Copper-Catalyzed [1,3]-Nitrogen Rearrangement of *O*-Aryl Ketoximes via Oxidative Addition of N−O Bond in Inversed Electron Flow

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Supporting Information

1. General Information

^{1}H and ^{13}C NMR spectra were recorded on a JEOL JNM-ECS600 (600 MHz for ^{1}H and 150 MHz for ^{13}C) spectrometer. Chemical shifts are reported in ppm relative to $CHCl_3$ (for ^{1}H, δ 7.26), and $CDCl_3$ (for ^{13}C, δ 77.00). ^{1}H NMR data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, sext = sextet, sept = septet, dd = double doublet, dt = double triplet, dq = double quartet, ddt = double double triplet, br = broad, m = multiplet) and coupling constants (Hz). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. High-resolution mass spectra analysis was performed on a Bruker Daltonics solariX FT-ICR-MS spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University. Flash column chromatography was performed with Kanto Chemical silica gel 60N (spherical, neutral, 40-50 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 F_{254}). All reactions were carried out under nitrogen atmosphere.

Materials

Anhydrous 1,2-dichloroethane, PhCl, toluene, MeCN, methanol, and chloroform were purchased from WAKO and used as received. IPrCuBr was prepared in accordance with the literature method.[1] $AgSbF_6$ was purchased from Aldrich and used as received. $BF_3{\cdot}OEt_2$ was purchased from TCI and used as received.

[1] D.-G. Silvia, C. E.-A. Eduardo, B.-B. Jordi, D. S. Edwin, M. Z. S. Alexandra, P. N. Steven, *Dalton*. *Trans*., **2010**, *39*, 7595.

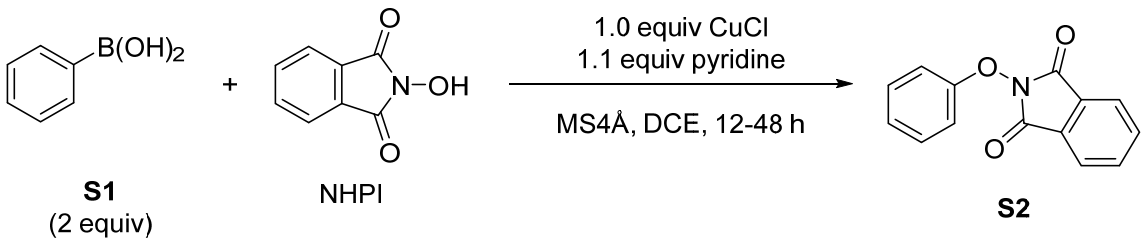
2. General procedure for preparation of starting materials 1

Compounds **1aa-1da, 1fa-1ia**, **1ab**, **1db**, **1dc**, **1dd**, **1hb**, **1hc**, **1ib**, **1ma**, **1na**, **1ob**, and **1qa-1sa** were synthesized by the synthetic route A, while compounds **1jb-1lb** and **1pb** were synthesized by the synthetic route B. Compound **1ea** was prepared by the synthetic route C. The deuterated substrate **1ba-*d*** was prepared according to the reported method.[1] The deuterated substrate **1ba-*d5*** was prepared according to the reported method.[2]

[1] J. Karthikeyan, R. Haridharan, C.-H. Cheng, *Angew. Chem. Int. Ed.* **2012**, *51*, 12343.

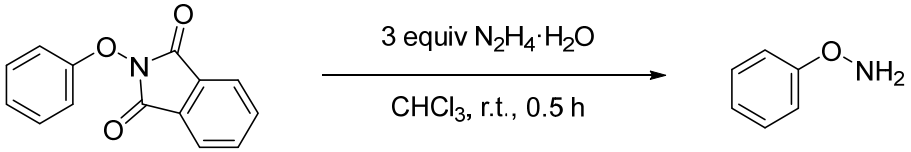
[2] C.-Z. Luo, P. Gandeepan, J. Jayakumar, K. Parthasarathy, Y.-W. Chang, C.-H. Cheng, *Chem. Eur. J.* **2013**, *19*, 14181

2-1. Synthetic route A via coupling between the arylboronic acid and NHPI



S1 (2 equiv) NHPI **S2**

The **S2** was prepared in accordance with the literature method.[3] To a mixture of *N*-hydroxyphthalimide (0.92 g, 5.0 mmol) and phenylboronic acid **S1** (2 equiv., 1.22 g, 10 mmol) in a 100 ml round-bottom flask were added copper (I) chloride (1 equiv., 0.50 g, 5 mmol) and freshly activated 4 Å molecular sieves inside a glovebox. Then, 1,2-dichloroethane (DCE, 0.25 M, 25 mL) followed by pyridine (1.1 equiv., 0.44 mL, 5.5 mmol) were added, resulting in a brown suspension. The reaction suspension was stirred open to the atmosphere for 24 h, then the color of the suspension turned from brown to green. The reaction mixture was absorbed onto ca. 6 g of silica gel and the solvents were removed under reduced pressure. The residue was purified by silica gel column chromatography using hexane/EtOAc (2/1) as eluent to afford **S2** as a colorless solid (86%, 1.03 g, 4.3 mmol).

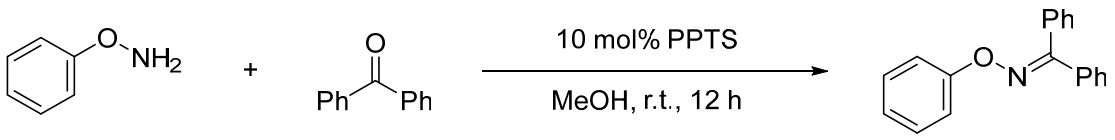


S2 **S3**

S3 was prepared in accordance with the literature method.[2] To a solution of **S2** (1.03 g, 4.3

mmol)、in chloroform (0.1 M, 43 mL) was added N_2H_4•H_2O (3 equiv., 0.64 mL, 13 mmol). The reaction mixture was stirred at rt for 0.5 h, then filtered through a short pad of Celite and extracted with dichloromethane. The combined organic layers were dried over Na_2SO_4 and the solvents were removed in vacuo. The crude product of the *O*-phenylhydroxylamine **S3** was used for the next step without further purification (ca. 83% yield, 3.5 mmol).

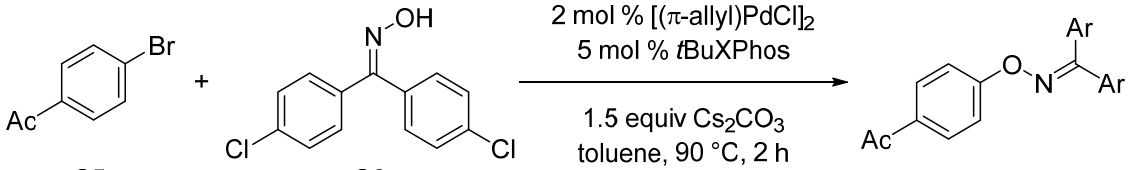
[3] H. M. Petrassi, K. B. Sharpless, W. Kelly, *Org. Lett.* **2001**, *3*, 1, 139.



S3 **S4** **1ba**

To a mixture of **S3** (1 equiv., 3.5 mmol)**, S4** (1 equiv., 0.645 g, 3.5 mmol), and PPTS (10 mol%, 89 mg, 0.35 mmol) in a 50 mL round-bottom flask was added methanol (0.5 M, 7.0 mL). The reaction mixture was stirred at r.t. for 12 h, then solvent was removed in vacuo. The residue was purified by silica gel column chromatography using hexane/EtOAc (20/1) as eluent afforded **1ba** (73%, 0.71 g, 2.6 mmol).

2-2. Synthetic route B via coupling between bromoarenes and ketooximes

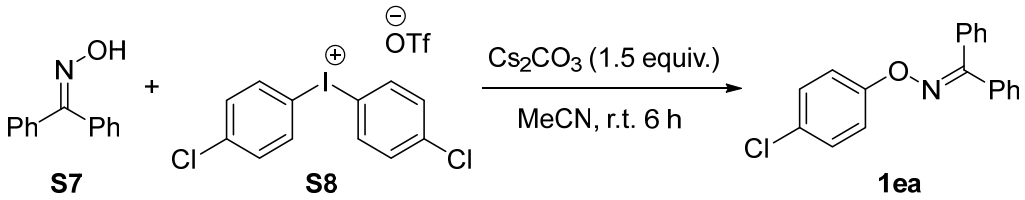


S5 **S6** **1jb**

This procedure is according to the literature method.[4] To a mixture of **S5** (1 equiv., 0.20 g, 1.0 mmol), **S6** (1.05 equiv., 0.28 g, 1.05 mmol), $[(allyl)PdCl]_2$ (2 mol%, 7.3 mg, 0.02 mmol), ^{t}BuXPhos (5 mol%, 21.25 mg, 0.05 mmol), and Cs_2CO_3 (1.5 equiv., 0.49 g, 1.5 mmol) in a 20 mL round-bottom flask was added toluene (0.25 M, 4.0 ml) in argon atmosphere. After stirring vigorously at 90 °C for 2 h, the reaction mixture was passed through a short pad of silica with EtOAc (50 mL), then solvent was removed in vacuo. The crude mixture was purified by flash silica gel column chromatography using hexane/EtOAc (30/1) as eluent to give **1jb** (39%, 0.15 g, 0.39 mmol) in an analytically pure form.

[4] Reeta, T. M. Rangarajan, R. P. Singh, R. P. Singh, M. Singh. *Chin. J. Chem.* **2020**, *38*, 830.

2-3. Synthetic route C via direct arylation of oximes with diaryliodonium salts

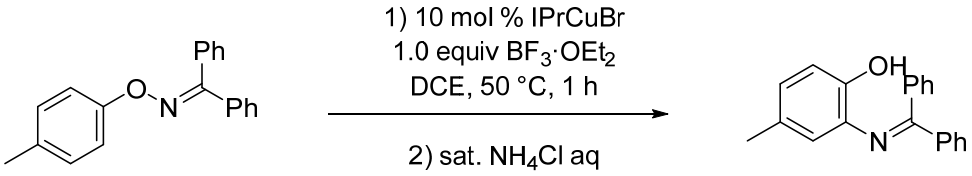


This procedure is according to the literature method.[5] The diaryliodonium salt was prepared according to the literature method.[6] A solution of cesium carbonate (1.5 equiv., 0.34 g, 0.85 mmol) and the **S7** (1 equiv., 0.14 g, 0.7 mmol) in acetonitrile anhydrous (0.25 M, 2.8 mL) was stirred for 5 min at room temperature. Then, diaryliodonium salt **S8** (1.2 equiv., 0.42 g, 0.84 mmol) was added in one portion at room temperature, and the mixture was stirred for 6 h at room temperature. The solvent was evaporated in vacuo. Then, the crude product was directly purified by flash silica gel column chromatography using hexane/EtOAc (10/1) to afford the desired product **1ea** (63%, 0.13 g, 0.44 mmol).

[5] Y. Y. Xunshen, W. J. Han, S. Mao, X. Qian, L. Wang, *Eur. J. Org. Chem.* **2014**, 6854.

[6] M. Bielawski, M. Zhu, B. Olofsson, *Adv. Synth. Catal.* **2007**, *349*, 2610.

3. General procedure for copper-catalyzed reaction of 1

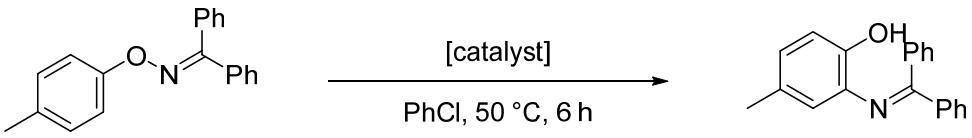


1aa **2aa**

To a mixture of **1aa** (1 equiv., 28.7 mg, 0.1 mmol), IPrCuBr (10 mol%, 5.34 mg, 0.01 mmol) in 1,2-DCE (0.7 mL, 0.14 M) in a 3 mL pressure vial was added BF_3•OEt_2 (1 equiv., 12.6 μL, 0.1 mmol) under argon atmosphere. After stirring at 50 °C for 1 h, the reaction mixture was extracted with dichloroethane and washed with sat. NH_4Cl aquation. After the combined organic layers were dried over Na_2SO_4, the organic solution was passed through a short pad of silica with EtOAc (50 mL), then solvent was removed in vacuo. The crude mixture was purified by flash silica gel column chromatography using hexane/EtOAc (30/1) as eluent to give **2aa** (82%, 23.5 mg, 0.082 mmol) in an analytically pure form.

4. Optimization of reaction conditions

4-1 Catalysts

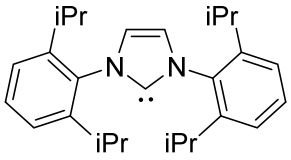


1aa **2aa**

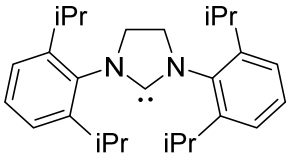
Table S1. Screening of catalysts

entry	catalysts. (mol%)	**2aa** (%)[a]	**1aa** (%)[a]
1	IPrCuBr (10), $AgSbF_6$ (10)	24	64
3	SIPrCuCl (10), $AgSbF_6$ (10)	25	32
4	I*t*BuCuCl (10), $AgSbF_6$ (10)	4	96
5	IPentCuCl (10), $AgSbF_6$ (10)	3	41
6	IMesCuCl (10), $AgSbF_6$ (10)	trace	76
7	$Yb(OTf)_3$ (20)	12	75
8	$CoCl_2$ (10), $AgNTf_2$ (20)	9	76

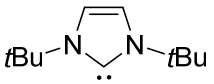
[a] NMR yields. The yields were determined using CH_2Br_2 as an internal standard.



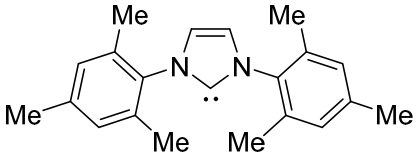
IPr



SIPr



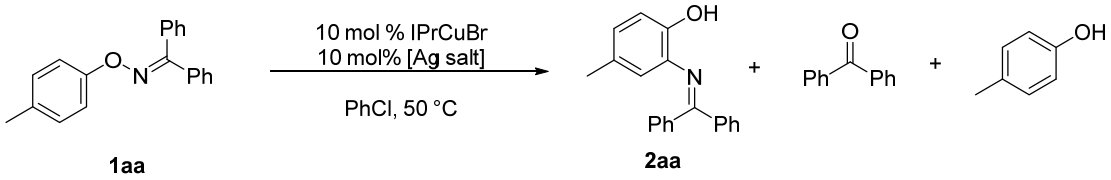
I*t*Bu



IMes

IPent (R = $CHEt_2$)

4-2 Silver salts



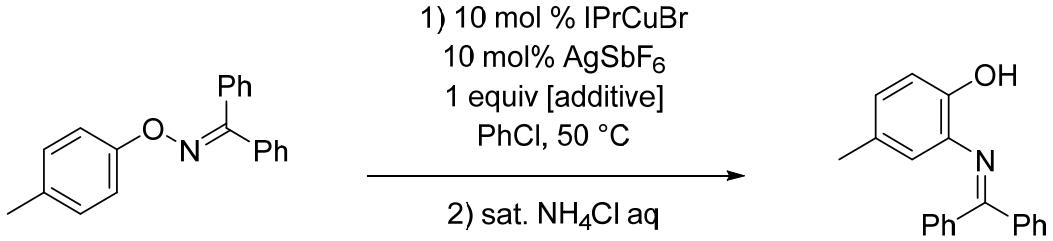
1aa **2aa**

Table S2. Screening of silver salts

entry	silver salt	time (h)	**2aa** (%)	**Benzophenone** (%)	***p*-cresol** (%)	**1aa** (%)
1	$AgSbF_6$	6	24	<1	<1	64
2	$AgSbF_6$	48	3	17	9	20
3	$AgNTf_2$	6	12	<1	<1	88
4	$AgBF_4$	6	9	<1	<1	89
5	$AgPF_6$	6	4	<1	<1	73
6	none	6	<1	<1	<1	94

[a] NMR yields. The yields were determined using CH_2Br_2 as an internal standard.

4-3 Additive



1aa **2aa**

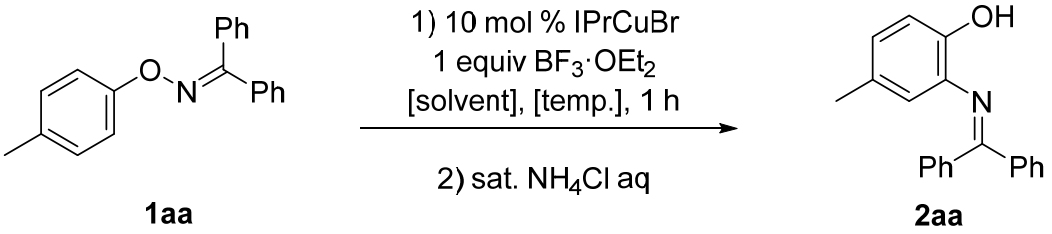
Table S3. Screening of additives

entry	additive	time (min.)	**2aa**	**1aa**
1[b]	none	360	24	64
2	BF_3•OEt_2	15	84	2
3	$EtB(OH)_2$	15	10	73
4	NaF	15	11	70
5	CaF_2	15	9	68
6	$Si(OMe)_4$	15	10	64

[a] NMR yields. The yields were determined using CH_2Br_2 as an internal standard.

[b] w/o work up process.

4-4 Solvent and temperature effect



1aa **2aa**

Table S4. Solvent and temperature effect

entry	solvent	T (°C)	**2aa**	**1aa**
1	1,2-DCE	50	86(82)	7
2	1,2-DCE	30	43	42
3	PhCl	50	85	2
4	toluene	50	10	68
5	THF	50	<1	91
6	MeCN	50	<1	99

[a] NMR yields. The yields were determined using CH_2Br_2 as an internal standard. Isolated yield in the parenthesis.

5. Substituent effect at the meta position

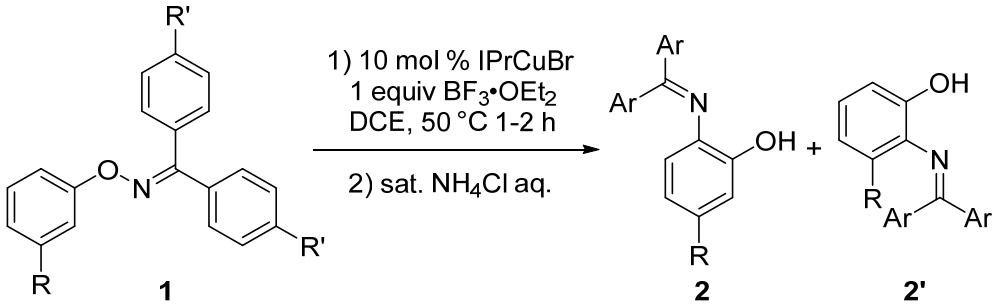
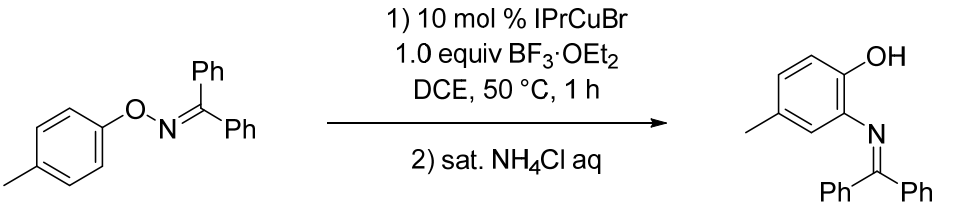


Table S4. Substituent effect at the meta position

1	R	R'	σ_{para} of R	A-value	**2**	yield (%)[a]	2:2'
1ma	OMe	H	-0.27	0.60	**2ma**	63	>20:1
1na	Cl	H	0.23	0.43	**2na**	39	>20:1
1ob	F	Cl	0.06	0.15	**2ob**	45	1.8:1
1pb	CO_2Me	Cl	0.45	1.27	**2pb**	70	1:2

[a] isolated yields.

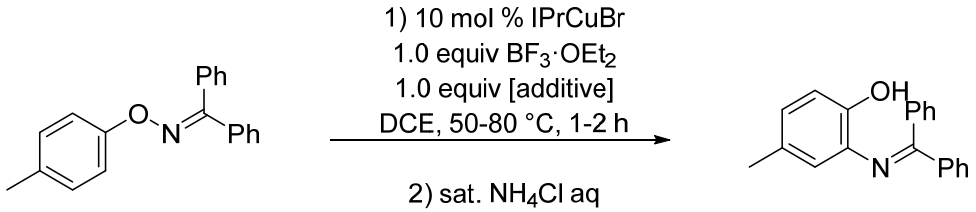
6. A larger scale experiment



1aa
1.0 mmol. 0.287 g

2aa, 68% yield
0.68 mmol, 0.194g

7 The reactions in the presence of radical-trapping reagents



1aa **2aa**

Table S6. The Cu-catalyzed reaction of 1aa in the presence of radical trapping reagents

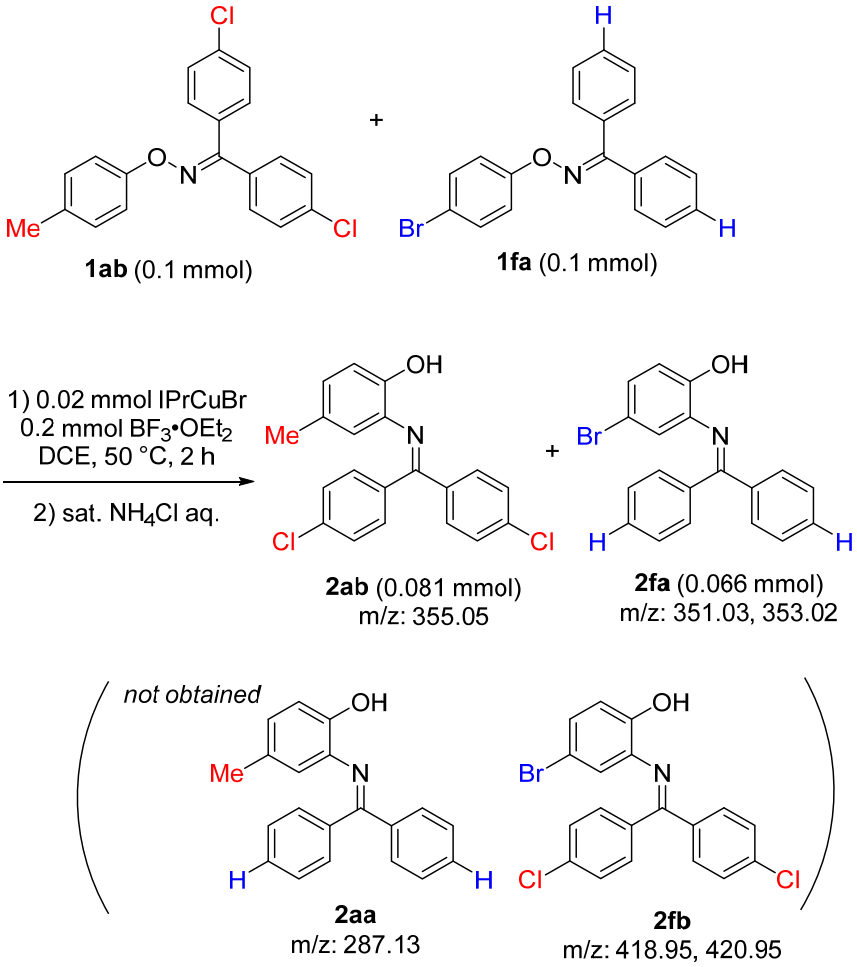
entry	additive	**2a** (%)[a]	**1a** (%)[a]	note
1	TEMPO	<1	87	
2	1,1-diphenylethylene	73	1	diphenylethylene: 87% recovery.
3	none	86(82)	7	

[a] NMR yields. CH_2Br_2 as an internal stansard. Isolated yield in parenthesis.

The reaction of **1aa** in the presence of TEMPO under the standard conditions resulted in recovery of considerable amounts of **1aa**, whereas that in the presence of 1,1-diphenylethylene gave **2aa** in the similar yield to that in the absence of the additive. At the present stage, we consider that TEMPO deactivates the cationic copper complex.

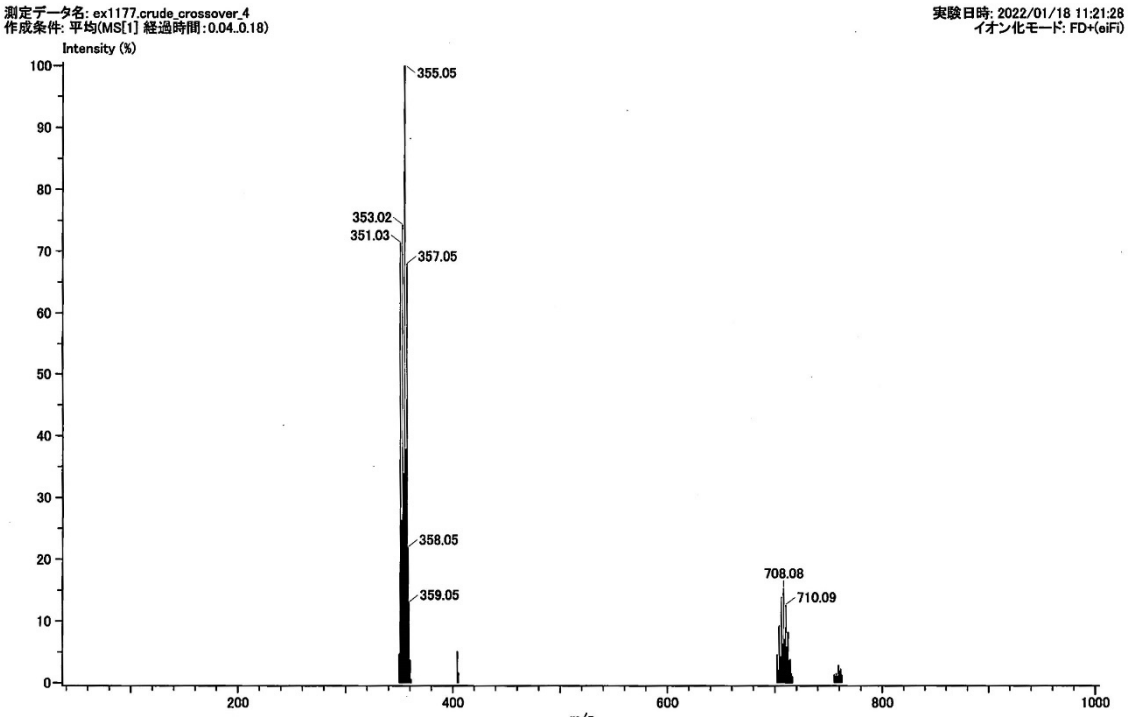
8 Competitive experiments

8-1. Crossover experiment

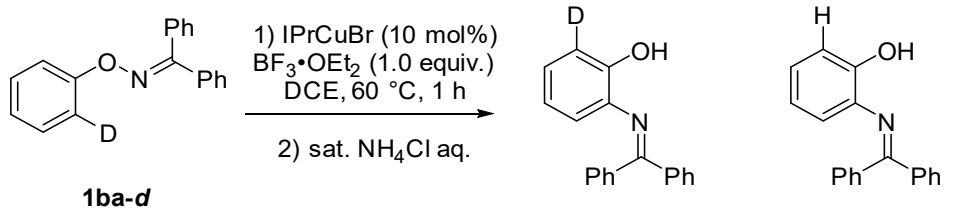


To a mixture of **1ab** (35.6 mg, 0.1 mmol), **1fa** (35.2 mg, 0.1 mmol), IPrCuBr (10.6 mg, 0.02 mmol) in 1,2-DCE (1.4 mL, 0.14 M) in a 3 mL pressure vial was added BF_3•OEt_2 (25.2 μL, 0.2 mmol) under argon atmosphere. After stirring at 50 °C for 2 h, the reaction mixture was extracted with dichloroethane and washed with sat. NH_4Cl aquation. After the combined organic layers were dried over Na_2SO_4, the organic solution was passed through a short pad of silica with EtOAc (50 ml), then solvent was removed in vacuo. The crude mixture was analyzed by ^1H NMR and HRMS. The products **2ab** and **2fa**, derived from the starting materials **1ab** and **1fa**, respectively in 81% and 66% yields respectively, whereas any crossover products **2aa** and **2fb** were not observed by HRMS (see HRMS chart of a mixture of the crude products).

HRMS chart of crossover experiment



8-2. Intramolecular competitive experiments

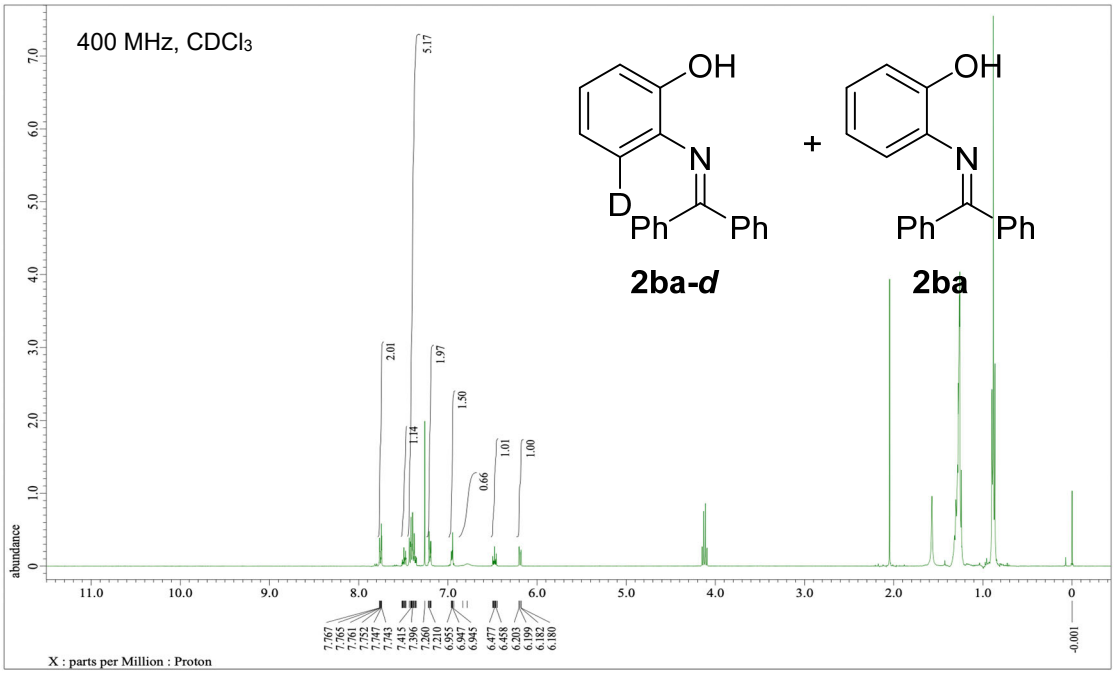


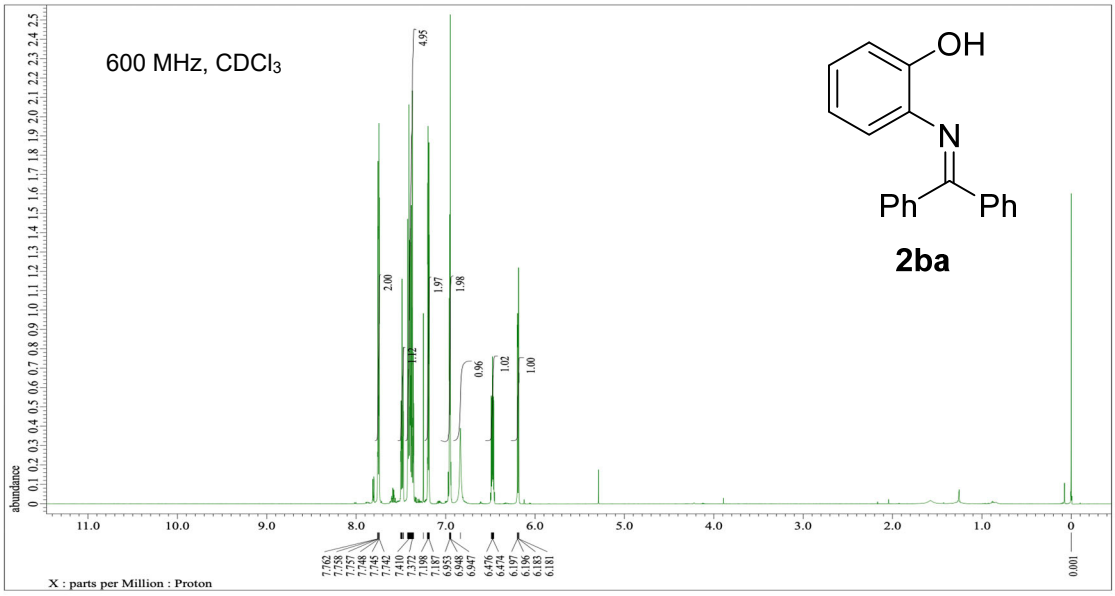
1ba-*d*
(99% D)

2ba-*d*
calcd: 274.1216
found: 274.1213

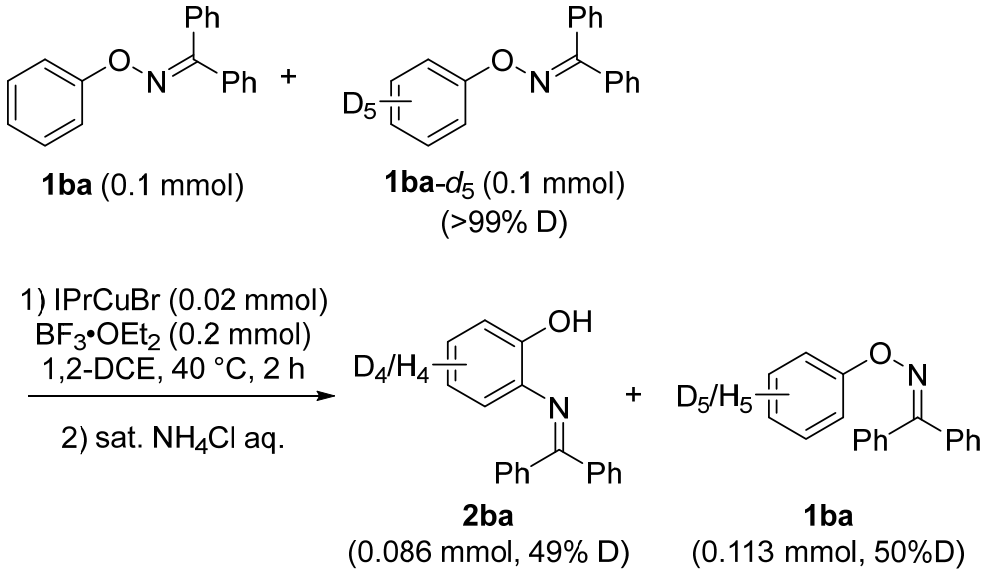
2ba
calcd: 273.1154
found: 273.1153

To a mixture of **1ba-*d*** (99% D, 1 equiv., 17.0 mg, 0.062 mmol), IPrCuBr (10 mol%, 3.29 mg, 0.00062 mmol) in 1,2-DCE (0.43 mL, 0.14 M) in a 3 mL pressure vial was added BF_3•OEt_2 (1.0 equiv., 7.81 μL, 0.062 mmol) under argon atmosphere. After stirring at 60 °C for 1 h, the reaction mixture was extracted with dichloroethane and washed with sat. NH_4Cl aquation. After the combined organic layers were dried over Na_2SO_4, the organic solution was passed through a short pad of silica with EtOAc (50 ml), then solvent was removed in vacuo. The crude mixture was analyzed by ^1H NMR and HRMS. The ratio between **2ba** and **2ba-*d*** was determined as 1:1, according to the integral at δ 6.945-6.955.

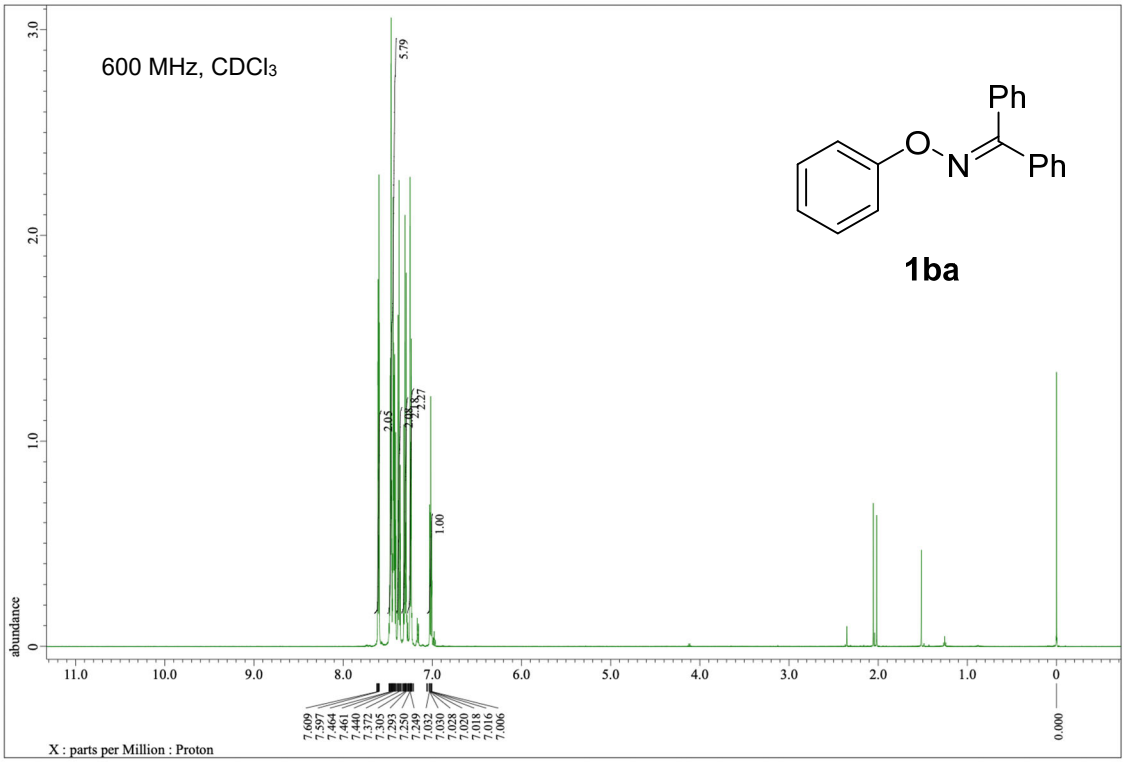


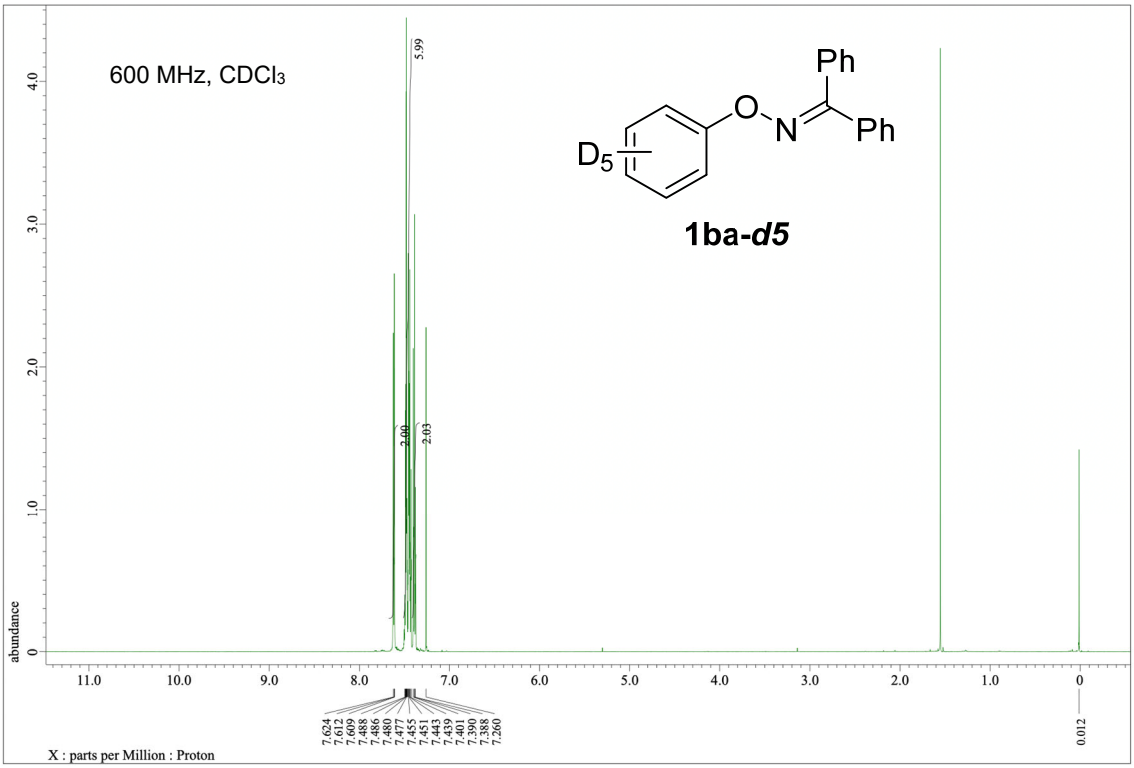

600 MHz, CDCl3
OH
N
Ph
Ph
2ba
abundance
X : parts per Million : Proton

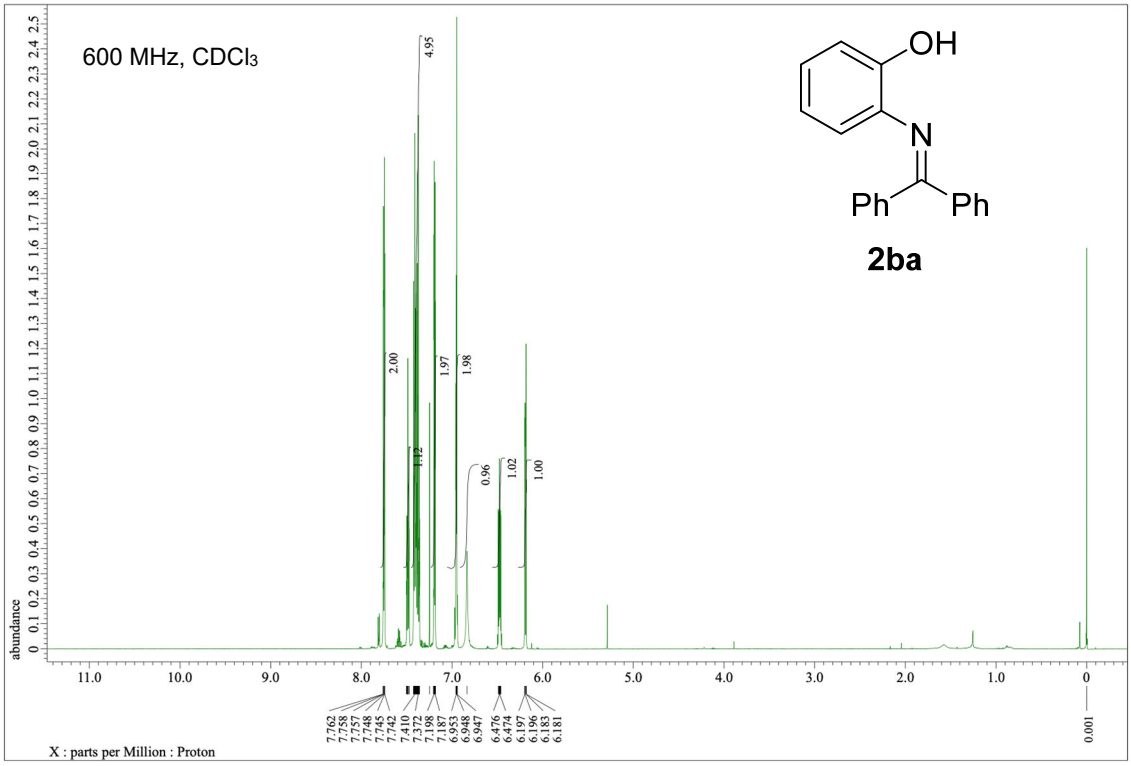
8-3. Intermolecular competitive experiments

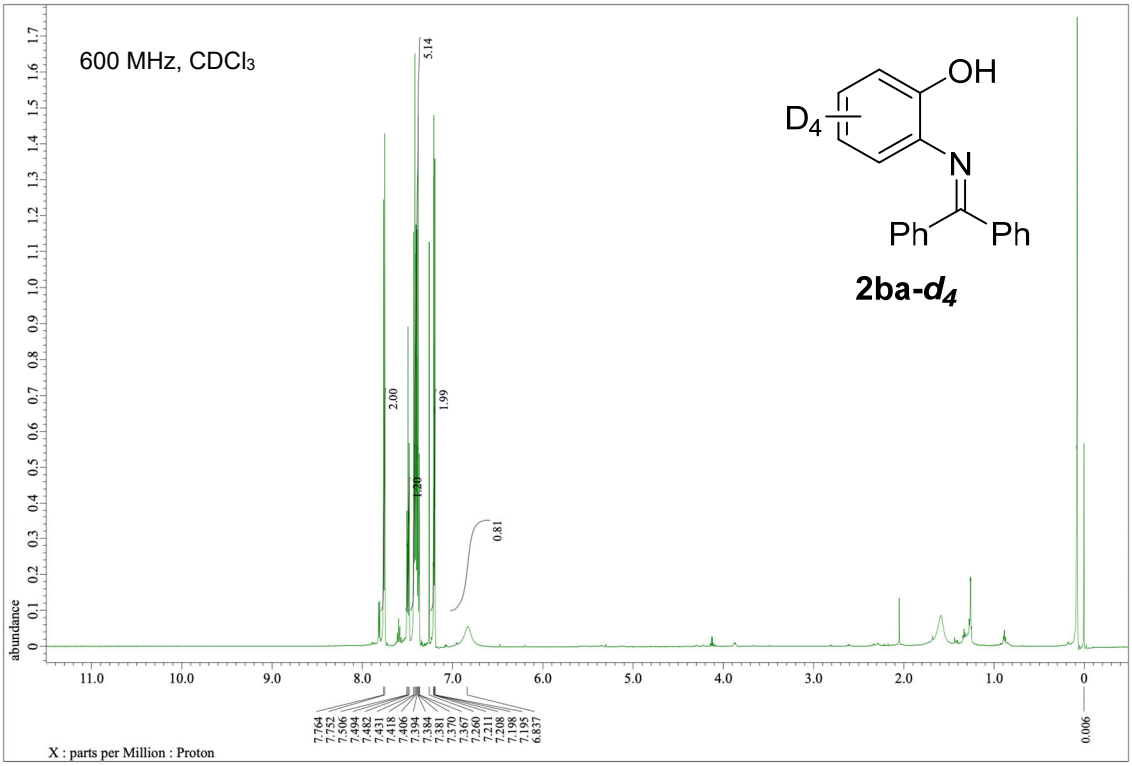


To a mixture of **1ba** (1 equiv., 27.3 mg, 0.1 mmol), **1ba-*d*$_5$** (99% D, 1 equiv., 27.8 mg, 0.1 mmol), IPrCuBr (10.6 mg, 0.002 mmol) in 1,2-DCE (1.4 mL, 0.14 M) in a 3 mL pressure vial was added BF_3•OEt_2 (25.2 μL, 0.2 mmol) under argon atmosphere. After stirring at 40 °C for 2 h, the reaction mixture was extracted with dichloroethane and washed with sat. NH_4Cl aquation. After the combined organic layers were dried over Na_2SO_4, the organic solution was passed through a short pad of silica with EtOAc (50 ml), then solvent was removed in vacuo. A mixture of the crude products was analyzed by ^1H NMR using dibromomethane as internal standard. The deuterium content of the obtained **2ba** and the recovered **1ba** were 49%D and 50%D, respectively.

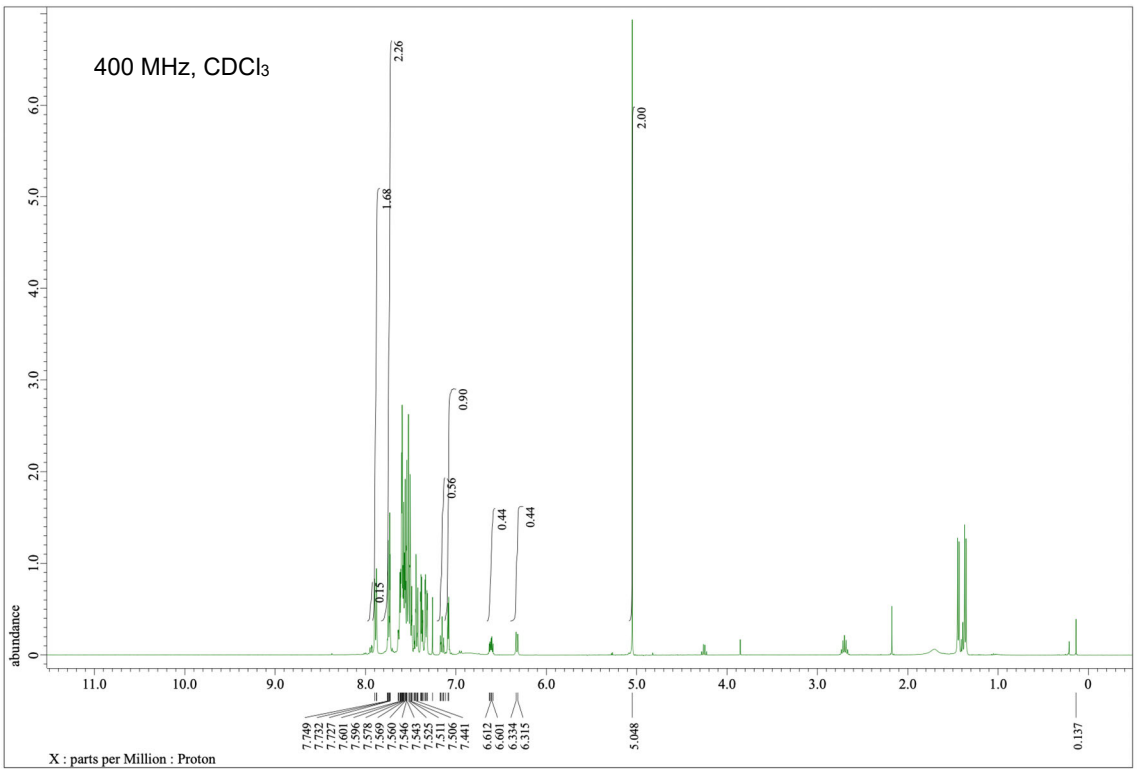

600 MHz, CDCl3
Ph
O
N
Ph
1ba
abundance
X : parts per Million : Proton


600 MHz, CDCl3
Ph
O
N
Ph
D5
1ba-d5
abundance
X : parts per Million : Proton


600 MHz, CDCl3
OH
N
Ph
Ph
2ba
abundance
X : parts per Million : Proton


600 MHz, CDCl3
OH
D4
N
Ph
Ph
2ba-d4
abundance
X : parts per Million : Proton

^{1}H-NMR chart of the crude products



9 Kinetic data for Hammett plot

9-1 General procedures

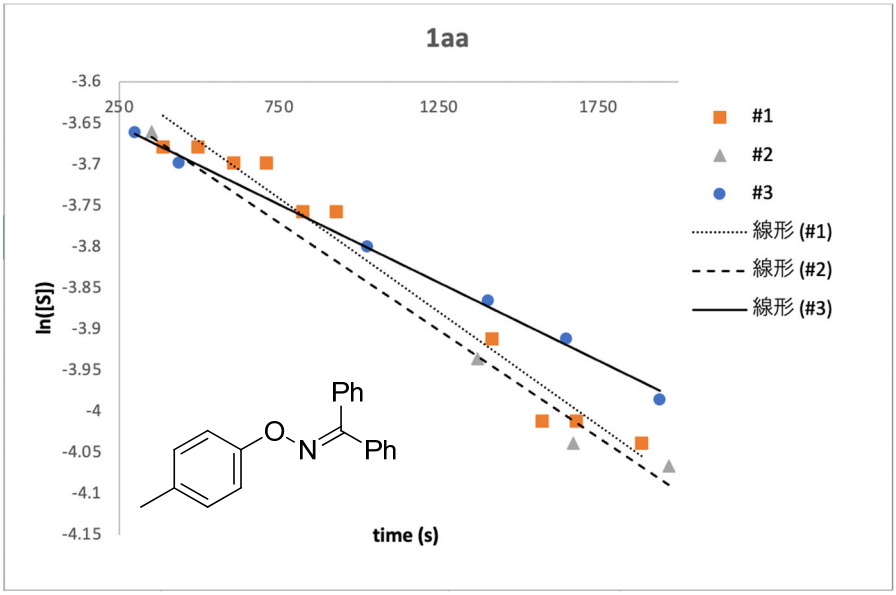
The procedure is according to the literature.[6] The rearrangement reactions were conducted in the presence of substrate **1** (0.01951 mmol), IPrCuBr (10 mol%, 1.0 mg, 0.001951 mmol), BF_3•OEt_2 (1 equiv., 0.1951 mmol, 2.5 μL) and CH_2Br_2 (7 μL) as an internal standard in $CDCl_3$ (0.028 M, 0.7 mL) in NMR tube at 50 °C in 400 Hz NMR and the consumption of **1** was monitored by ^1H NMR spectroscopy. The k_{obs} of each reaction was determined from a first-order plot of ln[SM] versus time. The σ and σ^+ values were according to the literature.[7]

[6]Lee, K. N. Lei, Z. Morales-Rivera. C. A. Liu, P. Ngai, M.-Y. *Org. Biomol. Chem*., **2016**, *14*, 5599.

[7]Hansch, C. Leo, A. Taft, R. W. *Chem*. Rev., **1991**, *91*, 165..

9-1-1 diphenylmethanone *O*-(*p*-tolyl) oxime (**1aa**).

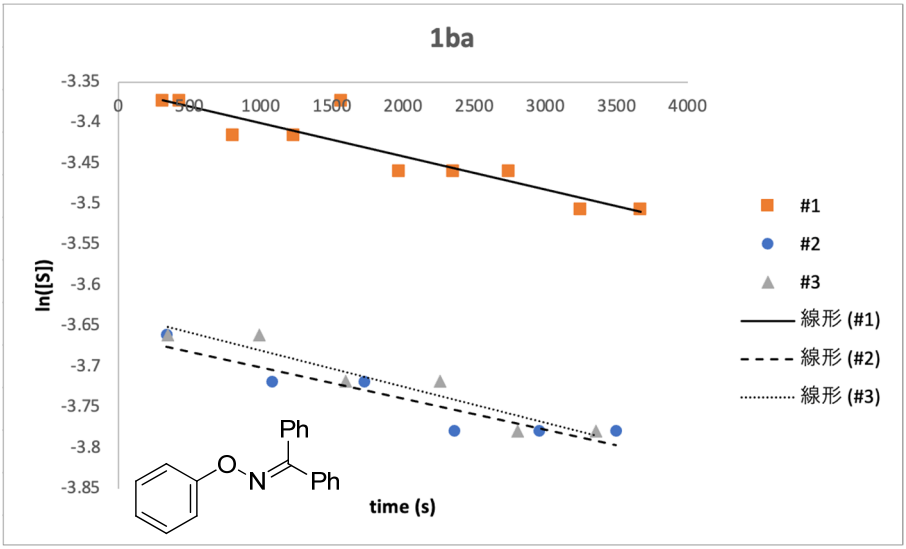
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.025238	$2.76316 * 10^{-4}$	ln[S] = 3.534158477-0.000276316t
2	0.025714189	$2.61280 * 10^{-4}$	ln[S] = 3.57481392-0.00026128t
3	0.02571489	$1.89357 * 10^{-4}$	ln[S] = 3.607181424-0.000189357t
average		$2.42318 * 10^{-4}$	



#1				#2			
time(s)	integral	[S] (mol/L)	Ln [S]	time(s)	integral	[S] (mol/L)	Ln [S]
387	0.53	0.025238	3.67940448	352	0.54	0.02571419	3.66071235
497	0.53	0.025238	3.67940448	1372	0.41	0.01952374	3.93612433
608	0.52	0.02476181	3.69845268	1672	0.37	0.01761898	4.03877848
710	0.52	0.02476181	3.69845268	1972	0.36	0.01714279	4.06617746
824	0.49	0.02333325	3.7578761	#3			
930	0.49	0.02333325	3.7578761	299	0.54	0.02571419	3.66071235
1417	0.42	0.01999992	3.91202678	437	0.52	0.02476181	3.69845268
1573	0.38	0.01809517	4.01211024	1025	0.47	0.02238087	3.7995488
1682	0.38	0.01809517	4.01211024	1403	0.44	0.0209523	3.86550676
1885	0.37	0.01761898	4.03877848	1650	0.42	0.01999992	3.91202678
				1942	0.39	0.01857136	3.98613475

9-1-2 diphenylmethanone *O*-phenyl oxime (**1ba**).

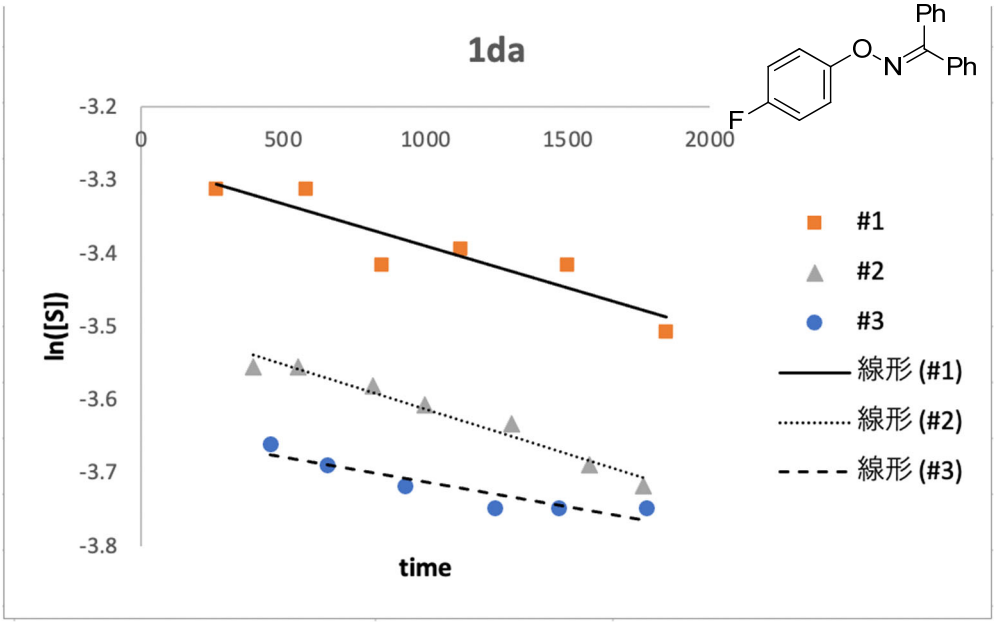
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.034286	$3.61195 * 10^{-5}$	ln[S] = -3.363660685-0.00003.61195t
2	0.025714	$4.20458 * 10^{-5}$	ln[S] = -3.654733312-0.0000420458t
3	0.025714	$4.53777 * 10^{-5}$	ln[S] = -3.635317458-0.0000453777t
average		$4.11810 * 10^{-5}$	



#1				#2			
time(s)	integral	concentration (mol/L)	ln(concentration)	time(s)	integral	concentration (mol/L)	ln(concentration)
313	0.24	0.034286	3.373018171	339	0.18	0.025714	-3.660719688
430	0.24	0.034286	3.373018171	1080	0.17	0.024285444	-3.717878102
808	0.23	0.032857417	3.415577786	1727	0.17	0.024285444	-3.717878102
1232	0.23	0.032857417	3.415577786	#3			
1565	0.24	0.034286	3.373018171	350	0.18	0.025714	-3.660719688
1972	0.22	0.031428833	3.460029548	989	0.18	0.025714	-3.660719688
				1600	0.17	0.024285444	-3.717878102

9-1-3 diphenylmethanone *O*-(4-fluorophenyl) oxime (**1da**).

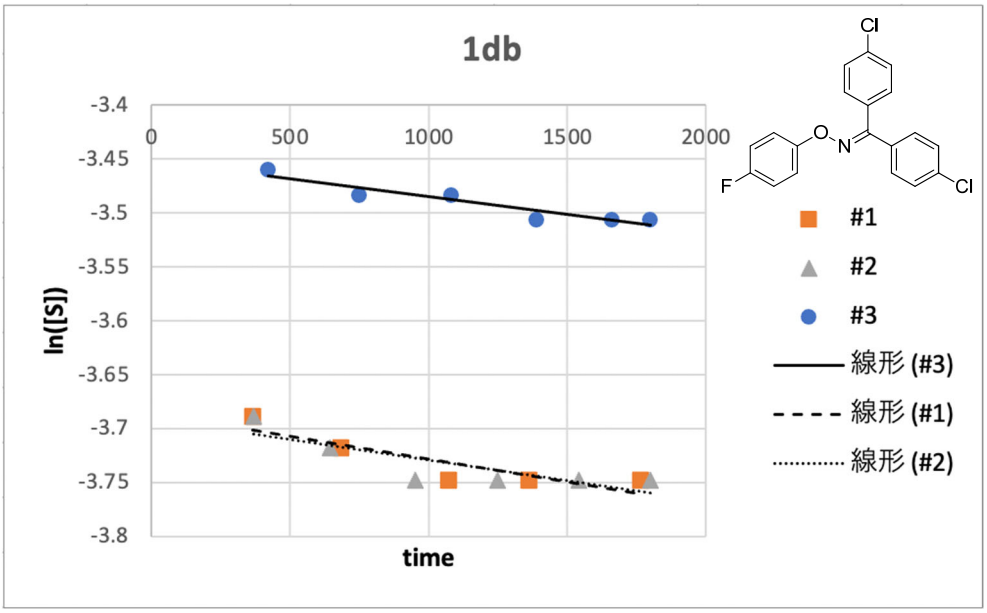
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.0364286	$1.14777 * 10^{-4}$	ln[S] = -3.274969627-0.000114777t
2	0.02857143	$1.22296 * 10^{-4}$	ln[S] = -3.490507712-0.000122296t
3	0.02571429	$6.77708 * 10^{-5}$	ln[S] = -3.644689771-0.0000677708t
average		$1.01615 * 10^{-4}$	



#1				#3			
time(s)	integral	concentration (mol/L)	ln(concentration)	time(s)	integral	concentration (mol/L)	ln(concentration)
264	0.51	0.036428578	-3.312401716	455	0.36	0.02571429	-3.66070841
580	0.51	0.036428578	-3.312401716	655	0.35	0.025000004	-3.688879287
845	0.46	0.032857148	-3.415585952	927	0.34	0.024285718	-3.717866824
1124	0.47	0.033571434	-3.394079747	1245	0.33	0.023571433	-3.747719787
1498	0.46	0.032857148	-3.415585952	1469	0.33	0.023571433	-3.747719787
1847	0.42	0.030000005	-3.506557731	1778	0.33	0.023571433	-3.747719787
#2							
394	0.4	0.028571433	-3.555347895				
550	0.4	0.028571433	-3.555347895				
815	0.39	0.027857148	-3.580665703				
996	0.38	0.027142862	-3.606641189				
1301	0.37	0.026428576	-3.633309436				
1576	0.35	0.025000004	-3.688879287				
1764	0.34	0.024285718	-3.717866824				

9-1-4. bis(4-chlorophenyl)methanone *O*-(4-fluorophenyl) oxime (**1db**).

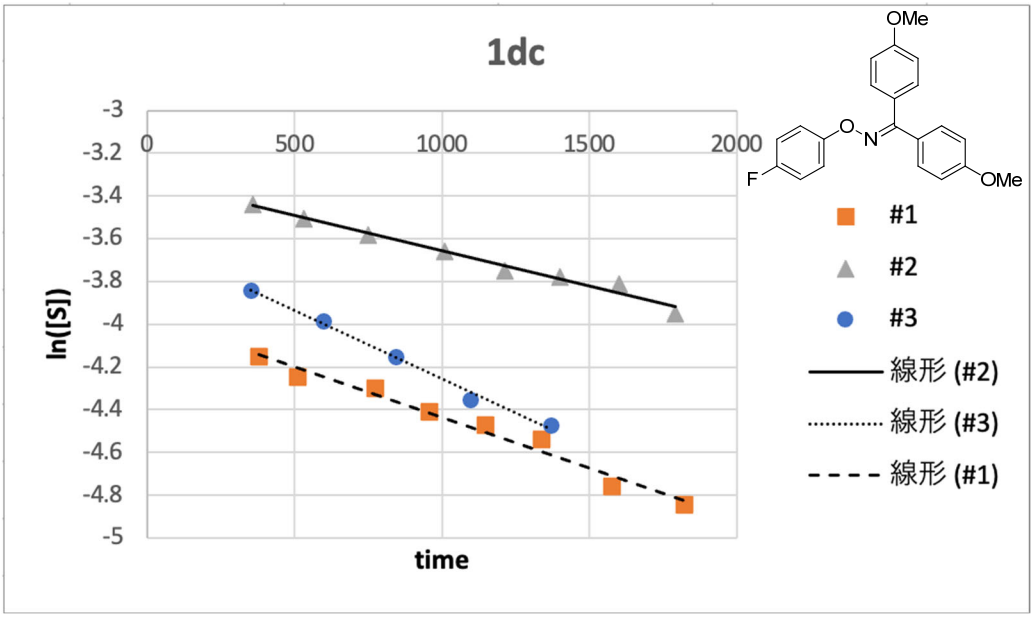
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.025	$4.22086 * 10^{-5}$	ln[S] = -3.685721211-0.0000422086t
2	0.025	$3.80276 * 10^{-5}$	ln[S] = -3.691455846-0.0000380276t
3	0.031428571	$3.75426 * 10^{-5}$	ln[S] = -3.448061411-0.0000375426t
average		$3.92596 * 10^{-5}$	



#1			
time(s)	integral	concentration (mol/L)	ln(concentration)
365	0.35	0.025	-3.688879454
681	0.34	0.024285718	-3.717866824
1071	0.33	0.023571433	-3.747719787
1362	0.33	0.023571433	-3.747719787
1764	0.33	0.023571433	-3.747719787
#2			
time(s)	integral	concentration (mol/L)	ln(concentration)
367	0.35	0.025	-3.688879454
642	0.34	0.024285718	-3.717866824
950	0.33	0.023571433	-3.747719787
1247	0.33	0.023571433	-3.747719787
1541	0.33	0.023571433	-3.747719787
1798	0.33	0.023571433	-3.747719787
#3			
time(s)	integral	concentration (mol/L)	ln(concentration)
420	0.44	0.031428571	-3.460037882
749	0.43	0.030714291	-3.483027233
1081	0.43	0.030714291	-3.483027233
1389	0.42	0.030000005	-3.506557731
1659	0.42	0.030000005	-3.506557731
1798	0.42	0.030000005	-3.506557731

9-1-5. bis(4-methoxyphenyl)methanone *O*-(4-fluorophenyl) oxime (**1dc**).

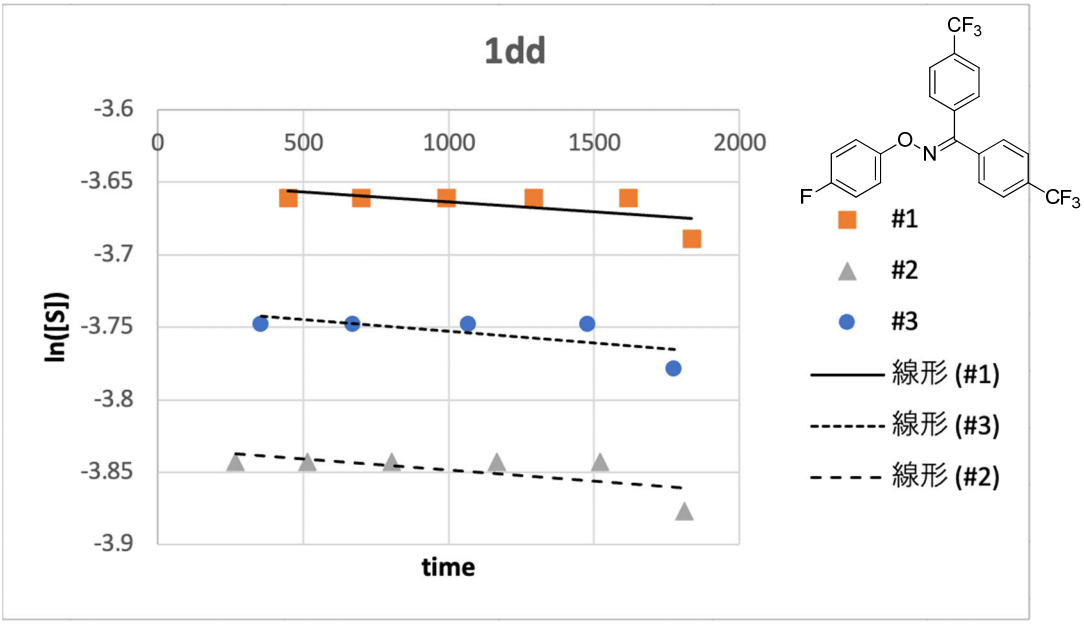
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.015714286	$4.73161 * 10^{-4}$	ln[S] = -4.016434153-0.000473161t
2	0.032142857	$3.29277 * 10^{-4}$	ln[S] = -3.327761928-0.000329277t
3	0.021428571	$6.41286 * 10^{-4}$	ln[S] = -3.614935509-0.000641286t
average		$4.81241 * 10^{-4}$	



#1			
time(s)	integral	concentration (mol/L)	ln(concentration)
379	0.22	0.015714286	-4.153185062
511	0.2	0.014285717	-4.248495075
775	0.19	0.013571431	-4.29978837
956	0.17	0.012142859	-4.411014005
1146	0.16	0.011428573	-4.471638627
1337	0.15	0.010714288	-4.536177148
1577	0.12	0.00857143	-4.759320699
1823	0.11	0.007857144	-4.846332076
#2			
time(s)	integral	concentration (mol/L)	ln(concentration)
357	0.45	0.032142857	-3.437565026
532	0.42	0.030000005	-3.506557731
748	0.39	0.027857148	-3.580665703
1009	0.36	0.02571429	-3.66070841
1214	0.33	0.023571433	-3.747719787
1401	0.32	0.022857147	-3.778491446
1599	0.31	0.022142861	-3.810240144
1790	0.27	0.019285718	-3.948390483
#3			
time(s)	integral	concentration (mol/L)	ln(concentration)
353	0.3	0.021428571	-3.843030134
598	0.26	0.018571432	-3.986130811
845	0.22	0.015714288	-4.153184896
1097	0.18	0.012857145	-4.353855591
1369	0.16	0.011428573	-4.471638627

9-1-6. bis(4-(trifluoromethyl)phenyl)methanone *O*-(4-(trifluoromethyl)phenyl) oxime (**1dd**).

Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.025714286	$1.35828 * 10^{-5}$	ln[S] = -3.649819538-0.0000135828t
2	0.021428575	$1.53102 * 10^{-5}$	ln[S] = -3.843030084-0.0000153102t
3	0.023571429	$1.62734 * 10^{-5}$	ln[S] = -3.736464818-0.0000162734t
average		$1.50555 * 10^{-5}$	

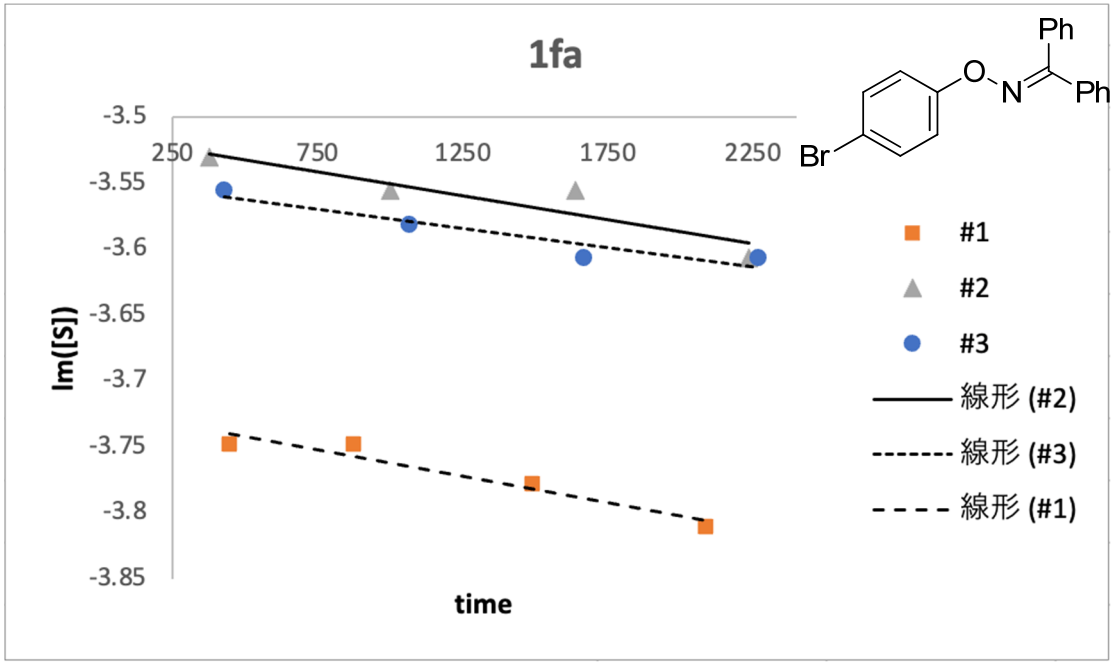


#1	time(s)	integral	concentration (mol/L)	ln(concentration)
	449	0.36	0.025714286	-3.660708577
	699	0.36	0.02571429	-3.66070841
	992	0.36	0.02571429	-3.66070841
	1291	0.36	0.02571429	-3.66070841
	1617	0.36	0.02571429	-3.66070841
	1836	0.35	0.025000004	-3.688879287
#2	time(s)	integral	concentration (mol/L)	ln(concentration)
	267	0.3	0.021428571	-3.843030134
	514	0.3	0.021428575	-3.843029967
	805	0.3	0.021428575	-3.843029967
	1166	0.3	0.021428575	-3.843029967
	1519	0.3	0.021428575	-3.843029967
	1809	0.29	0.020714289	-3.876931519
#3	time(s)	integral	concentration (mol/L)	ln(concentration)
	355	0.33	0.023571429	-3.747719954
	672	0.33	0.023571433	-3.747719787
	1067	0.33	0.023571433	-3.747719787
	1479	0.33	0.023571433	-3.747719787
	1776	0.32	0.022857147	-3.778491446

Because the reaction of **1dd** was too slow to obtain accurate rate constants, the data was not included in Hammett plot.

9-1-7. diphenylmethanone *O*-(4-bromophenyl) oxime (**1fa**).

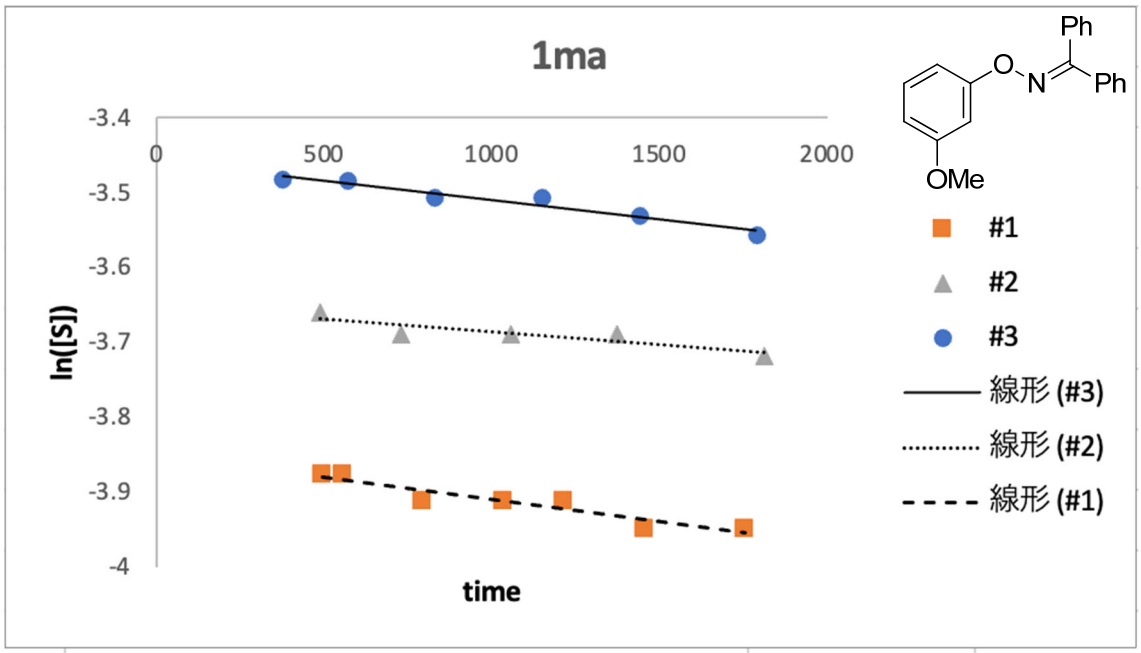
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.0235714	$4.0219 * 10^{-5}$	ln[S] = -3.721715561-0.000040219t
2	0.029286	$3.6448 * 10^{-5}$	ln[S] = -3.514067578-0.000036448t
3	0.028571707	$2.94754 * 10^{-5}$	ln[S] = -3.547265567-0.0000294754t
average		$3.53808 * 10^{-5}$	



#1	time(s)	integral	concentration (mol/L)	ln(concentration)
	448	0.33	0.0235714	-3.747721166
	876	0.33	0.0235714	-3.747721166
	1491	0.32	0.022857115	-3.778492825
	2091	0.31	0.02214283	-3.810241523
#2	time(s)	integral	concentration (mol/L)	ln(concentration)
	379	0.41	0.029286	-3.530645693
	1001	0.4	0.028571394	-3.555349274
	1641	0.4	0.028571394	-3.555349274
	2239	0.38	0.027142824	-3.606642568
#3	time(s)	integral	concentration (mol/L)	ln(concentration)
	430	0.4	0.028571707	-3.555338305
	1067	0.39	0.027857109	-3.580667082
	1669	0.38	0.027142824	-3.606642568
	2270	0.38	0.027142824	-3.606642568

9-1-8. diphenylmethanone *O*-(3-methoxyphenyl) oxime (**1ma**).

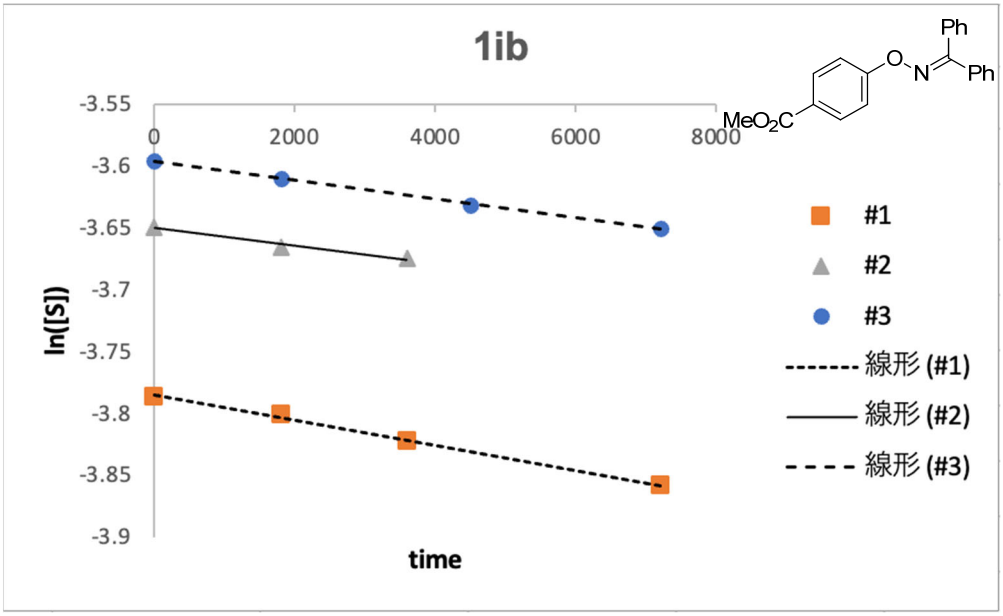
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.02071429	$5.91221 * 10^{-5}$	ln[S] = -3.850689307-0.0000591221t
2	0.02571429	$3.45884 * 10^{-5}$	ln[S] = -3.6151299786-0.0000345884t
3	0.030748464	$5.14318 * 10^{-5}$	ln[S] = -3.457959256-0.0000514318t
average		$4.82135 * 10^{-5}$	



#1	time(s)	integral	concentration (mol/L)	ln(concentration)	#2	time(s)	integral	concentration (mol/L)	ln(concentration)
	495	0.29	0.02071429	-3.876931479		488	0.36	0.02571429	-3.66070841
	555	0.29	0.02071429	-3.876931479		728	0.35	0.025000004	-3.688879287
	795	0.28	0.020000004	-3.912022799		1056	0.35	0.025000004	-3.688879287
	1035	0.28	0.020000004	-3.912022799		1373	0.35	0.025000004	-3.688879287
	1215	0.28	0.020000004	-3.912022799		1811	0.34	0.024285718	-3.717866824
	1455	0.27	0.019285718	-3.948390443	#3	time(s)	integral	concentration (mol/L)	ln(concentration)
	1755	0.27	0.019285718	-3.948390443		376	0.43	0.030748464	-3.481915241
						569	0.43	0.030714291	-3.483027233
						828	0.42	0.030000005	-3.506557731
						1148	0.42	0.030000005	-3.506557731
						1441	0.41	0.029285719	-3.530655282
						1788	0.4	0.028571433	-3.555347895

9-1-9. methyl 4-(((diphenylmethylene)amino)oxy)benzoate (**1ia**).

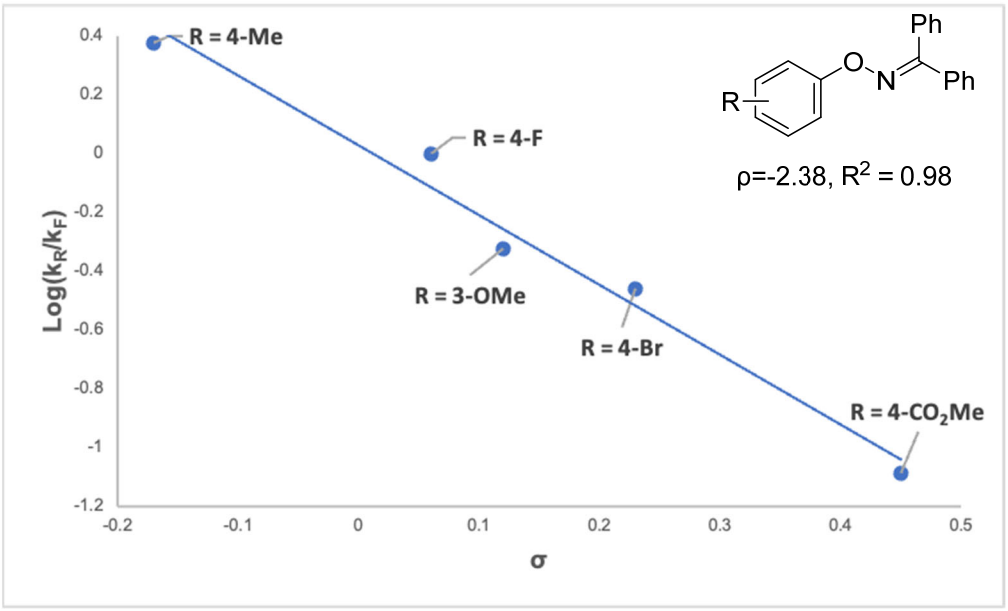
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.022685692	1.01989 * 10^{-5}	ln[S] = -3.784549684-0.0000101989t
2	0.02601426	7.10705 * 10^{-6}	ln[S] = -3.650290393-0.00000710705t
3	0.02744283	7.59955 * 10^{-6}	ln[S] = -3.596188873-0.00000759955t
average		8.30183 * 10^{-6}	



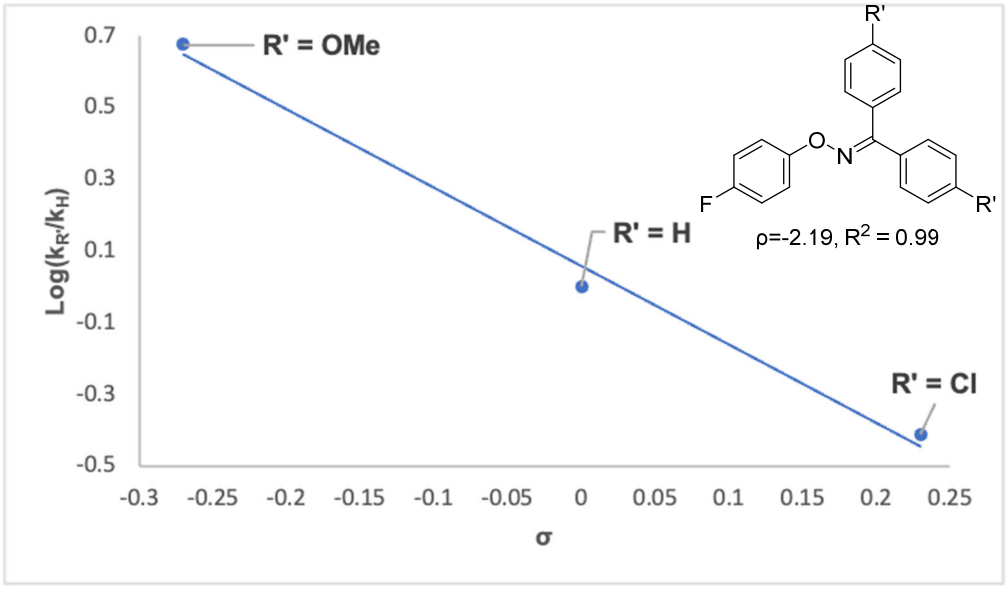
time(s)	integral	concentration (mol/L)	ln(concentration)
0	0.3176	0.022685692	-3.786020879
1800	0.3131	0.022364263	-3.80029098
3600	0.3063	0.02187855	-3.822248595
7200	0.2955	0.021107122	-3.858144772
time(s)	integral	concentration (mol/L)	ln(concentration)
0	0.3642	0.02601426	-3.649110441
1800	0.3583	0.025592832	-3.665442984
3600	0.355	0.025357118	-3.674695819
time(s)	integral	concentration (mol/L)	ln(concentration)
0	0.3842	0.02744283	-3.595650358
1800	0.3787	0.027049973	-3.610069274
4500	0.3707	0.026478545	-3.631420498
7200	0.3638	0.025985688	-3.650209343

9.2 Hammett Plot (σ)

(a) phenoxy group

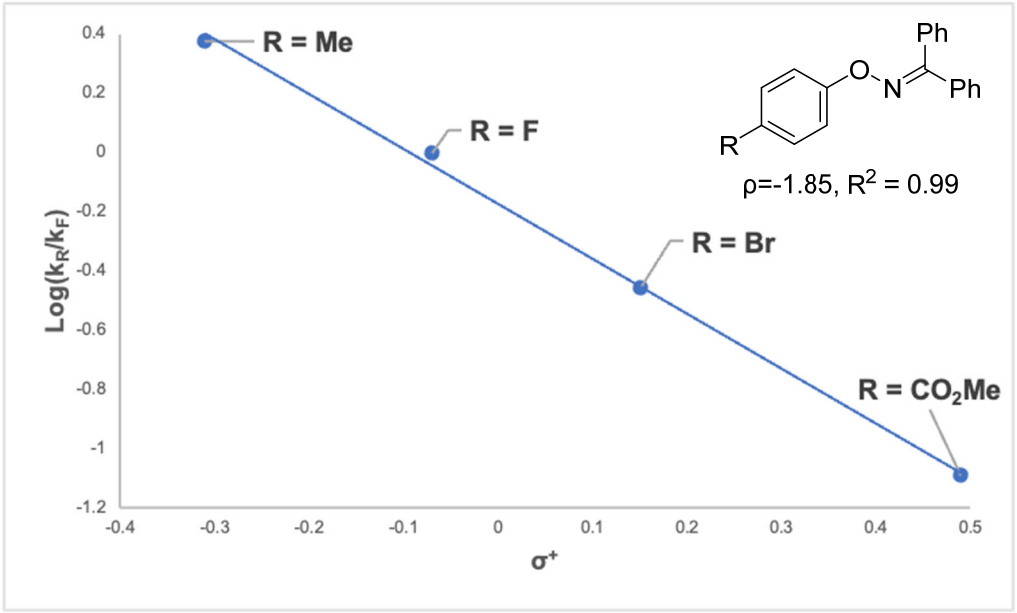


(b) aryl group at oxime carbon

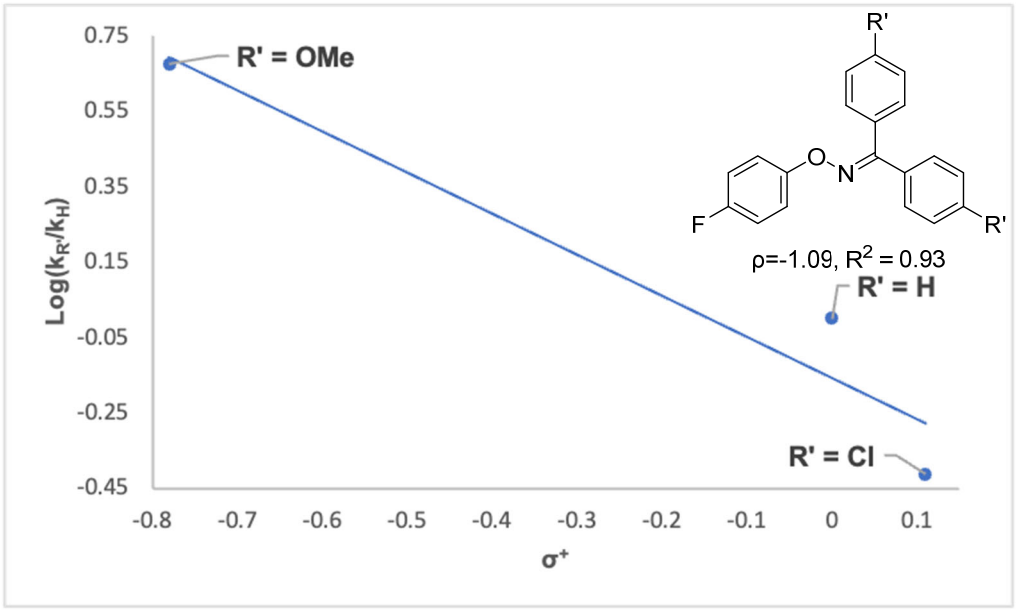


Hammett Plot (σ^+)

(a) phenoxy group



(b) aryl group at oxime carbon



9-3 General procedures under the conditions using IPrCuBr and $AgSbF_6$

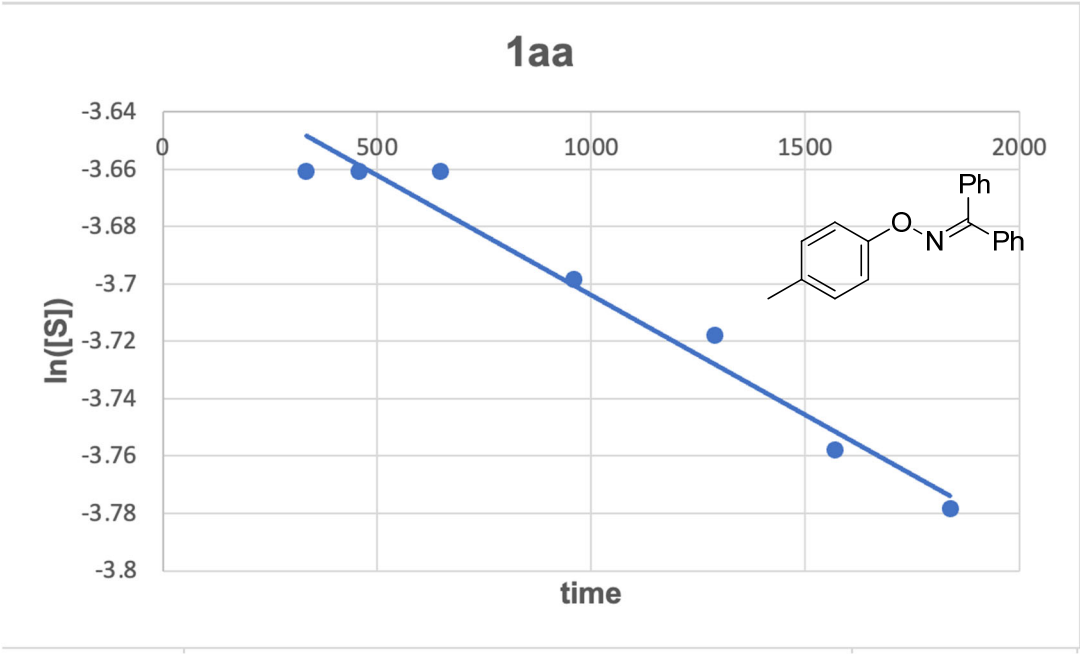
The procedure is according to the literature.[6] The rearrangement reactions were conducted in the presence of substrate (0.01951 mmol), IPrCuBr (10 mol%, 1.0 mg, 0.001951 mmol), $AgSbF_6$ (10 mol%, 0.67 mg, 0.001951 mmol) and CH_2Br_2 (7 μL) as an internal standard in $CDCl_3$ (0.028 M, 0.7 mL) in NMR tube at 50 °C in 400 Hz NMR and its reaction rate was monitored by ^1H NMR spectrocopy. The k_{obs} of each reaction was determined from a first-order plot of ln[SM] versus time. The σ value was according to the literature.[7]

[6]Lee, K. N. Lei, Z. Morales-Rivera. C. A. Liu, P. Ngai, M.-Y. *Org. Biomol. Chem*., **2016**, *14*, 5599.

[7]Hansch, C. Leo, A. Taft, R. W. *Chem*. Rev., **1991**, *91*, 165.

9-3-1 diphenylmethanone *O*-(*p*-tolyl) oxime (**1aa**).

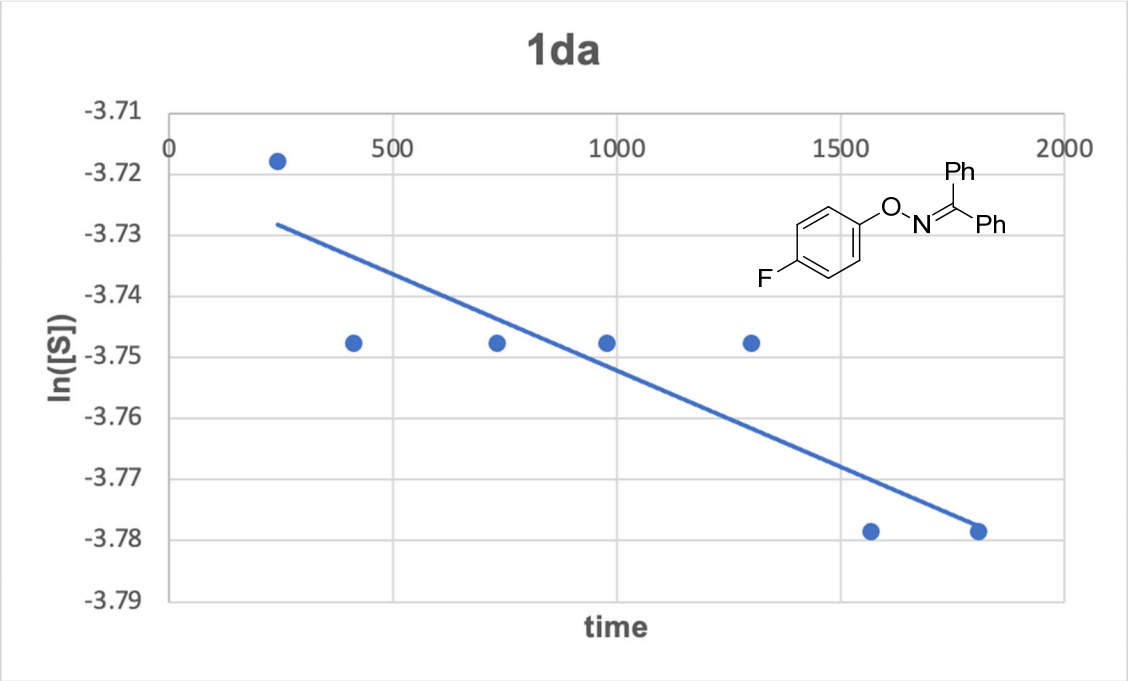
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.025714189	8.357 * 10^{-5}	ln[S] = -3.62022368-0.00008.357t



time(s)	integral	concentration (mol/L)	ln(concentration)
335	0.54	0.025714189	3.660712351
458	0.54	0.025714189	3.660712351
648	0.54	0.025714189	3.660712351
960	0.52	0.024761811	3.698452679
1290	0.51	0.024285623	3.717870765
1569	0.49	0.023333245	3.757876099
1839	0.48	0.022857057	3.778495386

9-3-2 diphenylmethanone *O*-(4-fluorophenyl) oxime (**1da**).

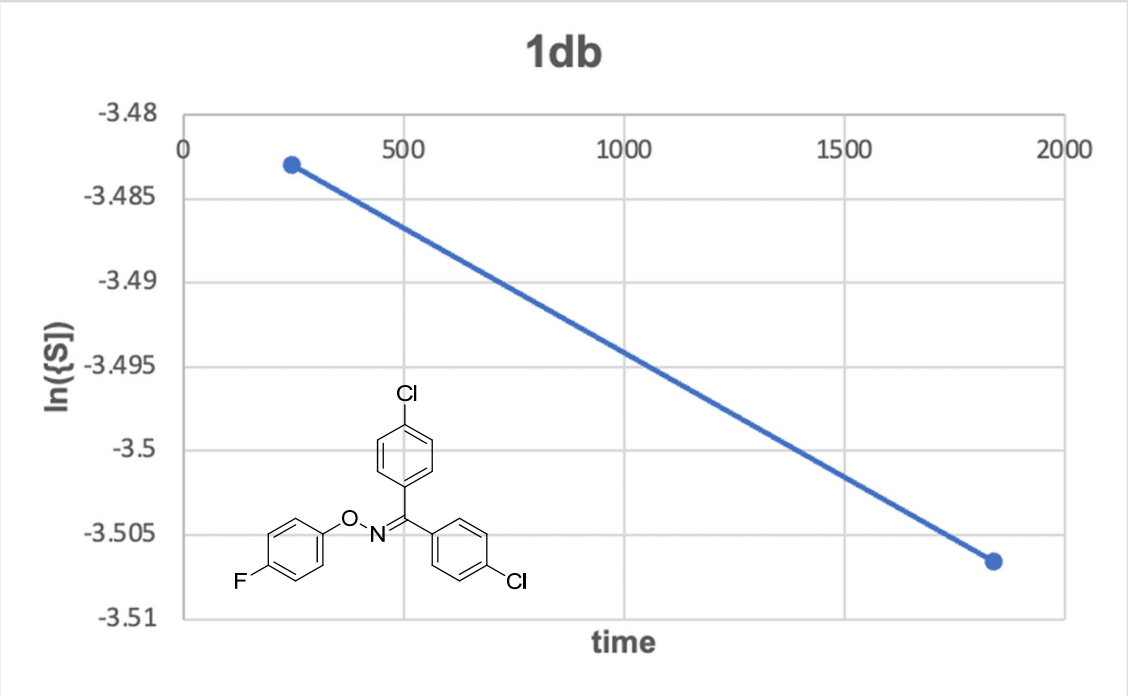
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.024285718	$3.14831 * 10^{-5}$	ln[S] = -3.720584193-0.0000314831t



time(s)	integral	concentration (mol/L)	ln(concentration)
241	0.34	0.024285718	-3.717866824
412	0.33	0.023571433	-3.747719787
733	0.33	0.023571433	-3.747719787
978	0.33	0.023571433	-3.747719787
1300	0.33	0.023571433	-3.747719787
1568	0.32	0.022857147	-3.778491446
1808	0.32	0.022857147	-3.778491446

9-3-3. bis(4-chlorophenyl)methanone *O*-(4-fluorophenyl) oxime (**1db**).

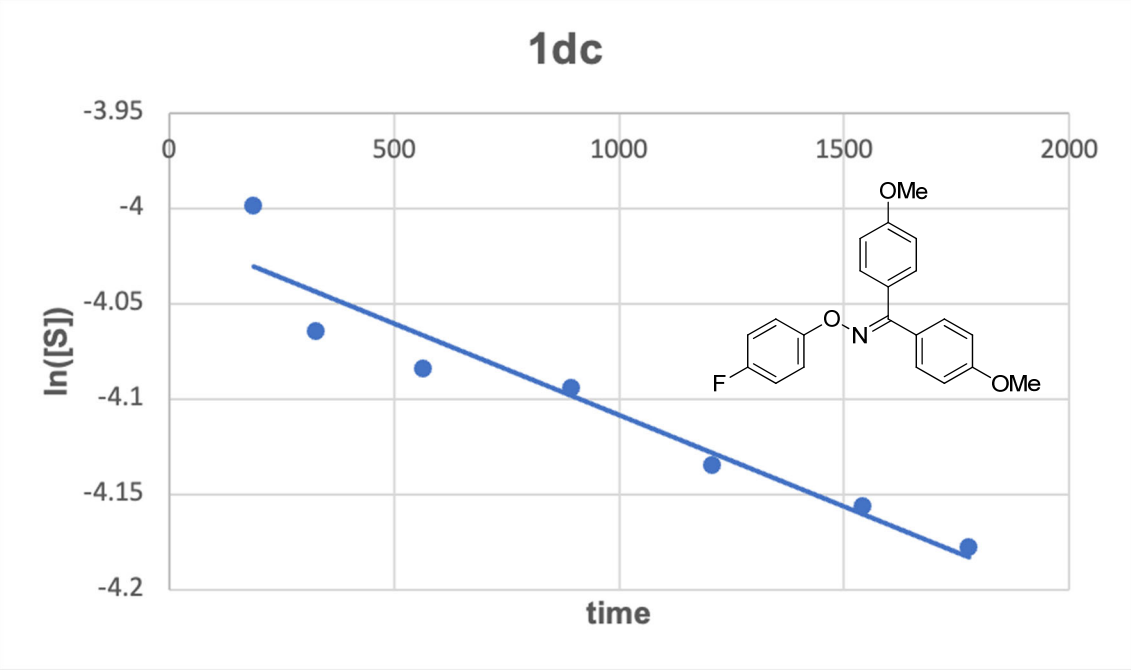
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.030714286	$1.47804 * 10^{-5}$	ln[S] = -3.479376651-0.0000147804t



time(s)	integral	concentration (mol/L)	ln(concentration)
247	0.43	0.030714286	-3.4830274
1839	0.42	0.030000005	-3.506557731

9-3-4. bis(4-methoxyphenyl)methanone *O*-(4-fluorophenyl) oxime (**1dc**).

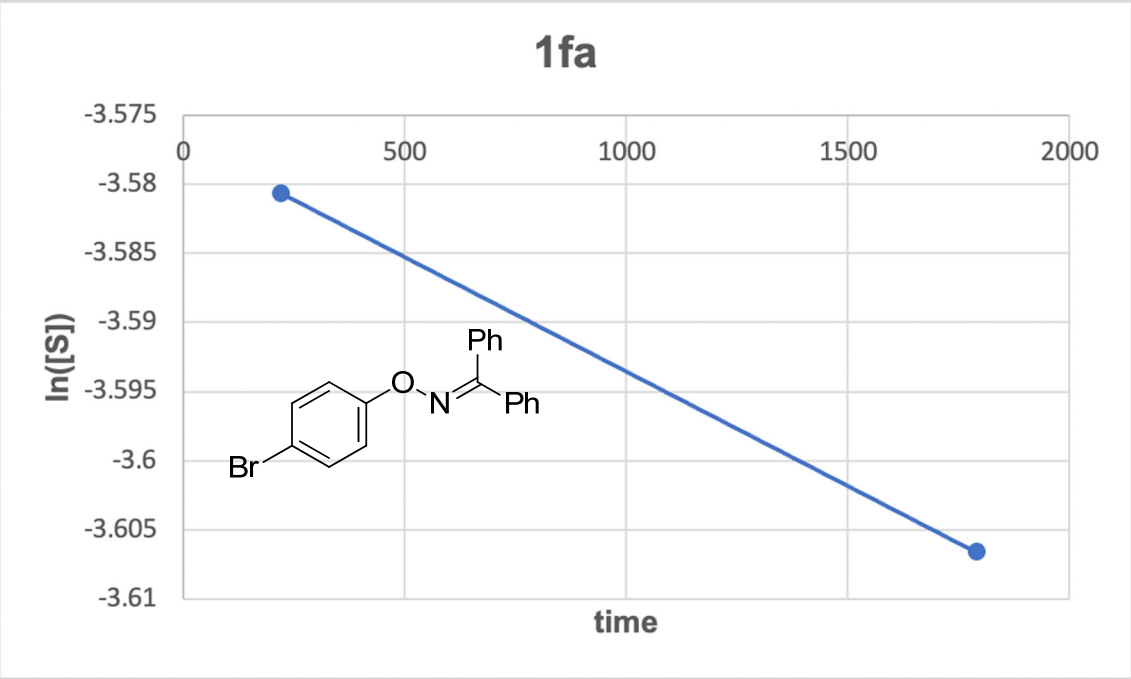
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.030714286	$9.55896 * 10^{-5}$	ln[S] = -4.003289834-0.0000955896t



time(s)	integral	concentration (mol/L)	ln(concentration)
188	1.1	0.018333333	-3.999034387
328	1.03	0.017166667	-4.064785764
565	1.01	0.016833333	-4.084394236
896	1	0.016666667	-4.094344567
1208	0.96	0.016	-4.135166561
1543	0.94	0.015666667	-4.15621997
1778	0.92	0.015333333	-4.177726176

9-3-5. diphenylmethanone *O*-(4-bromophenyl) oxime (**1fa**).

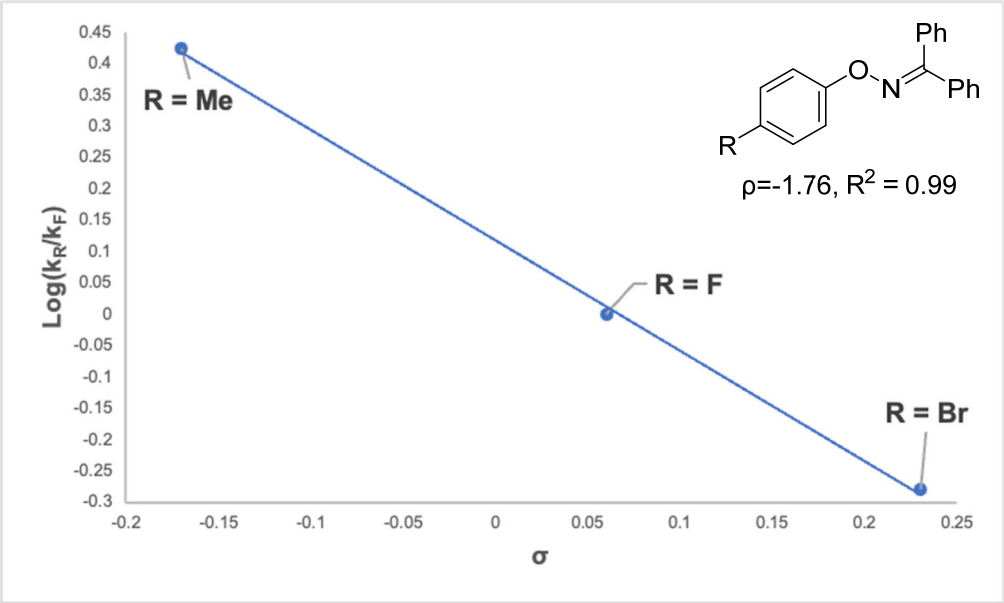
Trial	concentration (mole/L)	k (s^{-1})	approximate formula
1	0.027857109	1.65344 * 10^{-5}	ln[S] = -3.577012987-0.0000165344t



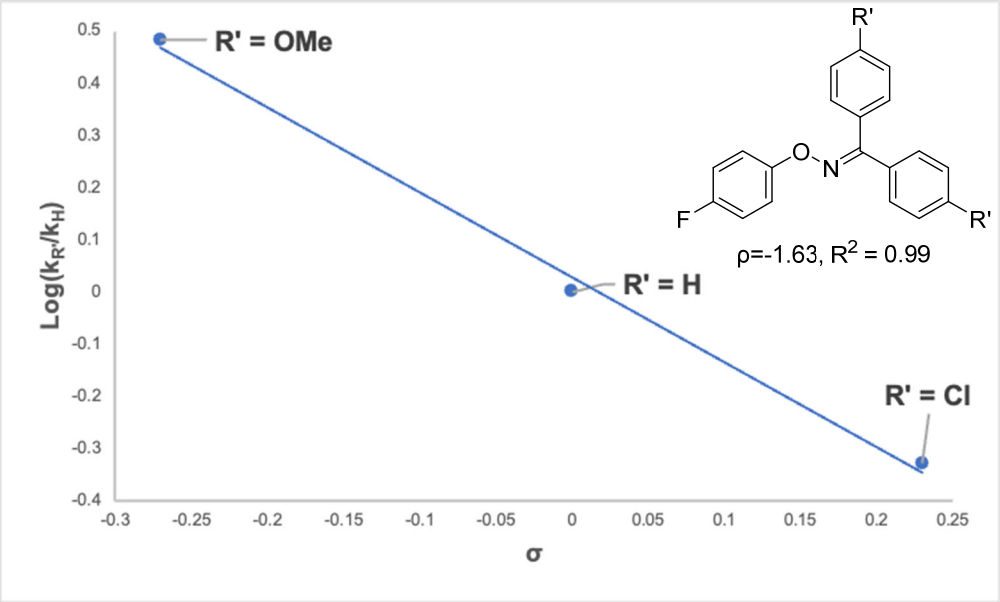
time(s)	integral	concentration (mol/L)	ln(concentration)
221	0.39	0.027857109	-3.580667082
1792	0.38	0.027142824	-3.606642568

9.4 Hammett Plot (σ)

(a) phenoxy group



(b) aryl group at oxime carbon



10 Computational Studies

10-1 General

Computations were carried out using B3LYP as implemented in the GAUSSIAN 09 software package.[1] Copper atom was described with the SDD basis set[2] with the associated effective core potential and other atoms were described with 6-31G+(d,p) basis in the geometry optimization and frequency calculations. Transition states were found by a Berny algorithm after scanning potential energy surface from reactants. All transition states were verified by the intrinsic reaction coordinate (IRC) method.

[1.] Gaussian 09, Revision C.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

2. A. Bergner, M. Dolg, W. Kuechle, H. Stoll, H. Preuss, *Mol. Phys.*, 1993, **80**, 1431.

10-2 Energy profile

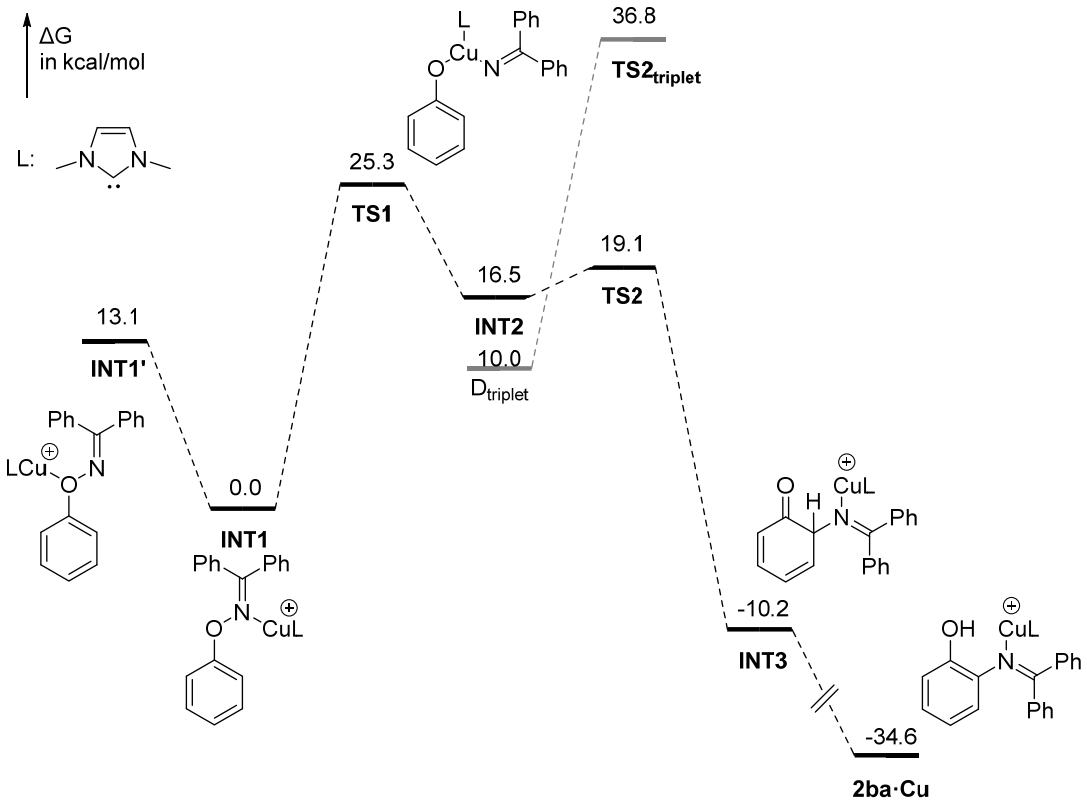


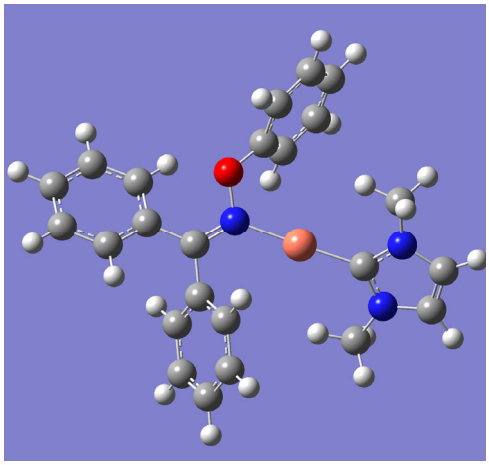
Figure S1. Reaction coordinate for the Cu-catalyzed reaction of **1ba** at the level of B3LYP/SDD(Cu),6-31+(d,p)(others).

Table S7. Calculated energies of intermediates and transition states

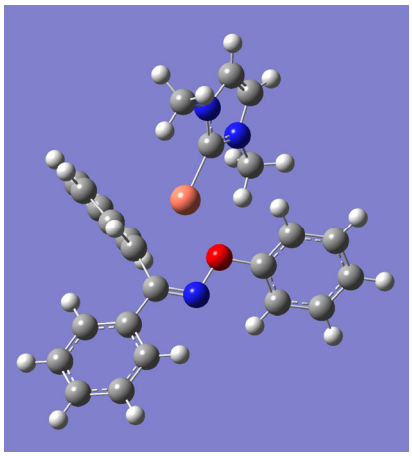
Compound	SCF energy / a.u.	E(ZPVE) / a.u.	H / a.u.	G(298) / a.u.	Imaginary frequency /cm^{-1}
INT1'	-1365.088506	-1364.669899	-1364.641754	-1364.732840	-
INT1	-1365.064391	-1364.647093	-1364.618385	-1364.711976	-
TS1	-1365.044464	-1364.629136	-1364.600865	-1364.692388	-218.16
INT2	-1365.058535	-1364.642340	-1364.613569	-1364.706537	-
TS2	-1365.054505	-1364.638882	-1364.610771	-1364.701511	-80.41
INT3	-1365.106002	-1364.687697	-1364.659522	-1364.749083	-
2ba·Cu	-1365.144167	-1364.725093	-1364.696725	-1364.749083	-
INT2$_{triplet}$	-1365.072599	-1364.658117	-1364.628489	-1364.726990	-
TS2$_{triplet}$	-1365.028222	-1364.612327	-1364.584617	-1364.674260	-278.74

Figure S2. Geometry of the computed intermediates and transition states

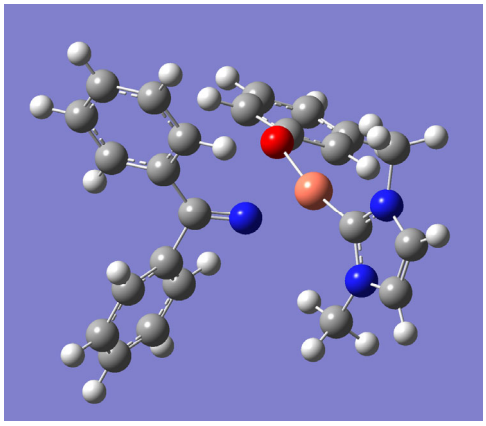
INT1'



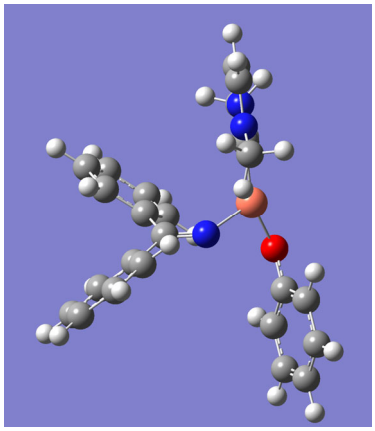
INT1



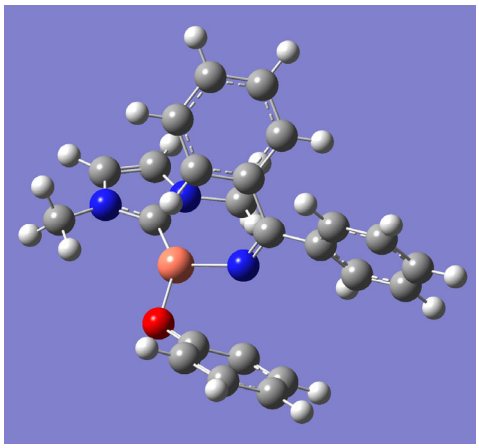
TS1



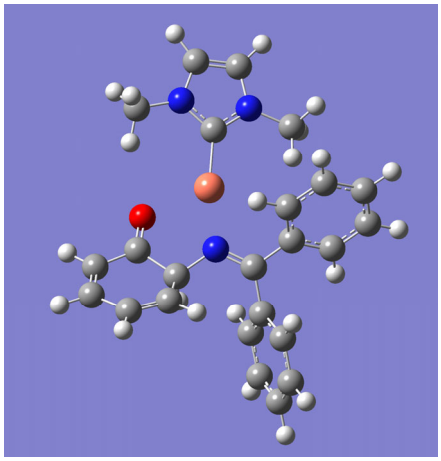
INT2



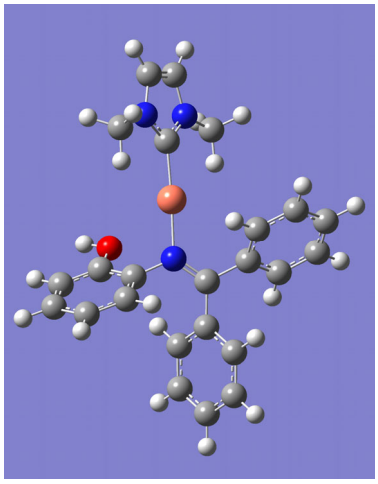
TS2



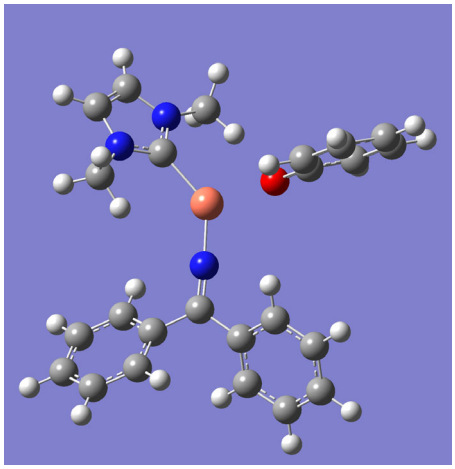
INT3



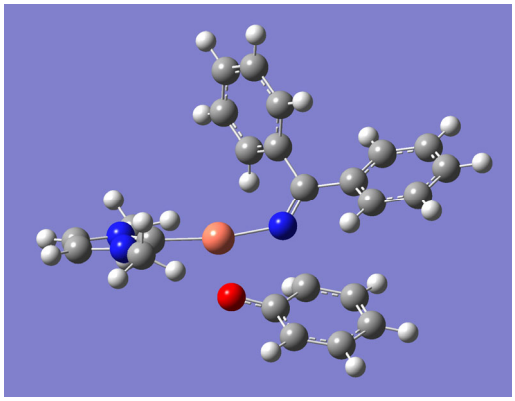
2ba·Cu



INT2$_{triplet}$



TS2$_{triplet}$

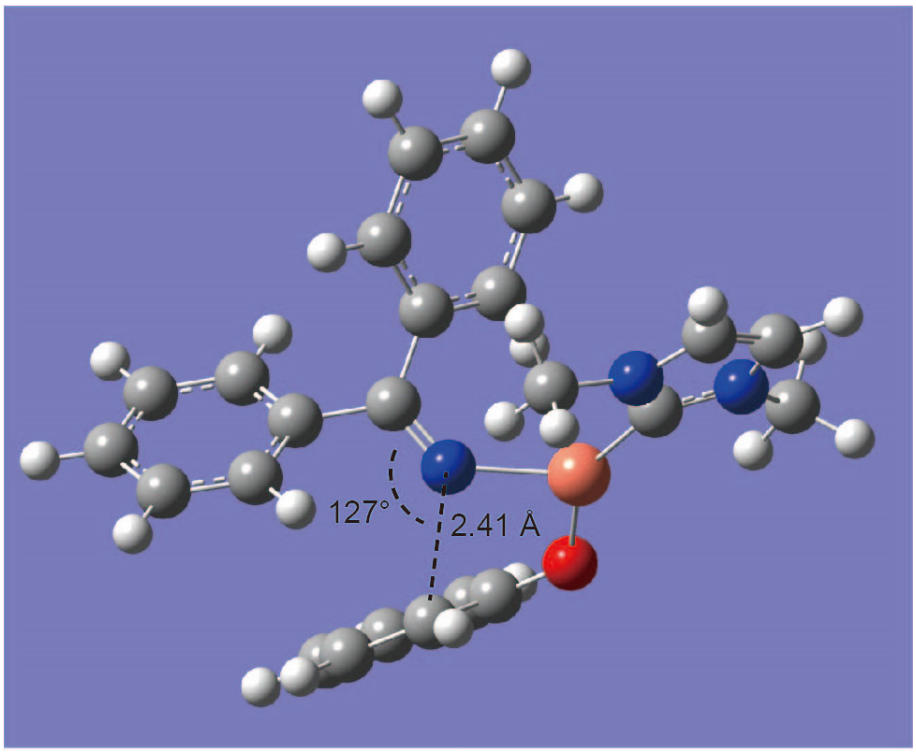


It should be noted that the triplet state of the intermediate **INT2$_{triplet}$**, which was formed after N-O bond cleavage, was calculated to be more stable than the singlet state **INT2**. However, the transition state **TS2$_{triplet}$** for the triplet state was calculated to be much higher than that for the singlet, suggesting that the C-N bond formation occurs in singlet state.

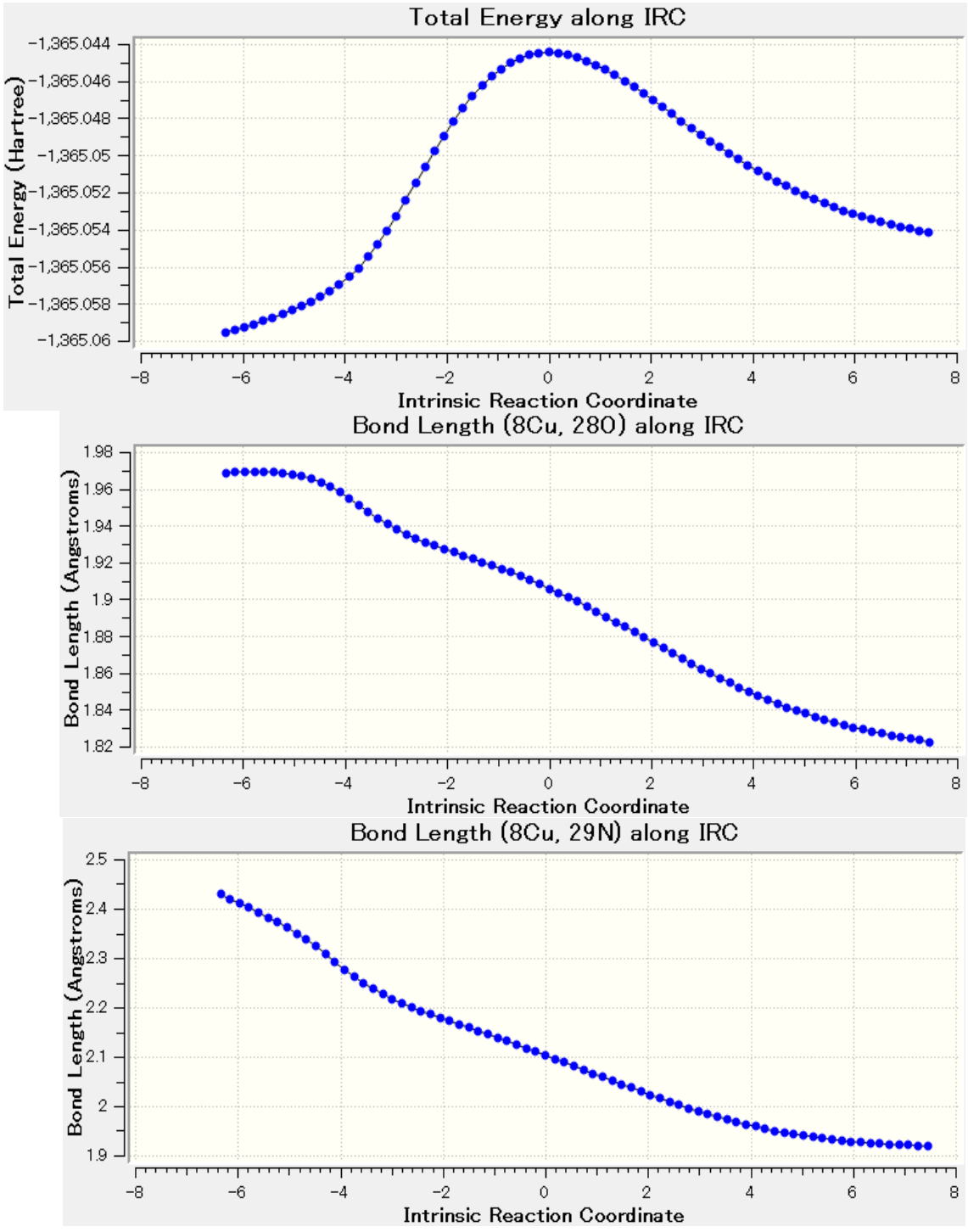
10-3. Stabilizing interaction from NBO calculations for the transition state **TS2**

	Stabilizing interaction (kcal/mol)
LP (N) → LP* (C_{ortho})	58.83
BD (C_{ortho}-C_{ipso}) → BD* (N-C)	0.51

Figure S3. Geometry of Figure **TS2**



10-4. IRC of **TS1**



Since the Cu-O bond (ca. 1.97 A) in the reactant before N-O bond cleavage was calculated to be much shorter than the Cu-N bond (ca. 2.42 A) according to the IRC analysis of **TS1**, we concluded that the N-O bond cleavage is initiated by coordination of the oxygen atom of the substrate **1** to the copper catalyst.

10-5. Cartesian Coordinates

INT1'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.201993	-0.770704	0.395996
2	1	0	6.157229	-0.439396	0.772830
3	6	0	4.877340	-1.825496	-0.398670
4	1	0	5.496494	-2.584362	-0.851431
5	7	0	4.018168	-0.113906	0.687720
6	7	0	3.503019	-1.787464	-0.566899
7	6	0	2.958142	-0.732375	0.098902
8	29	0	1.126072	-0.214838	0.180211
9	6	0	3.935185	1.069681	1.544490
10	1	0	4.651128	1.821303	1.204458
11	1	0	2.929103	1.483315	1.477903
12	1	0	4.150795	0.802017	2.582384
13	6	0	2.758825	-2.735449	-1.396068
14	1	0	3.046140	-3.756623	-1.135527
15	1	0	1.693122	-2.607309	-1.207615
16	1	0	2.965827	-2.557693	-2.454907
17	6	0	0.333365	3.682249	0.882090
18	6	0	-0.033663	2.611243	0.063466
19	6	0	0.437031	2.499962	-1.248089
20	6	0	1.308950	3.479734	-1.736598
21	6	0	1.686967	4.557723	-0.932214
22	6	0	1.191236	4.659284	0.373001
23	1	0	-0.063504	3.742528	1.890367
24	1	0	0.112785	1.682773	-1.883942
25	1	0	1.675593	3.404867	-2.755951
26	1	0	2.353100	5.320690	-1.322352
27	1	0	1.473549	5.500224	0.999169
28	8	0	-0.953758	1.720162	0.608038
29	7	0	-0.723708	0.369738	0.267271
30	6	0	-1.816645	-0.336713	0.161167
31	6	0	-3.192136	0.205955	0.132872
32	6	0	-3.521801	1.383049	-0.568955
33	6	0	-4.213597	-0.508207	0.788718
34	6	0	-4.841285	1.825996	-0.611636
35	1	0	-2.754515	1.940704	-1.092279
36	6	0	-5.527698	-0.041521	0.768477
37	1	0	-3.975285	-1.419606	1.327302
38	6	0	-5.845136	1.122827	0.064419
39	1	0	-5.087280	2.724153	-1.169568
40	1	0	-6.302014	-0.591076	1.294500
41	1	0	-6.870177	1.479957	0.037603
42	6	0	-1.613602	-1.807325	0.070989
43	6	0	-0.804273	-2.478918	1.005714
44	6	0	-2.249328	-2.543096	-0.945308
45	6	0	-0.626186	-3.862114	0.916489
46	1	0	-0.360763	-1.927386	1.829404

47	6	0	-2.051498	-3.920296	-1.041641
48	1	0	-2.890025	-2.034072	-1.658747
49	6	0	-1.242271	-4.582329	-0.110568
50	1	0	-0.023472	-4.376431	1.659012
51	1	0	-2.537624	-4.479226	-1.835300
52	1	0	-1.108077	-5.657888	-0.176610

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.001451	-0.936947	0.310602
2	1	0	5.909516	-0.663164	0.825139
3	6	0	4.802239	-1.707131	-0.791306
4	1	0	5.503649	-2.228287	-1.424319
5	7	0	3.751229	-0.505949	0.724923
6	7	0	3.434738	-1.729667	-1.017712
7	6	0	2.770095	-0.990960	-0.086015
8	29	0	0.878246	-0.665194	0.073639
9	6	0	3.533415	0.333482	1.902800
10	1	0	4.224817	1.178693	1.885039
11	1	0	2.512747	0.714718	1.880122
12	1	0	3.687853	-0.245274	2.817715
13	6	0	2.814442	-2.431270	-2.140098
14	1	0	3.121733	-3.479982	-2.139336
15	1	0	1.731932	-2.374515	-2.030500
16	1	0	3.107522	-1.967541	-3.085935
17	6	0	1.590995	2.716810	-0.951473
18	6	0	0.484052	2.525928	-0.127747
19	6	0	0.019870	3.521599	0.729630
20	6	0	0.695020	4.745198	0.756593
21	6	0	1.816556	4.957145	-0.051614
22	6	0	2.262761	3.942047	-0.902874
23	1	0	1.908831	1.925876	-1.622961
24	1	0	-0.855662	3.348203	1.344578
25	1	0	0.340654	5.533464	1.413701
26	1	0	2.333939	5.910889	-0.024314
27	1	0	3.123005	4.106134	-1.544766
28	8	0	-0.121241	1.255749	-0.164690
29	7	0	-1.541497	1.337535	-0.161337
30	6	0	-2.094466	0.179467	-0.043798
31	6	0	-1.348582	-1.108284	0.190420
32	6	0	-0.850578	-1.424929	1.480770
33	6	0	-1.348423	-2.120130	-0.799670
34	6	0	-0.425934	-2.732448	1.776666
35	1	0	-0.899380	-0.679475	2.269998
36	6	0	-0.918840	-3.413895	-0.492474
37	1	0	-1.744871	-1.896469	-1.785649
38	6	0	-0.477403	-3.727268	0.799242
39	1	0	-0.083543	-2.966206	2.780042
40	1	0	-0.957330	-4.184799	-1.256308
41	1	0	-0.174605	-4.741516	1.039750

42	6	0	-3.575431	0.135049	-0.133637
43	6	0	-4.282848	1.185472	-0.751196
44	6	0	-4.292668	-0.946741	0.408251
45	6	0	-5.673712	1.154172	-0.810706
46	1	0	-3.734470	2.013957	-1.185696
47	6	0	-5.687107	-0.970886	0.346854
48	1	0	-3.769339	-1.766586	0.889613
49	6	0	-6.380703	0.077818	-0.261364
50	1	0	-6.208408	1.966376	-1.293654
51	1	0	-6.229265	-1.808542	0.774712
52	1	0	-7.465018	0.055474	-0.313218-

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.278105	-1.423952	0.321839
2	1	0	6.248577	-1.484799	0.789586
3	6	0	4.732328	-2.149958	-0.690870
4	1	0	5.137870	-2.962210	-1.274071
5	7	0	4.321066	-0.501802	0.710141
6	7	0	3.456049	-1.653075	-0.893384
7	6	0	3.188096	-0.631949	-0.033998
8	29	0	1.580646	0.388339	0.080229
9	6	0	4.521631	0.475966	1.780031
10	1	0	3.627614	1.094539	1.859282
11	1	0	4.692702	-0.036304	2.730262
12	1	0	5.379335	1.112373	1.548632
13	6	0	2.538007	-2.158716	-1.915464
14	1	0	2.391747	-3.233374	-1.782230
15	1	0	1.580182	-1.649618	-1.811993
16	1	0	2.944724	-1.967212	-2.911858
17	6	0	0.499905	3.096853	-1.408220
18	6	0	-0.294206	2.566200	-0.366690
19	6	0	-1.582913	3.096895	-0.128138
20	6	0	-2.046339	4.158707	-0.897969
21	6	0	-1.251977	4.685494	-1.926199
22	6	0	0.019729	4.150924	-2.178227
23	1	0	1.489225	2.683433	-1.585495
24	1	0	-2.178283	2.678797	0.676922
25	1	0	-3.027170	4.580514	-0.700757
26	1	0	-1.619895	5.512225	-2.525863
27	1	0	0.634916	4.564952	-2.971239
28	8	0	0.151758	1.596272	0.441728
29	7	0	-0.368389	-0.158297	-0.489544
30	6	0	-1.378538	-0.637814	0.123773
31	6	0	-1.792178	-0.461833	1.538079
32	6	0	-0.842241	-0.306620	2.562039
33	6	0	-3.161351	-0.459193	1.858688
34	6	0	-1.255920	-0.154832	3.883371
35	1	0	0.216051	-0.324786	2.324462
36	6	0	-3.571108	-0.283830	3.180964

37	1	0	-3.901195	-0.582053	1.074449
38	6	0	-2.620307	-0.135566	4.194777
39	1	0	-0.516649	-0.051255	4.671694
40	1	0	-4.630181	-0.270509	3.418844
41	1	0	-2.939858	-0.010744	5.224970
42	6	0	-2.179210	-1.523040	-0.793304
43	6	0	-2.551780	-2.813016	-0.372732
44	6	0	-2.519649	-1.076286	-2.082015
45	6	0	-3.277325	-3.635838	-1.232275
46	1	0	-2.282792	-3.161276	0.619578
47	6	0	-3.257489	-1.903552	-2.930144
48	1	0	-2.222636	-0.082194	-2.398261
49	6	0	-3.632606	-3.182773	-2.509598
50	1	0	-3.571718	-4.628370	-0.905145
51	1	0	-3.538817	-1.549244	-3.917006
52	1	0	-4.203614	-3.826287	-3.172018

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.549730	-1.005982	-1.145786
2	1	0	-5.588118	-0.997276	-0.852525
3	6	0	-3.966861	-0.820403	-2.361524
4	1	0	-4.401638	-0.625576	-3.329667
5	7	0	-3.525018	-1.235832	-0.244267
6	7	0	-2.600993	-0.936889	-2.170655
7	6	0	-2.318075	-1.199088	-0.867805
8	29	0	-0.575781	-1.437771	-0.068023
9	6	0	-3.735033	-1.469571	1.186103
10	1	0	-4.488910	-2.248017	1.322215
11	1	0	-2.797664	-1.800366	1.632746
12	1	0	-4.060789	-0.548840	1.675949
13	6	0	-1.614798	-0.861254	-3.251519
14	1	0	-1.871469	-0.033154	-3.915268
15	1	0	-0.630932	-0.682623	-2.818968
16	1	0	-1.606964	-1.794367	-3.821368
17	6	0	2.492524	-2.829869	-0.547399
18	6	0	1.995803	-2.428530	0.724042
19	6	0	2.909796	-2.248010	1.799072
20	6	0	4.264479	-2.472064	1.604854
21	6	0	4.742783	-2.863702	0.342741
22	6	0	3.852533	-3.039171	-0.728669
23	1	0	1.788846	-2.979838	-1.360689
24	1	0	2.516598	-1.947360	2.764950
25	1	0	4.958767	-2.343222	2.429477
26	1	0	5.804498	-3.036696	0.196949
27	1	0	4.228854	-3.347453	-1.699248
28	8	0	0.710511	-2.242201	0.938539
29	7	0	0.418523	0.103316	-0.595132
30	6	0	0.348520	1.252810	-0.056257
31	6	0	-0.512648	1.594558	1.124869

32	6	0	-0.547467	0.754835	2.249535
33	6	0	-1.288922	2.764648	1.105240
34	6	0	-1.350527	1.086582	3.343847
35	1	0	0.076493	-0.133684	2.280745
36	6	0	-2.108825	3.076784	2.191448
37	1	0	-1.252217	3.425324	0.244517
38	6	0	-2.137469	2.242176	3.313879
39	1	0	-1.349896	0.450076	4.223946
40	1	0	-2.713620	3.978248	2.166506
41	1	0	-2.759612	2.499194	4.166023
42	6	0	1.221486	2.324412	-0.649061
43	6	0	1.464452	2.356660	-2.032878
44	6	0	1.837228	3.270558	0.187735
45	6	0	2.297076	3.335525	-2.574033
46	1	0	0.990188	1.622716	-2.675232
47	6	0	2.677334	4.241145	-0.359529
48	1	0	1.663475	3.246464	1.258528
49	6	0	2.907004	4.277175	-1.738822
50	1	0	2.469893	3.365137	-3.645550
51	1	0	3.149685	4.970765	0.291114
52	1	0	3.556543	5.037993	-2.160940

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.240763	-0.096958	0.662209
2	1	0	6.265497	-0.154250	0.329087
3	6	0	4.686387	0.543825	1.725941
4	1	0	5.136311	1.150252	2.496717
5	7	0	4.205212	-0.735416	0.000370
6	7	0	3.327035	0.280565	1.683644
7	6	0	3.014461	-0.510413	0.621725
8	29	0	1.284436	-1.190306	0.074185
9	6	0	4.387157	-1.544738	-1.204968
10	1	0	5.123203	-2.330233	-1.017602
11	1	0	3.434805	-2.006844	-1.466192
12	1	0	4.725408	-0.917416	-2.033842
13	6	0	2.373142	0.777145	2.674396
14	1	0	2.418758	1.868016	2.720959
15	1	0	1.371295	0.471276	2.375850
16	1	0	2.602462	0.360072	3.658585
17	6	0	-1.620636	-2.450845	0.665045
18	6	0	-0.986883	-2.703659	-0.616756
19	6	0	-1.822855	-2.944992	-1.760222
20	6	0	-3.188018	-2.963380	-1.618723
21	6	0	-3.796161	-2.728058	-0.348846
22	6	0	-3.023612	-2.484513	0.772164
23	1	0	-0.998322	-2.453785	1.550954
24	1	0	-1.339018	-3.118792	-2.715835
25	1	0	-3.821098	-3.159705	-2.478997
26	1	0	-4.877860	-2.767789	-0.264849

27	1	0	-3.492887	-2.343906	1.740033
28	8	0	0.287721	-2.633098	-0.735090
29	7	0	-0.481754	-0.350061	0.357951
30	6	0	-1.004552	0.769941	0.043827
31	6	0	-0.201120	1.793871	-0.705531
32	6	0	0.566506	1.419465	-1.820075
33	6	0	-0.217570	3.136772	-0.291673
34	6	0	1.304234	2.378787	-2.515978
35	1	0	0.552569	0.388624	-2.161631
36	6	0	0.540385	4.086891	-0.977291
37	1	0	-0.819959	3.433793	0.561229
38	6	0	1.299332	3.710850	-2.091123
39	1	0	1.872801	2.089131	-3.394650
40	1	0	0.529211	5.121984	-0.649634
41	1	0	1.874875	4.455933	-2.632053
42	6	0	-2.409120	1.109825	0.430561
43	6	0	-2.885681	0.786610	1.711410
44	6	0	-3.250227	1.774908	-0.477025
45	6	0	-4.184993	1.133940	2.082493
46	1	0	-2.228052	0.289024	2.416989
47	6	0	-4.557204	2.097452	-0.109064
48	1	0	-2.885860	2.031550	-1.466830
49	6	0	-5.024433	1.783124	1.171262
50	1	0	-4.540779	0.903919	3.082384
51	1	0	-5.206646	2.601754	-0.818006
52	1	0	-6.036399	2.050325	1.460360

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.409932	0.311985	-0.468947
2	1	0	6.352477	0.834002	-0.412254
3	6	0	5.125250	-0.974995	-0.801899
4	1	0	5.771126	-1.786400	-1.099505
5	7	0	4.201003	0.926132	-0.187193
6	7	0	3.749911	-1.113227	-0.705768
7	6	0	3.161111	0.055835	-0.325323
8	29	0	1.302044	0.438363	-0.074928
9	6	0	4.079020	2.319350	0.245209
10	1	0	4.787308	2.932311	-0.316246
11	1	0	3.067718	2.667485	0.038547
12	1	0	4.293420	2.407252	1.314337
13	6	0	3.037242	-2.345066	-1.036004
14	1	0	3.491725	-3.187690	-0.509530
15	1	0	1.999760	-2.243845	-0.720165
16	1	0	3.073583	-2.527508	-2.113827
17	6	0	-1.327106	1.816275	0.071592
18	6	0	-0.297098	2.914430	-0.198779
19	6	0	-0.690250	4.278723	0.126892
20	6	0	-1.710591	4.498449	0.997418
21	6	0	-2.475015	3.410487	1.589097

22	6	0	-2.272656	2.135733	1.204498
23	1	0	-1.952318	1.871682	-0.838497
24	1	0	-0.062270	5.081988	-0.244284
25	1	0	-1.943060	5.515025	1.303988
26	1	0	-3.208857	3.644572	2.353879
27	1	0	-2.844712	1.319719	1.632773
28	8	0	0.796061	2.631943	-0.699172
29	7	0	-0.678742	0.493187	0.174259
30	6	0	-1.393605	-0.596058	0.091515
31	6	0	-0.797625	-1.886925	0.522742
32	6	0	0.035919	-1.940215	1.657232
33	6	0	-1.108828	-3.080539	-0.154907
34	6	0	0.551586	-3.159278	2.095903
35	1	0	0.247806	-1.030185	2.208891
36	6	0	-0.568073	-4.294292	0.271310
37	1	0	-1.764589	-3.055933	-1.019318
38	6	0	0.257383	-4.337098	1.399760
39	1	0	1.171641	-3.192585	2.986627
40	1	0	-0.802937	-5.207105	-0.267449
41	1	0	0.657533	-5.286151	1.744066
42	6	0	-2.804542	-0.639713	-0.401161
43	6	0	-3.118164	-0.186814	-1.695171
44	6	0	-3.821364	-1.185787	0.400275
45	6	0	-4.429458	-0.260404	-2.168091
46	1	0	-2.332332	0.189256	-2.345248
47	6	0	-5.136150	-1.233106	-0.066765
48	1	0	-3.584452	-1.567041	1.389507
49	6	0	-5.442402	-0.771335	-1.350389
50	1	0	-4.657988	0.075024	-3.175055
51	1	0	-5.917506	-1.641626	0.566681
52	1	0	-6.463150	-0.820801	-1.716780

2ba·Cu

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.444732	0.716863	0.248475
2	1	0	6.293353	1.204926	0.702278
3	6	0	5.379351	-0.220597	-0.734263
4	1	0	6.160167	-0.704070	-1.300723
5	7	0	4.139367	0.988533	0.625325
6	7	0	4.036012	-0.496726	-0.930752
7	6	0	3.256054	0.243900	-0.095971
8	29	0	1.355777	0.239218	0.029082
9	6	0	3.777816	1.949009	1.667232
10	1	0	4.168832	2.938260	1.416432
11	1	0	2.690983	1.999887	1.732300
12	1	0	4.182882	1.630264	2.631241
13	6	0	3.538694	-1.456650	-1.915839
14	1	0	3.930389	-2.453713	-1.699191
15	1	0	2.450446	-1.479446	-1.862168
16	1	0	3.843290	-1.154422	-2.921086

17	6	0	-1.072619	1.675026	0.242620
18	6	0	-0.750256	2.600710	-0.764995
19	6	0	-1.151284	3.933560	-0.646166
20	6	0	-1.865073	4.351898	0.478999
21	6	0	-2.180565	3.440068	1.490056
22	6	0	-1.782172	2.108635	1.369041
23	1	0	-0.910283	4.640109	-1.437193
24	1	0	-2.172466	5.389556	0.561528
25	1	0	-2.730732	3.761717	2.368112
26	1	0	-2.014108	1.392624	2.151372
27	7	0	-0.575827	0.330674	0.150691
28	6	0	-1.380943	-0.700068	0.127630
29	6	0	-0.798418	-2.055396	0.300720
30	6	0	0.191479	-2.292487	1.273356
31	6	0	-1.239982	-3.124554	-0.500467
32	6	0	0.736803	-3.567659	1.430216
33	1	0	0.496703	-1.488835	1.936896
34	6	0	-0.673752	-4.391497	-0.358228
35	1	0	-2.013866	-2.957216	-1.242713
36	6	0	0.312572	-4.616412	0.608218
37	1	0	1.479383	-3.745689	2.202196
38	1	0	-1.009782	-5.205346	-0.993343
39	1	0	0.736607	-5.608595	0.730702
40	6	0	-2.848609	-0.602034	-0.086537
41	6	0	-3.373875	0.182682	-1.129739
42	6	0	-3.726693	-1.339104	0.728514
43	6	0	-4.750255	0.233093	-1.344370
44	1	0	-2.704425	0.729976	-1.784874
45	6	0	-5.105357	-1.259762	0.529603
46	1	0	-3.330735	-1.961174	1.525518
47	6	0	-5.618994	-0.477240	-0.508842
48	1	0	-5.145592	0.826588	-2.162989
49	1	0	-5.776046	-1.816211	1.176984
50	1	0	-6.691282	-0.427394	-0.672235
51	8	0	-0.061434	2.120236	-1.850897
52	1	0	0.131451	2.839728	-2.467680

INT2$_{\text{triplet}}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.910983	-4.306302	0.334501
2	1	0	3.673654	-4.914121	0.796252
3	6	0	2.056102	-4.577206	-0.687590
4	1	0	1.937496	-5.463059	-1.292116
5	7	0	2.637771	-3.012277	0.747943
6	7	0	1.279507	-3.443767	-0.865188
7	6	0	1.629673	-2.464706	0.014633
8	29	0	0.817872	-0.689706	0.179380
9	6	0	3.323121	-2.357105	1.862743
10	1	0	4.404273	-2.412790	1.713507
11	1	0	3.018666	-1.311914	1.897923

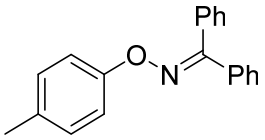
12	1	0	3.061860	-2.845980	2.805282
13	6	0	0.244820	-3.319558	-1.891747
14	1	0	-0.392323	-4.206742	-1.879597
15	1	0	-0.361806	-2.441550	-1.671373
16	1	0	0.699233	-3.212507	-2.880740
17	6	0	3.005655	1.801427	-1.210301
18	6	0	2.919680	1.625007	0.220626
19	6	0	3.676133	2.515601	1.070507
20	6	0	4.455170	3.510597	0.517046
21	6	0	4.521400	3.661394	-0.884812
22	6	0	3.793713	2.801443	-1.739182
23	1	0	2.438718	1.126823	-1.844783
24	1	0	3.598035	2.374269	2.143665
25	1	0	5.019736	4.181764	1.156747
26	1	0	5.138025	4.445811	-1.312710
27	1	0	3.860640	2.933269	-2.814765
28	8	0	2.200862	0.710454	0.748769
29	7	0	-0.862839	0.038585	0.055964
30	6	0	-2.063968	0.448121	0.066189
31	6	0	-3.188585	-0.541348	0.043523
32	6	0	-3.079588	-1.747988	0.755894
33	6	0	-4.340414	-0.290356	-0.721169
34	6	0	-4.112286	-2.684647	0.710351
35	1	0	-2.197591	-1.932731	1.360881
36	6	0	-5.363251	-1.238788	-0.776752
37	1	0	-4.430591	0.637085	-1.277612
38	6	0	-5.253384	-2.434024	-0.059351
39	1	0	-4.032034	-3.605062	1.281080
40	1	0	-6.247277	-1.041727	-1.375533
41	1	0	-6.056690	-3.163847	-0.093989
42	6	0	-2.352303	1.916136	0.097912
43	6	0	-1.510132	2.813383	-0.581040
44	6	0	-3.434563	2.413001	0.843466
45	6	0	-1.753249	4.185056	-0.522372
46	1	0	-0.682642	2.426784	-1.167273
47	6	0	-3.664285	3.788199	0.911404
48	1	0	-4.084867	1.728641	1.378649
49	6	0	-2.828248	4.675393	0.226912
50	1	0	-1.109922	4.871906	-1.064235
51	1	0	-4.497660	4.165506	1.496141
52	1	0	-3.016356	5.743843	0.273026

$TS2_{triplet}$

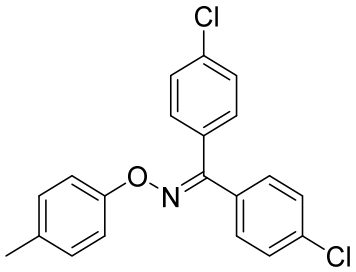
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.401063	0.065253	-0.172588
2	1	0	-6.293523	0.436214	-0.652233
3	6	0	-5.237365	-0.654028	0.971437
4	1	0	-5.961009	-1.022139	1.682020
5	7	0	-4.135915	0.270950	-0.694542
6	7	0	-3.879909	-0.873275	1.114512

7	6	0	-3.189372	-0.301797	0.094373
8	29	0	-1.241988	-0.404510	-0.147272
9	6	0	-3.885913	0.958120	-1.961417
10	1	0	-4.384269	1.930035	-1.958782
11	1	0	-2.813201	1.109802	-2.075788
12	1	0	-4.257124	0.357820	-2.796033
13	6	0	-3.276916	-1.598238	2.239237
14	1	0	-3.065486	-0.911391	3.063150
15	1	0	-3.975477	-2.364908	2.577939
16	1	0	-2.360125	-2.078946	1.897633
17	6	0	1.073396	-1.872474	-1.143260
18	6	0	0.229738	-2.728219	-0.302857
19	6	0	0.752088	-3.912289	0.234850
20	6	0	2.084542	-4.253567	0.003244
21	6	0	2.927558	-3.427860	-0.783426
22	6	0	2.440975	-2.273449	-1.355746
23	1	0	0.572005	-1.460554	-2.020326
24	1	0	0.108788	-4.535112	0.847506
25	1	0	2.484029	-5.163558	0.440576
26	1	0	3.954006	-3.730886	-0.965378
27	1	0	3.063824	-1.677306	-2.014484
28	8	0	-0.995185	-2.325162	-0.026549
29	7	0	0.646405	-0.208734	-0.292386
30	6	0	1.393153	0.820228	-0.080804
31	6	0	0.732145	2.161729	0.017811
32	6	0	1.020032	3.027988	1.086148
33	6	0	-0.206259	2.557940	-0.953486
34	6	0	0.359584	4.252710	1.194174
35	1	0	1.753432	2.737273	1.831962
36	6	0	-0.845986	3.796203	-0.855564
37	1	0	-0.378285	1.919903	-1.816914
38	6	0	-0.571773	4.640685	0.224168
39	1	0	0.578864	4.910085	2.030049
40	1	0	-1.538961	4.111916	-1.630105
41	1	0	-1.068176	5.603158	0.302014
42	6	0	2.862686	0.745605	0.120282
43	6	0	3.421600	-0.286965	0.893541
44	6	0	3.706204	1.729305	-0.429325
45	6	0	4.799017	-0.334109	1.110956
46	1	0	2.771595	-1.029682	1.343630
47	6	0	5.085019	1.661752	-0.233246
48	1	0	3.282949	2.537241	-1.018570
49	6	0	5.632706	0.633352	0.542013
50	1	0	5.220992	-1.123740	1.725198
51	1	0	5.730491	2.414853	-0.674657
52	1	0	6.704955	0.592147	0.708674

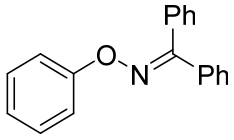
11 Analytical data of 1



diphenylmethanone *O*-(*p*-tolyl) oxime (1aa). Colorless solid. Melting point: 53.6 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 30.8% (3 steps, 0.963 mmol, 0.277 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.60 (m, 2H), 7.47-7.37 (m, 9H), 7.15-7.11 (m, 4H), 2.32 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 157.6, 136.1, 133.0, 131.7, 130.0, 129.7, 129.5, 129.3, 128.5, 128.4, 128.2, 114.9, 20.8. IR (neat) 3058, 3028, 2998, 2921, 2863, 2735, 2422, 2317, 1955, 1883, 1811, 1770, 1607, 1586, 1566, 1502, 1444, 1326, 1301, 1212, 1182, 1162, 1104, 1075, 1033, 1014, 983, 930, 847, 814, 772, 759, 692, 664, 648, 634, 606 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO$ (M^+): 287.1310, found: 287.1310.

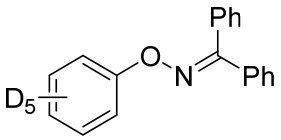


bis(4-chlorophenyl)methanone *O*-(*p*-tolyl) oxime (1ab). Colorless solid. Melting point: 101.9 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 21.6% (3 steps, 0.580 mmol, 0.207 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53-7.51 (m, 2H), 7.47-7.45 (m, 2H), 7.39-7.34 (m, 4H), 7.13-7.10 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.4, 157.2, 136.2, 135.4, 134.0, 132.0, 130.8, 130.7, 129.7, 129.5, 128.7, 128.6, 114.7, 20.6. IR (neat) 3031, 2923, 2862, 2358, 2342, 1605, 1594, 1503, 1491, 1398, 1323, 1297, 1213, 1161, 1092, 1015, 986, 933, 833, 816, 758, 729 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{15}Cl_2NO$ (M^+): 355.0531, found: 355.0531.

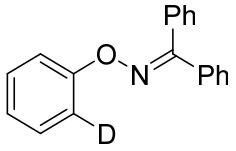


diphenylmethanone *O*-phenyl oxime (1ba). Brown oil. R_f = 0.4 [hexane/EtOAc = 10:1 (v/v)]. Yield: 67.0% (3 steps, 1.58 mmol, 0.431 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.60 (m, 2H), 7.49-7.41 (m, 6H), 7.39-7.36 (m, 2H), 7.32-7.29 (m, 2H), 7.25-7.23 (m, 2H), 7.03-7.00 (tt, *J* = 7.2, 1.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.9, 159.5, 153.9, 132.8, 129.9, 129.3, 129.2, 128.4, 128.3, 128.1, 122.2, 114.8, 77.9, 35.1, 14.0. IR (neat) 3027, 2364, 2314, 1955, 1811, 1748, 1658, 1592, 1489, 1456, 1444, 1396, 1327, 1301, 1274, 1211,

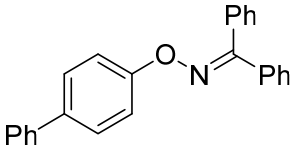
1183, 1158, 1073, 1023, 1000, 983, 929, 914, 832, 795, 772, 752, 689, 658, 608 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{15}NO$ (M^+): 273.1154, found: 273.1153.



diphenylmethanone *O*-phenyl-d_5 oxime (1ba-*d5*). Brown solid. Melting point: 55.3 °C. R_f = 0.4 [hexane/EtOAc = 10:1 (v/v)]. Yield: 14.2% (5 steps, 0.504 mmol, 0.141 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.61 (m, 2H), 7.50-7.43 (m, 6H), 7.40-7.38 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.0, 159.6, 133.0, 130.1, 129.5, 129.3, 129.0-128.7 (t, *J* = 24.6, 24.6 Hz), 128.6, 128.4, 128.2, 122.0-121.7 (t, *J* = 24.6 Hz), 114.7-114.4 (t, *J* = 24.6 Hz). IR (neat) 3058, 3029, 2979, 2931, 2359, 2279, 1958, 1893, 1814, 1720, 1558, 1493, 1444, 1373, 1324, 1170, 1076, 1042, 980, 959, 928, 812, 765, 696, 666 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{10}D_5NO$ (M^+): 278.1468, found: 278.1467.

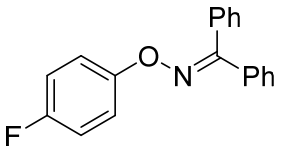


diphenylmethanone *O*-phenyl-2-*d* oxime (1ba-*d*). Brown oil. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 1.9% (5 steps, 0.134 mmol, 32.2 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.61 (m, 2H), 7.50-7.38 (m, 8H), 7.34-7.31 (m, 2H), 7.26-7.25 (m, 1H), 7.05-7.02 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.9, 159.5, 135.9, 132.8, 130.0, 129.3, 129.2, 129.1, 128.4, 128.3, 128.1, 122.2, 114.8, 114.7-114.4 (t, *J* = 24.6 Hz). IR (neat) 3350, 3149, 3061, 3026, 2918, 2858, 2415, 2359, 1811, 1747, 1705, 1658, 1586, 1542, 1491, 1466, 1444, 1327, 1308, 1277, 1214, 1183, 1156, 1116, 1075, 1033, 984, 930, 845, 771, 696, 658 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}D_1NO$ (M^+): 274.1216, found: 274.1216.

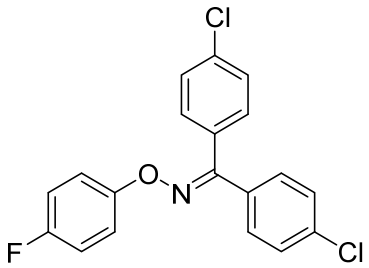


diphenylmethanone *O*-([1,1'-biphenyl]-4-yl) oxime (1ca). Colorless solid. Melting point: 104.7 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 6.5% (3 steps, 0.204 mmol, 70.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71-7.68 (m, 2H), 7.65-7.60 (m, 4H), 7.54-7.42 (m, 10H), 7.40-7.35 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.2, 159.2, 141.0, 136.0, 135.4,

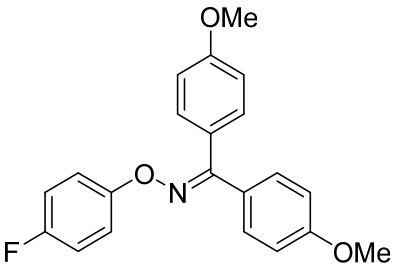
132.9, 130.2, 129.5, 129.4, 128.8, 128.6, 128.5, 128.3, 128.1, 127.8, 127.0, 126.9, 115.2. IR (neat) 1604, 1514, 1483, 1445, 1329, 1222, 1166, 984, 931, 836, 763, 696 cm^{-1}. HRMS (FD) calcd. for $C_{25}H_{19}NO$ (M^+): 349.1467, found: 349.1466.



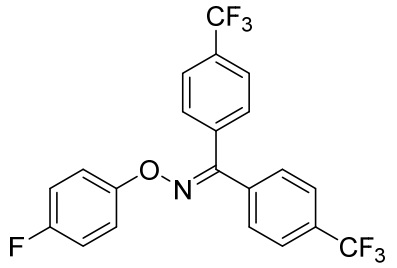
diphenylmethanone *O*-(4-fluorophenyl) oxime (1da). Orange oil. R_f = 0.6 [hexane/EtOAc = 10:1 (v/v)]. Yield: 23.0% (3 steps, 0.186 mmol, 54.2 mg). ^1H NMR (600 MHz, $CDCl_3$) δ 7.60-7.59 (m, 2H), 7.49-7.43 (m, 6H), 7.40-7.37 (m, 2H), 7.21-7.19 (m, 2H), 7.02-6.99 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.0, 159.0, 157.4, 155.6, 135.8, 132.7, 130.0, 129.3, 128.4, 128.3, 128.1, 116.1, 116.0, 115.6, 115.5. IR (neat) 1499, 1444, 1328, 1195, 1091, 1033, 985, 933, 831, 791, 764, 696 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}FNO$ (M^+): 291.1059, found: 291.1059.



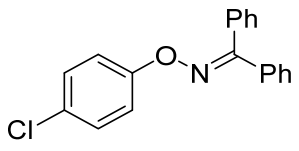
bis(4-chlorophenyl)methanone *O*-(4-fluorophenyl) oxime (1db). Colorless oil. R_f = 0.6 [hexane/EtOAc = 10:1 (v/v)]. Yield: 17.4% (3 steps, 0.140 mmol, 50.5 mg). ^1H NMR (600 MHz, $CDCl_3$) δ 7.51-7.50 (m, 2H), 7.48-7.46 (m, 2H), 7.37-7.35 (m, 4H), 7.18-7.15 (m, 2H), 7.02-6.99 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 157.9, 157.6, 155.3, 136.4, 135.6, 133.8, 130.7, 130.5, 129.5, 128.7-128.7 (d, *J* = 14.5 Hz), 116.1-116.0 (d, *J* = 8.7 Hz), 115.8-115.6 (d, J = 23.1). IR (neat) 3585, 3560, 3536, 3502, 3470, 3437, 2385, 2361, 1599, 1498, 1399, 1324, 1195, 1092, 1016, 986, 932, 831, 790 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2FNO$ (M^+): 359.0280, found: 359.0280.



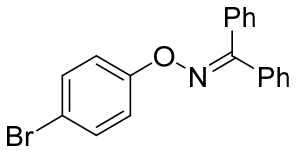
bis(4-methoxyphenyl)methanone *O*-(4-fluorophenyl) oxime (1dc). Yellow oil. R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. Yield: 31.6% (3 steps, 0.405 mmol, 0.142 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58-7.56 (m, 2H), 7.44-7.43 (m, 2H), 7.24-7.22 (m, 2H), 7.03-7.00 (m, 4H), 6.93-6.92 (m, 2H), 3.89 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.1, 160.2, 159.4, 158.8, 157.2, 155.7, 131.2, 130.0, 128.6, 124.9, 115.9-115.9 (d, J = 8.7 Hz), 115.5-115.4 (d, *J* = 23.1 Hz), 113.7-113.4 (d, *J* = 46.2 Hz), 55.3, 55.2. IR (neat) 3051, 3004, 2958, 2934, 2907, 2838, 2555, 2421, 2352, 2288, 2052, 1864, 1606, 1576, 1509, 1497, 1463, 1442, 1416, 1330, 1303, 1251, 1196, 1173, 1114, 1091, 1034, 983, 922, 832, 809, 795, 763, 740, 687cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{18}FNO_3$ (M^+): 351.1271, found: 351.1270.



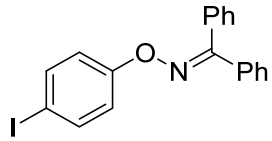
bis(4-(trifluoromethyl)phenyl)methanone *O*-(4-fluorophenyl) oxime (1dd). Colorless solid. R_f = 0.6 [hexane/EtOAc = 10:1 (v/v)]. Yield: 15.2% (3 steps, 0.0461 mmol, 19.7 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79-7.78 (d, *J* = 8.3 Hz, 2H), 7.70-7.65 (m, 4H), 7.56-7.54 (d, *J* = 7.9 Hz, 2H), 7.20-7.16 (m, 2H), 7.05-7.01 (m, 2H), 3.89 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.4, 157.8, 157.4, 155.1, 138.3, 135.6, 132.4-131.3 (multiplet), 129.6, 128.5, 125.51, 125.49, 124.7, 122.88-122.86 (d, *J* = 2.9 Hz), 116.2-116.1 (d, *J* = 8.7 Hz), 115.9-115.7 (d, J = 23.1). IR (neat) 3905, 3823, 2926, 2359, 1616, 1498, 1408, 1323, 1195, 1166, 1128, 1112, 1092, 1068, 1018, 990, 957, 941, 849, 833, 782, 761, 666cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{12}F_7NO$ (M^+): 427.0807, found: 427.0807.



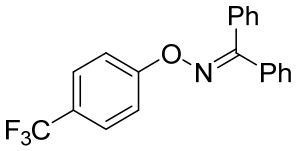
diphenylmethanone *O*-(4-chlorophenyl) oxime (1ea). Yellow oil. R_f = 0.6 [hexane/EtOAc = 10:1 (v/v)]. Yield: 34.9% (2 steps, 0.643 mmol, 0.198 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.7-7.58 (d, *J* = 7.2 Hz, 2H), 7.48-7.37 (m, 8H), 7.26-7.25 (m, 2H), 7.19-7.17 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.3, 158.1, 135.7, 132.6, 130.1, 129.3, 129.3, 129.1, 128.5, 128.4, 128.2, 127.0, 116.1, 123.8, 120.3, 115.3. IR (neat) 3060, 1880, 1745, 1676, 1590, 1482, 1444, 1404, 1329, 1307, 1280, 1217, 1157, 1095, 1033, 1008, 983, 930, 824, 774, 741, 695, 637, 619 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ (M^+): 307.0764, found: 307.0764.



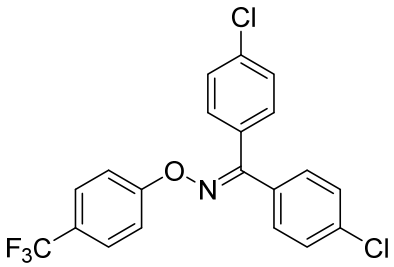
diphenylmethanone *O*-(4-bromophenyl) oxime (1fa). Colorless solid. Melting point: 78.6 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 30.1% (3 steps, 0.855 mmol, 0.301 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60-7.58 (m, 2H), 7.49-7.39 (m, 10H), 7.15-7.13 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 135.7, 132.7, 132.1, 130.3, 129.5, 129.4, 128.6, 128.5, 128.3, 116.6, 114.5. IR (neat) 2367, 2352, 1584, 1480, 1444, 1329, 1221, 1159, 1068, 984, 930, 822, 774, 696, 634, 614 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}BrNO$ (M^+): 351.0259, found: 351.0258.



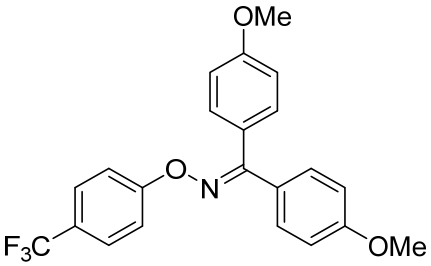
diphenylmethanone *O*-(4-iodophenyl) oxime (1ga). Brown oil. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 21.6% (3 steps, 0.4298 mmol, 0.172 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.61 (m, 4H), 7.51-7.49 (m, 3H), 7.48-7.43 (m, 3H), 7.42-7.40 (m, 2H), 7.07-7.05 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.4, 159.4, 138.0, 135.6, 132.6, 130.1, 129.3, 129.2, 128.4, 128.3, 128.1, 117.0, 84.6. IR (neat) 3059, 3027, 2924, 2853, 2359, 2342, 1579, 1477, 1444, 1396, 1328, 1295, 1278, 1219, 1162, 1093, 1076, 1056, 1032, 1002, 984, 930, 819, 774, 738, 695, 670 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}INO$ (M^+): 399.0120, found: 399.0119.



diphenylmethanone *O*-(4-(trifluoromethyl)phenyl) oxime (1ha). Colorless solid. Melting point: 68.0 °C. R_f = 0.7 [hexane/EtOAc = 10:1 (v/v)]. Yield: 15.8% (3 steps, 0.396 mmol, 0.135 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.60 (m, 2H), 7.57-7.56 (d, J = 8.6, 2H), 7.50-7.39 (m, 8H), 7.33-7.32 (d, *J* = 8.6 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161,8, 160.1, 135.4, 132.5, 130.4, 129.5, 129.2, 128.6, 128.4, 128.2, 126.7, 126.7, 123.8, 120.3, 115.3, 114.6. IR (neat) 3854, 3678, 3060, 1613, 1510, 1446, 1420, 1326, 1231, 1166, 1120, 1105, 1066, 1011, 984, 929, 839, 777, 696, 665, 617 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{14}F_3NO$ (M^+): 341.1028, found: 341.1026.

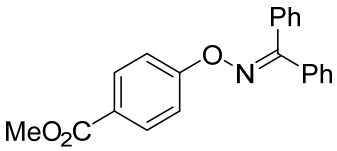


bis(4-chlorophenyl)methanone *O*-(4-(trifluoromethyl)phenyl) oxime (1hb). Colorless solid. Melting point: 128.7 °C. R_f = 0.8 [hexane/EtOAc = 10:1 (v/v)]. Yield: 28.8% (3 steps, 1.99 mmol, 0.817 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59-7.57 (d, *J* = 8.8 Hz, 2H), 7.54-7.52 (d, *J* = 8.6 Hz, 2H), 7.49-7.48 (d, *J* = 8.6 Hz, 2H), 7.39-7.35 (dd, *J* = 16.8, 8.6 Hz, 4H), 7.31-7.30 (d, *J* = 8.6 Hz, 2H), 7.16-7.14 (m, 2H), 7.10 (brs, 1H), 7.00-6.99 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.5, 159.0, 136.8, 135.8, 133.5, 130.7, 130.3, 129.7, 128.8, 128.7, 127.0, 126.77, 126.75, 114.6. IR (neat) 2369, 1905, 1611, 1596, 1510, 1491, 1420, 1324, 1228, 1164, 1122, 1105, 1092, 1066, 1014, 984, 929, 834, 730, 658, 620 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{12}Cl_2F_3NO$ (M^+): 409.0248, found: 409.0247.

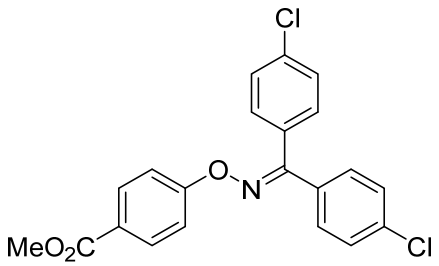


bis(4-methoxyphenyl)methanone *O*-(4-(trifluoromethyl)phenyl) oxime (1hc). Colorless solid. Melting point: 112.0 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 8.6% (3steps, 0.595 mmol, 0.239 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57-7.54 (m, 4H), 7.41-7.39 (m, 2H), 7.33-7.32 (d, *J* = 8.6 Hz, 2H), 7.00-6.98 (m, 2H), 6.93-6.91 (m, 2H), 3.89 (s, 3H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.0, 161.3, 160.6, 160.4, 131.3, 128.3,

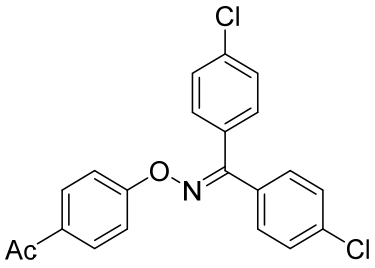
126.64, 126.61, 124.8, 114.5, 114.3, 113.8, 113.4, 55.4, 55.3. IR (neat) 3901, 3886, 3855, 3830, 3814, 3772, 3743, 3728, 3704, 3685, 3667, 3626, 3589, 3569, 3006, 2902, 2839, 2359, 2349, 2308, 1734, 1653, 1610, 1510, 1464, 1442, 1418, 1326, 1306, 1253, 1234, 1167, 1119, 1065, 1034, 983, 914, 837, 772 cm^{-1}. HRMS (FD) calcd. for $C_{22}H_{18}F_3NO_3$ (M^+): 401.1239, found: 401.1238.



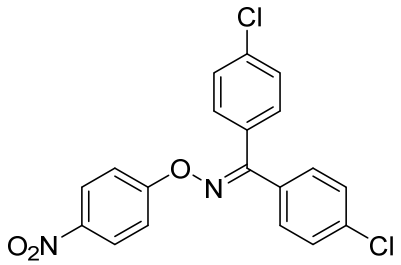
methyl 4-(((diphenylmethylene)amino)oxy)benzoate (1ia). Colorless solid. Melting point: 108.6 °C. R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. Yield: 14.3% (3 steps, 0.354 mmol, 0.117 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02-7.99 (m, 2H), 7.61-7.59 (m, 2H), 7.48-7.38 (m, 8H), 7.29-7.26 (m, 2H), 3.89 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.0, 163.2, 161.2, 135.6, 132.6, 131.5, 130.4, 129.6, 129.4, 128.7, 128.5, 128.3, 124.0, 114.3, 52.0. IR (neat) 1717, 1603, 1504, 1435, 1416, 1330, 1277, 1226, 1191, 1157, 1112, 1100, 1032, 984, 928, 853, 768, 739, 694, 676, 617 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{17}NO_3$ (M^+): 331.1208, found: 331.1208.



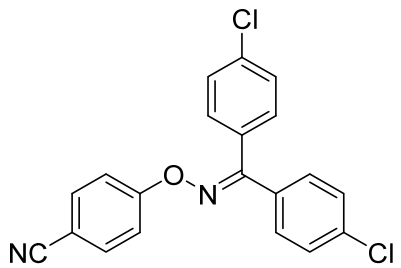
methyl 4-(((bis(4-chlorophenyl)methylene)amino)oxy)benzoate (1ib). Colorless solid. Melting point: 141.9 °C. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 14.6% (3 steps, 0.329 mmol, 0.132 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02-8.00 (m, 2H), 7.53-7.51 (m, 2H), 7.48-7.46 (m, 2H), 7.38-7.33 (m, 4H), 7.26-7.23 (m, 2H), 3.89 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.8, 162.8, 159.1, 136.9, 135.9, 133.6, 131.5, 130.8, 130.5, 129.8, 128.9, 128.8, 124.4, 114.2, 52.1. IR (neat) 2433, 2368, 1717, 1601, 1502, 1491, 1435, 1416, 1399, 1325, 1279, 1231, 1192, 1156, 1111, 1092, 1014, 985, 928, 835, 732, 695, 678, 655, 620, 607 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_3$ (M^+): 399.0429, found: 399.0428.



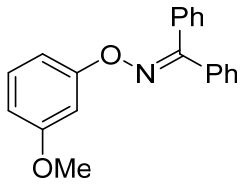
1-(4-(((bis(4-chlorophenyl)methylene)amino)oxy)phenyl)ethan-1-one (1jb). Colorless solid. Melting point: 132.0 °C. R_f = 0.1 [hexane/EtOAc = 10:1 (v/v)]. Yield: 39.4% (2 steps, 0.494 mmol, 0.151 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.54-7.52 (m, 2H), 7.49-7.48 (m, 2H), 7.39-7.35 (m, 4H), 7.28-7.27 (m, 2H), 2.58 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.8, 162.8, 159.1, 138.0, 136.8, 135.8, 133.5, 133.8, 130.7, 130.4, 130.3, 129.7, 128.8, 128.7, 114.2, 26.5. IR (neat) 2885, 2373, 2351, 2331, 1679, 1596, 1499, 1414, 1399, 1358, 1325, 1298, 1269, 1229, 1159, 1092, 1016, 984, 928, 834, 757, 726, 697, 680, 666 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_2$ (M^+): 383.0480, found: 383.0479.



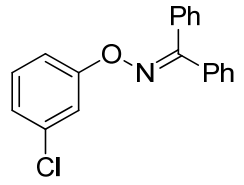
bis(4-chlorophenyl)methanone *O*-(4-nitrophenyl) oxime (1kb). Colorless solid. Melting point: 118.6 °C. R_f = 0.8 [hexane/EtOAc = 3:1 (v/v)]. Yield: 19.7% (2 steps, 0.198 mmol, 76.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97-7.95 (m, 2H), 7.54-7.52 (m, 2H), 7.49-7.48 (m, 2H), 7.39-7.35 (m, 4H), 7.28-7.27 (m, 2H), 2.58 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.7, 160.1, 142.7, 137.2, 136.1, 133.1, 130.6, 130.0, 129.8, 128.9, 128.8, 125.7, 114.5. IR (neat) 1589, 1516, 1487, 1399, 1342, 1234, 1158, 1111, 1092, 1016, 984, 924, 863, 835, 751, 732, 687 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2N_2O_3$ (M^+): 386.0225, found: 386.0225.



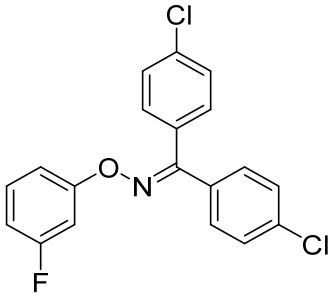
4-(((bis(4-chlorophenyl)methylene)amino)oxy)benzonitrile (1lb). Colorless solid. Melting point: 152.0 °C. R_f = 0.6 [hexane/EtOAc = 5:1 (v/v)]. Yield: 42.6% (2 steps, 0.426 mmol, 0.157 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.61 (m, 2H), 7.52-7.48 (m, 4H), 7.39-7.38 (m, 2H), 7.35-7.33 (m, 2H), 7.31-7.29 (m, 2H), 2.58 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 159.6, 137.0, 136.0, 133.9, 133.2, 130.6, 130.1, 129.7, 128.9, 128.8, 119.0, 115.2, 105.7. IR (neat) 3898, 3887, 3868, 3854, 3830, 3814, 3792, 3772, 3743, 3727, 3704, 3667, 3627, 3589, 3060, 2878, 2359, 2348, 2225, 1905, 1734, 1654, 1601, 1578, 1499, 1399, 1325, 1299, 1232, 1162, 1092, 1016, 984, 924, 835, 773, 730 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{12}Cl_2N2O$ (M^+): 366.0327, found: 366.0325.



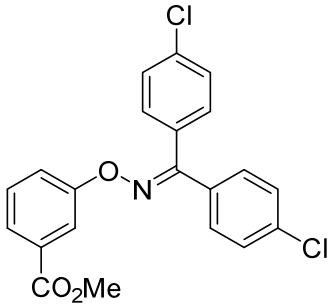
diphenylmethanone *O*-(3-methoxyphenyl) oxime (1ma). Colorless oil. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 16.6% (3 steps, 0.603 mmol, 0.183 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.61 (m, 2H), 7.50-7.48 (m, 3H), 7.45-7.43 (m, 3H), 7.40-7.38 (m, 2H), 7.23-7.21 (m, 1H), 6.86-6.84 (m, 2H), 6.61-6.59 (m, 1H), 3.81 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.7, 160.6, 159.9, 135.9, 132.8, 130.0, 129.7, 129.3, 129.2, 128.5, 128.3, 128.1, 128.4, 108.0, 107.14, 100.71, 55.3. IR (neat) 3060, 3022, 3001, 2943, 2905, 2835, 2367, 2339, 1591, 1490, 1444, 1328, 1281, 1264, 1194, 1168, 1137, 1076, 1042, 997, 984, 957, 921, 896, 837, 772, 696, 656 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO_2$ (M^+): 303.1259, found: 303.1259.



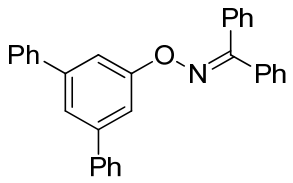
diphenylmethanone *O*-(3-chlorophenyl) oxime (1na). Colorless oil. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 15.3% (3 steps, 0.563 mmol, 0.173 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62-7.61 (m, 2H), 7.50-7.39 (m, 8H), 7.333-7.330 (m, 1H), 7.24-7.21 (t, *J* = 8.3 Hz, 1H), 7.110-7.096 (m, 1H), 7.02-7.00 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.6, 160.1, 135.5, 134.7, 132.6, 130.2, 130.0, 129.4, 129.2, 128.5, 128.4, 122.3, 115.2, 113.0. IR (neat) 3593, 3575, 3504, 3458, 3399, 3062, 2362, 1773, 1589, 1470, 1444, 1431, 1328, 1303, 1266, 1213, 1088, 1066, 984, 940, 873, 781, 778, 696, 680 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ (M^+): 307.0764, found: 307.0763.



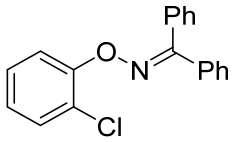
bis(4-chlorophenyl)methanone *O*-(3-fluorophenyl) oxime (1ob). Colorless oil. R_f = 0.6 [hexane/EtOAc = 10:1 (v/v)]. Yield: 6.7% (3 steps, 0.138 mmol, 49.7 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53-7.51 (m, 2H), 7.48-7.46 (m, 2H), 7.39-7.34 (m, 4H), 7.27-7.23 (m, 1H), 7.05-7.02 (dt, *J* = 10.7, 2.4 Hz 1H), 6.95-6.93 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.76-6.73 (td, *J* = 8.4, 2.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 164.2, 162.6, 160.4-160.3 (d, *J* = 11.6 Hz), 158.4, 136.6, 135.7, 133.6, 130.7, 130.4, 130.1-130.3 (d, *J* = 10.1 Hz), 129.6, 128.8-128.7 (d, J = 17.3 Hz), 110.3, 109.3-109.2 (d, *J* = 21.7 Hz), 102.6-102.4 (d, *J* = 27.5 Hz). IR (neat) 3072, 3033, 2985, 2883, 2409, 2370, 2339, 1913, 1786, 1700, 1666, 1606, 1596, 1560, 1530, 1485, 1453, 1400, 1324, 1297, 1257, 1220, 1159, 1119, 1092, 1071, 1016, 1004, 965, 910, 834, 772, 730 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2FNO$ (M^+): 359.0280, found: 359.0280.



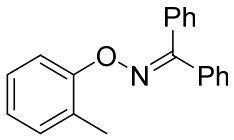
methyl 3-(((bis(4-chlorophenyl)methylene)amino)oxy)benzoate (1pb). Colorless solid. Melting point: 98.6 °C. R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. Yield: 2.9% (2 steps, 0.0834 mmol, 33.4 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86-7.85 (m, 1H), 7.73-7.72 (m, 1H), 7.54-7.53 (m, 2H), 7.49-7.47 (m, 2H), 7.43-7.42 (m, 1H), 7.40-7.36 (m, 5H), 3.92 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.6, 166.6, 150.4, 140.2, 138.2, 137.1, 136.1, 133.3, 130.9, 130.5, 129.1, 128.7, 128.1, 121.4, 119.7, 115.9, 52.1. IR (neat) 3069, 2951, 2386, 1724, 1591, 1489, 1445, 1399, 1295, 1272, 1207, 1092, 1017, 1001, 983, 935, 835, 756 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_3$ (M^+): 399.0429, found: 399.0429.



diphenylmethanone *O*-([1,1':3',1''-terphenyl]-5'-yl) oxime (1qa). Colorless solid. Melting point: 171.9 °C. R_f = 0.4 [hexane/EtOAc = 10:1 (v/v)]. Yield: 49.2% (3 steps, 0.492 mmol, 0.210 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.68-7.66 (m, 4H), 7.53-7.44 (m, 13H), 7.42-7.36 (m, 4H), 7.49-7.47 (m, 2H), 7.43-7.42 (m, 1H), 7.40-7.36 (m, 5H), 3.92 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.24, 160.21, 142.9, 141.0, 135.8, 132.9, 130.1, 129.33, 129.27, 128.7, 128.5, 128.3, 128.2, 127.5, 127.3, 120.2, 112.6. IR (neat) 3544, 3463, 3409, 3370, 3344, 3334, 3310, 3295, 3266, 3255, 3244, 3221, 3060, 2354, 1734, 1589, 1575, 1498, 1444, 1409, 1343, 1173, 986, 949, 866, 761, 743, 698 cm^{-1}. HRMS (FD) calcd. for $C_{31}H_{23}NO$ (M^+): 425.1780, found: 425.1779.



diphenylmethanone *O*-(2-chlorophenyl) oxime (1ra). Colorless oil. R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. Yield: 4.2% (3 steps, 0.159 mmol, 48.8 mg). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.68-7.67 (d, *J* = 8.3 Hz, 1H), 7.63-7.61 (m, 2H), 7.56-7.55 (m, 2H), 7.49-7.44 (m, 4H), 7.41-7.39 (m, 2H), 7.33-7.32 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.28-7.25 (m, 1H), 6.98-6.95 (td, *J* = 7.6, 1.4 Hz, 1 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.0, 155.1, 135.7, 132.3, 130.2, 129.9, 129.8, 129.5, 128.7, 128.4, 128.3, 128.0, 127.6, 122.9, 120.9, 116.3. IR (neat) 3063, 3032, 2938, 2358, 2336, 2307, 1748, 1659, 1583, 1492, 1473, 1447, 1329, 1304, 1264, 1228, 1157, 1127, 1060, 1034, 982, 930, 795, 778, 752, 695 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ (M^+): 307.0764, found: 307.0763.



diphenylmethanone *O*-(*o*-tolyl) oxime (1sa). Brown oil. R_f = 0.8 [hexane/EtOAc = 10:1 (v/v)]. Yield: 66.1% (2.01 mmol, 0.58 g). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.74 (m, 2H), 7.73-7.71 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.57-7.46 (m, 8H), 7.33-7.30 (td, *J* = 7.2, 1.4 Hz, 1H), 7.210-7.198 (d, *J* = 7.2 Hz, 1H), 7.05-7.02 (td, *J* = 7.6, 1.0 Hz, 1H), 2.15 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.9, 157.5, 140.1, 135.8, 133.0, 130.5, 129.9, 129.2, 129.1, 128.33,

128.28, 128.0, 126.8, 124.7, 122.1, 121.9, 121.7, 113.9, 15.8. IR (neat) 3059, 3026, 2978, 2947, 2917, 2858, 2736, 2602, 2446, 2405, 2359, 2058, 1954, 1893, 1814, 1766, 1590, 1561, 1484, 1462, 1381, 1330, 1308, 1274, 1225, 1183, 1113, 1076, 1042, 935, 839, 797, 765, 752, 695, 665, 655 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO$ (M^+): 287.1310, found: 287.1309.

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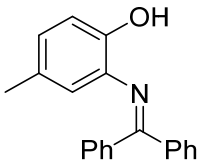
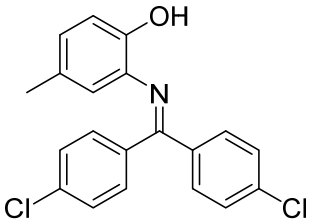
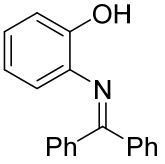


2-((diphenylmethylene)amino)-4-methylphenol (2aa). Yellow solid. Melting point: 168.6 °C. Yield: 82% (0.082 mmol, 23.5 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61-7.75 (m, 2H), 7.50-7.47 (m, 1H), 7.42-7.36 (m, 5H), 7.20-7.19 (m, 2H), 6.84-6.982 (d, *J* = 8.3 Hz, 2H), 6.77-6.75 (m, 1H), 1.93 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.1, 149.4, 139.7, 136.4, 135.3, 130.9, 129.3, 129.1, 128.9, 128.5, 128.3, 128.2, 127.2, 126.3, 120.9, 114.0, 20.6. IR (neat) 3063, 3028, 2919, 2364, 2309, 1747, 1716, 1659, 1648, 1592, 1568, 1502, 1446, 1319, 1279, 1244, 1193, 1109, 1075, 1001, 970, 930, 868, 795, 700, 639 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO$ (M^+): 287.1310, found: 287.1310.

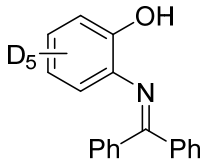


2-((bis(4-chlorophenyl)methylene)amino)-4-methylphenol (2ab). Yellow solid. Melting point: 68.6 °C. Yield: 88% (0.0876 mmol, 31.2 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66-7.64 (m, 2H), 7.39-7.36 (m, 4H), 7.13-7.11 (m, 2H), 6.85-6.83 (d, J = 8.3 Hz, 2H), 6.80-6.78 (dd, *J* = 8.3, 1.4 Hz, 2H), 6.43 (brs, 1H), 5.99-5.98 (d, *J* = 1.4 Hz, 1H), 1.98 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.8, 149.1, 137.9, 137.4, 135.1, 134.2, 130.5, 130.5, 129.0, 128.6, 127.6, 120.6, 114.4, 20.6. IR (neat) 1587, 1562, 1499, 1399, 1307, 1279, 1239, 1219, 1092, 1015, 964, 838, 772 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{15}Cl_2NO$ (M^+): 355.0531, found: 355.0531.

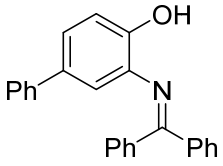


2-((diphenylmethylene)amino)phenol (2ba). Orange solid. Melting point: 153.6 °C. Yield: 69.5% (0.0695 mmol, 19.0 mg, 0.1 mmol scale). R_f = 0.2 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.74 (m, 2H), 7.50-7.47 (m, 1H), 7.42-7.36 (m, 5H), 7.20-

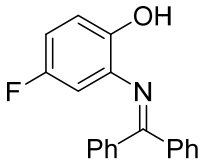
7.18 (m, 2H), 6.96-6.95 (m, 2H), 6.84 (bs, 1H), 6.49-6.46 (m, 1H), 6.12-6.18 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.4, 151.7, 139.7, 136.3, 135.7, 129.4, 129.2, 129.0, 128.8, 128.6, 128.2, 126.7, 120.4, 119.2, 114.4. IR (neat) 3059, 1593, 1580, 1567, 1484, 1446, 1321, 1285, 1255, 1232, 1188, 1035, 967, 795, 772, 741, 698 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{15}NO$ (M^+): 273.1154, found: 273.1152.



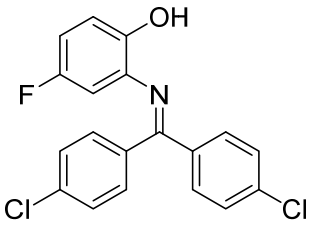
2-((diphenylmethylene)amino)phen-3,4,5,6-*d*$_4$-ol (2ba-*d5*). Yellow solid. Melting point: 155.4 °C. Yield: 71.0% (0.0710 mmol, 19.7 mg, 0.1 mmol scale). R_f = 0.2 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (m, 2H), 7.51-7.48 (m, 1H), 7.43-7.37 (m, 5H), 7.21-7.20 (m, 2H), 6.84 (brs, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.3, 151.7, 139.7, 136.3, 135.6, 131.0, 129.4, 129.2, 129.0, 128.6, 128.2, 126.4-126.1 (t, *J* = 23.1 Hz), 120.1-119.8 (t, *J* = 24.6 Hz), 118.8-118.5 (t, *J* = 24.6, 24.6 Hz), 114.2-113.9 (t, *J* = 24.6, 24.6 Hz). IR (neat) 3980, 3943, 3923, 3864, 3852, 3842, 3825, 3780, 3751, 3734, 3715, 3690, 3671, 3649, 3597, 3547, 3501, 2929, 2368, 2345, 2334, 1748, 1261, 1029, 793, 697 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{10}D_5NO$ (M^+): 277.1405, found: 277.1404.



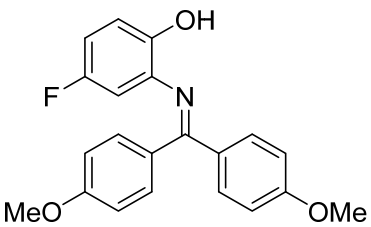
3-((diphenylmethylene)amino)-[1,1'-biphenyl]-4-ol (2ca). Yellow solid. Melting point: 152.0 °C. Yield: 70% (0.0695 mmol, 24.3 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.81-7.80 (m, 2H), 7.52-7.42 (m, 6H), 7.27-7.24 (m, 4H), 7.22-7.18 (m, 2H), 7.04-7.01 (m, 3H), 6.92 (brs, 1H), 6.46-6.45 (d, *J* = 2.1 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.7, 151.4, 140.8, 139.5, 136.5, 135.6, 132.2, 131.2, 129.4, 129.3, 129.0, 128.8, 128.4, 128.3, 126.5, 126.3, 125.5, 119,5, 114.7. IR (neat) 2364, 2349, 2307, 1594, 1508, 1482, 1446, 1268, 931, 761, 699, 633 cm^{-1}. HRMS (FD) calcd. for $C_{25}H_{19}NO$ (M^+): 349.1467, found: 349.1466.



2-((diphenylmethylene)amino)-4-fluorophenol (2da). Yellow solid. Melting point: 155.4 °C. Yield: 57.7% (0.0288 mmol, 8.4 mg, 0.05 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (m, 2H), 7.52-7.50 (m, 1H), 7.46-7.39 (m, 5H), 7.19-7.18 (m, 2H), 6.88-6.85 (dd, *J* = 8.8, 5.2 Hz, 1H), 6.69-6.65 (td, *J* = 8.8, 3.0 Hz, 1H), 6.49 (brs, 1H), 5.92-5.90 (dd, *J* = 10.0, 3.0 Hz, 1H), 1.98 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.8, 156.5, 155.0, 147.7, 139.3, 136.0, 135.6, 131.4, 129.7, 129.5, 128.81, 128.77, 128.3, 114.5, 114.5, 112.9, 112.7, 107.4, 107.2. IR (neat) 3060, 2988, 2368, 2358, 2308, 1592, 1571, 1496, 1446, 1320, 1257, 1230, 1168, 1130, 1028, 978, 855, 795, 700 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}FNO$ (M^+): 291.1059, found: 291.1058.

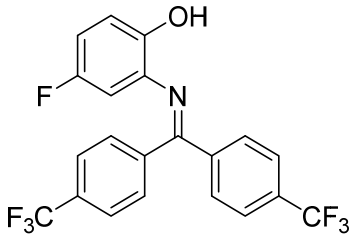


2-((bis(4-chlorophenyl)methylene)amino)-4-fluorophenol (2db). Yellow oil. Yield: 66.2% (0.389 mmol, 14.0 mg, 0.583 mmol scale). R_f = 0.5 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66-7.64 (m, 2H), 7.41-7.39 (m, 4H), 7.13-7.12 (m, 2H), 6.89-6.86 (dd, *J* = 8.9, 5.5 Hz, 1H), 6.72-6.69 (td, *J* = 8.3, 3.1 Hz, 1H), 6.28 (s, 1H), 5.93-5.91 (dd, *J* = 9.6, 3.1 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.4, 156.5, 155.0, 147.5, 138.0, 137.4, 136.1, 133.4, 130.7, 130.3, 129.3, 128.7, 115.03-114.96 (d, *J* = 10.1 Hz), 113.4-113.3 (d, *J* = 23.1 Hz), 107.1-107.0 (d, *J* = 24.6 Hz). IR (neat) 3409, 3071, 2763, 2288, 1913, 1789, 1604, 1586, 1563, 1490, 1432, 1399, 1346, 1308, 1290, 1256, 1227, 1167, 1130, 1091, 952, 936, 838, 813, 799, 773, 739, 703, 671cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2FNO$ (M^+): 359.0280, found: 359.0280.

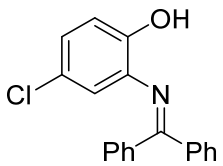


2-((bis(4-methoxyphenyl)methylene)amino)-4-fluorophenol (2dc). Yellow oil. Yield:

42.5% (0.0425 mmol, 15.3 mg, 0.1 mmol scale). R_f = 0.5 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72-7.70 (m, 2H), 7.11-7.10 (m, 2H), 6.93-6.91 (m, 2H), 6.89-6.88 (m, 2H), 6.86-6.84 (dd, J = 8.9, 5.2, 1H), 6.66-6.62 (td, *J* = 8.6, 3.1 Hz, 1H), 5.96-5.93 (dd, *J* = 10.0, 3.1 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.3, 162.3, 160.5, 156.6, 155.0, 147.5, 136.8-136.7 (d, *J* = 8.7 Hz), 132.3, 131.5, 130.8, 127.6, 114.33-114.28 (d, *J* = 8.7 Hz), 114.0, 113.6, 112.1-111.9 (d, *J* = 24.6 Hz), 107.3-107.1 (d, *J* = 24.6 Hz), 55.5, 55.3. IR (neat) 3073, 3005, 2959, 2934, 2905, 2839, 2905, 2839, 2374, 2336, 1605, 1587, 1567, 1509, 1491, 1463, 1442, 1418, 1319, 1306, 1254, 1173, 1130, 1116, 1088, 1032, 977, 949, 840, 794, 683 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{18}FNO_3$ (M^+): 351.1271, found: 351.1270.

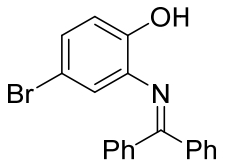


2-((bis(4-(trifluoromethyl)phenyl)methylene)amino)-4-fluorophenol (2dd). Yellow oil. Yield: 39.7% (0.0288 mmol, 12.3 mg, 0.1 mmol scale). R_f = 0.4 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82-7.81 (d, *J* = 7.9 Hz, 2H), 7.22-7.69 (m, 4H), 7.35-7.34 (d, *J* = 7.9 Hz, 2H), 6.91-6.89 (dd, *J* = 8.9, 5.2, 1H), 6.76-6.73 (td, *J* = 8.3, 3.1, 1H), 6.25 (s, 1H), 5.90-5.88 (dd, *J* = 9.5, 3.1, 1H), 3.87 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.6, 156.5, 154.9, 147.6, 141.8, 138.6, 135.03-134.98 (d, *J* = 8.7 Hz), 133.3-133.1 (d, *J* = 33.2 Hz), 132.2-131.9 (d, *J* = 31.8 Hz), 130.2, 129.6, 129.3, 126.12-126.10 (d, *J* = 2.9), 125.49-125.47 (d, *J* = 2.9 Hz), 115.43-115.38 (d, *J* = 8.7 Hz), 114.2-114.1 (d, *J* = 23.1 Hz), 107.1-106.9 (d, *J* = 26.0 Hz). IR (neat) 3518, 3479, 3448, 3420, 3397, 3385, 3363, 3294, 3145, 3084, 2934, 2362, 2339, 1619, 1576, 1493, 1434, 1410, 1326, 1275, 1258, 1227, 1169, 1131, 1112, 1090, 1067, 1018, 976, 942, 852, 801, 761, 739, 687, 671, 656cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{12}F_7NO$ (M^+): 427.0807, found: 427.0806.

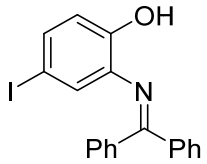


4-chloro-2-((diphenylmethylene)amino)phenol (2ea). Yellow solid. Melting point: 171.9 °C. Yield: 59% (0.059 mmol, 18.2 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc =

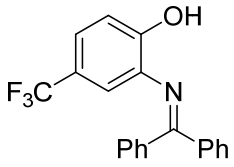
10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (m, 2H), 7.52-7.40 (m, 7H), 7.19-7.17 (m, 2H), 6.92-6.90 (dd, *J* = 8.6, 2.4, 1H), 6.87-6.86 (d, *J* = 8.6 Hz, 1H), 6.62 (brs, 1H), 6.14-6.14 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.0, 150.1, 139.3, 136.526, 136.531, 131.4, 129.7, 129.5, 129.3, 128.8, 128.7, 128.3, 126.2, 123.8, 120.3, 115.3. IR (neat) 3052, 1701, 1593, 1571, 1484, 1445, 1321, 1279, 1234, 1150, 1110, 1085, 970, 895, 795, 702 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ (M^+): 307.0764, found: 307.0763.



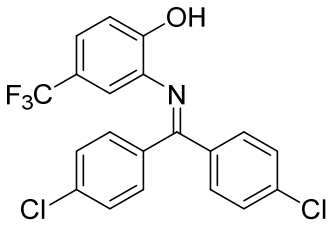
4-bromo-2-((diphenylmethylene)amino)phenol (2fa). Yellow solid. Melting point: 185.2 °C. Yield: 72% (0.0715 mmol, 25.2 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (m, 2H), 7.53-7.50 (m, 1H), 7.47-7.40 (m, 5H), 7.18-7.17 (d, *J* = 6.9, 2H), 7.06-7.04 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.83-6.82 (d, *J* = 8.6 Hz, 1H), 6.71 (brs, 1H), 6.273-6.270 (d, *J* = 2.1 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.1, 150.7, 139.3, 137.0, 135.6, 131.6, 129.8, 129.7, 129.2, 128.9, 128.8, 128.4, 123.3, 116.0, 111.1. IR (neat) 2366, 2354, 1592, 1569, 1481, 1445, 1320, 1228, 1234, 1178, 1028, 970, 879, 776, 702, 634, 623, 607 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}BrNO$ (M^+): 351.0259, found: 351.0258.



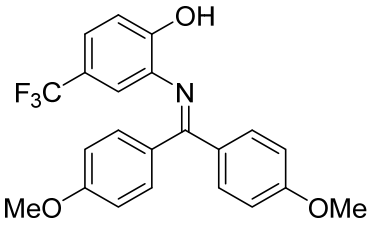
2-((diphenylmethylene)amino)-4-iodophenol (2ga). Yellow solid. Yield: 66% (0.06613 mmol, 26.4 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75-7.74 (m, 2H), 7.52-7.50 (m, 1H), 7.47-7.45 (m, 1H), 7.44-7.41 (m, 4H), 7.23-7.21 (m, 1H), 7.17-7.16 (m, 2H), 6.77 (brs, 1H), 6.72-6.71 (d, *J* = 8.6 Hz, 1H), 6.44-6.43 (d, *J* = 2.1 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.9, 151.4, 139.3, 139.2, 137.3, 135.5, 135.1, 131.4, 129.7, 129.5, 129.2, 128.8, 128.7, 128.3, 116.5, 80.6. IR (neat) 3916, 3872, 3840, 3726, 3706, 3625, 3597, 3567, 3060, 2363, 2348, 1591, 1567, 1478, 1445, 1398, 1321, 1299, 1273, 1253, 1234, 1177, 1150, 1112, 1075, 1002, 969, 917, 875, 774, 701 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}INO$ (M^+): 399.0120, found: 399.0119.



diphenylmethanone *O*-(4-(trifluoromethyl)phenyl) oxime (2ha). Yellow solid. Melting point: 177.5 °C. Yield: 52% (0.0516 mmol, 17.6 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75-7.76 (m, 2H), 7.53-7.51 (m, 1H), 7.44-7.42 (m, 3H), 7.40-7.37 (m, 2H), 7.21-7.19 (m, 1H), 7.16-7.14 (m, 2H), 7.10 (brs, 1H), 7.00-6.99 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.8, 154,3, 139.2, 135.8, 135.5, 131.7, 129.8, 129.7, 128.9, 128.8, 128.5, 123.7, 123.6, 118.0, 118.0, 114.6. IR (neat) 3067, 1658, 1591, 1568, 1509, 1446, 1424, 1325, 1284, 1232, 1163, 1113, 1072, 973, 908, 889, 780, 719, 703, 637 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{14}F_3NO$ (M^+): 341.1028, found: 341.1027.

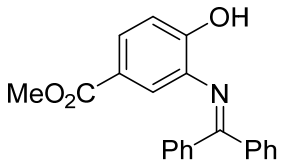


2-((bis(4-chlorophenyl)methylene)amino)-4-(trifluoromethyl)phenol (2hb). Yellow solid. Melting point: 108.7 °C. Yield: 58% (0.0576 mmol, 23.6 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69-7.67 (m, 2H), 7.42-7.38 (m, 4H), 7.25-7.24 (m, 1H), 7.10-7.08 (m, 2H), 7.02-7.01 (d, *J* = 8.6 Hz, 1H), 6.88 (brs, 1H), 6.41 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.9, 138.2, 137.2, 136.2, 135.4, 133.2, 130.7, 130.2, 129.3, 128.8, 124.0, 123.9, 121.9, 117.7, 117.6, 114.9. IR (neat) 1588, 1561, 1490, 1400, 1328, 1287, 1236, 1164, 1121, 1093, 1071, 1015, 969, 833, 666 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{12}Cl_2F_3NO$ (M^+): 409.0248, found: 409.0247.

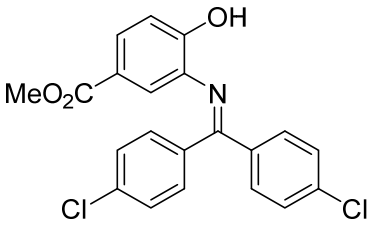


2-((bis(4-methoxyphenyl)methylene)amino)-4-(trifluoromethyl)phenol (2hc). Colorless oil. Yield: 38% (0.0378 mmol, 15.2 mg, 0.1 mmol scale). R_f = 0.5 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90-7.89 (brs, 1H), 7.44-7.43 (brs, 2H), 7.12-

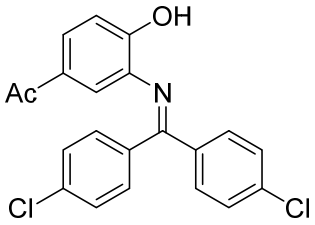
7.11 (brs, 1H), 6.93-6.90 (m, 3H), 6.77-6.76 (d, *J* = 8.3, 3H),3.84 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.2, 157.7, 156.9, 150.6, 138.3, 131.5, 130.7, 127.1, 124.9, 124.7, 124.2, 122.5, 121.9, 116.6, 114.0, 113.9, 55.4, 55.3. IR (neat) 3006, 2959, 2908, 2838, 1654, 1608, 1577, 1513, 1465, 1442, 1419, 1327, 1248, 1223, 1168, 1122, 1108, 1067, 1037, 1004, 912, 837, 806, 766 cm^{-1}. HRMS (FD) calcd. for $C_{22}H_{18}F_3NO_3$ (M^+): 401.1238, found: 401.1239.



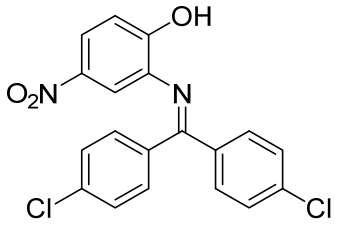
methyl 3-((diphenylmethylene)amino)-4-hydroxybenzoate (2ia). Colorless solid. Melting point: 80.6 °C. Yield: 47% (0.0471 mmol, 15.6 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (m, 2H), 7.68-7.65 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.50-7.48 (m, 1H), 7.43-7.38 (m, 5H), 7.18-7.16 (m, 2H), 6.96-6.94 (d, *J* = 8.7 Hz, 1H), 6.90-6.89 (d, *J* = 1.8 Hz, 1H), 3.69 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.2, 166.6, 155.7, 139.3, 135.7, 135.5, 131.4, 129.5, 129.5, 128.73, 128.71, 128.5, 128.3, 122.2, 121.3, 114.2, 51.7. IR (neat) 2251, 1712, 1652, 1598, 1537, 1499, 1437, 1282, 1218, 1184, 1114, 1093, 1030, 993, 960, 909, 835, 785, 767, 732, 695, 648, 610 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{17}NO_3$ (M^+): 331.1208, found: 331.1208.



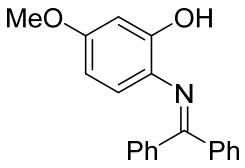
methyl 3-((bis(4-chlorophenyl)methylene)amino)-4-hydroxybenzoate (2ib). Yellow solid. Melting point: 71.9 °C. Yield: 65% (0.650 mmol, 26.0 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71-7.69 (dd, *J* = 8.6, 2.1, 1H), 7.67-7.65 (m, 2H), 7.41-7.37 (m, 4H), 7.11-7.09 (m, 2H), 6.97-6.96 (d, *J* = 8.6 Hz, 1H), 6.891-6.888 (d, *J* = 1.7 Hz, 1H), 3.74 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.0, 166.4, 155.3, 138.0, 137.4, 135.9, 135.2, 135.6, 130.7, 130.2, 129.2, 128.9, 128.7, 121.9, 121.6, 114.6, 51.8. IR (neat) 1714, 1587, 1564, 1489, 1437, 1399, 1289, 1216, 1181, 1092, 1015, 993, 961, 944, 903, 838, 796, 758, 741, 707, 672, 623 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_3$ (M^+): 399.0429, found: 399.0428.



1-(3-((bis(4-chlorophenyl)methylene)amino)-4-hydroxyphenyl)ethan-1-one (2ib). Yellow solid. Melting point: 65.3 °C. Yield: 49% (0.495 mmol, 19 mg, 0.1 mmol scale). R_f = 0.4 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67-7.64 (m, 3H), 7.41-7.38 (t, *J* = 8.9 Hz, 4H), 7.26 (brs, 1H), 7.12-7.10 (m, 2H), 6.99-6.98 (d, *J* = 8.6 Hz, 1H), 6.82-6.81 (d, *J* = 2.1 Hz, 1H), 2.21 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.4, 168.0, 155.7, 138.1, 137.3, 136.0, 135.1, 133.7, 130.7, 130.2, 129.3, 129.1, 128.7, 127.9, 121.2, 114.8, 26.0. IR (neat) 1671, 1588, 1488, 1422, 1399, 1358, 1287, 1275, 1215, 1180, 1091, 1015, 961, 927, 837, 758, 671 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_2$ (M^+): 383.0480, found: 383.0479.

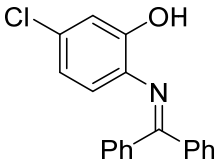


2-((bis(4-chlorophenyl)methylene)amino)-4-nitrophenol (2kb). Orange solid. Melting point: 68.7 °C. Yield: 44% (0.0439 mmol, 17.0 mg, 0.1 mmol scale). R_f = 0.2 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96-7.93 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.69-7.67 (m, 2H), 7.44-7.40 (m, 4H), 7.13-7.11 (m, 3H), 7.04-7.01 (d, *J* = 9.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.0, 156.8, 140.5, 138.7, 136.9, 136.6, 135.4, 132.7, 130.9, 130.1, 129.6, 128.9, 123.0, 116.0, 114.7. IR (neat) 3383, 3089, 1586, 1518, 1489, 1433, 1400, 1335, 1288, 1232, 1184, 1144, 1092, 1014, 966, 928, 836, 758 cm^{-1}. HRMS (FD) calcd. for (M^+): 386.0225, found: 386.0225.

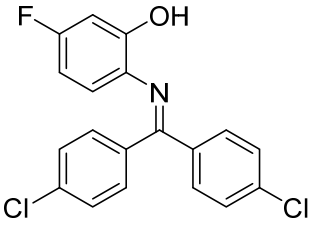


2-((diphenylmethylene)amino)-5-methoxyphenol (2ma). Yellow oil. Yield: 63% (0.0630 mmol, 19.1 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72-7.71 (m, 2H), 7.47-7.42 (m, 4H), 7.41-7.38 (m, 2H), 7.24-7.23 (m,

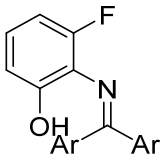
2H), 3.73 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.2, 154.2, 140.1, 137.1, 130.5, 129.1, 128.91, 128.89, 128.7, 128.2, 128.1, 121.3, 105.1, 99.6, 55.28. IR (neat) 2365, 2349, 2309, 1747, 1689, 1680, 1658, 1648, 1621, 1582, 1542, 1498, 1445, 1319, 1281, 1219, 1199, 1152, 1032, 956, 834, 770, 697 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO_2$ (M^+): 303.1259, found: 303.1258.



5-chloro-2-((diphenylmethylene)amino)phenol (2na). Yellow soilid. Yield: 39% (0.0195 mmol, 6.0 mg, 0.05 mmol scale). R_f = 0.4 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74-7.73 (m, 2H), 7.51-7.49 (m, 1H), 7.45-7.39 (m, 5H), 7.19-7.17 (m, 2H), 6.961-6.958 (d, *J* = 2.2 Hz, 1H), 6.46-6.45 (dd, *J* = 9.1, 2.2 Hz, 1 H), 6.09-6.08 (d, *J* = 9.1 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 168.9, 152.5, 139.5, 136.0, 134.2, 131.7, 131.3, 129.5, 129.4, 128.9, 128.8, 128.3, 121.1, 119.3, 114.8. IR (neat) 3384, 3060, 2362, 1776, 1745, 1601, 1570, 1478, 1446, 1259, 1220, 1191, 1148, 1112, 1076, 1001, 966, 906, 855, 809, 785, 766, 698, 676 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ (M^+): 307.0764, found: 307.0763.

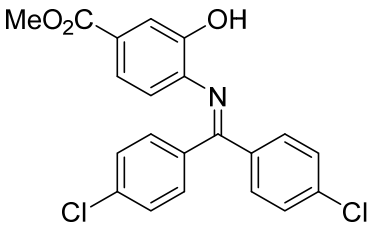


2-((bis(4-chlorophenyl)methylene)amino)-5-fluorophenol (2ob). Yellow oil. Yield: 29% (0.0144 mmol, 5.2 mg, 0.05 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64-7.62 (m, 2H), 7.42-7.38 (m, 4H), 7.14-7.12 (m, 2H), 6.99 (brs, 1H), 6.70-6.68 (dd, *J* = 9.6, 2.8 Hz, 1H), 6.26-6.22 (td, *J* = 8.9, 2.8 Hz, 1H), 6.14-6.11 (dd, *J* = 8.9, 6.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 165.3, 162.6, 160.9, 153.4-153.3 (d, *J* = 30.3 Hz), 137.8-137.5 (d, *J* = 30.3 Hz), 135.8, 134.1, 131.4-131.1 (d, *J* = 31.8 Hz), 130.4, 130.3, 129.4, 128.6, 121.0-120.9 (d, *J* = 10.1 Hz), 106.2-106.0 (d, *J* = 23.1 Hz), 102.4-102.3 (d, *J* = 26.0 Hz). IR (neat) 3743, 3700, 3627, 3607, 3378, 3310, 3073, 2883, 2361, 2340, 1768, 1593, 1560, 1527, 1494, 1400, 1308, 1290, 1267, 1235, 1175, 1135, 1092, 1015, 969, 942, 909, 840, 804, 765, 738 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2FNO$ (M^+): 359.0280, found: 359.0279.

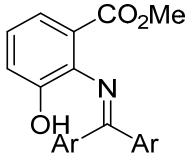


(Ar = 4-ClC$_6$H$_4$)

2-((bis(4-chlorophenyl)methylene)amino)-3-fluorophenol (2ob'). Yellow oil. Yield: 16% (0.00805 mmol, 2.9 mg, 0.05 mmol scale). R_f = 0.2 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69-7.68 (m, 2H), 7.41-7.40 (m, 2H), 7.30-7.28 (m, 2H), 7.10-7.08 (m, 2H), 6.93-6.89 (ddd, *J* = 9.2, 8.3, 5.8 Hz, 1H), 6.76-6.74 (dt, J = 8.3, 1.0 Hz, 1H), 6.38-6.35 (ddd, *J* = 9.2, 9.2, 1.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 171.8, 138.1, 137.1, 135.9, 134.5, 131.3, 131.1, 129.9, 128.8, 128.61, 128.57, 125.9, 125.8, 110.4, 107.6-107.4 (d, *J* = 20.2 Hz). IR (neat) 3412, 3098, 2361, 1787, 1700, 1667, 1589, 1560, 1513, 1469, 1401, 1292, 1220, 1220, 1192, 1173, 1142, 1092, 1059, 1014, 964, 910, 841, 772, 736 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{12}Cl_2FNO$ (M^+): 359.0280, found: 359.0280

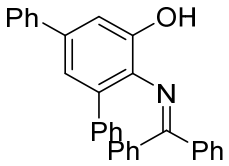


methyl 4-((bis(4-chlorophenyl)methylene)amino)-3-hydroxybenzoate (2pb). Yellow solid. Melting point: 172.52 °C. Yield: 24% (0.0117 mmol, 4.7 mg, 0.05 mmol scale). R_f = 0.3 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69-7.68 (m, 2H), 7.609-7.606 (d, *J* = 1.7 Hz, 1H), 7.42-7.41 (m, 2H), 7.35-7.34 (m, 2H), 7.27-7.25 (m, 1H), 7.10-7.09 (m, 2H), 6.22-6.21 (d, *J* = 8.3 Hz, 1H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.4, 140.2, 138.2, 137.1, 136.1, 133.3, 130.9, 130.5, 129.1, 128.7, 128.1, 121.4, 119.7, 115.9, 52.1. IR (neat) 3961, 3919, 3902, 3872, 3817, 1798, 3760, 3737, 3714, 3646, 3612, 3566, 3545, 3467, 3017, 2363, 1715, 1587, 1489, 1437, 1291, 1219, 1092, 1015, 772 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_3$ (M^+): 399.0429, found: 399.0428.

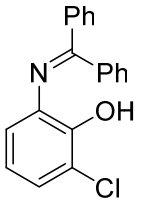


(Ar = 4-ClC$_6$H$_4$)

methyl 2-((bis(4-chlorophenyl)methylene)amino)-3-hydroxybenzoate (2pb'). Colorless oil. Yield: 47% (0.0235 mmol, 9.4 mg, 0.05 mmol scale). R_f = 0.5 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40-7.39 (m, 4H), 7.35-7.33 (m, 4H), 7.30-7.28 (dd, *J* = 8.3 Hz, 1.4, 1H), 6.87-6.86 (d, *J* = 7.6 Hz, 1H), 6.68-6.66 (t, *J* = 8.3 Hz, 1H), 6.42 (s, 1H), 3.89 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.4, 140.7, 139.7, 134.9, 131.3, 128.8, 128.7, 127.7, 121.4, 118.6, 110.9, 109.7, 102.1, 51.8. IR (neat) 3980, 3943, 3903, 3858, 3841, 3748, 3714, 3646, 3613, 3567, 3545, 3524, 3505, 3479, 2360, 2308, 1689, 1595, 1478, 1293, 1249, 1220, 1092, 1056, 772 cm^{-1}. HRMS (FD) calcd. for $C_{21}H_{15}Cl_2NO_3$ (M^+): 399.0429, found: 399.0429.

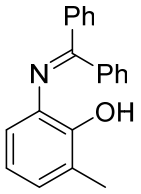


4'-((diphenylmethylene)amino)-[1,1':3',1''-terphenyl]-5'-ol (2qa). Yellow soilid. Melting point: 83.1 °C. Yield: 76% (0.0757 mmol, 32.2 mg, 0.1 mmol scale). R_f = 0.5 [hexane/EtOAc = 3:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66-7.65 (m, 2H), 7.62-7.60 (m, 2H), 7.50-7.48 (m, 1H), 7.42-7.30 (m, 5H), 7.268-7.265 (d, *J* = 1.7 Hz, 1H), 7.02-7.00 (t, *J* = 7.7 Hz, 2H), 6.94-6.93 (m, 2H), 6.910-6.907 (d, *J* = 2.1 Hz, 1H), 6.45-6.43 (m, 2H), 6.14 (brs, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.4, 140.7, 139.7, 134.9, 131.3, 128.8, 128.7, 127.7, 121.4, 118.6, 110.9, 109.7, 102.1, 51.8. IR (neat) 3060, 3029, 2922, 2372, 2360, 2345, 1597, 1564, 1497, 1467, 1444, 1409, 1321, 1302, 1196, 1151, 1061, 1030, 1001, 964, 935, 868, 789, 762, 697 cm^{-1}. HRMS (FD) calcd. for $C_{31}H_{23}NO$ (M^+): 425.1780, found: 425.1779.

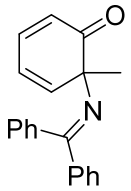


2-chloro-6-((diphenylmethylene)amino)phenol (2ra). Yellow soilid. Melting point: 122.1 °C. Yield: 31% (0.0156 mmol, 4.8 mg, 0.05 mmol scale). R_f = 0.3 [hexane/EtOAc = 10:1 (v/v)]. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63-7.75 (m, 2H), 7.52-7.50 (m, 1H), 7.44-7.36 (m, 5H), 7.19-7.18 (m, 2H), 7.01-6.99 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.47-6.44 (t, *J* = 8.0, 1H), 6.15-6.13 (dd, *J* = 7.9, 1.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 170.1, 147.0, 139.3, 137.4, 135.9, 131.4, 130.1, 129.6, 129.4, 128.9, 128.5, 128.3, 126.3, 119.4, 118.9. IR (neat) 3987, 3974, 3915, 3900, 3869, 3851, 3830, 3814, 3764, 3743, 3730, 3699, 3686, 3673, 3645,

3626, 3603, 3585, 3565, 3544, 3517, 3052, 2359, 1785, 1567, 1320, 795, 704 cm^{-1}. HRMS (FD) calcd. for $C_{19}H_{14}ClNO$ M^+ 307.0764, found 307.0764.

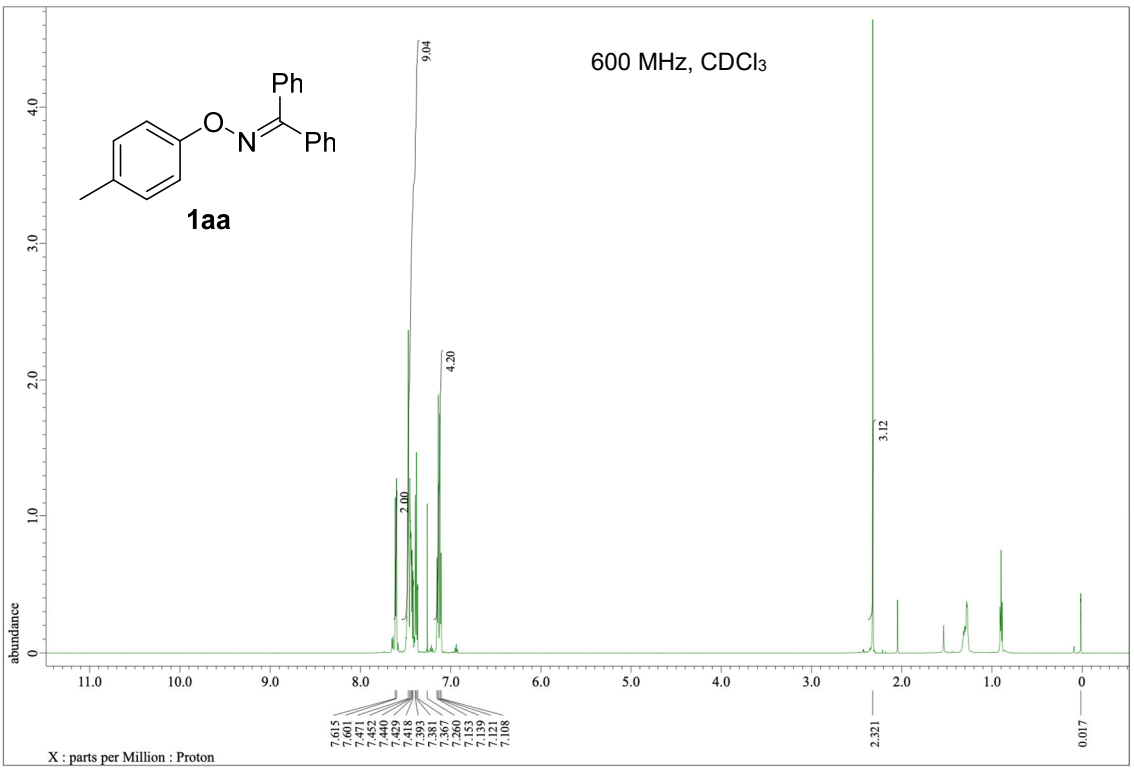


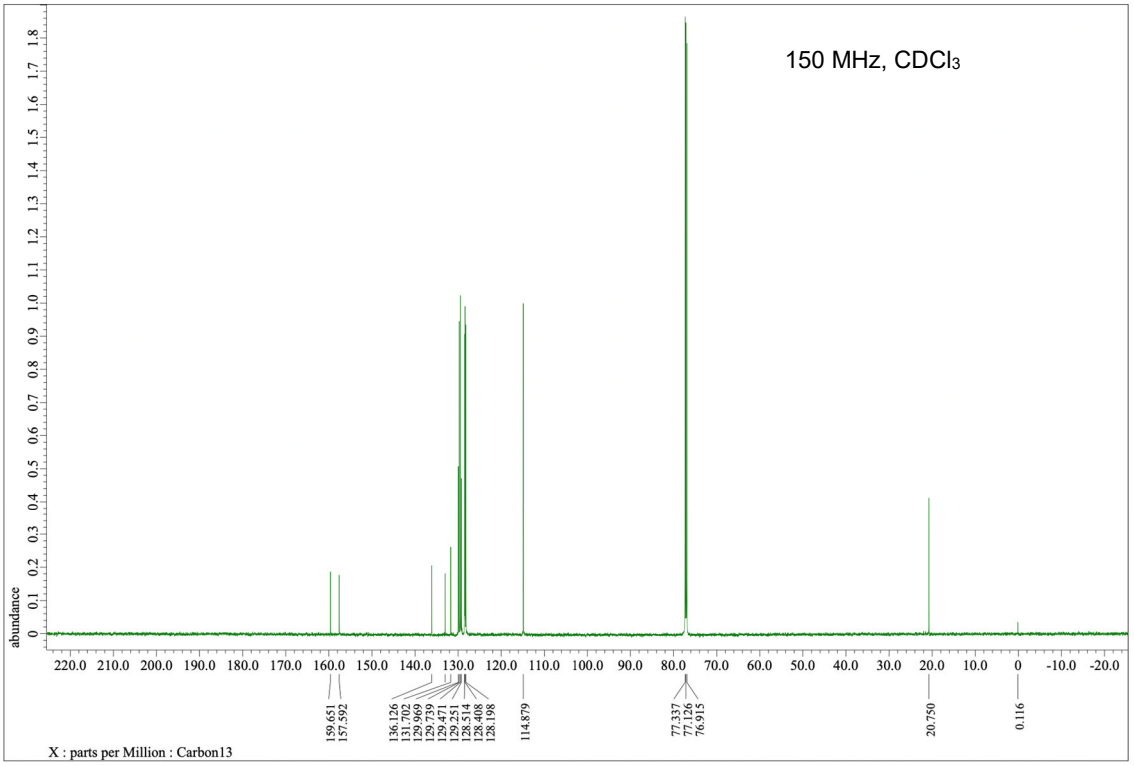
2-((diphenylmethylene)amino)-6-methylphenol (2sa). Yellow solid. Melting point: 118.7 °C. Yield: 61% (0.0613 mmol, 17.6 mg, 0.1 mmol scale). R_f = 0.5 [hexane/EtOAc = 10:1 (v/v)]. ^1H NMR (600 MHz, $CDCl_3$) δ 7.76-7.75 (d, *J* = 7.6 Hz, 2H), 7.51-7.47 (m, 1H), 7.43-7.37 (m, 5H), 7.22-7.20 (m, 2H), 6.98 (brs, 1H), 6.84-6.82 (d, *J* = 7.6, 1H), 6.40-6.37 (t, *J* = 7.9 Hz, 1H), 6.05-6.04 (d, *J* = 7.9 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 167.8, 150.2, 139.9, 136.5, 134.9, 130.9, 129.3, 129.2, 129.0, 128.6, 128.2, 128.1, 123.6, 118.3, 117.9, 15.7. IR (neat) 3914, 3901, 3886, 3855, 3829, 3814, 3772, 3743, 3727, 3697, 3652, 3627, 3589, 3404, 3059, 3027, 2977, 2948, 2916, 2851, 2359, 1899, 1656, 1592, 1571, 1482, 1445, 1318, 1258, 1222, 1181, 1159, 1113, 1076, 1029, 1010, 961, 934, 835, 770, 743, 696 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO$ (M^+): 287.1310, found: 287.1310.

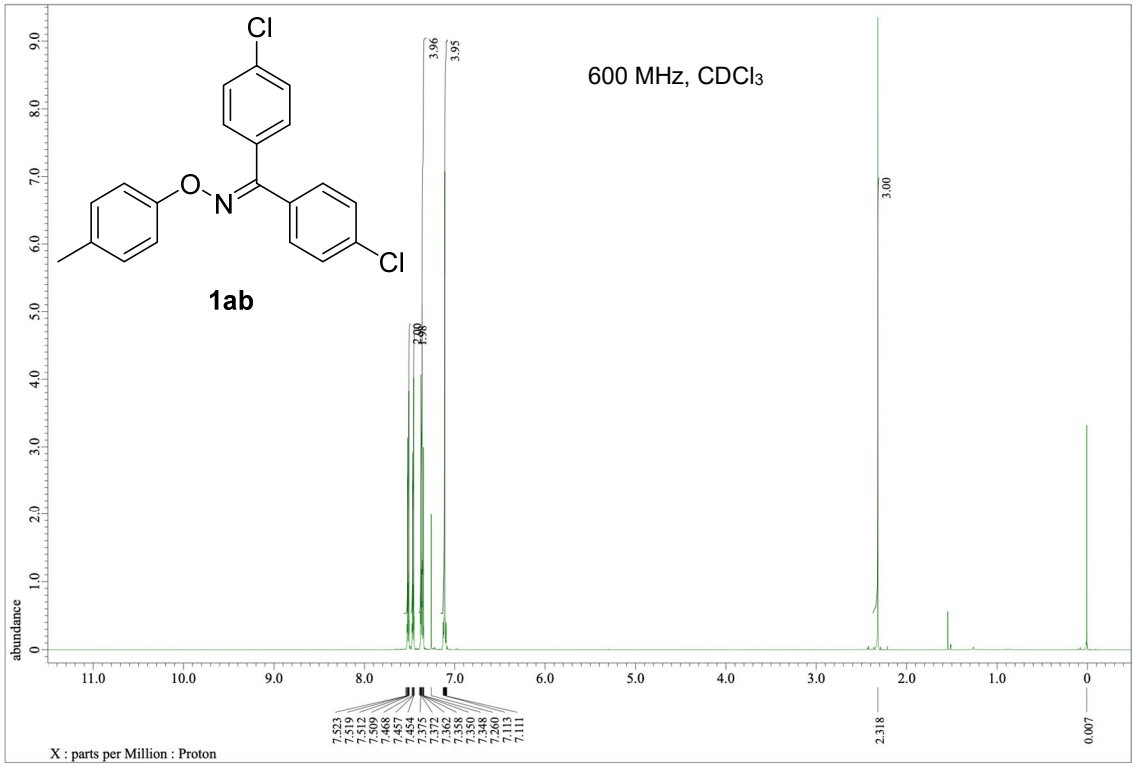


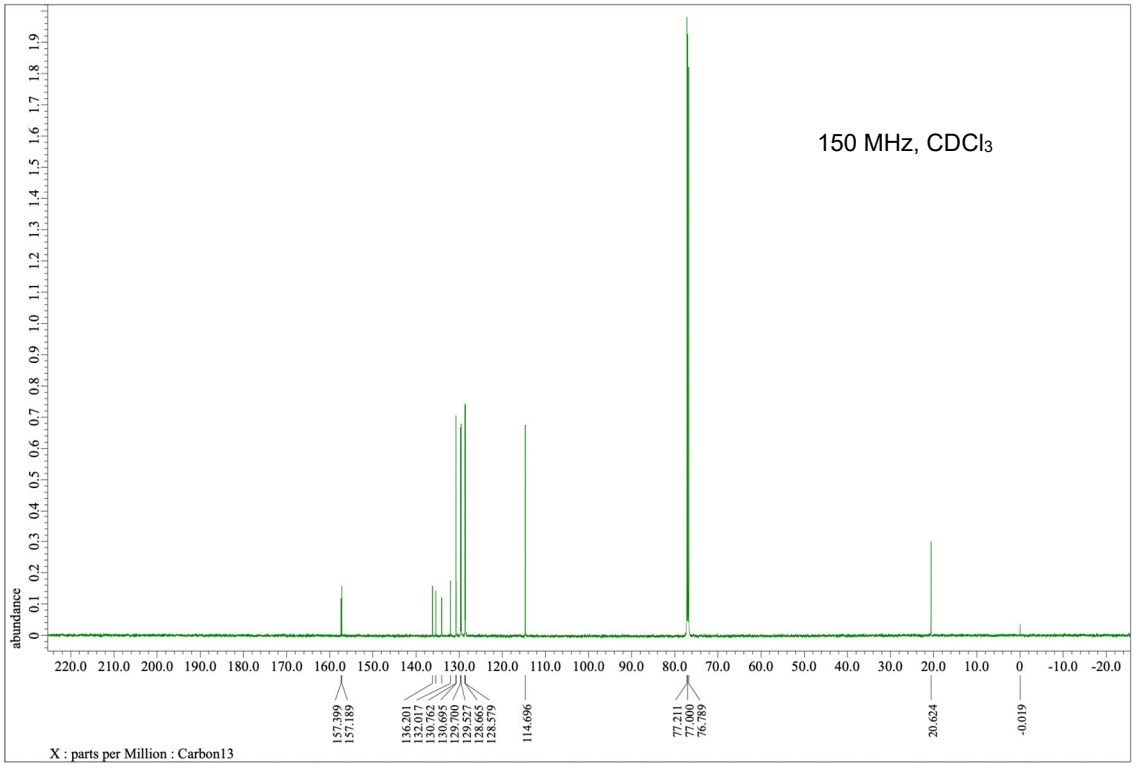
6-((diphenylmethylene)amino)-6-methylcyclohexa-2,4-dien-1-one (3sa). Yellow oil. Yield: 6% (0.006 mmol, 1.7 mg, 0.1 mmol scale). R_f = 0.3 [hexane/EtOAc = 3:1 (v/v)]. ^1H NMR (600 MHz, $CDCl_3$) δ 7.62-7.60 (m, 2H), 7.39-7.36 (m, 1H), 7.31-7.29 (m, 2H), 7.28-7.25 (m, 1H), 7.21-7.18 (m, 2H), 6.98-6.97 (m, 2H), 6.60-6.57 (ddd, *J* = 9.6, 6.2, 1.7 Hz, 1H), 6.34-6.32 (m, 1H), 5.80-5.78 (ddd, *J* = 9.6, 5.9, 1.0 Hz, 1H), 5.66-5.65 (m, 1H), 1.68 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 204.2, 146.7, 140.4, 139.7, 138.8, 130.4, 128.8, 128.6, 128.3, 127.9, 127.5, 125.5, 118.1, 69.5, 29.9. IR (neat) 3989, 3969, 3950, 3905, 3891, 3880, 3863, 3842, 3820, 3785, 3761, 3737, 3680, 3643, 3612, 3592, 3567, 3504, 3055, 2924, 2367, 2349, 2310, 1663, 1628, 1554, 1490, 1445, 1413, 1314, 1281, 1036, 769, 699, 636 cm^{-1}. HRMS (FD) calcd. for $C_{20}H_{17}NO$ M^+ 287.1310, found 287.1309

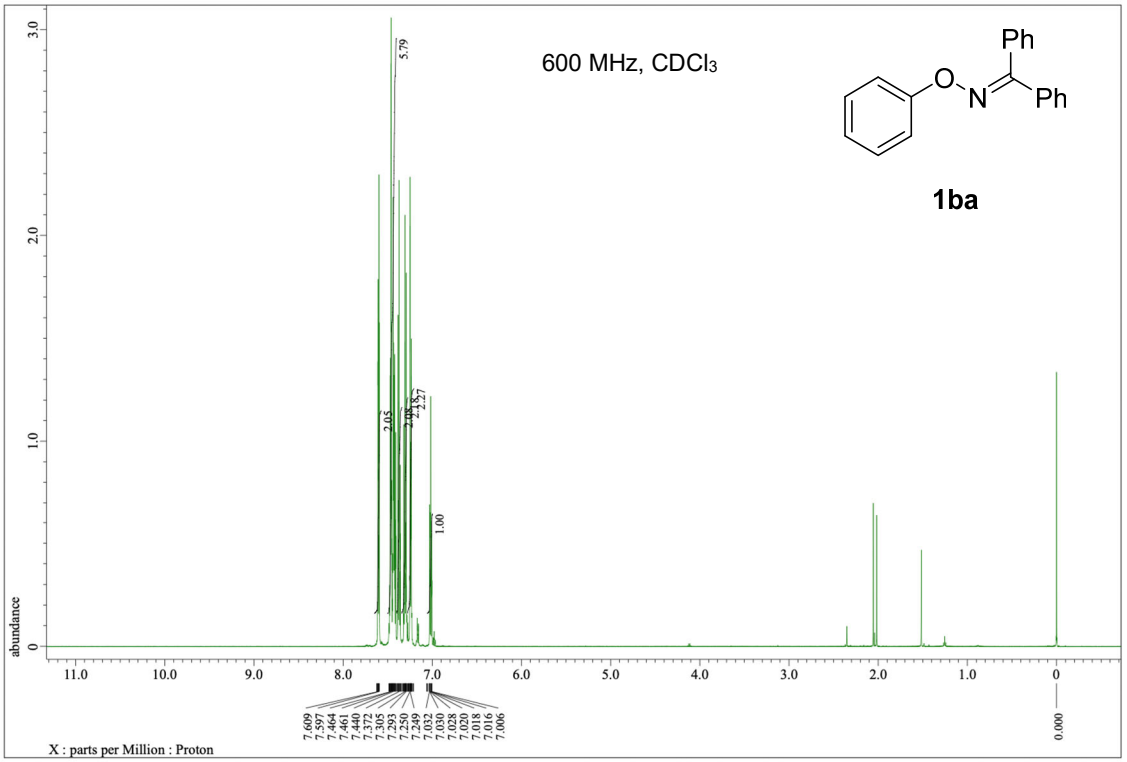
13. ^{1}H and ^{13}C NMR chart of 1

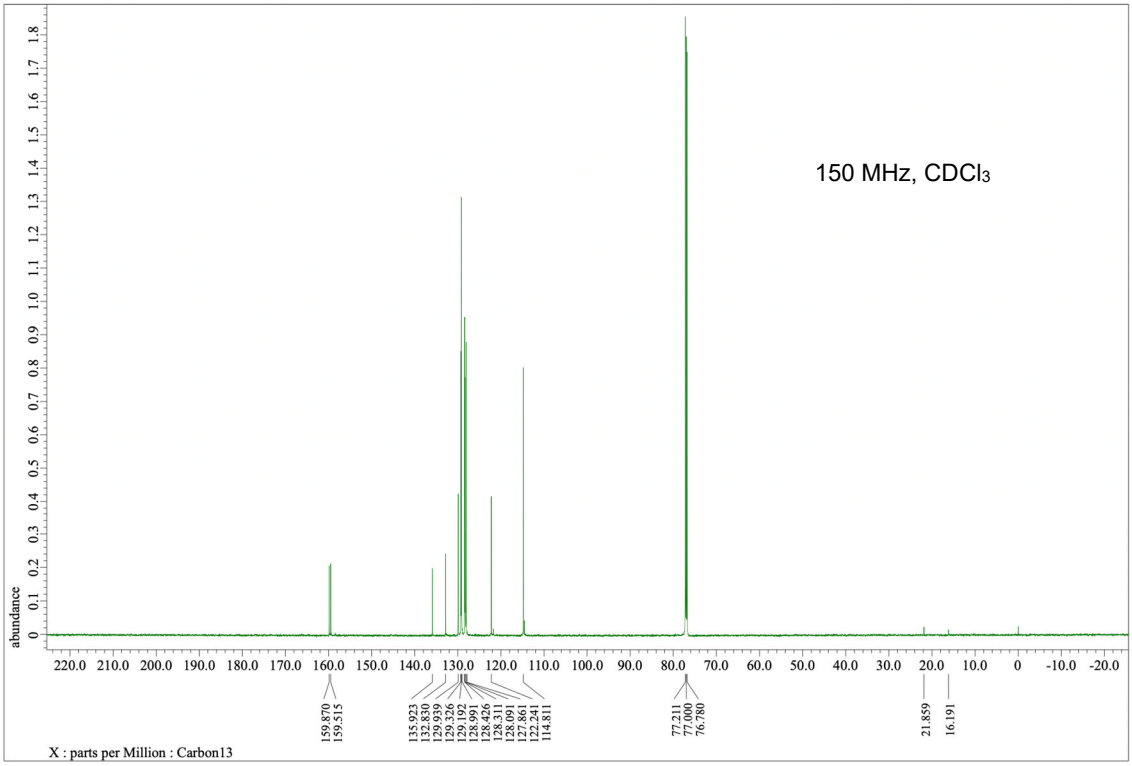


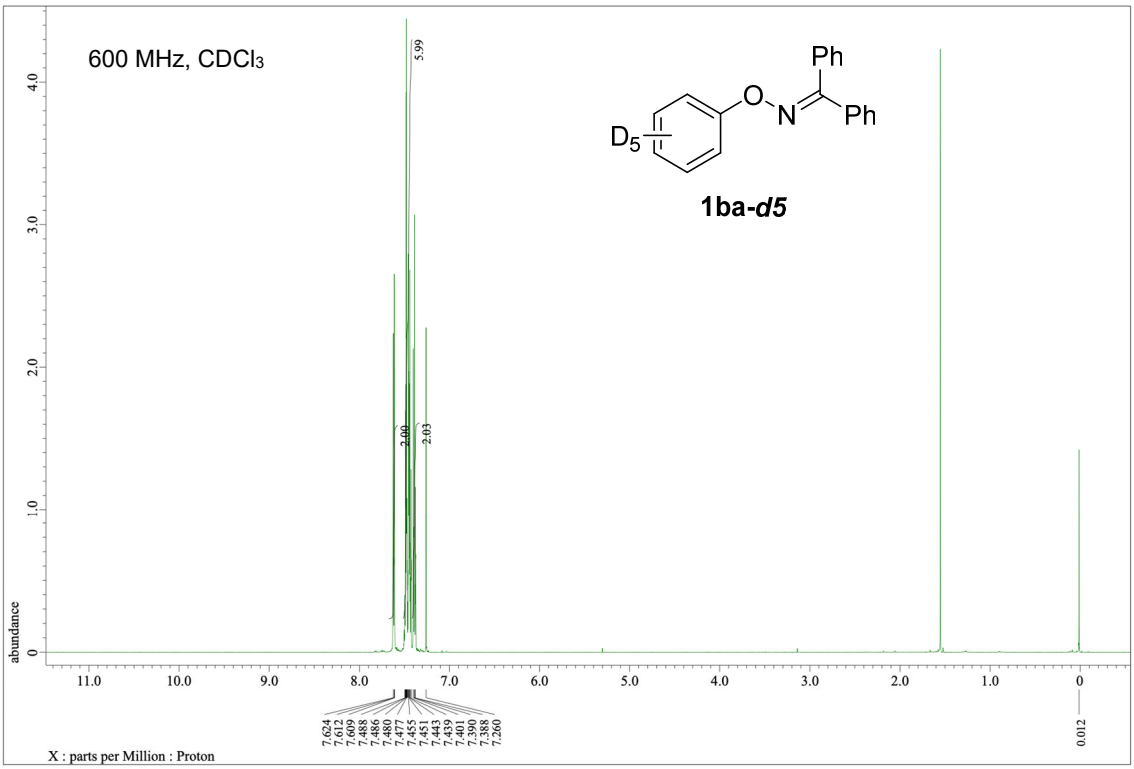


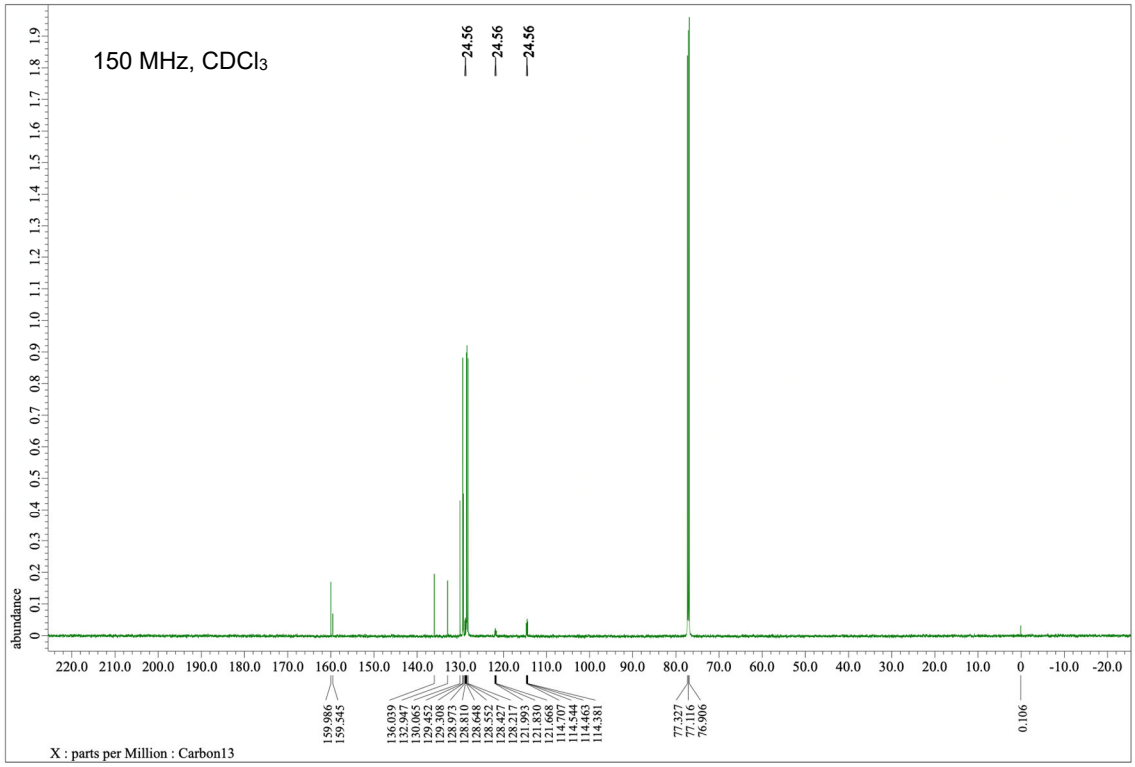

Cl
O
N
Cl
1ab
600 MHz, CDCl3
3.96
3.95
3.00
2.00
1.98
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.523
7.519
7.512
7.509
7.468
7.457
7.454
7.375
7.372
7.362
7.358
7.350
7.348
7.260
7.113
7.111
2.318
0.007
X : parts per Million : Proton

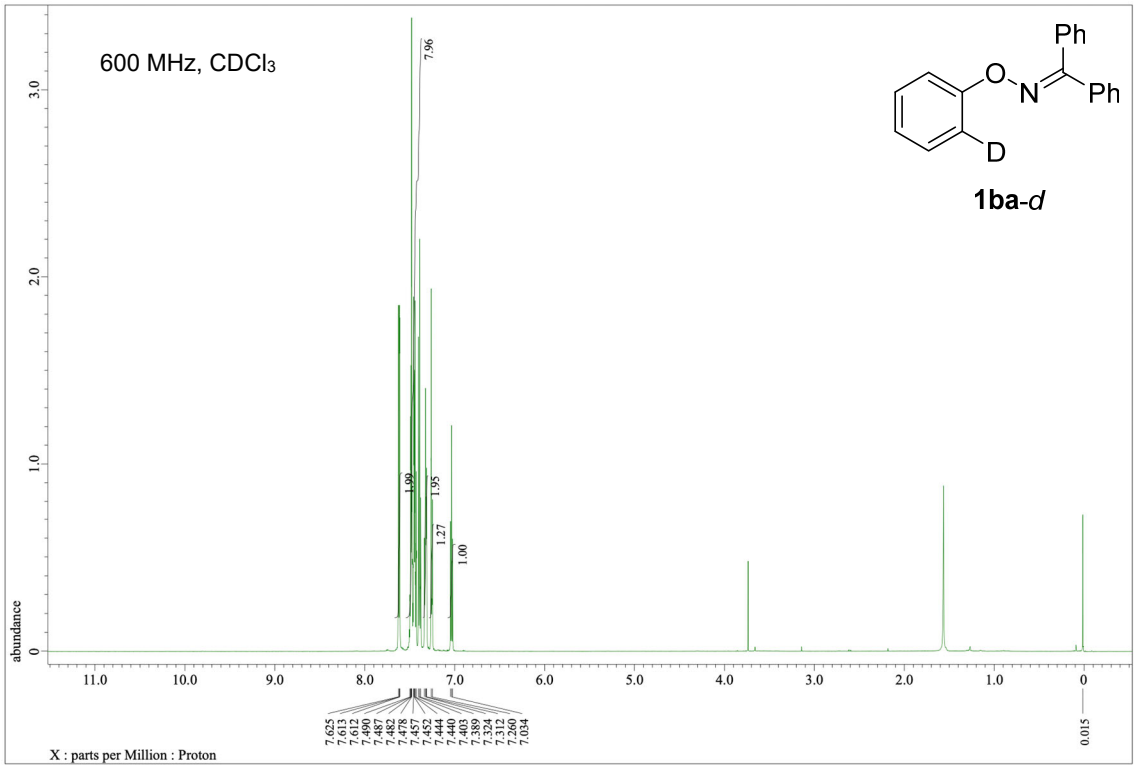

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
157.399
157.189
136.201
135.017
130.762
130.695
129.700
129.527
128.665
128.579
114.696
77.211
77.000
76.789
20.624
-0.019
X : parts per Million : Carbon13

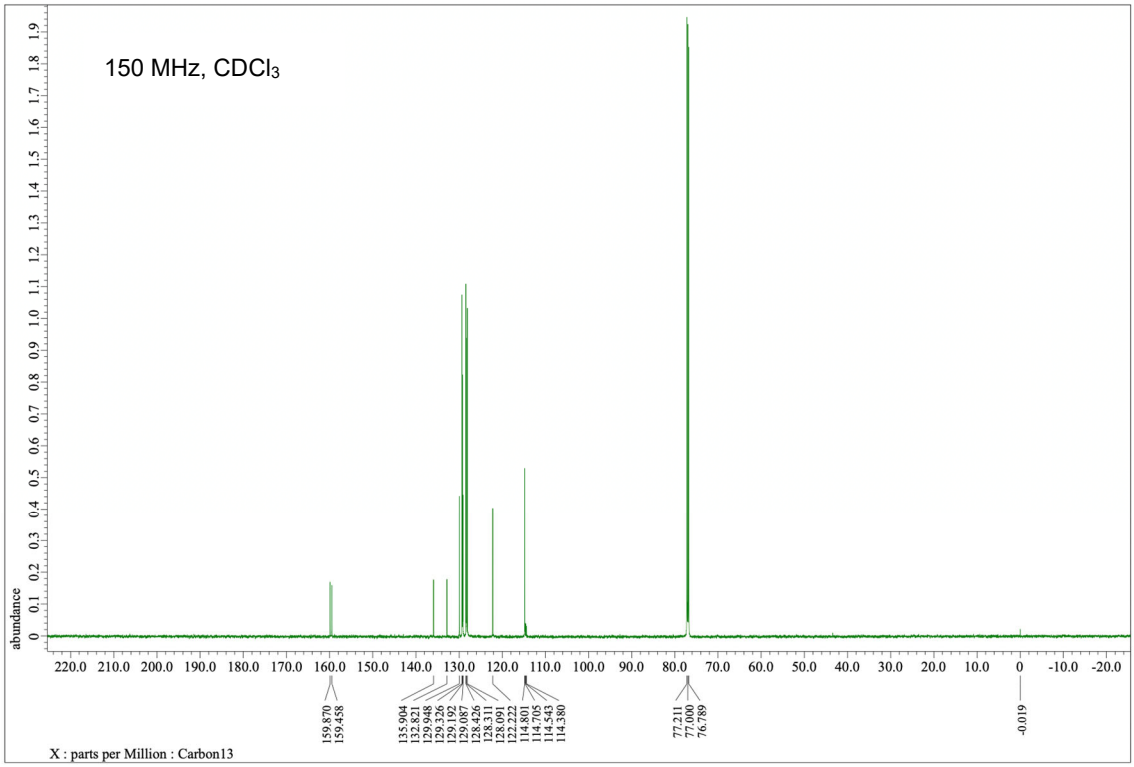

600 MHz, CDCl3
Ph
O
N
Ph
1ba
abundance
X : parts per Million : Proton

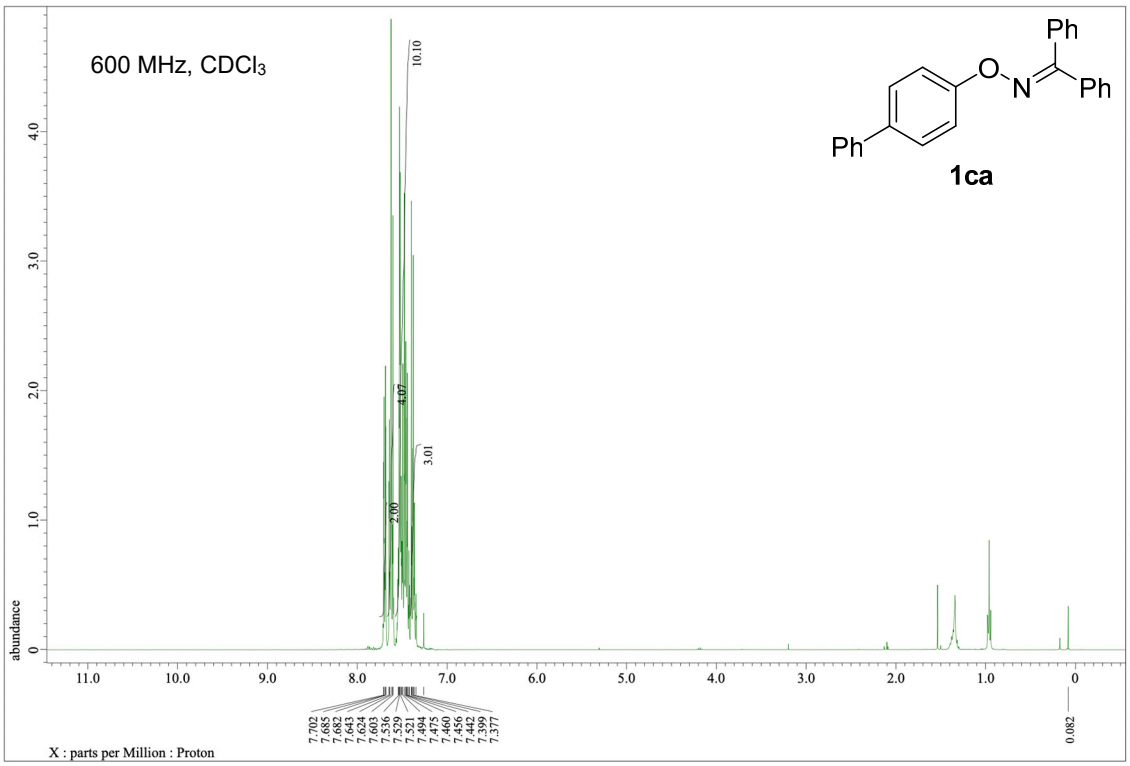

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

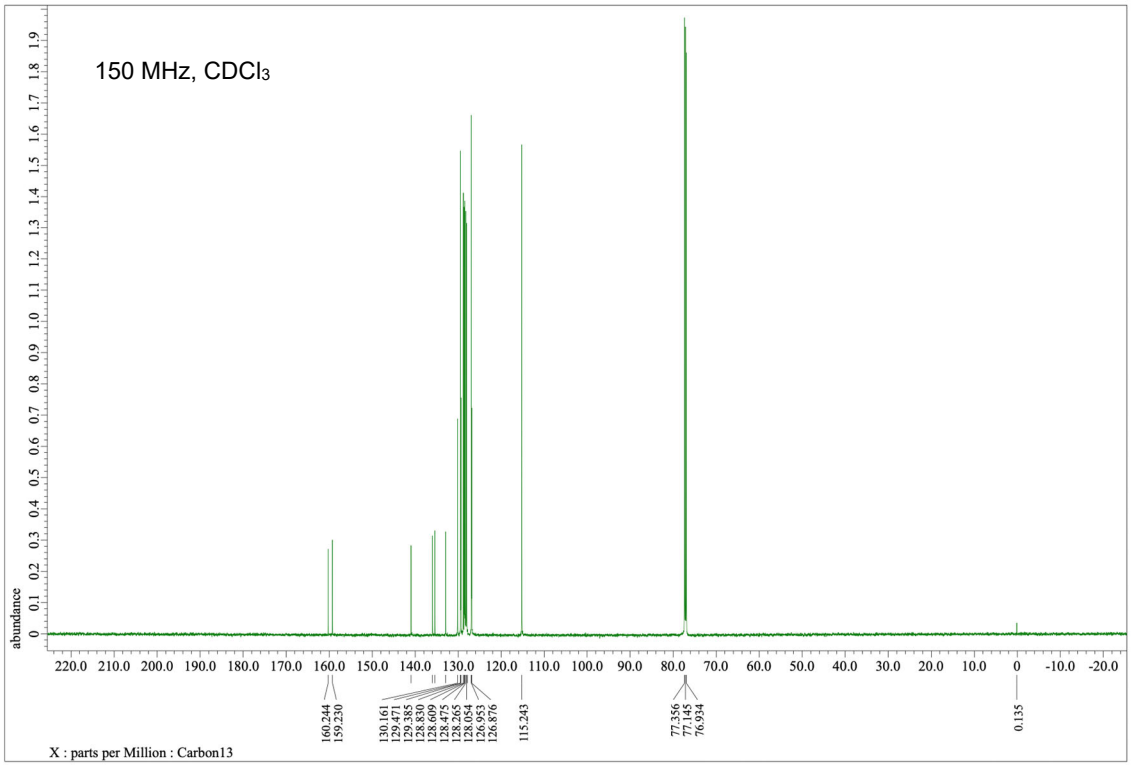

600 MHz, CDCl3
Ph
O
N
Ph
D5
1ba-d5
abundance
X : parts per Million : Proton

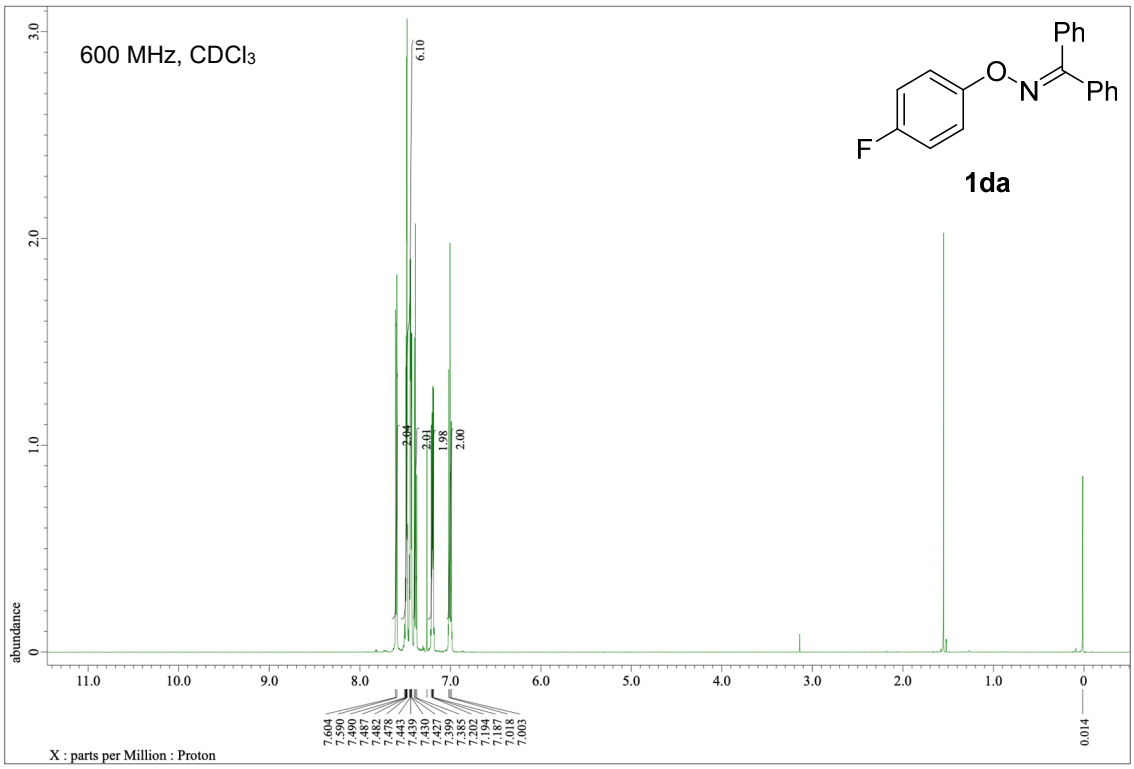

150 MHz, CDCl3
24.56
24.56
24.56
abundance
X : parts per Million : Carbon13

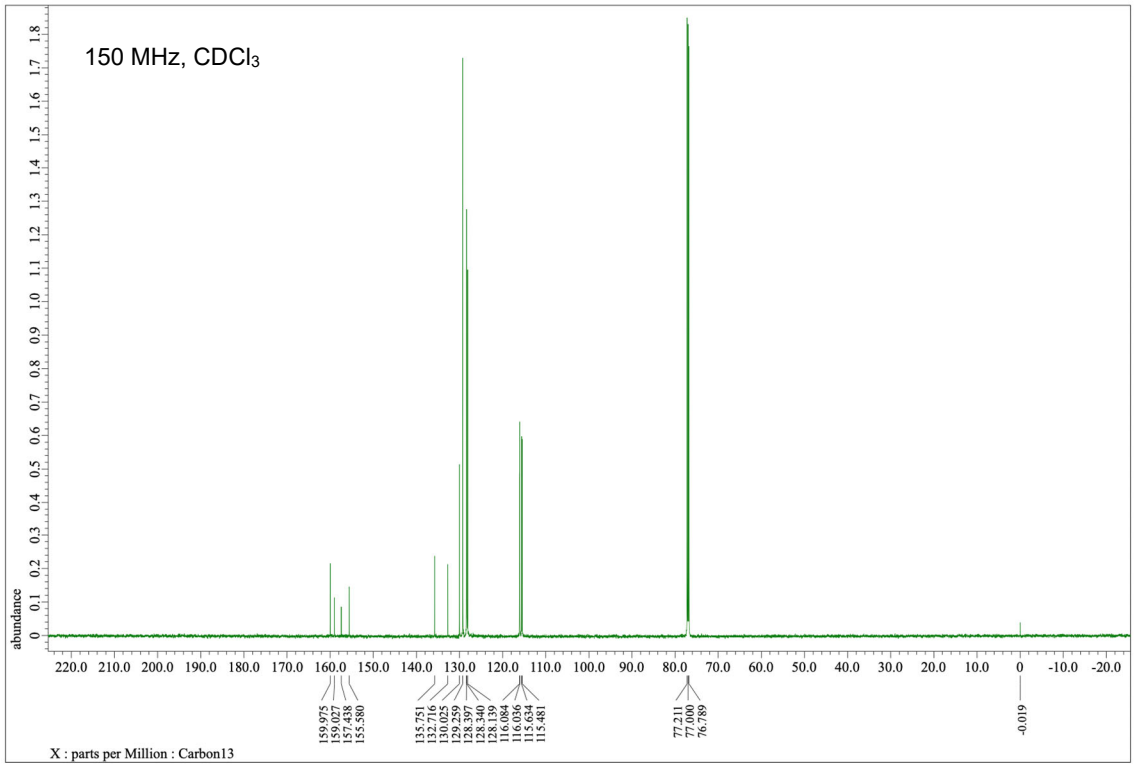

600 MHz, CDCl3
Ph
O
N
Ph
D
1ba-d
abundance
X : parts per Million : Proton


150 MHz, CDCl3
abundance
X : parts per Million : Carbon13


600 MHz, CDCl3
Ph
O
N
Ph
Ph
1ca
10.10
4.07
3.01
2.00
abundance
X : parts per Million : Proton


150 MHz, CDCl3
abundance
X : parts per Million : Carbon13


600 MHz, CDCl3
Ph
O
N
Ph
F
1da
6.10
2.04
2.01
1.98
2.00
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.604
7.590
7.490
7.487
7.482
7.478
7.443
7.439
7.430
7.427
7.399
7.395
7.202
7.194
7.187
7.018
7.003
0.014
X : parts per Million : Proton


150 MHz, CDCl3
abundance
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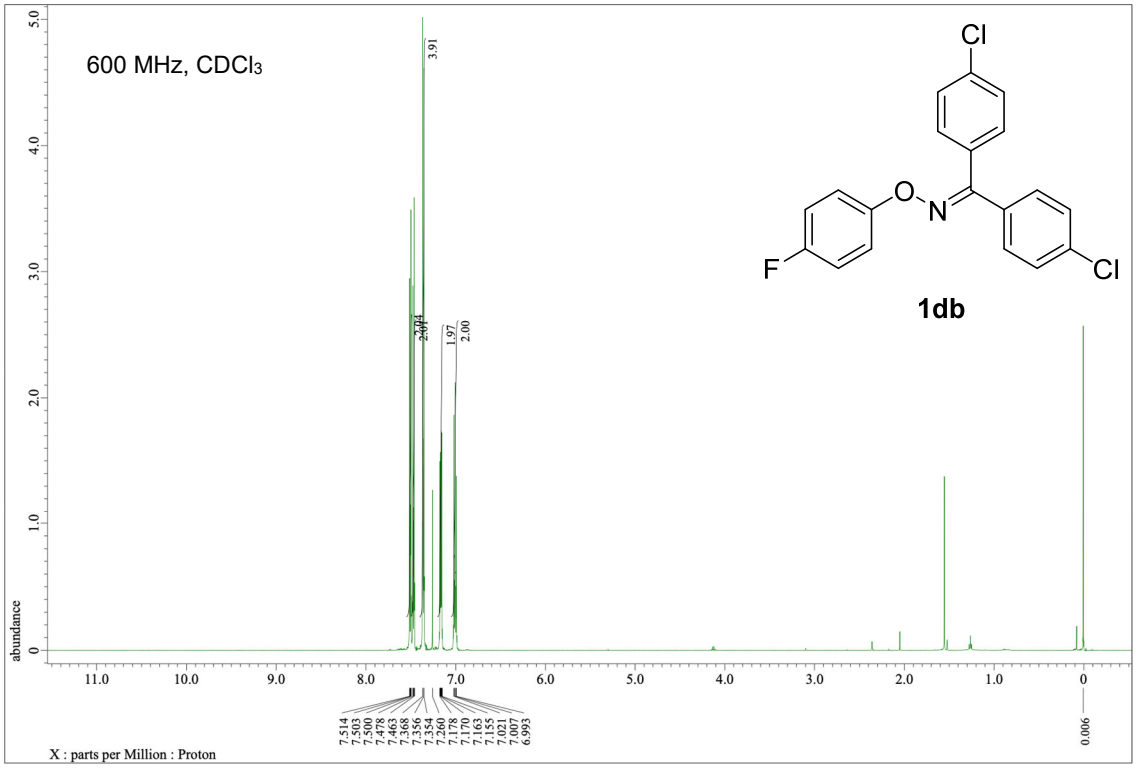
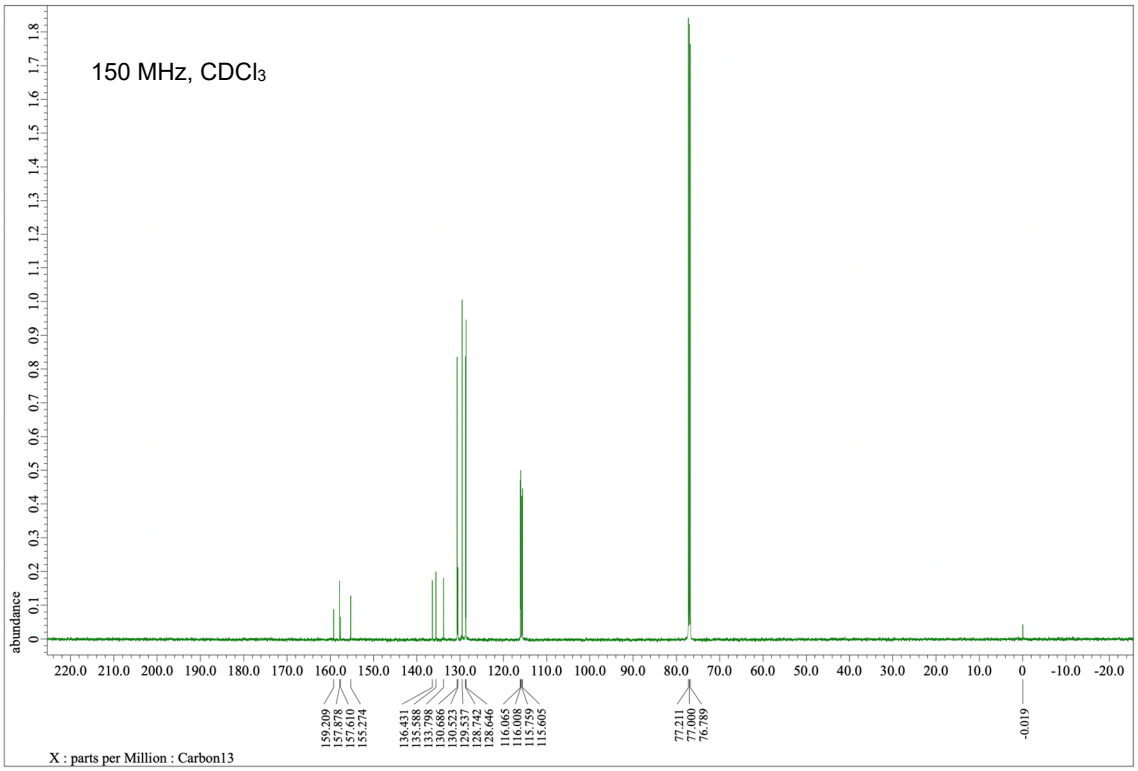
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
159.975
157.077
157.438
155.580
135.751
132.716
130.025
129.259
128.397
128.340
128.139
116.084
115.656
115.634
115.481
77.211
77.000
76.789
-0.019
X : parts per Million : Carbon13


600 MHz, CDCl3
Cl
O
N
F
Cl
1db
3.91
2.04
2.01
1.97
2.00
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.514
7.503
7.500
7.478
7.463
7.348
7.356
7.354
7.260
7.178
7.170
7.163
7.155
7.031
7.007
6.993
0.006
X : parts per Million : Proton


150 MHz, CDCl3
abundance
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210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
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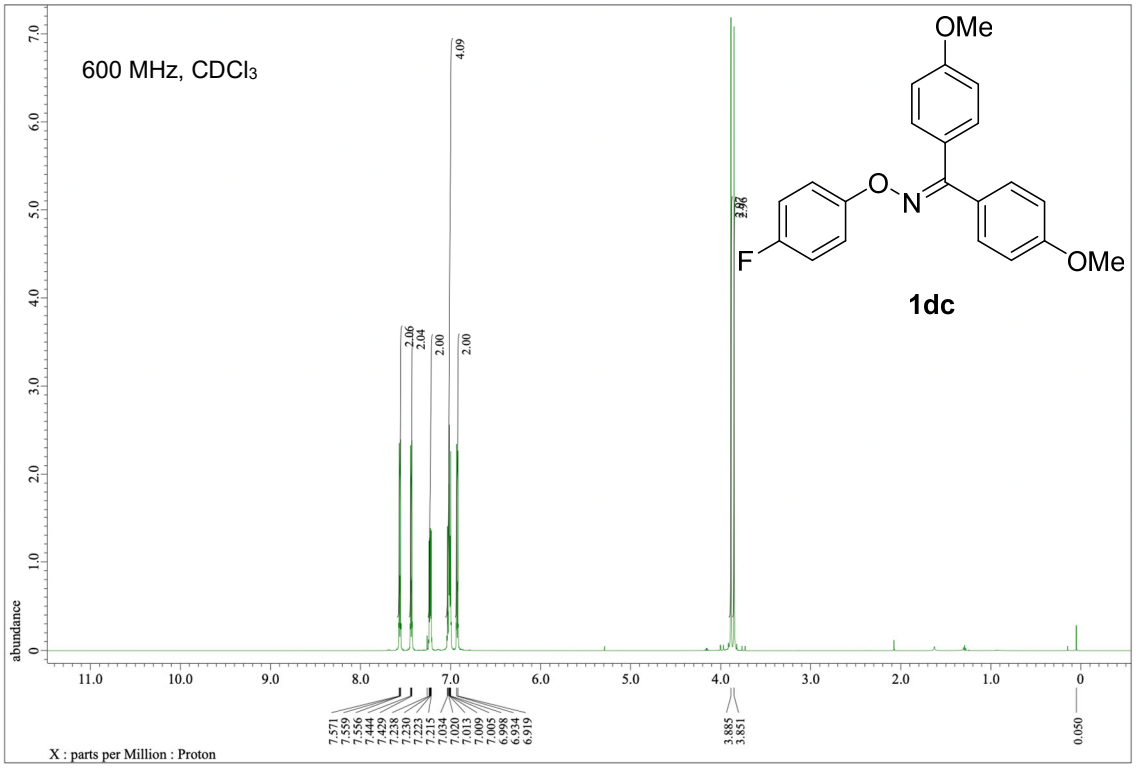
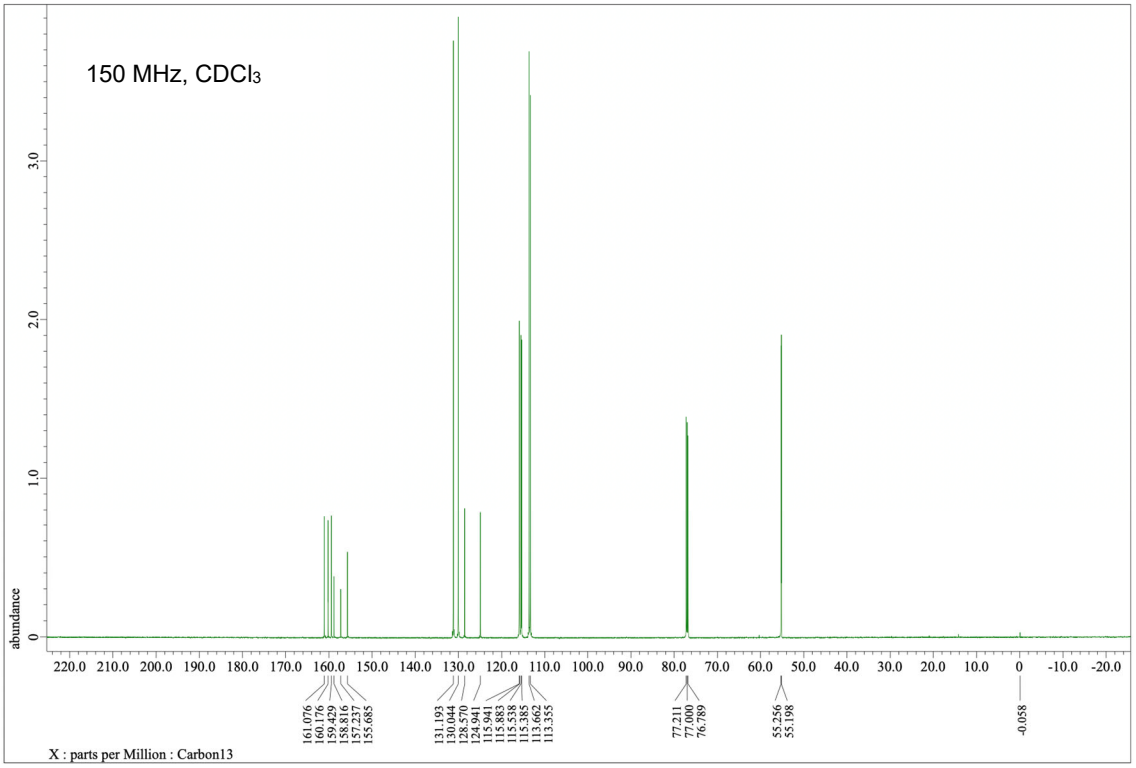
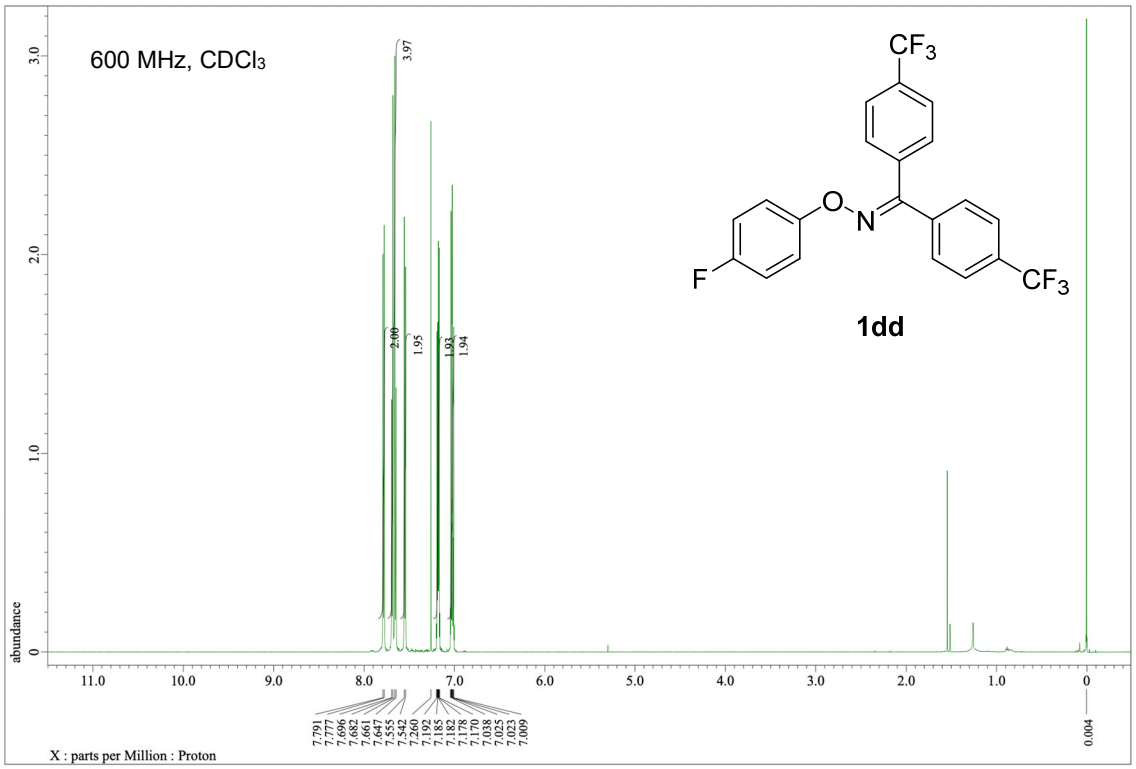
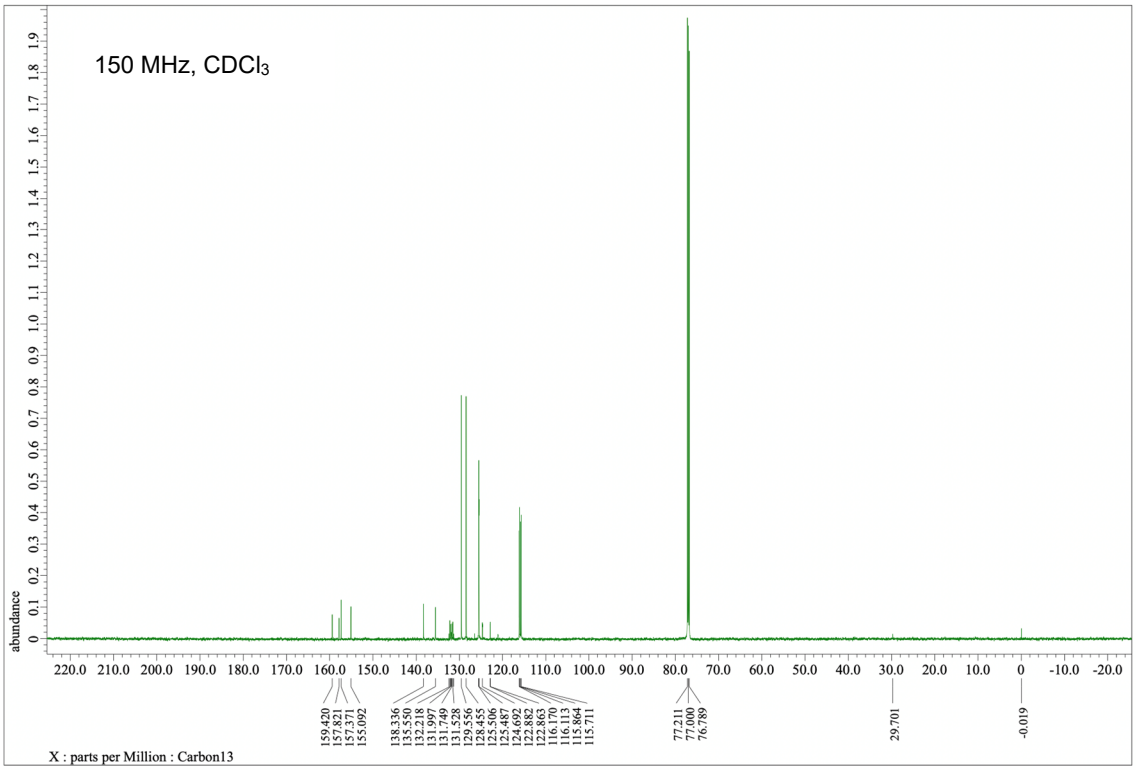
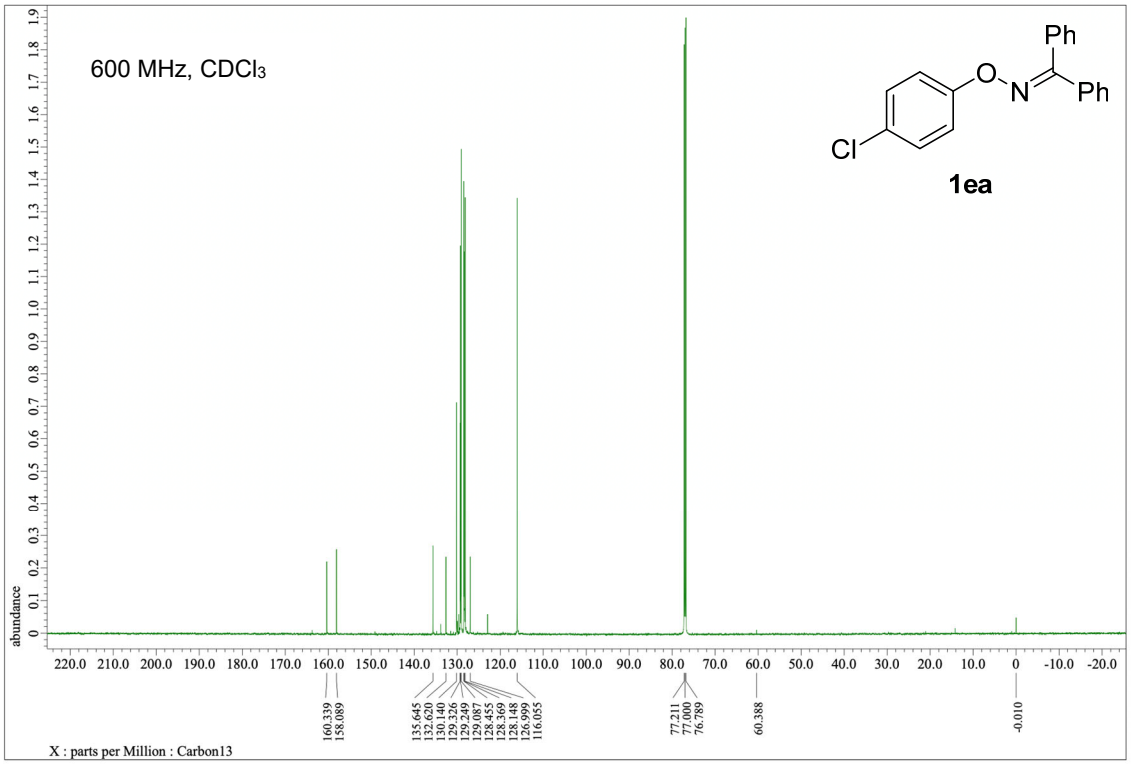
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
159.209
157.878
157.610
155.274
136.431
135.588
133.798
130.686
130.523
129.537
128.742
128.646
116.065
116.008
115.759
115.605
77.211
77.000
76.789
-0.019
X : parts per Million : Carbon13

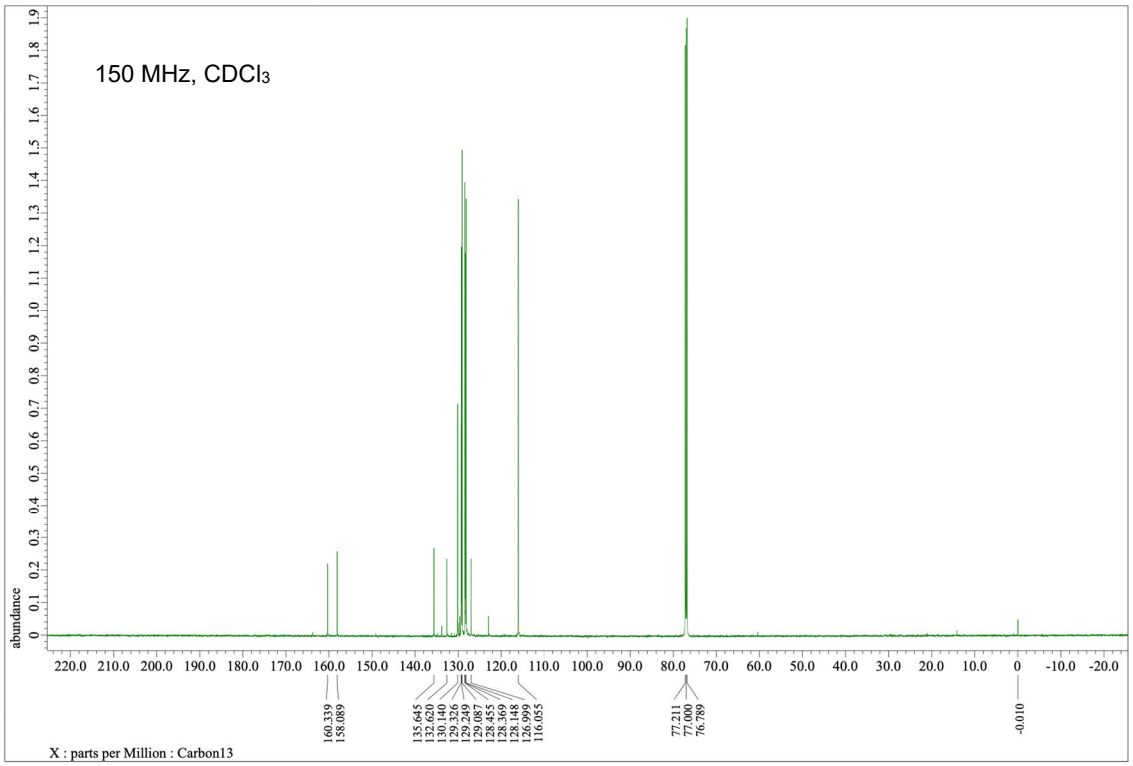

600 MHz, CDCl3
OMe
O
N
F
OMe
1dc
4.09
2.06
2.04
2.00
2.00
abundance
X : parts per Million : Proton

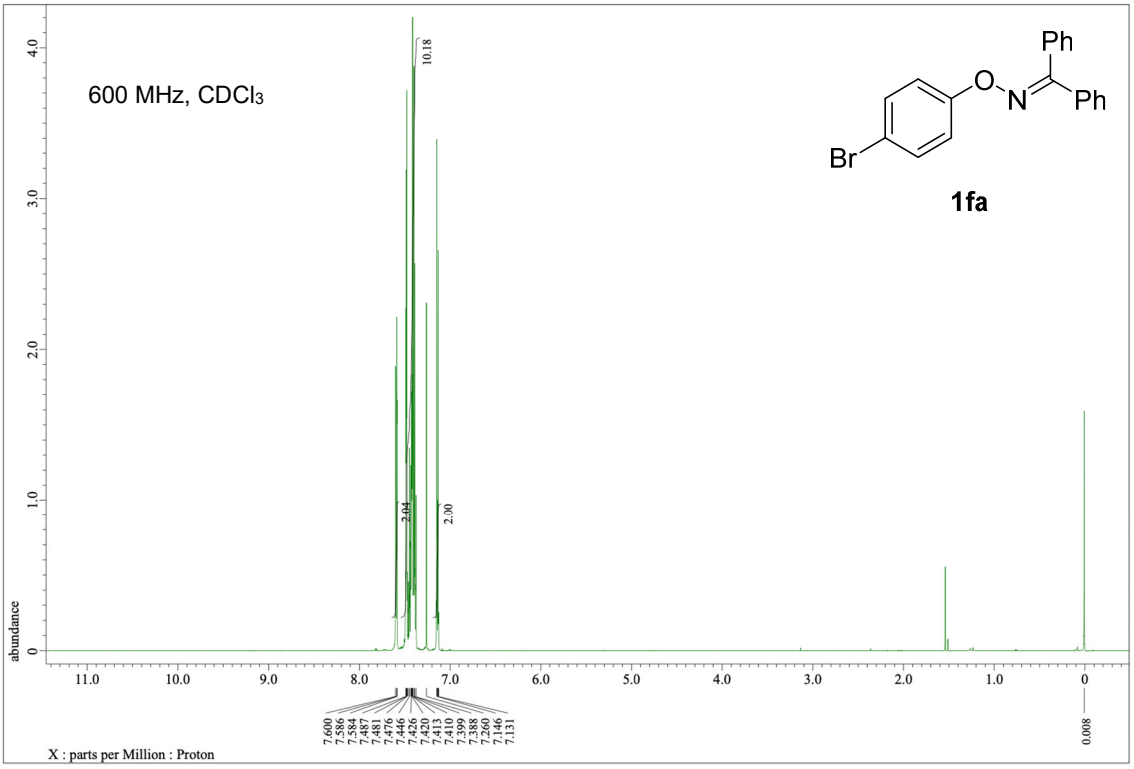

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

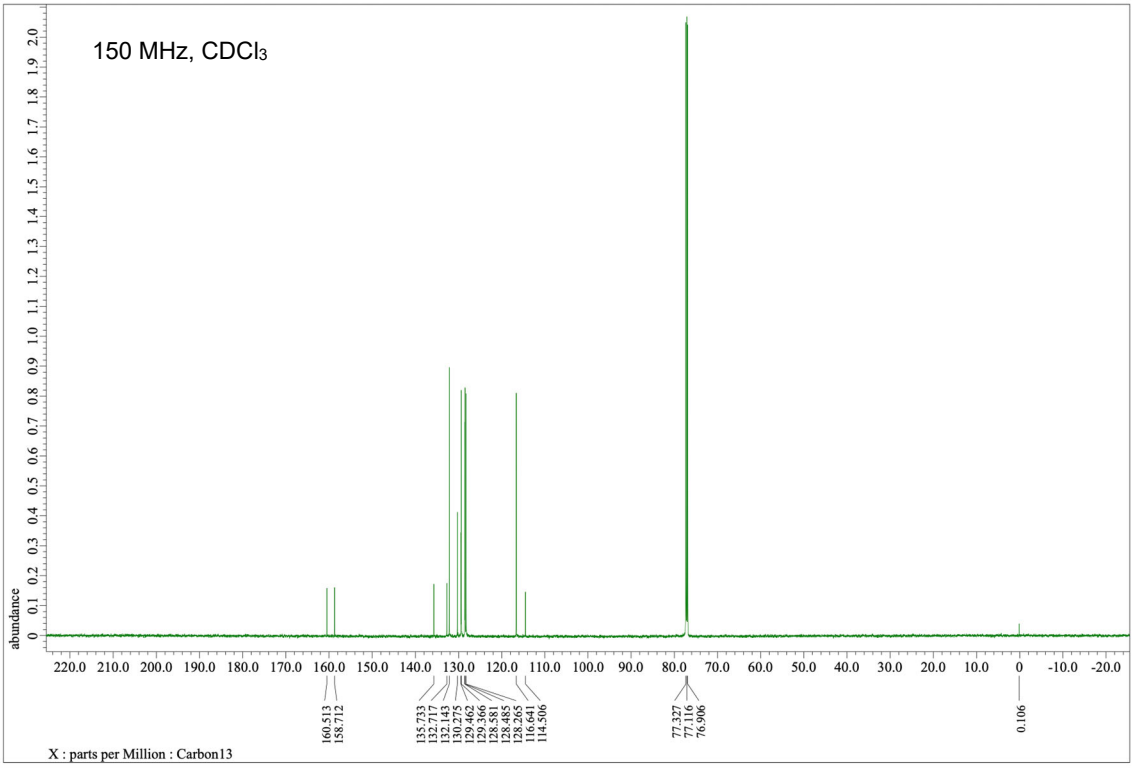

600 MHz, CDCl3
CF3
O
N
F
CF3
1dd
3.97
2.00
1.95
1.92
1.94
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.791 7.777 7.696 7.682 7.661 7.647 7.555 7.542 7.260 7.192 7.185 7.182 7.178 7.170 7.038 7.025 7.023 7.009
0.004
X : parts per Million : Proton

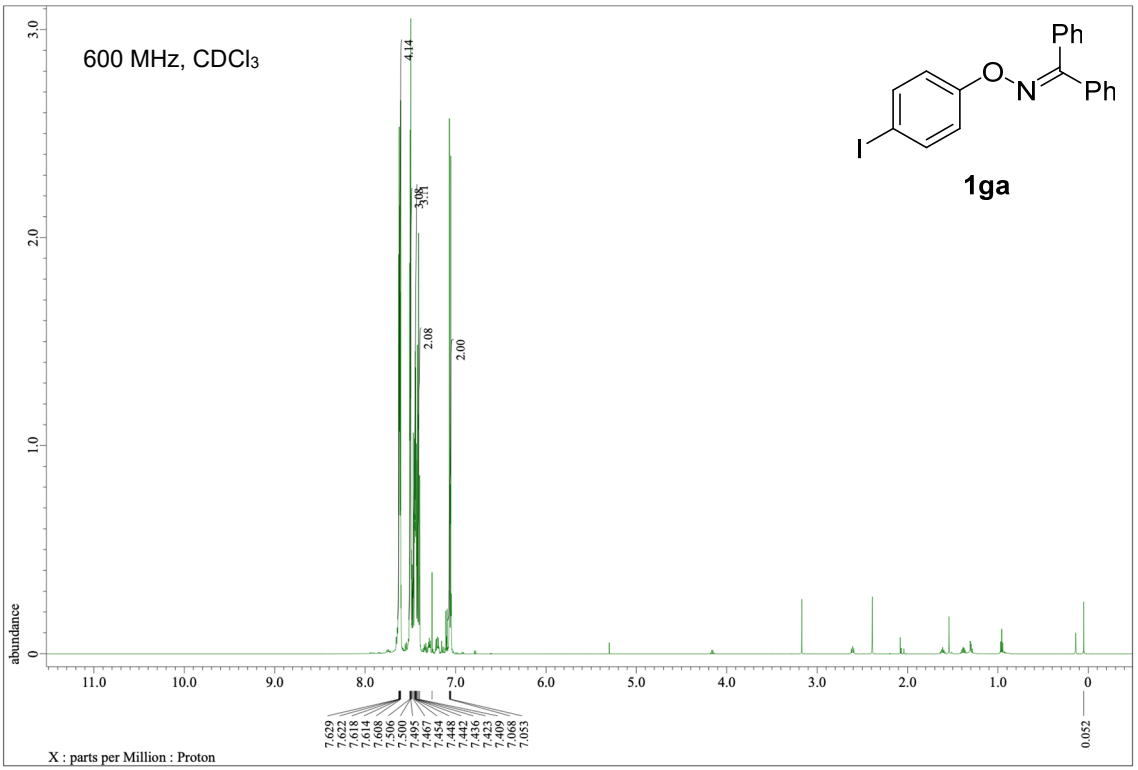

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
159.420 157.821 157.771 155.092
138.336 135.550 131.938 131.697 131.749 131.528 129.556 128.455 125.506 125.487 124.469 122.882 122.863 116.170 116.113 115.864 115.711
77.211 77.000 76.789
29.701
-0.019
X : parts per Million : Carbon13

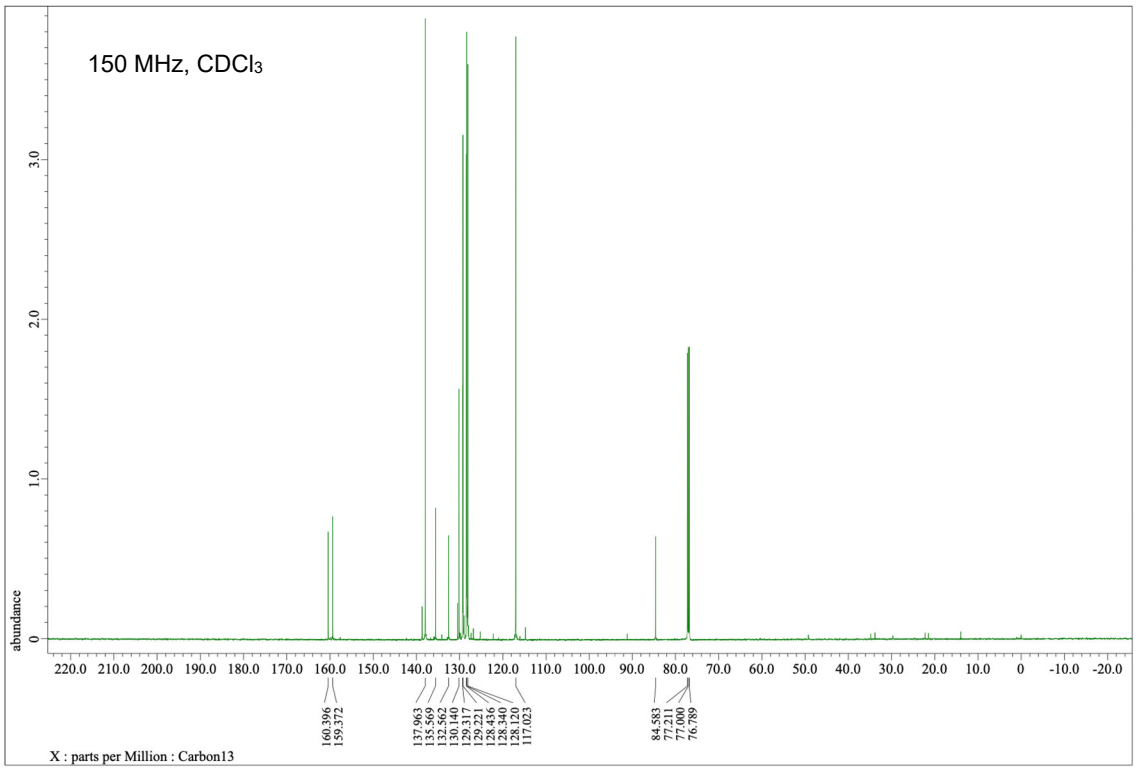

600 MHz, CDCl3
Ph
O
N
Ph
Cl
1ea
abundance
X : parts per Million : Carbon13

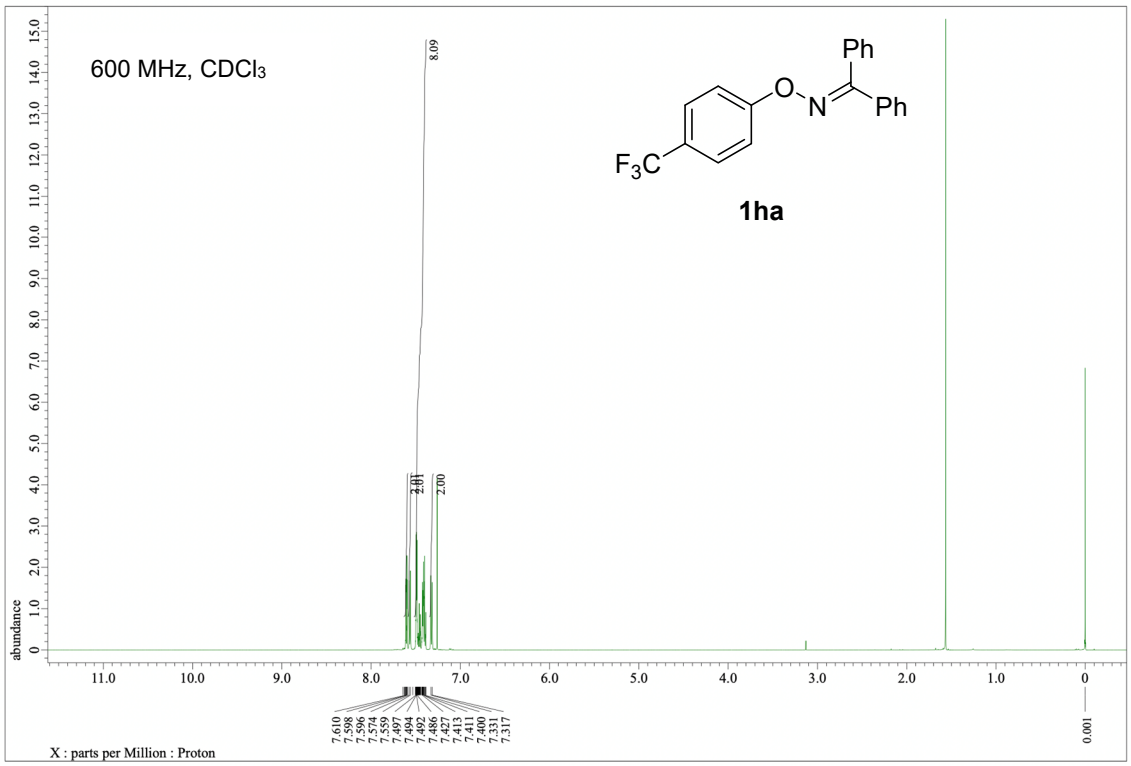

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

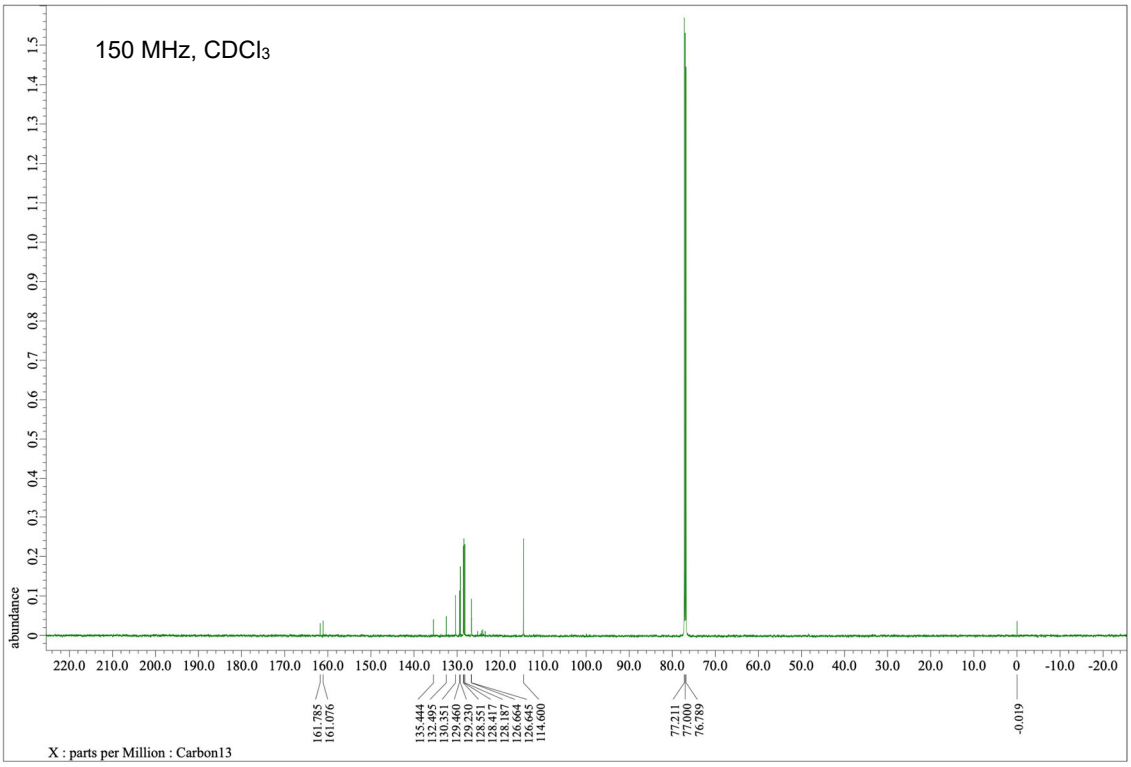

600 MHz, CDCl3
Ph
O
N
Ph
Br
1fa
10.18
2.04
2.00
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.600 7.586 7.584 7.487 7.481 7.476 7.446 7.426 7.420 7.413 7.410 7.399 7.388 7.260 7.146 7.131
0.008
X : parts per Million : Proton

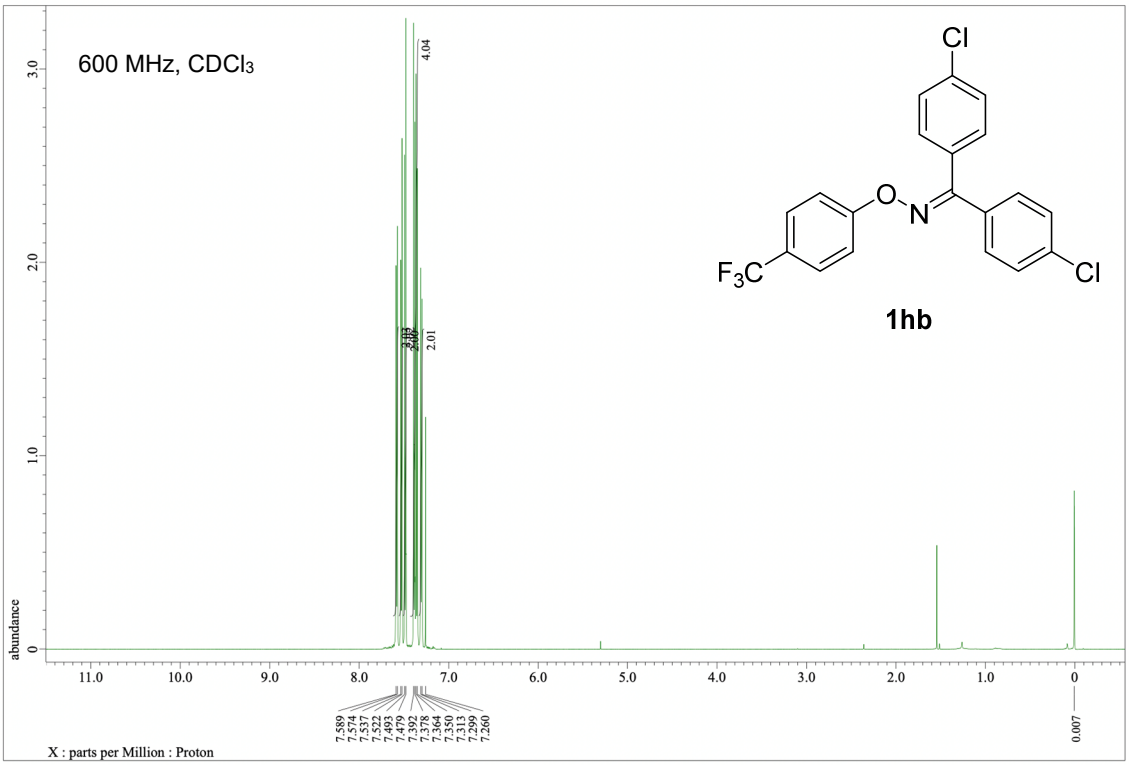

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
160.513 158.712
135.733 132.717 132.145 130.275 129.462 129.366 128.581 128.485 128.265 116.641 114.506
77.327 77.116 76.906
0.106
X : parts per Million : Carbon13

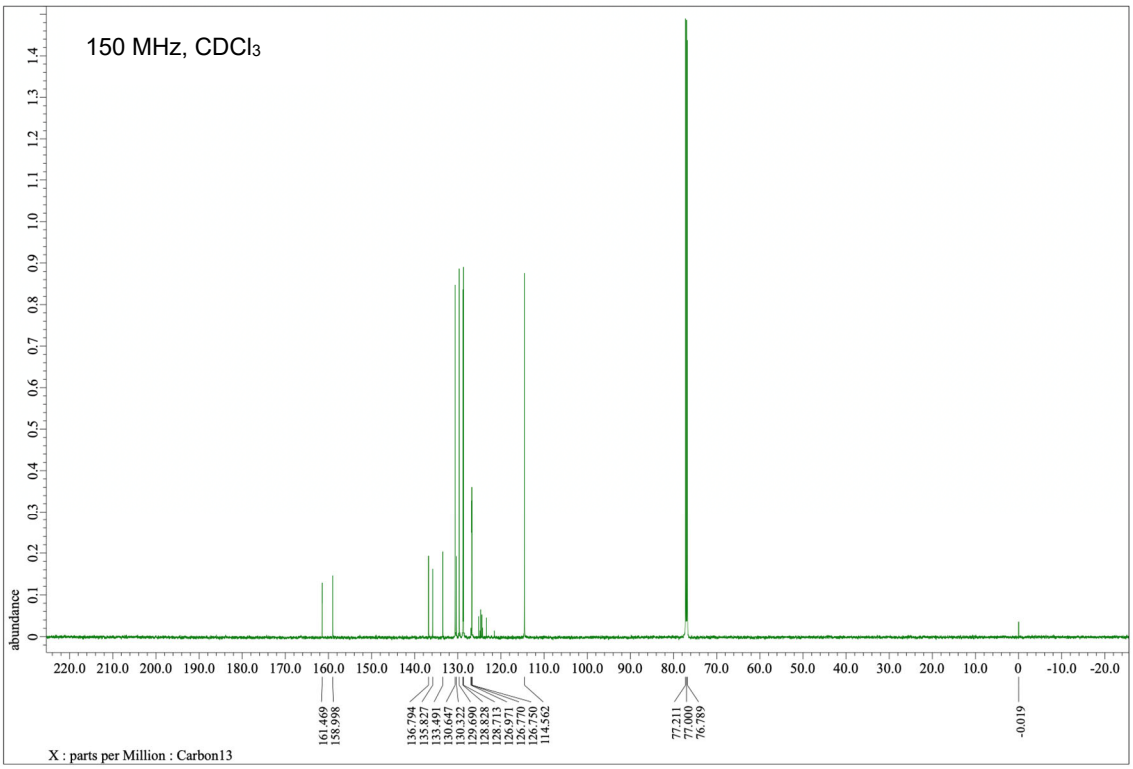

600 MHz, CDCl3
Ph
O
N
Ph
I
1ga
4.14
3.08
3.04
2.08
2.00
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.629 7.622 7.618 7.614 7.608 7.506 7.500 7.495 7.467 7.454 7.448 7.442 7.436 7.423 7.409 7.068 7.053
0.052
X : parts per Million : Proton

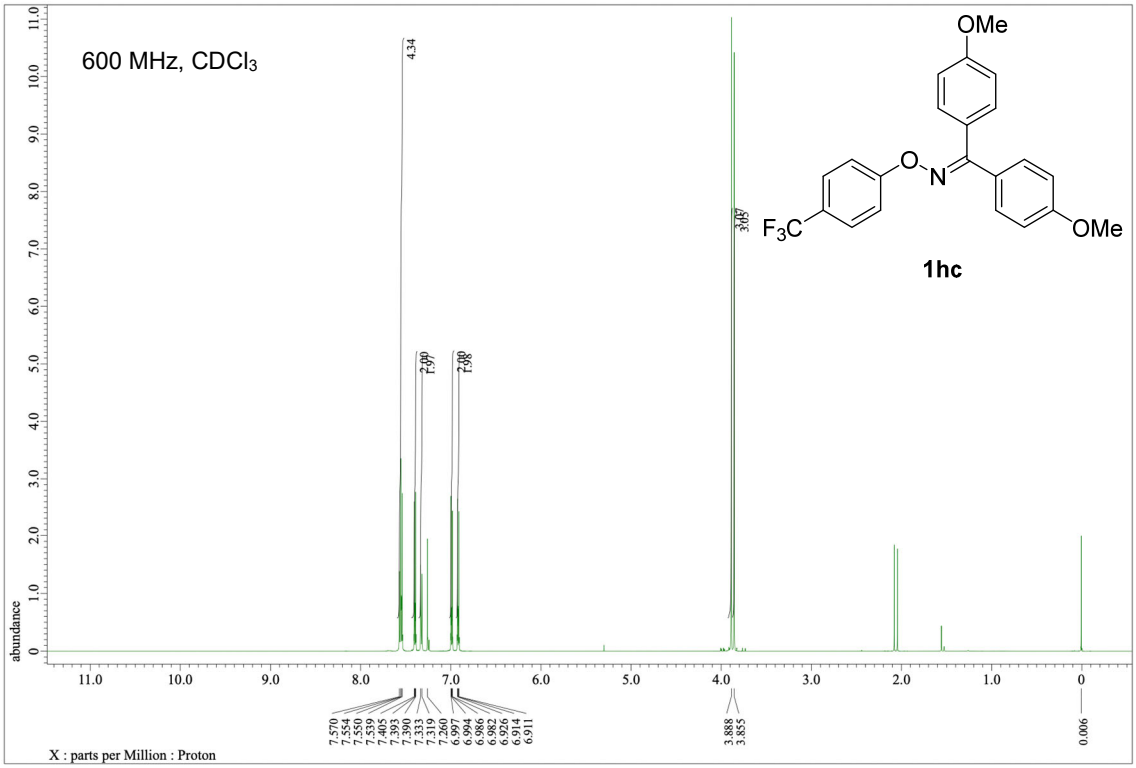

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
160.396 159.372
137.963 135.569 132.562 130.140 129.317 129.221 128.436 128.340 128.120 117.023
84.583 77.211 77.000 76.789
X : parts per Million : Carbon13

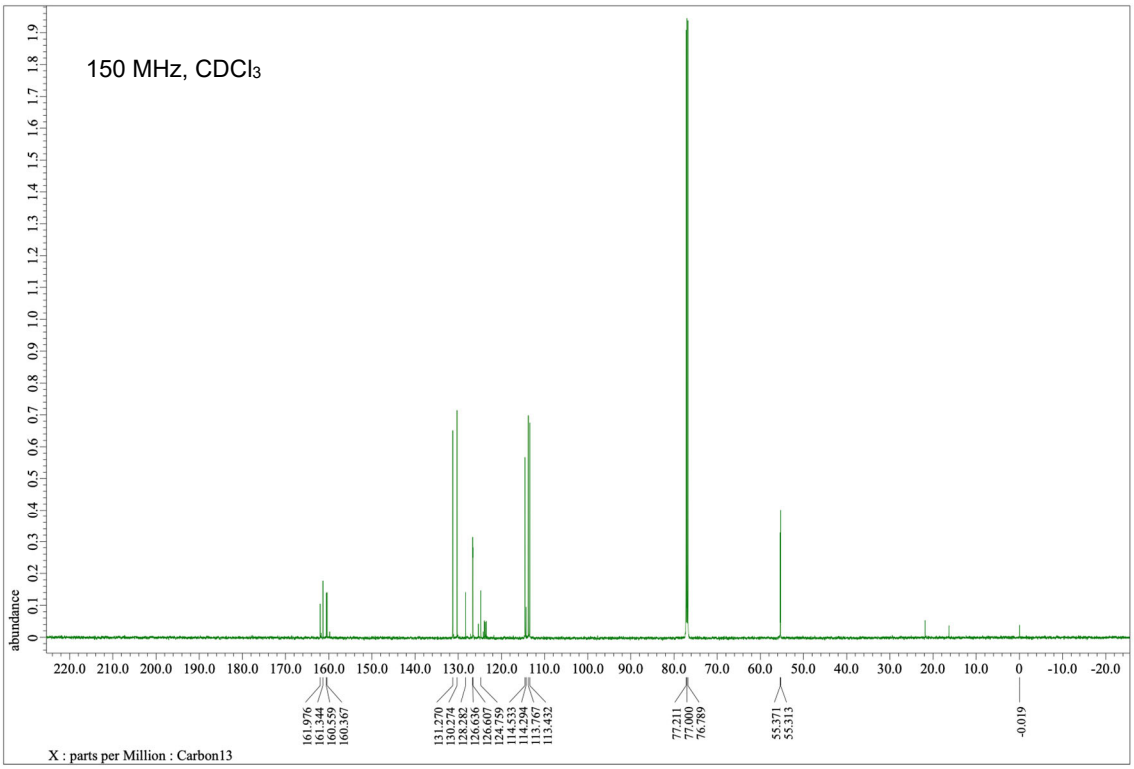

600 MHz, CDCl3
Ph
O
N
Ph
F3C
1ha
8.09
2.01
2.01
2.00
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.610
7.598
7.596
7.594
7.559
7.497
7.494
7.492
7.486
7.427
7.413
7.411
7.400
7.331
7.317
0.001
X : parts per Million : Proton

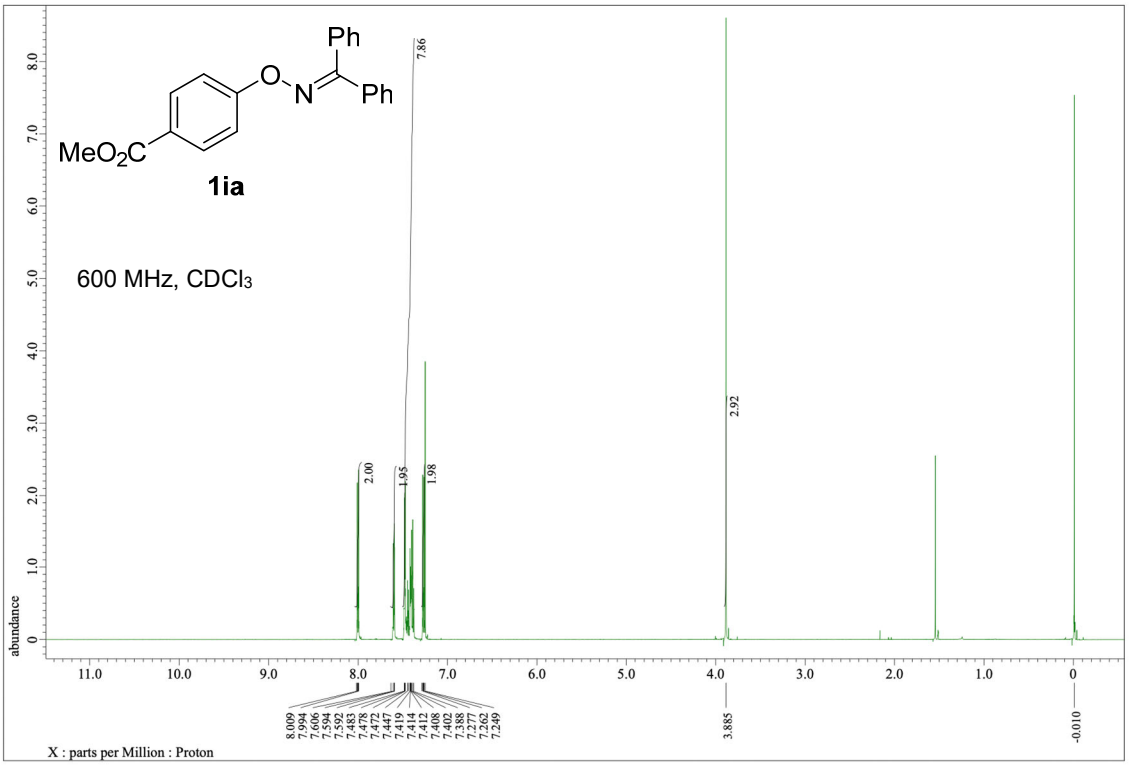

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
161.785
161.076
135.444
132.495
130.155
129.460
129.230
128.551
128.417
128.187
126.664
126.645
114.600
77.211
77.000
76.789
-0.019
X : parts per Million : Carbon13

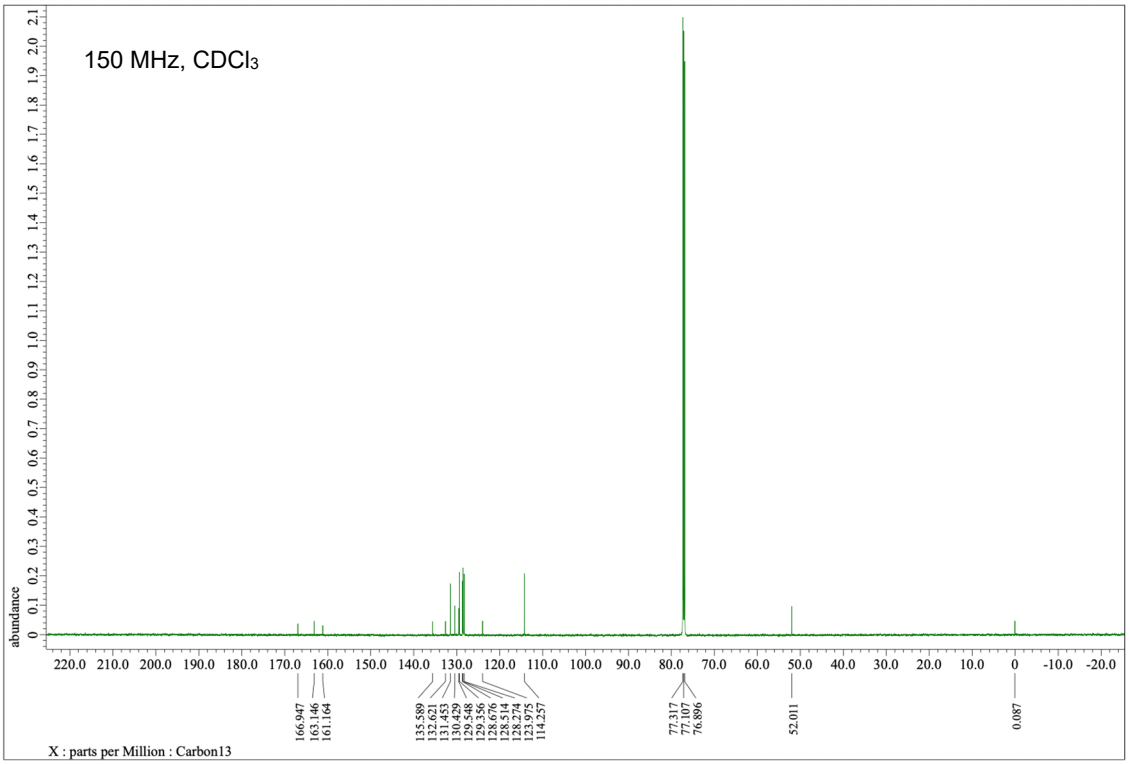

600 MHz, CDCl3
Cl
O
N
F3C
Cl
1hb
4.04
2.01
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.589 7.574 7.537 7.522 7.493 7.479 7.392 7.378 7.364 7.350 7.313 7.299 7.260
0.007
X : parts per Million : Proton

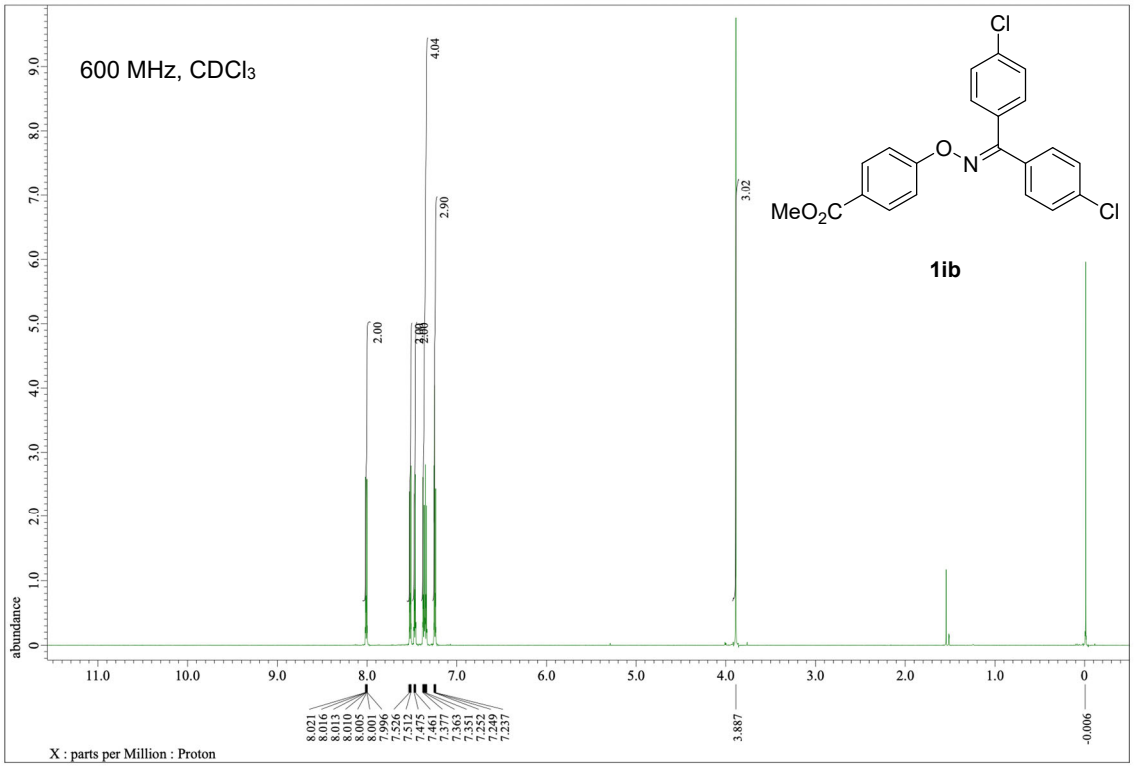

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
161.469 158.998
136.794 135.827 133.491 130.647 130.322 129.690 128.828 128.713 126.971 126.770 126.750 114.562
77.211 77.000 76.789
-0.019
X : parts per Million : Carbon13

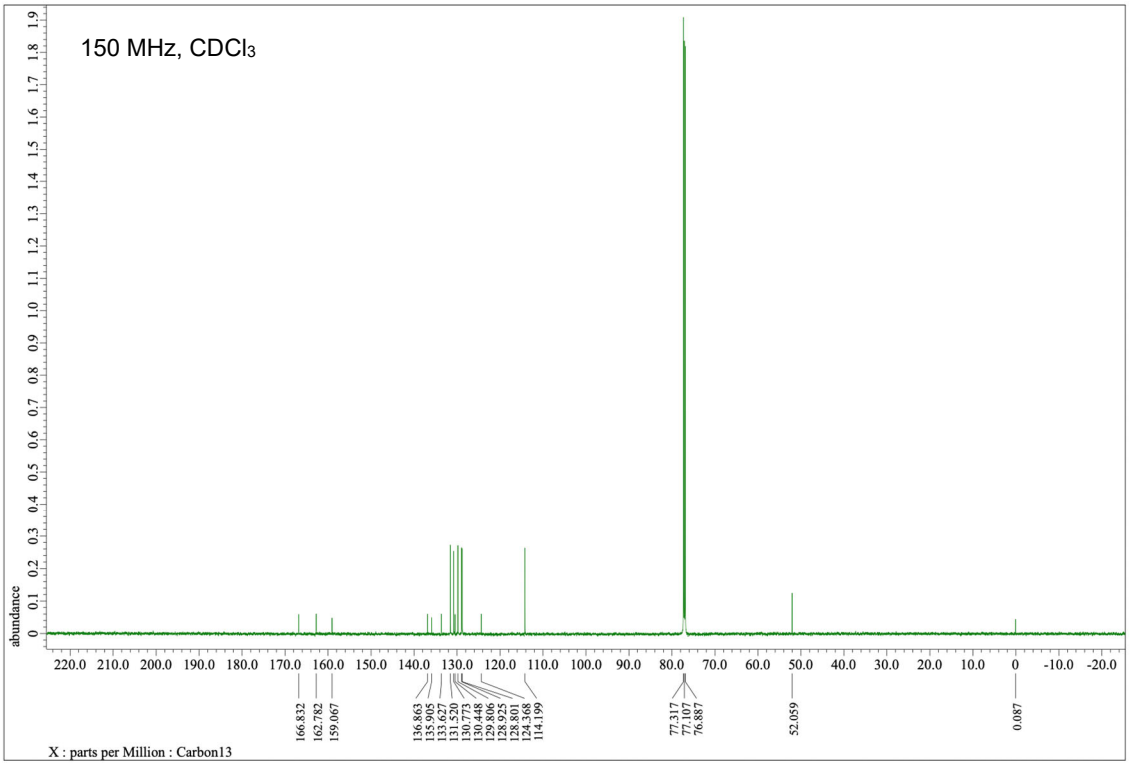

600 MHz, CDCl3
OMe
O
N
F3C
OMe
1hc
abundance
X : parts per Million : Proton

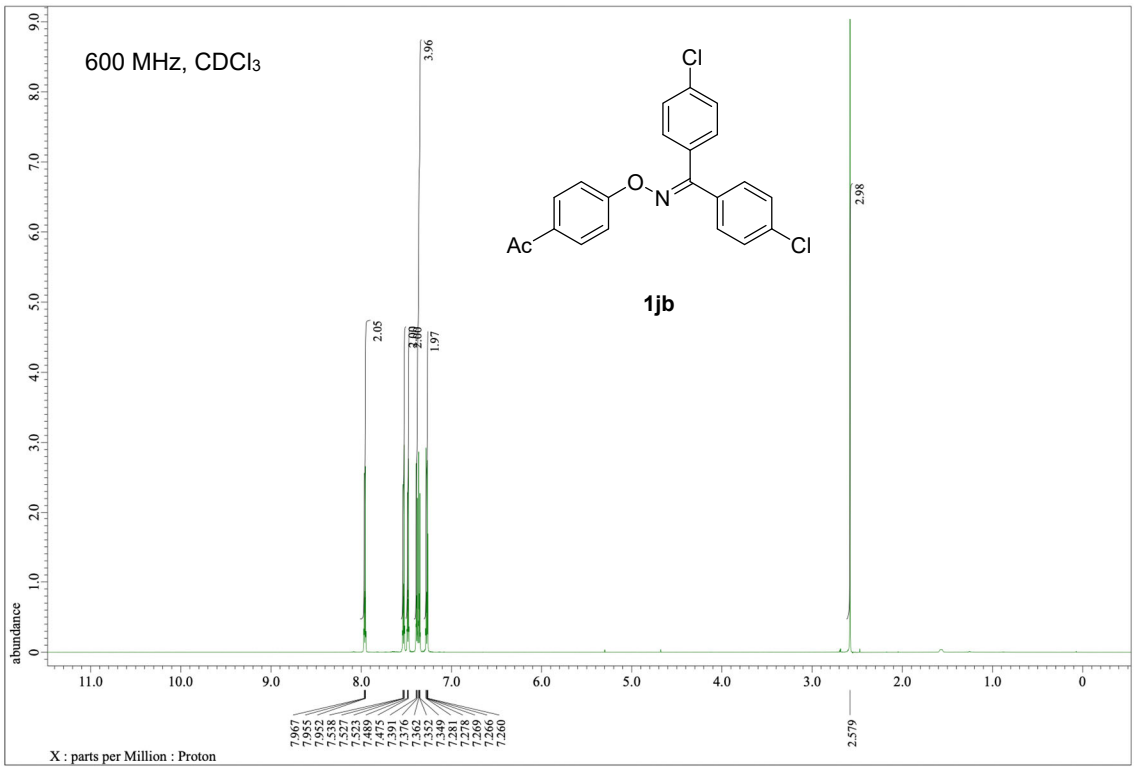

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

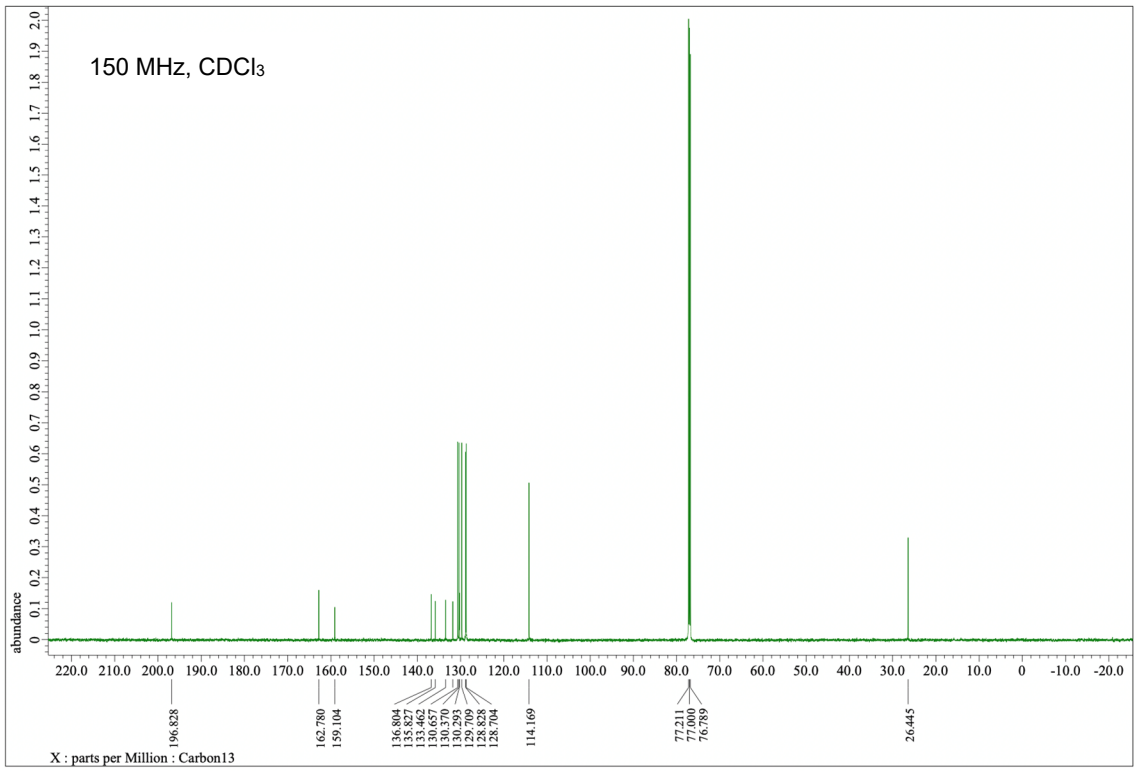

Ph
O
N
Ph
MeO2C
1ia
600 MHz, CDCl3
7.86
2.92
2.00
1.95
1.98
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.009
7.994
7.606
7.594
7.592
7.483
7.478
7.472
7.447
7.419
7.414
7.412
7.408
7.402
7.388
7.277
7.260
7.249
3.885
-0.010
X : parts per Million : Proton

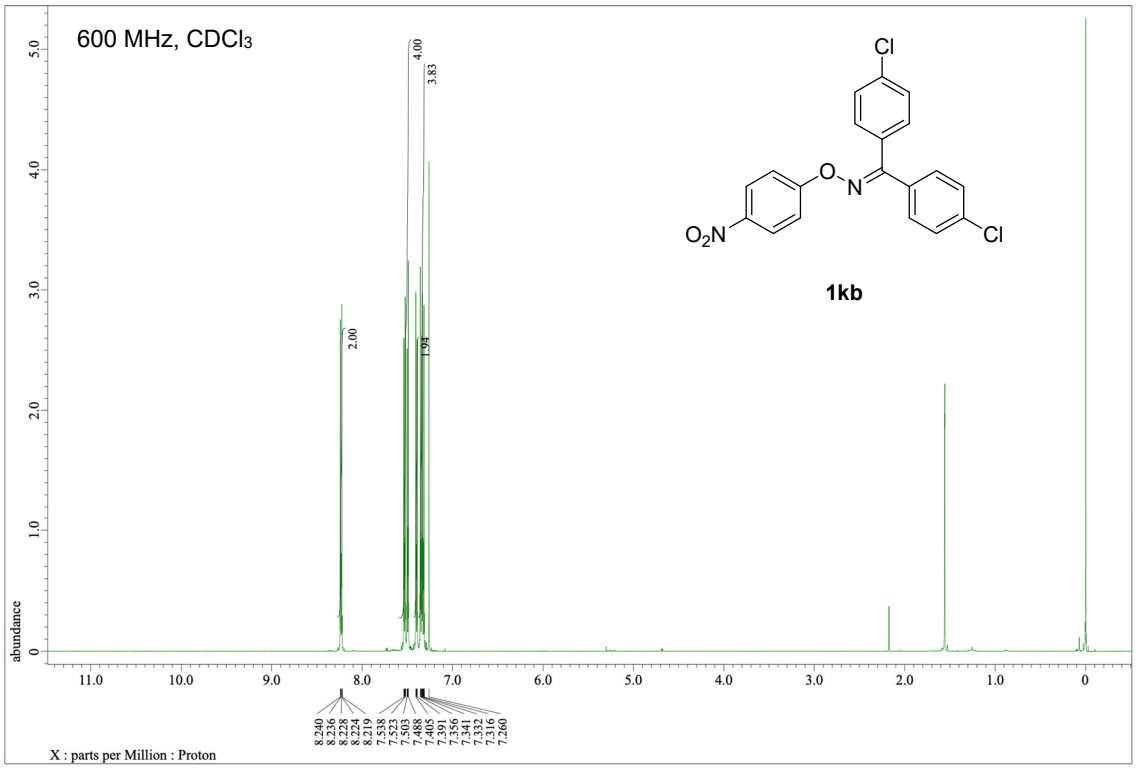

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
166.947
163.146
161.164
135.589
132.621
131.453
130.448
129.548
129.356
128.676
128.514
128.274
123.975
114.257
77.317
77.107
76.896
52.011
0.087
X : parts per Million : Carbon13

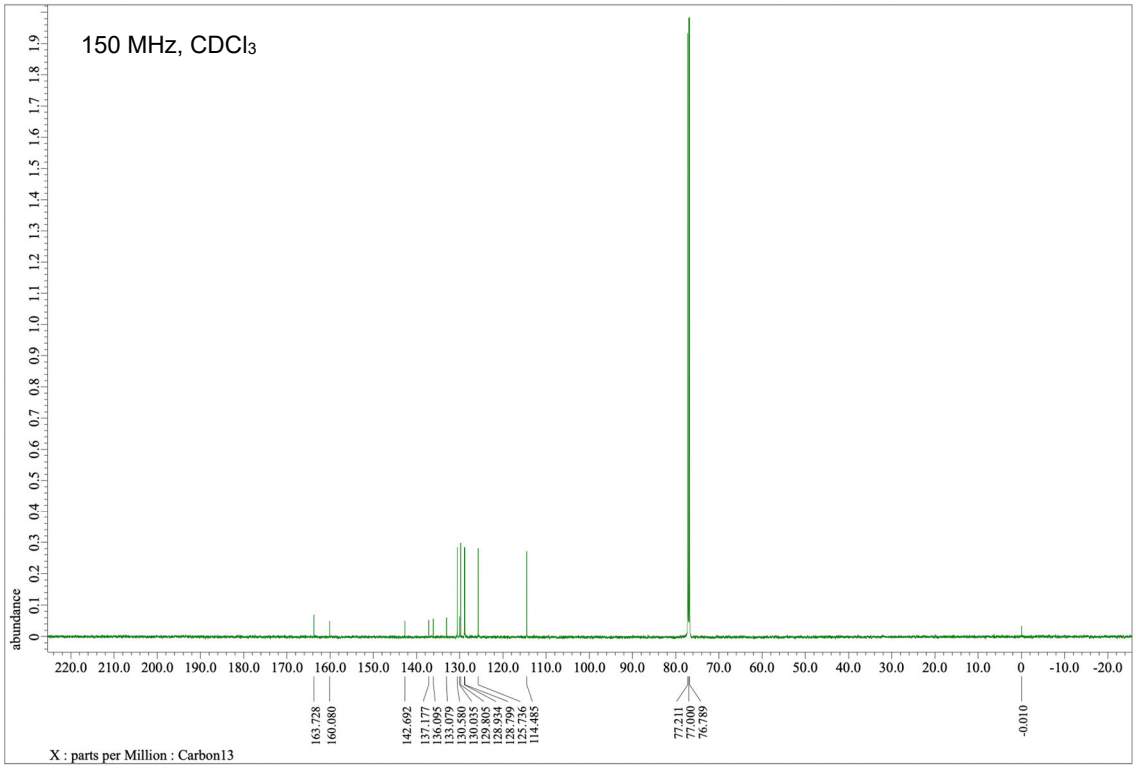

600 MHz, CDCl3
Cl
O
N
MeO2C
Cl
1ib
4.04
3.02
2.90
2.00
abundance
X : parts per Million : Proton
8.021
8.016
8.013
8.010
8.005
8.001
7.996
7.526
7.512
7.475
7.466
7.377
7.363
7.351
7.252
7.249
7.237
3.887
-0.006

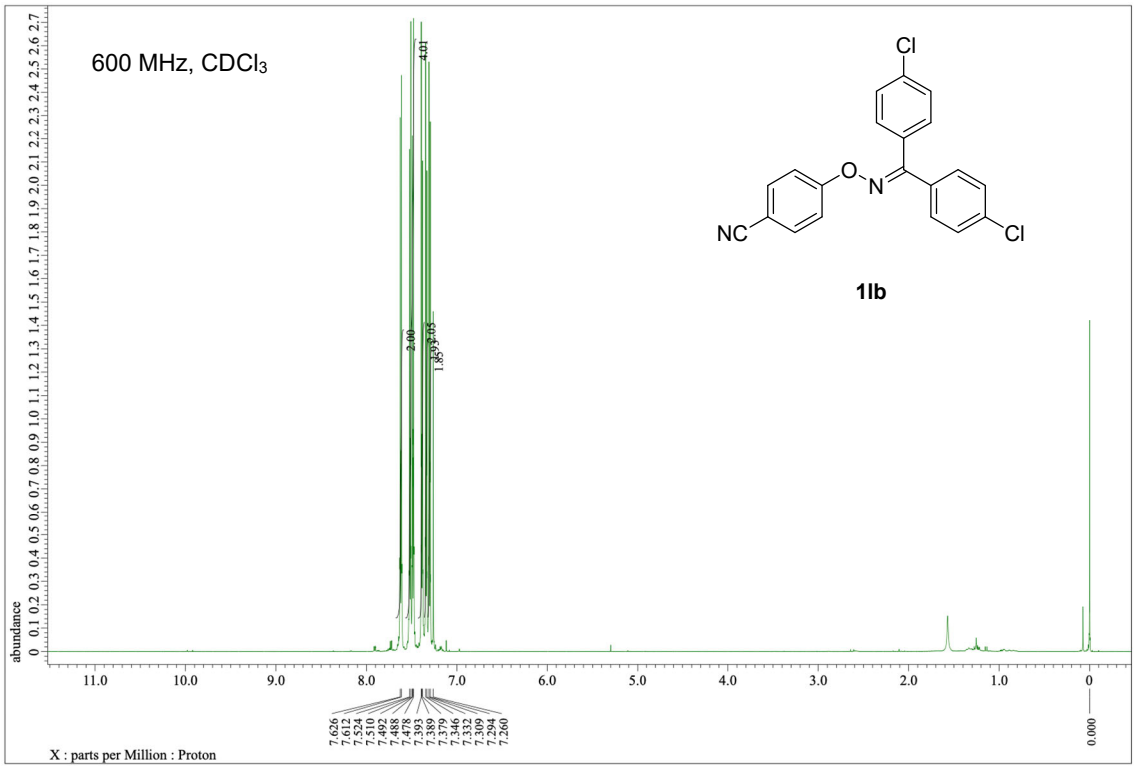

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13
166.832
162.782
159.067
136.865
135.905
135.227
131.520
130.773
130.448
129.806
128.925
128.301
124.468
114.199
77.317
77.107
76.887
52.059
0.087

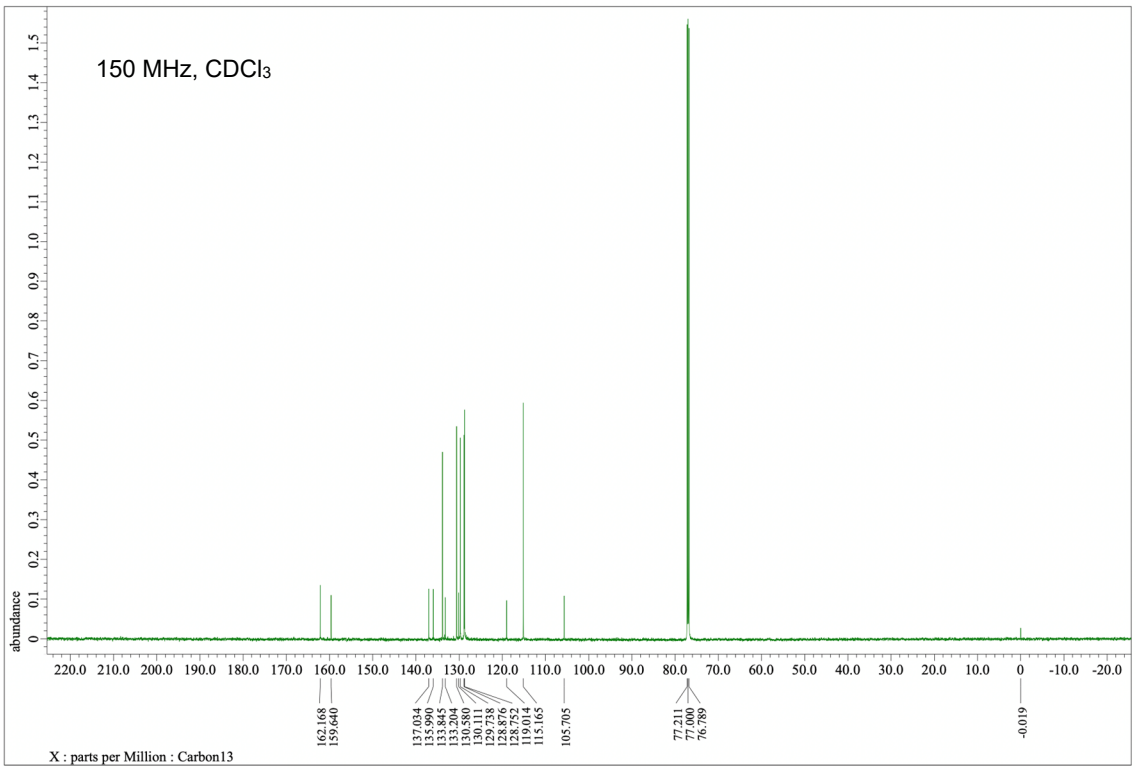

600 MHz, CDCl3
Cl
O
N
Ac
Cl
1jb
3.96
2.98
2.05
1.97
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.967
7.955
7.952
7.538
7.527
7.523
7.489
7.475
7.391
7.376
7.362
7.352
7.349
7.281
7.278
7.269
7.266
7.260
2.579
X : parts per Million : Proton

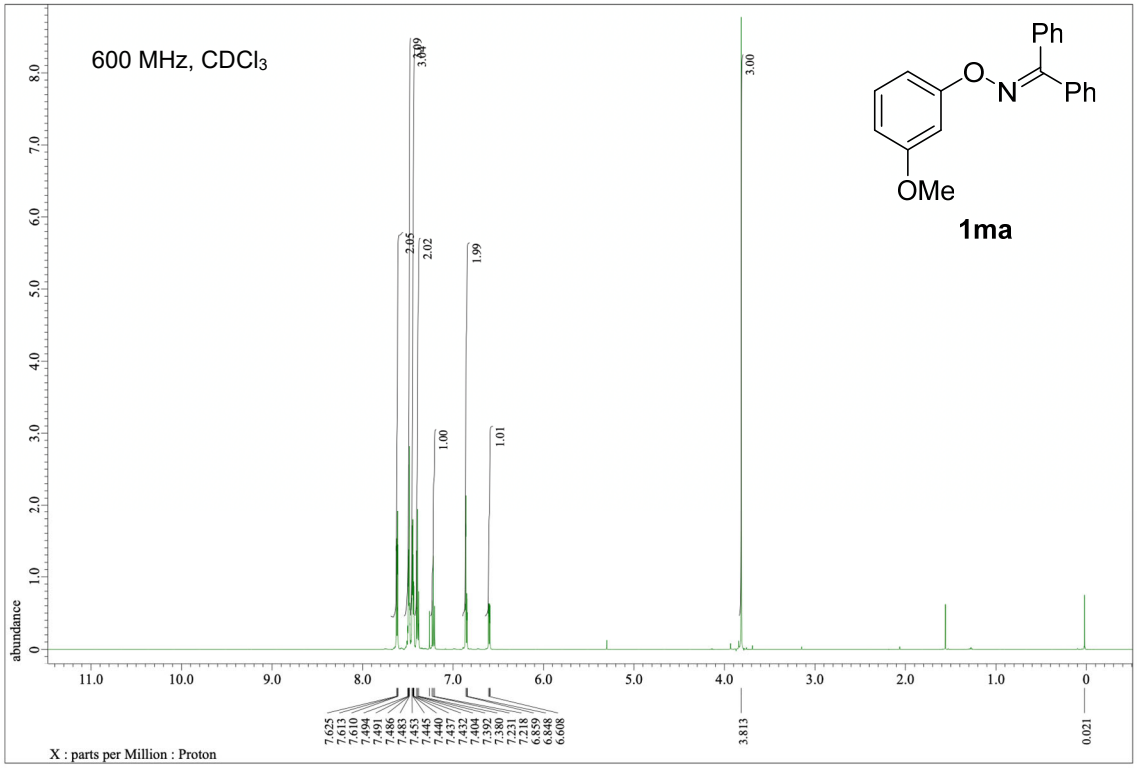

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
196.828
162.780
159.104
136.804
135.827
133.462
130.657
130.370
130.293
129.709
128.828
128.704
114.169
77.211
77.000
76.789
26.445
X : parts per Million : Carbon13

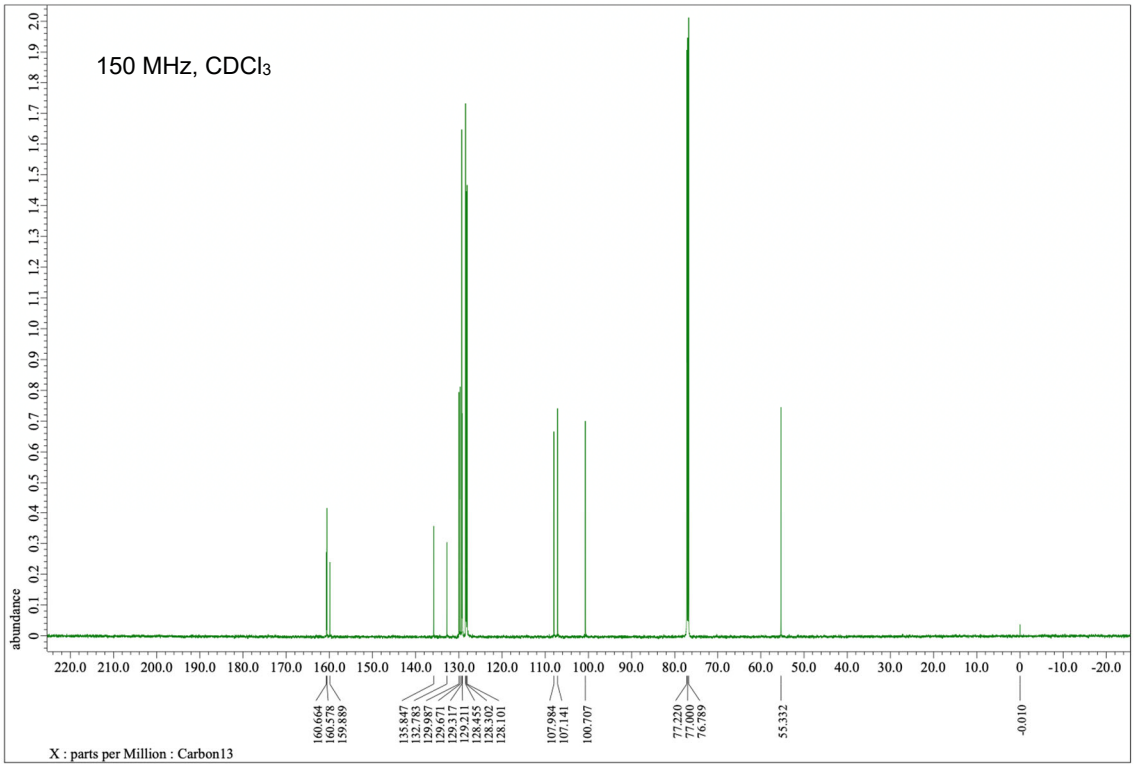

600 MHz, CDCl3
Cl
O
N
O2N
Cl
1kb
4.00
3.83
2.00
1.94
abundance
X : parts per Million : Proton

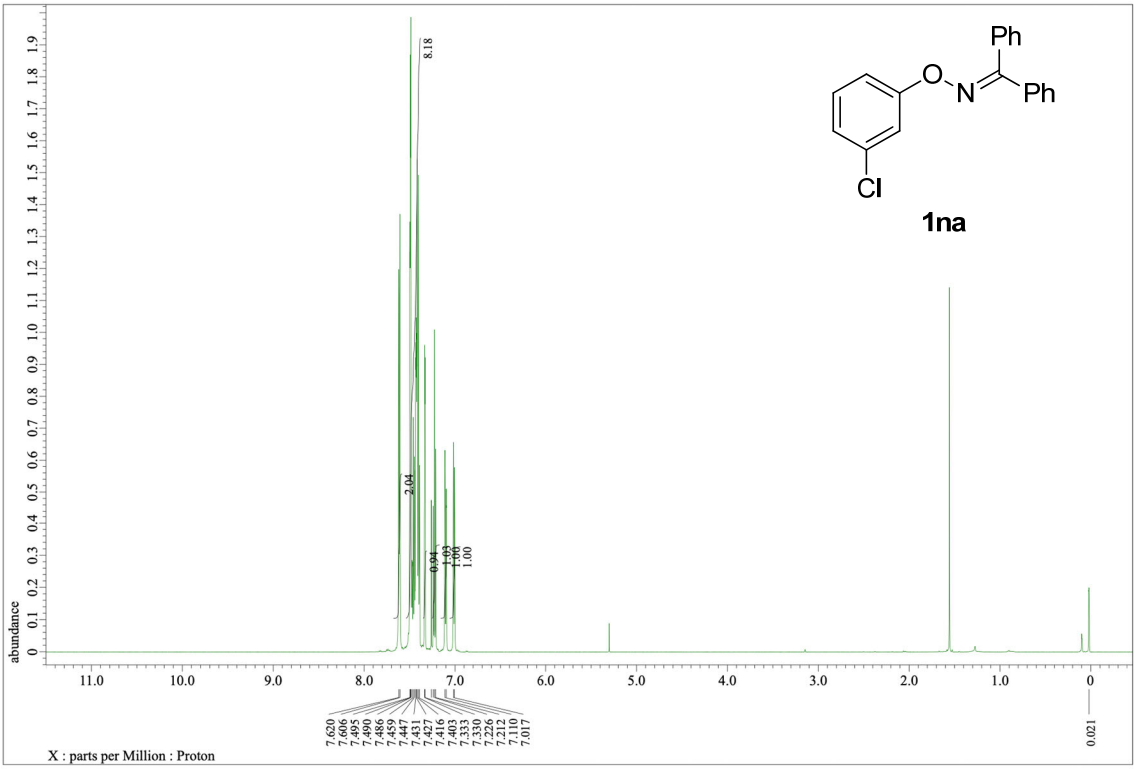

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

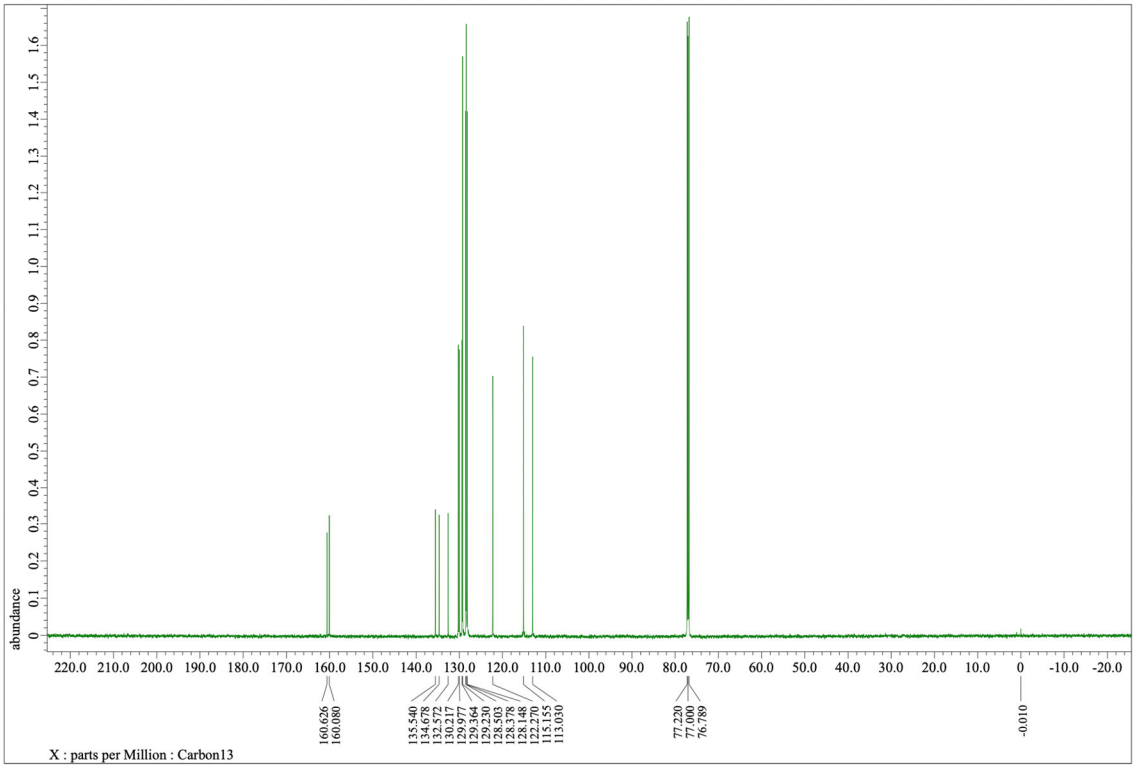

600 MHz, CDCl3
Cl
O
N
NC
Cl
1lb
abundance
X : parts per Million : Proton

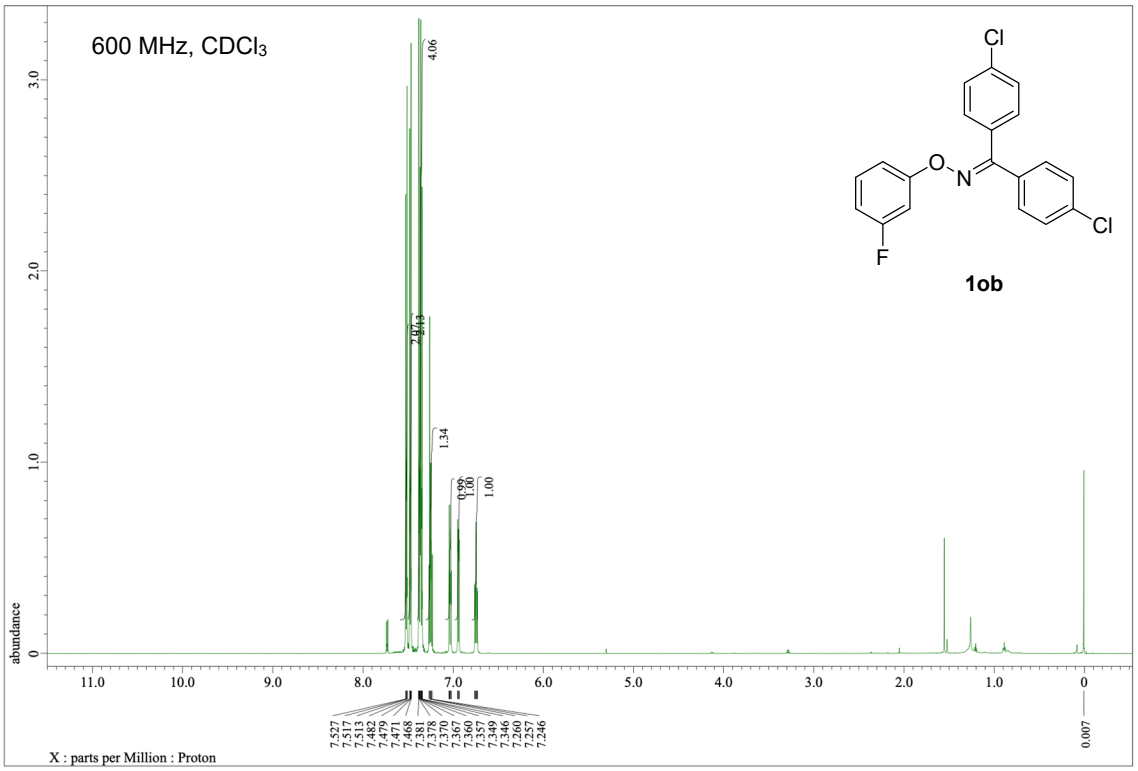

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

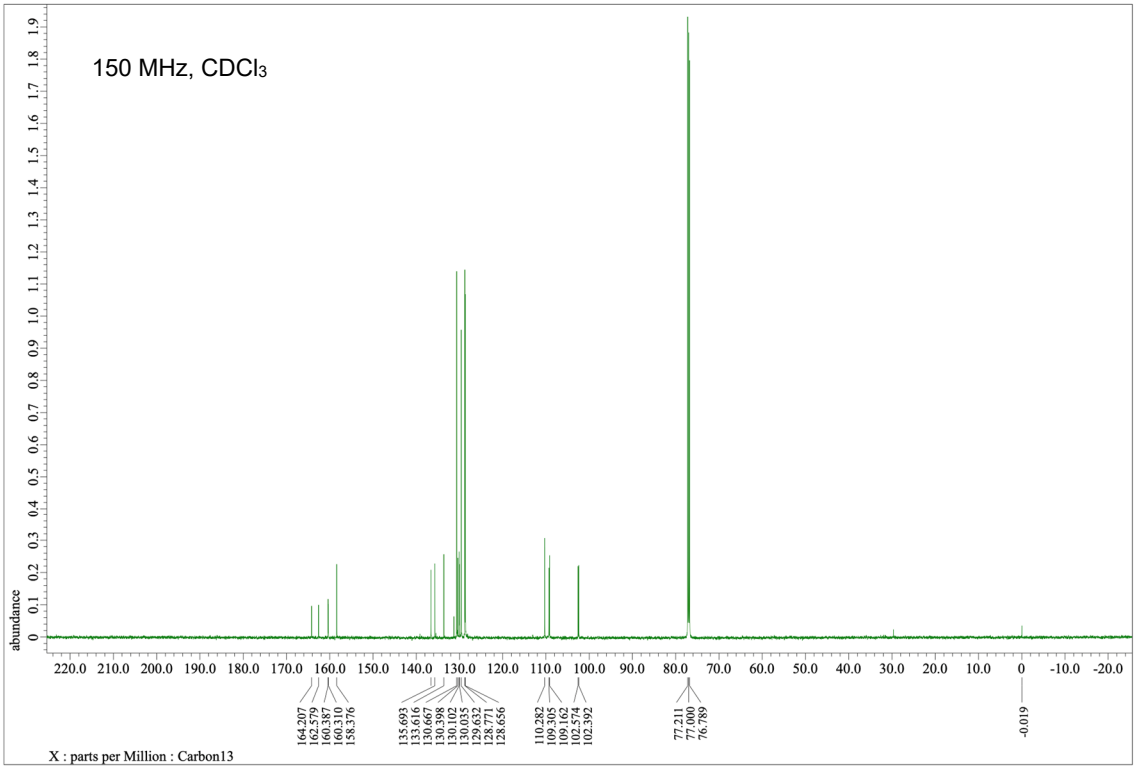

600 MHz, CDCl3
Ph
O
N
Ph
OMe
1ma
3.00
3.04
3.09
2.05
2.02
1.99
1.00
1.01
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.625 7.613 7.610 7.494 7.491 7.486 7.483 7.453 7.445 7.440 7.437 7.432 7.414 7.392 7.380 7.231 7.218 6.859 6.848 6.608
3.813
0.021
X : parts per Million : Proton

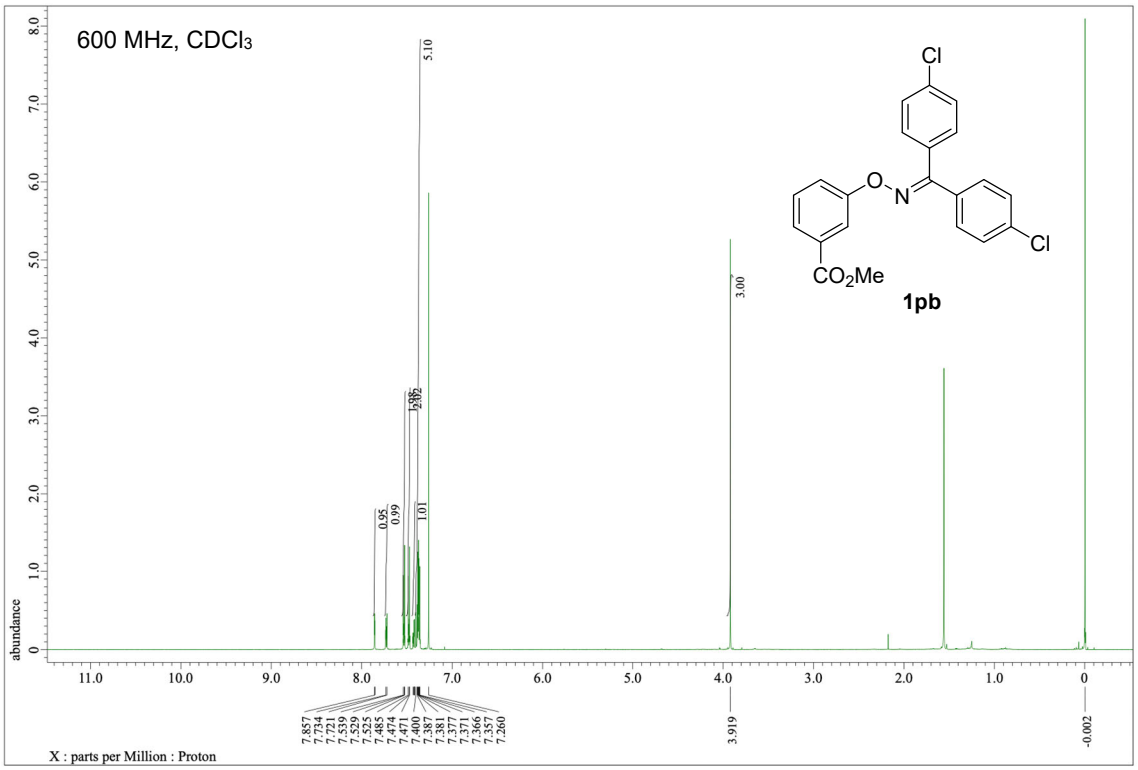

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
160.664 160.578 159.889
135.847 132.783 129.987 129.671 129.317 129.211 128.455 128.107 128.101
107.984 107.141
100.707
77.220 77.000 76.789
55.332
-0.010
X : parts per Million : Carbon13

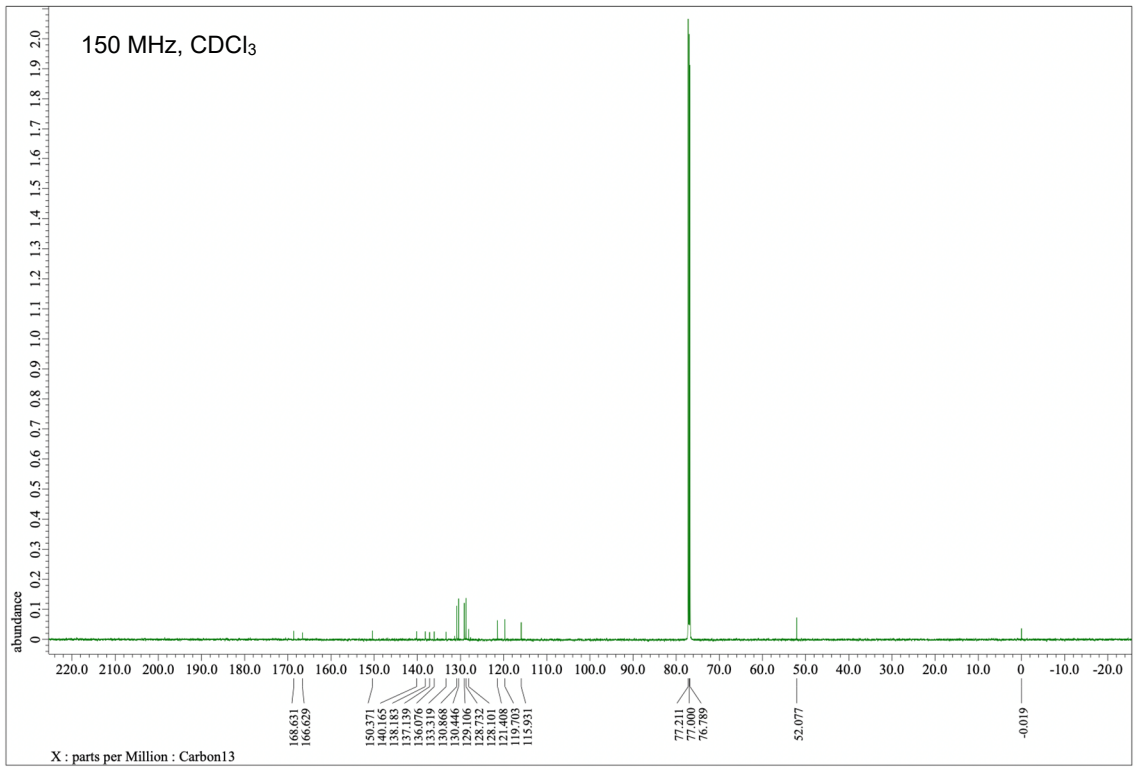

Ph
O
N
Ph
Cl
1na
8.18
2.04
0.94
1.43
1.00
1.00
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.620
7.606
7.495
7.490
7.486
7.459
7.447
7.431
7.427
7.416
7.403
7.333
7.330
7.226
7.212
7.110
7.017
0.021
X : parts per Million : Proton

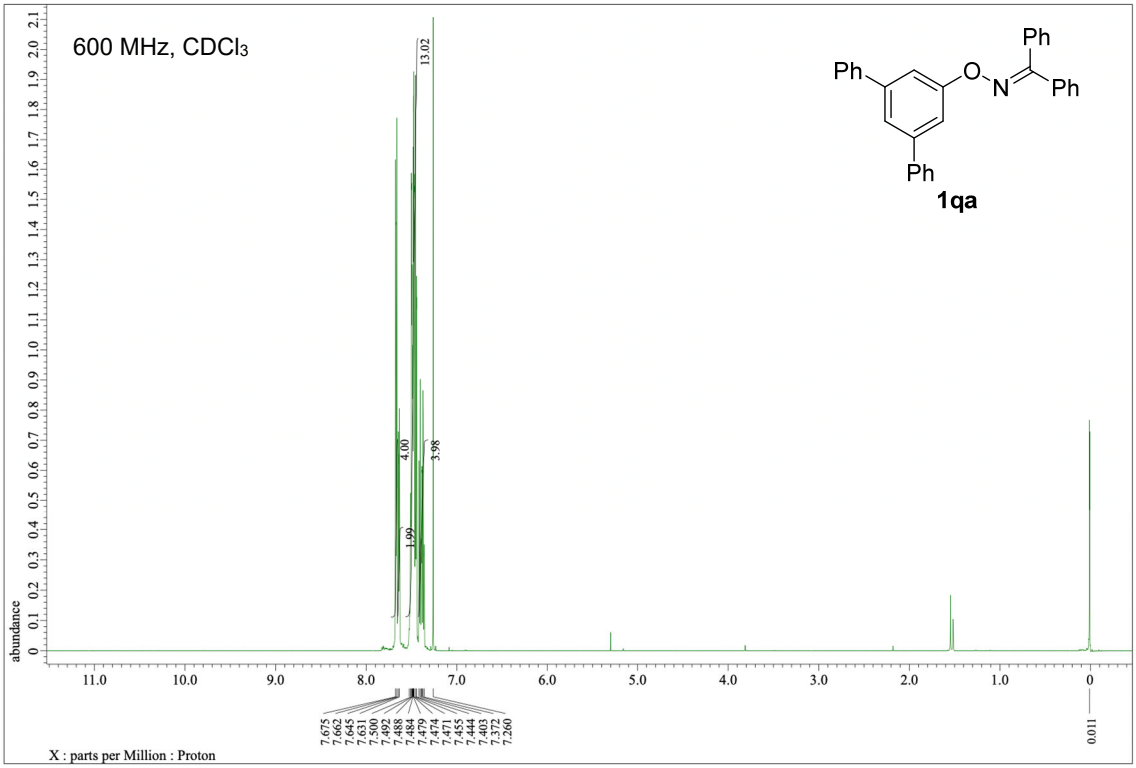

abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
160.626
160.080
135.540
134.678
132.572
130.217
129.964
129.377
129.230
128.503
128.378
128.148
122.270
115.155
113.030
77.220
77.000
76.789
-0.010
X : parts per Million : Carbon13

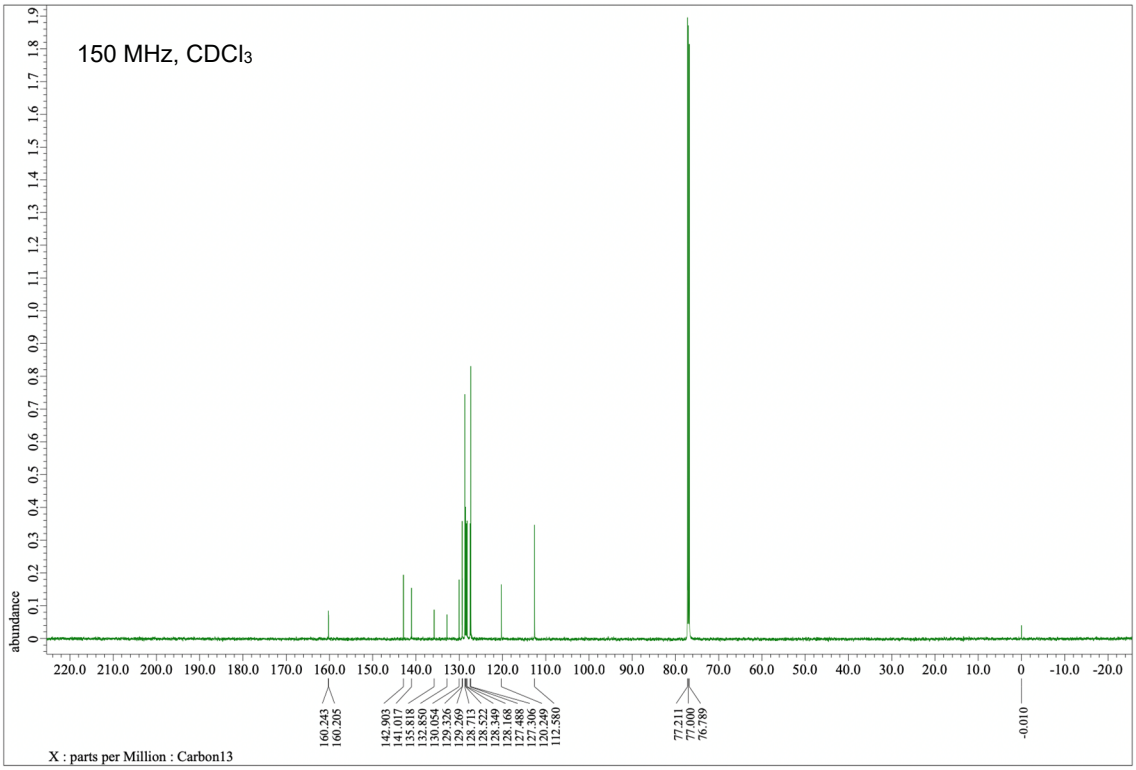

600 MHz, CDCl3
Cl
O
N
Cl
F
1ob
4.06
2.13
1.34
1.00
abundance
X : parts per Million : Proton

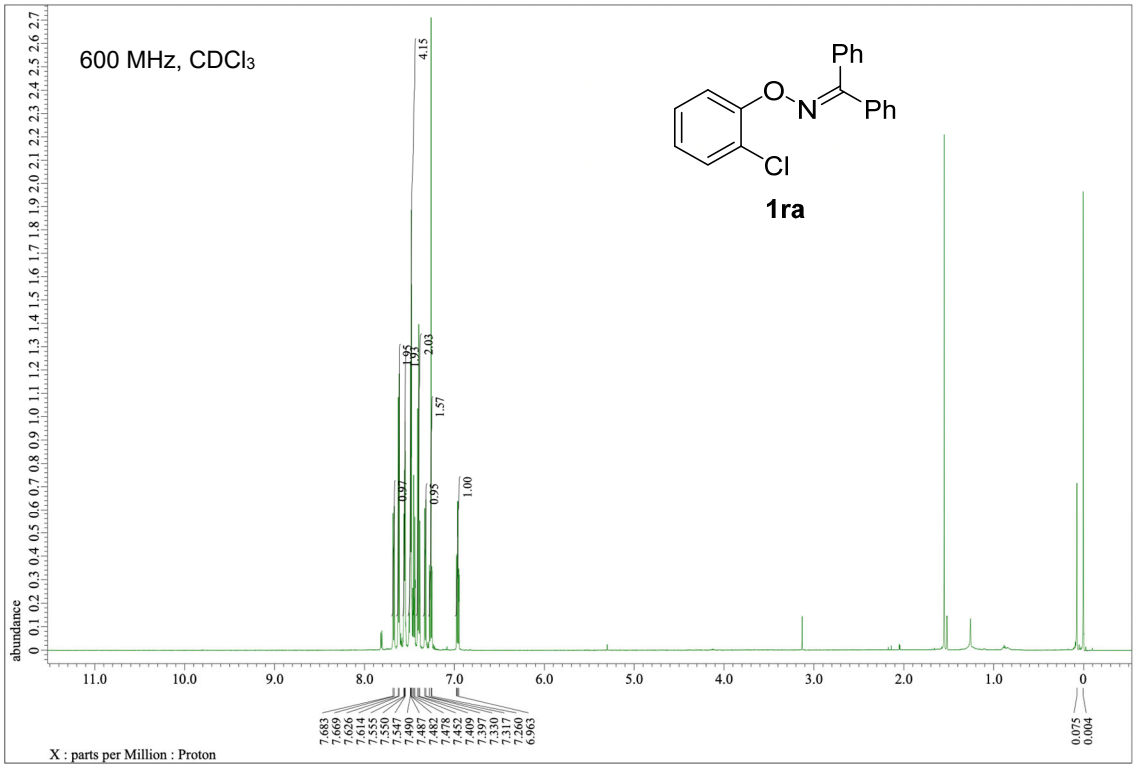

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

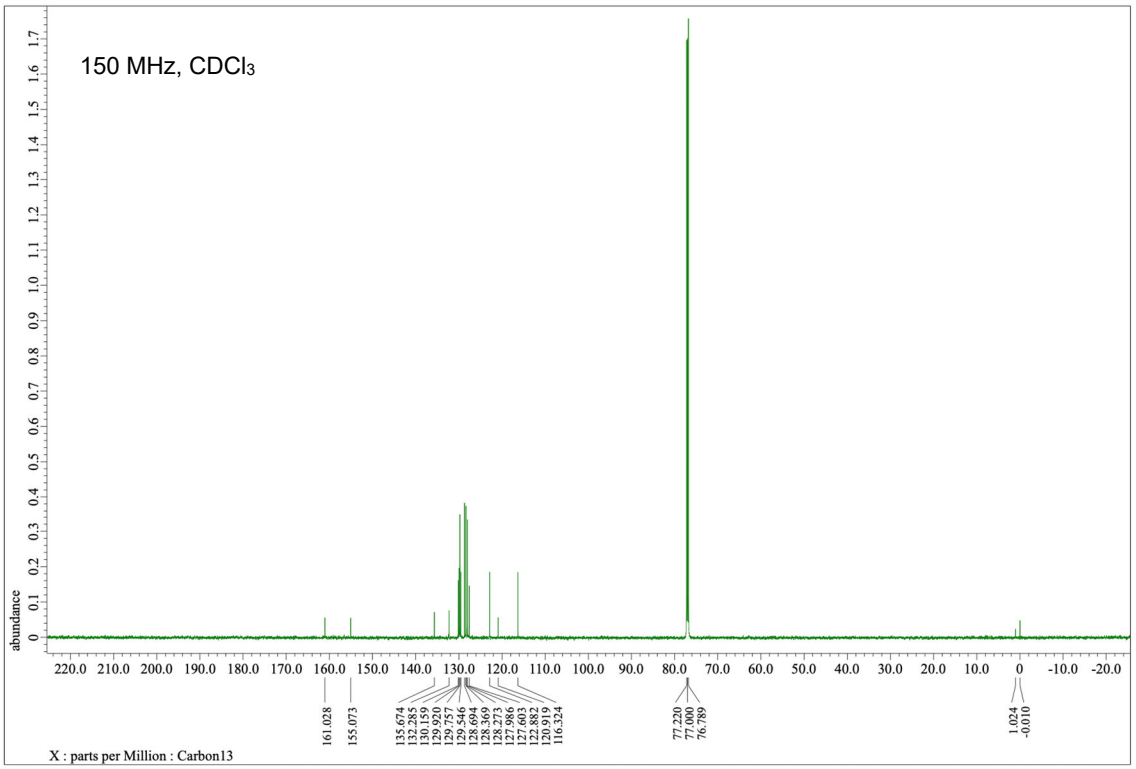

600 MHz, CDCl3
Cl
O
N
Cl
CO2Me
1pb
abundance
X : parts per Million : Proton

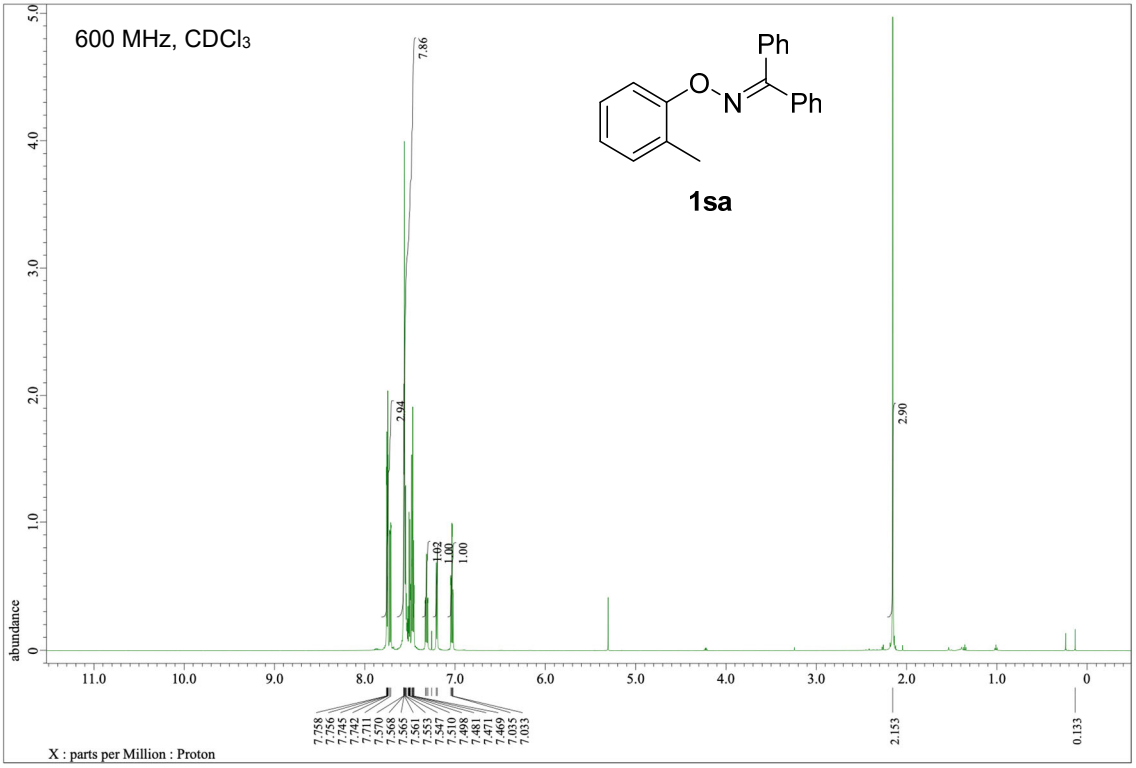

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

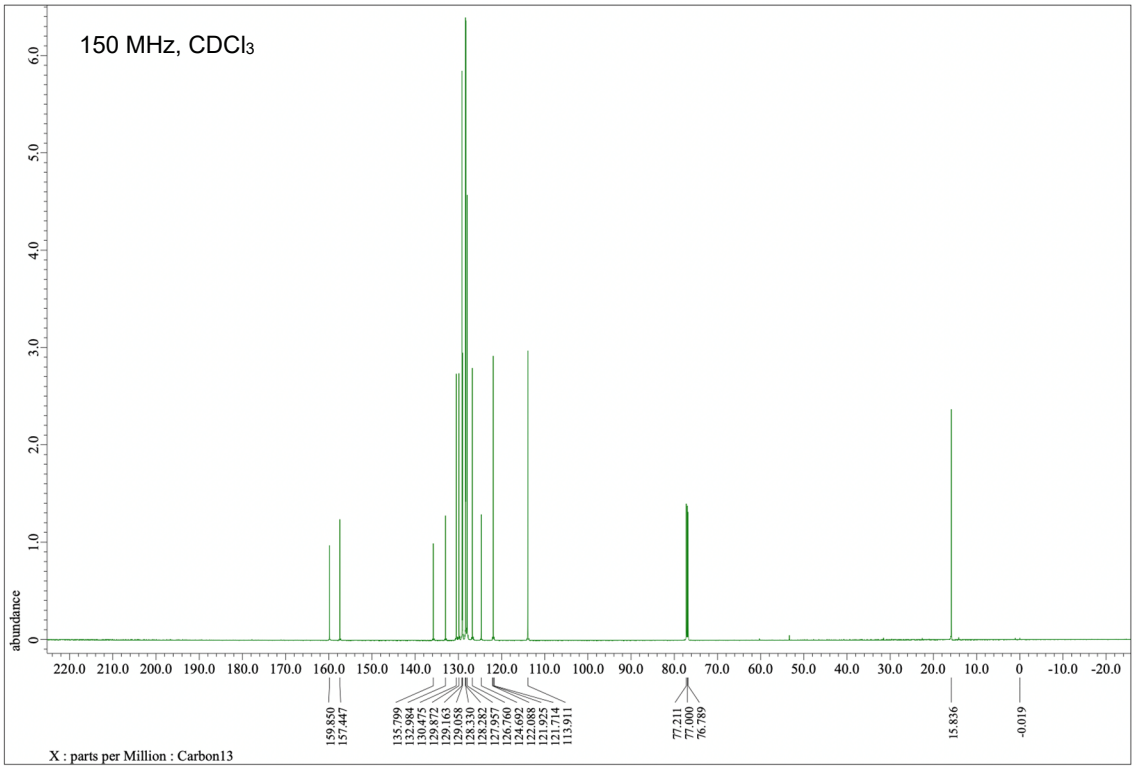

600 MHz, CDCl3
Ph
Ph
O
N
Ph
Ph
1qa
13.02
4.00
3.98
1.99
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.675
7.662
7.645
7.631
7.500
7.492
7.488
7.484
7.479
7.474
7.471
7.455
7.444
7.403
7.372
7.260
0.011
X : parts per Million : Proton


150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
160.243
160.205
142.903
141.017
135.818
132.850
130.054
129.326
129.269
128.713
128.522
128.349
128.168
127.488
127.306
120.249
112.580
77.211
77.000
76.789
-0.010
X : parts per Million : Carbon13

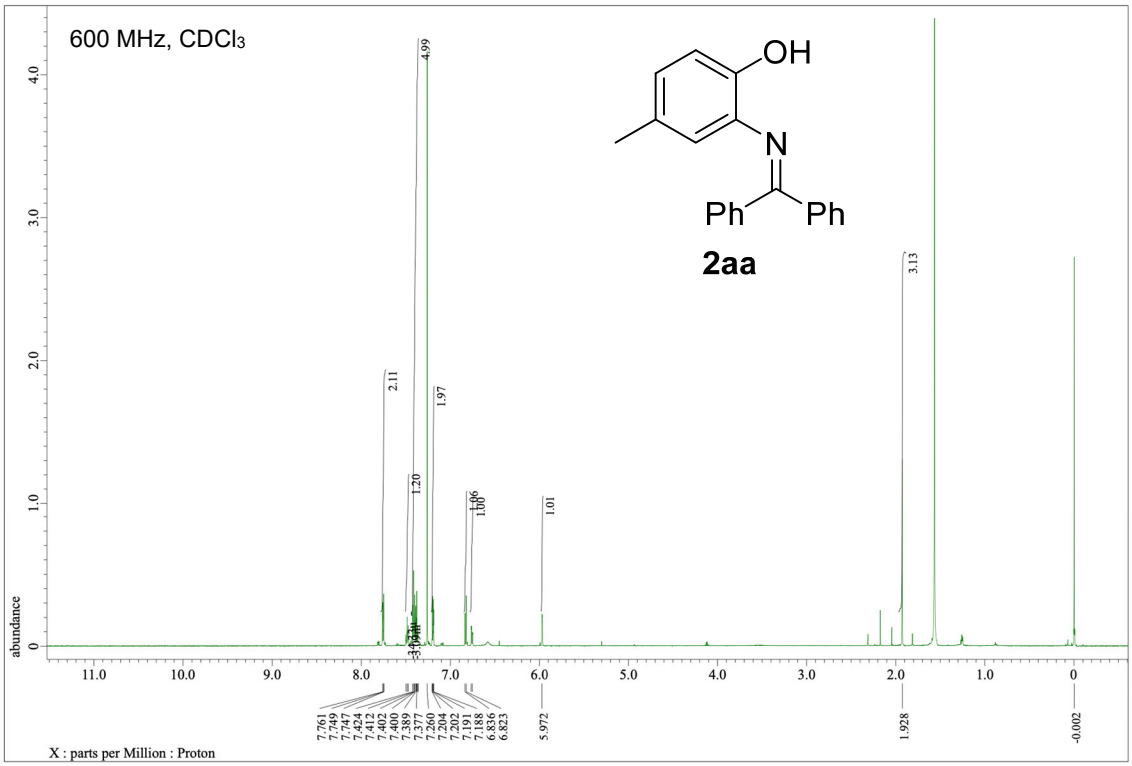

600 MHz, CDCl3
Ph
O
N
Ph
Cl
1ra
4.15
2.03
1.95
1.93
1.57
1.00
0.97
0.95
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.683
7.669
7.626
7.614
7.555
7.550
7.547
7.490
7.487
7.482
7.478
7.452
7.409
7.397
7.330
7.317
7.260
6.965
0.075
0.004
X : parts per Million : Proton

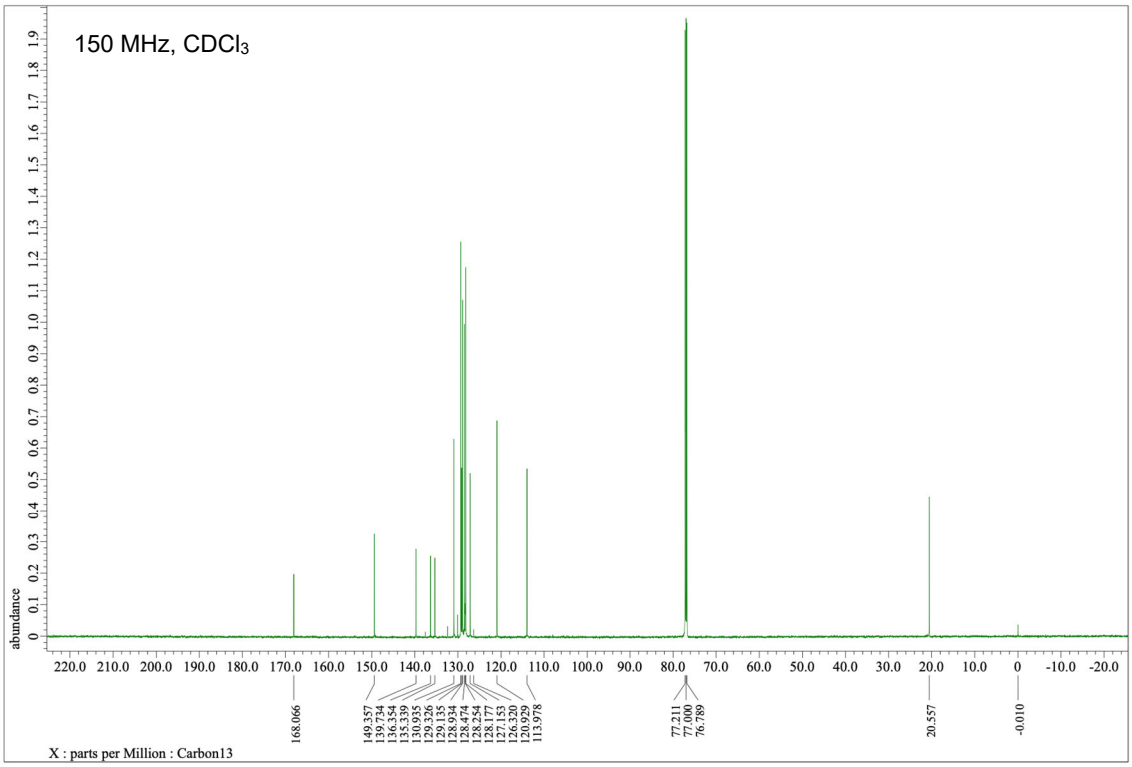

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
161.028
155.073
135.674
132.285
130.159
129.920
129.757
129.546
129.264
128.369
128.273
127.986
127.603
122.882
120.919
116.324
77.220
77.000
76.789
1.024
-0.010
X : parts per Million : Carbon13

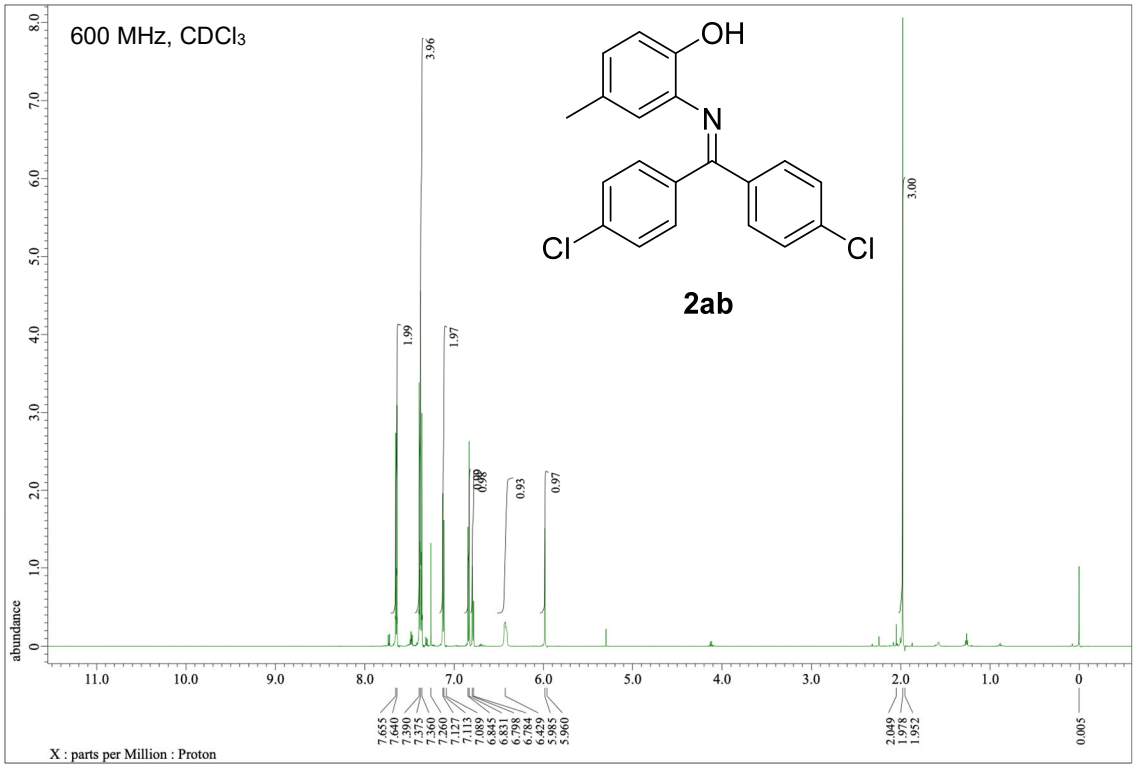

600 MHz, CDCl3
Ph
O
N
Ph
1sa
7.86
2.94
2.90
1.02
1.00
1.00
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.758 7.756 7.745 7.742 7.711 7.570 7.568 7.565 7.561 7.553 7.547 7.510 7.498 7.481 7.471 7.469 7.035 7.033
2.153
0.133
X : parts per Million : Proton

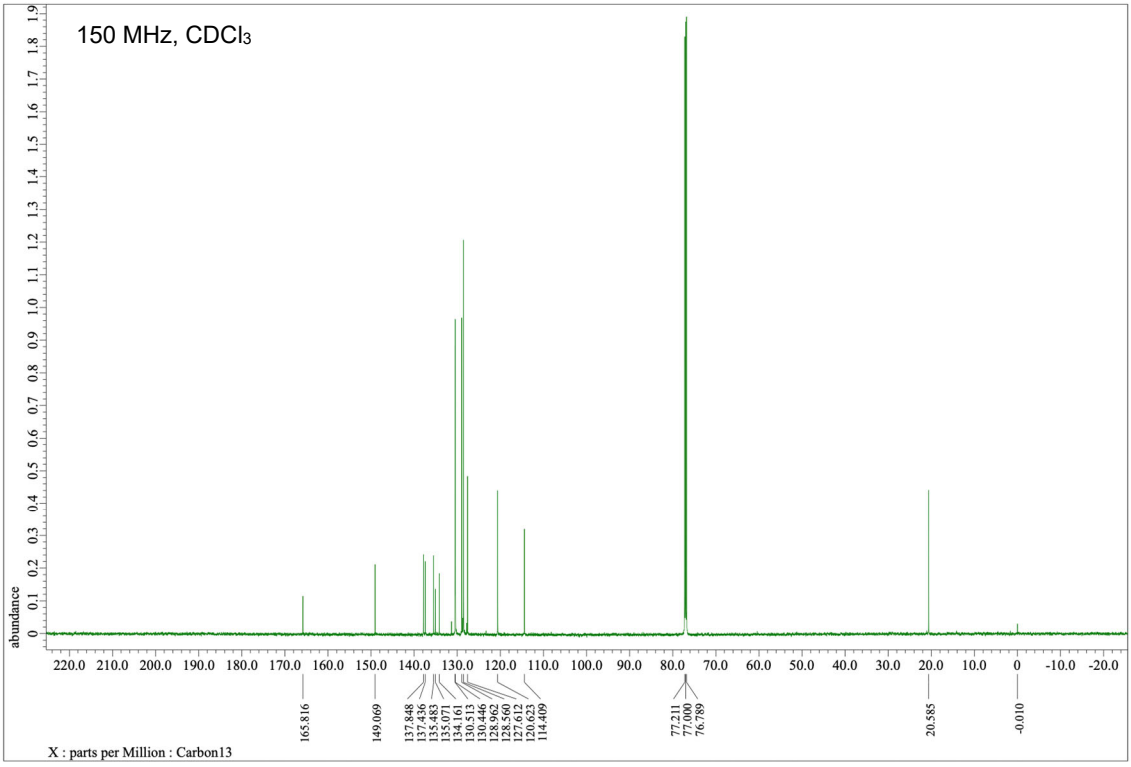

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
159.850 157.447 135.799 132.984 130.475 129.872 129.165 129.058 128.330 128.282 127.957 126.760 124.692 121.928 121.714 113.911
77.211 77.000 76.789
15.836
-0.019
X : parts per Million : Carbon13

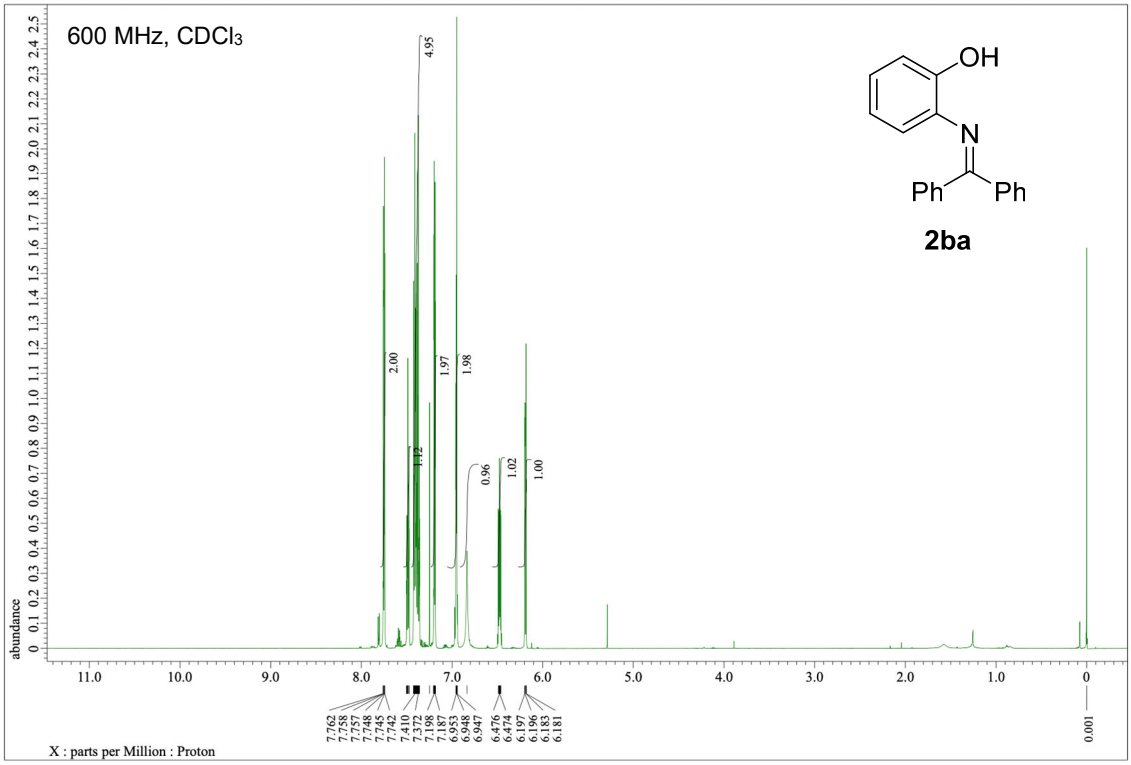
14. ^{1}H and ^{13}C NMR chart of 2

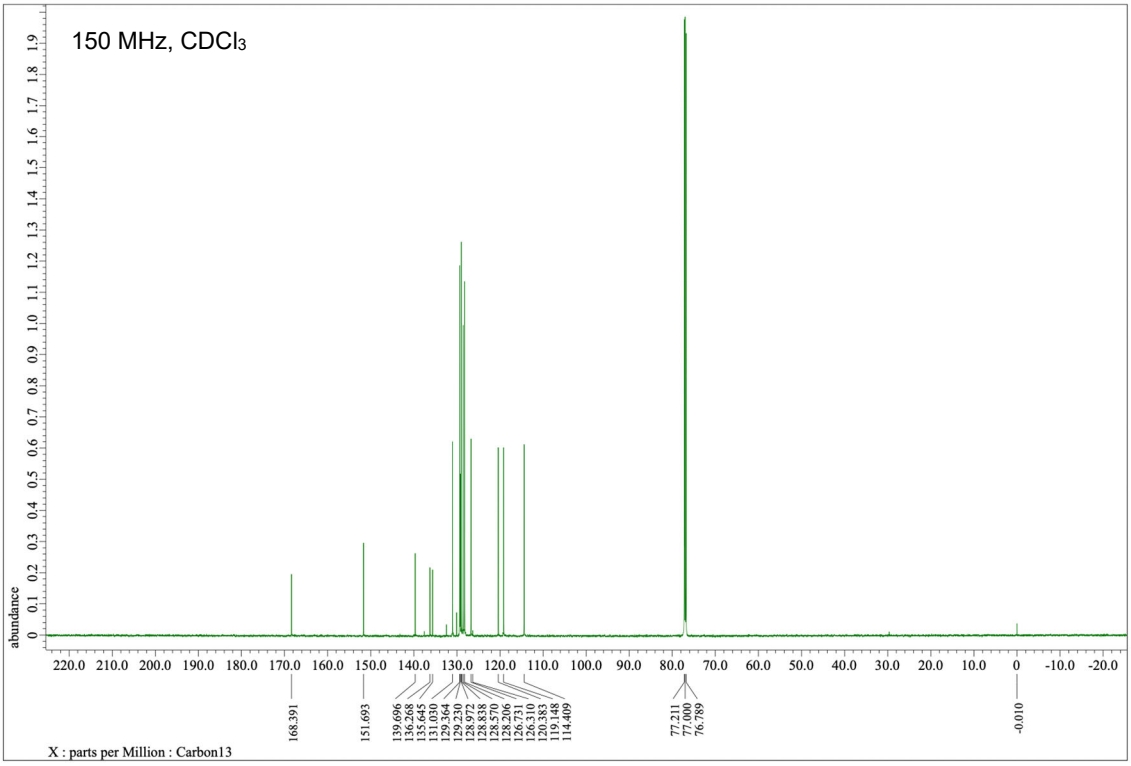


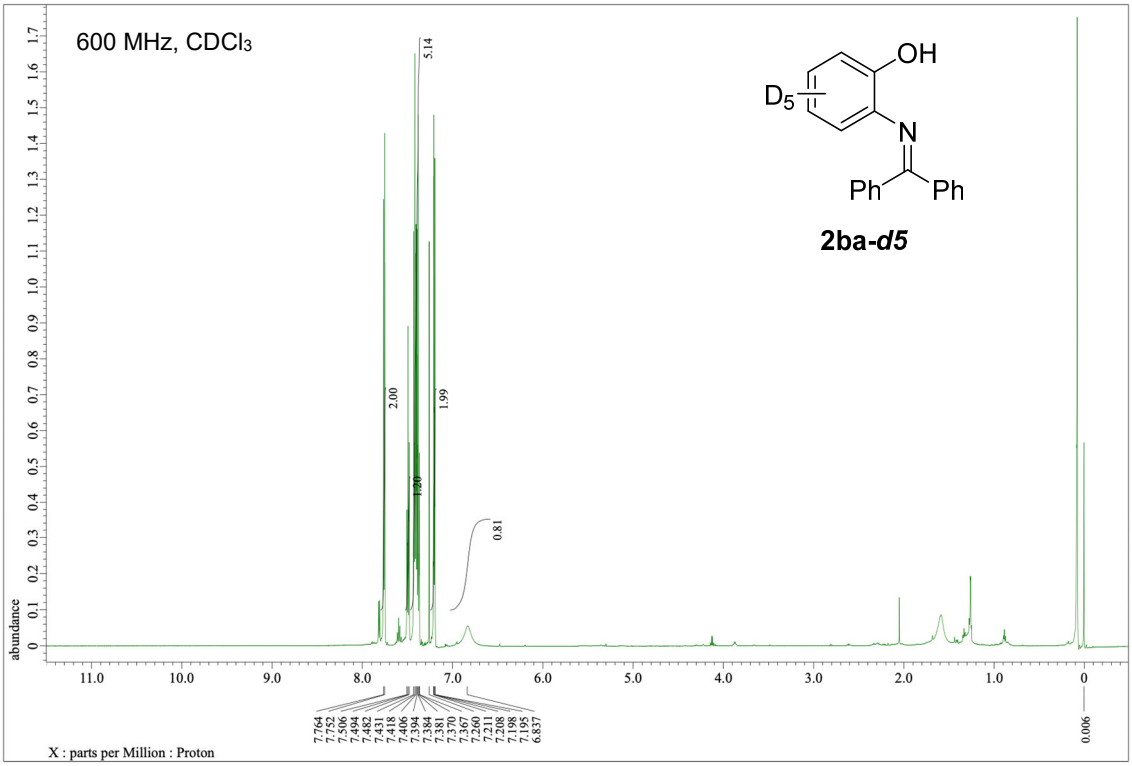


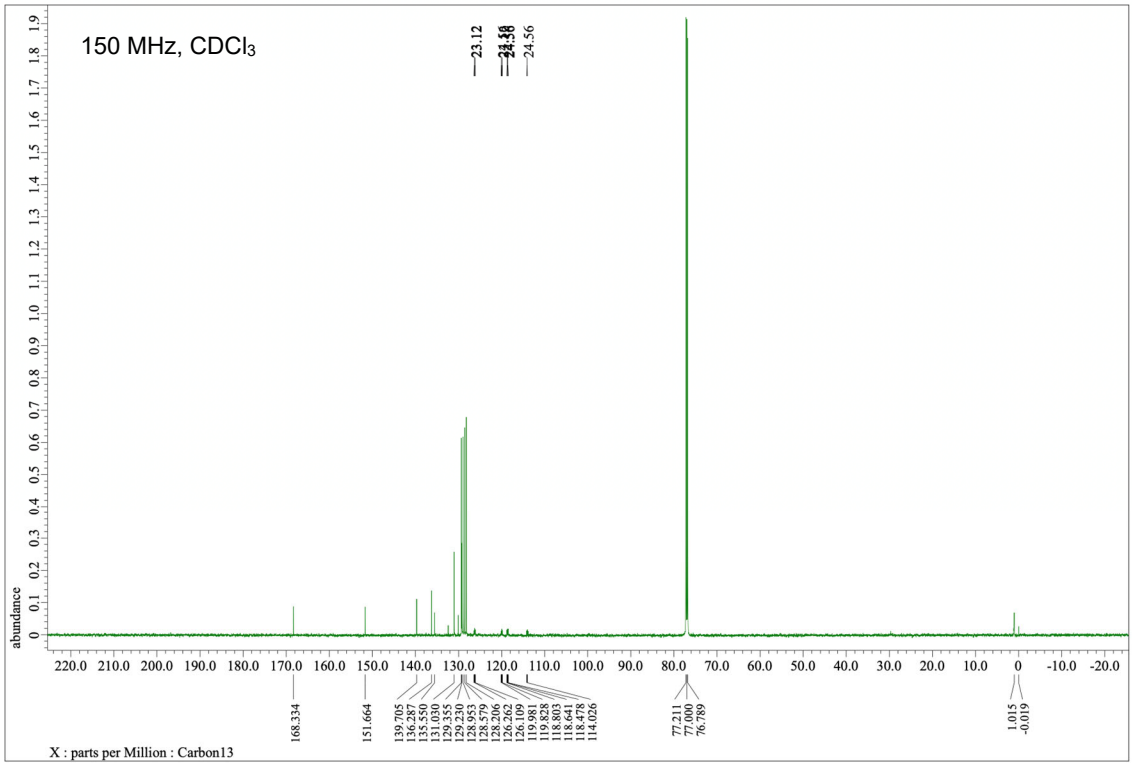

600 MHz, CDCl3
OH
N
Cl
Cl
2ab
3.96
3.00
1.99
1.97
0.93
0.97
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.655 7.640 7.390 7.375 7.360 7.260 7.127 7.113 7.089 6.845 6.831 6.798 6.784 6.429 5.985 5.960
2.049 1.978 1.952
0.005
X : parts per Million : Proton

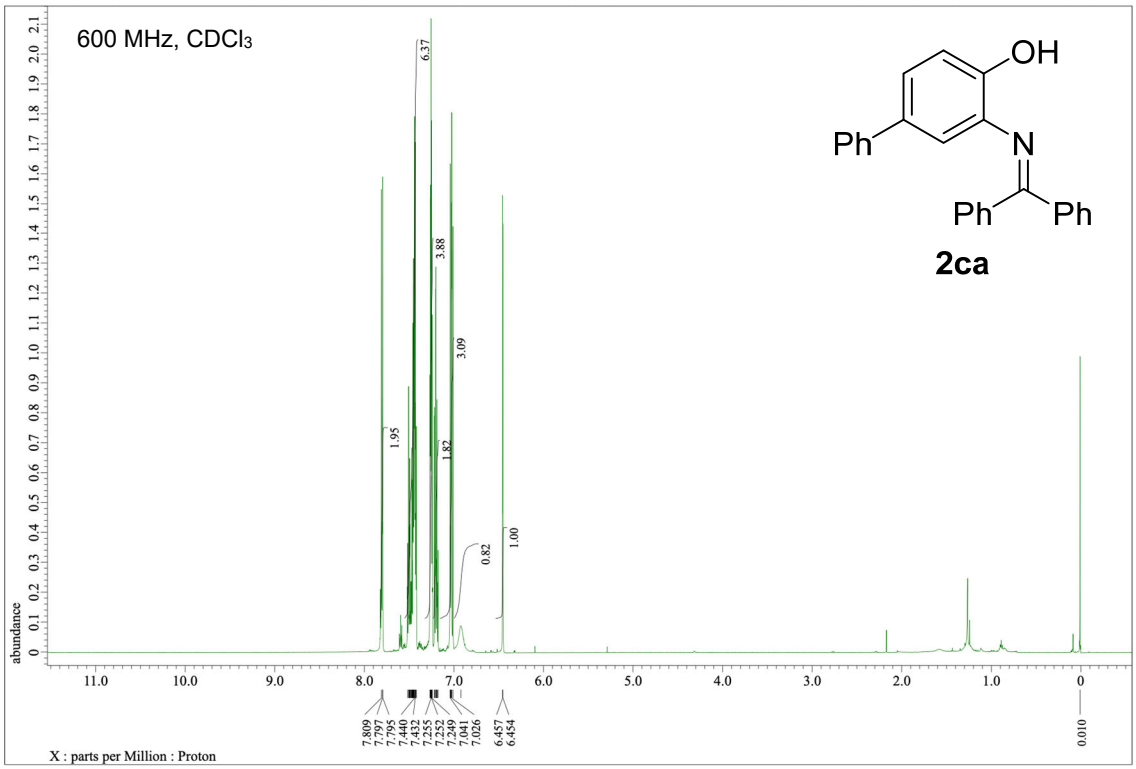

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.816
149.069
137.848 137.436 135.483 135.071 134.464 130.513 130.446 128.962 128.560 127.612 120.623 114.469
77.211 77.000 76.789
20.585
-0.010
X : parts per Million : Carbon13

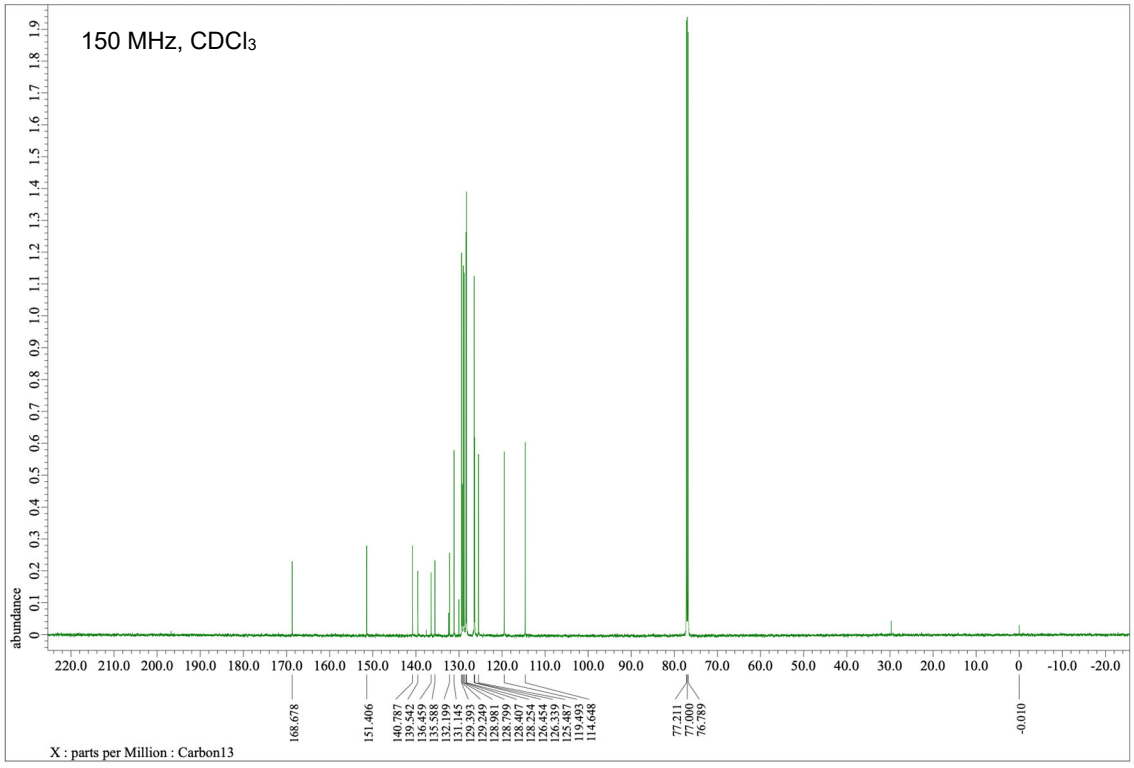

600 MHz, CDCl3
OH
N
Ph
Ph
2ba
abundance
X : parts per Million : Proton

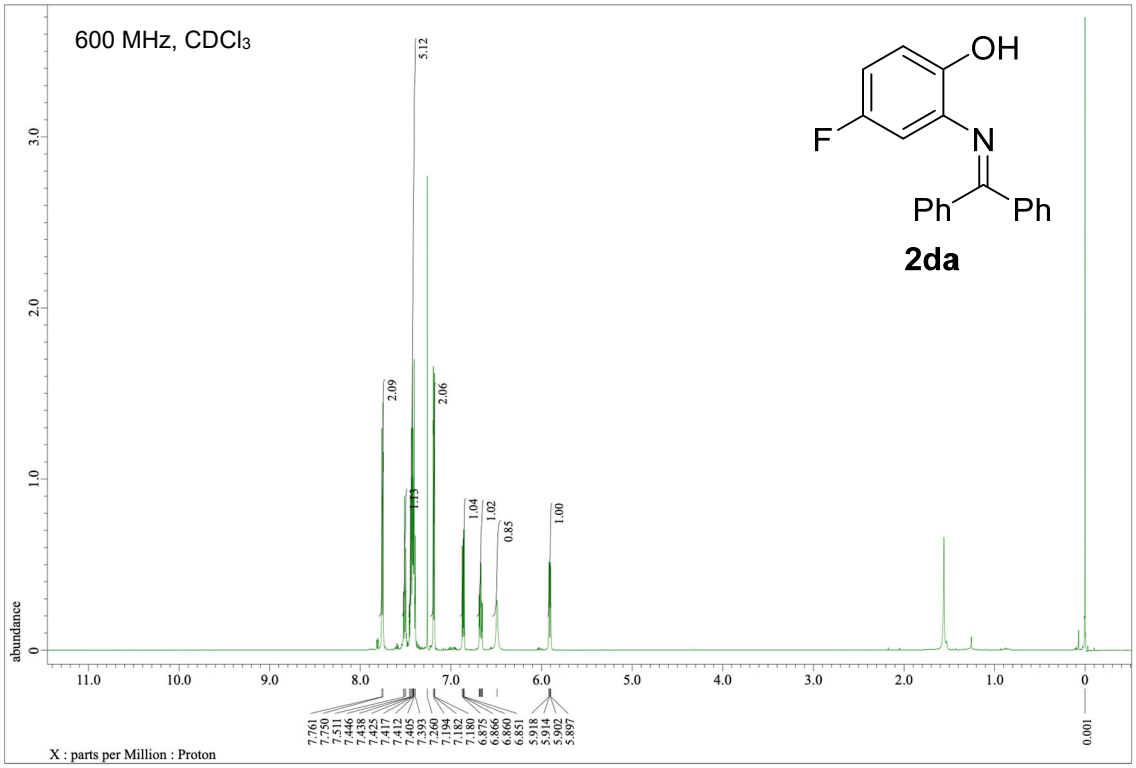

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

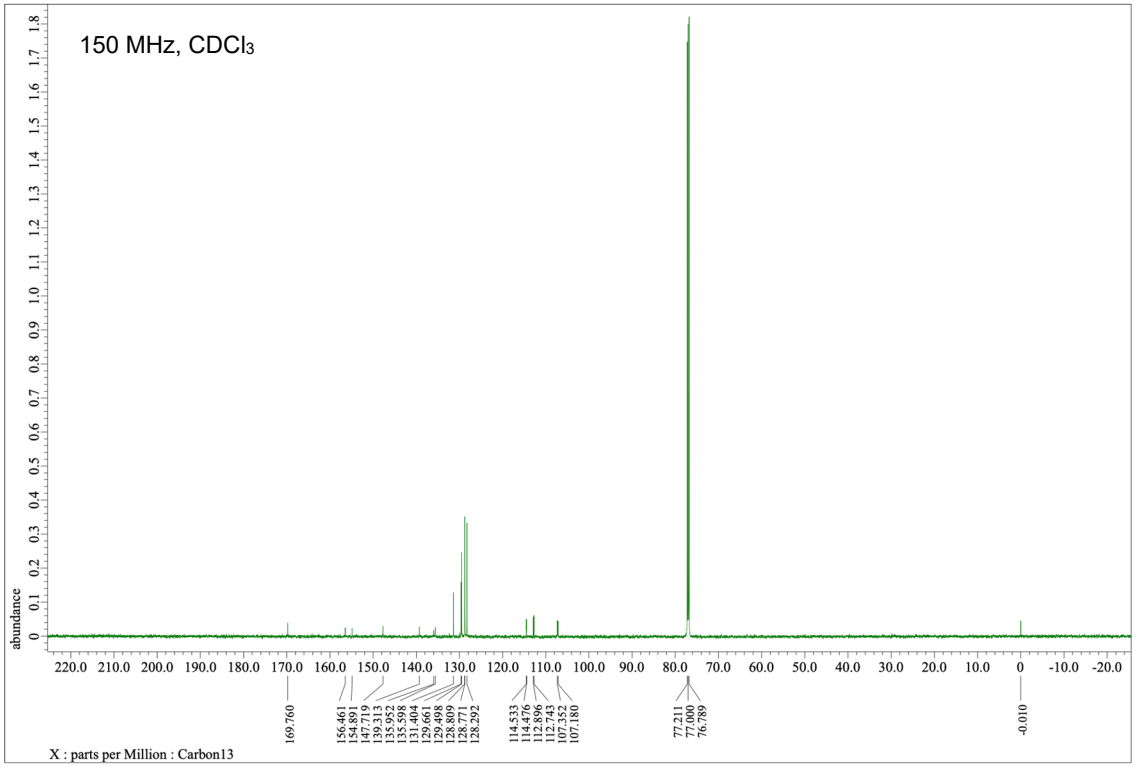

600 MHz, CDCl3
OH
D5
N
Ph
Ph
2ba-d5
abundance
X : parts per Million : Proton

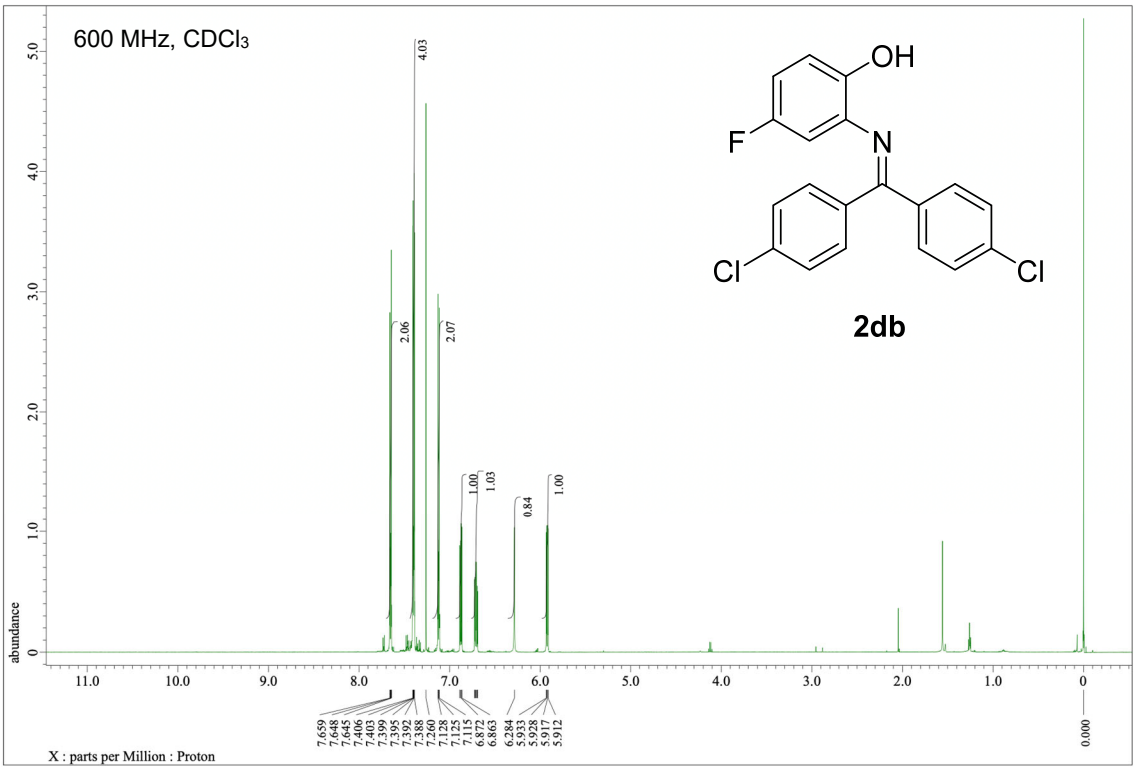

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

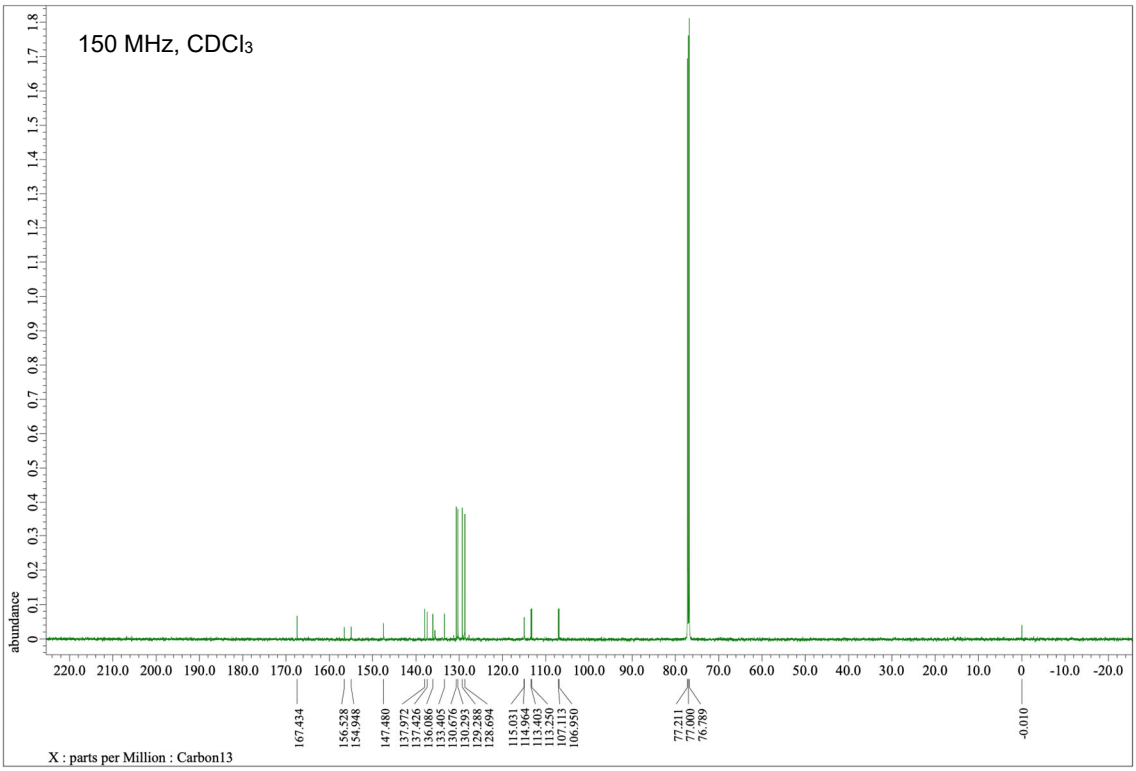

600 MHz, CDCl3
OH
Ph
N
Ph
Ph
2ca
6.37
3.88
3.09
1.95
1.82
0.82
1.00
abundance
X : parts per Million : Proton

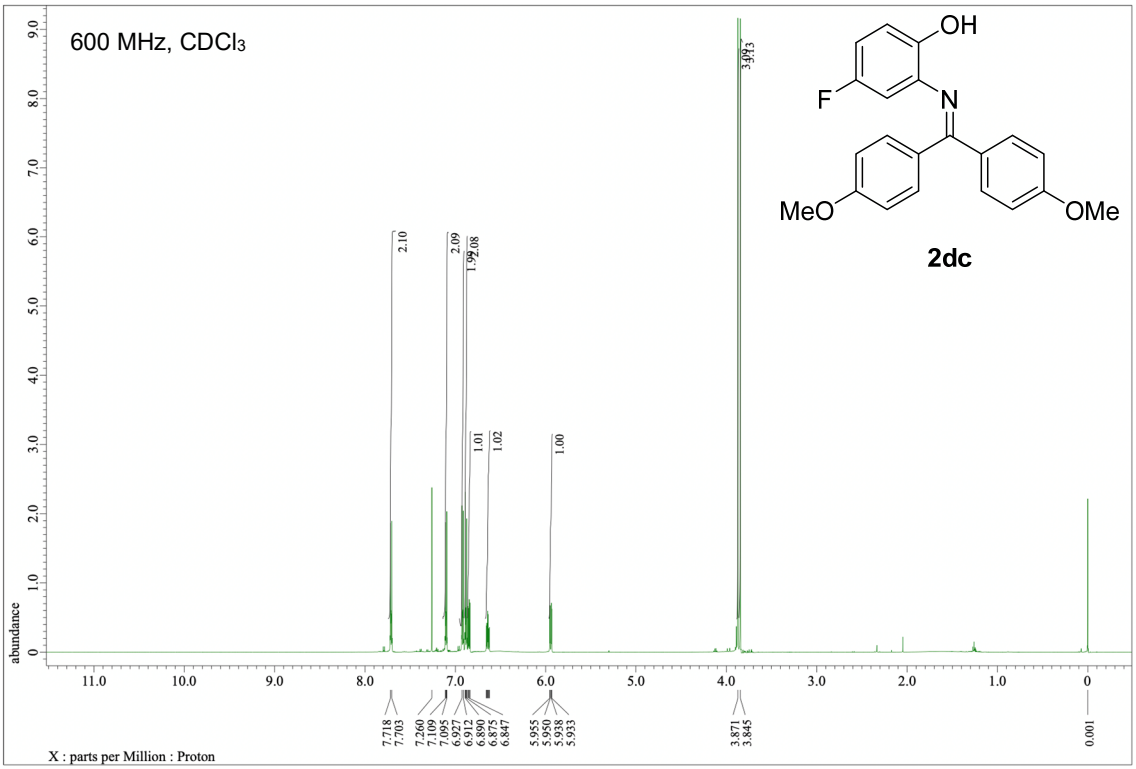

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

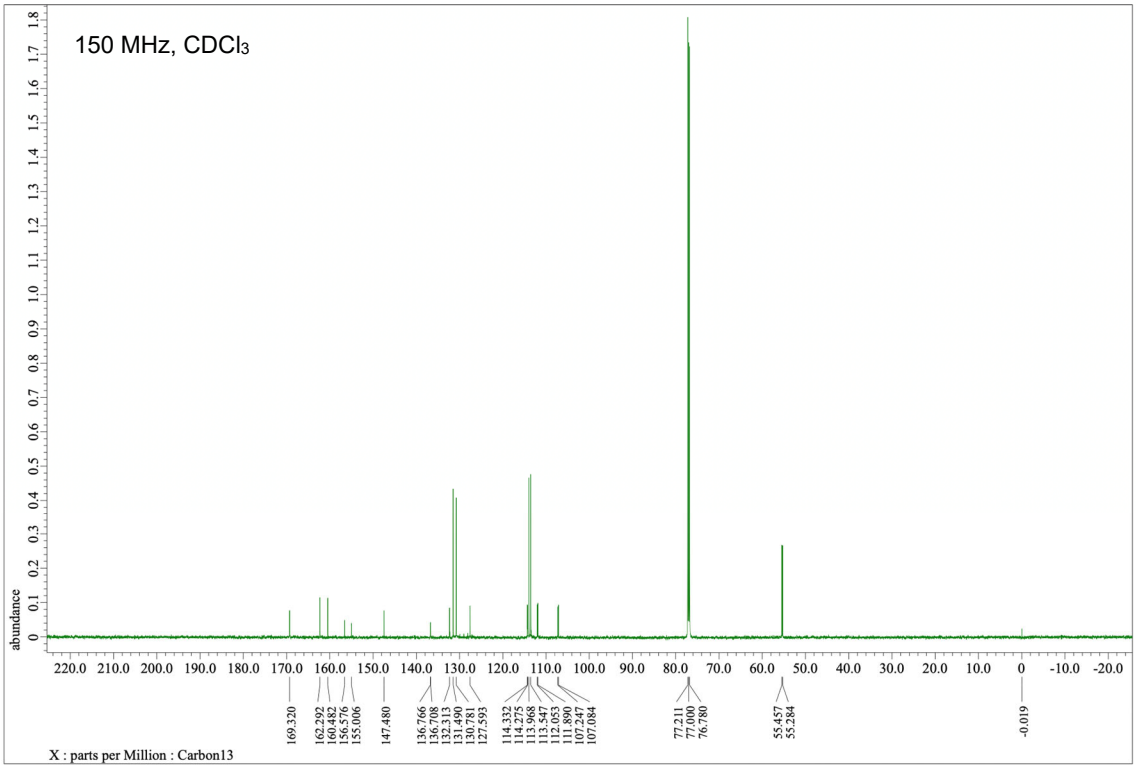

600 MHz, CDCl3
OH
F
N
Ph
Ph
2da
abundance
X : parts per Million : Proton

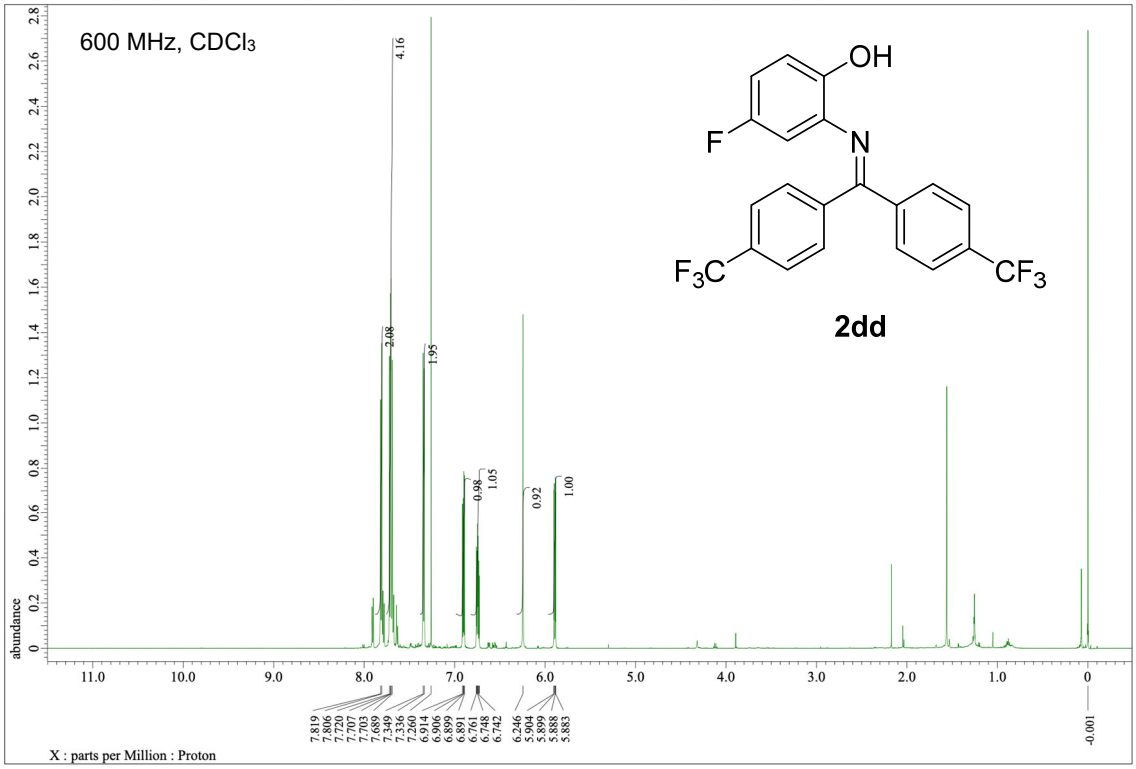

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

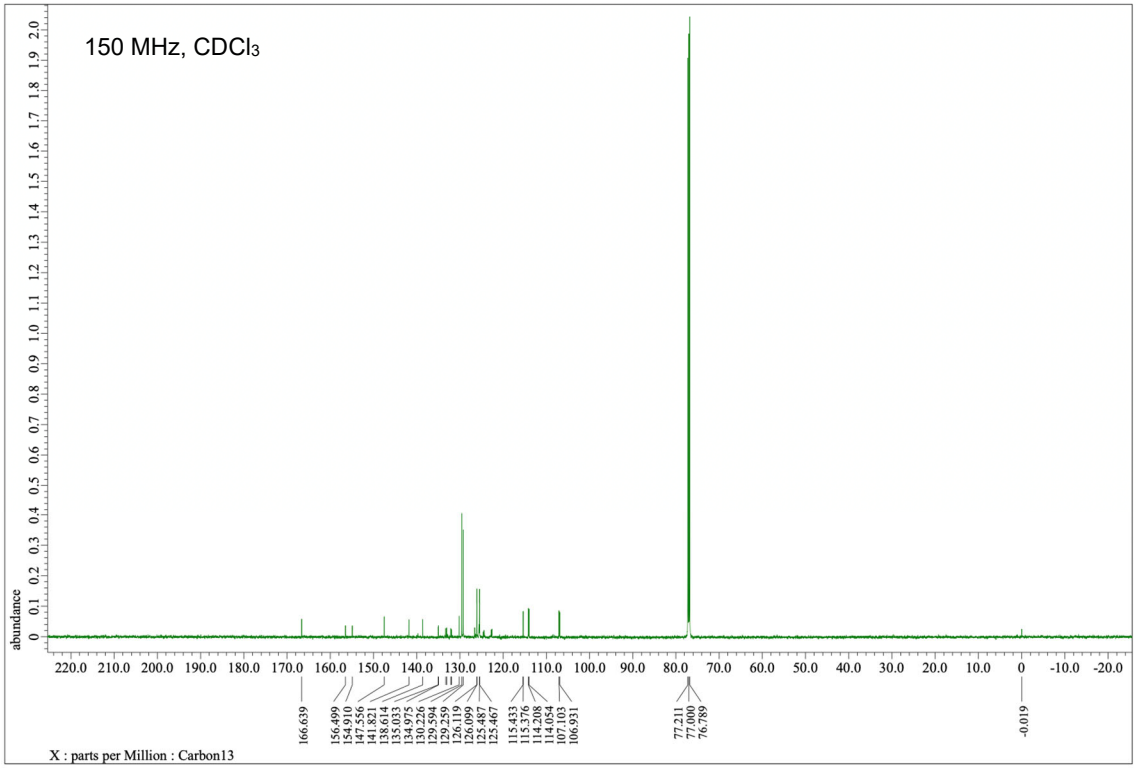

600 MHz, CDCl3
OH
F
N
Cl
Cl
2db
4.03
2.06
2.07
1.00
1.03
0.84
1.00
abundance
X : parts per Million : Proton

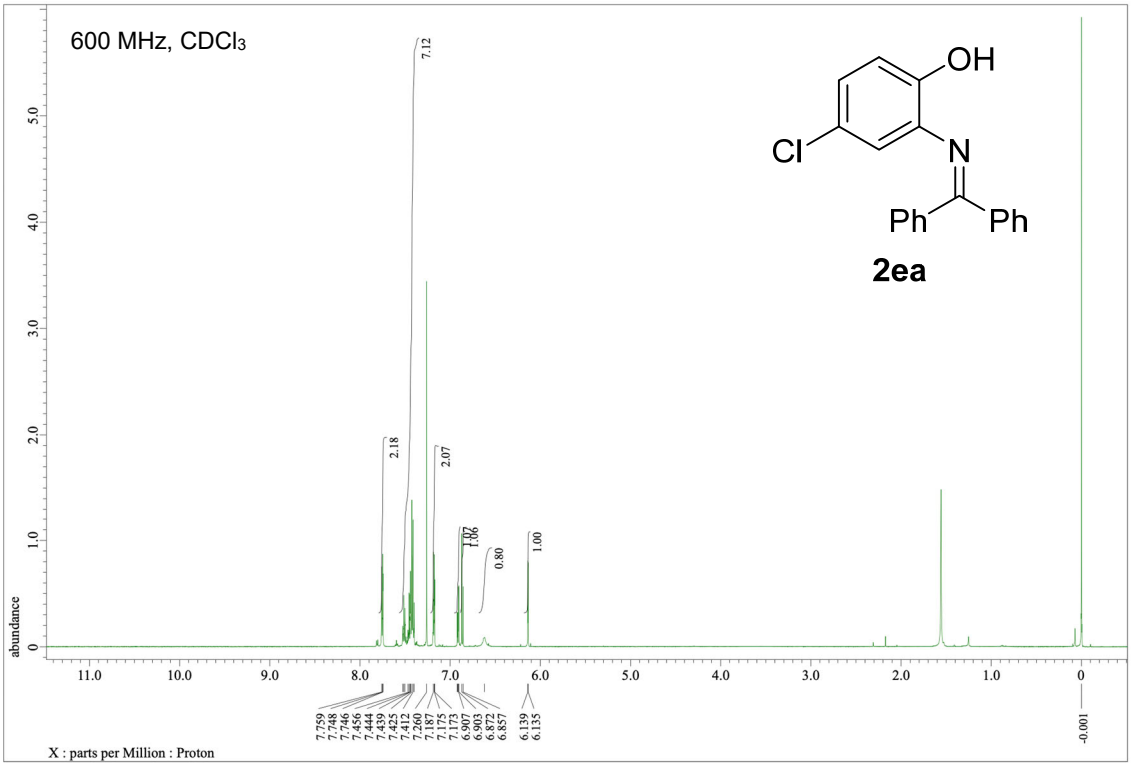

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

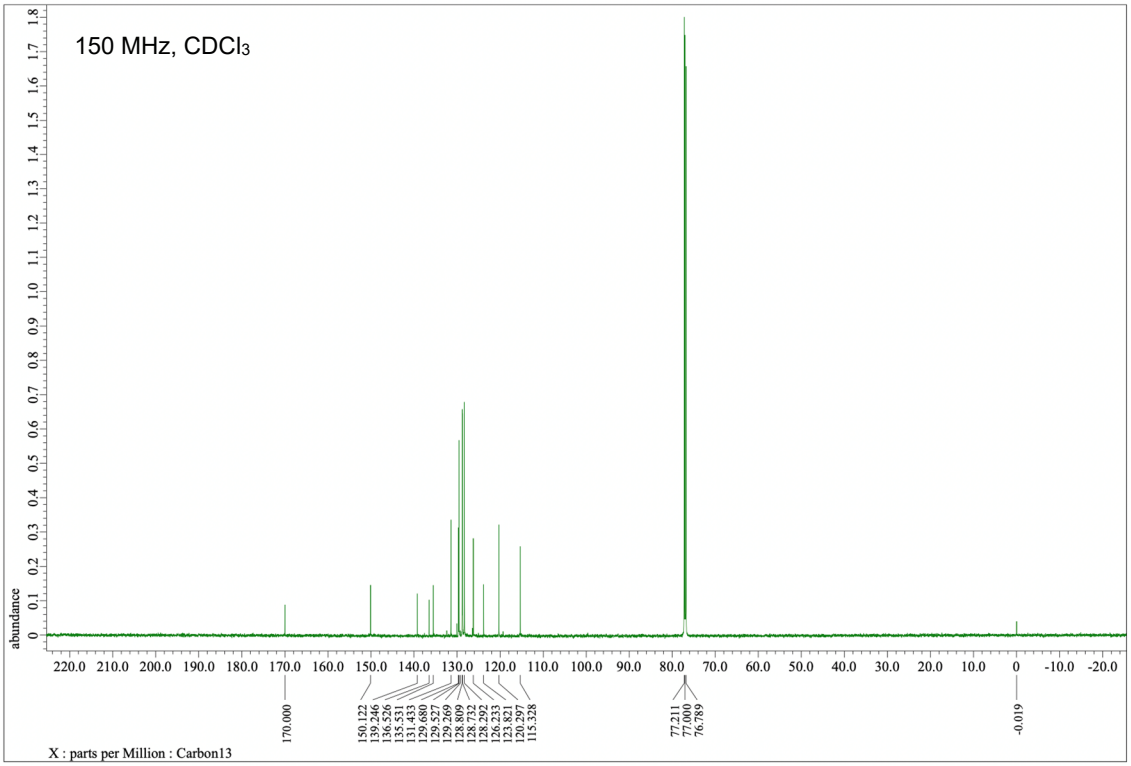

600 MHz, CDCl3
OH
F
N
MeO
OMe
2dc
abundance
X : parts per Million : Proton

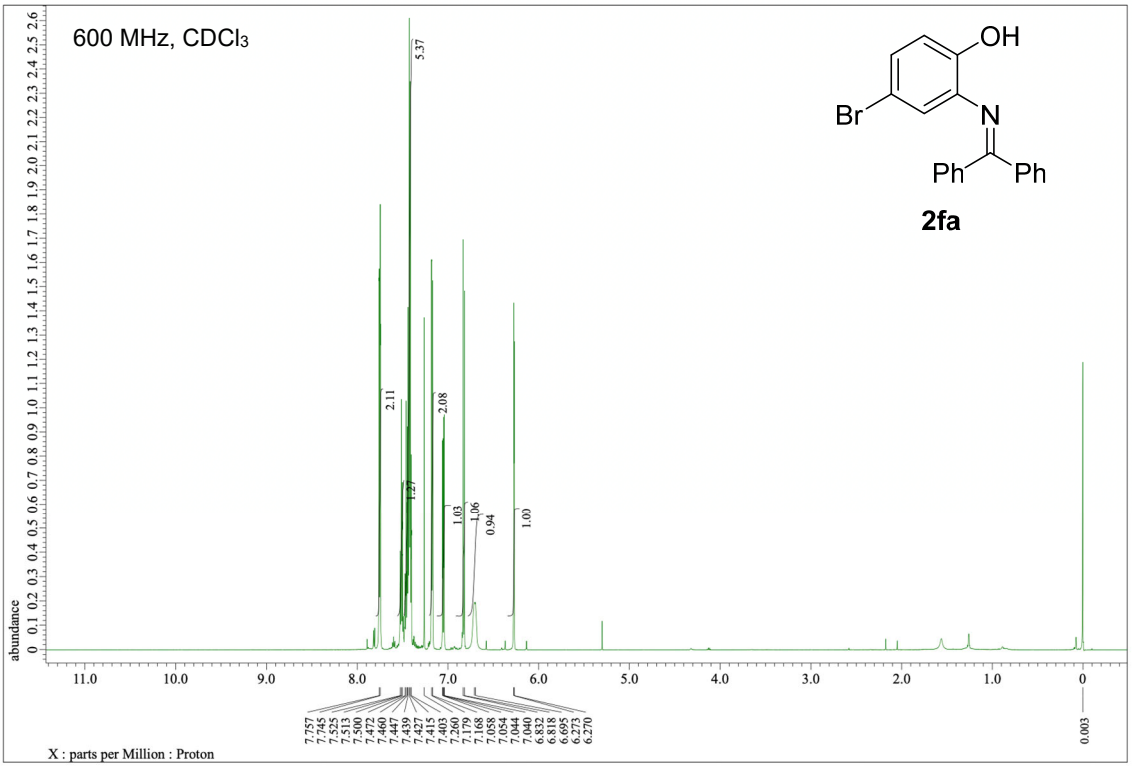

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

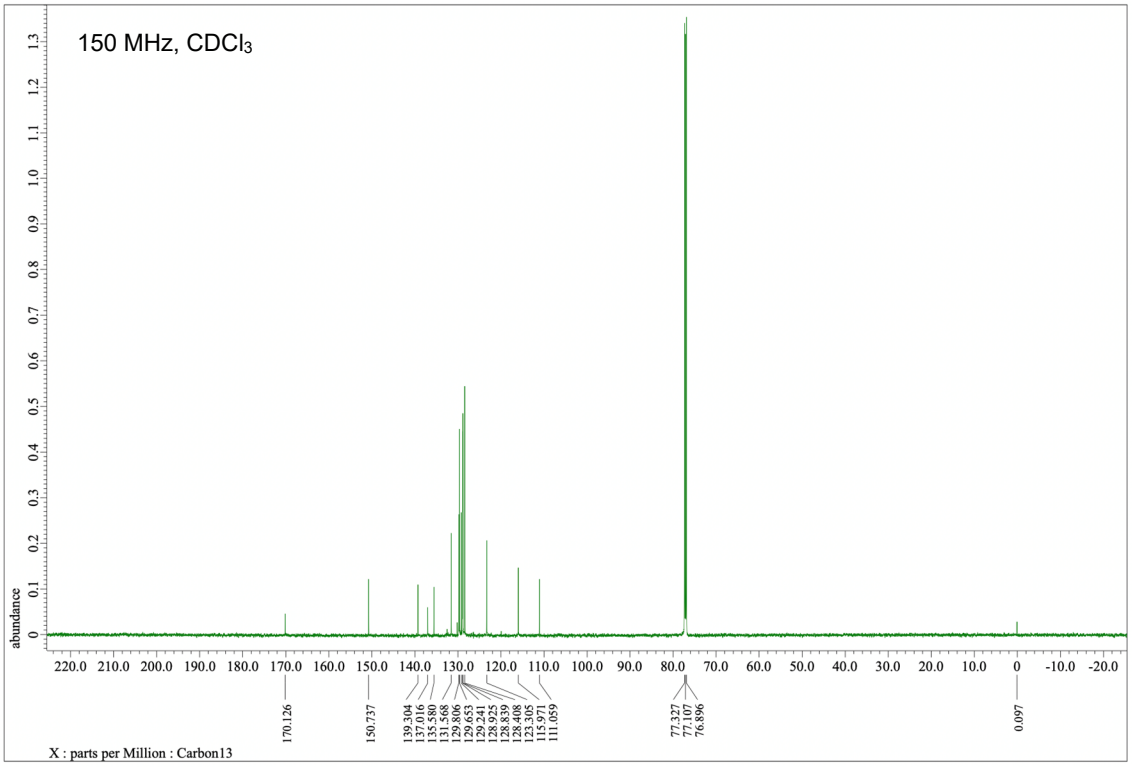

600 MHz, CDCl3
OH
F
N
F3C
CF3
2dd
4.16
2.08
1.95
0.98
1.05
0.92
1.00
abundance
X : parts per Million : Proton

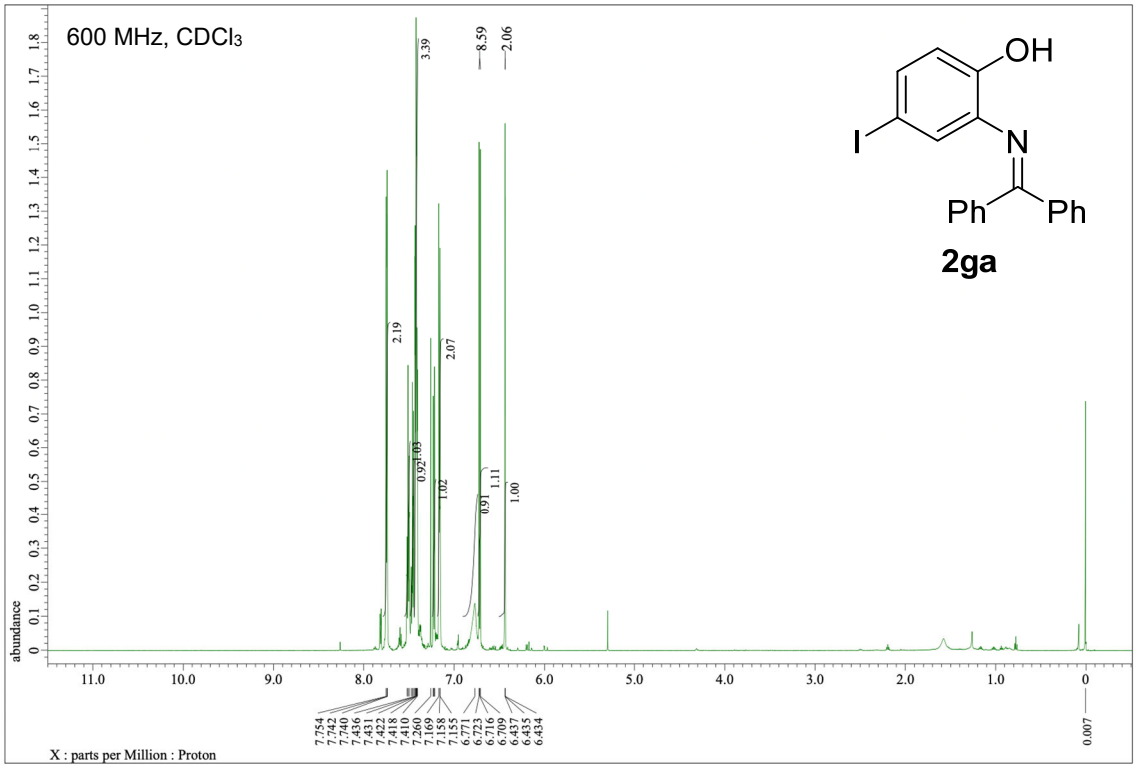

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

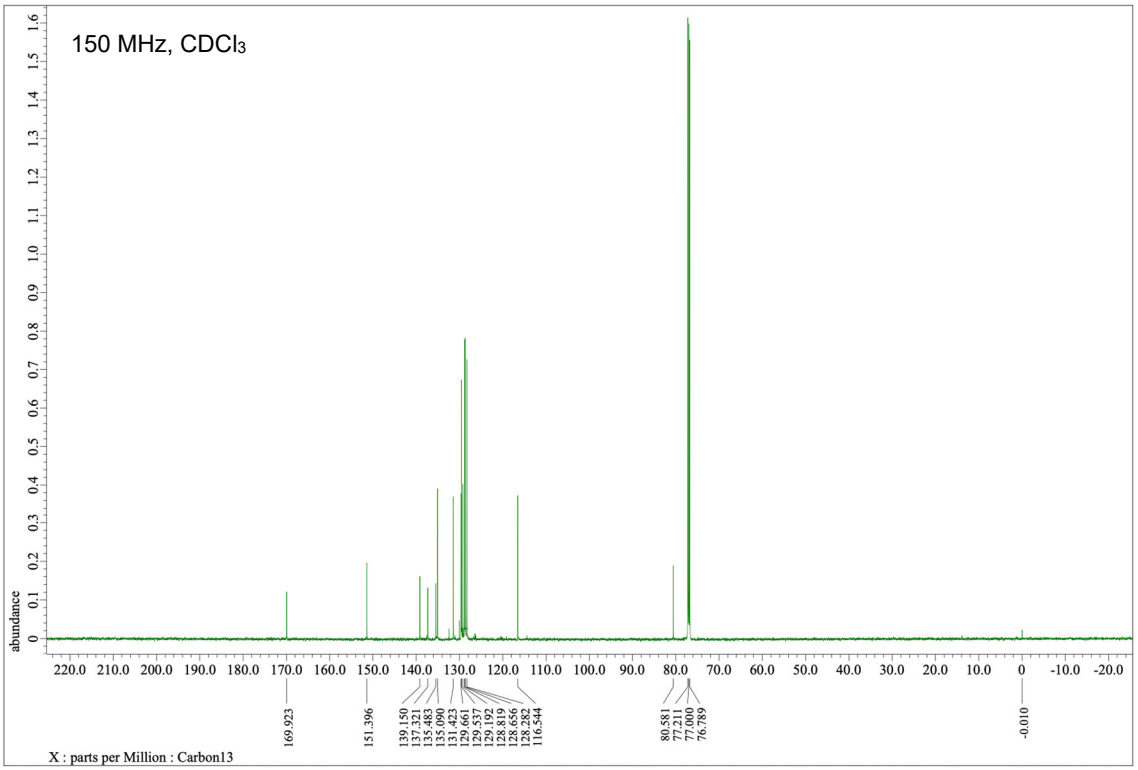

600 MHz, CDCl3
OH
Cl
N
Ph
Ph
2ea
abundance
X : parts per Million : Proton

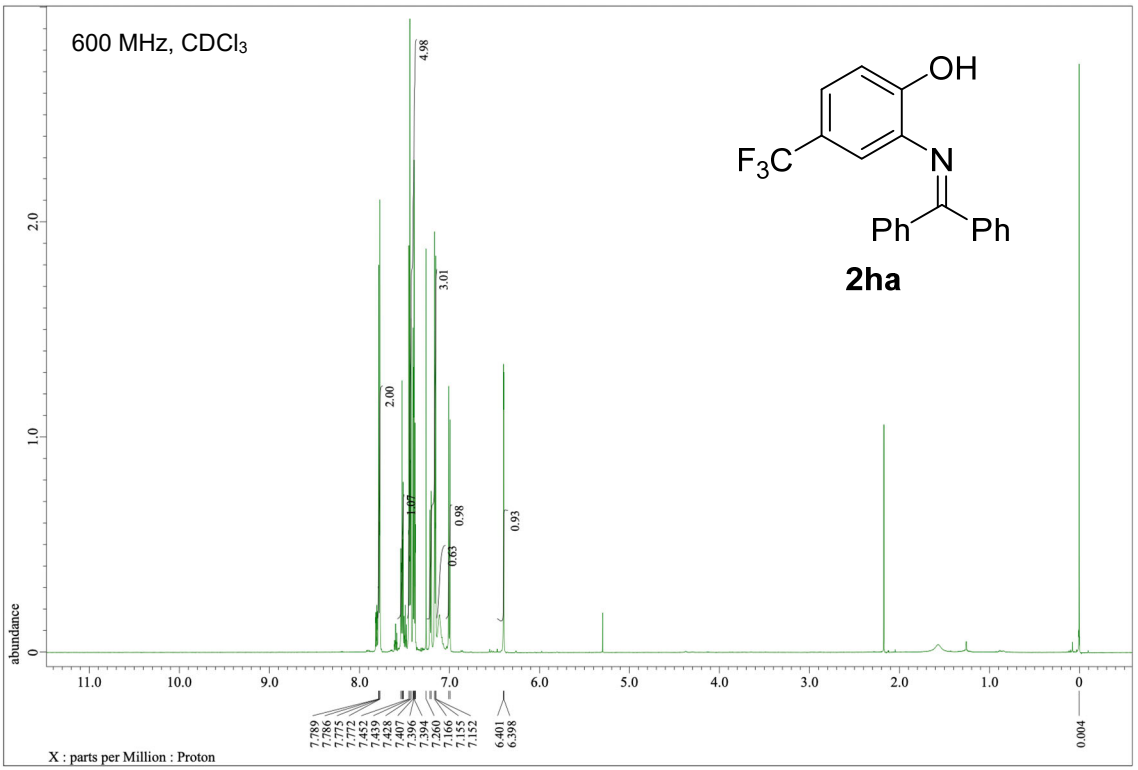

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

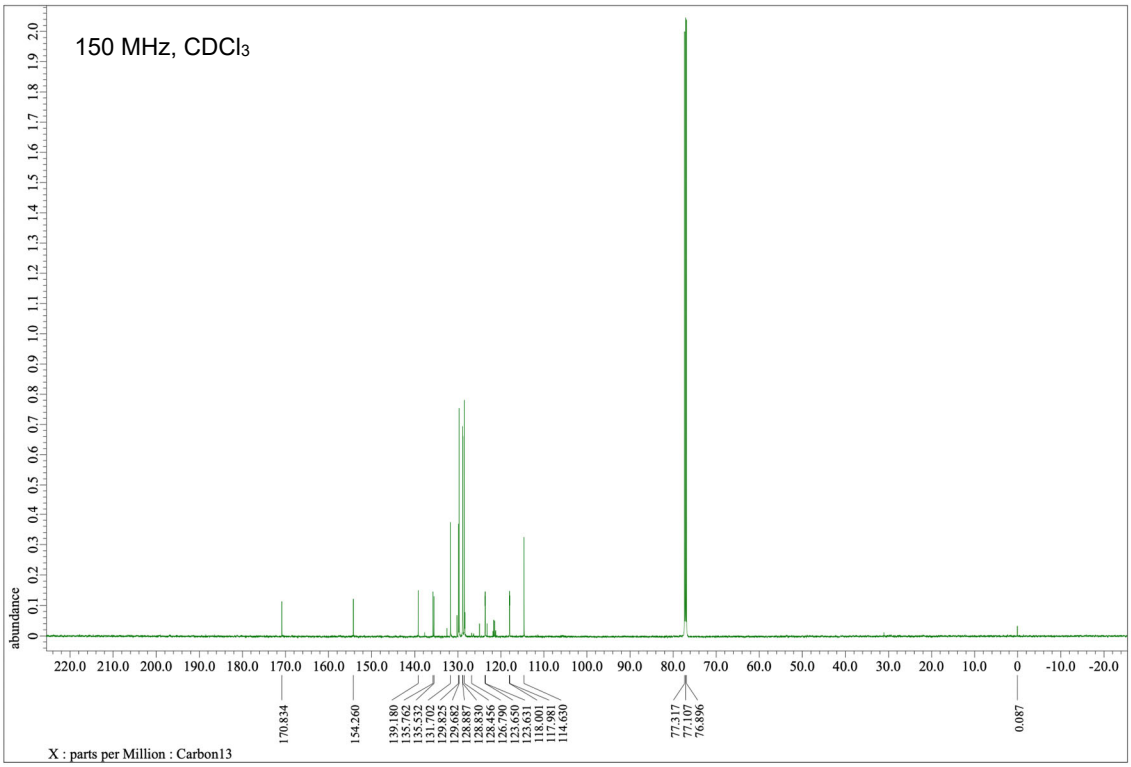

600 MHz, CDCl3
OH
Br
N
Ph
Ph
2fa
abundance
X : parts per Million : Proton

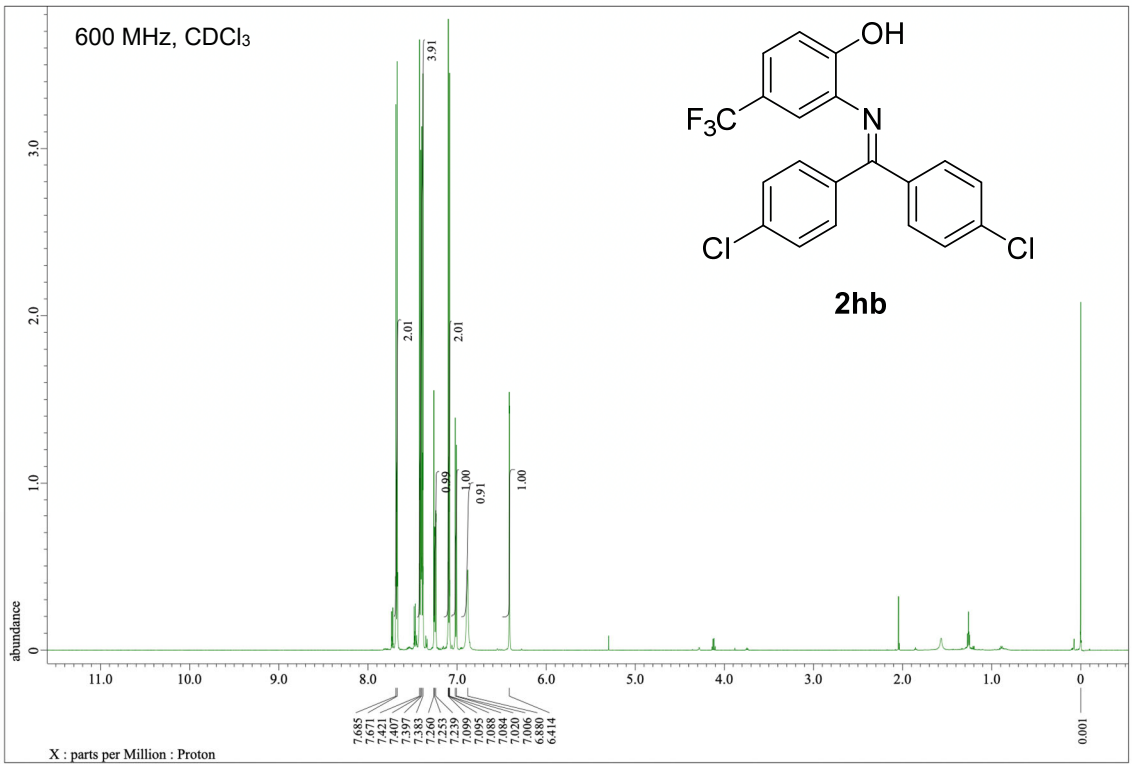

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

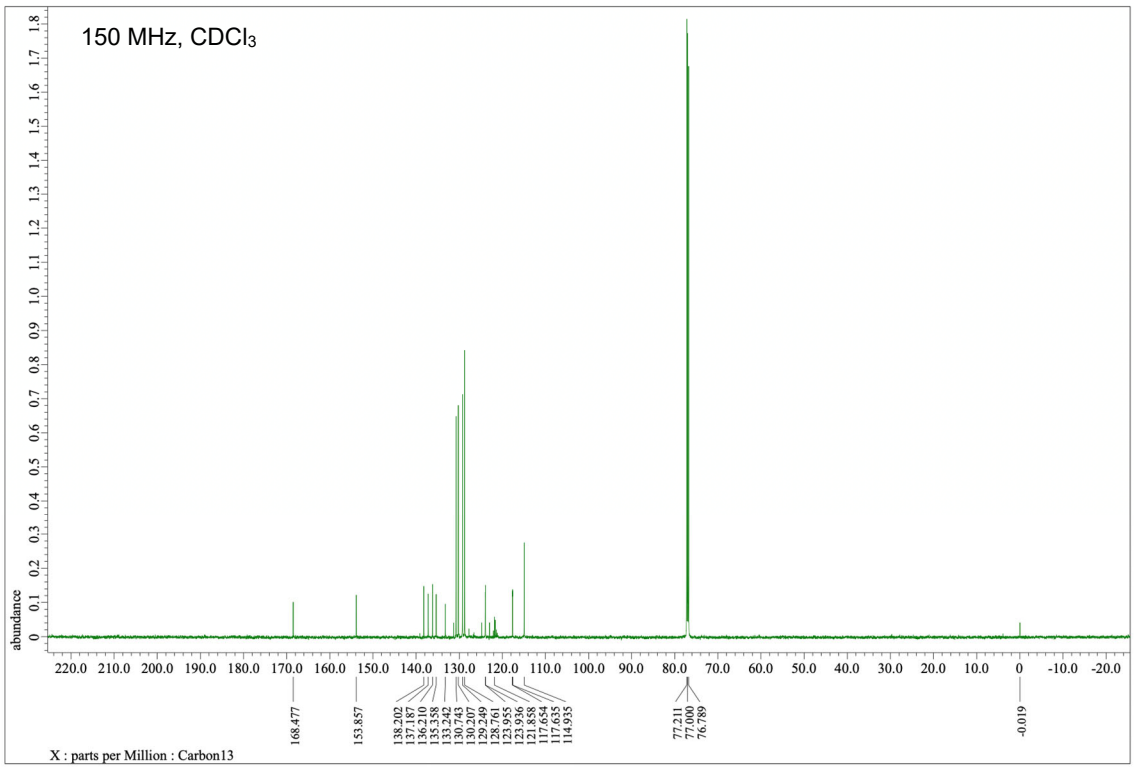

600 MHz, CDCl3
OH
I
N
Ph
Ph
2ga
abundance
X : parts per Million : Proton

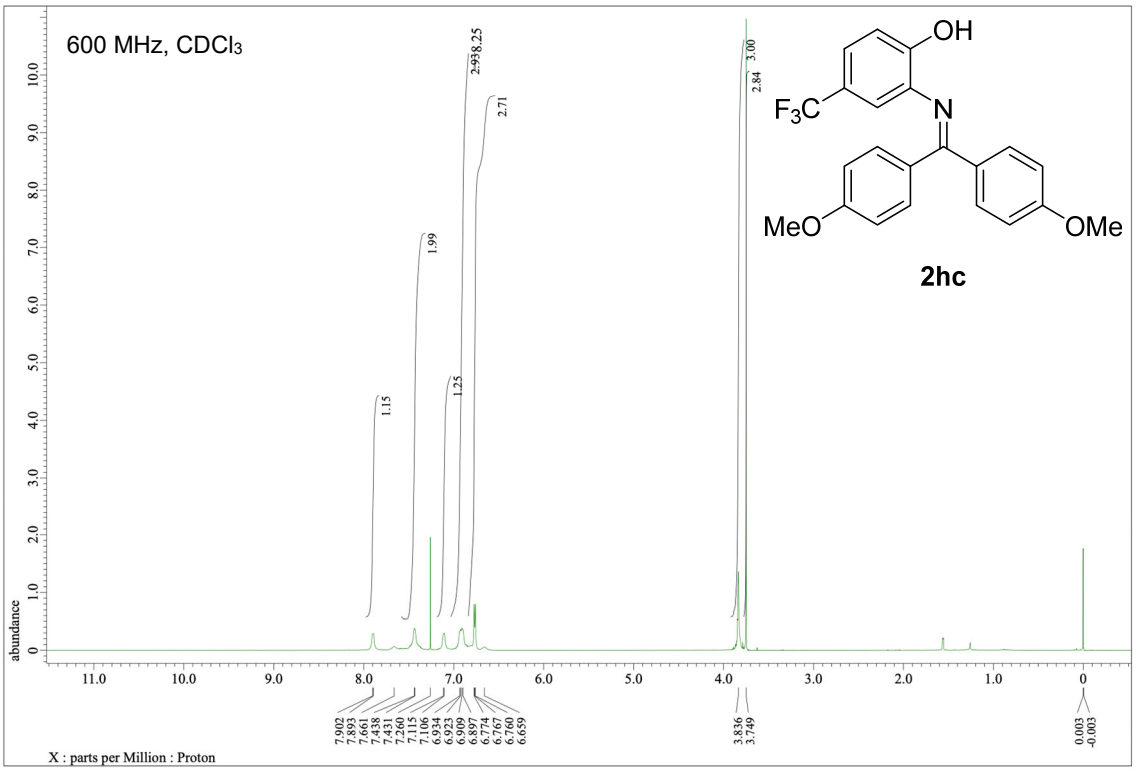

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

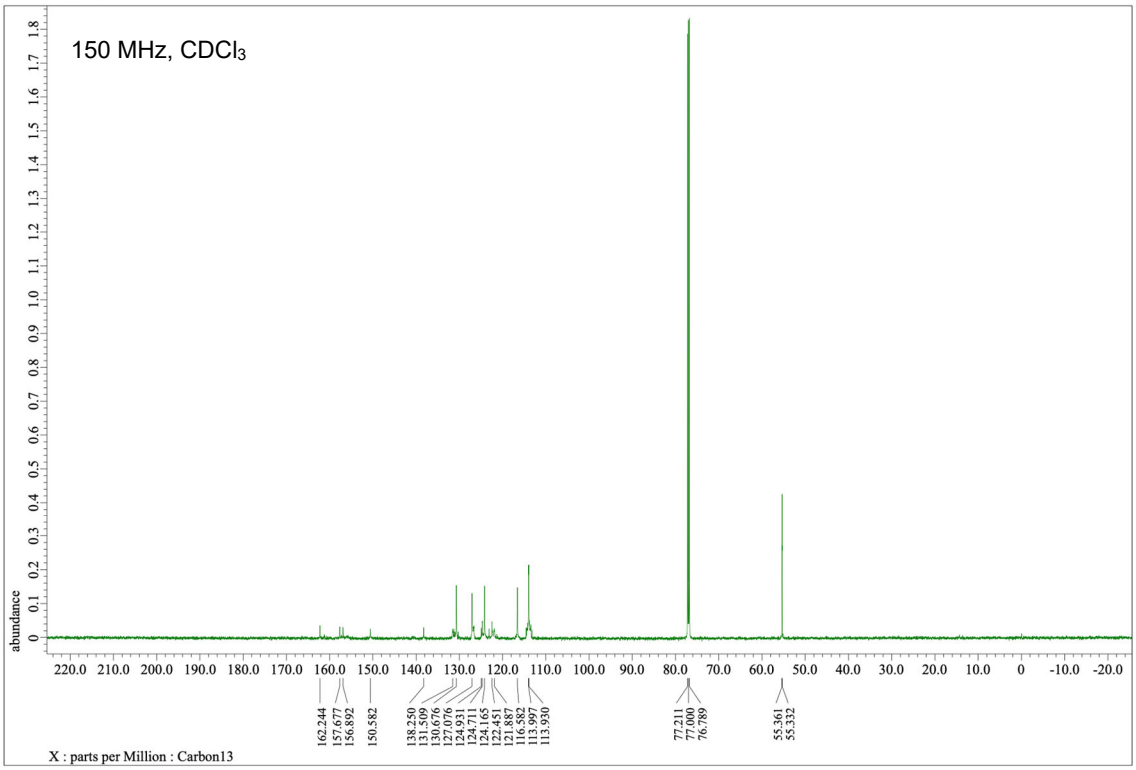

600 MHz, CDCl3
OH
F3C
N
Ph
Ph
2ha
4.98
3.01
2.00
1.07
0.98
0.93
0.63
abundance
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.789 7.786 7.775 7.772 7.439 7.428 7.407 7.396 7.394 7.260 7.166 7.155 7.152
6.401 6.398
0.004
X : parts per Million : Proton

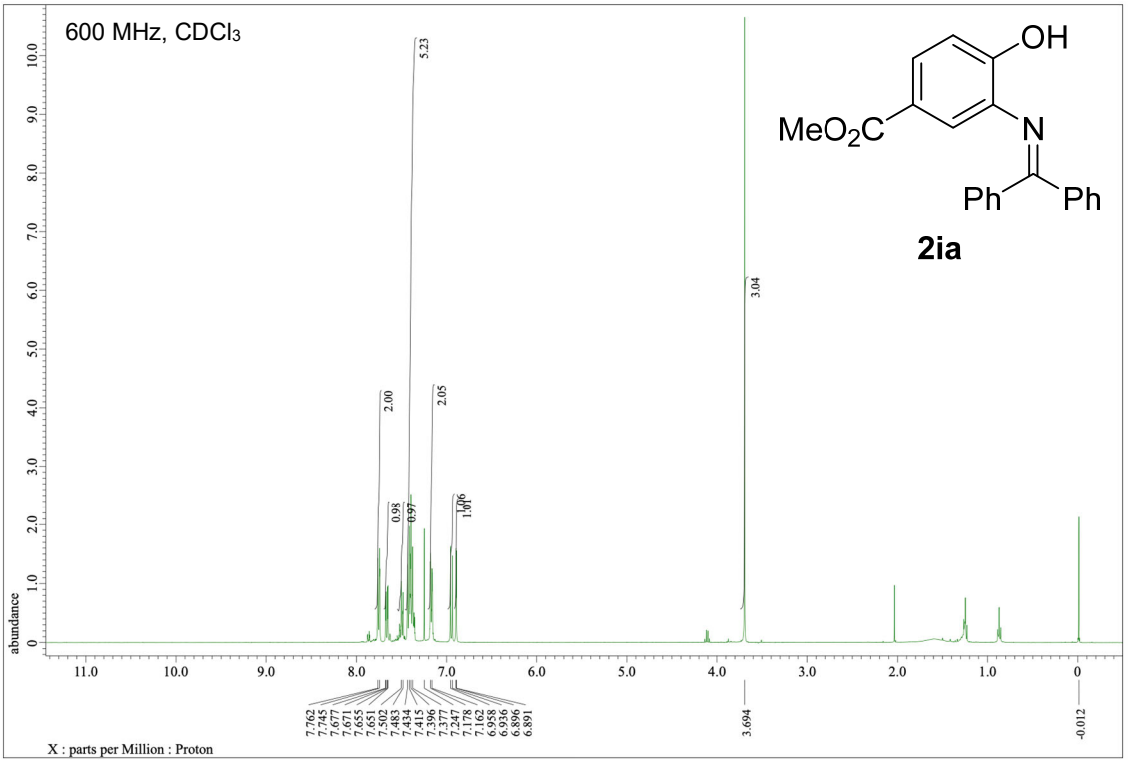

150 MHz, CDCl3
abundance
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
170.834
154.260
139.180 135.762 135.532 131.702 131.325 129.682 128.887 128.830 128.456 126.790 123.650 123.451 118.001 117.981 114.630
77.317 77.107 76.896
0.087
X : parts per Million : Carbon13

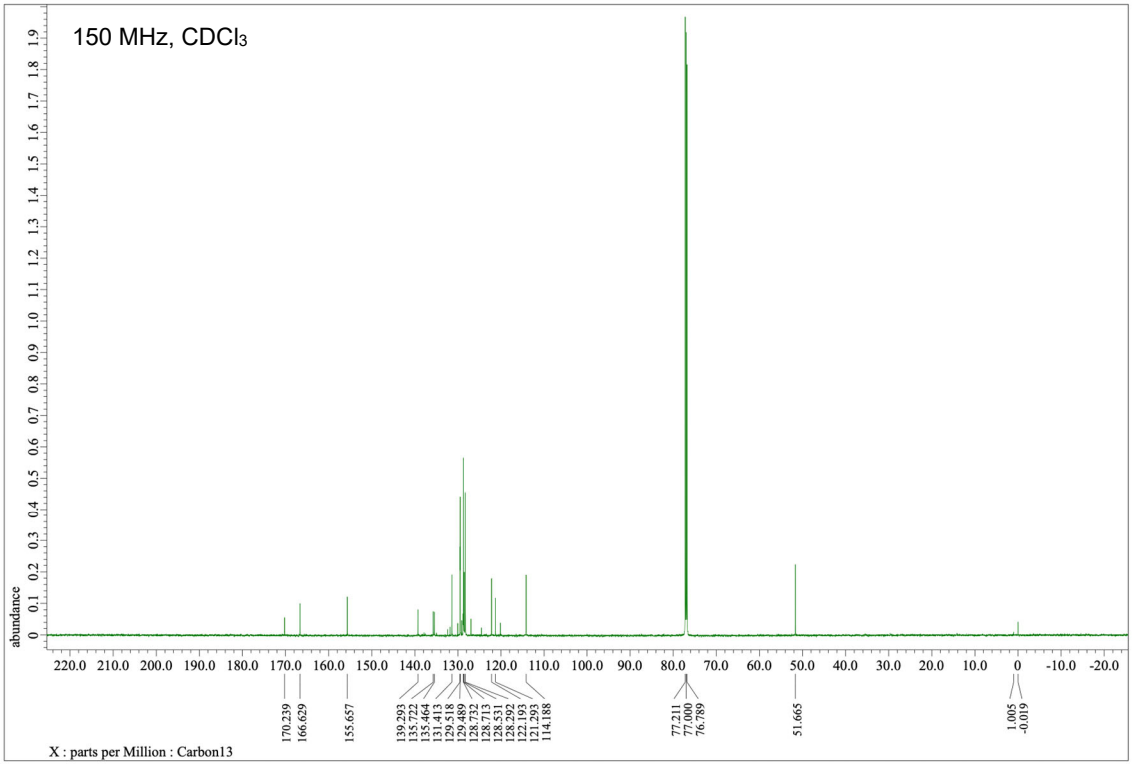

600 MHz, CDCl3
OH
F3C
N
Cl
Cl
2hb
abundance
X : parts per Million : Proton

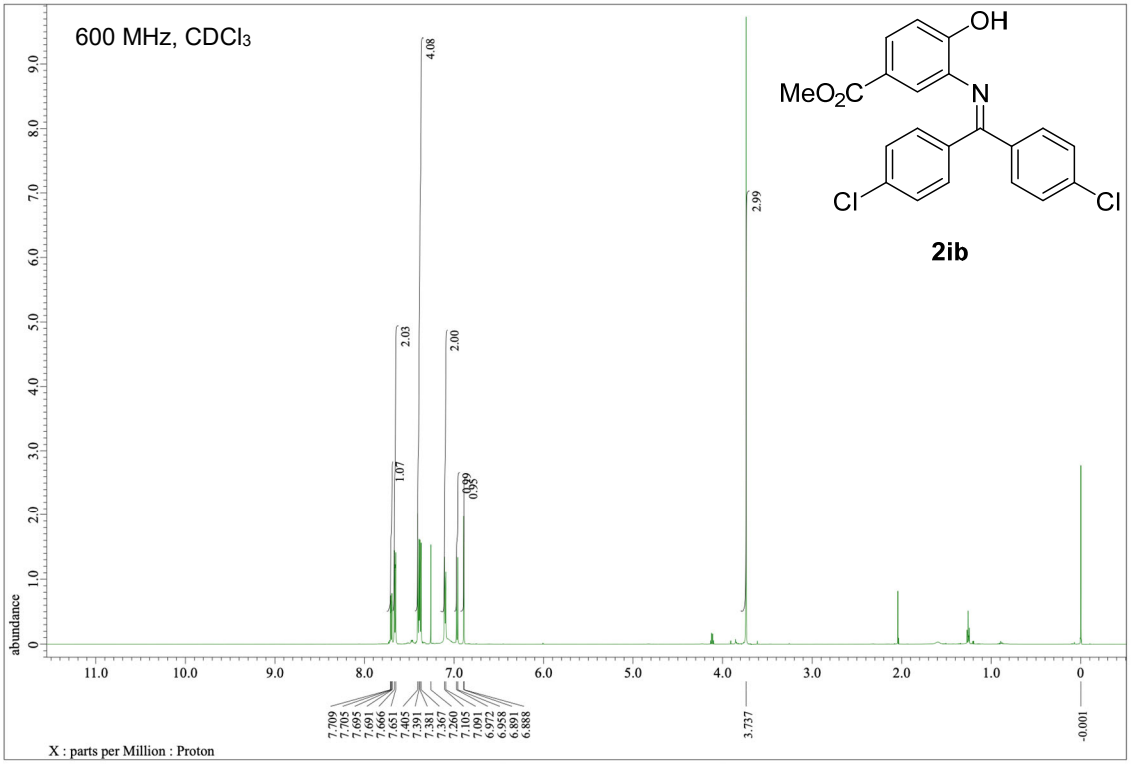

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

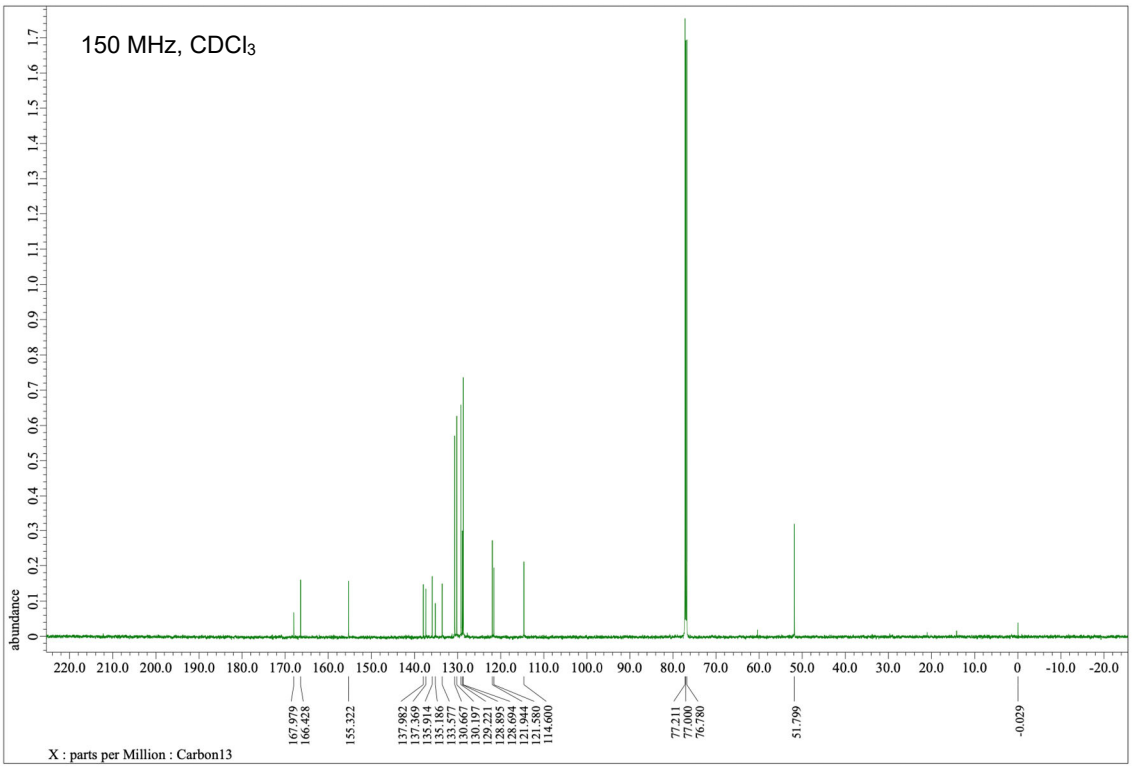

600 MHz, CDCl3
OH
F3C
N
MeO
OMe
2hc
abundance
X : parts per Million : Proton

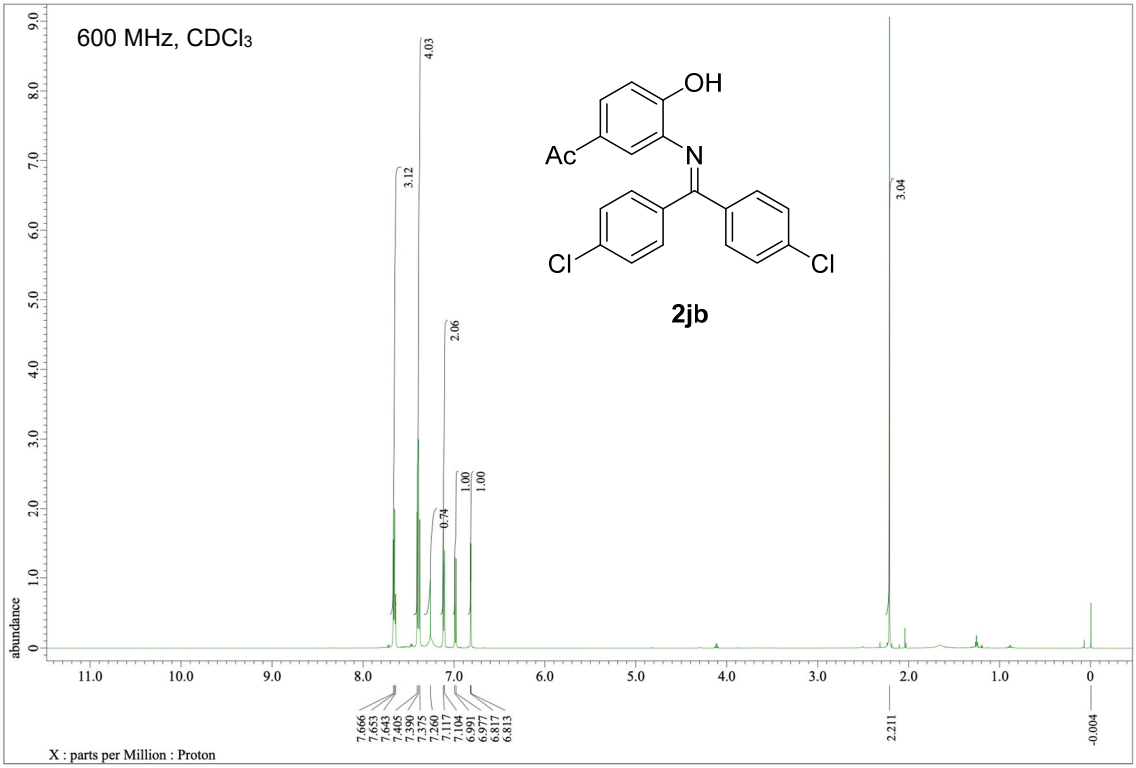

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

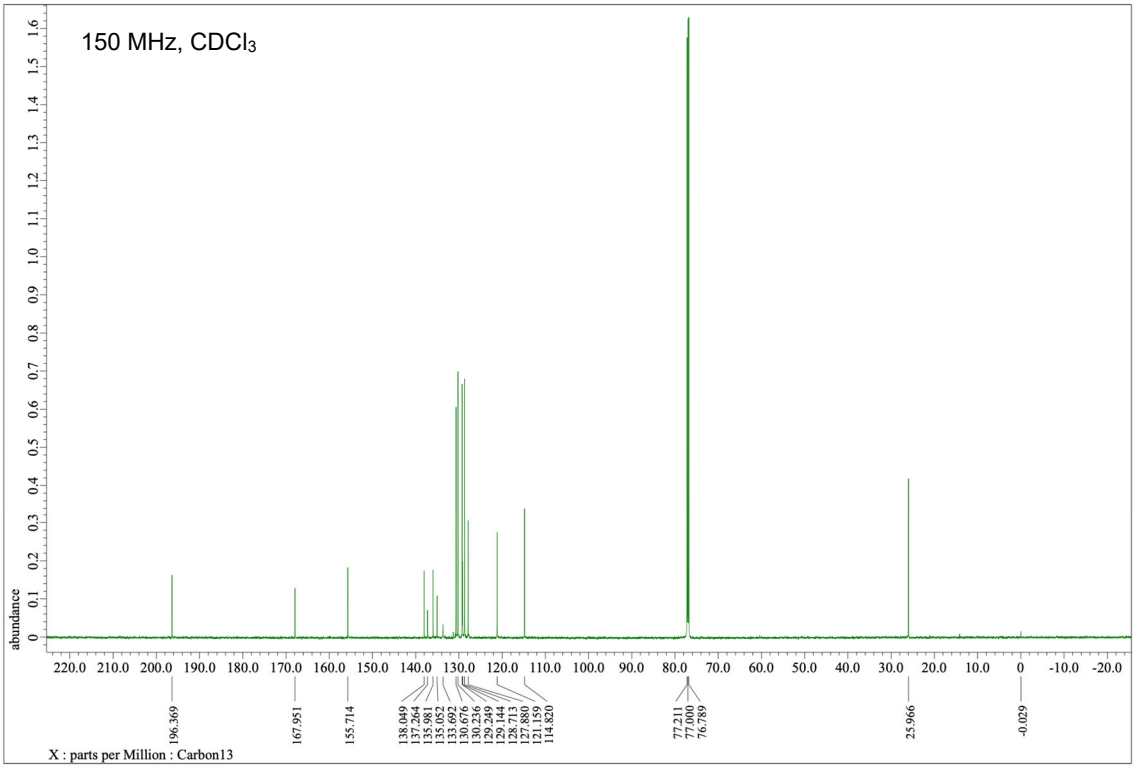

600 MHz, CDCl3
OH
MeO2C
N
Ph
Ph
2ia
abundance
X : parts per Million : Proton

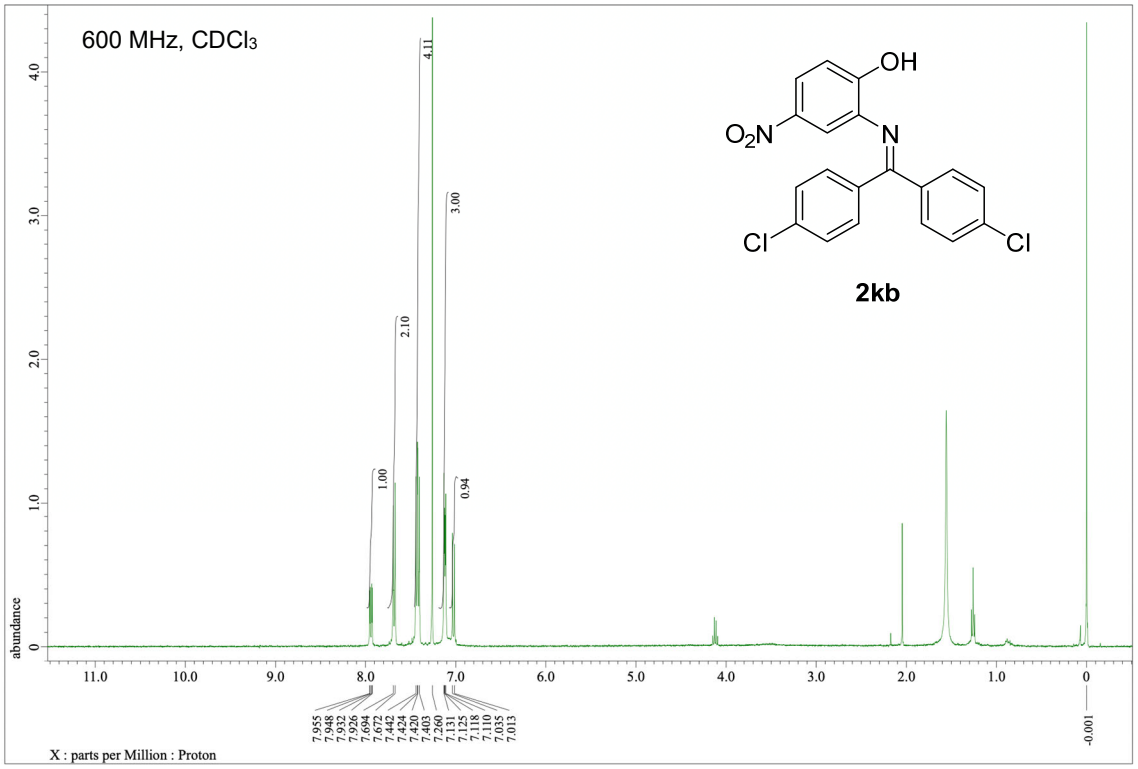

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

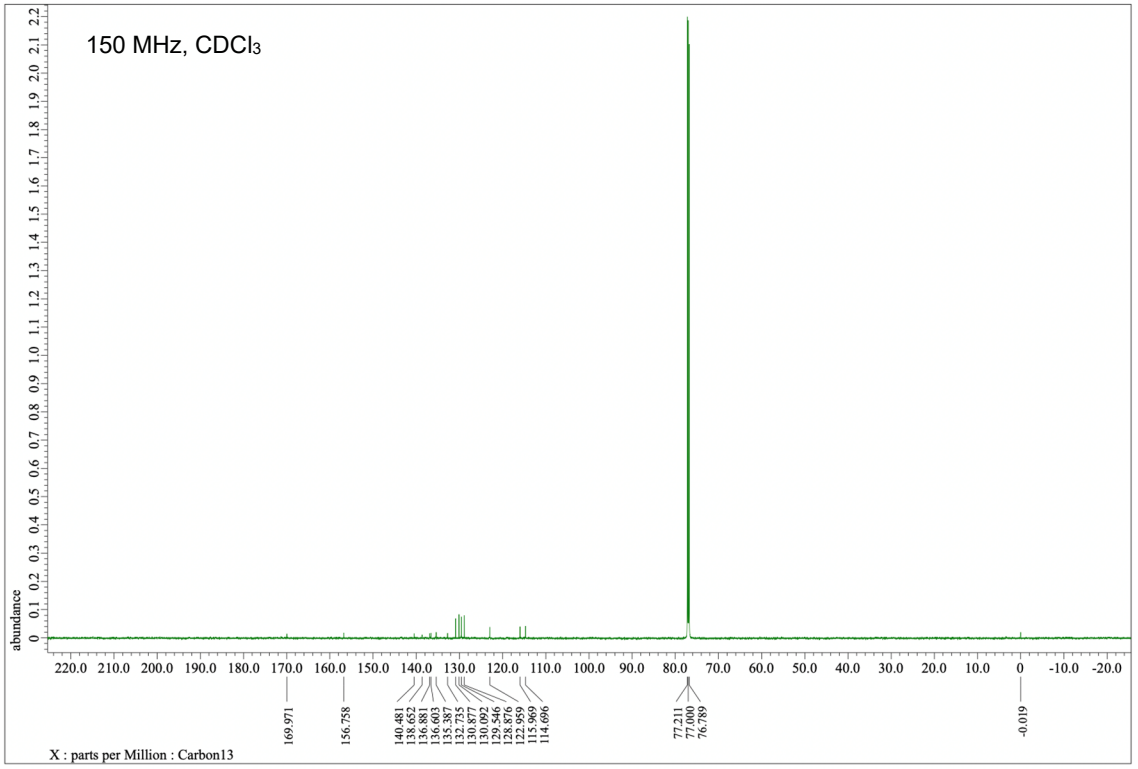

600 MHz, CDCl3
OH
MeO2C
N
Cl
Cl
2ib
4.08
2.99
2.03
2.00
1.07
0.99
0.95
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.709
7.705
7.695
7.691
7.666
7.651
7.405
7.391
7.381
7.367
7.260
7.105
7.091
6.972
6.958
6.901
6.888
3.737
-0.001
X : parts per Million : Proton

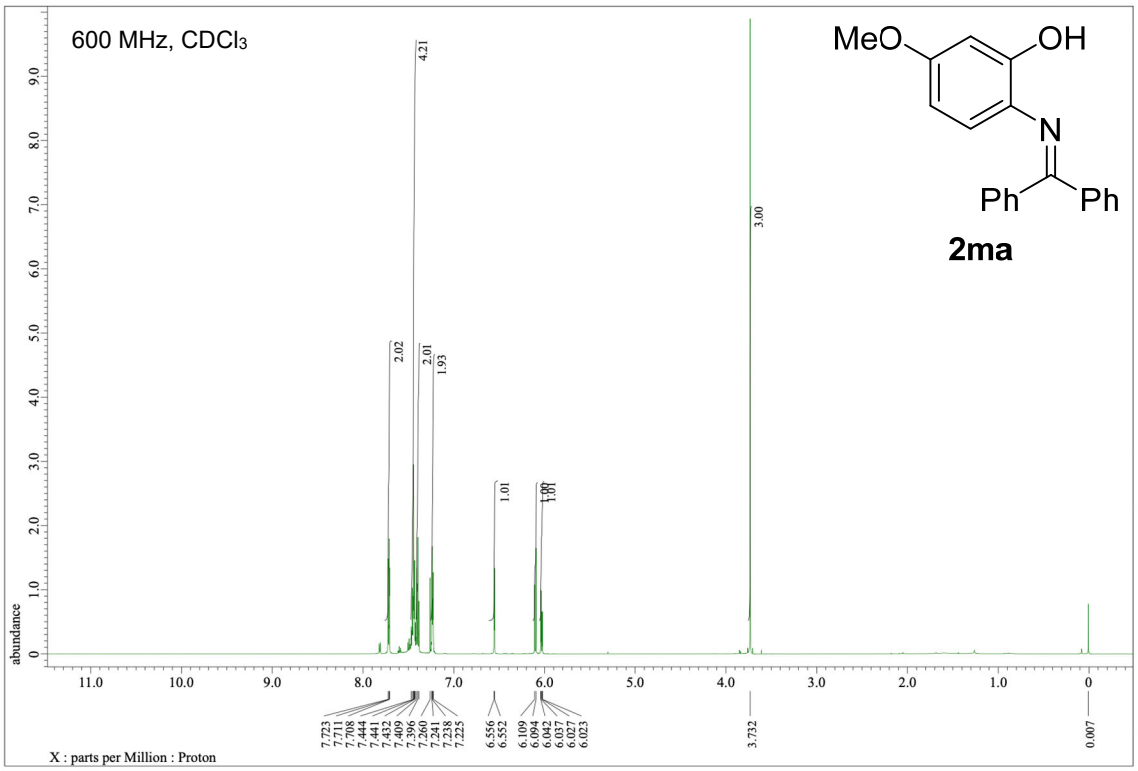

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
167.979
166.428
155.322
137.982
137.369
135.914
135.186
133.577
130.667
130.197
129.271
128.895
128.694
121.944
121.580
114.600
77.211
77.000
76.780
51.799
-0.029
X : parts per Million : Carbon13

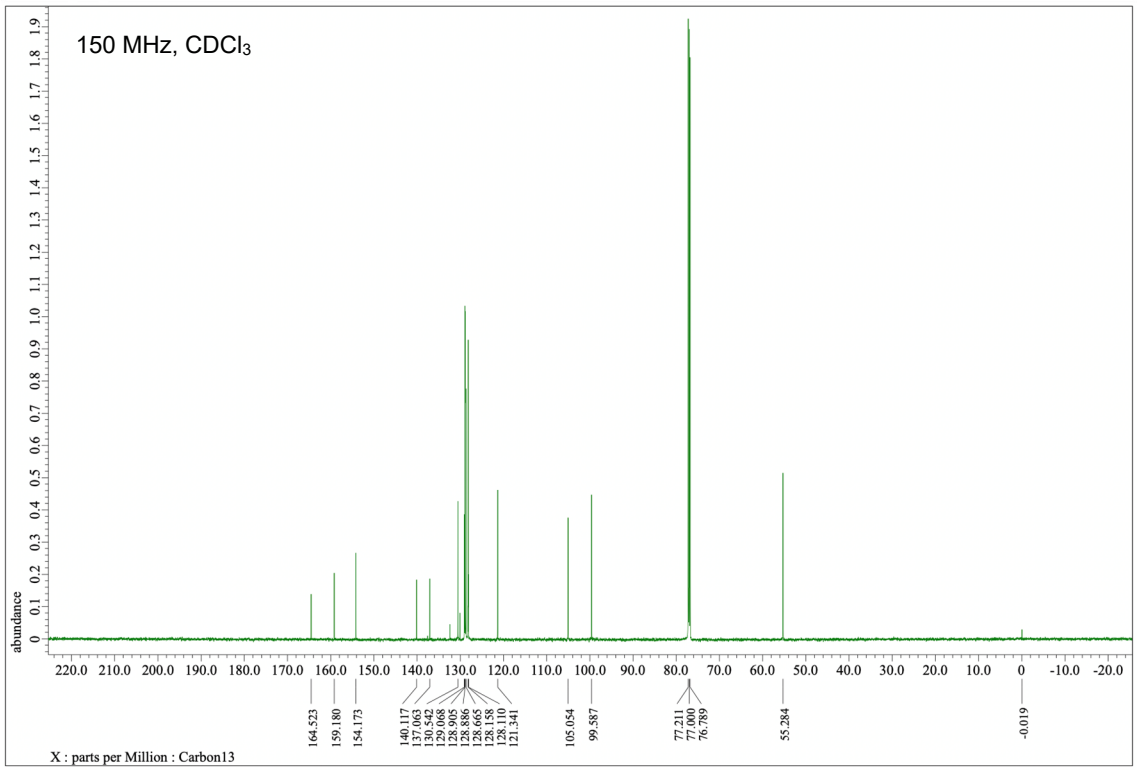

600 MHz, CDCl3
OH
Ac
N
Cl
Cl
2jb
4.03
3.12
3.04
2.06
1.00
1.00
0.74
abundance
X : parts per Million : Proton

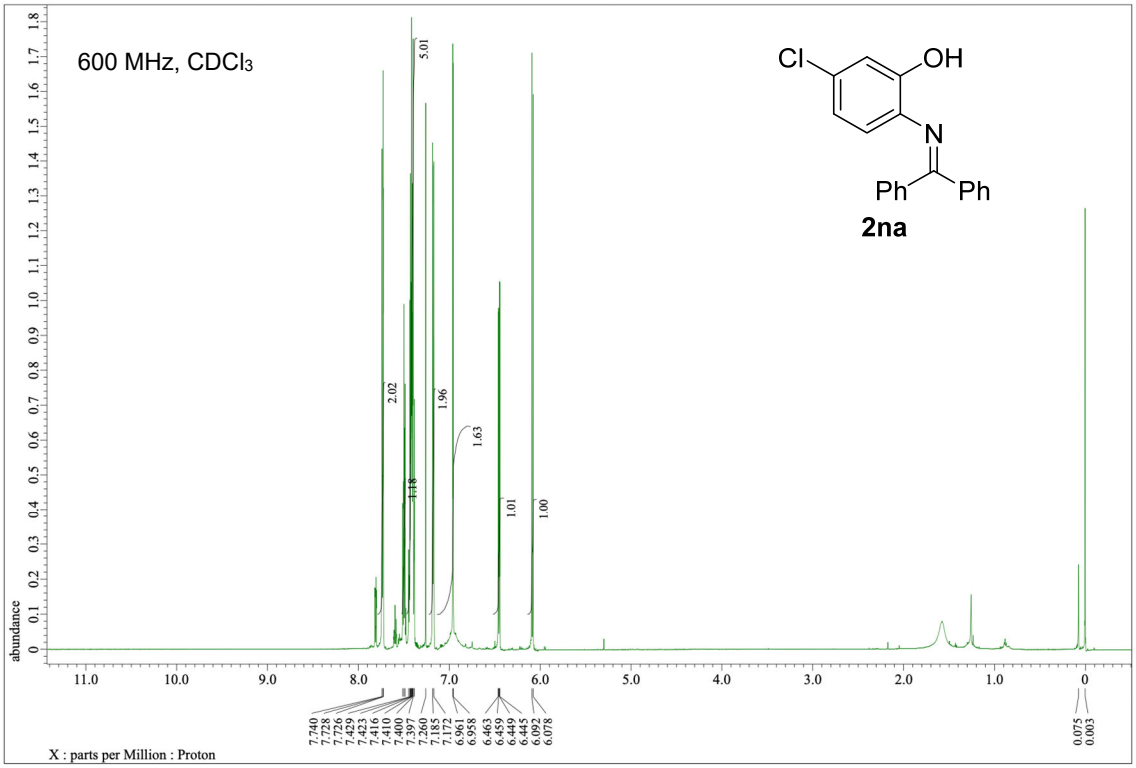

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

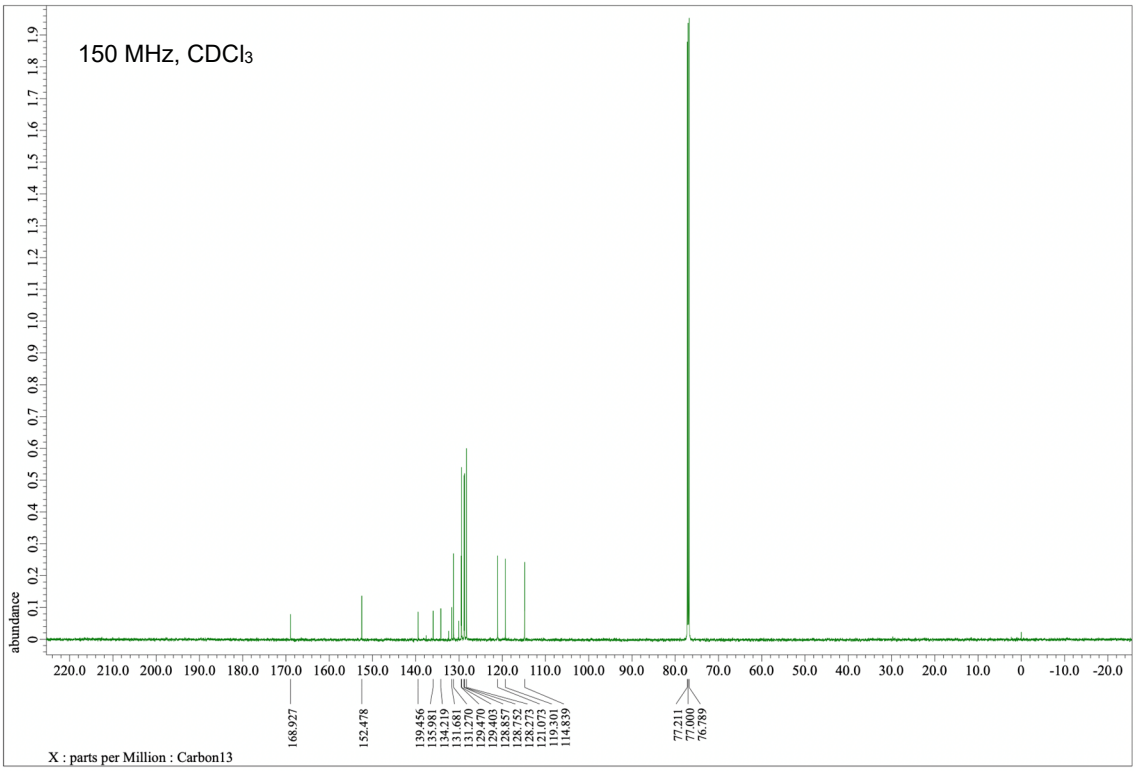

600 MHz, CDCl3
OH
O2N
N
Cl
Cl
2kb
4.11
3.00
2.10
1.00
0.94
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.955
7.948
7.932
7.926
7.694
7.672
7.442
7.424
7.420
7.403
7.260
7.131
7.125
7.118
7.110
7.035
7.013
-0.001
X : parts per Million : Proton

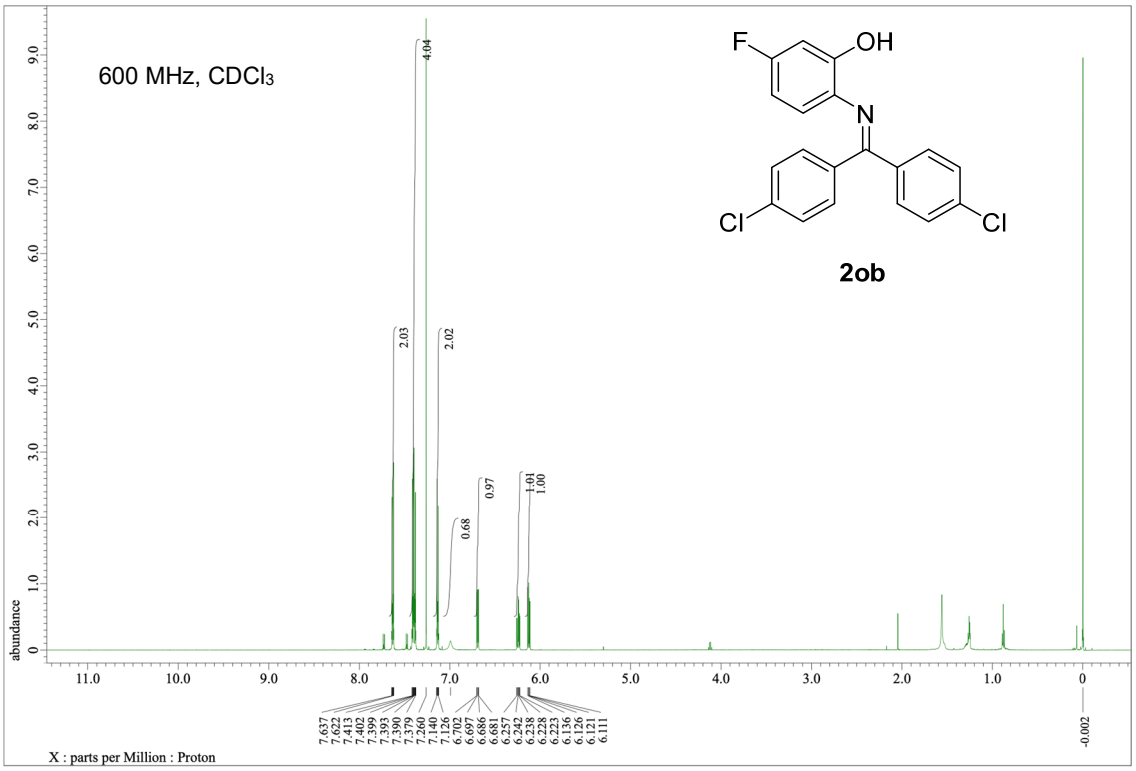

150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
169.971
156.758
140.481
138.652
136.881
136.603
135.587
132.755
130.877
130.092
129.546
128.876
122.959
115.969
114.696
77.211
77.000
76.789
-0.019
X : parts per Million : Carbon13

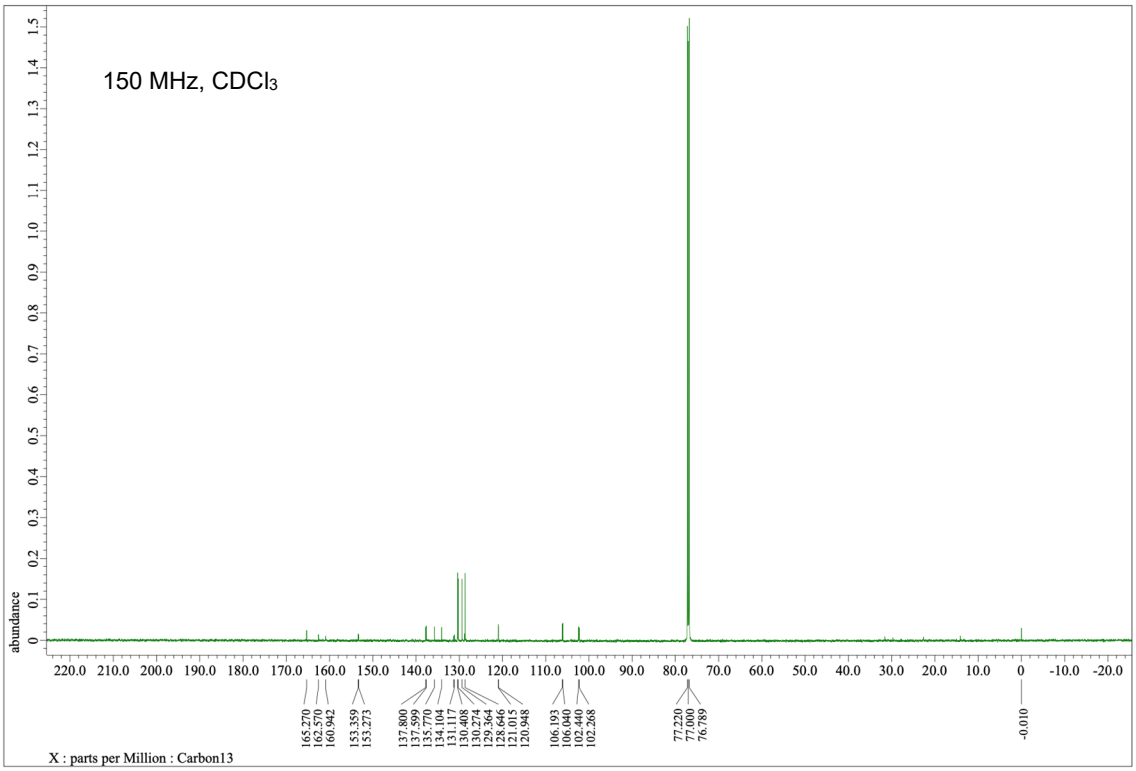

600 MHz, CDCl3
MeO
OH
N
Ph
Ph
2ma
4.21
3.00
2.02
2.01
1.93
1.01
abundance
X : parts per Million : Proton

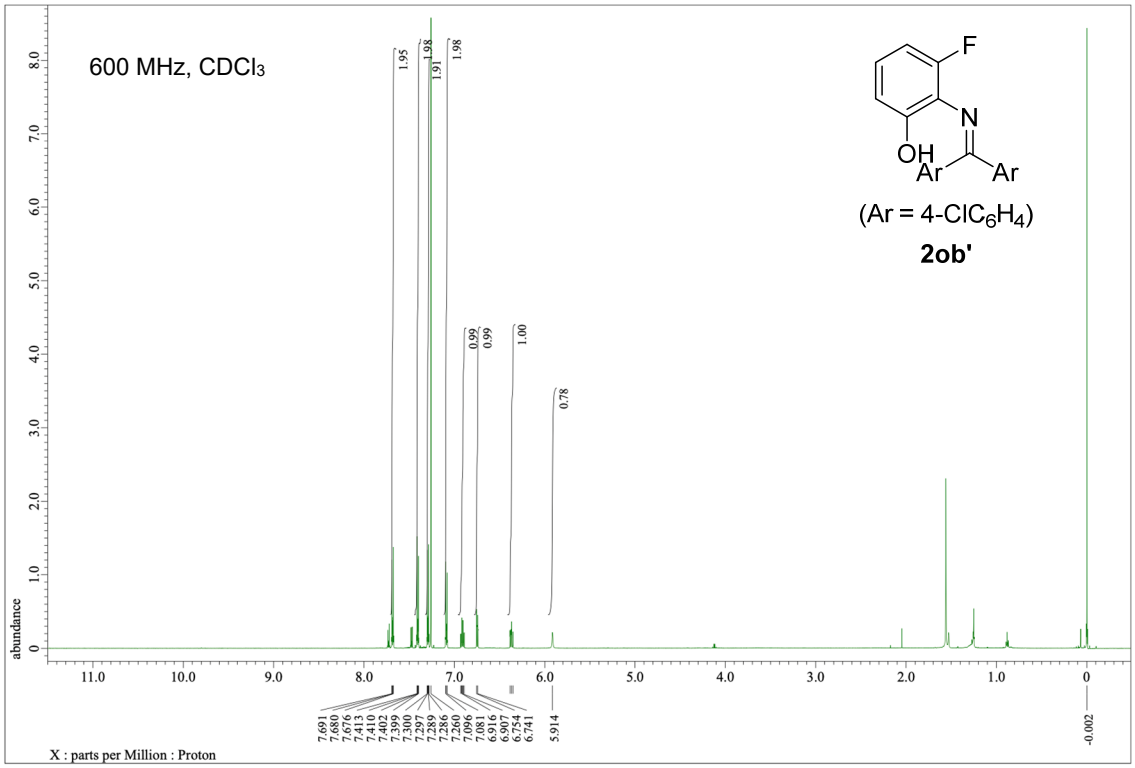

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

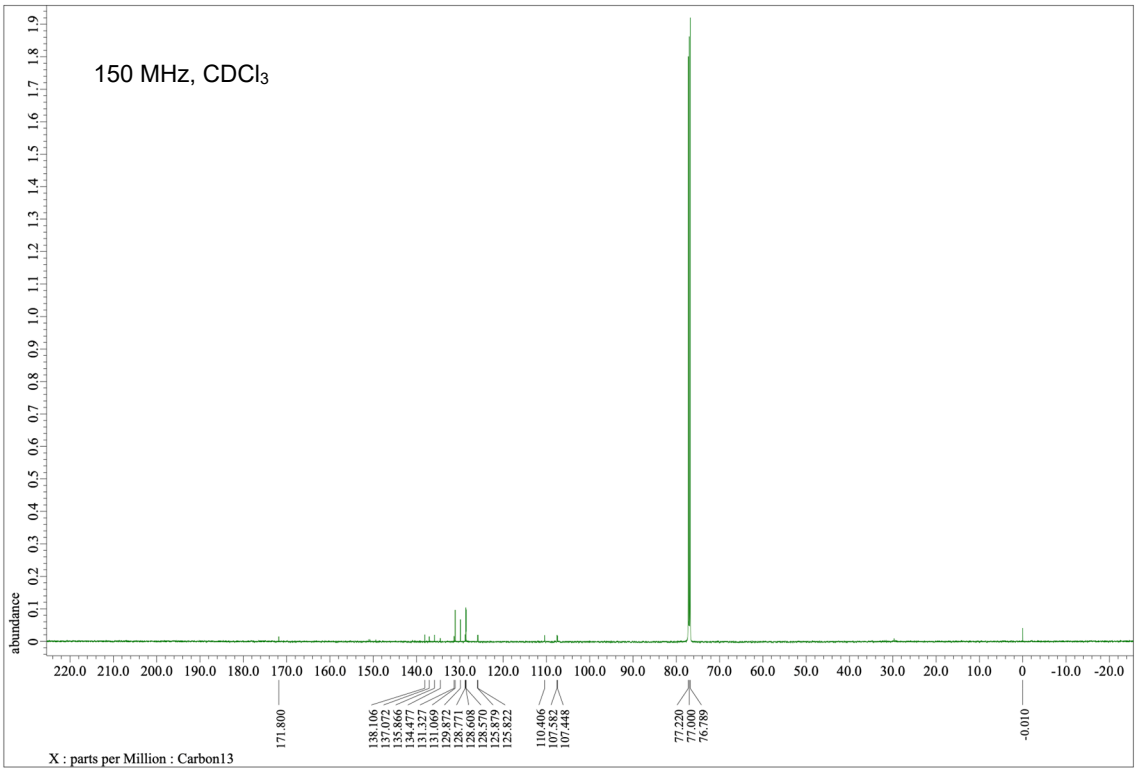

600 MHz, CDCl3
Cl
OH
N
Ph
Ph
2na
abundance
X : parts per Million : Proton

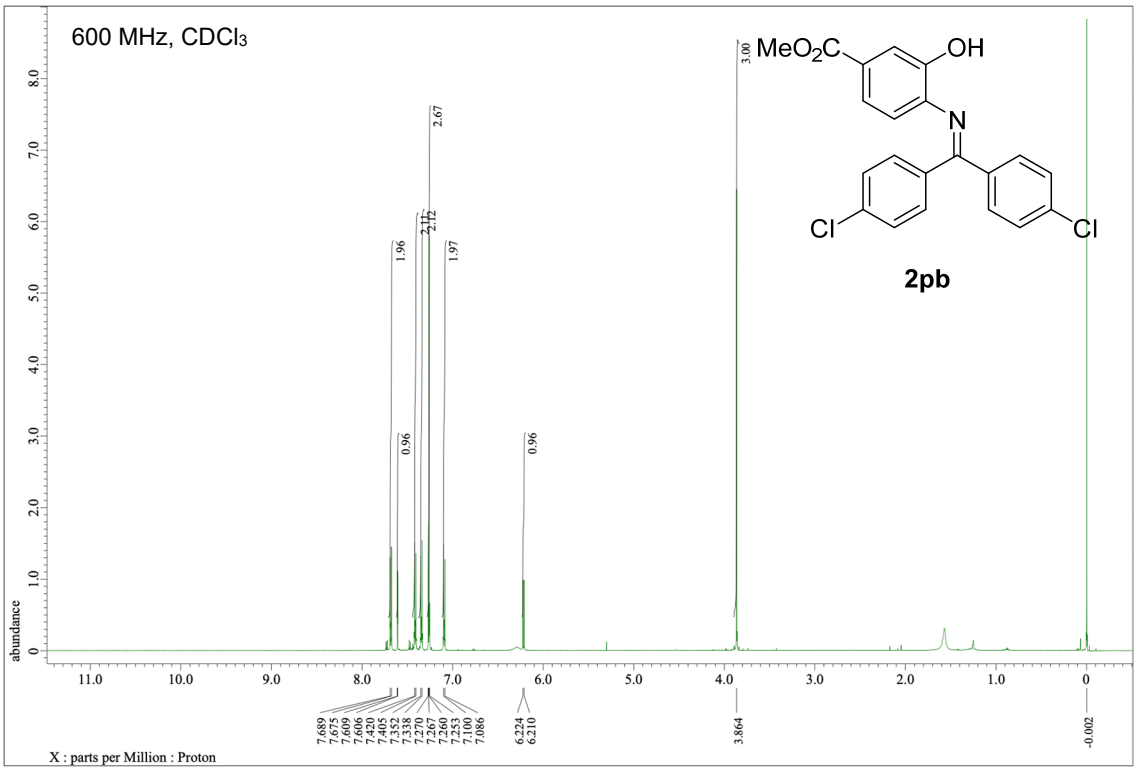

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

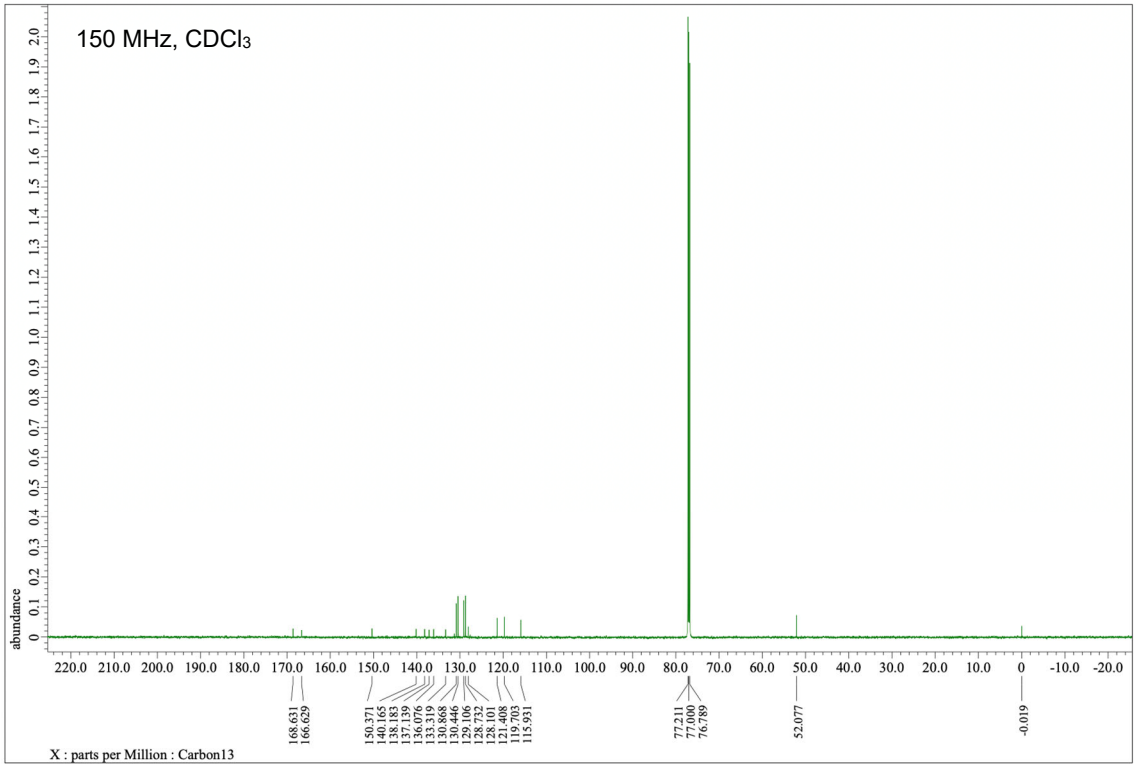

600 MHz, CDCl3
F
OH
N
Cl
Cl
2ob
4.04
2.03
2.02
0.97
1.01
1.00
0.68
abundance
X : parts per Million : Proton

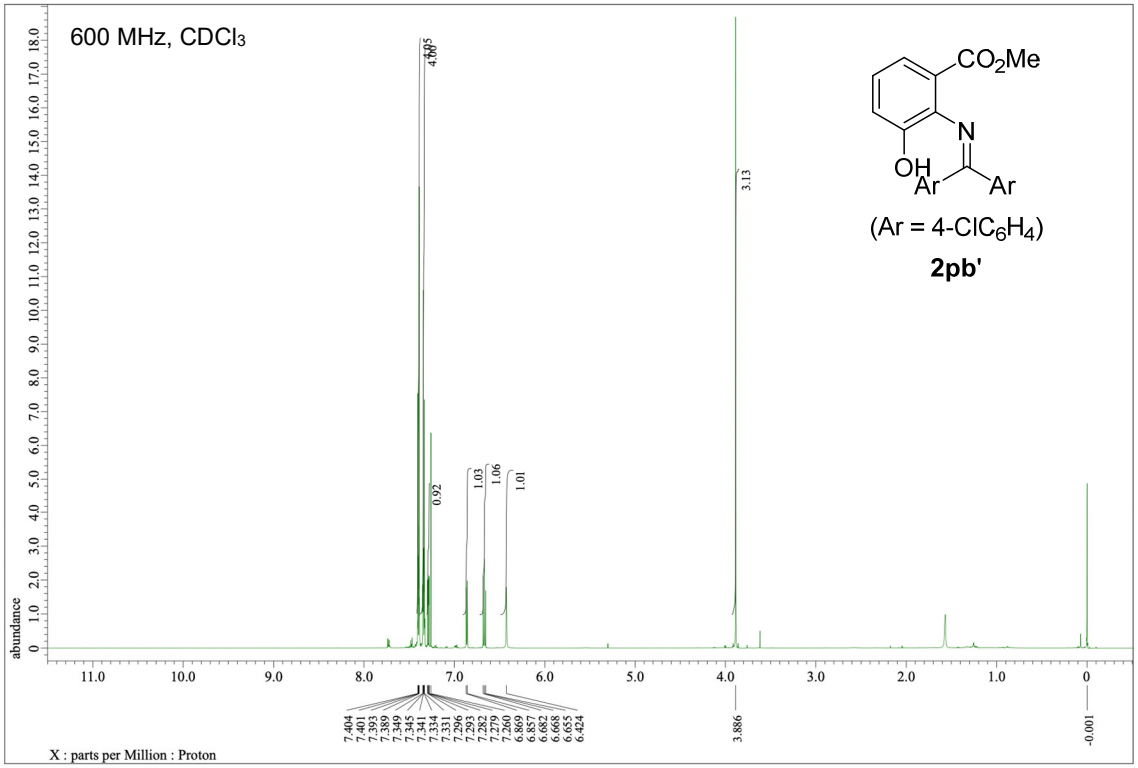

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

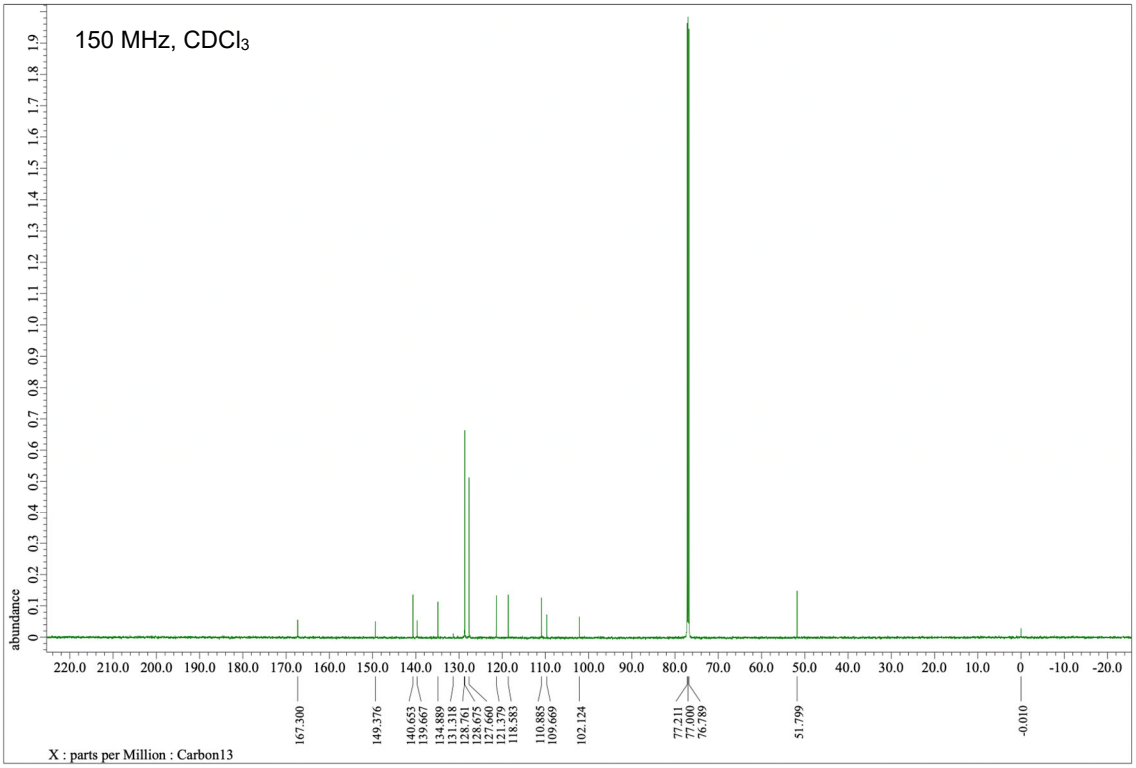

600 MHz, CDCl3
F
N
OH
Ar
Ar
(Ar = 4-ClC6H4)
2ob'
abundance
X : parts per Million : Proton

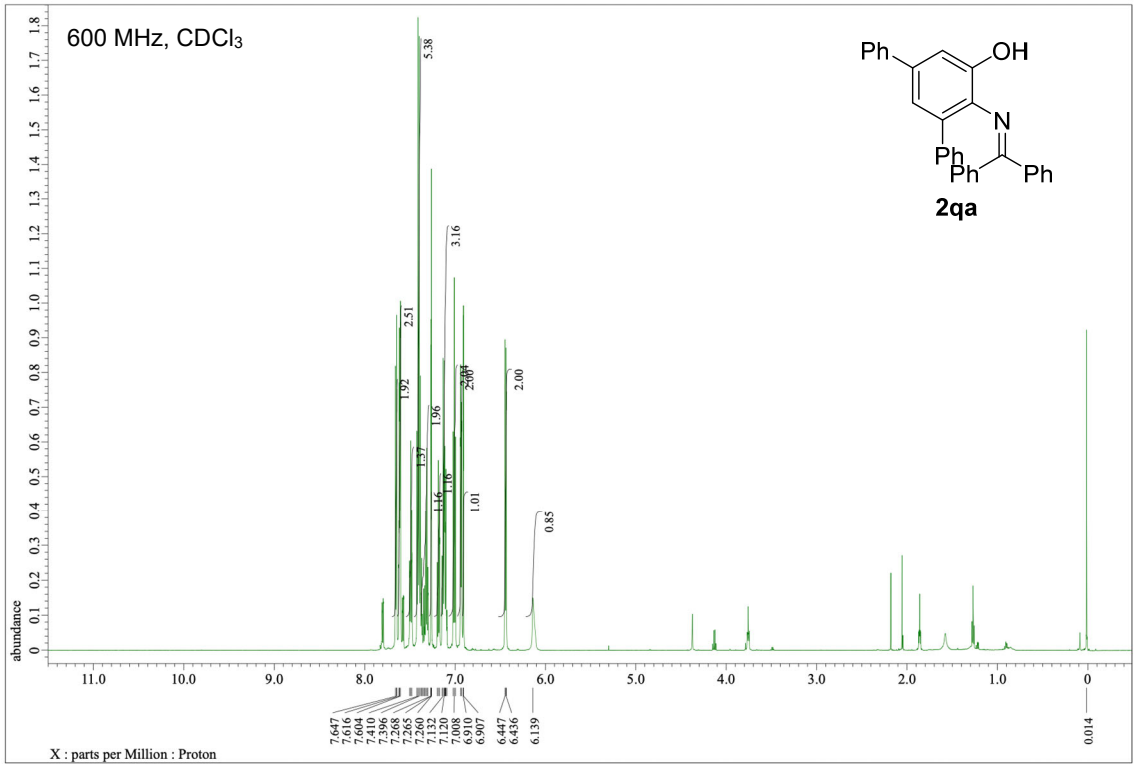

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

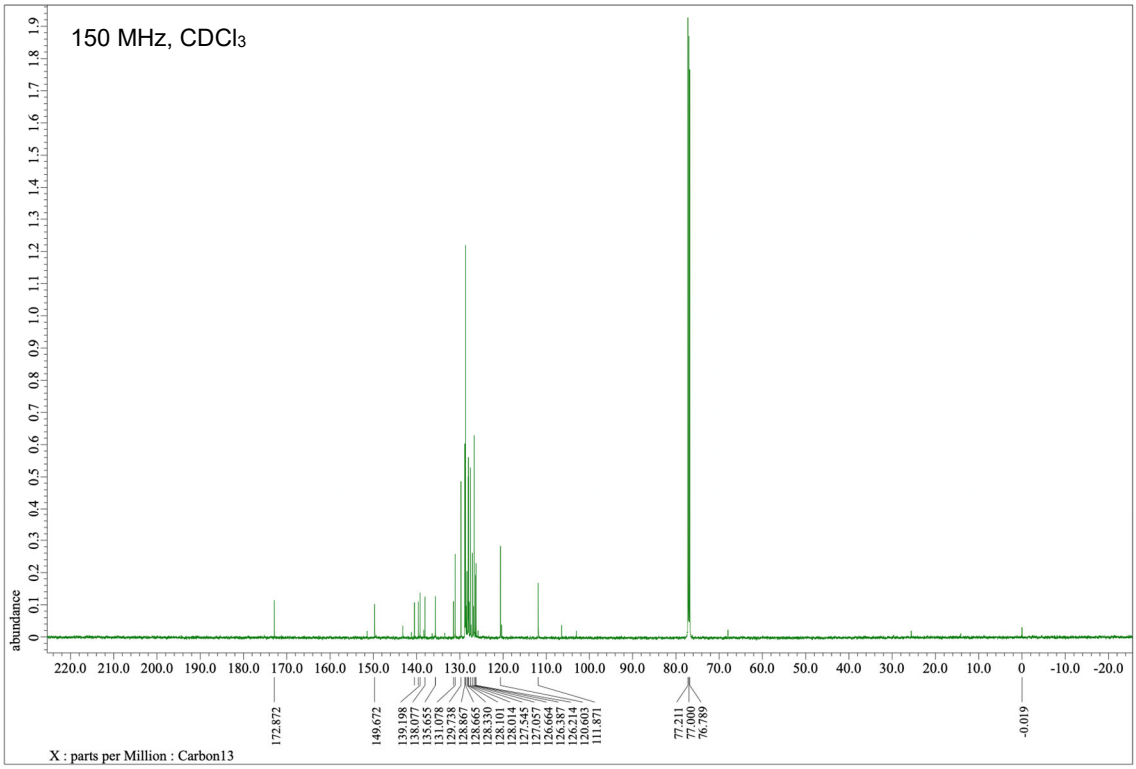

600 MHz, CDCl3
MeO2C
OH
N
Cl
Cl
2pb
abundance
X : parts per Million : Proton

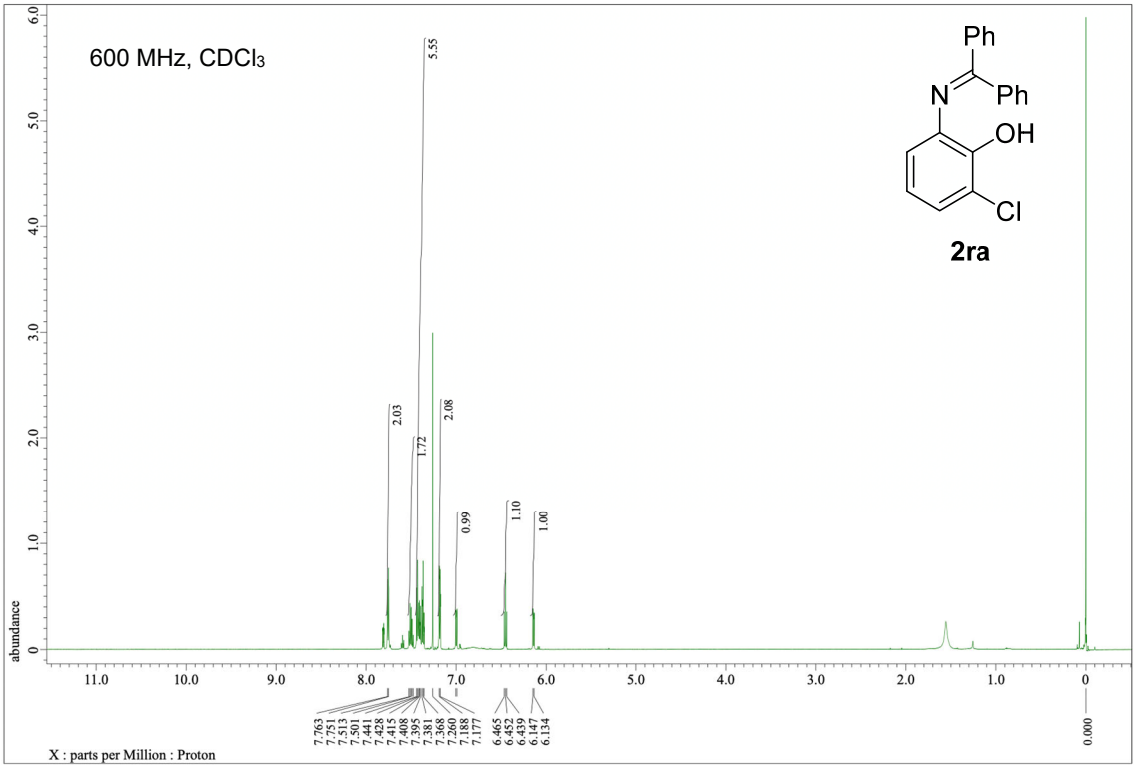

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

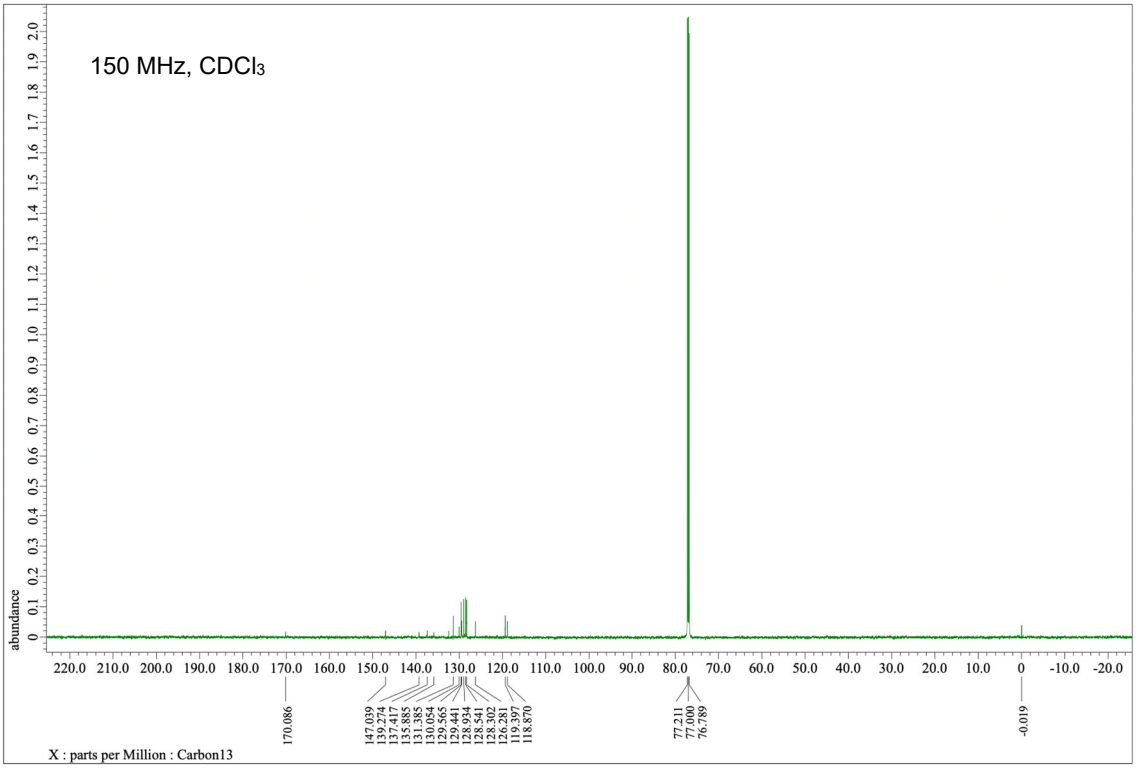

600 MHz, CDCl3
CO2Me
N
OH
Ar
Ar
(Ar = 4-ClC6H4)
2pb'
4.005
3.13
0.92
1.03
1.06
1.01
abundance
X : parts per Million : Proton
7.404
7.401
7.393
7.389
7.349
7.345
7.341
7.334
7.331
7.296
7.293
7.282
7.279
7.260
6.869
6.657
6.682
6.668
6.655
6.424
3.886
-0.001

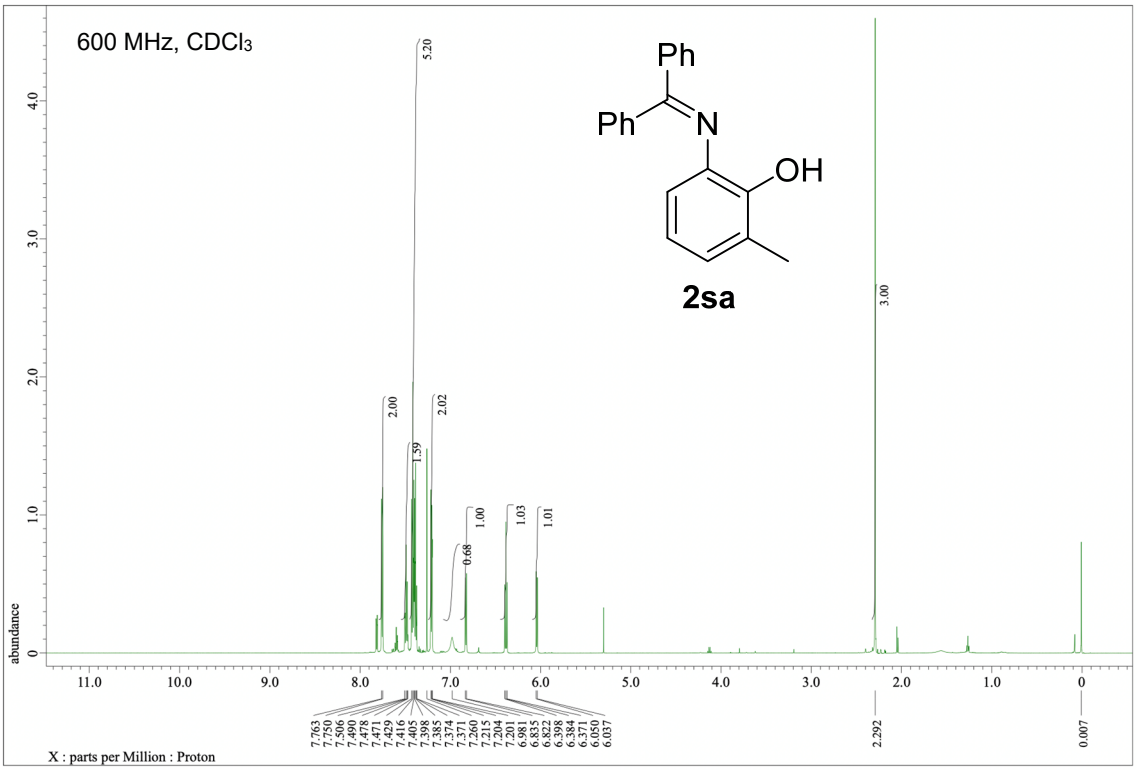

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13
167.300
149.376
140.653
139.667
134.889
131.318
128.761
128.675
127.660
121.379
118.583
110.885
109.669
102.124
77.211
77.000
76.789
51.799
-0.010

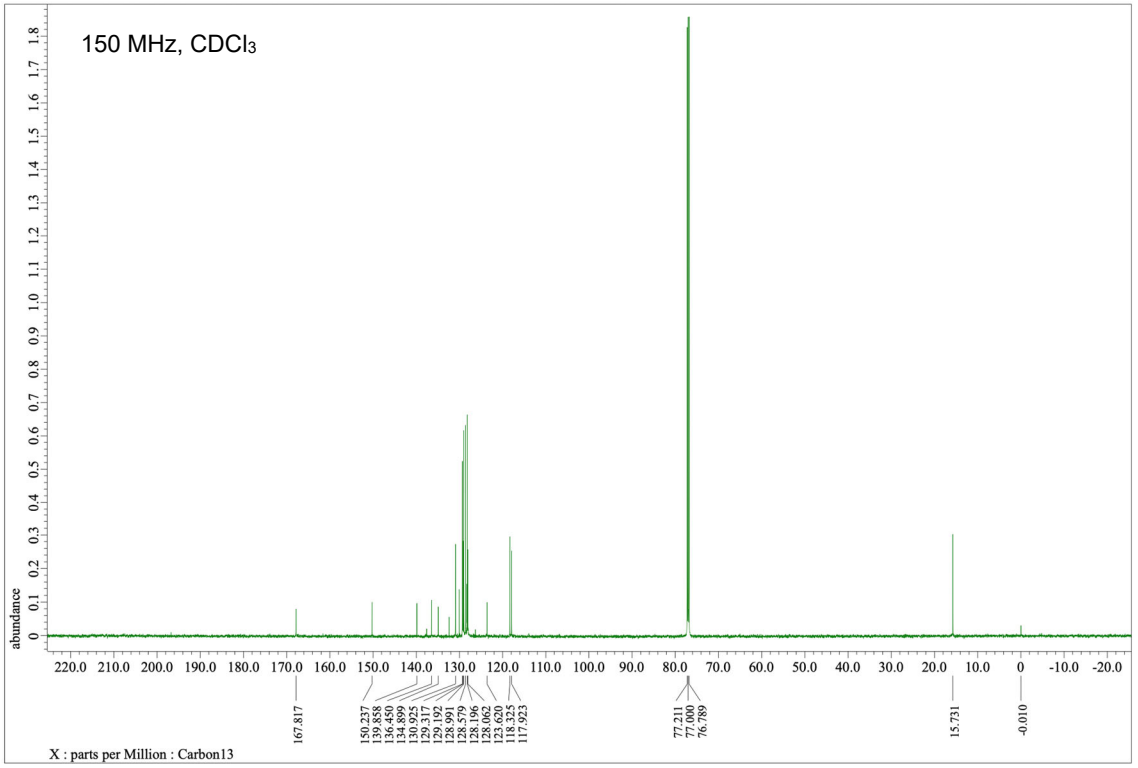

600 MHz, CDCl3
Ph
OH
N
Ph
Ph
Ph
2qa
abundance
X : parts per Million : Proton

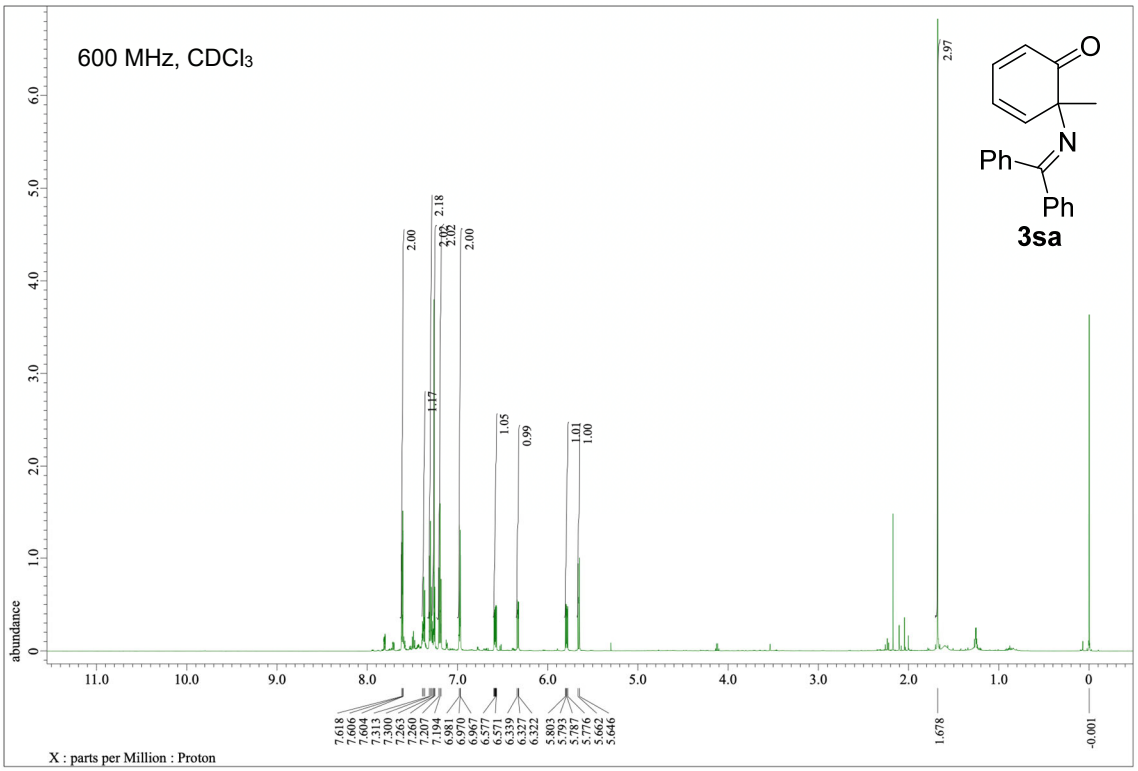

150 MHz, CDCl3
abundance
X : parts per Million : Carbon13

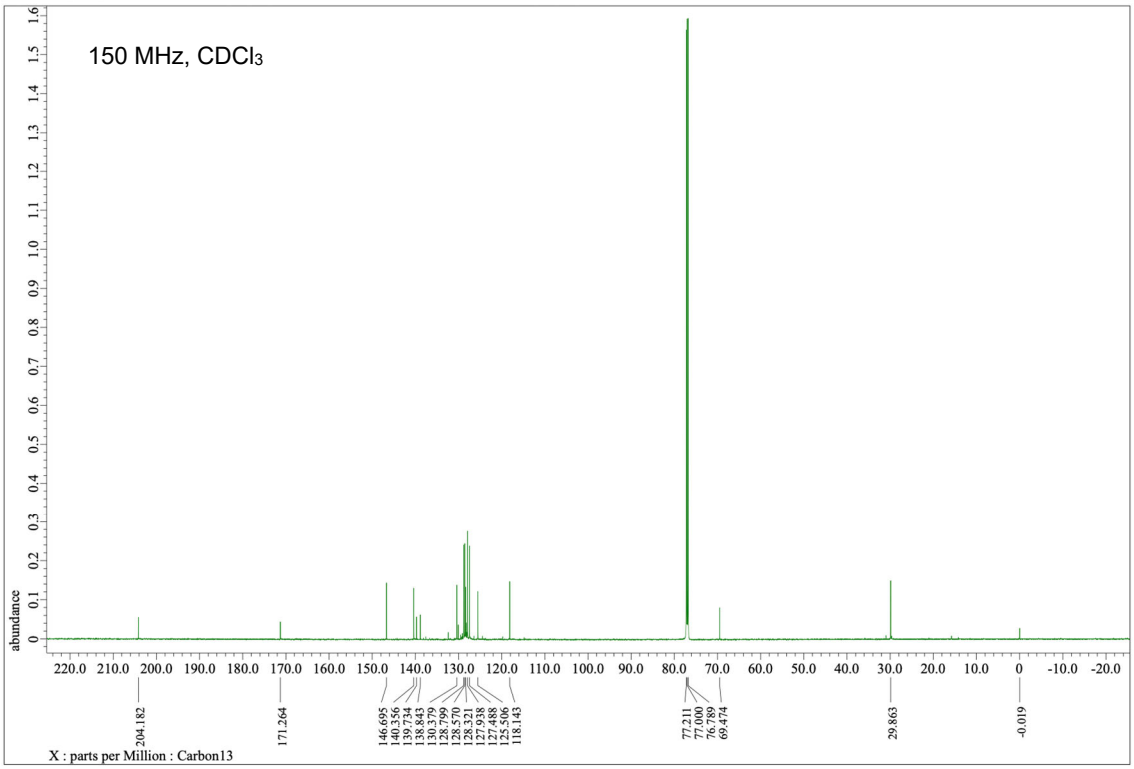

600 MHz, CDCl3
Ph
N
Ph
OH
Cl
2ra
5.55
2.03
1.72
2.08
0.99
1.10
1.00
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.763
7.751
7.513
7.501
7.441
7.428
7.415
7.408
7.395
7.381
7.368
7.260
7.188
7.177
6.465
6.452
6.439
6.147
6.134
0.000
X : parts per Million : Proton


150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
170.086
147.039
139.274
137.417
133.885
131.135
130.054
129.565
129.441
128.934
128.541
128.302
126.781
119.397
118.870
77.211
77.000
76.789
-0.019
X : parts per Million : Carbon13


600 MHz, CDCl3
Ph
Ph
N
OH
2sa
5.20
3.00
2.00
1.59
2.02
1.00
1.03
1.01
0.68
abundance
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.763
7.750
7.506
7.490
7.478
7.471
7.429
7.416
7.405
7.398
7.385
7.374
7.371
7.260
7.215
7.204
7.201
6.981
6.835
6.822
6.398
6.384
6.371
6.050
6.037
2.292
0.007
X : parts per Million : Proton


150 MHz, CDCl3
abundance
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
-20.0
167.817
150.237
139.858
136.450
134.899
130.925
129.317
129.192
128.999
128.579
128.196
128.062
123.620
118.325
117.923
77.211
77.000
76.789
15.731
-0.010
X : parts per Million : Carbon13


600 MHz, CDCl3
O
N
Ph
Ph
3sa
abundance
X : parts per Million : Proton


150 MHz, CDCl3
abundance
X : parts per Million : Carbon13