Supporting Information

Stereoselective Synthesis of 1,3- and 1,4-Dicarbonyl-alkenes from Cyclopropenes in Catalytic Zinc System

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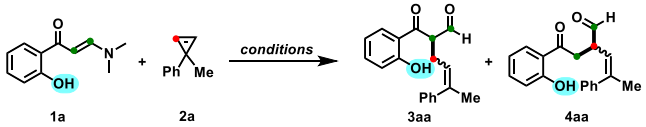
General methods:

All reactions were carried out in flame or oven-dried glassware under nitrogen atmosphere with freshly distilled dry solvents under anhydrous conditions unless otherwise indicated. Flash column chromatography was performed with silica gel 60 (230 – 400 mesh). Chromatograms were visualized by fluorescence quenching with UV light at 254 nm or by staining with base solution of potassium permanganate and molybdate. NMR spectra were recorded at RT on 300 or 400 MHz Bruker spectrometers. The residual solvent signals were taken as the reference (0.00 ppm for ^{1}H NMR spectra and 77.0 ppm for ^{13}C NMR spectra in $CDCl_3$). Chemical shift (δ) is reported in ppm, coupling constants (*J*) are given in Hz. The following abbreviations classify the multiplicity: s = singlet, d = doublet, t = triplet, m = multiplet, dd = doublet of doublet, q = quartet and br = broad signal. HRMS (ESI) spectra were recorded on a Waters Q-Tof premier TM mass spectrometer.

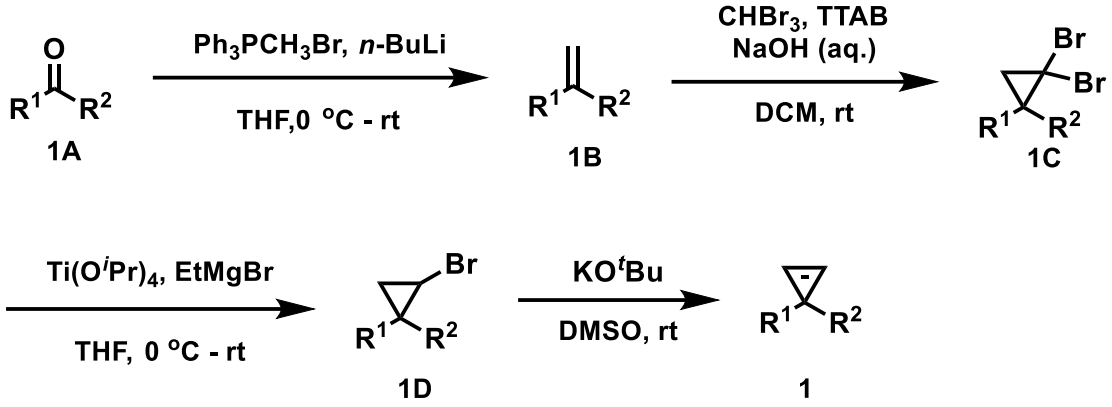
Table S1. Optimization of reaction conditions[a]



entry	catalyst	additive	solvent	yield of **3aa** (%)[b]	yield of **4aa** (%)[b]
1	$Rh_2(OAc)_4$	-	DCE	-	30 (*E*/*Z* = 75:25)
2	$Cu(OH)_2$	-	DCE	-	5
3	$AgNO_3$	-	DCE	-	12 (*E*/*Z* = 75:25)
4	$ZnBr_2$	-	DCE	-	33 (*E*/*Z* = 94:6)
5	$ZnBr_2$	BF_3	DCE	71 (*E*/*Z* > 99:1)	8
6	$ZnCl_2$	BF_3	DCE	66 (*E*/*Z* > 99:1)	-
7	$Zn(OAc)_2$	BF_3	DCE	46 (*E*/*Z* > 99:1)	-
8	$ZnBr_2$	BF_3	DCM	68 (*E*/*Z* > 99:1)	-
9	$ZnBr_2$	BF_3	ACN	10	20
10	$ZnBr_2$	BF_3	THF	-	15
11[c]	$ZnBr_2$	BF_3	DCE	62 (*E*/*Z* > 99:1)	-
12[d]	$ZnBr_2$	BF_3	DCE	80 (*E*/*Z* > 99:1)	-
13	**$ZnBr_2$**	**BF_3[e]**	DCE	**87 (*E*/*Z* > 99:1)**	**-**
14	$ZnBr_2$	$Sc(OTf)_2$	DCE	-	51 (*E*/*Z* = 95:5)
15	$ZnBr_2$	$Cu(OTf)_2$	DCE	-	34 (*E*/*Z* = 95:5)
16	$ZnBr_2$	$In(OTf)_3$	DCE		62 (*E*/*Z* = 95:5)
17	$ZnBr_2$[f]	-	DCE	-	80 (*E*/*Z* = 95:5)
18	**$ZnBr_2$[f]**	**-**	**TCE**	**-**	**83 (*E*/*Z* = 95:5)**
19	$ZnBr_2$[f]	BF_3[e]	DCE	52 (*E*/*Z* > 99:1)	-
20[c]	$ZnBr_2$[f]	-	TCE		52 (*E*/*Z* = 95:5)

[a]Unless otherwise noted, reactions were performed as follows: **1a** (0.20 mmol, 1.0 equiv.), **2a** (0.60 mmol, 3.0 equiv.), catalyst (10 mol %) and additive (1.2 equiv.) were mixed with 2.0 mL solvent and reacted at room temperature (25 ^{o}C) under nitrogen atmosphere for about 10 hours. [b]Isolated yields, *E*/*Z* ratio was determined by ^{1}H NMR analysis. [c]**1a**/**2a** = 1:2. [d]**1a**/**2a** = 1:4. [e]BF_3•Et_2O (1.5 equiv.). [f]$ZnBr_2$ (1.0 equiv.). DCE = dichloroethane, DCM = dichloromethane, THF = tetrahydrofuran, TCE = tetrachloroethane.

General procedure for the synthesis of cyclopropenes[1]:



To a stirred solution of Ph_3PCH_3Br (100 mmol) in THF (150 mL) at 0 °C was added 1.6 M *n*-butyllitium (90 mmol) dropwise over 60 minutes. The reaction mixture was stirred for 2 hours at room temperature. Ketone **1A** (50 mmol) in THF (15 mL) was added dropwise to the cooled reaction mixture at 0 °C via cannular. The reaction was then stirred at room temperature for 24 - 48 hours, quenched with saturated NH_4Cl (40 mL), diluted with water (30 mL) and extracted with EtOAc (3 x 30 mL). The combined organic extracts were washed with brine (2 x 30 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was dissolved in hexane and triphenylphosphine oxide was filtered off. The filtrate solution was then concentrated under reduced pressure. The product **1B** was isolated by flash column chromatography (eluent: PE).

A solution of 10 M aqueous sodium hydroxide (200 mmol) was added to alkyltrimethylammonium bromide (2.0 g). To the stirring reaction mixture was added a solution of alkene **1B** (50 mmol) in DCM (2 mL). Bromoform (100 mmol) in DCM (10 mL) was added dropwise over 1 hour. The reaction was allowed to stir vigorously

[1] A. Parra, L. Amenós, M. Guisán-Ceinos, A. López, J. L. García Ruano and M. Tortosa, *J. Am. Chem. Soc.*, 2014, **136**, 15833-15836.

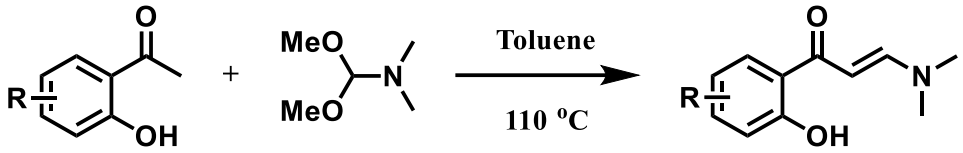
at 25 °C for 24 hours, after which the mixture was extracted with DCM (3 x 100 mL). The combined organic layers were washed with brine (2 x 100 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The product **1C** was purified by flash column chromatography (eluent: PE)

A solution of ethylmagnesium bromide (75 mmol) was added dropwise over an hour to a stirring solution of 2, 2-dibromocyclopropane **1C** (50 mmol), $Ti(O^iPr)_4$ (5.0 mmol) and Et_2O (50 mL) and the resulting mixture was stirred for 3 hours at 25 °C. The reaction was quenched by slow addition of water (20 mL) and 1 M HCl (30 mL), stirred for a further few minutes followed by the addition of Et_2O (30 mL). The aqueous layer was washed with Et_2O (3 x 20 mL), combined organic layers washed with saturated sodium bicarbonate (10 mL), brine (10 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The crude oil was purified by flash column chromatography to afford **1D** (eluent: PE).

Potassium *tert*-butoxide (10 mmol) and dimethyl sulfoxide (10 mL) were heated to 55 °C and allowed to stir for 30 minutes at this temperature until the mixture was homogenous. The solution was then cooled to 25 °C. 2-Bromocyclopropane **1D** (5 mmol) in DMSO (5 mL) was added to the reaction mixture over 3 hours and allowed to stir at 25 °C for 20 hours. The reaction was quenched with brine (50 mL) and PE (50 mL) and layers partitioned. The aqueous layer was washed with PE (3 x 50 mL) and combined organic layers washed with brine (2 x 50 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The product was purified by flash column chromatography (eluent: PE) to afford cyclopropenes **3a-3l**, **4f**, **4j**, **4k.**

The spectroscopic properties of these compounds were consistent with literature data: 3a – 3f, **4f**;[2] **3g – 3i**, **4j**, **4k**;[3] **3j – 3k**.[4]

General procedure for the synthesis of enaminones[5]:



To a stirred solution of ketone (5.0 mmol, 1.0 equiv.) in toluene (5.0 mL), 1,1-dimethoxy-N,N-dimethylmethanamine (7.0 mmol, 1.4 equiv.) was added and stirred at 110 ºC. After completion of the reaction (monitored by TLC), it was quenched with water, extracted with ethyl acetate and dried with anhydrous Na_2SO_4. Then the reaction mixture was concentrated under reduced pressure and purified by column chromatography (petroleum ether : ethyl acetate = 1 : 1) to give the desired product.

The spectroscopic properties of these compounds were consistent with literature data.[6]

(*E*)-3-(Dimethylamino)-1-(2-hydroxyphenyl)prop-2-en-1-one (1a)[6]:

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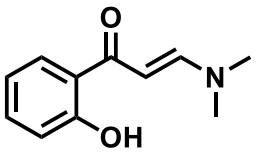
[2] J. Chen, J. Han, T. Wu, J. Zhang, M. Li, Y. Xu, J. Zhang, Y. Jiao, Y. Yang and Y. Jiang, *Org. Chem. Front*., 2022, **9**, 1820–1825.

[3] J. Chen, P. Guo, J. Zhang, J. Rong, W. Sun, Y. Jiang and T.-P. Loh, *Angew. Chem., Int. Ed.*, 2019, **58**, 12674–12679.

[4] J. Chen, J. Han, J. Zhang, L. Li, Z. Zhang, Y. Yang and Y. Jiang, *ACS Catal*., 2022, **12**, 14748−14753.

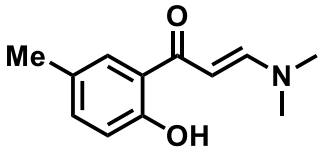
[5] Y. Jiang, V. Y. K. Zhong, L. Emmanuvel and C.-M. Park, *Chem. Commun*., 2012. **48**, 3133-3135.

[6] M. Akram, S. Bera and N. Patil, *Chem. Commun*., 2016. **52**, 12306-12309.



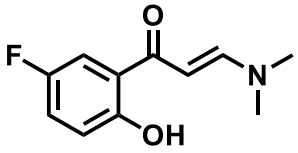
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1a** as yellow solid in 89% yield (851.0mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.96 (s, 1H), 7.87 (d, J = 12.2 Hz, 1H), 7.70 (dd, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1H), 7.39 - 7.32 (m, 1H), 6,96 - 6.89 (m, 1H), 6.85 - 6.78 (m, 1H), 5.78 (d, J = 12.2 Hz, 1H), 3.20 (s, 3H), 2.97 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(2-hydroxy-5-methylphenyl)prop-2-en-1-one (1b)[6]:



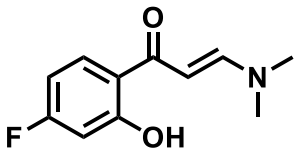
Purification by column chromatography (TLC R_f = 0.3) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1b** as yellow solid in 92% yield (944.2mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13,73 (s, 1H), 7.88 (d, J = 12.1 Hz, 1H), 7.47 (s, 1H), 7.16 (d, J = 8.3 Hz, 1H), 6.84 (d, J = 8.3 Hz, 1H), 5.78 (d, J = 12.3 Hz, 1H), 3.19 (s, 3H), 2.99 (s, 3H), 2.30 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(5-fluoro-2-hydroxyphenyl)prop-2-en-1-one (1c)[6]:



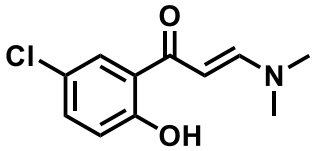
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1c** as yellow solid in 67% yield (700.9mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.04 (s, 1H), 8.00 (d, J = 12.1 Hz, 1H), 7.87 (d, J = 2.3 Hz, 1H), 7.51 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.93 (d, J = 8.8 Hz, 1H), 5.77 (d, J = 12.0 Hz, 1H), 3.32 (s, 3H), 3.10 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(4-fluoro-2-hydroxyphenyl)prop-2-en-1-one (1c')[6]:



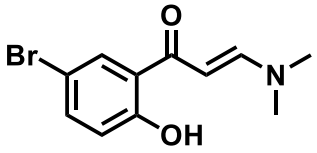
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1c'** as yellow solid in 76% yield (795.0mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.93 (s, 1H), 7.90 (d, J = 12.0 Hz, 1H), 7.62 (d, J = 2.6 Hz, 1H), 7.28 (dd, J_1 = 9.0 Hz, J_2 = 2.6 Hz, 1H), 6.87 (d, J = 8.9 Hz, 1H), 5.67 (d, J = 12.1 Hz, 1H), 3.21 (s, 3H), 3.00 (s, 3H).

(*E*)-1-(5-Chloro-2-hydroxyphenyl)-3-(dimethylamino)prop-2-en-1-one (1d)[6]:



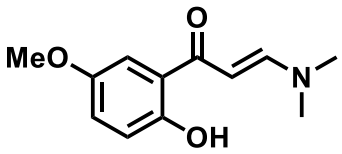
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1d** as yellow solid in 83% yield (936.5mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.93 (s, 1H), 7.90 (d, J = 12.1 Hz, 1 H), 7.62 (d, J = 2.4 Hz, 1H), 7.28 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 6.87 (d, J = 8.8 Hz, 1H), 5.68 (d, J = 12.1 Hz, 1H), 3.21 (s, 3H), 3.00 (s, 3H).

(*E*)-1-(5-Bromo-2-hydroxyphenyl)-3-(dimethylamino)prop-2-en-1-one (1e)[6]:



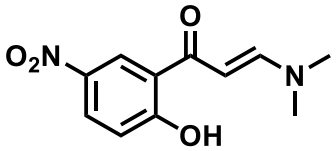
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1e** as yellow solid in 84% yield (1134.5mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.94 (s, 1H), 7.89 (d, J = 12.1 Hz, 1H), 7.76 (d, J = 2.4 Hz, 1H), 7.41 (dd, J_1 = 8.8 Hz, J_2 = 2.3 Hz, 1H), 6.83 (d, J = 8.8 Hz, 1H), 5.67 (d, J = 12.1 Hz, 1H), 3.21(s, 3H), 3.00(s, 3H).

(*E*)-3-(Dimethylamino)-1-(2-hydroxy-5-methoxyphenyl)prop-2-en-1-one (1f)[6]:



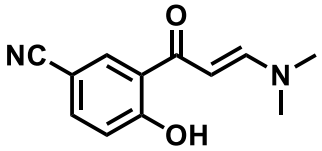
Purification by column chromatography (TLC R_f = 0.3) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1f** as yellow solid in 72% yield (796.5mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.49 (s, 1H), 7.84 (d, J = 12.0 Hz, 1H), 7.60 (d, J = 8.7 Hz, 1H), 6.50 – 6.30 (m, 2H), 5.68 (d, J = 12.0 Hz, 1H), 3.81 (s, 3H), 3.17 (s, 3H), 2.95 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(2-hydroxy-5-nitrophenyl)prop-2-en-1-one (1g)[6]:



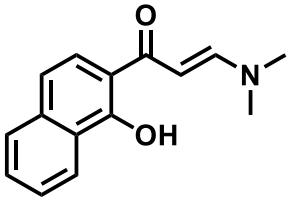
Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1g** as yellow solid in 80% yield (944.9mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.23 (s, 1 H), 8.63 (d, J = 2.8 Hz, 1H), 8.22 (dd, J_1 = 9.2 Hz, J_2 = 2.7 Hz, 1H), 7.98 (d, J = 11.9 Hz, 1H), 6.98 (d, J = 9.2 Hz, 1H), 5.79 (d, J = 12.0 Hz, 1H), 3.27 (s, 3H), 3.07 (s, 3H).

(*E*)-3-(3-(Dimethylamino)acryloyl)-4-hydroxybenzonitrile (1h)[6]:



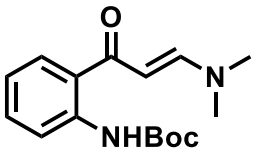
Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1h** as yellow solid in 70% yield (7456.8mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.82 (s, 1 H), 7.99 (d, J = 2.0 Hz, 1 H), 7.94 (d, J = 12.0 Hz, 1H), 7.56 (dd, J_1 = 8.7 Hz, J_2 = 1.8 Hz, 1H), 6.96 (d, J = 8.7 Hz, 1H), 5.68 (d, J = 11.9 Hz, 1H), 3.25 (s, 3H), 3.03 (s, 3H).

(*E*)-3-(Dimethylamino)-1-(1-hydroxynaphthalen-2-yl)prop-2-en-1-one (1i)[6]:



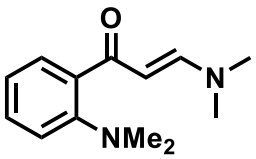
Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc/PE (1:1) as the eluent the desired product **1i** as yellow solid in 65% yield (784.2mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 15.66 (s, 1 H), 8.44 (d, J = 8.3 Hz, 1H), 7.96 (d, J = 12.1 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.68 (d, J = 8.8 Hz, 1H), 7.58 - 7.54 (m, 1H), 7.51 - 7.46 (m, 1H), 7.21 (d, J = 8.9 Hz, 1H), 5.85 (d, J = 12.1 Hz, 1H), 3.22 (s, 3H), 3.01 (s, 3H).

***tert*-butyl-(*E*)-(2-(3-(dimethylamino)acryloyl)phenyl)carbamate (1j)[7]:**



Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc/PE (1:4) as the eluent the desired product **1j** as yellow oil in 75% yield (1088.9mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.95 (s, 1 H), 8.31 (dd, J_1 = 8.5 Hz, J_2 = 1.2 Hz, 1H), 7.73 (d, J = 12.2 Hz, 1H), 7.68 (dd, J_1 = 7.9 Hz, J_2 = 1.6 Hz, 1H), 7.36 (ddd, J_1 = 8.7 Hz, J_2 = 7.3 Hz, J_3 = 1.6 Hz, 1H), 6.96 – 6.92 (m, 1H), 5.62 (d, J = 12.2 Hz, 1H), 3.11 (s, 3H), 2.88 (s, 3H), 1.48 (s, 3H).

(*E*)-3-(dimethylamino)-1-(2-(dimethylamino)phenyl)prop-2-en-1-one (1k):

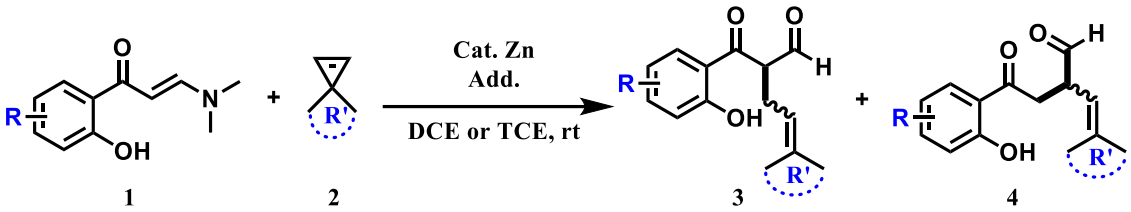


Purification by column chromatography (TLC R_f = 0.2) on silica gel using EtOAc as the eluent the desired product **1k** as yellow oil in 42% yield (458.4mg); ^{1}H NMR (400

[7] J. Joussot, A. Schoenfelder, L. Larquetoux, M. Nicolas, J. Suffert and G. Blond, *Synthesis*, 2016, **48(19)**: 3364–3372.

MHz, $CDCl_3$) δ 732. (s, 1 H), 7.317.16 (m, 2H), 6.866.77 (m, 2H), 5.48 (d, J = 12.2 Hz, 1H), 3.012.74 (m, 12H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 129.5, 129.3, 119.0, 115.9, 43.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{13}H_{19}N_2O$: 219.1497. Found: 219.1493.

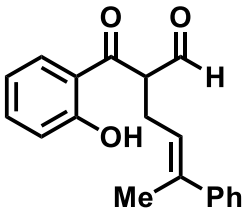
General procedure for the synthesis of 1,*n*-Dicarbonyl-alkenes:



1,3-Dicarbonyl-alkenes: A mixture of **1** (0.2 mmol, 1.0 equiv.), **2** (0.6 mmol, 3.0 equiv.), $BF_3 \cdot Et_2O$ (0.3 mmol, 1.5 equiv.) and $ZnBr_2$ (0.02 mmol, 10 mol %) was dissolved in DCE (2.0 mL) in a Schlenk tube under N_2 protection. The mixture was stirred until the **1** was consumed completely about 10 hours at room temperature. Then the reaction mixture was diluted with saturated NH_4Cl and extracted with DCM. The organic phase dried over $MgSO_4$ and concentrated under reduced pressure. The product was purified by column chromatography to give the desired product **3**.

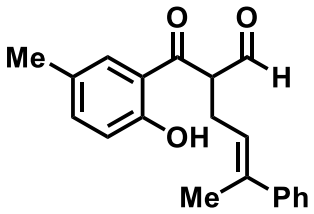
1,4-Dicarbonyl-alkenes: A mixture of **1** (0.2 mmol, 1.0 equiv.), **2** (0.6 mmol, 3.0 equiv.) and $ZnBr_2$ (0.2 mmol, 1.0 equiv.) was dissolved in TCE (2.0 mL) in a Schlenk tube under N_2 protection. The mixture was stirred until the **1** was consumed completely about 24 hours at room temperature. Then the reaction mixture was concentrated under reduced pressure and purified by column chromatography to give the desired product **4**.

(*E*)-2-(2-Hydroxybenzoyl)-5-phenylhex-4-enal (3aa):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3aa** as yellow oil in 87% yield (51.2 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.11 (s, 1H), 9.84 (s, 1H), 7.83 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.48 (ddd, J_1 = 18.7 Hz, J_2 = 7.3 Hz, J_3 = 1.6 Hz, 1H), 7.34 – 7.26 (m, 5H), 6.99 (dd, J_1 = 8.5 Hz, J_2 = 1.1 Hz, 1H), 6.90 (ddd, J_1 = 8.2 Hz, J_2 = 7.1 Hz, J_3 = 1.1 Hz, 1H), 5.67 (dd, J_1 = 10.2 Hz, J_2 = 1.3 Hz, 1H), 4.93 (td, J_1 = 9.6 Hz, J_2 = 9.6 Hz, J_3 = 4.4 Hz, 1H), 3.37 (dd, J_1 = 18.5 Hz, J_2 = 9.0 Hz, 1H), 2.72 (dd, J_1 = 18.5 Hz, J_2 = 4.4 Hz, 1H), 2.27 (d, *J* = 1.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 199.8, 163.0, 142.1, 138.5, 136.7, 130.0, 128.3, 127.6, 125.8, 124.1, 119.0, 118.6, 118.6, 45.4, 41.5, 16.5; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{19}O_3$: 294.1334. Found: 294.1342.

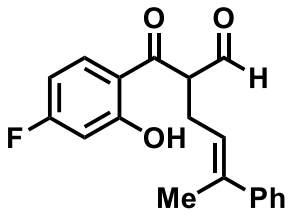
(*E*)-2-(2-Hydroxy-5-methylbenzoyl)-5-phenylhex-4-enal (3ba):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ba** as yellow oil in 92% yield (56.7 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.94 (s, 1H), 9.84 (s, 1H), 7.61 (d, *J* = 2.2 Hz, 1H), 7.34 – 7.25 (m, 6H), 6.90 (d, *J* = 8.5 Hz, 1H), 5.65 (dd, J_1 = 10.3 Hz, J_2 = 1.4 Hz, 1H), 4.93 (ddd, J_1 = 10.3 Hz, J_2 = 8.9 Hz, J_3 = 4.6 Hz, 1H), 3.36 (ddd, J_1 = 18.5 Hz, J_2 = 9.0 Hz, J_3 = 0.7 Hz, 1H), 2.72 (dd, J_1 = 18.5 Hz, J_2 = 4.6 Hz, 1H), 2.29 (s, 3H), 2.29

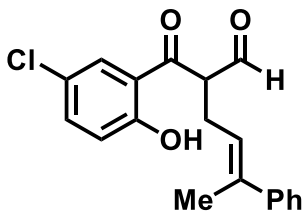
(d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 199.9, 160.9, 142.2, 138.3, 137.7, 129.7, 128.3, 127.9, 127.6, 125.8, 124.2, 118.3, 118.1, 45.4, 41.4, 20.7, 16.5; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_3$: 309.1491. Found: 309.1491.

(*E*)-2-(4-Fluoro-2-hydroxybenzoyl)-5-phenylhex-4-enal (3ca):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ca** as yellow oil in 62% yield (38.7 mg, E/Z > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.43 (s, 1H), 9.83 (s, 1H), 7.84 (dd, J_1 = 9.0 Hz, J_2 = 6.4 Hz, 1H), 7.32 – 7.26 (m, 5H), 6.68 – 6.60 (m, 2H), 5.65 (dd, J_1 = 10.2 Hz, J_2 = 1.4 Hz, 1H), 4.88 – 4.82 (m, 1H), 3.38 (dd, J_1 = 18.6 Hz, J_2 = 9.3 Hz, 1H), 2.71 (dd, J_1 = 18.6 Hz, J_2 = 4.3 Hz, 1H), 2.26 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 199.7, 167.5 (d, J = 257.5 Hz), 165.6 (d, J = 257.5 Hz), 142.0, 138.7, 132.4 (d, J = 11.8 Hz), 128.4, 127.7, 125.8, 123.9, 115.7, 107.4 (d, J = 22.7 Hz), 105.2 (d, J = 23.5 Hz), 45.4, 41.6, 16.5.; ^{19}F NMR (376Hz,$CDCl_3$) δ -123.5; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}FO_3$: 313.1240. Found: 313.1234.

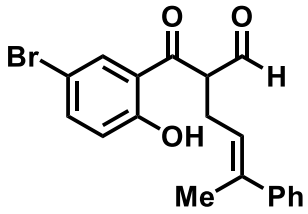
(*E*)-2-(5-Chloro-2-hydroxybenzoyl)-5-phenylhex-4-enal (3da):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3da** as yellow oil in 84% yield (55.2 mg, E/Z > 99:1); ^{1}H

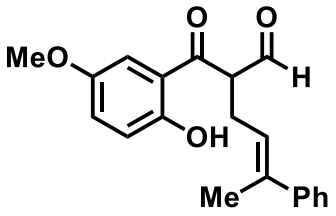
NMR (400 MHz, $CDCl_3$) δ 11.97 (s, 1H), 9.83 (s, 1H), 7.79 (d, J = 2.5 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.35 – 7.27 (m, 5H), 6.95 (d, J = 8.95 Hz, 1H), 5.62 – 5.58 (m, 1H), 4.84 (ddd, J_1 = 10.4 Hz, J_2 = 9.3 Hz, J_3 = 4.3 Hz, 1H), 3.40 (dd, J_1 = 18.7 Hz, J_2 = 9.3 Hz, 1H), 2.73 (dd, J_1 = 18.7 Hz, J_2 = 4.2 Hz, 1H), 2.3 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 199.5, 161.4, 142.0, 139.2, 136.4, 129.3, 128.4, 127.7, 125.8, 123.6, 123.4, 120.2, 119.0, 45.4, 41.6, 16.5; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}ClO_3$: 329.0944. Found: 329.0937.

(*E*)-2-(5-Bromo-2-hydroxybenzoyl)-5-phenylhex-4-enal (3ea):



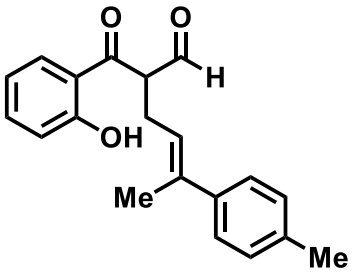
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ea** as yellow oil in 95% yield (70.9 mg, E/Z > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.97 (s, 1H), 9.83 (s, 1H), 7.95 (d, J = 2.4 Hz, 1H), 7.54 (dd, J_1 = 8.9 Hz, J_2 = 2.4 Hz, 1H), 7.33 – 7.26 (m, 5H), 6.90 (d, J = 8.9 Hz, 1H), 5.59 (dd, J_1 = 10.4 Hz, J_2 = 1.5 Hz, 1H), 4.87 – 4.81 (m, 1H), 3.40 (dd, J_1 = 18.7 Hz, J_2 = 9.2 Hz, 1H), 2.73 (dd, J_1 = 18.7 Hz, J_2 = 4.2 Hz, 1H), 2.3 (d, J = 1.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.1, 199.5, 161.8, 142.1, 139.2, 139.1, 132.4, 128.4, 127.8, 125.8, 123.4, 120.6, 119.7, 110.5, 45.3, 41.7, 16.6; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}BrO_3$: 373.0439. Found: 373.0443.

(*E*)-2-(2-Hydroxy-5-methoxybenzoyl)-5-phenylhex-4-enal (3fa):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.6) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3fa** as yellow oil in 28% yield (18.2 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.59 (s, 1H), 9.84 (s, 1H), 7.72 (d, J = 8.7 Hz, 1H), 7.34 – 7.26 (m, 5H), 6.46 – 6.42 (m, 2H), 5.69 (dd, J_1 = 10.1 Hz, J_2 = 1.5 Hz, 1H), 4.83 (ddd, J_1 = 10.2 Hz, J_2 = 8.8 Hz, J_3 = 4.6 Hz, 1H), 3.83 (s, 3H), 3.32 (dd, J_1 = 18.3 Hz, J_2 = 8.8 Hz, 1H), 2.69 (dd, J_1 = 18.3 Hz, J_2 = 4.6 Hz, 1H), 2.25 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.9, 199.9, 166.3, 166.0, 142.3, 138.0, 131.6, 128.3, 127.6, 125.8, 124.6, 112.7, 107.9, 101.0, 55.6, 45.3, 41.3, 16.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_4$: 325.1440. Found: 325.1444.

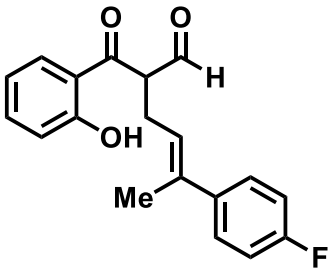
(*E*)-2-(2-Hydroxybenzoyl)-5-(p-tolyl)hex-4-enal (3ab):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ab** as yellow oil in 77% yield (47.5 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.12 (s, 1H), 9.84 (s, 1H), 7.83 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.47 (ddd, J_1 = 8.6 Hz, J_2 = 7.1 Hz, J_3 = 1.6 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.12 – 7.09 (m, 2H), 6.99 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.90 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.64 (dd, J_1 = 10.2 Hz, J_2 = 1.4 Hz, 1H), 4.92 (ddd, J_1 = 10.2 Hz, J_2 = 9.0 Hz, J_3 = 4.5 Hz, 1H), 3.36 (ddd, J_1 = 18.5 Hz, J_2 = 9.0 Hz, J_3 = 0.7

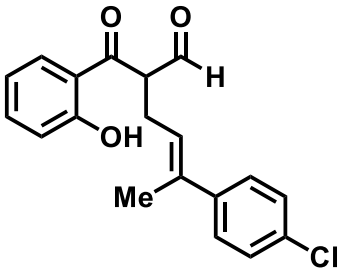
Hz, 1H), 2.74 – 2.68 (m, 1H), 2.32 (s, 3H), 2.25 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.1, 199.9, 163.0, 139.2, 138.3, 137.5, 136.6, 130.0, 129.0, 125.7, 123.2, 119.0, 118.6, 118.5, 45.4, 41.5, 21.0, 16.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_3$: 309.1491. Found: 309.1482.

(*E*)-5-(4-Fluorophenyl)-2-(2-hydroxybenzoyl)hex-4-enal (3ac):



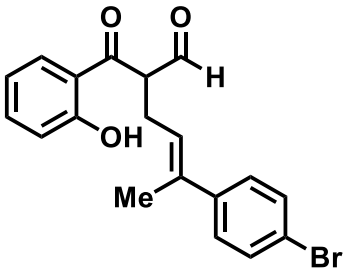
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ac** as yellow oil in 78% yield (48.7 mg, E/Z > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.09 (s, 1H), 9.83 (s, 1H), 7.82 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.48 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.7 Hz, 1H), 7.30 – 7.26 (m, 2H), 7.01 – 6.95 (m, 3H), 6.91 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.62 – 5.59 (m, 1H), 4.92 (ddd, J_1 = 10.2 Hz, J_2 = 8.8 Hz, J_3 = 4.6 Hz, 1H), 3.35 (dd, J_1 = 18.5 Hz, J_2 = 8.8 Hz, 1H), 2.72 (dd, J_1 = 18.5 Hz, J_2 = 4.5 Hz, 1H), 2.24 (d, J_1 = 1.4 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 199.6, 163.5, 163.1, 161.1, 138.3 (d, J = 3.4 Hz), 137.6, 136.7, 129.9, 127.4 (d, J = 8.2 Hz), 124.1, 118.9 (d, J = 35.2 Hz), 118.5, 115.1 (d, J = 21.5 Hz), 45.5, 41.4, 16.6; ^{19}F NMR (376Hz,$CDCl_3$) δ -114.6; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}FO_3$: 313.1240. Found: 313.1230.

(*E*)-5-(4-Chlorophenyl)-2-(2-hydroxybenzoyl)hex-4-enal (3ad):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ad** as yellow oil in 87% yield (57.2 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.10 (s, 1H), 9.84 (s, 1H), 7.82 (dd, J_1 = 8.1 Hz, J_2 = 1.7 Hz, 1H), 7.50 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 7.27 – 7.26 (m, 4H), 7.01 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.92 (ddd, J_1 = 8.2 Hz, J_2 = 7.1 Hz, J_3 = 1.2 Hz,1H), 5.66 (dd, J_1 = 10.2 Hz, J_2 = 1.4 Hz, 1H), 4.94 (ddd, J_1 = 10.2 Hz, J_2 = 8.9 Hz, J_3 = 4.6 Hz, 1H), 3.38 (dd, J_1 = 18.5 Hz, J_2 = 8.9 Hz, 1H), 2.74 (dd, J_1 = 18.6 Hz, J_2 = 4.6 Hz, 1H), 2.25 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 199.5, 163.0, 140.6, 137.4, 136.7, 133.4, 129.9, 128.4, 127.1, 124.6, 119.1, 118.7, 118.5, 45.4, 41.4, 16.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}ClO_3$: 329.0944. Found: 329.0940.

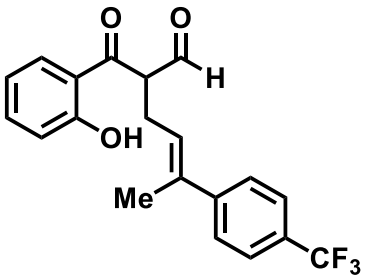
(*E*)-5-(4-Bromophenyl)-2-(2-hydroxybenzoyl)hex-4-enal (3ae):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ae** as yellow oil in 94% yield (70.2 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.08 (s, 1H), 9.83 (s, 1H), 7.81 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.48 (ddd, J_1 = 8.7 Hz, J_2 = 7.2 Hz, J_3 = 1.6 Hz, 1H), 7.43 – 7.39 (m, 2H), 7.20 – 7.16 (m, 2H), 7.00 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.91 (ddd, J_1 = 8.2 Hz, J_2

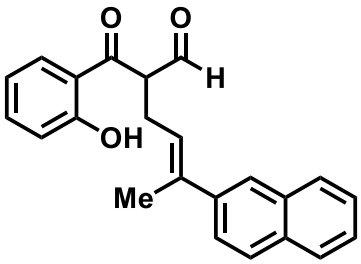
= 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.66 (dd, J_1 = 10.2 Hz, J_2 = 1.4 Hz, 1H), 4.92 (ddd, J_1 = 10.2 Hz, J_2 = 8.9 Hz, J_3 = 4.6 Hz, 1H), 3.36 (dd, J_1 = 18.5 Hz, J_2 = 8.9 Hz, 1H), 2.72 (dd, J_1 = 18.5 Hz, J_2 = 4.6 Hz, 1H), 2.22 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 199.5, 163.0, 141.0, 137.5, 136.7, 131.4, 129.9, 127.4, 124.7, 121.6, 119.1, 118.7, 118.5, 45.4, 41.4, 16.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}BrO_3$: 373.0439. Found: 373.0439.

(*E*)-2-(2-Hydroxybenzoyl)-5-(4-(trifluoromethyl)phenyl)hex-4-enal (3af):



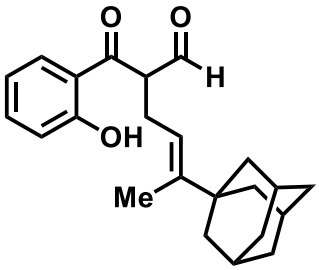
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3af** as yellow oil in 64% yield (46.4 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.08 (s, 1H), 9.84 (s, 1H), 7.82 (dd, J_1 = 8.1 Hz, J_2 = 1.7 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.49 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.7 Hz, 1H), 7.42 (d, J = 7.9 Hz, 2H), 7.01 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.92 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.74 (dd, J_1 = 10.2 Hz, J_2 = 1.4 Hz, 1H), 4.99 – 4.93 (m, 1H), 3.38 (dd, J_1 = 18.6 Hz, J_2 = 8.9 Hz, 1H), 2.75 (dd, J_1 = 18.5 Hz, J_2 = 4.6 Hz, 1H), 2.28 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 199.4, 163.1, 145.7, 137.5, 136.8, 130.0, 129.8, 126.2, 126.1, 125.3 (d, J = 3.9 Hz), 119.1, 118.8, 118.5, 45.4, 41.3, 16.4; ^{19}F NMR (376Hz,$CDCl_3$) δ -62.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{18}F_3O_3$: 363.1208. Found: 363.1206.

(*E*)-2-(2-Hydroxybenzoyl)-5-(naphthalen-2-yl)hex-4-enal (3ag):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ag** as yellow oil in 39% yield (26.9 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.14 (s, 1H), 9.87 (s, 1H), 7.88 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.81 – 7.75 (m, 4H), 7.50 – 7.44 (m, 4H), 7.01 (d, J = 8.4 Hz, 1H), 6.93 (t, J_1 = 7.6 Hz, 1H), 5.83 (dd, J_1 = 10.1 Hz, J_2 = 1.5 Hz, 1H), 4.99 (td, J_1 = 9.7 Hz, J_2 = 9.6 Hz, J_3 = 4.5 Hz, 1H), 3.42 (dd, J_1 = 18.5 Hz, J_2 = 9.0 Hz, 1H), 2.77 (dd, J_1 = 18.5 Hz, J_2 = 4.5 Hz, 1H), 2.38 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.1, 199.8, 163.1, 139.3, 138.4, 136.7, 133.2, 132.7, 130.0, 128.1, 127.9, 127.5, 126.3, 126.0, 124.7, 124.6, 124.0, 119.1, 118.7, 118.6, 45.5, 41.6, 16.5; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{23}H_{21}O_3$: 345.1491. Found: 345.1484.

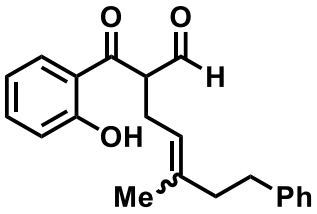
(*E*)-5-((3r,5r,7r)-Adamantan-1-yl)-2-(2-hydroxybenzoyl)hex-4-enal (3ah):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ah** as yellow oil in 65% yield (45.8 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.16 (s, 1H), 9.79 (s, 1H), 7.72 (dd, J_1 = 8.1 Hz, J_2 = 1.7 Hz, 1H), 7.46 (ddd, J_1 = 8.6 Hz, J_2 = 7.1 Hz, J_3 = 1.7 Hz, 1H), 6.97 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.87 (ddd, J_1 = 8.2 Hz, J_2 = 7.1 Hz, J_3 = 1.2 Hz, 1H), 5.09 (dd, J_1 = 9.9 Hz, J_2 = 1.4 Hz, 1H), 4.73 (td, J_1 = 9.6 Hz, J_2 = 9.5 Hz, J_3 = 4.5 Hz, 1H), 3.22 (dd,

J_1 = 18.3 Hz, J_2 = 9.1 Hz, 1H), 2.55 (dd, J_1 = 18.2 Hz, J_2 = 4.5 Hz, 1H), 1.97 (s, 3H), 1.81 (d, J = 1.3 Hz, 3H), 1.71 – 1.58 (m, 13H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.1, 200.3, 162.9, 147.9, 136.4, 130.1, 118.7, 118.7, 118.6, 118.5, 45.5, 41.2, 40.6, 38.1, 36.8, 28.5, 12.4; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{23}H_{29}O_3$: 353.2117. Found: 353.2112.

2-(2-Hydroxybenzoyl)-5-methyl-7-phenylhept-4-enal (3ai):



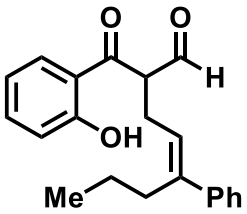
The title compound was prepared according to the general procedure. Purification by column chromatography on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ai** as yellow oil in 92% yield (59.3 mg, *E*/*Z* = 66:34).

(TLC R_{f1} = 0.5, *major* of **3ai**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.08 (s, 1H), 9.55 (s, 1H), 7.71 – 7.68 (m, 1H), 7.47 – 7.43 (m, 1H), 7.31 – 7.27 (m, 2H), 7.22 – 7.18 (m, 3H), 6.95 (d, J = 8.4 Hz, 1H), 6.88 – 6.84 (m, 1H), 5.04 (d, J = 10.5 Hz, 1H), 4.55 (td, J_1 = 9.9 Hz, J_2 = 9.8 Hz, J_3 = 4.0 Hz, 1H), 3.00 (dd, J_1 = 18.7 Hz, J_2 = 9.5 Hz, 1H), 2.85 – 2.78 (m, 1H), 2.78 – 2.61 (m, 2H), 2.47 – 2.41 (m, 1H), 1.85 – 1.83 (m, 1H), 1.77 (d, J = 1.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.5, 200.1, 163.0, 141.2, 138.7, 136.5, 130.0, 128.3, 128.2, 125.9, 122.1, 118.9, 118.6, 118.5, 45.6, 41.2, 40.8, 34.0, 16.8; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{23}O_3$: 323.1647. Found: 323.1641.

(TLC R_{f2} = 0.2, *minor* of **3ai**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.10 (s, 1H), 9.71 (s, 1H), 7.73 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.47 (ddd, J_1 = 8.6 Hz, J_2 = 7.1 Hz, J_3 = 1.7 Hz, 1H), 7.25 – 7.11 (m, 3H), 7.06 – 7.04 (m, 2H), 6.98 (dd, J_1 = 8.4 Hz, J_2 = 1.1 Hz, 1H), 6.90 – 6.86 (m, 1H), 4.99 – 4,96 (m, 1H), 4.73 – 4,67 (m, 1H), 3.13 (dd, J_1 = 18.4 Hz, J_2 = 8.7 Hz, 1H), 2.68 – 2.65 (m, 2H), 2.50 (dd, J_1 = 18.4 Hz, J_2 = 4.8 Hz,

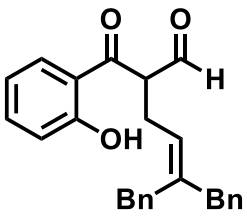
1H), 2.29 (t, J_1 = 7.7 Hz, 2H), 1.85 (d, J = 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.6, 199.8, 162.9, 141.5, 138.2, 136.4, 130.0, 128.6, 128.6, 128.3, 126.2,122.8, 118.9, 118.5, 45.9, 40.3, 34.5, 35.5, 23.2; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{23}O_3$: 323.1647. Found: 323.1642.

(*E*)-2-(2-Hydroxybenzoyl)-5-phenyloct-4-enal (3aj):



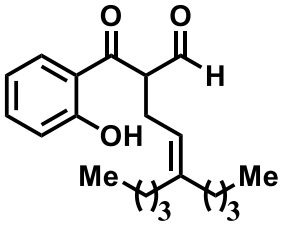
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3aj** as yellow oil in 92% yield (59.3 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.11 (s, 1H), 9.83 (s, 1H), 7.90 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.49 (ddd, J_1 = 8.6 Hz, J_2 = 7.1 Hz, J_3 = 1.7 Hz, 1H), 7.29 – 7.22 (m, 5H), 7.00 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.92 (ddd, J_1 = 8.3 Hz, J_2 = 7.1 Hz, J_3 = 1.2 Hz, 1H), 5.52 (d, J = 10.2 Hz, 1H), 4.97 (td, J_1 = 9.8 Hz, J_2 = 9.8 Hz, J_3 = 4.2 Hz, 1H), 3.40 (dd, J_1 = 18.5 Hz, J_2 = 9.3 Hz, 1H), 2.73 – 2.65 (m, 2H), 1.43 – 1.26 (m, 3H), 0.93 (t, J_1 = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 199.8, 163.0, 144.1, 141.6, 136.7, 130.1, 128.3, 127.5, 126.5, 124.6, 118.9, 118.6, 118.5, 46.2, 41.0, 32.2, 21.4, 14.2; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{23}O_3$: 323.1647. Found: 323.1654.

5-Benzyl-2-(2-hydroxybenzoyl)-6-phenylhex-4-enal (3ak):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3ak** as yellow oil in 88% yield (67.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.08 (s, 1H), 9.76 (s, 1H), 7.71 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.48 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.7 Hz, 1H), 7.29 – 7.20 (m, 6H), 7.08 – 7.06 (m, 2H), 7.01 – 6.96 (m, 3H), 6.79 (ddd, J_1 = 8.4 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.42 (d, J = 10.2 Hz, 1H), 4.89 (td, J_1 = 9.8 Hz, J_2 = 9.7 Hz, J_3 = 4.2 Hz, 1H), 3.55 – 3.42 (m, 2H), 3.34 (dd, J_1 = 18.5 Hz, J_2 = 9.3 Hz, 1H), 3.26 (s, 2H), 2.60 (dd, J_1 = 18.5 Hz, J_2 = 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 199.6, 163.0, 141.6, 138.7, 138.3, 136.6, 130.3, 128.9, 128.7, 128.6, 128.4, 126.5, 126.4, 125.2, 118.9, 118.6, 118.5, 46.0, 43.4, 40.8, 35.6; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{26}H_{25}O_3$: 385.1804. Found: 385.1801.

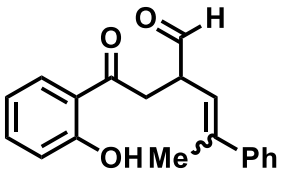
5-Ethyl-2-(2-hydroxybenzoyl)hept-4-enal (3al):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **3al** as yellow oil in 93% yield (58.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.12 (s, 1H), 9.78 (s, 1H), 7.80 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.46 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.7 Hz, 1H), 6.97 (dd, J_1 = 8.4 Hz, J_2 = 1.7 Hz, 1H), 6.87 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.04 (d, J = 10.1 Hz, 1H), 4.79 (ddd, J_1 = 9.7 Hz, J_2 = 9.7 Hz, J_3 = 4.3 Hz, 1H), 3.27 (dd, J_1 = 18.5 Hz, J_2 = 9.2 Hz, 1H), 2.57 (dd, J_1 = 18.4 Hz, J_2 = 4.3 Hz, 1H), 2.22 – 2.13 (m, 2H), 2.00 – 1.936 (m, 2H), 1.39 – 1.17 (m, 8H), 0.96 – 0.92 (m, 3H), 0.83 (t, J_1 = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 200.2, 162.9, 144.4, 136.5, 130.2, 120.8, 118.7,

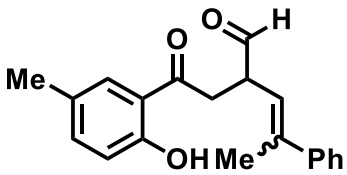
118.5, 46.4, 40.5, 36.1, 30.2, 30.2, 29.9, 23.1, 22.3, 14.1, 13.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{29}O_3$: 317.2117. Found: 317.2119.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4aa):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4aa** as yellow oil in 83% yield (48.9 mg, *E*/*Z* = 95:5); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.03 & 11.98 (s, 1H), 9.75 & 9.65 (s, 1H), 7.81 & 7.72 (dd, J_1 = 8.1 Hz & 8.1Hz, J_2 = 1.7 Hz & 1.7Hz, 1H), 7.48 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_3 = 1.6 Hz, 1H), 7.40 – 7.25 (m, 5H), 6.99 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.92 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.55 & 5.28 (dd, J_1 = 9.7 Hz & 10.0 Hz, J_2 = 1.4 Hz & 1.6 Hz, 1H), 4.21 – 4.15 (m, 1H), 3.74 & 3.57 (dd, J_1 = 17.8 Hz & 17.7 Hz, J_2 = 7.6 Hz & 7.5 Hz, 1H), 3.23 & 3.11 (dd, J_1 = 17.9 Hz & 17.7 Hz, J_2 = 5.0 Hz & 5.1 Hz, 1H), 2.24 & 2.10 (d, J = 1.4 Hz &1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 198.7, 162.3, 142.5, 141.8, 136.6, 129.9, 128.4, 127.7, 125.9, 120.5, 119.2, 119.1, 118.6, 47.5, 38.1, 17.0; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{19}O_3$: 295.1334. Found: 295.1326.

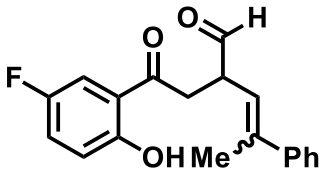
2-(2-(2-Hydroxy-5-methylphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4ba):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ba** as yellow oil in 83% yield (51.2 mg, *E*/*Z* = 95:5); ^{1}H

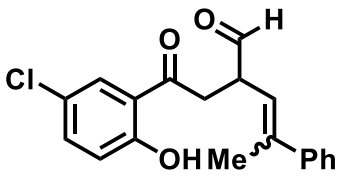
NMR (400 MHz, $CDCl_3$) δ 11.87 & 11.81 (s, 1H), 9.75 & 9.65 (s, 1H), 7.60 (d, J = 2.3 Hz, 1H), 7.42 – 7.26 (m, 6H), 6.90 (d, J = 8.5 Hz, 1H), 5.56 & 5.28 (dd, J_1 = 9.7 Hz & 10.0 Hz, J_2 = 1.5 Hz & 1.5 Hz, 1H), 4.22 – 4.16 & 3.84 – 3.78 (m, 1H), 3.74 & 3.57 (dd, J_1 = 17.9 Hz & 17.8 Hz, J_2 = 7.6 Hz & 7.5 Hz, 1H), 3.23 & 3.12 (dd, J_1 = 18.0 Hz & 17.7 Hz, J_2 = 5.2 Hz & 5.3 Hz, 1H), 2.32 & 2.30 (s, 3H), 2.25 & 2.11 (d, J = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.2, 198.8, 160.2, 142.5, 141.6, 137.7, 129,6, 128.3, 128.2, 127.7, 125.8, 120.5, 118.7, 118.3, 47.5, 38.1, 20.5, 16.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_3$: 309.1491. Found: 309.1493.

2-(2-(5-Fluoro-2-hydroxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4ca):



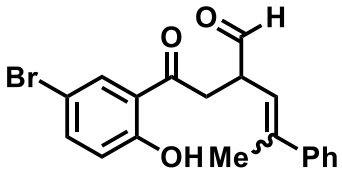
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.6) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ca** as yellow oil in 78% yield (48.7 mg, E/Z = 96:4); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 & 12.30 (d, J = 1.5 Hz & 1.5 Hz, 1H), 9.74 & 9.64 (s, 1H), 7.83 & 7.72 (dd, J_1 = 8.9 Hz & 9.0 Hz, J_2 = 6.3 Hz & 6.4 Hz, 1H), 7.40 – 7.29(m, 5H), 6.68 – 6.61 (m, 2H) 5.53 & 5.26 (dd, J_1 = 9.7 Hz & 10.1 Hz, J_2 = 1.5 Hz & 1.6 Hz, 1H), 4.22 – 4.16 & 3.87 – 3.73 (m, 1H), 3.69 & 3.52 (dd, J_1 = 17.8 Hz & 17.6 Hz, J_2 = 7.6 Hz & 7.5 Hz, 1H), 3.17 & 3.05 (dd, J_1 = 17.8 Hz & 17.5 Hz, J_2 = 5.1 Hz & 5.3 Hz, 1H), 2.25 & 2.11 (d, J = 1.5 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.2, 198.5, 167.5 (d, J = 257.3 Hz), 164.9 (d, J = 14.4 Hz), 142.4, 141.9, 132.2 (d, J = 11.9 Hz), 128.4, 127.7, 125.8, 120.2, 116.3, 107.4 (d, J = 23.0 Hz), 105.1 (d, J = 23.6 Hz), 47.5, 38.0, 17.0; ^{19}F NMR (376Hz,$CDCl_3$) δ -98.7; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}FO_3$: 313.1240. Found: 313.1230.

2-(2-(5-Chloro-2-hydroxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4da):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4da** as yellow oil in 77% yield (50.6 mg, *E*/*Z* = 97:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.91 & 11.85 (s, 1H), 9.72 & 9.62 (s, 1H), 7.77 & 7.69 (d, *J* = 2.5 Hz & 2.5 Hz, 1H), 7.46 – 7.36 (m, 3H), 7.36 – 7.27 (m, 3H), 6.94 (d, *J* = 8.9 Hz, 1H), 5.52 & 5.25 (dd, J_1 = 9.8 Hz & 10.1 Hz, J_2 = 1.4 Hz & 1.6 Hz, 1H), 4.21 – 4.15 & 3.82 – 3.77 (m, 1H), 3.70 & 3.52 (dd, J_1 = 18.0 Hz & 17.9 Hz, J_2 = 7.7 Hz & 7.7 Hz, 1H), 3.16 & 3.05 (dd, J_1 = 18.0 Hz & 18.0 Hz, J_2 = 5.0 Hz & 5.0 Hz, 1H), 2.25 & 2.10 (d, *J* = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 198.3, 160.8, 142.3, 142.0, 136.5, 129.1, 128.4, 127.8, 125.8, 123.7, 120.2, 120.0, 119.7, 47.4, 38.0, 17.0; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}ClO_3$: 329.0944. Found: 329.0934.

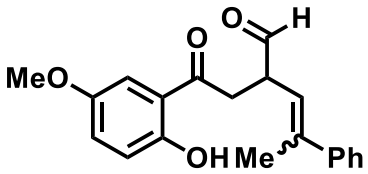
2-(2-(5-Bromo-2-hydroxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4ea):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ea** as yellow oil in 77% yield (57.5 mg, *E*/*Z* = 97:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.94 & 11.88 (s, 1H), 9.72 & 9.62 (s, 1H), 7.91 & 7.83 (d, *J* = 2.4 Hz & 2.4 Hz, 1H), 7.55 (dd, J_1 = 8.9 Hz, J_2 = 2.4 Hz, 1H), 7.40 – 7.28 (m, 5H), 6.90 (d, *J* = 8.9 Hz, 1H), 5.52 & 5.25 (dd, J_1= 9.8 Hz & 10.2 Hz, J_2 = 1.5 Hz & 1.5 Hz, 1H), 4.21 – 4.16 (m, 1H), 3.70 & 3.53 (dd, J_1 = 18.1 Hz & 18.0 Hz, J_2 = 7.8 Hz & 7.7 Hz, 1H), 3.17 & 3.05 (dd, J_1 = 18.1 Hz & 18.0 Hz, J_2 = 4.9 Hz & 5.0 Hz, 1H), 2.25 & 2.11 (d, *J* = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.6, 198.3, 161.3,

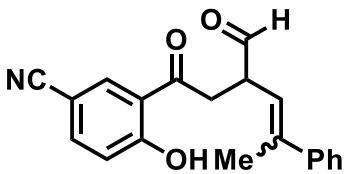
142.4, 142.1, 139.3, 132.2, 128.4, 127.8, 125.9, 120.6, 120.4, 120.0, 110.6, 47.4, 38.0, 17.0; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}BrO_3$: 373.0439. Found: 373.0443.

2-(2-(2-Hydroxy-5-methoxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4fa):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4fa** as yellow oil in 53% yield (34.4 mg, *E*/*Z* = 92:8); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.51 & 12.46 (s, 1H), 9.75 & 9.65 (s, 1H), 7.70 & 7.61 (d, *J* = 8.8 Hz & 8.9 Hz, 1H), 7.40 – 7.26 (m, 5H), 6.48 – 6.40 (m, 2H), 5.54 & 5.27 (dd, J_1 = 9.7 Hz & 10.1 Hz, J_2 = 1.4 Hz & 1.6 Hz, 1H), 4.18 – 4.11 & 3.79 – 3.71 (m, 1H), 3.79 & 3.71 (s, 3H), 3.63 & 3.47 (dd, J_1 = 17.5 Hz & 17.4 Hz, J_2 = 7.6 Hz & 7.6 Hz, 1H), 3.15 & 3.04 (dd, J_1 = 17.6 Hz & 17.4 Hz, J_2 = 5.2 Hz & 5.3 Hz, 1H), 2.22 & 2.09 (d, *J* = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 201.3, 198.9, 166.2, 165.2, 142.5, 141.5, 131.5, 128.3, 127.6, 125.8, 120.7, 113.3, 107.9, 100.9, 55.6, 47.6, 37.7, 16.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_4$: 325.1440. Found: 325.1430.

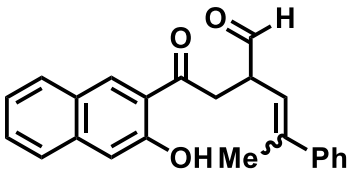
2-(2-(2-Hydroxy-5-methoxyphenyl)-2-oxoethyl)-4-phenylpent-3-enal (4ga):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ga** as yellow oil in 83% yield (53.0 mg, *E*/*Z* = 97:3); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.48 & 12.42 (s, 1H), 9.71 & 9.62 (s, 1H), 8.18 (d, *J* =

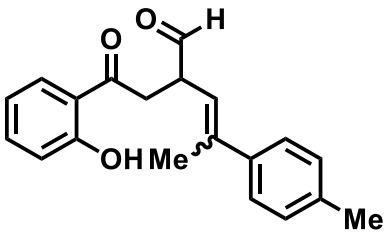
1.9 Hz, 1H). 7.72 (dd, J_1 = 8.8 Hz, J_2 = 1.9 Hz, 1H), 7.44 – 7.29 (m, 5H), 7.08 (d, J = 8.8 Hz, 1H), 5.53 & 5.26 (dd, J_1 = 9.9 Hz & 9.9Hz, J_2 = 1.4 Hz & 1.4 Hz, 1H), 4.27 – 4.18 & 3.88 – 3.81 (m, 1H), 3.75 (dd, J_1 = 18.1 Hz, J_2 = 8.0 Hz, 1H), 3.05 & 3.18 (dd, J_1 = 18.1 Hz & 17.2 Hz, J_2 = 4.6 Hz & 5.0 Hz, 1H), 2.27 & 2.13 (d, J = 1.5 Hz & 1.5Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.7, 198.0, 165.3, 142.4, 142.2, 138.8, 135.0, 128.4, 127.9, 125.8, 120.2, 119.5, 119.3, 118.1, 102.8, 47.4, 37.8, 17.0; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{18}NO_3$: 320.1287. Found: 320.1288.

2-(2-(1-Hydroxynaphthalen-2-yl)-2-oxoethyl)-4-phenylpent-3-enal (4ha):



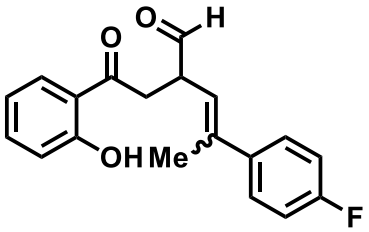
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.6) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ha** as yellow oil in 73% yield (50.3 mg, E/Z = 94:6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.74 & 13.68 (s, 1H), 9.78 & 9.68 (s, 1H), 8.44 (d, J = 7.8 Hz, 1H), 7.73 (dd, J_1 = 19.7 Hz, J_2 = 8.6 Hz, 2H), 7.65 – 7.61 (m, 1H), 7.54 – 7.50 (m, 1H), 7.40 – 7.38 (m, 2H), 7.35 – 7.25 (m, 4H), 5.58 & 5.31 (dd, J_1 = 9.7 Hz & 10.2 Hz, J_2 = 1.4 Hz & 1.6 Hz, 1H), 4.26 – 4.20 (m, 1H), 3.80 & 3.63 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 7.6 Hz & 7.5 Hz, 1H), 3.30 & 3.20 (dd, J_1 = 17.8 Hz & 17.6 Hz, J_2 = 5.1 Hz & 5.3 Hz, 1H), 2.25 & 2.10 (d, J = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.0, 198.8, 162.5, 142.5, 141.7, 137.4, 130.2, 128.4, 127.7, 127.4, 126.0, 125.9, 125.2, 124.5, 124.0, 120.6, 118.6, 112.7, 47.6, 38.4, 17.0.; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{23}H_{21}O_3$: 345.1491. Found: 345.1483.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-(p-tolyl)pent-3-enal (4ab):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ab** as yellow oil in 70% yield (43.2 mg, *E*/*Z* = 91:9); ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.05 & 11.99 (s, 1H), 9.74 & 9.65 (s, 1H), 7.82 & 7.74 (dd, J_1 = 8.0 Hz & 8.0 Hz, J_2 = 1.6 Hz & 1.8 Hz, 1H), 7.52 – 6.89 (m, 7H), 5.52 & 5.25 (dd, J = 9.6 Hz & 10.0 Hz, 1.4 Hz & 1.6 Hz, 1H), 4.18 & 3.83 (ddd, J_1 = 9.6 Hz & 10.1 Hz, J_2 = 7.6 Hz & 7.6 Hz, J_3 = 5.1 Hz & 5.1 Hz, 1H), 3.74 & 3.58 (dd, J_1 = 18.0 Hz & 17.6 Hz, J_2 = 7.7 Hz & 7.6 Hz, 1H), 3.22 & 3.11 (dd, J_1 = 17.8 Hz & 17.7 Hz, J_2 = 5.0 Hz & 5.1 Hz, 1H), 2.36 & 2.35 (s, 3H), 2.23 & 2.09 (d, *J* = 1.4 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.2, 198.8, 160.2, 142.5, 141.6, 137.7, 129,6, 128.3, 128.2, 127.7, 125.8, 120.5, 118.7, 118.3, 47.5, 38.1, 20.5, 16.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_3$: 309.1491. Found: 309.1487.

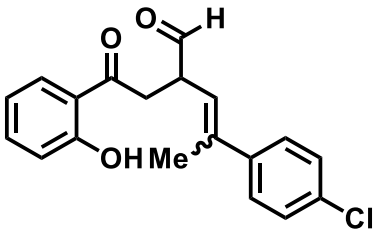
4-(4-Fluorophenyl)-2-(2-(2-hydroxyphenyl)-2-oxoethyl)pent-3-enal (4ac):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ac** as yellow oil in 61% yield (38.1 mg, *E*/*Z* = 94:6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.02 & 11.97 (s, 1H), 9.73 & 9.62 (s, 1H), 7.81 (dd, J_1 = 8.0, J_2 = 1.6 Hz, 1H), 7.52 – 7.31 (m, 3H), 7.04 – 6.89 (m, 4H), 5.50 & 5.29 (dd, J_1 = 9.6 Hz & 10.0 Hz, J_2 = 1.4 Hz & 1.5 Hz, 1H), 4.16 (ddd, J_1 = 9.8 Hz, J_2 = 7.4 Hz, J_3 =

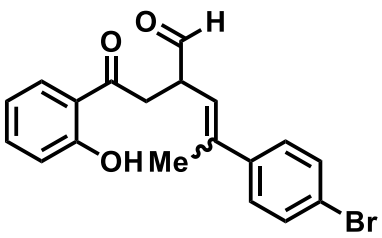
5.2 Hz, 1H), 3.73 & 3.57 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 7.4 Hz & 7.1 Hz, 1H), 3.24 & 3.12 (dd, J_1 = 17.8 Hz & 17.6 Hz, J_2 = 5.1 Hz & 5.4 Hz, 1H), 2.22 & 2.08 (d, J = 1.3 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.3, 198.6, 163.6, 162.4, 161.1, 140.7, 138.5 (d, J = 3.4 Hz), 136.7, 127.5 (d, J = 8.1 Hz), 120.5, 119.1, 119.1, 118.6, 115.2 (d, J = 21.4 Hz), 47.5, 38.1, 17.1; ^{19}F NMR (376Hz,$CDCl_3$) δ -114.6; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}FO_3$: 313.1240. Found: 313.1230.

4-(4-Chlorophenyl)-2-(2-(2-hydroxyphenyl)-2-oxoethyl)pent-3-enal (4ad):



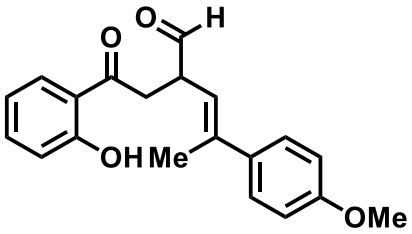
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ad** as yellow oil in 82% yield (53.9 mg, E/Z = 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.01 & 11.96 (s, 1H), 9.74 & 9.63 (s, 1H), 7.81 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.55 – 7.27 (m, 5H), 7.02 – 6.88 (m, 2H), 5.55 & 5.29 (dd, J_1 = 9.8 Hz & 10.3 Hz, J_2 = 1.5 Hz & 1.6 Hz, 1H), 4.20 – 4.13 (m, 1H). 3.74 & 3.57 (dd, J = 17.8 Hz & 17.8 Hz, J2 = 7.4 Hz & 7.2 Hz, 1H), 3.24 & (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 5.3 Hz & 5.4 Hz, 1H), 2.22 & 2.08 (d, J = 1.2 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.2, 198.6, 162.3, 140.9, 140.6, 136.7, 133.5, 129.8, 128.8, 128.5, 127.2, 121.1, 119.1, 118.6, 47.5, 38.1, 16.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}ClO_3$: 329.0944. Found: 329.0940.

4-(4-Bromophenyl)-2-(2-(2-hydroxyphenyl)-2-oxoethyl)pent-3-enal (4ae):



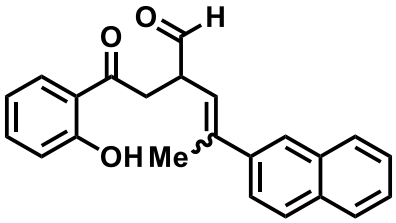
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ae** as yellow oil in 87% yield (64.9 mg, *E*/*Z* = 93:7); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.00 & 11.95 (s, 1H), 9.74 & 9.63 (s, 1H), 7.81 (dd, J_1 = 8.0 Hz, *J2* = 1.6 Hz, 1H), 7.52 – 7.22 (m, 5H), 7.02 – 6.89 (m, 2H), 5.55 & 5.30 (dd, J_1 = 9.6 Hz & 10.3 Hz, J_2 = 1.5 Hz & 1.6 Hz, 1H), 4.22 – 4.11 (m, 1H), 3.73 & 3.56 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 7.5 Hz & 7.1 Hz, 1H), 3.24 & 3.12 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 5.3 Hz & 5.4 Hz, 1H), 2.21 & 2.08 (d, *J* = 1.4 Hz & 1.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 198.3, 162.2, 141.2, 140.5, 136.6, 131.3, 129.7, 127.3, 121.6, 121.0, 119.1, 119.0, 118.5, 47.4, 38.0, 16.7; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{18}BrO_3$: 373.0439. Found: 373.0443.

(*E*)-2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-(4-methoxyphenyl)pent-3-enal (4af):



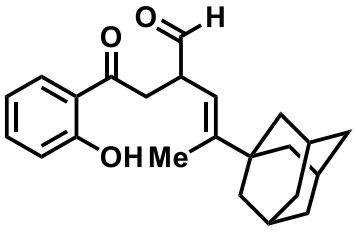
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4af** as yellow oil in 55% yield (35.7 mg, *E*/*Z* = 99 > 1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.06 (s, 1H), 9.73 (s, 1H), 7.82 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.48 (ddd, J_1 = 8.5 Hz, J_2 = 7.1 Hz, J_3 = 1.5 Hz, 1H), 7.34 (d, *J* = 8.8 Hz, 2H), 6.99 (dd, J_1 = 8.4 Hz, J_2 = 1.1 Hz, 1H), 6.92 (ddd, J_1 = 8.1 Hz, J_2 = 7.1 Hz, J_3 = 1.1 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 2H), 5.47 (dd, J_1 = 9.7 Hz, J_2 = 1.4 Hz, 1H), 4.20 – 4.15 (m, 1H), 3.81 (s, 3H), 3.74 (dd, J_1 = 17.9 Hz, J_2 = 7.7 Hz, 1H), 3.22 (dd, J_1 = 17.9 Hz, J_2 = 5.2 Hz, 1H), 3.22 (d, *J* = 1.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 198.7, 162.3, 159.2, 141.0, 136.6, 134.8, 129.9, 126.9, 119.1, 119.0, 118.7, 118.5, 113.6, 55.3, 47.5, 38.1, 16.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{20}H_{21}O_4$: 325.1440. Found: 325.1435.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-(naphthalen-2-yl)pent-3-enal (4ag):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ag** as yellow oil in 63% yield (43.4 mg, *E*/*Z* = 92:8); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.05 & 11.98 (s, 1H), 9.80 & 9.68 (s, 1H), 7.87 – 7.77 (m, 5H), 7.59 – 7.41 (m, 4H), 7.04 – 6.84 (m, 2H), 5.71 & 5.37 (dd, J_1 = 9.9 Hz & 10.0 Hz, J_2 = 1.5 Hz & 1.5 Hz, 1H), 4.31 – 4.21 & 3.89 – 3.83 (m, 1H), 3.79 & 3.58 (dd, J_1 = 17.8 Hz & 17.6 Hz, J_2 = 7.6 Hz & 7.2 Hz, 1H), 3.28 & 3.15 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 5.0 Hz & 5.4 Hz, 1H), 2.36 & 2.19 (d, J = 1.3 Hz & 1.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.3, 198.6, 162.3, 141.5, 139.6, 136.6, 133.2, 132.8, 129.9, 128.1, 127.9, 127.5, 126.3, 126.0, 124.7, 124.0, 120.9, 119.1, 119.0, 118.5, 47.6, 38.1, 17.0; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{23}H_{21}O_3$: 345.1491. Found: 345.1485.

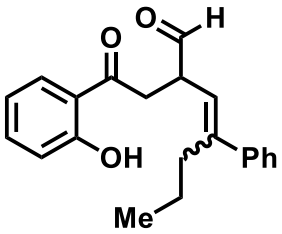
4-((3r,5r,7r)-Adamantan-1-yl)-2-(2-(2-hydroxyphenyl)-2-oxoethyl)pent-3-enal (4ah):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ah** as yellow oil in 57% yield (40.2 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.07 (s, 1H), 9.59 (s, 1H), 7.80 (dd, J_1 = 8.1 Hz, J_2 = 1.7

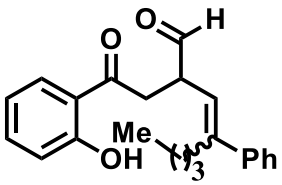
Hz, 1H), 7.48 – 7.44 (m, 1H), 6.96 (dd, J_1 = 8.4 Hz, J_2 = 1.4 Hz, 1H), 6.90 (ddd, J_1 = 8.3 Hz, J_2 = 7.1 Hz, J_2 = 1.2 Hz, 1H), 4.89 (dd, J_1 = 9.4 Hz, J_2 = 1.3 Hz, 1H), 4.04 – 3.98 (m, 1H), 3.61 (dd, J_1 = 17.7 Hz, J_2 = 7.9 Hz, 1H), 3.06 (dd, J_1 = 17.6 Hz, J_2 = 5.0 Hz, 1H), 1.99 (s, 3H), 1.76 – 1.61 (m, 15H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 199.3, 162.3, 151.7, 136.5, 130.0, 119.3, 119.0, 118.5, 114.2, 47.0, 40.7, 38.4, 38.1, 36.8, 28.5, 12.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{23}H_{29}O_3$: 353.2117. Found: 353.2114.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-phenylhept-3-enal (4ai):



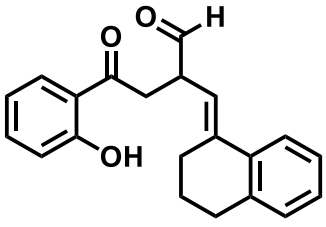
The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ai** as yellow oil in 84% yield (54.2 mg, *E*/*Z* = 94:6); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.06 & 12.01 (s, 1H), 9.75 & 9.64 (s, 1H), 7.81 & 7.73 (dd, J_1 = 8.0 Hz & 8.0 Hz, J_2 = 1.7 Hz & 1.8 Hz, 1H), 7.54 – 7.27 (m, 6H), 7.03 – 6.88 (m, 2H), 5.39 & 5.24 (d, J = 10.0 Hz & 10.0 Hz, 1H), 4.20 (ddd, J_1 = 10.2 Hz, J_2 = 7.9 Hz, J_3 = 5.0 Hz, 1H), 3.75 & 3.57 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 7.9 Hz & 7.6 Hz, 1H), 3.21 & 3.11 (dd, J_1 = 17.9 Hz & 17.6 Hz, J_2 = 5.0 Hz & 5.4 Hz, 1H), 2.66 & 2.37 (t, J = 7.3 Hz & 7.1 Hz, 2H), 1.42 (qd, J_1 = 7.6 Hz, J_2 = 3.0 Hz, 2H), 0.93 & 0.88 (t, J = 7.5 Hz & 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 199.0, 162.6, 147.8, 142.1, 136.8, 130.1, 128.6, 127.8, 126.7, 120.7, 119.4, 119.3, 118.8, 47.6, 38.5, 31.3, 22.9, 14.1; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{23}O_3$: 323.1647. Found: 323.1652.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-phenyloct-3-enal (4aj):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.4) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4aj** as yellow oil in 61% yield (41.0 mg, *E*/*Z* = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.03 & 11.98 (s, 1H), 9.73 & 9.62 (s, 1H), 7.80 & 7.72 (dd, J_1 = 8.1 Hz & 8.1 Hz, J_2 = 1.7 Hz & 1.7 Hz, 1H), 7.48 (ddd, J_1 = 8.7 Hz, J_2 = 7.2 Hz, J_3 = 1.7 Hz, 1H), 7.35 – 7.26 (m, 5H), 6.98 (dd, J_1 = 10.0 Hz, J_1 = 1.2 Hz, 1H), 6.91 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.36 & 5.23 (d, *J* = 10.1 Hz & 10.0 Hz, 1H), 4.20 – 4.14 (m, 1H), 3.73 & 3.55 (dd, J_1 = 17.6 Hz & 17.5 Hz, J_2 = 7.7 Hz & 7.4 Hz, 1H), 3.18 & 3.09 (dd, J_1 = 17.6 Hz & 17.5 Hz, J_2 = 7.7 Hz & 7.4 Hz, 1H), 2.68 – 2.63 & 2.39 – 2.35 (m, 2H), 1.38 – 1.28 (m, 4H), 0.88 – 0.84 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 198.8, 162.4, 147.6, 141.9, 136.6, 129.9, 128.4, 127.6, 126.5, 120.5, 119.2, 119.1, 118.6, 47.4, 38.3, 31.1, 30.5, 22.7, 13.9; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{22}H_{25}O_3$: 337.1804. Found: 337.1794.

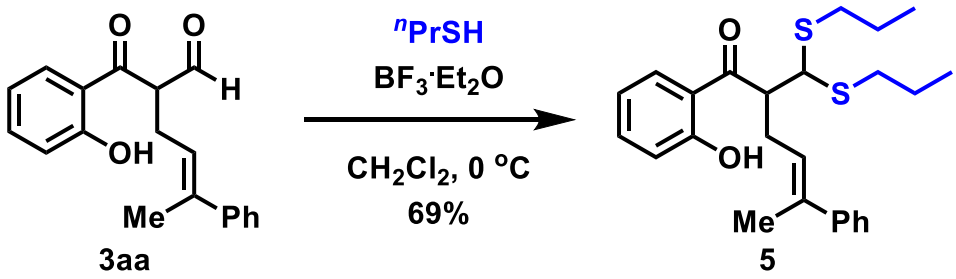
2-((3,4-Dihydronaphthalen-1(2H)-ylidene)methyl)-4-(2-hydroxyphenyl)-4-oxobut anal (4ak):



The title compound was prepared according to the general procedure. Purification by column chromatography (TLC R_f = 0.5) on silica gel using EtOAc /PE (2:8) as the eluent the desired product **4ak** as yellow oil in 73% yield (46.8 mg, *E*/*Z* > 99:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.04 (s, 1H), 9.72 (s, 1H), 7.82 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.57 – 7.45 (m, 2H), 7.22 – 7.10 (m, 3H), 7.01 – 6.88 (m, 2H), 5.74 (dt, J_1 = 9.8 Hz, J_2 = 1.8 Hz, 1H), 4.30 – 4.16 (m, 1H), 3.75 (dd, J_1 = 18.0 Hz, J_2 = 7.6 Hz, 1H),

3.23 (dd, J_1 = 17.9 Hz, J_2 = 5.1 Hz, 1H), 2.87 – 2.60 (m, 4H), 2.02 – 1.83 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 198.6, 162.3, 140.9, 137.8, 136.6, 134.9, 129.8, 129.0, 127.8, 126.2, 124.0, 119.1, 119.0, 118.5, 116.1, 46.9, 38.1, 30.2, 27.4, 23.2; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{21}H_{21}O_3$: 321.1491. Found: 321.1490.

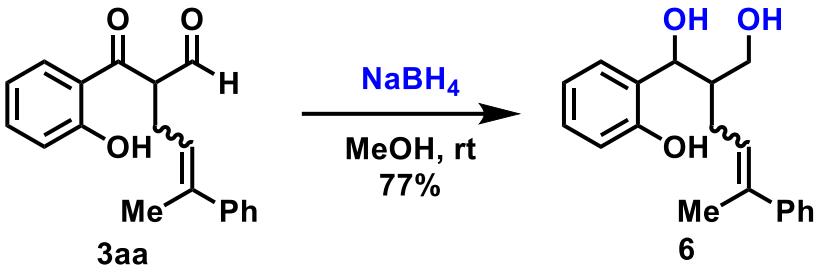
(*E*)-2-(Bis(propylthio)methyl)-1-(2-hydroxyphenyl)-5-phenylhex-4-en-1-one (5)[8]:



A flame-dried round-bottomed flask was charged with 3aa (0.1 mmol, 1.0 equiv., 29.4 mg), ^{n}PrSH (0.22 mmol, 2.2 equiv., 16.8 mg) and CH_2Cl_2 (1 mL), then cooled to 0 °C. BF_3·Et_2O (0.10 mmol, 1.0 equiv., 14.2 mg) was added dropwise and the mixture was stirred at 0 °C for 2 h. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (2 × 5 mL). The combined organic layers were washed with brine (10 mL), then dried (Na_2SO_4). After removal of the solvent, the residue was subjected to column chromatography (PE:EtOAc = 9:1) to give **5** (29.6 mg, 69% yield) as yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.35 (s, 1H), 7.92 (dd, J_1 = 8.1 Hz, J_2 = 1.6 Hz, 1H), 7.47 (ddd, J_1 = 8.6 Hz, J_2 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 7.49 – 7.45 (m, 5H), 6.98 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 6.92 (ddd, J_1 = 8.2 Hz, J_2 = 7.2 Hz, J_3 = 1.2 Hz, 1H), 5.74 (dd, J_1 = 10.0 Hz, J_2 = 1.4 Hz, 1H), 4.96 – 4.90 (m, 1H), 3.73 (dd, J_1 = 8.0 Hz, J_2 = 6.6 Hz, 1H), 2.70 – 2.50 (m, 5H), 2.25 (d, J = 1.4 Hz, 3H), 2.11 – 2.04 (m, 1H), 1.64 – 1.55 (m, 4H), 1.00 (t, J = 17.4 Hz, 3H), 0.93 (t, J = 17.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.6, 163.2, 142.6, 138.6, 136.6, 130.0, 128.3, 127.5, 125.8, 125.4, 119.0, 119.0, 118.7, 49.5, 44.8, 38.9, 32.4, 32.4, 22.8, 22.7, 16.8, 13.7, 13.6; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{25}H_{33}O_2S_2$: 429.1922. Found: 429.1927.

1-(2-Hydroxyphenyl)-2-(3-phenylbut-2-en-1-yl)propane-1,3-diol (6)[9]:

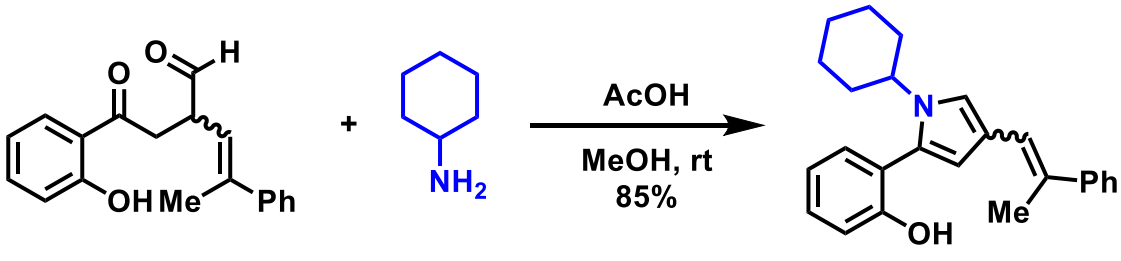
[8] S. Hanessian, T. Focken and R. Oza, *Tetrahedron*, 2011, **67**, 9870–9884.



3aa 6

A mixture of 3aa (0.1 mmol, 1.0 equiv., 29.4 mg) in MeOH (1.00 mL) was cooled to 0 ℃, $NaBH_4$ (0.4 mmol, 4.0 equiv., 15.1 mg) was added and the reaction mixture was stirred at the same temperature for 30 min under nitrogen atmosphere. The mixture was poured into H_2O (5 mL) and extracted with EtOAc (10 mL). The organic layer was washed with brine (10 mL) and dried with Na_2SO_4. After removal of the solvent, the residue was subjected to column chromatography to give **6** (23.0 mg, 77% yield) as yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 & 8.30 (s, 1H), 7.39 – 7.12 (m, 6H), 6.99 – 6.96 (m, 1H), 6.85 – 6.79 & 6.76 – 6.72 (m, 2H), 5.68 & 5.44 (d, J = 10.3 Hz & 10.2 Hz, 1H), 4.77 & 4.66 (d, J = 6.6 Hz & 8.2 Hz, 1H), 4.13 – 4.07 & 3.85 – 3.77 (m, 1H), 3.69 – 3.63 & 3.58 – 3.52 (m, 2H), 3.13 – 3.06 (m, 1H), 2.03 & 1.92 (s, 3H), 1.79 – 1.62 (m, 2H), 1.26 – 1.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 143.8, 143.2, 140.0, 137.9, 128.8, 128.6, 128.3, 128.3, 128.1, 127.9, 127.2, 126.8, 126.4, 125.8, 125.7, 125.2, 119.4, 119.2, 117.2, 116.8, 79.0, 78.8, 77.3, 77.0, 76.7, 60.6, 60.5, 43.3, 42.9, 34.7, 34.6, 21.0, 16.4, 16.0, 14.1; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{23}O_3$: 299.1647. Found: 299.1644.

2-(1-Cyclohexyl-4-(2-phenylprop-1-en-1-yl)-1H-pyrrol-2-yl)phenol (7)[10]:



4aa 7

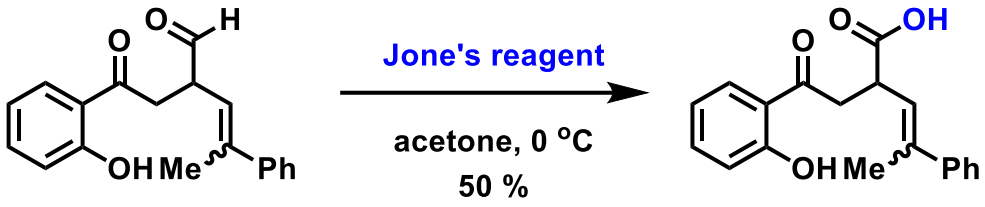
Acetic acid (0.2 mmol, 2.0 equiv., 12.0 mg) was added to the mixture of 4aa (0.1

[9] G. Zhong, *Angew. Chem., Int. Ed*., 2003, **42**, 4247−4250.

[10] S. G. Salamone and G. B. Dudley, *Org. Lett*., 2005, **7**, 20, 4443–4445.

mmol, 1.0equiv., 29.4 mg), cyclohexanamine (0.2 mmol, 2.0 equiv., 19.8 mg) in MeOH (1 mL). Then the reaction mixture was stirred at room temperature for 4 h. Brine (2 mL) was added, and extracted with DCM (5 ml × 3). The combined organic layer were dried over Na_2SO_4, and concentrated in *vacuo*. The residue was purified by flash column chromatography on silica gel give the desired product **7** as yellow oil (30.4 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 2H), 7.37 – 7.30 (m, 3H), 7.26 – 7.24 (m, 1H), 7.18 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 7.09 – 6.98 (m, 3H), 6.70 (s, 1H), 6,42 (d, J = 1.8 Hz, 1H), 5.72 (s, 1H), 3.78 – 3.70 (m, 1H), 2.37 (s, 3H), 1.98 – 1.95 (m, 2H), 1.84 – 1.81 (m, 2H), 1.69 – 1.63 (m, 3H), 1.27 – 1.21 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 145.0, 132.5, 130.9, 130.0, 128.2, 126.5, 126.3, 125.8, 122.3, 120.9, 120.2, 119.6, 118.8, 115.4, 109.6, 55.5, 34.7, 25.7, 25.3, 18.2; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{25}H_{28}NO$: 358.2171. Found: 358.2176.

2-(2-(2-Hydroxyphenyl)-2-oxoethyl)-4-phenylpent-3-enoic acid (8)[11]:



4aa **8**

A mixture of 4aa (0.1 mmol, 1.0 equiv., 29.4 mg) in acetone was cooled to 0 ℃. Jone's reagent (2.67 M, 0.1 mL) was added dropwise and the reaction mixture was stirred at 0 ℃ until 4aa was completely converted. Then the reaction mixture was quenched with 2-Propanol (2 mL). Brine (2 mL) was added, and extracted with DCM (5 ml × 3). The combined organic layer were dried over Na_2SO_4, and concentrated in *vacuo*. The residue was purified by flash column chromatography on silica gel give the desired product **8** as yellow oil (15.5 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.91 (s, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.48 – 7.37 (m, 6H), 6.89 – 6.82 (m, 2H), 3.76 (d, J = 5.7 Hz, 2H), 3.5 (s, 1H), 1.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 201.3, 171.4, 162.4, 137.9, 129.8, 128.5, 128.5, 124.3, 119.4, 118.8, 117.8,

[11] N. Waizumi, T. Itoh and T. Fukuyama, *J. Am. Chem. Soc*., 2000, **122**, 7825–7826.

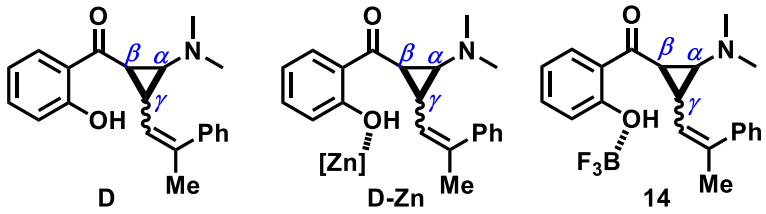
90.0, 69.5, 44.3, 29.7, 27.8; HRMS (ESI) m/z $[M+H]^+$: Calcd for $C_{19}H_{19}O_4$: 311.1283. Found: 311.1275.

Computational details

In this work, the involved structures are optimized at M06/6-31G(d,p)/LANL2DZ(Zn,Br)/IEF-PCM$_{dichloroethane}$ level using density functional theory (DFT), followed by a single-point energy correction of the structures at M06/6-311+G(d,p)/SDD(Zn,Br)/IEF-PCM$_{dichloroethane}$ level. All calculations are performed by Gaussian 16 program. In addition, Laplacian bond order (LBO) were carried out for key intermediates by Multiwfn. In addition, CYLview[1] software was used for the optimized 3D structure drawing.

To understand how the reaction controls its selectivity, we calculated the Laplacian bond order (LBO) of the key intermediates. As shown in **Scheme 1**, the LBO of C_β-C_α and C_α-C_γ for intermediate **D** are 0.754/0.735, respectively, so it is difficult to occur ring opening to obtain the corresponding products. When there is only zinc catalyst in the system, it can be seen that the LBO of C_β-C_α is reduced to 0.546, while the LBO of C_α-C_γ is 0.913, so the C_β-C_α bond can be broken more easily to form α-vinyl-1,4-ketoaldehyde **4aa**. With the addition of Lewis acid BF_3 to this reaction, the LBO of C_α-C_γ and C_β-C_α were 0.679/0.855, respectively, and it can be seen that the C_α-C_γ bond is more easily broken to generate 1,3-dicarbonyl compound **3aa**. In summary, different Lewis acid catalysis regulate the chemoselectivity of the reaction.

LBO	D	D-Zn	14
C_β-C_α	0.754	0.546	0.855
C_α-C_γ	0.735	0.913	0.679



Scheme 1. Laplacian bond order (LBO) at different sites in intermediates D, D-Zn and 14.

Cartesian coordinates

1a

Zero-point correction= 0.220792
Thermal correction to Energy= 0.234777
Thermal correction to Enthalpy= 0.235721
Thermal correction to Gibbs Free Energy= 0.178846
Sum of electronic and zero-point Energies= -631.556272
Sum of electronic and thermal Energies= -631.542287
Sum of electronic and thermal Enthalpies= -631.541343

Sum of electronic and thermal Free Energies= -631.598218

Cartesian coordinates

C	3.743179	0.994249	0.439088
C	2.413513	1.332109	0.245390
C	1.432590	0.382159	-0.064060
C	1.845576	-0.955006	-0.210750
C	3.186542	-1.301006	-0.025426
C	4.127811	-0.337332	0.303215
H	4.473915	1.757700	0.691816
H	2.082036	2.363897	0.330593
H	3.484557	-2.341803	-0.149205
H	5.165059	-0.630123	0.447515
C	0.032880	0.906944	-0.225617
O	-0.107703	2.106937	-0.499527
C	-1.086596	0.024765	0.010496
C	-2.349012	0.537659	-0.088085
H	-0.908458	-1.010224	0.276172
H	-2.447187	1.591229	-0.352581
O	0.941570	-1.903172	-0.563524
H	1.391348	-2.753719	-0.643203
N	-3.502531	-0.119808	0.101400
C	-4.783847	0.554309	0.050442
H	-5.447709	0.070179	-0.675806
H	-5.276799	0.540122	1.030868
H	-4.640257	1.594778	-0.249660
C	-3.489461	-1.521713	0.466599
H	-3.039689	-1.671529	1.457233
H	-4.513762	-1.899992	0.486569
H	-2.915316	-2.104790	-0.263456

Vibrational frequencies

28.3439	37.8512	78.1701
81.3102	117.2030	138.8689
174.5981	214.2272	235.0209
252.2449	268.9448	323.4924
361.2436	373.6181	386.9926
442.0673	453.1241	517.8795
541.8509	563.3294	594.3946
649.0938	695.4666	756.5915
774.3446	808.5615	814.2852
851.9709	853.7523	919.1891
959.2154	982.4475	1003.2313
1065.5257	1076.9120	1090.9670
1105.9826	1107.4621	1133.1417
1142.8687	1155.3235	1179.0518

1218.8427	1265.3321	1291.4021
1312.0266	1325.9526	1371.3090
1384.9670	1422.6896	1434.2865
1443.1921	1449.9576	1453.0867
1480.0150	1485.8515	1521.5217
1533.9773	1632.0088	1656.1193
1671.7528	1729.2325	3014.3726
3020.3245	3092.1994	3094.6655
3150.6728	3153.5241	3158.6862
3160.4214	3180.3063	3190.9778
3200.7315	3244.0302	3861.6862

r2

Zero-point correction= 0.164836
Thermal correction to Energy= 0.173557
Thermal correction to Enthalpy= 0.174502
Thermal correction to Gibbs Free Energy= 0.131136
Sum of electronic and zero-point Energies= -386.539952
Sum of electronic and thermal Energies= -386.531230
Sum of electronic and thermal Enthalpies= -386.530286
Sum of electronic and thermal Free Energies= -386.573652
Cartesian coordinates

C	2.269377	-0.981134	0.645632
C	2.269404	-0.981141	-0.645617
C	1.498547	0.138397	-0.000019
H	2.543832	-1.426781	1.590970
H	2.543844	-1.426997	-1.590862
C	-0.003416	0.062257	0.000001
C	-0.657031	-1.177054	0.000003
C	-0.797378	1.214425	0.000007
C	-2.043187	-1.262136	-0.000006
H	-0.065459	-2.090448	-0.000004
C	-2.187238	1.132307	0.000000
H	-0.329798	2.196024	0.000013
C	-2.819063	-0.105681	0.000001
H	-2.521645	-2.239317	0.000007
H	-2.777566	2.046199	-0.000002
H	-3.904505	-0.170506	-0.000023
C	2.093775	1.531566	-0.000016
H	1.791175	2.106791	-0.885039
H	1.791192	2.106754	0.885040
H	3.186189	1.467441	-0.000022

Vibrational frequencies

40.8888	139.0073	223.3637

269.8629	340.6015	341.9263
372.3220	414.6156	421.8054
509.8333	548.8005	626.1868
635.6046	710.0488	712.6531
765.0337	827.2239	845.5847
855.4247	886.0888	921.4415
969.0558	973.0234	993.7451
997.7403	1003.9697	1057.1250
1073.4529	1090.3315	1108.0758
1156.8223	1191.4467	1258.9023
1285.8480	1330.3982	1371.5527
1391.0937	1462.3743	1472.0583
1480.8371	1531.1504	1646.1935
1674.8151	1751.0670	3017.5731
3092.7721	3127.0957	3165.9034
3172.5603	3182.1138	3188.6214
3195.4089	3241.8557	3291.1727

BF_3

Zero-point correction= 0.012621
Thermal correction to Energy= 0.016111
Thermal correction to Enthalpy= 0.017056
Thermal correction to Gibbs Free Energy= -0.011824
Sum of electronic and zero-point Energies= -324.447237
Sum of electronic and thermal Energies= -324.443747
Sum of electronic and thermal Enthalpies= -324.442802
Sum of electronic and thermal Free Energies= -324.471682
Cartesian coordinates

B	0.000000	0.000000	0.000000
F	0.000000	1.309591	0.000000
F	1.134139	-0.654795	0.000000
F	-1.134139	-0.654795	0.000000

Vibrational frequencies

482.9664	483.0868	679.6603
907.3945	1493.4502	1493.5543

9

Zero-point correction= 0.236254
Thermal correction to Energy= 0.254161
Thermal correction to Enthalpy= 0.255106
Thermal correction to Gibbs Free Energy= 0.188540
Sum of electronic and zero-point Energies= -956.042753
Sum of electronic and thermal Energies= -956.024846
Sum of electronic and thermal Enthalpies= -956.023902

Sum of electronic and thermal Free Energies= -956.090467

Cartesian coordinates

C	-3.464371	-0.689131	1.031370
C	-2.236044	-0.061594	0.921569
C	-1.183742	-0.623861	0.182500
C	-1.412934	-1.849798	-0.475745
C	-2.657915	-2.471696	-0.377489
C	-3.672427	-1.900240	0.374912
H	-4.256506	-0.238338	1.621772
H	-2.063640	0.889833	1.415107
H	-2.822100	-3.411403	-0.902593
H	-4.632879	-2.404639	0.444712
C	0.116758	0.064743	0.185793
O	0.175624	1.351173	0.289905
C	1.315727	-0.660746	0.198477
C	2.525722	0.015352	0.182552
H	1.271530	-1.742797	0.203926
H	2.507237	1.103055	0.125252
O	-0.424901	-2.392131	-1.221577
H	-0.745591	-3.202082	-1.638765
N	3.724842	-0.540020	0.226150
C	4.939054	0.257930	0.165371
H	5.546683	0.086226	1.060024
H	5.526998	-0.017067	-0.716781
H	4.682965	1.317049	0.106005
C	3.878895	-1.985633	0.311174
H	3.474796	-2.470710	-0.584094
H	4.939675	-2.225904	0.393894
H	3.358679	-2.375002	1.192559
B	-0.740924	2.437260	-0.283296
F	0.123343	3.413524	-0.724317
F	-1.481072	1.903999	-1.313332
F	-1.537298	2.909293	0.744635

Vibrational frequencies

22.2081	28.9797	49.2636
64.5791	70.5882	87.3305
121.2347	133.0605	166.4899
169.7606	203.9285	227.3781
243.3608	262.4345	290.2853
297.1678	355.9012	384.4402
398.3063	421.3009	428.8030
461.8881	468.8122	495.6770
513.9691	537.0020	545.0998
575.1078	610.3488	653.5898

685.3936	723.6125	756.1670
776.6735	819.1988	835.2062
853.9171	859.0667	893.0418
935.5799	961.6444	986.5868
998.2143	1074.7223	1076.2948
1101.1088	1113.9510	1124.8000
1144.7360	1159.3097	1163.5070
1183.5908	1193.3946	1214.5478
1237.6264	1276.9889	1300.7000
1308.4376	1334.8536	1386.7339
1393.1411	1424.2152	1428.7654
1441.7744	1455.2425	1458.9816
1474.7399	1486.4203	1526.4524
1544.4832	1572.4445	1654.8501
1667.1954	1684.8265	3036.3245
3040.3209	3122.6246	3124.6122
3167.1139	3169.0810	3171.5816
3175.9565	3188.1925	3202.8578
3219.4924	3247.4817	3856.5937

$ZnBr_2$

Zero-point correction= 0.001372
Thermal correction to Energy= 0.005907
Thermal correction to Enthalpy= 0.006851
Thermal correction to Gibbs Free Energy= -0.028396
Sum of electronic and zero-point Energies= -91.877600
Sum of electronic and thermal Energies= -91.873065
Sum of electronic and thermal Enthalpies= -91.872121
Sum of electronic and thermal Free Energies= -91.907368
Cartesian coordinates

Zn	-0.000000	-0.000000	0.230874
Br	0.000000	-2.395290	-0.098946
Br	0.000000	2.395290	-0.098946

Vibrational frequencies

129.2226	178.6703	294.5472

A

Zero-point correction= 0.168693
Thermal correction to Energy= 0.183911
Thermal correction to Enthalpy= 0.184856
Thermal correction to Gibbs Free Energy= 0.121595
Sum of electronic and zero-point Energies= -478.418310
Sum of electronic and thermal Energies= -478.403091
Sum of electronic and thermal Enthalpies= -478.402147

Sum of electronic and thermal Free Energies= -478.465408

Cartesian coordinates

C	-1.107516	-0.757057	0.116829
C	0.108050	-1.339809	0.364977
C	-2.377131	-1.380177	0.199071
H	-1.100653	0.289529	-0.188029
H	0.105592	-2.383202	0.691542
C	-2.511218	-2.841906	0.415722
H	-3.278405	-3.062783	1.163720
H	-1.575075	-3.314603	0.710334
C	-3.575203	-0.593422	0.023567
C	-3.551028	0.815029	0.146834
C	-4.809137	-1.219370	-0.262021
C	-4.707484	1.556242	-0.013083
H	-2.630463	1.329502	0.407631
C	-5.956682	-0.470642	-0.446214
H	-4.860163	-2.298755	-0.370154
C	-5.908581	0.917765	-0.319381
H	-4.676667	2.635627	0.101873
H	-6.893107	-0.964644	-0.688046
Zn	1.820839	-0.194864	0.108794
Br	1.135961	2.255039	0.092414
Br	4.187046	-0.903404	-0.248802
H	-2.832706	-3.316593	-0.521197
H	-6.813207	1.504734	-0.455722

Vibrational frequencies

34.8075	38.0941	43.1963
47.3868	78.5982	94.1028
111.4859	134.7767	150.4484
170.7723	203.7192	215.9909
247.8508	286.2973	371.1671
400.1571	403.5085	467.5440
547.8121	565.7752	616.4524
650.3293	676.1510	760.5777
773.4882	790.7755	843.7772
945.4567	958.9047	983.1987
991.4230	1004.1749	1017.6846
1025.9945	1054.9380	1082.7168
1122.6853	1163.0173	1167.9260
1199.0550	1297.7212	1344.0404
1349.7341	1369.5018	1396.6792
1398.3090	1430.9159	1460.0685
1492.7241	1527.6377	1557.8332
1628.3601	1660.7344	3045.8920

3125.5299	3140.9741	3160.4120
3189.3257	3192.7556	3201.2235
3205.4122	3212.4871	3217.1052

10-ts

Zero-point correction= 0.406857
Thermal correction to Energy= 0.440482
Thermal correction to Enthalpy= 0.441426
Thermal correction to Gibbs Free Energy= 0.337608
Sum of electronic and zero-point Energies= -1434.451476
Sum of electronic and thermal Energies= -1434.417851
Sum of electronic and thermal Enthalpies= -1434.416907
Sum of electronic and thermal Free Energies= -1434.520725
Cartesian coordinates

C	2.934959	-2.061684	-2.215560
C	1.651782	-1.888194	-1.734665
C	1.333046	-2.089394	-0.375541
C	2.375251	-2.480585	0.499572
C	3.666707	-2.668155	0.003400
C	3.944634	-2.460366	-1.337095
H	3.153459	-1.886814	-3.264704
H	0.861892	-1.569249	-2.407888
H	4.453963	-2.979887	0.687274
H	4.959842	-2.604568	-1.698560
C	-0.039355	-1.828538	0.049018
O	-1.011142	-1.849167	-0.782812
C	-0.346988	-1.387283	1.373147
C	-1.697736	-1.427020	1.777886
H	0.448648	-1.399365	2.105704
H	-2.446866	-1.611573	1.006051
O	2.107314	-2.700515	1.801693
H	2.904319	-3.006561	2.254320
N	-2.166455	-1.220445	2.984024
C	-3.603209	-1.234546	3.245186
H	-3.847722	-2.075002	3.902512
H	-3.884533	-0.300038	3.741559
H	-4.150948	-1.314675	2.304620
C	-1.336288	-0.953719	4.151693
H	-1.395753	0.108086	4.416262
H	-1.714657	-1.541996	4.992329
H	-0.298856	-1.235475	3.972079
B	-1.336182	-2.722925	-2.031006
F	-0.527392	-3.829423	-2.001228
F	-2.660361	-3.029278	-1.870838

F	-1.116438	-1.927314	-3.135631
C	1.193334	1.011397	0.572903
C	-0.134226	0.843034	1.038752
C	2.317907	1.205972	1.346905
H	1.326280	1.055656	-0.509331
H	-0.261975	0.942281	2.120192
C	2.275711	1.218066	2.838514
H	3.102055	0.629546	3.251505
H	1.337822	0.832145	3.241741
C	3.619520	1.444431	0.714827
C	3.893989	0.974121	-0.581017
C	4.639095	2.125416	1.401924
C	5.133539	1.179747	-1.166439
H	3.146789	0.397278	-1.121067
C	5.872376	2.349016	0.806148
H	4.460955	2.504269	2.405059
C	6.125297	1.875409	-0.478908
H	5.327403	0.785550	-2.161482
H	6.641537	2.892747	1.348458
Zn	-1.721671	1.348372	-0.190947
Br	-4.128514	0.601666	-0.041625
Br	-1.387581	3.449502	-1.516567
H	2.392494	2.240788	3.219736
H	7.095689	2.041376	-0.940034

Vibrational frequencies

-276.1164	22.4793	28.1078
32.4137	38.3057	43.8729
49.2649	56.8289	58.5548
62.8695	68.3214	70.4230
77.0161	83.1223	85.1172
91.2179	96.2962	101.7684
105.7075	119.3931	136.2858
144.6175	147.6214	176.0817
180.4184	214.0095	228.8308
230.7372	240.1751	250.9245
254.5763	267.1066	275.0483
282.2233	296.4433	342.8155
365.5677	368.9742	394.7546
409.1988	411.7188	419.7196
433.0878	456.2359	457.3236
476.3744	480.0304	507.0086
512.6483	537.3693	540.1426
553.2991	577.0792	578.3827
613.6332	621.7200	646.7137

658.0646	675.9933	695.1816
709.8119	764.7689	767.5054
772.8319	782.7472	824.8979
834.1493	850.6547	856.5360
860.1176	868.5365	912.5335
931.9244	941.1668	957.7294
980.0509	980.9074	984.5232
997.5924	1001.7530	1005.0996
1006.0948	1037.6665	1053.6166
1055.3355	1082.4063	1084.1612
1101.4877	1112.9096	1119.5844
1127.7706	1147.0152	1151.9453
1159.1344	1161.0456	1173.9058
1189.9165	1192.6694	1208.2472
1220.2467	1237.2665	1254.1830
1270.2183	1287.7496	1311.1211
1321.6316	1324.8817	1357.4735
1361.5589	1383.1965	1396.4751
1403.5011	1406.2608	1414.9279
1425.7540	1426.9102	1444.8566
1450.6491	1453.6603	1458.6866
1462.1729	1476.5910	1486.9767
1524.6608	1525.1123	1541.8824
1563.4848	1578.2155	1640.5874
1646.8979	1664.9935	1673.4491
1696.8507	3044.2730	3044.5668
3049.3192	3117.2806	3132.6706
3135.7223	3139.6814	3149.1633
3164.7562	3168.7721	3174.9571
3177.4030	3177.5640	3185.4811
3186.1804	3193.9685	3194.5698
3197.9330	3203.7749	3208.1885
3220.3995	3280.3684	3849.4771

11

Zero-point correction= 0.406628
Thermal correction to Energy= 0.433294
Thermal correction to Enthalpy= 0.434238
Thermal correction to Gibbs Free Energy= 0.348972
Sum of electronic and zero-point Energies= -1342.625190
Sum of electronic and thermal Energies= -1342.598524
Sum of electronic and thermal Enthalpies= -1342.597580
Sum of electronic and thermal Free Energies= -1342.682847
Cartesian coordinates

C	0.380654	-1.610756	-0.511673
C	-1.064778	-1.676579	-0.802134
C	1.287899	-0.983251	-1.285652
H	0.707660	-2.054724	0.429241
H	-1.347710	-1.900586	-1.831939
C	0.903800	-0.239231	-2.531795
H	0.955153	0.847303	-2.370781
H	-0.118604	-0.460846	-2.848910
C	2.715877	-0.965170	-0.901743
C	3.292921	-2.026319	-0.190525
C	3.533756	0.120991	-1.241315
C	4.628335	-1.992214	0.187520
H	2.690554	-2.901159	0.045227
C	4.870189	0.157071	-0.860563
H	3.116956	0.959974	-1.795404
C	5.423645	-0.898321	-0.143253
H	5.054017	-2.830732	0.733664
H	5.481670	1.016182	-1.126336
H	1.583235	-0.472196	-3.359757
H	6.470352	-0.873190	0.149582
C	0.510628	3.382312	-0.774739
C	0.188959	2.248986	-0.049526
C	-1.121675	1.741438	-0.046073
C	-2.119858	2.424037	-0.769780
C	-1.795123	3.580467	-1.476079
C	-0.488679	4.046188	-1.485754
H	1.533265	3.747230	-0.788479
H	0.959741	1.707928	0.492318
H	-2.575928	4.110277	-2.017973
H	-0.250197	4.942439	-2.052500
C	-1.344041	0.428628	0.559330
O	-0.773586	0.049387	1.614545
C	-2.043997	-0.590215	-0.210613
C	-2.076656	-2.009727	0.248929
H	-2.765105	-0.227842	-0.933561
H	-1.637625	-2.157846	1.238422
O	-3.380937	1.950058	-0.718085
H	-3.967212	2.506448	-1.247824
N	-3.212432	-2.857678	0.030939
C	-2.782088	-4.244419	-0.025330
H	-3.656957	-4.903448	-0.036743
H	-2.170476	-4.464531	-0.921398
H	-2.183525	-4.485317	0.860398
C	-4.060056	-2.523278	-1.095572

H	-3.546276	-2.575630	-2.075497
H	-4.891073	-3.235579	-1.128980
H	-4.490688	-1.524332	-0.976744
B	0.073594	0.782599	2.733721
F	1.380240	0.656588	2.329901
F	-0.354302	2.076719	2.812324
F	-0.207521	0.055753	3.851679

Vibrational frequencies

14.9169	33.2463	41.5888
48.9673	58.2387	68.5987
72.5521	79.1151	95.2295
100.3092	104.6056	126.4962
143.6853	152.4564	181.5768
186.9145	194.1185	213.6862
237.2631	250.8522	255.2342
260.7562	284.5583	298.0766
322.3385	343.0961	363.9588
385.6102	389.3606	396.7085
415.3479	420.1905	427.9046
454.9728	470.1646	483.6708
499.9043	513.0967	529.1938
537.3990	560.5389	567.9453
573.2549	590.8431	611.3502
626.1380	640.5902	678.0481
706.4190	711.0553	728.7801
768.5870	771.5145	777.0894
812.5425	843.8030	856.1303
861.2954	865.0738	868.8927
879.3355	910.0206	922.9508
935.8319	948.7749	976.3127
981.7509	985.1805	998.2409
1005.7636	1010.4113	1036.7904
1054.3895	1057.5018	1065.4557
1075.8996	1081.3648	1088.9370
1102.2764	1108.5777	1110.4397
1117.0578	1129.5437	1157.9403
1163.8414	1166.5470	1175.7090
1188.4415	1194.8826	1214.0199
1231.4387	1234.8623	1261.6907
1270.1397	1271.5192	1312.7119
1315.7663	1319.2221	1337.4268
1344.2512	1354.6411	1373.1687
1389.8714	1400.0048	1402.8747
1417.0170	1443.5769	1448.3650

1452.9343	1457.3918	1466.5475
1468.6133	1477.1664	1480.8147
1492.3375	1503.6288	1529.6897
1539.7650	1633.9459	1642.2524
1655.5421	1671.2332	1675.6077
1705.9273	2940.2778	2948.9607
3025.2279	3070.9068	3079.7003
3098.3917	3123.0736	3124.4845
3130.4708	3140.7262	3145.1557
3155.3923	3170.7585	3175.1004
3178.4718	3182.5580	3187.8279
3191.8365	3197.4195	3204.1108
3213.9683	3245.8911	3856.5380

12

Zero-point correction= 0.235535
Thermal correction to Energy= 0.253755
Thermal correction to Enthalpy= 0.254699
Thermal correction to Gibbs Free Energy= 0.187930
Sum of electronic and zero-point Energies= -956.016647
Sum of electronic and thermal Energies= -955.998427
Sum of electronic and thermal Enthalpies= -955.997482
Sum of electronic and thermal Free Energies= -956.064251
Cartesian coordinates

C	-3.547030	-2.012178	0.094310
C	-2.194653	-2.193685	-0.151961
C	-1.248641	-1.185489	0.069880
C	-1.754021	0.028214	0.540055
C	-3.103477	0.248004	0.768346
C	-4.007942	-0.784144	0.557439
H	-4.244171	-2.826918	-0.080993
H	-1.816778	-3.138591	-0.531870
H	-3.436957	1.229578	1.098945
H	-5.065718	-0.621239	0.743568
C	0.188446	-1.538868	-0.256497
O	0.373294	-2.558679	-0.931487
C	1.264958	-0.722384	0.239341
C	2.548600	-1.065712	-0.090955
H	1.059753	0.148605	0.846986
H	2.697954	-1.964485	-0.690036
O	-0.880535	1.110382	0.768437
H	-1.182289	1.621125	1.536717
N	3.660607	-0.398039	0.236455
C	4.979465	-0.906689	-0.084157

H	5.550813	-0.162537	-0.651221
H	5.538658	-1.150014	0.827940
H	4.888578	-1.812324	-0.687953
C	3.580652	0.823863	1.014183
H	3.288321	0.617981	2.052554
H	4.557301	1.312759	1.016716
H	2.845135	1.507664	0.575115
B	-0.556396	2.208663	-0.542131
F	-1.623315	3.033489	-0.470588
F	0.616261	2.739285	-0.139187
F	-0.515510	1.385241	-1.600947

Vibrational frequencies

21.9094	39.4475	50.7400
76.1259	83.0602	93.0199
107.8816	116.7843	153.0330
178.6581	192.5623	196.1604
232.9904	248.1684	270.7567
280.3679	321.8243	338.0242
368.1554	402.7604	445.2238
448.1157	456.4078	483.9846
497.5063	534.0417	577.7088
581.9296	591.5784	643.8431
649.9902	688.5158	759.7195
785.0285	803.6551	837.3097
843.5576	870.9404	875.5143
918.4368	964.4804	1000.7596
1008.1577	1064.2529	1078.6799
1093.0005	1106.9041	1111.4452
1137.8772	1144.7477	1156.5134
1199.4254	1221.3803	1230.9381
1266.8985	1295.1153	1312.5225
1319.2092	1361.1454	1378.1669
1384.4590	1425.9180	1434.8527
1444.5185	1455.6074	1457.0805
1478.5459	1481.6420	1519.1155
1529.3449	1632.4622	1650.9285
1681.1600	1733.4536	3018.7382
3023.7543	3097.8107	3106.1366
3154.2788	3155.7256	3166.0738
3181.0660	3189.4302	3201.9068
3207.8768	3260.4782	3798.4749

13-ts

Zero-point correction= 0.407322

Thermal correction to Energy= 0.439998
Thermal correction to Enthalpy= 0.440943
Thermal correction to Gibbs Free Energy= 0.340778
Sum of electronic and zero-point Energies= -1434.442667
Sum of electronic and thermal Energies= -1434.409990
Sum of electronic and thermal Enthalpies= -1434.409046
Sum of electronic and thermal Free Energies= -1434.509211
Cartesian coordinates

C	-1.294939	4.982917	-0.649960
C	-0.509524	4.059047	0.023631
C	-0.953515	2.757255	0.291795
C	-2.244096	2.444234	-0.154065
C	-3.051655	3.353507	-0.817639
C	-2.571966	4.631309	-1.077274
H	-0.911808	5.982219	-0.838303
H	0.487044	4.319748	0.369383
H	-4.051713	3.044766	-1.110038
H	-3.198325	5.348553	-1.600346
C	0.025169	1.858186	1.011378
O	1.140151	2.313858	1.292985
C	-0.314809	0.479759	1.291080
C	0.587231	-0.280658	2.033886
H	-1.316207	0.113395	1.124366
H	1.580349	0.144258	2.190055
O	-2.801230	1.185966	0.116373
H	-2.891541	0.561120	-0.648939
N	0.388631	-1.476791	2.551574
C	1.484045	-2.236257	3.136762
H	1.225274	-2.537260	4.157329
H	1.660584	-3.136284	2.534201
H	2.392481	-1.630957	3.156535
C	-0.887124	-2.179098	2.515858
H	-0.826188	-3.018360	1.809968
H	-1.089633	-2.581290	3.513886
H	-1.705198	-1.513613	2.236403
B	-3.829343	0.972694	1.392462
F	-5.035389	1.405371	0.955168
F	-3.740063	-0.371411	1.591464
F	-3.262020	1.734148	2.357113
C	2.048221	0.034865	-0.654266
C	0.678721	-0.101871	-0.899410
C	2.818853	1.167625	-0.873644
H	2.561064	-0.839740	-0.246197
H	0.170756	0.780541	-1.303352

C	2.306987	2.364077	-1.600376
H	2.629976	3.285817	-1.106771
H	1.219567	2.378115	-1.688361
C	4.230494	1.173144	-0.484755
C	4.700406	0.348858	0.553851
C	5.151044	2.022760	-1.122541
C	6.034721	0.364011	0.928042
H	4.007085	-0.288718	1.096749
C	6.489603	2.025307	-0.757852
H	4.822946	2.672855	-1.929129
C	6.936097	1.196708	0.268165
H	6.373443	-0.271734	1.741772
H	7.187677	2.677633	-1.275826
Zn	-0.346491	-1.877045	-1.023220
Br	0.682533	-4.081502	-0.413395
Br	-2.755752	-1.432615	-1.798962
H	2.714430	2.378803	-2.620327
H	7.983750	1.203953	0.558148

Vibrational frequencies

-127.7139	25.5760	26.6409
37.2461	39.7054	44.4377
53.8273	55.6345	58.9556
72.6296	79.6495	82.5548
89.5123	97.7541	108.0817
112.4257	119.1255	128.6356
140.4924	151.7879	157.0920
180.0212	192.2806	199.3056
213.0865	219.7034	237.3884
245.1088	251.6409	255.7374
280.6488	286.9400	296.7795
318.4489	329.2036	343.9485
361.4095	365.1166	395.9295
406.4050	412.2123	415.1845
437.9507	459.7573	462.3314
478.1530	484.6221	492.6672
515.3077	536.9811	549.7795
573.7278	581.0058	598.6461
611.1054	612.9574	623.4970
647.7078	667.6834	694.7992
696.2150	766.7241	769.8885
774.3651	798.6823	807.3664
838.0785	849.2971	860.4038
870.9895	879.9498	895.4782
910.9564	941.1558	958.6230

979.2335	981.3792	982.5326
1006.9380	1007.3561	1008.5093
1019.5823	1035.2299	1056.3951
1062.8221	1065.8701	1084.7224
1090.0960	1113.1787	1114.6604
1118.9088	1140.5090	1156.7747
1159.8835	1161.6069	1162.8794
1195.3043	1212.1552	1222.2174
1247.8961	1255.6101	1276.7479
1278.4974	1288.6997	1294.9689
1326.0182	1337.5870	1346.2537
1362.0521	1369.1345	1377.2105
1384.9569	1402.5944	1417.4007
1429.9684	1439.8255	1449.7747
1453.0660	1454.6570	1464.2681
1479.0803	1481.4306	1495.8147
1515.7912	1520.6612	1527.9773
1558.8771	1638.1680	1640.7126
1659.8826	1666.0622	1674.3047
1717.7733	3032.4114	3038.4594
3039.5000	3117.3830	3120.7013
3123.1109	3123.3345	3134.0119
3163.1354	3167.7729	3170.6623
3177.1196	3184.7730	3190.1335
3192.4449	3200.0524	3200.7379
3207.2072	3208.5343	3212.3913
3212.8626	3306.2461	3363.0471

14

Zero-point correction= 0.406017
Thermal correction to Energy= 0.432945
Thermal correction to Enthalpy= 0.433889
Thermal correction to Gibbs Free Energy= 0.347242
Sum of electronic and zero-point Energies= -1342.619156
Sum of electronic and thermal Energies= -1342.592229
Sum of electronic and thermal Enthalpies= -1342.591284
Sum of electronic and thermal Free Energies= -1342.677931
Cartesian coordinates

C	2.482976	-3.691097	1.674055
C	1.933891	-2.500484	2.122133
C	1.544759	-1.496391	1.227874
C	1.677471	-1.768858	-0.136431
C	2.209381	-2.956370	-0.608063
C	2.629002	-3.913859	0.306724

H	2.796982	-4.447257	2.387455
H	1.809154	-2.304317	3.183814
H	2.275004	-3.116307	-1.679934
H	3.055673	-4.845441	-0.053979
C	1.011277	-0.224029	1.801053
O	0.432475	-0.227342	2.874214
C	1.218665	1.018096	1.004721
C	0.609547	2.290571	1.442973
H	2.142970	1.043998	0.431052
H	0.008582	2.202381	2.351166
O	1.232241	-0.871082	-1.116176
H	0.602407	-0.216844	-0.751297
N	1.290452	3.544859	1.347610
C	0.329764	4.624378	1.195656
H	0.838943	5.589596	1.289027
H	-0.187551	4.598778	0.217608
H	-0.430109	4.559674	1.982328
C	2.346186	3.630163	0.357268
H	2.001414	3.467053	-0.682995
H	2.782095	4.633519	0.399716
H	3.146771	2.915835	0.573192
B	2.354054	-0.071457	-2.137408
F	2.639891	-1.001291	-3.064024
F	1.585053	0.970071	-2.541040
F	3.368540	0.253670	-1.303609
C	-1.314032	0.926654	0.349946
C	-0.014344	1.604980	0.241739
C	-2.159443	0.623987	-0.655351
H	-1.601655	0.653269	1.366265
H	0.260064	2.025802	-0.726285
C	-1.911403	1.003290	-2.087708
H	-2.227476	0.199789	-2.762355
H	-0.859567	1.216407	-2.296662
C	-3.421917	-0.089874	-0.359900
C	-3.507473	-1.011160	0.693880
C	-4.565339	0.123776	-1.140531
C	-4.696921	-1.670277	0.973374
H	-2.618958	-1.234314	1.282665
C	-5.757504	-0.534071	-0.859664
H	-4.529238	0.826542	-1.970277
C	-5.830174	-1.432099	0.199943
H	-4.735410	-2.385615	1.791590
H	-6.634269	-0.342868	-1.474039
H	-2.484282	1.897072	-2.368293

H	-6.760265	-1.952091	0.415629

Vibrational frequencies

13.5480	28.7080	36.1712
39.6177	49.2632	55.3910
77.0964	83.1552	85.9423
95.8766	108.1330	118.5955
139.6409	147.9655	168.1895
188.4486	189.7852	218.9977
243.5193	255.4565	261.7251
266.4303	283.0210	292.8375
307.4023	329.6477	354.0841
364.7383	374.8102	389.9828
413.4865	420.0457	440.2397
448.4056	468.6194	481.6217
485.1175	494.6546	528.5470
551.3858	554.7830	564.1114
579.2167	586.0794	606.2050
626.2258	628.8247	643.4702
694.3908	706.6118	734.8300
768.1091	771.6076	775.0700
810.6019	827.3512	852.1759
853.7988	863.0924	877.5814
884.4958	900.6567	928.8405
933.0375	959.8731	970.7687
975.2282	985.8025	997.6466
1001.8247	1005.6469	1038.7123
1052.0413	1053.9727	1059.7327
1066.6112	1073.5226	1088.4069
1096.3137	1102.0319	1106.3395
1109.8334	1119.3606	1157.9720
1158.3992	1163.1401	1181.7028
1190.6549	1211.5644	1215.8298
1235.1922	1238.8757	1262.2736
1271.7067	1294.2564	1318.5193
1322.3938	1323.0476	1337.6734
1358.3430	1361.1938	1369.5716
1384.9534	1404.2881	1410.1092
1418.0394	1443.7467	1451.4221
1460.7939	1465.5867	1469.1317
1470.4420	1478.2520	1481.0490
1492.6554	1498.0488	1518.3545
1530.0499	1642.9538	1647.2841
1670.8502	1685.7520	1718.2458
1794.1219	2945.4449	2952.1062

3033.4366	3072.8748	3081.4750
3105.7941	3123.4554	3125.4438
3131.3312	3146.4452	3149.7404
3163.6433	3167.1849	3172.8686
3180.9451	3187.7099	3189.4997
3191.4649	3197.0529	3199.5285
3207.9868	3216.7428	3635.2700

15-ts

Zero-point correction= 0.401652
Thermal correction to Energy= 0.428121
Thermal correction to Enthalpy= 0.429065
Thermal correction to Gibbs Free Energy= 0.343478
Sum of electronic and zero-point Energies= -1342.599453
Sum of electronic and thermal Energies= -1342.572985
Sum of electronic and thermal Enthalpies= -1342.572040
Sum of electronic and thermal Free Energies= -1342.657627
Cartesian coordinates

C	2.697947	-3.674971	1.376579
C	2.043792	-2.570193	1.890992
C	1.735797	-1.459154	1.091638
C	2.084682	-1.522302	-0.267652
C	2.729174	-2.632009	-0.797815
C	3.047413	-3.700899	0.027177
H	2.936973	-4.515790	2.021090
H	1.760807	-2.525143	2.939132
H	2.970450	-2.632929	-1.856104
H	3.562361	-4.562675	-0.388659
C	1.070187	-0.315115	1.775138
O	0.580074	-0.434368	2.883652
C	1.013484	1.004811	1.045667
C	0.191911	2.059409	1.567968
H	1.997461	1.286371	0.661024
H	-0.682970	1.779431	2.151527
O	1.768128	-0.508832	-1.153078
H	0.905836	0.098148	-0.812690
N	0.438810	3.373574	1.450152
C	-0.713027	4.260575	1.383842
H	-0.430936	5.262656	1.717080
H	-1.094254	4.319184	0.351869
H	-1.509790	3.882434	2.029388
C	1.620621	3.839513	0.744121
H	1.539550	3.673408	-0.341875
H	1.733344	4.911487	0.920847

H	2.517332	3.336695	1.114296
B	2.914685	0.436551	-1.743765
F	3.584071	-0.302716	-2.666645
F	2.194598	1.478270	-2.258164
F	3.690386	0.797906	-0.670269
C	-1.309463	0.301085	0.055990
C	-0.047277	1.012685	-0.072894
C	-2.366078	0.399273	-0.781443
H	-1.396872	-0.366971	0.917087
H	0.045587	1.819229	-0.801483
C	-2.337703	1.346198	-1.949452
H	-3.046145	1.049122	-2.729099
H	-1.345270	1.380667	-2.413046
C	-3.593165	-0.378258	-0.535067
C	-3.562278	-1.630820	0.098794
C	-4.845857	0.119283	-0.925714
C	-4.729258	-2.338277	0.353321
H	-2.603123	-2.068683	0.369196
C	-6.014612	-0.589579	-0.672946
H	-4.909236	1.088434	-1.417010
C	-5.965034	-1.821761	-0.029076
H	-4.671918	-3.309445	0.840226
H	-6.971555	-0.172625	-0.979416
H	-2.589242	2.376182	-1.653723
H	-6.878112	-2.379461	0.164183

Vibrational frequencies

-716.6767	16.9274	24.6453
34.0805	50.2349	58.5236
64.1916	70.9358	80.3942
83.7264	93.2507	108.0104
130.1960	136.0871	146.1286
151.5048	203.3193	215.2569
227.7159	242.9105	248.9084
255.1888	270.6088	283.3744
287.0502	326.7211	338.2627
359.1701	386.4811	392.9999
401.3765	416.8410	438.0526
443.7450	464.2091	485.4476
488.1853	495.9905	521.7136
526.3921	551.5554	574.3067
582.7336	594.6844	616.4601
626.1550	644.5881	679.4133
693.6652	707.3531	715.7357
758.2018	766.6018	781.3773

786.1618	824.7646	840.0840
851.0379	876.5908	880.6543
886.7224	899.7571	920.1468
948.7439	954.9143	970.9909
976.7211	991.7157	993.5161
1002.1781	1003.7954	1029.1195
1037.1698	1055.2163	1067.8392
1069.4532	1083.2193	1094.8491
1103.2129	1107.0750	1124.3716
1135.5500	1149.6948	1155.5765
1156.8159	1162.1992	1181.1993
1191.0897	1211.9597	1225.6892
1233.0016	1243.2028	1266.3725
1279.8558	1285.8508	1296.5111
1317.0095	1340.0028	1357.4583
1368.9425	1374.8362	1385.7302
1392.7920	1409.2174	1424.5727
1442.5042	1446.4004	1450.5601
1459.0307	1466.8060	1469.0928
1472.1062	1476.4375	1481.3490
1488.8365	1519.4016	1529.8003
1556.7922	1617.0632	1638.6067
1653.1911	1669.6178	1678.6357
1712.2718	1799.2196	2997.8392
3003.3980	3010.4165	3087.2671
3108.3464	3113.1302	3127.3441
3127.3893	3131.6114	3158.1232
3160.7900	3163.3327	3166.3377
3170.1844	3179.6013	3183.4736
3189.0268	3191.2163	3194.9839
3199.1941	3208.1904	3219.3257

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Zero-point correction= 0.407433
Thermal correction to Energy= 0.434188
Thermal correction to Enthalpy= 0.435132
Thermal correction to Gibbs Free Energy= 0.348822
Sum of electronic and zero-point Energies= -1342.657220
Sum of electronic and thermal Energies= -1342.630465
Sum of electronic and thermal Enthalpies= -1342.629521
Sum of electronic and thermal Free Energies= -1342.715831
Cartesian coordinates

C	-4.137982	-3.168691	-1.013960
C	-2.836620	-2.739016	-1.182967

C	-2.343846	-1.610440	-0.504869
C	-3.186065	-0.936823	0.413294
C	-4.512096	-1.369505	0.560129
C	-4.978525	-2.465133	-0.145260
H	-4.506760	-4.034797	-1.556412
H	-2.164026	-3.248646	-1.868631
H	-5.144865	-0.830631	1.258997
H	-6.008960	-2.787072	-0.010333
C	-0.986925	-1.161616	-0.873569
O	-0.209423	-1.873272	-1.497615
C	-0.564801	0.265407	-0.528007
C	0.318844	0.800808	-1.579358
H	-1.450367	0.892001	-0.416473
H	0.903574	0.093550	-2.170811
O	-2.698653	0.036410	1.179680
H	-0.374118	-0.289967	1.534287
N	0.480443	2.053157	-1.832365
C	1.432626	2.505748	-2.850500
H	0.887794	3.041221	-3.631902
H	2.148097	3.186649	-2.381467
H	1.956934	1.650578	-3.276549
C	-0.213980	3.138520	-1.126532
H	0.483957	3.598605	-0.419489
H	-0.508318	3.885744	-1.866564
H	-1.100828	2.777744	-0.603105
B	-3.239791	1.414464	1.179142
F	-4.511728	1.465940	1.723319
F	-2.338686	2.176873	1.905502
F	-3.272482	1.873360	-0.153614
C	1.604801	-0.275678	0.687221
C	0.227108	0.287380	0.821520
C	2.773183	0.376447	0.827190
H	1.638621	-1.330160	0.407575
H	0.217238	1.317821	1.192196
C	2.875899	1.844766	1.127377
H	3.606581	2.031364	1.922925
H	1.924187	2.279855	1.441884
C	4.054771	-0.352656	0.668042
C	4.165741	-1.713661	0.986063
C	5.201449	0.305456	0.204053
C	5.364057	-2.394652	0.818826
H	3.306001	-2.238625	1.396952
C	6.401579	-0.375462	0.034015
H	5.156964	1.363914	-0.042516

C	6.488742	-1.729765	0.337691
H	5.423415	-3.448729	1.079741
H	7.273682	0.158017	-0.336923
H	3.221425	2.409480	0.250184
H	7.428532	-2.261605	0.211507

Vibrational frequencies

18.8713	25.5862	31.5079
43.2767	54.6654	60.5207
70.2815	87.8634	90.6363
92.6256	114.1903	124.1002
135.5442	142.1757	172.4621
180.6546	182.4468	195.7155
208.5654	229.3563	240.1613
271.7023	295.3124	307.8334
327.8148	336.0827	358.7164
376.8666	395.2332	399.5610
411.9525	421.5619	442.7634
446.1180	471.5628	481.6934
498.8238	512.2715	526.2819
558.2783	568.0687	579.2160
593.9223	611.2644	626.3960
635.1087	655.4599	704.6838
712.5453	744.6399	747.0670
768.7609	779.6036	786.5988
804.9624	851.1047	863.3679
872.9574	884.3667	886.1065
911.1969	919.1558	929.9200
970.8047	973.2468	973.7101
986.3743	994.0492	996.3947
996.7133	1005.7165	1035.9239
1041.0317	1046.5224	1056.4137
1067.0411	1082.3814	1099.6736
1106.2069	1109.0039	1110.2264
1120.1985	1131.5666	1153.6602
1158.1397	1158.8056	1160.6000
1177.3836	1191.5436	1205.1622
1219.4934	1232.5365	1240.8821
1270.5826	1302.0554	1320.7254
1327.0229	1342.7423	1357.3852
1369.4948	1380.6545	1384.1089
1404.1109	1411.1388	1424.0588
1429.8575	1434.7103	1443.7473
1452.5342	1461.3663	1467.8515
1473.5586	1477.4875	1480.0830

1490.2423	1524.4050	1530.9553
1625.2886	1643.1469	1668.2536
1672.6648	1729.8531	1750.9745
1768.1014	3028.0606	3058.3580
3060.5787	3066.1676	3097.9160
3123.1689	3149.0524	3151.3392
3152.7388	3156.8424	3160.7957
3161.9440	3170.4869	3174.4043
3176.0755	3183.7850	3188.0981
3188.9465	3189.6358	3192.8465
3196.8345	3200.7537	3214.7430

17

Zero-point correction= 0.420830
Thermal correction to Energy= 0.452331
Thermal correction to Enthalpy= 0.453276
Thermal correction to Gibbs Free Energy= 0.356444
Sum of electronic and zero-point Energies= -1667.090346
Sum of electronic and thermal Energies= -1667.058845
Sum of electronic and thermal Enthalpies= -1667.057901
Sum of electronic and thermal Free Energies= -1667.154733
Cartesian coordinates

C	-2.866338	3.638169	-0.615854
C	-2.059917	2.946856	0.269326
C	-1.636845	1.637606	-0.018260
C	-1.989942	1.077776	-1.258489
C	-2.791006	1.770909	-2.151547
C	-3.240889	3.042174	-1.819819
H	-3.207844	4.638805	-0.370430
H	-1.765182	3.390883	1.215875
H	-3.033259	1.304389	-3.102379
H	-3.874620	3.580788	-2.518779
C	-0.942530	0.878685	1.018298
O	-0.103865	1.396232	1.801466
C	-1.226888	-0.537784	1.165404
C	-0.573698	-1.344710	2.238553
H	-2.174246	-0.869865	0.752438
H	0.078143	-0.758495	2.889182
O	-1.545884	-0.153867	-1.673773
H	-0.745709	-0.434089	-1.199407
N	-1.290406	-2.351071	2.959324
C	-0.348716	-3.281662	3.562948
H	-0.883645	-3.960046	4.235634
H	0.186287	-3.890111	2.809425

H	0.395913	-2.733078	4.149776
C	-2.326658	-3.058918	2.231669
H	-1.945835	-3.652061	1.377866
H	-2.815061	-3.757783	2.918193
H	-3.096228	-2.372124	1.866231
B	-2.892366	-1.724472	-1.844919
F	-3.244547	-1.498653	-3.095128
F	-1.979934	-2.652810	-1.574165
F	-3.705710	-1.341086	-0.867697
C	1.283100	-1.003118	0.454429
C	-0.024087	-1.535428	0.856955
C	2.022485	-1.429455	-0.591044
H	1.689209	-0.214310	1.090252
H	-0.402107	-2.401634	0.313398
C	1.613029	-2.558201	-1.493711
H	1.892649	-2.344555	-2.530961
H	0.538121	-2.757211	-1.473565
C	3.334067	-0.800945	-0.863573
C	3.549540	0.563135	-0.620715
C	4.391225	-1.557093	-1.386473
C	4.788748	1.139960	-0.866887
H	2.728279	1.186450	-0.271657
C	5.632154	-0.979093	-1.626870
H	4.249799	-2.616207	-1.591506
C	5.837280	0.371801	-1.365588
H	4.931815	2.201501	-0.679201
H	6.442071	-1.588323	-2.021201
H	2.117675	-3.492411	-1.214360
H	6.805641	0.826529	-1.559657
B	0.876757	2.635030	1.583719
F	0.289699	3.707649	2.189632
F	2.014076	2.206647	2.202633
F	1.032230	2.777672	0.230449

Vibrational frequencies

20.9859	26.1540	30.2714
39.7589	42.8379	56.7765
62.9182	65.7057	69.9063
78.2228	87.3680	91.0404
94.9951	104.5523	105.5994
129.7797	148.2662	159.2666
171.5002	187.4944	192.6635
201.9432	212.2163	232.6638
256.5180	264.2617	272.1673
282.9357	300.0711	308.7951

323.0018	355.7520	368.9320
373.7132	400.1684	414.4080
415.0408	424.2247	429.8740
454.1598	477.2577	482.8431
484.3755	490.4188	506.6197
512.9420	518.6266	527.7613
557.9976	564.6596	570.6556
581.5498	595.8184	607.9817
624.3067	632.1820	671.3934
692.7007	708.1600	728.3650
769.1783	772.1794	774.5603
811.7078	834.2457	854.6443
858.2277	865.3495	876.1734
883.0788	887.0772	916.1249
925.4993	944.4197	950.7734
976.8363	979.4596	988.6546
1000.7798	1005.1501	1005.8261
1039.2764	1055.5790	1060.3651
1062.7435	1070.8441	1081.6970
1093.8231	1103.4403	1110.0617
1113.9437	1120.8121	1135.5332
1159.2166	1163.3627	1165.1740
1183.3825	1196.6269	1218.5780
1222.5554	1231.7588	1238.3784
1256.4763	1266.9830	1278.7026
1287.1283	1323.6790	1328.1689
1330.3494	1342.7920	1365.2255
1382.7368	1389.0023	1401.1845
1409.7312	1415.1308	1419.8043
1445.9190	1446.7015	1455.0303
1459.9867	1468.4517	1470.6803
1474.3394	1479.3045	1485.0958
1495.7900	1504.8481	1521.2271
1531.3217	1628.6536	1642.7269
1648.6154	1670.1434	1683.9147
1709.0111	2949.3860	2954.4821
3033.8873	3077.3025	3085.6564
3108.4812	3129.7956	3134.0607
3135.0647	3143.7112	3159.7824
3169.6365	3169.9377	3176.3544
3183.8493	3188.6232	3193.7852
3195.6811	3204.2111	3209.3975
3217.3914	3225.5206	3757.7474

18-ts

Zero-point correction= 0.415980
Thermal correction to Energy= 0.446774
Thermal correction to Enthalpy= 0.447718
Thermal correction to Gibbs Free Energy= 0.352995
Sum of electronic and zero-point Energies= -1667.065776
Sum of electronic and thermal Energies= -1667.034982
Sum of electronic and thermal Enthalpies= -1667.034038
Sum of electronic and thermal Free Energies= -1667.128760
Cartesian coordinates

C	-2.547332	3.662595	-0.837095
C	-1.876525	2.941117	0.129270
C	-1.630848	1.562292	-0.031021
C	-2.061867	0.947800	-1.228248
C	-2.700045	1.681988	-2.215566
C	-2.959140	3.029759	-2.009896
H	-2.749491	4.717684	-0.682949
H	-1.555407	3.423302	1.047666
H	-2.991617	1.175736	-3.129593
H	-3.482106	3.593222	-2.777533
C	-0.998403	0.856067	1.070792
O	-0.232325	1.399793	1.898242
C	-1.210767	-0.607425	1.231097
C	-0.529784	-1.335950	2.265864
H	-2.233617	-0.908553	0.996165
H	0.403126	-0.932341	2.652816
O	-1.807684	-0.375447	-1.496876
H	-1.019255	-0.804188	-0.855184
N	-0.994291	-2.448893	2.844110
C	-0.027832	-3.376336	3.415956
H	-0.484151	-3.913814	4.251103
H	0.303443	-4.102793	2.660311
H	0.842603	-2.826426	3.781041
C	-2.253446	-3.040888	2.421926
H	-2.163790	-3.514800	1.431602
H	-2.538461	-3.807627	3.145308
H	-3.048428	-2.292050	2.389329
B	-3.012355	-1.454327	-1.629225
F	-3.654164	-1.162944	-2.785428
F	-2.321515	-2.629685	-1.627820
F	-3.778232	-1.266932	-0.508597
C	1.153657	-0.849246	0.078814
C	-0.200740	-1.335480	0.313600
C	1.998900	-1.333204	-0.856834

H	1.502759	-0.027822	0.708240
H	-0.474247	-2.362394	0.067786
C	1.601173	-2.472834	-1.752188
H	2.059070	-2.376940	-2.742818
H	0.515147	-2.516941	-1.895099
C	3.355174	-0.772262	-1.005266
C	3.647231	0.560456	-0.670364
C	4.400708	-1.564730	-1.500557
C	4.933692	1.064446	-0.802388
H	2.849825	1.220484	-0.332165
C	5.688831	-1.058292	-1.632951
H	4.208289	-2.601142	-1.770935
C	5.964348	0.258743	-1.281790
H	5.130409	2.102305	-0.542507
H	6.481525	-1.699621	-2.012106
H	1.911874	-3.447315	-1.348978
H	6.969809	0.658394	-1.389349
B	0.839831	2.616944	1.742932
F	0.261059	3.697519	2.331746
F	1.905512	2.109772	2.414099
F	1.056620	2.748532	0.402743

Vibrational frequencies

-802.9243	16.6464	34.8111
35.9714	43.6854	49.5158
58.0608	62.1862	70.9024
74.9373	78.0907	81.5995
94.2208	103.1549	112.2436
136.2403	147.9892	165.9374
172.0002	175.0321	182.8308
215.2902	222.6341	238.4444
243.0328	261.2718	268.6965
281.3164	295.5239	305.4810
314.9377	348.6494	353.1249
378.0844	396.0581	401.0189
409.8529	417.0162	424.0712
445.5433	464.3500	476.9136
483.2940	486.8568	500.5695
509.5593	521.0369	534.3649
554.3758	558.3663	580.5683
589.1678	606.3751	619.9348
625.7825	644.0903	655.0332
668.8161	710.2035	722.5232
764.9728	767.8237	782.2373
796.6660	815.0530	832.9678

854.5099	858.5658	882.5930
884.9536	892.7547	906.0632
931.7305	938.6071	959.3716
978.5252	992.2880	993.2213
999.6016	1004.4290	1012.1354
1035.8903	1053.5320	1058.5370
1070.3186	1077.7149	1083.6818
1091.5103	1101.6179	1110.0509
1112.2646	1136.2147	1144.5952
1151.0116	1157.2756	1170.3208
1172.3566	1193.8986	1228.0229
1237.8431	1238.6548	1256.2810
1259.9129	1274.7945	1281.3102
1285.0122	1291.1214	1315.8721
1321.2619	1335.3723	1361.4836
1377.4645	1379.1267	1388.5379
1398.3853	1410.7111	1425.4408
1444.7723	1447.7286	1452.1422
1460.4988	1464.6208	1468.4487
1476.3607	1477.7888	1482.2106
1496.3866	1518.4255	1531.4370
1569.0268	1632.8892	1638.5571
1647.2524	1653.2123	1670.7611
1689.0120	1712.6685	3008.3439
3015.1600	3017.3572	3091.7778
3115.7776	3118.5416	3122.6471
3136.7570	3142.1664	3162.0399
3162.3245	3163.8925	3166.6722
3171.2529	3180.0316	3184.1944
3194.3395	3194.6697	3195.3299
3208.8159	3218.5909	3224.4498

19-ts

Zero-point correction= 0.404548
Thermal correction to Energy= 0.431461
Thermal correction to Enthalpy= 0.432405
Thermal correction to Gibbs Free Energy= 0.346903
Sum of electronic and zero-point Energies= -1342.591372
Sum of electronic and thermal Energies= -1342.564458
Sum of electronic and thermal Enthalpies= -1342.563514
Sum of electronic and thermal Free Energies= -1342.649017
Cartesian coordinates

C	4.100546	-2.595426	-0.245334
C	3.116919	-1.830755	0.354293

C	2.631904	-0.642555	-0.229697
C	3.205490	-0.248116	-1.463192
C	4.185314	-1.030426	-2.068995
C	4.634216	-2.197257	-1.468767
H	4.454030	-3.499356	0.242222
H	2.719375	-2.133910	1.316804
H	4.597680	-0.707178	-3.023740
H	5.404558	-2.789338	-1.955680
C	1.660391	0.134651	0.524182
O	1.046134	-0.332273	1.558315
C	1.331289	1.534026	0.214710
C	0.591252	2.334003	1.181855
H	2.118312	2.063016	-0.318362
H	-0.049455	1.812697	1.890390
O	2.777995	0.890503	-2.056063
H	3.223019	0.999160	-2.906593
N	0.554539	3.645772	1.200139
C	-0.468019	4.355083	1.961380
H	0.002692	5.140325	2.559032
H	-1.192789	4.811463	1.278191
H	-0.986736	3.659254	2.622371
C	1.344589	4.447889	0.274870
H	0.953929	4.336463	-0.745178
H	1.277824	5.495948	0.569233
H	2.393589	4.143140	0.296522
B	0.344452	-1.669540	1.817789
F	1.116850	-2.390738	2.706182
F	-0.860677	-1.308091	2.394098
F	0.162800	-2.324105	0.624431
C	-1.020089	0.567355	-0.452278
C	0.195478	1.229557	-0.749335
C	-2.071233	0.395083	-1.314509
H	-1.139417	0.173890	0.557058
H	0.375700	1.612504	-1.749592
C	-2.052859	0.962949	-2.705244
H	-2.543070	0.287782	-3.416918
H	-1.035042	1.127533	-3.070276
C	-3.290857	-0.298860	-0.886905
C	-3.305916	-1.213271	0.185337
C	-4.510613	-0.075554	-1.552804
C	-4.478642	-1.841942	0.577271
H	-2.382138	-1.455288	0.705587
C	-5.683146	-0.709122	-1.158440
H	-4.548231	0.623364	-2.385646

C	-5.679268	-1.596410	-0.087564
H	-4.451676	-2.546931	1.406059
H	-6.608210	-0.503370	-1.693631
H	-2.577829	1.927903	-2.773602
H	-6.594411	-2.096619	0.220414

Vibrational frequencies

-153.9678	25.2262	36.5614
41.4686	49.9660	59.7169
62.8503	74.5334	80.9825
88.1832	100.3365	106.7371
118.7810	136.0436	153.9594
162.8923	165.9826	180.0908
213.2600	219.5972	238.6605
253.3577	265.7669	277.3080
278.3076	321.0925	356.9886
362.1739	378.5560	392.2865
401.0361	411.4007	418.4418
432.6706	444.9751	456.9079
476.3426	484.6498	512.8804
517.4741	534.5137	543.2370
552.3785	571.8621	600.5732
611.4774	624.1109	626.1738
652.4840	705.3730	706.1569
714.0588	721.9732	762.3901
766.7388	777.5598	824.0411
848.3313	851.2079	856.2581
879.8324	896.0498	906.5347
923.9836	957.5670	957.6589
968.7170	986.9362	988.0362
993.2838	998.7479	1000.4331
1037.3119	1056.4477	1062.7087
1067.4775	1083.4941	1094.1028
1096.8162	1110.5866	1114.5643
1133.8594	1140.2755	1150.0967
1155.5831	1164.8664	1174.8914
1196.2853	1200.3808	1210.9069
1212.5841	1227.6876	1256.2139
1284.5274	1287.3901	1305.1455
1323.2836	1336.6345	1346.9992
1364.4701	1379.9523	1392.9227
1394.1666	1413.3930	1421.0457
1425.7474	1442.3152	1443.5456
1454.5903	1455.9709	1465.5731
1470.2852	1477.4017	1481.1471

1490.3448	1519.8780	1531.2552
1546.0273	1612.3529	1633.6493
1645.2318	1665.6995	1669.1502
1671.0461	3006.8607	3031.7413
3041.4602	3081.8836	3130.0978
3131.3763	3134.9646	3162.3066
3166.5366	3168.1906	3169.9775
3173.7315	3175.1809	3182.0412
3182.2083	3188.5075	3189.8484
3194.5421	3202.0912	3206.6790
3208.8107	3228.1276	3853.4321

H_20

Zero-point correction= 0.021691
Thermal correction to Energy= 0.024527
Thermal correction to Enthalpy= 0.025471
Thermal correction to Gibbs Free Energy= 0.004044
Sum of electronic and zero-point Energies= -76.370584
Sum of electronic and thermal Energies= -76.367749
Sum of electronic and thermal Enthalpies= -76.366804
Sum of electronic and thermal Free Energies= -76.388232
Cartesian coordinates

O	-0.000000	0.000000	0.119176
H	0.000000	0.754965	-0.476705
H	-0.000000	-0.754965	-0.476705

Vibrational frequencies

1641.7381	3881.4128	3998.2886

NH_4Cl

Zero-point correction= 0.049596
Thermal correction to Energy= 0.053715
Thermal correction to Enthalpy= 0.054659
Thermal correction to Gibbs Free Energy= 0.024198
Sum of electronic and zero-point Energies= -517.278101
Sum of electronic and thermal Energies= -517.273982
Sum of electronic and thermal Enthalpies= -517.273038
Sum of electronic and thermal Free Energies= -517.303499
Cartesian coordinates

N	-1.827304	0.000019	-0.000013
H	-2.173638	-0.954944	0.080718
H	-0.747507	-0.000149	-0.000743
H	-2.175074	0.407697	-0.866789
H	-2.173740	0.547023	0.786929
Cl	1.180064	0.000014	-0.000001

Vibrational frequencies

269.8056	308.6765	321.8529
1372.0626	1464.1167	1467.6623
1675.3825	1676.6302	2542.4080
3471.6736	3599.1404	3600.6554

NH_2Me_2Cl

Zero-point correction= 0.107068
Thermal correction to Energy= 0.113502
Thermal correction to Enthalpy= 0.114446
Thermal correction to Gibbs Free Energy= 0.076350
Sum of electronic and zero-point Energies= -595.771387
Sum of electronic and thermal Energies= -595.764953
Sum of electronic and thermal Enthalpies= -595.764009
Sum of electronic and thermal Free Energies= -595.802105
Cartesian coordinates

N	-0.968441	-0.000014	-0.489562
H	0.099487	-0.000504	-0.507565
H	-1.308779	0.000154	-1.452259
Cl	1.972434	-0.000294	0.036834
C	-1.388056	1.237338	0.207231
H	-2.474599	1.255030	0.307001
H	-0.916978	1.240843	1.192437
H	-1.044558	2.100748	-0.363015
C	-1.389498	-1.236783	0.207330
H	-0.916701	-1.241715	1.191709
H	-2.475914	-1.252090	0.308976
H	-1.048923	-2.100691	-0.363909

Vibrational frequencies

73.9323	119.1240	172.7023
220.1680	319.5830	411.2184
856.1644	906.8412	1024.2270
1036.5980	1098.0966	1238.7545
1256.8822	1393.8077	1411.3967
1434.9854	1443.5967	1455.9446
1464.8327	1479.2418	1481.9418
1583.6548	2722.4204	3068.7207
3072.5669	3181.0399	3181.7330
3189.9862	3190.2018	3506.8420

$BF_3{\cdot}NH_3$

Zero-point correction= 0.052617
Thermal correction to Energy= 0.058168
Thermal correction to Enthalpy= 0.059112

Thermal correction to Gibbs Free Energy= 0.023848
Sum of electronic and zero-point Energies= -380.976533
Sum of electronic and thermal Energies= -380.970982
Sum of electronic and thermal Enthalpies= -380.970037
Sum of electronic and thermal Free Energies= -381.005302
Cartesian coordinates

N	1.466618	-0.001316	-0.000529
H	1.838966	-0.330315	-0.889724
H	1.838931	-0.606986	0.728975
H	1.839575	0.933049	0.159273
B	-0.186746	-0.000037	-0.000024
F	-0.549495	0.825312	-1.031605
F	-0.551659	-1.305508	-0.198169
F	-0.548853	0.481713	1.230363

Vibrational frequencies

115.3996	277.9199	279.2391
457.1994	457.8670	473.9145
691.9817	808.0666	810.8510
920.0213	1260.8868	1261.3772
1350.4687	1620.3419	1623.3852
3477.4654	3604.2434	3605.3459

3aa

Zero-point correction= 0.322778
Thermal correction to Energy= 0.342817
Thermal correction to Enthalpy= 0.343761
Thermal correction to Gibbs Free Energy= 0.271809
Sum of electronic and zero-point Energies= -959.558344
Sum of electronic and thermal Energies= -959.538305
Sum of electronic and thermal Enthalpies= -959.537361
Sum of electronic and thermal Free Energies= -959.609313
Cartesian coordinates

C	3.544181	-2.639009	0.661549
C	2.675804	-1.646639	1.075383
C	2.632975	-0.385251	0.460385
C	3.521579	-0.141560	-0.605872
C	4.408058	-1.139126	-1.018333
C	4.416748	-2.375737	-0.394078
H	3.546730	-3.608239	1.151389
H	1.986688	-1.815689	1.898585
H	5.094070	-0.931085	-1.837965
H	5.111320	-3.139138	-0.735566
C	1.646422	0.578101	1.017708
O	1.092973	0.342285	2.084457

C	1.224475	1.812316	0.248127
C	0.519049	2.767386	1.180159
H	2.119878	2.341535	-0.111243
H	0.992047	2.872779	2.180586
O	3.518741	1.065351	-1.215526
H	1.033541	0.967885	-1.715498
C	-0.762749	0.520716	-0.655553
C	0.369443	1.442038	-0.980156
C	-2.081461	0.762215	-0.747607
H	-0.458748	-0.464383	-0.291583
H	0.017621	2.378238	-1.424012
C	-2.660488	2.083286	-1.164055
H	-3.496006	1.941898	-1.859845
H	-1.922368	2.731881	-1.639725
C	-3.054754	-0.301248	-0.398913
C	-2.766904	-1.656977	-0.609999
C	-4.305471	0.022903	0.143467
C	-3.677062	-2.647738	-0.265308
H	-1.824052	-1.935650	-1.076460
C	-5.217140	-0.967525	0.491427
H	-4.565922	1.065400	0.312944
C	-4.907234	-2.308595	0.291361
H	-3.429275	-3.691344	-0.446010
H	-6.176141	-0.687503	0.921512
H	-3.050336	2.633445	-0.297885
H	-5.622160	-3.083543	0.557017
O	-0.448097	3.425767	0.875297
H	4.181355	1.078955	-1.918213

Vibrational frequencies

15.4211	22.8179	35.3985
55.0559	59.4305	75.1186
93.5753	129.6323	132.6966
149.0027	185.4673	205.8020
242.0114	253.0446	261.5321
304.2775	312.1735	333.3161
364.7914	382.5767	386.6346
391.3804	412.7646	422.1477
453.8550	510.1529	537.7997
542.8040	559.9227	562.5861
587.0756	626.1360	639.3296
651.2630	706.0249	712.9597
739.0034	761.5693	762.7058
769.6355	797.5236	839.0661
850.8361	853.5544	857.6370

900.2465	911.7862	928.5634
964.8793	973.0126	973.2674
991.8147	994.7072	995.2285
1005.1765	1038.1134	1049.4917
1056.8013	1066.4118	1078.1245
1089.7501	1105.7436	1115.9661
1149.0124	1157.3546	1158.8193
1181.3198	1187.3924	1207.7627
1221.0883	1243.1527	1294.9013
1304.9632	1318.5073	1325.9778
1330.9667	1357.0140	1367.9564
1383.4494	1393.8135	1405.6448
1420.0212	1445.5806	1456.3570
1470.4493	1478.9949	1491.3603
1529.4119	1531.1769	1642.2910
1652.9751	1671.8279	1672.5594
1737.2349	1763.6818	1854.6840
2928.2958	3033.0849	3046.3250
3049.5447	3101.9677	3118.1501
3129.8363	3158.6039	3167.5090
3168.3578	3173.8482	3181.7457
3187.3821	3187.5604	3195.5200
3197.6691	3208.0508	3855.6053

D

Zero-point correction= 0.391438
Thermal correction to Energy= 0.414313
Thermal correction to Enthalpy= 0.415257
Thermal correction to Gibbs Free Energy= 0.336694
Sum of electronic and zero-point Energies= -1018.149635
Sum of electronic and thermal Energies= -1018.126760
Sum of electronic and thermal Enthalpies= -1018.125816
Sum of electronic and thermal Free Energies= -1018.204378
Cartesian coordinates

C	-1.322500	-0.667343	0.001627
C	-0.127284	-1.461289	0.297811
C	-2.376806	-0.446791	0.809547
H	-1.336951	-0.232831	-0.995771
H	-0.124571	-2.022823	1.232181
C	-2.500804	-1.031816	2.187140
H	-2.880743	-0.287390	2.897149
H	-1.544998	-1.398527	2.569973
C	-3.500630	0.391719	0.335602
C	-3.299769	1.420104	-0.597958

C	-4.800808	0.198244	0.820926
C	-4.357376	2.197225	-1.048800
H	-2.291606	1.627269	-0.953407
C	-5.861252	0.976597	0.370004
H	-4.992505	-0.584105	1.552444
C	-5.646755	1.978263	-0.569899
H	-4.171042	2.990769	-1.769140
H	-6.861887	0.796959	0.757236
H	-3.203512	-1.876149	2.208405
H	-6.474249	2.591261	-0.918996
C	3.276821	3.584019	0.026932
C	2.352640	2.638058	-0.382170
C	2.576545	1.264033	-0.228357
C	3.802870	0.851609	0.323534
C	4.741428	1.802412	0.728229
C	4.478022	3.156402	0.587982
H	3.067830	4.643549	-0.089266
H	1.409650	2.937357	-0.832402
H	5.688511	1.466816	1.148918
H	5.220653	3.880368	0.914312
C	1.486336	0.358972	-0.698469
O	0.724164	0.742948	-1.577700
C	1.300759	-0.955835	-0.038917
C	0.682026	-2.072630	-0.813963
H	2.030538	-1.213301	0.719169
H	0.342917	-1.763821	-1.806389
O	4.077870	-0.472971	0.421267
H	4.964517	-0.589738	0.784483
N	1.188680	-3.413912	-0.798677
C	0.103155	-4.358367	-0.985119
H	0.507331	-5.365359	-1.139321
H	-0.589059	-4.390935	-0.121118
H	-0.480128	-4.084353	-1.871566
C	2.025657	-3.775962	0.324015
H	1.507286	-3.738124	1.303575
H	2.373476	-4.805445	0.183539
H	2.907874	-3.129616	0.370011

Vibrational frequencies

15.1013	21.7567	28.1203
35.0316	56.5373	58.2911
72.9048	100.0689	116.6858
141.1774	151.9344	167.8188
194.1438	198.2956	221.0872
244.0412	250.9088	279.4911

294.2665	303.6603	326.3163
360.5777	370.6332	374.9906
376.5762	413.9208	417.5816
439.8432	463.4701	483.0963
486.5443	530.4490	544.9284
556.0530	560.6347	566.1699
603.9651	626.2334	653.6394
699.2783	707.8157	745.6070
762.2533	770.0505	771.7812
817.4485	840.3448	851.8166
855.1848	860.1022	866.5636
906.4587	928.7954	940.7745
952.5367	962.6538	973.9228
983.4568	986.0640	994.5843
1004.7228	1039.3126	1047.6079
1055.5636	1060.4477	1070.0251
1074.6814	1085.7938	1090.8154
1104.5765	1107.6379	1108.9709
1122.7984	1157.8864	1159.8434
1164.8885	1180.7489	1182.2880
1192.7533	1222.3285	1236.8678
1249.4106	1275.9994	1295.4980
1318.7565	1323.5744	1327.7602
1338.6125	1362.0175	1374.4290
1385.8410	1394.7411	1408.3058
1416.7961	1441.3144	1452.9461
1456.4445	1465.5023	1466.8159
1470.1635	1477.2486	1481.4261
1490.7145	1496.2727	1531.1002
1534.4598	1642.0303	1656.0539
1671.7354	1674.8636	1724.3524
1766.8703	2927.5412	2944.2868
3024.3011	3066.5133	3074.1510
3093.6743	3114.9867	3119.3368
3129.5927	3138.6590	3153.1887
3161.4675	3163.9484	3168.3513
3177.2346	3183.3683	3183.9980
3186.7342	3192.7517	3193.5048
3205.1199	3227.8741	3863.7086

D-Zn

Zero-point correction= 0.395677
Thermal correction to Energy= 0.423961
Thermal correction to Enthalpy= 0.424906

Thermal correction to Gibbs Free Energy= 0.333011
Sum of electronic and zero-point Energies= -1109.999706
Sum of electronic and thermal Energies= -1109.971422
Sum of electronic and thermal Enthalpies= -1109.970478
Sum of electronic and thermal Free Energies= -1110.062372
Cartesian coordinates

C	3.283248	-1.025378	-0.121414
C	2.024966	-1.587192	-0.645196
C	4.412887	-0.820439	-0.822048
H	3.274785	-0.764373	0.933925
H	2.116665	-2.194602	-1.543948
C	4.565339	-1.174183	-2.273588
H	5.073133	-0.369740	-2.819062
H	3.603850	-1.351953	-2.762527
C	5.589094	-0.222933	-0.150950
C	5.429026	0.707942	0.886256
C	6.893001	-0.550267	-0.544969
C	6.529828	1.262709	1.525490
H	4.424250	1.018643	1.168995
C	7.995831	0.004249	0.095832
H	7.050639	-1.261347	-1.353828
C	7.820153	0.910650	1.136480
H	6.379239	1.986681	2.323425
H	8.998538	-0.274681	-0.221095
H	5.173823	-2.078934	-2.407846
H	8.682169	1.348713	1.634258
C	-0.327018	4.025338	-1.329430
C	0.363349	2.972223	-0.748483
C	-0.135046	1.664492	-0.771605
C	-1.383842	1.472431	-1.362902
C	-2.105535	2.516094	-1.926589
C	-1.563911	3.795877	-1.926135
H	0.093980	5.026690	-1.312154
H	1.322568	3.131509	-0.263020
H	-3.091532	2.323726	-2.348116
H	-2.119731	4.613756	-2.376581
C	0.717767	0.604481	-0.134501
O	1.446852	0.921348	0.796877
C	0.717145	-0.753803	-0.693215
C	0.920737	-1.944150	0.263890
H	0.097986	-0.940424	-1.566743
H	1.048979	-1.602677	1.295228
O	-1.969572	0.203099	-1.297436
H	-2.556450	0.068189	-2.058888

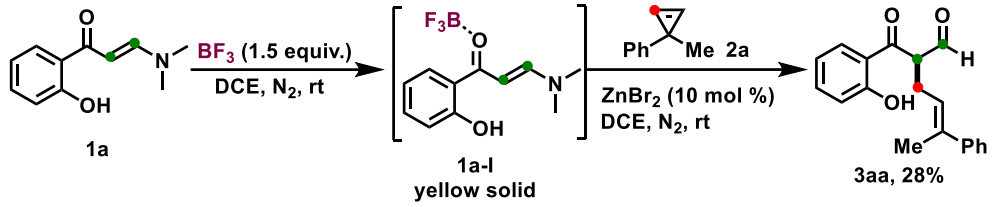
N	0.158704	-3.143464	0.166248
C	0.210900	-3.864035	-1.087107
H	-0.370632	-4.786423	-0.985386
H	-0.214501	-3.299902	-1.940767
H	1.238901	-4.147545	-1.331024
C	-1.195734	-2.968345	0.634287
H	-1.810283	-2.381902	-0.089033
H	-1.684614	-3.940021	0.764238
H	-1.200325	-2.442448	1.597012
Zn	-3.167924	-0.100018	0.491383
Br	-5.244452	-0.683332	-0.602810
Br	-1.955433	0.631152	2.423883

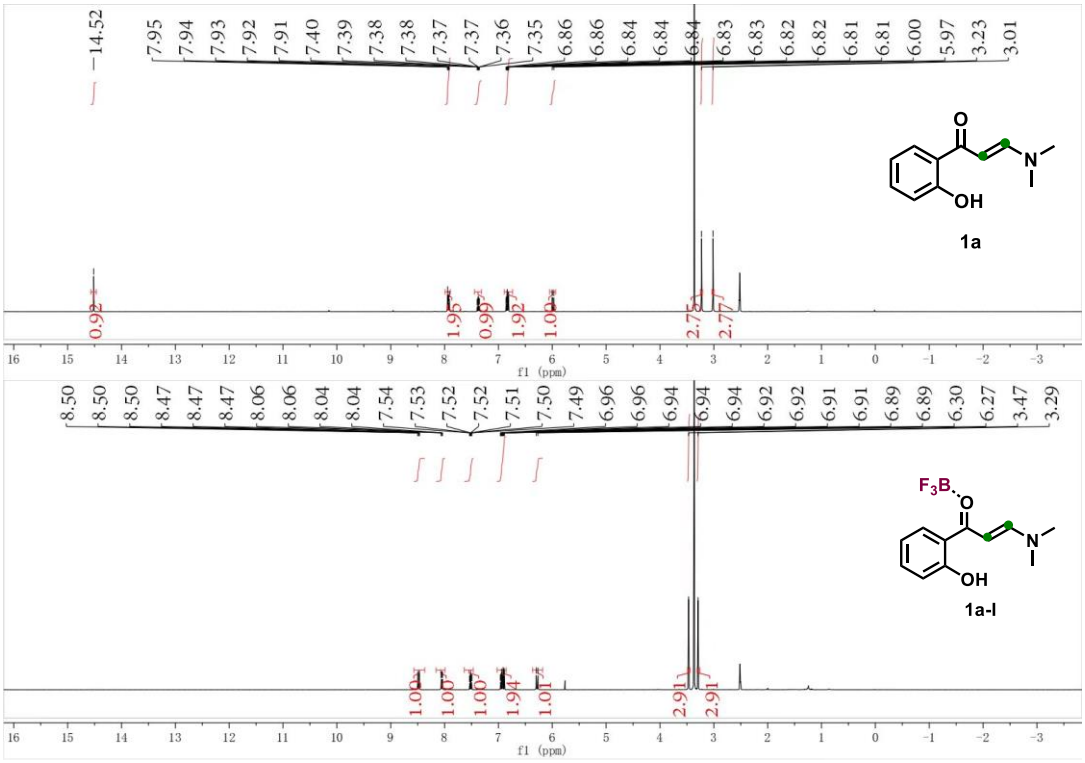
Vibrational frequencies

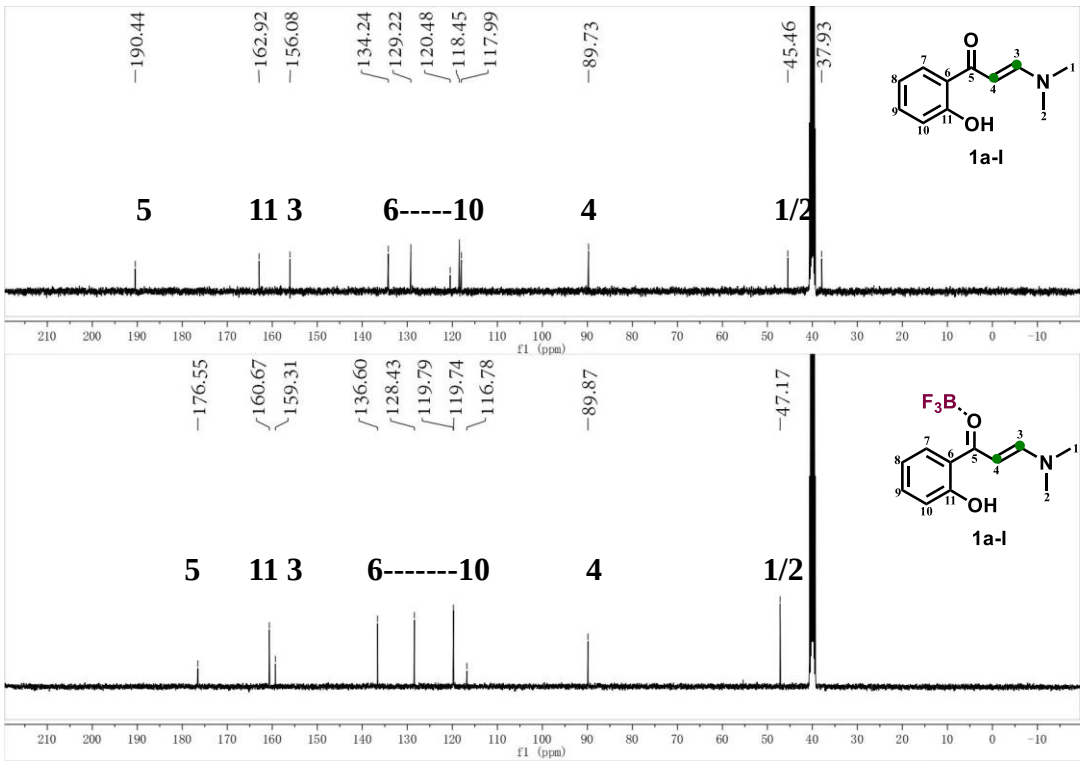
17.9260	20.5765	27.1906
47.7743	52.6783	56.8692
61.6373	63.6091	73.6500
78.9595	83.5438	92.6733
108.1003	120.0925	140.6621
157.4894	175.0668	186.9898
188.2962	203.8616	218.0522
235.7710	237.0570	263.2839
278.5409	298.0139	307.8425
312.4631	338.0441	364.4302
371.6056	383.1010	395.1006
417.3258	428.6521	442.4386
478.5498	487.7211	503.9157
522.7440	545.4653	559.8010
562.0968	564.4219	581.1077
614.9067	626.0504	654.9449
703.3790	709.2707	736.8018
767.6805	770.2081	772.8374
811.2180	828.2306	852.3565
856.4295	865.2531	878.9123
898.0268	906.4796	929.9612
951.1889	965.5277	975.2455
985.7488	996.6812	996.7120
1005.4230	1038.3948	1042.8794
1054.5732	1070.0634	1071.9967
1073.2699	1084.3819	1096.9501
1106.6374	1109.5536	1120.3478
1123.1716	1156.9462	1161.3274
1164.9436	1189.5834	1190.5641
1192.0676	1226.8049	1235.1054
1242.2388	1245.2293	1284.0534

1305.2539	1320.0710	1327.5011
1351.0460	1361.6061	1374.4321
1383.5877	1391.4995	1405.8551
1419.9629	1443.1714	1448.6599
1459.8040	1466.2909	1468.3450
1472.0837	1478.9538	1482.7681
1498.9483	1523.5675	1527.3545
1531.4593	1643.1368	1652.1740
1673.0359	1681.9681	1729.9697
1769.2885	2927.9344	2940.6494
3028.8835	3064.9668	3083.6033
3099.4705	3112.3898	3126.8664
3136.9305	3142.7558	3166.7465
3167.3081	3169.6190	3171.4936
3179.5412	3186.0530	3191.7456
3195.5116	3197.8089	3199.8363
3202.6611	3209.8744	3792.0307

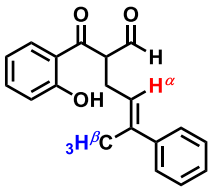
NMR spectra for intermediate 1a-I.





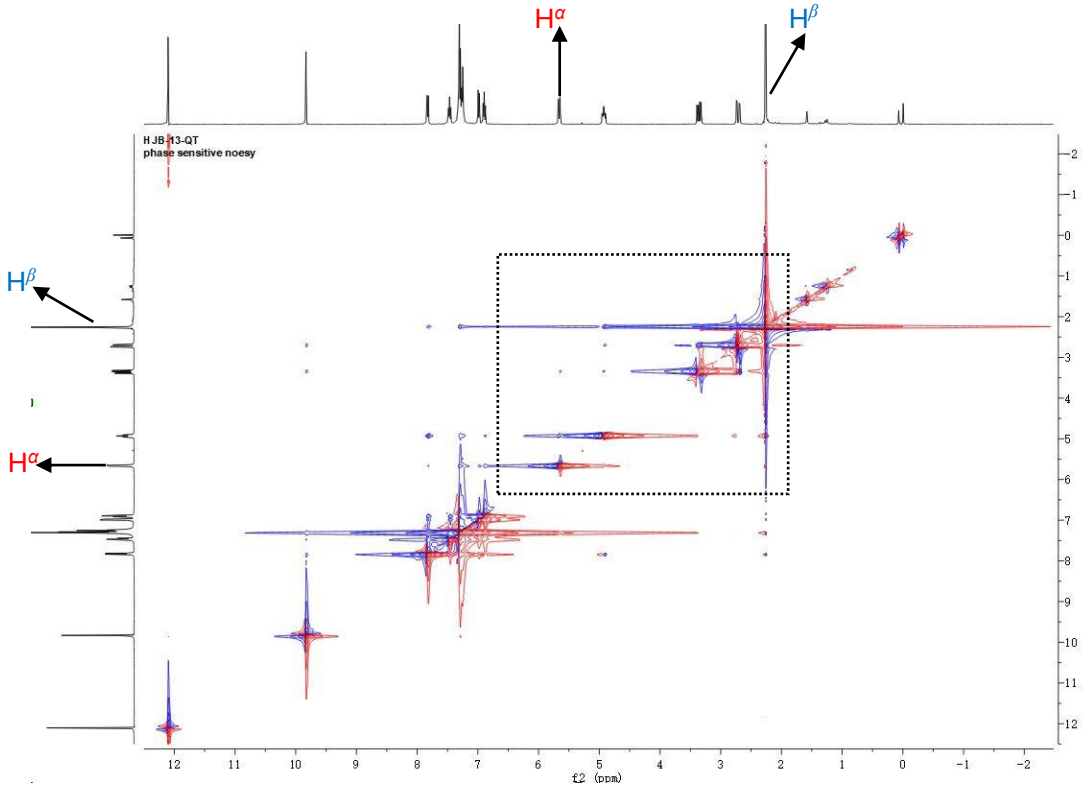


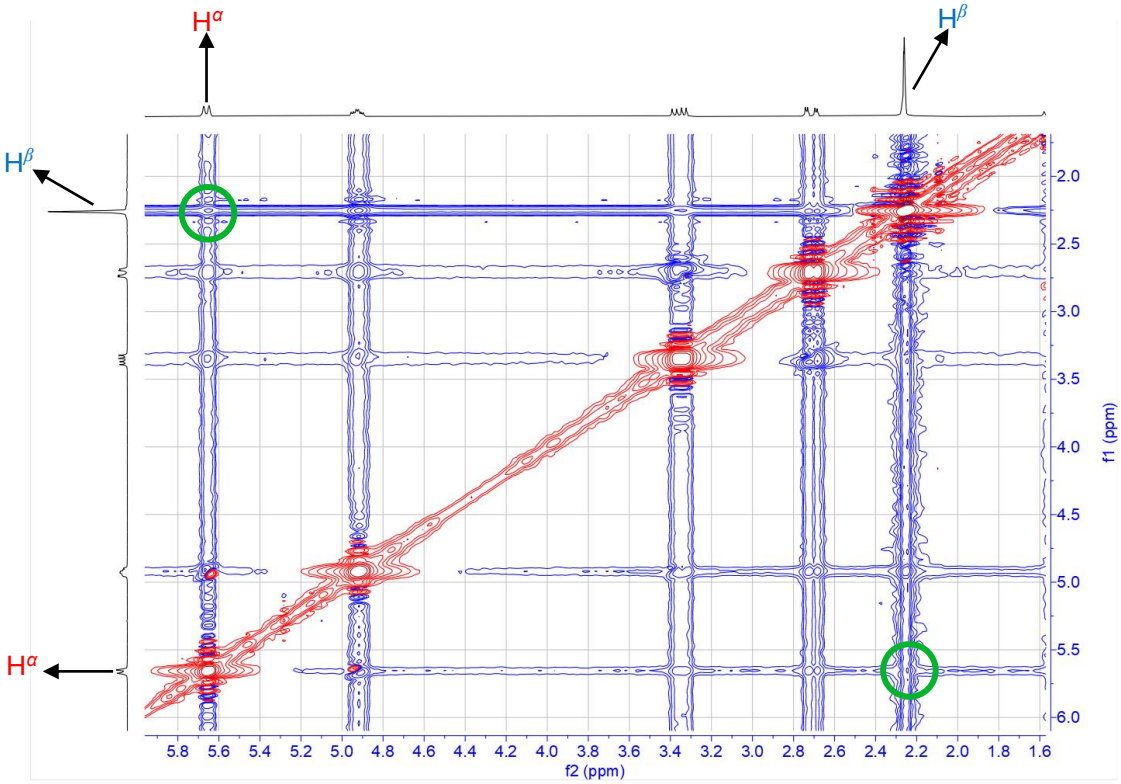
NOESY NMR spectra of product:

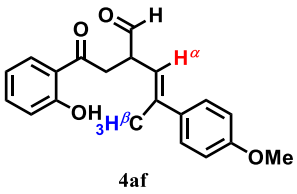


3aa

No NOE was observed between H^{α} and H^{β}

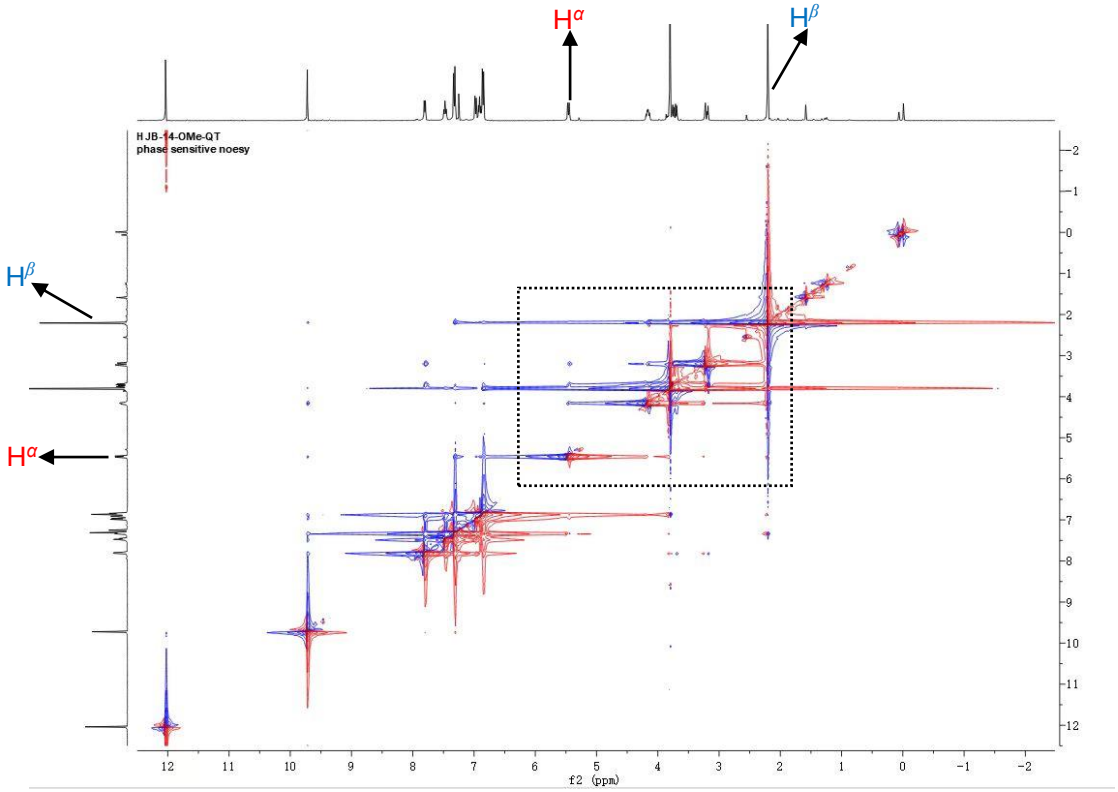


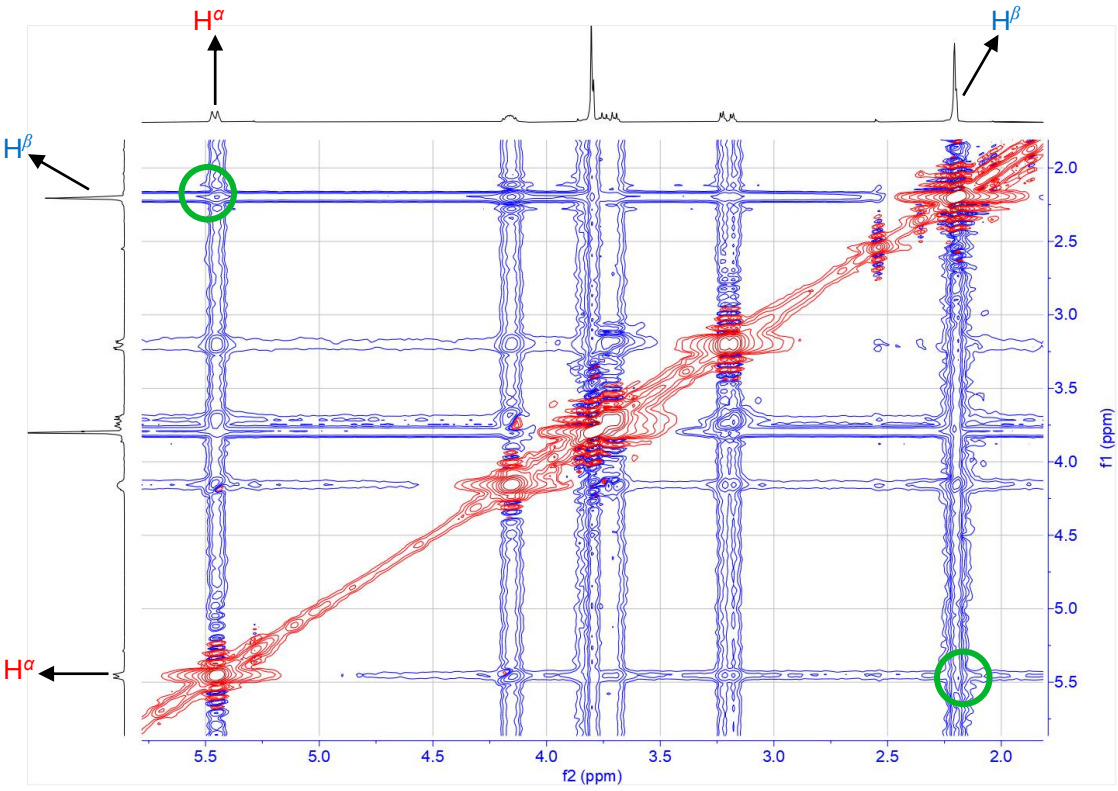




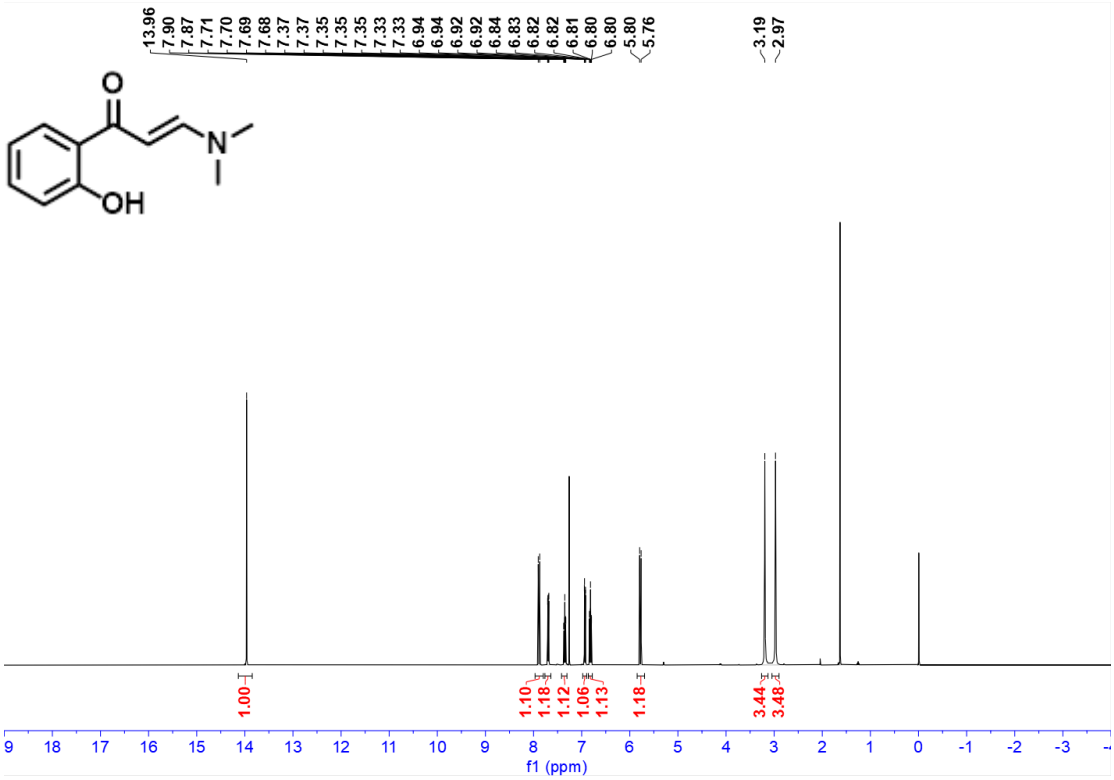
4af

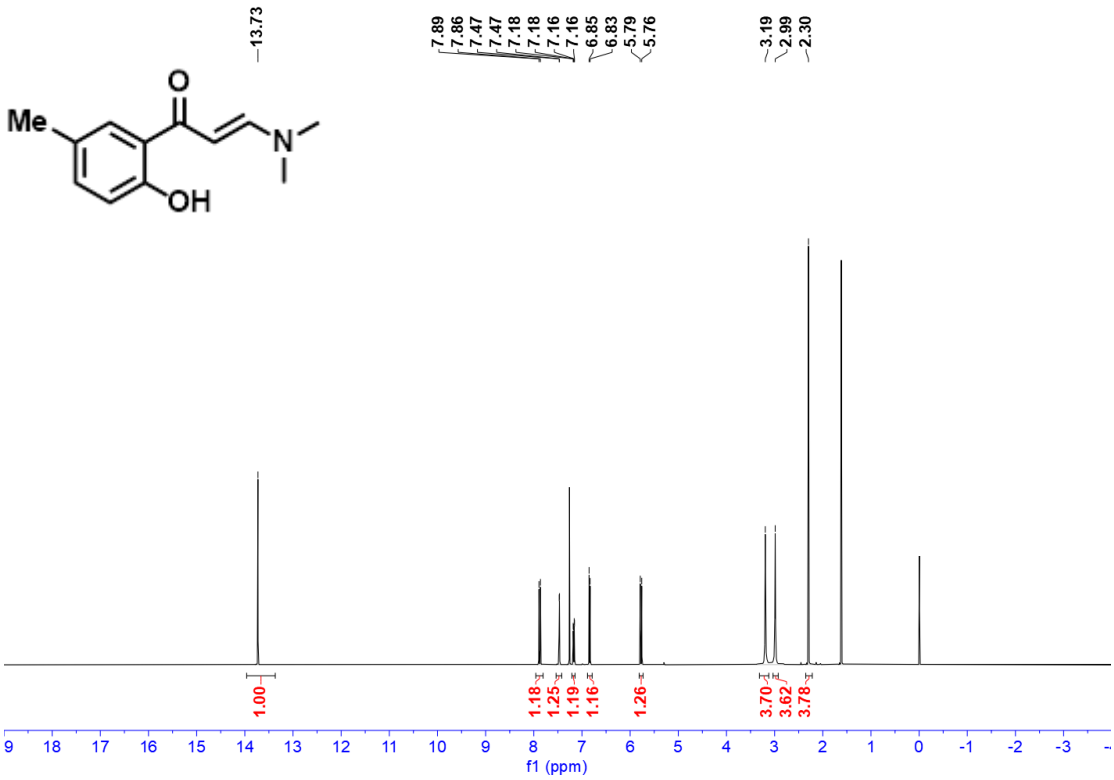
No NOE was observed between H$^{\alpha}$ and H$^{\beta}$

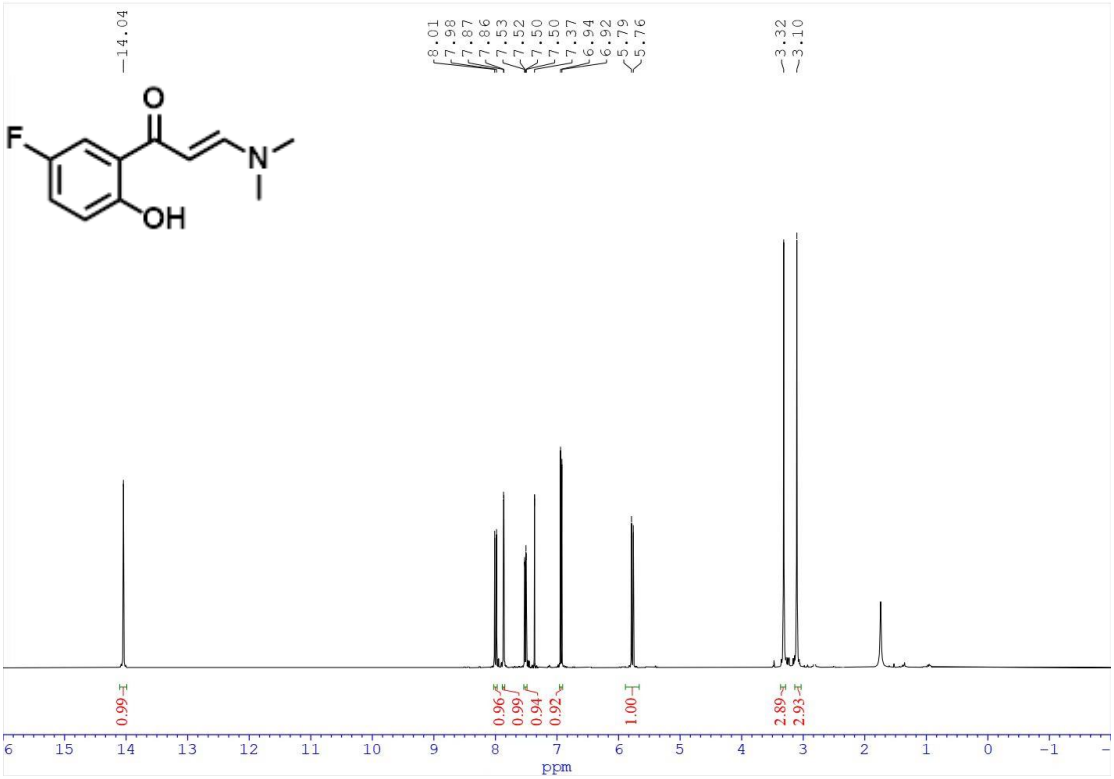


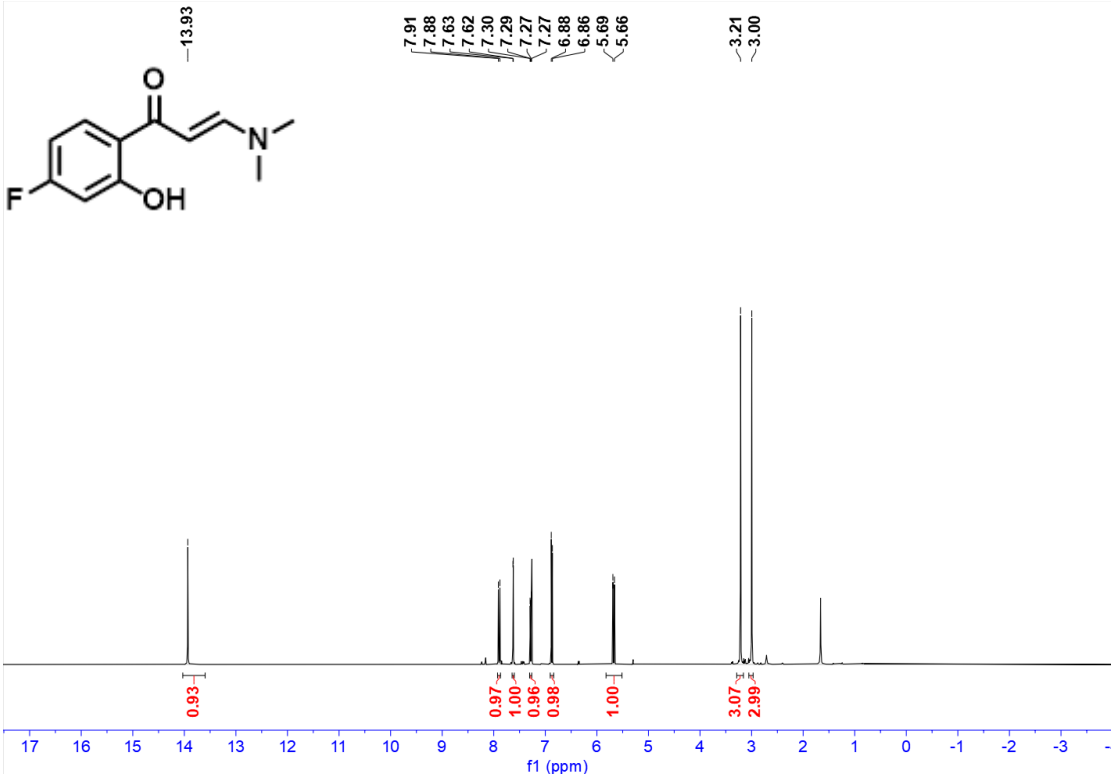


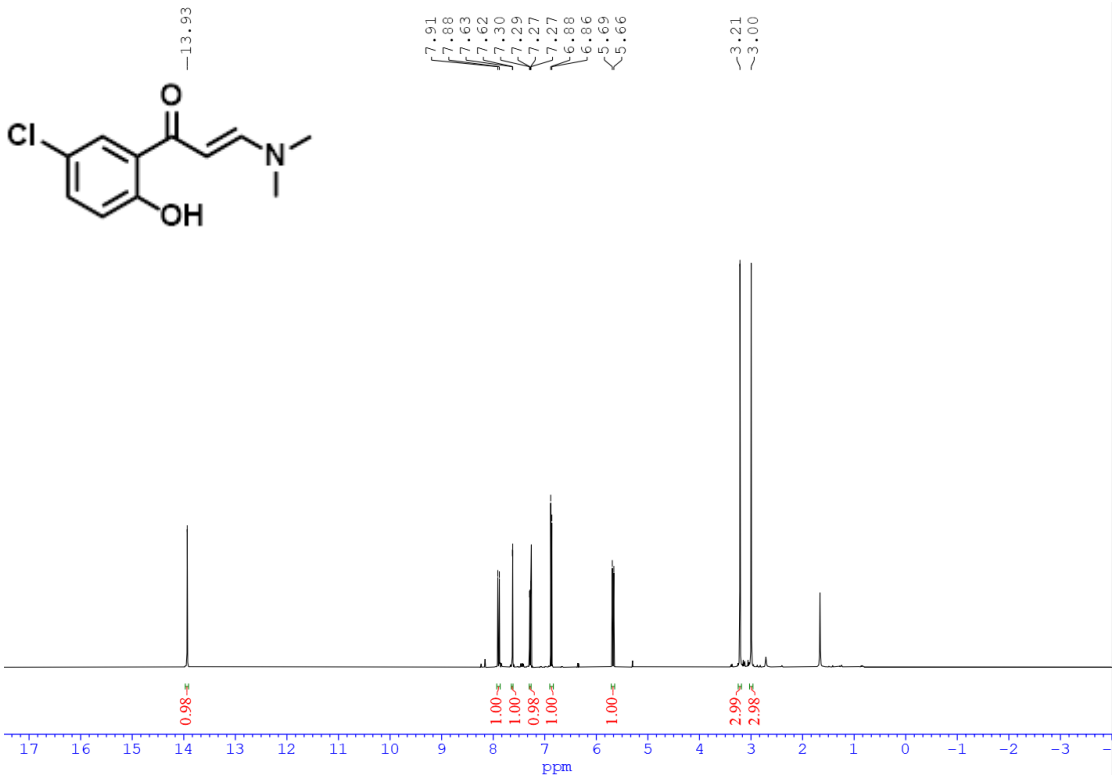
NMR spectra for enamides:

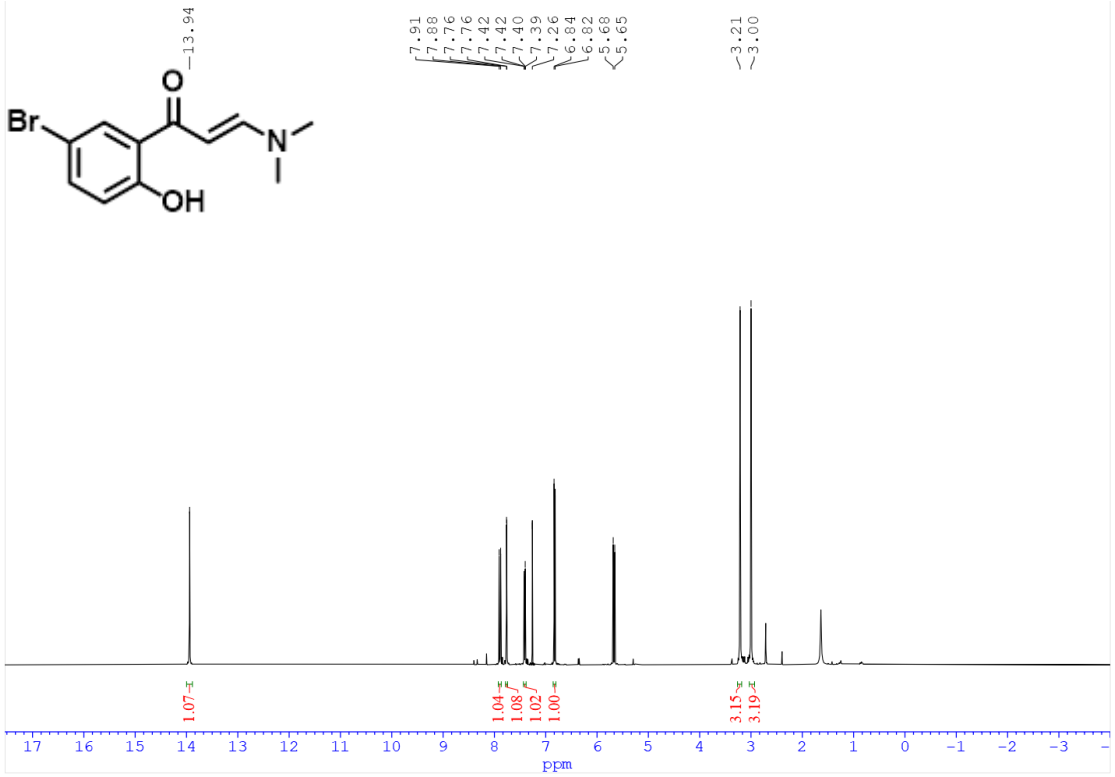


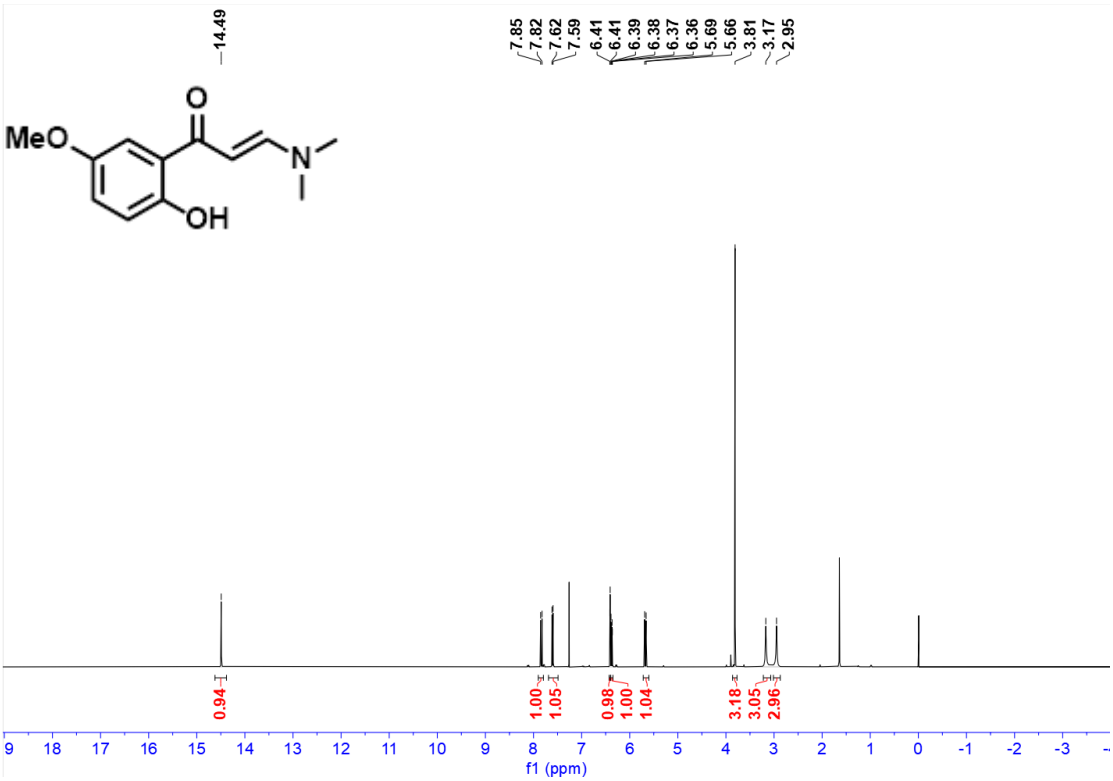


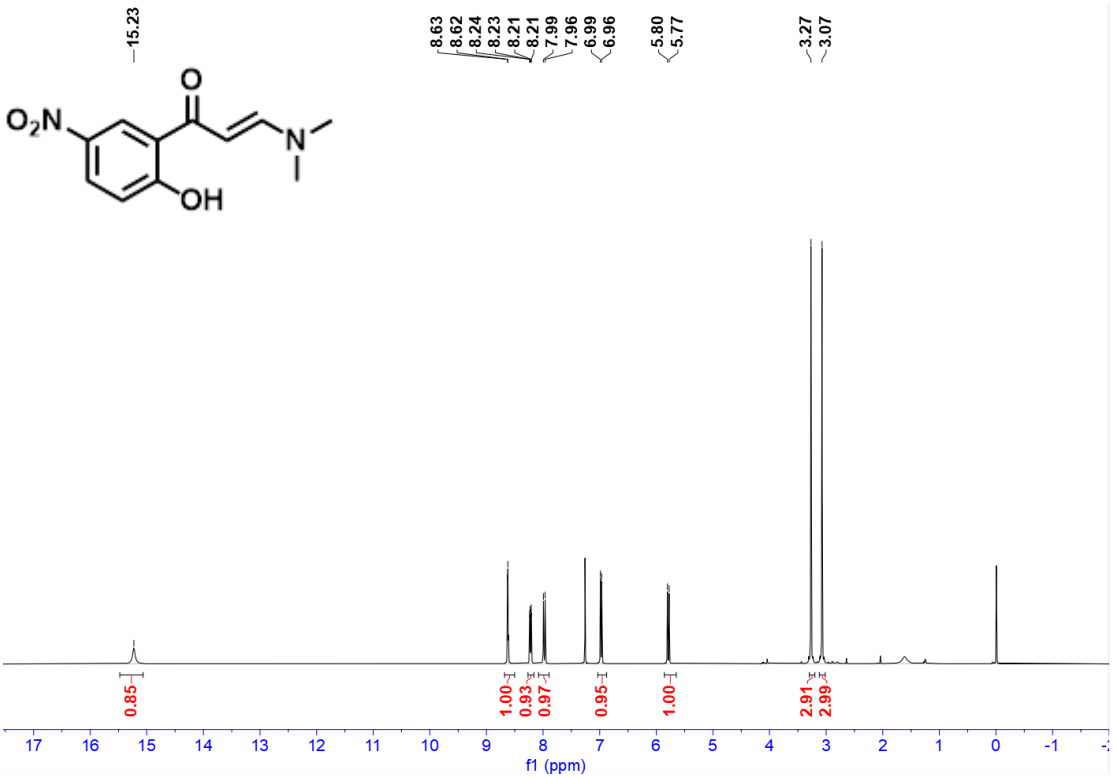

14.04
8.01
7.98
7.87
7.86
7.53
7.52
7.50
7.50
7.37
6.94
6.92
5.79
5.76
3.32
3.10
F
O
N
OH
0.99
0.96
0.99
0.94
0.92
1.00
2.89
2.93
ppm

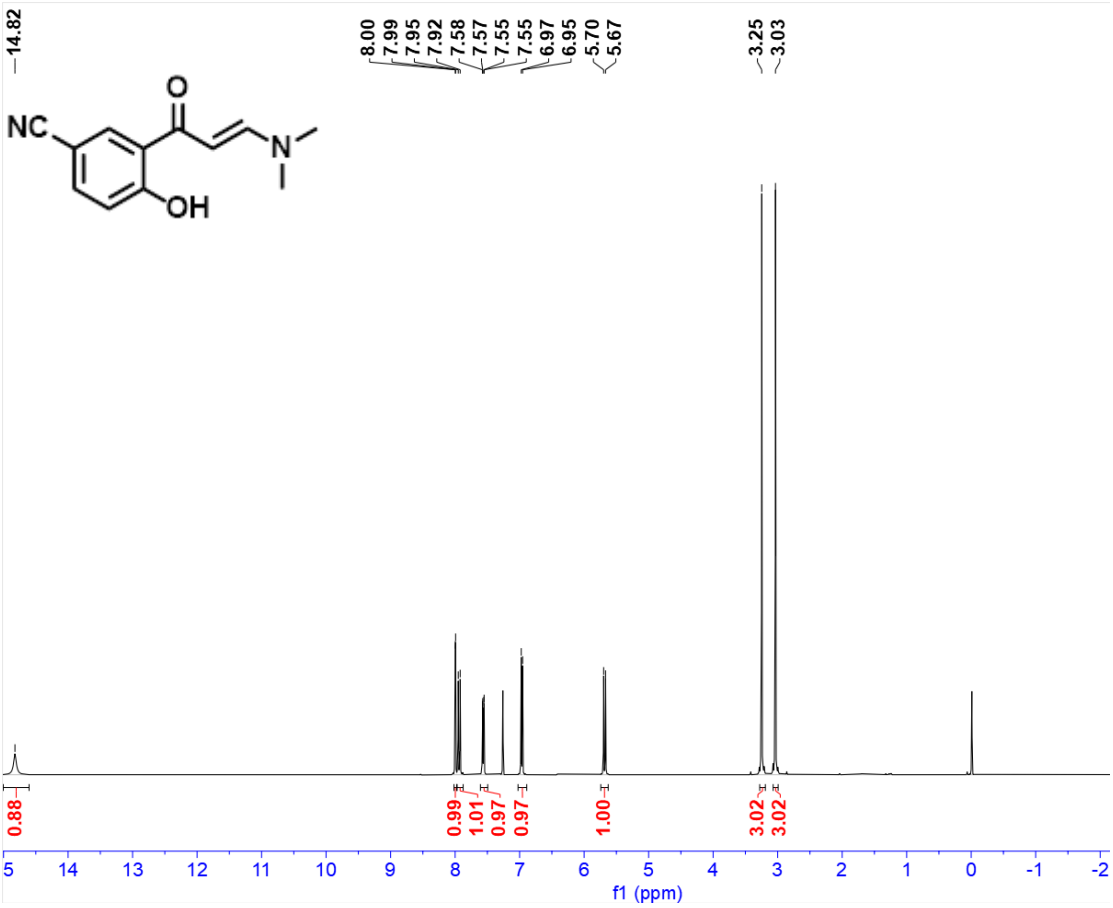

13.93
7.91
7.88
7.63
7.62
7.30
7.29
7.27
7.27
6.88
6.86
5.69
5.66
3.21
3.00
F
O
N
OH
0.93
0.97
1.00
0.96
0.98
1.00
3.07
2.99
f1 (ppm)

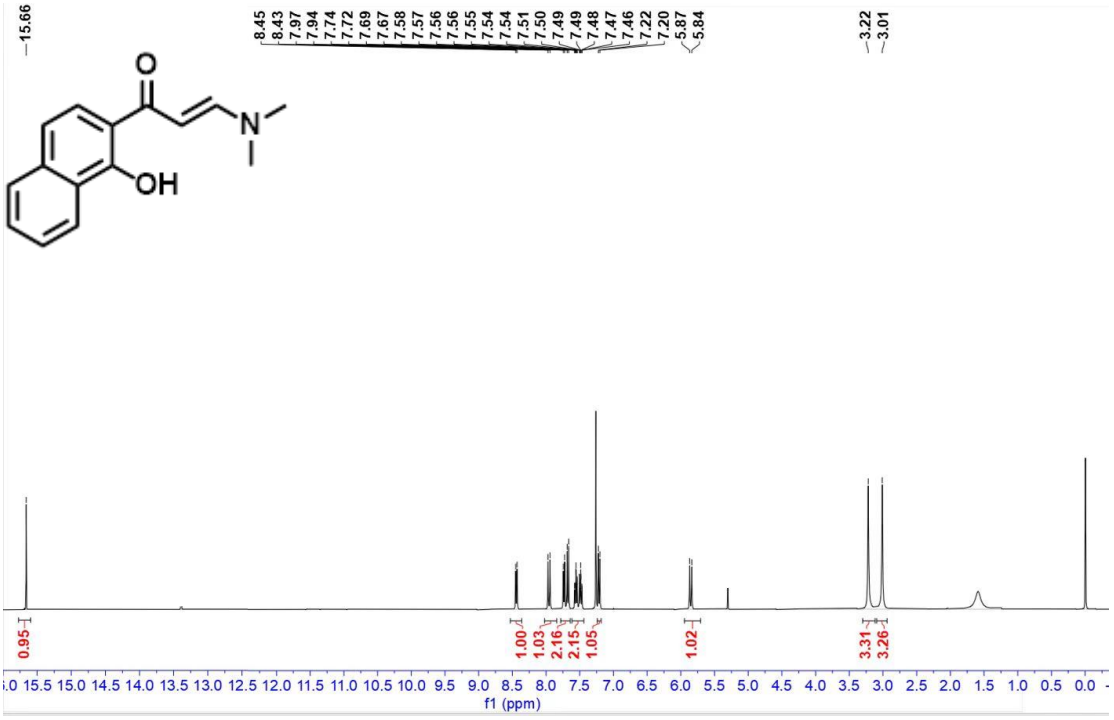

13.93
7.91
7.88
7.63
7.62
7.30
7.29
7.27
7.27
6.88
6.86
5.69
5.66
3.21
3.00
Cl
O
N
OH
0.98
1.00
1.00
0.98
1.00
1.00
2.99
2.98
ppm

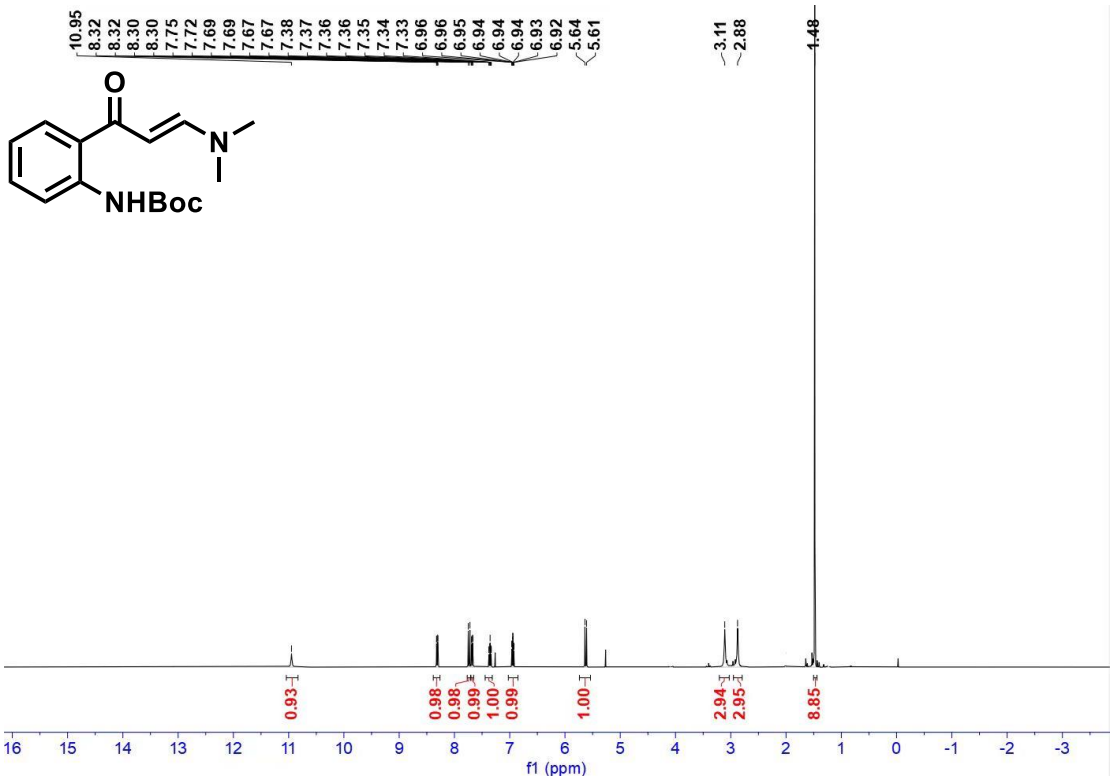

13.94
7.91
7.88
7.76
7.76
7.42
7.42
7.40
7.39
7.26
6.84
6.82
5.68
5.65
3.21
3.00
Br
O
N
OH
1.07
1.04
1.08
1.02
1.00
3.15
3.19
ppm

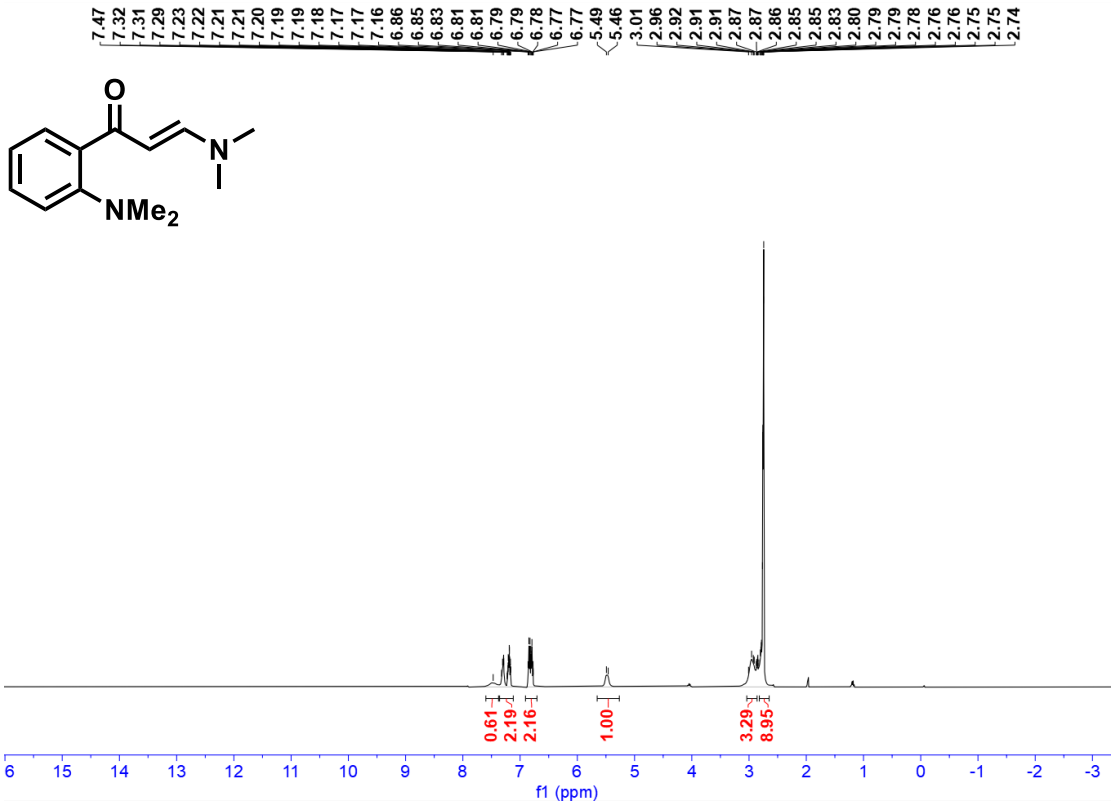

14.49
7.85
7.82
7.62
7.59
6.41
6.41
6.39
6.38
6.37
6.36
5.69
5.66
3.81
3.17
2.95
MeO
O
N
OH
0.94
1.00
1.05
0.98
1.00
1.04
3.18
3.05
2.96
f1 (ppm)

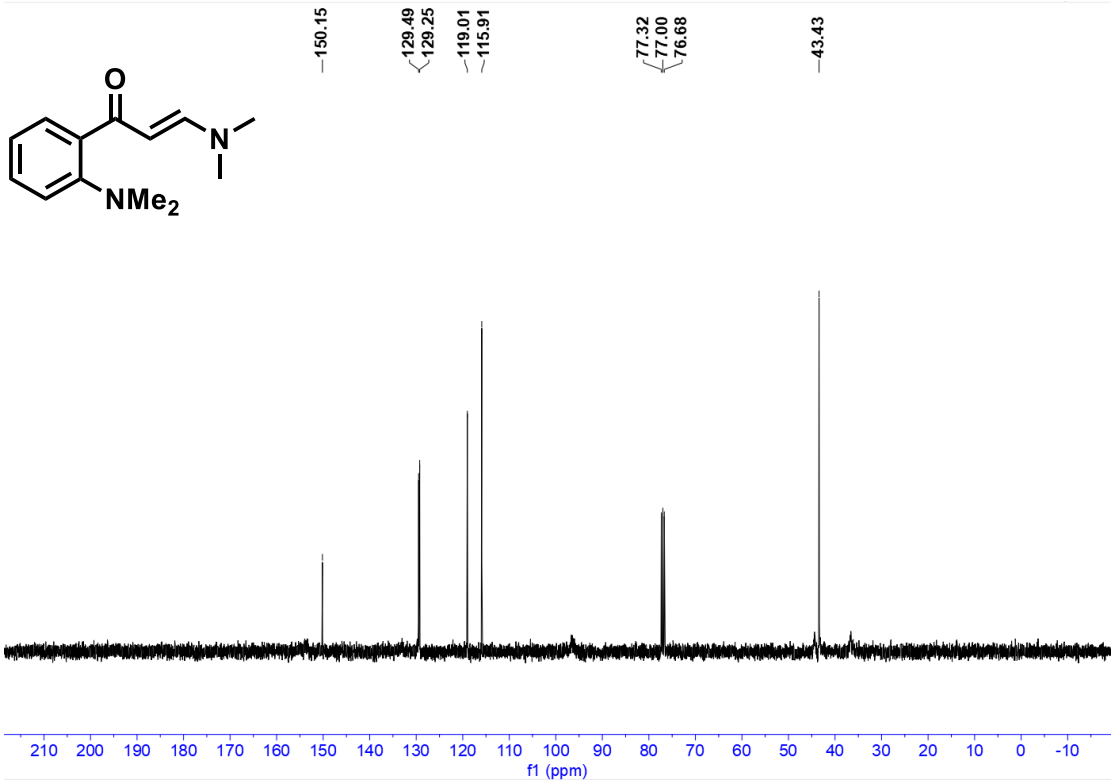

15.23
8.63
8.62
8.24
8.23
8.21
8.21
7.99
7.96
6.99
6.96
5.80
5.77
3.27
3.07
O2N
O
N
OH
0.85
1.00
0.93
0.97
0.95
1.00
2.91
2.99
f1 (ppm)


14.82
8.00
7.99
7.95
7.92
7.58
7.57
7.55
7.55
6.97
6.95
5.70
5.67
3.25
3.03
NC
O
N
OH
0.88
0.99
1.01
0.97
0.97
1.00
3.02
3.02
f1 (ppm)

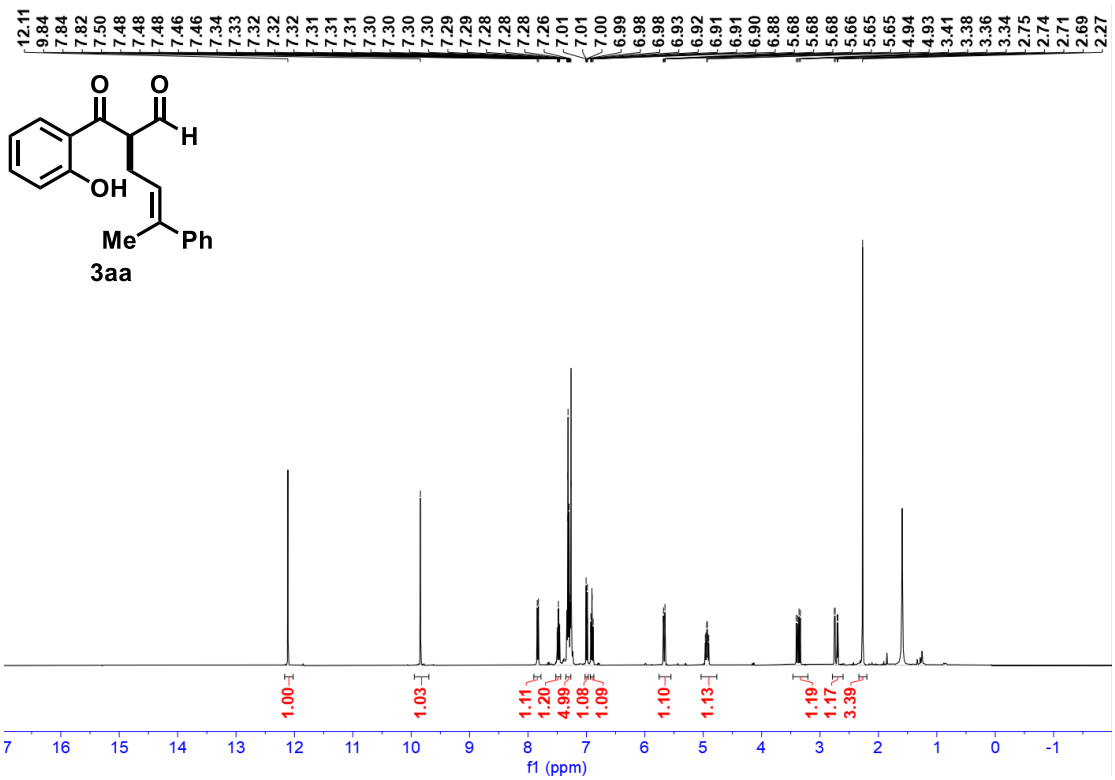

15.66
8.45
8.43
7.97
7.94
7.74
7.72
7.69
7.67
7.58
7.57
7.56
7.56
7.55
7.54
7.54
7.51
7.50
7.49
7.49
7.48
7.47
7.46
7.22
7.20
5.87
5.84
3.22
3.01
O
N
OH
0.95
1.00
1.03
2.16
2.15
1.05
1.02
3.31
3.26
f1 (ppm)

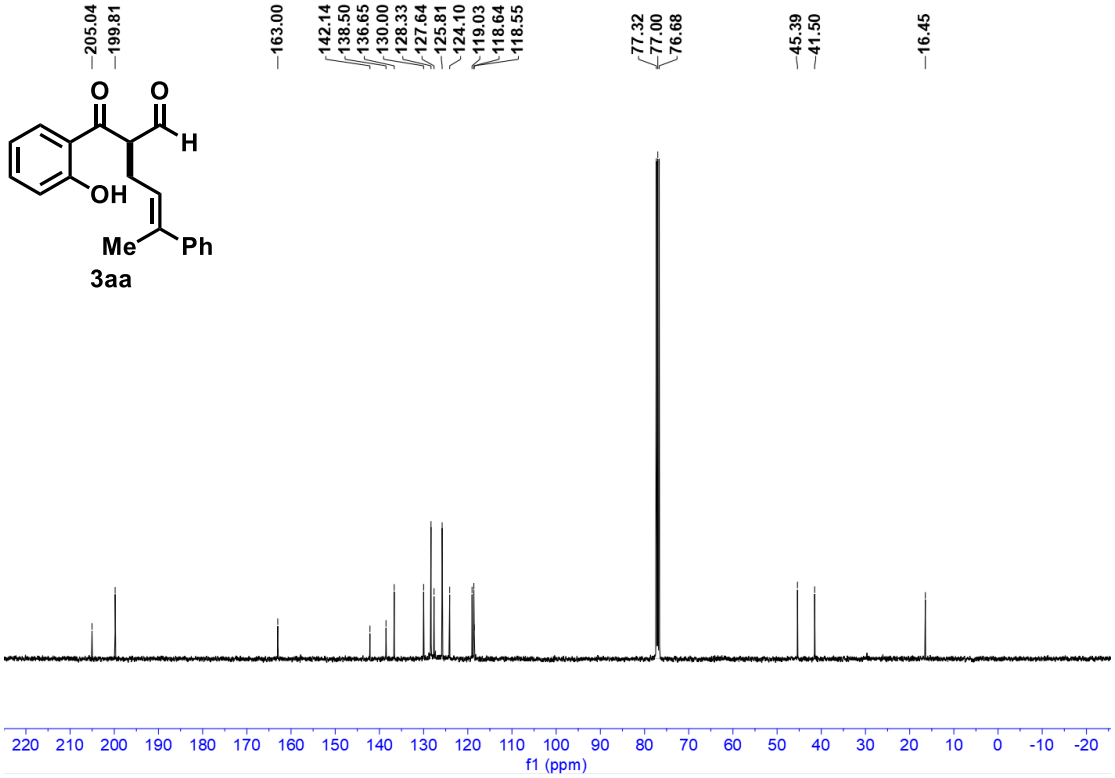

10.95
8.32
8.32
8.30
8.30
7.75
7.72
7.69
7.69
7.67
7.67
7.38
7.37
7.36
7.36
7.35
7.34
7.33
6.96
6.96
6.95
6.94
6.94
6.94
6.93
6.92
5.64
5.61
3.11
2.88
1.48
O
N
NHBoc
0.93
0.98
0.98
0.99
1.00
0.99
1.00
2.94
2.95
8.85
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

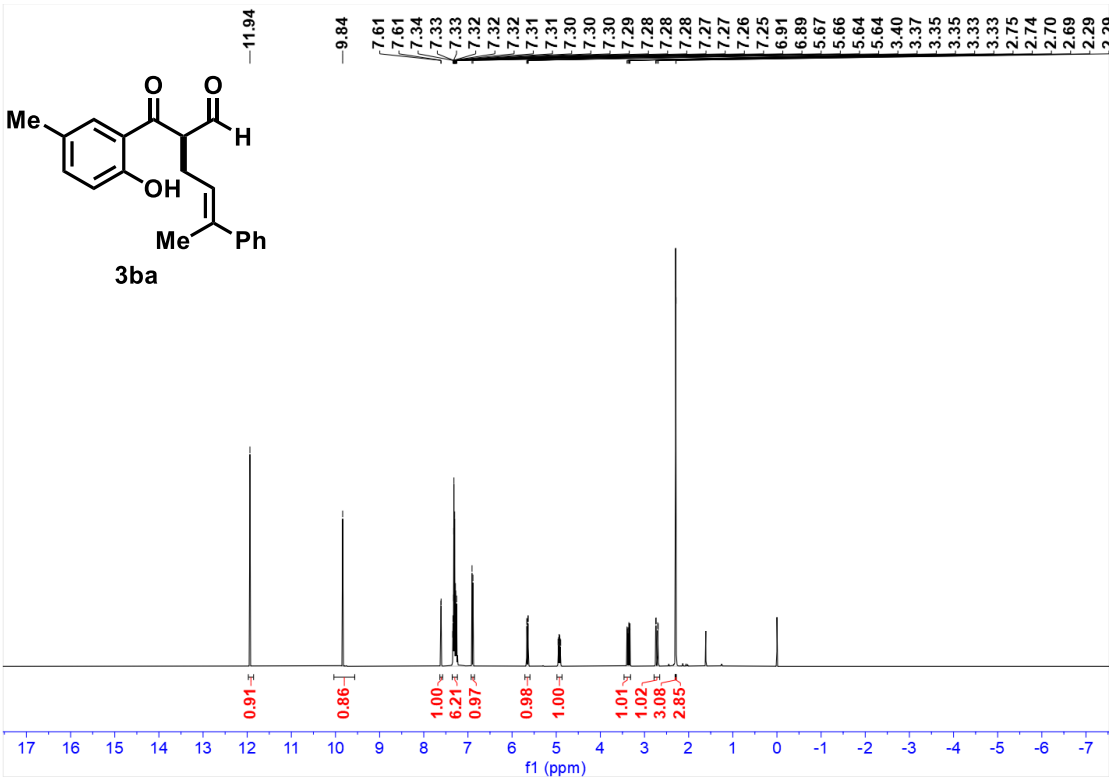

7.47
7.32
7.31
7.29
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.18
7.17
7.17
7.16
6.86
6.85
6.83
6.81
6.81
6.79
6.78
6.77
6.77
5.49
5.46
3.01
2.96
2.92
2.91
2.91
2.87
2.87
2.86
2.85
2.85
2.83
2.80
2.79
2.79
2.78
2.76
2.76
2.75
2.75
2.74
O
N
NMe2
0.61
2.19
2.16
1.00
3.29
8.95
6 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

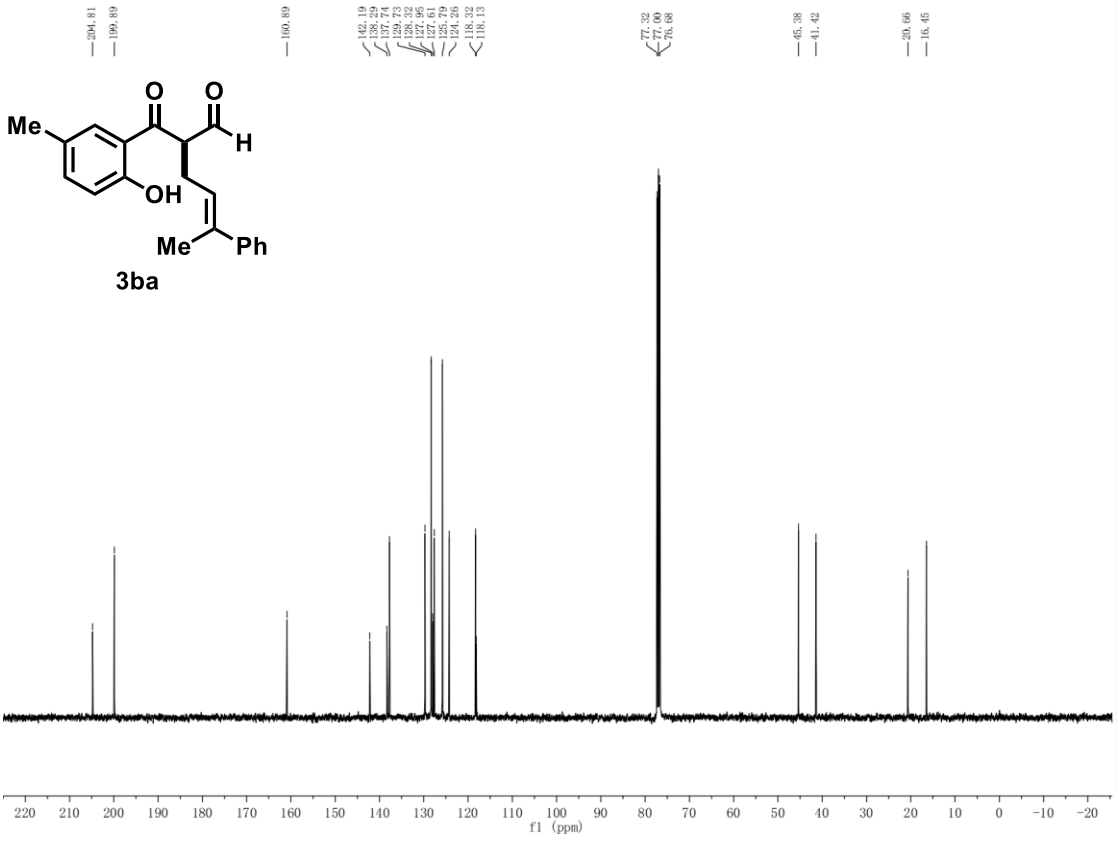

150.15
129.49
129.25
119.01
115.91
77.32
77.00
76.68
43.43
O
N
NMe2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

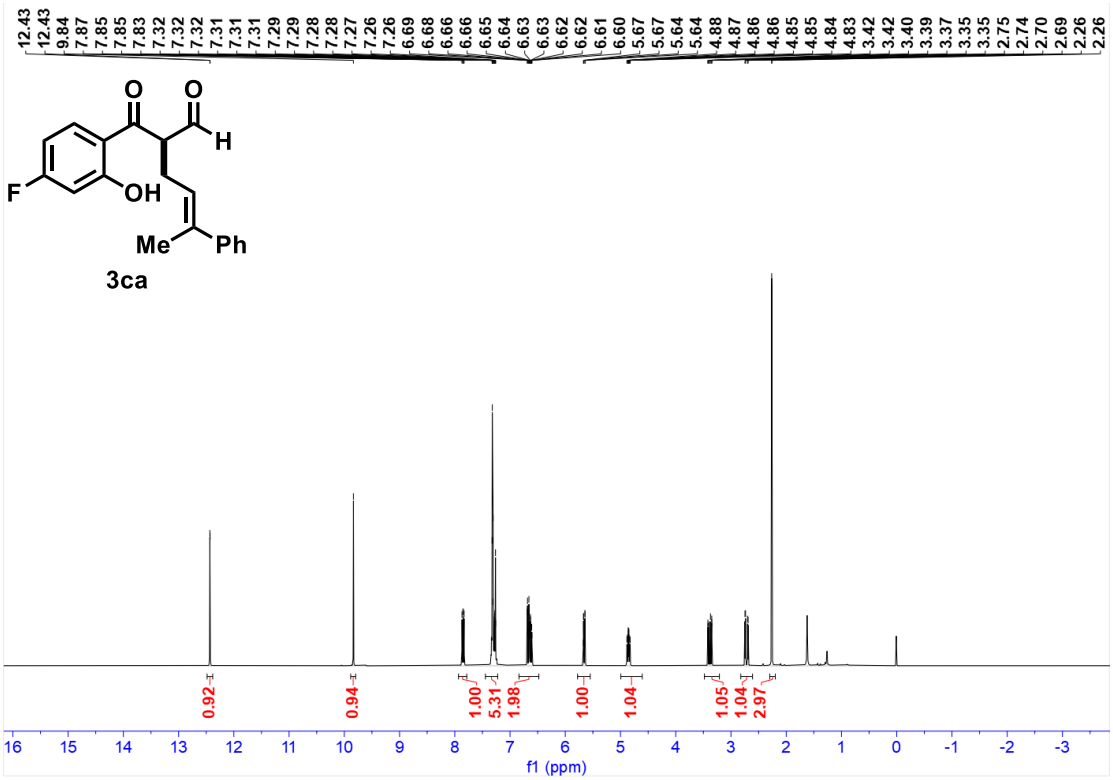
NMR spectra for 1,3-dicarbonyl-alkenes:

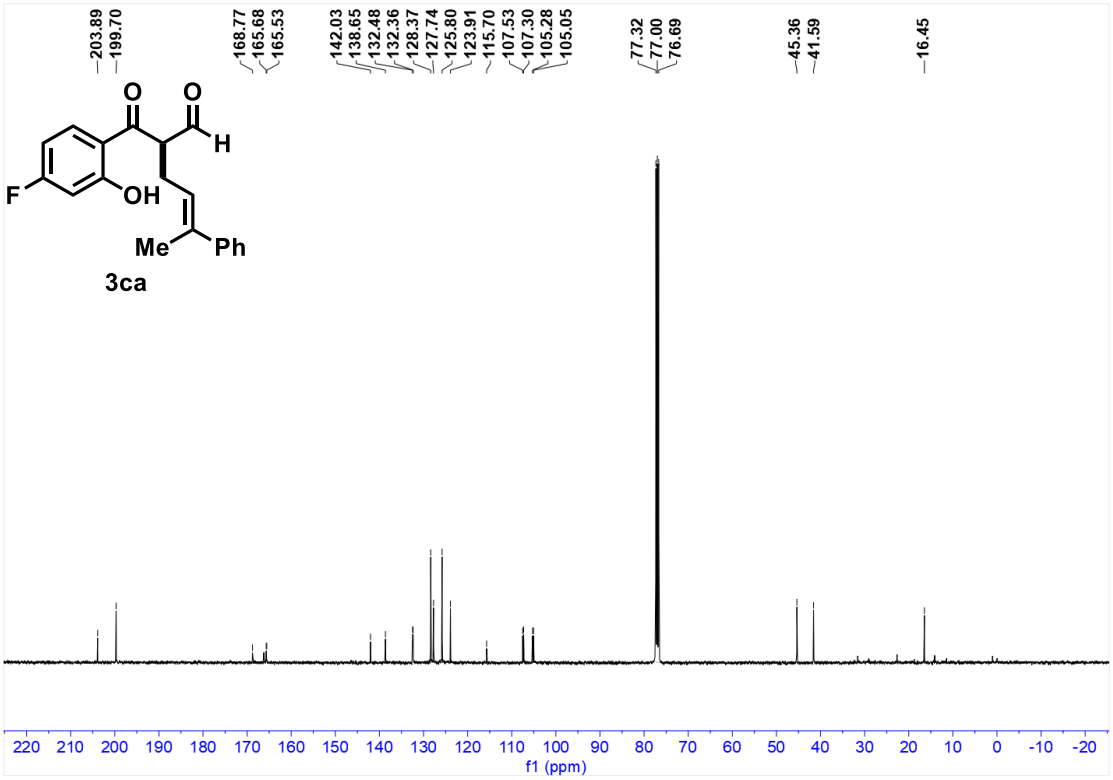


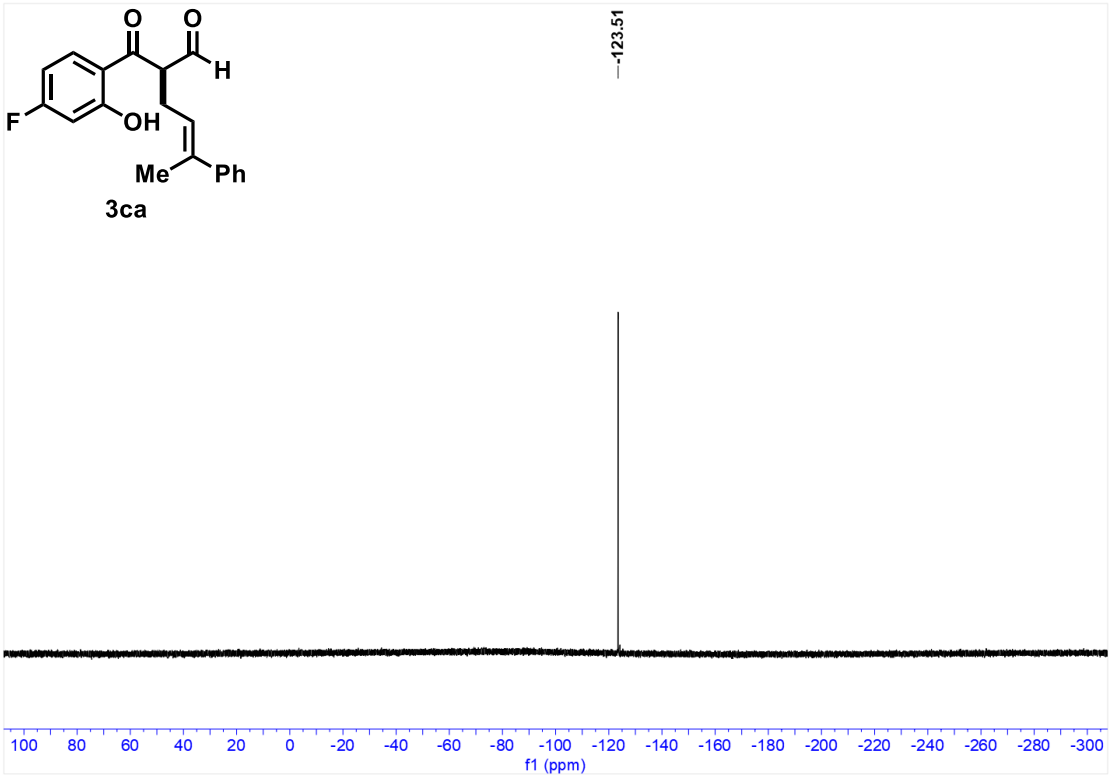


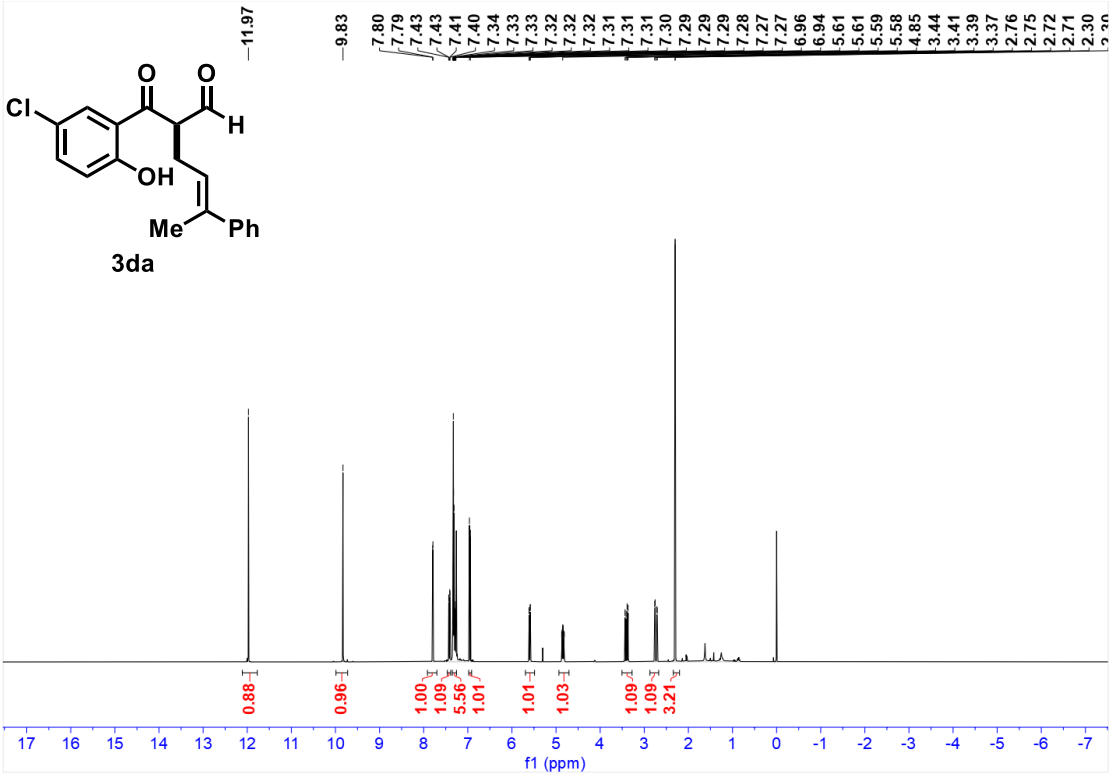

Me
O
O
H
OH
Me
Ph
3ba
11.94
9.84
7.61
7.61
7.34
7.33
7.33
7.32
7.32
7.32
7.31
7.31
7.30
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.27
7.26
7.25
6.91
6.89
5.67
5.66
5.64
5.64
3.40
3.37
3.35
3.35
3.33
3.33
2.75
2.74
2.70
2.69
0.91
0.86
1.00
6.21
0.97
0.98
1.00
1.01
1.02
3.08
2.85
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)

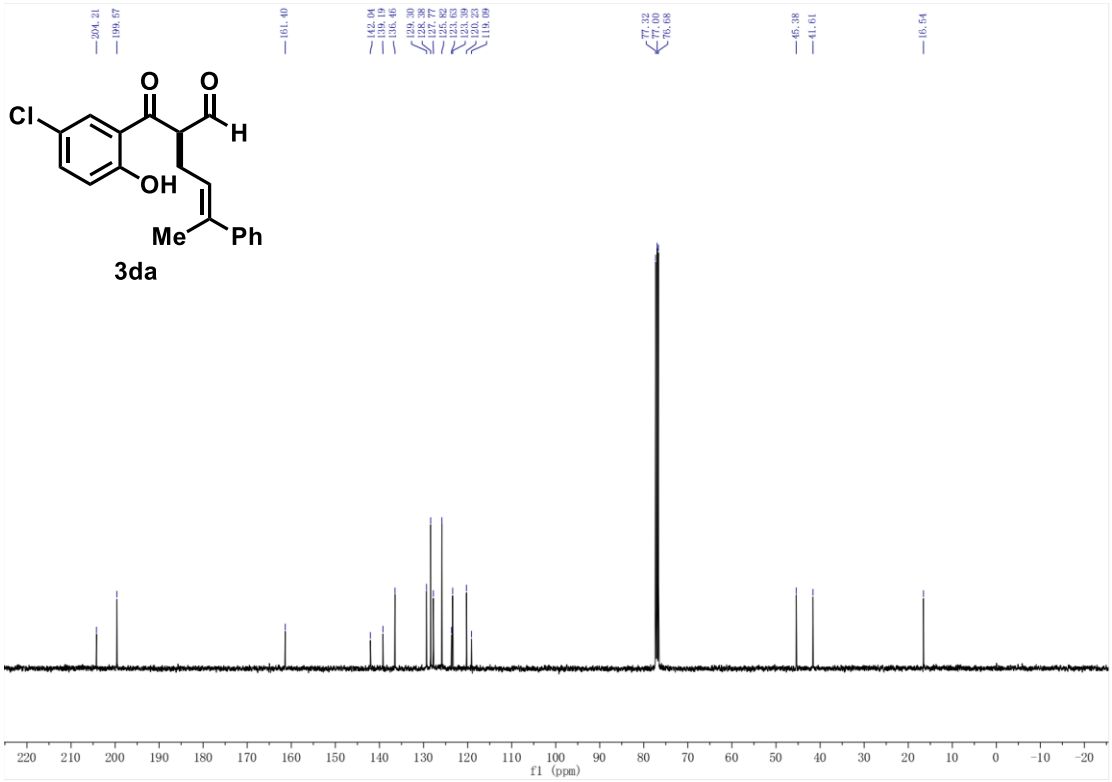

Me
O
O
H
OH
Me
Ph
3ba
204.81
199.89
160.89
142.19
138.29
137.74
129.73
128.92
127.95
127.61
125.79
124.26
118.32
118.13
77.32
77.00
76.68
45.38
41.42
20.66
16.45
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

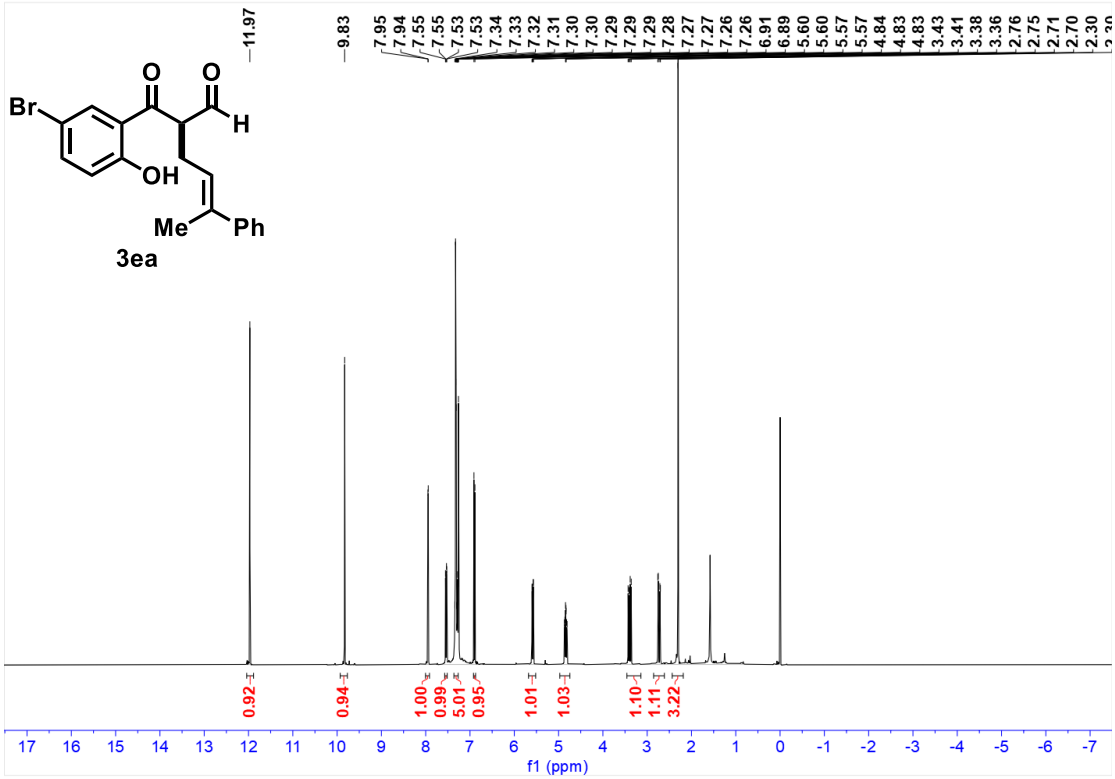

12.43 12.43 9.84 7.87 7.85 7.85 7.83 7.32 7.32 7.32 7.31 7.31 7.31 7.29 7.29 7.28 7.28 7.27 7.26 7.26 6.69 6.68 6.66 6.66 6.65 6.64 6.63 6.63 6.62 6.62 6.61 6.60 5.67 5.67 5.64 5.64 4.88 4.87 4.86 4.86 4.85 4.85 4.84 4.83 3.42 3.42 3.40 3.39 3.37 3.35 3.35 2.75 2.74 2.70 2.69 2.26 2.26
O
O
H
F
OH
Me
Ph
3ca
0.92
0.94
1.00
5.31
1.98
1.00
1.04
1.05
1.04
2.97
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

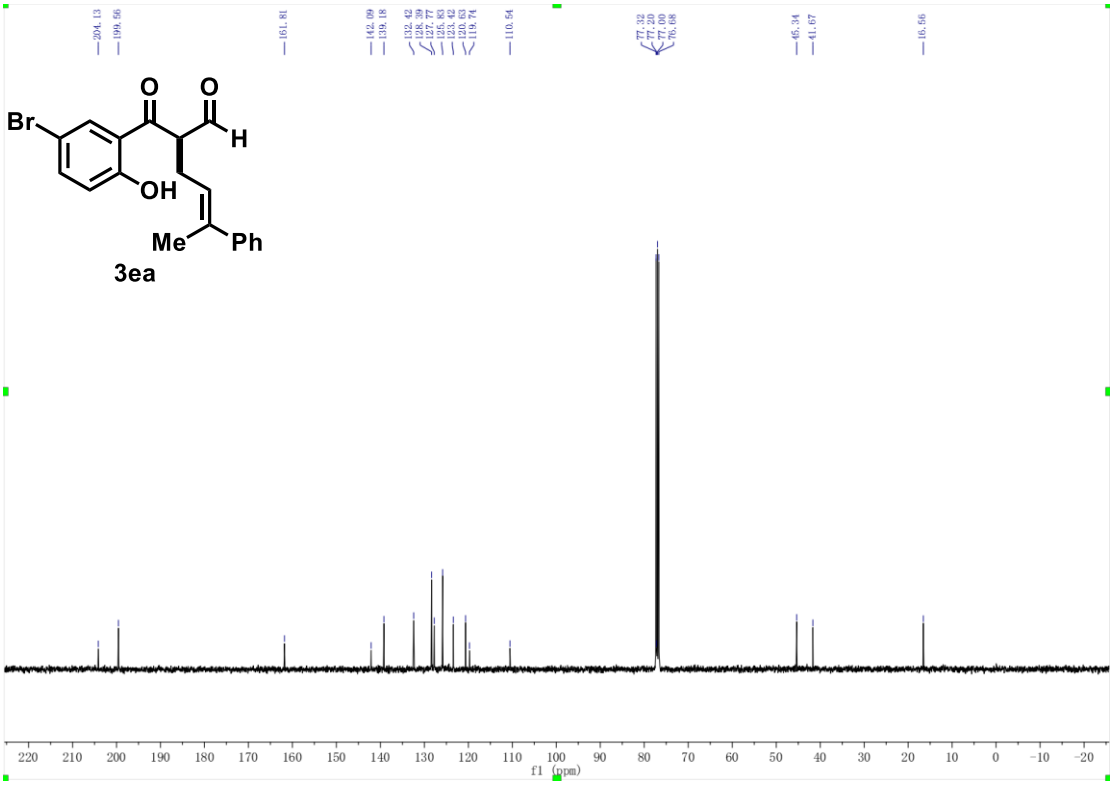

203.89 199.70 168.77 165.68 165.53 142.03 138.65 132.48 132.36 128.37 127.74 125.80 123.91 115.70 107.53 107.30 105.28 105.05 77.32 77.00 76.69 45.36 41.59 16.45
O
O
H
F
OH
Me
Ph
3ca
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

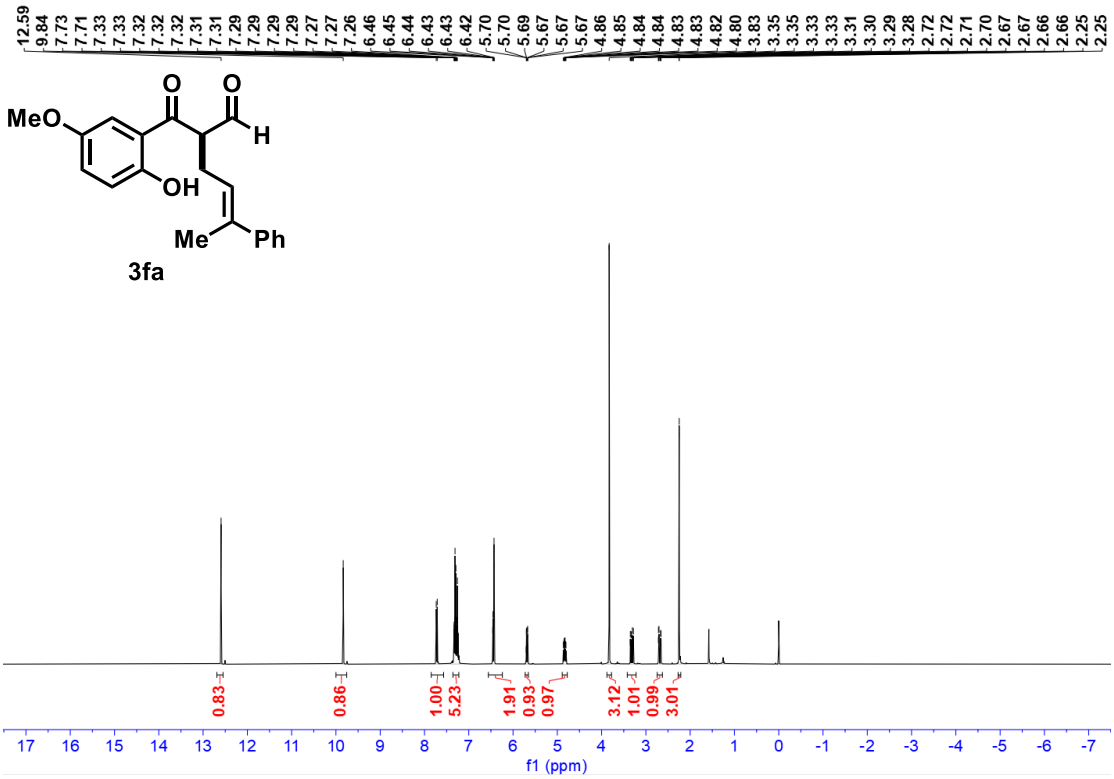

O
O
H
F
OH
Me
Ph
3ca
-123.51
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

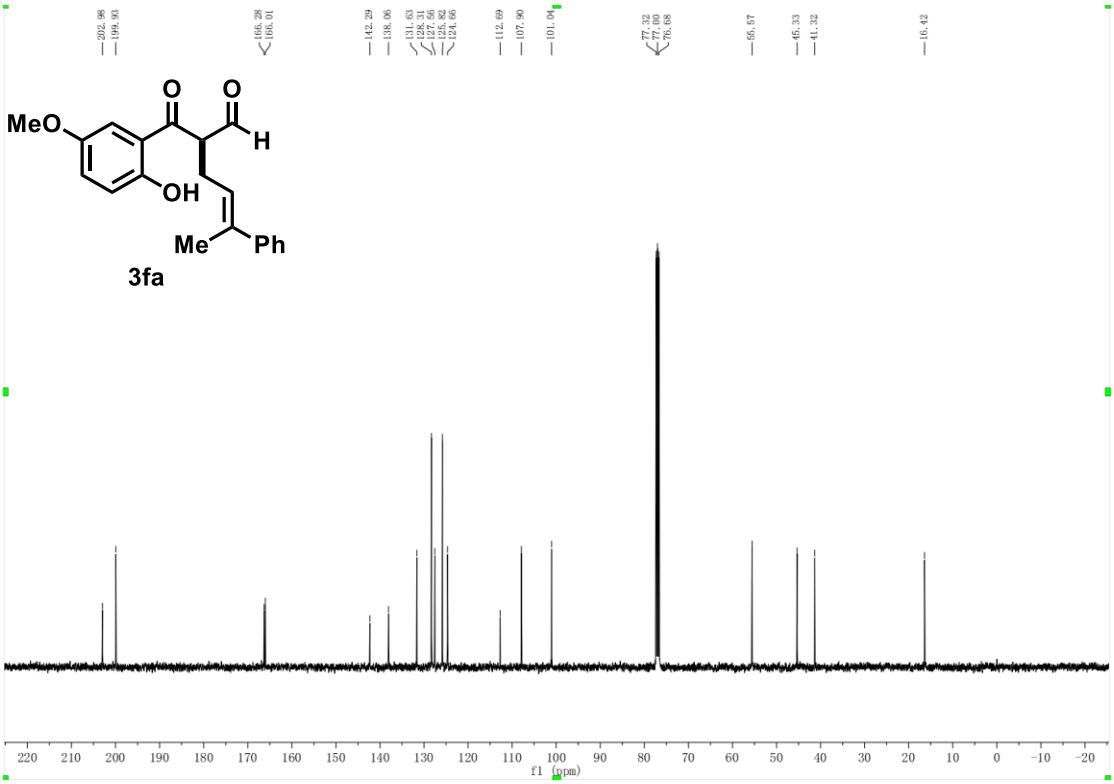

11.97
9.83
7.80 7.79 7.43 7.43 7.41 7.40 7.34 7.33 7.33 7.32 7.32 7.32 7.31 7.31 7.31 7.30 7.29 7.29 7.29 7.28 7.27 7.27 6.96 6.94 5.61 5.59 5.58 4.85 3.44 3.41 3.39 3.37 2.76 2.75 2.72 2.71 2.30
Cl
O
O
H
OH
Me
Ph
3da
0.88 0.96 1.00 1.09 5.56 1.01 1.01 1.03 1.09 1.09 3.21
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)

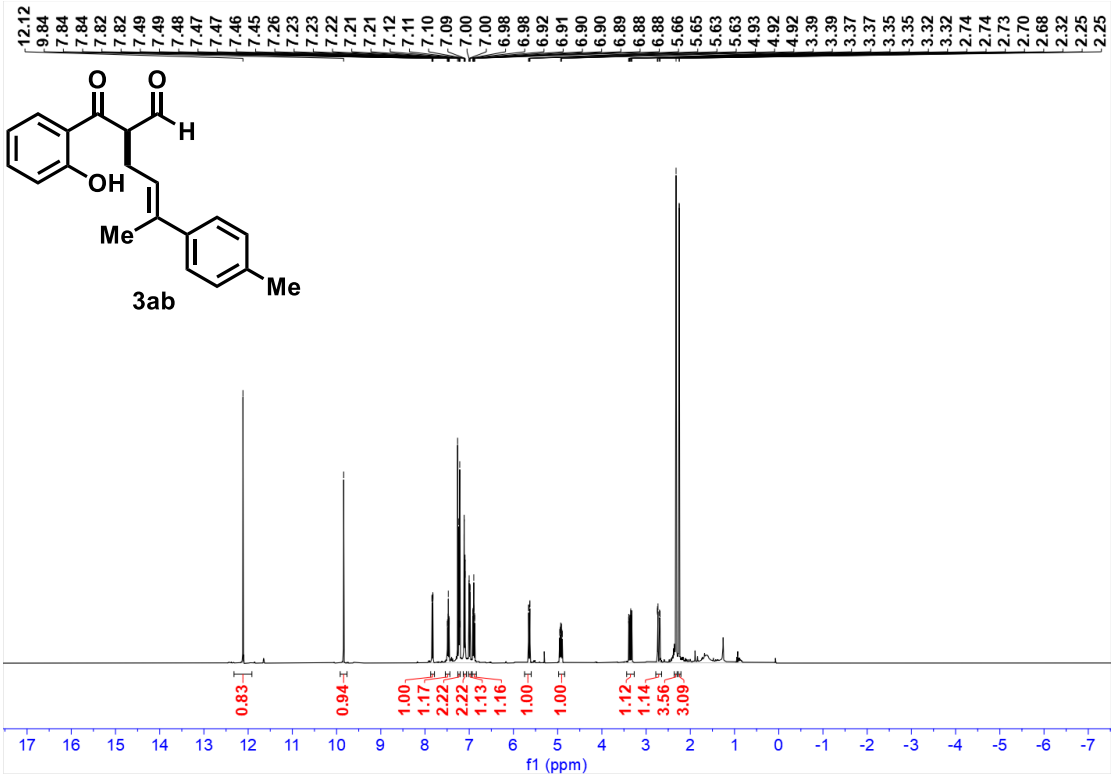

Cl
O
O
H
OH
Me
Ph
3da
f1 (ppm)

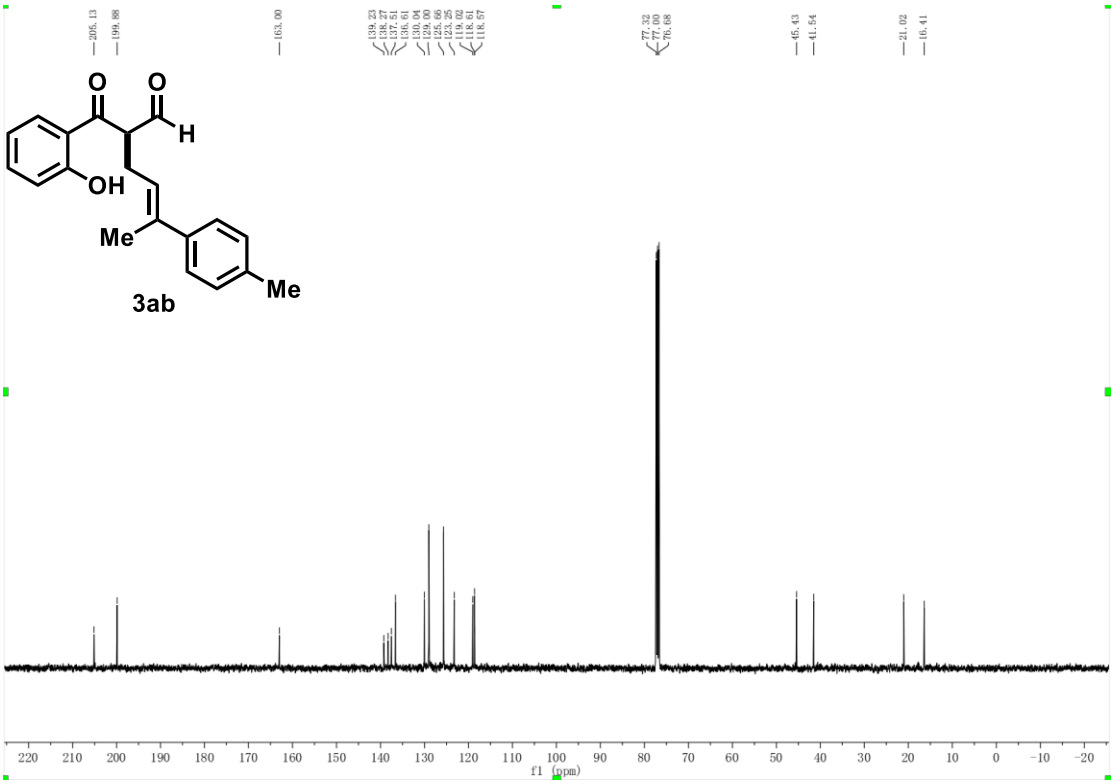

Br
O
O
H
OH
Me
Ph
3ea
f1 (ppm)


Br
O
O
H
OH
Me
Ph
3ea
f1 (ppm)


MeO
O
O
H
OH
Me
Ph
3fa
f1 (ppm)


MeO
O
O
H
OH
Me
Ph
3fa
f1 (ppm)


O
O
H
OH
Me
Me
3ab
f1 (ppm)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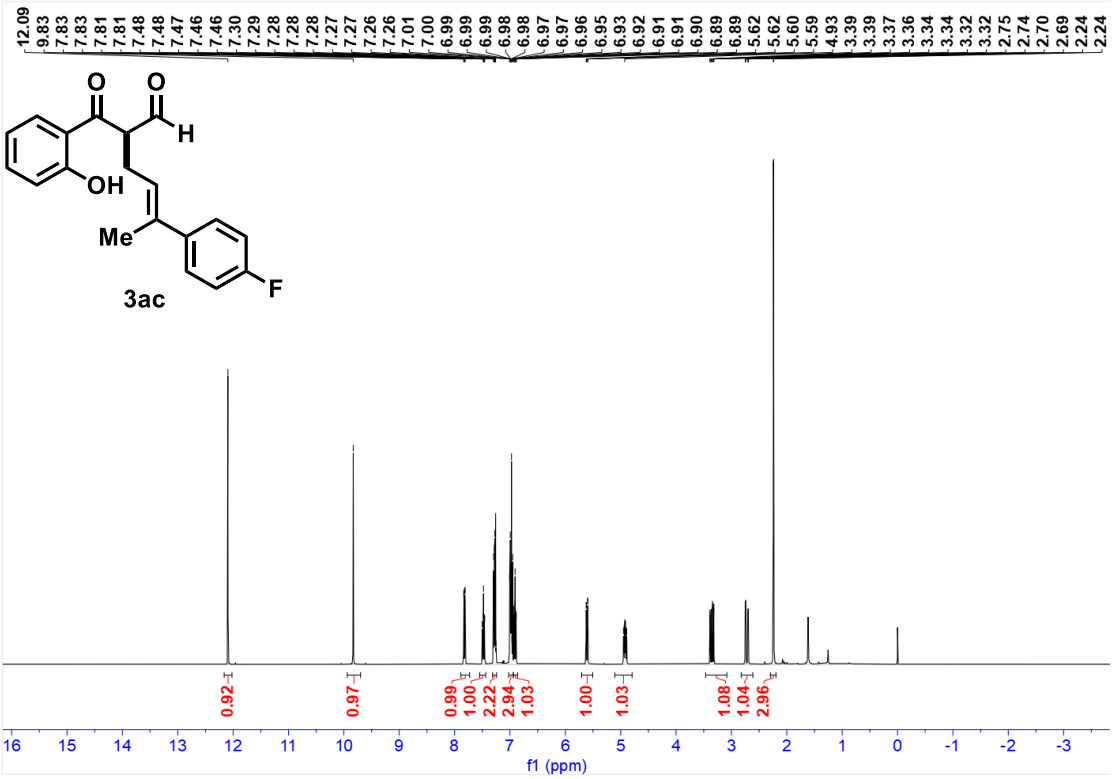
137.61
136.61
130.04
129.00
125.96
123.35
119.02
118.61
118.57
77.32
77.00
76.68
45.43
41.54
21.02
16.41
O
O
H
OH
Me
Me
3ab
f1 (ppm)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7.83
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7.81
7.48
7.48
7.47
7.46
7.46
7.30
7.29
7.28
7.28
7.28
7.27
7.27
7.26
7.26
7.01
7.00
6.99
6.99
6.99
6.98
6.98
6.97
6.97
6.96
6.95
6.93
6.92
6.91
6.91
6.90
6.89
6.89
5.62
5.60
5.59
4.93
3.39
3.39
3.37
3.36
3.34
3.34
3.32
3.32
2.75
2.74
2.70
2.69
2.24
2.24
O
O
H
OH
Me
F
3ac
0.92
0.97
0.99
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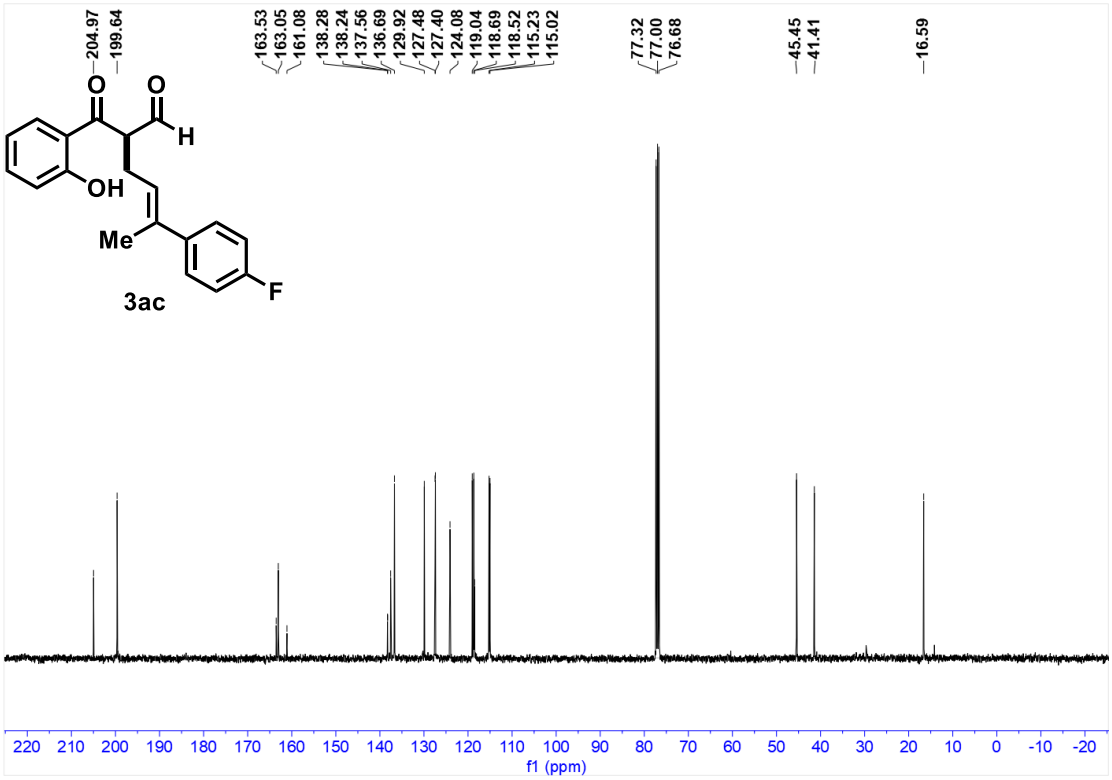
2.22
2.94
1.03
1.00
1.03
1.08
1.04
2.96
f1 (ppm)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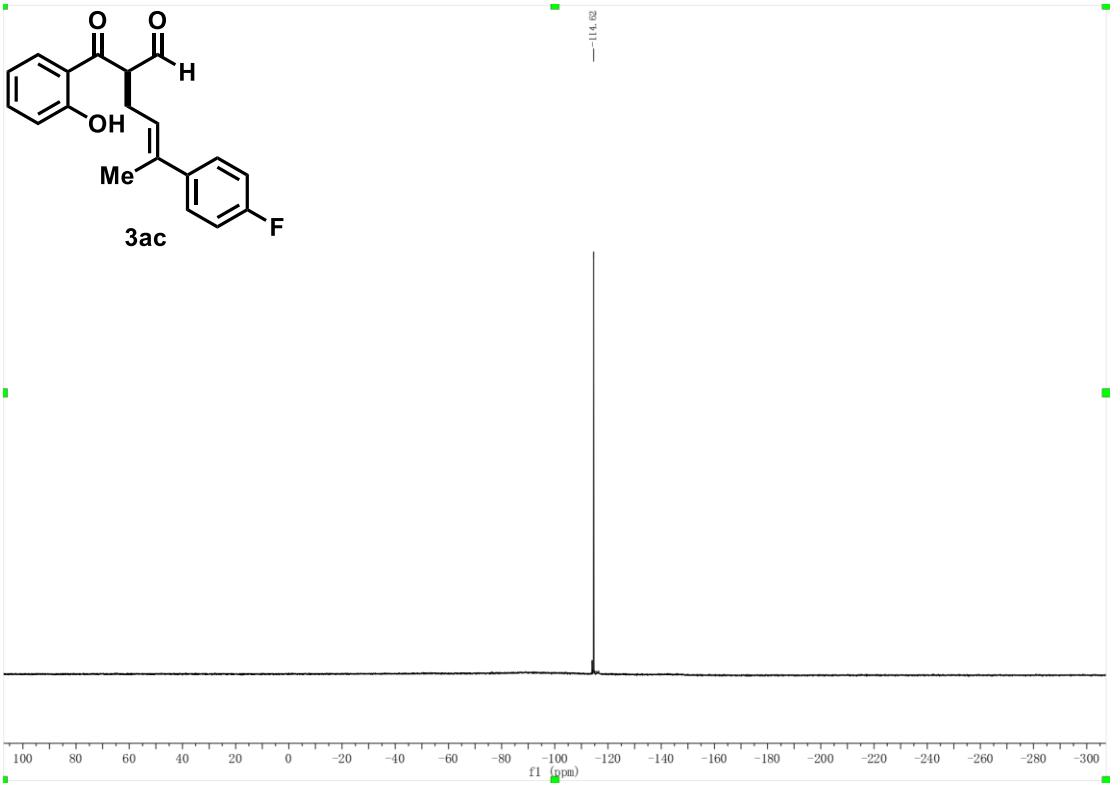
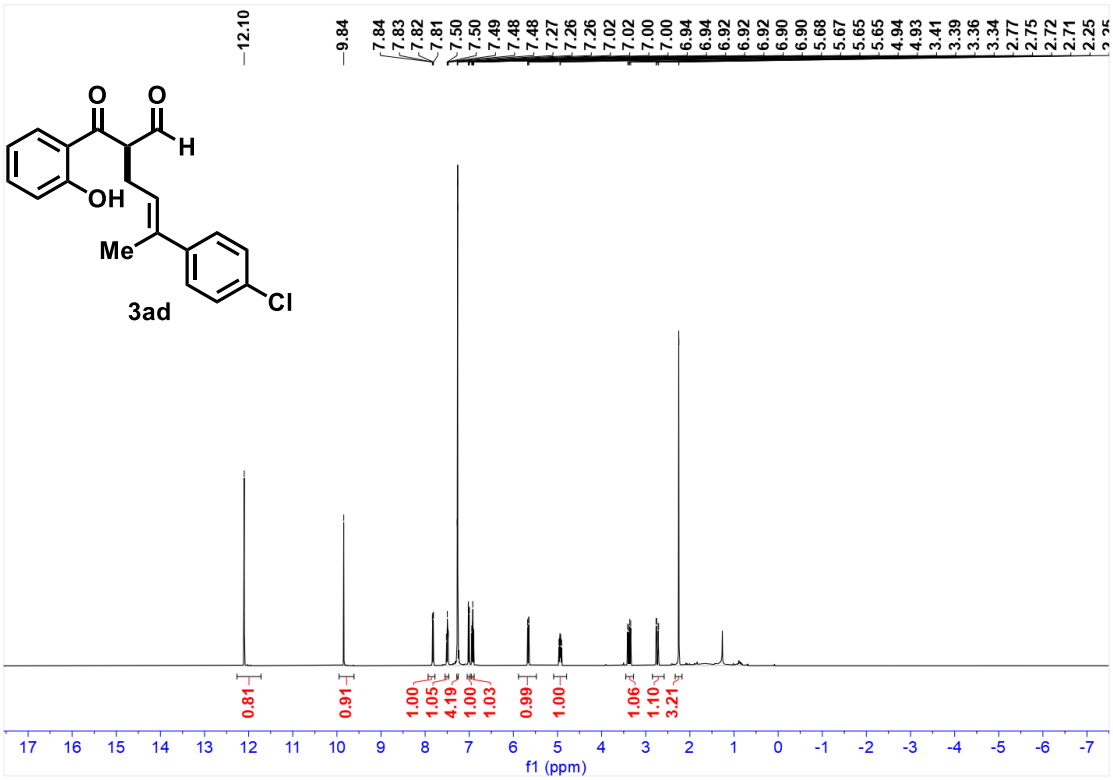
163.05
161.08
138.28
138.24
137.56
136.69
129.92
127.48
127.40
124.08
119.04
118.69
118.52
115.23
115.02
77.32
77.00
76.68
45.45
41.41
16.59
O
O
H
OH
Me
F
3ac
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


O
O
H
OH
Me
F
3ac
-114.62
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)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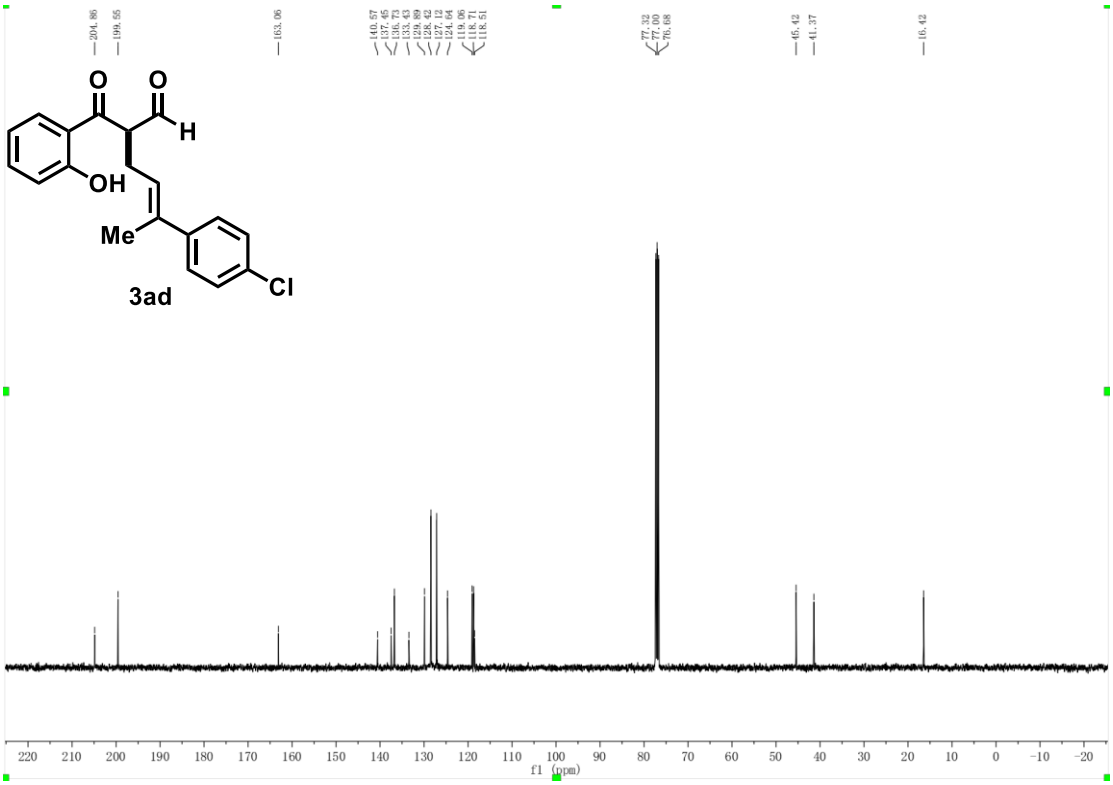
7.83
7.82
7.81
7.50
7.49
7.48
7.27
7.26
7.02
7.00
6.94
6.92
6.90
5.68
5.67
5.65
4.94
4.93
3.41
3.39
3.36
3.34
2.77
2.75
2.72
2.71
2.25
O
O
H
OH
Me
Cl
3ad
0.81
0.91
1.00
1.05
4.19
1.00
1.03
0.99
1.00
1.06
1.10
3.21
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)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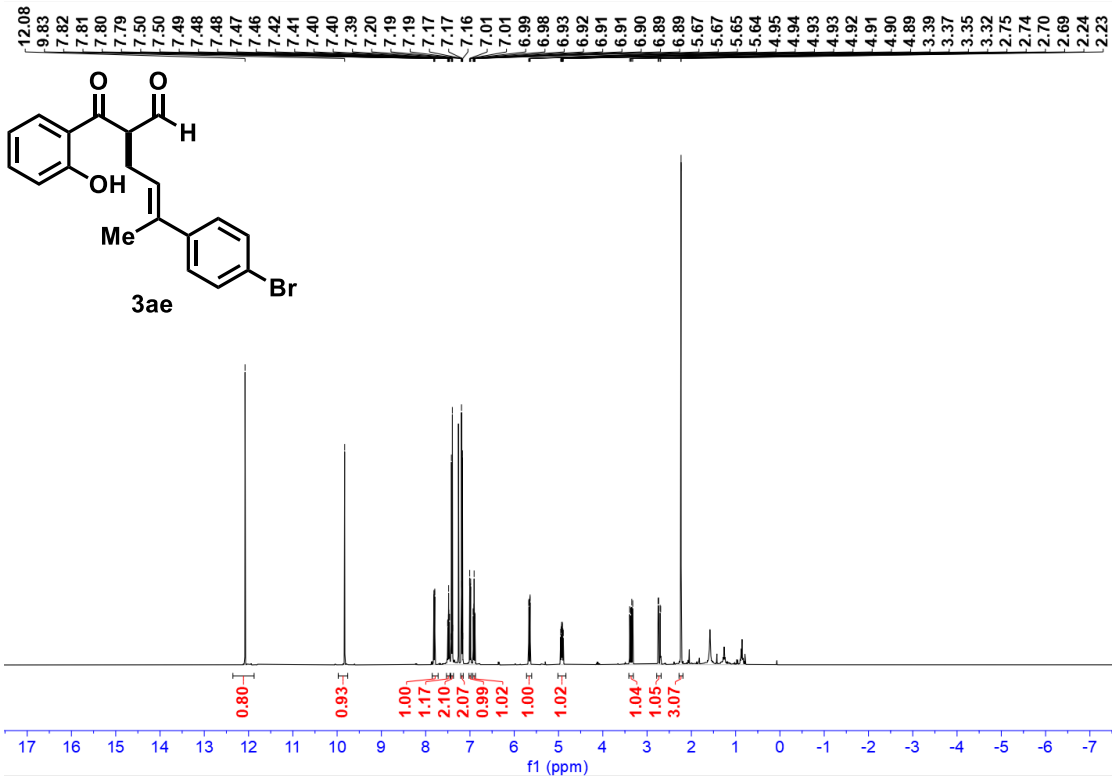
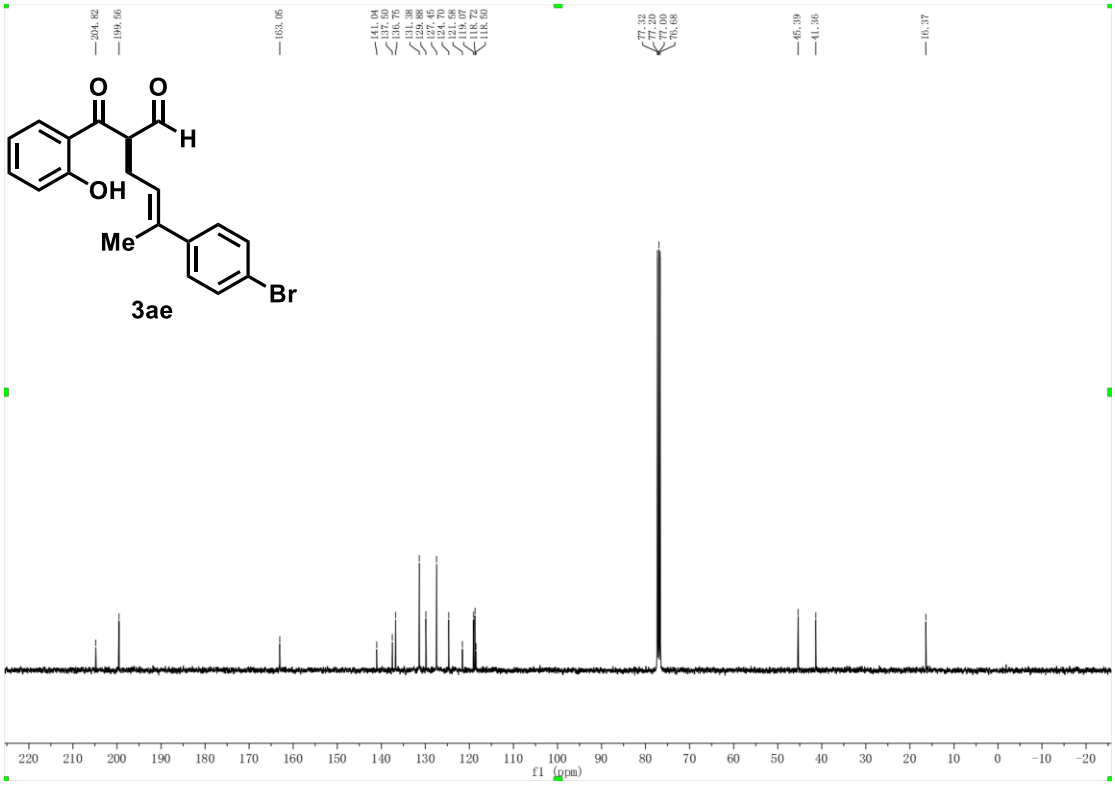
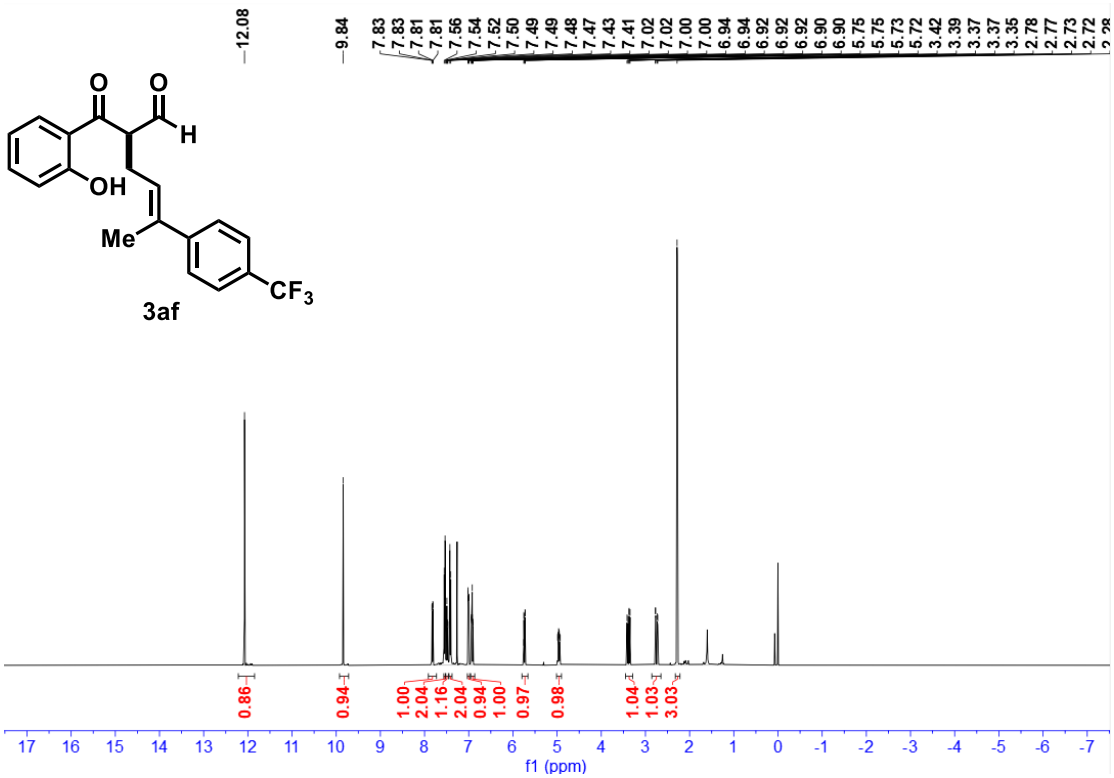
129.89
128.42
127.12
124.64
118.96
118.71
118.51
77.33
77.00
76.68
45.42
41.37
16.42
O
O
H
OH
Me
Cl
3ad
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


12.08 9.83 7.82 7.81 7.80 7.79 7.50 7.50 7.49 7.48 7.48 7.47 7.46 7.42 7.41 7.40 7.40 7.39 7.20 7.19 7.19 7.17 7.17 7.16 7.01 7.01 6.99 6.98 6.93 6.92 6.91 6.91 6.90 6.89 6.89 5.67 5.65 5.64 4.95 4.94 4.93 4.93 4.92 4.91 4.90 4.89 3.39 3.37 3.35 3.32 2.75 2.74 2.70 2.69 2.24 2.23
O
O
H
OH
Me
Br
3ae
0.80 0.93 1.00 1.17 2.10 2.07 0.99 1.02 1.00 1.02 1.04 1.05 3.07
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)


204.82 199.96 153.05 141.04 137.50 136.75 131.38 129.36 127.45 124.70 121.08 114.97 118.72 118.50 77.32 77.20 77.00 76.68 45.39 41.36 16.37
O
O
H
OH
Me
Br
3ae
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.54
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7.50
7.49
7.49
7.48
7.47
7.43
7.41
7.02
7.02
7.00
7.00
6.94
6.94
6.92
6.92
6.90
6.90
5.75
5.75
5.73
5.72
3.42
3.39
3.37
3.37
3.35
2.78
2.77
2.73
2.72
O
O
H
OH
Me
CF3
3af
0.86
0.94
1.00
2.04
1.16
2.04
0.94
1.00
0.97
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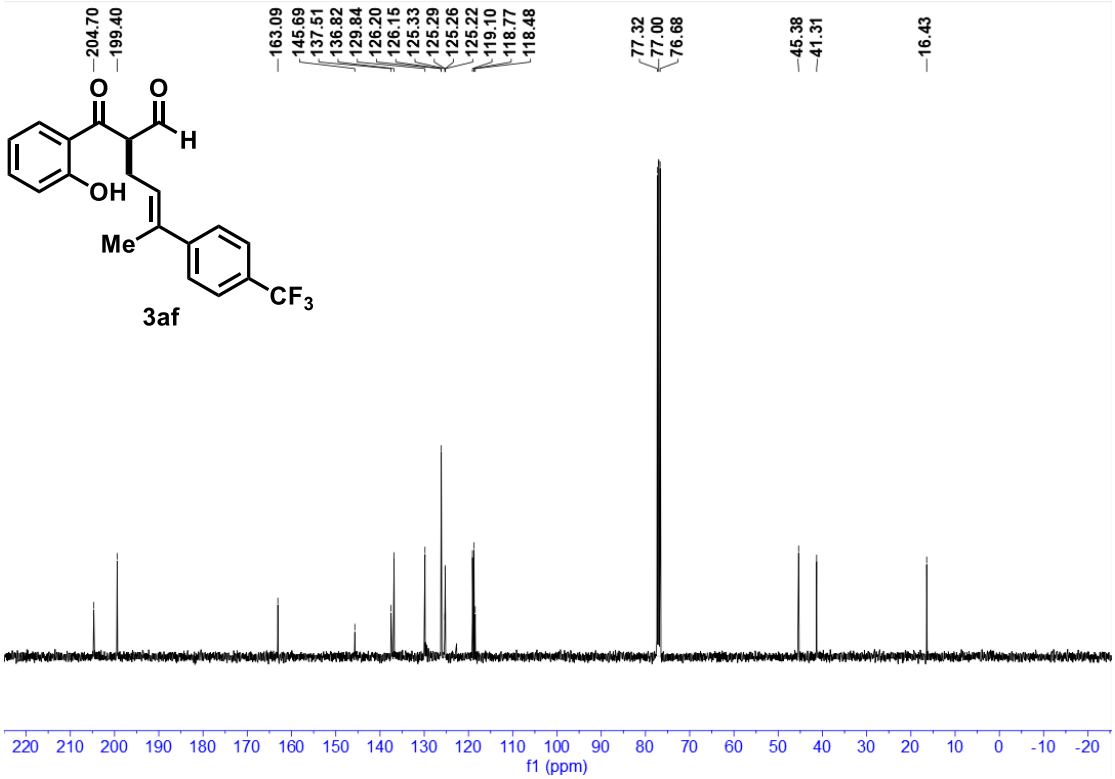
1.04
1.03
3.03
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)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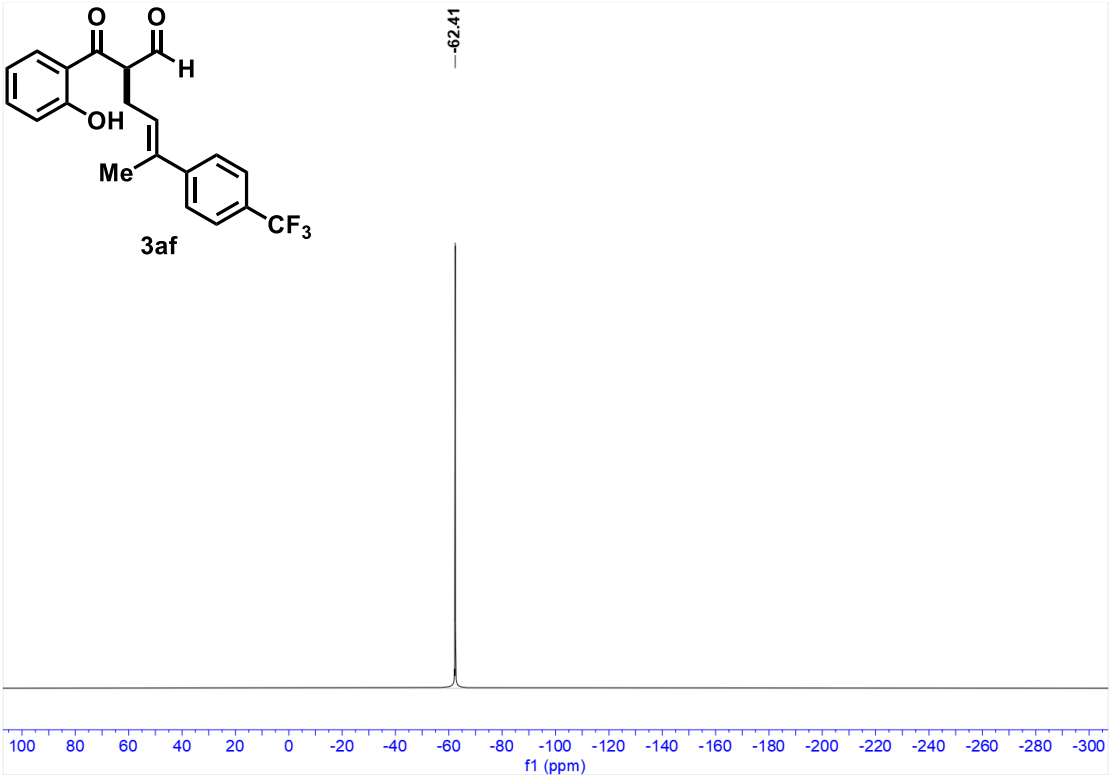
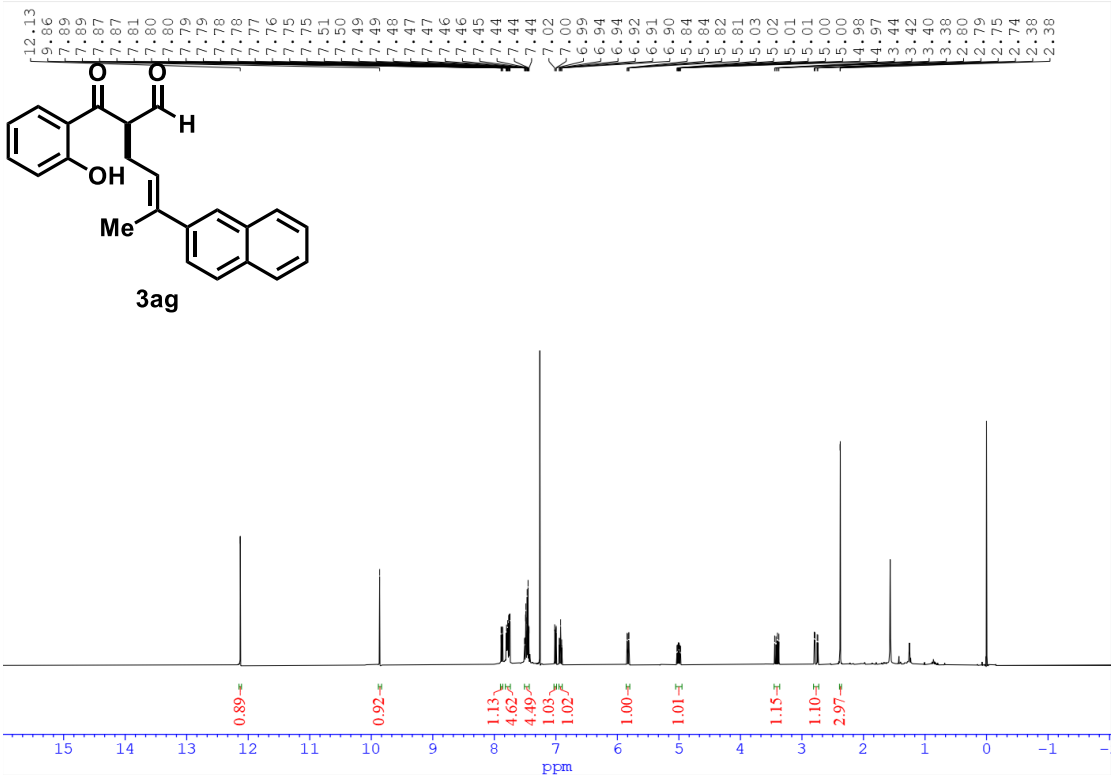
136.82
129.84
126.20
126.15
125.33
125.29
125.26
125.22
119.10
118.77
118.48
77.32
77.00
76.68
45.38
41.31
16.43
O
O
H
OH
Me
CF3
3af
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


O
O
H
OH
Me
CF3
3af
-62.41
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)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7.77
7.76
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5.00
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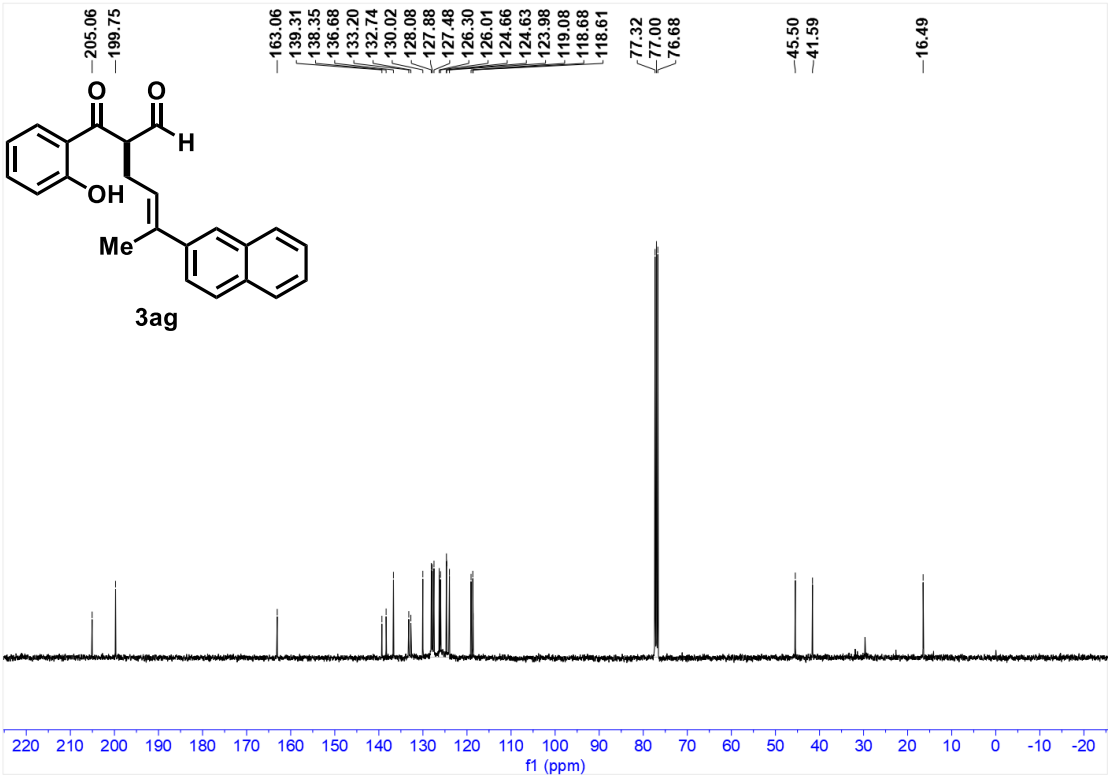
3.40
3.38
2.80
2.79
2.75
2.74
2.38
2.38
O
O
H
OH
Me
3ag
0.89
0.92
1.13
4.62
4.49
1.03
1.02
1.00
1.01
1.15
1.10
2.97
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
ppm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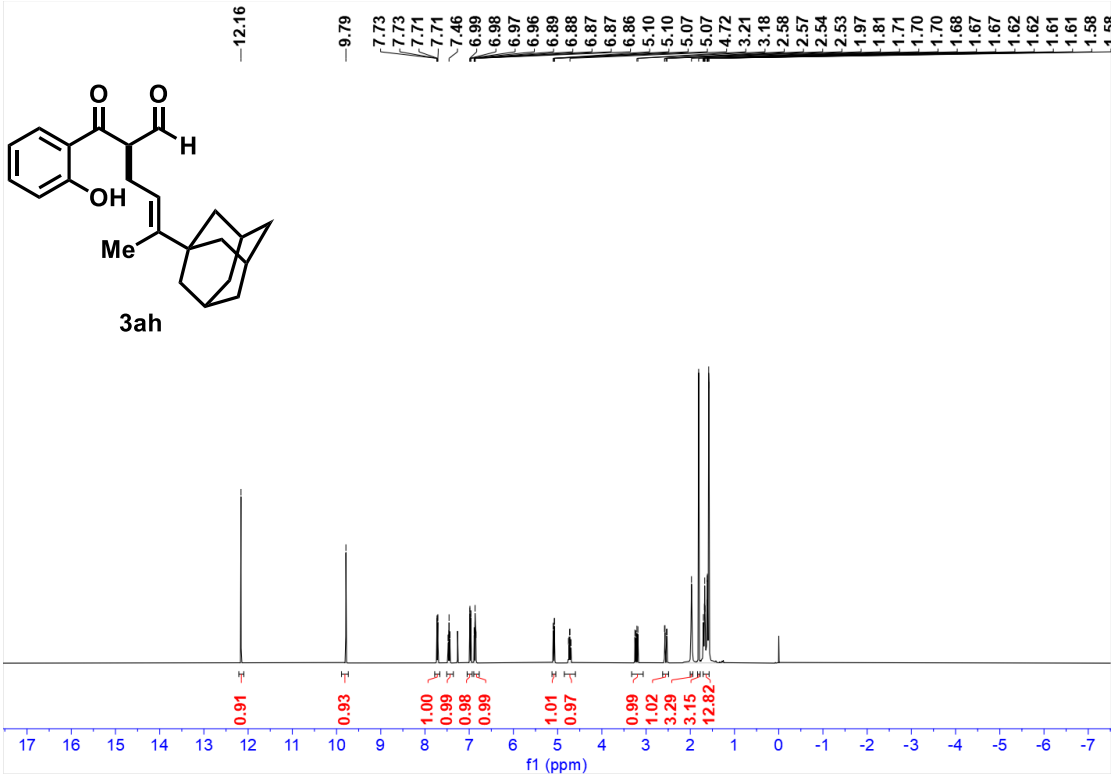
199.75
163.06
139.31
138.35
136.68
133.20
132.74
130.02
128.08
127.88
127.48
126.30
126.01
124.66
124.63
123.98
119.08
118.68
118.61
77.32
77.00
76.68
45.50
41.59
16.49
O
O
H
OH
Me
3ag
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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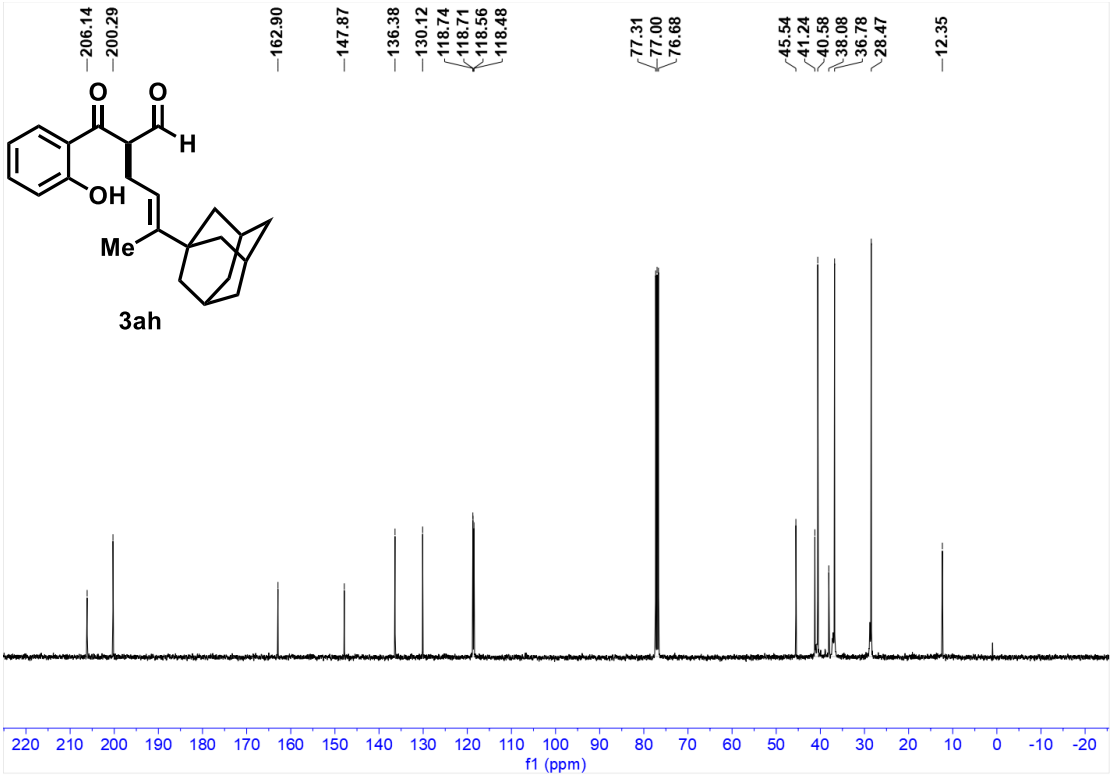
7.73
7.73
7.71
7.71
7.46
6.99
6.98
6.97
6.96
6.89
6.88
6.87
6.87
6.86
5.10
5.10
5.07
5.07
4.72
3.21
3.18
2.58
2.57
2.54
2.53
1.97
1.81
1.71
1.70
1.70
1.68
1.67
1.67
1.62
1.62
1.61
1.61
1.58
O
O
H
OH
Me
3ah
0.91
0.93
1.00
0.99
0.98
0.99
1.01
0.97
0.99
1.02
3.29
3.15
12.82
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)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200.29
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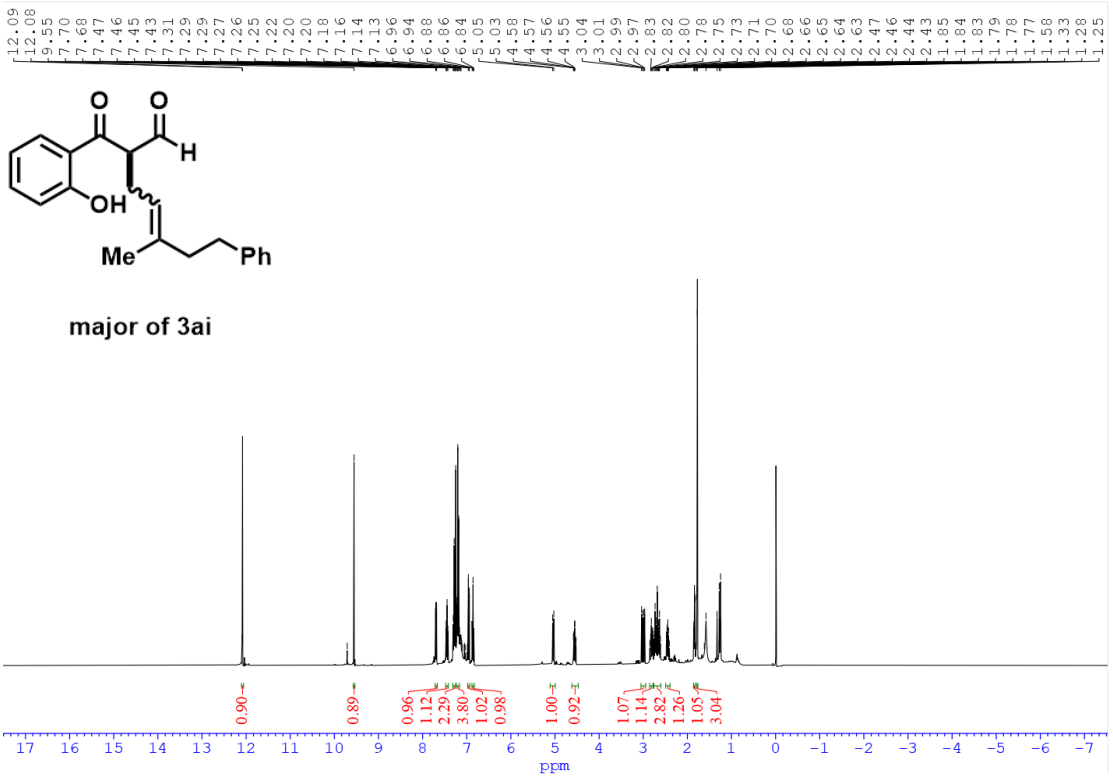
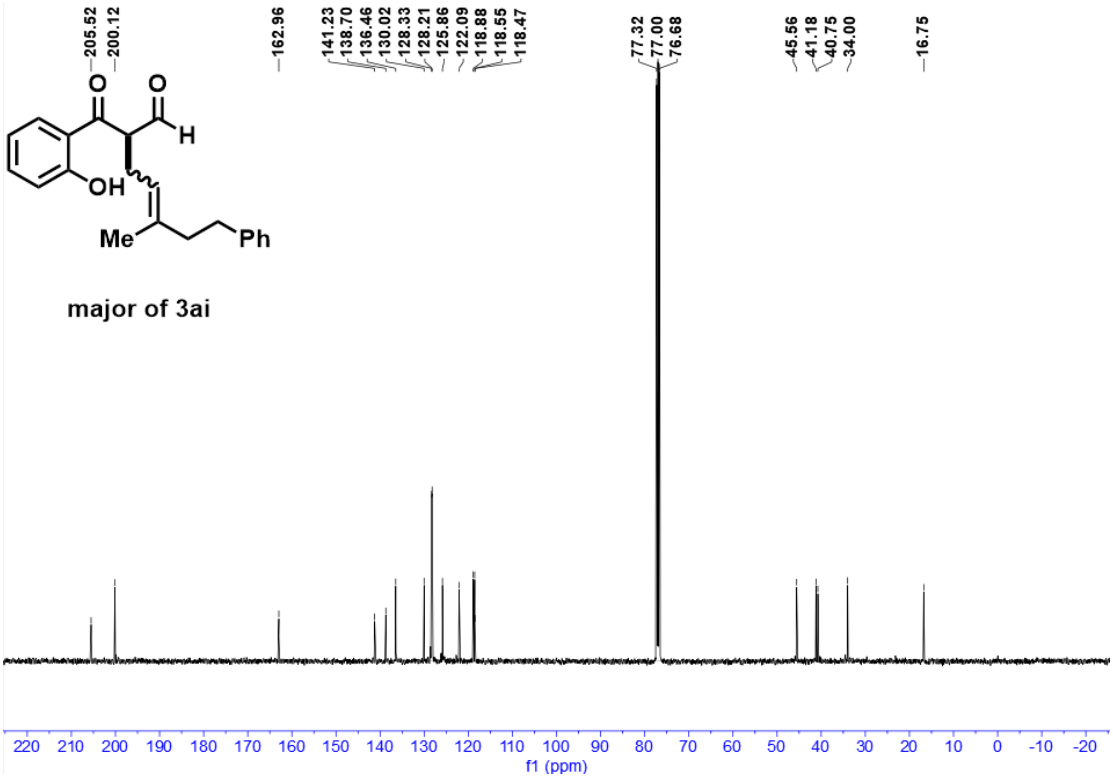
130.12
118.74
118.71
118.56
118.48
77.31
77.00
76.68
45.54
41.24
40.58
38.08
36.78
28.47
12.35
O
O
H
OH
Me
3ah
f1 (ppm)


O
O
H
OH
Me
Ph
major of 3ai
ppm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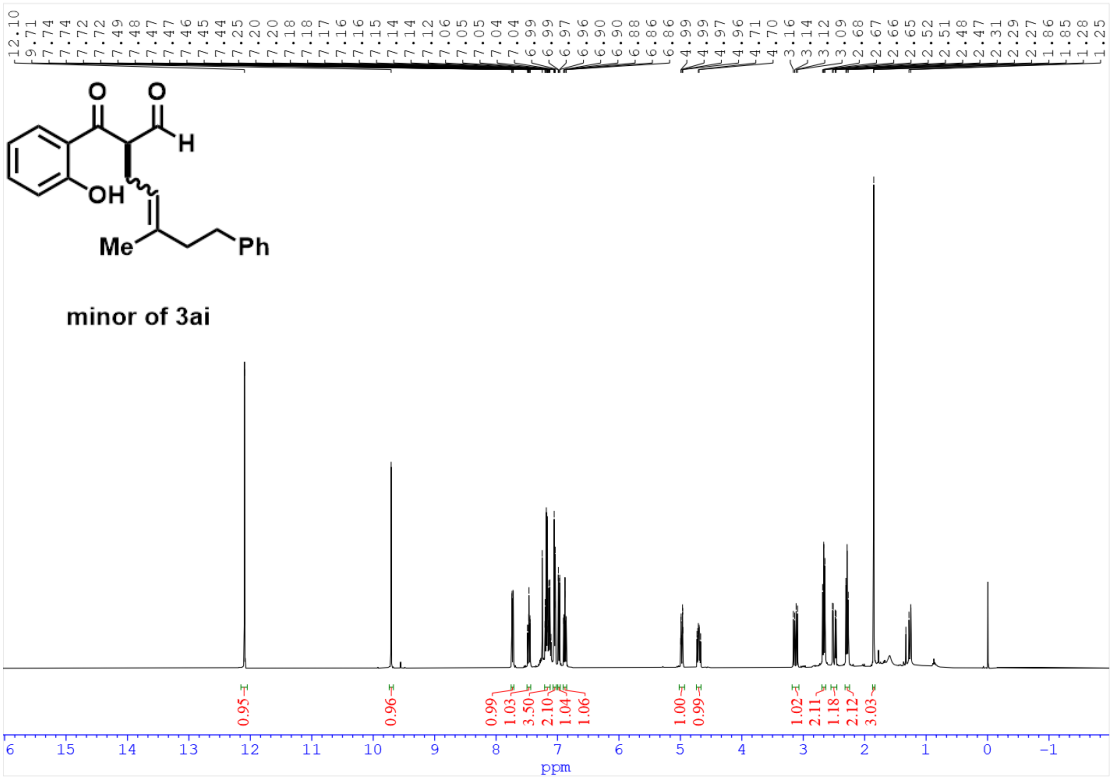
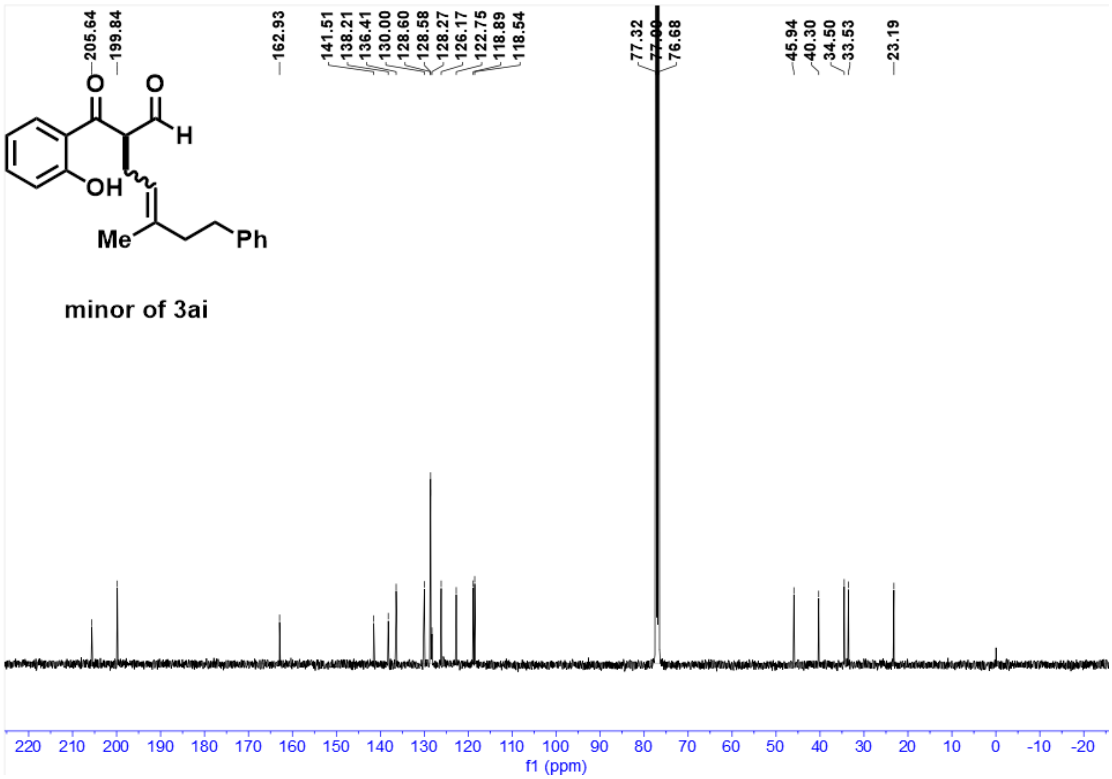
136.46
130.02
128.33
128.21
125.86
122.09
118.88
118.55
118.47
77.32
77.00
76.68
45.56
41.18
40.75
34.00
16.75
O
O
H
OH
Me
Ph
major of 3ai
f1 (ppm)


O
O
H
OH
Me
Ph
minor of 3ai
ppm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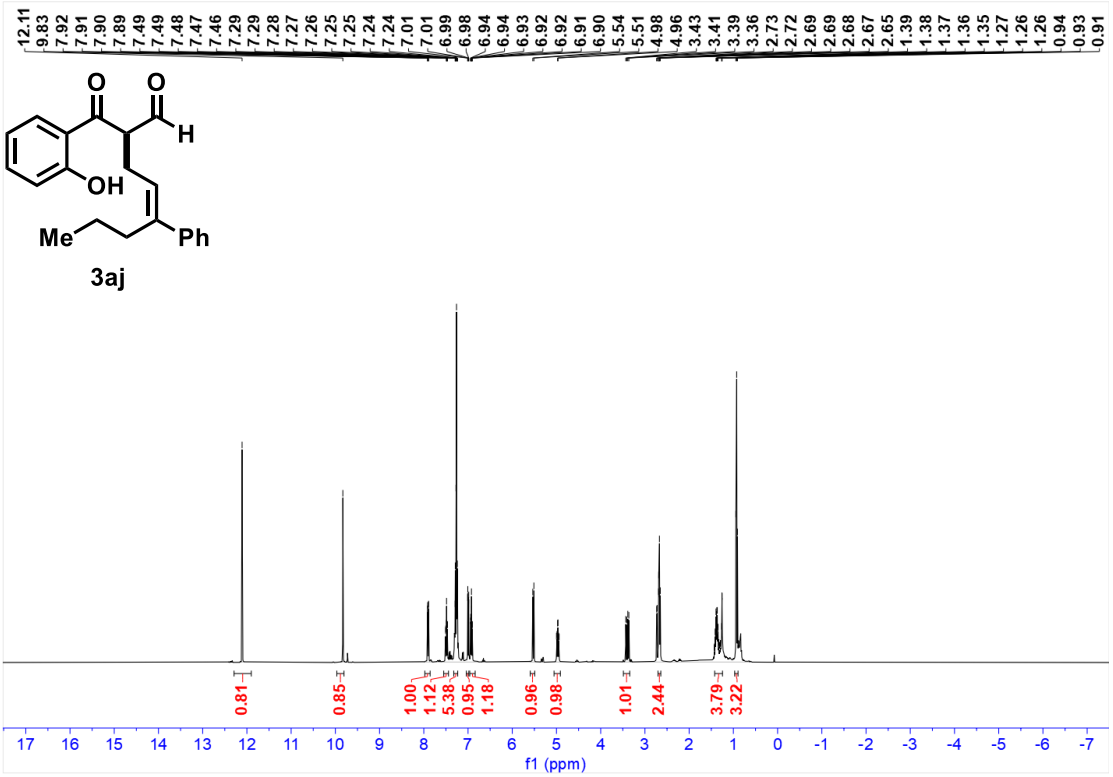
128.27
126.17
122.75
118.89
118.54
77.32
77.00
76.68
45.94
40.30
34.50
33.53
23.19
O
O
H
OH
Me
Ph
minor of 3ai
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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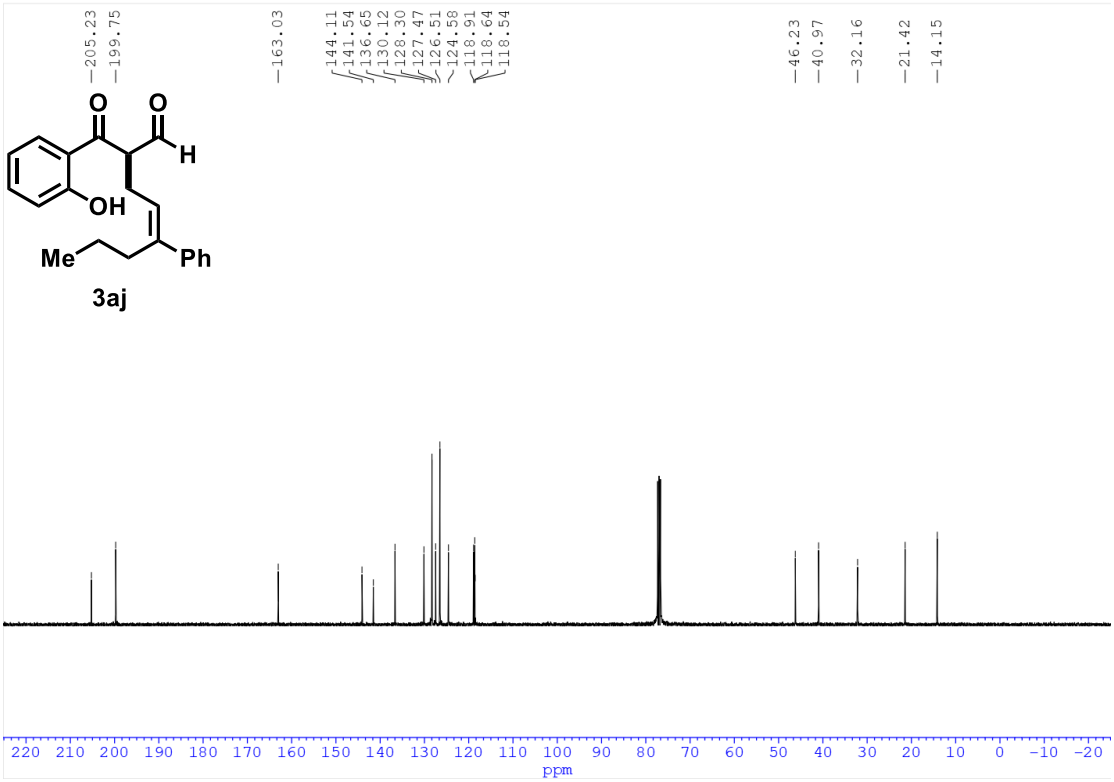
7.92
7.91
7.90
7.89
7.49
7.49
7.48
7.47
7.46
7.29
7.29
7.28
7.27
7.26
7.25
7.25
7.24
7.24
7.01
7.01
6.99
6.98
6.94
6.94
6.93
6.92
6.92
6.91
6.90
5.54
5.51
4.98
4.96
3.43
3.41
3.39
3.36
2.73
2.72
2.69
2.69
2.68
2.67
2.65
1.39
1.38
1.37
1.36
1.35
1.27
1.26
1.26
0.94
0.93
0.91
O
O
H
OH
Me
Ph
3aj
0.81
0.85
1.00
1.12
5.38
0.95
1.18
0.96
0.98
1.01
2.44
3.79
3.22
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)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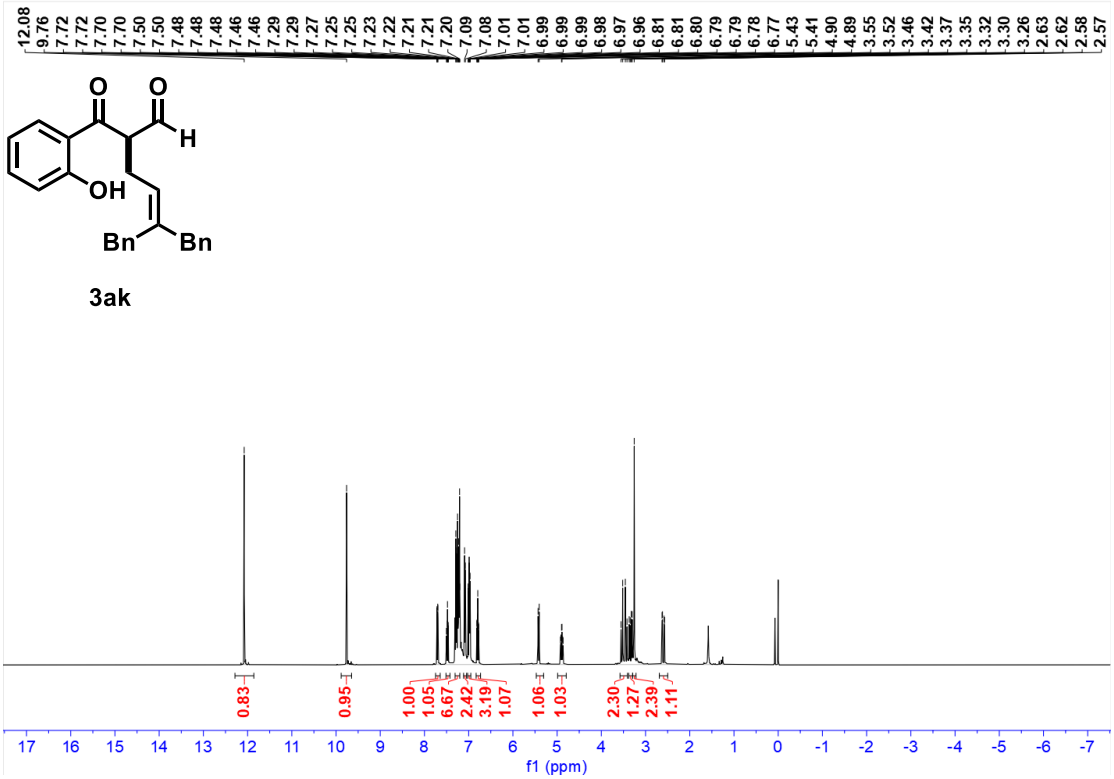
199.75
163.03
144.11
141.54
136.65
130.12
128.30
127.47
126.51
124.58
118.91
118.64
118.54
46.23
40.97
32.16
21.42
14.15
O
O
H
OH
Me
Ph
3aj
ppm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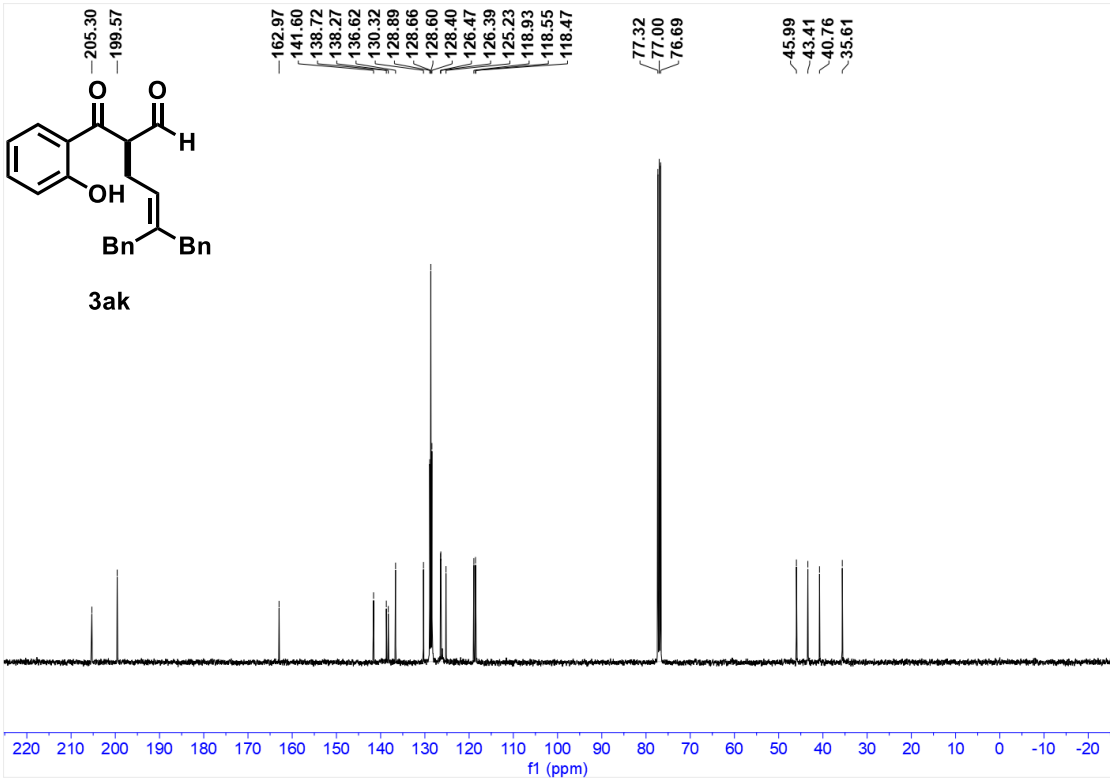
9.76
7.72
7.72
7.70
7.70
7.50
7.50
7.48
7.48
7.48
7.46
7.46
7.29
7.29
7.27
7.25
7.25
7.23
7.22
7.21
7.21
7.20
7.09
7.08
7.01
7.01
6.99
6.99
6.99
6.98
6.97
6.96
6.81
6.81
6.80
6.79
6.79
6.78
6.77
5.43
5.41
4.90
4.89
3.55
3.52
3.46
3.42
3.37
3.35
3.32
3.30
3.26
2.63
2.62
2.58
2.57
O
O
H
OH
Bn
Bn
3ak
0.83
0.95
1.00
1.05
6.67
2.42
3.19
1.07
1.06
1.03
2.30
1.27
2.39
1.11
f1 (ppm)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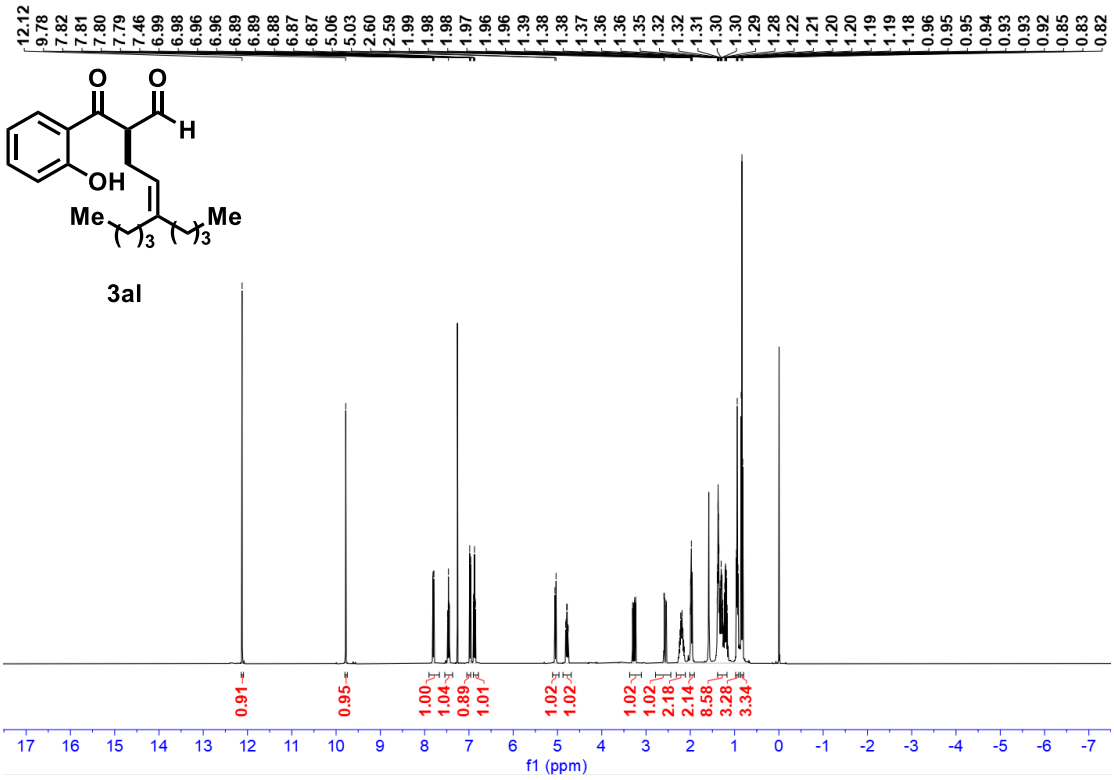
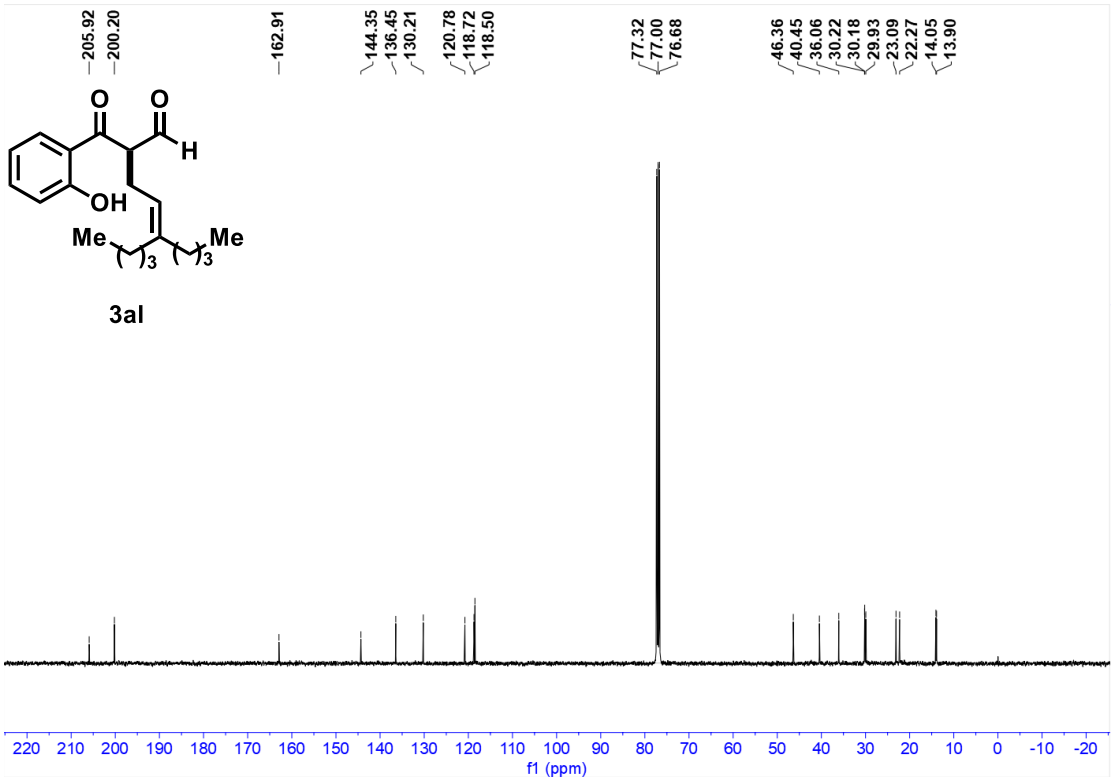
199.57
162.97
141.60
138.72
138.27
136.62
130.32
128.89
128.66
128.60
128.40
126.47
126.39
125.23
118.93
118.55
118.47
77.32
77.00
76.69
45.99
43.41
40.76
35.61
O
O
H
OH
Bn
Bn
3ak
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


12.12
9.78
7.82
7.81
7.80
7.79
7.46
6.99
6.98
6.96
6.96
6.89
6.89
6.88
6.87
6.87
5.06
5.03
2.60
2.59
1.99
1.98
1.98
1.97
1.96
1.96
1.39
1.38
1.38
1.37
1.36
1.36
1.35
1.32
1.32
1.31
1.30
1.30
1.29
1.28
1.22
1.21
1.20
1.20
1.19
1.19
1.18
0.96
0.95
0.95
0.94
0.93
0.93
0.92
0.85
0.83
0.82
O
O
H
OH
Me
Me
3
3
3al
0.91
0.95
1.00
1.04
0.89
1.01
1.02
1.02
1.02
1.02
2.18
2.14
8.58
3.28
3.34
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)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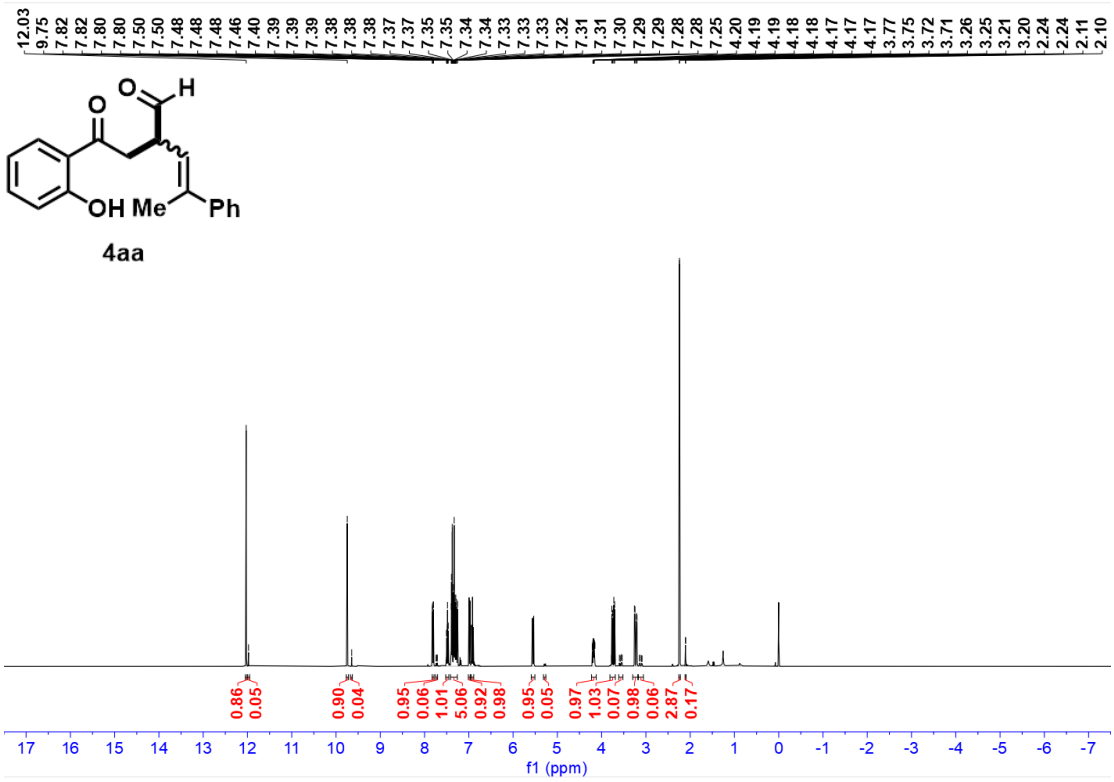
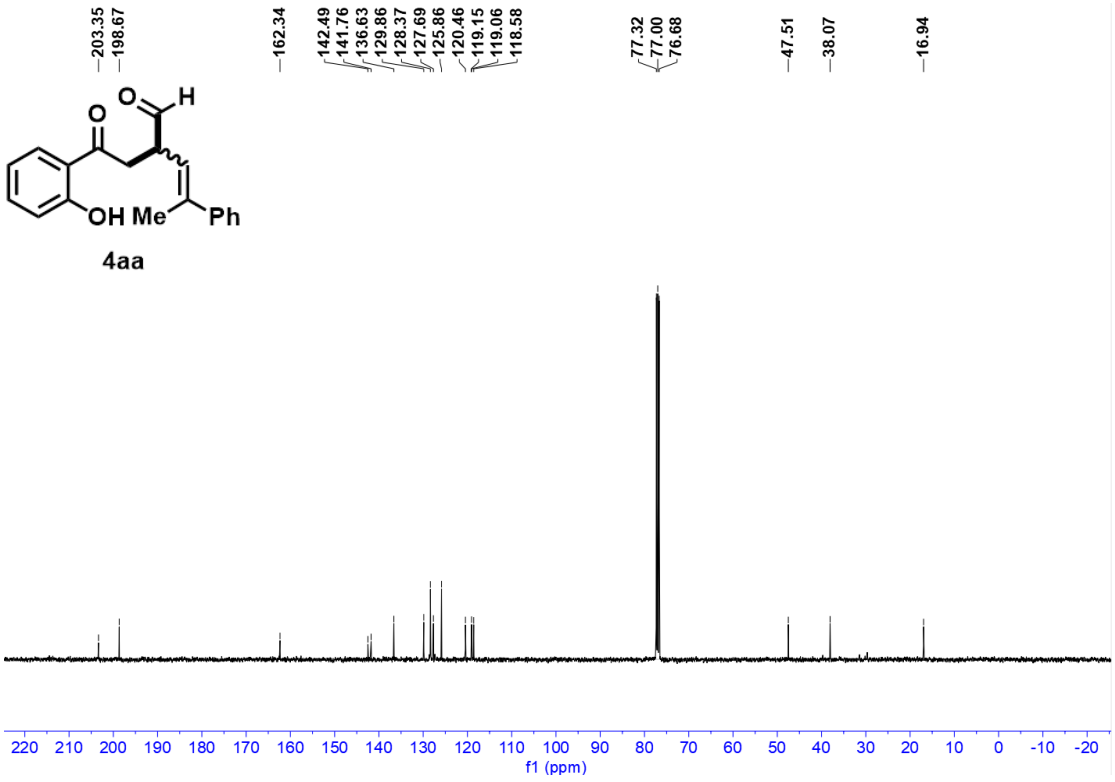
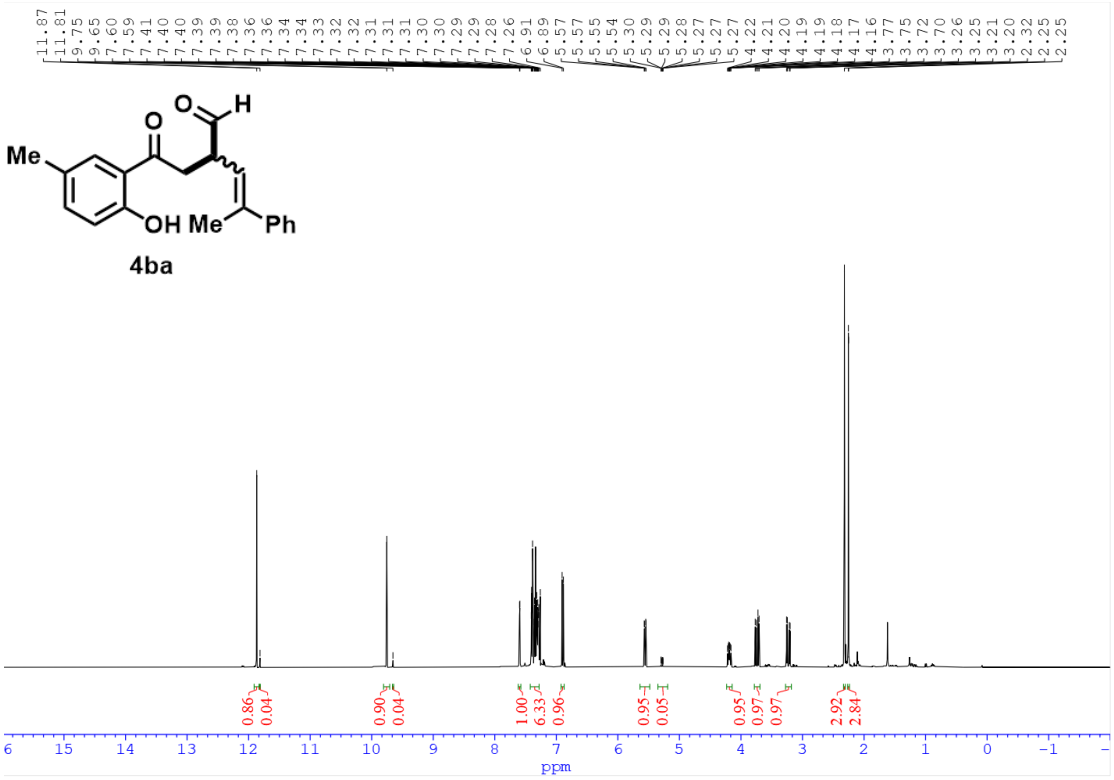
136.45
130.21
120.78
118.72
118.50
77.32
77.00
76.68
46.36
40.45
36.06
30.22
30.18
29.93
23.09
22.27
14.05
13.90
O
O
H
OH
Me
3
3
Me
3al
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

NMR spectra for 1,4-dicarbonyl-alkenes:



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7.59
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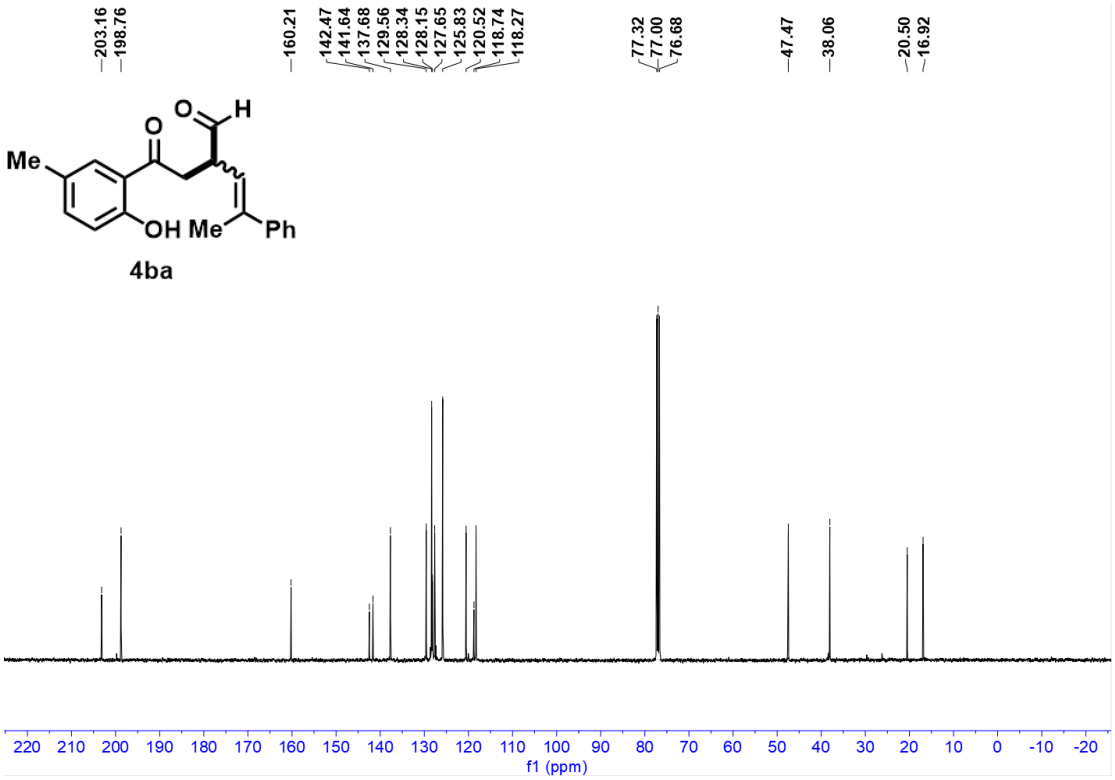
7.40
7.40
7.39
7.39
7.38
7.36
7.36
7.34
7.34
7.33
7.32
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.26
6.91
6.89
5.57
5.57
5.55
5.54
5.30
5.29
5.29
5.28
5.27
5.27
5.27
4.22
4.21
4.20
4.19
4.19
4.18
4.17
4.16
3.77
3.75
3.72
3.70
3.26
3.25
3.21
3.20
2.32
2.25
2.25
O
H
O
Me
OH Me
Ph
4ba
0.86
0.04
0.90
0.04
1.00
6.33
0.96
0.95
0.05
0.95
0.97
0.97
2.92
2.84
6
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm


203.16
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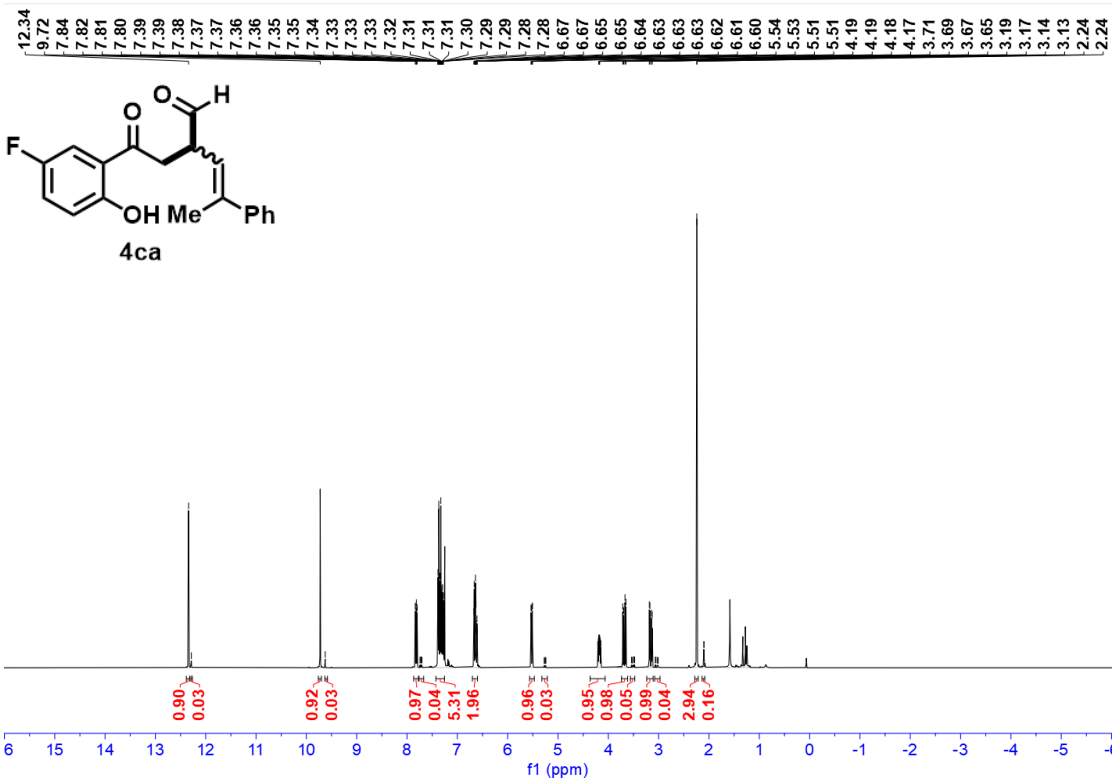
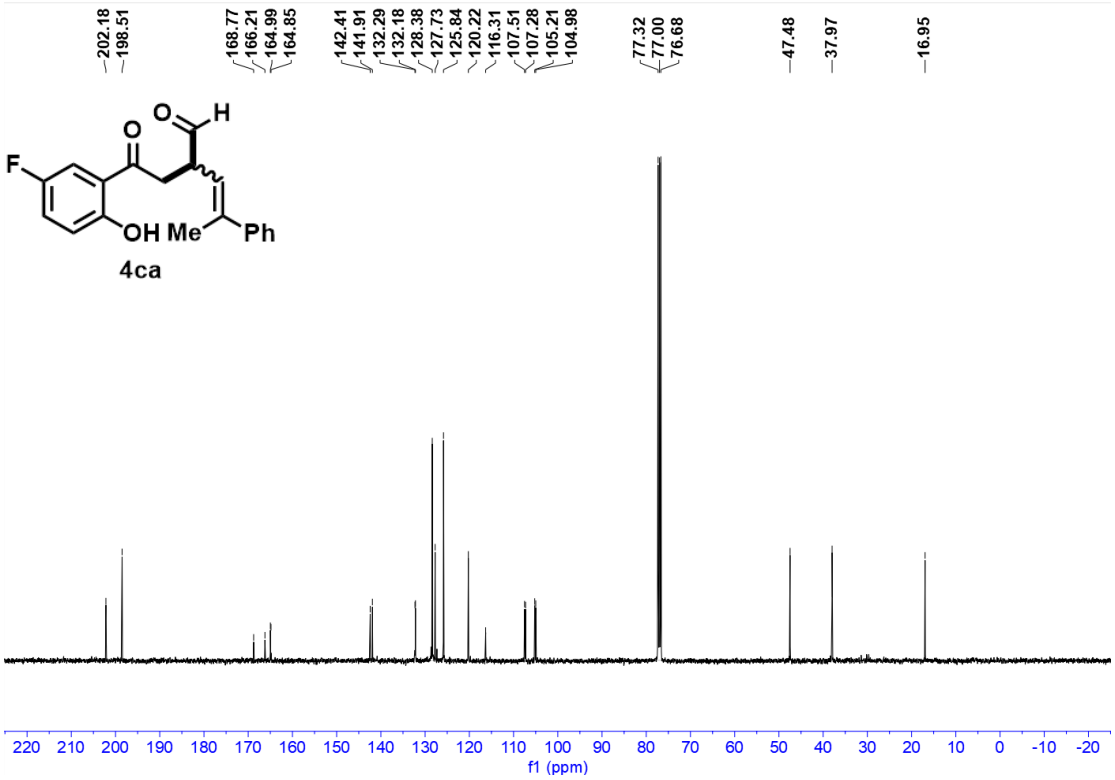
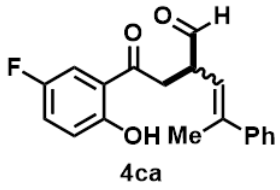
141.64
137.68
129.56
128.34
128.15
127.65
125.83
120.52
118.74
118.27
77.32
77.00
76.68
47.47
38.06
20.50
16.92
O
H
O
Me
OH Me
Ph
4ba
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

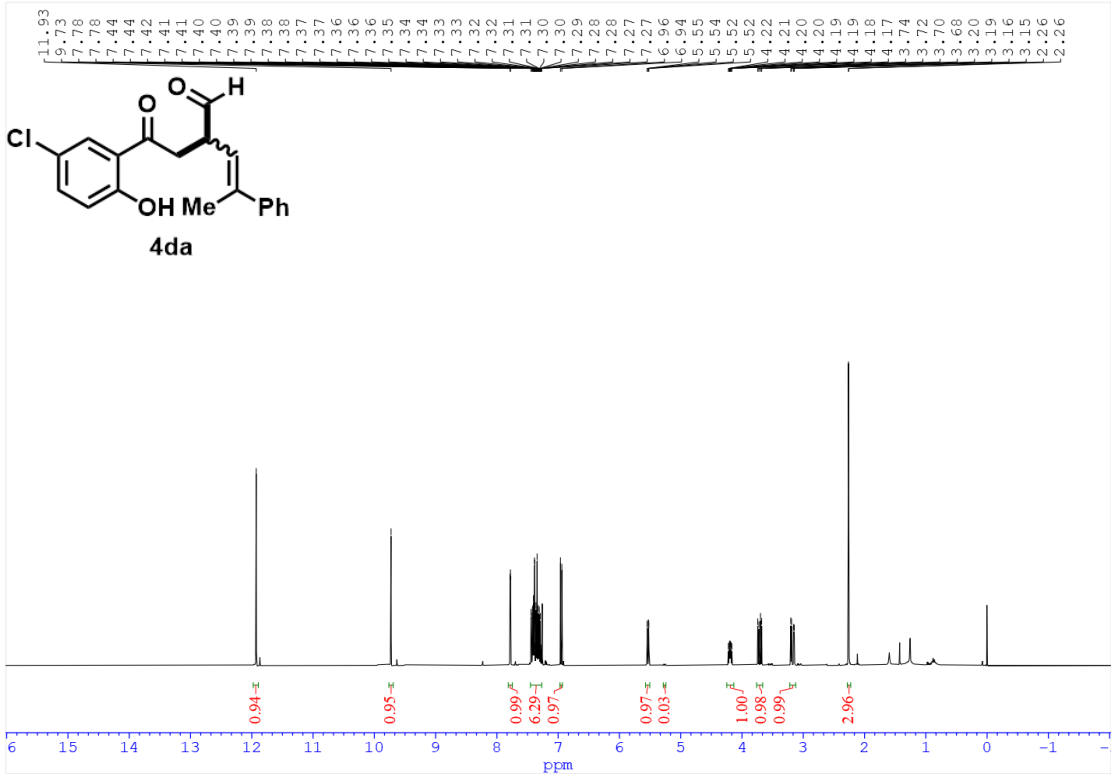

12.34 9.72 7.84 7.82 7.81 7.80 7.39 7.39 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.31 7.31 7.31 7.30 7.29 7.29 7.28 7.28 6.67 6.65 6.65 6.64 6.63 6.63 6.63 6.62 6.61 6.60 5.54 5.53 5.51 5.51 4.19 4.19 4.18 4.17 3.71 3.69 3.67 3.65 3.19 3.17 3.14 3.13 2.24 2.24
O
H
O
F
OH Me
Ph
4ca
0.90 0.03 0.92 0.03 0.97 0.04 5.31 1.96 0.96 0.03 0.95 0.98 0.05 0.99 0.04 2.94 0.16
6 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5
f1 (ppm)


202.18 198.51 168.77 166.21 164.99 164.85 142.41 141.91 132.29 132.18 128.38 127.73 125.84 120.22 116.31 107.51 107.28 105.21 104.98 77.32 77.00 76.68 47.48 37.97 16.95
O
H
O
F
OH Me
Ph
4ca
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


O
H
O
F
OH Me
Ph

4ca

-98.67
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
ppm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7.40
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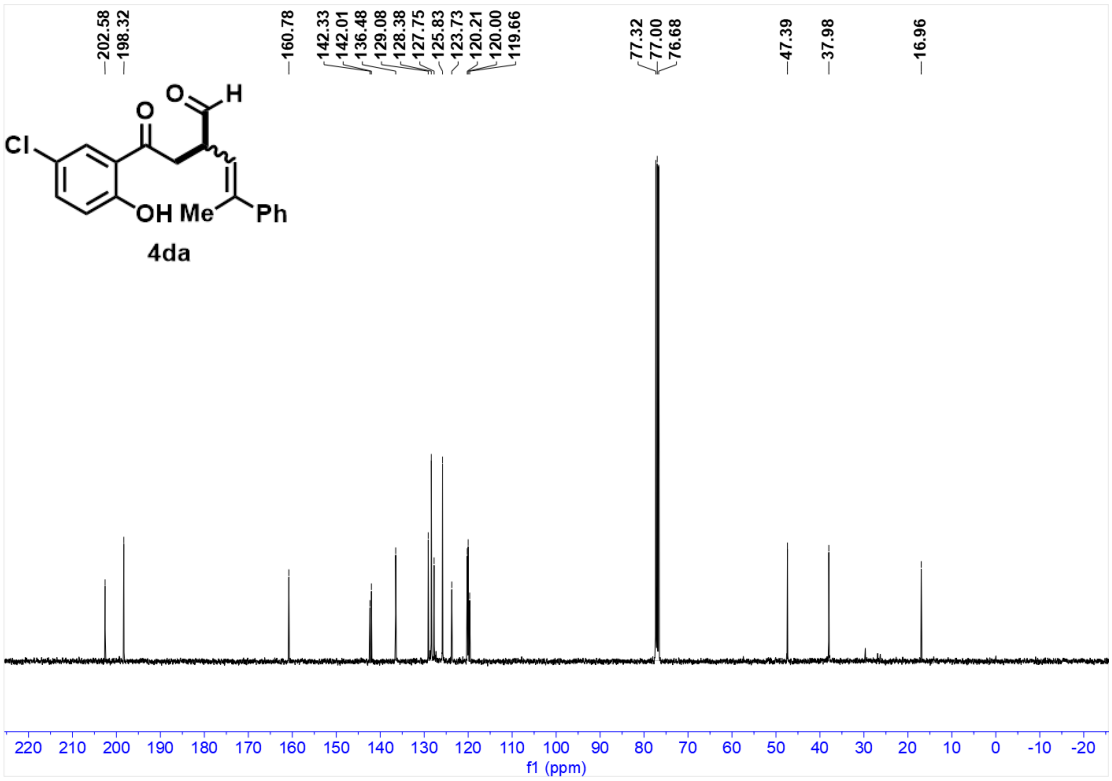
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.27
7.27
6.96
6.94
5.55
5.54
5.52
5.52
4.22
4.21
4.20
4.20
4.19
4.19
4.18
4.17
3.74
3.72
3.70
3.68
3.20
3.19
3.16
3.15
2.26
2.26
O
H
O
Cl
OH Me
Ph
0.94
0.95
0.99
6.29
0.97
0.97
0.03
1.00
0.98
0.99
2.96
6 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
ppm

4da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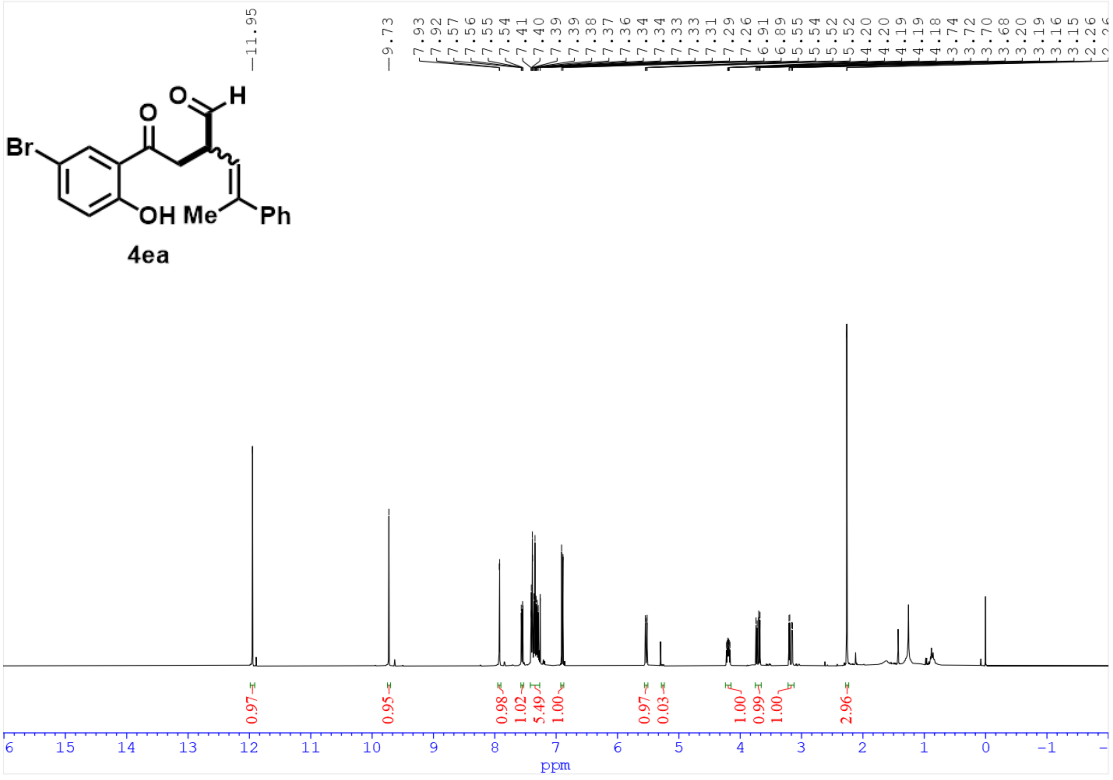
142.01
136.48
129.08
128.38
127.75
125.83
123.73
120.21
120.00
119.66
77.32
77.00
76.68
47.39
37.98
16.96
Cl
O
O
H
OH Me
Ph
4da
f1 (ppm)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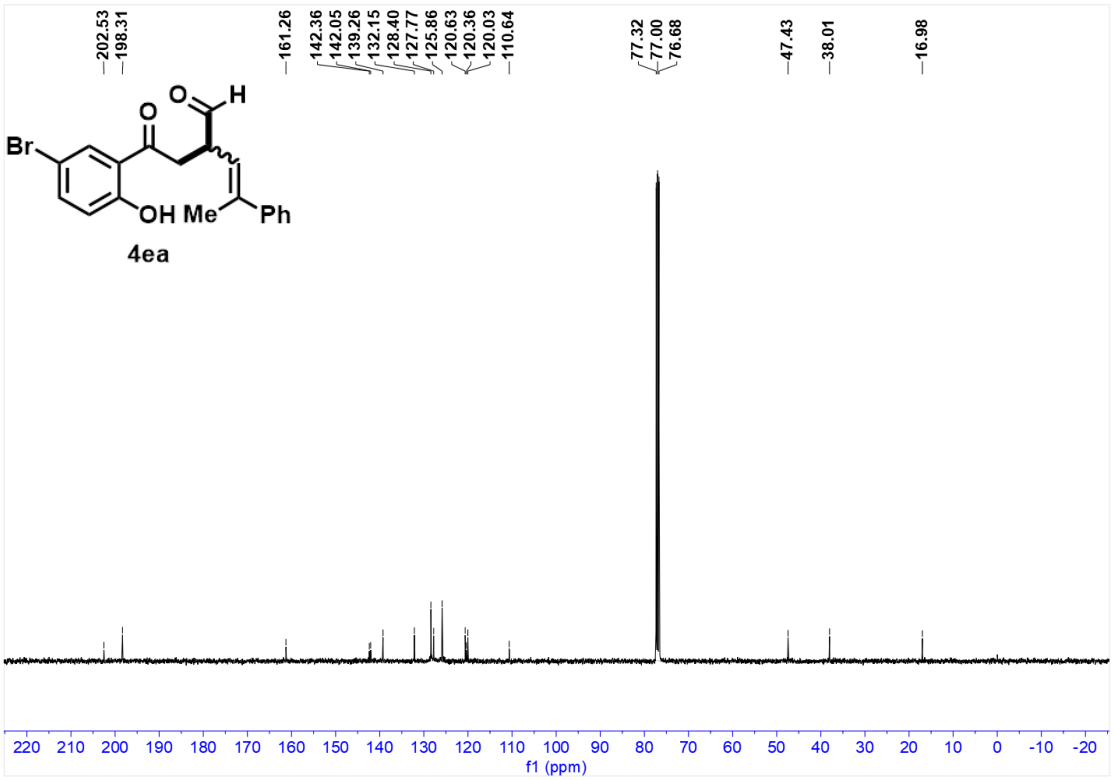
7.54
7.41
7.40
7.39
7.39
7.38
7.37
7.36
7.34
7.34
7.33
7.33
7.31
7.29
7.26
6.91
6.89
5.55
5.54
5.52
5.52
4.20
4.20
4.19
4.19
4.18
3.74
3.72
3.70
3.68
3.20
3.19
3.16
3.15
2.26
Br
O
O
H
OH Me
Ph
4ea
0.97
0.95
0.98
1.02
5.49
1.00
0.97
0.03
1.00
0.99
1.00
2.96
ppm


202.53
198.31
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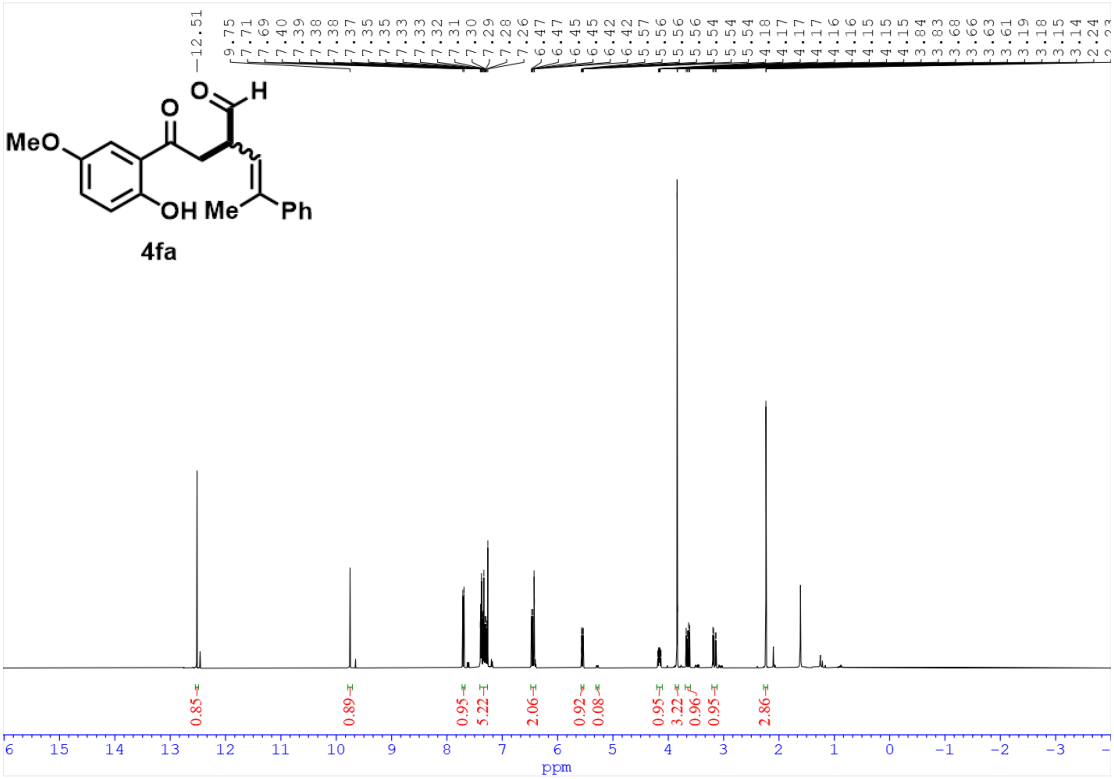
142.36
142.05
139.26
132.15
128.40
127.77
125.86
120.63
120.36
120.03
110.64
77.32
77.00
76.68
47.43
38.01
16.98
Br
O
H
OH Me
Ph
4ea
f1 (ppm)


12.51
9.75
7.71
7.69
7.40
7.39
7.38
7.38
7.37
7.35
7.35
7.33
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7.31
7.30
7.29
7.28
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6.47
6.45
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6.42
6.42
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5.56
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5.54
5.54
4.18
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4.17
4.17
4.16
4.16
4.15
4.15
4.15
3.84
3.83
3.68
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3.63
3.61
3.19
3.18
3.15
3.14
2.24
MeO
O
H
OH Me
Ph
4fa
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0.95
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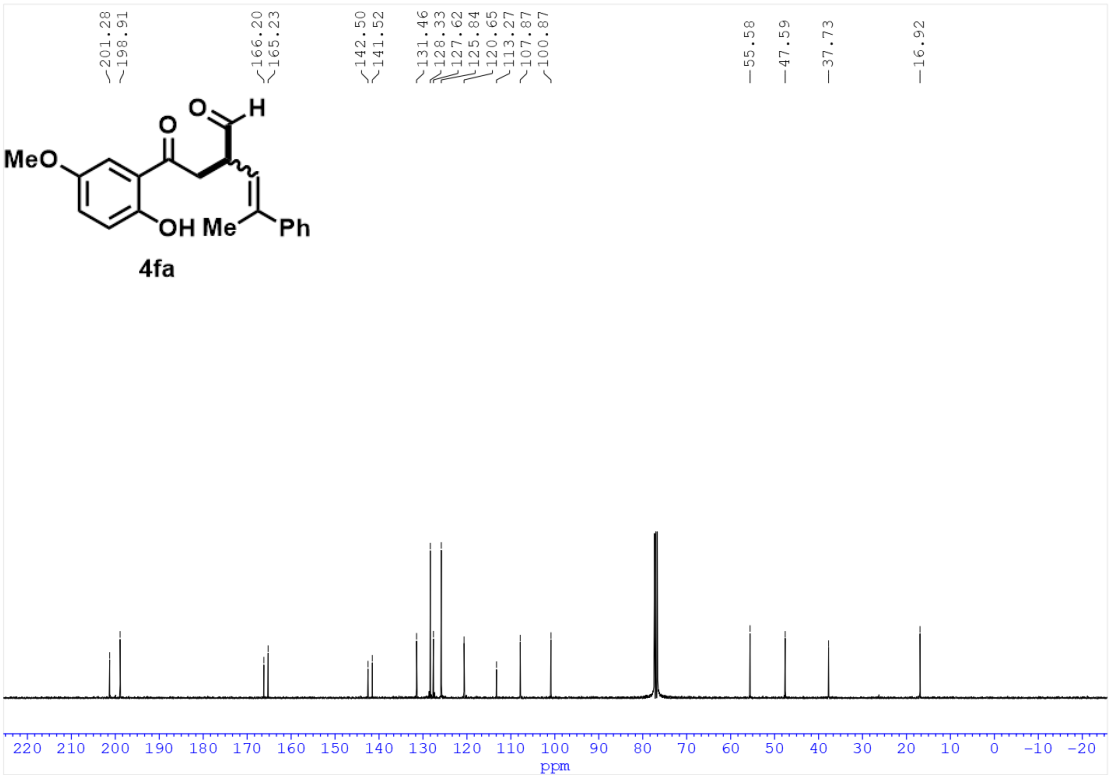
ppm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100.87
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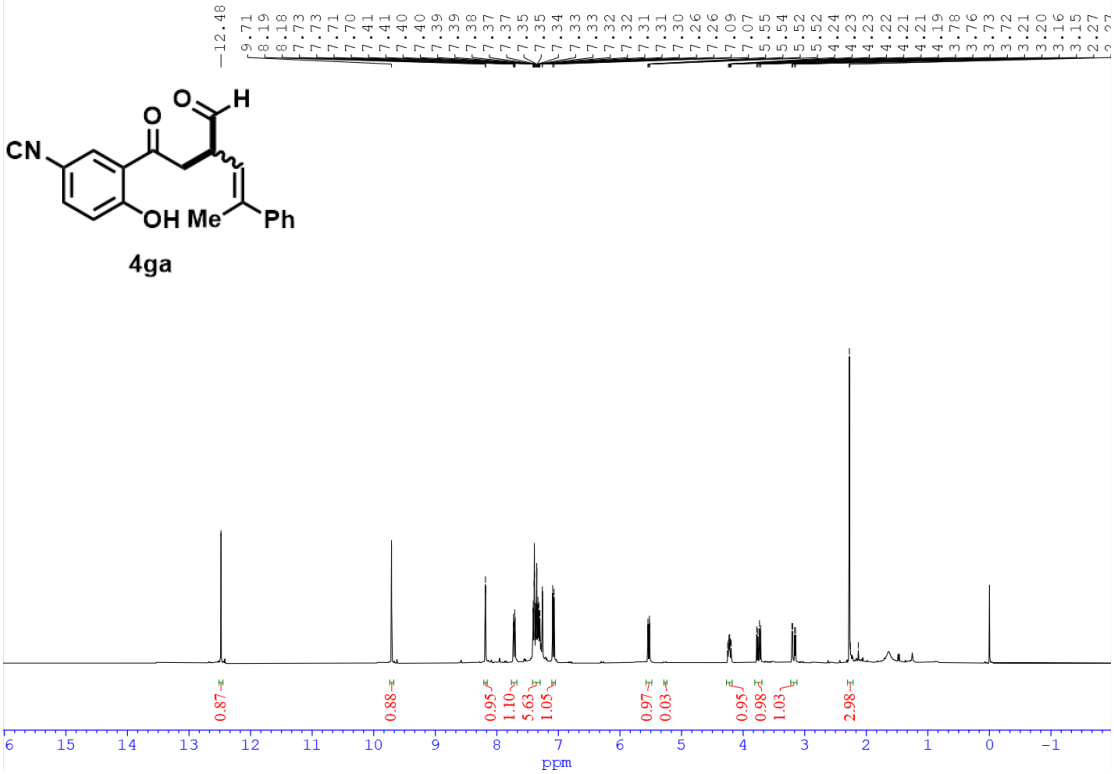
37.73
16.92
MeO
O
H
OH Me
Ph
4fa
ppm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7.39
7.39
7.38
7.37
7.37
7.35
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.26
7.26
7.09
7.07
5.55
5.54
5.52
5.52
4.24
4.23
4.22
4.21
4.21
4.19
3.78
3.76
3.73
3.72
3.21
3.20
3.16
3.15
2.27
CN
O
H
OH Me
Ph
4ga
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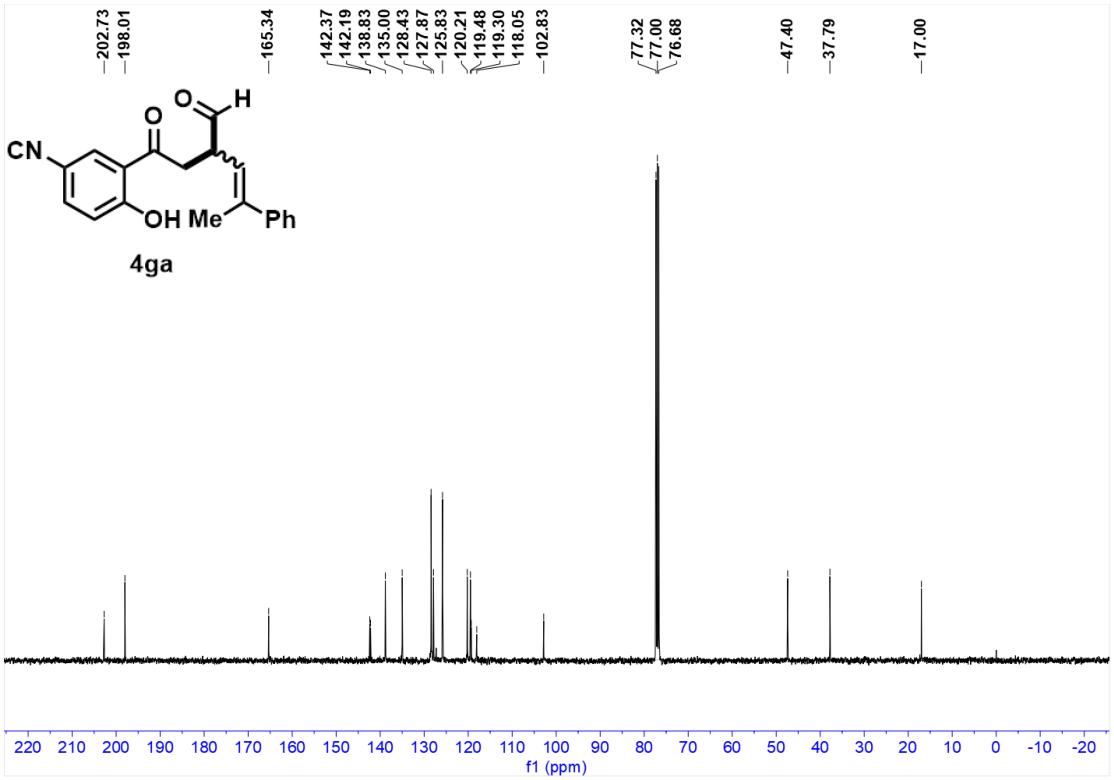
1.10
5.63
1.05
0.97
0.03
0.95
0.98
1.03
2.98
ppm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119.30
118.05
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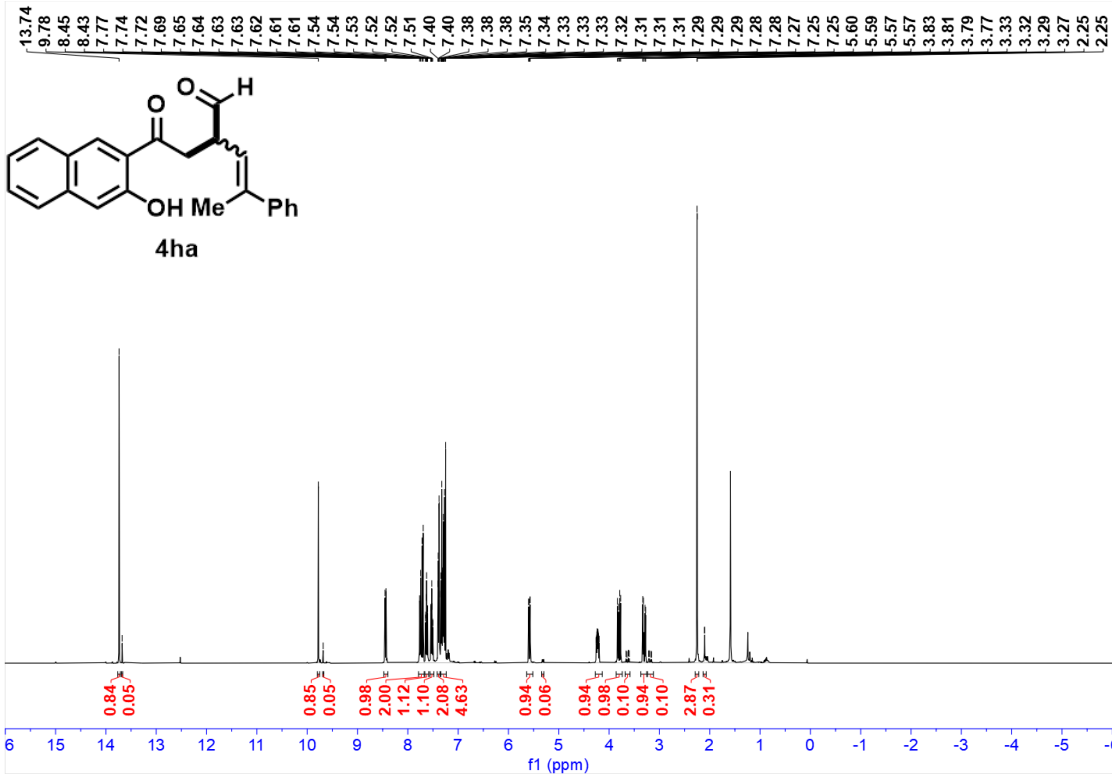
76.68
47.40
37.79
17.00
CN
O
H
OH Me
Ph
4ga
f1 (ppm)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7.61
7.61
7.54
7.54
7.53
7.52
7.52
7.51
7.40
7.40
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7.38
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7.33
7.33
7.33
7.32
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7.29
7.29
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7.25
7.25
5.60
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5.57
5.57
3.83
3.81
3.79
3.77
3.33
3.32
3.29
3.27
2.25
2.25
O
H
OH Me
Ph
4ha
0.84
0.05
0.85
0.05
0.98
2.00
1.12
1.10
2.08
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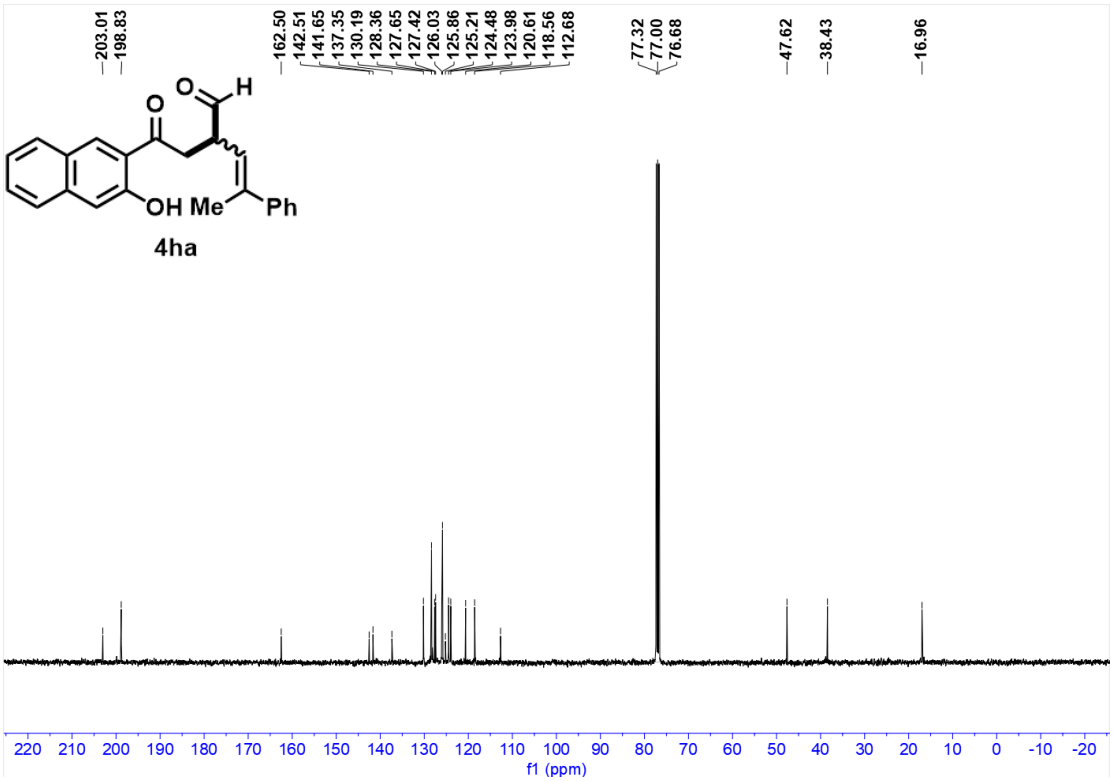
0.06
0.94
0.98
0.10
0.94
0.10
2.87
0.31
f1 (ppm)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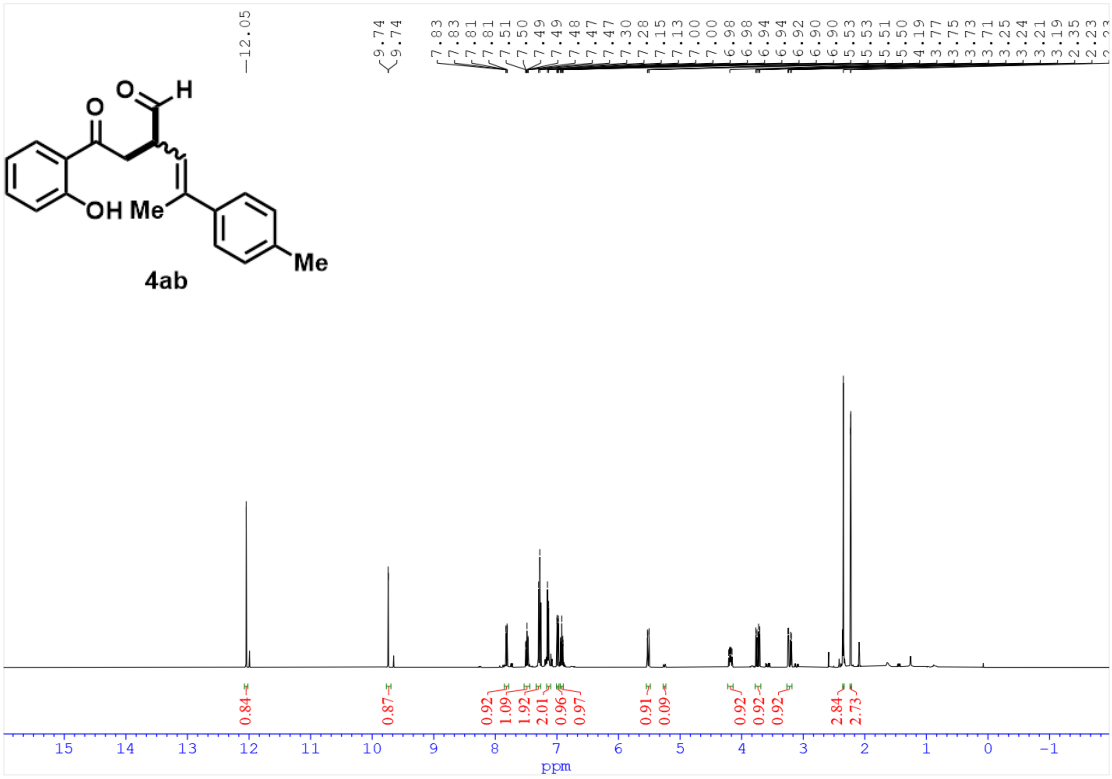
125.21
124.48
123.98
120.61
118.56
112.68
77.32
77.00
76.68
47.62
38.43
16.96
O
H
O
OH Me
Ph
4ha
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.48
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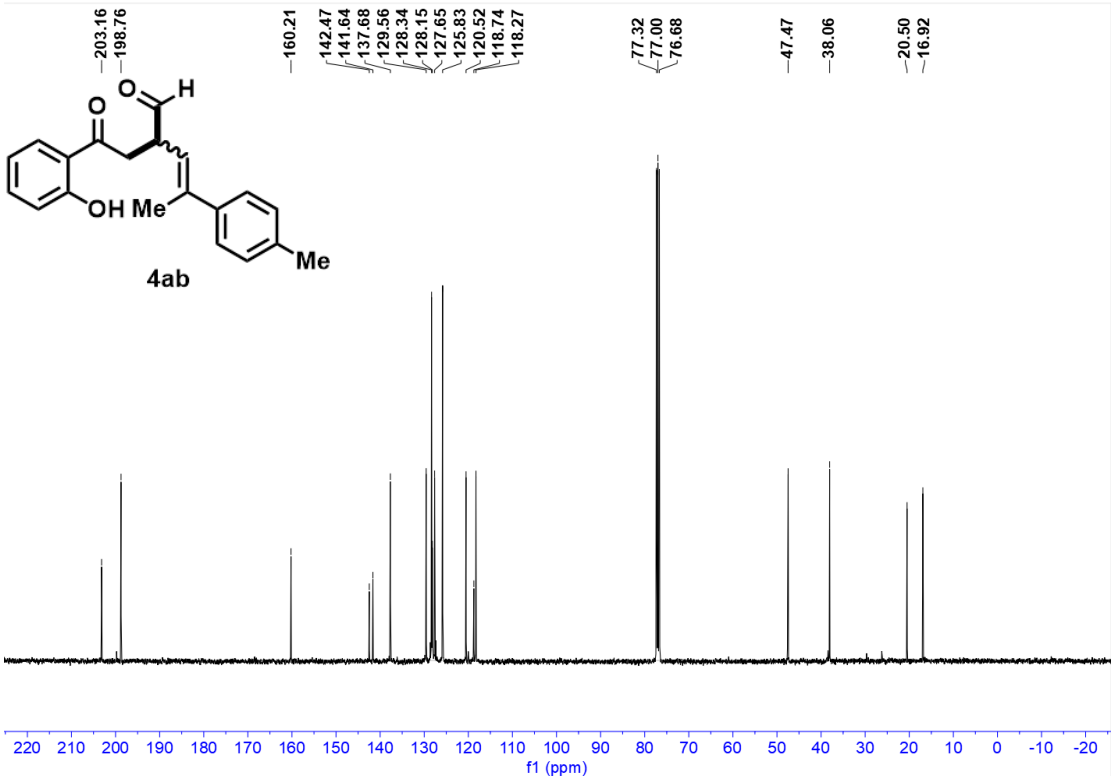
7.47
7.30
7.28
7.15
7.13
7.00
7.00
6.98
6.98
6.94
6.94
6.92
6.90
6.90
5.53
5.53
5.51
5.50
4.19
3.77
3.75
3.73
3.71
3.25
3.24
3.21
3.19
2.35
2.23
O
H
O
OH Me
Me
4ab
0.84
0.87
0.92
1.09
1.92
2.01
0.96
0.97
0.91
0.09
0.92
0.92
0.92
2.84
2.73
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
ppm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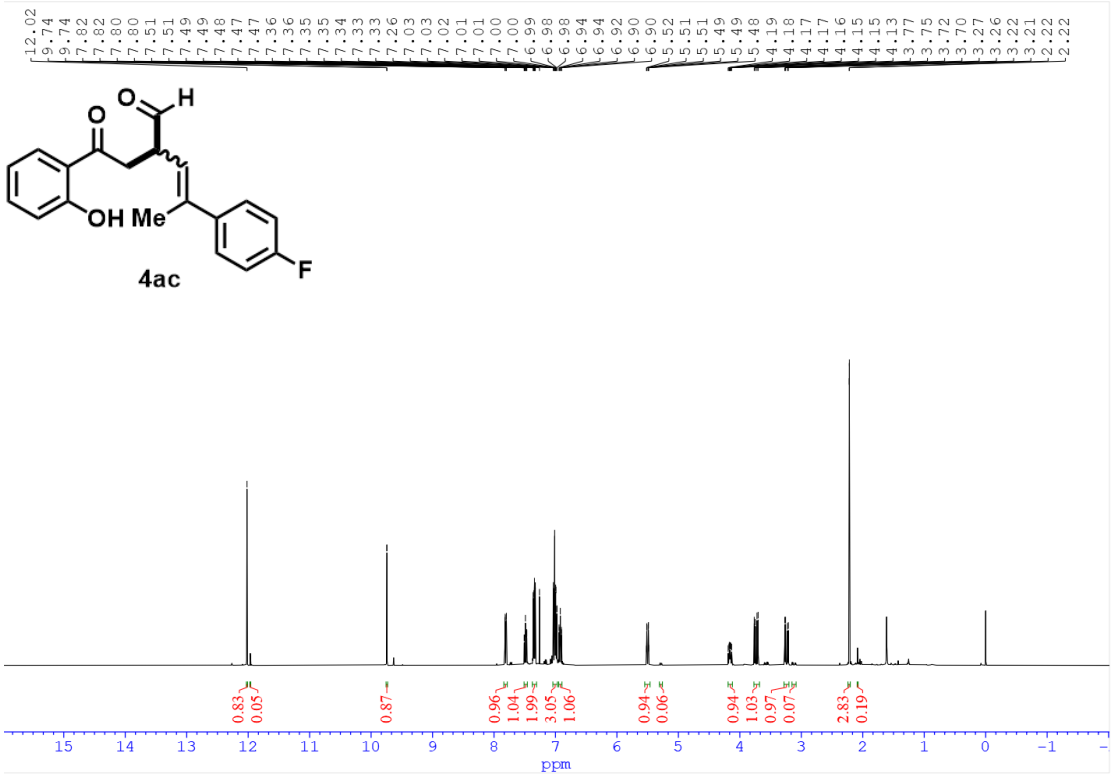
128.15
127.65
125.83
120.52
118.74
118.27
77.32
77.00
76.68
47.47
38.06
20.50
16.92
O
H
O
OH Me
Me
4ab
f1 (ppm)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7.47
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.26
7.03
7.03
7.02
7.01
7.01
7.00
7.00
6.99
6.98
6.98
6.94
6.94
6.92
6.90
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5.52
5.51
5.51
5.49
5.49
5.48
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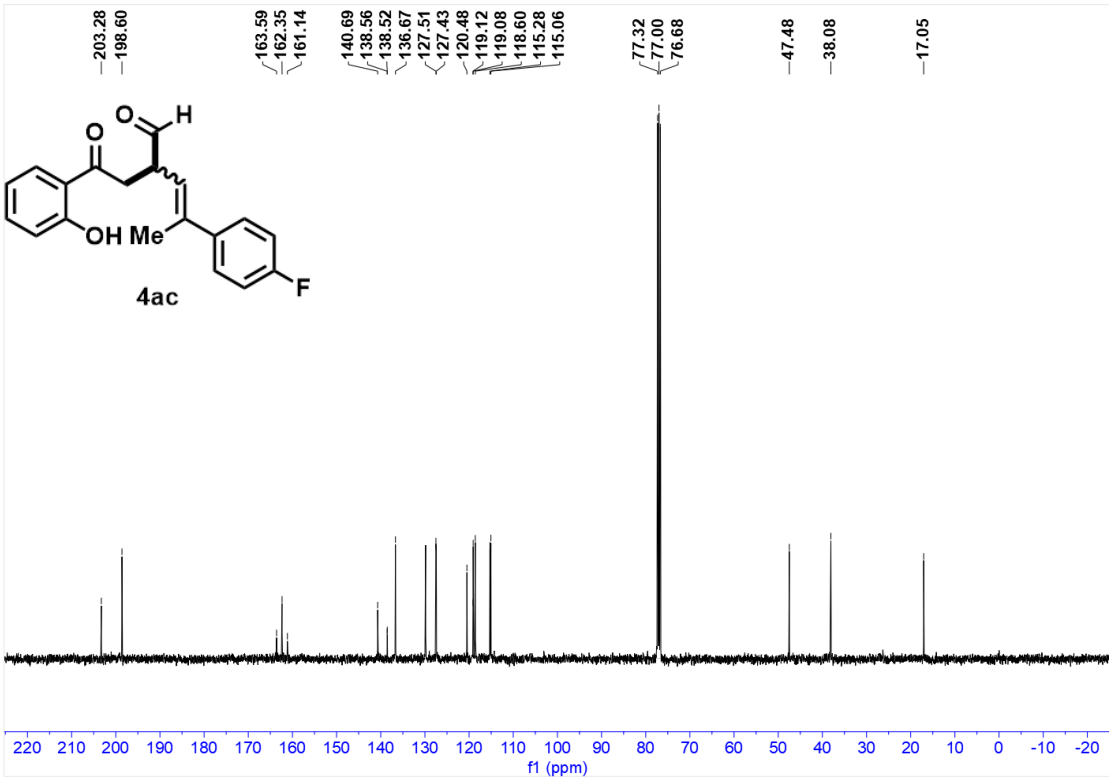
4.18
4.17
4.17
4.16
4.15
4.15
4.13
3.77
3.75
3.72
3.70
3.27
3.26
3.22
3.21
2.22
2.22
O
H
O
OH Me
F
4ac
0.83
0.05
0.87
0.96
1.04
1.99
3.05
1.06
0.94
0.06
0.94
1.03
0.97
0.07
2.83
0.19
ppm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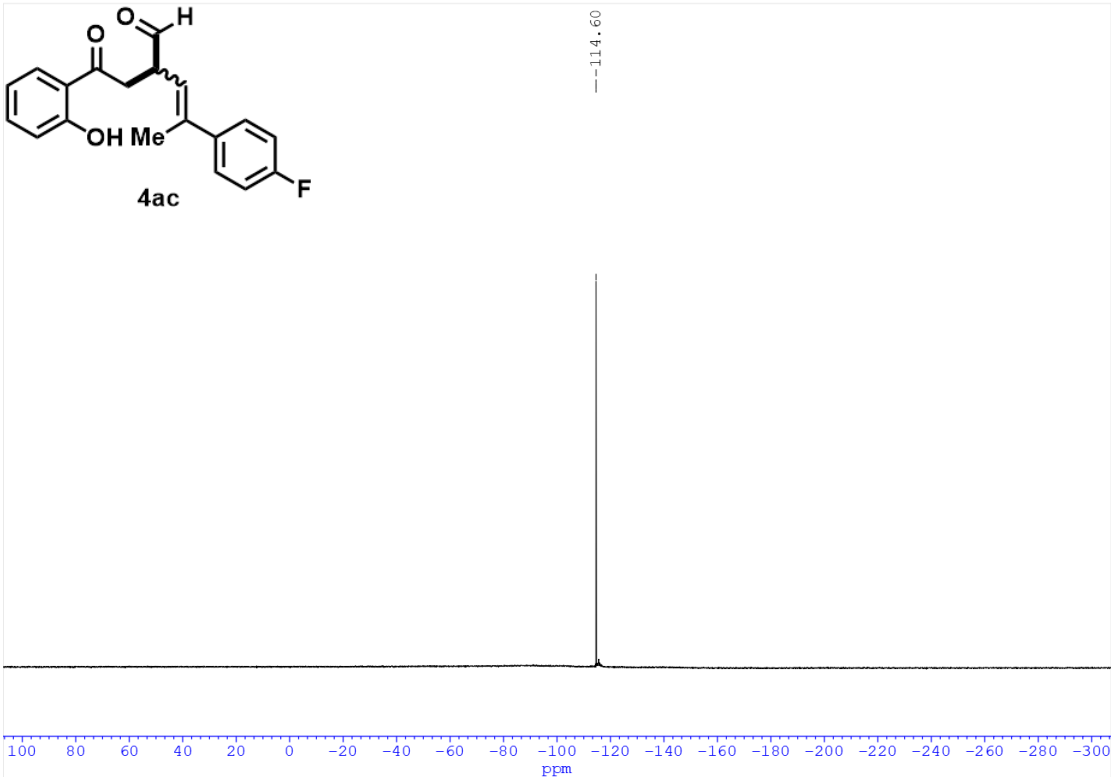
127.43
120.48
119.12
119.08
118.60
115.28
115.06
77.32
77.00
76.68
47.48
38.08
17.05
O
H
O
OH Me
F
4ac
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


O
H
O
OH Me
F
4ac
-114.60
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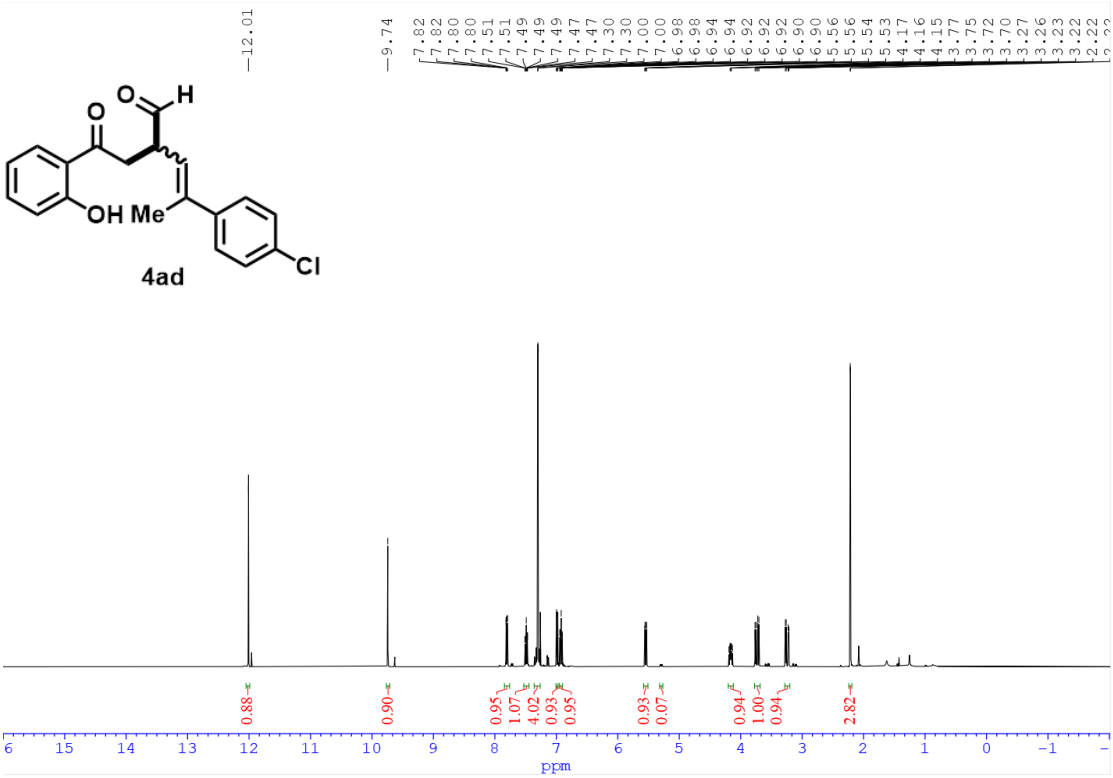
ppm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7.82
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7.80
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7.51
7.49
7.49
7.49
7.49
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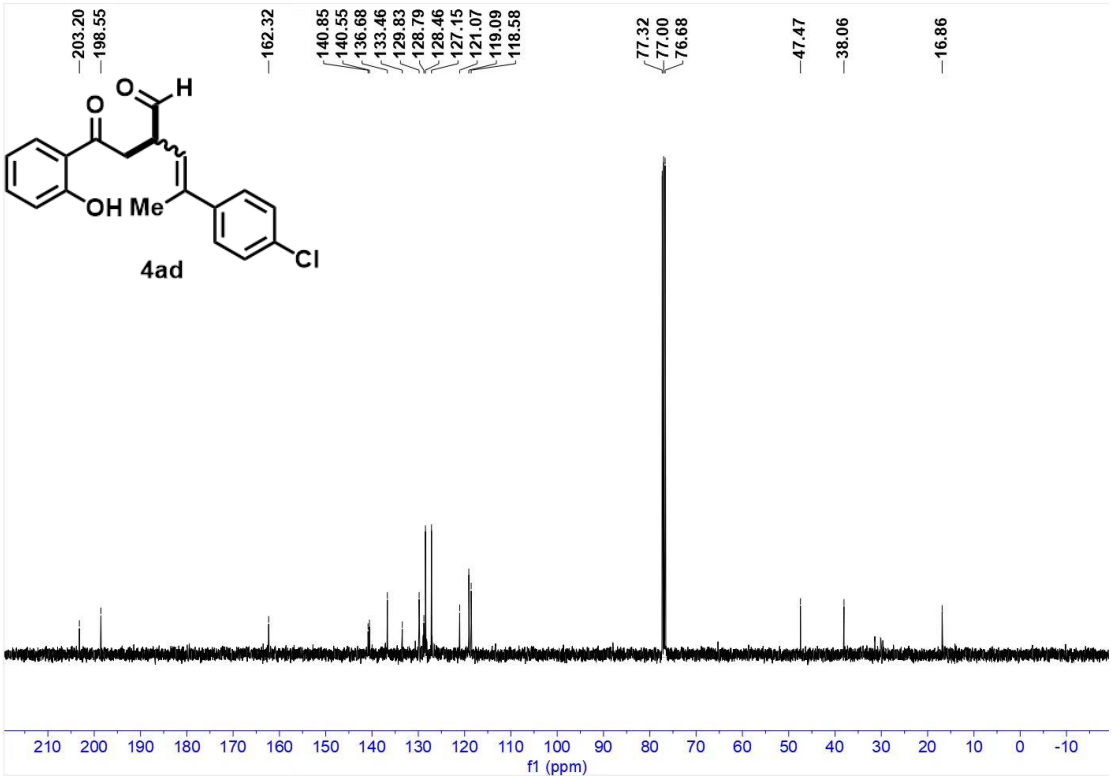
7.47
7.30
7.30
7.00
7.00
6.98
6.98
6.94
6.94
6.92
6.92
6.90
6.90
5.56
5.56
5.54
5.53
4.17
4.16
4.15
3.77
3.75
3.72
3.70
3.27
3.26
3.23
3.22
2.22
O
H
O
OH Me
Cl
4ad
0.88
0.90
0.95
1.07
4.02
0.93
0.95
0.93
0.07
0.94
1.00
0.94
2.82
ppm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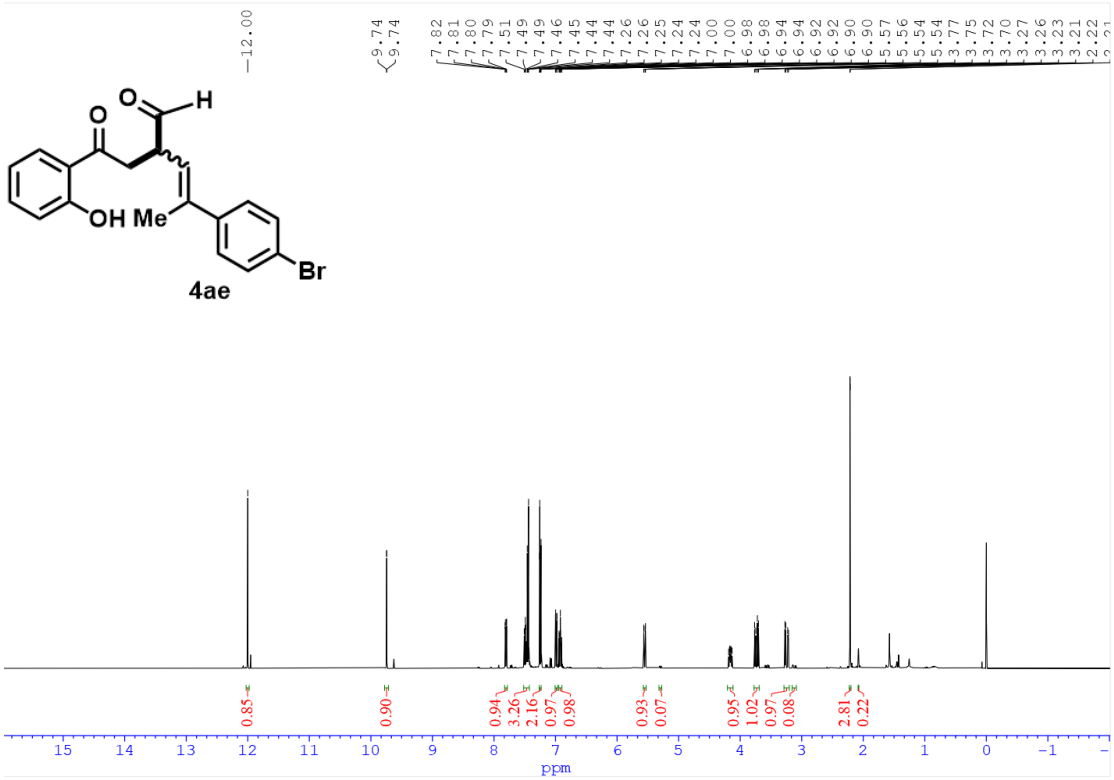
128.46
127.15
121.07
119.09
118.58
77.32
77.00
76.68
47.47
38.06
16.86
O
H
O
OH Me
Cl
4ad
f1 (ppm)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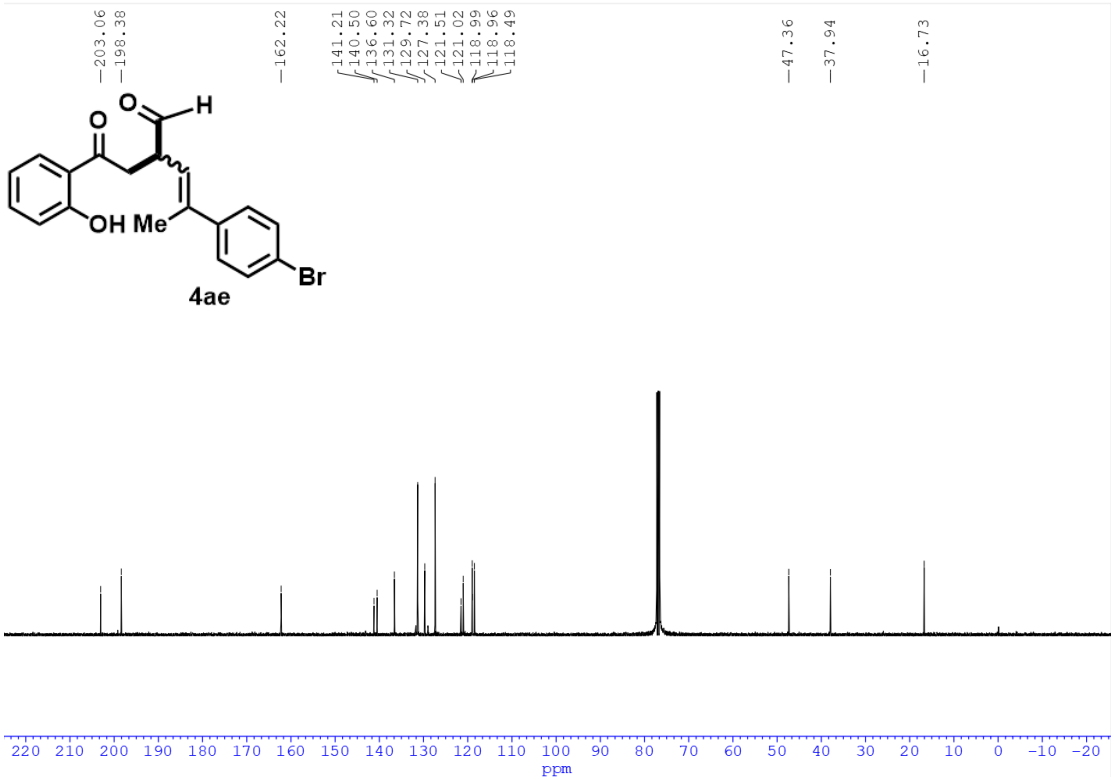
7.49
7.46
7.45
7.44
7.44
7.26
7.26
7.25
7.24
7.24
7.00
7.00
6.98
6.98
6.94
6.94
6.92
6.92
6.90
6.90
5.57
5.56
5.54
5.54
3.77
3.75
3.72
3.70
3.27
3.26
3.23
3.21
2.22
O
H
O
OH Me
Br
4ae
0.85
0.90
0.94
3.26
2.16
0.97
0.98
0.93
0.07
0.95
1.02
0.97
0.08
2.81
0.22
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
ppm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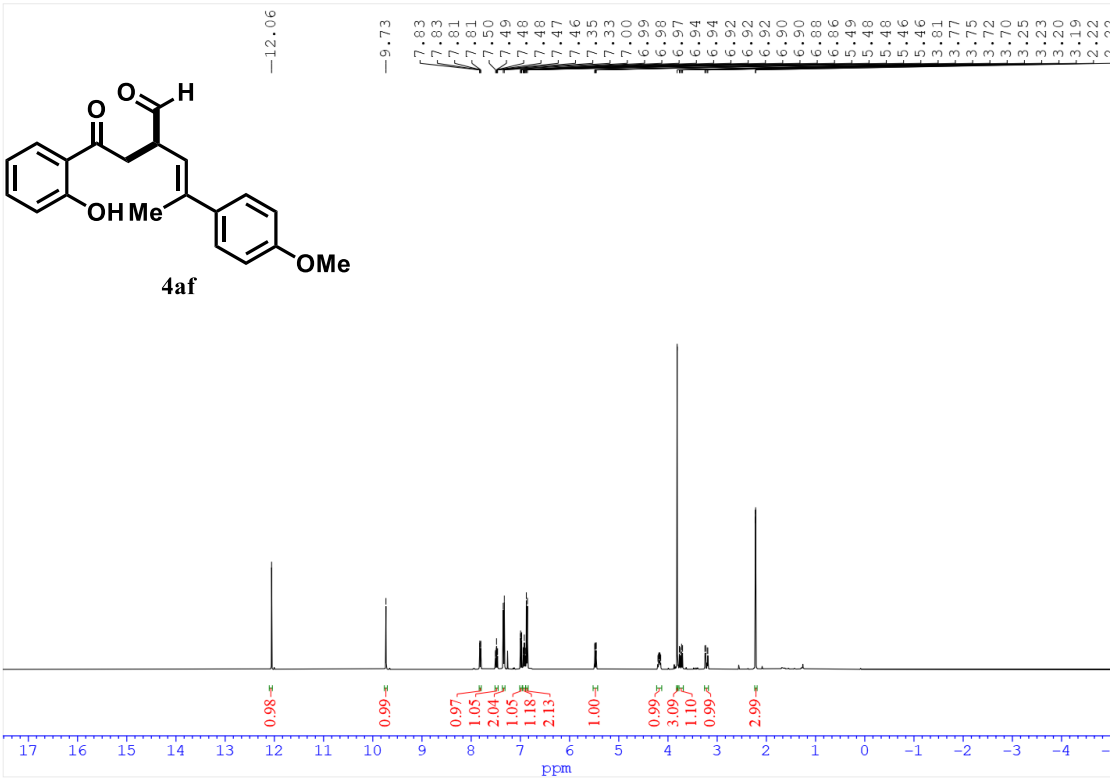
121.51
121.02
118.99
118.96
118.49
47.36
37.94
16.73
O
H
O
OH Me
Br
4ae
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
ppm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7.47
7.46
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7.33
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6.94
6.92
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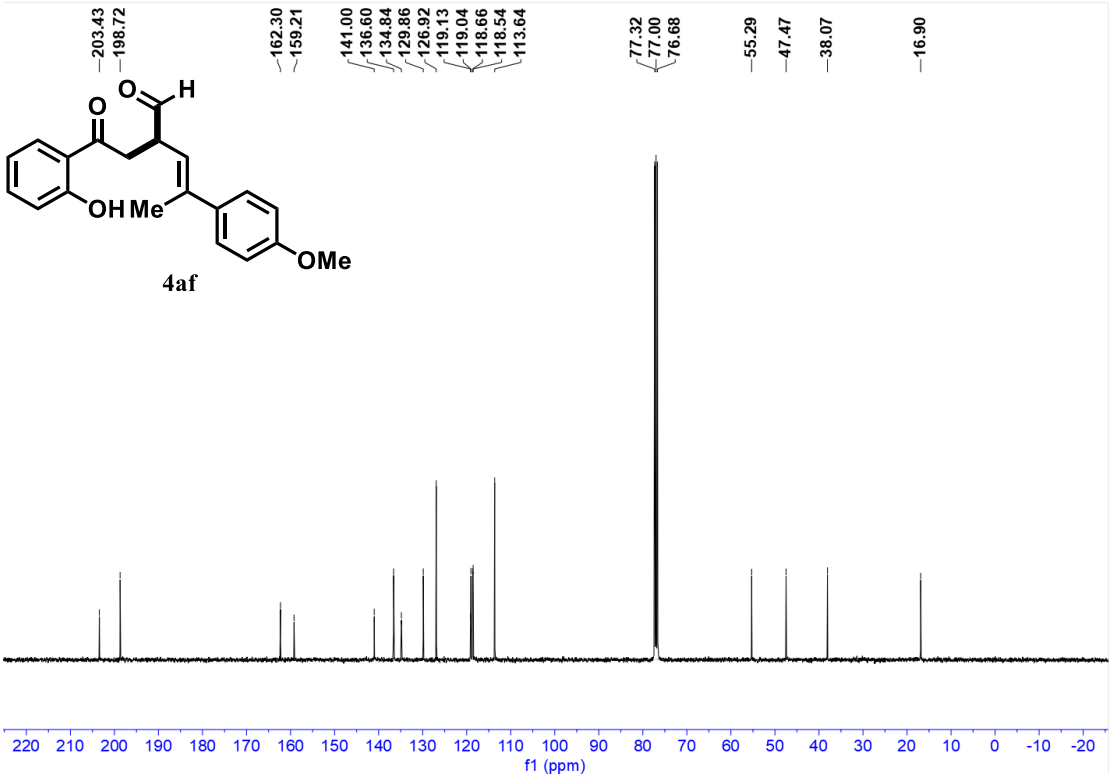
3.70
3.25
3.23
3.20
3.19
2.22
O
H
O
OH
Me
OMe
4af
0.98
0.99
0.97
1.05
2.04
1.05
1.18
2.13
1.00
0.99
3.09
1.10
0.99
2.99
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3 −4
ppm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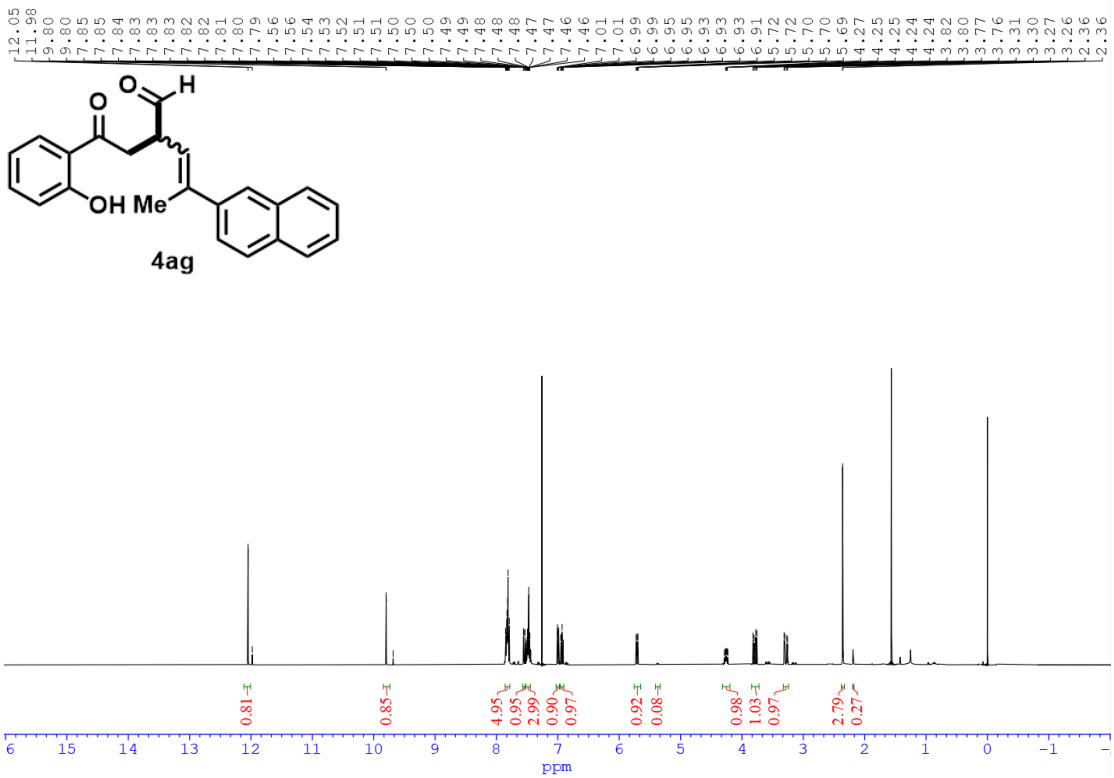
119.13
119.04
118.66
118.54
113.64
77.32
77.00
76.68
55.29
47.47
38.07
16.90
O
H
O
OH
Me
OMe
4af
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.83
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7.82
7.81
7.80
7.79
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7.54
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7.51
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7.50
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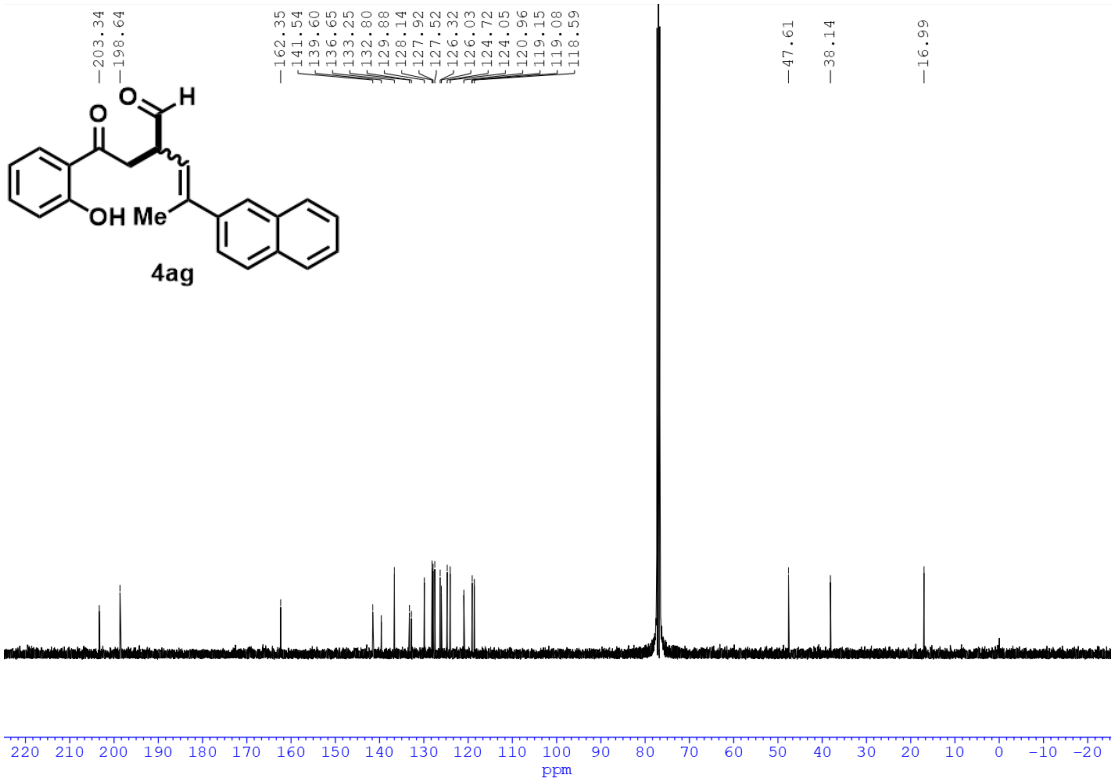
6.99
6.95
6.95
6.93
6.93
6.93
6.91
5.72
5.72
5.70
5.70
5.69
4.27
4.25
4.25
4.24
4.24
3.82
3.80
3.77
3.76
3.31
3.30
3.27
3.26
2.36
2.36
O
H
O
OH Me
4ag
0.81
0.85
4.95
0.95
2.99
0.90
0.97
0.92
0.08
0.98
1.03
0.97
2.79
0.27
6 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
ppm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132.80
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128.14
127.92
127.52
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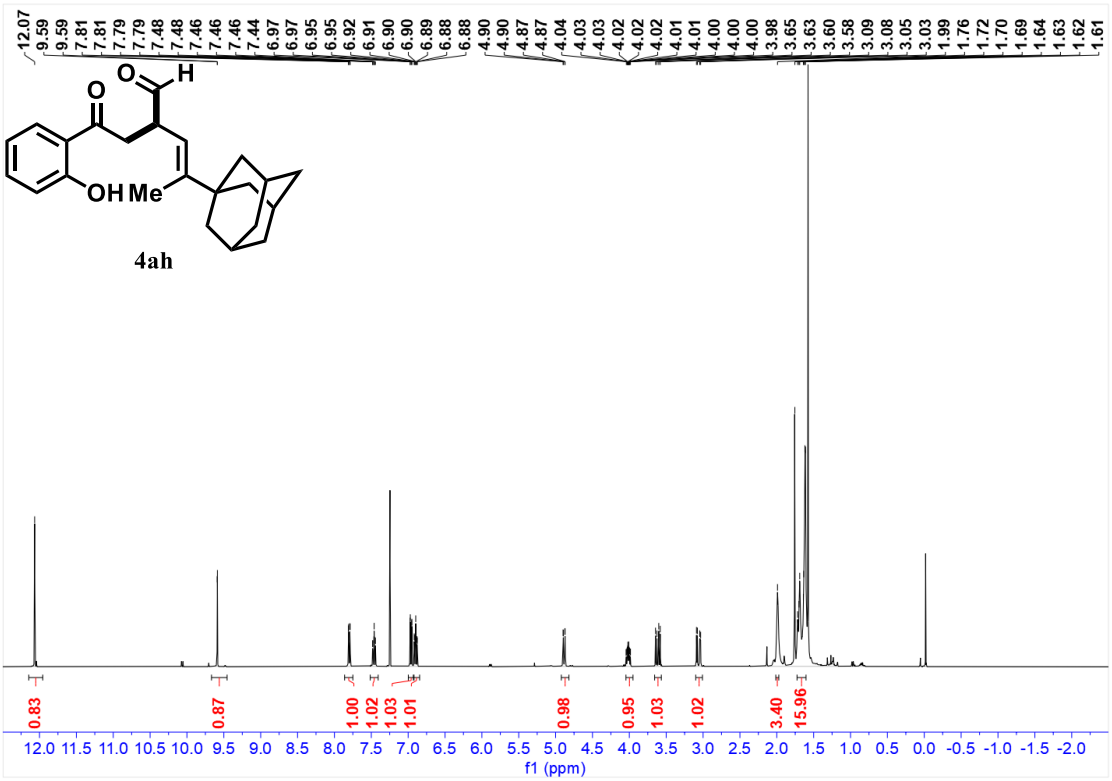
126.03
124.72
124.05
120.96
119.15
119.08
118.59
47.61
38.14
16.99
O
H
O
OH Me
4ag
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
ppm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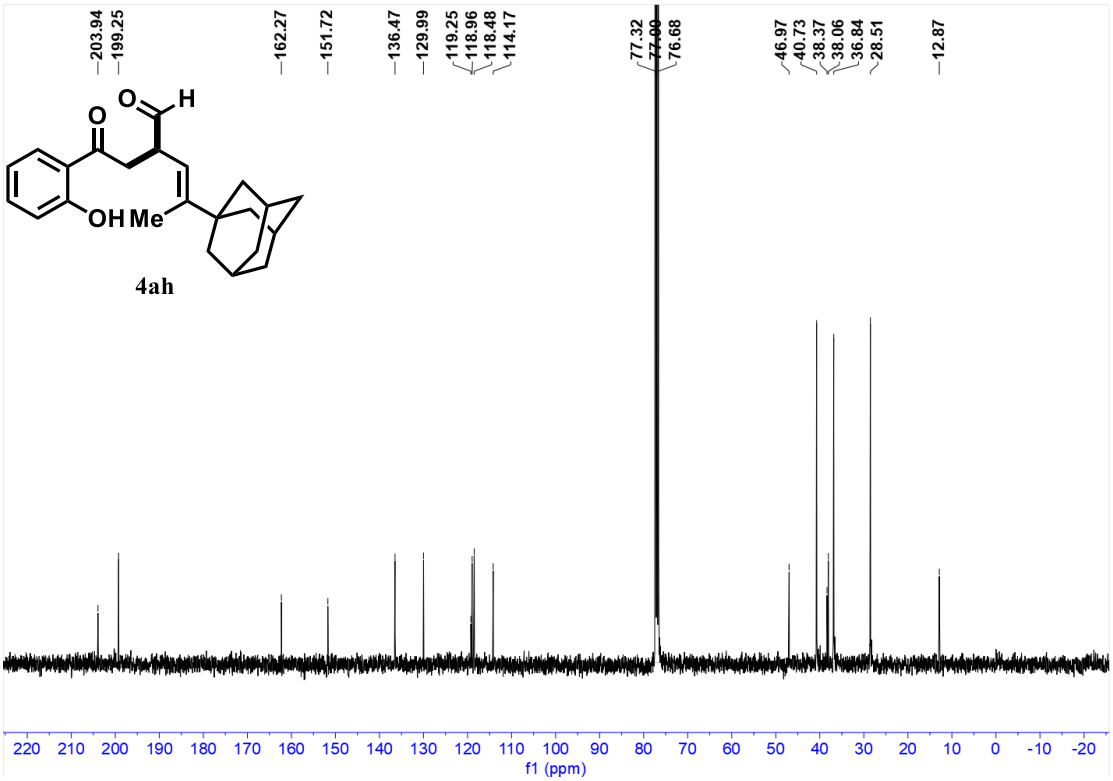
O
H
O
OH Me
4ah
0.83 0.87 1.00 1.02 1.03 1.01 0.98 0.95 1.03 1.02 3.40 15.96
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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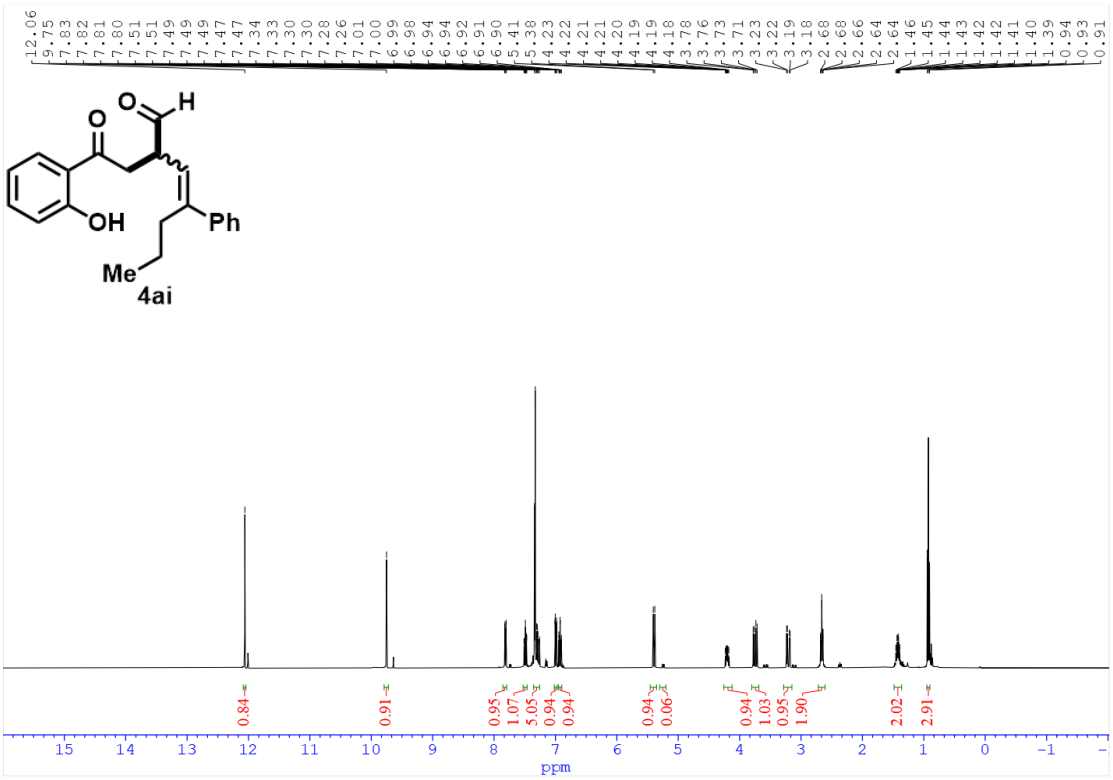
O
H
O
OH Me
4ah
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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7.47
7.34
7.33
7.30
7.30
7.28
7.26
7.01
7.00
6.99
6.98
6.94
6.94
6.92
6.91
6.90
5.41
5.38
4.23
4.22
4.21
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4.20
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4.19
4.18
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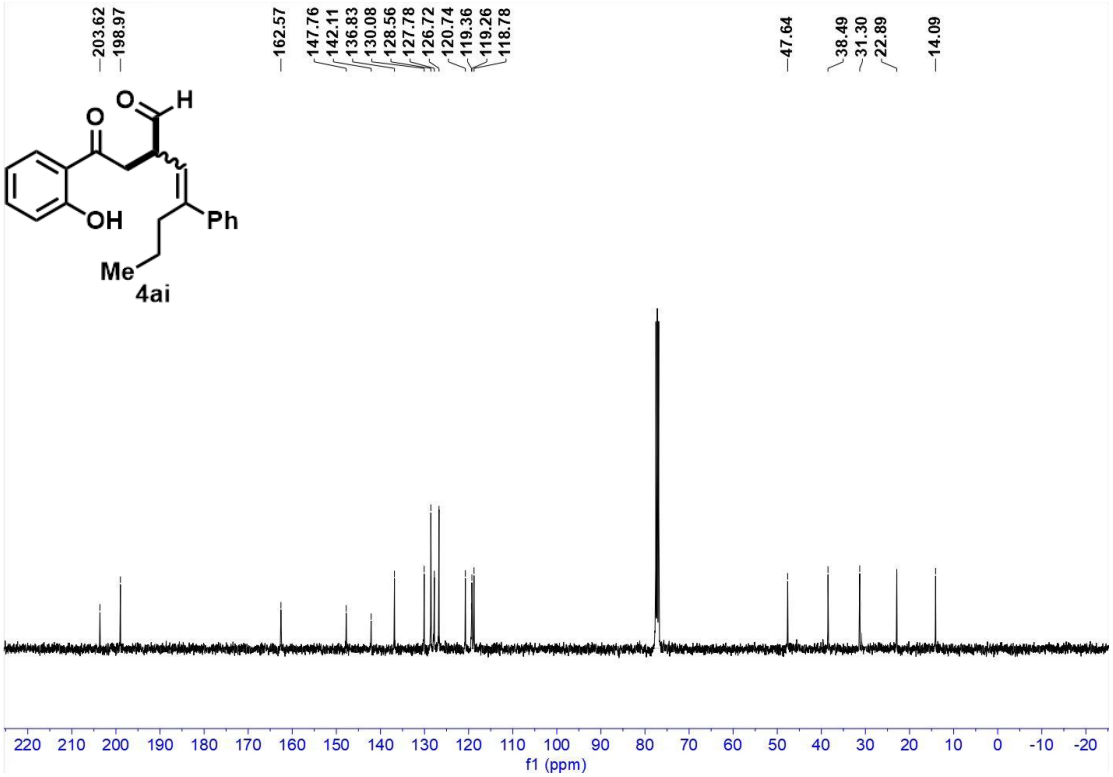
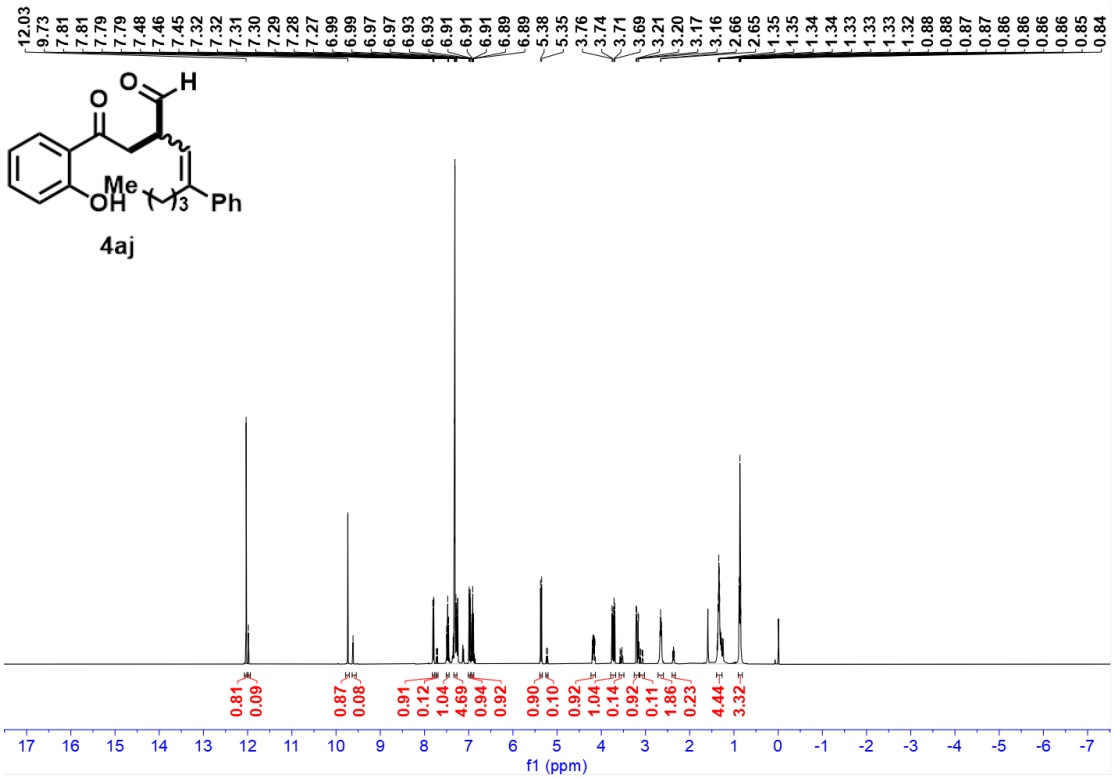
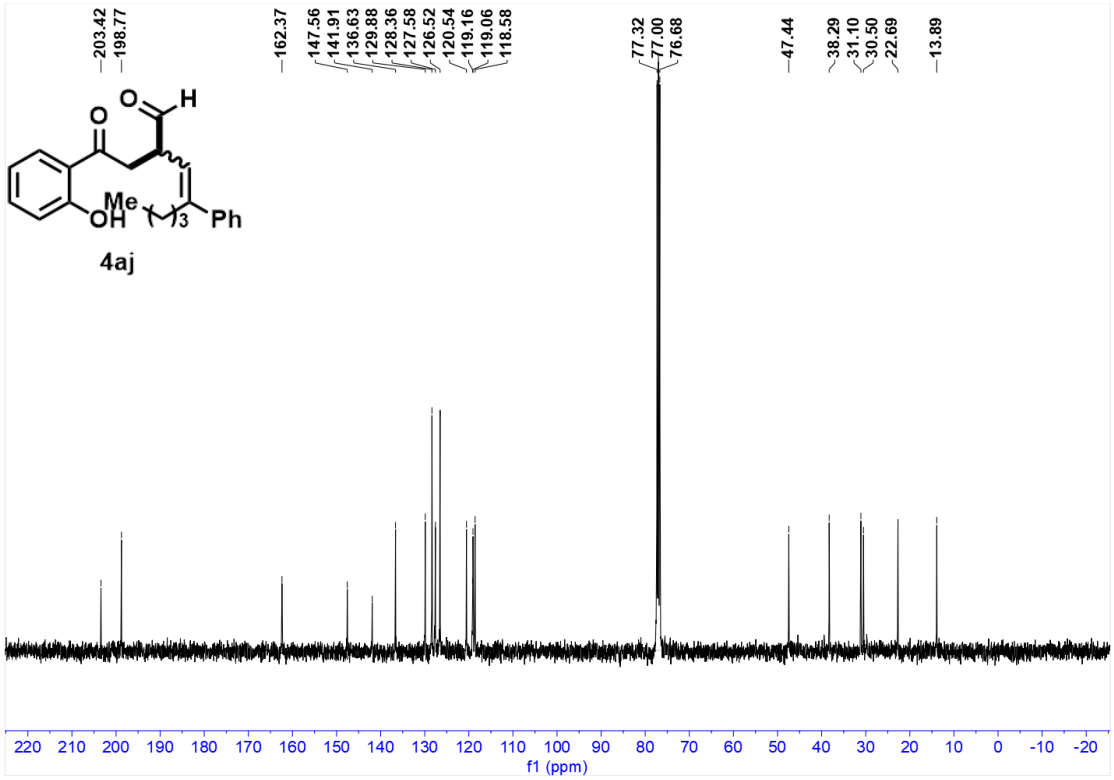
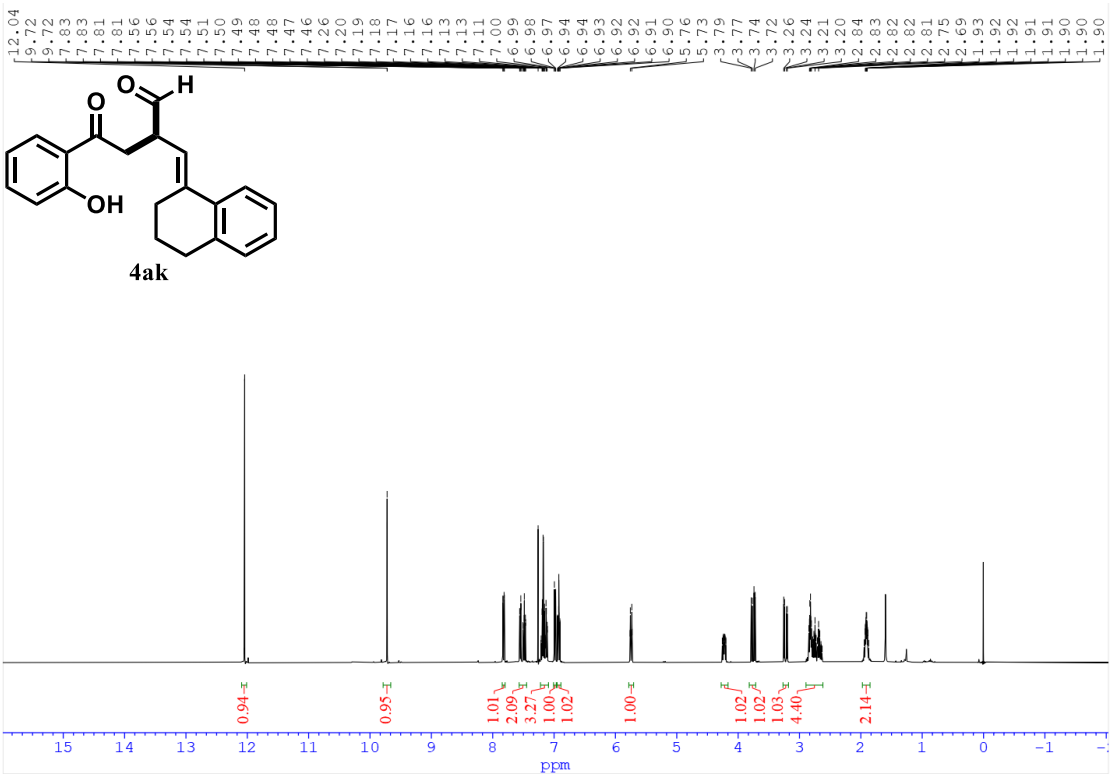
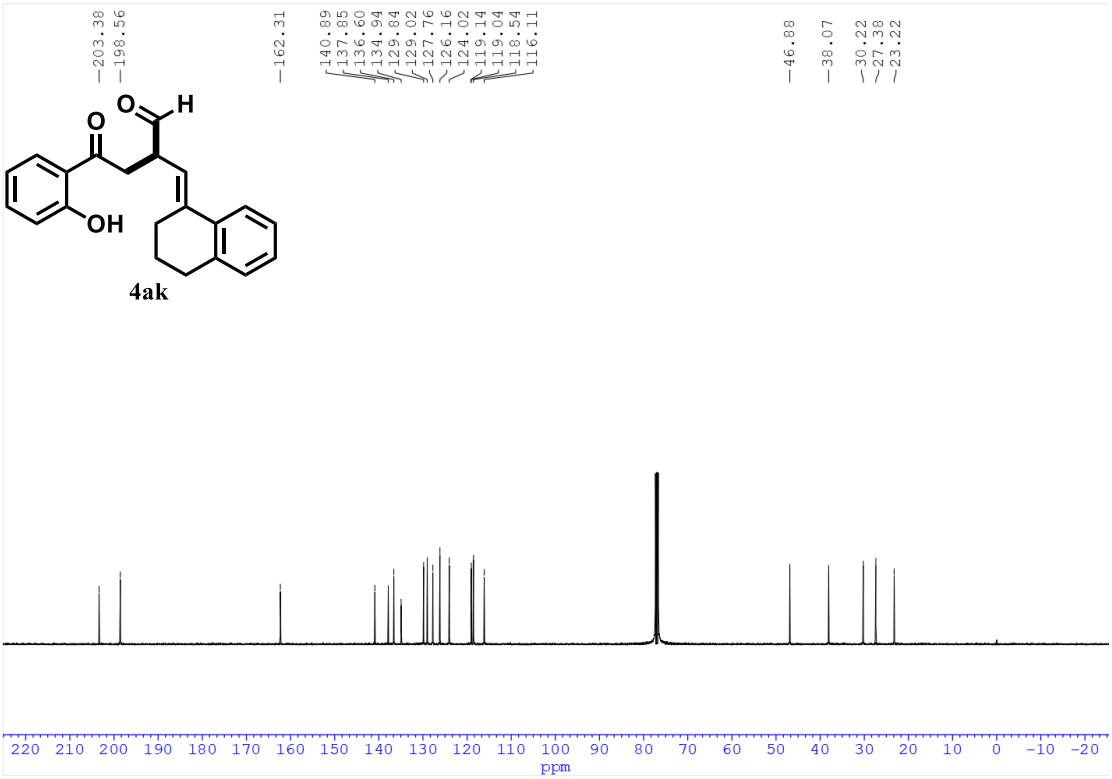
3.76
3.73
3.71
3.23
3.22
3.19
3.18
2.68
2.68
2.66
2.64
2.64
1.46
1.45
1.44
1.43
1.42
1.42
1.41
1.40
1.39
0.94
0.93
0.91
O
H
O
OH
Ph
Me
4ai
0.84
0.91
0.95
1.07
5.05
0.94
0.94
0.94
0.06
0.94
1.03
0.95
1.90
2.02
2.91
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm


203.62
198.97
162.57
147.76
142.11
136.83
130.08
128.56
127.78
126.72
120.74
119.36
119.26
118.78
47.64
38.49
31.30
22.89
14.09
O
H
O
OH
Ph
Me
4ai
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

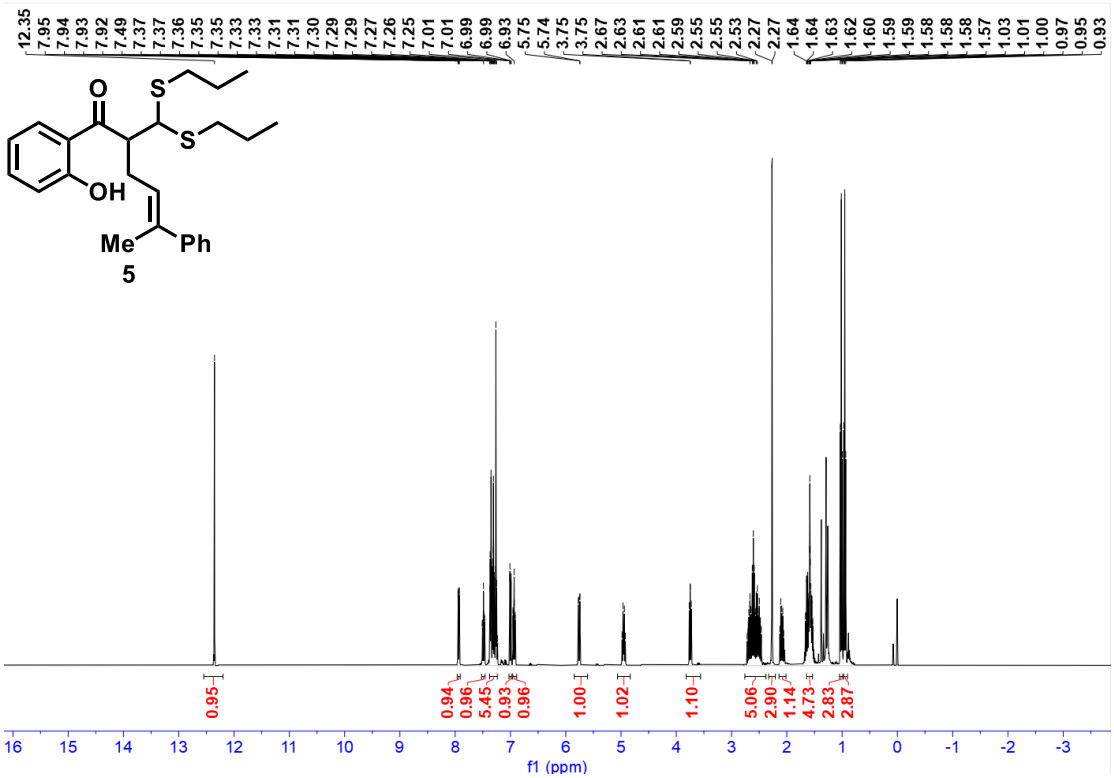

12.03
9.73
7.81
7.81
7.79
7.79
7.48
7.46
7.45
7.32
7.32
7.31
7.30
7.29
7.28
7.27
6.99
6.99
6.97
6.97
6.93
6.93
6.91
6.91
6.91
6.89
6.89
5.38
5.35
3.76
3.74
3.71
3.69
3.21
3.20
3.17
3.16
2.66
2.65
1.35
1.35
1.34
1.34
1.33
1.33
1.33
1.32
0.88
0.88
0.87
0.87
0.86
0.86
0.86
0.86
0.85
0.84
O
H
O
Me
OH
3
Ph
4aj
0.81
0.09
0.87
0.08
0.91
0.12
1.04
4.69
0.94
0.92
0.90
0.10
0.92
1.04
0.14
0.92
0.11
1.86
0.23
4.44
3.32
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6 -7
f1 (ppm)

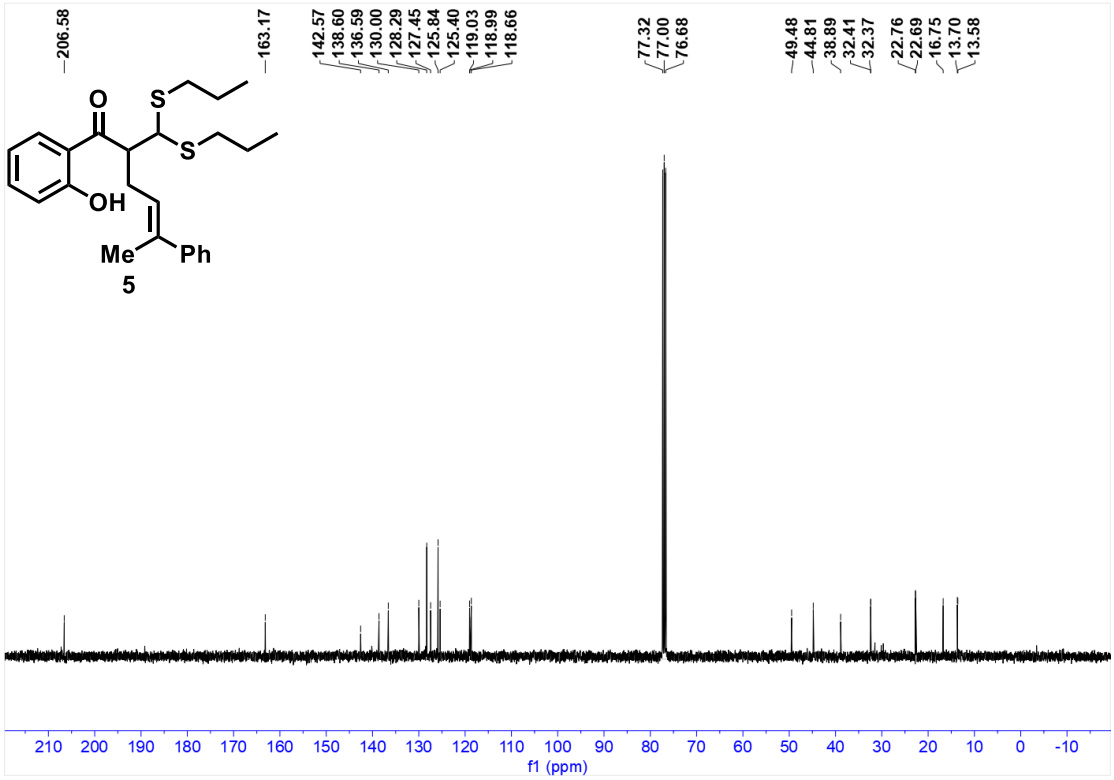

203.42
198.77
162.37
147.56
141.91
136.63
129.88
128.36
127.58
126.52
120.54
119.16
119.06
118.58
77.32
77.00
76.68
47.44
38.29
31.10
30.50
22.69
13.89
O
H
O
Me
OH
3
Ph
4aj
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

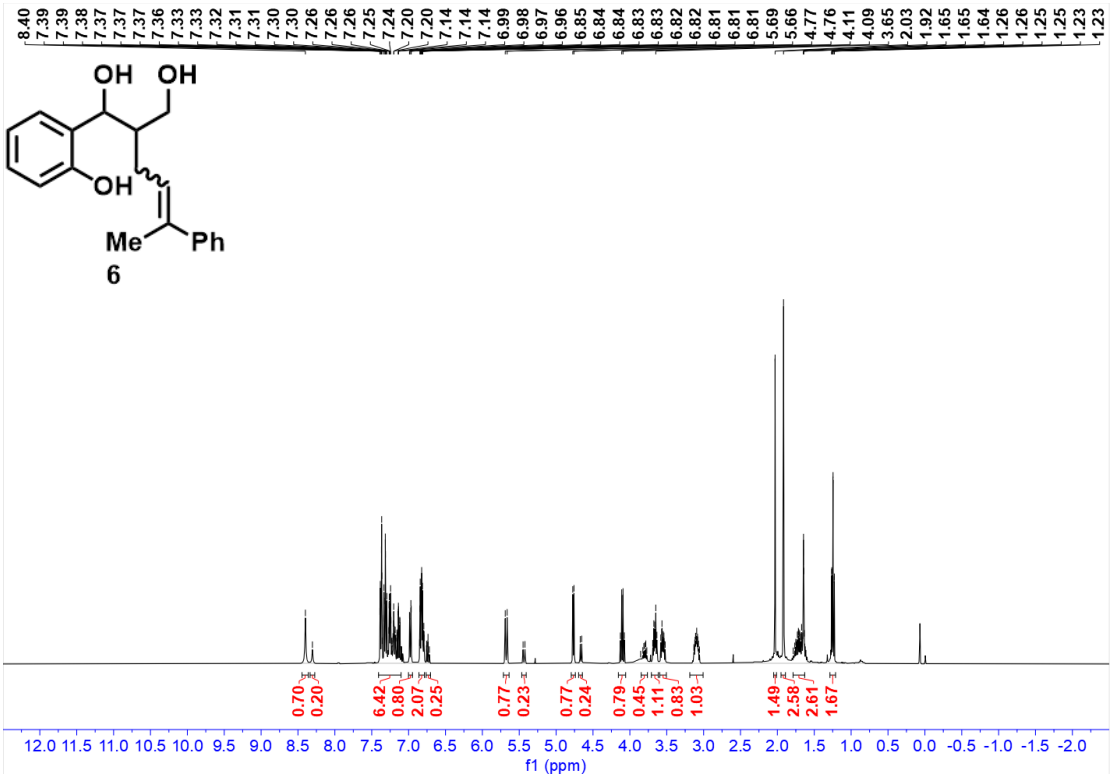

12.04
9.72
7.83
7.83
7.81
7.81
7.56
7.56
7.54
7.54
7.51
7.50
7.49
7.48
7.48
7.47
7.46
7.26
7.20
7.19
7.18
7.17
7.16
7.16
7.13
7.11
7.00
6.99
6.98
6.97
6.94
6.94
6.93
6.92
6.92
6.91
6.90
5.76
5.73
3.79
3.77
3.74
3.72
3.26
3.24
3.21
3.20
2.84
2.83
2.82
2.82
2.81
2.75
2.69
1.93
1.92
1.92
1.91
1.91
1.90
1.90
1.90
O
H
O
OH
4ak
0.94
0.95
1.01
2.09
3.27
1.00
1.02
1.00
1.02
1.02
1.03
4.40
2.14
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1
ppm

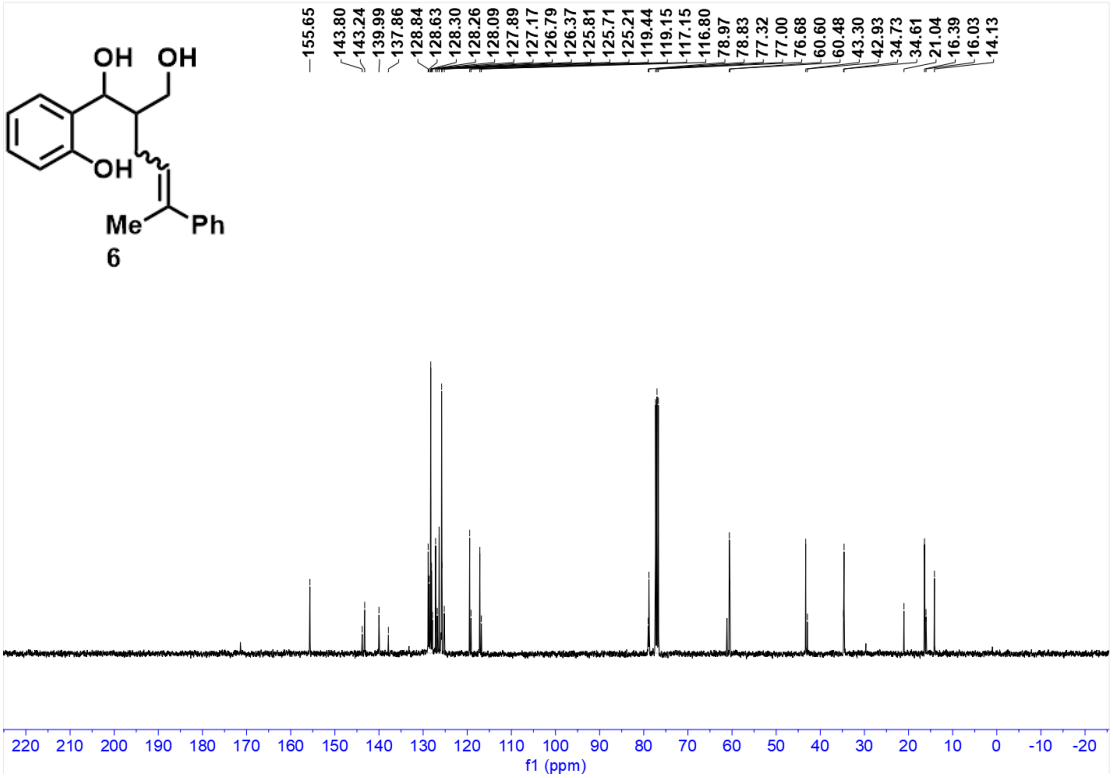

203.38
198.56
162.31
140.89
137.85
136.60
134.94
129.84
129.02
127.76
126.16
124.02
119.14
119.04
118.54
116.11
46.88
38.07
30.22
27.38
23.22
O
H
O
OH
4ak
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
ppm

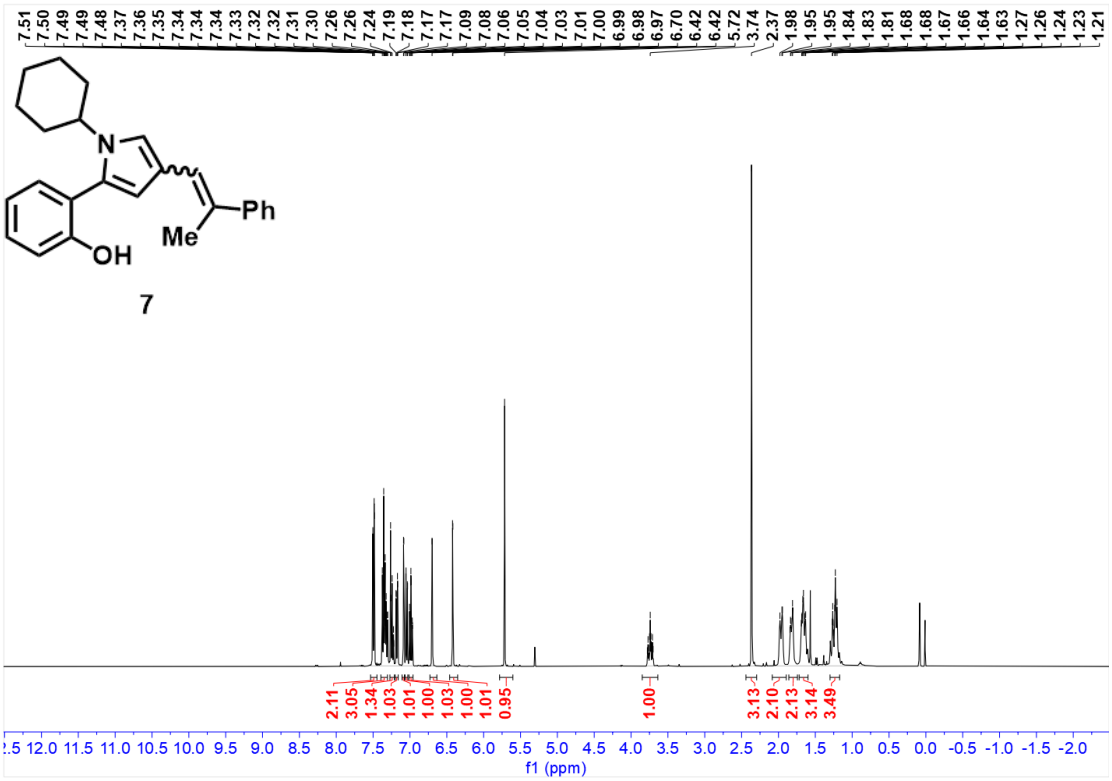
NMR spetra for diverse transformations:

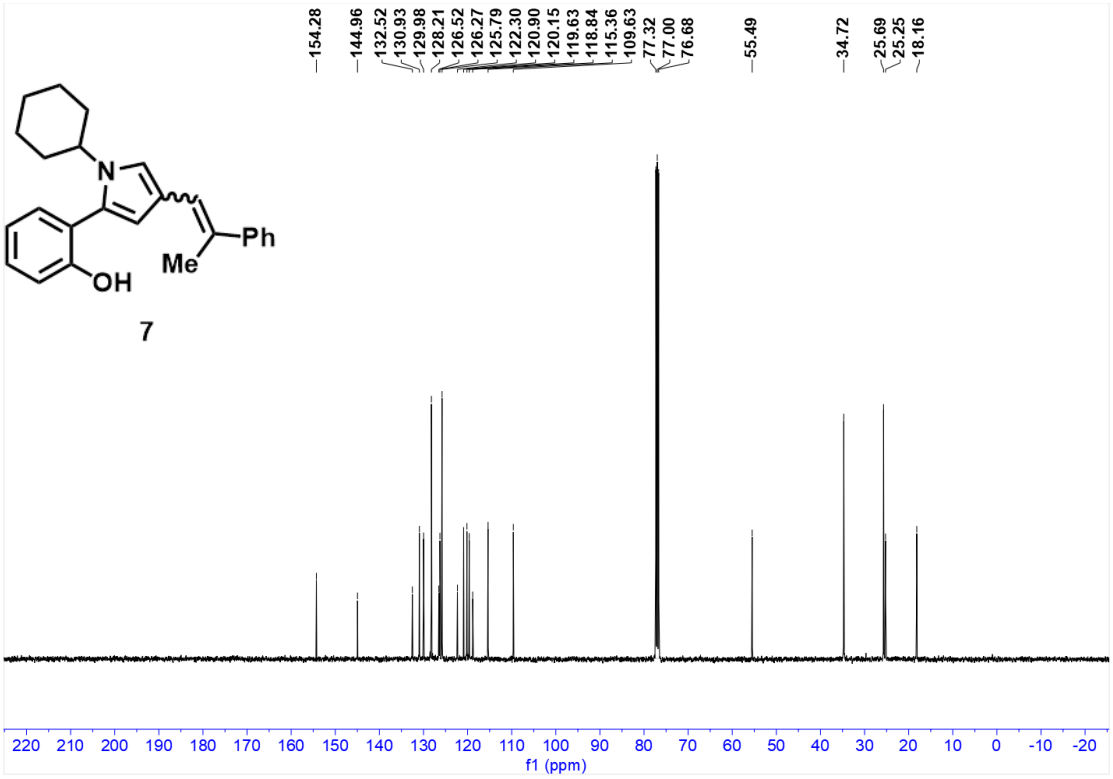


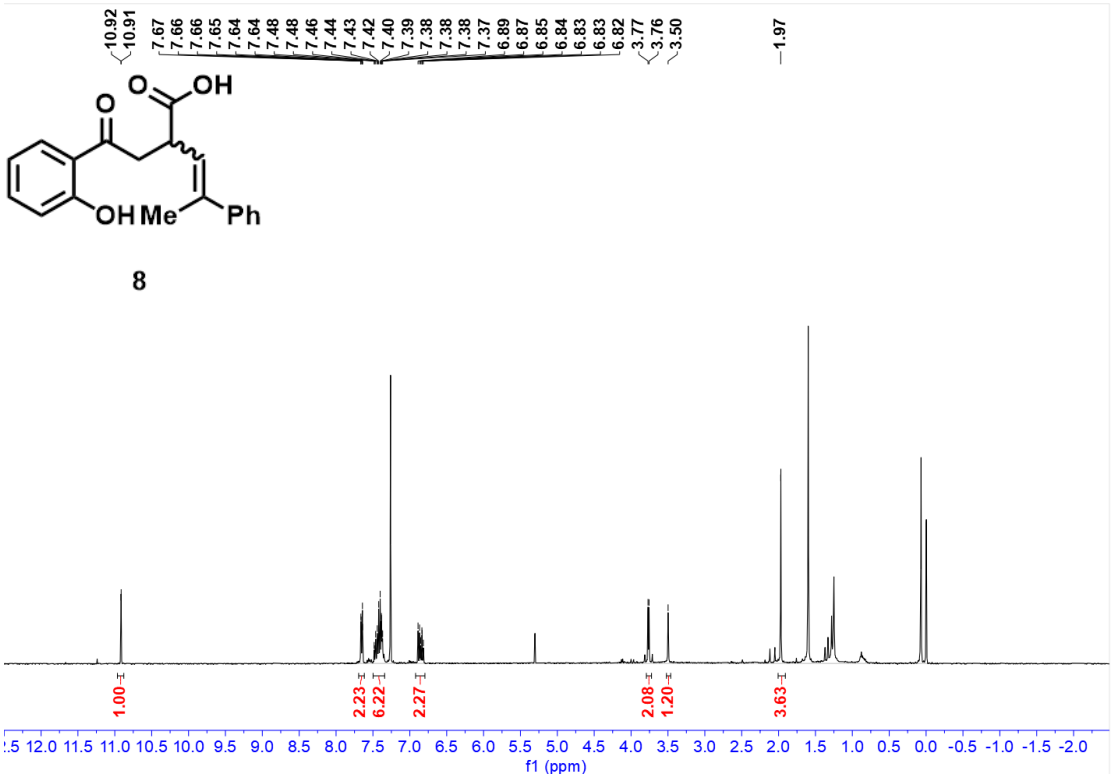


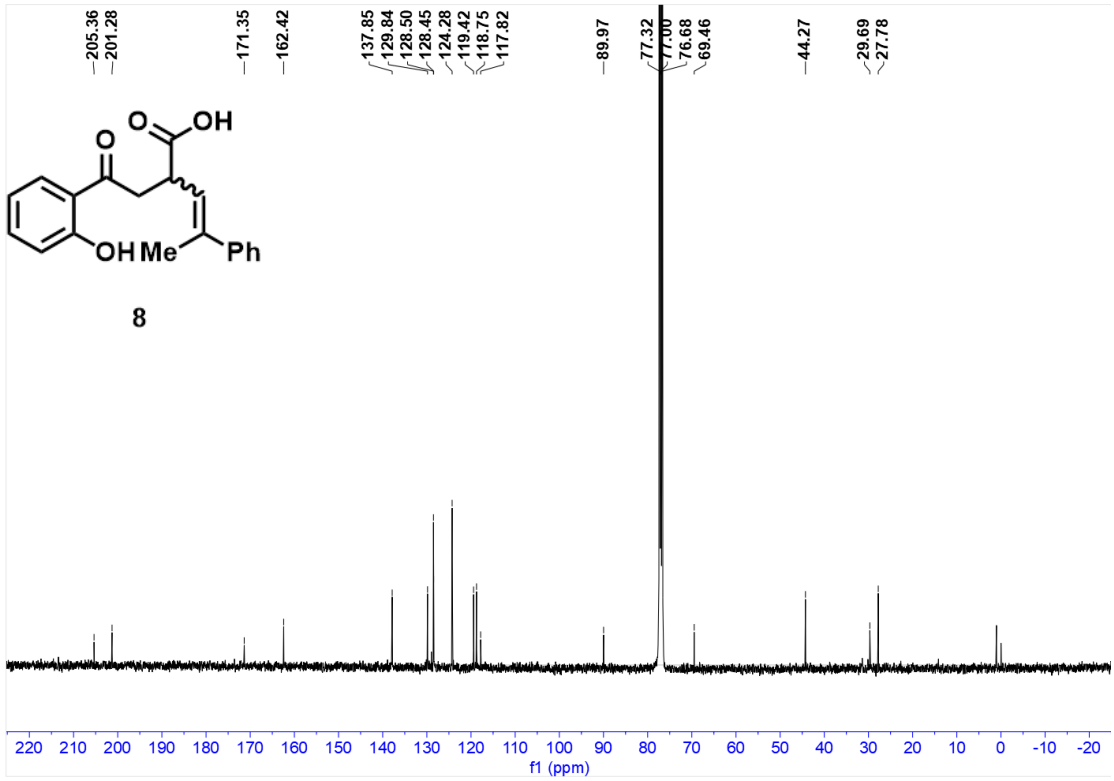

OH
OH
OH
Me
Ph
6
f1 (ppm)


OH
OH
OH
Me
Ph
6
f1 (ppm)


7.51 7.50 7.49 7.49 7.48 7.37 7.36 7.35 7.34 7.34 7.33 7.32 7.31 7.30 7.26 7.26 7.24 7.19 7.18 7.17 7.17 7.09 7.08 7.06 7.05 7.04 7.03 7.01 7.00 6.99 6.98 6.97 6.70 6.42 6.42 5.72 3.74 2.37 1.98 1.95 1.95 1.84 1.83 1.81 1.68 1.68 1.67 1.66 1.64 1.63 1.27 1.26 1.24 1.23 1.21
N
Ph
Me
OH
7
2.11 3.05 1.34 1.03 1.01 1.00 1.03 1.00 1.01 0.95 1.00 3.13 2.10 2.13 3.14 3.49
f1 (ppm)


154.28 144.96 132.52 130.93 129.98 128.21 126.52 126.27 125.79 122.30 120.90 120.15 119.63 118.84 115.36 109.63 77.32 77.00 76.68 55.49 34.72 25.69 25.25 18.16
N
Ph
Me
OH
7
f1 (ppm)


10.92
10.91
7.67
7.66
7.66
7.65
7.64
7.64
7.48
7.48
7.46
7.44
7.43
7.42
7.40
7.39
7.38
7.38
7.37
6.89
6.87
6.85
6.84
6.83
6.83
6.82
3.77
3.76
3.50
1.97
O
OH
O
OH
Me
Ph
8
1.00
2.23
6.22
2.27
2.08
1.20
3.63
f1 (ppm)


205.36
201.28
171.35
162.42
137.85
129.84
128.50
128.45
124.28
119.42
118.75
117.82
89.97
77.32
77.00
76.68
69.46
44.27
29.69
27.78
O
OH
O
OH
Me
Ph
8
f1 (ppm)