Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Nitrate Promoted Mild and Versatile Pd-catalysed C(sp^2)-H Oxidation with Carboxylic Acids

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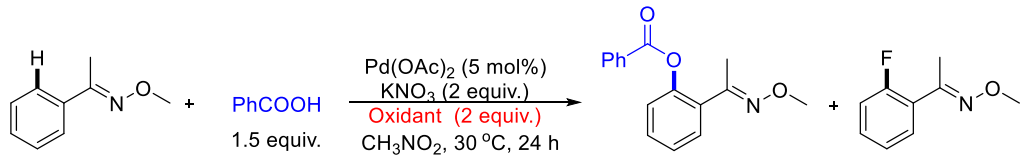
I. General

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without purification. Most ^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker AVANCE III 500 instrument in $CDCl_3$ using TMS as an internal standard, operating at 500 MHz and 126 MHz, respectively. Some ^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker ASCEND (600M) instrument in $CDCl_3$ using TMS as an internal standard, operating at 600 MHz and 151 MHz, respectively. Chemical shifts are expressed in ppm and coupling constants *J* are given in Hz. For $CDCl_3$ or DMSO-d_6 solutions the chemical shifts are reported as parts per million (ppm) to residual protium or carbon of the solvents; $CHCl_3$ H (7.28 ppm) and $CDCl_3$ C (77.03 ppm). GC experiments were carried out using Agilent 7890B GC. GC-MS experiments that used dodecane as an internal standard were performed with a Thermo DSQ II, Trace GC Ultra. High resolution mass spectra (HRMS (ESI-TOF)) were obtained on an Agilent 6545 Q-TOF LCMS spectrometer equipped with an ESI source.

II. Conditions Screening for the C-H bond oxidation of O-methyl oxime

Table S1. Screening of oxidants[a]

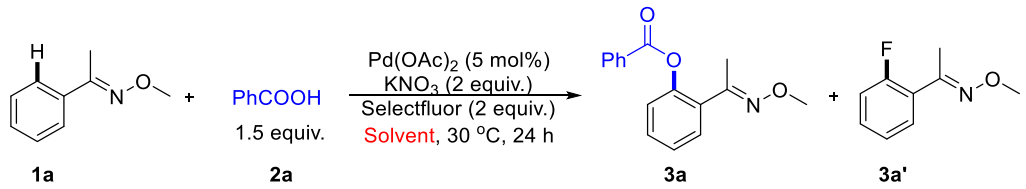


1a **2a** **3a** **3a'**

Entry	Oxidant	Conv. of 1a (%)	Yield of 3a (%)[b]	Yield of 3a' (%)[b]
1	**Selectfluor**	**99**	**74**	**8**
2[c]	Selectfluor	95	72	11
3	O_2	NR	--	--
4	NFSI	86	59	26
5	Air	NR	--	--
6	$Na_2S_2O_8$	12	2	--
7	$(NH_4)_2S_2O_8$	NR	--	--
8	$PhI(OAc)_2$	40	--	--
9	$Cu(OAc)_2$	NR	--	--
10	BQ	15	--	--
11	CAN	92	65	--

[a]Reaction conditions: **1a** (0.1 mmol, 14.9 mg), PhCOOH (0.15 mmol, 18.3 mg), Oxidant (0.2 mmol), KNO_3 (0.2 mmol, 20.2 mg), $Pd(OAc)_2$ (5 mol%, 1.2 mg), CH_3NO_2 (1 mL), 30 °C, 24 h, [b]GC yields, [c]Under N_2 atmosphere.

Table S2. Screening of solvents[a]

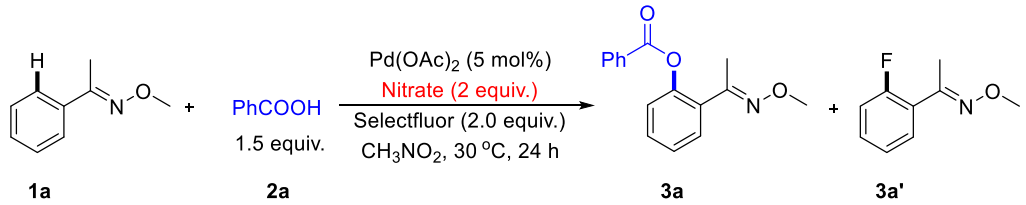


1a **2a** **3a** **3a'**

Entry	Solvent	Conv. of 1a (%)	Yield of 3a (%)[b]	Yield of 3a' (%)[b]
1	**CH_3NO_2**	**99**	**74**	**8**
2	DCE	45	44	--
3	DCM	35	34	--
4	DMF	NR	--	--
5	Toluene	16	15	--
6	MeOH	NR	--	--
7	Dioxane	NR	--	--
8	THF	NR	--	--
9	EtOAc	NR	--	--
10	MeCN	45	44	--
11	Acetone	NR	--	--

[a]Reaction conditions: **1a** (0.1 mmol, 14.9 mg), PhCOOH (0.15 mmol, 18.3 mg), Selectfluor (0.2 mmol, 70.8 mg), KNO_3 (0.2 mmol, 20.2 mg), $Pd(OAc)_2$ (5 mol%, 1.2 mg), Solvent (1 mL), 30 °C, 24 h, under air, [b]GC yields.

Table S3. Screening of nitrate additives[a]



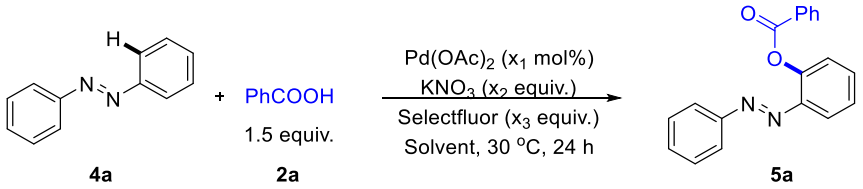
1a **2a** **3a** **3a'**

Entry	Nitrate	Conv. of 1a (%)	Yield of 3a (%)[b]	Yield of 3a' (%)[b]
1	**KNO_3**	**99**	**74**	**8**
2	/	21	13	0
3	$AgNO_3$	99	73	16
4	$LiNO_3$	99	54	5
5	$NaNO_3$	95	73	18
6	$Mg(NO_3)_2 \cdot 6H_2O$	99	30	--
7	$Fe(NO_3)_3 \cdot 9H_2O$	99	23	16
8	$Cu(NO_3)_2$	97	40	--
9	$Ba(NO_3)_3$	99	38	--

[a]Reaction conditions: **1a** (0.1 mmol, 14.9 mg), PhCOOH (0.15 mmol, 18.3 mg), Selectfluor (0.2 mmol, 70.8 mg), Nitrate (0.2 mmol), $Pd(OAc)_2$ (5 mol%, 1.2 mg), CH_3NO_2 (1 mL), 30 °C, 24 h, [b]GC yields.

III. Conditions Screening for the C-H bond oxidation of Azobenzene

Table S4. Screening of azobenzene oxidation conditions[a]



4a **2a** **5a**

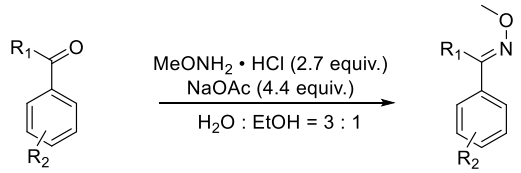
Entry	$Pd(OAc)_2$	KNO_3	Solvent	Selectfluor	Yield of 5a (%)[b]
1	5 mol%	0.2 equiv.	CH_3NO_2	2.0 equiv.	57
2	5 mol%	0.2 equiv.	DCE	2.0 equiv.	74
3	5 mol%	0.4 equiv.	DCE	2.0 equiv.	76
4	5 mol%	1.0 equiv.	DCE	2.0 equiv.	62
5	5 mol%	2.0 equiv.	DCE	2.0 equiv.	66
6	5 mol%	0 equiv.	DCE	2.0 equiv.	32
7	5 mol%	0.4 equiv.	DCE	1.5 equiv.	51
8	5 mol%	0.4 equiv.	DCE	2.0 equiv.	74
9	5 mol%	0.4 equiv.	DCE	2.5 equiv.	86
10	10 mol%	0.4 equiv.	DCE	2.0 equiv.	84
11	15 mol%	0.4 equiv.	DCE	2.0 equiv.	80
12[c]	**10 mol%**	**0.4 equiv.**	**DCE**	**2.5 equiv.**	**88**
13[c]	15 mol%	0 equiv.	DCE	2.5 equiv.	19

[a]Reaction conditions: **4a** (0.1 mmol, 18.2 mg), PhCOOH (0.15 mmol, 18.3 mg), Selectfluor (x_3 *equiv.*), KNO_3 (x_2 *equiv.*), $Pd(OAc)_2$ (x_1 mol%.), Solvent (1 mL), 30 °C, 24 h, under air, [b]GC yields, [c]$AgNO_3$ instead of KNO_3 and $PdCl_2$ instead of $Pd(OAc)_2$.

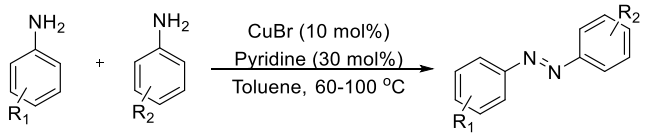
IV. Typical experimental procedure for synthesis of products

A. Typical experimental procedure for synthesis of 1 and 4

O-methyl oximes **1** and azobenzenes **4** were prepared according to the literature procedure.[1]



In a 50 mL round bottom flask equipped with a stir bar, acetophenone (1.7 mmol, 1 *equiv.*), $MeONH_2$•HCl (384.2 mg, 4.6 mmol, 2.7 *equiv.*), NaOAc (615 mg, 7.5 mmol, 4.4 *equiv.*), H_2O (15 mL), and EtOH (5 mL). The flask was equipped with a reflux condenser and heated at 70 ^oC for 2 h. After cooling, the mixture was extracted with EtOAc (3 x 15 mL). The organic layers were combined, dried with $MgSO_4$, and concentrated to afford the desired product oximes.



In a 100 mL round bottom flask equipped with a stir bar, CuBr (143 mg, 1.0 mmol, 0.2 *equiv.*), pyridine (253.1 mg, 3.2 mmol, 0.6 *equiv.*), aniline-R_1 (5 mmol, 1.0 *equiv.*) and aniline-R_2 (5 mmol, 1.0 *equiv.*) were mixed in toluene (60 mL). The reaction mixture was vigorously stirred at 60-100 ^oC for 24 h. After cooling down to room temperature and concentrating under vacuum, the residue was purified by silica gel chromatography (petroleum ether) to afford the desired product azobenzenes.

B. Typical experimental procedure for synthesis of 3

In a 10 mL test tube equipped with a stir bar, O-methyl oxime **1** (0.3 mmol, 1.0 *equiv.*), **2** (0.45 mmol, 1.5 *equiv.*), $Pd(OAc)_2$ (3.4 mg, 0.015 mmol, 5 mol%), Selectfluor (212.4 mg, 0.6 mmol, 2.0 *equiv.*), KNO_3 (60.6 mg, 0.6 mmol, 2.0 *equiv.*) and CH_3NO_2 (3.0 mL) were added successively. Then the tube was sealed at indicated temperature for 24 h under stirring. Upon completion, the residue was purified by silica gel chromatography (petroleum ether / EtOAc = 30:1) to afford the desired products **3.**

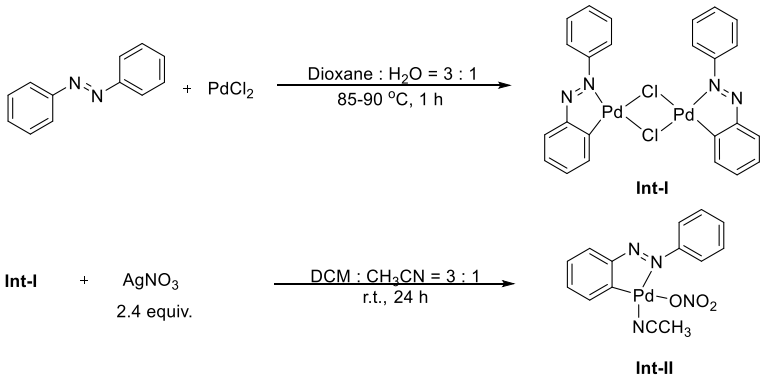
C. Typical experimental procedure for synthesis of 5

In a 10 mL test tube equipped with a stir bar, azobenzene **4** (0.3 mmol, 1.0 *equiv.*), **2** (0.45 mmol, 1.5 *equiv.*), $PdCl_2$ (5.1 mg, 0.03 mmol, 10 mol%), Selectfluor (258.8 mg, 0.75 mmol, 2.5 *equiv.*), $AgNO_3$ (20.4 mg, 0.12 mmol, 0.4 *equiv.*) and DCE (3.0 mL) were added successively. Then the tube was sealed at indicated temperature for 24 h under stirring. Upon completion, the residue was purified by silica gel chromatography (petroleum ether / EtOAc = 30:1) to afford the desired products **5.**

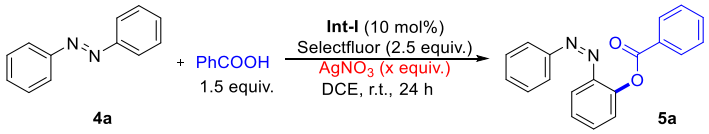
V. Reactivities of the Pd complexes in the oxidation reactions

(A) Preparation of Pd(II) complexes

Int-I, Int-II were prepared according to the literature procedures.[1]



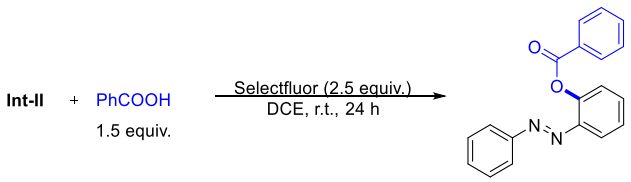
(B) Catalytic activity of Int-I



Entry	[Pd]	$AgNO_3$	Yield of 5a[b]
1	**Int-I**	0	27
2	**Int-I**	0.1 equiv.	69
3	**Int-I**	0.2 equiv.	**77**
4	**Int-I**	**0.4 equiv.**	70
5	**Int-I**	0.5 equiv.	68

[a]Reaction conditions: **4a** (0.1 mmol, 18.2 mg), PhCOOH (0.15 mmol, 18.3 mg), Selectfluor (0.25 mmol, 88.5 mg), $AgNO_3$ (x mmol), [Pd] (0.01 mmol), DCE (1 mL), room temperature, 24 h, under air, [b]GC yields.

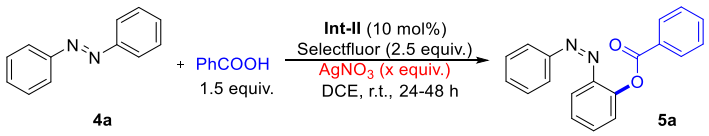
(C) Stoichiometric transformation of Int-II



In a 10 mL test tube equipped with a stir bar, **Int-II** (39 mg, 0.1 mmol, 1.0 *equiv.*), PhCOOH (18.3 mg, 0.15 mmol, 1.5 *equiv.*), Selectfluor (88.5 mg, 0.25 mmol, 2.5 *equiv.*) and DCE (1.0 mL) were added successively. Then the tube was sealed and stirred at room temperature for 24 h. Upon completion, CH_3COOH (0.5 mL) was added to the resulting mixture and stirred vigorously for the indicated time. The resulting acidic mixture was neutralized by NaOH aqueous, extracted with EtOAc and separated.

The organic layer was filtered, the yield was determined by GC (82% yield).

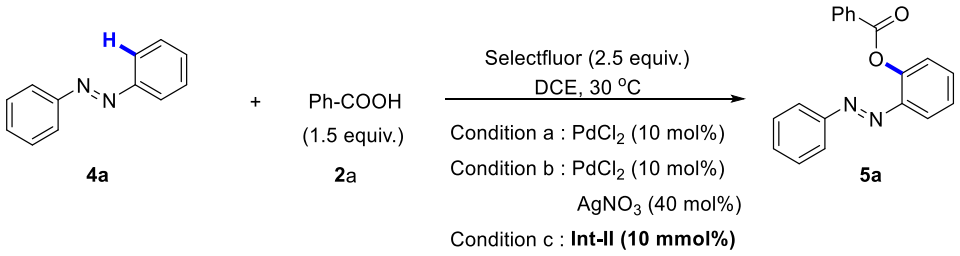
(D) Catalytic activity of Int-II



Entry	[Pd]	$AgNO_3$	Yield of 5a[b]
1	**Int-II**	0	58
2	**Int-II**	0.1 equiv.	79
3	**Int-II**	0.2 equiv.	84
4	**Int-II**	**0.4 equiv.**	**86**
5	**Int-II**	0.5 equiv.	84

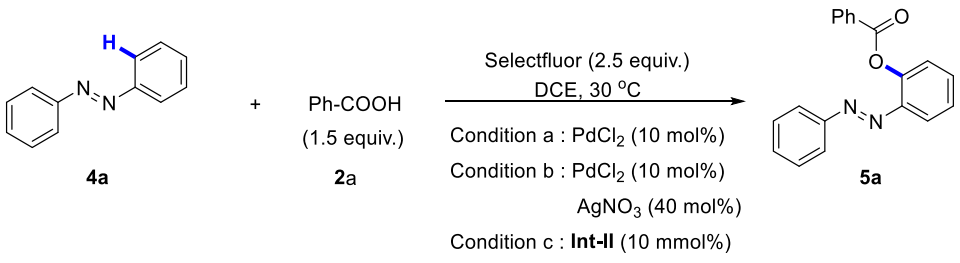
[a]Reaction conditions: **4a** (0.1 mmol, 18.2 mg), PhCOOH (0.15 mmol, 18.3 mg), Selectfluor (0.25 mmol, 88.5 mg), $AgNO_3$ (x mmol), [Pd] (0.01 mmol), DCE (1 mL), room temperature, 24 h, under air, [b]GC yields.

(E) Kinetic study for the oxidation of azobenzene with benzoic acid



Reaction condition : In a 10 mL test tube equipped with a stir bar, **4a** (54.6 mg, 0.3 mmol, 1.0 *equiv.*), PhCOOH (54.9 mg, 0.45 mmol, 1.5 *equiv.*), Selectfluor (265.2 mg, 0.2 mmol, 2.5 *equiv.*) and DCE (3 mL) [a] $PdCl_2$ (5.3 mg, 0.03 mmol, 10 mmol%), [b] $PdCl_2$ (5.3 mg, 0.03 mmol, 10 mmol%), AgNO3 (10.2 mg, 0.12mmol, 40 mmol%) [c] **Int-II** (11.7 mg, 0.03 mmol, 10 mmol%) were added successively. Then the tube was sealed and stirred at 30 °C oil bath for the indicated time. The resulting mixture diluted with EtOAc and filtered, followed by GC experiments. The data of kinetic curves from reaction a, b and c are included below. Each data point is an average of three independent GC injections using biphenyl as an internal standard.

Table S5. Kinetic study for the oxidation of azobenzene with benzoic acid



Time / min.	Conv. / % (GC)		
	a	b	c
5	0	0	0
10	0	0	1.4
20	0	4.5	2.4
30	0	20.5	5.2
60	0	30.3	10.6
90	0	36.8	12.2
150	0	40.1	19
210	0	43.7	23.5
330	0	46.3	31
450	0	50.8	39.2
570	0	56.4	48.5
750	0	61.4	55.8
930	1.4	64.3	56.8

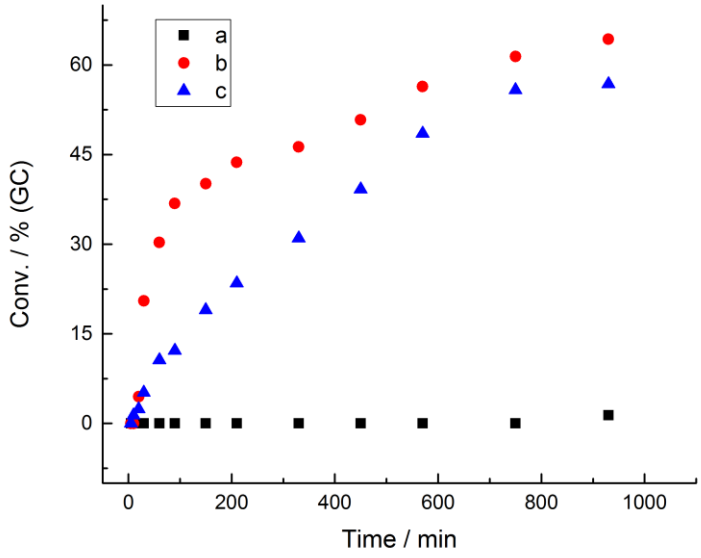


Figure S1 Kinetic plots for the oxidation reaction of **4a**

As shown in Figure S1, the time-conversion curves of oxidation reaction displayed a lack of induction period, indicating that the palladacycle complex **Int-II** might be involved in the catalytic cycle.

VI. Computational Studies

Computational Details

All calculations were carried out with Gaussian 16 program.[2] The geometry optimizations were performed at the B3LYP[3]/BSI level. In the basis set BSI, the 6-31G(d) basis set was considered for all nonmetallic atoms, and the Stuttgart/Dresden effective core potential (ECP) together with associated

basis set (MWB28)[4] was used for Pd atom. Each optimized structure was subsequently analyzed by harmonic vibration frequencies at the same level to characterize a minimum without imaginary frequency (N_{imag} = 0) or a transition state with only one imaginary frequency (N_{imag} = 1) and to obtain the thermodynamic corrections to Gibbs free energy. The connection of transition states was generally confirmed via intrinsic reaction coordinate (IRC) calculations, while some of transition states were confirmed to connect corresponding minima via separate geometrical optimization along with the reaction coordinates due to the failure in IRC following (Figures S3-S5 and S7-S10). All the structures were optimized without any symmetry restrictions. The subsequent single-point calculations were carried out at the level of M06[5]/BSII together with SMD model[6] for considering the dichloroethane (DCE) solvation effect. Gibbs free energies in solution described in the study were obtained from such single-point calculations, including gas-phase free energy corrections.

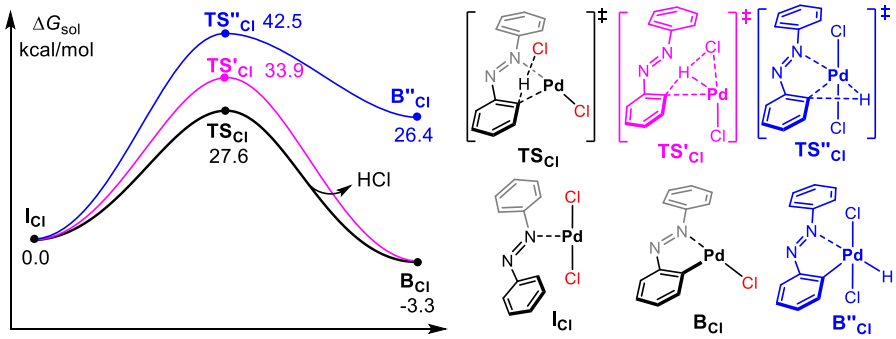


Fig. S2 Compared different processes of C–H activation of **4a** catalyzed by $PdCl_2$. The free energies are given in kcal/mol.

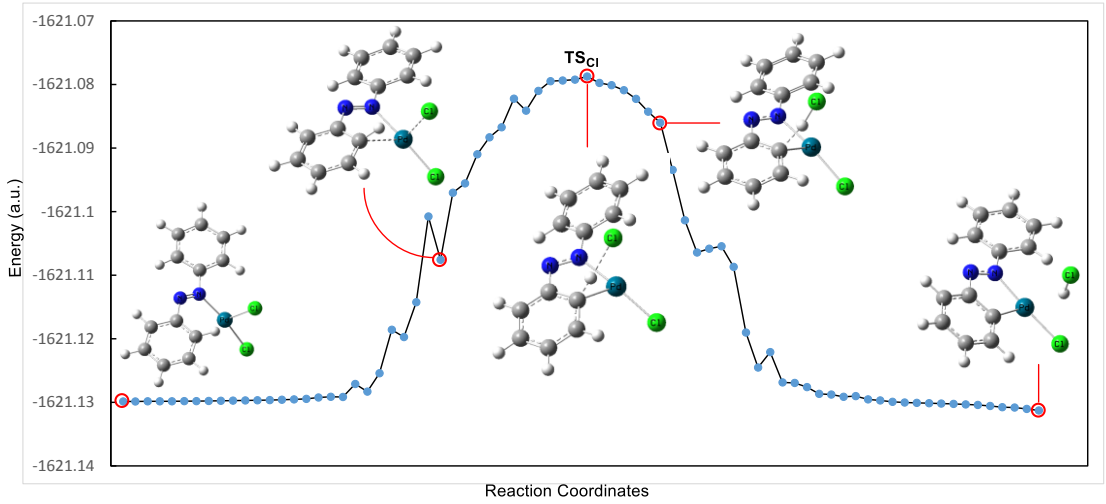


Fig. S3 Geometrical optimization curves along with the reaction coordinates at the both sides of transition state $\mathbf{TS_{Cl}}$. It is shown that such optimizations can reach the corresponding reactants and products.

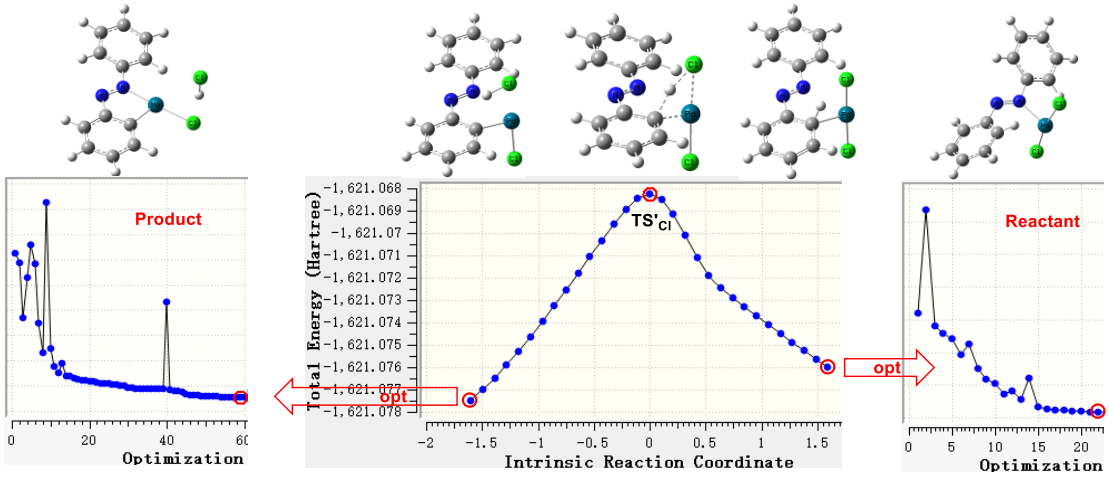


Fig. S4 IRC calculations of $\mathbf{TS'_{Cl}}$ and the geometrical optimization curves along with the reaction coordinates at the both sides. It is shown that such optimizations can reach the corresponding reactants and products.

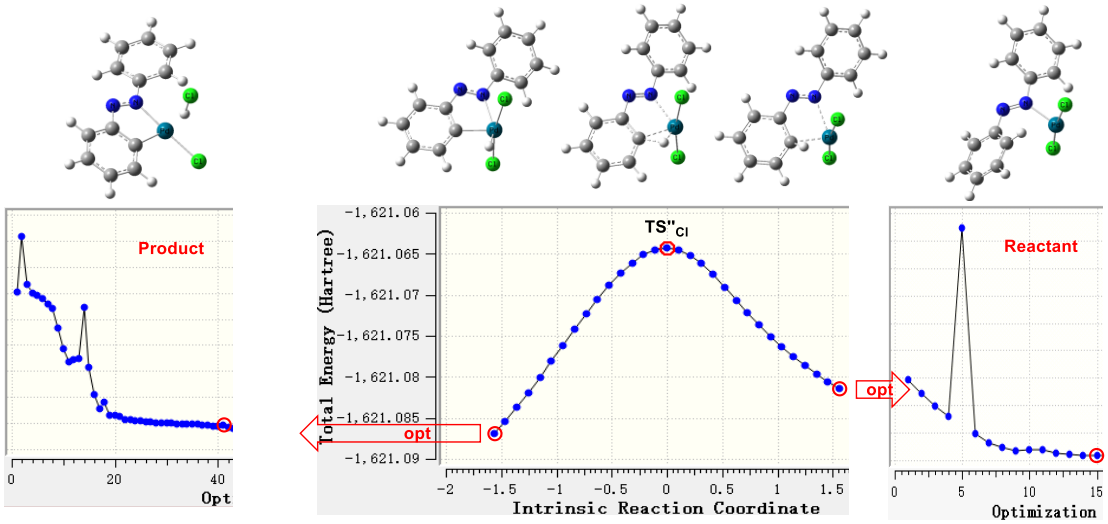


Fig. S5 IRC calculations of $\mathbf{TS''_{Cl}}$ and the geometrical optimization curves along with the reaction coordinates at the both sides. It is shown that such optimizations can reach the corresponding reactants and products.

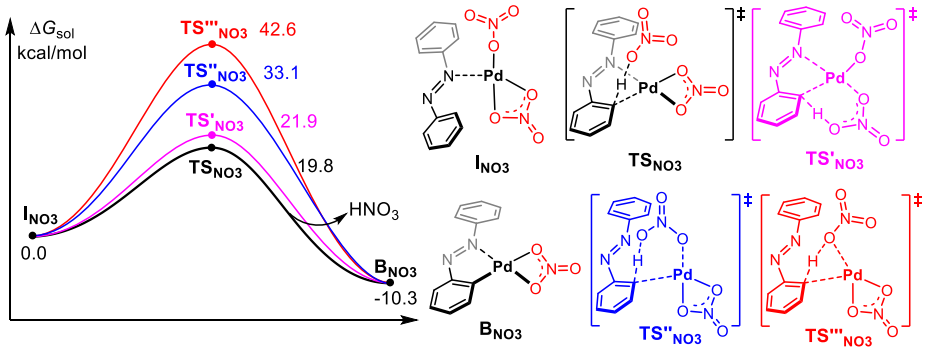


Fig. S6 Compared different processes of C–H activation of **4a** catalyzed by $Pd(NO_3)_2$. The free energies are given in kcal/mol.

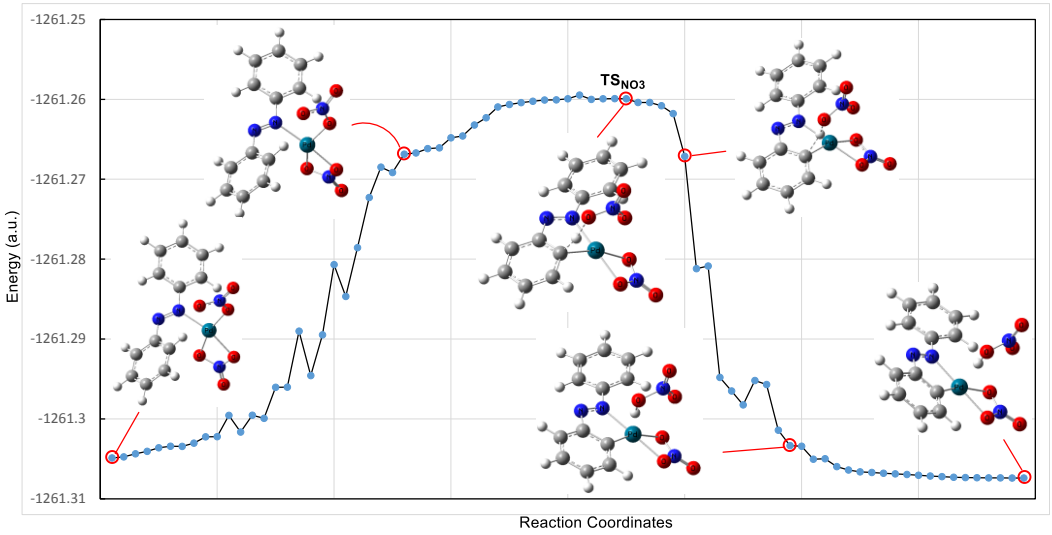


Fig. S7 Geometrical optimization curves along with the reaction coordinates at the both sides of transition state $\mathbf{TS_{Cl}}$. It is shown that such optimizations can reach the corresponding reactants and products.

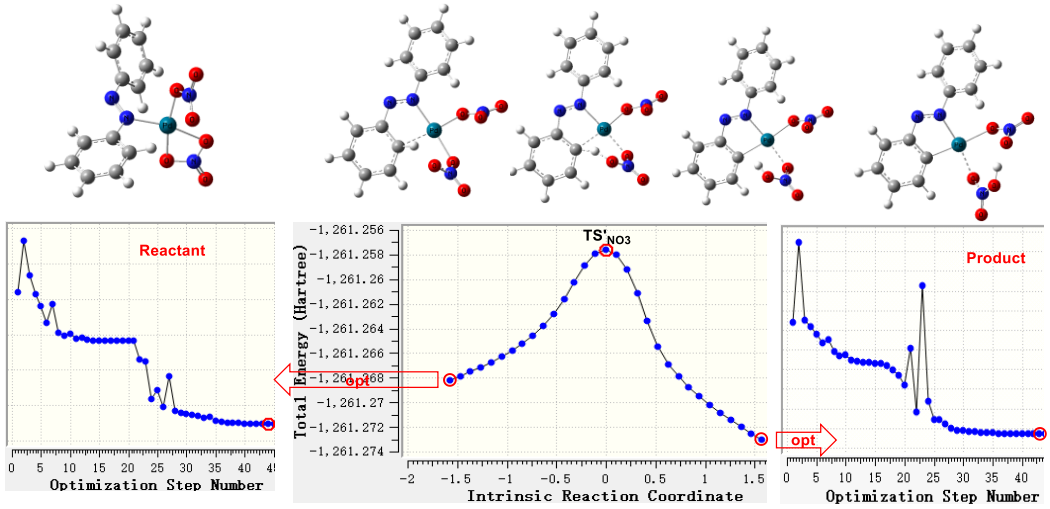


Fig. S8 IRC calculations of $\mathbf{TS'_{NO3}}$ and the geometrical optimization curves along with the reaction coordinates at the both sides. It is shown that such optimizations can reach the corresponding reactants and products.

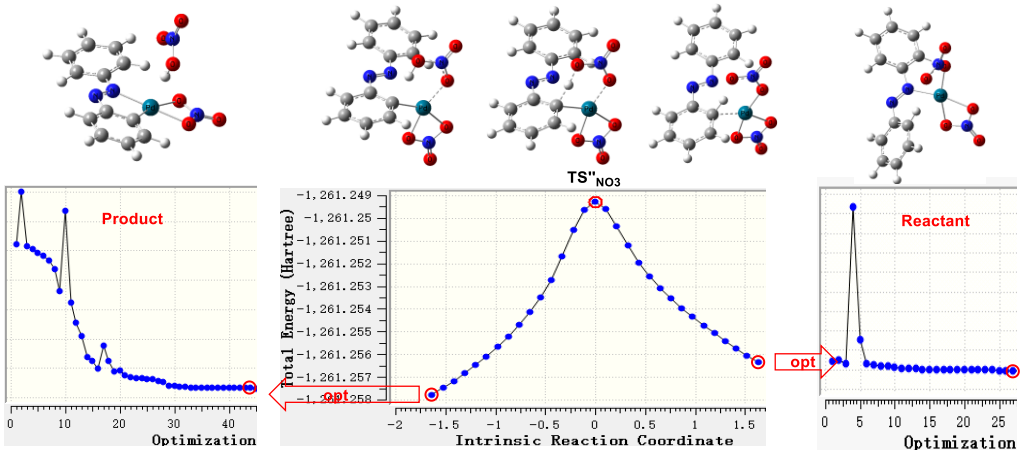


Fig. S9 IRC calculations of $\mathbf{TS''_{NO3}}$ and the geometrical optimization curves along with the reaction

coordinates at the both sides. It is shown that such optimizations can reach the corresponding reactants and products.

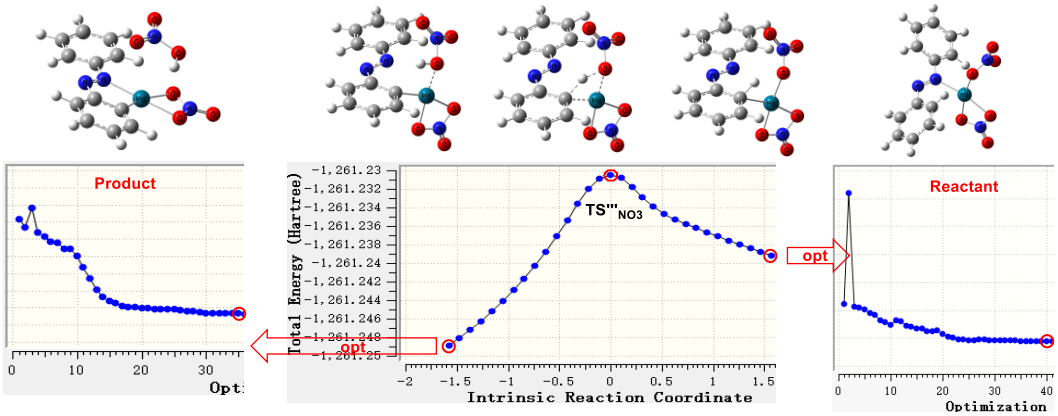


Fig. S10 IRC calculations of **TS'''$_{NO3}$** and the geometrical optimization curves along with the reaction coordinates at the both sides. It is shown that such optimizations can reach the corresponding reactants and products.

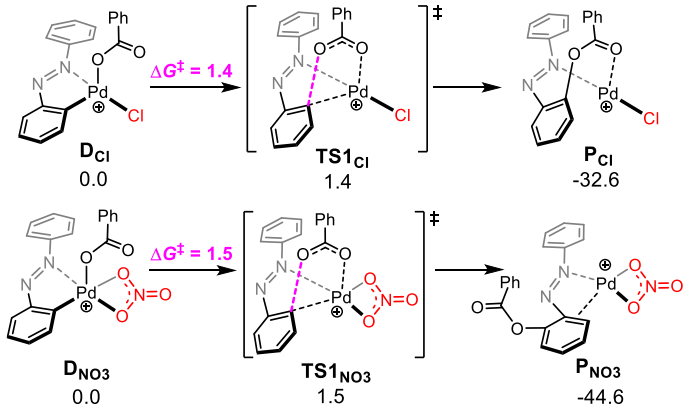
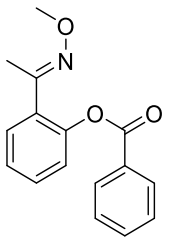


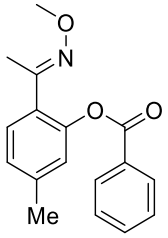
Fig. S11 Computed reductive elimination processes (C–O bond coupling) of the species **D$_{Cl}$** and **D$_{NO3}$**. The relative free energies and energy barriers are given in kcal/mol.

VII. Characterization of the products

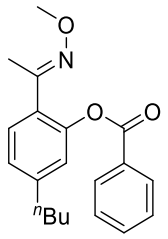


(Z)-2-(1-(methoxyimino)ethyl)phenyl benzoate (3a): Colorless oil (70%, 56.5 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1) ; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25-8.19 (m, 2H), 7.69-7.62 (m, 1H), 7.57-7.49 (m, 3H), 7.44 (td, J_1 = 7.8 Hz, J_2 = 1.7 Hz, 1H), 7.32 (td, J_1 = 7.6 Hz, J_2 = 1.3 Hz, 1H), 7.29-7.22 (m, 1H), 3.76 (s, 3H), 2.17 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.1, 153.2, 148.3, 133.6, 130.4, 130.3 (2C), 129.7, 129.6, 129.5, 128.6 (2C), 126.1, 123.4, 61.7, 15.1 ppm; HRMS

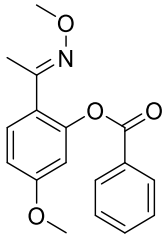
(ESI-TOF) for $C_{16}H_{15}NO_3$: calcd. $[M+Na]^+$ 292.0944; found: 292.0948.



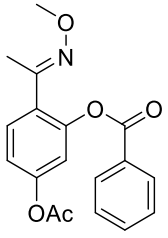
(Z)-2-(1-(methoxyimino)ethyl)-5-methylphenyl benzoate (3b): Colorless oil (80%, 67.9 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.26-8.16 (m, 2H), 7.72-7.58 (m, 1H), 7.56-7.49 (m, 2H), 7.40 (d, J = 7.9 Hz, 1H), 7.15-7.10 (m, 1H), 7.07 (s, 1H), 3.73 (s, 3H), 2.41 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.3, 151.9, 147.5, 139.6, 133.4, 129.5 (2C), 129.0, 128.8, 128.4 (2C), 126.9, 126.4, 123.6, 60.9, 20.5, 14.4 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_3$: calcd. $[M+Na]^+$ 306.1101; found: 306.1104.



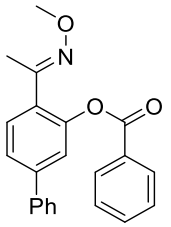
(Z)-5-butyl-2-(1-(methoxyimino)ethyl)phenyl benzoate (3c): Brown oil (80%, 78.3 mg); R_f = 0.29 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.22-8.17 (m, 2H), 7.63 (ddt, J_1 = 8.8 Hz, J_2 = 7.1 Hz, J_3 = 1.4 Hz, 1H), 7.54-7.46 (m, 2H), 7.39 (d, J = 7.9 Hz, 1H), 7.11 (dd, J_1 = 7.9 Hz, J_2 = 1.7 Hz, 1H), 7.04 (d, J = 1.7 Hz, 1H), 3.71 (s, 3H), 2.72-2.57 (m, 2H), 2.13 (s, 3H), 1.61 (m, 2H), 1.41-1.33 (m, 2H), 0.92 (t, J = 7.3 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.1, 153.2, 148.1, 145.2, 133.5, 130.2 (2C), 129.7, 129.2, 128.5 (2C), 127.6, 126.2, 123.2, 61.6, 35.2, 33.2, 22.2, 15.0, 13.9 ppm; HRMS (ESI-TOF) for $C_{20}H_{23}NO_3$: calcd. $[M+Na]^+$ 348.1570; found: 348.1573.



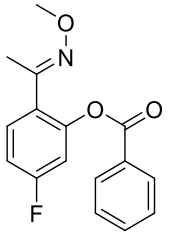
(Z)-5-methoxy-2-(1-(methoxyimino)ethyl)phenyl benzoate (3d): Yellow solid (90%, 80.7 mg); R_f = 0.25 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.22-8.18 (m, 2H), 7.69-7.61 (m, 1H), 7.56-7.49 (m, 2H), 7.43 (d, J = 8.7 Hz, 1H), 6.86 (dd, J_1 = 8.7 Hz, J_2 = 2.6 Hz, 1H), 6.78 (d, J = 2.6 Hz, 1H), 3.84 (s, 3H), 3.70 (s, 3H), 2.14 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 160.7, 152.9, 149.3, 133.6, 130.3 (2C), 130.1, 129.6, 128.6 (2C), 122.9, 112.1, 109.0, 61.6, 55.6, 15.0 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_4$: calcd. $[M+Na]^+$ 322.0554; found: 322.1057.



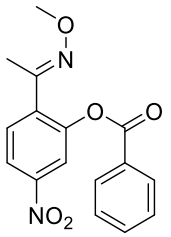
(Z)-5-acetoxy-2-(1-(methoxyimino)ethyl)phenyl benzoate (3e): White solid (85%, 83.4 mg, E/Z = 19:1); R_f = 0.20 (petroleum ether-EtOAc = 20:1); Major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25-8.16 (m, 2H), 7.98 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.92 (d, J = 1.6 Hz, 1H), 7.70-7.63 (m, 1H), 7.59 (d, J = 8.1 Hz, 1H), 7.53 (t, J = 7.8 Hz, 2H), 3.94 (s, 3H), 3.76 (s, 3H), 2.17 (s, 3H) ppm; ^{13}C NMR (126 MHz, DMSO) δ = 164.8, 164.2, 151.6, 147.6, 134.1, 133.8, 130.8, 129.7 (2C), 129.6, 128.6 (2C), 128.5, 126.6, 124.2, 61.3, 52.1, 14.4 ppm; HRMS (ESI-TOF) for $C_{18}H_{17}NO_5$: calcd. $[M+Na]^+$ 350.0999; found: 350.1003.



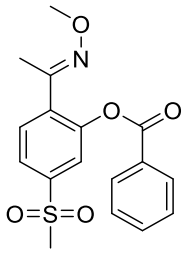
(Z)-4-(1-(methoxyimino)ethyl)-[1,1'-biphenyl]-3-yl benzoate (3f): White solid (60%, 62.1 mg); R_f = 0.24 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.32-8.18 (m, 2H), 7.71-7.61 (m, 3H), 7.60 (d, J = 8.1 Hz, 1H), 7.59-7.52 (m, 3H), 7.52-7.44 (m, 3H), 7.43-7.36 (m, 1H), 3.77 (s, 3H), 2.22 (s, 3H) ppm; ^{13}C NMR (126 MHz, CDCl3) δ = 165.1, 152.9, 148.6, 143.0, 139.5, 133.6, 130.3 (2C), 129.8, 129.5, 129.0, 128.8 (2C), 128.6 (2C), 127.9, 127.1 (2C), 124.7, 122.0, 61.7, 14.9 ppm; HRMS (ESI-TOF) for $C_{22}H_{19}NO_3$: calcd. $[M+Na]^+$ 368.1257; found: 368.1259.



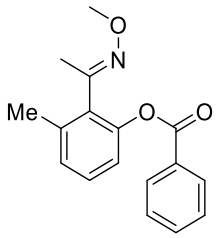
(Z)-5-fluoro-2-(1-(methoxyimino)ethyl)phenyl benzoate (3g): Colorless oil (86%, 74.0 mg, E/Z = 20:1); R_f = 0.27 (petroleum ether-EtOAc = 30:1); Major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.21 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 7.76-7.62 (m, 1H), 7.58-7.42 (m, 3H), 7.14-6.91 (m, 2H), 3.75 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.6, 162.7 (d, J = 250.2 Hz), 152.4, 149.2 (d, J = 11.0 Hz), 133.8, 130.5 (d, J = 9.4 Hz), 130.3 (2C), 129.1, 128.6 (2C), 126.8(d, J = 3.7 Hz), 113.2 (d, J = 21.3 Hz), 111.3 (d, J = 24.5 Hz), 61.7, 15.1 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}FNO_3$: calcd. $[M+Na]^+$ 310.0850; found: 310.0853.



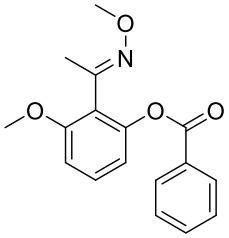
(Z)-2-(1-(methoxyimino)ethyl)-5-nitrophenyl benzoate(3h): White solid (48%, 45.2 mg); R_f = 0.25 (petroleum ether-EtOAc = 20:1); 1H NMR (500 MHz, CDCl3) δ = 8.21 (d, J = 1.3 Hz, 1H), 8.20 (d, J = 1.4 Hz, 1H), 8.17 (dd, J_1 = 8.5 Hz, J_2 = 2.3 Hz, 1H), 8.15 (d, J = 2.2 Hz, 1H), 7.73-7.66 (m, 2H), 7.59-7.52 (m, 2H), 3.78 (s, 3H), 2.19 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.5, 151.6, 148.6, 148.0, 136.8, 134.1, 130.3 (2C), 130.2, 128.7 (2C), 128.6, 120.9, 119.3, 62.1, 14.8 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}N_2O_5$: calcd. $[M+Na]^+$ 337.0795; found: 337.0790



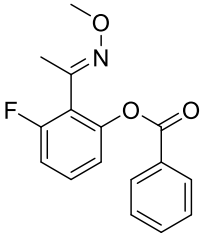
(E)-2-(1-(methoxyimino)ethyl)-5-(methylsulfonyl)phenyl benzoate (3i): Pale yellow solid (66%, 69.2 mg); R_f = 0.33 (petroleum ether-EtOAc = 3:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25-8.14 (m, 2H), 7.87 (dd, J_1 = 8.1 Hz, J_2 = 1.8 Hz, 1H), 7.84 (d, J = 1.8 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.71-7.64 (m, 1H), 7.54 (t, J = 7.8 Hz, 2H), 3.77 (s, 3H), 3.10 (s, 3H), 2.18 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.6, 151.9, 148.7, 141.5, 135.9, 134.1, 130.7, 130.3 (2C), 128.8 (2C), 128.7, 124.8, 123.0, 62.1, 44.5, 14.9 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_5S$: calcd. $[M+Na]^+$ 370.0720; found: 370.0726.



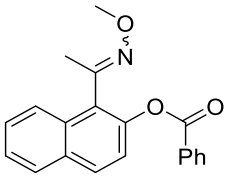
(E)-2-(1-(methoxyimino)ethyl)phenyl benzoate (3j): Pale yellow oil (79%, 67.0 mg, E/Z = 20:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.17 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.69-7.62 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.32 (t, J = 7.9 Hz, 1H), 7.16 (d, J = 7.7 Hz, 1H), 7.12 (d, J = 8.1 Hz, 1H), 3.84 (s, 3H), 2.36 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 153.0, 148.8, 138.0, 133.6, 130.5, 130.1 (2C), 129.5, 129.0, 128.6 (2C), 127.9, 120.2, 61.7, 19.5, 16.1 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_3$: calcd. $[M+Na]^+$ 306.1101; found: 306.1094.



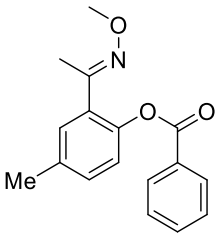
(Z)-3-methoxy-2-(1-(methoxyimino)ethyl)phenyl benzoate(3k): Pale yellow oil (90%, 80.7 mg); R_f = 0.25 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25-8.13 (m, 2H), 7.72-7.59 (m, 1H), 7.55-7.48 (m, 2H), 7.37 (t, J = 8.3 Hz, 1H), 6.91 (dd, J_1 = 8.2 Hz, J_2 = 1.0 Hz, 1H), 6.86 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 3.86 (s, 3H), 3.72 (s, 3H), 2.12 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 158.5, 151.4, 149.1, 133.4, 130.1 (2C), 129.7, 129.5, 128.4 (2C), 120.4, 115.1, 108.6, 61.5, 55.9, 15.7 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_4$: calcd. $[M+Na]^+$ 322.0554; found: 322.0726.



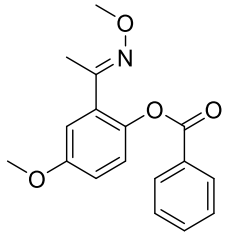
(Z)-3-fluoro-2-(1-(methoxyimino)ethyl)phenyl benzoate (3l): Colorless oil (73%, 62.9 mg, E/Z = 20:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); Major (E-isomer)*:* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.18 (dd, J_1 = 8.4 Hz, J_2 = 1.4 Hz, 2H), 7.70-7.62 (m, 1H), 7.56-7.50 (m, 2H), 7.42-7.37 (m, 1H), 7.13-7.03 (m, 2H), 3.71 (s, 3H), 2.16 (d, J = 1.8 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.9, 161.0 (d, J = 249.4 Hz), 149.2 (d, J = 6.3 Hz), 148.9, 133.7, 130.3 (2C), 129.9 (d, J = 10.0 Hz), 129.2, 128.6 (2C), 120.0 (d, J = 17.7 Hz), 118.9 (d, J = 3.4 Hz), 113.5 (d, J = 22.0 Hz), 61.8, 15.8 (d, J = 3.0 Hz) ppm; HRMS (ESI-TOF) for $C_{16}H_{14}FNO_3$: calcd. $[M+Na]^+$ 310.0857; found: 310.0850.



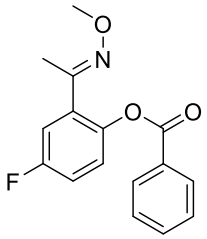
(E)-3-(1-(methoxyimino)ethyl)naphthalen-2-yl benzoate (3m): Pale yellow solid (65%, 62.2 mg, E/Z = 10:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); *Major (E-isomer)*: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.31-8.25 (m, 2H), 8.00 (s, 1H), 7.91 (d, J = 7.2 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 7.73 (s, 1H), 7.71-7.64 (m, 1H), 7.59-7.48 (m, 4H), 3.77 (s, 3H), 2.28 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.3, 153.4, 146.0, 133.6, 133.6, 131.3, 130.3 (2C), 129.7, 129.7, 129.4, 128.6 (2C), 128.1, 127.3, 127.2, 126.2, 120.8, 61.8, 15.2 ppm; HRMS (ESI-TOF) for $C_{20}H_{17}NO_3$: calcd. $[M+Na]^+$ 342.1101; found: 342.1103.



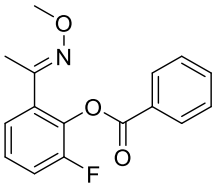
(Z)-2-(1-(methoxyimino)ethyl)-4-methylphenyl benzoate (3n): Pale yellow oil (81%, 68.8 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.19 (dd, J_1 = 8.3 Hz, J_2 =1.4 Hz, 2H), 7.65-7.58 (m, 1H), 7.53-7.46 (m, 2H), 7.28 (d, J = 2.3 Hz, 1H), 7.22-7.19 (m, 1H), 7.10 (d, J = 8.2 Hz, 1H), 3.75 (s, 3H), 2.38 (s, 3H), 2.13 (s, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 165.3, 153.5, 146.1, 135.8, 133.6, 130.4, 130.3 (2C), 130.0, 129.9, 129.6, 128.6 (2C), 123.1, 61.7, 20.9, 15.2 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_3$: calcd. $[M+Na]^+$ 306.1101; found: 306.1102.



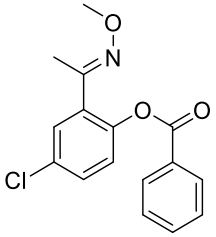
(Z)-4-methoxy-2-(1-(methoxyimino)ethyl)phenyl benzoate (3o): Pale yellow oil (91%, 81.6 mg); R_f = 0.25 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.24-8.17 (m, 2H), 7.69-7.61 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.15 (d, J = 8.9 Hz, 1H), 7.02 (d, J = 3.0 Hz, 1H), 6.96 (dd, J_1 = 8.8 Hz, J_2 = 3.1 Hz, 1H), 3.86 (s, 3H), 3.77 (s, 3H), 2.15 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.4, 157.3, 153.2, 141.7, 133.5, 131.1, 130.2 (2C), 129.6, 128.5 (2C), 124.2, 115.0, 114.4, 61.7, 55.7, 15.0 ppm; HRMS (ESI-TOF) for $C_{17}H_{17}NO_4$: calcd. $[M+Na]^+$ 322.0554; found: 322.1056.



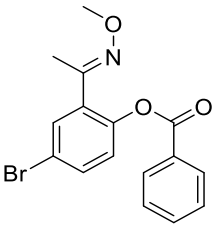
(Z)-4-fluoro-2-(1-(methoxyimino)ethyl)phenyl benzoate (3p): Pale yellow oil (60%, 51.7 mg, E/Z = 15:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); *Major (E-isomer):* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.32-8.15 (m, 2H), 7.66 (m, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.26-7.17 (m, 2H), 7.17-7.08 (m, 1H), 3.76 (s, 3H), 2.15 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.0, 155.0 (d, *J* = 249.3 Hz), 152.3 (d, *J* = 2.8 Hz), 136.4 (d, *J* = 14.2 Hz), 133.8, 132.8, 130.5 (2C), 128.8, 128.6 (2C), 126.7 (d, *J* = 8.0 Hz), 124.4 (d, *J* = 3.5 Hz), 116.8 (d, *J* = 19.0 Hz), 61.9, 14.9 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}FNO_3$: calcd. $[M+Na]^+$ 310.0850; found: 310.0858.



(Z)-2-fluoro-6-(1-(methoxyimino)ethyl)phenyl benzoate (3p'): Pale yellow oil (30%, 25.8 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.32-8.15 (m, 2H), 7.66 (m, 1H), 7.53 (t, *J* = 7.8 Hz, 2H), 7.26-7.17 (m, 2H), 7.17-7.08 (m, 1H), 3.76 (s, 3H), 2.15 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.1, 160.1 (d, *J* = 245.4 Hz), 152.2 (d, *J* = 1.8 Hz), 144.1 (d, *J* = 2.9 Hz), 133.7, 131.9 (d, *J* = 8.0 Hz), 130.3 (2C), 129.3, 128.6 (2C), 124.9 (d, *J* = 8.7 Hz), 116.3 (d, *J* = 23.3 Hz), 116.1 (d, *J* = 24.5 Hz), 61.9, 14.8 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}FNO_3$: calcd. $[M+Na]^+$ 310.0850; found: 310.0853.

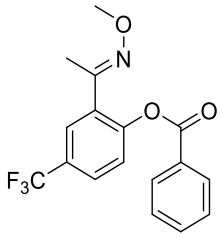


(Z)-4-chloro-2-(1-(methoxyimino)ethyl)phenyl benzoatee (3q): Pale yellow oil (86%, 78.2 mg); R_f = 0.38 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.23-8.16 (m, 2H), 7.70-7.62 (m, 1H), 7.57-7.48 (m, 3H), 7.39 (dd, J_1 = 8.6 Hz, J_2 = 2.6 Hz, 1H), 7.19 (d, *J* = 8.7 Hz, 1H), 3.77 (s, 3H), 2.15 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.8, 152.1, 146.8, 133.8, 131.9, 131.5, 130.3 (2C), 129.6, 129.4, 129.2, 128.6 (2C), 124.8, 61.9, 14.9 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}ClNO_3$: calcd. $[M+Na]^+$ 326.0554; found: 326.0556.

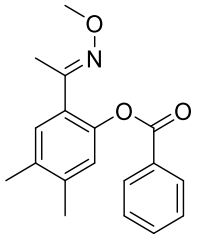


(Z)-4-bromo-2-(1-(methoxyimino)ethyl)phenyl benzoate (3r): Yellow oil (80%, 83.3 mg); R_f = 0.38

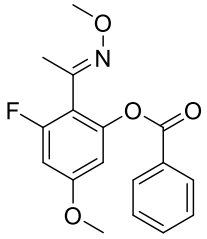
(petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, CDCl3) δ = 8.20 (dd, J_1 = 8.3 Hz, J_2 = 1.3 Hz, 2H), 7.70-7.63 (m, 2H), 7.57-7.49 (m, 3H), 7.13 (d, J = 8.6 Hz, 1H), 3.77 (s, 3H), 2.14 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.7, 152.0, 147.4, 133.8, 132.5, 132.3 (2C), 130.3 (2C), 129.1, 128.6 (2C), 125.1, 119.1, 61.9, 14.9 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}BrNO_3$: calcd. $[M+Na]^+$ 370.0049; found: 370.0055.



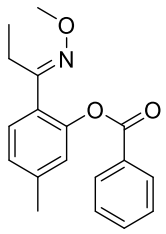
(Z)-2-(1-(methoxyimino)ethyl)-4-(trifluoromethyl)phenyl benzoate (3s): Colorless oil (82%, 82.9 mg); R_f = 0.40 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.24-8.19 (m, 2H), 7.80 (d, J = 2.3 Hz, 1H), 7.73-7.65 (m, 2H), 7.55 (t, J = 7.8 Hz, 2H), 7.39 (d, J = 8.4 Hz, 1H), 3.79 (s, 3H), 2.19 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.6, 152.1, 150.9, 134.0, 131.3, 130.4 (2C), 128.9, 128.7 (2C), 128.5 (q, J = 32.8 Hz), 126.9 (q, J = 3.7 Hz), 126.7 (q, J = 3.6 Hz), 124.2, 123.7 (q, J = 273.42 Hz), 62.0, 15.0 ppm; HRMS (ESI-TOF) for $C_{17}H_{14}F_3NO_3$: calcd. $[M+Na]^+$ 360.0818; found: 360.0825.



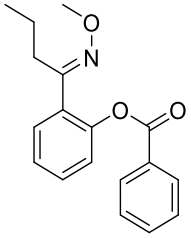
(Z)-2-(1-(methoxyimino)ethyl)-4,5-dimethylphenyl benzoate (3t): Pale yellow oil (83%, 74.0 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.23-8.17 (m, 2H), 7.69-7.59 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.26 (s, 1H), 7.01 (s, 1H), 3.75 (s, 3H), 2.30 (s, 6H), 2.14 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.3, 153.4, 146.0, 138.7, 134.5, 133.4, 130.3 (2C), 130.2, 129.8, 128.5 (2C), 127.5, 124.2, 61.6, 19.7, 19.2, 15.0 ppm; HRMS (ESI-TOF) for $C_{18}H_{19}NO_3$: calcd. $[M+Na]^+$ 320.1257; found: 320.1264.



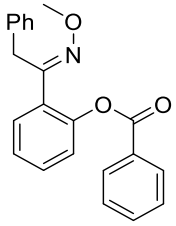
(Z)-3-fluoro-5-methoxy-2-(1-(methoxyimino)ethyl)phenyl benzoate (3u): Pale orange solid (80%, 76.0 mg, E/Z = 15:1); R_f = 0.40 (petroleum ether-EtOAc = 20:1); *Major (E-isomer):* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.21-8.12 (m, 2H), 7.70-7.62 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 6.68-6.56 (m, 2H), 3.83 (s, 3H), 3.67 (s, 3H), 2.12 (d, J = 1.9 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.8, 161.7 (d, J = 228.8 Hz), 160.7 (d, J = 5.1 Hz), 149.9 (d, J = 9.3 Hz), 149.0, 133.7, 130.3 (2C), 129.2, 128.6 (2C), 112.5 (d, J = 18.0 Hz), 105.0 (d, J = 3.0 Hz), 100.2 (d, J = 26.0 Hz), 61.7, 55.8, 15.9 (d, J = 3.4 Hz) ppm; HRMS (ESI-TOF) for $C_{17}H_{16}FNO_4$: calcd. $[M+Na]^+$ 349.0956; found: 349.0959.



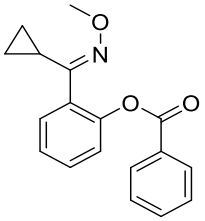
(Z)-2-(1-(methoxyimino)propyl)-5-methylphenyl benzoate (3v): Pale yellow oil (68%, 60.6 mg, E/Z = 15:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); *Major (E-isomer):* ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.20-8.13 (m, 2H), 7.68-7.58 (m, 1H), 7.50 (td, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 2H), 7.33 (dd, J_1 = 7.9 Hz, J_2 = 1.4 Hz, 1H), 7.11 (t, J = 6.5 Hz, 1H), 7.06 (s, 1H), 3.68 (d, J = 1.5 Hz, 3H), 2.64 (q, J = 7.6 Hz, 2H), 2.39 (s, 3H), 1.03 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 165.2, 158.2, 148.3, 140.1, 133.5, 130.3 (2C), 129.7, 129.5, 128.5(2C), 126.9, 126.4, 124.0, 61.6, 22.1, 21.2, 10.6 ppm; HRMS (ESI-TOF) for $C_{18}H_{19}NO_3$: calcd. $[M+Na]^+$ 320.1257; found: 320.1261.



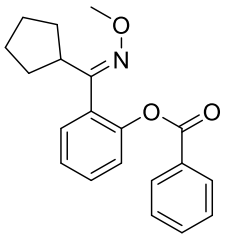
(Z)-2-(1-(methoxyimino)butyl)phenyl benzoate (3w): Pale yellow oil (65%, 57.9 mg, E/Z = 10:1); R_f = 0.22 (petroleum ether-EtOAc = 30:1); *Major (E-isomer):* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.21 (dd, J_1 = 8.4 Hz, J_2 = 1.3 Hz, 2H), 7.69-7.61 (m, 1H), 7.57-7.49 (m, 2H), 7.49-7.40 (m, 2H), 7.31 (td, J_1 = 7.6 Hz, J_2 = 1.3 Hz, 1H), 7.30-7.24 (m, 1H), 3.72 (s, 3H), 2.68-2.62 (m, 2H), 1.57-1.45 (m, 2H), 0.89 (t, J = 7.4 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 157.1, 148.5, 133.5, 130.2 (2C), 129.8, 129.6, 129.6, 129.6, 128.5 (2C), 126.0, 123.5, 61.6, 30.7, 19.4, 14.1 ppm; HRMS (ESI-TOF) for $C_{18}H_{19}NO_3$: calcd. $[M+Na]^+$ 320.1257; found: 320.1300.



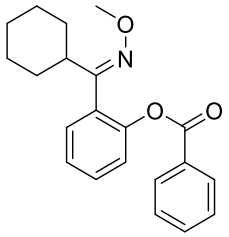
(Z)-2-(1-(methoxyimino)-2-phenylethyl)phenyl benzoate (3x): Pale yellow solid (64%, 66.2 mg, E/Z = 20:1); R_f = 0.24 (petroleum ether-EtOAc = 30:1); *Major (E-isomer):* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.20-8.13 (m, 2H), 7.69-7.62 (m, 1H), 7.53 (t, J = 7.8 Hz, 2H), 7.45-7.37 (m, 1H), 7.36 (dd, J_1 = 7.8 Hz, J_2 = 1.7 Hz, 1H), 7.28-7.20 (m, 4H), 7.20-7.15 (m, 3H), 4.08 (s, 2H), 3.75 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.1, 152.9, 148.6, 143.0, 139.5, 133.6, 130.3 (2C), 129.8, 129.5, 129.0, 128.8 (2C), 128.6 (2C), 127.9, 127.1 (2C), 124.7, 122.0, 61.7, 14.9 ppm; HRMS (ESI-TOF) for $C_{22}H_{19}NO_3$: calcd. $[M+Na]^+$ 368.1257; found: 368.1262.



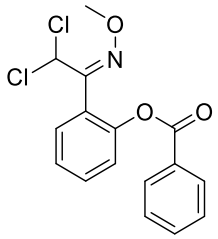
(Z)-2-(cyclopropyl(methoxyimino)methyl)phenyl benzoate (3y): Colorless oil (62%, 54.9 mg); R_f = 0.40 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.21 (dd, J_1 = 8.4 Hz, J_2 = 1.4 Hz, 2H), 7.69-7.62 (m, 1H), 7.57-7.48 (m, 2H), 7.47-7.40 (m, 1H), 7.33 (dd, J_1 = 8.1 Hz, J_2 = 1.1 Hz, 1H), 7.31-7.25(m, 2H), 3.87 (s, 3H), 2.41-2.23 (m, 1H), 0.83 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 2H), 0.57 (dd, J_1 = 5.3 Hz, J_2 = 1.9 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.7, 158.6, 149.2, 133.6, 130.8, 130.2 (2C), 129.8, 129.6, 128.6 (2C), 126.5, 125.6, 123.0, 61.9, 10.0, 5.4 (2C) ppm; HRMS (ESI-TOF) for $C_{18}H_{17}NO_3$: calcd. $[M+Na]^+$ 318.1101; found: 318.1105.



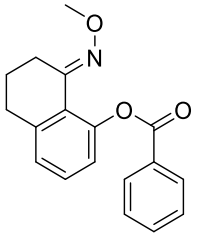
(Z)-2-(cyclopentyl(methoxyimino)methyl)phenyl benzoate (3z): Pale yellow oil (55%, 53.3 mg); R_f = 0.25 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.22-8.15 (m, 2H), 7.68-7.60 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.47-7.39 (m, 1H), 7.33 (dd, J_1 = 7.5 Hz, J_2 = 1.8 Hz, 2H), 7.29 (dd, J_1 = 7.3 Hz, J_2 = 1.2 Hz, 1H), 3.80 (s, 3H), 3.46-3.28 (m, 1H), 2.04-1.80 (m, 2H), 1.65-1.42 (m, 6H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.7, 160.5, 148.8, 133.5, 130.3, 130.2 (2C), 129.6, 129.4, 129.1, 128.6 (2C), 125.5, 123.0, 61.6, 39.9, 29.8 (2C), 25.2 (2C) ppm; HRMS (ESI-TOF) for $C_{20}H_{21}NO_3$: calcd. $[M+Na]^+$ 346.1414; found: 346.1546.



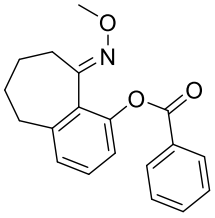
(Z)-2-(cyclohexyl(methoxyimino)methyl)phenyl benzoate (3aa): Yellow oil (60%, 60.7 mg, E/Z = 15:1); R_f = 0.24 (petroleum ether-EtOAc = 30:1); *Major (E-isomer):* ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8 .21-8.16 (m, 2H), 7.68-7.61 (m, 1H), 7.52 (t, J = 7.8 Hz, 2H), 7.47-7.40 (m, 1H), 7.35 (dd, J_1 = 7.7 Hz, J_2 = 1.8 Hz, 1H), 7.34-7.25 (m, 2H), 3.78 (s, 3H), 3.27-3.05 (m, 1H), 1.80 (d, J = 11.4 Hz, 2H), 1.74-1.60 (m, 3H), 1.38-1.24 (m, 4H), 1.17-1.06 (m, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.9, 160.4, 148.9, 133.5, 130.4, 130.2 (2C), 129.6, 129.3, 128.9, 128.5 (2C), 125.4, 123.2, 61.6, 39.1, 29.1 (2C), 26.1 (2C), 25.9 ppm; HRMS (ESI-TOF) for $C_{21}H_{23}NO_3$: calcd. $[M+Na]^+$ 360.1570; found: 360.1682.



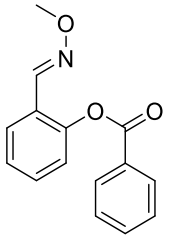
(E)-2-(2,2-dichloro-1-(methoxyimino)ethyl)phenyl benzoate (3ab): Colorless oil (90%, 91.0 mg); R_f = 0.35 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.25-8.19 (m, 2H), 7.83 (dd, J_1 = 8.2 Hz, J_2 = 1.6 Hz, 1H), 7.69-7.62 (m, 1H), 7.58-7.50 (m, 3H), 7.39 (d, J = 7.9 Hz, 2H), 7.18 (s, 1H), 3.81 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.7, 149.8, 149.3, 133.5, 130.9, 130.7, 130.2 (2C), 129.3, 128.5 (2C), 125.5, 124.3, 123.5, 63.0, 60.3 ppm; HRMS (ESI-TOF) for $C_{16}H_{13}Cl_2NO_3$: calcd. $[M+Na]^+$ 360.0165; found: 360.0165.



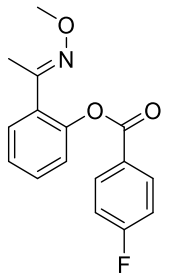
(E)-8-(methoxyimino)-5,6,7,8-tetrahydronaphthalen-1-yl benzoate (3ac): Pale red oil (73%, 64.6 mg, E/Z = 19:1); R_f = 0.35 (petroleum ether-EtOAc = 20:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.29-8.23 (m, 2H), 7.66-7.59 (m, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.30 (t, J = 7.8 Hz, 1H), 7.12 (d, J = 7.6 Hz, 1H), 7.07 (d, J = 8.0 Hz, 1H), 3.36 (s, 3H), 2.78 (t, J = 4.0 Hz, 2H), 2.73 (t, J = 6.7 Hz, 2H), 1.87-1.78 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.6, 152.2, 148.1, 142.6, 133.0, 130.5, 130.4 (2C), 129.0, 128.3 (2C), 126.4, 123.6, 122.2, 61.4, 30.5, 24.7, 21.0 ppm; HRMS (ESI-TOF) for $C_{18}H_{17}NO_3$: calcd. $[M+Na]^+$ 318.1101; found: 318.1104.



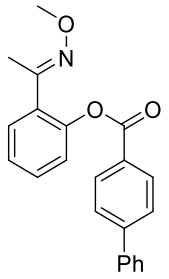
(E)-9-(methoxyimino)-6,7,8,9-tetrahydro-5H-benzo[7]annulen-1-yl benzoate (3ad): Pale yellow solid (47%, 43.6 mg); R_f = 0.22 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.22-8.14 (m, 2H), 7.67-7.58 (m, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 7.8 Hz, 1H), 7.12 (dd, J_1 = 8.2 Hz, J_2 = 1.2 Hz, 1H), 7.08 (d, J = 7.1 Hz, 1H), 3.59 (s, 3H), 2.78 (t, J = 6.6 Hz, 2H), 2.64-2.56 (m, 2H), 1.82-1.73 (m, 2H), 1.71-1.63 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 157.2, 148.0, 141.8, 133.3, 130.2 (2C), 129.9, 129.5, 128.8, 128.4 (2C), 126.3, 120.8, 61.6, 32.3, 26.5, 26.3, 22.1 ppm; HRMS (ESI-TOF) for $C_{19}H_{19}NO_3$: calcd. $[M+Na]^+$ 332.1257; found: 332.1260.



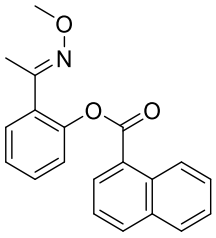
(Z)-2-((methoxyimino)methyl)phenyl benzoate (3ae): Pale yellow solid (64%, 49.0 mg); R_f = 0.40 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.27-8.21 (m, 2H), 8.20 (s, 1H), 7.87 (dd, J_1 = 7.9 Hz, J_2 = 1.7 Hz, 1H), 7.72-7.64 (m, 1H), 7.54 (t, J = 7.8 Hz, 2H), 7.46 (td, J_1 = 7.8 Hz, J_2 = 1.7 Hz, 1H), 7.32 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.25 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 3.87 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 164.9, 148.9, 143.8, 133.8, 130.7, 130.3 (2C), 129.1, 128.6 (2C), 127.7, 126.3, 124.9, 123.1, 62.0 ppm; HRMS (ESI-TOF) for $C_{15}H_{13}NO_3$: calcd. $[M+Na]^+$ 278.0788; found: 278.0793.



(Z)-2-(1-(methoxyimino)ethyl)phenyl 4-fluorobenzoate (3af): Pale yellow oil (90%, 77.5 mg); R_f = 0.20 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.27-8.20 (m, 2H), 7.51 (dd, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.44 (td, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.32 (td, J_1 = 7.6 Hz, J_2 = 1.3 Hz, 1H), 7.26-7.17 (m, 3H), 3.74 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.1 (d, J = 255.1 Hz), 164.1, 153.1, 148.1, 132.9 (d, J = 9.3 Hz, 2C), 130.4, 129.8, 129.5, 126.2, 125.8 (d, J = 2.9 Hz), 123.4, 115.8 (d, J = 22.0 Hz, 2C), 61.7, 15.0 ppm; HRMS (ESI-TOF) for $C_{16}H_{14}FNO_3$: calcd. $[M+Na]^+$ 310.0850; found: 310.0859.

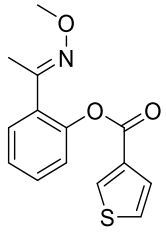


(Z)-2-(1-(methoxyimino)ethyl)phenyl [1,1'-biphenyl]-4-carboxylate (3ag): Pale yellow oil (60%, 62.1 mg); R_f = 0.20 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.31-8.26 (m, 2H), 7.79-7.73 (m, 2H), 7.69 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 7.52 (m, 3H), 7.45(m, 2H), 7.33 (td, J_1 = 7.6 Hz, J_2 = 1.3 Hz, 1H), 7.27 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 3.80 (s, 3H), 2.20 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 153.3, 148.3, 146.3, 139.8, 130.8 (2C), 130.5, 129.8, 129.5, 129.0 (2C), 128.3, 128.2, 127.3 (2C), 127.2 (2C), 126.1, 123.4, 61.8, 15.1 ppm; HRMS (ESI-TOF) for $C_{22}H_{19}NO_3$: calcd. $[M+Na]^+$ 368.1257; found: 368.1266.

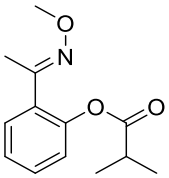


(Z)-2-(1-(methoxyimino)ethyl)phenyl 1-naphthoate (3ah): Pale yellow oil (89%, 85.2 mg); R_f = 0.30 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.11 (dd, J_1 = 8.7 Hz, J_2 = 1.1 Hz, 1H), 8.54 (dd, J_1 = 7.3 Hz, J_2 = 1.4 Hz, 1H), 8.13 (d, J = 8.2 Hz, 1H), 7.95 (d, J = 8.1 Hz, 1H),

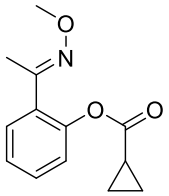
7.70-7.65 (m, 1H), 7.63-7.56 (m, 2H), 7.55 (dd, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.53-7.46 (m, 1H), 7.40-7.31 (m, 2H), 3.77 (s, 3H), 2.23 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 153.3, 148.2, 134.3, 133.9, 131.7, 131.4, 130.8, 129.7, 129.5, 128.6, 128.1, 126.4, 126.1, 125.8, 125.7, 124.5, 123.5, 61.7, 15.2 ppm; HRMS (ESI-TOF) for $C_{20}H_{17}NO_3$: calcd. $[M+Na]^+$ 342.1101; found: 342.1102.



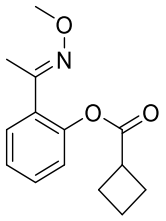
(Z)-2-(1-(methoxyimino)ethyl)phenyl thiophene-3-carboxylate (3ai): Pale yellow oil (80%, 66.0 mg); R_f = 0.30 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.32 (dd, J_1 = 3.0 Hz, J_2 = 1.1 Hz, 1H), 7.68 (dd, J_1 = 5.0 Hz, J_2 = 1.1 Hz, 1H), 7.50 (dd, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.43 (td, J_1 = 7.7 Hz, J_2 = 1.5 Hz, 1H), 7.39 (dd, J_1 = 5.0 Hz, J_2 = 3.1 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.24 (d, J = 8.1 Hz, 1H), 3.79 (s, 3H), 2.17 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 160.9, 153.3, 148.0, 134.1, 132.9, 130.4, 129.7, 129.5, 128.3, 126.4, 126.1, 123.4, 61.7, 15.1 ppm; HRMS (ESI-TOF) for $C_{14}H_{13}NO_3S$: calcd. $[M+Na]^+$ 298.0508; found: 298.0519.



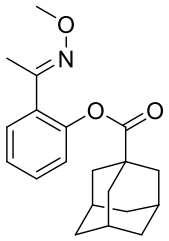
(Z)-2-(1-(methoxyimino)ethyl)phenyl isobutyrate (3aj): Yellow oil (88%, 62.0 mg); R_f = 0.40 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, CDCl3) δ = 7.44-7.34 (m, 2H), 7.25 (td, J_1 = 7.6 Hz, J_2 = 1.2, 1H), 7.09 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 3.97 (s, 3H), 2.87-2.75 (m, 1H), 2.16 (s, 3H), 1.33 (s, 3H), 1.32 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 175.2, 153.6, 148.2, 130.7, 129.6, 129.4, 125.9, 123.0, 61.8, 34.2, 18.8 (2C), 15.5 ppm; HRMS (ESI-TOF) for $C_{13}H_{17}NO_3$: calcd. $[M+Na]^+$ 258.101; found: 258.1237.



(Z)-2-(1-(methoxyimino)ethyl)phenyl cyclopropanecarboxylate (3ak): Yellow oil (89%, 62.2 mg, E/Z = 15:1); R_f = 0.20 (petroleum ether-EtOAc = 20:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.43 (dd, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.40-7.33 (m, 1H), 7.25 (td, J_1 = 7.6 Hz, J_2 = 1.3, 1H), 7.11 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 4.00 (s, 3H), 2.17 (s, 3H), 1.91-1.82 (m, 1H), 1.22-1.15 (m, 2H), 1.06-0.97 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 173.2, 153.6, 148.1, 130.5, 129.6, 129.4, 125.9, 123.2, 61.9, 15.2, 13.0, 9.1 (2C) ppm; HRMS (ESI-TOF) for $C_{13}H_{15}NO_3$: calcd. $[M+Na]^+$ 256.0944; found: 256.1091.



(Z)-2-(1-(methoxyimino)ethyl)phenyl cyclobutanecarboxylate (3al): Colorless oil (84%, 62.2 mg); R_f = 0.30 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.42 (dd, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.41-7.34 (m, 1H), 7.25 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.11 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 3.97 (s, 3H), 3.45-3.30 (m, 1H), 2.51-2.40 (m, 2H), 2.38-2.27 (m, 2H), 2.15 (s, 3H), 2.07 (dt, J_1 = 11.3 Hz, J_2 = 8.8 Hz, 1H), 2.04-1.94 (m, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 173.5, 153.7, 148.1, 130.6, 129.6, 129.4, 125.9, 123.0, 61.8, 38.1, 25.2 (2C), 18.4, 15.4 ppm; HRMS (ESI-TOF) for $C_{14}H_{17}NO_3$: calcd. $[M+Na]^+$ 270.1208; found: 270.1256.



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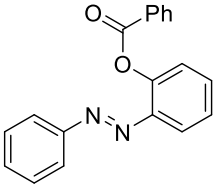
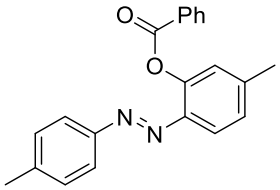
2-((Z)-1-(methoxyimino)ethyl)phenyl (3r,5r,7r)-adamantane-1-carboxylate (3am): Colorless oil (84%, 82.4 mg); R_f = 0.40 (petroleum ether-EtOAc = 20:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.42-7.33 (m, 2H), 7.24 (td, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1H), 7.03 (dd, J_1 = 8.1 Hz, J_2 = 1.2 Hz, 1H), 3.98 (s, 3H), 2.15 (s, 3H), 2.10 (s, 3H), 2.06 (d, J = 2.9 Hz, 6H), 1.78 (s, 6H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 175.8, 153.7, 148.5, 130.9, 129.6, 129.4, 125.7, 123.0, 61.8, 41.0, 38.7 (3C), 36.4 (3C), 27.9 (3C), 15.8 ppm; HRMS (ESI-TOF) for $C_{20}H_{25}NO_3$: calcd. $[M+Na]^+$ 350.1727; found: 350.1737

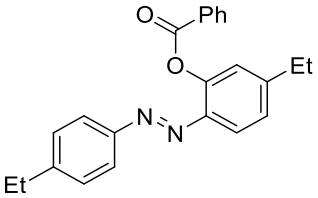


(E)-2-(phenyldiazenyl)phenyl benzoate (5a): Orange solid (80%, 72.5 mg); R_f = 0.33 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.31 (d, J = 7.2 Hz, 2H), 7.92 (dd, J_1 = 8.3 Hz, J_2 = 1.6 Hz, 1H), 7.75 (dd, J_1 = 2.5 Hz, J_2 = 1.5 Hz, 2H), 7.73-7.66 (m, 1H), 7.61-7.53 (m, 3H), 7.46-7.36 (m, 5H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 152.7, 149.3, 144.0, 133.6, 132.1, 131.2, 130.4 (2C), 129.5, 129.0 (2C), 128.6 (2C), 126.6, 123.6, 123.1 (2C), 117.9 ppm; HRMS (ESI-TOF) for $C_{19}H_{14}N_2O_2$: calcd. $[M+Na]^+$ 325.0947; found: 325.0952.

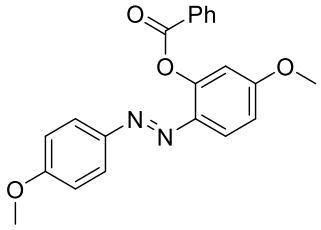


(E)-5-methyl-2-(p-tolyldiazenyl)phenyl benzoate (5b): Orange solid (70%, 69.3 mg); R_f = 0.37 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.30 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.73-7.65 (m, 1H), 7.62 (d, J = 8.3 Hz, 2H), 7.56 (t, J = 7.8 Hz, 2H),

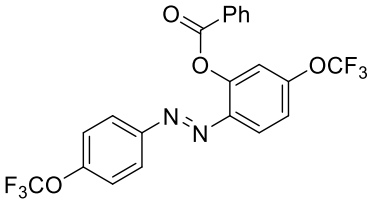
7.24-7.12 (m, 4H), 2.48 (s, 3H), 2.38 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.6, 150.9, 149.0, 142.8, 141.8, 141.5, 133.5, 130.3 (2C), 129.9, 129.6 (2C), 128.6 (2C), 127.4, 123.8, 122.9 (2C), 117.6, 21.5, 21.4 ppm; HRMS (ESI-TOF) for $C_{21}H_{18}N_2O_2$: calcd. $[M+Na]^+$ 353.1260; found: 353.1263.



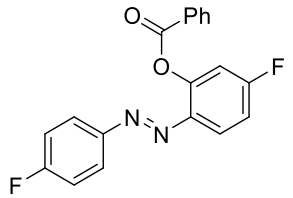
(E)-5-ethyl-2-((4-ethylphenyl)diazenyl)phenyl benzoate (5c): Orange solid (75%, 80.6 mg); R_f = 0.40 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.32 (dd, J_1 = 9.5 Hz, J_2 = 1.5 Hz, 2H), 7.86(d, J = 8.8 Hz, 1H), 7.72-7.64 (m, 3H), 7.57 (t, J = 7.8 Hz, 2H), 7.27-7.19 (m, 4H), 2.80 (q, J = 7.6 Hz, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.35 (t, J = 7.6 Hz, 3H), 1.26 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.6, 151.1, 149.1, 149.0, 147.7, 142.0, 133.5, 130.3 (2C), 129.6, 128.6 (2C), 128.4 (2C), 126.1, 123.0 (2C), 122.6, 117.7, 28.7, 28.7, 15.3, 15.0 ppm; HRMS (ESI-TOF) for $C_{23}H_{22}N_2O_2$: calcd. $[M+Na]^+$ 381.1537; found: 381.1582.



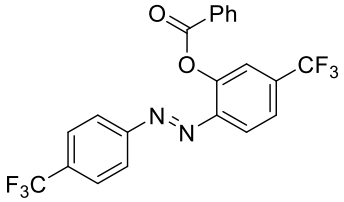
(E)-5-methoxy-2-((4-methoxyphenyl)diazenyl)phenyl benzoate (5d): Orange solid (83%, 90.1 mg); R_f = 0.33 (petroleum ether-EtOAc = 10:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.31-8.26 (m, 2H), 7.89 (d, J = 8.9 Hz, 1H), 7.71-7.67 (m, 1H), 7.66-7.63 (m, 2H), 7.56 (dd, J_1 = 8.4 Hz, J_2 = 7.1 Hz, 2H), 6.94-6.89 (m, 2H), 6.87-6.83 (m, 2H), 3.91 (s, 3H), 3.83 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.4, 162.3, 161.7, 150.4, 147.2, 138.2, 133.6, 130.4 (2C), 129.5, 128.6 (2C), 124.5 (2C), 118.9, 114.0 (2C), 112.8, 108.1, 55.8, 55.5 ppm; HRMS (ESI-TOF) for $C_{21}H_{18}N_2O_4$: calcd. $[M+Na]^+$ 385.1159; found: 385.1165.



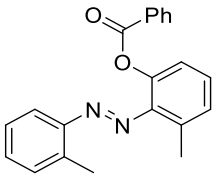
(E)-5-(trifluoromethoxy)-2-((4-(trifluoromethoxy)phenyl)diazenyl)phenyl benzoate (5e): Pale pink solid (70%, 98.7 mg, E/Z = 19:1); R_f = 0.50 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.27 (dd, J_1 = 8.3 Hz, J_2 = 1.3 Hz, 2H), 7.95 (d, J = 8.9 Hz, 1H), 7.78-7.68 (m, 3H), 7.62-7.55 (m, 2H), 7.31 (d, J = 1.5 Hz, 1H), 7.30-7.24 (m, 1H), 7.23 (dd, J_1 = 9.0 Hz, J_2 = 1.0 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.0, 151.6, 151.3, 150.6, 150.1, 142.2, 134.1, 130.4 (2C), 128.8 (2C), 128.8, 124.6 (2C), 121.2 (2C), 120.4 (q, J = 258.3 Hz), 119.2 (q, J = 258.3 Hz), 118.7, 118.1, 116.2 ppm; HRMS (ESI-TOF) for $C_{21}H_{12}F_6N_2O_4$: calcd. $[M+Na]^+$ 493.0593; found: 493.0606.



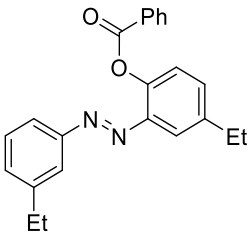
(E)-5-fluoro-2-((4-fluorophenyl)diazenyl)phenyl benzoate (5f): Yellow solid (72%, 73.0 mg, E/Z = 14:1); R_f = 0.43(petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.27 (dd, J_1 = 8.3 Hz, J_2 = 1.3 Hz, 2H), 8.01-7.85 (m, 1H), 7.78-7.64 (m, 2H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.25-7.18 (m, 1H), 7.19-7.12 (m, 1H), 7.14-7.08 (m, 1H), 7.06 (dd, J_1 = 9.0 Hz, J_2 = 8.2 Hz, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) *δ* = 165.5 (d, *J* = 2.2 Hz), 164.4 (d, *J* = 251.9 Hz), 164.3 (d, *J* = 201.7 Hz), 150.4 (d, *J* = 11.7 Hz), 149.2 (d, *J* = 3.2 Hz), 140.6 (d, *J* = 3.8 Hz), 133.9, 130.4 (2C), 129.0, 128.7 (2C), 125.0 (d, *J* = 9.1 Hz), 124.8 (d, *J* = 9.0 Hz), 119.2 (d, *J* = 10.1 Hz), 116.1 (d, *J* = 22.9 Hz), 116.0 (d, *J* = 22.8 Hz), 113.9 (d, *J* = 22.6 Hz), 111.3 (d, *J* = 25.1 Hz) ppm; HRMS (ESI-TOF) for $C_{19}H_{12}F_2N_2O_2$: calcd. $[M+Na]^+$ 361.0759; found: 361.0769.



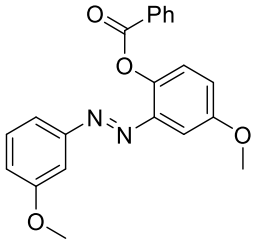
(E)-5-(trifluoromethyl)-2-((4-(trifluoromethyl)phenyl)diazenyl)phenyl benzoate (5g): Yellow solid (68%, 89.4 mg, E/Z = 28:1); R_f = 0.50 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) *δ* = 8.27 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.99 (dd, J_1 = 8.4 Hz, J_2 = 1.0 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 2H), 7.77-7.69 (m, 2H), 7.72-7.65 (m, 3H), 7.62-7.55 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) *δ* = 165.1, 154.2, 149.5, 145.7, 134.2(q, *J* = 32.8 Hz), 134.2, 133.2(q, *J* = 32.8 Hz), 130.4 (2C), 128.9 (2C), 128.6, 126.4 (q, *J* = 3.7 Hz, 2C), 123.7 (q, *J* = 273.4 Hz), 123.6 (q, *J* = 3.7 Hz), 123.4 (2C), 123.3 (q, *J* = 237.4 Hz), 121.4 (q, *J* = 3.7 Hz), 118.5 ppm; HRMS (ESI-TOF) for $C_{21}H_{12}F_6N_2O_2$: calcd. $[M+Na]^+$ 461.0695; found: 461.0698.



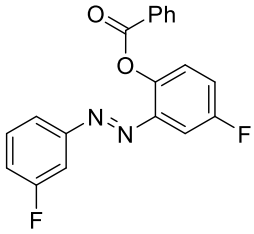
(E)-3-methyl-2-(o-tolyldiazenyl)phenyl benzoate (5h): Red brown solid (61%, 60.4 mg, E/Z = 20:1); R_f = 0.40 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) *δ* = 8.15 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.65-7.58 (m, 1H), 7.50-7.43 (m, 2H), 7.42 (dd, J_1 = 8.1 Hz, J_2 = 1.4 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.33-7.25 (m, 2H), 7.24-7.15 (m, 2H), 7.16-7.09 (m, 1H), 2.58 (s, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) *δ* = 165.4, 151.3, 143.8, 142.8, 138.3, 134.8, 133.4, 131.2, 131.1, 130.3 (2C), 129.6, 129.4, 129.3, 128.4 (2C), 126.2, 121.5, 115.2, 19.3, 17.4 ppm; HRMS (ESI-TOF) for $C_{21}H_{18}N_2O_2$: calcd. $[M+Na]^+$ 353.1260; found: 353.1267.



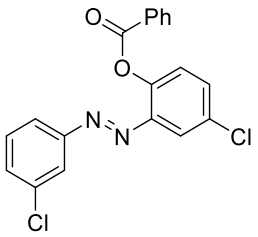
(E)-4-ethyl-2-((3-ethylphenyl)diazenyl)phenyl benzoate (5i): Orange solid (80%, 85.9 mg); R_f = 0.43(petroleum ether-EtOAc = 30:1); ^{1}H NMR (600 MHz, $CDCl_3$) ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.31 (dd, J_1 = 8.4 Hz, J_2 = 1.3 Hz, 2H), 7.75 (d, J = 2.2 Hz, 1H), 7.71-7.66 (m, 1H), 7.62-7.59 (m, 1H), 7.58-7.55 (m, 2H), 7.54-7.52 (m, 1H), 7.42 (dd, J_1 = 8.2 Hz, J_2 = 2.2 Hz, 1H), 7.36-7.30 (m, 2H), 7.26-7.23 (m, 1H), 2.79 (q, J = 7.6 Hz, 2H), 2.59 (q, J = 7.6 Hz, 2H), 1.35 (t, J = 7.7 Hz, 3H), 1.13 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 165.8, 153.0, 147.4, 145.1, 143.4, 142.7, 133.5, 131.6, 130.9, 130.4 (2C), 129.6, 128.8, 128.6 (2C), 116.7, 28.6, 28.5, 15.5, 15.2 ppm; HRMS (ESI-TOF) for $C_{23}H_{22}N_2O_2$: calcd. $[M+Na]^+$ 381.1573; found: 381.1583.



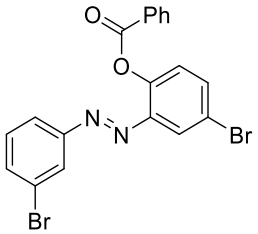
(E)-4-methoxy-2-((3-methoxyphenyl)diazenyl)phenyl benzoate (5j): Orange solid (65%, 70.6 mg, E/Z = 6:1); R_f = 0.33 (petroleum ether-EtOAc = 10:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.30 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.70-7.63 (m, 1H), 7.54 (t, J = 7.8 Hz, 2H), 7.52-7.46 (m, 1H), 7.44 (d, J = 3.1 Hz, 1H), 7.37-7.29 (m, 2H), 7.18-7.10 (m, 2H), 7.00-6.94 (m, 1H), 3.92 (s, 3H), 3.43 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 162.4, 161.7, 150.4, 147.3, 138.2, 133.6, 130.4 (2C), 129.5, 128.6 (2C), 124.5 (2C), 118.9, 114.0 (2C), 112.9, 108.1, 55.8, 55.5 ppm; HRMS (ESI-TOF) for $C_{21}H_{18}N_2O_4$: calcd. $[M+Na]^+$ 385.1159; found: 385.1167.



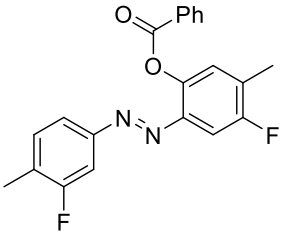
(E)-4-fluoro-2-((3-fluorophenyl)diazenyl)phenyl benzoate (5k): Yellow solid (77%, 78.1 mg, major regioisomer: minor regioisomer = 15:1); R_f = 0.40 (petroleum ether-EtOAc = 30:1); major regioisomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.28 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.74-7.67 (m, 1H), 7.62 (dd, J_1 = 9.2 Hz, J_2 = 2.9 Hz, 2H), 7.61-7.54 (m, 2H), 7.44-7.35 (m, 2H), 7.35 (dt, J_1 = 9.7 Hz, J_2 = 2.3 Hz, 1H), 7.34-7.26 (m, 1H), 7.18-7.15 (m, 1H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 163.1 (d, J = 248.1 Hz), 160.7 (d, J = 247.1 Hz), 153.8 (d, J = 7.0 Hz), 145.8 (d, J = 3.3 Hz), 144.5 (d, J = 6.3 Hz), 133.9, 130.3 (2C), 130.3 (d, J = 8.3 Hz), 129.0, 128.7 (2C), 124.8 (d, J = 8.6 Hz), 121.0 (d, J = 2.9 Hz), 119.1 (d, J = 24.3 Hz), 118.5 (d, J = 22.0 Hz), 108.2 (d, J = 23.1 Hz), 104.3 (d, J = 24.8 Hz) ppm; HRMS (ESI-TOF) for $C_{19}H_{12}F_2N_2O_2$: calcd. $[M+Na]^+$ 361.0759; found: 361.0765.



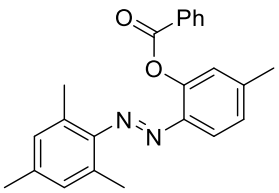
(E)-4-chloro-2-((3-chlorophenyl)diazenyl)phenyl benzoate (5l): Pale pink oil (68%, 75.5 mg, E/Z = 13:1); R_f = 0.40 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.27 (dd, J_1 = 8.3 Hz, J_2 = 1.4 Hz, 2H), 7.88 (d, J = 2.5 Hz, 1H), 7.74-7.67 (m, 1H), 7.69-7.61 (m, 2H), 7.61-7.52 (m, 3H), 7.43-7.33 (m, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.4, 153.2, 148.3, 144.0, 135.2, 134.0, 132.5, 132.2, 131.5, 130.4 (2C), 130.1, 128.9, 128.8 (2C), 124.9, 122.7, 122.1, 117.8 ppm; HRMS (ESI-TOF) for $C_{19}H_{12}Cl_2N_2O_2$: calcd. $[M+Na]^+$ 393.0168; found: 393.2096.



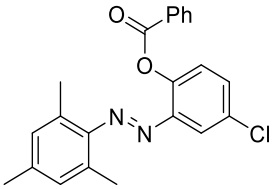
(E)-4-bromo-2-((3-bromophenyl)diazenyl)phenyl benzoate (5m): Yellow solid (75%, 103.3 mg); R_f = 0.43 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.30-8.24 (m, 2H), 8.02 (d, J = 2.4 Hz, 1H), 7.78 (t, J = 1.9 Hz, 1H), 7.74-7.67 (m, 3H), 7.61-7.54 (m, 2H), 7.57-7.51 (m, 1H), 7.35-7.26 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.3, 153.3, 148.8, 144.1, 135.1, 134.3, 134.0, 130.4, 130.4 (2C), 128.9, 128.8 (2C), 125.2, 124.9, 123.3, 123.1, 120.7, 120.0 ppm; HRMS (ESI-TOF) for $C_{19}H_{12}Br_2N_2O_2$: calcd. $[M+Na]^+$ 482.9158; found: 482.9148.



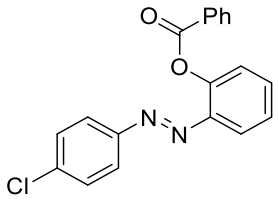
(E)-4-fluoro-2-((3-fluoro-4-methylphenyl)diazenyl)-5-methylphenyl benzoate (5n): Yellow solid (62%, 68.1 mg, major regioisomer: minor regioisomer = 9: 1); R_f = 0.40 (petroleum ether-EtOAc = 30:1); major regioisomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.33-8.20 (m, 2H), 7.73-7.66 (m, 1H), 7.61-7.55 (m, 3H), 7.49 (dd, J_1 = 8.0 Hz, J_2 = 1.9 Hz, 1H), 7.28 (dd, J_1 = 10.5 Hz, J_2 = 1.9 Hz, 1H), 7.26-7.18(m, 2H), 2.40 (d, J = 2.0 Hz, 3H), 2.30 (d, J = 2.1 Hz, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.7, 161.5 (d, J = 246.8 Hz), 159.3 (d, J = 245.9 Hz), 152.2 (d, J = 7.0 Hz), 145.3 (d, J = 2.9 Hz), 142.6 (d, J = 6.5 Hz), 133.8, 131.5 (d, J = 5.6 Hz), 130.5 (2C), 129.9 (d, J = 20.2 Hz), 129.2, 128.7 (d, J = 28.0 Hz), 128.7 (2C), 125.7 (d, J = 5.3 Hz), 120.7 (d, J = 3.2 Hz), 107.6 (d, J = 23.8 Hz), 103.7 (d, J = 25.8 Hz), 15.0 (d, J = 2.9 Hz), 14.8 (d, J = 3.4 Hz) ppm; HRMS (ESI-TOF) for $C_{21}H_{16}F_2N_2O_2$: calcd. $[M+Na]^+$ 389.1072; found: 389.1079.



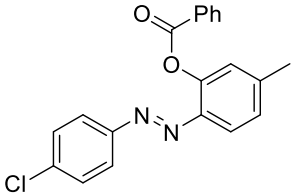
(E)-2-(mesityldiazenyl)-5-methylphenyl benzoate (5o): Orange solid (88%, 94.5 mg); R_f = 0.40 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.33-8.17 (m, 2H), 7.84-7.69 (m, 2H), 7.55-7.48 (m, 2H), 7.23-7.18 (m, 2H), 6.86(s, 2H), 2.49 (s, 3H), 2.32 (s, 6H), 2.29 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.3, 149.3, 148.0, 142.9, 142.5, 139.1, 133.5, 132.8, 130.3 (2C), 130.0 (2C), 129.5, 129.1, 128.5 (2C), 127.5, 124.0, 116.5, 21.4, 21.1, 19.8 (2C) ppm; HRMS (ESI-TOF) for $C_{23}H_{22}N_2O_2$: calcd. $[M+Na]^+$ 381.1573; found: 381.1581.



(E)-4-chloro-2-(mesityldiazenyl)phenyl benzoate (5p): Red brown solid (66%, 74.8 mg, E/Z = 11:1); R_f = 0.47 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.23 (dd, J_1 = 8.3 Hz, J_2 = 1.3 Hz, 2H), 7.79 (d, J = 2.5 Hz, 1H), 7.70-7.62 (m, 1H), 7.55-7.45 (m, 3H), 7.32 (d, J = 8.6 Hz, 1H), 6.88 (s, 2H), 2.34 (s, 6H), 2.29 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.1, 147.9, 147.5, 145.3, 140.4, 133.7, 133.7, 132.5, 131.0, 130.4 (2C), 130.2 (2C), 129.2, 129.1, 128.6 (2C), 124.9, 116.8, 21.2, 20.2 (2C) ppm; HRMS (ESI-TOF) for $C_{22}H_{19}ClN_2O_2$: calcd. $[M+Na]^+$ 401.1027; found: 401.1033.

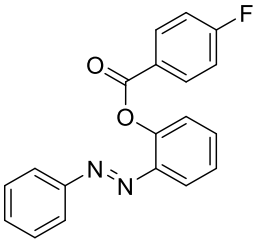


(E)-2-((4-chlorophenyl)diazenyl)phenyl benzoate (5q): Orange solid (67%, 67.5 mg); R_f = 0.30 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.31-8.24 (m, 2H), 7.89 (dd, J_1 = 8.3 Hz, J_2 = 1.6 Hz, 1H), 7.72-7.68 (m, 1H), 7.67-7.64 (m, 2H), 7.59-7.54 (m, 3H), 7.43-7.39 (m, 2H), 7.37-7.33 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 165.5, 151.1, 149.4, 143.8, 137.2, 133.7, 132.4, 130.3 (2C), 129.4, 129.3 (2C), 128.7 (2C), 126.6, 124.2 (2C), 123.6, 117.9 ppm; HRMS (ESI-TOF) for $C_{19}H_{13}ClN_2O_2$: calcd. $[M+Na]^+$ 359.0558; found: 359.0564.

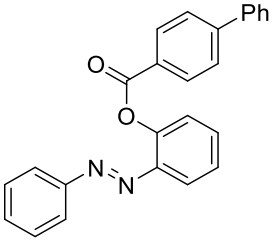


(E)-2-((4-chlorophenyl)diazenyl)-5-methylphenyl benzoate (5r): Yellow solid (58%, 60.8 mg, E/Z = 6:1); R_f = 0.37 (petroleum ether-EtOAc = 30:1); major *E*-isomer: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.28 (dd, J = 8.3, 1.4 Hz, 2H), 7.71-7.64 (m, 4H), 7.58-7.54 (m, 2H), 7.40 (ddd, J_1 = 8.2 Hz, J_2 = 2.2 Hz, J_3 = 0.8 Hz, 1H), 7.37-7.34 (m, 2H), 7.29 (d, J = 9.0 Hz, 1H), 2.48 (s, 3H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 165.7, 151.1, 147.3, 143.3, 137.1, 136.6, 133.6, 133.1, 130.3(2C), 129.4, 129.3 (2C), 128.6 (2C),

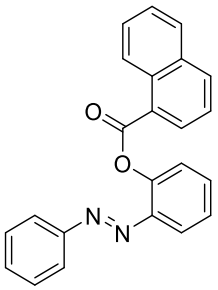
124.2 (2C), 123.2, 118.0, 21.1 ppm; HRMS (ESI-TOF) for $C_{20}H_{15}N_2O_2$: calcd. $[M+Na]^+$ 373.0714; found: 373.0718.



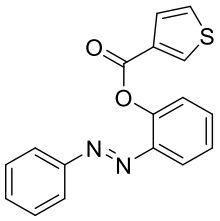
(E)-2-(phenyldiazenyl)phenyl 4-fluorobenzoate (5s): Orange solid (82%, 78.7 mg); R_f = 0.37 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.35-8.28 (m, 2H), 7.91 (dd, J_1 = 8.0 Hz, J_2 = 1.6, 1H), 7.74 (dd, J_1 = 7.8 Hz, J_2 = 1.9 Hz, 2H), 7.57 (td, J_1 = 7.7 Hz, J_2 = 1.7 Hz, 1H), 7.46-7.38 (m, 5H), 7.27-7.20 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.2 (d, J = 254.9 Hz), 164.5, 152.7, 149.1, 143.9, 133.0 (d, J = 9.5 Hz, 2C), 132.1, 131.3, 129.0 (2C), 126.7, 125.7 (d, J = 2.9 Hz), 123.5, 123.0 (2C), 118.0, 115.9 (d, J = 22.2 Hz, 2C,) ppm; HRMS (ESI-TOF) for $C_{19}H_{13}FN_2O_2$: calcd. $[M+Na]^+$ 343.0853; found: 343.0857.



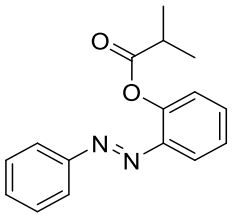
(E)-2-(phenyldiazenyl)phenyl [1,1'-biphenyl]-4-carboxylate (5t): Orange solid (46%, 52.1 mg); R_f = 0.27 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.36 (d, J = 8.4 Hz, 2H), 7.92 (dd, J_1 = 8.4 Hz, J_2 = 1.7 Hz, 1H), 7.79 (d, J = 8.4 Hz, 2H), 7.76 (dd, J_1 = 7.7 Hz, J_2 = 2.1 Hz, 2H), 7.72 (dd, J_1 = 8.2 Hz, J_2 = 1.3 Hz, 2H), 7.62-7.57 (m, 1H), 7.53 (dd, J_1 = 8.4 Hz, J_2 = 6.9 Hz, 2H), 7.48-7.44 (m, 2H), 7.44-7.40 (m, 4H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 165.4, 152.7, 149.3, 146.3, 144.0, 139.9, 132.1, 131.3, 130.9 (2C), 129.0 (2C), 129.0 (2C), 128.4, 128.1, 127.4 (2C), 127.3 (2C), 126.6, 123.6, 123.1 (2C), 117.8 ppm; HRMS (ESI-TOF) for $C_{25}H_{18}N_2O_2$: calcd. $[M+Na]^+$ 401.1260; found: 401.1268.



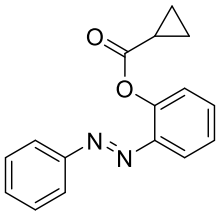
(E)-2-(phenyldiazenyl)phenyl 1-naphthoate (5u): Orange solid (82%, 86.6 mg); R_f = 0.30 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.11 (d, J = 8.5 Hz, 1H), 8.62 (d, J = 7.2 Hz, 1H), 8.16 (d, J = 8.3 Hz, 1H), 8.04-7.96 (m, 2H), 7.86 (d, J = 8.0 Hz, 2H), 7.69-7.58 (m, 4H), 7.52 (d, J = 7.9 Hz, 1H), 7.51-7.44 (m, 1H), 7.44-7.34 (m, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 166.1, 152.6, 149.4, 144.1, 134.1, 133.8, 132.1, 131.6, 131.2, 131.2, 128.9 (2C), 128.6, 128.0, 126.6, 126.4, 126.1, 125.8, 124.5, 123.6, 123.1 (2C), 117.5 ppm; HRMS (ESI-TOF) forrre $C_{23}H_{16}N_2O_2$: calcd. $[M+Na]^+$ 375.1104; found: 375.1104.



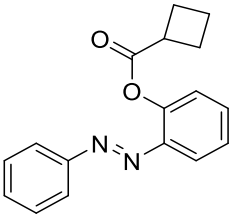
(E)-2-(phenyldiazenyl)phenyl thiophene-3-carboxylate (5v): Orange solid (81%, 74.8 mg); R_f = 0.27 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.42 (dd, J_1 = 3.0 Hz, J_2 = 1.2 Hz, 1H), 7.91 (dd, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 7.78-7.74 (m, 3H), 7.61-7.53 (m, 1H), 7.45-7.38 (m, 6H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 161.2, 152.7, 148.9, 144.0, 134.2, 132.6, 132.0, 131.2, 129.0 (2C), 128.3, 126.5, 126.4, 123.5, 123.0 (2C), 117.8 ppm; HRMS (ESI-TOF) for $C_{17}H_{12}N_2O_2S$: calcd. $[M+Na]^+$ 331.0512; found: 331.0513.



(E)-2-(phenyldiazenyl)phenyl isobutyrate (5w): Orange solid (65%, 52.3 mg); R_f = 0.37 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.91-7.85 (m, 2H), 7.82 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.56-7.47 (m, 4H), 7.39-7.32 (m, 1H), 7.25 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 2.95 (m, J = 7.0 Hz, 1H), 1.40 (s, 3H), 1.39 (s, 3H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 175.5, 152.9, 149.2, 144.3, 132.0, 131.2, 129.0 (2C), 126.4, 123.4, 123.0 (2C), 117.3, 34.2, 19.1 (2C) ppm; HRMS (ESI-TOF) for $C_{16}H_{16}N_2O_2$: calcd. $[M+Na]^+$ 291.1104; found: 291.1109.



(E)-2-(phenyldiazenyl)phenyl cyclopropanecarboxylate (5x): Orange solid (66%, 52.7 mg); R_f = 0.30 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.92-7.86 (m, 2H), 7.80 (dd, J = 8.1, 1.9 Hz, 1H), 7.54-7.45 (m, 4H), 7.33 (t, J = 7.7 Hz, 1H), 7.26-7.22 (m, 1H), 2.02-1.92 (m, 1H), 1.27-1.20 (m, 2H), 1.11-1.00 (m, 2H) ppm; ^{13}C NMR (151 MHz, $CDCl_3$) δ = 173.6, 152.8, 149.2, 144.0, 132.0, 131.3, 129.1 (2C), 126.4, 123.4, 123.1 (2C), 117.4, 13.0, 9.2 (2C) ppm; HRMS (ESI-TOF) for $C_{16}H_{14}N_2O_2$: calcd. $[M+Na]^+$ 289.0947; found: 289.0954.



(E)-2-(phenyldiazenyl)phenyl cyclobutanecarboxylate (5y): Orange solid (60%, 50.4 mg); R_f = 0.33 (petroleum ether-EtOAc = 30:1); ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.91-7.85 (m, 2H), 7.83 (dd, J_1 = 8.1

Hz, J_2 = 1.6 Hz, 1H), 7.56-7.47 (m, 4H), 7.39-7.32 (m, 1H), 7.26 (dd, J_1 = 8.0 Hz, J_2 = 1.3 Hz, 1H), 3.59-3.48 (m, 1H), 2.61-2.50 (m, 2H), 2.45-2.34 (m, 2H), 2.15-1.98 (m, 2H) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ = 173.9, 152.9, 149.2, 144.2, 132.0, 131.3, 129.0 (2C), 126.4, 123.4, 123.0 (2C), 117.3, 38.1, 25.4 (2C), 18.6 ppm; HRMS (ESI-TOF) for $C_{17}H_{16}N_2O_2$: calcd. $[M+Na]^+$ 303.1104; found: 303.1111.

VIII. References

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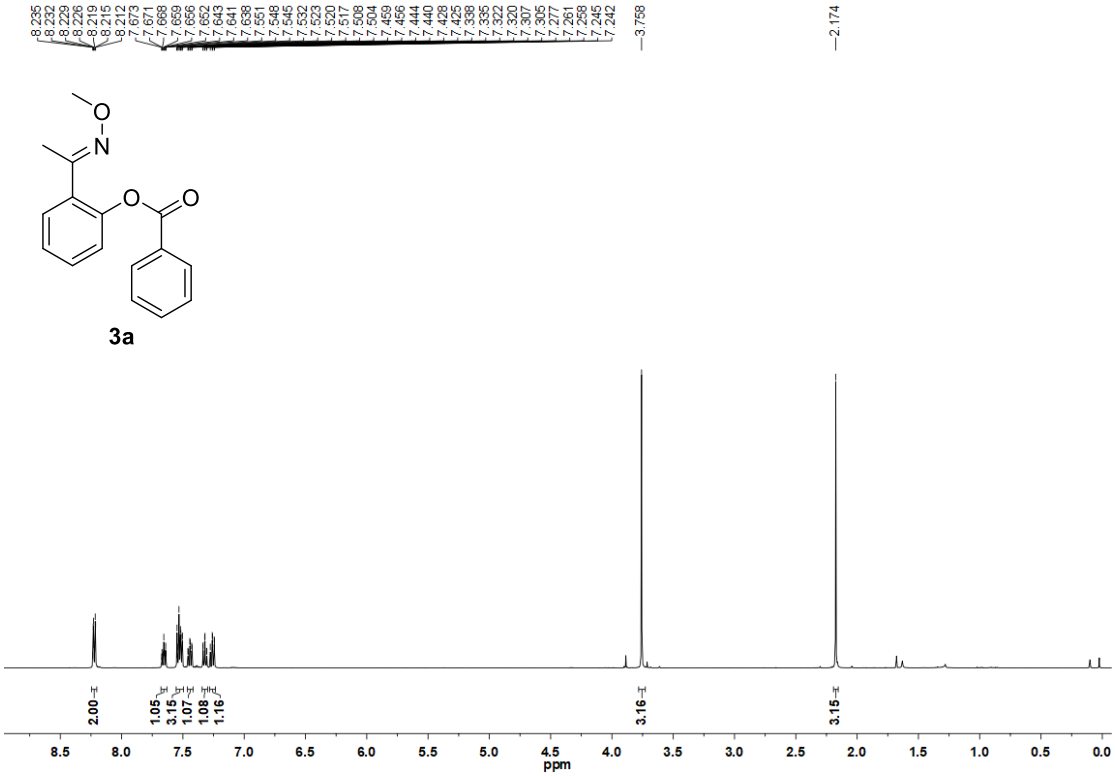
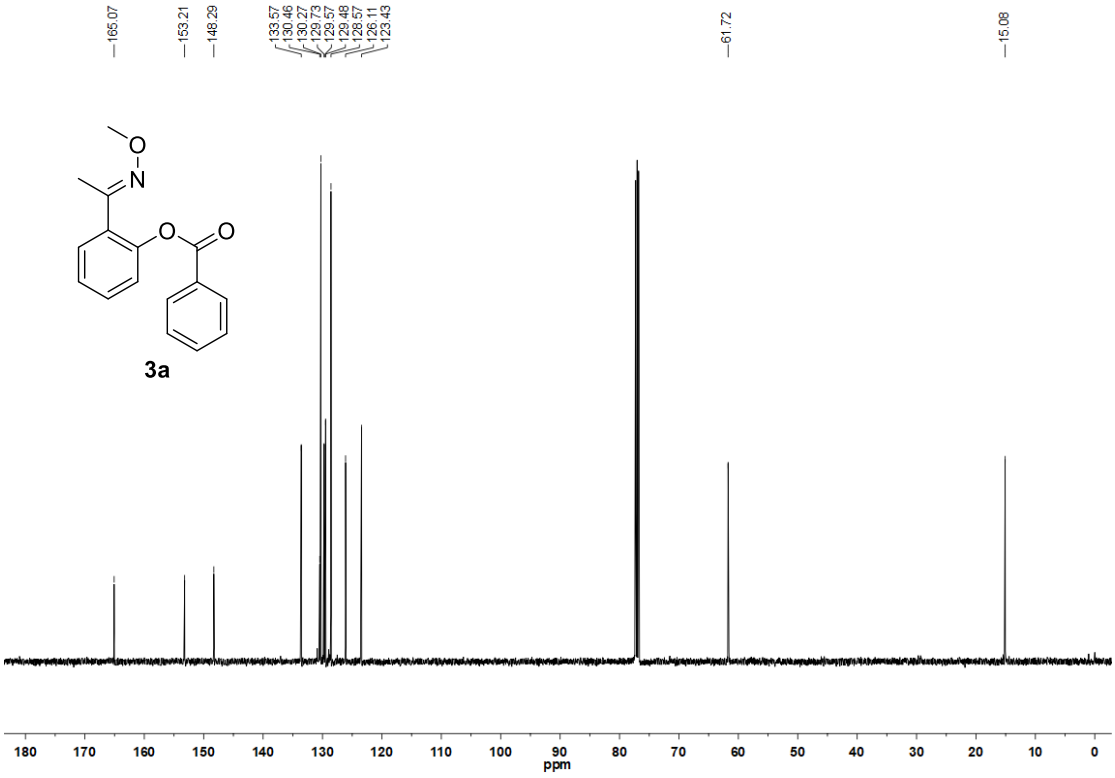
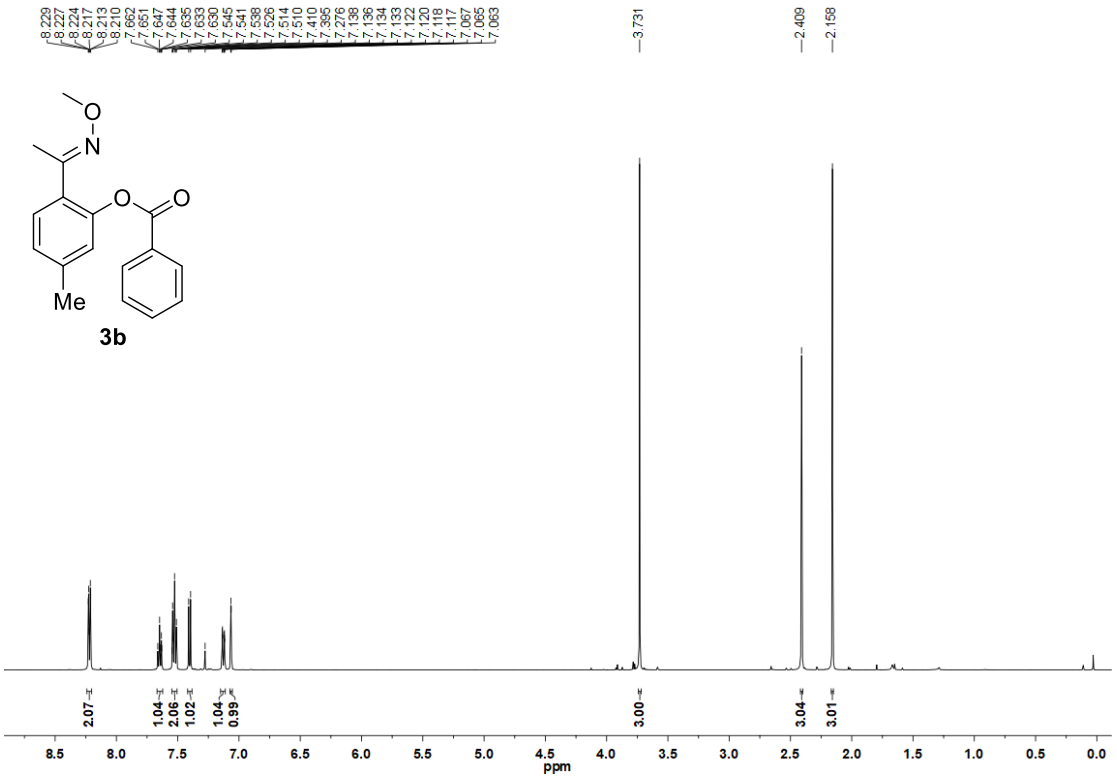
IX. NMR spectra



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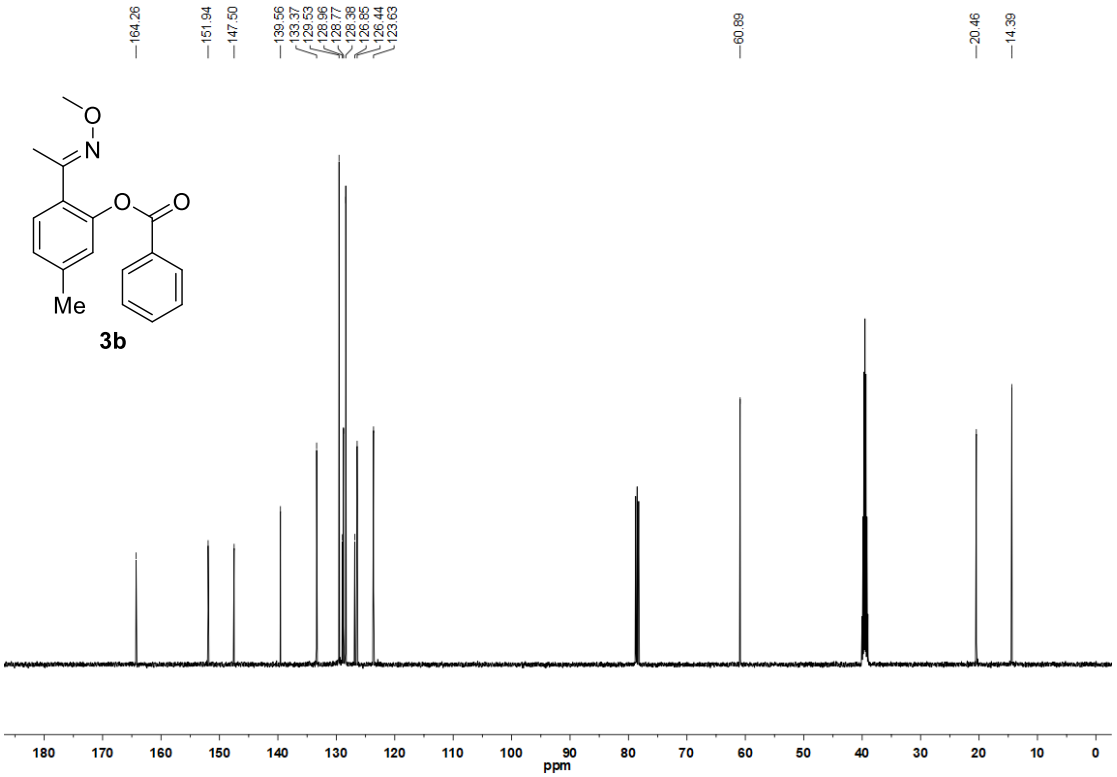
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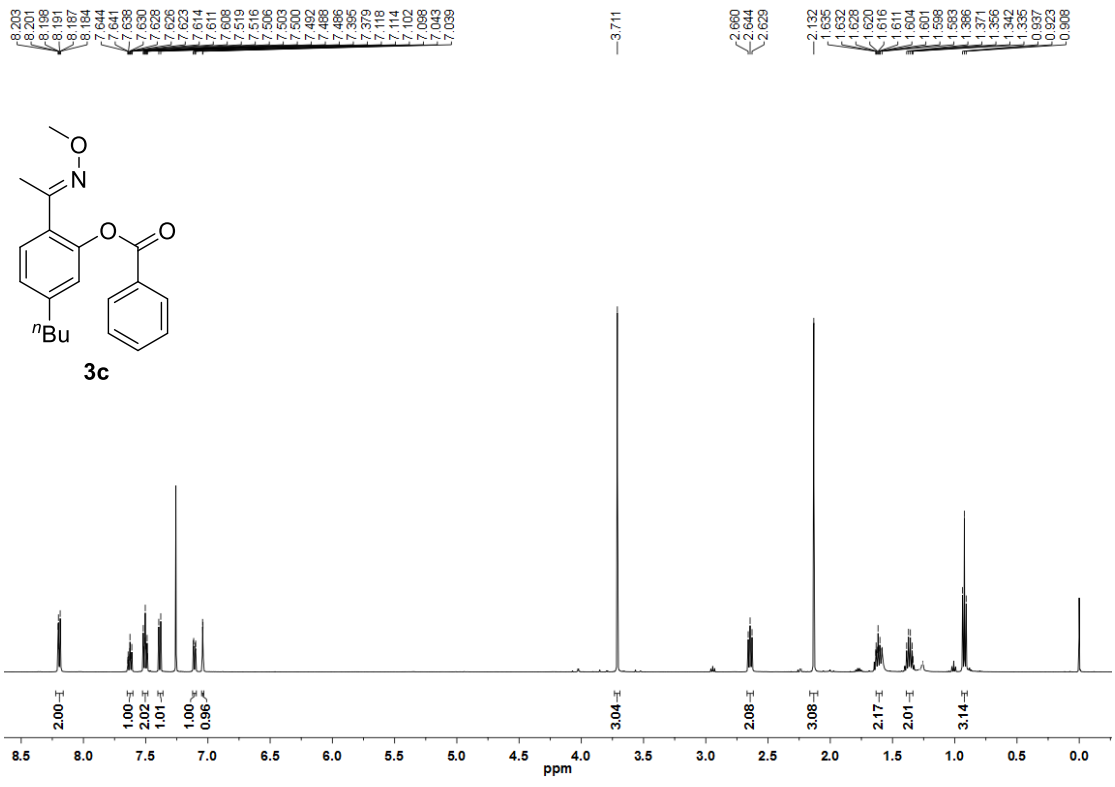
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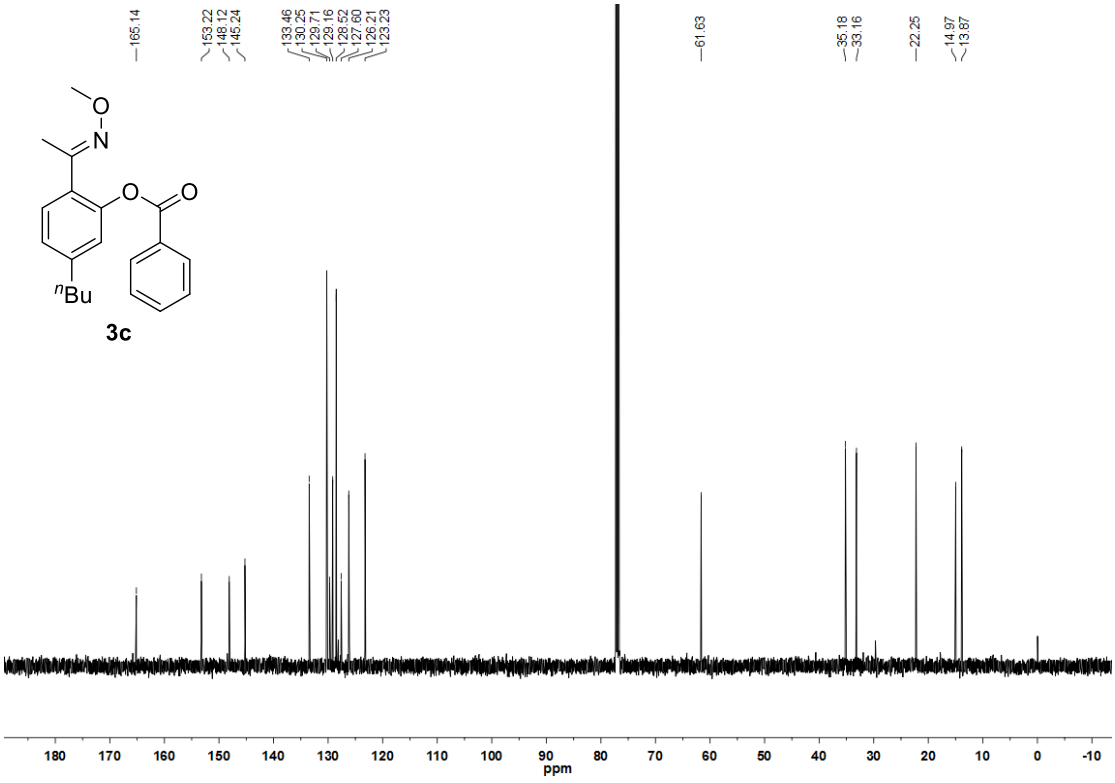
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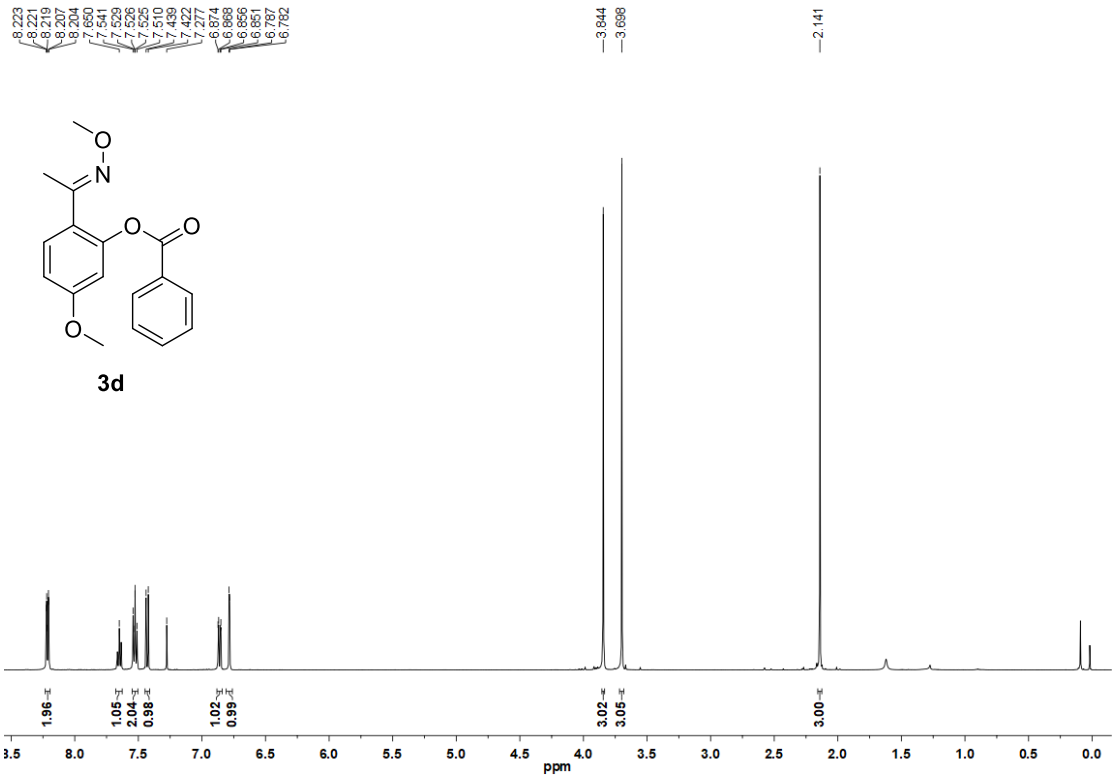
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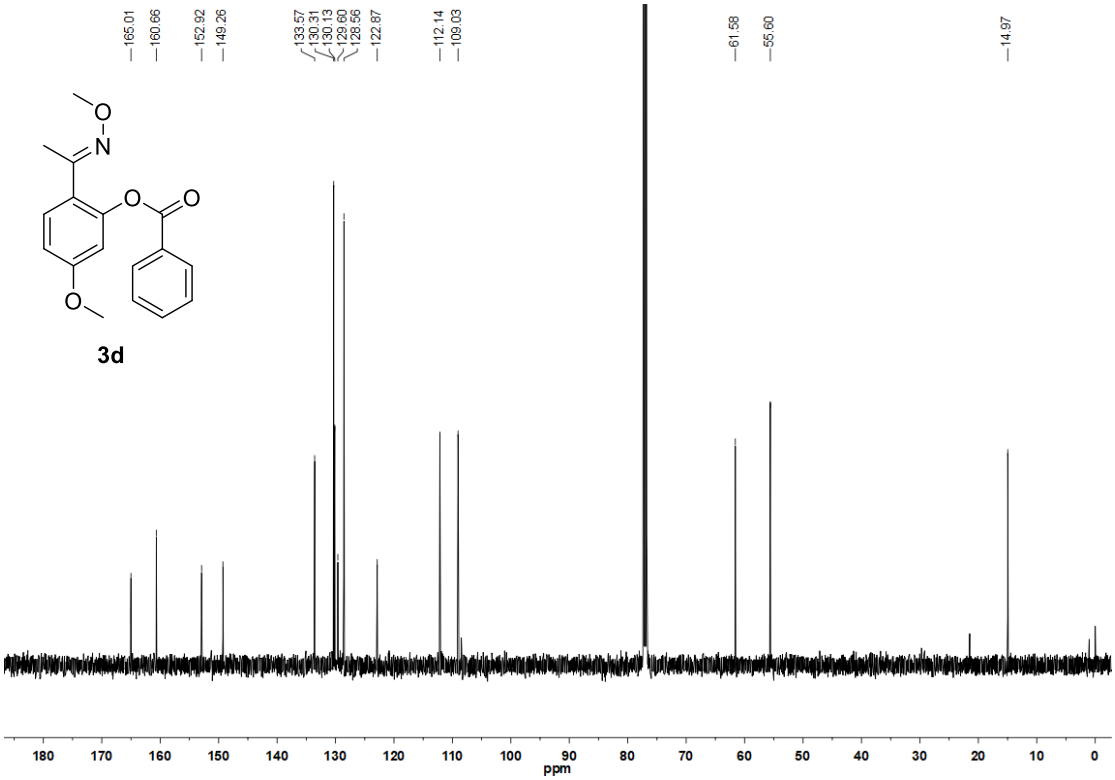
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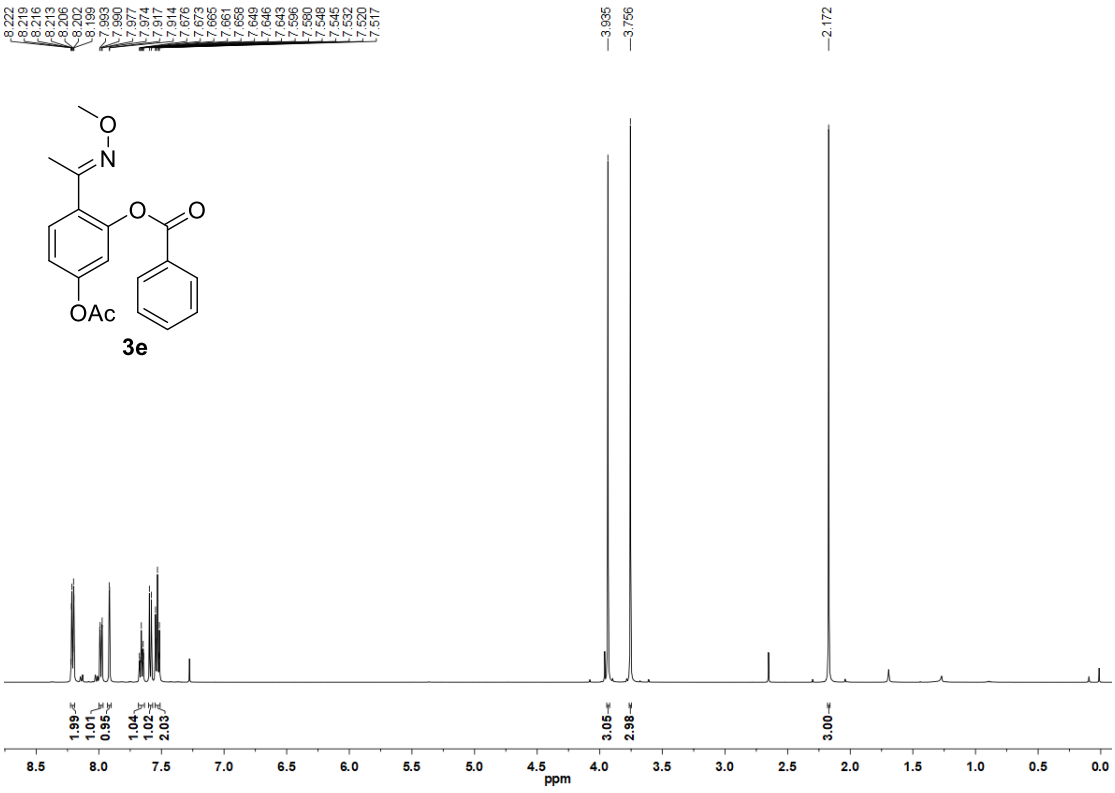
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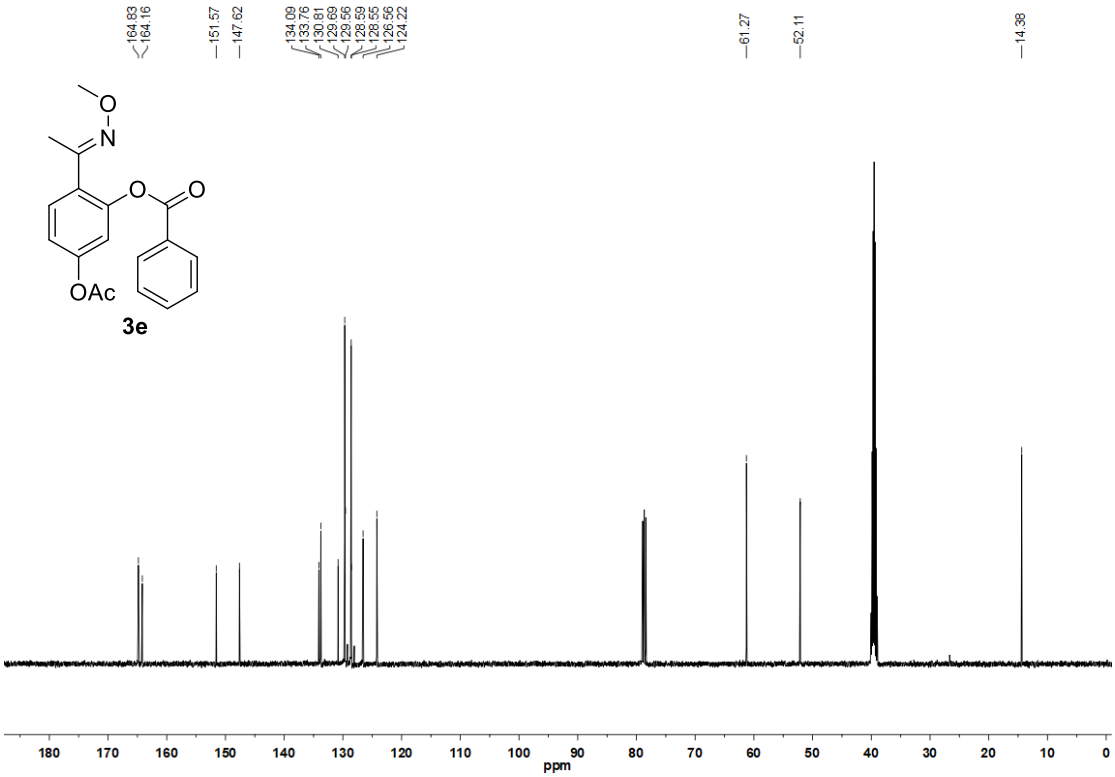
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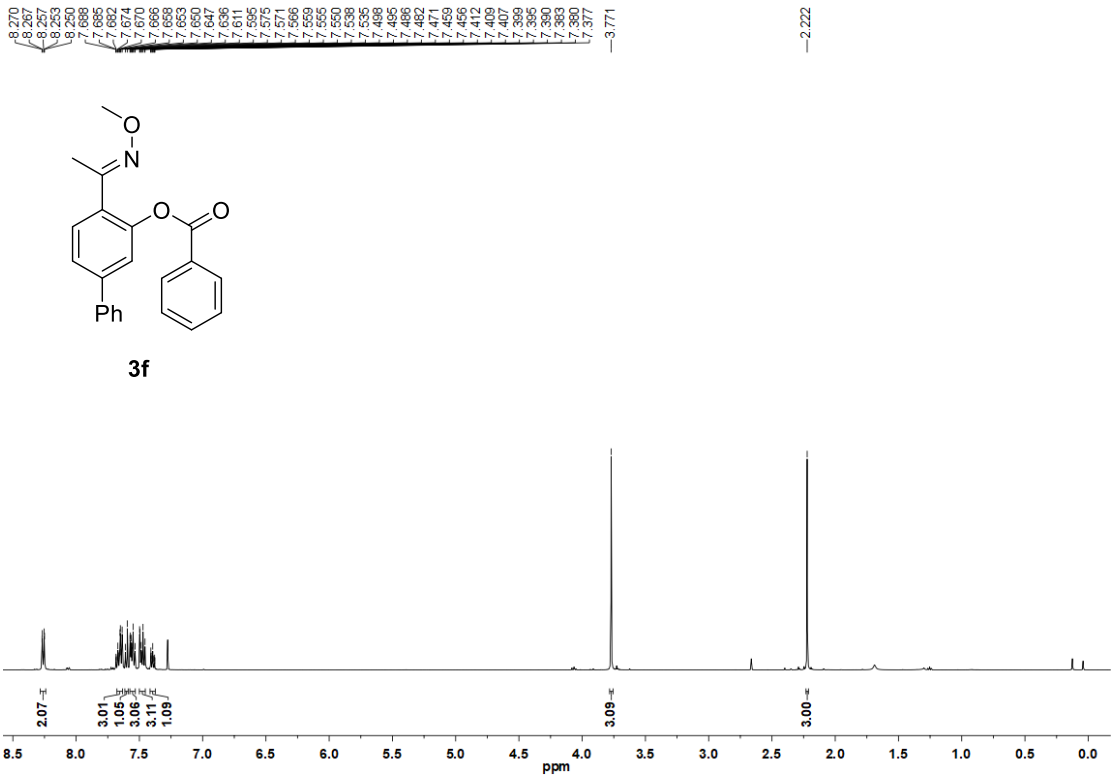
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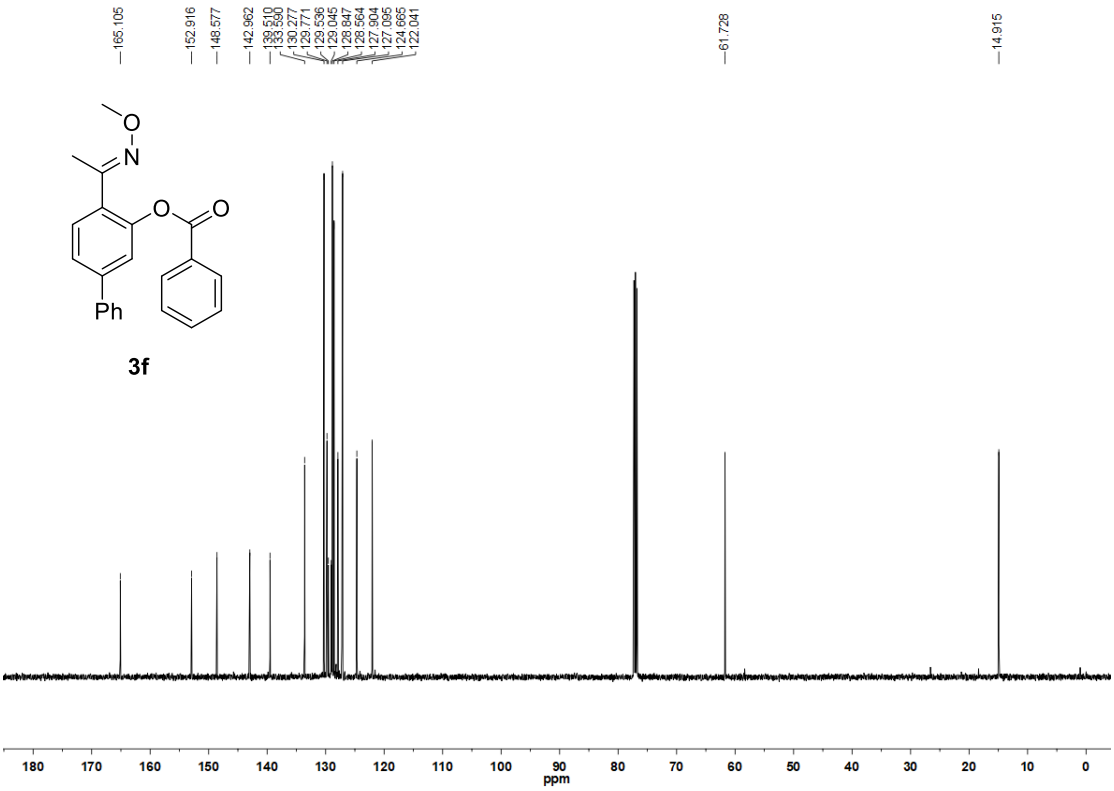
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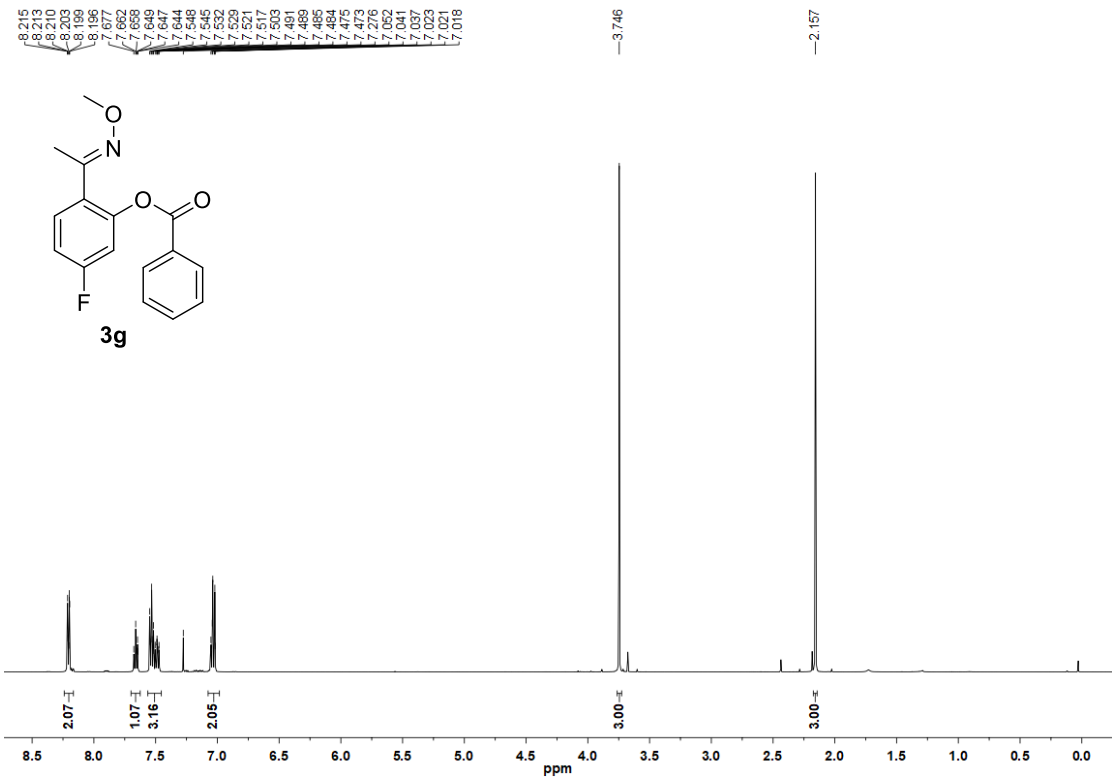
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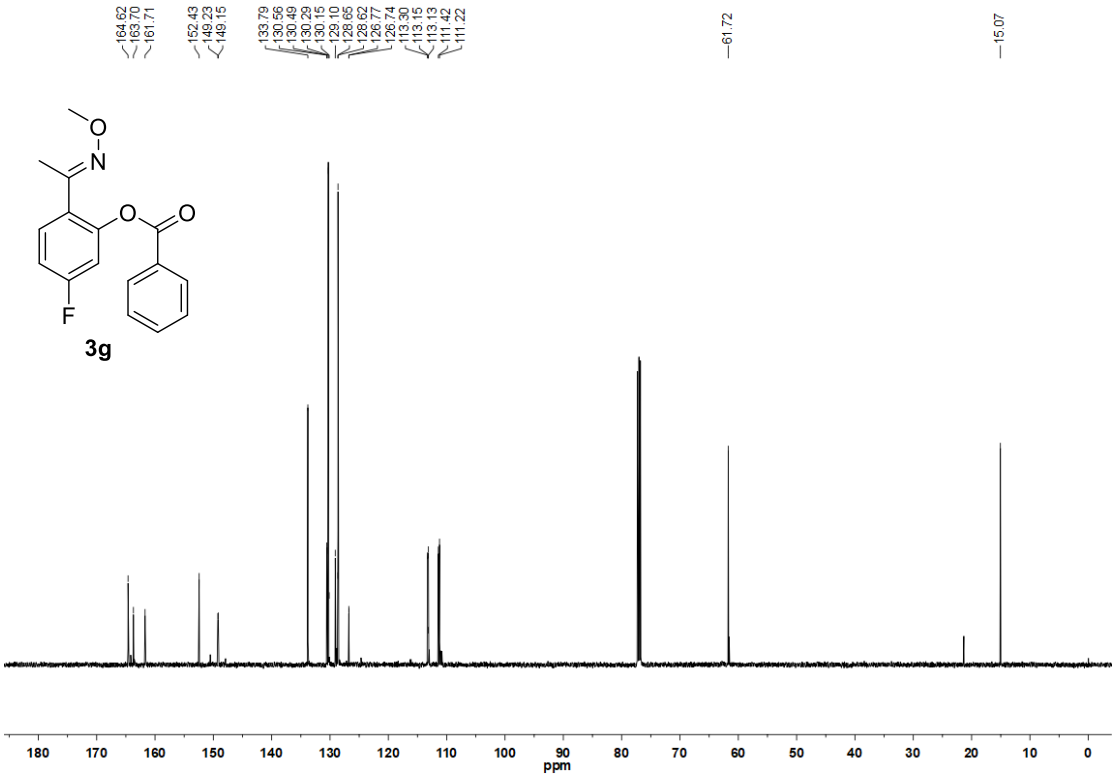
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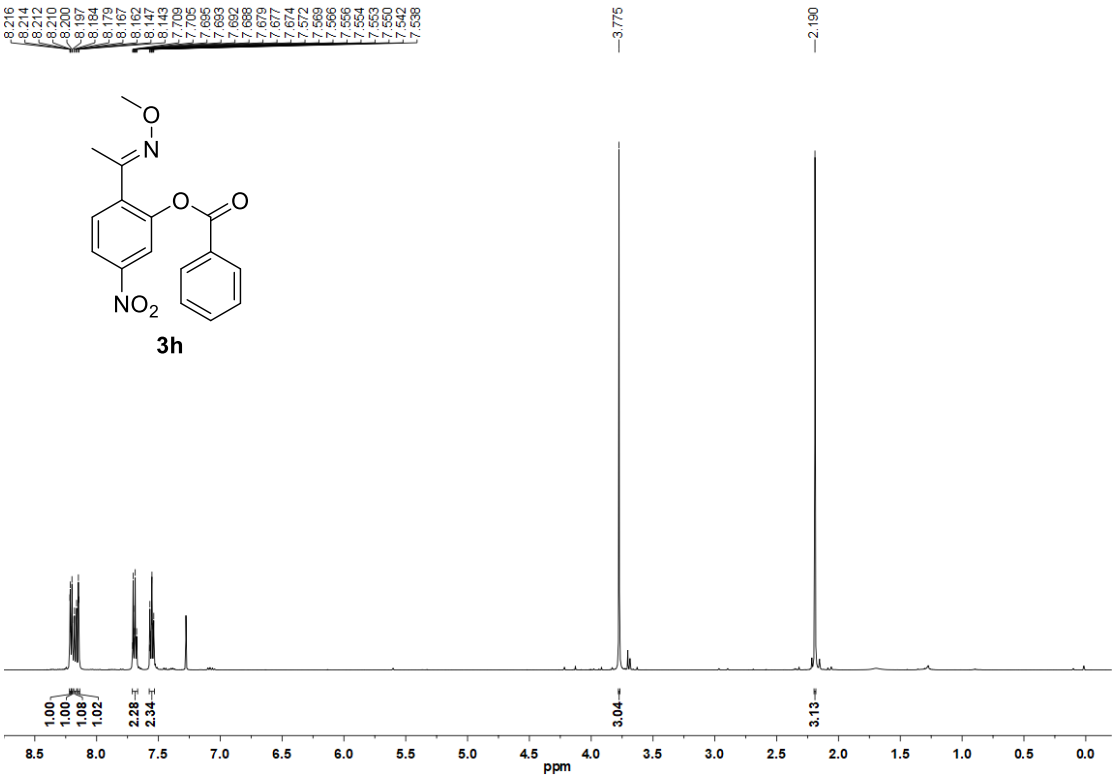
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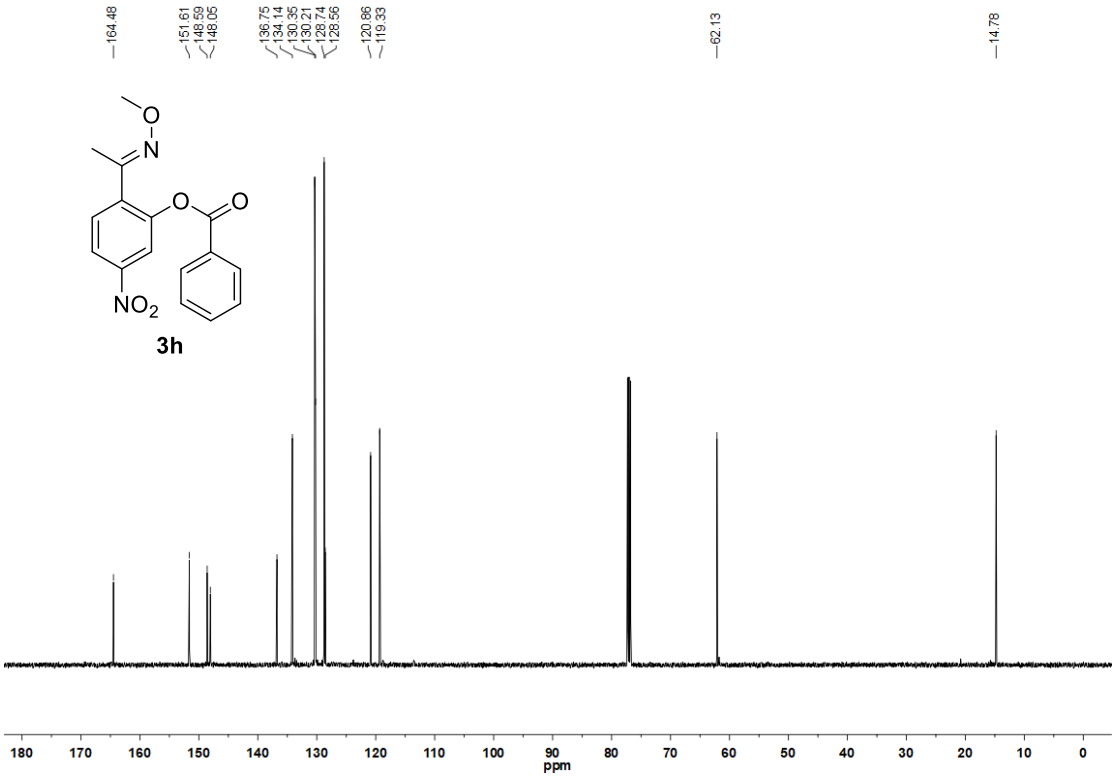
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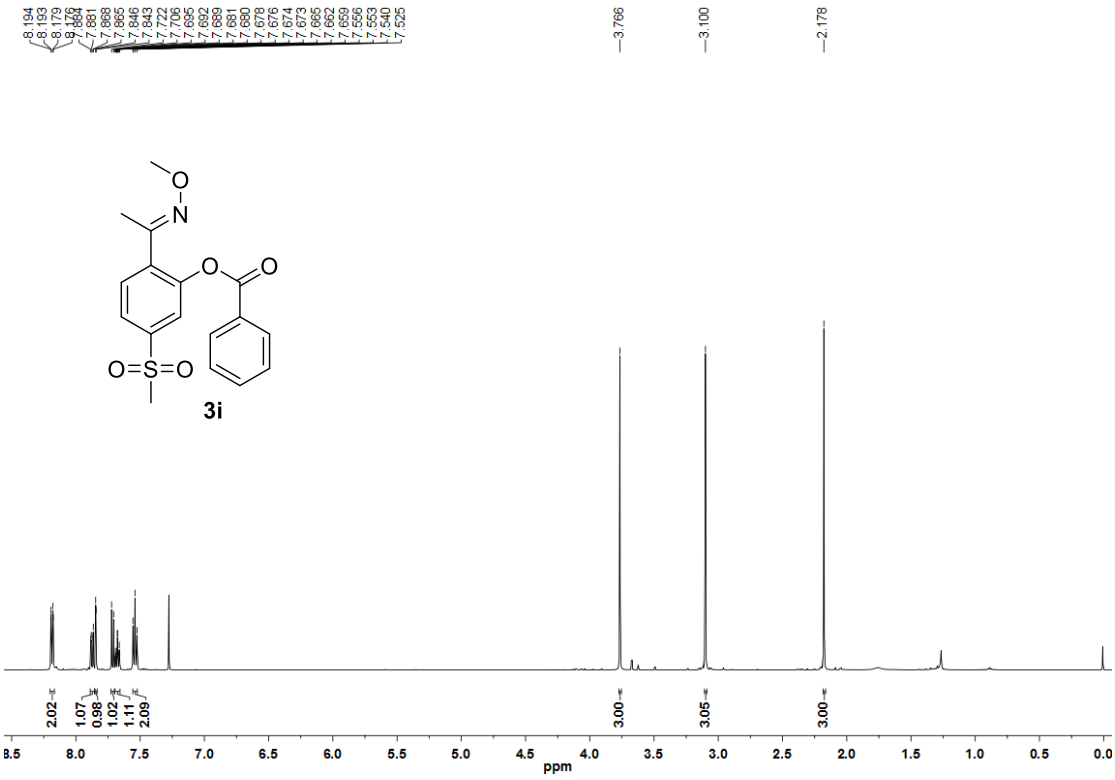
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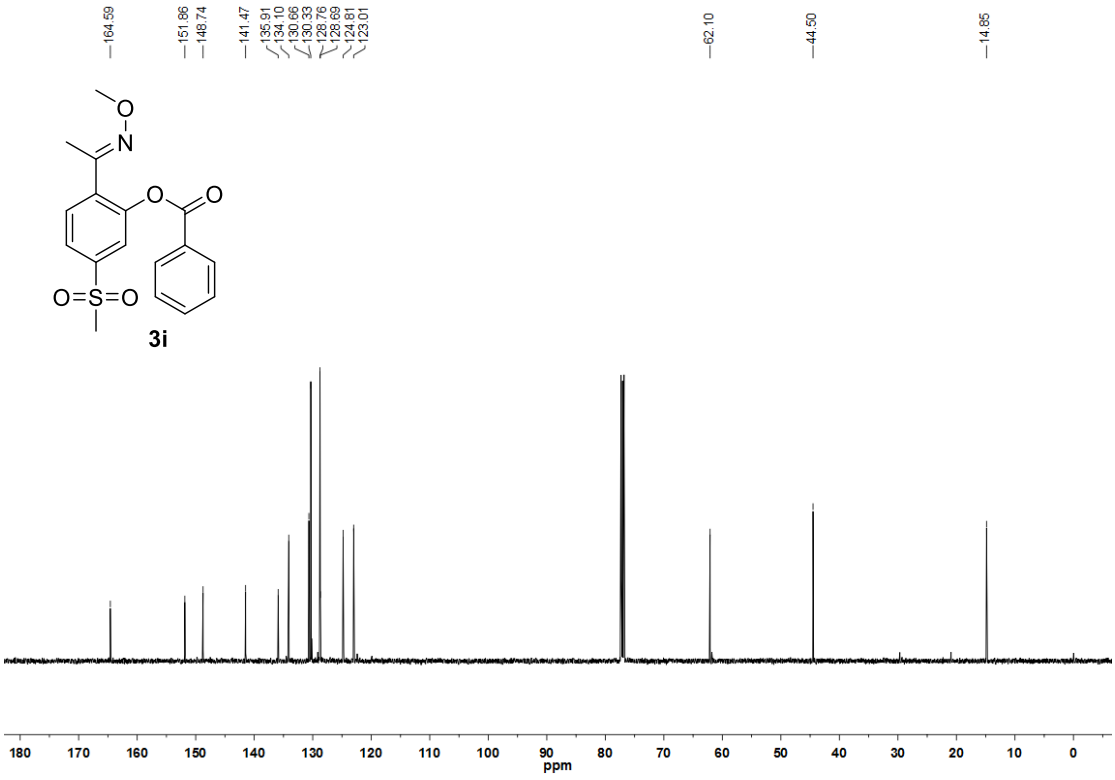
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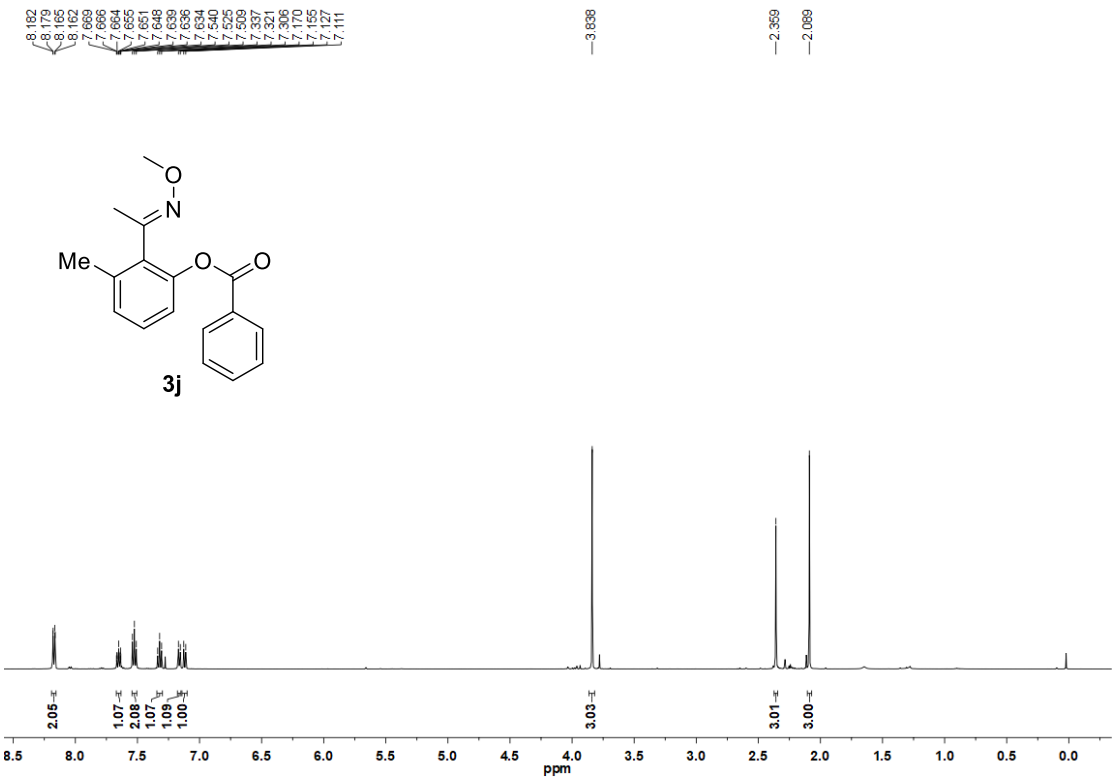
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7.111
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Me
O
N
O
O
3j
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2.08
1.07
1.09
1.00
3.03
3.01
3.00
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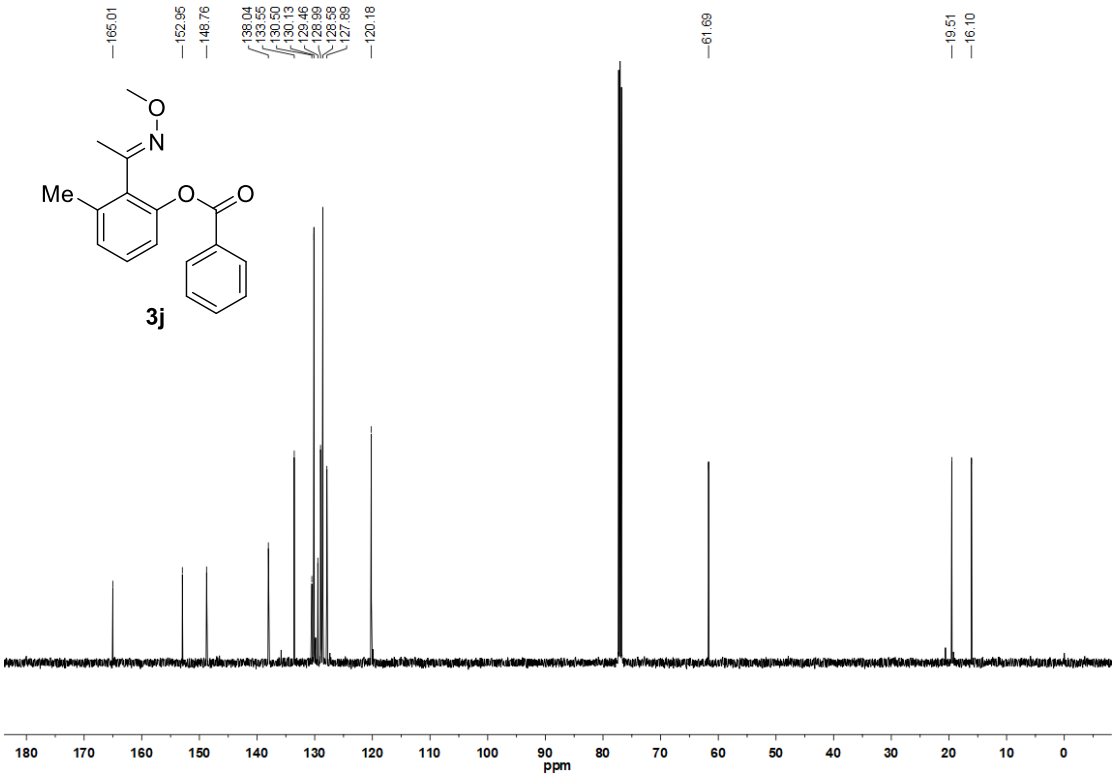
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16.10
Me
O
N
O
O
3j
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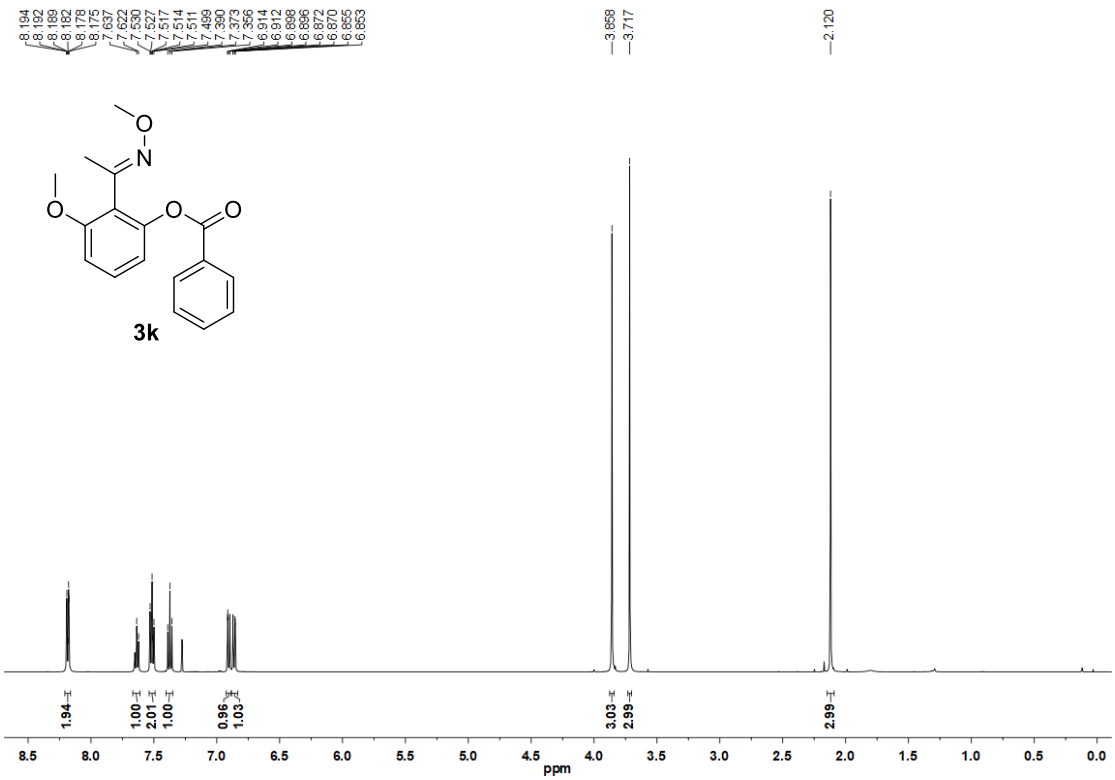
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6.912
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6.870
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6.853
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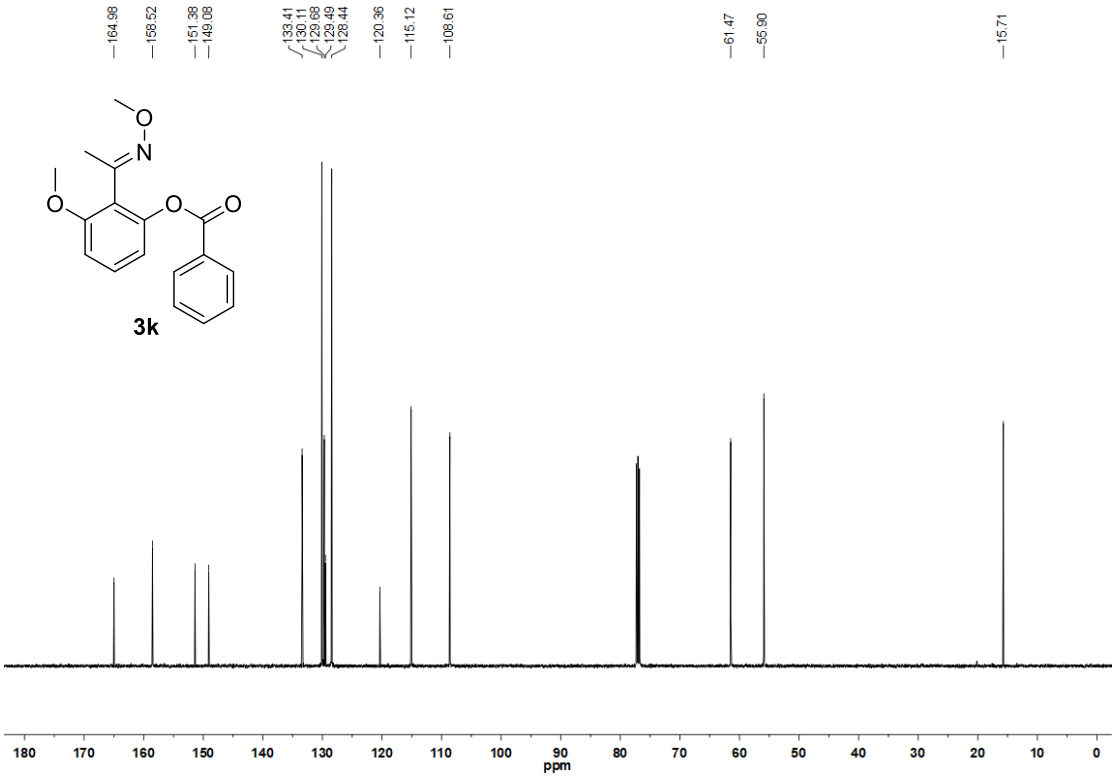
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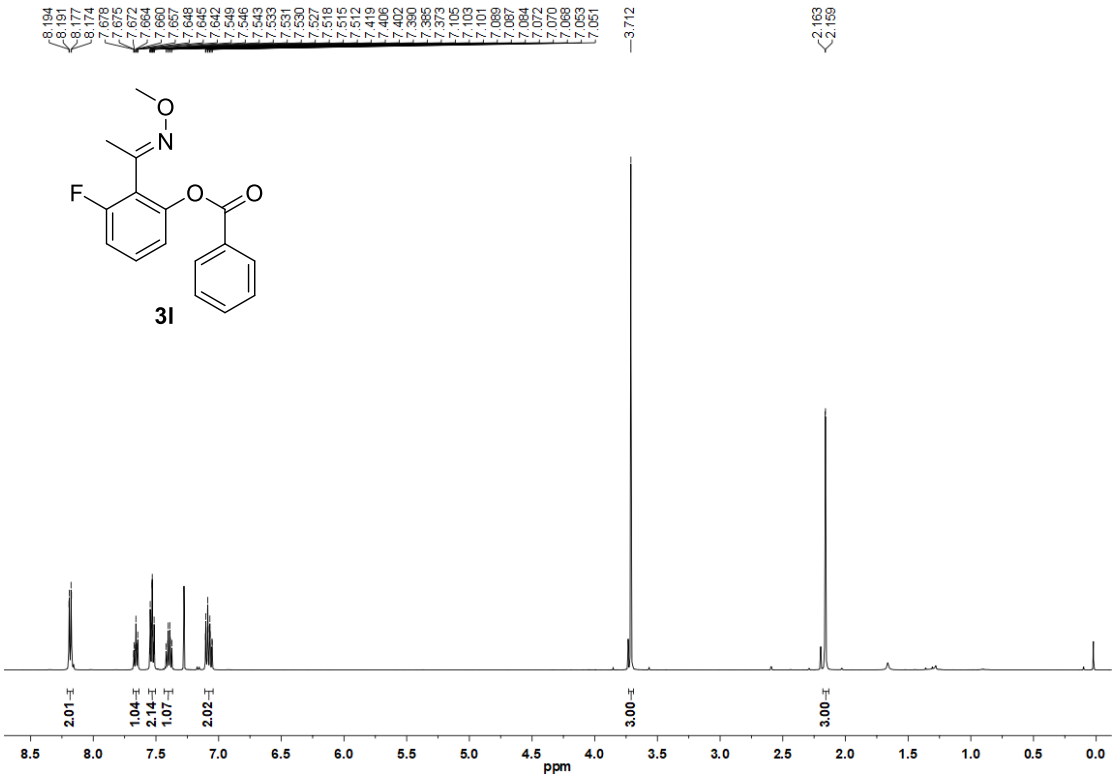
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7.543
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7.518
7.515
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7.419
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7.402
7.390
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7.373
7.105
7.103
7.101
7.089
7.087
7.084
7.072
7.070
7.068
7.053
7.051
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2.163
2.159
O
N
F
O
O
3l
2.01
1.04
2.14
1.07
2.02
3.00
3.00
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6.0
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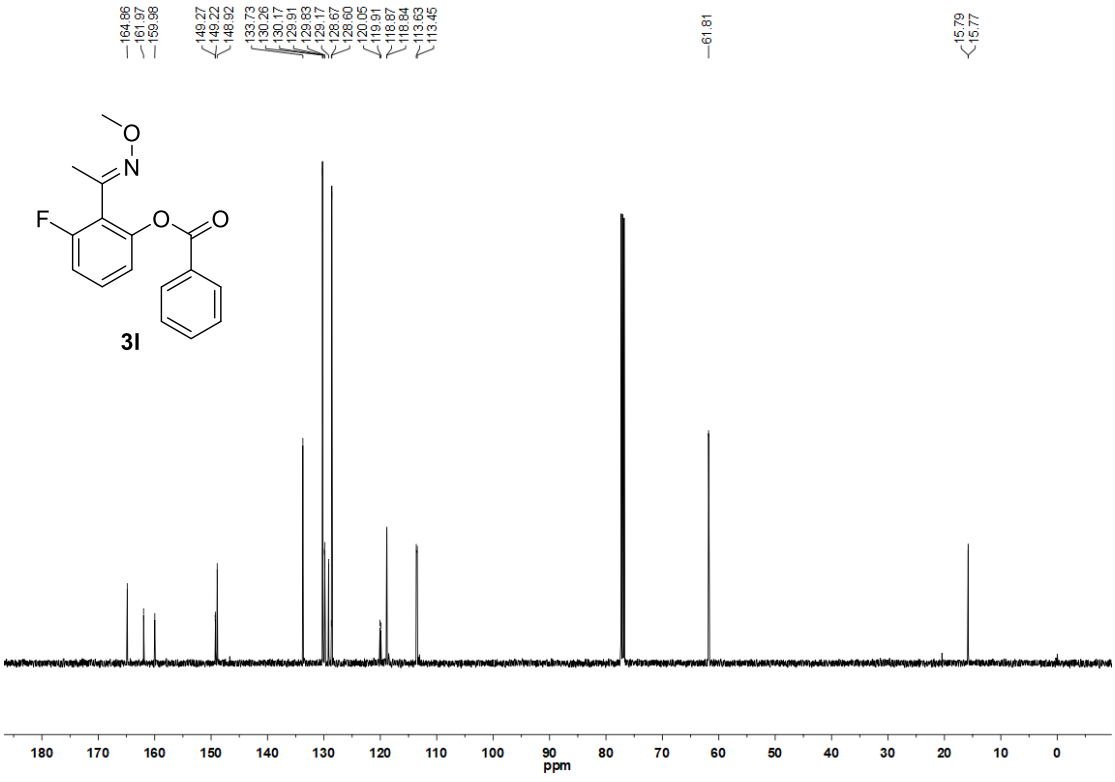
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O
3l
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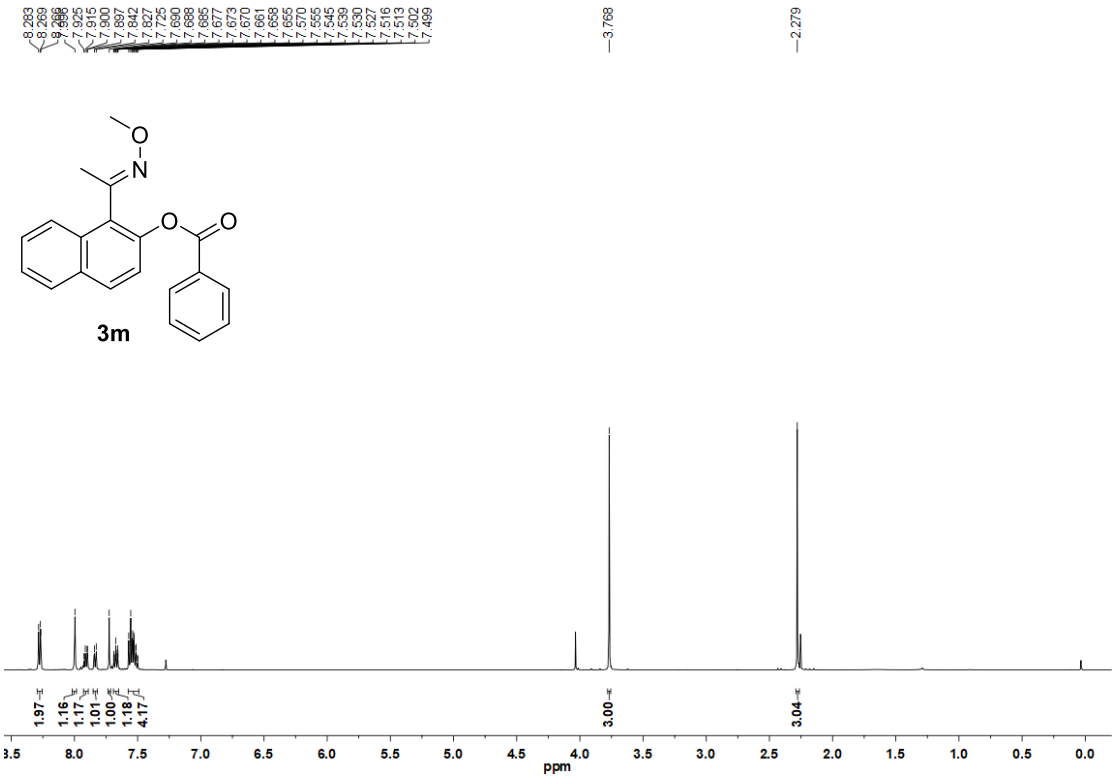
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7.673
7.670
7.661
7.658
7.655
7.570
7.565
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7.539
7.530
7.527
7.516
7.513
7.502
7.499
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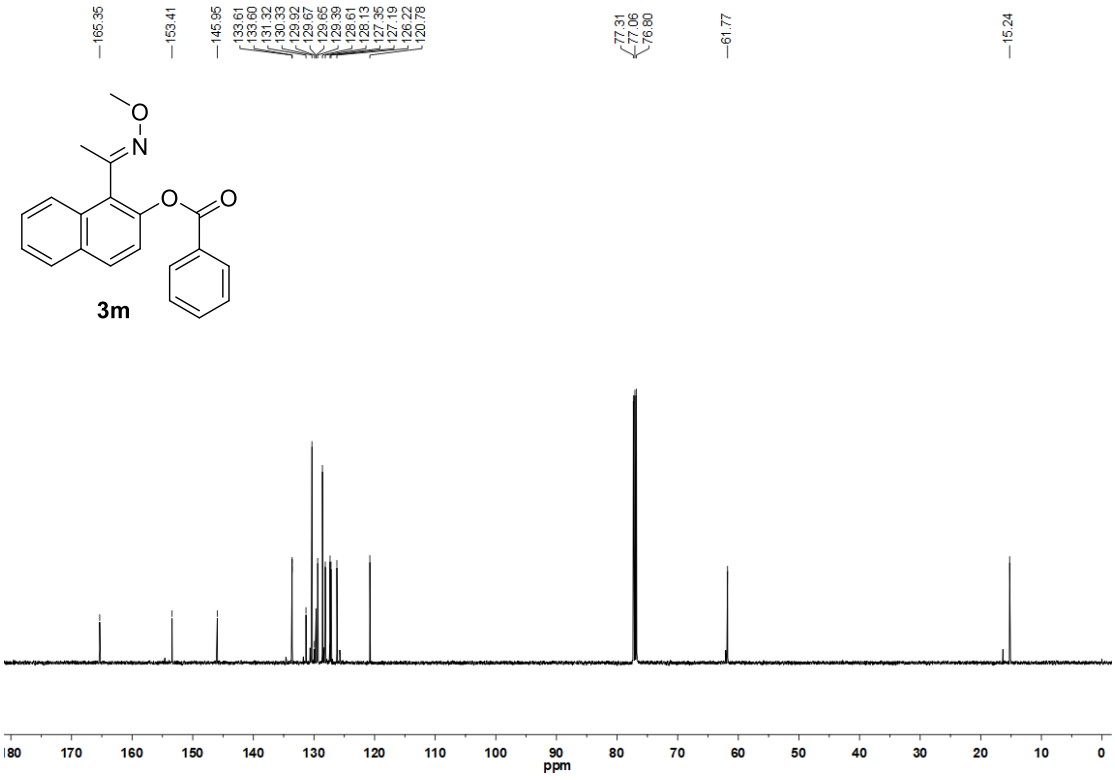
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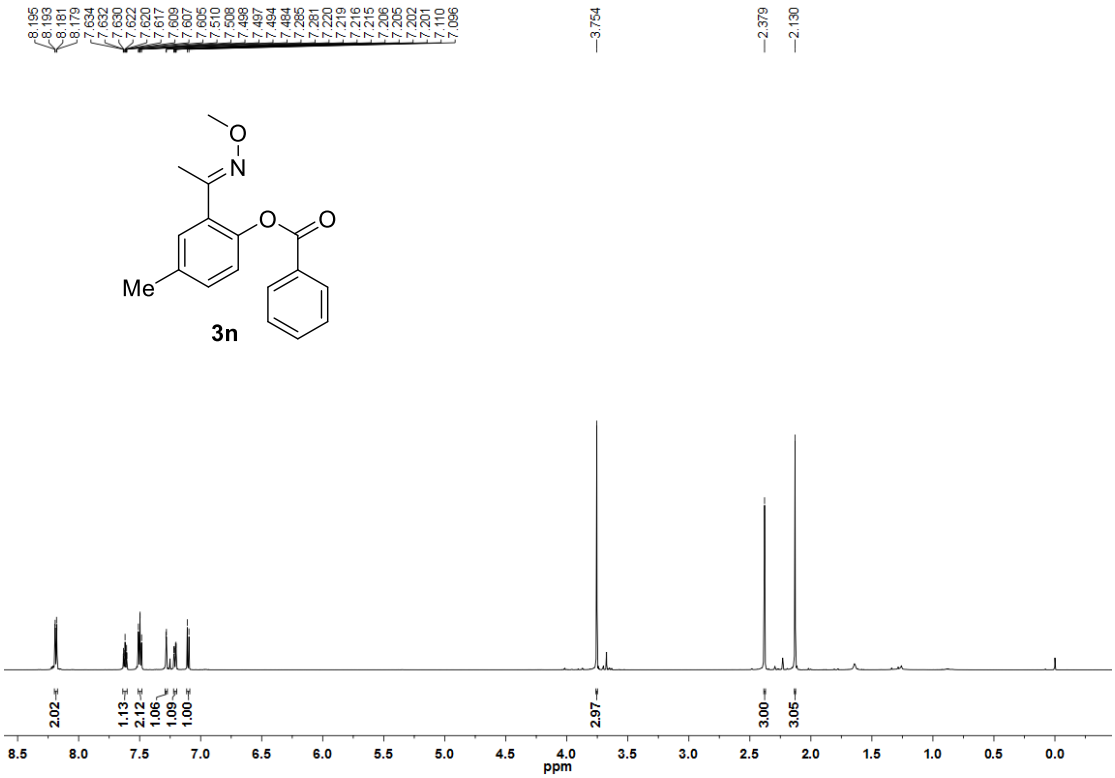
3m
ppm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7.605
7.510
7.508
7.498
7.497
7.494
7.484
7.285
7.281
7.220
7.219
7.216
7.215
7.206
7.205
7.202
7.201
7.110
7.096
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2.130
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N
O
O
Me
3n
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1.13
2.12
1.06
1.09
1.00
2.97
3.00
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7.0
6.5
6.0
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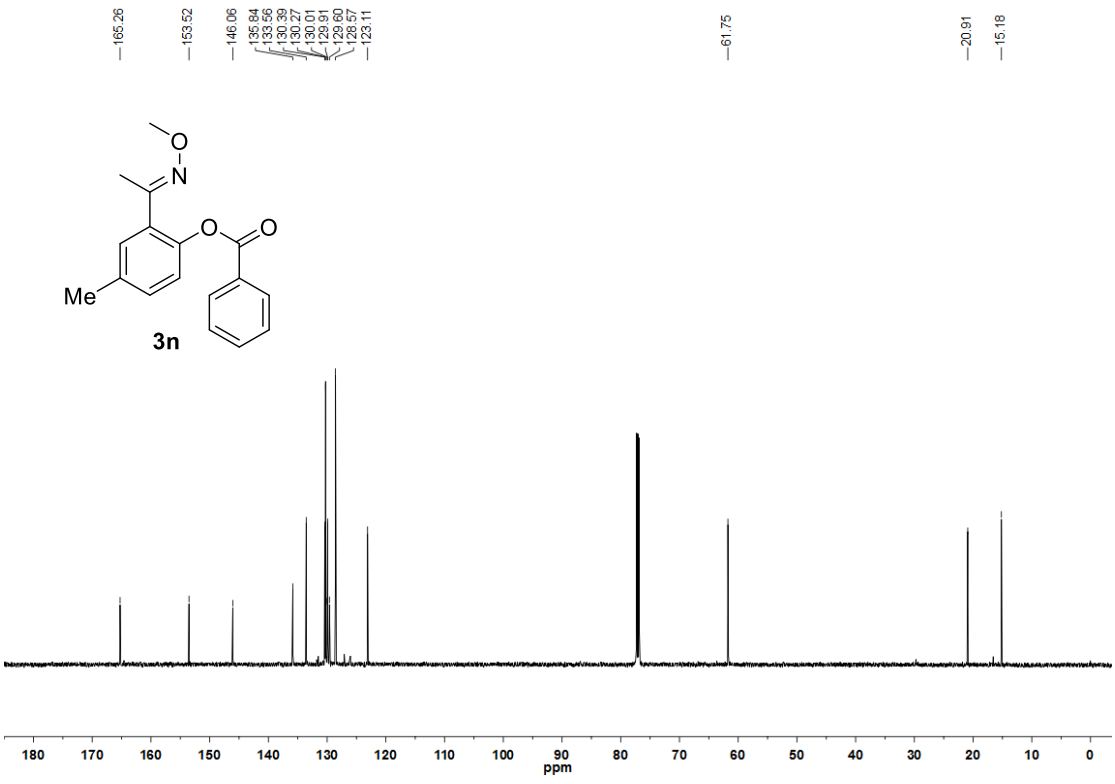
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128.57
123.11
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O
O
Me
3n
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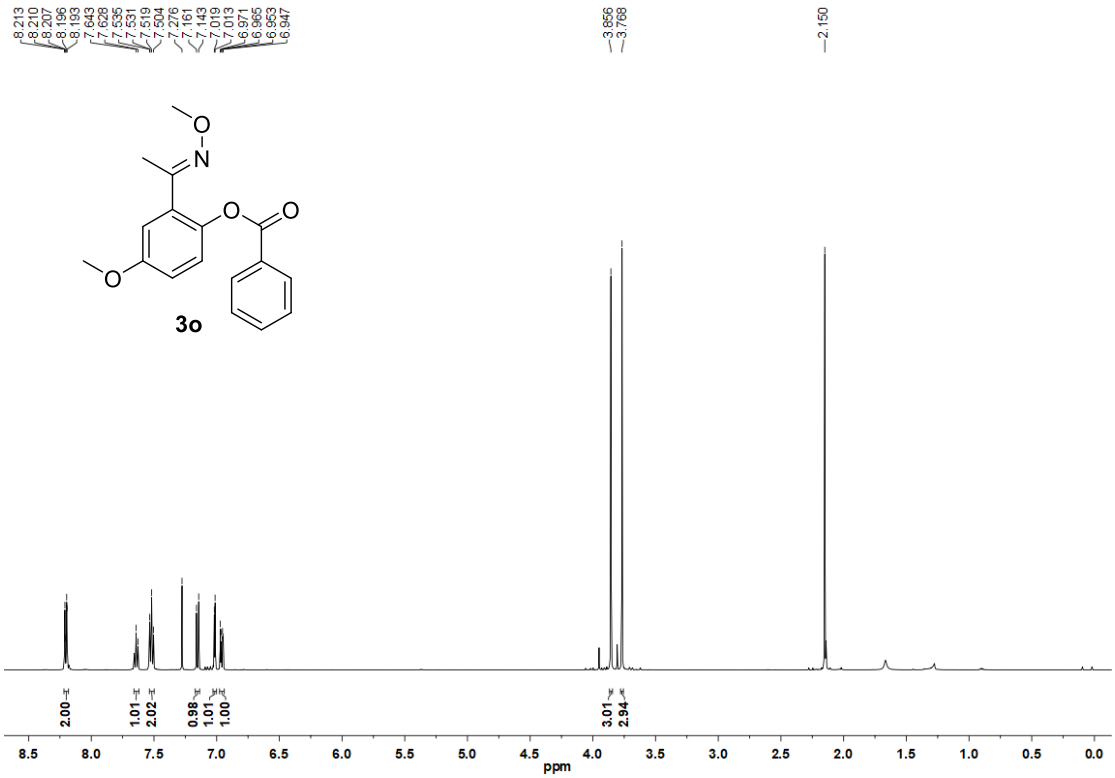
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7.161
7.143
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7.013
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6.953
6.947
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2.02
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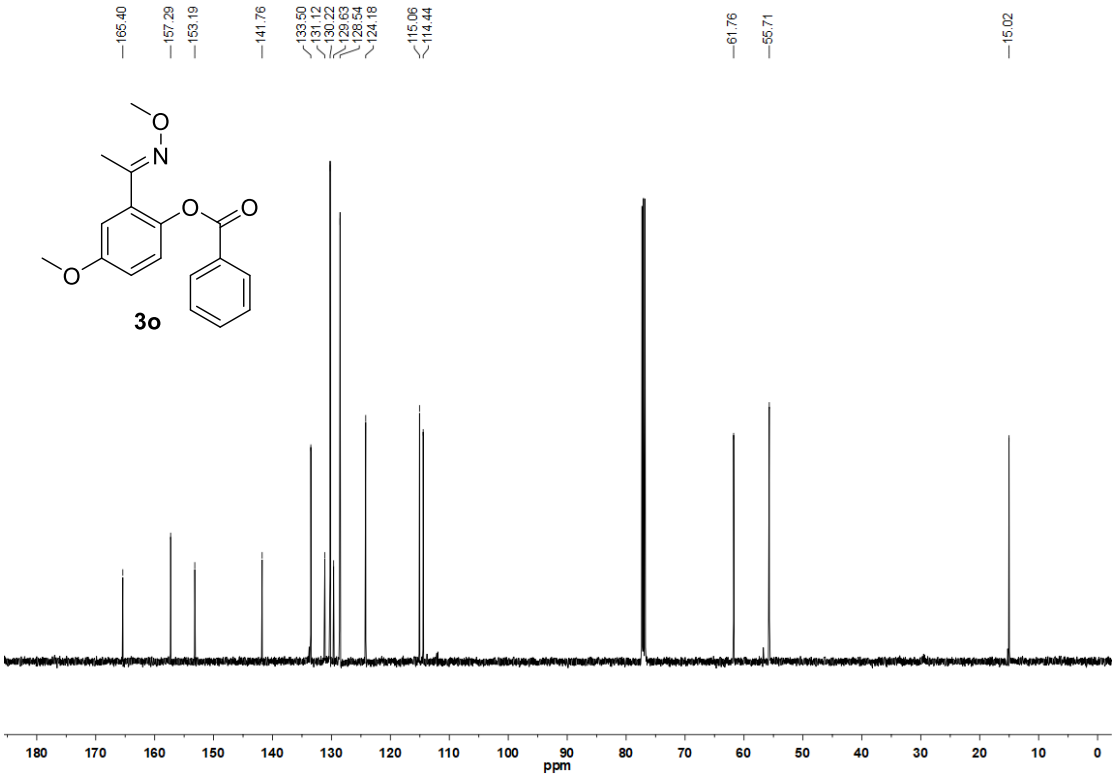
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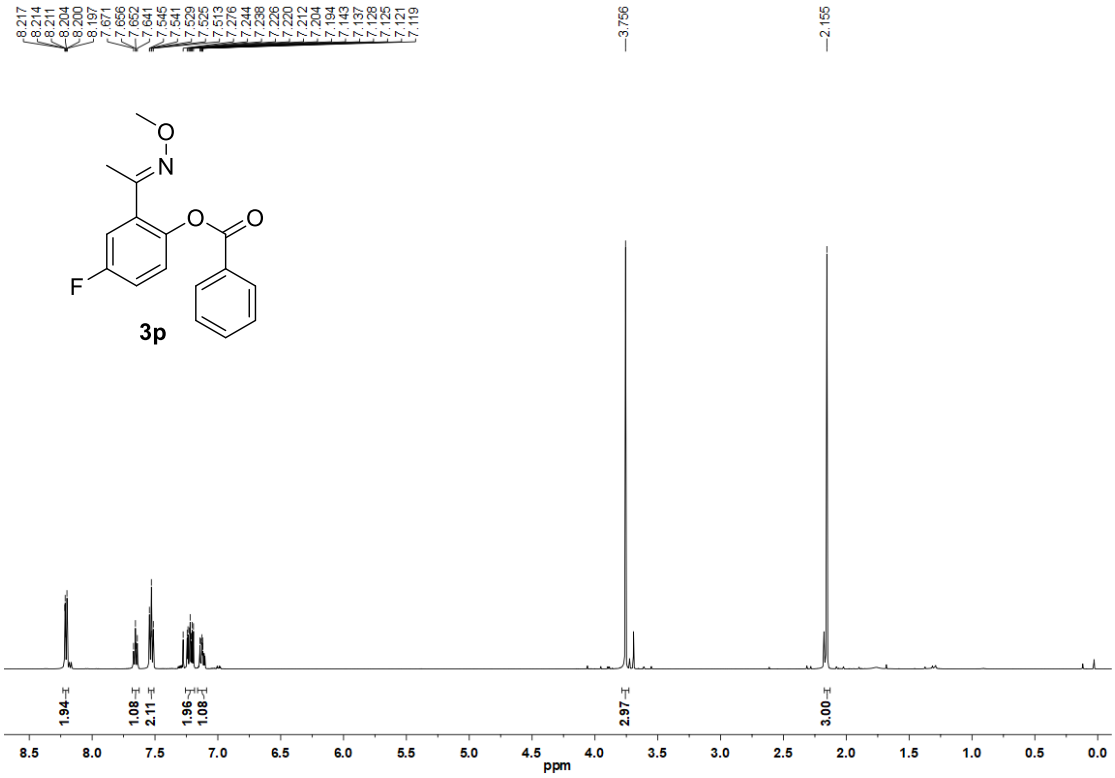
15.02
3o
ppm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7.525
7.513
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F
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1.08
2.97
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7.0
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6.0
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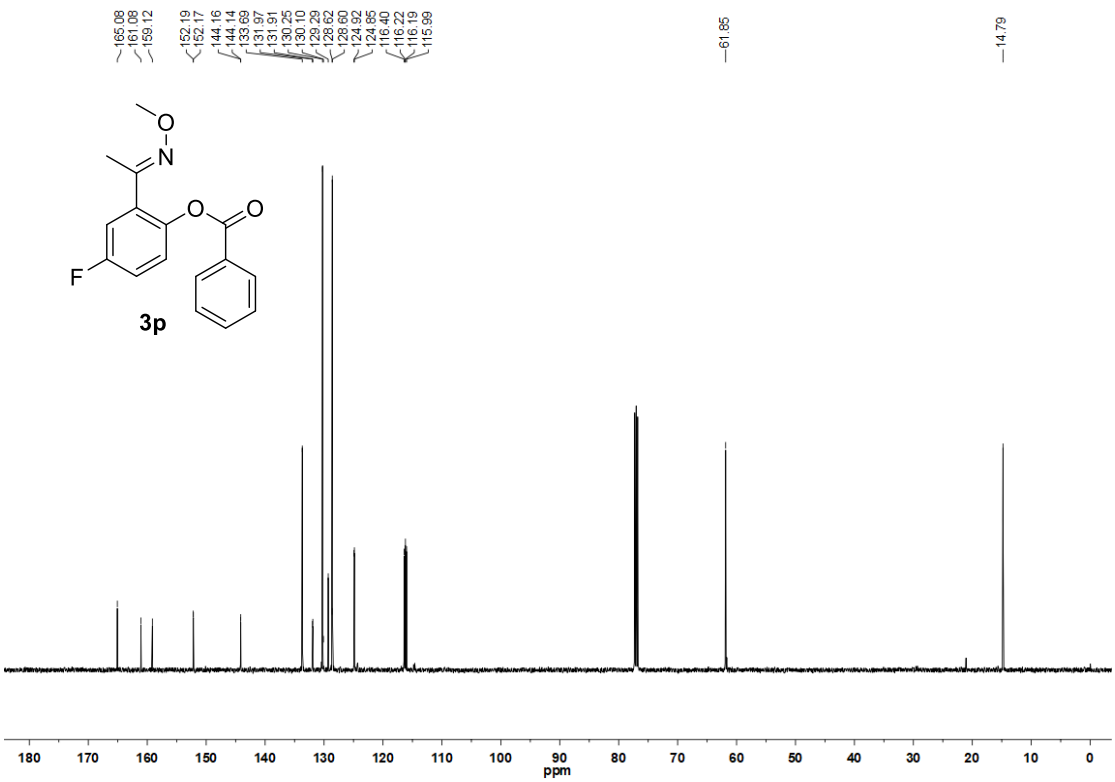
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F
3p
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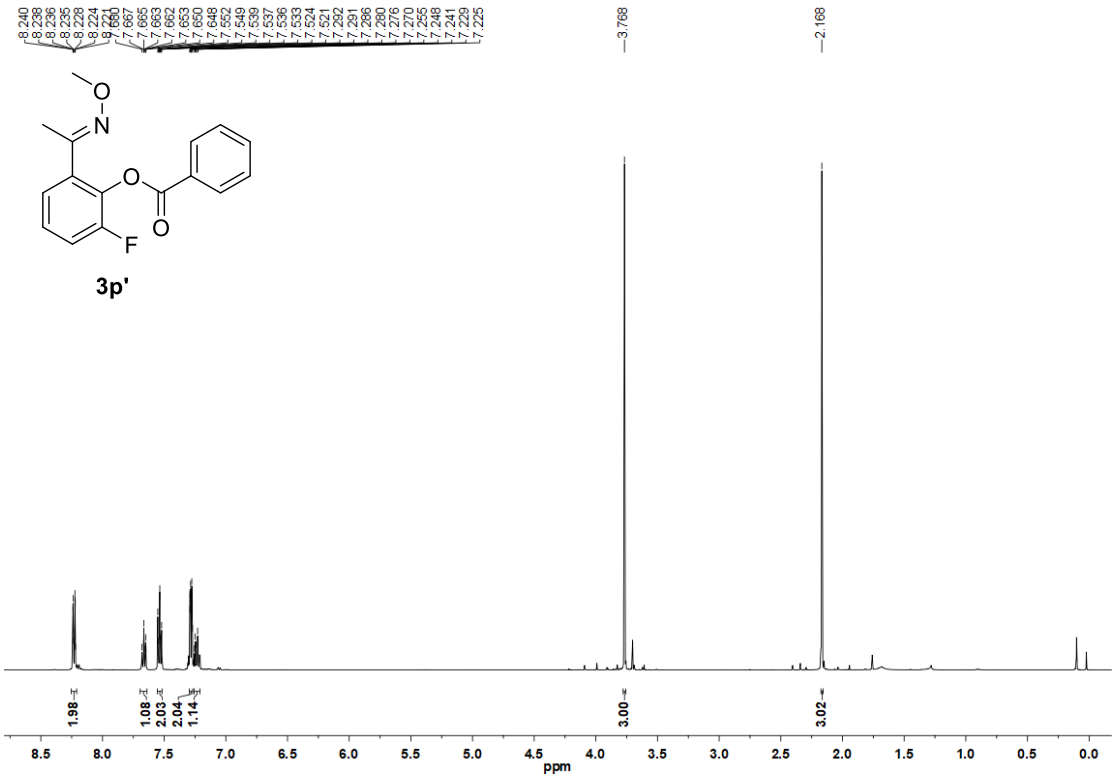
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7.521
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7.241
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7.225
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O
N
O
O
F
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2.04
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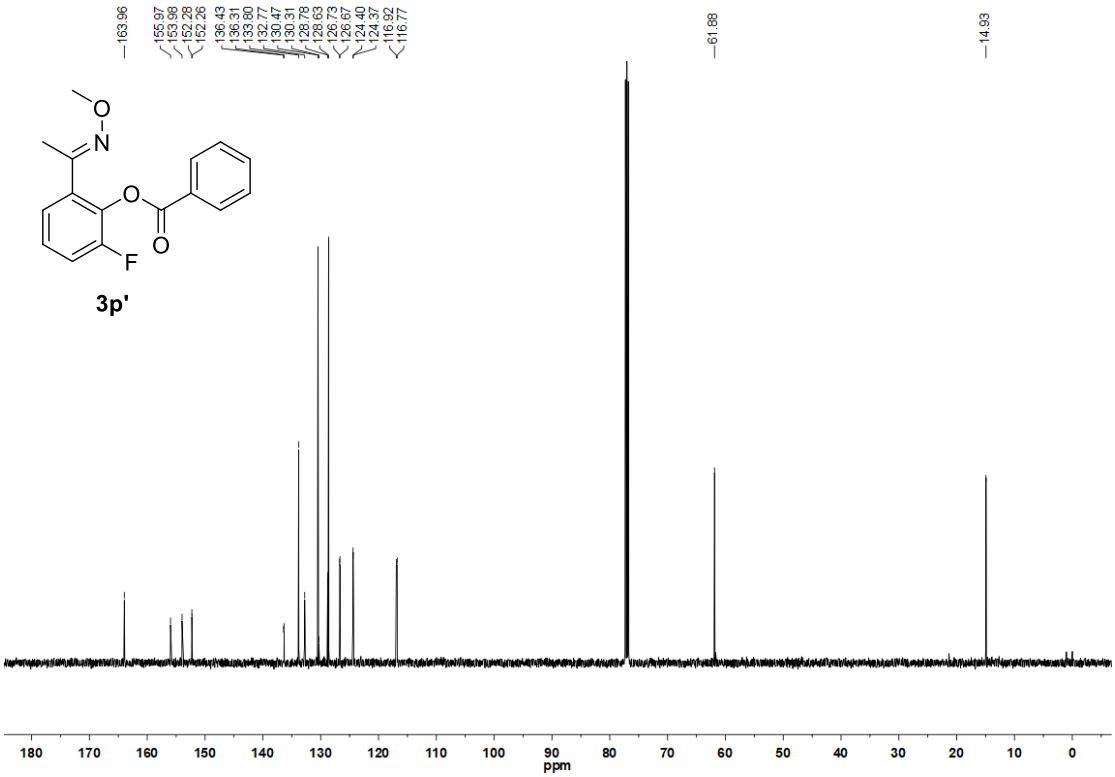
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O
N
O
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F
3p'
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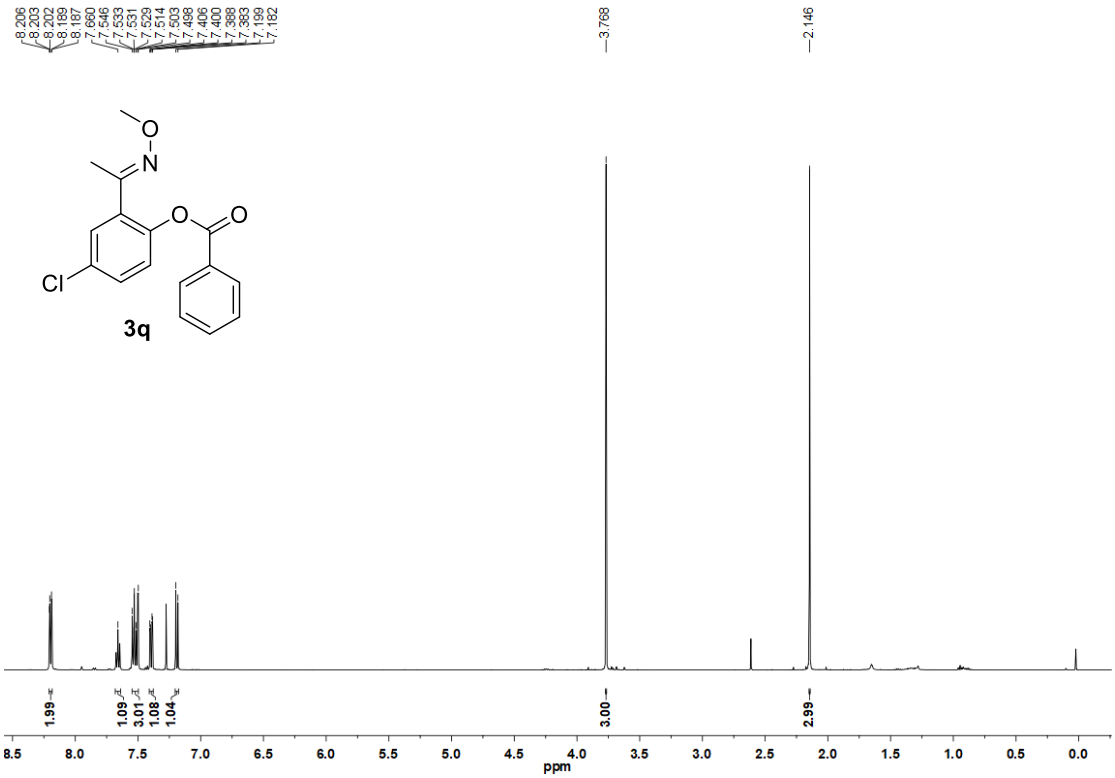
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7.406
7.400
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7.383
7.199
7.182
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2.146
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N
O
O
Cl
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1.09
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1.08
1.04
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2.99
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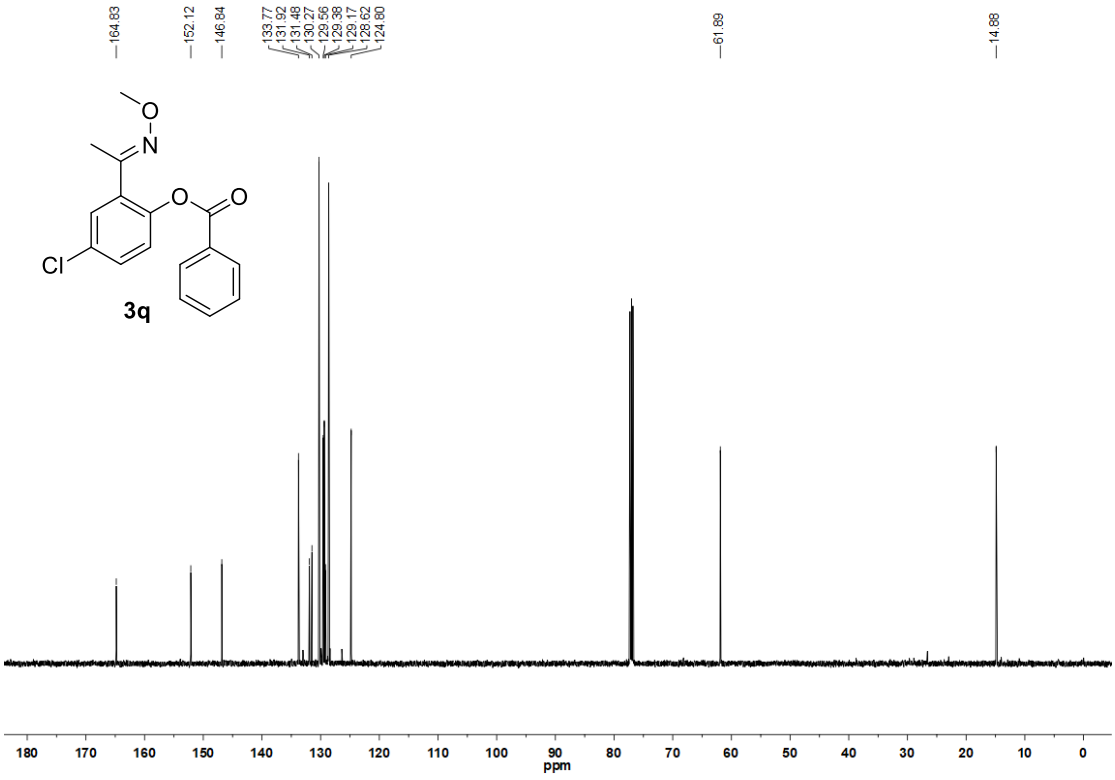
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O
Cl
3q
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ppm


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3.09
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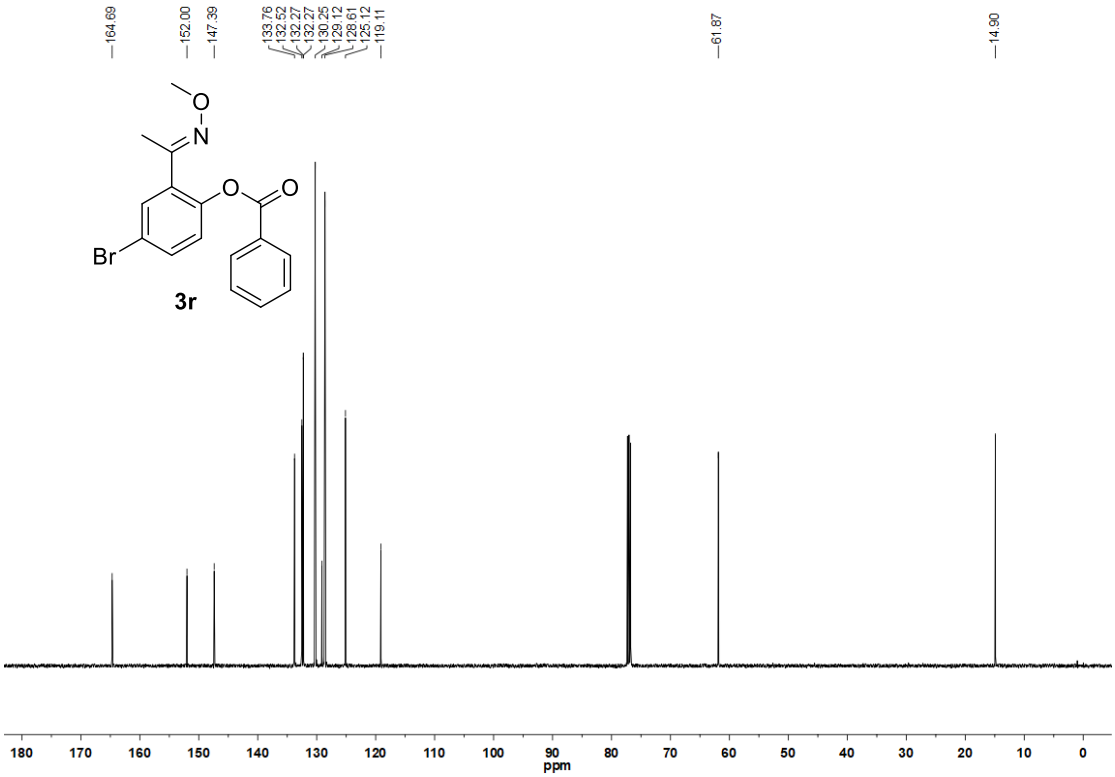
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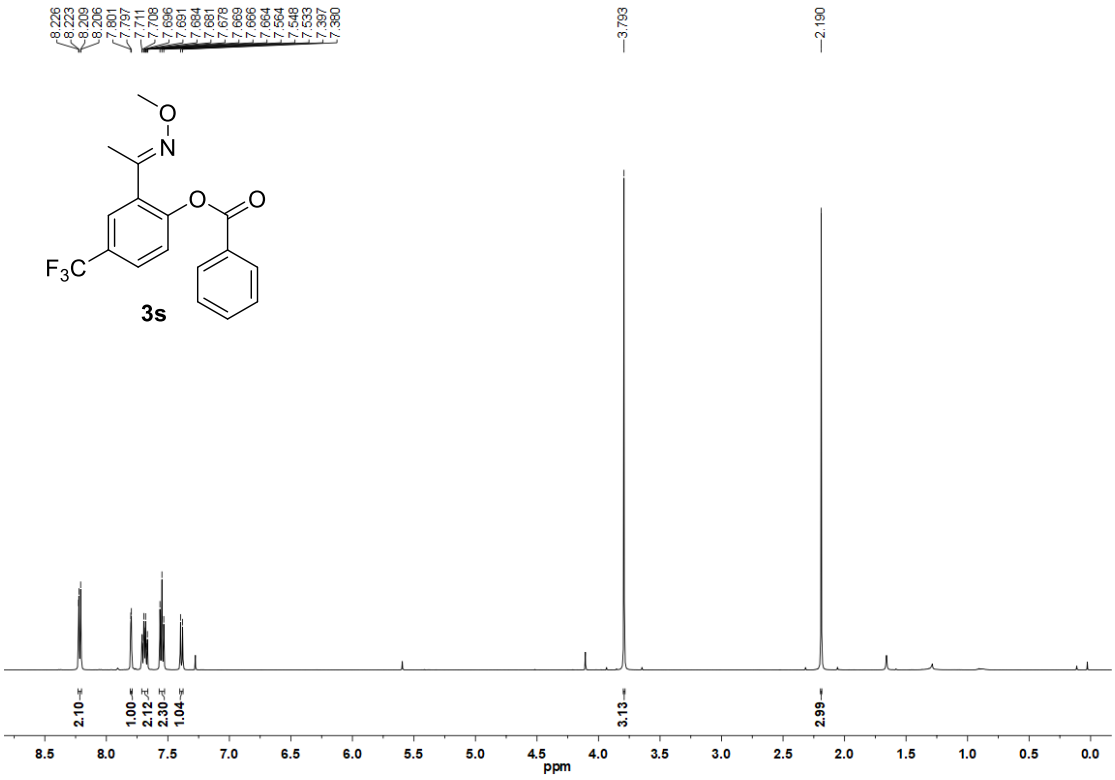
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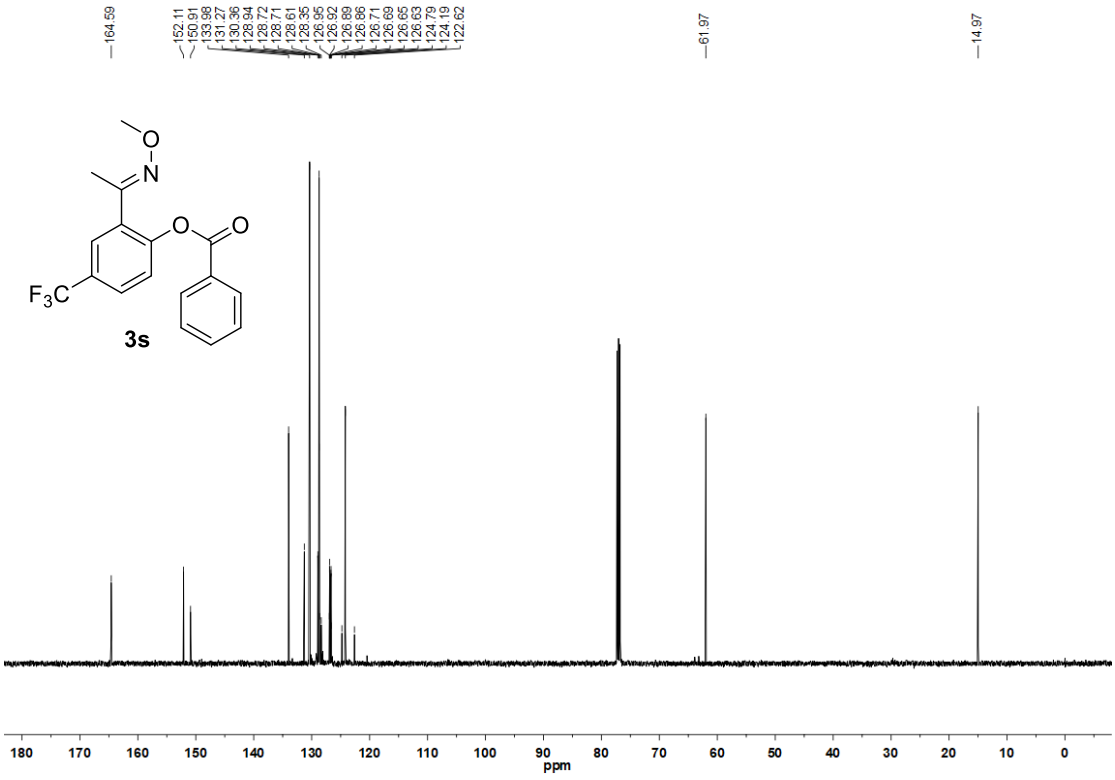
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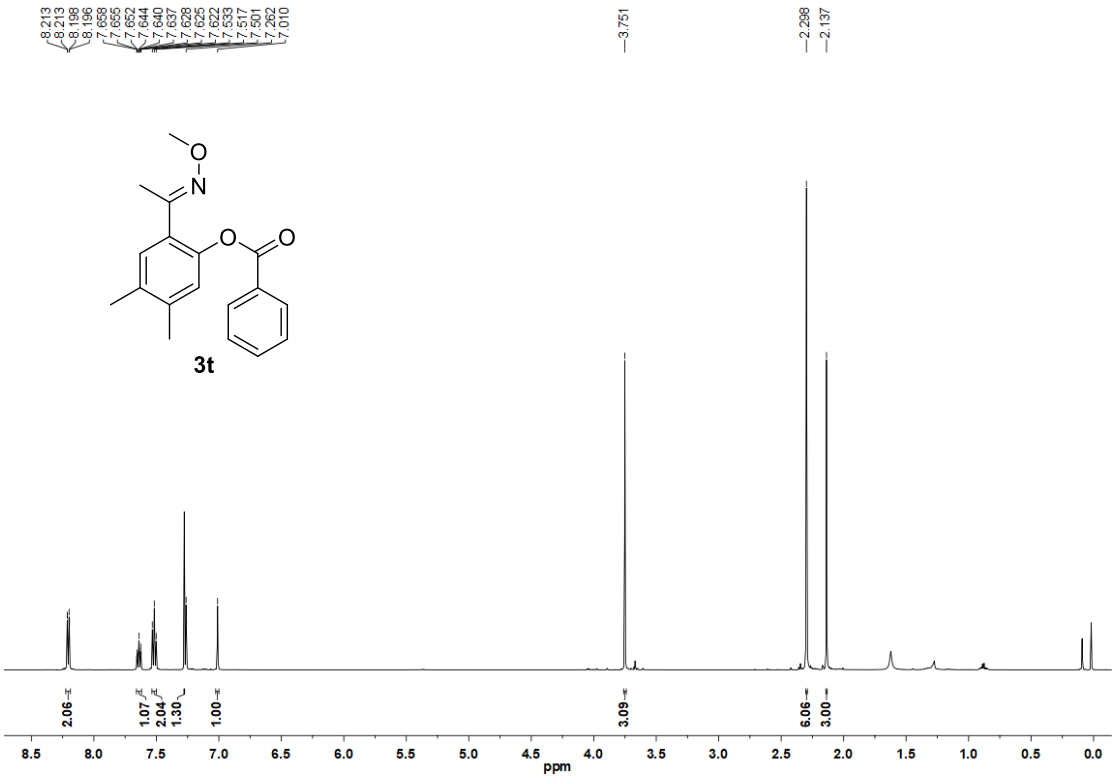
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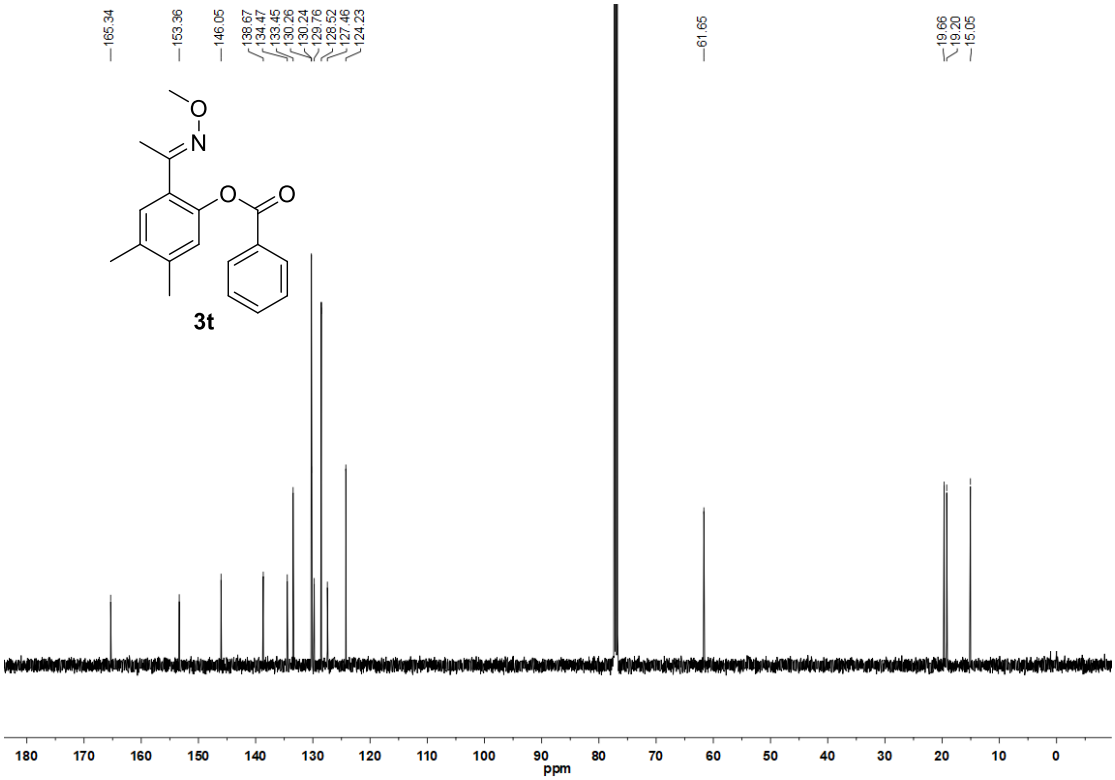
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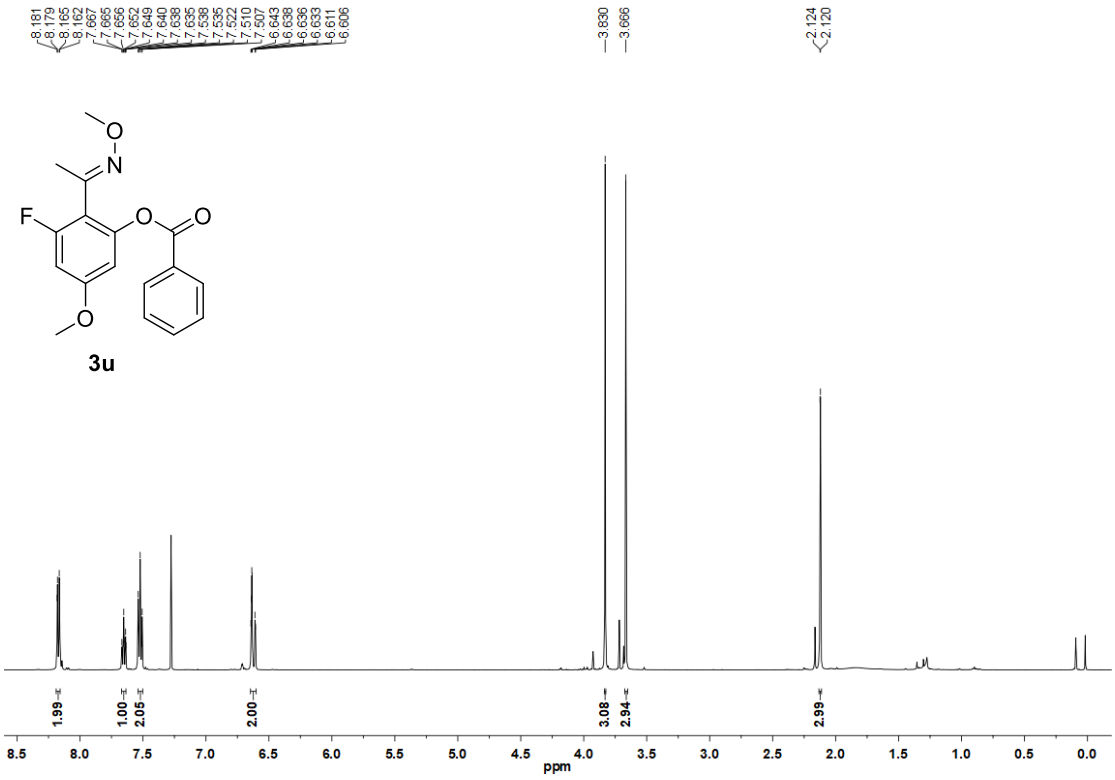
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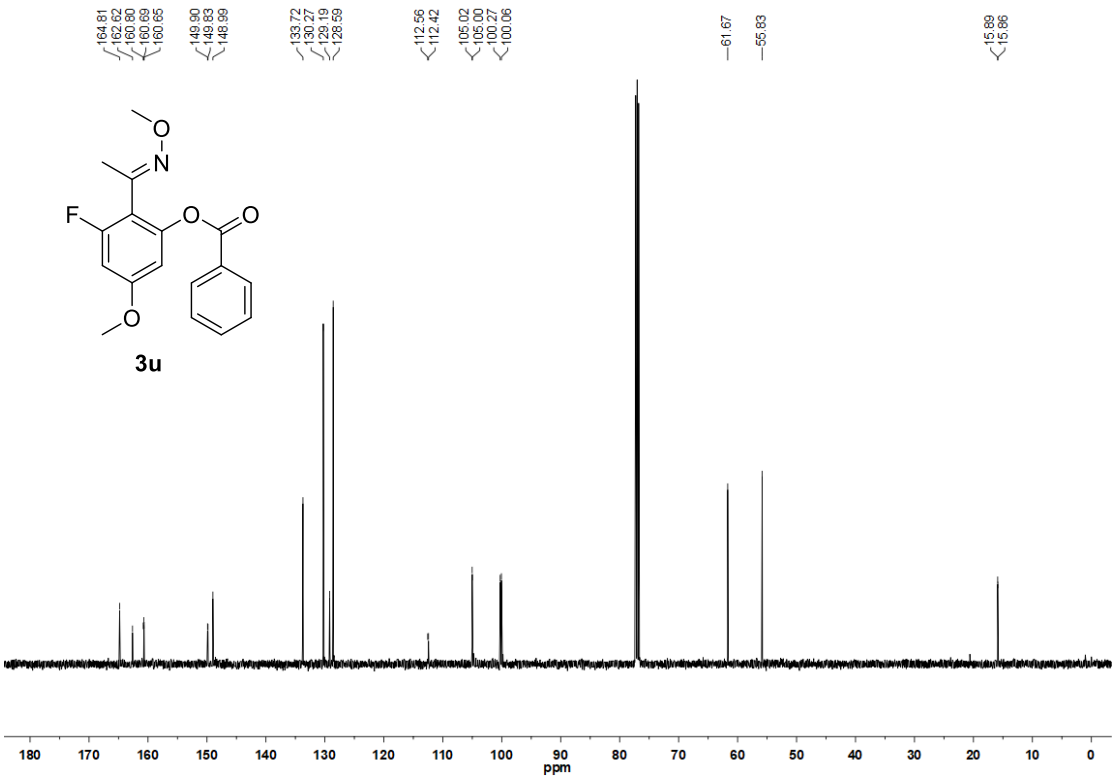
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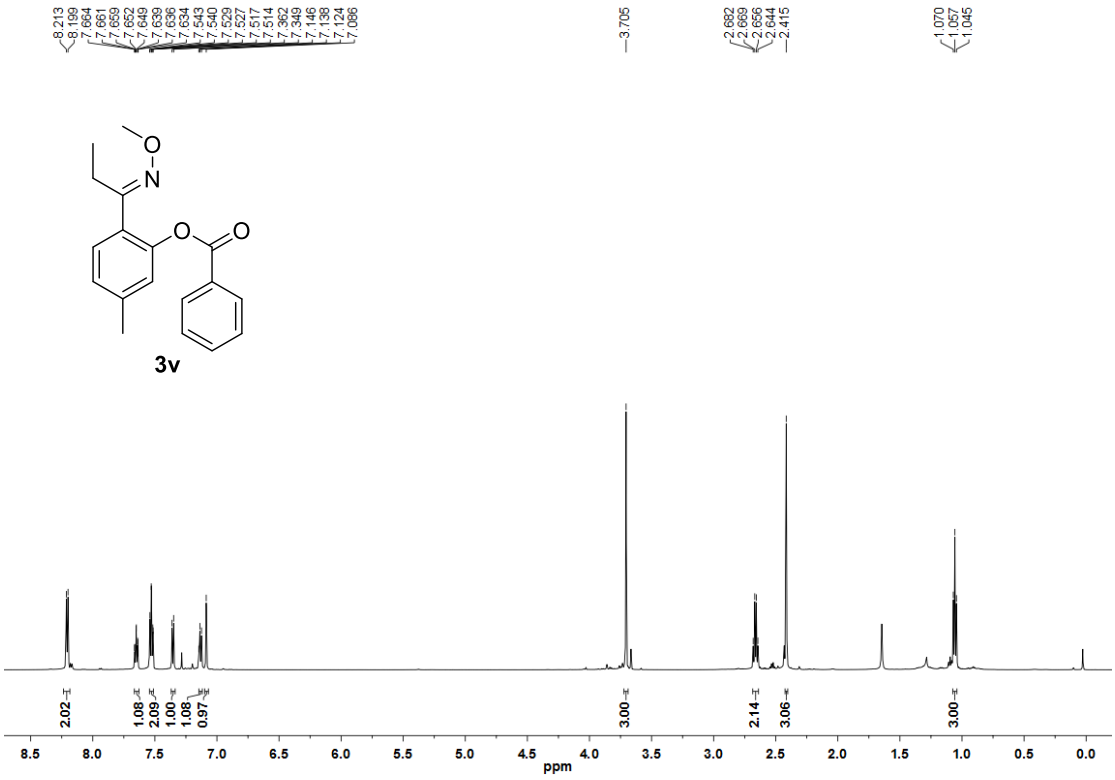
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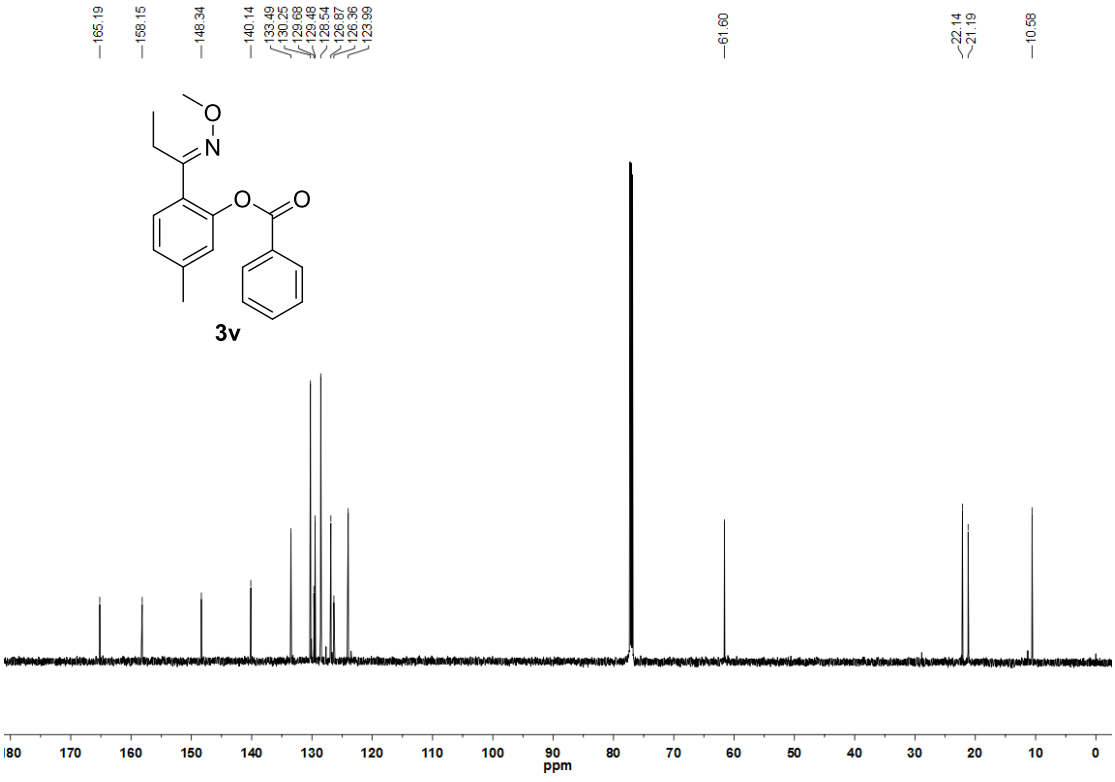
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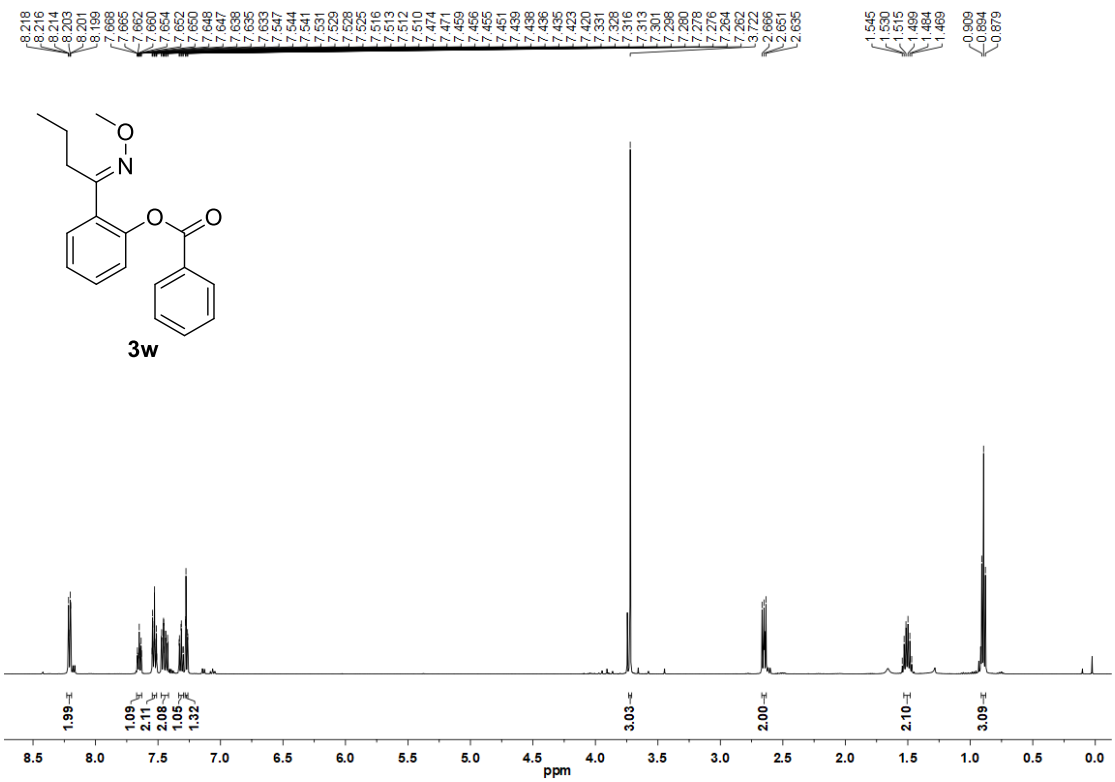
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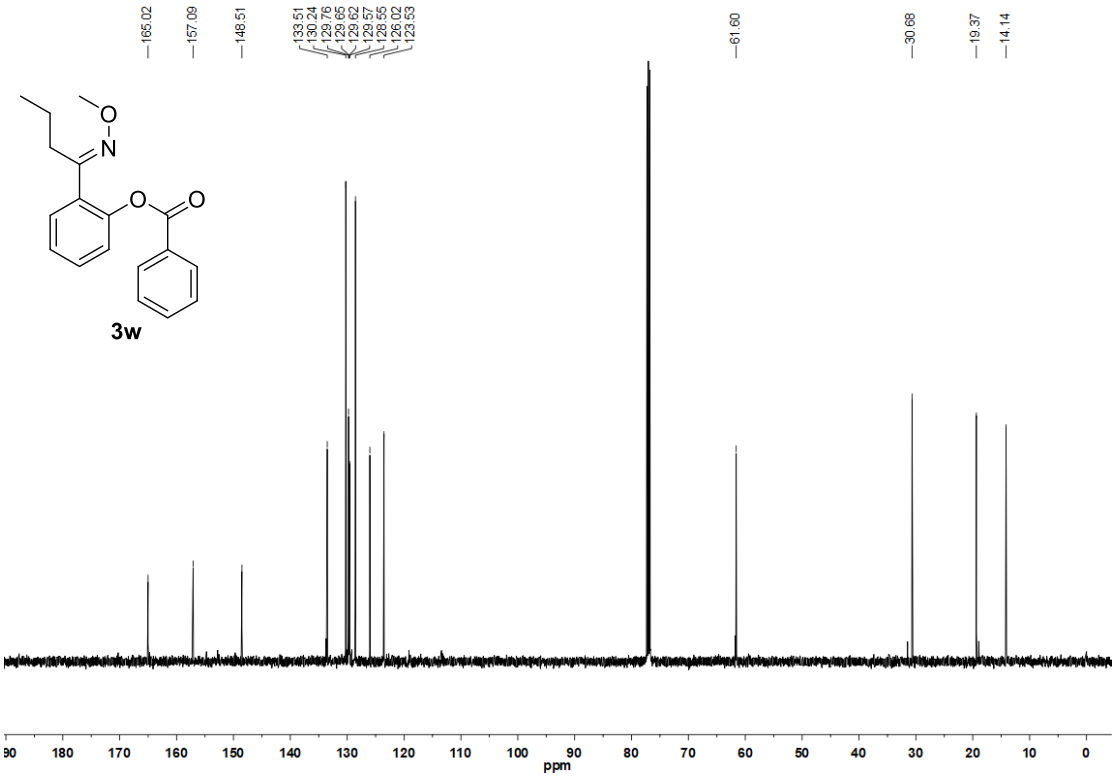
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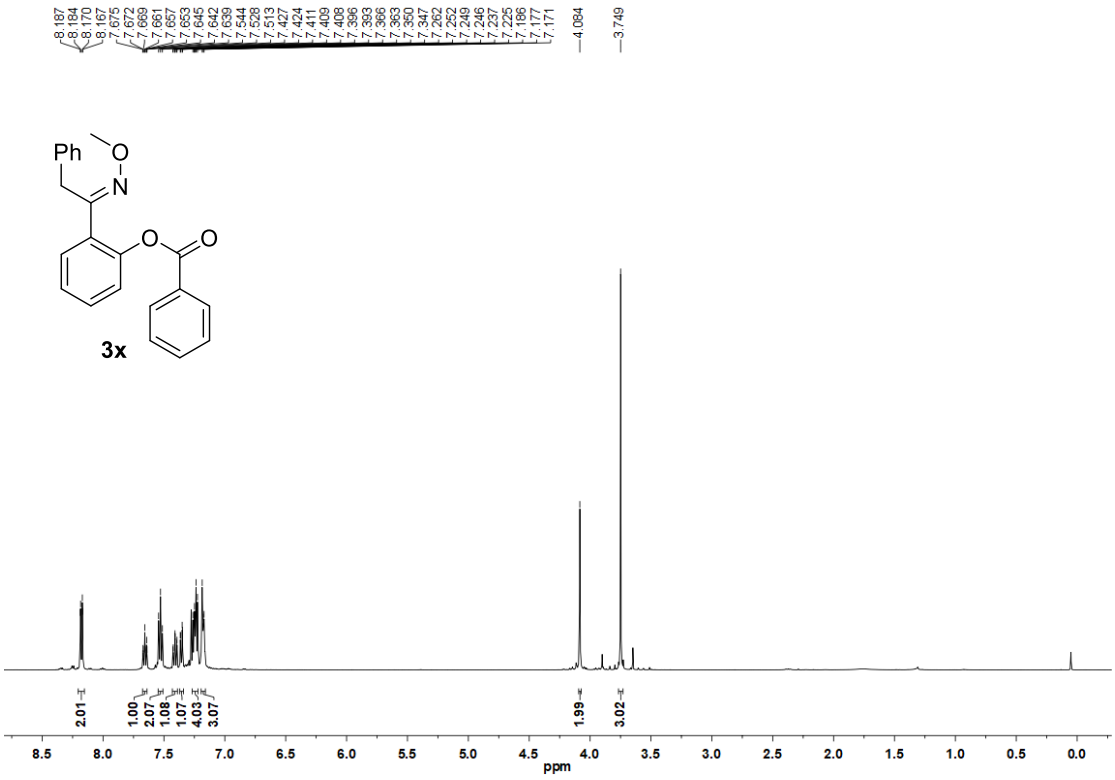
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7.408
7.396
7.393
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7.252
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7.177
7.171
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Ph
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N
O
O
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1.00
2.07
1.08
1.07
4.03
3.07
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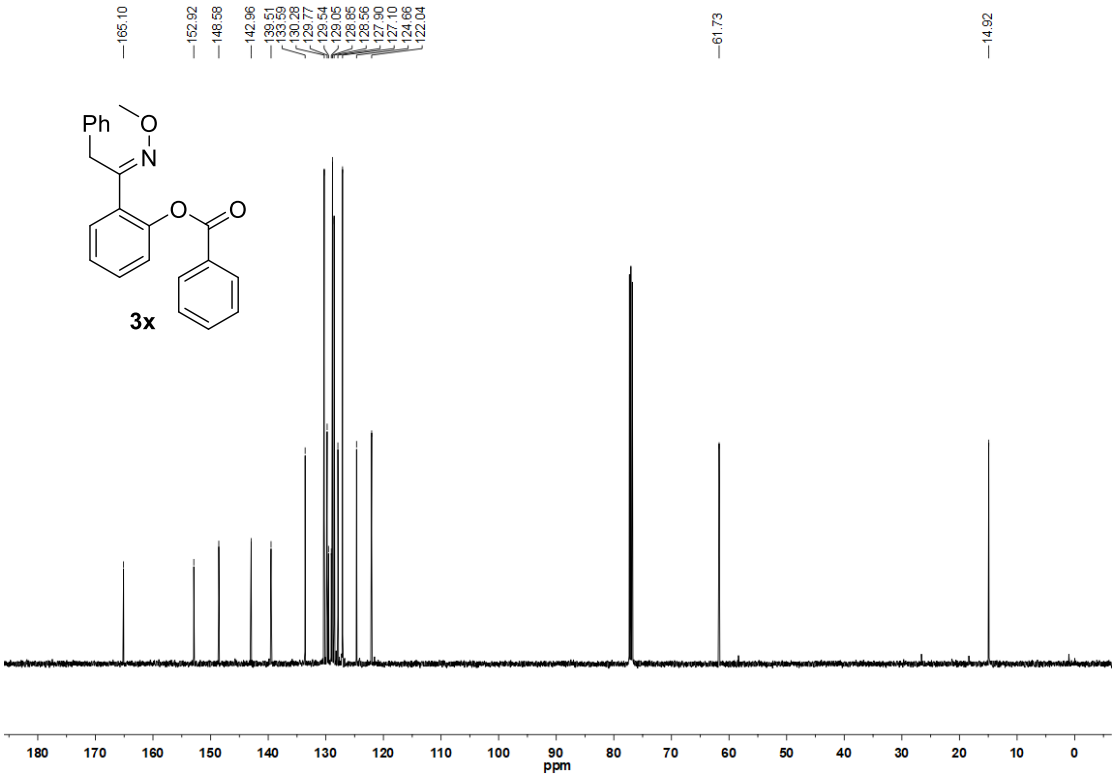
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128.56
127.90
127.10
124.66
122.04
61.73
14.92
Ph
O
N
O
O
3x
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130
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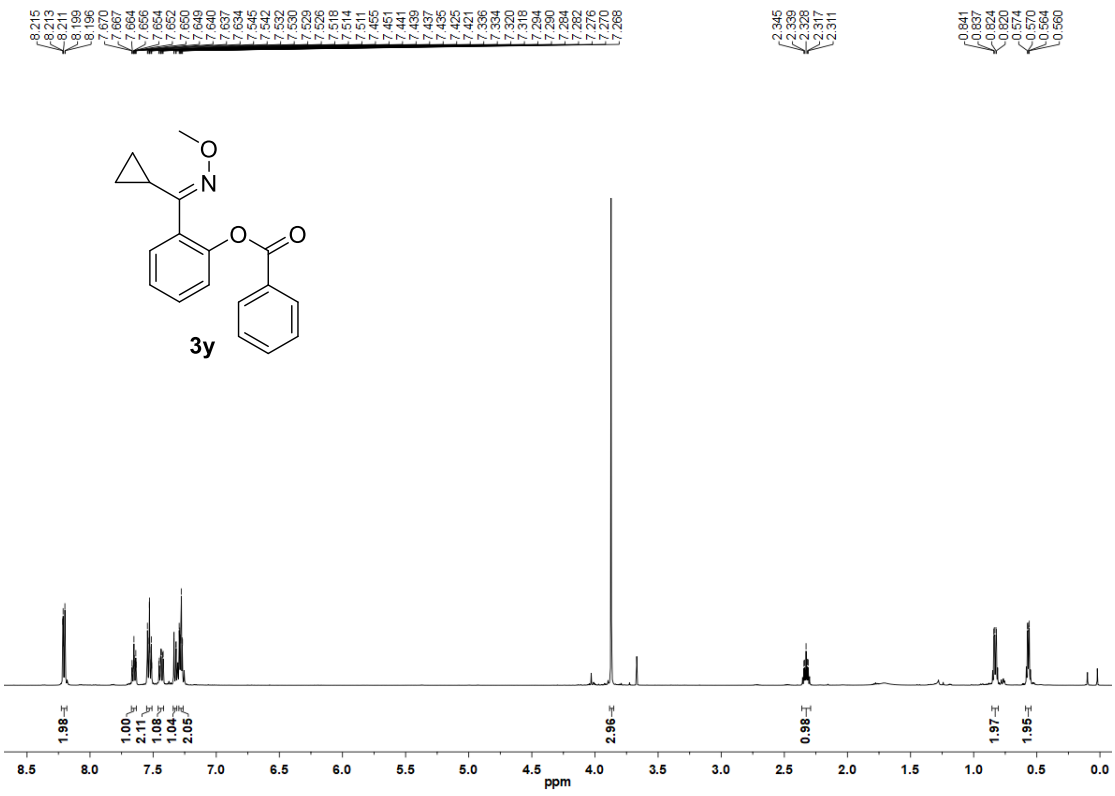
ppm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7.282
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0.564
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O
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O
O
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1.04
2.05
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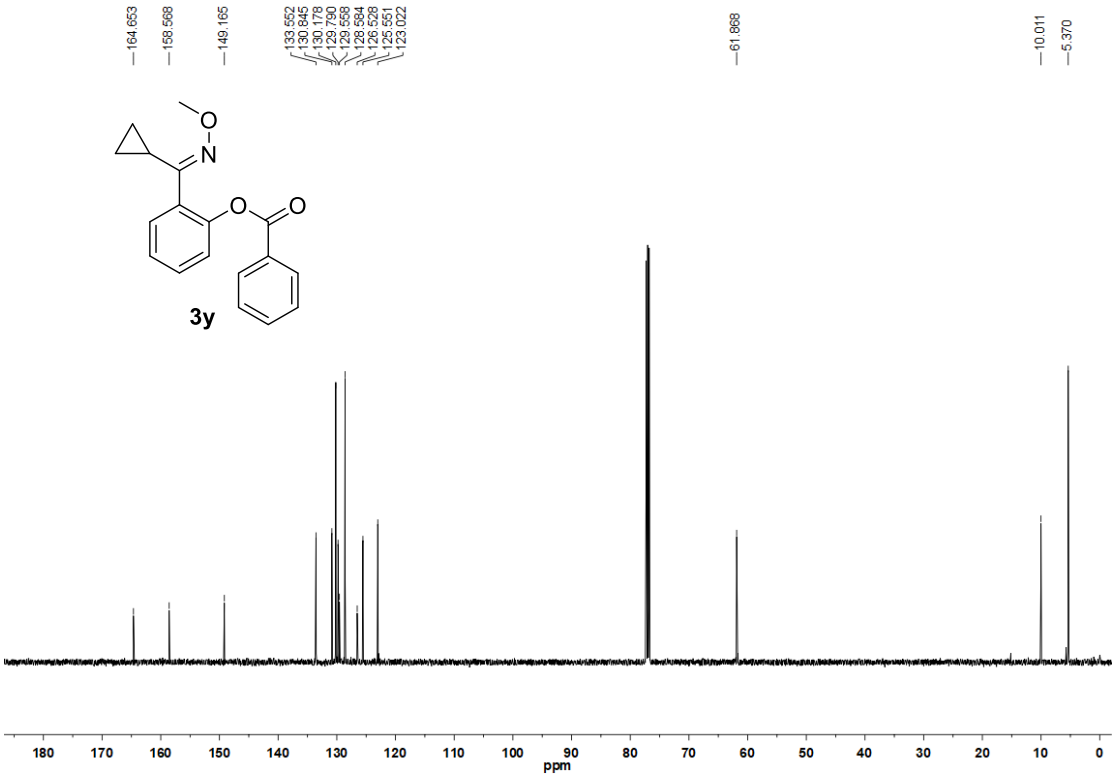
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O
N
O
O
3y
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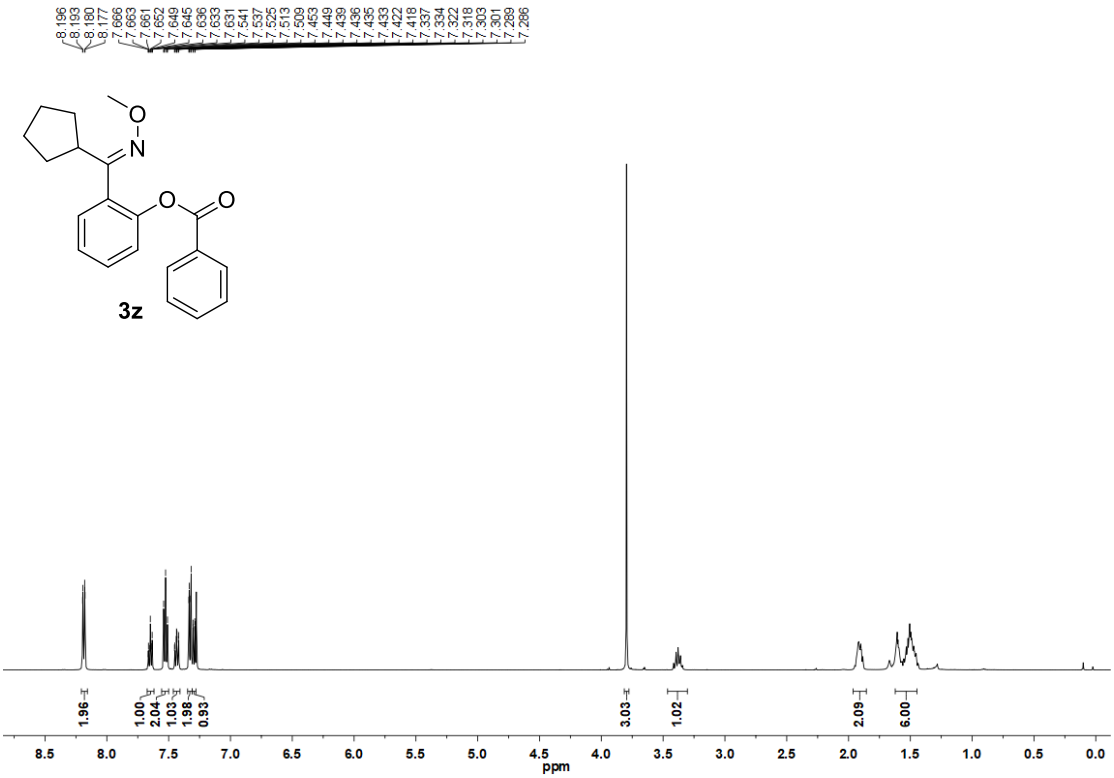
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7.525
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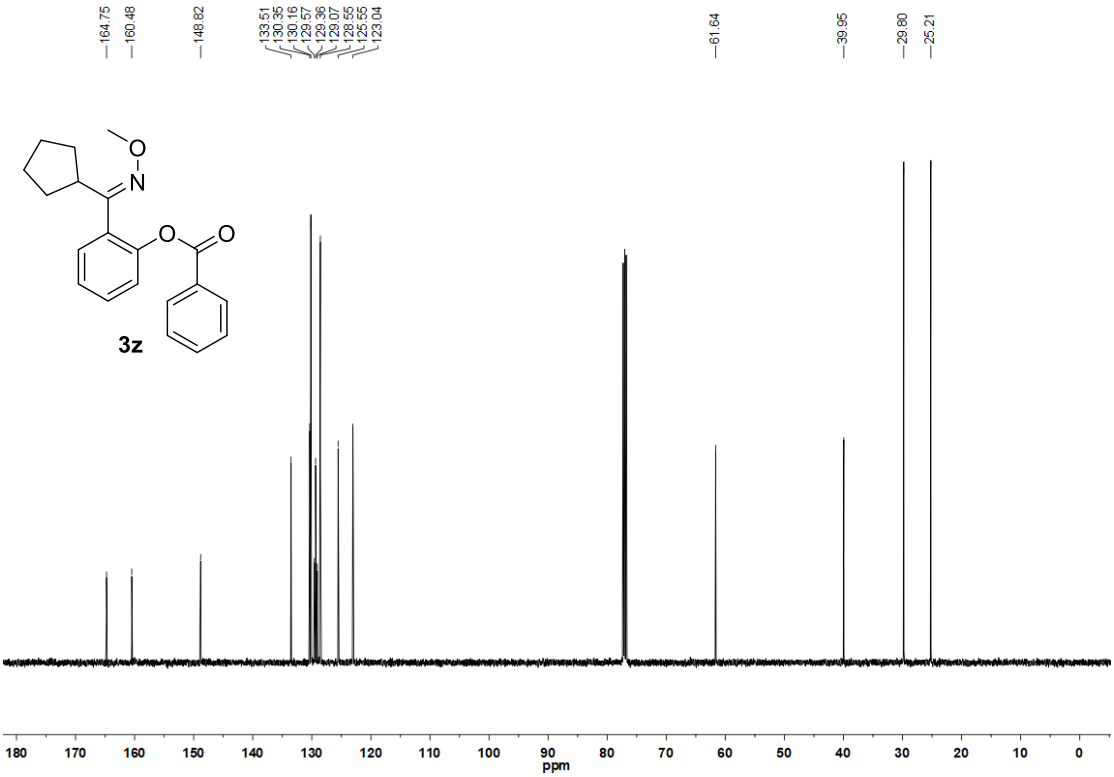
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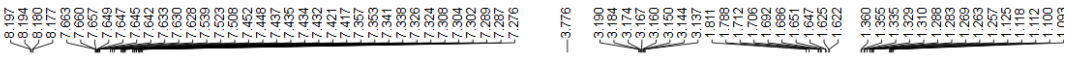
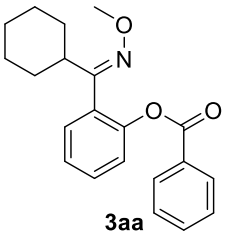
ppm





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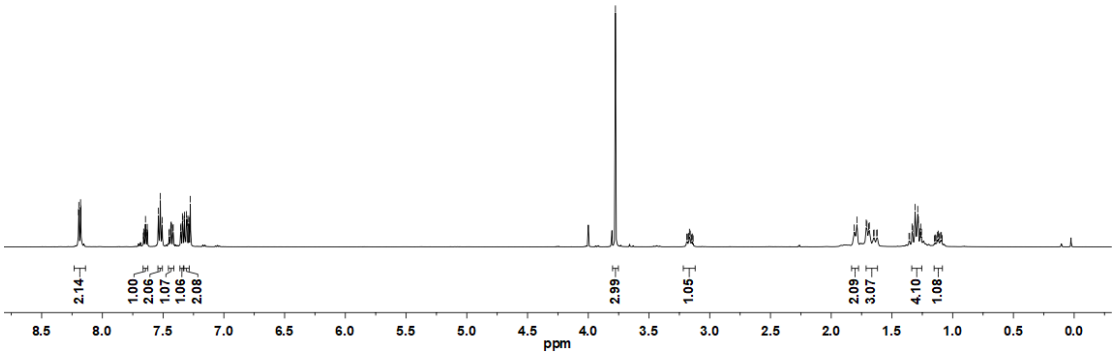

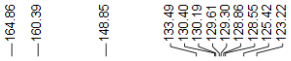

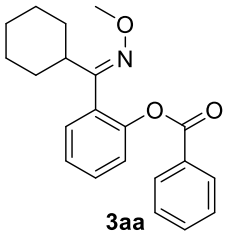

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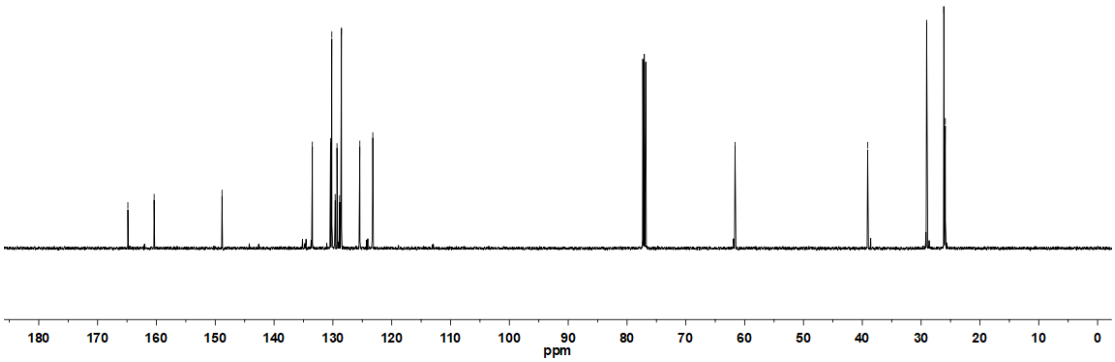

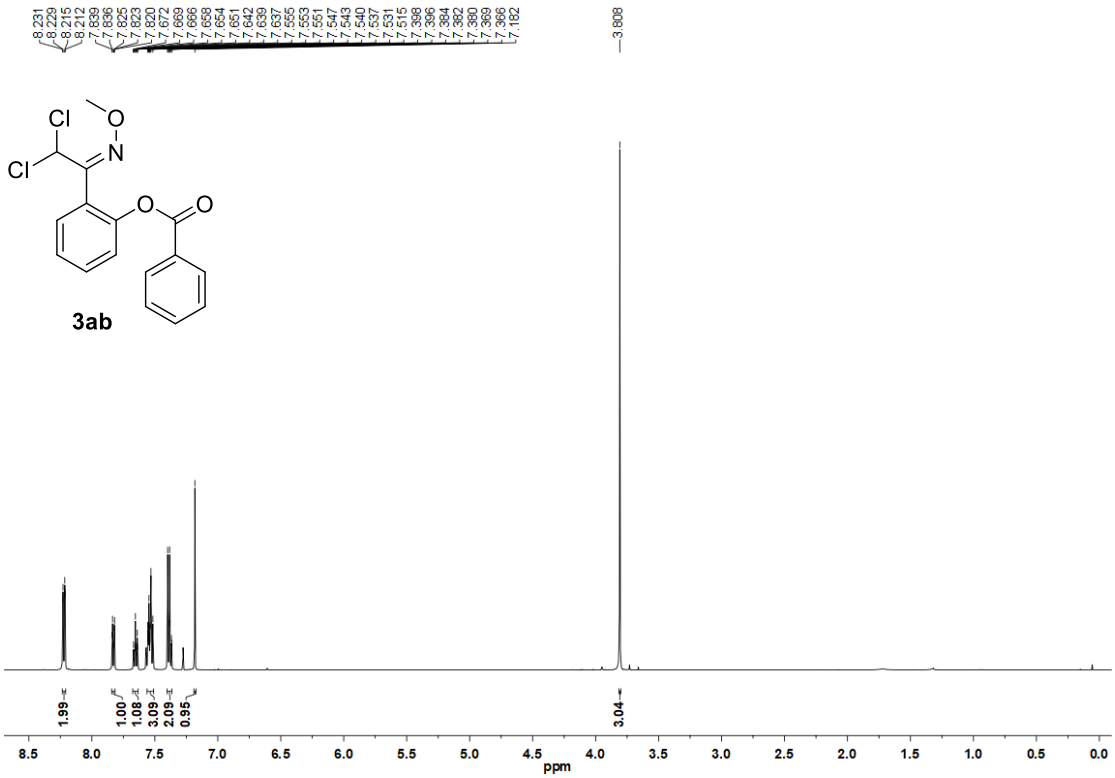
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1.00
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2.09
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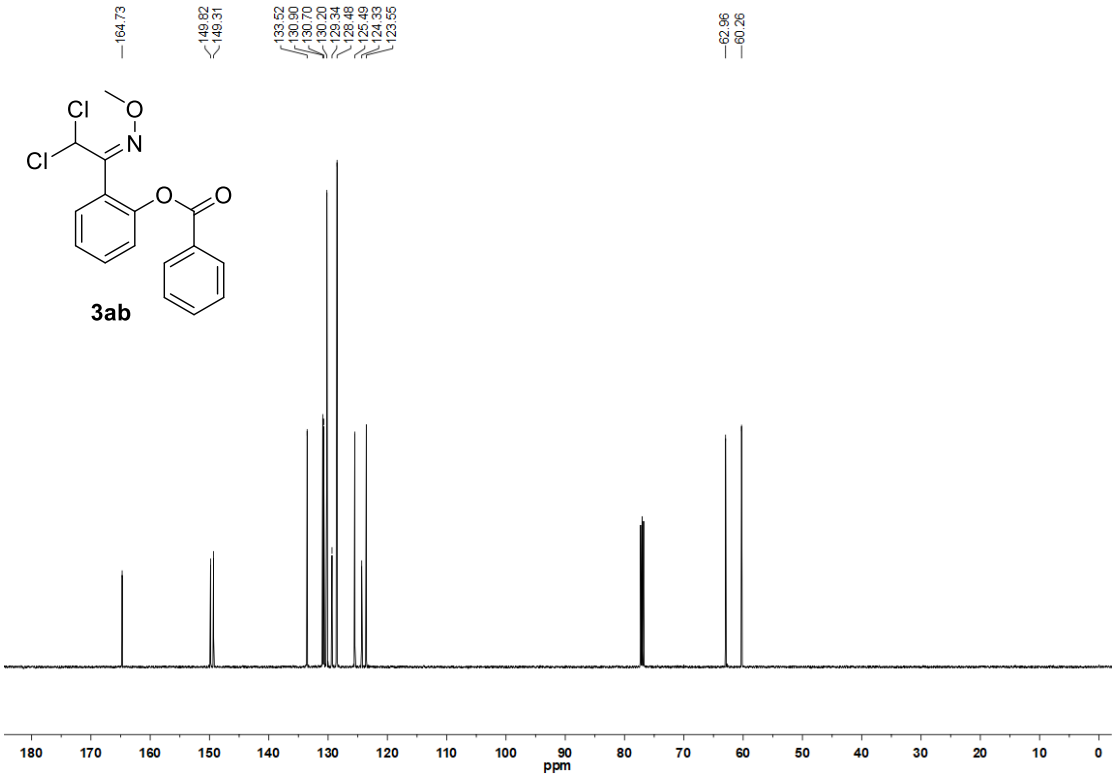
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Cl
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O
3ab
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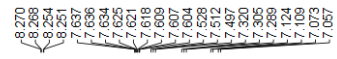
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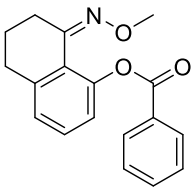
1.801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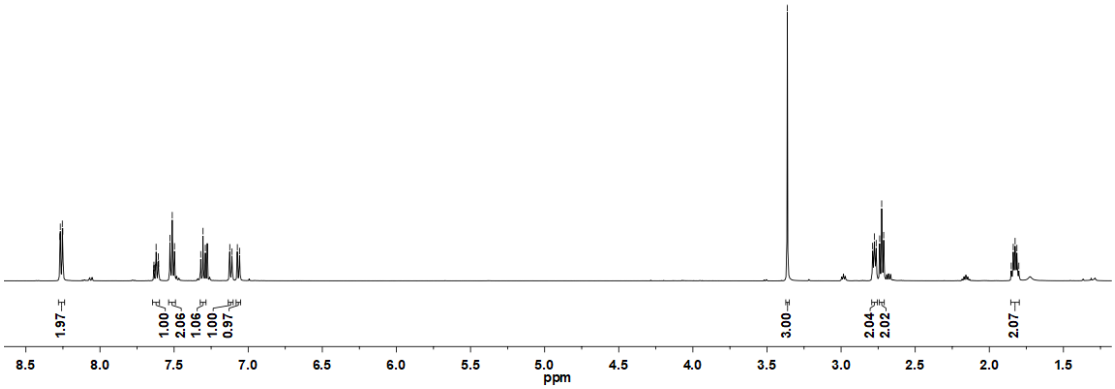
O

3ac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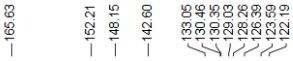
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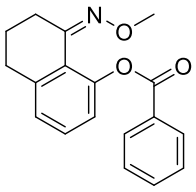
20.98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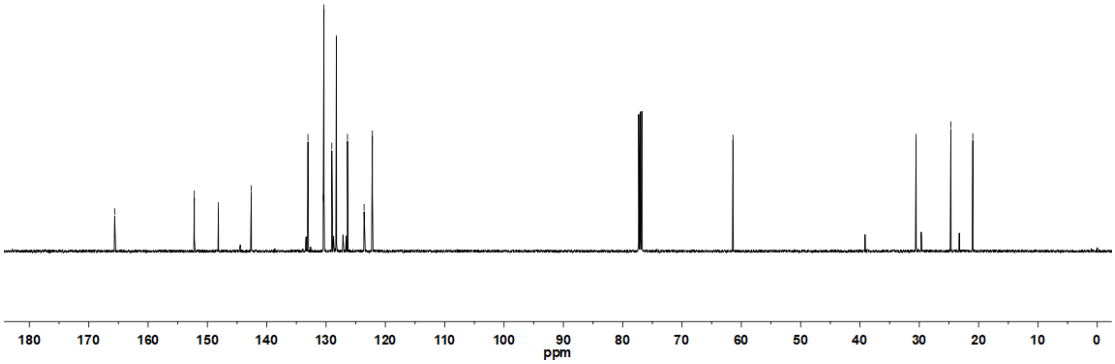
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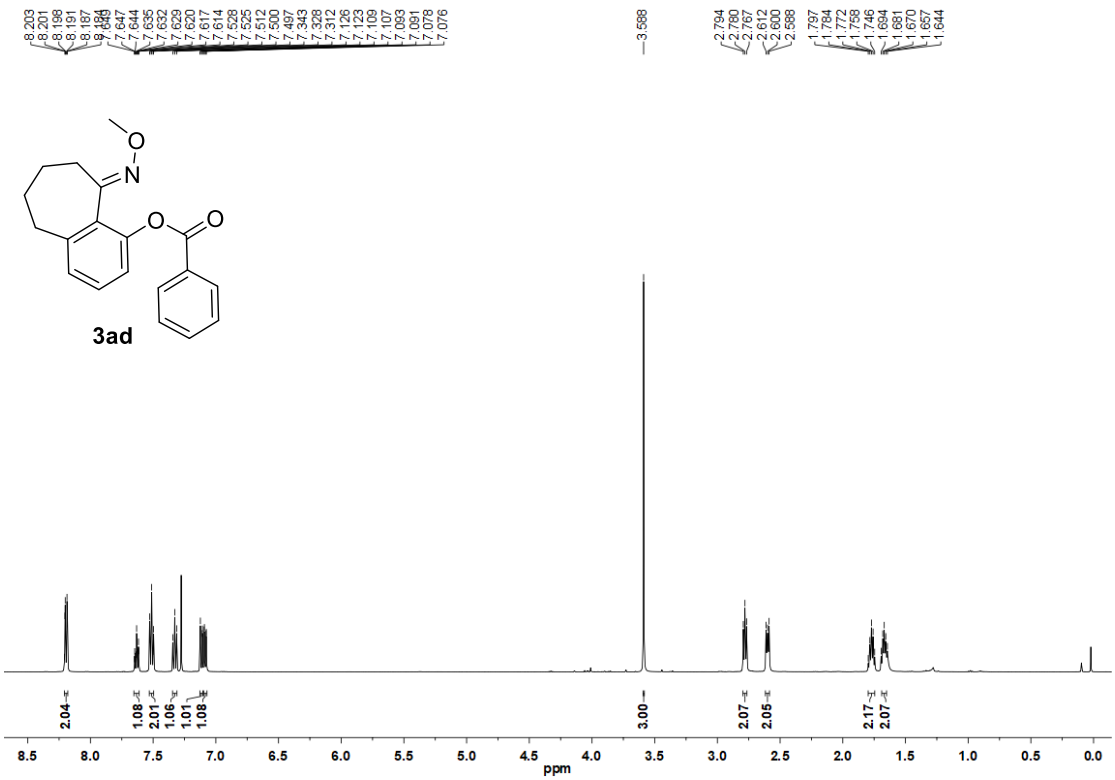
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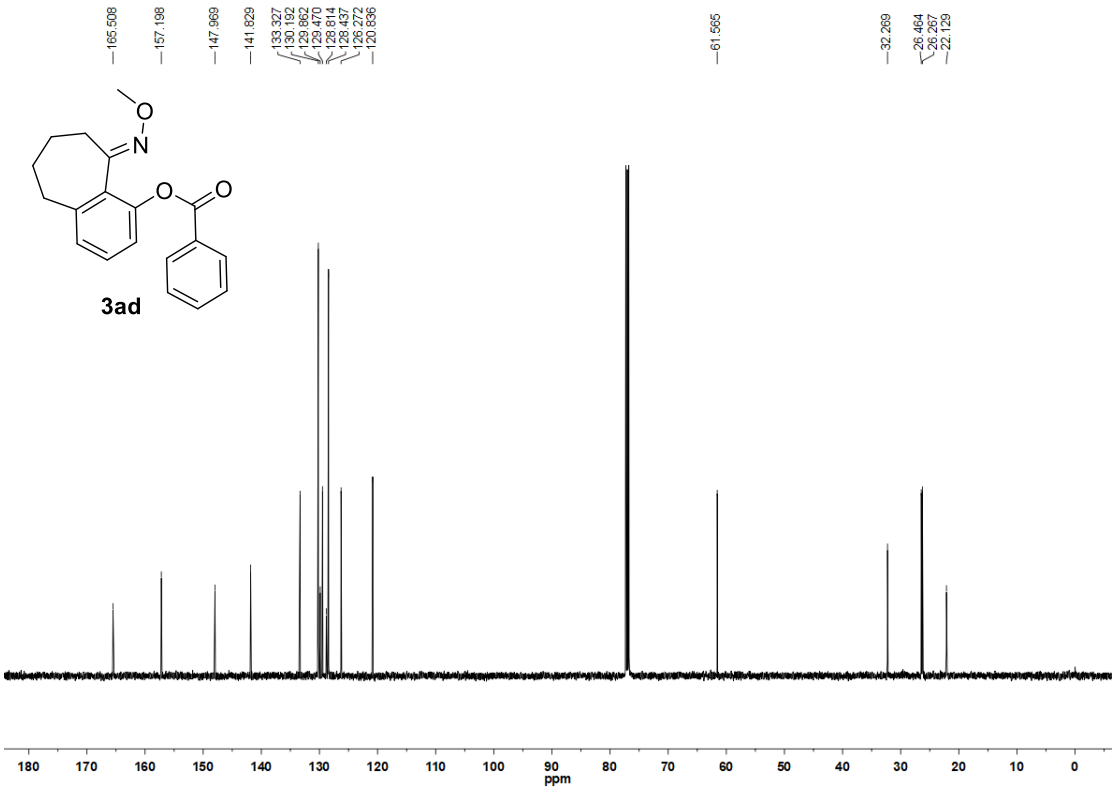
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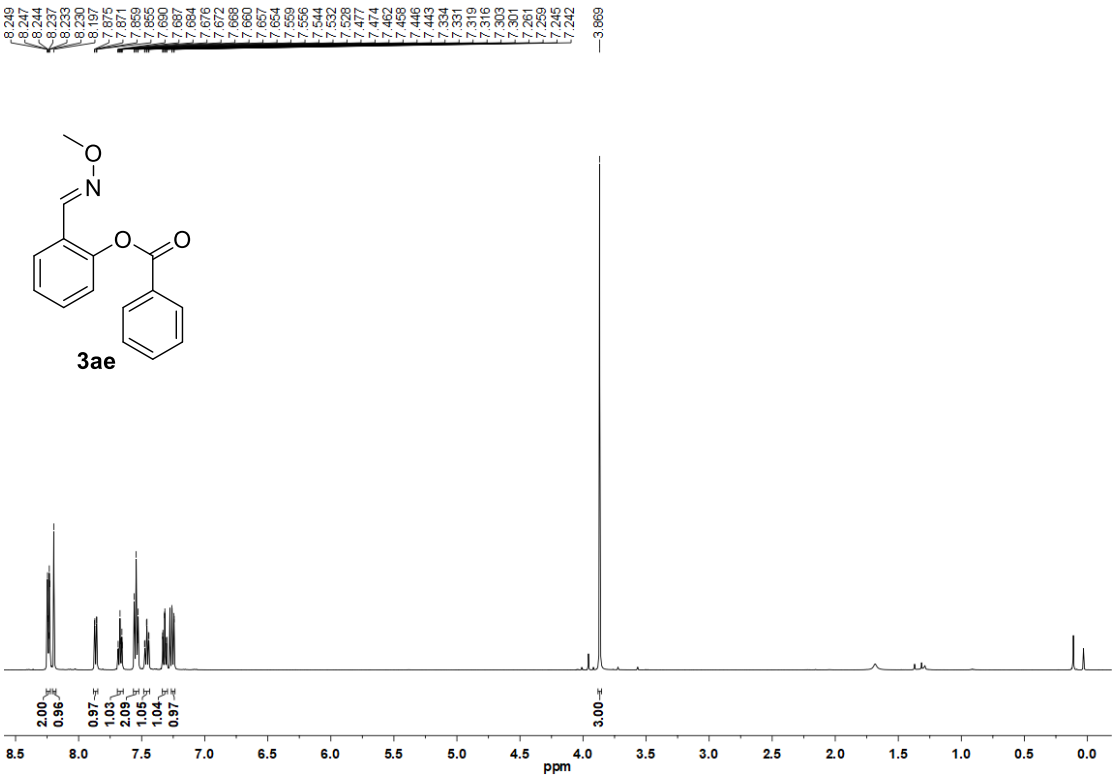
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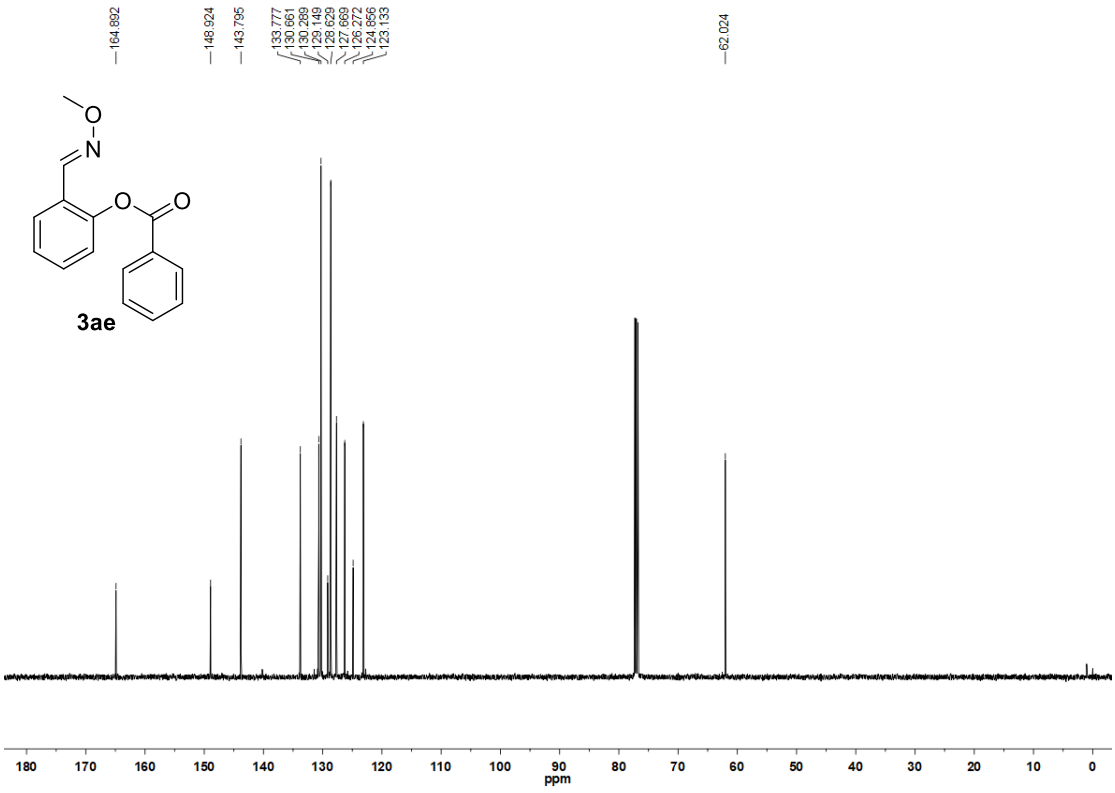
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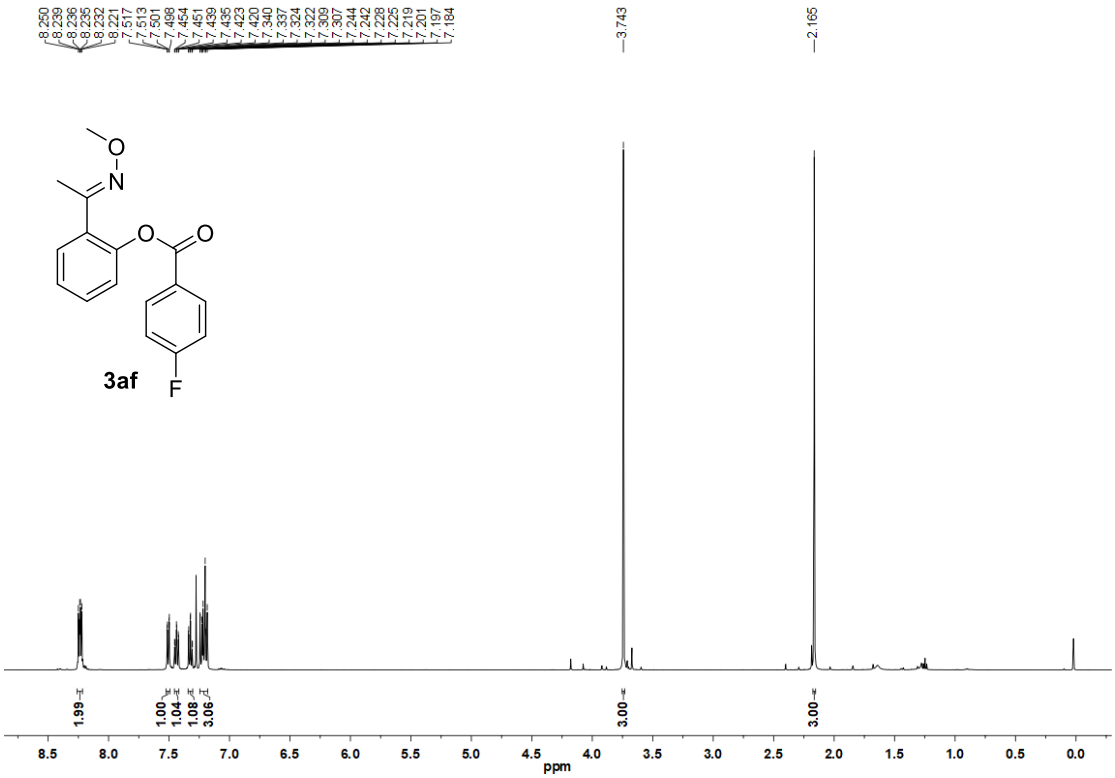
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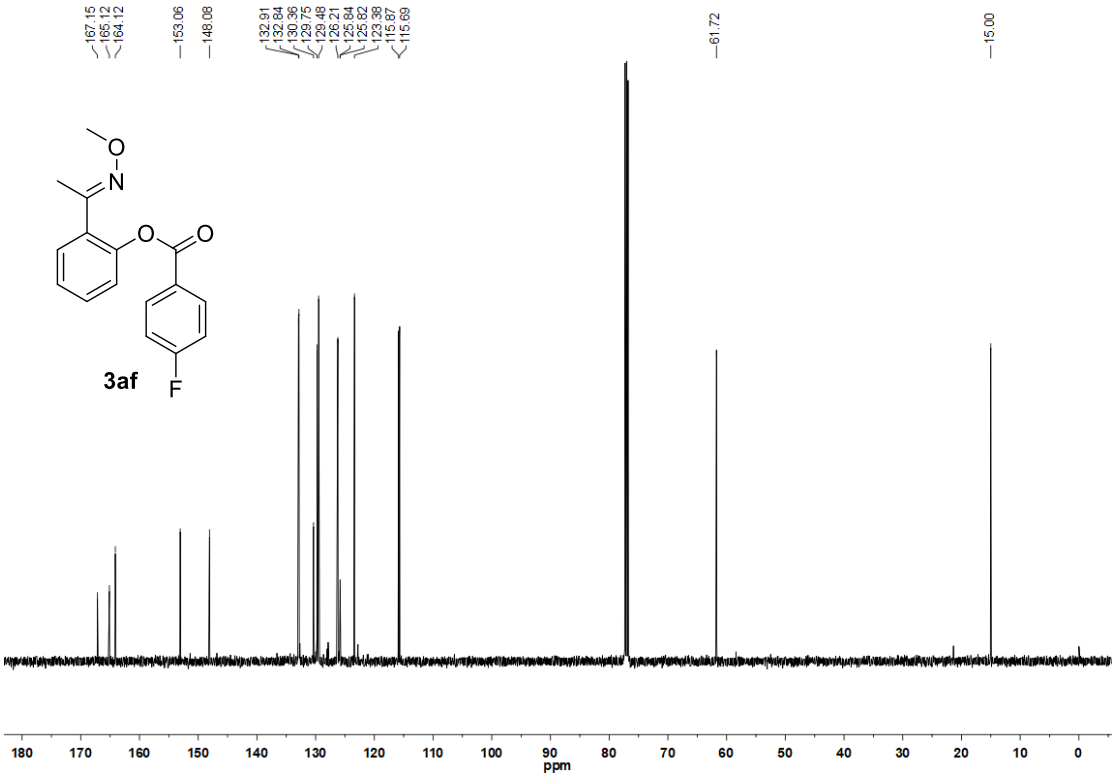
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O
O
F
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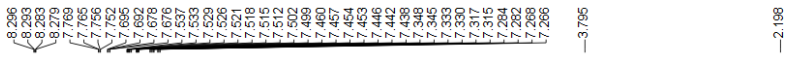
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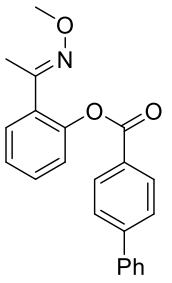
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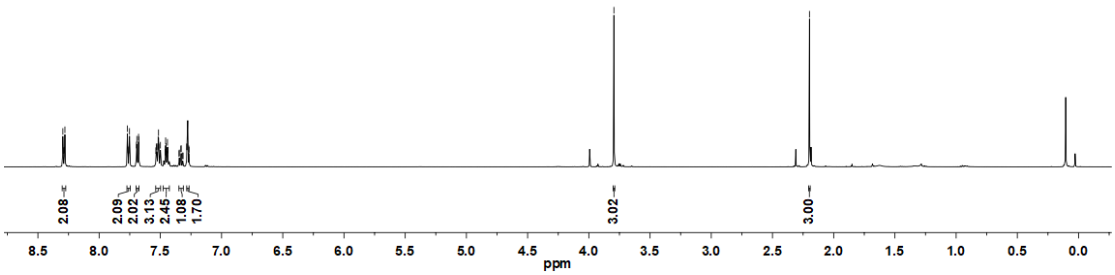
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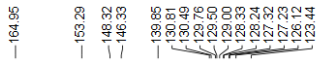
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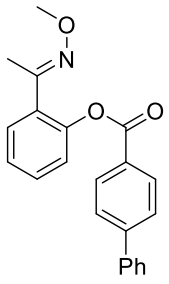
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Ph

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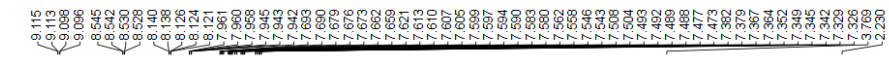
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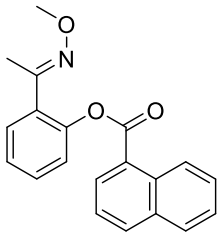

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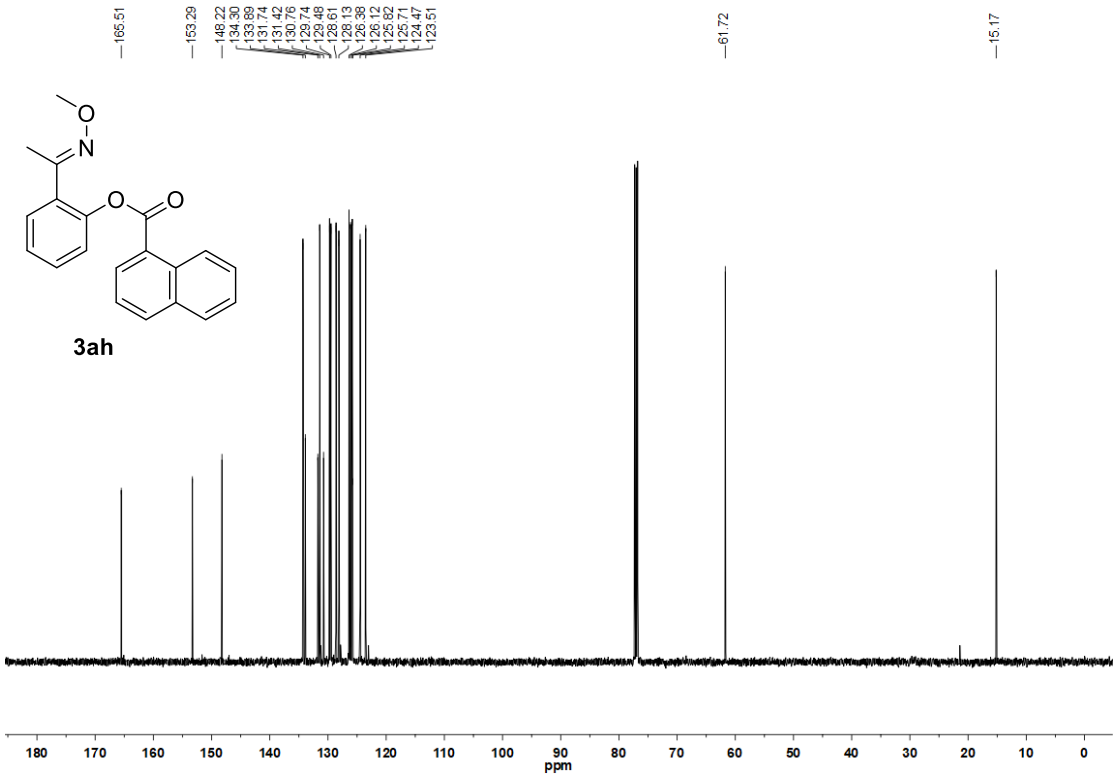
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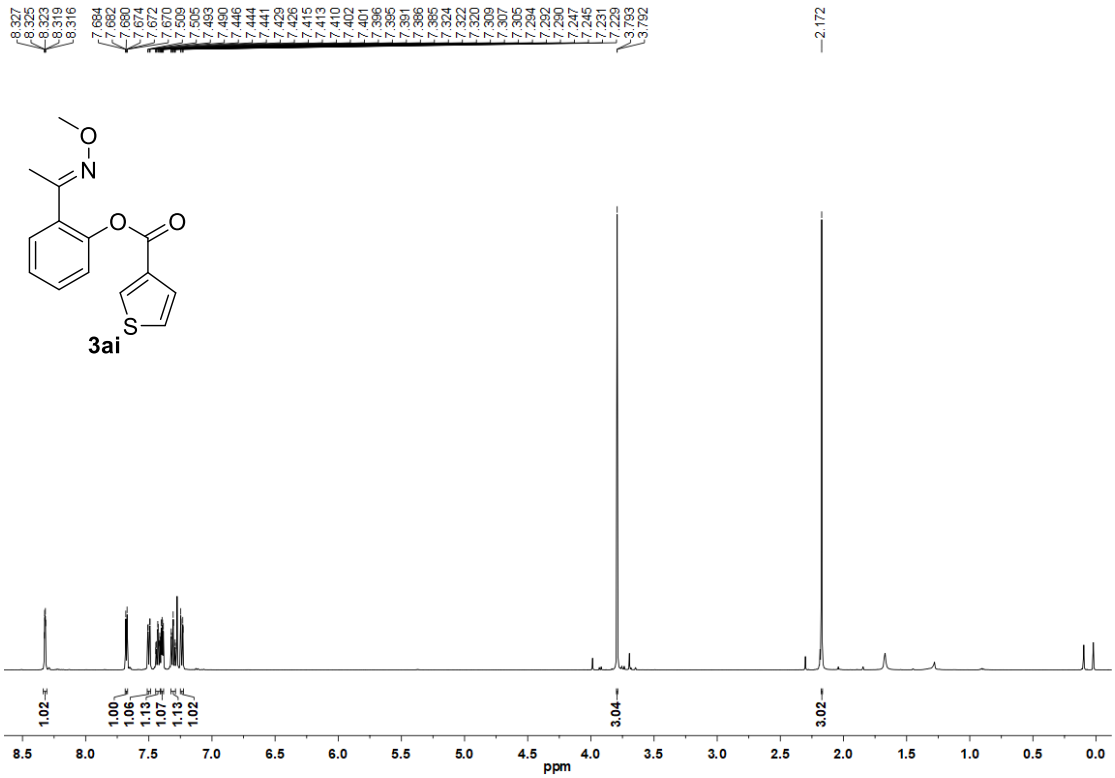
3ah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7.410
7.402
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7.385
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7.305
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7.292
7.290
7.247
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1.02
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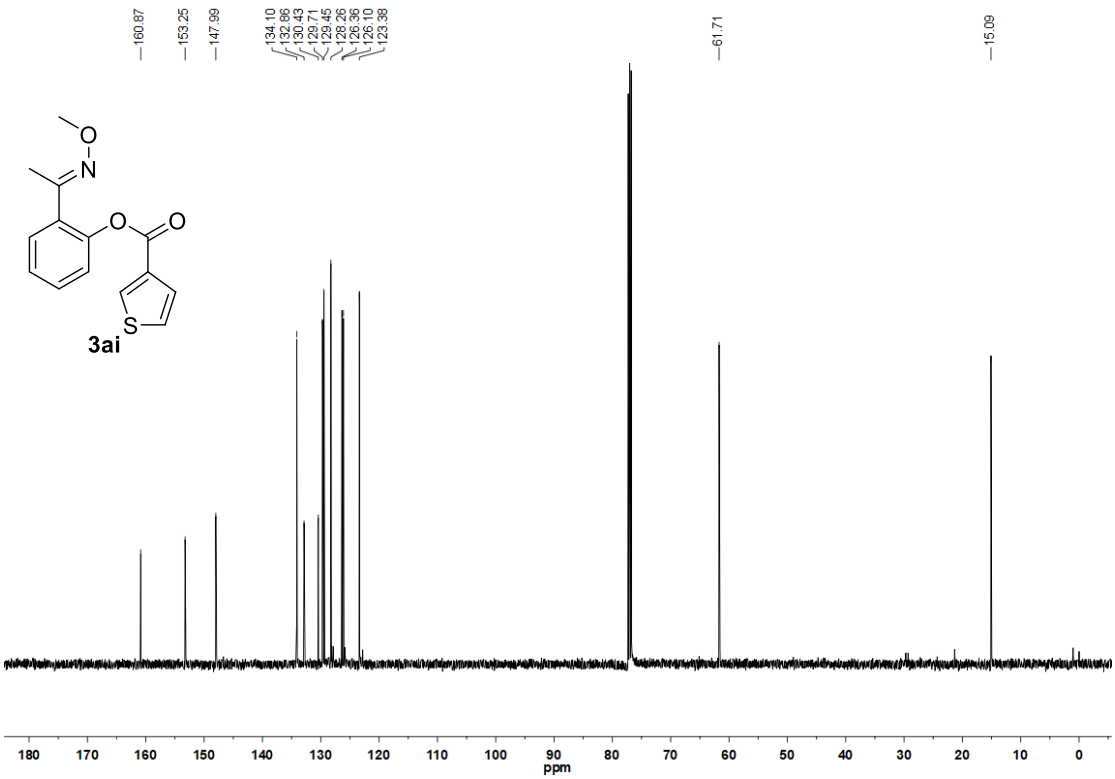
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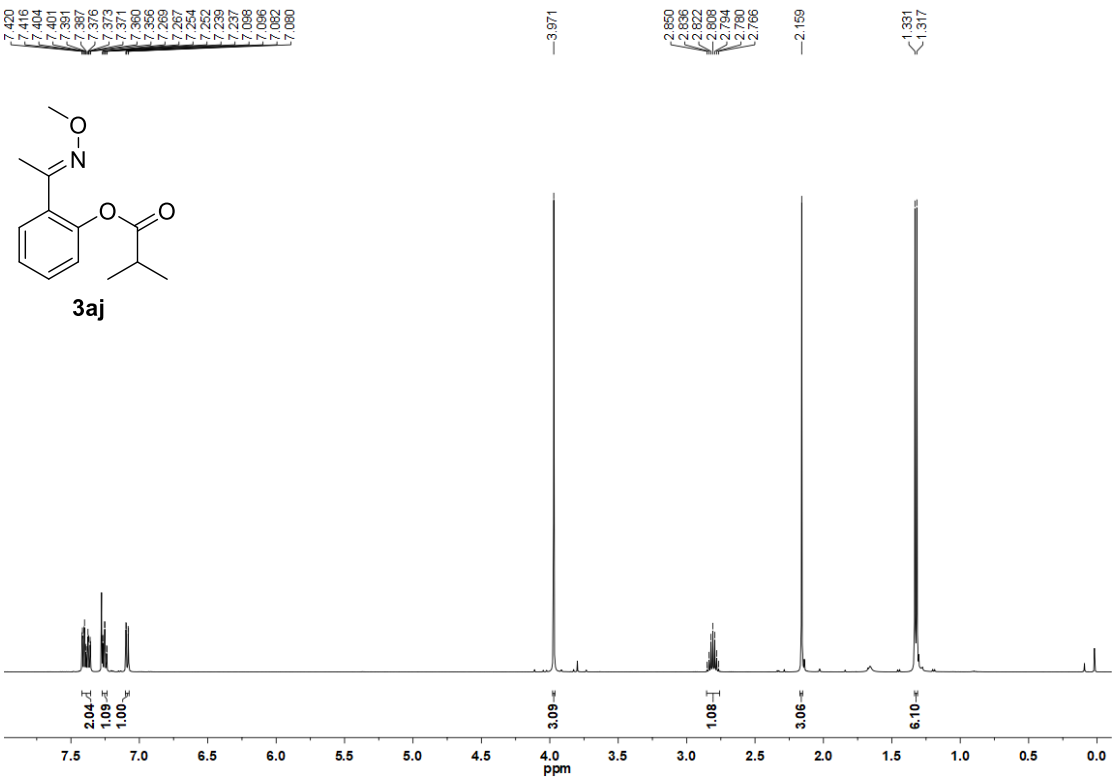
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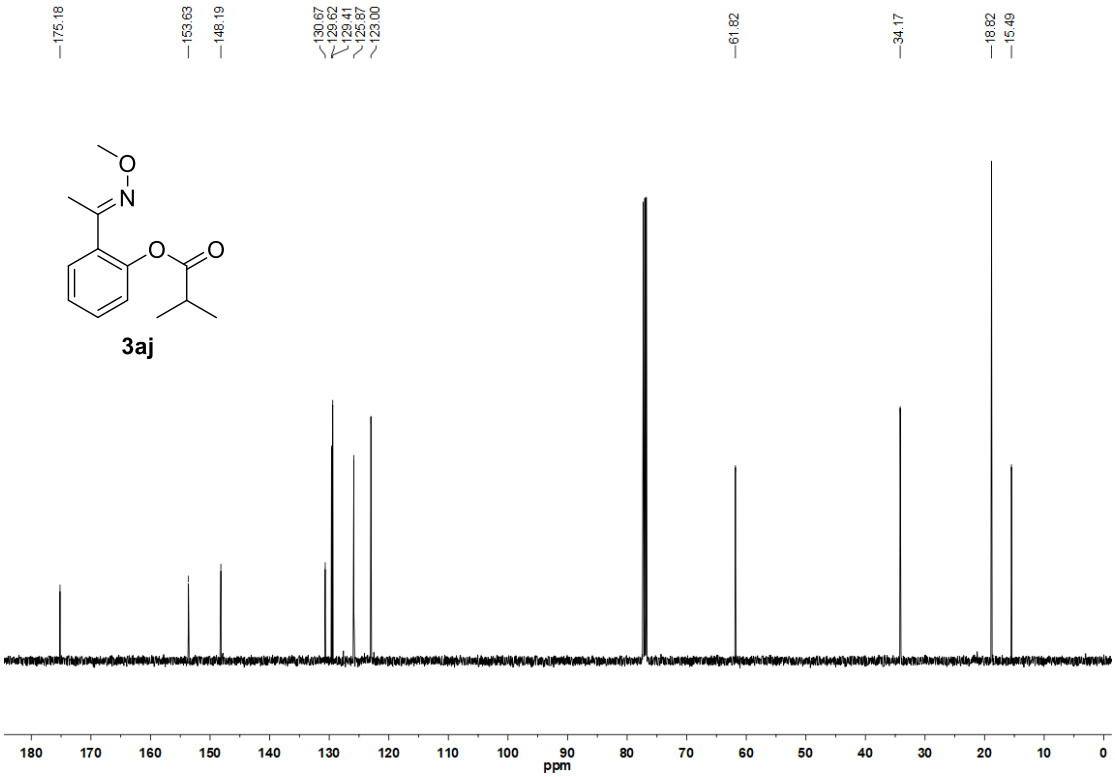
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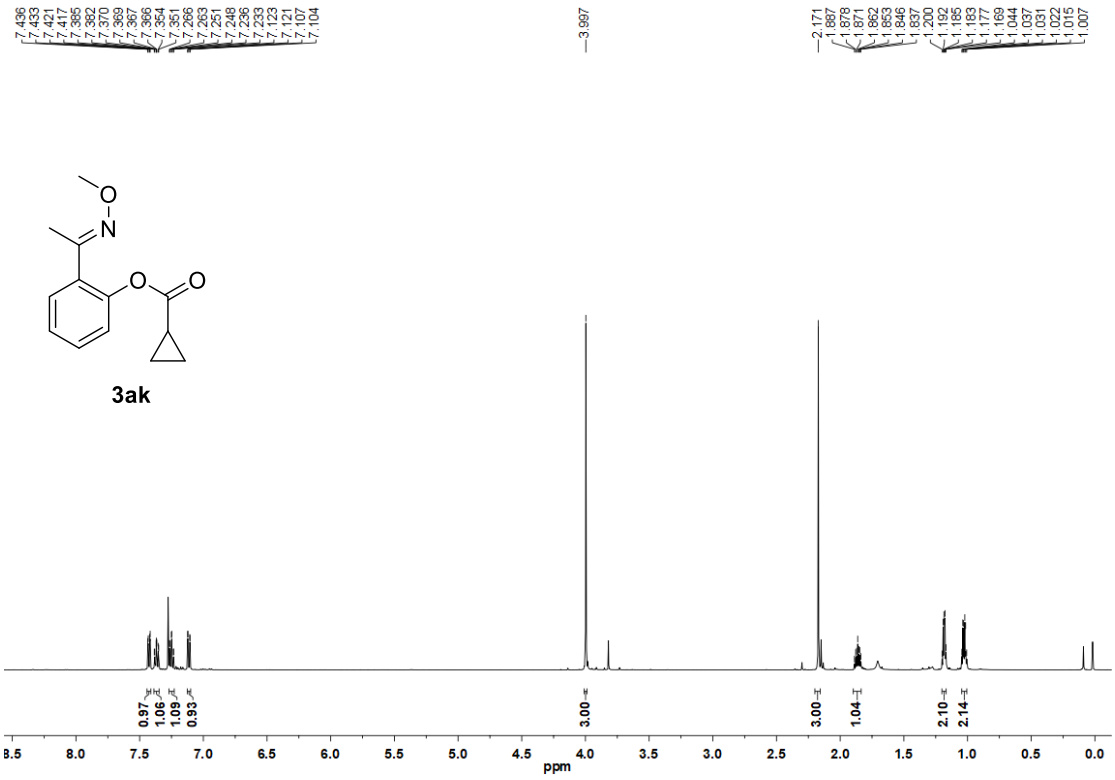
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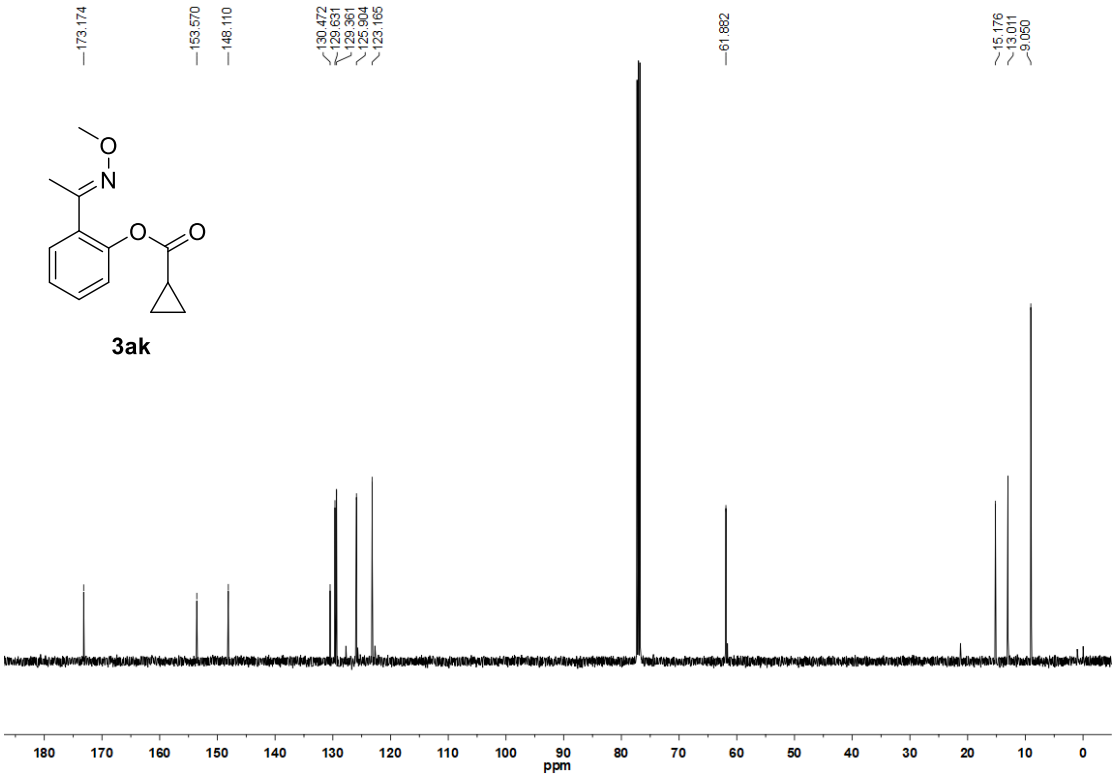
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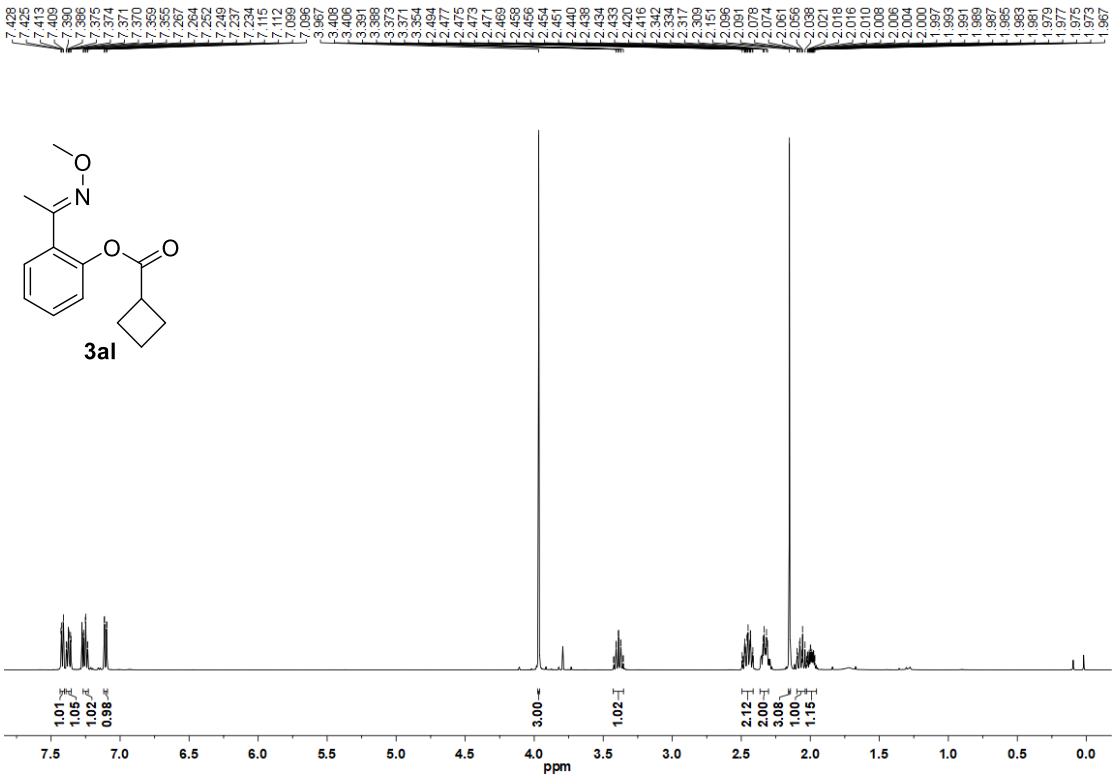
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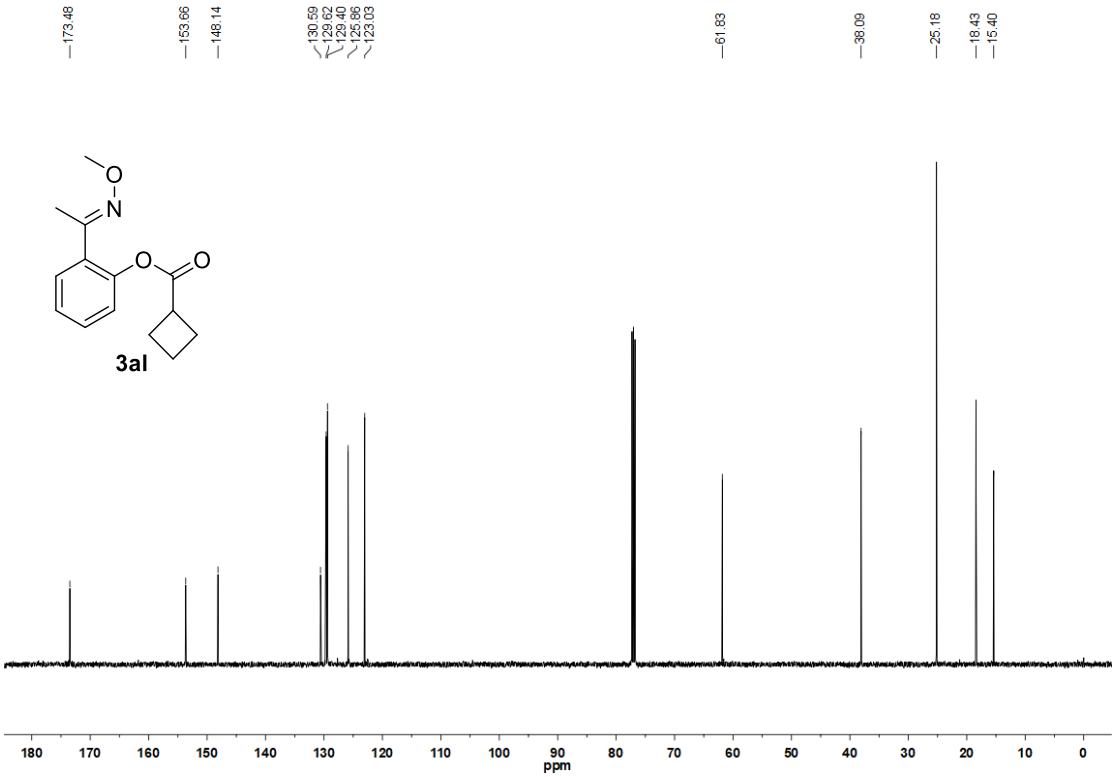
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O
O
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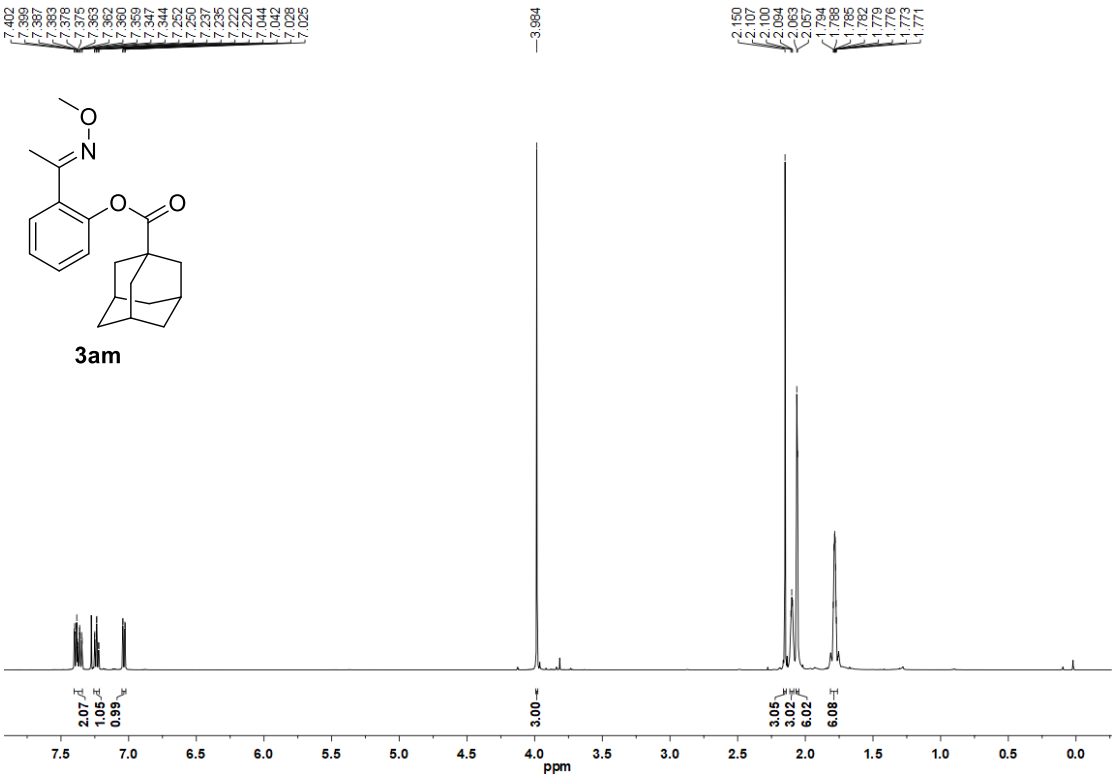
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O
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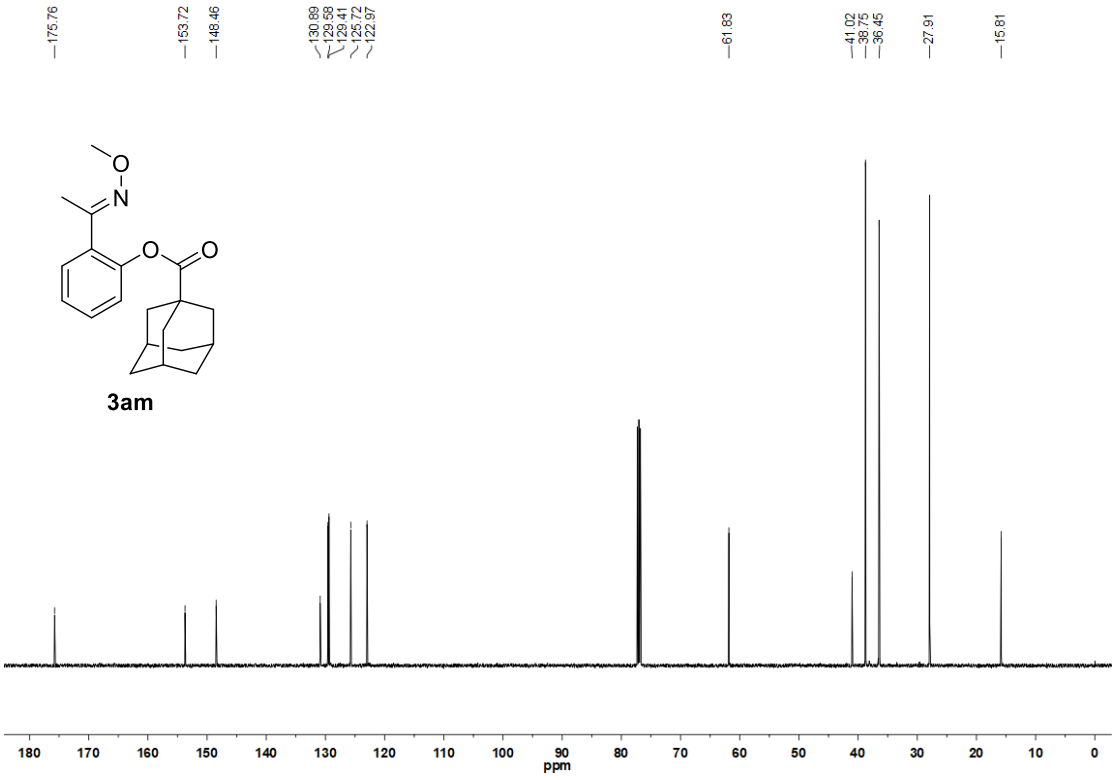
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O
3am
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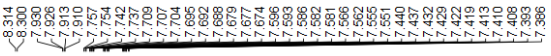
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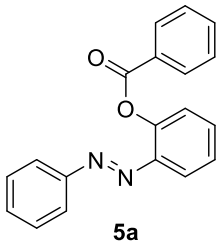
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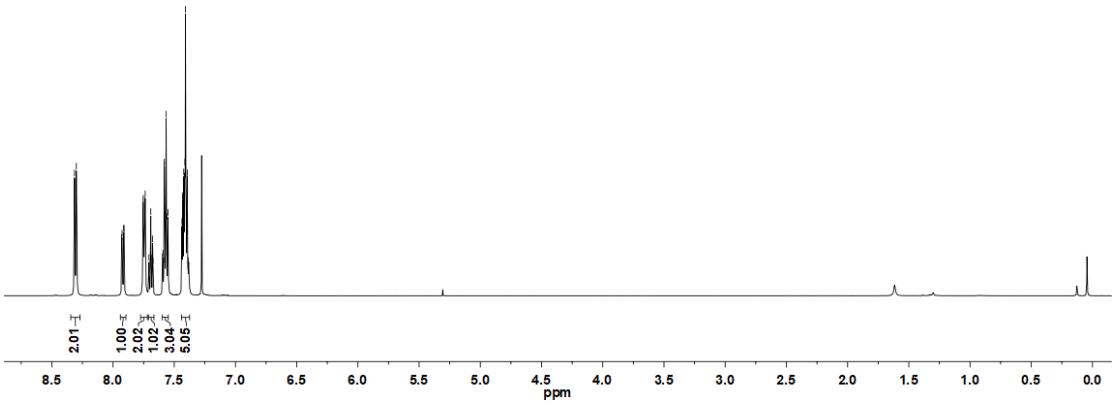
5a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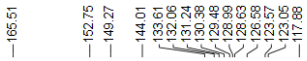
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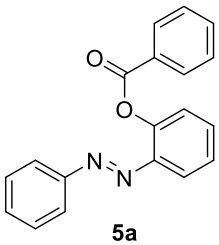
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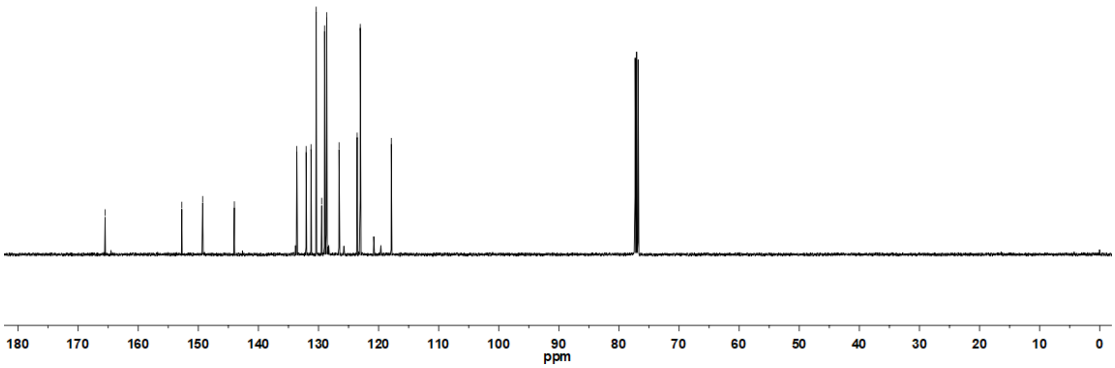
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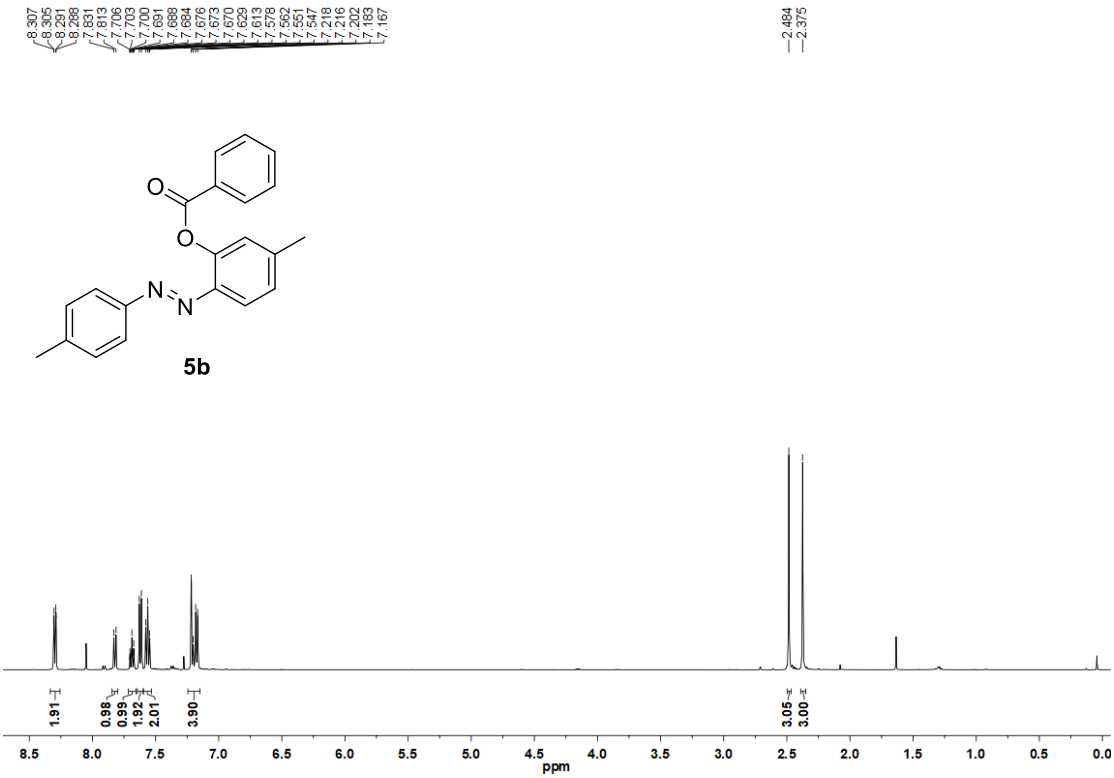
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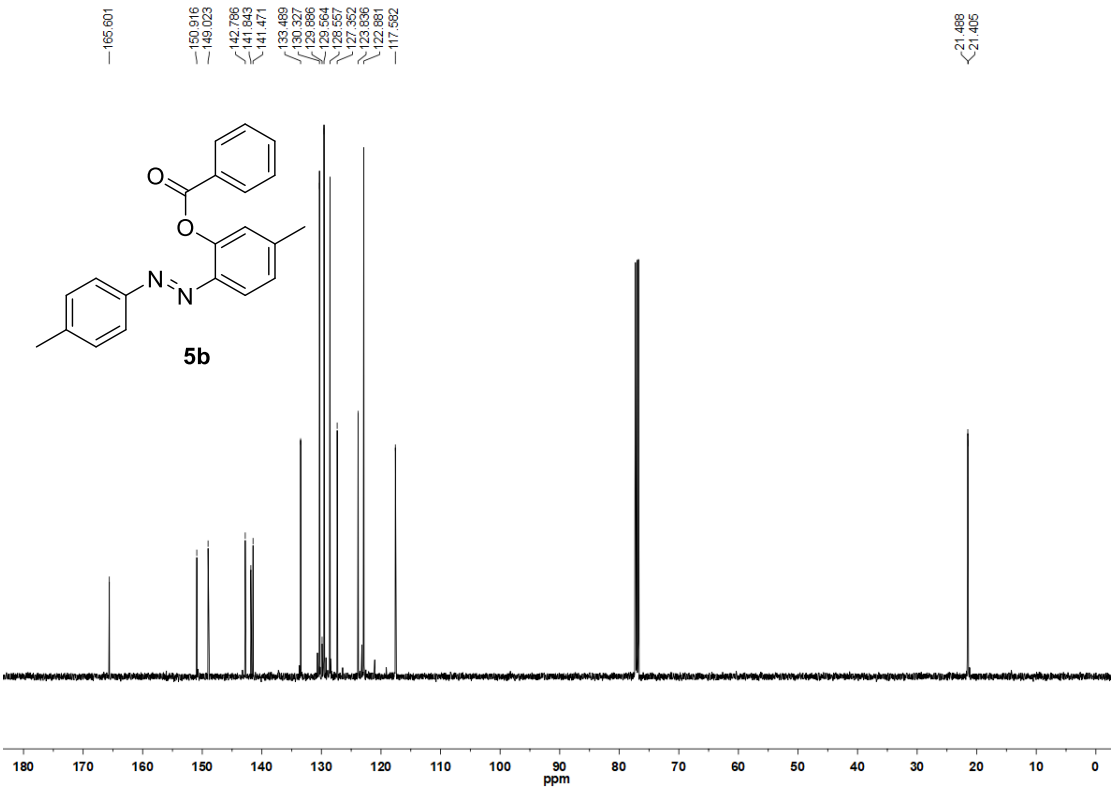
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21.405
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O
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N
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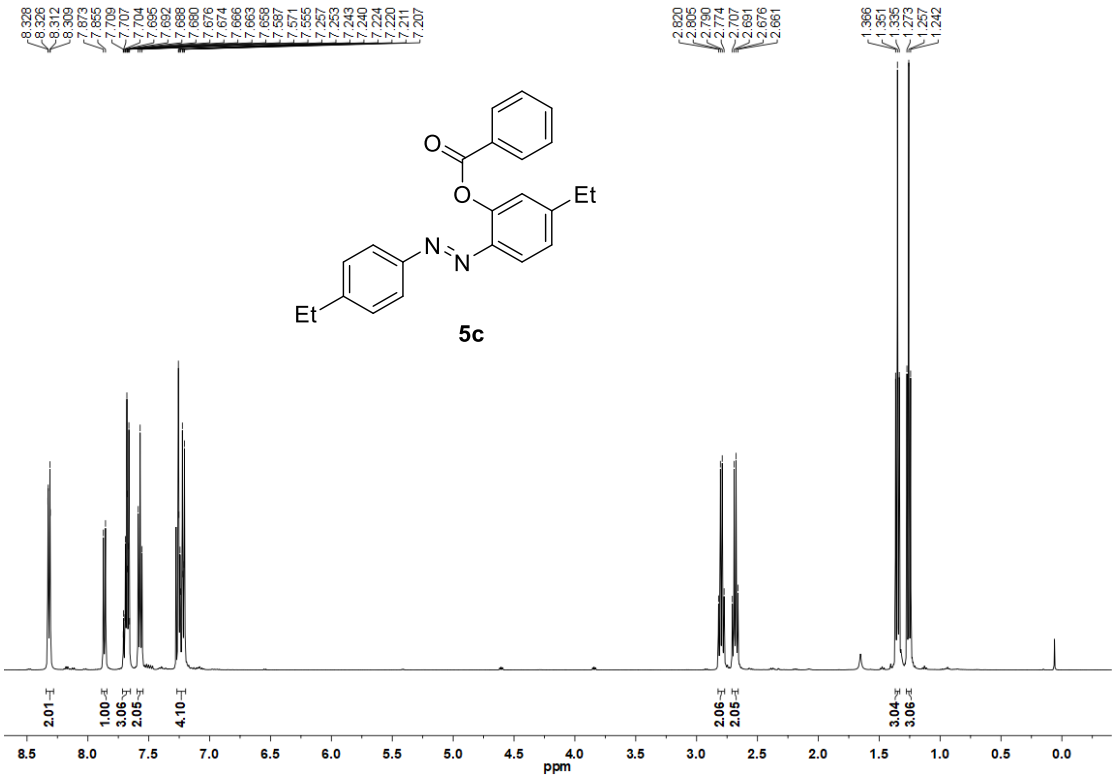
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1.242
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O
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N
Et
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2.05
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2.05
3.04
3.06
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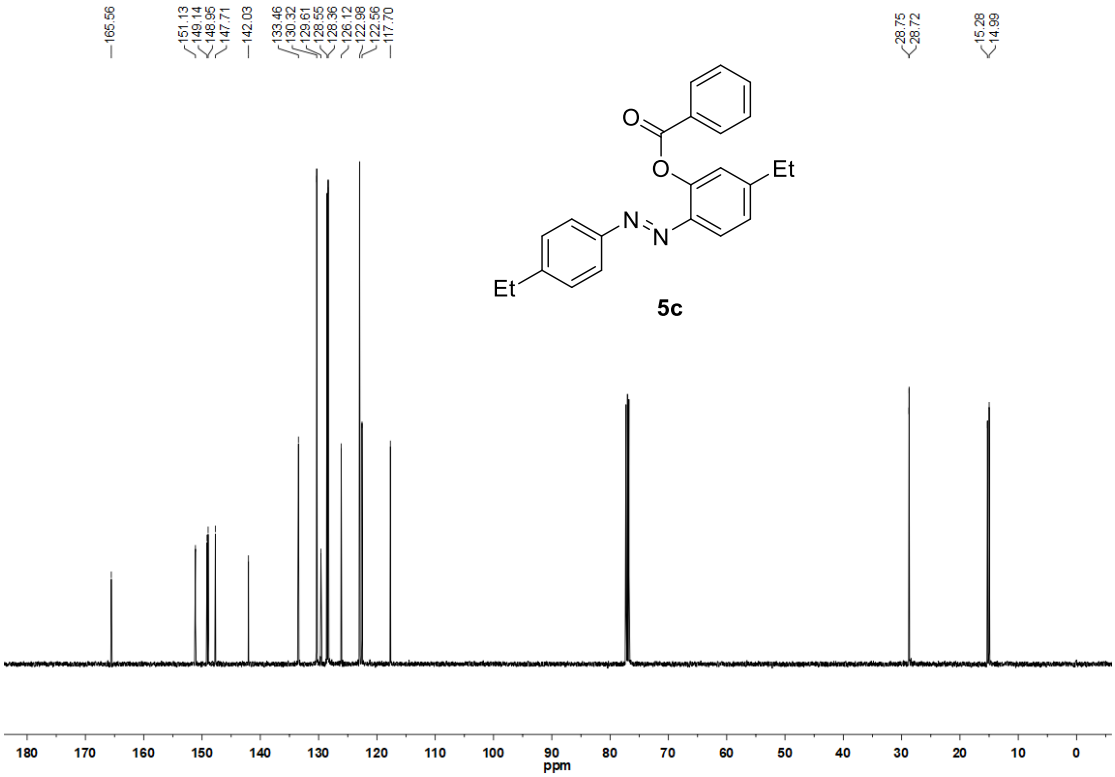
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28.72
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O
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N
N
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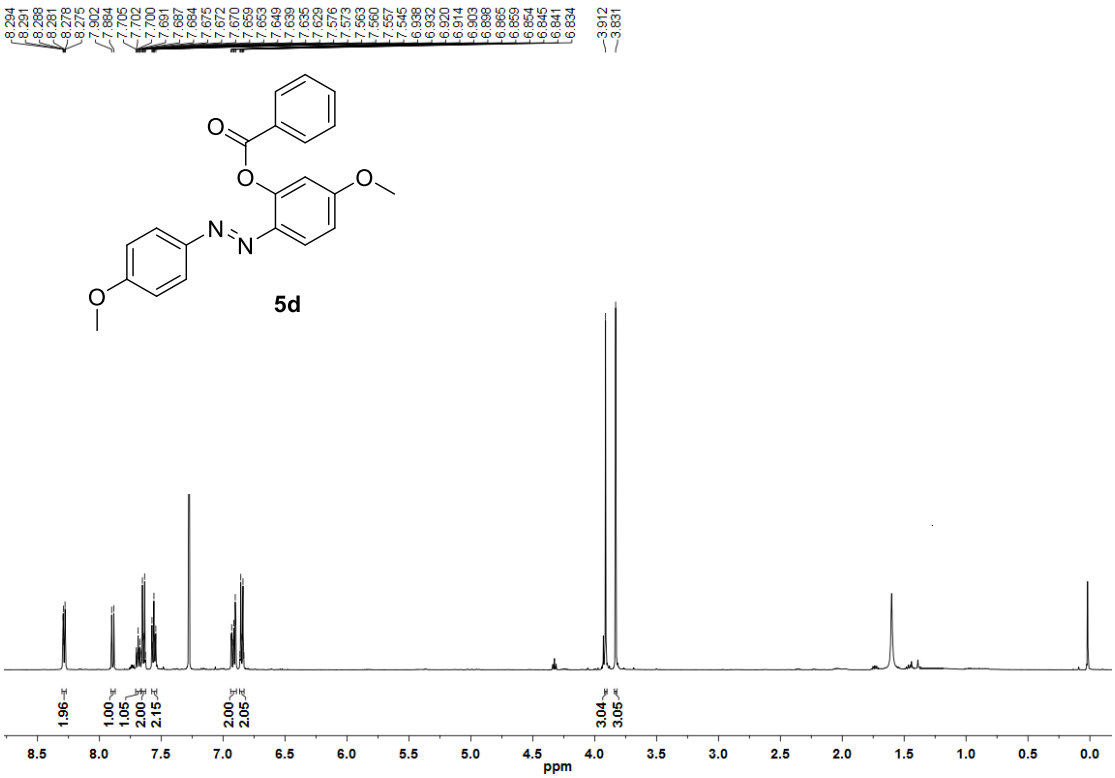
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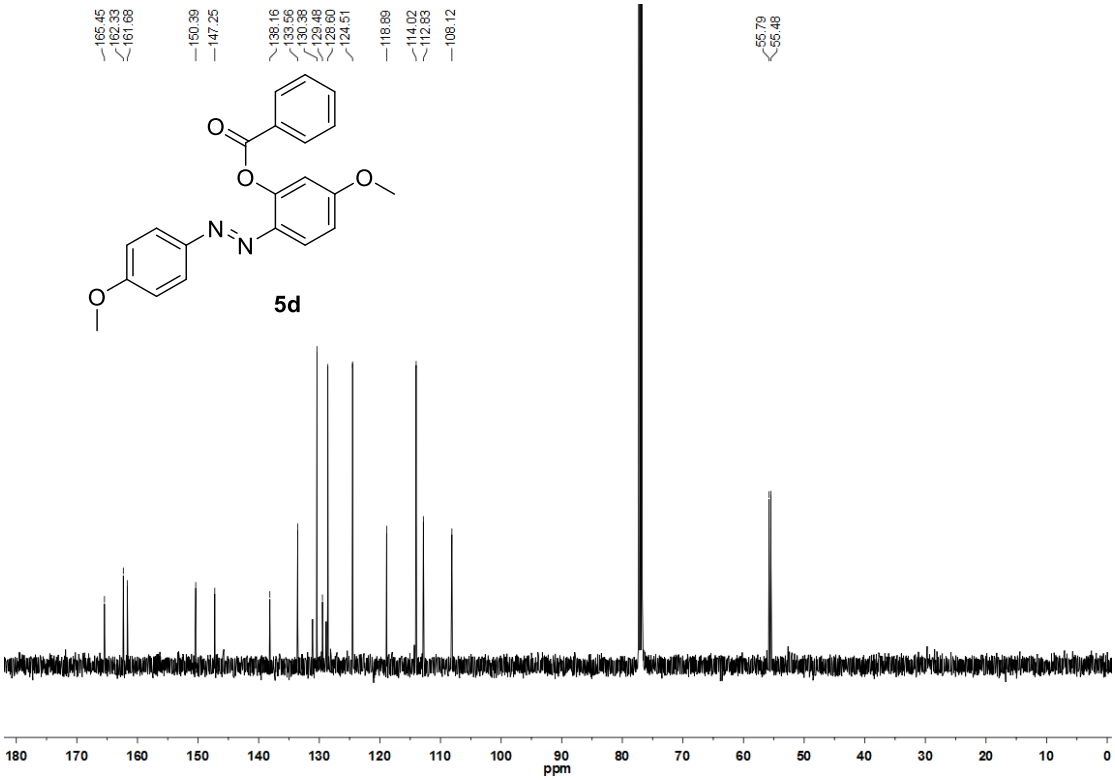
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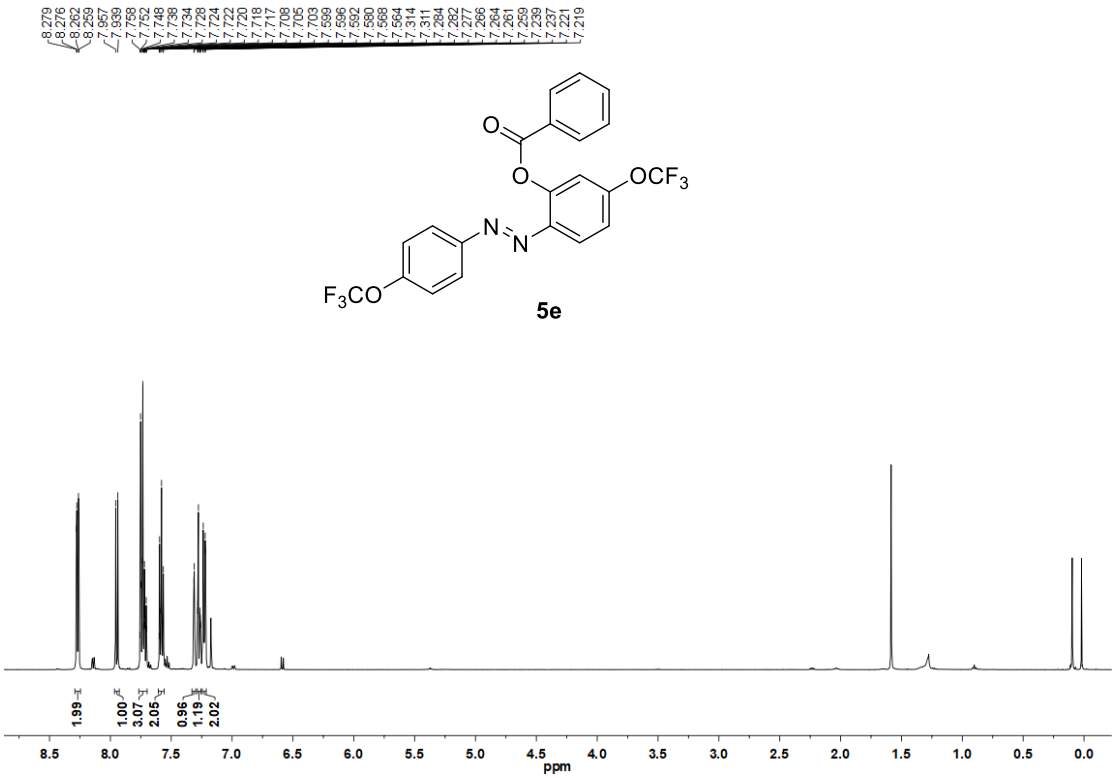
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7.237
7.221
7.219
O
O
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1.00
3.07
2.05
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1.19
2.02
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7.5
7.0
6.5
6.0
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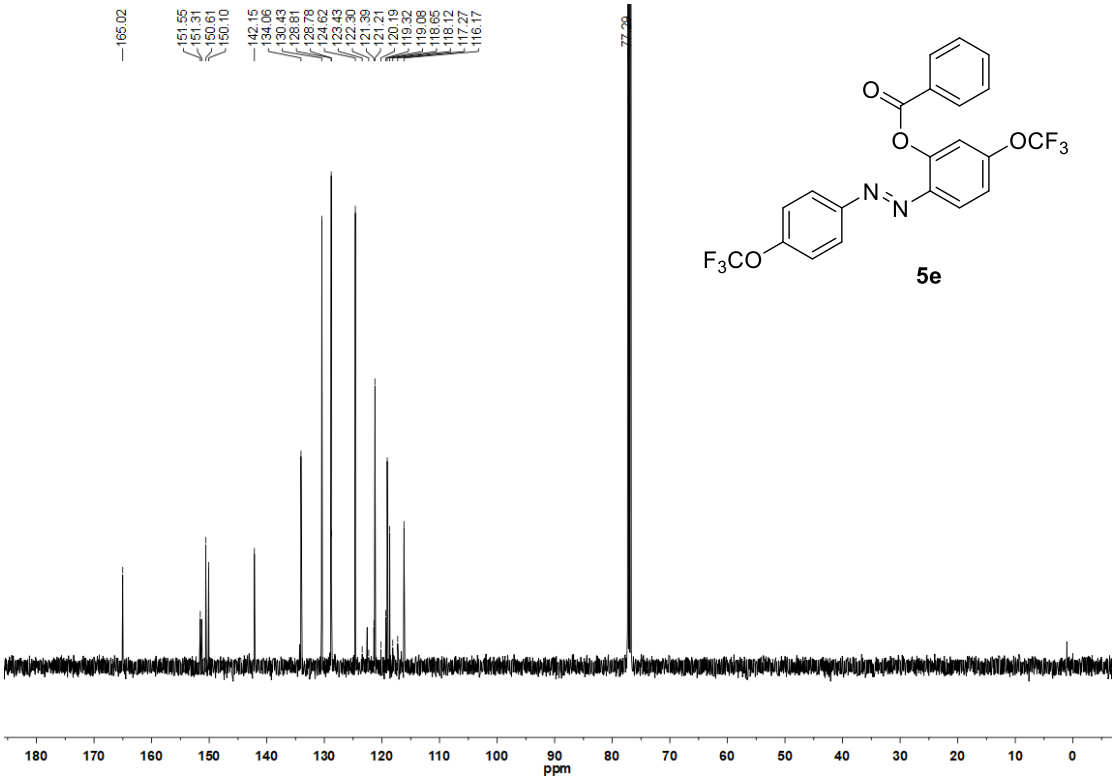
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N
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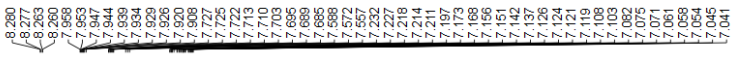
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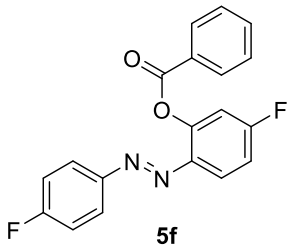
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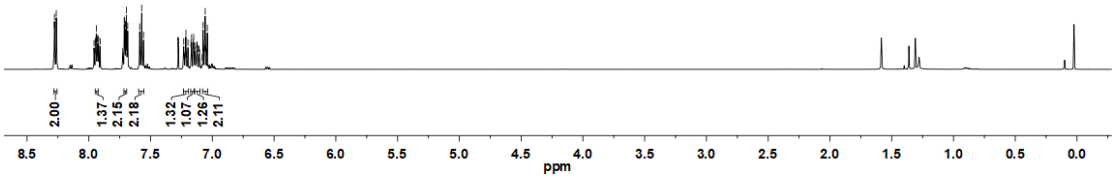
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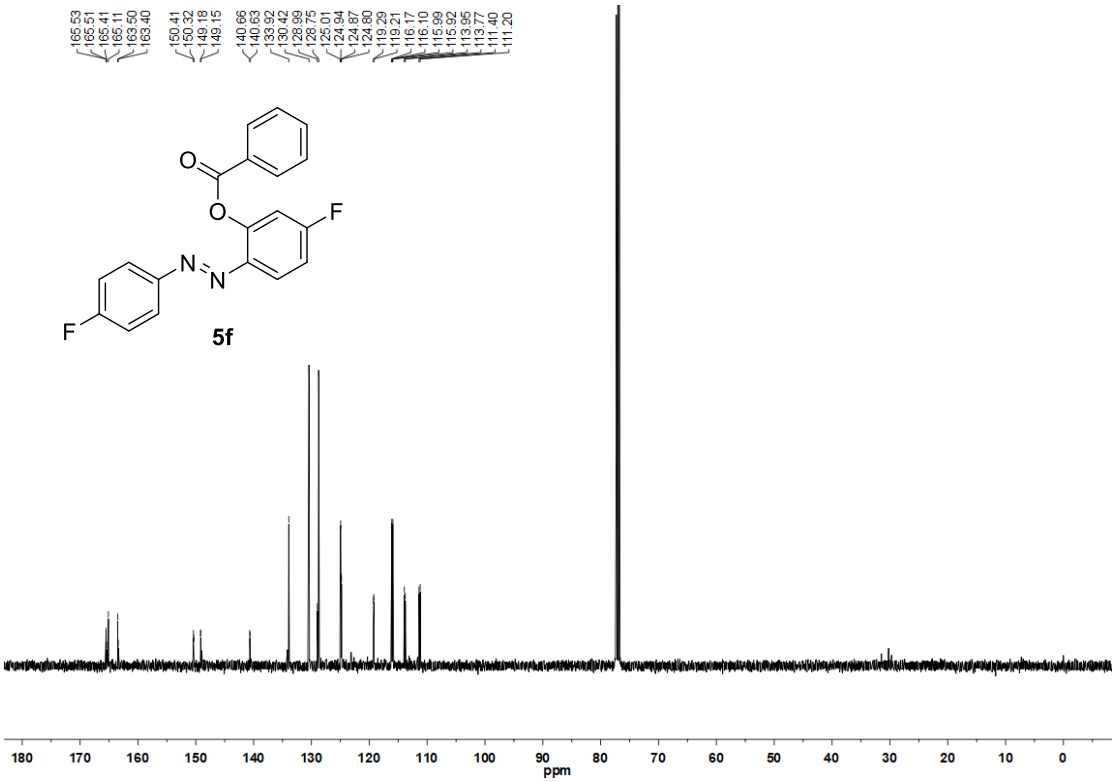
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O
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N
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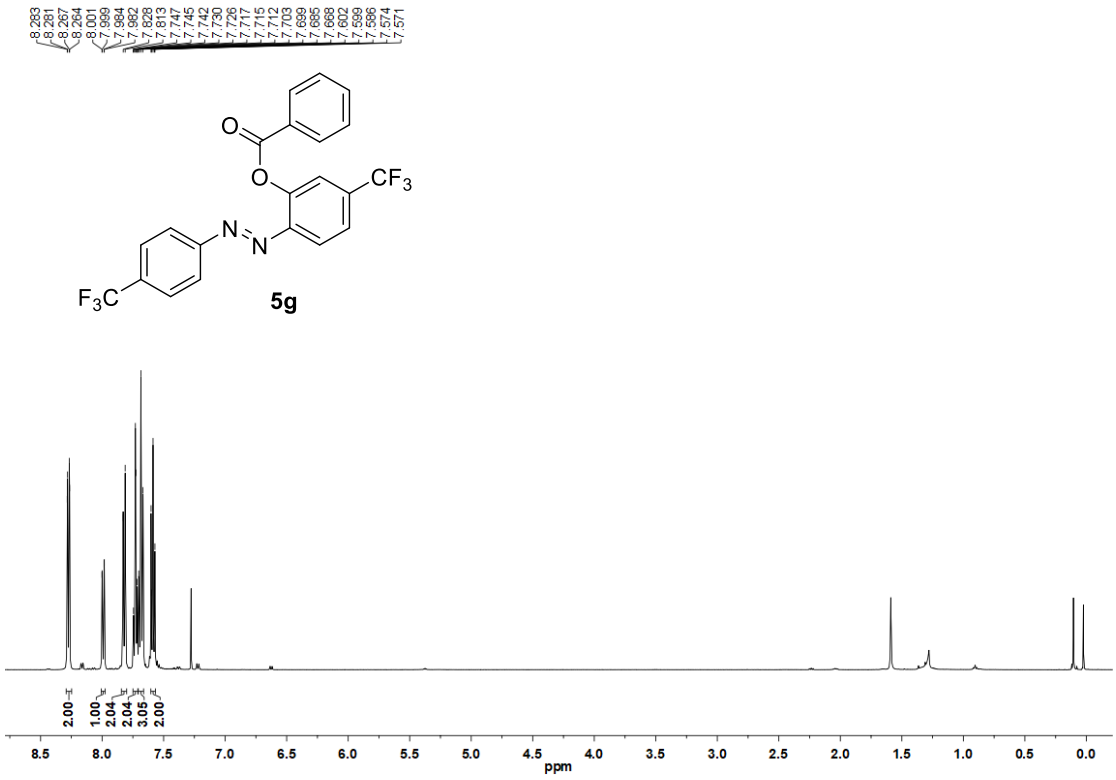
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7.668
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7.571
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N
F3C
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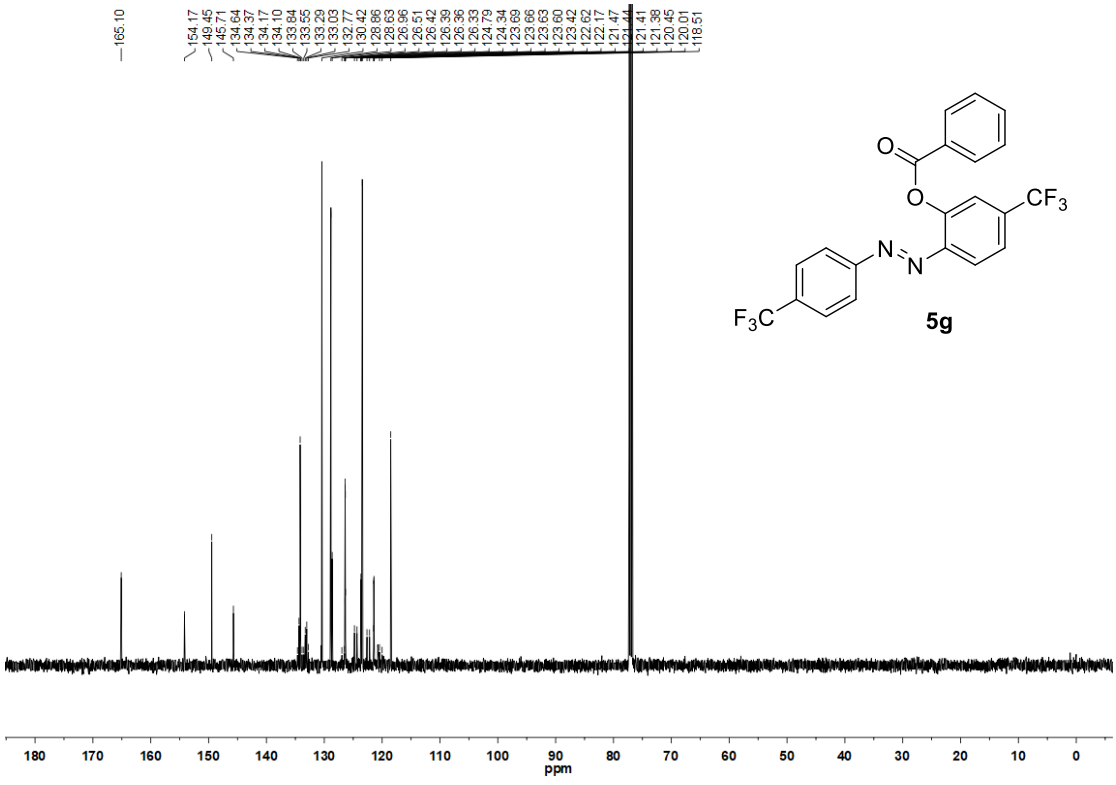
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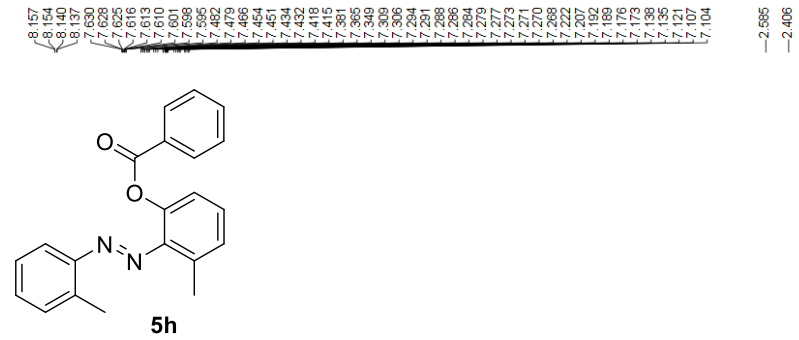
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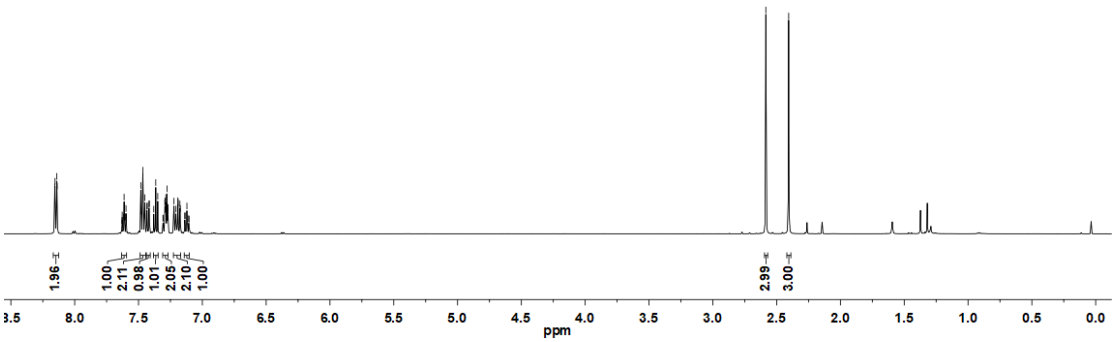
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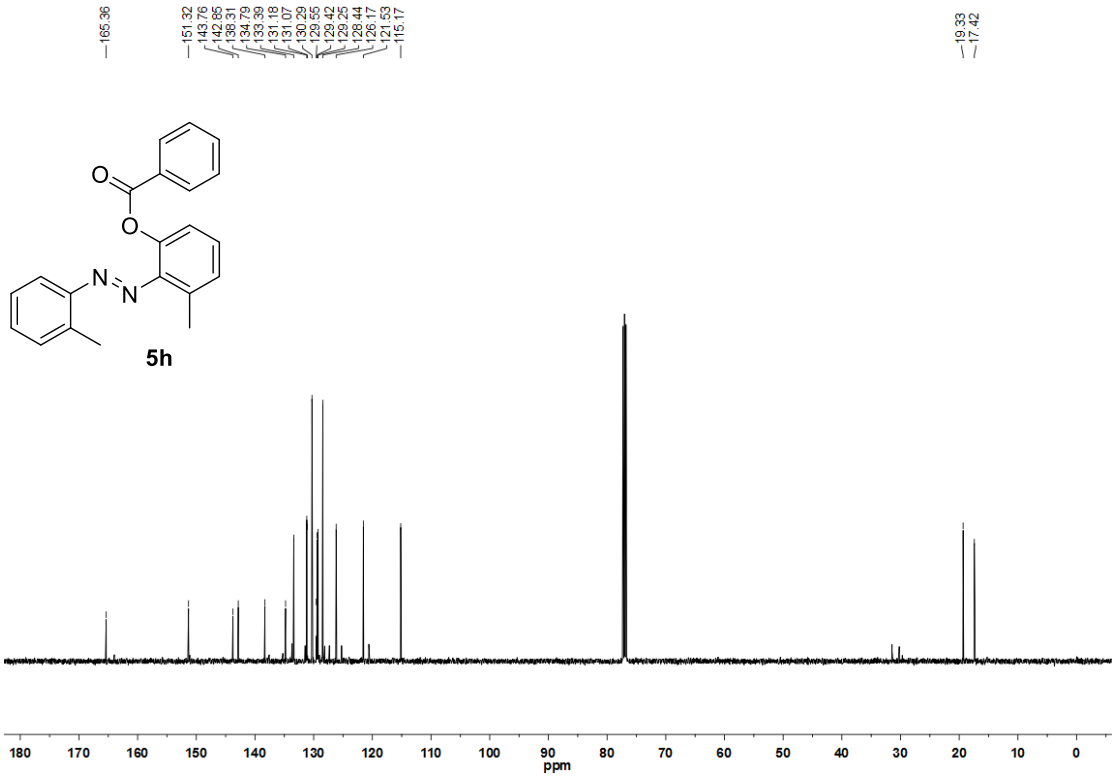
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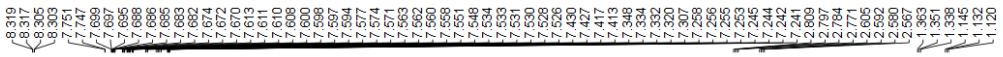

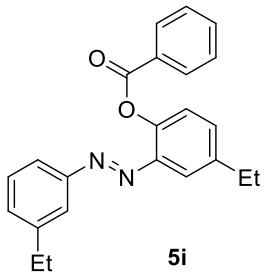

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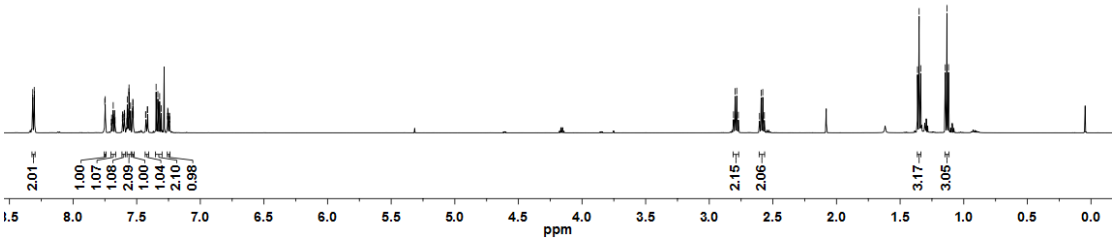

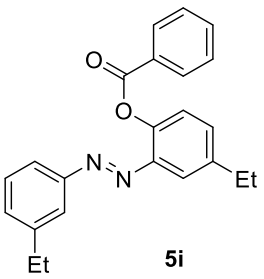

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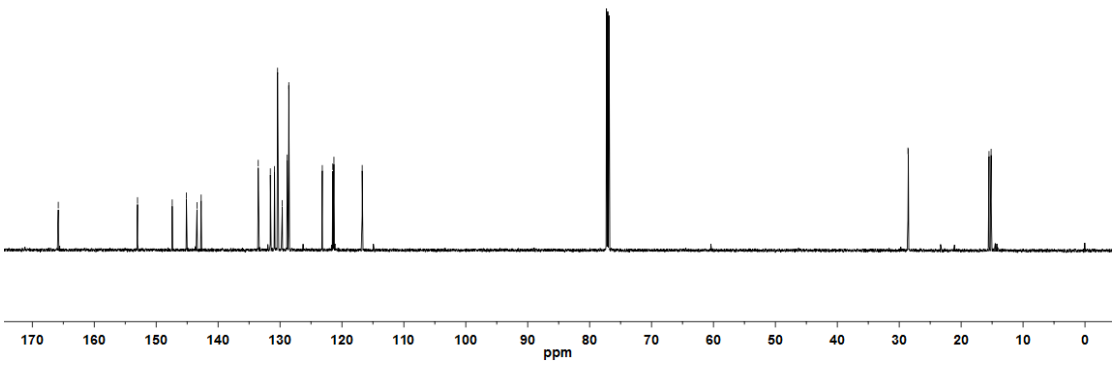

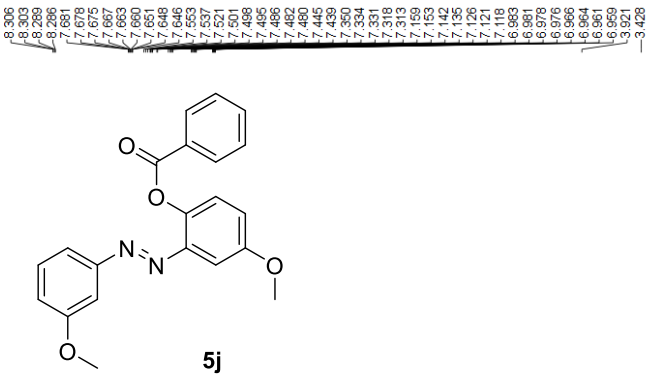
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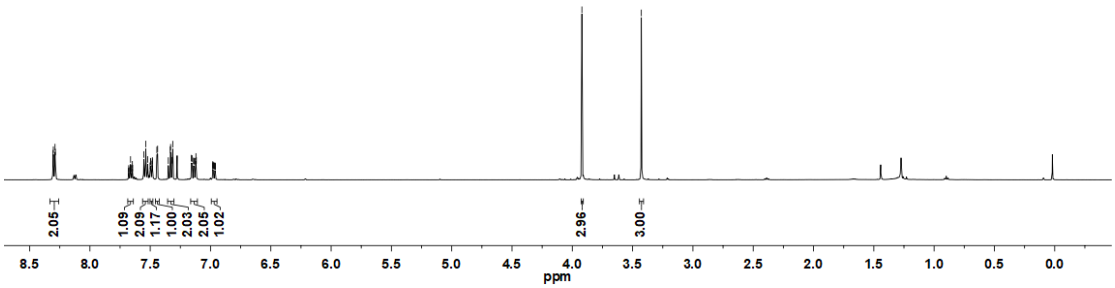
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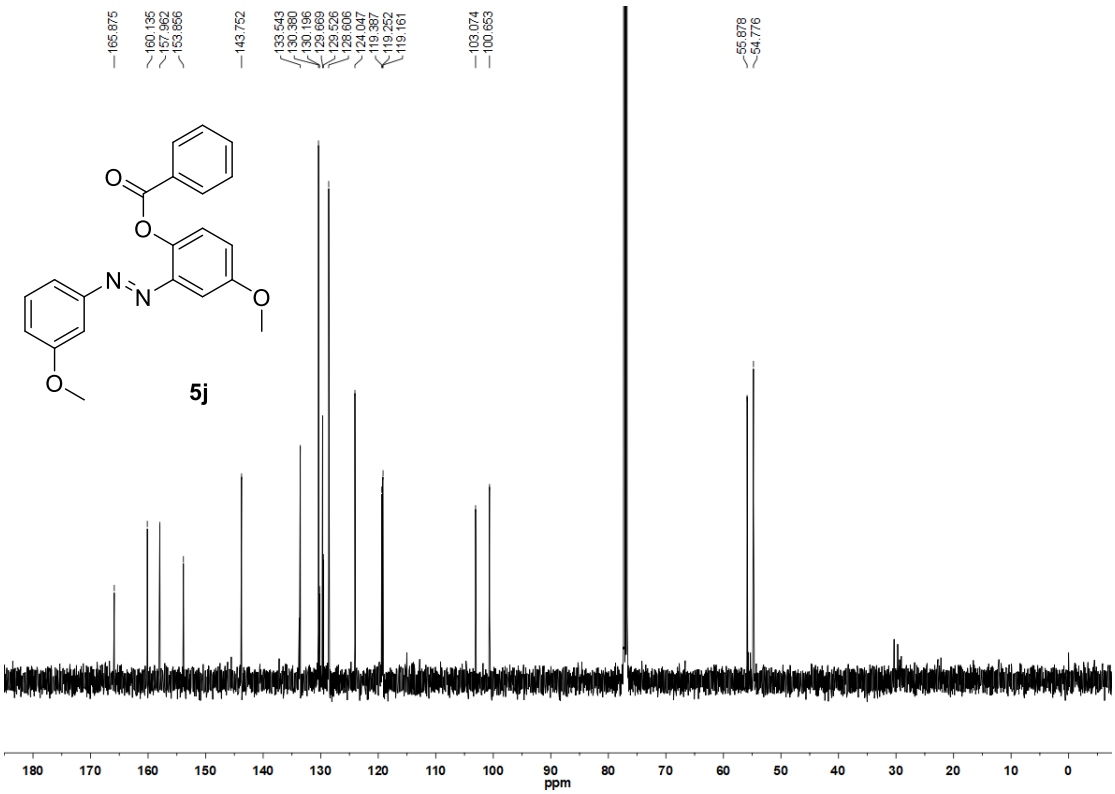
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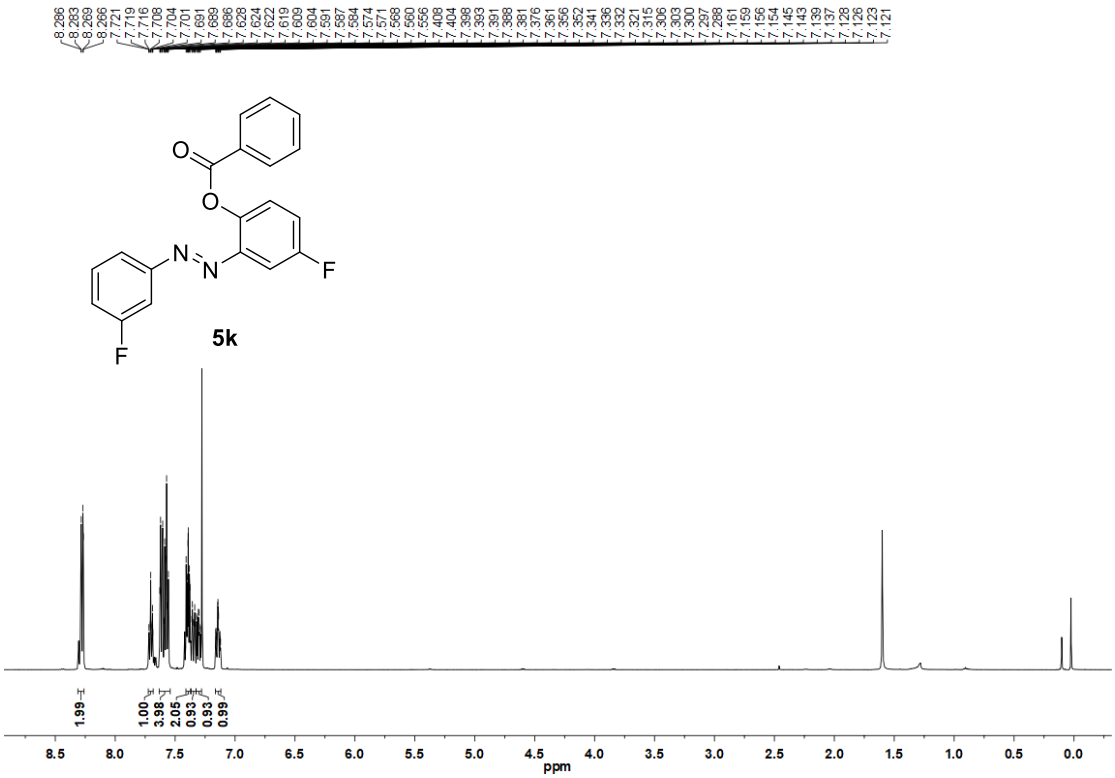
5j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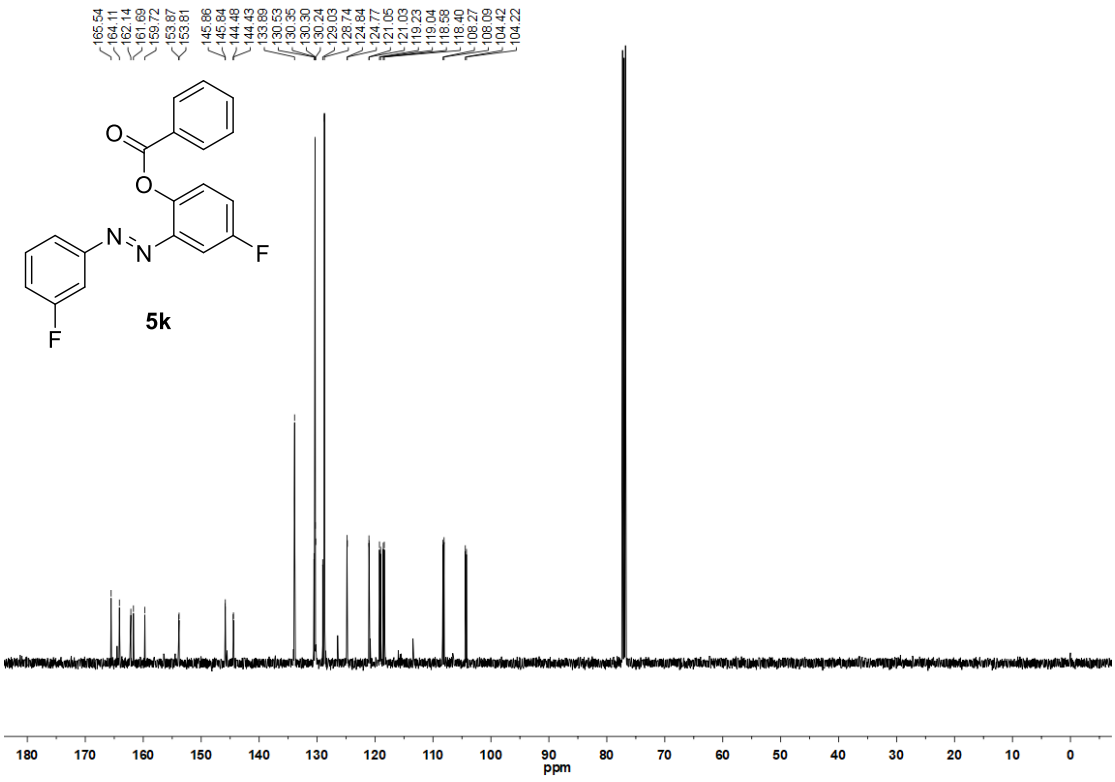
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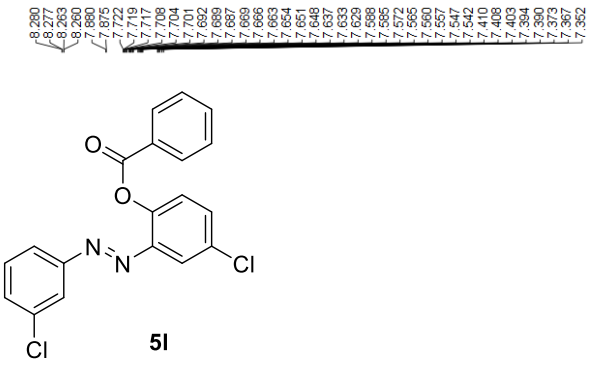
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Cl
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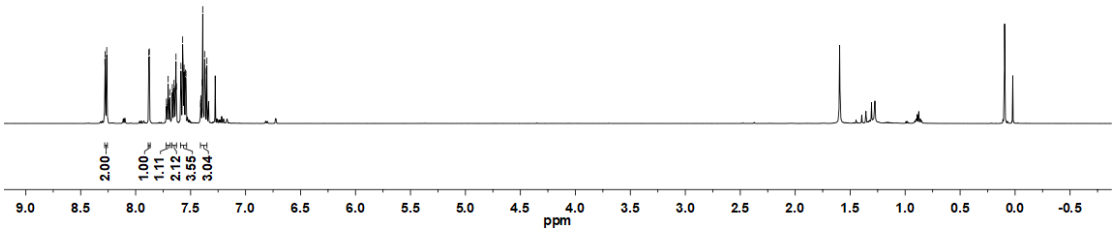
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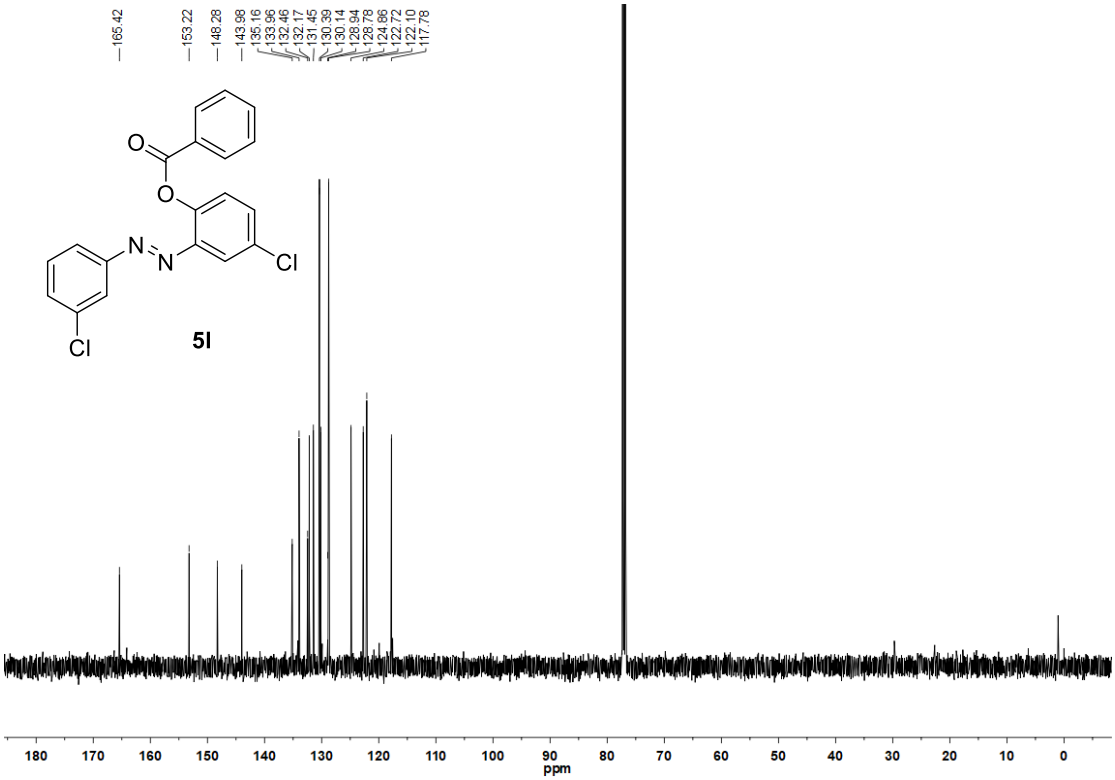
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122.10
117.78
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O
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N
Cl
Cl
5l
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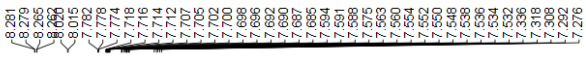
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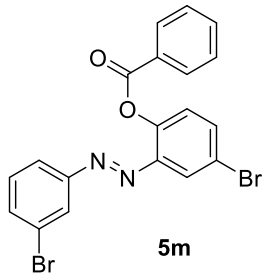
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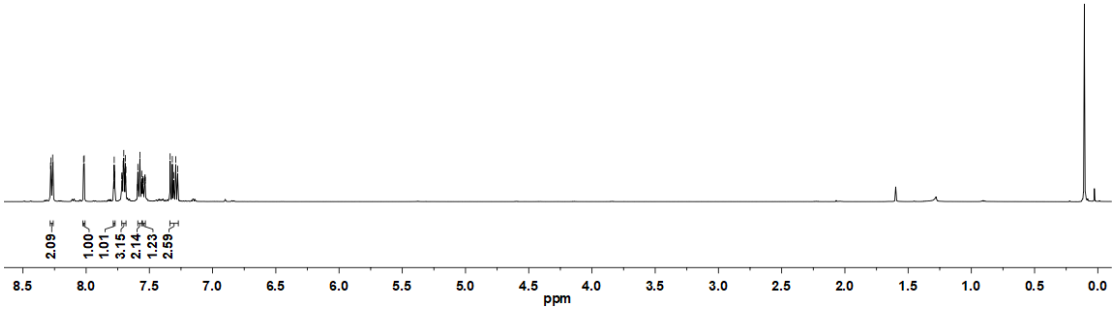
N
Br
Br

5m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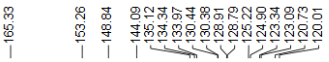
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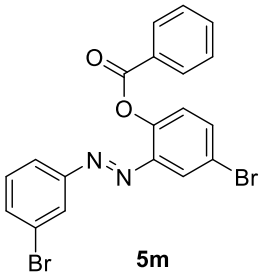
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Br
Br

5m

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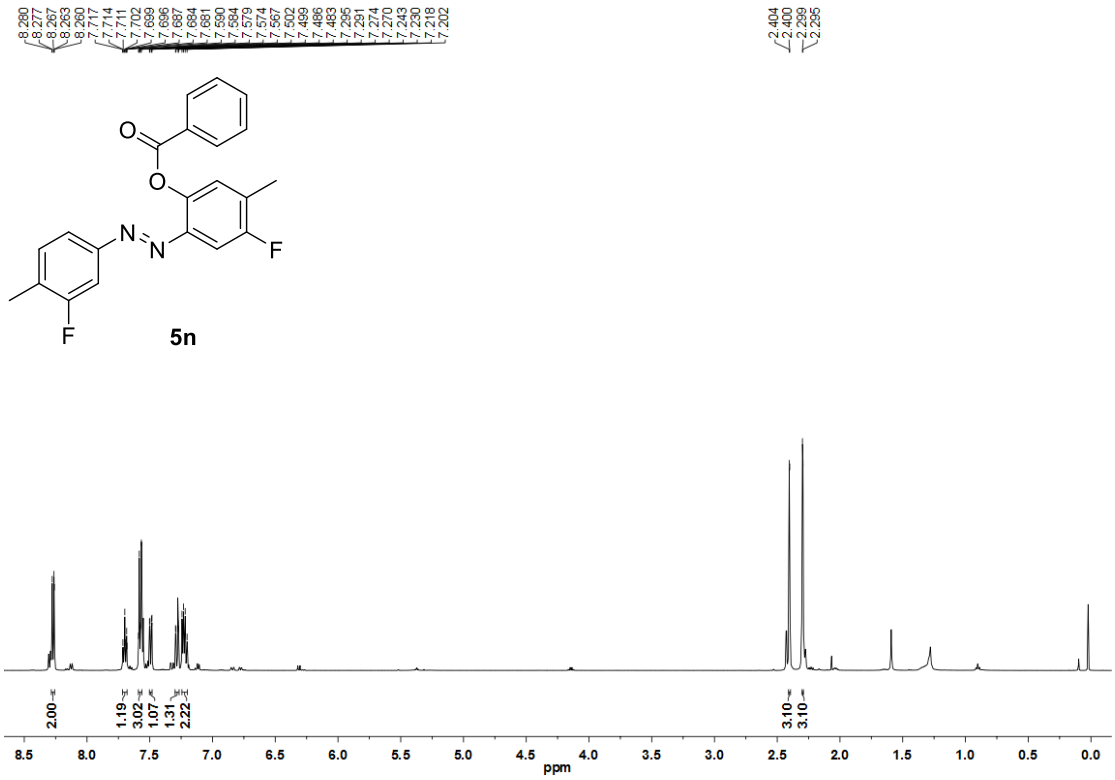
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7.584
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7.483
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7.270
7.243
7.230
7.218
7.202
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2.400
2.299
2.295
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O
N
N
F
F
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1.07
1.31
2.22
3.10
3.10
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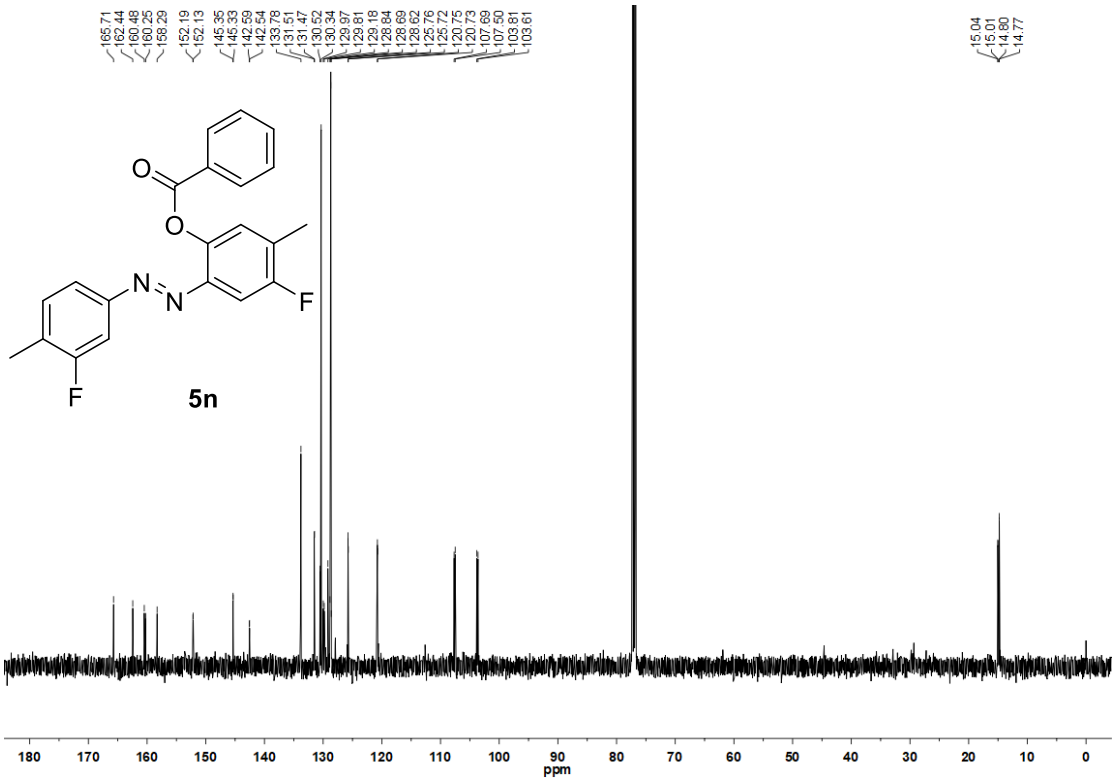
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131.47
130.52
130.34
129.97
129.81
129.18
128.84
128.69
128.62
125.76
125.72
120.75
120.73
107.69
107.50
103.81
103.61
15.04
15.01
14.80
14.77
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N
N
F
F
5n
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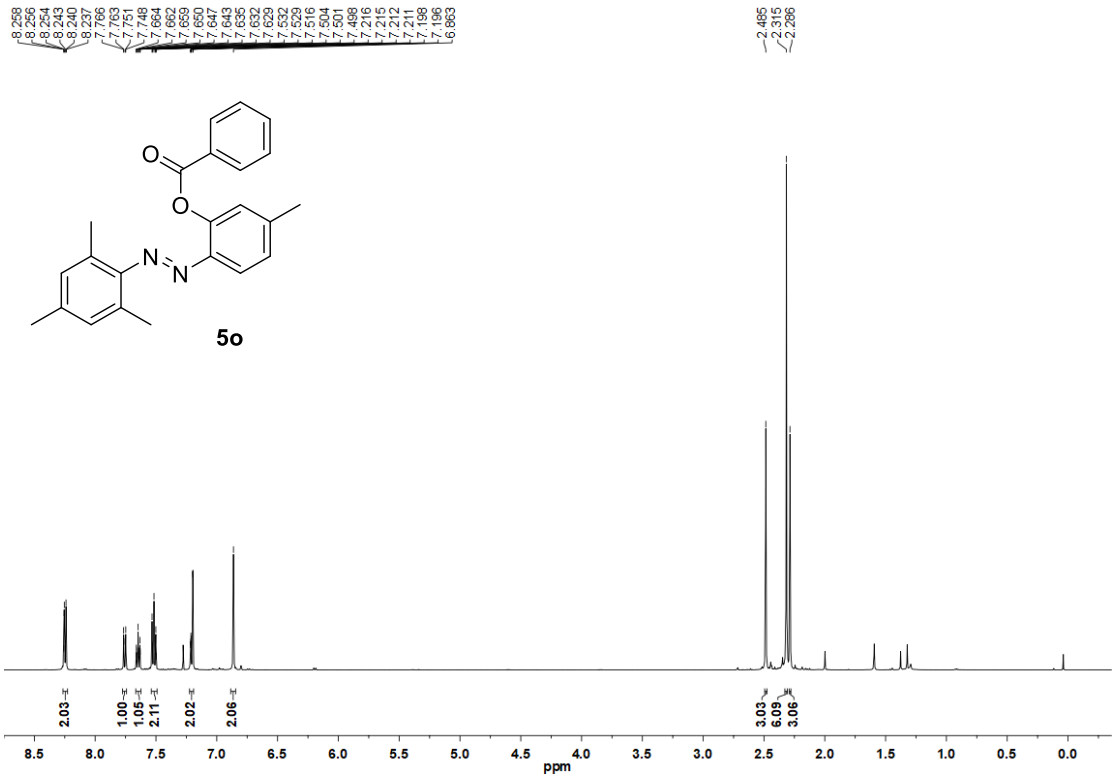
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N
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3.03
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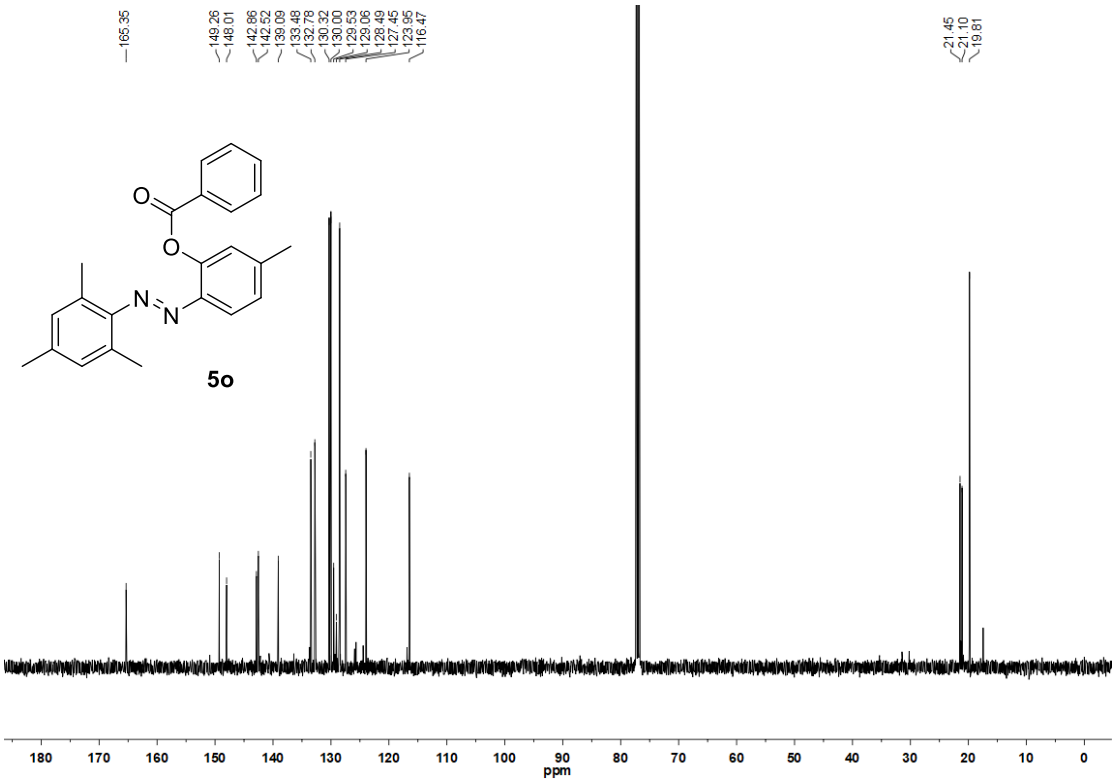
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123.95
116.47
21.45
21.10
19.81
O
O
N
N
5o
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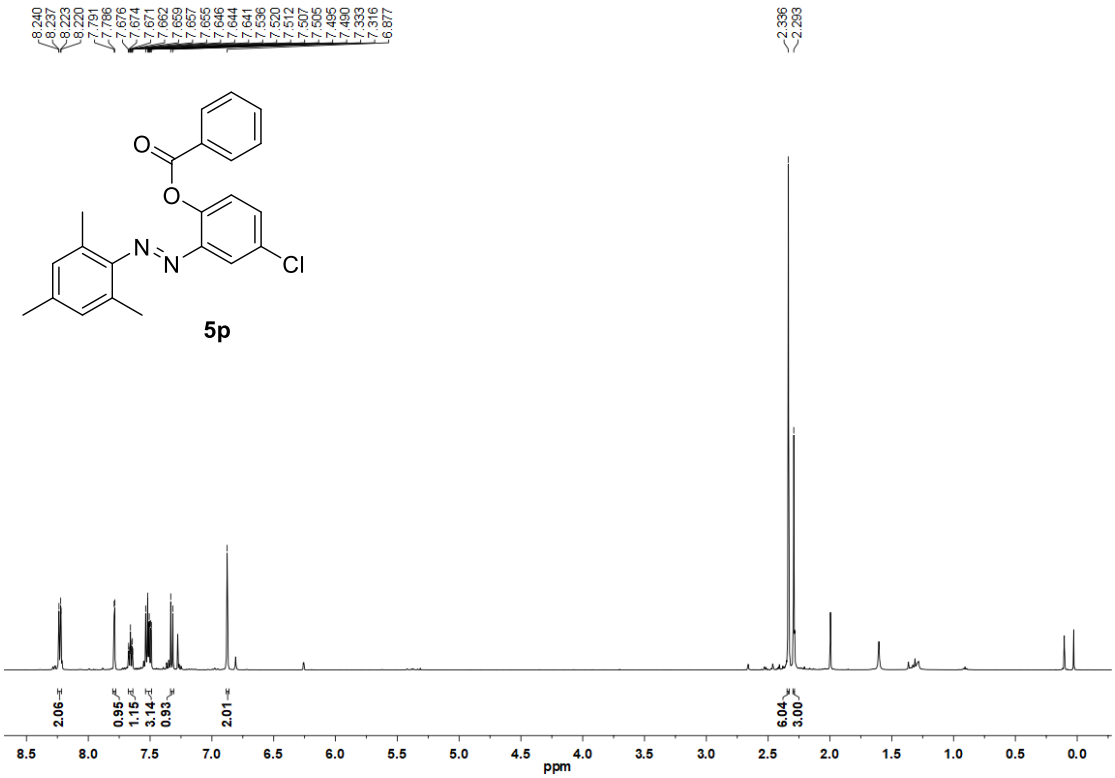
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7.641
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6.04
3.00
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6.0
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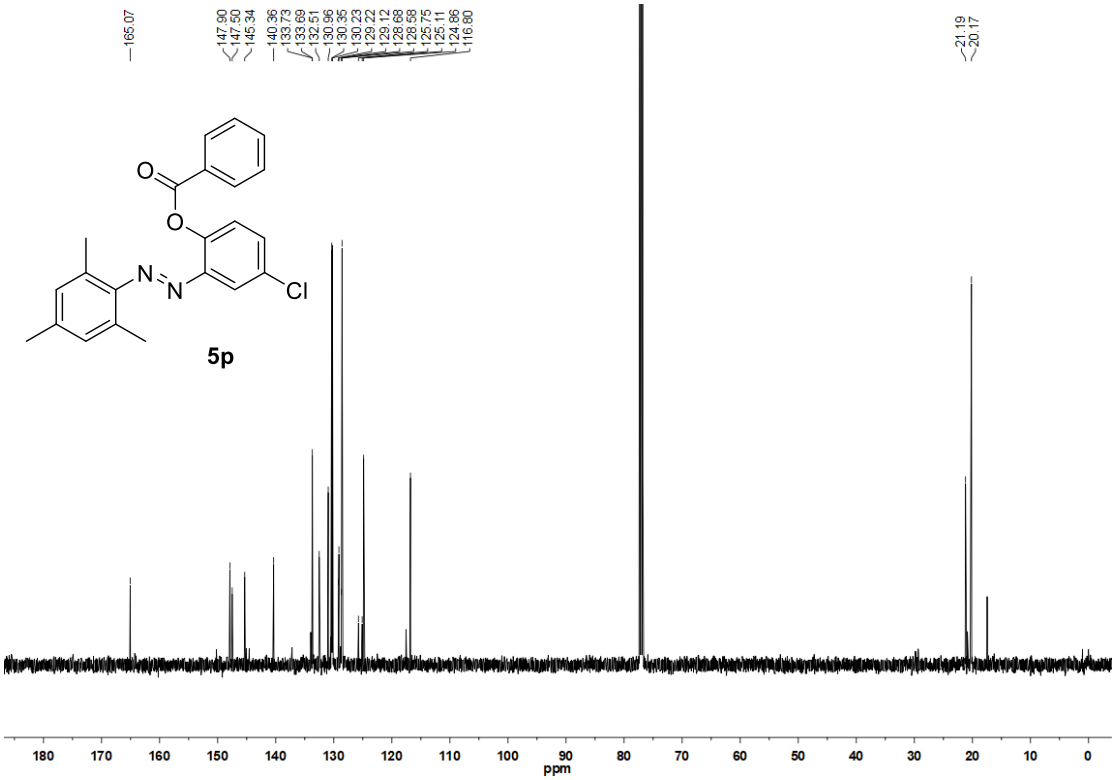
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125.11
124.86
116.80
21.19
20.17
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O
N
N
Cl
5p
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100
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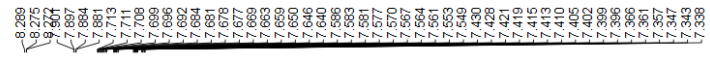
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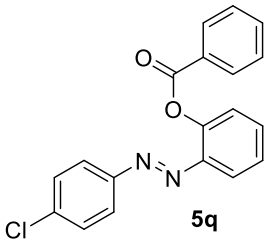
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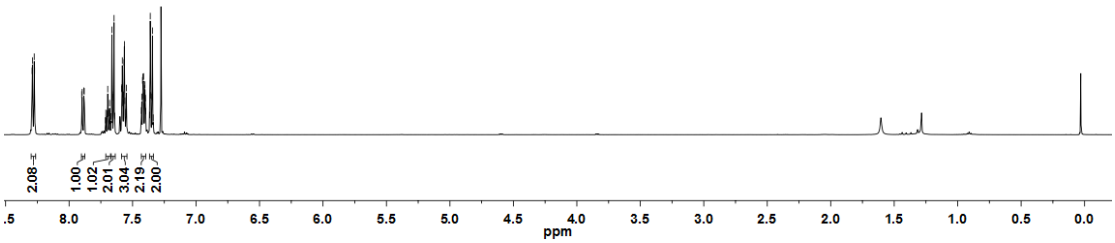
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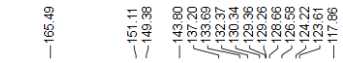
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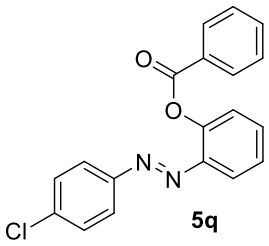
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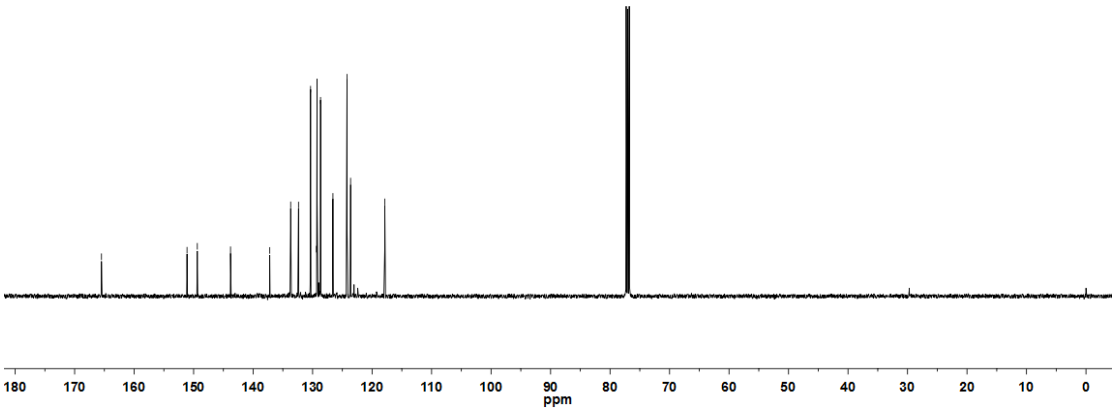
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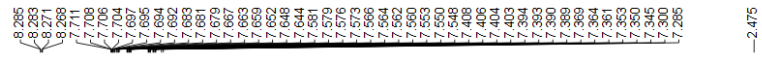
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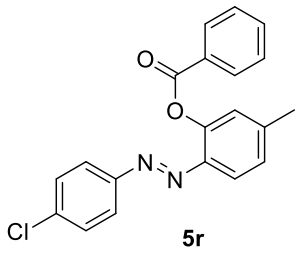
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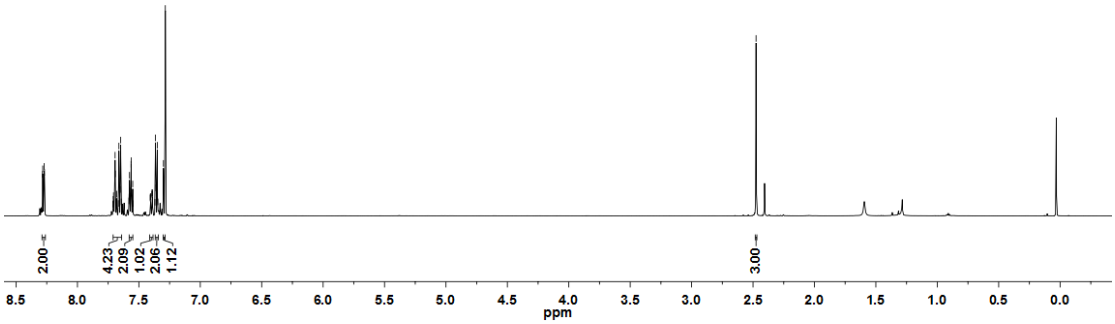
5r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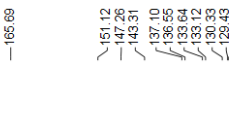
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123.24
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N
Cl

5r

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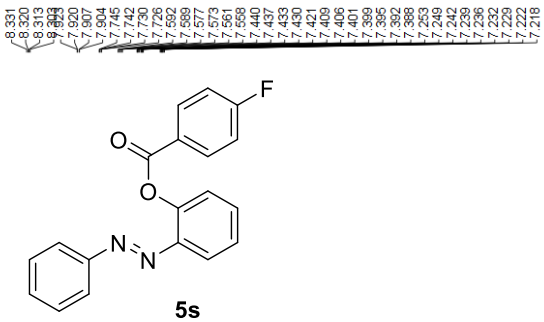
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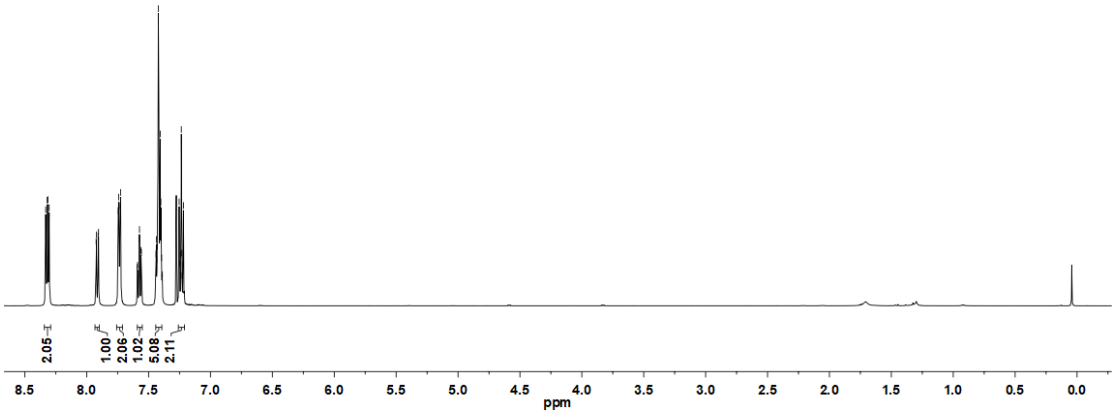
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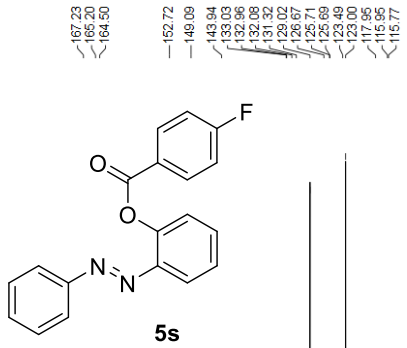
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125.69
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123.00
117.95
115.95
115.77
F
O
O
N
N
5s

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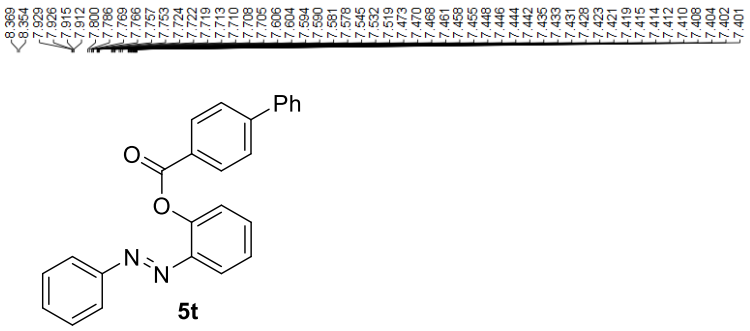
10
0
ppm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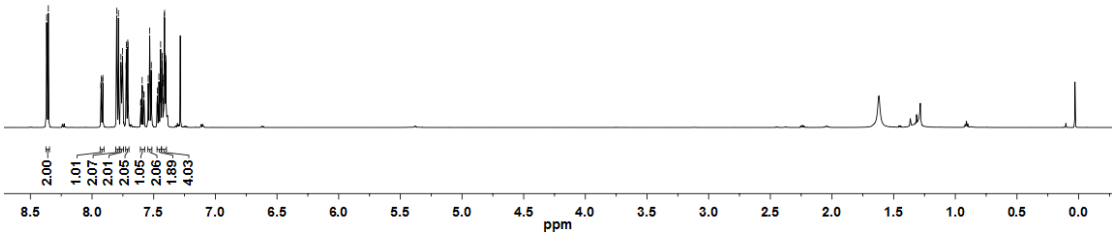
7.402
7.401
Ph
O
O
N
N
5t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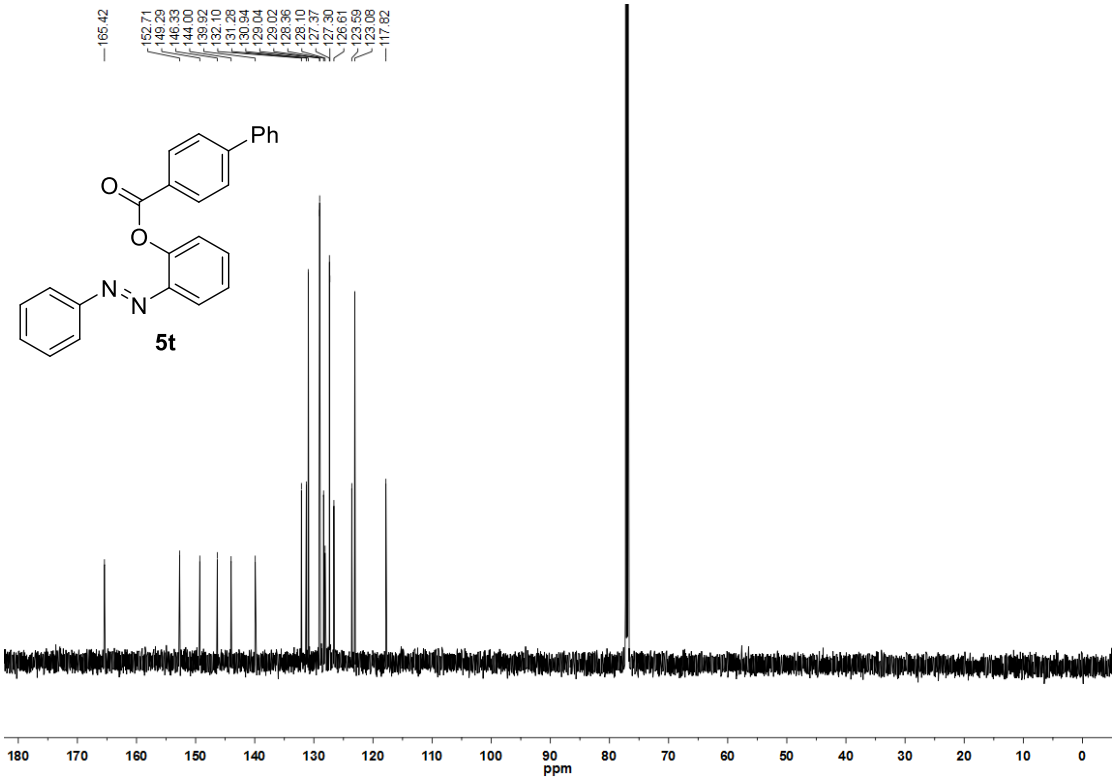
1.01
2.07
2.01
2.05
1.05
2.06
1.89
4.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


165.42
152.71
149.29
146.33
144.00
139.92
132.10
131.28
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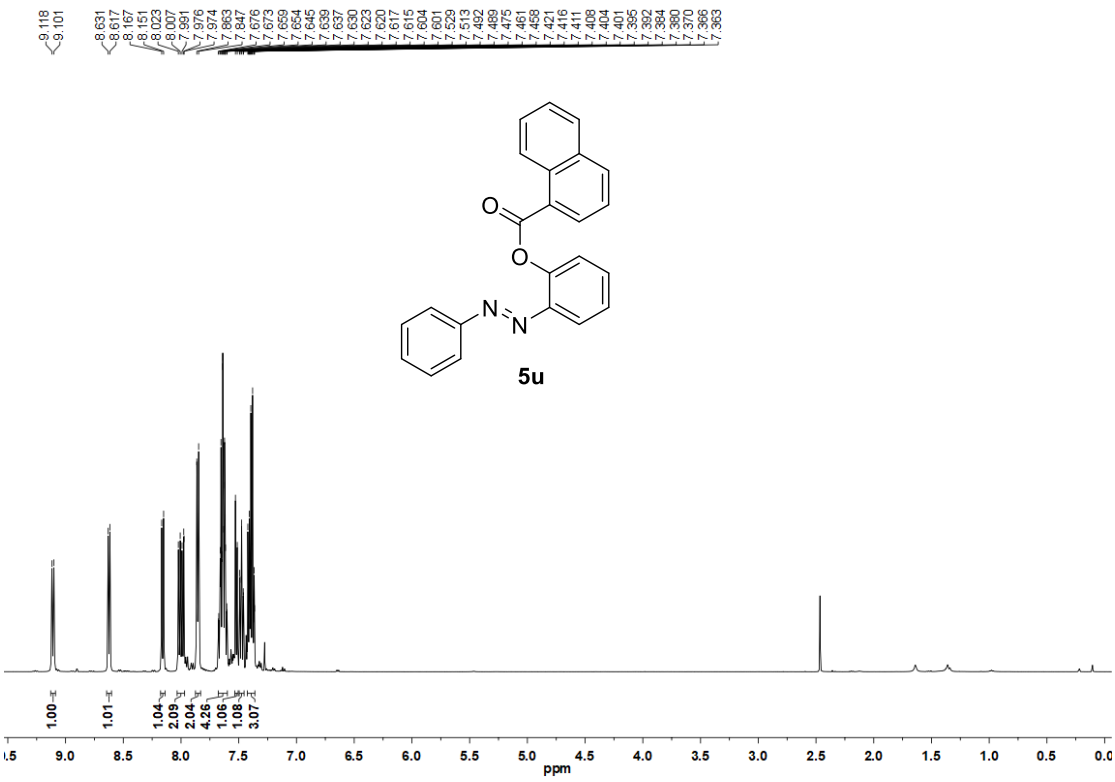
129.04
129.02
128.36
128.10
127.37
127.30
126.61
123.59
123.08
117.82
Ph
O
O
N
N
5t
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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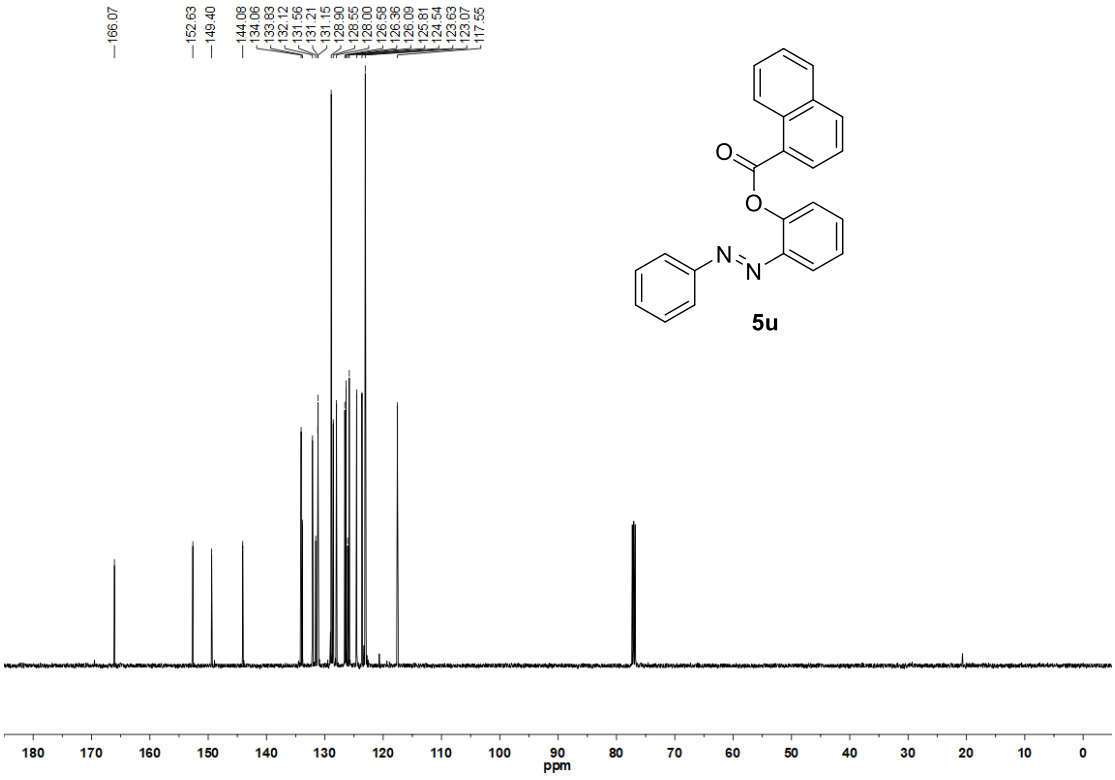
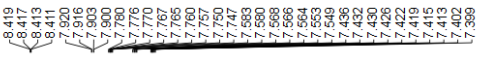
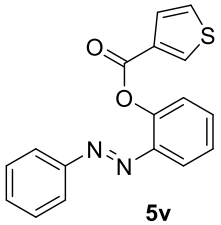
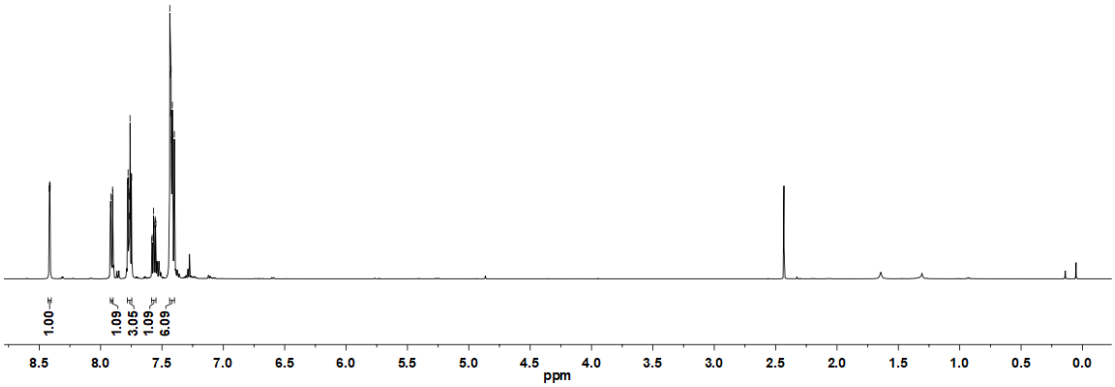
9.101
8.631
8.617
8.157
8.151
8.023
8.007
7.991
7.976
7.974
7.863
7.847
7.676
7.673
7.659
7.654
7.645
7.639
7.637
7.630
7.623
7.620
7.617
7.615
7.604
7.601
7.529
7.513
7.492
7.489
7.475
7.461
7.458
7.421
7.416
7.411
7.408
7.404
7.401
7.395
7.392
7.384
7.380
7.370
7.366
7.363
O
O
N
N
5u
1.00
1.01
1.04
2.09
2.04
4.26
1.06
1.08
3.07
ppm

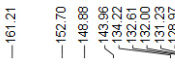

166.07
152.63
149.40
144.08
134.06
133.83
132.12
131.56
131.21
131.15
128.90
128.55
128.00
126.58
126.36
126.09
125.81
124.54
123.63
123.07
117.55
O
O
N
N
5u
ppm

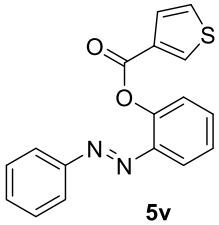

8.419
8.417
8.413
8.411
7.920
7.916
7.903
7.900
7.780
7.776
7.770
7.767
7.765
7.760
7.757
7.750
7.747
7.583
7.580
7.568
7.566
7.564
7.553
7.549
7.436
7.432
7.430
7.426
7.422
7.419
7.415
7.413
7.402
7.399


O
S
O
N
N

5v

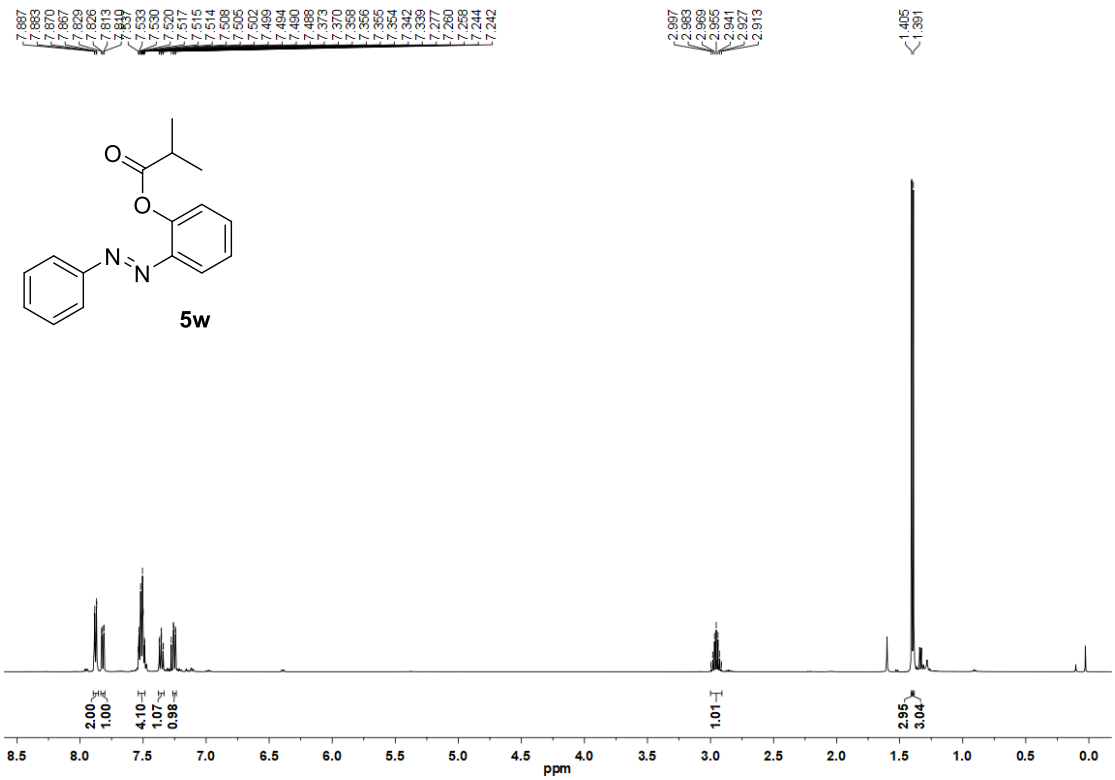

1.00
1.09
3.05
1.09
6.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

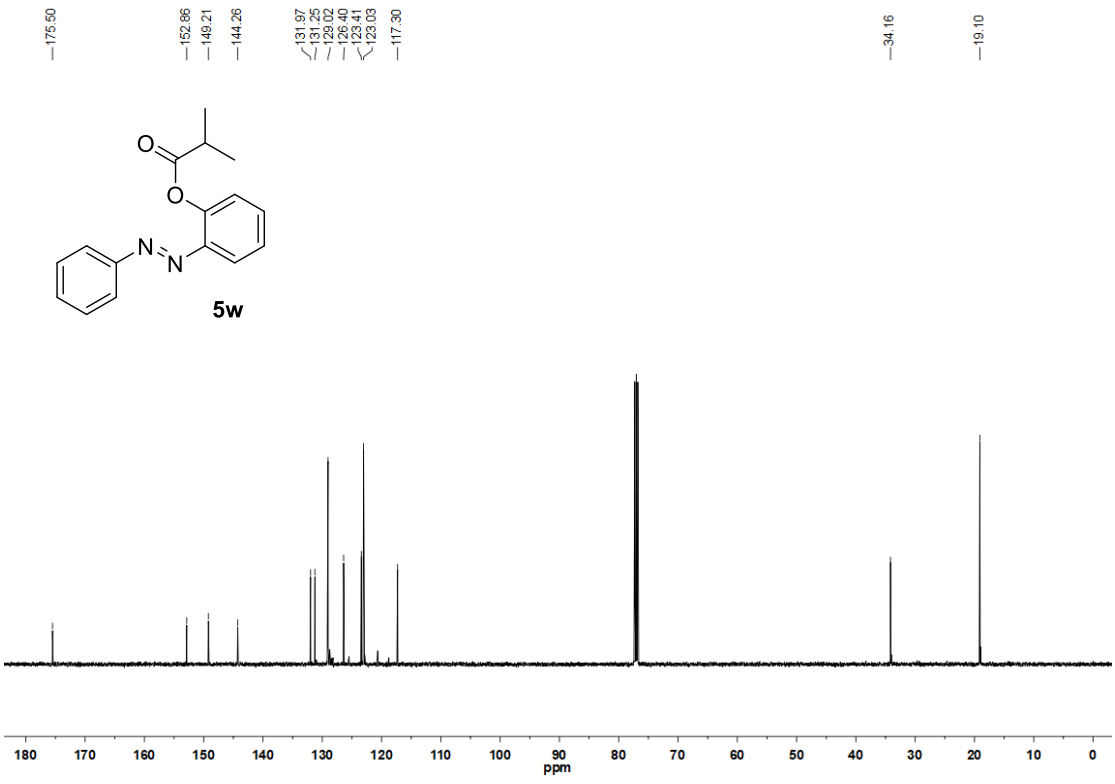

161.21
152.70
148.88
143.96
134.22
132.61
132.00
131.23
128.97
128.34
126.54
126.37
123.51
123.01
117.81

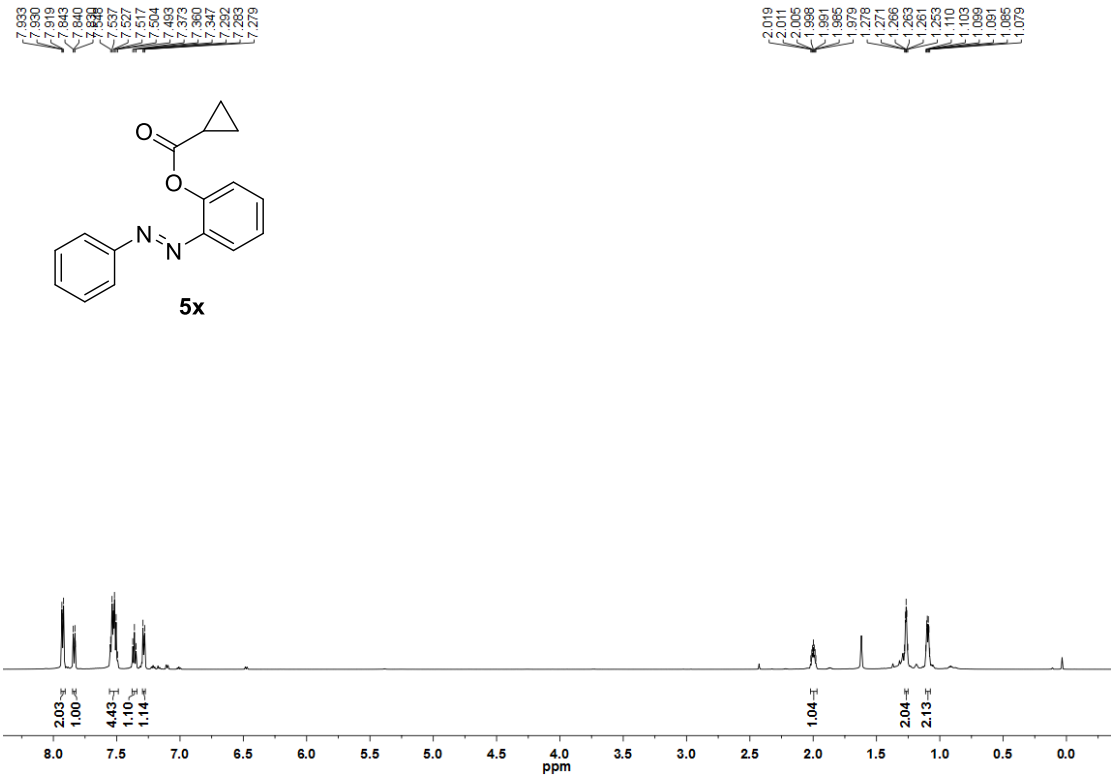

O
S
O
N
N

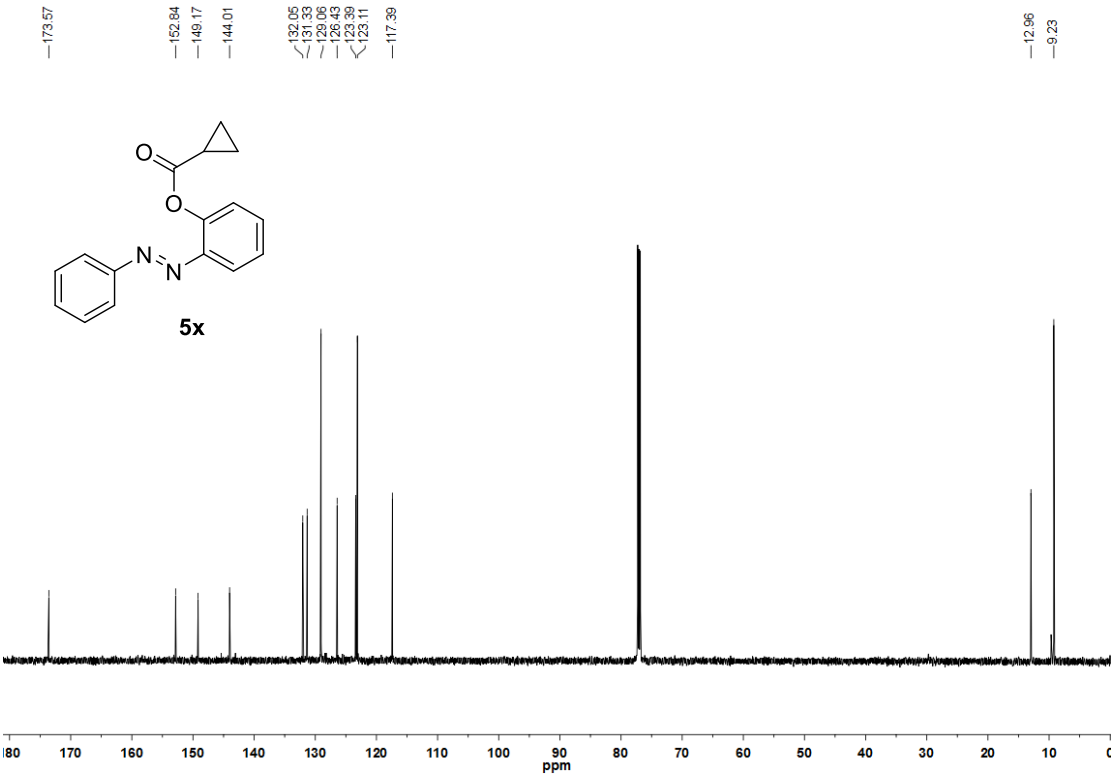
5v

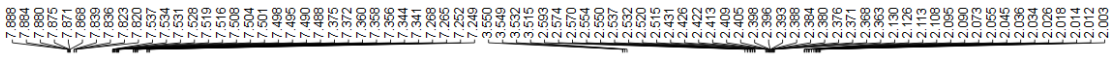
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

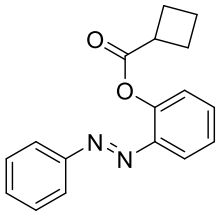

7.887
7.883
7.870
7.867
7.829
7.826
7.813
7.810
7.533
7.530
7.520
7.517
7.515
7.514
7.508
7.505
7.502
7.496
7.494
7.490
7.488
7.373
7.370
7.369
7.368
7.366
7.365
7.354
7.342
7.339
7.277
7.260
7.259
7.244
7.242
2.997
2.983
2.969
2.955
2.941
2.927
2.913
1.405
1.391
5w
2.00
1.00
4.10
1.07
0.98
1.01
2.95
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


175.50
152.86
149.21
144.26
131.97
131.25
129.02
126.40
123.41
123.03
117.30
34.16
19.10
5w
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

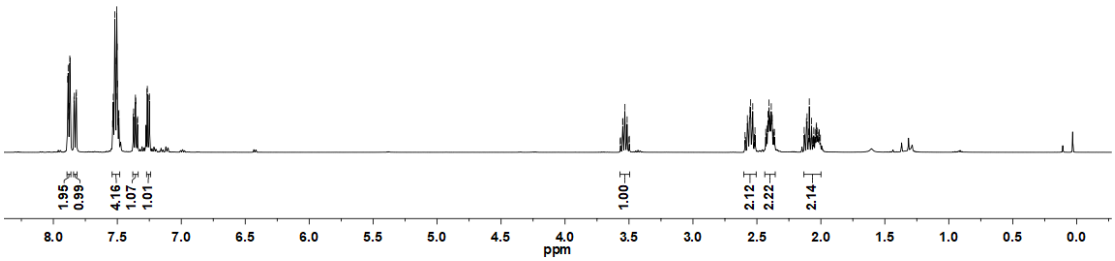

7.933
7.930
7.919
7.843
7.840
7.527
7.517
7.504
7.493
7.373
7.360
7.347
7.282
7.263
7.279
2.019
2.011
2.005
1.998
1.991
1.985
1.979
1.278
1.271
1.266
1.263
1.261
1.253
1.110
1.103
1.099
1.091
1.085
1.079
O
O
N
N
5x
2.03
1.00
4.43
1.10
1.14
1.04
2.04
2.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

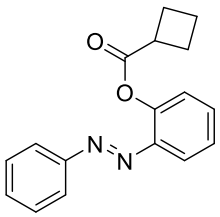

173.57
152.84
149.17
144.01
132.05
131.33
129.06
126.43
123.39
123.11
117.39
12.96
9.23
O
O
N
N
5x
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



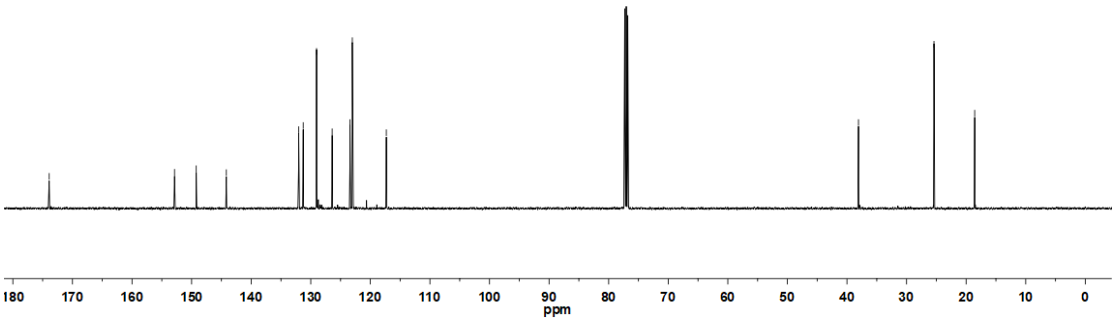


5y


1.95
0.99
4.16
1.07
1.01
1.00
2.12
2.22
2.14
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm



5y


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

X. DFT optimized Cartesian coordinates of all structures

Optimized Cartesian coordinates and single-point calculation energies ($\Delta E_{(SCF\ Done)}$, a.u.) for all of the stationary as well as the imaginary frequencies (IF, cm^{-1}) of transition states.

I_{Cl}, $\Delta E_{(SCF\ Done)}$ = -1620.848646 a.u.

N	-0.439509000	-0.568795000	-0.034504000
N	0.375900000	-1.512287000	0.009465000
C	-1.832273000	-0.917321000	-0.033895000
C	-2.252114000	-2.130898000	0.530579000
C	-2.751842000	-0.030339000	-0.603869000
C	-3.604656000	-2.452532000	0.512342000
H	-1.522301000	-2.792510000	0.981976000
C	-4.102417000	-0.371231000	-0.623580000
H	-2.405158000	0.901857000	-1.038296000
C	-4.531159000	-1.577126000	-0.064840000
H	-3.938877000	-3.384467000	0.958410000
H	-4.818268000	0.309381000	-1.073712000
H	-5.586672000	-1.833187000	-0.071571000
C	1.757488000	-1.322711000	0.130859000
C	2.356097000	-0.346472000	0.950387000
C	2.547603000	-2.256304000	-0.564678000
C	3.746419000	-0.286670000	1.018950000
C	3.932564000	-2.157776000	-0.513026000
H	2.056079000	-3.020366000	-1.157989000
C	4.533671000	-1.171891000	0.277888000
H	4.214492000	0.452202000	1.662495000
H	4.544776000	-2.855380000	-1.076292000
H	5.616630000	-1.108480000	0.332958000
Pd	0.009478000	1.387881000	-0.086540000
Cl	0.578079000	1.393927000	-2.316376000
Cl	-0.501386000	1.775380000	2.137980000
H	1.748509000	0.305413000	1.568185000

TS_{Cl}, $\Delta E_{(SCF\ Done)}$ = -1620.802987 a.u., IF = -215.46 cm^{-1}

N	0.785821000	0.702669000	-0.009215000
N	0.239088000	1.840167000	0.134012000
C	2.193813000	0.631372000	-0.084664000
C	2.962561000	1.710262000	-0.554541000
C	2.795238000	-0.575999000	0.310214000
C	4.341679000	1.566613000	-0.633236000
H	2.468899000	2.627384000	-0.854730000
C	4.180664000	-0.697456000	0.232756000
H	2.178957000	-1.366453000	0.729165000

C	4.951579000	0.366048000	-0.242890000
H	4.947578000	2.388433000	-1.002924000
H	4.656693000	-1.618981000	0.552680000
H	6.030958000	0.264417000	-0.309172000
C	-1.151423000	1.748215000	0.145305000
C	-1.776215000	0.478764000	0.408138000
C	-1.914284000	2.889247000	-0.107653000
C	-3.180178000	0.386851000	0.275680000
C	-3.302134000	2.764698000	-0.194563000
H	-1.419327000	3.840768000	-0.271636000
C	-3.930908000	1.520936000	-0.020237000
H	-3.660790000	-0.570137000	0.450291000
H	-3.903246000	3.643231000	-0.410118000
H	-5.011541000	1.450000000	-0.099081000
Pd	-0.380759000	-0.902615000	-0.461950000
Cl	-1.661938000	-2.613641000	-1.235701000
Cl	-0.200992000	-1.123530000	2.593858000
H	-1.300137000	-0.143644000	1.297143000

TS_{Cl}', $\Delta E_{(SCF\ Done)}$ = -1620.785548 a.u., IF = -995.53 cm^{-1}

N	1.140595000	0.488507000	-0.082556000
N	0.628132000	1.639357000	-0.129335000
C	2.551694000	0.447382000	-0.099508000
C	3.379135000	1.586069000	-0.122284000
C	3.118742000	-0.836047000	-0.093244000
C	4.758593000	1.426684000	-0.139341000
H	2.922892000	2.569245000	-0.126385000
C	4.503915000	-0.986164000	-0.111954000
H	2.457214000	-1.696698000	-0.078284000
C	5.324156000	0.143591000	-0.134412000
H	5.402762000	2.301479000	-0.156424000
H	4.941722000	-1.979976000	-0.109386000
H	6.404612000	0.029519000	-0.147913000
C	-0.781352000	1.678117000	-0.083285000
C	-1.652939000	0.582447000	0.190851000
C	-1.331880000	2.952937000	-0.273096000
C	-3.045491000	0.798178000	0.199319000
C	-2.711481000	3.147556000	-0.250679000
H	-0.647517000	3.776762000	-0.449950000
C	-3.572241000	2.072673000	-0.009810000
H	-3.710289000	-0.038478000	0.389061000
H	-3.116763000	4.141435000	-0.417315000
H	-4.647566000	2.222581000	0.010517000
Pd	-0.984754000	-1.314019000	0.023255000

Cl	-1.514397000	-1.600110000	-2.175184000
Cl	-0.780503000	-0.984030000	2.500529000
H	-1.321289000	0.073787000	1.533403000

TS_{Cl}'', $\Delta E_{(SCF\ Done)}$ = -1620.776233 a.u., IF = -1013.91 cm^{-1}

N	0.857161000	0.547638000	-0.296950000
N	0.249493000	1.622647000	-0.049676000
C	2.270531000	0.601184000	-0.305943000
C	3.008880000	1.716467000	0.125901000
C	2.924710000	-0.544145000	-0.780247000
C	4.396620000	1.674333000	0.071550000
H	2.483359000	2.587919000	0.498856000
C	4.316382000	-0.574352000	-0.834982000
H	2.330314000	-1.392216000	-1.108250000
C	5.052839000	0.533066000	-0.408735000
H	4.974737000	2.529695000	0.409503000
H	4.823988000	-1.459883000	-1.205362000
H	6.138402000	0.508534000	-0.443824000
C	-1.155531000	1.566695000	0.003766000
C	-1.952274000	0.399006000	0.139398000
C	-1.794550000	2.804682000	-0.180386000
C	-3.335066000	0.476203000	-0.051981000
C	-3.177066000	2.883686000	-0.305580000
H	-1.165112000	3.684724000	-0.266619000
C	-3.943908000	1.718428000	-0.259061000
H	-3.943170000	-0.420584000	-0.011079000
H	-3.653189000	3.846783000	-0.461726000
H	-5.023104000	1.764353000	-0.371915000
Pd	-0.676733000	-1.218029000	0.245041000
Cl	-1.406728000	-1.935199000	-1.813491000
Cl	0.159252000	-0.973340000	2.393785000
H	-2.045397000	-0.898339000	0.967711000

B_{Cl}, $\Delta E_{(SCF\ Done)}$ = -1160.036225 a.u.

N	-0.780453000	0.589176000	-0.030183000
N	-0.255916000	1.749073000	-0.036712000
C	-2.196049000	0.505662000	-0.018044000
C	-3.014514000	1.635468000	0.148643000
C	-2.768670000	-0.764806000	-0.170899000
C	-4.395545000	1.479450000	0.158990000
H	-2.555654000	2.609306000	0.269616000
C	-4.154985000	-0.908743000	-0.160458000
H	-2.131607000	-1.635228000	-0.311521000
C	-4.970666000	0.211539000	0.005333000

H	-5.030838000	2.350603000	0.290865000
H	-4.593912000	-1.894281000	-0.282424000
H	-6.051038000	0.100458000	0.016866000
C	1.125297000	1.691535000	-0.030165000
C	1.766636000	0.422853000	-0.010126000
C	1.879330000	2.876598000	-0.044279000
C	3.153488000	0.350867000	-0.002457000
C	3.267687000	2.795618000	-0.038709000
H	1.361368000	3.830597000	-0.058794000
C	3.894560000	1.543651000	-0.018264000
H	3.654169000	-0.609848000	0.013966000
H	3.865187000	3.702007000	-0.050029000
H	4.979985000	1.486657000	-0.014980000
Pd	0.475452000	-1.041570000	0.010460000
Cl	1.786276000	-2.907878000	0.070363000

HCl, **$\Delta E_{(\text{SCF Done})}$ = -460.798054 a.u.**

Cl	0.000000000	0.000000000	0.071636000
H	0.000000000	0.000000000	-1.217812000

B_{Cl}'', $\Delta E_{(\text{SCF Done})}$ = -1620.804947 a.u.

N	0.773879000	0.616245000	0.000095000
N	0.143501000	1.711385000	0.000345000
C	2.185735000	0.672747000	0.000162000
C	2.900227000	1.883980000	-0.000070000
C	2.868131000	-0.551737000	0.000425000
C	4.288790000	1.853964000	-0.000007000
H	2.355900000	2.820797000	-0.000314000
C	4.261215000	-0.569891000	0.000506000
H	2.305385000	-1.480381000	0.000590000
C	4.972904000	0.630894000	0.000291000
H	4.845694000	2.786547000	-0.000206000
H	4.787599000	-1.519409000	0.000733000
H	6.059096000	0.618148000	0.000339000
C	-1.244061000	1.563773000	0.000264000
C	-1.883151000	0.306338000	-0.000065000
C	-2.038590000	2.721718000	0.000536000
C	-3.257654000	0.178942000	-0.000044000
C	-3.425939000	2.613694000	0.000538000
H	-1.538391000	3.685179000	0.000718000
C	-4.029151000	1.353817000	0.000249000
H	-3.737361000	-0.792014000	-0.000339000
H	-4.039207000	3.509291000	0.000744000
H	-5.112099000	1.267918000	0.000268000

Pd	-0.571444000	-1.173802000	-0.000249000
Cl	-0.529242000	-1.378302000	-2.302590000
Cl	-0.529764000	-1.379716000	2.301982000
H	-1.649476000	-2.257706000	-0.000530000

I_{NO3}, $\Delta E_{(SCF\ Done)}$ = -1260.923318 a.u.

N	0.612138000	0.835380000	-0.344351000
N	-0.017384000	1.923086000	-0.321675000
C	2.017116000	0.944698000	-0.609353000
C	2.714818000	2.111170000	-0.260714000
C	2.678229000	-0.130499000	-1.215866000
C	4.075173000	2.197379000	-0.535636000
H	2.187704000	2.921291000	0.229266000
C	4.038788000	-0.026253000	-1.495904000
H	2.129812000	-1.030921000	-1.471480000
C	4.738962000	1.132989000	-1.155365000
H	4.622283000	3.092787000	-0.256172000
H	4.551566000	-0.855924000	-1.972430000
H	5.802854000	1.204403000	-1.362038000
C	-1.365850000	1.974360000	0.060409000
C	-1.925962000	1.207751000	1.101358000
C	-2.138343000	2.940889000	-0.609185000
C	-3.270868000	1.385040000	1.420069000
C	-3.487453000	3.077377000	-0.303378000
H	-1.668032000	3.547575000	-1.376420000
C	-4.055976000	2.298281000	0.710554000
H	-3.703810000	0.812623000	2.235236000
H	-4.092925000	3.800422000	-0.841485000
H	-5.105209000	2.421034000	0.963407000
Pd	-0.214788000	-1.035901000	-0.144305000
H	-1.297749000	0.549513000	1.691678000
O	-1.796945000	-0.982448000	-1.495624000
N	-2.123699000	-2.223548000	-1.263440000
O	-1.351277000	-2.793188000	-0.394196000
O	-3.044702000	-2.770569000	-1.802357000
O	0.613077000	-0.173570000	2.585548000
N	1.376692000	-1.097927000	2.285448000
O	1.242071000	-1.675068000	1.079651000
O	2.263745000	-1.548828000	2.985063000

TS_{NO3}, $\Delta E_{(SCF\ Done)}$ = -1260.889536 a.u., IF = -107.08 cm^{-1}

N	-0.022360000	-2.195212000	-0.204112000
N	-0.653800000	-1.095770000	-0.199757000
C	1.362303000	-2.016651000	-0.202190000

C	2.178670000	-3.063905000	-0.633178000
C	1.908030000	-0.758326000	0.209019000
C	3.553868000	-2.844551000	-0.736038000
H	1.732938000	-4.011338000	-0.917895000
C	3.294812000	-0.567793000	0.064306000
H	1.447194000	-0.275376000	1.208335000
C	4.108242000	-1.600613000	-0.404900000
H	4.198755000	-3.645958000	-1.084231000
H	3.732005000	0.379522000	0.367073000
H	5.179799000	-1.448470000	-0.493475000
C	-2.070263000	-1.133817000	-0.231452000
C	-2.753106000	-2.232395000	-0.781710000
C	-2.763858000	-0.036374000	0.302789000
C	-4.141841000	-2.220841000	-0.797187000
C	-4.156754000	-0.050389000	0.289912000
H	-2.213428000	0.778396000	0.763513000
C	-4.844996000	-1.132831000	-0.262977000
H	-4.681170000	-3.057897000	-1.230351000
H	-4.702218000	0.785898000	0.715588000
H	-5.931055000	-1.132169000	-0.280228000
Pd	0.395317000	0.623266000	-0.443047000
H	-2.189618000	-3.062111000	-1.192370000
O	1.117317000	-0.021894000	2.715869000
N	0.190314000	0.855325000	2.921520000
O	-0.306836000	1.457201000	1.923963000
O	-0.180966000	1.076853000	4.065388000
O	1.340483000	2.394152000	-0.909142000
N	0.299508000	2.922931000	-1.495762000
O	-0.716354000	2.131015000	-1.535816000
O	0.308350000	4.032580000	-1.951185000

TS_{NO3}', $\Delta E_{(SCF\ Done)}$ = -1260.886655 a.u., IF = -1380.50 cm^{-1}

N	-0.191028000	2.286583000	-0.338103000
N	-0.773028000	1.180021000	-0.131257000
C	1.191355000	2.248903000	-0.196967000
C	1.847672000	3.482216000	-0.091630000
C	1.889987000	1.012638000	-0.058081000
C	3.205336000	3.512236000	0.220707000
H	1.272312000	4.394213000	-0.212947000
C	3.242419000	1.084175000	0.303665000
H	1.898787000	-0.125242000	-0.866851000
C	3.894261000	2.316581000	0.436981000
H	3.720134000	4.463729000	0.311749000
H	3.812236000	0.169650000	0.437319000

H	4.949032000	2.337072000	0.695303000
C	-2.195805000	1.191893000	-0.207890000
C	-2.912883000	2.318771000	0.224504000
C	-2.854426000	0.074894000	-0.737233000
C	-4.299775000	2.316894000	0.128254000
C	-4.243329000	0.097805000	-0.845074000
H	-2.285608000	-0.780968000	-1.083833000
C	-4.966952000	1.209592000	-0.407785000
H	-4.862969000	3.177726000	0.476252000
H	-4.758564000	-0.760210000	-1.265472000
H	-6.050800000	1.213074000	-0.478509000
Pd	0.384847000	-0.435919000	0.325180000
H	-2.378397000	3.166208000	0.638227000
O	2.424636000	-1.208636000	-1.469015000
N	2.433622000	-2.170563000	-0.596191000
O	1.726718000	-2.026114000	0.481946000
O	3.095060000	-3.162641000	-0.770178000
O	-1.085032000	-1.561525000	1.179802000
N	-1.431002000	-2.640708000	0.467404000
O	-1.016554000	-2.717706000	-0.699396000
O	-2.154356000	-3.447117000	1.021944000

TS_{NO3}'', $\Delta E_{(SCF\ Done)}$ = -1260.863171 a.u., IF = -1211.96 cm^{-1}

N	-0.815581000	-1.808778000	-0.747371000
N	-1.243896000	-0.688625000	-0.360724000
C	0.586114000	-1.977327000	-0.666889000
C	1.079152000	-3.092800000	-1.353738000
C	1.464759000	-1.156154000	0.102757000
C	2.442714000	-3.383770000	-1.338134000
H	0.376084000	-3.713324000	-1.900765000
C	2.836982000	-1.495118000	0.112793000
H	1.001425000	-1.040372000	1.366611000
C	3.326107000	-2.589918000	-0.599074000
H	2.816061000	-4.240416000	-1.892209000
H	3.523184000	-0.899280000	0.709452000
H	4.384916000	-2.830435000	-0.570805000
C	-2.646404000	-0.522108000	-0.383650000
C	-3.557094000	-1.514552000	-0.792236000
C	-3.111731000	0.732821000	0.038610000
C	-4.918216000	-1.239077000	-0.775206000
C	-4.479634000	0.999092000	0.053221000
H	-2.388142000	1.480076000	0.350813000
C	-5.382789000	0.014979000	-0.353425000
H	-5.626723000	-2.000374000	-1.089721000

H	-4.839025000	1.970137000	0.380594000
H	-6.449721000	0.220067000	-0.343043000
Pd	1.039876000	0.897169000	0.170790000
H	-3.178140000	-2.477737000	-1.114132000
O	0.576550000	-1.092009000	2.558384000
N	0.405086000	0.118770000	2.988473000
O	0.620288000	1.098751000	2.178836000
O	0.058294000	0.325512000	4.125786000
O	1.471155000	1.264112000	-1.811848000
N	1.236060000	2.546752000	-1.721166000
O	0.894991000	2.917488000	-0.534208000
O	1.333015000	3.289727000	-2.659176000

TS_{NO3}''', $\Delta E_{(SCF\ Done)}$ = -1260.848494 a.u., IF = -1348.43 cm^{-1}

N	1.103857000	0.902106000	-0.158263000
N	0.577494000	1.883955000	-0.749690000
C	2.491956000	0.741698000	-0.362407000
C	3.271797000	1.580422000	-1.182590000
C	3.084474000	-0.339982000	0.308687000
C	4.629578000	1.327513000	-1.321306000
H	2.796105000	2.410108000	-1.692428000
C	4.449092000	-0.583812000	0.162792000
H	2.466119000	-0.969080000	0.940659000
C	5.221416000	0.246755000	-0.650890000
H	5.236522000	1.970031000	-1.953174000
H	4.906729000	-1.420072000	0.682778000
H	6.284892000	0.056569000	-0.766944000
C	-0.817973000	2.021274000	-0.576787000
C	-1.681884000	1.082019000	0.065579000
C	-1.348524000	3.198817000	-1.116016000
C	-3.062617000	1.372614000	0.111177000
C	-2.716910000	3.462134000	-1.040582000
H	-0.667487000	3.894807000	-1.595381000
C	-3.580442000	2.552504000	-0.424505000
H	-3.733019000	0.666689000	0.595023000
H	-3.110167000	4.380807000	-1.466881000
H	-4.645263000	2.757781000	-0.366969000
Pd	-1.127090000	-0.937227000	0.151199000
H	-1.310014000	0.695130000	1.334409000
O	-1.363017000	-1.634707000	-1.773933000
N	-0.985727000	-2.852710000	-1.480143000
O	-0.686674000	-3.001349000	-0.236561000
O	-0.931018000	-3.727040000	-2.301169000
O	-1.085653000	-0.238310000	2.162267000

N	0.187141000	-0.116104000	2.765353000
O	0.450385000	0.984108000	3.194644000
O	0.841296000	-1.135553000	2.811508000

B_{NO3}, $\Delta E_{(SCF\ Done)}$ = -980.074700 a.u.

N	0.737922000	-0.915922000	-0.030884000
N	0.219934000	-2.078303000	-0.035040000
C	2.158119000	-0.841277000	-0.016970000
C	2.758957000	0.407833000	-0.226975000
C	2.951175000	-1.981860000	0.203449000
C	4.149689000	0.513263000	-0.224034000
H	2.147635000	1.286600000	-0.396846000
C	4.334951000	-1.860402000	0.207126000
H	2.470870000	-2.938185000	0.369981000
C	4.940129000	-0.615356000	-0.006940000
H	4.610746000	1.482165000	-0.390231000
H	4.948098000	-2.739912000	0.381824000
H	6.022942000	-0.529394000	0.000032000
C	-1.162462000	-2.047229000	-0.028933000
C	-1.803844000	-0.782075000	-0.013713000
C	-1.898800000	-3.242416000	-0.039966000
C	-3.191721000	-0.728682000	-0.007591000
C	-3.289011000	-3.172243000	-0.035262000
H	-1.374683000	-4.193178000	-0.051482000
C	-3.927330000	-1.925450000	-0.019331000
H	-3.706163000	0.228436000	0.004941000
H	-3.879303000	-4.083426000	-0.043863000
H	-5.013438000	-1.880208000	-0.016489000
Pd	-0.531098000	0.706430000	0.003999000
O	-1.759953000	2.384717000	0.047809000
N	-0.791407000	3.263545000	0.054758000
O	0.382911000	2.747003000	0.037286000
O	-1.008015000	4.448458000	0.076300000

HNO_3, **$\Delta E_{(SCF\ Done)}$ = -280.846432 a.u.**

H	-1.729078000	0.197181000	-0.000963000
O	-1.122821000	-0.571419000	0.000147000
N	0.147604000	0.038209000	-0.000053000
O	0.146921000	1.255007000	0.000062000
O	1.062882000	-0.741668000	-0.000043000

D_{Cl}, $\Delta E_{(SCF\ Done)}$ = -1579.820675 a.u.

N	1.448434000	0.819990000	-0.462367000
N	2.059884000	0.244954000	-1.404333000

C	1.517475000	2.218078000	-0.311923000
C	0.553018000	2.847815000	0.498788000
C	2.543770000	2.960973000	-0.931638000
C	0.614876000	4.225611000	0.680083000
H	-0.251845000	2.271267000	0.943159000
C	2.586120000	4.333971000	-0.740362000
H	3.282267000	2.452127000	-1.540031000
C	1.628212000	4.968023000	0.065323000
H	-0.128784000	4.720814000	1.295789000
H	3.371678000	4.916736000	-1.210789000
H	1.676497000	6.042299000	0.214476000
C	2.048810000	-1.129235000	-1.307139000
C	1.421618000	-1.762253000	-0.201670000
C	2.654276000	-1.927885000	-2.287593000
C	1.321344000	-3.133651000	-0.079223000
C	2.593770000	-3.315080000	-2.165421000
H	3.149869000	-1.445373000	-3.123805000
C	1.940451000	-3.907728000	-1.078736000
H	0.811620000	-3.603668000	0.752478000
H	3.049055000	-3.941813000	-2.925109000
H	1.897671000	-4.989640000	-0.995101000
Pd	0.765058000	-0.414170000	1.084879000
O	-1.143877000	-0.033340000	0.644522000
C	-1.644685000	-0.379941000	-0.548862000
O	-1.002200000	-0.761519000	-1.506262000
C	-3.122363000	-0.138236000	-0.530223000
C	-3.728474000	0.270910000	-1.729956000
C	-3.886462000	-0.311491000	0.640314000
C	-5.103200000	0.473895000	-1.761381000
H	-3.122265000	0.391627000	-2.621303000
C	-5.263824000	-0.108735000	0.593519000
H	-3.405091000	-0.622310000	1.560609000
C	-5.870379000	0.288809000	-0.600423000
H	-5.584988000	0.761969000	-2.690796000
H	-5.862346000	-0.259003000	1.486521000
H	-6.943546000	0.452039000	-0.633726000
Cl	0.508930000	-1.649062000	2.960186000

$TS1_{Cl}$, $\Delta E_{(SCF\ Done)}$ = -1579.820544 a.u., IF = -139.86 cm^{-1}

N	-1.536146000	-0.501183000	-0.578641000
N	-1.829066000	0.236554000	-1.565545000
C	-2.002009000	-1.826160000	-0.527651000
C	-1.410806000	-2.700286000	0.407358000
C	-3.051345000	-2.260733000	-1.365992000

C	-1.866805000	-4.010780000	0.493377000
H	-0.581678000	-2.366284000	1.022440000
C	-3.490689000	-3.571617000	-1.265151000
H	-3.499271000	-1.567691000	-2.068191000
C	-2.904717000	-4.446861000	-0.337209000
H	-1.411852000	-4.693372000	1.203544000
H	-4.298022000	-3.917630000	-1.902647000
H	-3.262311000	-5.469217000	-0.262160000
C	-1.455700000	1.552982000	-1.382873000
C	-0.659402000	1.923468000	-0.255527000
C	-1.902527000	2.552684000	-2.254956000
C	-0.262722000	3.241574000	-0.031228000
C	-1.554921000	3.880245000	-2.003789000
H	-2.529121000	2.274045000	-3.095995000
C	-0.760461000	4.220192000	-0.896279000
H	0.398925000	3.495979000	0.787253000
H	-1.895854000	4.659625000	-2.677456000
H	-0.494935000	5.257959000	-0.719417000
Pd	-0.774332000	0.478147000	1.103781000
O	1.031651000	-0.522387000	0.882879000
C	1.707664000	0.068967000	-0.044007000
O	1.274748000	1.040523000	-0.718184000
C	3.072376000	-0.471258000	-0.311556000
C	3.787049000	0.010052000	-1.420559000
C	3.635096000	-1.441306000	0.534735000
C	5.062988000	-0.482652000	-1.678512000
H	3.340400000	0.761330000	-2.061667000
C	4.914129000	-1.922092000	0.268359000
H	3.079396000	-1.798050000	1.394426000
C	5.626180000	-1.446559000	-0.836643000
H	5.620523000	-0.111317000	-2.532929000
H	5.356574000	-2.666052000	0.923689000
H	6.623461000	-1.825330000	-1.040428000
Cl	-0.271878000	1.556436000	3.023290000

P_{Cl}, $\Delta E_{(SCF\ Done)}$ = -1579.876497 a.u.

N	1.487230000	0.321534000	-0.625740000
N	1.482481000	-0.384561000	-1.664530000
C	2.063232000	1.621212000	-0.691118000
C	1.993001000	2.421018000	0.462076000
C	2.695206000	2.087830000	-1.858954000
C	2.562754000	3.691486000	0.449717000
H	1.489851000	2.057109000	1.354731000
C	3.258191000	3.356302000	-1.854357000

H	2.738660000	1.456497000	-2.738312000
C	3.195216000	4.158255000	-0.704964000
H	2.511942000	4.313491000	1.337318000
H	3.751058000	3.726544000	-2.747708000
H	3.640813000	5.148278000	-0.714017000
C	0.875600000	-1.659624000	-1.524842000
C	-0.469429000	-1.820339000	-1.139450000
C	1.634850000	-2.794484000	-1.839660000
C	-1.026813000	-3.088155000	-1.015517000
C	1.086365000	-4.065788000	-1.682852000
H	2.658117000	-2.661229000	-2.175744000
C	-0.237092000	-4.213608000	-1.259355000
H	-2.076000000	-3.183890000	-0.754802000
H	1.690177000	-4.940151000	-1.902277000
H	-0.669509000	-5.202747000	-1.150197000
Pd	0.988673000	-0.516593000	1.211258000
O	-1.003575000	-0.005050000	1.022265000
C	-1.695014000	-0.041803000	-0.018829000
O	-1.342954000	-0.716046000	-1.121114000
C	-2.955727000	0.684552000	-0.117908000
C	-3.789253000	0.535068000	-1.244964000
C	-3.338750000	1.530530000	0.943150000
C	-4.988585000	1.234717000	-1.306671000
H	-3.494235000	-0.120339000	-2.056233000
C	-4.542171000	2.220410000	0.870684000
H	-2.693964000	1.630921000	1.809311000
C	-5.365108000	2.074157000	-0.252178000
H	-5.633275000	1.125174000	-2.172838000
H	-4.842594000	2.870939000	1.685745000
H	-6.305332000	2.615238000	-0.304744000
Cl	0.823573000	-1.556057000	3.197090000

D_{NO3}, $\Delta E_{(SCF\ Done)}$ = -1399.85299 a.u.

N	1.591608000	0.504028000	-0.751016000
N	2.048922000	-0.256002000	-1.650998000
C	1.890003000	1.879016000	-0.759276000
C	1.111228000	2.740586000	0.038833000
C	2.954211000	2.376627000	-1.543128000
C	1.392774000	4.102151000	0.038201000
H	0.290503000	2.352527000	0.631030000
C	3.217765000	3.736873000	-1.528794000
H	3.546458000	1.693172000	-2.139860000
C	2.442191000	4.601446000	-0.739793000
H	0.794772000	4.773488000	0.645525000

H	4.033709000	4.131446000	-2.125867000
H	2.663164000	5.664367000	-0.730167000
C	1.812596000	-1.595694000	-1.418329000
C	1.059284000	-1.968657000	-0.273522000
C	2.312925000	-2.585921000	-2.271141000
C	0.748766000	-3.290234000	0.003108000
C	2.038487000	-3.923171000	-1.976415000
H	2.903364000	-2.300122000	-3.135574000
C	1.276924000	-4.271726000	-0.851703000
H	0.134874000	-3.564013000	0.855824000
H	2.412491000	-4.703296000	-2.631394000
H	1.073960000	-5.317425000	-0.640919000
Pd	0.733537000	-0.434468000	0.901382000
O	0.061856000	-1.325109000	2.621781000
N	0.070321000	-0.230885000	3.380712000
O	0.504364000	0.802307000	2.768934000
O	-0.299438000	-0.267624000	4.515049000
O	-1.126500000	0.174503000	0.368647000
C	-1.710294000	-0.390004000	-0.681726000
O	-1.187287000	-1.133957000	-1.492641000
C	-3.128112000	0.102575000	-0.774499000
C	-3.688146000	0.221909000	-2.056338000
C	-3.873049000	0.435829000	0.371546000
C	-5.007634000	0.642881000	-2.183341000
H	-3.098320000	-0.045987000	-2.926037000
C	-5.196192000	0.849297000	0.229803000
H	-3.425335000	0.349442000	1.354788000
C	-5.760494000	0.960112000	-1.042851000
H	-5.459034000	0.708497000	-3.168722000
H	-5.783236000	1.089076000	1.110839000
H	-6.789386000	1.290037000	-1.151910000

$TS1_{NO3}$, $\Delta E_{(SCF\ Done)}$ = -1399.852805 a.u., IF = -47.6 cm^{-1}

N	-1.487003000	-0.368409000	-0.915495000
N	-1.724835000	0.443194000	-1.857474000
C	-1.939580000	-1.695465000	-0.994850000
C	-1.408806000	-2.639739000	-0.091819000
C	-2.910312000	-2.069262000	-1.951842000
C	-1.841792000	-3.958611000	-0.159845000
H	-0.658175000	-2.346916000	0.633044000
C	-3.328301000	-3.388709000	-2.001646000
H	-3.311780000	-1.324161000	-2.628141000
C	-2.798898000	-4.334576000	-1.108243000
H	-1.434969000	-4.693114000	0.527191000

H	-4.074098000	-3.688580000	-2.730832000
H	-3.139987000	-5.364420000	-1.151571000
C	-1.370783000	1.744978000	-1.559209000
C	-0.664424000	2.005531000	-0.348051000
C	-1.734548000	2.807931000	-2.390900000
C	-0.280967000	3.296920000	0.011709000
C	-1.389708000	4.106785000	-2.007785000
H	-2.289804000	2.609627000	-3.301885000
C	-0.689268000	4.349849000	-0.814014000
H	0.305264000	3.478877000	0.906843000
H	-1.661904000	4.941459000	-2.645701000
H	-0.433669000	5.368205000	-0.537599000
Pd	-0.787774000	0.466620000	0.859321000
O	-0.264675000	1.261234000	2.665384000
N	-0.583477000	0.201145000	3.407156000
O	-1.084361000	-0.754595000	2.725713000
O	-0.401718000	0.201411000	4.586210000
O	1.069503000	-0.411725000	0.585386000
C	1.796741000	0.207183000	-0.299350000
O	1.423664000	1.177401000	-0.979441000
C	3.172791000	-0.368037000	-0.473135000
C	3.945505000	0.079691000	-1.556081000
C	3.679366000	-1.325790000	0.419973000
C	5.227854000	-0.431175000	-1.737746000
H	3.539361000	0.822519000	-2.232908000
C	4.965744000	-1.824624000	0.229392000
H	3.077034000	-1.661311000	1.256219000
C	5.737834000	-1.381631000	-0.847971000
H	5.832417000	-0.081546000	-2.569178000
H	5.365324000	-2.559157000	0.921933000
H	6.739785000	-1.774813000	-0.993033000

P_{NO3}, $\Delta E_{(SCF\ Done)}$ = -1399.926669 a.u.

N	-0.822740000	-0.855811000	-0.931880000
N	0.151834000	-0.272087000	-1.489471000
C	-0.857893000	-2.262743000	-0.871697000
C	-2.043710000	-2.870482000	-0.422690000
C	0.258002000	-3.034186000	-1.255342000
C	-2.116159000	-4.258386000	-0.366567000
H	-2.893988000	-2.263583000	-0.130094000
C	0.167973000	-4.416188000	-1.189321000
H	1.164460000	-2.543672000	-1.589095000
C	-1.014364000	-5.029778000	-0.747324000
H	-3.028278000	-4.736751000	-0.025553000

H	1.019664000	-5.023857000	-1.477808000
H	-1.071613000	-6.112900000	-0.697645000
C	-0.038577000	1.128235000	-1.421194000
C	1.020737000	1.976453000	-1.057515000
C	-1.328639000	1.678956000	-1.723004000
C	0.797802000	3.349848000	-0.992698000
C	-1.517341000	3.081952000	-1.648573000
H	-2.013869000	1.093368000	-2.337959000
C	-0.462575000	3.902265000	-1.279759000
H	1.625480000	3.987144000	-0.696902000
H	-2.481611000	3.501962000	-1.916413000
H	-0.597290000	4.977398000	-1.224325000
Pd	-2.010823000	0.464892000	0.069410000
O	-3.162703000	1.674367000	1.256841000
N	-3.515036000	0.696246000	2.051410000
O	-2.985872000	-0.437468000	1.684320000
O	-4.231527000	0.828357000	2.990180000
O	1.437225000	0.351235000	1.016352000
C	2.403667000	0.663421000	0.356896000
O	2.268138000	1.493009000	-0.767003000
C	3.801686000	0.272621000	0.587786000
C	4.846602000	0.666200000	-0.265939000
C	4.072460000	-0.522882000	1.715137000
C	6.149732000	0.261144000	0.009609000
H	4.637498000	1.281601000	-1.133415000
C	5.377913000	-0.920342000	1.984022000
H	3.254426000	-0.813018000	2.366051000
C	6.415870000	-0.529337000	1.131861000
H	6.959106000	0.563048000	-0.647944000
H	5.589300000	-1.531249000	2.856218000
H	7.434982000	-0.839582000	1.343988000