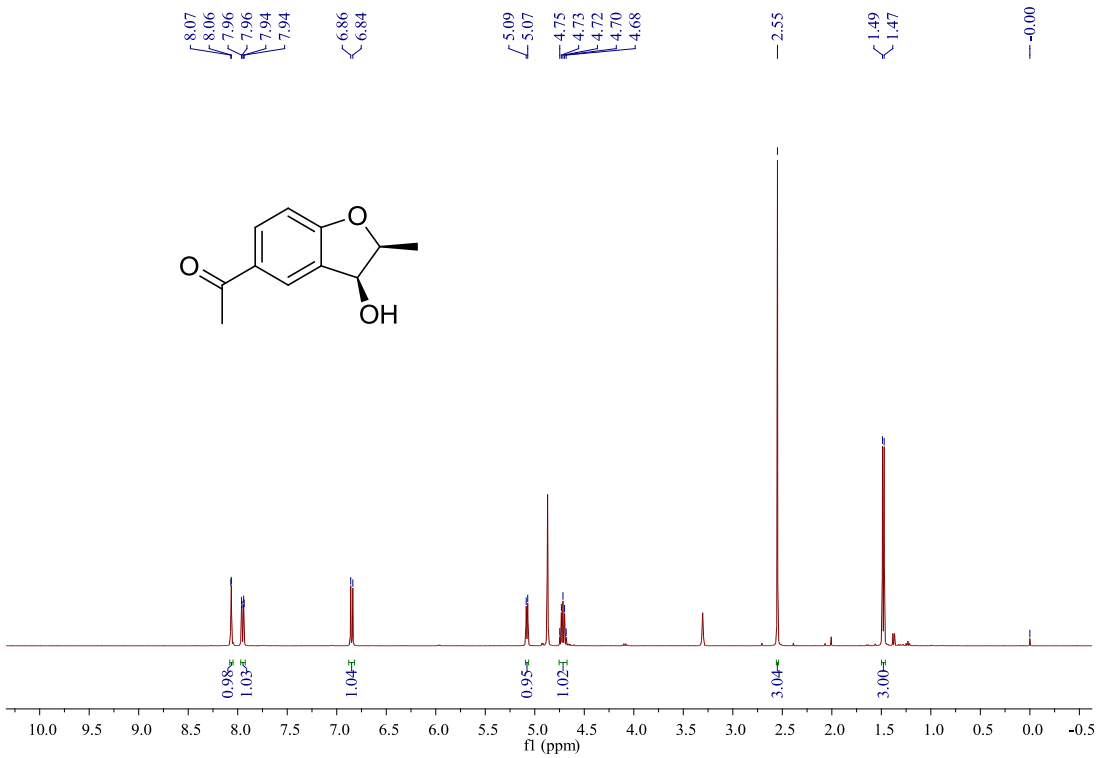
Reduction of **1a** with **3a** and **3c** could give the *cis*-product and the enantiomer respectively with similar yield, %ee and dr (Scheme S2), that means the reduce

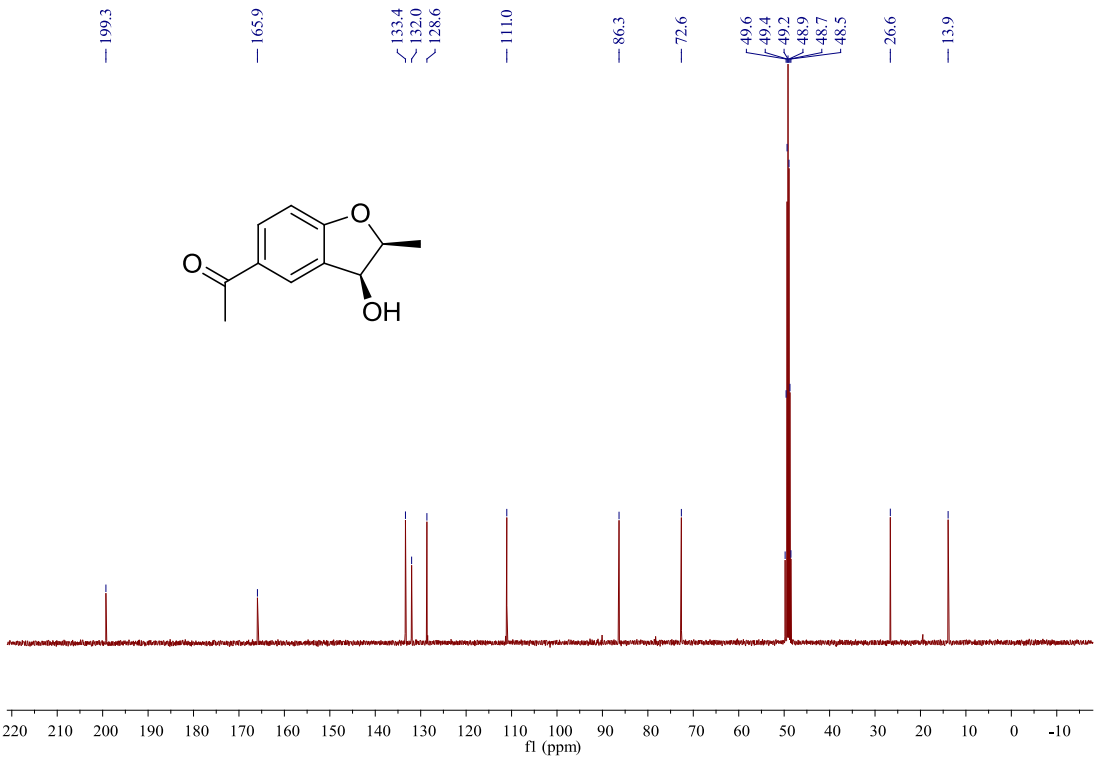
system shows high stereoselectivity for the substrates, the stereo configuration of products is closely related to the chiral catalyst. The following reduction of the mono-reduced intermediate (**TS-VI**) with the **3a** and **3c** gave the corrosponding products with different yield and dr values (scheme S3), but reduction of the mono-reduced intermediate (**TS-VI**) with **3a** could give the final *cis*- product with almost the same yield and %ee that obtained from the starting material **10a** (scheme S3), it indicated that the substrate and the catalyst probably formed the substrate/metal complexation from the beginning of the reaction as we proposed, it was essential for the stereoselectivity, and the yield and %ee were not affected if the favoured configuration of the complexion could be kept. Moreover, the reaction could go on with the intermediate and gave the similar yield, %ee and dr values at last, this result showed the reaction actually was one pot reaction although it appeared to be a two-step process because of the intermediate obtained. In addition, the acetophenone could be reduced by the cataylst to provide the almost optically pure phenylethanol(scheme S4), it proved that the reduction of acetophenone really via an ATH process as we believed.

NMR Spectra and HPLC analysis for the above products in Scheme S2-S4.

NMR Spectra





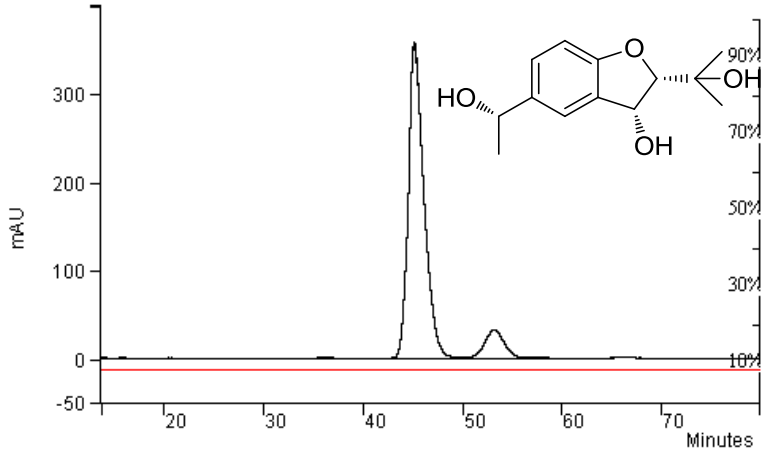


HPLC Analysis Spectra

(2*S*,3*R*)-5-((*S*)-1-hydroxyethyl)-2-(2-hydroxypropan-2-yl)-2,3-dihydrobenzofuran -3-ol (The product prepared from **1a** with catalyst **3a)**

HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector:

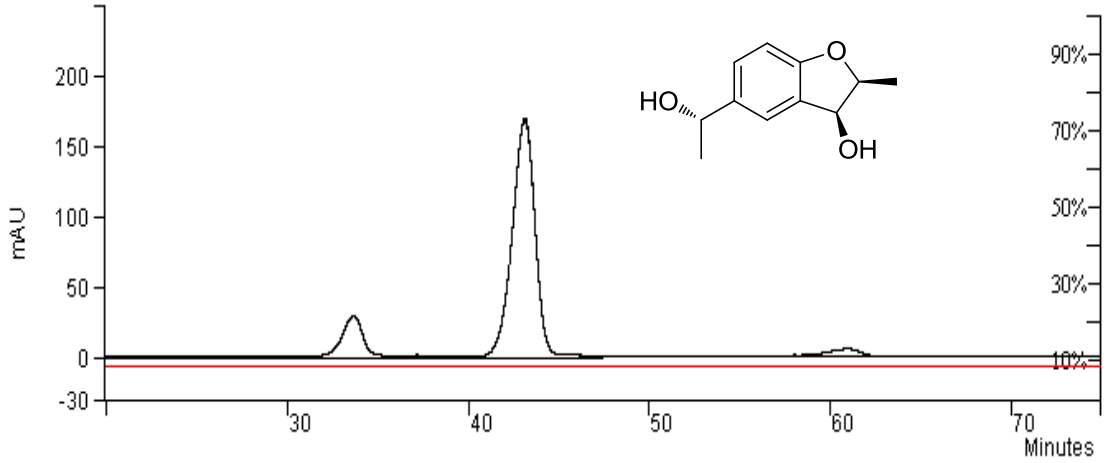
280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		89.8709	45.079	0.000	96.0	393176416
2		10.1291	53.083	0.000	125.6	44313944
	Totals	**100.0000**		**0.000**		**437490368**

(2*S*,3*S*)-5-((*S*)-1-hydroxyethyl)-2-methyl-2,3-dihydrobenzofuran-3-ol (The product prepared from **17** with catalyst **3c)**

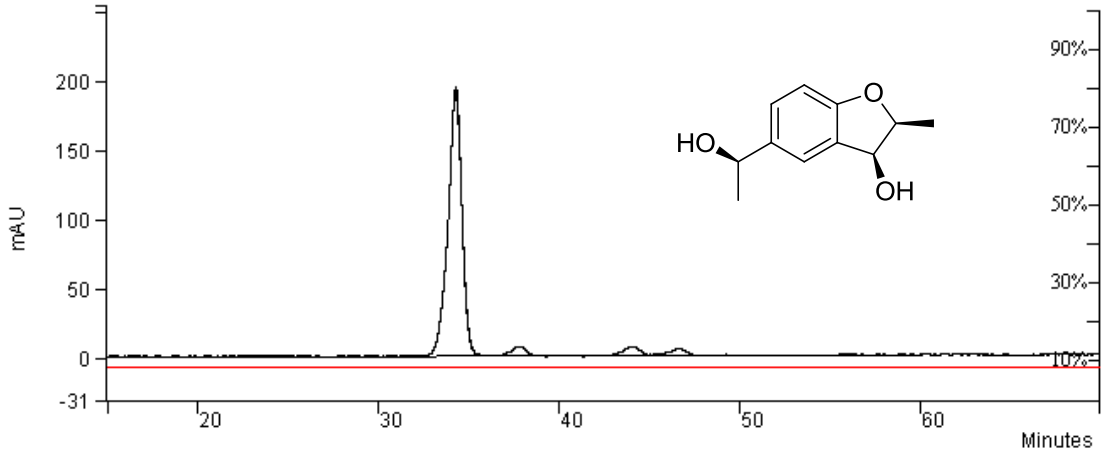
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		13.7892	33.598	0.000	69.6	25308732
2		81.1963	43.066	0.000	79.8	149027792
3		5.0145	60.912	0.000	116.2	9203616
	Totals	**100.0000**		**0.000**		**183540144**

(2*S*,3*S*)-5-((*R*)-1-hydroxyethyl)-2-methyl-2,3-dihydrobenzofuran-3-ol(The product prepared from **17** with catalyst **3a)**

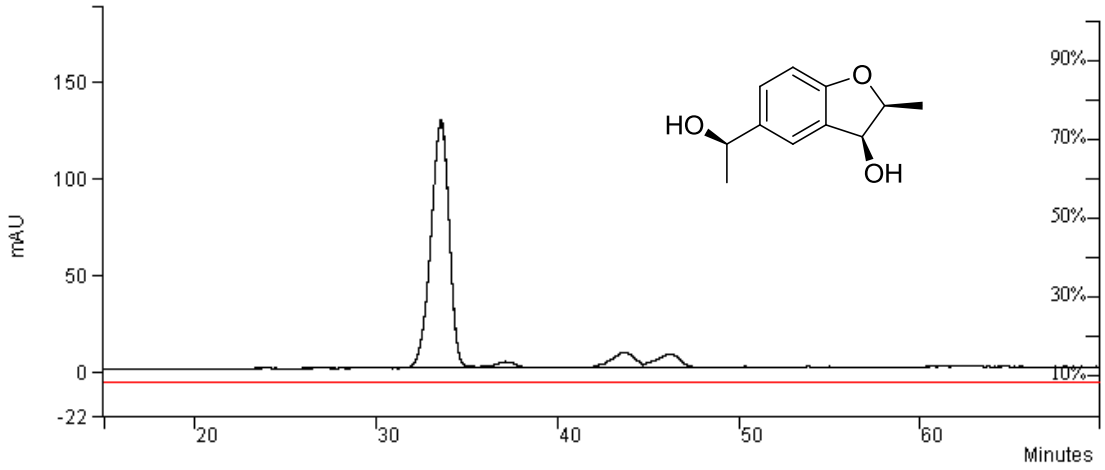
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		88.8856	34.205	0.000	48.0	105466832
2		3.7668	37.731	0.000	55.9	4469510
3		4.1502	43.988	0.000	66.7	4924464
4		3.1974	46.551	0.000	79.3	3793831
	Totals	**100.0000**		**0.000**		**118654640**

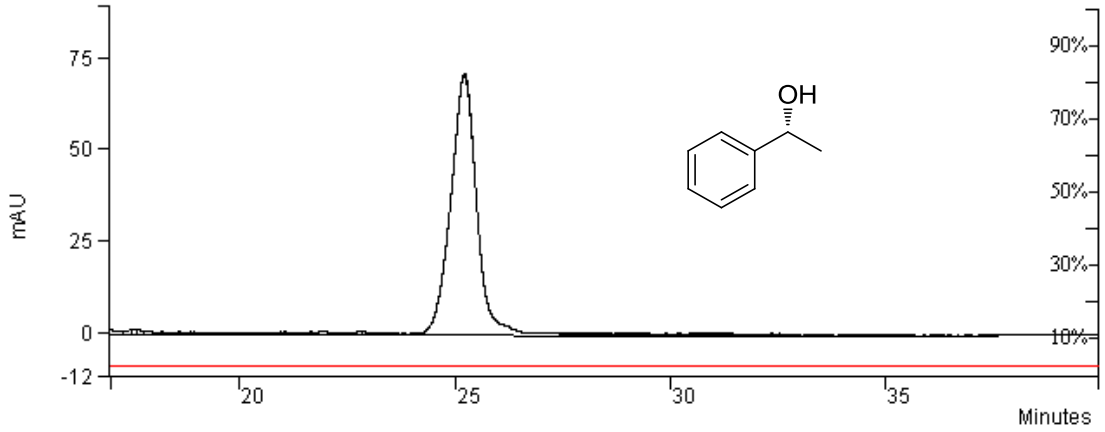
(2*S*,3*S*)-5-((*R*)-1-hydroxyethyl)-2-methyl-2,3-dihydrobenzofuran-3-ol(The product prepared from **10a** with catalyst **3a)**

HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =92/8, detector: 280 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		84.9049	33.533	0.000	65.1	90049528
2		2.1341	37.093	0.000	0.0	2263414
3		6.7177	43.665	0.000	87.7	7124721
4		6.2433	46.157	0.000	91.5	6621650
	Totals	**100.0000**		**0.000**		**106059312**

(*R*)-1-phenylethanol(The product prepared from **19** with catalyst **3a)**
HPLC (DAICEL CHIRALPAK® IA column, eluent: Hexanes/i-PrOH =98/2, detector: 254 nm, flow rate: 0.5 mL/min, 35 ˚C)



Peak No	Peak Name	Result (ug/ml)	Ret. Time (min)	Time Offset (min)	Width 1/2 (sec)	Area (counts)
1		100.0000	25.202	0.000	35.2	31413250
	Totals	**100.0000**		**0.000**		**31413250**

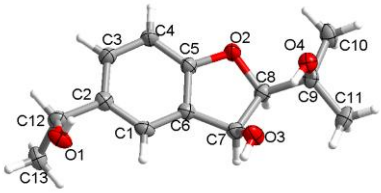
4. References

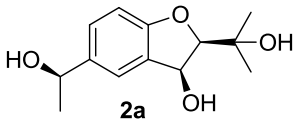
1. Fang, L.-Z.; Liu, S.-S.; Han, L.-L.; Li, H.-H.; Zhao, F.-F. Ruthenium -Catalyzed Synthesis of cis-2,3-Dihydrobenzofuran-3-ols by Aqueous Transfer Hydrogenation

via Dynamic Kinetic Resolution. *Organometallics* **2017**, *36*, 1217-1219.
2. Fang, L.-Z.; Lyu, Q.-H.; Lu, C.-J.; Li, H.-H.; Liu, S.-S.; Han, L.-L. Synthesis of Chiral Dihydrobenzofurans and Phthalides by Asymmetric Transfer Hydrogenation via Dynamic Kinetic Resolution:A Strategy for Total Synthesis of Daldinins A, B, and C and Concentricolide. *Adv. Synth. Catal*. **2016**, *358*, 3196-3200.
3. Cheng, T.-Y.; Ye, Q.-Q.; Zhao, Q.-K.; Liu, G.-H. Dynamic Kinetic Resolution of Phthalides via Asymmetric Transfer Hydro-genation: A Strategy Constructs 1,3-Distereocentered 3-(2-Hydroxy-2 arylethyl)isobenzofuran-1(3H)-one. *Org. Lett*. **2015**, *17*, 4972-4975.

5. X-Ray crystallography

X-Ray crystallography and structural formula of compound **2a**





Original data see the cif files.
Displacement ellipsoids are drawn at the 40% probabil-ity level.
Crystal structure at the Cambridge Crystallographic Data Centre. Deposition Number:
CCDC 1506041
Formula: $C_{13}H_{18}O_4$
Unit Cell Parameters: a 6.8682(2) b 9.6210(4) c 18.8039(8) $P2_12_12_1$

Chemical formula	$C_{13}H_{18}O_4$	
Formula weigh	238.27	
Temperature	293K	
Wavelength	1.54184	
Crystal system	Orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a=6.8682(2)	α=90°
	b=9.6210(4)	β=90°
	c=18.8039(8)	γ=90°
Volume	1242.55(8)	
Z	4	
Density diffrn	1.274	
Absorpt coefficient	0.771	
F(000)	512	

Theta range for data collection	4.703 to 67.053
Index ranges	-8<=h<=5,-7<=k<11，-22<=l<=21
R (reflections)	0.0376 (2062)
wR_2 (reflections)	0.1024 (2203)
Flack parameter	-0.233(330)
	by classical fit to all intensities
	-0.086(129)
	from 777 selected quotients (Parsons' method)