

Electronic Supplementary Information

Iron-catalyzed regioselective alkylation of 1,4-quinones and coumarins with functionalized alkyl bromides

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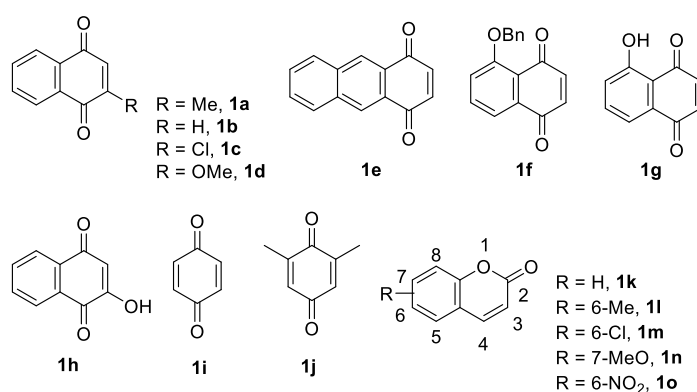
I. General Information

All the solvents and commercially available reagents were purchased from Sigma-Aldrich, TCI, Alfa Aesar, Energy Chemical or Adamas-beta (purity $\geq$ 95%) and used without further purification unless otherwise stated. ^1H NMR, ^{13}C NMR or ^{19}F NMR spectra were recorded on a 400 MHz Bruker FT-NMR spectrometer. All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; q, quartet. The coupling constants, J , are reported in Hertz (Hz). High Resolution Mass (MS) analysis was obtained using on a LC/MSD TOF spectrometer system with Electrospray Ionization (ESI). Reactions were monitored by thin-layer chromatography (TLC) carried out on commercial silica gel plates (GF254) under UV light. Flash chromatography was performed on silica gel 60 (200–300 mesh).

II. Preparation of Starting Materials

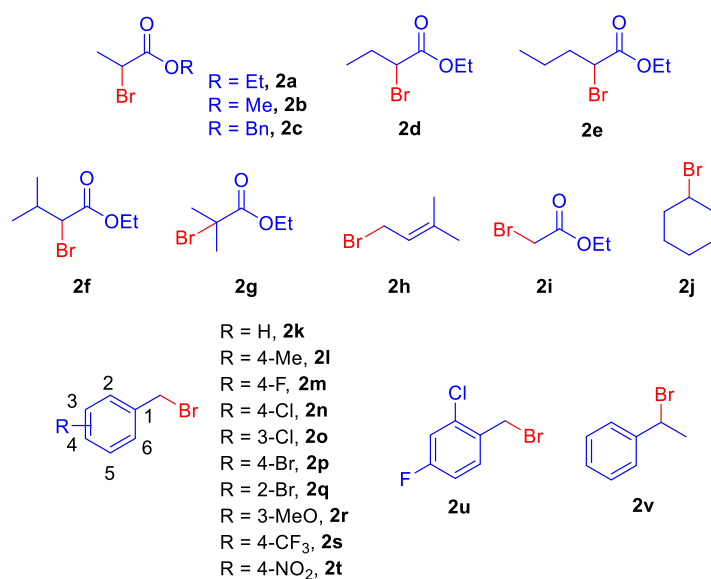
2.1 Preparation of the 1,4-quinone and coumarin substrates

Substrates **1a-1e**, **1g-1l** and **1n-1o** were purchased from commercial sources and used as received without further purification. **1f**¹ and **1m**² were prepared according to literature procedures.



2.2. Preparation of the alkyl halides

The alkyl halides **2a-2v** in the reaction were obtained from commercial sources and used without further purification.



III. Optimization of the Reaction Conditions and the General Procedure

3.1 Optimization of the reaction conditions

Under air atmosphere, ethyl 2-bromopropanoate (**2a**, 2.0 equiv, 0.40 mmol, 72.4 mg) was added to a mixture of 2-methylnaphthalene-1,4-dione (**1a**, 1.0 equiv, 0.20 mmol, 34.4 mg), [Fe] (10 mol%), DIPEA (*N,N*-Diisopropylethylamine, 2.0 equiv, 0.40 mmol, 51.7 mg) in solvent (1.5 mL) in a dry 10 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 100 °C for 18-30 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 15/1, R_f = 0.30) to give the desired product **3a** as a yellow liquid.

Table S1. Optimization of the reaction conditions^a

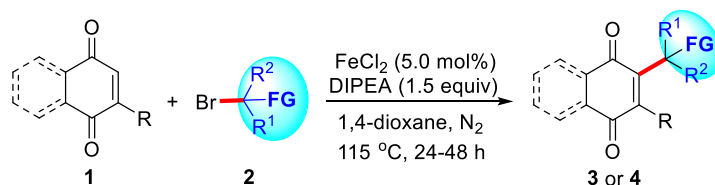
					
Entry	Catalyst (mol%)	Base (equiv)	Solvent	T(°C) / t(h)	Yield (%) ^b
1	FeCl ₂ (10)	DIPEA (2.0)	1,4-dioxane	100 / 24	48
2	FeCl ₂ (10)	--	1,4-dioxane	100 / 18	n.d.
3	--	DIPEA (2.0)	1,4-dioxane	100 / 30	n.d.
4	FeCl ₂ (10)	DIPEA (2.0)	1,4-dioxane	85 / 30	< 5
5	FeCl ₂ (10)	DIPEA (2.0)	DCE	100 / 28	27
6	FeCl ₂ (10)	DIPEA (2.0)	toluene	100 / 28	36
7	FeCl ₂ (10)	DIPEA (2.0)	CH ₃ CN	100 / 24	28
8	FeCl ₂ (10)	DIPEA (2.0)	DMF	100 / 18	< 5

9	FeCl ₂ (10)	DIPEA (2.0)	DMSO	100 / 24	n.d.
10	FeCl ₂ (10)	DIPEA (2.0)	NMP	100 / 24	< 5
11	FeCl ₃ (10)	DIPEA (2.0)	1,4-dioxane	100 / 24	46
12	Fe(acac) ₃ (10)	DIPEA (2.0)	1,4-dioxane	100 / 22	20
13	Fe(acac) ₂ (10)	DIPEA (2.0)	1,4-dioxane	100 / 22	24
14	Fe(OTf) ₂ (10)	DIPEA (2.0)	1,4-dioxane	100 / 24	36
15	Fe(OAc) ₂ (10)	DIPEA (2.0)	1,4-dioxane	100 / 24	25
16	FeCl ₂ (10)	DIPEA (2.0)	1,4-dioxane	115 / 24	57 ^c
17	FeCl ₂ (10)	DABCO (2.0)	1,4-dioxane	115 / 22	n.d.
18	FeCl ₂ (10)	NEt ₃ (2.0)	1,4-dioxane	115 / 22	19
19	FeCl ₂ (10)	PMDTA (2.0)	1,4-dioxane	115 / 22	n.d.
20	FeCl ₂ (10)	Na ₂ CO ₃ (2.0)	1,4-dioxane	115 / 22	22
21	FeCl ₂ (7.5)	DIPEA (2.0)	1,4-dioxane	115 / 24	68 ^c
22	FeCl₂ (5.0)	DIPEA (1.5)	1,4-dioxane	115 / 28	69^c
23	FeCl ₂ (5.0)	DIPEA (1.5)	1,4-dioxane	115 / 28	60 ^{c, d}
24	FeCl ₂ (3.0)	DIPEA (1.5)	1,4-dioxane	115 / 28	59 ^c

^a Reaction conditions: In N₂ atmosphere, **1a** (1.0 equiv, 0.20 mmol), **2a** (2.0 equiv, 0.40 mmol), [Fe], base (2.0 equiv, 0.40 mmol) in solvent (1.5 mL) at 100 °C for 18-28 h; ^b Isolated yield; ^c 0.40 mmol scale of **1a** was used; ^d **2a** (1.5 equiv) was used. Unless otherwise noted, DIPEA = *N,N*-Diisopropylethylamine; DABCO = Triethylenediamine; PMDTA = Pentamethyldiethylenetriamine; n.d. = not detected.

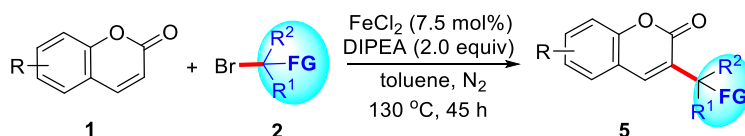
3.2 General Procedures

3.2.1 General Procedures for the Synthesis of 3 or 4



Under air atmosphere, functionalized alkyl halides (**2**, 2.0 equiv, 0.40 mmol) was added to a mixture of 1,4-quinones (**1**, 1.0 equiv, 0.20 mmol), FeCl₂ (5.0 mol%, 1.3 mg), DIPEA (*N,N*-Diisopropylethylamine, 1.5 equiv, 0.30 mmol, 38.8 mg) in 1,4-dioxane (1.5 mL) in a dry 10 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 115 °C for 24-48 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give the desired product **3** or **4**.

3.2.2 General Procedures for the Synthesis of 5

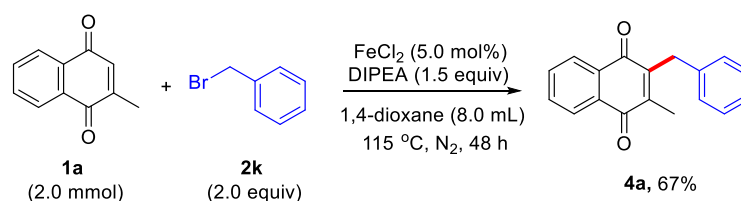


Under air atmosphere, functionalized alkyl halides (**2**, 2.0 equiv, 0.40 mmol) was added to a mixture of coumarins (**1**, 1.0 equiv, 0.20 mmol), FeCl₂ (7.5 mol%, 1.9 mg), DIPEA (*N,N*-Diisopropylethylamine, 2.0 equiv, 0.40 mmol, 51.7 mg) in toluene (2.0 mL) in a dry 10 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 130 °C for 45 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give the desired product **5**.

3.3 Large-scale synthesis of 4

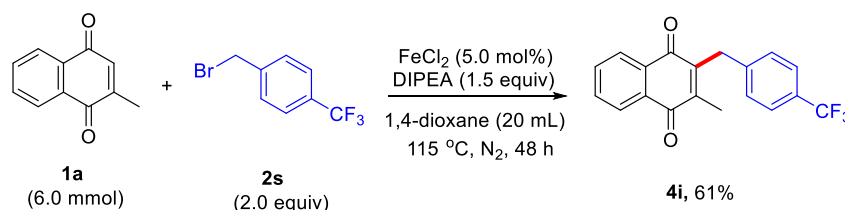
3.3.1 Large-scale synthesis of 4a (2.0 mmol scale)

Under air atmosphere, (bromomethyl)benzene (**2k**, 2.0 equiv, 4.0 mmol, 684.0 mg) was added to a mixture of 2-methylnaphthalene-1,4-dione (**1a**, 1.0 equiv, 2.0 mmol, 344.0 mg), FeCl₂ (5.0 mol%, 13.0 mg), DIPEA (*N,N*-Diisopropylethylamine, 1.5 equiv, 3.0 mmol, 387.7 mg) in 1,4-dioxane (8.0 mL) in a dry 35 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 115 °C for 48 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate; R_f = 0.50, petroleum ether/ethyl acetate = 30:1) to give the desired product **4a** (350.0 mg, yellow solid, 67% yield).



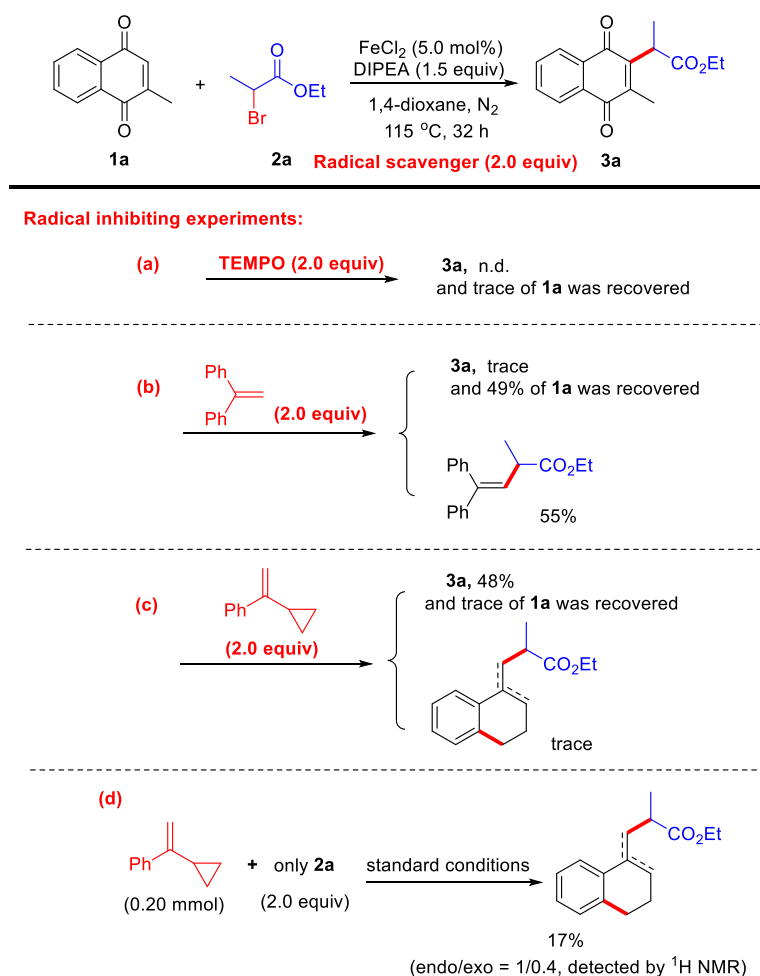
3.3.2 Large-scale synthesis of 4i (6.0 mmol scale)

Under air atmosphere, 1-(bromomethyl)-4-(trifluoromethyl)benzene (**2s**, 2.0 equiv, 12.0 mmol, 2868.0 mg) was added to a mixture of 2-methylnaphthalene-1,4-dione (**1a**, 1.0 equiv, 6.0 mmol, 1032.0 mg), FeCl₂ (5.0 mol%, 39.0 mg), DIPEA (*N,N*-Diisopropylethylamine, 1.5 equiv, 9.0 mmol, 1163.2 mg) in 1,4-dioxane (20.0 mL) in a dry 100 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 115 °C for 48 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate; R_f = 0.30, petroleum ether/ethyl acetate = 30:1) to give the desired product **4i** (1210.0 mg, yellow solid, 61% yield).

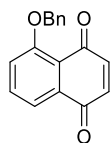


IV. Mechanistic Studies

Under air atmosphere, ethyl 2-bromopropanoate (**2a**, 2.0 equiv, 0.40 mmol, 72.4 mg) was added to a mixture of 2-methylnaphthalene-1,4-dione (**1a**, 1.0 equiv, 0.20 mmol, 34.4 mg), FeCl₂ (5.0 mol%, 1.3 mg), DIPEA (*N,N*-Diisopropylethylamine, 1.5 equiv, 0.30 mmol, 38.8 mg) and a radical scavenger, such as, 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO, 2.0 equiv, 0.40 mmol, 62.5 mg), or 1,1-diphenylethylene (2.0 equiv, 0.4 mmol, 72.1 mg) or (1-cyclopropylvinyl)benzene (2.0 equiv, 0.40 mmol, 57.7 mg) in 1,4-dioxane (1.5 mL) in a dry 10 mL Schlenk tube. Then the tube was degassed with N₂ for three times and the mixture was heated at 115 °C for 32 h (monitored by TLC). After completion of the reaction, it was cooled to room temperature and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate) to give the desired products.

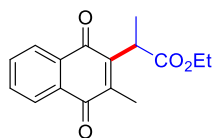


V. Characterization Data



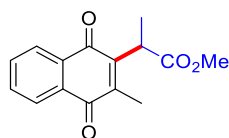
5-(Benzyloxy)naphthalene-1,4-dione (1f)

Yellow solid (1.0 mmol scale, 82.0 mg, 31% yield) $R_f = 0.40$ (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.74-7.72 (m, 1H), 7.66-7.62 (m, 1H), 7.59-7.57 (m, 2H), 7.43-7.39 (m, 2H), 7.34-7.31 (m, 2H), 6.88 (s, 2H), 5.29 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): 185.17, 184.12, 158.42, 140.83, 136.17, 135.95, 134.81, 134.03, 128.64, 127.92, 126.58, 120.13, 119.55, 119.40, 70.76; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{12}\text{NaO}_3^+$ $[\text{M}+\text{Na}]^+$ 287.0679, found 287.0677.



Ethyl 2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)propanoate (3a)³

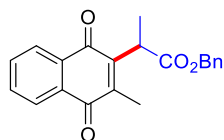
Yellow liquid (0.4 mmol scale, 75.0 mg, 69% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.11-8.03 (m, 2H), 7.73-7.68 (m, 2H), 4.22-4.08 (m, 2H), 3.88 (q, $J = 7.2$ Hz, 1H), 2.19 (s, 3H), 1.44 (d, $J = 7.2$ Hz, 3H), 1.18 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.09, 183.46, 172.75, 146.43, 143.72, 133.58, 133.57, 131.94, 131.90, 126.40, 126.33, 60.98, 38.73, 15.21, 14.09, 12.73.



Methyl 2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)propanoate (3b)

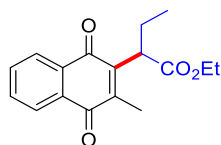
Yellow liquid (0.2 mmol scale, 32.0 mg, 62% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.09-8.02 (m, 2H), 7.72-7.68 (m, 2H), 3.88 (q, $J = 7.1$ Hz, 1H), 3.66 (s, 3H), 2.19 (s, 3H), 1.44 (d, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.99, 183.46, 173.26, 146.17, 143.79, 133.60, 133.59, 131.87,

131.78, 126.43, 126.33, 52.16, 38.54, 15.22, 12.69; HRMS (ESI) calcd for $C_{15}H_{15}O_4^+$ $[M+H]^+$ 259.0965, found 259.0962.



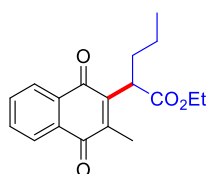
Benzyl 2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)propanoate (3c)

Yellow liquid (0.2 mmol scale, 23.2 mg, 35% yield) R_f = 0.25 (petroleum ether/ethyl acetate = 15:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.10-8.01 (m, 2H), 7.73-7.69 (m, 2H), 7.29-7.25 (m, 5H), 5.14 (s, 2H), 3.94 (q, J = 7.2 Hz, 1H), 2.15 (s, 3H), 1.48 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 184.98, 183.47, 172.64, 146.17, 143.81, 135.68, 133.60, 133.57, 131.86, 131.78, 128.39, 128.24, 128.11, 126.40, 126.33, 66.73, 38.78, 15.24, 12.72; HRMS (ESI) calcd for $C_{21}H_{19}O_4^+$ $[M+H]^+$ 335.1278, found 335.1277.



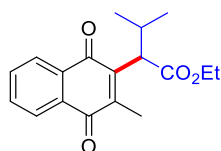
Ethyl 2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)butanoate (3d)

Yellow liquid (0.2 mmol scale, 31.2 mg, 54% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 20:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.12-8.04 (m, 2H), 7.74-7.69 (m, 2H), 4.21-4.07 (m, 2H), 3.77 (dd, J = 5.7 Hz, 3.2 Hz, 1H), 2.37-2.26 (m, 1H), 2.21 (s, 3H), 1.82-1.70 (m, 1H), 1.16 (t, J = 7.1 Hz, 3H), 0.93 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 185.07, 183.71, 172.28, 145.04, 144.84, 133.60, 133.58, 131.97, 131.82, 126.48, 126.34, 60.88, 45.64, 23.50, 14.09, 13.27, 12.31; HRMS (ESI) calcd for $C_{17}H_{19}O_4^+$ $[M+H]^+$ 287.1278, found 287.1275.

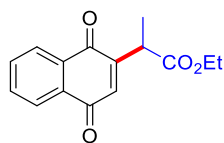


Ethyl 2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)pentanoate (3e)

Yellow liquid (0.2 mmol scale, 23.0 mg, 38% yield) $R_f = 0.35$ (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.11-8.03 (m, 2H), 7.73-7.68 (m, 2H), 4.20-4.06 (m, 2H), 3.85 (dd, $J = 5.7$ Hz, 2.9 Hz, 1H), 2.29-2.22 (m, 1H), 2.20 (s, 3H), 1.73-1.64 (m, 1H), 1.40-1.33 (m, 2H), 1.16 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.08, 183.71, 172.34, 145.40, 144.56, 133.57, 131.96, 131.81, 126.47, 126.31, 60.90, 43.98, 32.48, 21.07, 14.09, 13.23; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{21}\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 301.1434, found 301.1432.

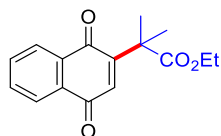
**Ethyl 3-methyl-2-(3-methyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)butanoate (3f)**

Yellow liquid (0.2 mmol scale, 12.8 mg, 21% yield) $R_f = 0.40$ (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.12-8.05 (m, 2H), 7.74-7.69 (m, 2H), 4.17-4.05 (m, 2H), 3.72 (d, $J = 9.1$ Hz, 1H), 2.65-2.53 (m, 1H), 2.23 (s, 3H), 1.20 (d, $J = 6.4$ Hz, 3H), 1.15 (t, $J = 7.1$ Hz, 3H), 0.77 (t, $J = 6.9$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.13, 183.95, 171.85, 145.09, 144.86, 133.61, 131.99, 131.68, 126.63, 126.31, 60.73, 50.46, 28.65, 23.08, 20.33, 14.09, 13.42; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{21}\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 301.1434, found 301.1431.

**Ethyl 2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)propanoate (3g)**

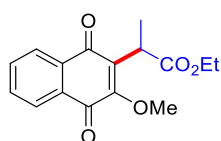
Yellow liquid (0.4 mmol scale, 47.2 mg, 46% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.11-8.06 (m, 2H), 7.77-7.72 (m, 2H), 6.87 (d, $J = 1.1$ Hz, 1H), 4.16 (q, $J = 7.1$ Hz, 2H), 3.93 (qd, $J = 6.2$ Hz, 1.0 Hz, 1H), 1.48 (d, $J = 7.2$ Hz, 3H), 1.23 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.97, 184.10, 172.68, 149.67, 134.89, 133.92, 133.86, 131.93, 131.91, 126.78,

126.15, 61.31, 39.41, 15.87, 14.05; HRMS (ESI) calcd for $C_{15}H_{15}O_4^+$ $[M+H]^+$ 259.0965, found 259.0963.



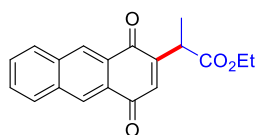
Ethyl 2-(1,4-dioxo-1,4-dihydronaphthalen-2-yl)-2-methylpropanoate (3h)³

Yellow liquid (0.2 mmol scale, 16.0 mg, 29% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 15:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.10-8.05 (m, 2H), 7.76-7.72 (m, 2H), 6.87 (s, 1H), 4.13 (q, J = 7.1 Hz, 2H), 1.49 (s, 6H), 1.16 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 185.37, 184.06, 175.19, 154.19, 133.89, 133.82, 133.17, 132.27, 131.73, 126.85, 125.99, 61.05, 44.45, 25.06, 13.96.



Ethyl 2-(3-methoxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)propanoate (3i)

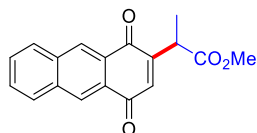
Yellow liquid (0.2 mmol scale, 16.1 mg, 28% yield) R_f = 0.25 (petroleum ether/ethyl acetate = 15:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.10-8.04 (m, 2H), 7.75-7.69 (m, 2H), 4.15 (q, J = 7.5 Hz, 2H), 4.14 (s, 3H), 4.07 (q, J = 7.1 Hz, 1H), 1.38 (d, J = 7.1 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 183.97, 181.58, 173.13, 157.11, 134.33, 134.03, 133.41, 131.65, 131.40, 126.40, 126.21, 61.20, 60.84, 35.12, 15.24, 14.17; HRMS (ESI) calcd for $C_{16}H_{17}O_5^+$ $[M+H]^+$ 289.1071, found 289.1070.



Ethyl 2-(1,4-dioxo-1,4-dihydroanthracen-2-yl)propanoate (3j)

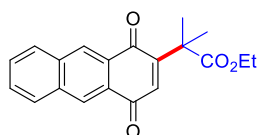
Yellow solid (0.2 mmol scale, 27.4 mg, 44% yield) R_f = 0.35 (petroleum ether/ethyl acetate = 7:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.62-8.59 (m, 2H), 8.06-8.02 (m, 2H), 7.70-7.66 (m, 2H), 6.97 (d, J = 1.1 Hz, 1H), 4.18 (q, J = 7.1 Hz, 2H), 3.99 (qd, J = 7.1

Hz, 1.1 Hz, 1H), 1.51 (d, $J = 7.2$ Hz, 3H), 1.24 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.59, 183.69, 172.74, 151.08, 136.38, 134.81, 134.78, 130.18, 130.15, 129.57, 129.51, 129.31, 128.51, 128.42, 128.33, 61.29, 39.61, 15.90, 14.06; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{16}\text{NaO}_4^+$ $[\text{M}+\text{Na}]^+$ 331.0941, found 331.0942.



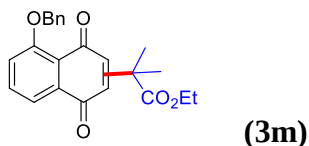
Methyl 2-(1,4-dioxo-1,4-dihydroanthracen-2-yl)propanoate (3k)

Yellow solid (0.2 mmol scale, 26.8 mg, 46% yield) $R_f = 0.35$ (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 8.62-8.59 (m, 2H), 8.06-8.02 (m, 2H), 7.69-7.67 (m, 2H), 6.97 (d, $J = 1.0$ Hz, 1H), 4.01 (qd, $J = 7.2$ Hz, 0.8 Hz, 1H), 3.72 (s, 3H), 1.52 (d, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.55, 183.67, 173.21, 150.89, 136.47, 134.80, 134.78, 130.19, 130.16, 129.60, 129.54, 129.38, 128.55, 128.39, 128.27, 52.48, 39.39, 15.91; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{14}\text{NaO}_4^+$ $[\text{M}+\text{Na}]^+$ 317.0784, found 317.0785.



Ethyl 2-(1,4-dioxo-1,4-dihydroanthracen-2-yl)-2-methylpropanoate (3l)

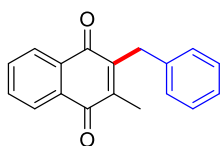
Yellow solid (0.2 mmol scale, 13.7 mg, 21% yield) $R_f = 0.35$ (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 8.62-8.61 (m, 2H), 8.08-8.03 (m, 2H), 7.71-7.67 (m, 2H), 6.98 (s, 1H), 4.16 (q, $J = 7.2$ Hz, 2H), 1.53 (s, 6H), 1.18 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.08, 183.68, 175.30, 155.63, 134.90, 134.78, 134.70, 130.20, 130.15, 129.57, 129.53, 129.44, 128.68, 128.38, 128.30, 61.07, 44.62, 25.10, 14.01; HRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{NaO}_4^+$ $[\text{M}+\text{Na}]^+$ 345.1097, found 345.1096.



Ethyl 2-(8-(benzyloxy)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)-2-methylpropanoate and

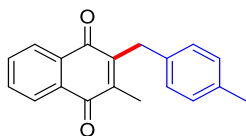
Ethyl 2-(5-(benzyloxy)-1,4-dioxo-1,4-dihydronaphthalen-2-yl)-2-methylpropanoate

Yellow solid (0.1 mmol scale, 10.0 mg, 26% yield, regioselectivity = 1/0.4) R_f = 0.40 (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.74-7.71 (m, 1.4H), 7.64-7.60 (m, 1.2H), 7.58-7.56 (m, 2H), 7.53-7.49 (m, 0.8H), 7.44-7.37 (m, 3H), 7.35-7.29 (m, 3H), 6.81 (s, 0.4H), 6.79 (s, 1H), 5.33 (s, 2H), 5.30 (s, 0.8H), 4.16 (q, J = 7.0 Hz, 0.8H), 4.13 (q, J = 7.0 Hz, 2H), 1.51 (s, 2.4H), 1.49 (s, 6H), 1.17 (t, J = 7.1 Hz, 1.2H), 1.16 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.57, 184.46, 184.23, 175.41, 175.31, 158.22, 156.17, 151.65, 136.04, 135.36, 134.74, 134.64, 134.59, 134.02, 131.14, 128.68, 128.62, 127.94, 127.87, 126.59, 126.56, 120.12, 119.92, 119.86, 119.48, 119.00, 70.80, 61.00, 44.61, 44.03, 25.37, 24.94, 13.98; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{22}\text{NaO}_5^+$ $[\text{M}+\text{Na}]^+$ 401.1359, found 401.1356.



2-Benzyl-3-methylnaphthalene-1,4-dione (4a)^{4, 6}

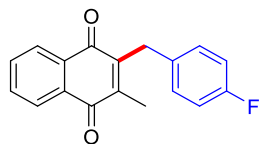
Yellow solid (0.2 mmol scale, 36.4 mg, 69% yield; 2.0 mmol scale, 350.0 mg, 67% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.06 (m, 2H), 7.71-7.67 (m, 2H), 7.29-7.17 (m, 5H), 4.04 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.31, 184.57, 145.23, 144.34, 137.97, 133.43, 133.40, 132.00, 131.91, 128.58, 128.53, 126.39, 126.36, 126.19, 32.34, 13.23.



2-Methyl-3-(4-methylbenzyl)naphthalene-1,4-dione (4b)⁴

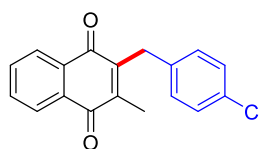
Yellow solid (0.2 mmol scale, 44.2 mg, 80% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.06 (m, 2H), 7.71-7.67 (m, 2H), 7.14-7.12 (m, 2H), 7.09-7.07 (m, 2H), 3.99 (s, 2H), 2.29 (s, 3H), 2.26 (s, 3H); ^{13}C

NMR (100 MHz, CDCl₃): 185.39, 184.63, 145.45, 144.15, 135.94, 134.88, 133.41, 133.38, 132.02, 131.96, 129.28, 128.43, 126.40, 126.18, 31.94, 20.95, 13.22.



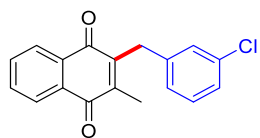
2-(4-Fluorobenzyl)-3-methylnaphthalene-1,4-dione (4c)⁴

Yellow solid (0.2 mmol scale, 37.5 mg, 67% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 50:1) ¹H NMR (400 MHz, CDCl₃): δ 8.08-8.06 (m, 2H), 7.71-7.68 (m, 2H), 7.21-7.17 (m, 2H), 6.97-6.92 (m, 2H), 3.99 (s, 2H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 185.26, 184.57, 161.42 (d, J = 243.3 Hz), 145.04, 144.31, 133.62 (d, J = 3.1 Hz), 133.51, 131.99, 131.87, 129.99 (d, J = 7.9 Hz), 126.42, 126.26, 115.39 (d, J = 21.2 Hz), 31.60, 13.23; ¹⁹F NMR (376 MHz, CDCl₃) -116.44 to -116.51 (m, 1F).



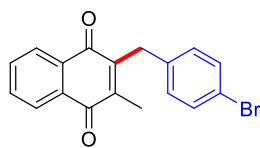
2-(4-Chlorobenzyl)-3-methylnaphthalene-1,4-dione (4d)⁴

Yellow solid (0.2 mmol scale, 43.0 mg, 72% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 50:1) ¹H NMR (400 MHz, CDCl₃): δ 8.10-8.05 (m, 2H), 7.73-7.68 (m, 2H), 7.24-7.21 (m, 2H), 7.17-7.15 (m, 2H), 3.98 (s, 2H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 185.20, 184.52, 144.77, 144.50, 136.47, 133.55, 133.20, 131.99, 131.85, 129.89, 128.70, 126.44, 126.29, 31.79, 13.28.



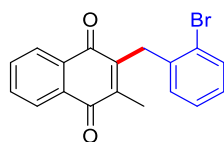
2-(3-Chlorobenzyl)-3-methylnaphthalene-1,4-dione (4e)

Yellow solid (0.2 mmol scale, 34.1 mg, 57% yield) R_f = 0.45 (petroleum ether/ethyl acetate = 50:1) ¹H NMR (400 MHz, CDCl₃): δ 8.12-8.07 (m, 2H), 7.73-7.69 (m, 2H), 7.22-7.15 (m, 3H), 7.13-7.10 (m, 1H), 4.01 (s, 2H), 2.24 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 185.20, 184.48, 144.75, 144.48, 139.98, 134.38, 133.59, 132.03, 131.86, 129.84, 128.56, 126.76, 126.68, 126.52, 126.34, 32.07, 13.34; HRMS (ESI) calcd for C₁₈H₁₄ClO₂⁺ [M+H]⁺ 297.0677, found 297.0669.



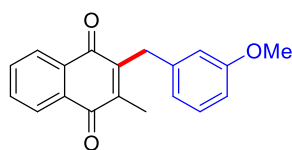
2-(4-Bromobenzyl)-3-methylnaphthalene-1,4-dione (4f)⁴

Yellow solid (0.2 mmol scale, 48.0 mg, 70% yield) $R_f = 0.45$ (petroleum ether/ethyl acetate = 50:1) ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.04 (m, 2H), 7.73-7.67 (m, 2H), 7.39-7.35 (m, 2H), 7.11-7.09 (m, 2H), 3.96 (s, 2H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.16, 184.48, 144.66, 144.50, 136.98, 133.54, 131.96, 131.82, 131.63, 130.26, 126.42, 126.28, 120.23, 31.84, 13.28.



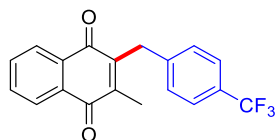
2-(2-Bromobenzyl)-3-methylnaphthalene-1,4-dione (4g)

Yellow solid (0.2 mmol scale, 46.5 mg, 68% yield) $R_f = 0.40$ (petroleum ether/ethyl acetate = 50:1) ^1H NMR (400 MHz, CDCl_3): δ 8.14-8.07 (m, 2H), 7.75-7.70 (m, 2H), 7.60-7.57 (m, 1H), 7.17-7.13 (m, 1H), 7.08-7.04 (m, 1H), 6.92-6.90 (m, 1H), 4.12 (s, 2H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.04, 184.34, 145.87, 144.52, 137.27, 133.59, 133.56, 132.86, 132.10, 131.92, 128.55, 127.95, 127.55, 126.54, 126.34, 124.66, 32.64, 13.30; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{14}\text{BrO}_2^+$ $[\text{M}+\text{H}]^+$ 341.0172, found 341.0164.



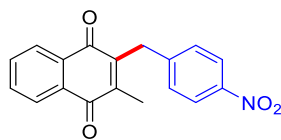
2-(3-Methoxybenzyl)-3-methylnaphthalene-1,4-dione (4h)⁵

Yellow solid (0.2 mmol scale, 43.1 mg, 74% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.06 (m, 2H), 7.71-7.67 (m, 2H), 7.20-7.16 (m, 1H), 6.82-6.71 (m, 3H), 4.01 (s, 2H), 3.76 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.31, 184.56, 159.66, 145.05, 144.46, 139.50, 133.44, 133.42, 132.02, 131.92, 129.53, 126.42, 126.20, 120.89, 114.58, 111.30, 55.09, 32.29, 13.25.



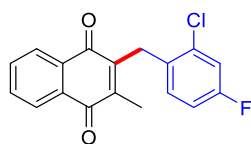
2-Methyl-3-(4-(trifluoromethyl)benzyl)naphthalene-1,4-dione (4i)⁴

Yellow solid (0.2 mmol scale, 43.3 mg, 66% yield; 6.0 mmol scale, 1210.0 mg, 61% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.10-8.05 (m, 2H), 7.72-7.68 (m, 2H), 7.53-7.51 (m, 2H), 7.36-7.34 (m, 2H), 4.08 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.07, 184.44, 144.81, 144.32, 142.15, 133.62, 131.98, 131.80, 128.84, 128.72 (q, $J = 32.3$ Hz), 124.08 (q, $J = 270.4$ Hz), 126.46, 126.34, 125.53 (q, $J = 3.7$ Hz), 32.29, 13.32; ^{19}F NMR (376 MHz, CDCl_3) -62.43 (s, 3F).



2-Methyl-3-(4-nitrobenzyl)naphthalene-1,4-dione (4j)⁴

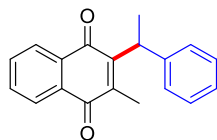
Yellow solid (0.2 mmol scale, 32.4 mg, 53% yield) $R_f = 0.35$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.13-8.11 (m, 2H), 8.10-8.04 (m, 2H), 7.74-7.69 (m, 2H), 7.40-7.38 (m, 2H), 4.12 (s, 2H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.88, 184.32, 146.54, 145.79, 145.10, 143.72, 133.75, 133.71, 131.92, 131.68, 129.33, 126.48, 126.40, 123.83, 32.42, 13.40.



2-(2-Chloro-4-fluorobenzyl)-3-methylnaphthalene-1,4-dione (4k)

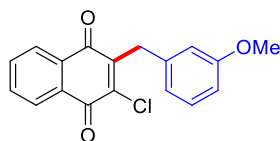
Yellow solid (0.2 mmol scale, 48.6 mg, 77% yield) $R_f = 0.50$ (petroleum ether/ethyl acetate = 30:1) ^1H NMR (400 MHz, CDCl_3): δ 8.14-8.06 (m, 2H), 7.75-7.70 (m, 2H), 7.15-7.13 (m, 1H), 6.97-6.93 (m, 1H), 6.86-6.82 (m, 1H), 4.07 (s, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 184.95, 184.37, 161.02 (d, $J = 247.1$ Hz), 145.80, 144.13, 134.37 (d, $J = 10.2$ Hz), 133.63, 132.05, 131.87, 131.47 (d, $J = 3.6$ Hz), 129.74 (d, $J = 8.6$ Hz), 126.52, 126.37, 116.87 (d, $J = 24.6$ Hz), 114.09 (d, $J = 20.9$ Hz).

Hz), 29.27, 13.25; ^{19}F NMR (376 MHz, CDCl_3) -114.26 to -114.32 (m, 1F); HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{13}\text{ClFO}_2^+ [\text{M}+\text{H}]^+$ 315.0583, found 315.0575.



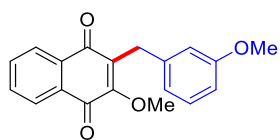
2-Methyl-3-(1-phenylethyl)naphthalene-1,4-dione (4l)

Yellow solid (0.2 mmol scale, 17.3 mg, 31% yield) R_f = 0.45 (petroleum ether/ethyl acetate = 50:1) ^1H NMR (400 MHz, CDCl_3): δ 8.09-8.01 (m, 2H), 7.71-7.66 (m, 2H), 7.32-7.28 (m, 4H), 7.23-7.17 (m, 1H), 4.74 (q, J = 7.2 Hz, 1H), 2.09 (s, 3H), 1.69 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.78, 184.35, 150.15, 144.08, 142.95, 133.50, 133.31, 132.25, 131.89, 128.33, 126.97, 126.48, 126.11, 126.04, 36.54, 16.73, 12.98; HRMS (ESI) calcd for $\text{C}_{19}\text{H}_{17}\text{O}_2^+ [\text{M}+\text{H}]^+$ 277.1223, found 277.1219.



2-Chloro-3-(3-methoxybenzyl)naphthalene-1,4-dione (4m)

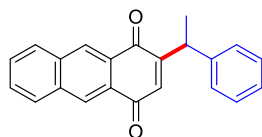
Yellow solid (0.2 mmol scale, 42.7 mg, 68% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.15-8.09 (m, 2H), 7.76-7.71 (m, 2H), 7.21-7.17 (m, 1H), 6.96-6.91 (m, 2H), 6.76-6.74 (m, 1H), 4.14 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 182.30, 177.88, 159.62, 146.18, 143.68, 138.05, 134.24, 133.96, 131.51, 131.21, 129.55, 127.12, 127.10, 121.50, 115.01, 111.98, 55.12, 33.83; HRMS (ESI) calcd for $\text{C}_{18}\text{H}_{13}\text{ClNaO}_3^+ [\text{M}+\text{Na}]^+$ 335.0445, found 335.0437.



2-Methoxy-3-(3-methoxybenzyl)naphthalene-1,4-dione (4n)

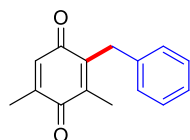
Yellow oil (0.2 mmol scale, 28.2 mg, 46% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 8.07-8.01 (m, 2H), 7.71-7.65 (m, 2H), 7.19-7.16 (m, 1H), 6.93-6.89 (m, 2H), 6.73-6.71 (m, 1H), 4.14 (s, 3H), 3.92 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 185.03, 181.73, 159.52, 157.60, 140.52,

133.83, 133.44, 133.23, 131.73, 131.41, 129.31, 126.27, 126.04, 121.40, 114.80, 111.44, 61.18, 55.09, 29.25; HRMS (ESI) calcd for $C_{19}H_{17}O_4^+$ $[M+H]^+$ 309.1121, found 309.1119.



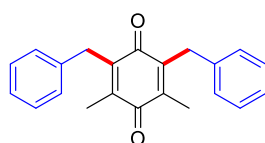
2-(1-Phenylethyl)anthracene-1,4-dione (4o)

Yellow solid (0.2 mmol scale, 30.5 mg, 49% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 15:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.57-8.56 (m, 2H), 8.03-8.00 (m, 2H), 7.68-7.63 (m, 2H), 7.33-7.30 (m, 4H), 7.25-7.21 (m, 1H), 6.89 (d, J = 1.1 Hz, 1H), 4.56 (qd, J = 7.2 Hz, 1.0 Hz, 1H), 1.58 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 185.10, 184.08, 156.32, 142.75, 135.50, 134.80, 134.69, 130.12, 130.08, 129.41, 129.38, 129.23, 128.70, 128.44, 128.25, 127.71, 126.85, 38.10, 20.01; HRMS (ESI) calcd for $C_{22}H_{16}NaO_2^+$ $[M+Na]^+$ 335.1043, found 335.1045.



2-Benzyl-3,5-dimethylcyclohexa-2,5-diene-1,4-dione (4p)⁷

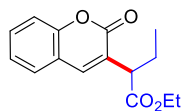
Yellow sticky solid (0.2 mmol scale, 15.0 mg, 33% yield) R_f = 0.60 (petroleum ether/ethyl acetate = 30:1) 1H NMR (400 MHz, $CDCl_3$): δ 7.28-7.24 (m, 2H), 7.20-7.16 (m, 3H), 6.58 (q, J = 1.6 Hz, 1H), 3.85 (s, 2H), 2.10 (s, 3H), 2.04 (d, J = 1.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 188.32, 187.18, 145.40, 142.69, 141.76, 137.97, 133.06, 128.57, 128.52, 126.35, 31.67, 15.91, 12.73.



2,6-Dibenzyl-3,5-dimethylcyclohexa-2,5-diene-1,4-dione (4q)

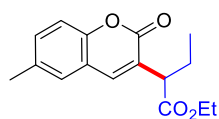
Yellow sticky solid (0.2 mmol scale, 13.1 mg, 21% yield) R_f = 0.65 (petroleum ether/ethyl acetate = 30:1) 1H NMR (400 MHz, $CDCl_3$): δ 7.27-7.23 (m, 4H), 7.20-7.13 (m, 6H), 3.87 (s, 4H), 2.09 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): 188.24,

186.82, 142.48, 141.43, 138.16, 128.57, 128.47, 126.30, 32.06, 12.76; HRMS (ESI) calcd for $C_{22}H_{21}O_2^+$ $[M+H]^+$ 317.1536, found 317.1532.



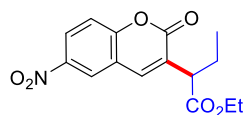
Ethyl 2-(2-oxo-2H-chromen-3-yl)butanoate (5a)

Pale yellow liquid (0.2 mmol scale, 26.1 mg, 50% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 7:1) 1H NMR (400 MHz, $CDCl_3$): δ 7.73 (s, 1H), 7.53-7.49 (m, 2H), 7.34-7.27 (m, 2H), 4.25-4.13 (m, 2H), 3.78 (t, J = 7.6 Hz, 1H), 2.11-2.01 (m, 1H), 1.94-1.83 (m, 1H), 1.26 (t, J = 7.1 Hz, 3H), 1.00 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 172.91, 161.10, 153.06, 139.53, 131.26, 127.78, 127.02, 124.41, 119.10, 116.45, 61.08, 46.63, 24.95, 14.12, 12.05; HRMS (ESI) calcd for $C_{15}H_{17}O_4^+$ $[M+H]^+$ 261.1121, found 261.1122.



Ethyl 2-(6-methyl-2-oxo-2H-chromen-3-yl)butanoate (5b)

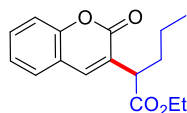
Pale yellow liquid (0.2 mmol scale, 22.1 mg, 40% yield) R_f = 0.30 (petroleum ether/ethyl acetate = 7:1) 1H NMR (400 MHz, $CDCl_3$): δ 7.65 (s, 1H), 7.31-7.26 (m, 2H), 7.21-7.19 (m, 1H), 4.23-4.11 (m, 2H), 3.75 (t, J = 7.5 Hz, 1H), 2.39 (s, 3H), 2.08-1.97 (m, 1H), 1.91-1.80 (m, 1H), 1.24 (t, J = 7.1 Hz, 3H), 0.97 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 172.94, 161.30, 151.18, 139.50, 134.07, 132.23, 127.58, 126.84, 118.83, 116.13, 61.03, 46.62, 24.93, 20.71, 14.11, 12.03; HRMS (ESI) calcd for $C_{16}H_{19}O_4^+$ $[M+H]^+$ 275.1278, found 275.1277.



Ethyl 2-(6-nitro-2-oxo-2H-chromen-3-yl)butanoate (5c)

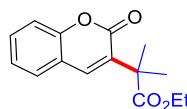
Pale yellow sticky solid (0.2 mmol scale, 16.3 mg, 27% yield) R_f = 0.40 (petroleum ether/ethyl acetate = 5:1) 1H NMR (400 MHz, $CDCl_3$): δ 8.44-8.43 (m, 1H), 8.38-8.35 (m, 1H), 7.81 (s, 1H), 7.46-7.44 (m, 1H), 4.26-4.13 (m, 2H), 3.77 (t, J = 7.4 Hz, 1H), 2.12-2.02 (m, 1H), 1.95-1.84 (m, 1H), 1.26 (t, J = 7.1 Hz, 3H), 1.01 (t, J = 7.4 Hz,

3H); ^{13}C NMR (100 MHz, CDCl_3): 172.22, 159.55, 156.47, 144.04, 138.32, 129.53, 126.01, 123.66, 119.16, 117.64, 61.39, 46.84, 24.88, 14.12, 12.02; HRMS (ESI) calcd for $\text{C}_{15}\text{H}_{16}\text{NO}_6^+$ $[\text{M}+\text{H}]^+$ 306.0972, found 306.0970.



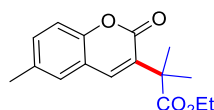
Ethyl 2-(2-oxo-2H-chromen-3-yl)pentanoate (5d)

Pale yellow liquid (0.2 mmol scale, 22.7 mg, 41% yield) R_f = 0.35 (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.73 (s, 1H), 7.53-7.49 (m, 2H), 7.34-7.27 (m, 2H), 4.25-4.12 (m, 2H), 3.87 (t, J = 7.5 Hz, 1H), 2.05-1.96 (m, 1H), 1.86-1.77 (m, 1H), 1.44-1.35 (m, 2H), 1.26 (t, J = 7.2 Hz, 3H), 0.96 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 173.05, 161.07, 153.04, 139.46, 131.23, 127.76, 127.23, 124.40, 119.11, 116.43, 61.09, 44.84, 33.79, 20.71, 14.11, 13.76; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{19}\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 275.1278, found 275.1277.



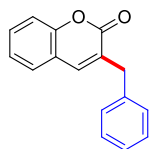
Ethyl 2-methyl-2-(2-oxo-2H-chromen-3-yl)propanoate (5e)⁸

Pale yellow solid (0.2 mmol scale, 16.4 mg, 32% yield) R_f = 0.40 (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.60 (s, 1H), 7.52-7.48 (m, 2H), 7.34-7.26 (m, 2H), 4.15 (q, J = 7.1 Hz, 2H), 1.56 (s, 6H), 1.20 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 175.41, 160.35, 153.05, 136.48, 133.37, 131.05, 127.75, 124.35, 119.09, 116.40, 61.12, 44.63, 24.57, 14.02.



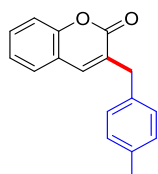
Ethyl 2-methyl-2-(6-methyl-2-oxo-2H-chromen-3-yl)propanoate (5f)⁸

Pale yellow solid (0.2 mmol scale, 16.2 mg, 30% yield) R_f = 0.40 (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.54 (s, 1H), 7.31-7.29 (m, 2H), 7.22-7.20 (m, 1H), 4.14 (q, J = 7.2 Hz, 2H), 2.40 (s, 3H), 1.55 (s, 6H), 1.19 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 175.48, 160.55, 151.16, 136.45, 133.98, 133.19, 132.00, 127.59, 118.82, 116.07, 61.07, 44.59, 24.57, 20.76, 14.00.



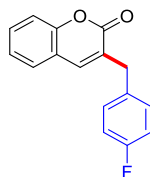
3-Benzyl-2*H*-chromen-2-one (5g)^{3, 6}

Pale yellow solid (0.2 mmol scale, 27.1 mg, 57% yield) $R_f = 0.45$ (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.48-7.44 (m, 1H), 7.38-7.32 (m, 4H), 7.31-7.26 (m, 4H), 7.24-7.20 (m, 1H), 3.90 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): 161.69, 152.99, 139.24, 137.57, 130.76, 129.37, 128.74, 127.35, 126.80, 124.24, 119.35, 116.38, 36.50.



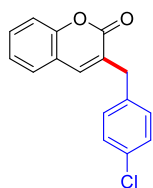
3-(4-Methylbenzyl)-2*H*-chromen-2-one (5h)^{3, 6}

White solid (0.2 mmol scale, 26.3 mg, 53% yield) $R_f = 0.50$ (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.48-7.43 (m, 1H), 7.37-7.34 (m, 1H), 7.32-7.26 (m, 2H), 7.24-7.20 (m, 1H), 7.19-7.15 (m, 4H), 3.86 (s, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 161.73, 152.97, 139.08, 136.38, 134.42, 130.68, 129.60, 129.42, 129.25, 127.31, 124.20, 119.41, 116.36, 36.07, 21.06.



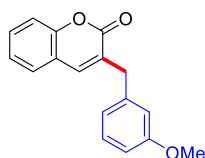
3-(4-Fluorobenzyl)-2*H*-chromen-2-one (5i)^{3, 6}

White solid (0.2 mmol scale, 15.7 mg, 31% yield) $R_f = 0.50$ (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.49-7.45 (m, 1H), 7.39-7.37 (m, 1H), 7.33-7.22 (m, 5H), 7.07-7.01 (m, 2H), 3.87 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): 161.79 (d, $J = 243.5$ Hz), 161.58, 153.05, 139.27, 133.25 (d, $J = 3.1$ Hz), 130.87 (d, $J = 6.3$ Hz), 130.76, 129.17, 127.37, 124.33, 119.28, 116.45, 115.57 (d, $J = 21.2$ Hz), 35.83; ^{19}F NMR (376 MHz, CDCl_3): -116.01 to -116.08 (m, 1F).



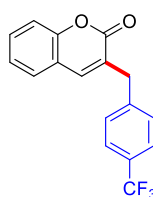
3-(4-Chlorobenzyl)-2H-chromen-2-one (5j)^{3, 6}

Pale yellow solid (0.2 mmol scale, 30.0 mg, 55% yield) R_f = 0.45 (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.49-7.45 (m, 1H), 7.39-7.37 (m, 1H), 7.33-7.30 (m, 4H), 7.26-7.21 (m, 3H), 3.85 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): 161.49, 153.04, 139.38, 136.08, 132.64, 130.94, 130.64, 128.83, 128.77, 127.38, 124.34, 119.21, 116.42, 35.97.



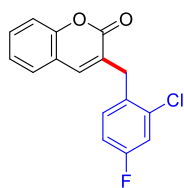
3-(3-Methoxybenzyl)-2H-chromen-2-one (5k)³

White solid (0.2 mmol scale, 30.0 mg, 56% yield) R_f = 0.55 (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.48-7.43 (m, 1H), 7.37-7.35 (m, 1H), 7.32-7.25 (m, 3H), 7.24-7.20 (m, 1H), 6.89-6.87 (m, 1H), 6.85-6.81 (m, 2H), 3.86 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 161.66, 159.80, 152.96, 139.29, 139.13, 130.75, 129.70, 129.11, 127.35, 124.23, 121.66, 119.33, 116.34, 115.03, 112.06, 55.15, 36.46.



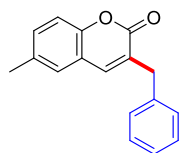
3-(4-(Trifluoromethyl)benzyl)-2H-chromen-2-one (5l)³

Pale yellow solid (0.2 mmol scale, 43.2 mg, 71% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 7:1) ^1H NMR (400 MHz, CDCl_3): δ 7.60-7.58 (m, 2H), 7.50-7.46 (m, 1H), 7.44-7.39 (m, 3H), 7.36 (s, 1H), 7.32-7.30 (m, 1H), 7.27-7.23 (m, 1H), 3.95 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3): 161.41, 153.12, 141.84, 139.71, 131.10, 129.54, 129.09 (q, J = 32.0 Hz), 128.21, 127.43, 125.60 (q, J = 3.7 Hz), 124.41, 124.12 (q, J = 270.2 Hz), 119.13, 116.45, 36.47; ^{19}F NMR (376 MHz, CDCl_3): -62.39 (s, 3F).



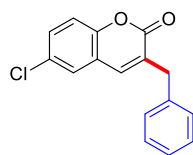
3-(2-Chloro-4-fluorobenzyl)-2H-chromen-2-one (5m)³

Pale yellow solid (0.2 mmol scale, 41.0 mg, 71% yield) ¹H NMR (400 MHz, CDCl₃): δ 7.49-7.45 (m, 1H), 7.40-7.36 (m, 2H), 7.33-7.31 (m, 1H), 7.25-7.21 (m, 2H), 7.18-7.15 (m, 1H), 7.02-6.97 (m, 1H), 3.97 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): 161.55 (d, J = 247.8 Hz), 161.47, 153.01, 139.40, 135.01 (d, J = 10.2 Hz), 132.70 (d, J = 8.6 Hz), 131.09 (d, J = 3.6 Hz), 130.97, 127.47, 126.94, 124.33, 119.18, 117.05 (q, J = 24.5 Hz), 116.42, 114.36 (d, J = 20.9 Hz), 33.57; ¹⁹F NMR (376 MHz, CDCl₃): -113.11 to -113.17 (m, 1F).



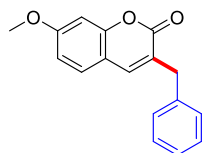
3-Benzyl-6-methyl-2H-chromen-2-one (5n)⁶

Pale yellow solid (0.2 mmol scale, 28.4 mg, 57% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 7:1) ¹H NMR (400 MHz, CDCl₃): δ 7.37-7.33 (m, 2H), 7.29-7.25 (m, 4H), 7.21-7.19 (m, 2H), 7.14 (s, 1H), 3.88 (s, 2H), 2.35 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): 161.92, 151.13, 139.26, 137.68, 133.88, 131.74, 129.38, 129.21, 128.72, 127.21, 126.77, 119.10, 116.09, 36.51, 20.71.



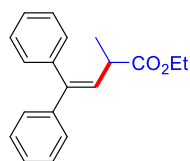
3-Benzyl-6-chloro-2H-chromen-2-one (5o)

White solid (0.2 mmol scale, 26.8 mg, 49% yield) R_f = 0.50 (petroleum ether/ethyl acetate = 7:1) ¹H NMR (400 MHz, CDCl₃): δ 7.43-7.36 (m, 4H), 7.33-7.28 (m, 4H), 7.19 (s, 1H), 3.91 (d, J = 0.8 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): 161.06, 151.34, 137.93, 137.08, 130.79, 130.66, 129.47, 129.39, 128.83, 126.99, 126.64, 120.39, 117.80, 36.55; HRMS (ESI) calcd for C₁₆H₁₂ClO₂⁺ [M+H]⁺ 271.0520, found 271.0518.



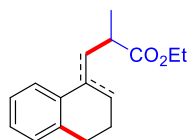
3-Benzyl-7-methoxy-2H-chromen-2-one (5p)⁹

Pale yellow solid (0.2 mmol scale, 17.1 mg, 32% yield) $R_f = 0.45$ (petroleum ether/ethyl acetate = 5:1) ^1H NMR (400 MHz, CDCl_3): δ 7.37-7.33 (m, 2H), 7.30-7.22 (m, 5H), 6.81-6.78 (m, 2H), 3.85 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): 162.03, 161.95, 154.70, 139.39, 137.97, 129.32, 128.68, 128.22, 126.69, 125.69, 112.99, 112.37, 100.38, 55.68, 36.34.



Ethyl 2-methyl-4,4-diphenylbut-3-enoate¹⁰

Yellow liquid (0.4 mmol scale, 62.0 mg, 55% yield) $R_f = 0.30$ (petroleum ether/ethyl acetate = 50:1) ^1H NMR (400 MHz, CDCl_3): δ 7.40-7.31 (m, 3H), 7.28-7.20 (m, 7H), 6.12 (d, $J = 10.2$ Hz, 1H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.27 (qd, $J = 7.1$ Hz, 10.2 Hz, 1H), 1.27 (d, $J = 7.0$ Hz, 3H), 1.25 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 174.92, 142.90, 141.85, 139.35, 129.73, 128.29, 128.10, 127.87, 127.33, 127.29, 60.59, 40.39, 18.47, 14.18.



Ethyl 3-(3,4-dihydronaphthalen-1-yl)-2-methylpropanoate

Colorless liquid (0.2 mmol scale, 8.2 mg, 17% yield; *endo/exo* = 1/0.4, detected by ^1H NMR) $R_f = 0.40$ (petroleum ether/ethyl acetate = 15:1) ^1H NMR (400 MHz, CDCl_3): δ 7.36-7.30 (m, 4.3H), 7.29-7.24 (m, 0.7H), 7.15-7.12 (m, 0.7H), 5.68 (t, $J = 7.2$ Hz, 1H), 5.49 (t, $J = 7.2$ Hz, 0.4H), 4.08-4.00 (m, 2.8H), 3.45 (dt, $J = 7.0$ Hz, 1.5 Hz, 2H), 3.31 (t, $J = 7.0$ Hz, 0.8H), 2.95-2.90 (m, 0.8H), 2.83-2.78 (m, 2H), 2.75-2.68 (m, 0.4H), 2.63-2.58 (m, 1H), 2.51-2.46 (m, 0.8H), 2.44-2.35 (m, 2H), 1.20 (t, $J = 7.1$ Hz, 4.2H), 1.10 (d, $J = 6.6$ Hz, 1.2H), 1.07 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3): 176.18, 141.84, 141.37, 140.42, 139.57, 128.34, 128.30, 128.27, 127.35, 127.22, 127.05, 126.60, 125.80, 60.31, 60.21, 43.37, 38.02, 37.80, 33.50, 32.78, 32.44,

32.10, 31.92, 16.74, 16.60, 14.23, 14.16. HRMS (ESI) calcd for C₁₆H₂₁O₂⁺ [M+H]⁺ 245.1536, found 245.1534.

VI. References

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VII. Copies of ^1H , ^{13}C and ^{19}F NMR Spectra

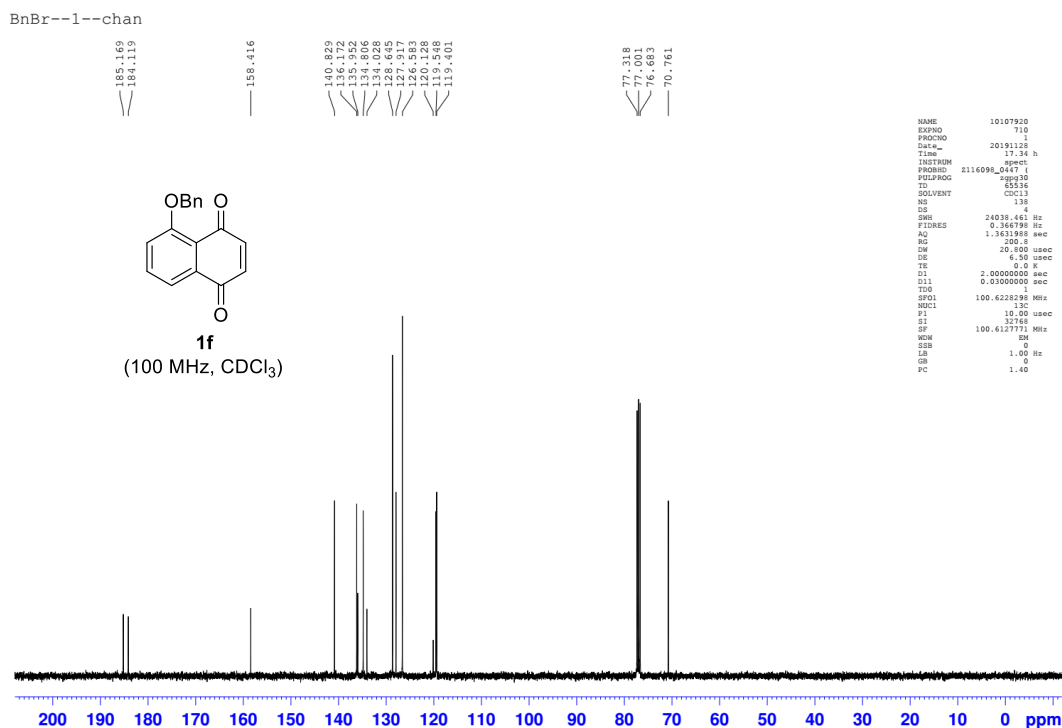
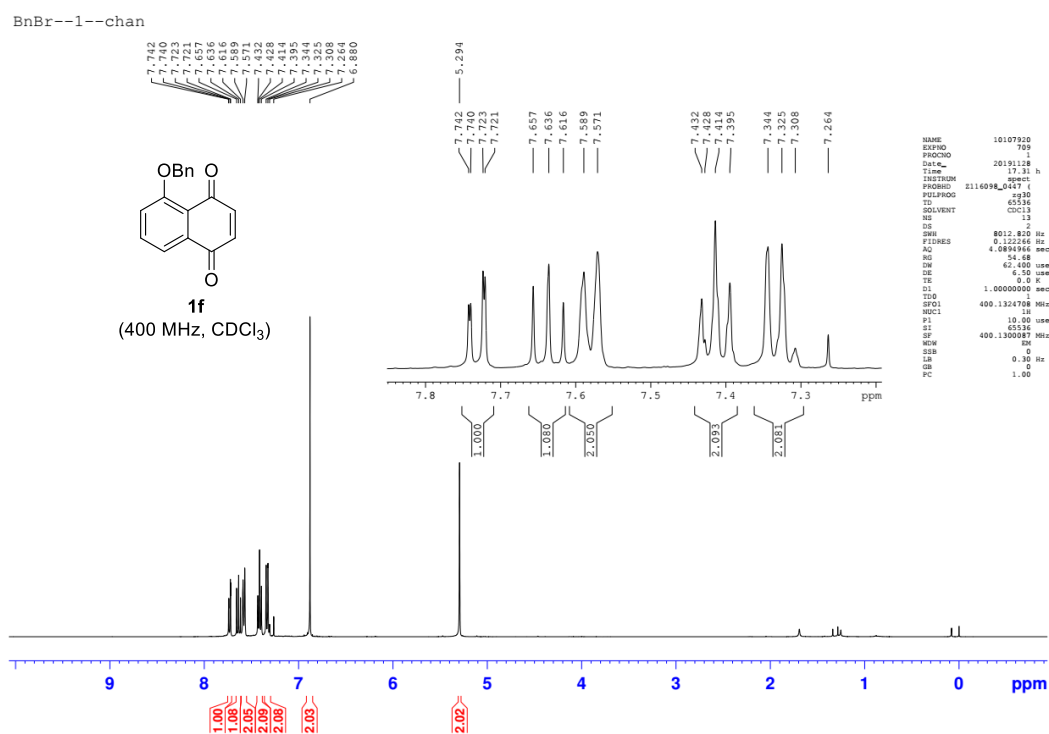


Figure 1 is a dendrogram illustrating the hierarchical clustering of 20 samples based on their genetic profiles. The samples are numbered 1 through 20. The dendrogram shows two main clusters joining at a high distance. The first main cluster consists of a group of samples (1-10) and a group of samples (11-20). The second main cluster consists of a group of samples (1-10) and a group of samples (11-20). The samples are numbered 1 through 20. The dendrogram shows two main clusters joining at a high distance. The first main cluster consists of a group of samples (1-10) and a group of samples (11-20). The second main cluster consists of a group of samples (1-10) and a group of samples (11-20).

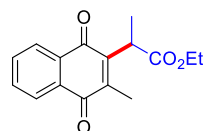
Year	Population (millions)
1980	20
1985	22
1990	24
1995	26
2000	28

—2.193

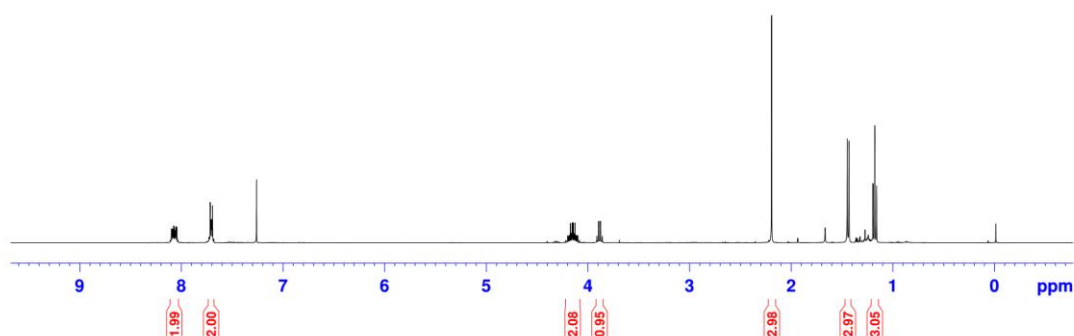
1.449
1.431
1.195
1.178
1.160



NAME	101079-6	
EXPNO	443	
PROCN0	1	
Date_	20190403	
Time	19:44	h
INSTRUM	spect	
PROBHD	Z116098	4447
TD	400.0	MHz
TD0	65536	
NUC1	C13	
NS	16	
DW	8012.820	Hz
FIDRES	0.122264	Hz
AQ	4.0809966	sec
RG	54.68	
DW	62.400	usec
DE	6.50	usec
TE	295.2	K
TD0	1.0000000	MHz
SF01	400.1324708	MHz
NUC1	1H	
P1	10.00	usec
S1	65536	
SCF	400.1300101	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



3a
(400 MHz, CDCl₃)



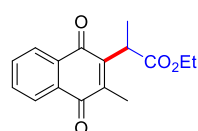
—	185.086
—	183.458
—	172.752
—	146.432
—	143.717
—	133.583
—	135.570
—	131.944
—	131.899
—	126.404
—	126.334

$$\begin{array}{r} 77.316 \\ 76.998 \\ 76.681 \\ \hline \end{array}$$

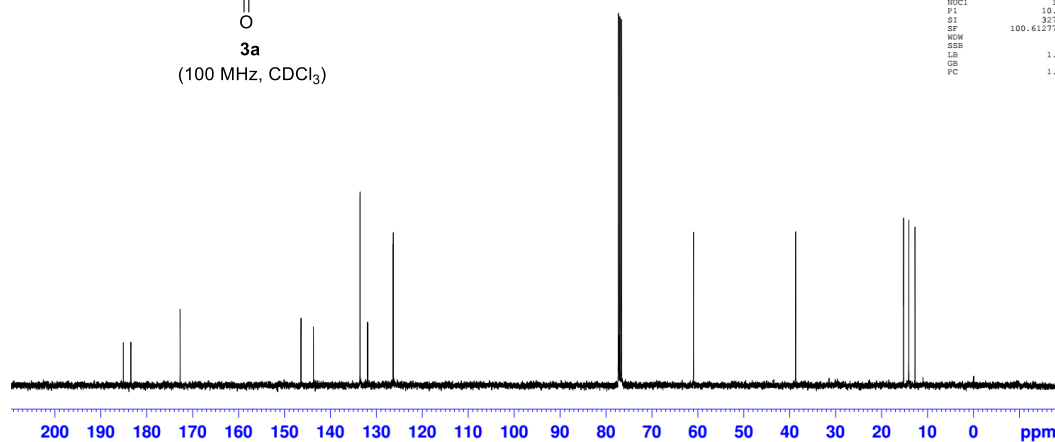
—38.731

$$\begin{array}{r} 15.210 \\ 14.087 \\ 12.731 \end{array}$$

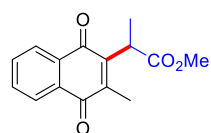
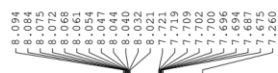
NAME	101079-6
EXPNO	444
PROCNO	
Date_	20100403
Time	20.03
INSTRUM	spect
PROBHD	z116098_0447
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	275
DSH	4
SWH	24038.461
F2FILES	0.3667798
AQ	1.3631988
RG	200.8
DW	20.800
DE	6.50
TE	295.7
D1	2.00000000
D11	0.03000000
TD0	
SI	100.6228298
NUC1	13C
SF01	SI 10.00
SI	32768
NF	612730
SDW	EM
SSB	0
LB	1.00
GB	0
PC	1.40



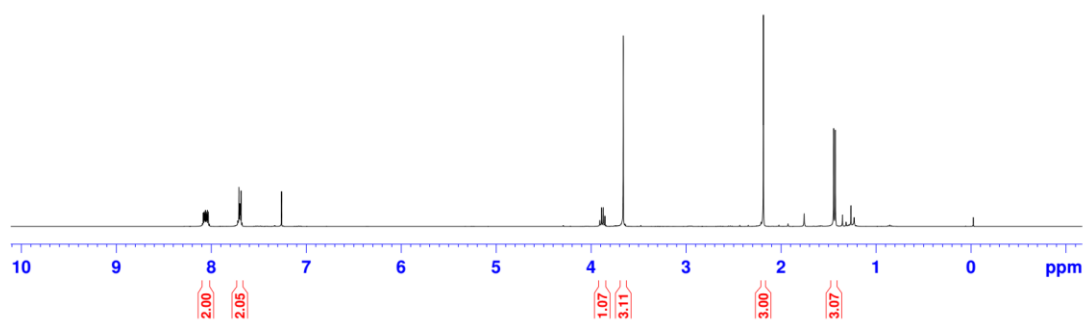
3a
(100 MHz, CDCl₃)



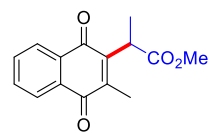
ldk-2019-15 Me-ester TM h23



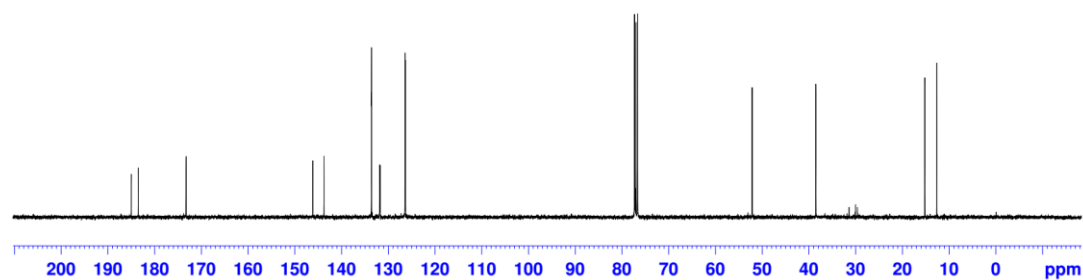
NAME	10107919
EXPNO	23
PROCNO	1
Date_	20190620
Time	18.12 h
INSTRUM	spect
PROBHD	2116098_0447 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122566 Hz
AQ	4.0894966 sec
RG	31
DW	62.400 usec
DE	6.50 usec
TE	290.4 K
D1	1.00000000 sec
TDO	1
SFO1	400.1324708 MHz
NUC1	13
P1	10.00 usec
S1	45536
SF	400.1300100 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



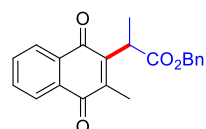
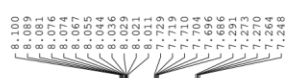
ldk-2019-15 Me-ester TM c24



NAME	10107919
EXPNO	24
PROCNO	1
Date_	20190620
Time	18.30
INSTRUM	spect
PROBHD	2116098_0447 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	300
DS	4
SWH	24038.461
FIDRES	0.366798
AQ	1.3631988
RG	200.8
DW	20.800
DE	6.50
TE	291.1
D1	2.00000000
D11	0.03000000
TDO	1
SFO1	100.6228298
NUC1	13C
P1	10.00
S1	32768
SF	100.6127764
WDW	EM
SSB	0
LB	1.00
GB	0
PC	1.40



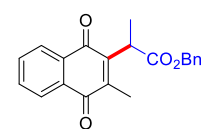
ldk-2019-22 BnOH-ester h 39



3c
(400 MHz, CDCl₃)

```
NAME      10107919
EXPNO     39
PROCNO    1
Date_     20190624
Time      22.43 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg
TD         65536
SOLVENT    CDCl3
NS         16
DS         2
SWH        8812.820 Hz
FIDRES     0.122566 Hz
AQ         4.0894966 sec
RG         31
DM         62.400 usec
DE         6.50 usec
TE         290.2 K
D1         1.00000000 sec
TDS         1
SFO1       400.1324708 MHz
NUC1       13
P1         10.00 usec
B1         60.336
SF         400.1300087 MHz
WDW         0
SSB         0
GB         0.20 Hz
PC         1.00
```

ldk-2019-22 BnOH-ester c 40



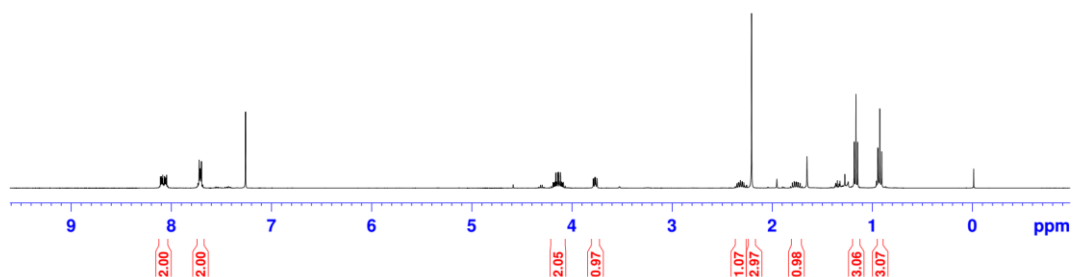
3c
(100 MHz, CDCl₃)

```
NAME      10107919
EXPNO     40
PROCNO    1
Date_     20190624
Time      22.55 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg
TD         65536
SOLVENT    CDCl3
NS         200
DS         2
SWH        24839.461 Hz
FIDRES     0.364798 Hz
AQ         1.3411988 sec
RG         256
DM         20.000 usec
DE         6.50 usec
TE         290.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TDS         1
SFO1       100.6228218 MHz
NUC1       13
P1         10.00 usec
B1         60.32768
SF         100.6177969 MHz
WDW         DM
SSB         0
GB         1.00 Hz
PC         1.40
```

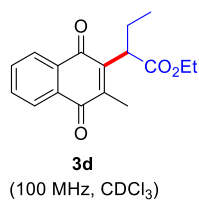
ldk-2019-18 Butyl-ester h29



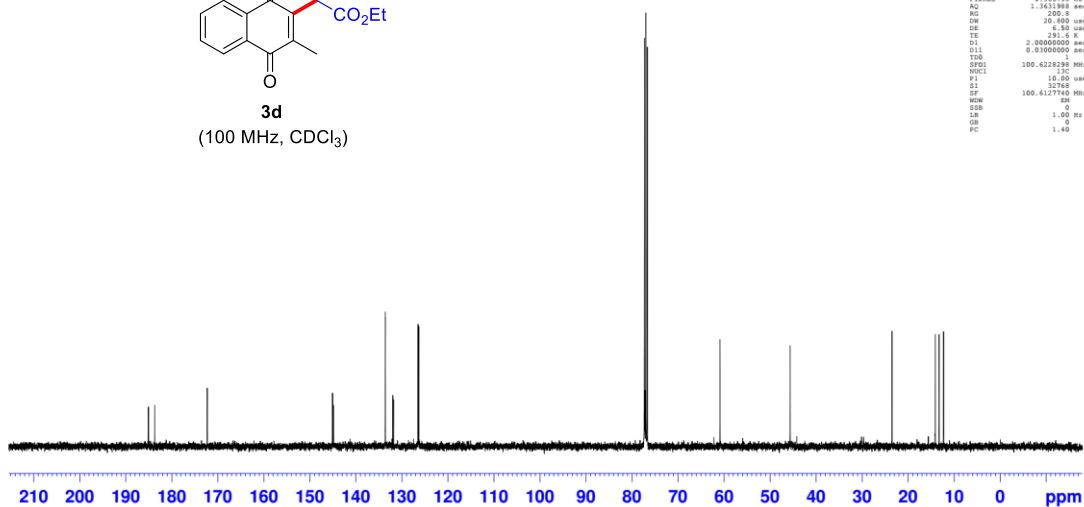
NAME 10107919
EXPNO 29
PROCNO 1
Date_ 20190622
Time 17.22 h
INSTRUM spect
PROBHD 511609H_0471
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 8012.822 Hz
FIDRES 0.122268 Hz
AQ 1.088961 sec
RG 64.00
WDW EM
SSB 0.000000
LB 62.100 uHz
GB 0.00
PC 1.000000000
TD 400.1324700 MHz
NUC1 13C
P1 10.00 uHz
PI 65536
RG 400.1300000 MHz
SOLV CDCl3
LB 0.30 Hz
GB 0.00
PC 1.00



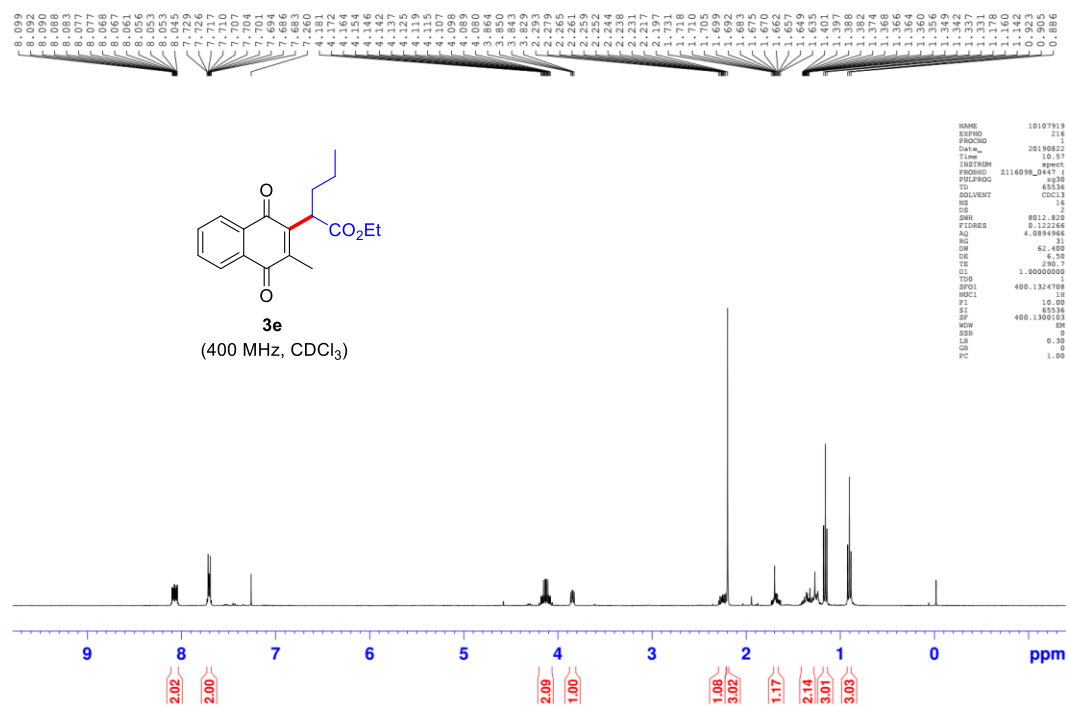
ldk-2019-18 Butyl-ester c36 new



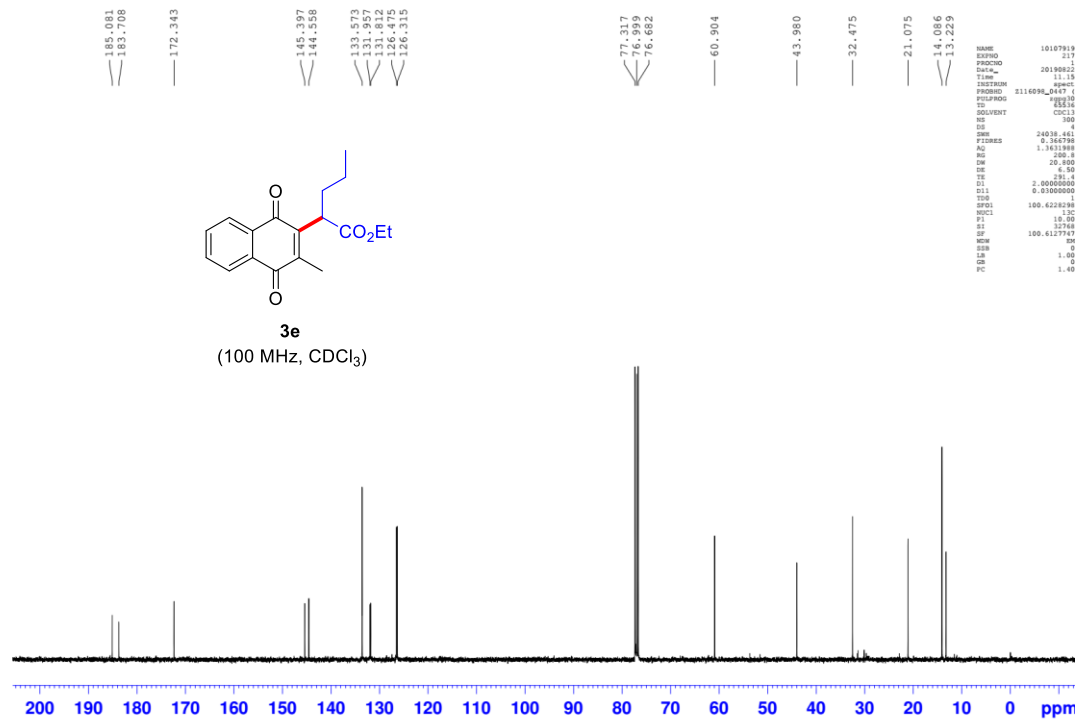
NAME 10107919
EXPNO 36
PROCNO 1
Date_ 20190622
Time 18.33 h
INSTRUM spect
PROBHD 511609H_0471
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24039.461 Hz
FIDRES 0.264798 Hz
AQ 1.361180 sec
RG 64.00
WDW EM
SSB 0.000000
LB 62.100 uHz
GB 0.00
PC 1.000000000
TD 100.6228290 MHz
NUC1 13C
P1 10.00 uHz
PI 65536
RG 100.6127740 MHz
SOLV CDCl3
LB 0.30 Hz
GB 0.00
PC 1.40



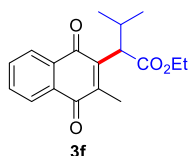
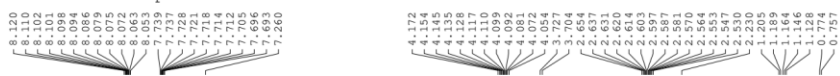
ldk-2019-107 BQ wu-ester 216 h



ldk-2019-107 BQ wu-ester 217c

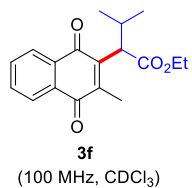


ldk-2019-119 new iso-pro ester 235 h



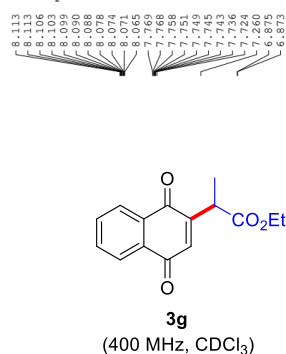
NAME 10107919
EXPNO 219
PROCNO 1
Date_ 20190802
Time 15.24 h
INSTRUM spect
PROBHD 5116098_0447 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
F2FILES 8012.820 Hz
AQ 0.122564 Hz
RG 4.0893965 Hz
DE 2.19
TE 300.2 K
DE 62.500 MHz
TE 300.2 K
D1 1.00000000 Hz
D11 10.00
HQC1 400.1324798 MHz
P1 10.00
RF 400.1324798 MHz
WDSW 400.1324798 MHz
SFO 400.1324798 MHz
GB 0.00
PC 1.00

ldk-2019-108 BQ iso-pro ester 219 c



NAME 10107919
EXPNO 219
PROCNO 1
Date_ 20190802
Time 12.44 h
INSTRUM spect
PROBHD 5116098_0447 (1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
F2FILES 240.981461 Hz
AQ 0.366798 Hz
RG 1.3631985 Hz
DE 200.8 Hz
TE 300.2 K
DE 62.500 MHz
TE 300.2 K
D1 2.00000000 Hz
D11 10.00
HQC1 100.6238235 MHz
P1 10.00
RF 100.6238235 MHz
WDSW 100.6238235 MHz
SFO 100.6238235 MHz
GB 0.00
PC 1.00

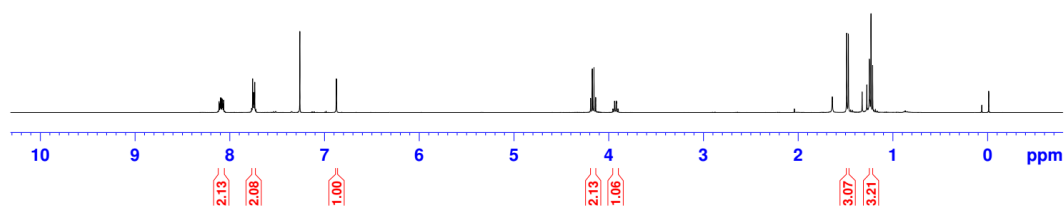
ldk-2019-01 naph 07 h new



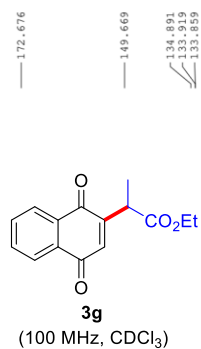
```

NAME      10107919
EXPNO     7
PROCNO    1
Date_     20190608
Time      17.53 h
INSTRUM   spect
PROBHD    z116098_0417
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        8012.410 Hz
FIDRES     0.122566 Hz
AQ         4.0894966 sec
RG          72.26
DW         62.400 usec
DE         6.50 usec
TE         291.5 K
D1         1.00000000 sec
TDO        1
SFO1       400.1324708 MHz
NUC1       1H
P1         10.00 usec
SI         65536
SF         400.1300102 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00

```



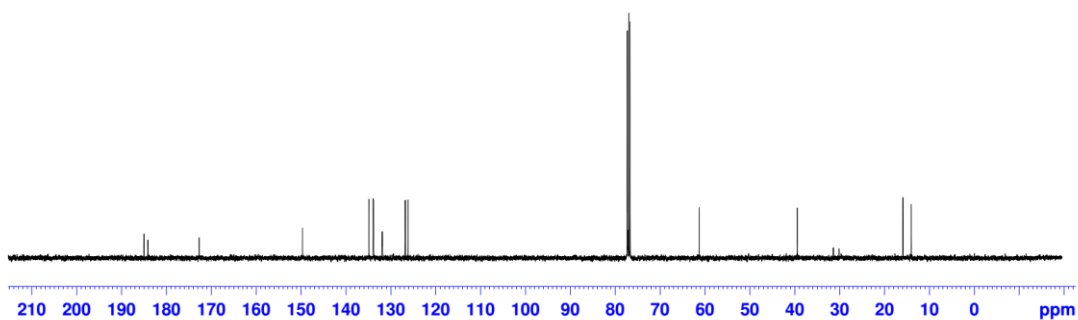
ldk-2019-01 naph 08 C new



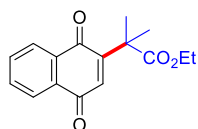
```

NAME      10107919
EXPNO     8
PROCNO    1
Date_     20190608
Time      18.03 h
INSTRUM   spect
PROBHD    z116098_0417
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         150
DS         4
SWH       24038.461 Hz
FIDRES     9.366798 Hz
AQ        1.3631998 sec
RG         289.8
DW        20.800 usec
DE         6.50 usec
TE         291.7 K
D1         2.00000000 sec
D11        0.01000000 sec
TDO        1
SFO1       100.6228298 MHz
NUC1       13C
P1         10.00 usec
SI         32768
SF         100.6127740 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40

```

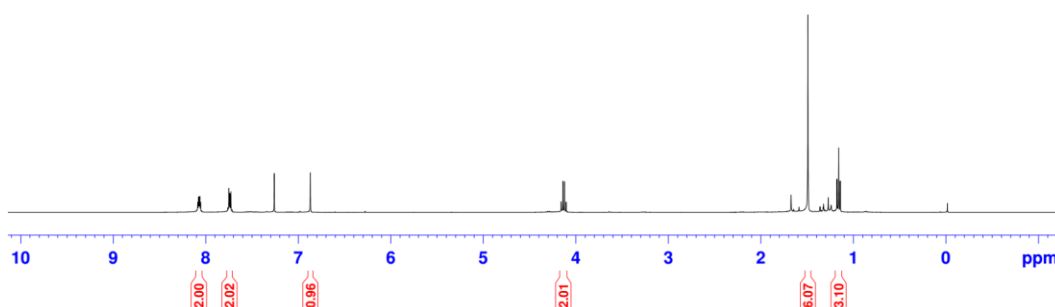


ldk-2019-09 naph-diMe h 15

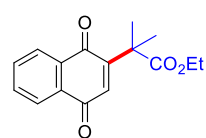


(400 MHz, CDCl₃)

```
NAME 10107919
EXPNO 15
PROCNO 1
Date_ 20190612
Time 17.23
INSTRUM spect
PROBHD 5116098_0447
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.810 Hz
FIDRES 0.122246 Hz
AQ 4.0884948 sec
RG 54.68
DM 62.400 um
DE 6.50 um
TE 301.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1324708 MHz
NUC1 13
P1 10.00 um
S1 45334
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

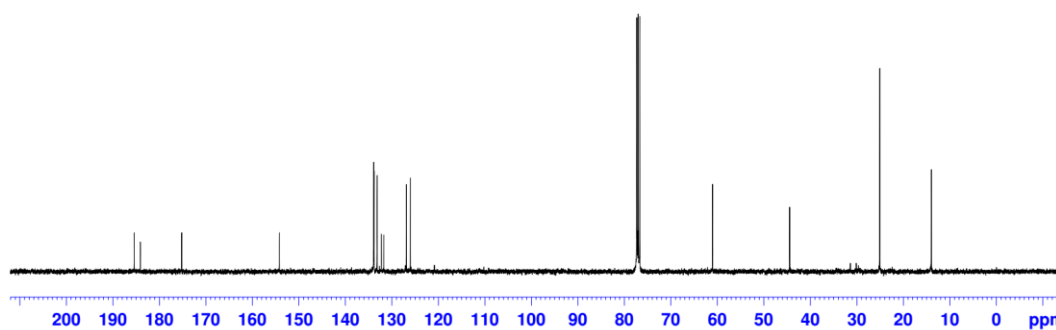


ldk-2019-09 naph-diMe c 16

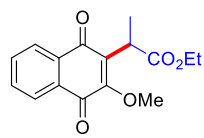
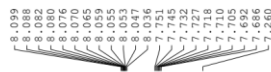


(100 MHz, CDCl₃)

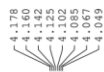
```
NAME 10107919
EXPNO 16
PROCNO 1
Date_ 20190612
Time 17.13
INSTRUM spect
PROBHD 5116098_0447
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 560
DS 2
SWH 24618.641 Hz
FIDRES 0.1364798 Hz
AQ 1.361188 sec
RG 200.8
DM 30.000 um
DE 6.50 um
TE 301.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SF01 100.6228288 MHz
NUC1 13
P1 10.00 um
S1 32766
SF 100.6127748 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```



ldk-2019-97 BQ MeO ester 196 h



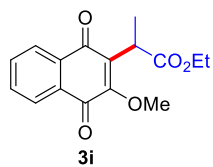
3i
(400 MHz, CDCl₃)



```

NAME      10107919
EXPNO    196
PROCNO    1
Date_     20190814
Time      18.22 h
INSTRUM   spect
PROBHD    511699H_01
PULPROG    zgpg30
TD        65536
SOLVENT    CDCl3
NS         1624
DS         4
SWH        8012.820 Hz
FIDRES     0.122144 Hz
AQ         4.0059365 sec
RG         65.87
DM         62.400 usec
DE         390.3 K
TE         1.00000000 sec
D11        0.00000000 sec
TOD        400.1324704 MHz
SFO1       100.6228198 MHz
P1         18.00 usec
SI         0.00000000 sec
SF         400.1324704 MHz
WDW         0
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```

ldk-2019-97 BQ MeO ester 197 c

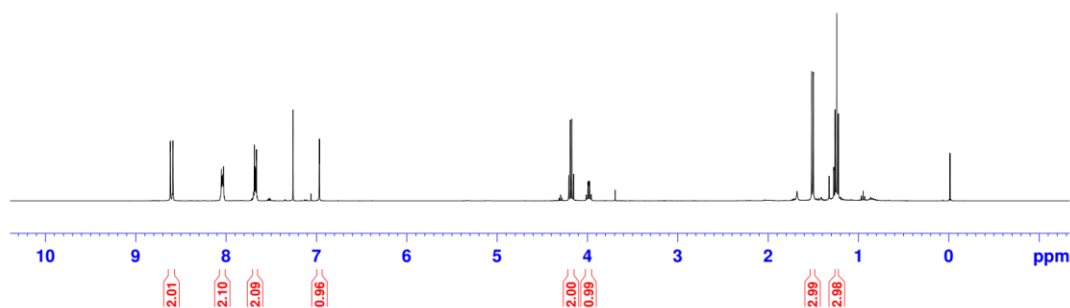
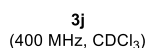


3i
(100 MHz, CDCl₃)

```

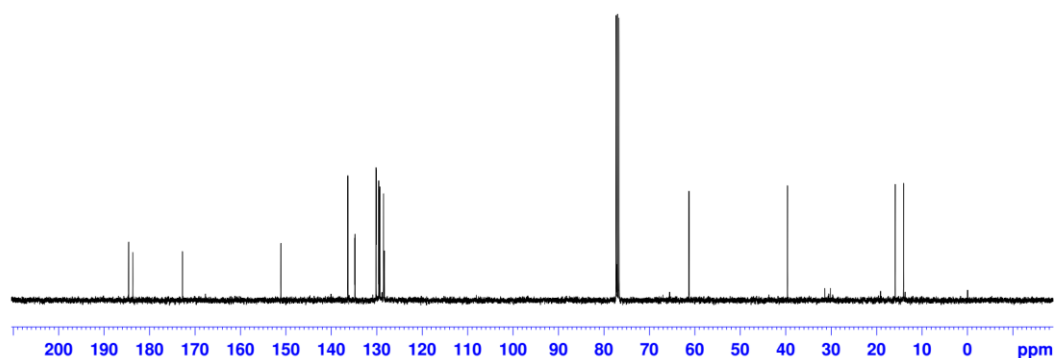
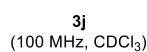
NAME      10107919
EXPNO    197
PROCNO    1
Date_     20190814
Time      19.21 h
INSTRUM   spect
PROBHD    511699H_01
PULPROG    zgpg30
TD        65536
SOLVENT    CDCl3
NS         1624
DS         4
SWH        24038.46 Hz
FIDRES     0.346798 Hz
AQ         1.3631388 sec
RG         200.8
DM         62.400 usec
DE         390.3 K
TE         1.00000000 sec
D11        0.00000000 sec
TOD        100.6228198 MHz
SFO1       100.6228198 MHz
P1         18.00 usec
SI         0.00000000 sec
SF         100.6127732 MHz
WDW         0
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```


8.618
8.597
8.589
8.065
8.054
8.046
8.038
8.030
8.019
7.697
7.689
7.681
7.673
7.665
7.658
7.657
7.655
7.260
6.970
6.967



NAME	10107920
EDNO	23
PROCNO	1
Date_	20191127
Time	3.59 hr
INSTRUM	sp
PROBHD	2116098.0447
PULPRG	n330
PRG	65336
TO SOLVENT	CDCl3
DS	16
NS	2
SWH	801.2 820 Hz
FIDRES	0.1222466
RG	4.00 18465 sec
RG	48.69
DW	62.400 usec
DE	6.50 usec
TE	0.0 K
T0	1.00000000 MHz
TD1	1
SFO1	400.1324798 MHz
NUC1	1H
F1	10.400 usec
SI	65336
SF	400.1300103 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
RB	1.00

184.593
183.689
182.740
181.804
180.866
179.928
178.990
178.052
177.114
176.176
175.238
174.300
173.362
172.424
171.486
170.548
169.610
168.672
167.734
166.796
165.858
164.920
163.982
163.044
162.106
161.168
160.230
159.292
158.354
157.416
156.478
155.540
154.602
153.664
152.726
151.788
150.850
149.912
148.974
148.036
147.098
146.160
145.222
144.284
143.346
142.408
141.470
140.532
139.594
138.656
137.718
136.780
135.842
134.904
133.966
133.028
132.090
131.152
130.214
129.276
128.338
127.400
126.462
125.524
124.586
123.648
122.710
121.772
120.834
119.896
118.958
118.020
117.082
116.144
115.206
114.268
113.330
112.392
111.454
110.516
109.578
108.640
107.702
106.764
105.826
104.888
103.950
103.012
102.074
101.136
100.198
99.260
98.322
97.384
96.446
95.508
94.570
93.632
92.694
91.756
90.818
89.880
88.942
88.004
87.066
86.128
85.190
84.252
83.314
82.376
81.438
80.500
79.562
78.624
77.686
76.748
75.810
74.872
73.934
72.996
72.058
71.120
70.182
69.244
68.306
67.368
66.430
65.492
64.554
63.616
62.678
61.740
60.802
59.864
58.926
57.988
57.050
56.112
55.174
54.236
53.298
52.360
51.422
50.484
49.546
48.608
47.670
46.732
45.794
44.856
43.918
42.980
42.042
41.104
40.166
39.228
38.290
37.352
36.414
35.476
34.538
33.600
32.662
31.724
30.786
29.848
28.910
27.972
27.034
26.096
25.158
24.220
23.282
22.344
21.406
20.468
19.530
18.592
17.654
16.716
15.778
14.840
13.902
12.964
12.026
11.088
10.150
9.212
8.274
7.336
6.398
5.460
4.522
3.584
2.646
1.708
0.770
-0.168
-1.130
-2.092
-3.054
-4.016
-4.978
-5.940
-6.902
-7.864
-8.826
-9.788
-10.750
-11.712
-12.674
-13.636
-14.598
-15.560
-16.522
-17.484
-18.446
-19.408
-20.370
-21.332
-22.294
-23.256
-24.218
-25.180
-26.142
-27.104
-28.066
-29.028
-29.990
-30.952
-31.914
-32.876
-33.838
-34.800
-35.762
-36.724
-37.686
-38.648
-39.610
-40.572
-41.534
-42.496
-43.458
-44.420
-45.382
-46.344
-47.306
-48.268
-49.230
-50.192
-51.154
-52.116
-53.078
-54.040
-55.002
-55.964
-56.926
-57.888
-58.850
-59.812
-60.774
-61.736
-62.698
-63.660
-64.622
-65.584
-66.546
-67.508
-68.470
-69.432
-70.394
-71.356
-72.318
-73.280
-74.242
-75.204
-76.166
-77.128
-78.090
-79.052
-80.014
-80.976
-81.938
-82.900
-83.862
-84.824
-85.786
-86.748
-87.710
-88.672
-89.634
-90.596
-91.558
-92.520
-93.482
-94.444
-95.406
-96.368
-97.330
-98.292
-99.254
-100.216
-101.178
-102.140
-103.102
-104.064
-105.026
-105.988
-106.950
-107.912
-108.874
-109.836
-110.798
-111.760
-112.722
-113.684
-114.646
-115.608
-116.570
-117.532
-118.494
-119.456
-120.418
-121.380
-122.342
-123.304
-124.266
-125.228
-126.190
-127.152
-128.114
-129.076
-130.038
-130.999
-131.961
-132.923
-133.885
-134.847
-135.809
-136.771
-137.733
-138.695
-139.657
-140.619
-141.581
-142.543
-143.505
-144.467
-145.429
-146.391
-147.353
-148.315
-149.277
-150.239
-151.201
-152.163
-153.125
-154.087
-155.049
-156.011
-156.973
-157.935
-158.897
-159.859
-160.821
-161.783
-162.745
-163.707
-164.669
-165.631
-166.593
-167.555
-168.517
-169.479
-170.441
-171.403
-172.365
-173.327
-174.289
-175.251
-176.213
-177.175
-178.137
-179.099
-180.061
-181.023
-181.985
-182.947
-183.909
-184.871
-185.833
-186.795
-187.757
-188.719
-189.681
-190.643
-191.605
-192.567
-193.529
-194.491
-195.453
-196.415
-197.377
-198.339
-199.301
-200.263
-201.225
-202.187
-203.149
-204.111
-205.073
-206.035
-206.997
-207.959
-208.921
-209.883
-210.845
-211.807
-212.769
-213.731
-214.693
-215.655
-216.617
-217.579
-218.541
-219.503
-220.465
-221.427
-222.389
-223.351
-224.313
-225.275
-226.237
-227.199
-228.161
-229.123
-230.085
-231.047
-232.009
-232.971
-233.933
-234.895
-235.857
-236.819
-237.781
-238.743
-239.705
-240.667
-241.629
-242.591
-243.553
-244.515
-2



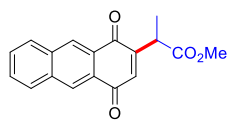
NAME	10107920
EXPNO	24
PROCNO	1
Date_	20191127
Time	12.2 h
INSTRUM	apert
PROBHD	E116098-047
SOLVENT	apert
PULPROG	205536
FOV	220
NS	C23
DS	4
SWH	24038.461 Hz
FIDRES	0.36678 Hz
AQ	1.3631988 sec
RG	200.8
DW	20.860 usec
DE	6.50 usec
TE	0.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	
SI	100.6228298 MHz
NUC1	13C
P1	10.60 usec
PI	3.7668
SD	100.6127747 MHz
RF	EM
SSB	0
LS	1.00 Hz
PC	0
RC	1.40

ldk-2020-18 enBQ-Me-ester h29

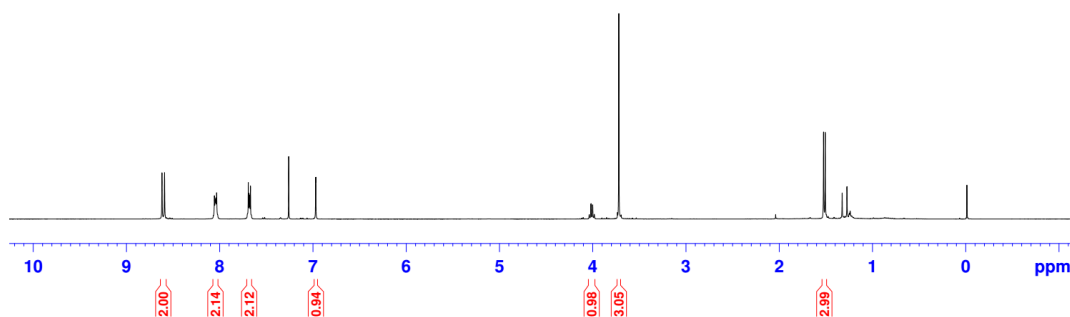
8.619
8.591
8.056
8.048
8.033
8.022
7.993
7.978
7.670
7.560
6.971
6.969

4.037
4.033
4.003
3.984
3.721
3.721

1.525
1.507



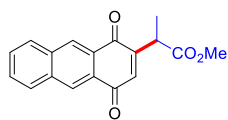
3k
(400 MHz, CDCl₃)



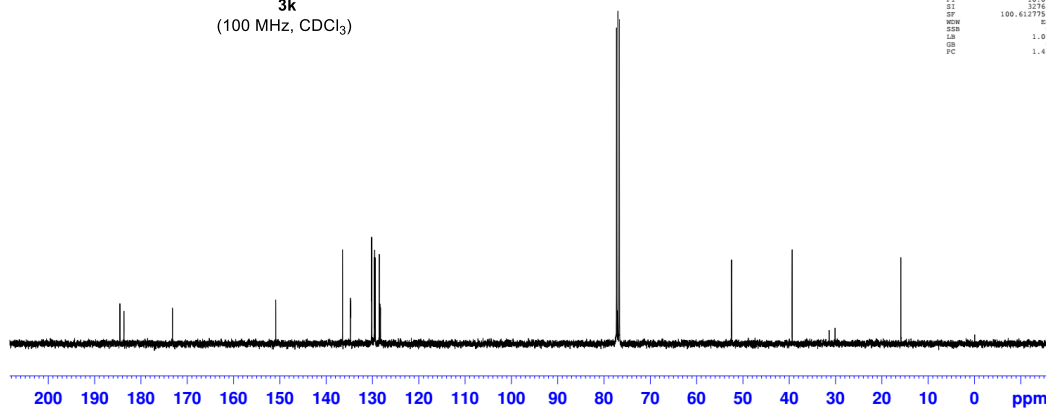
NAME 10107920
EXPNO 29
PROCNO 1
DATE_ 20191130
TIME 17.29 h
INSTRUM spect
PROBHD z116099_0447 f
PULPROG zgpg30
TD 65516
SOLVENT CDCl3
NS 14
DS 1
SWH 8012.820 Hz
FIDRES 0.122164 Hz
AQ 4.0894966 sec
RG 64.68
DW 62.400 usec
DE 6.50 usec
TE 0.0 K
D1 1.00000000 sec
TD0
SFO1 400.1324705 MHz
NUC1 13C
P1 10.00 usec
SI 65516
SF 400.1306103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ldk-2020-18 enBQ-Me-ester c30

186.552
185.676
173.207
150.893
136.471
136.462
134.780
130.188
130.159
130.159
127.539
127.383
126.596
126.596
126.271
77.313
76.996
76.678
52.477
39.388
15.909

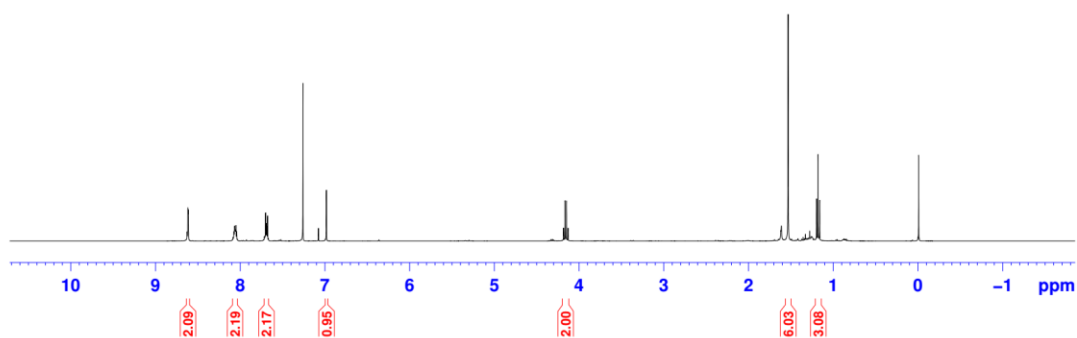
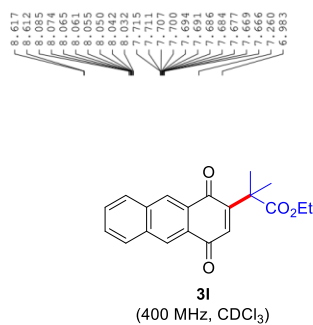


3k
(100 MHz, CDCl₃)



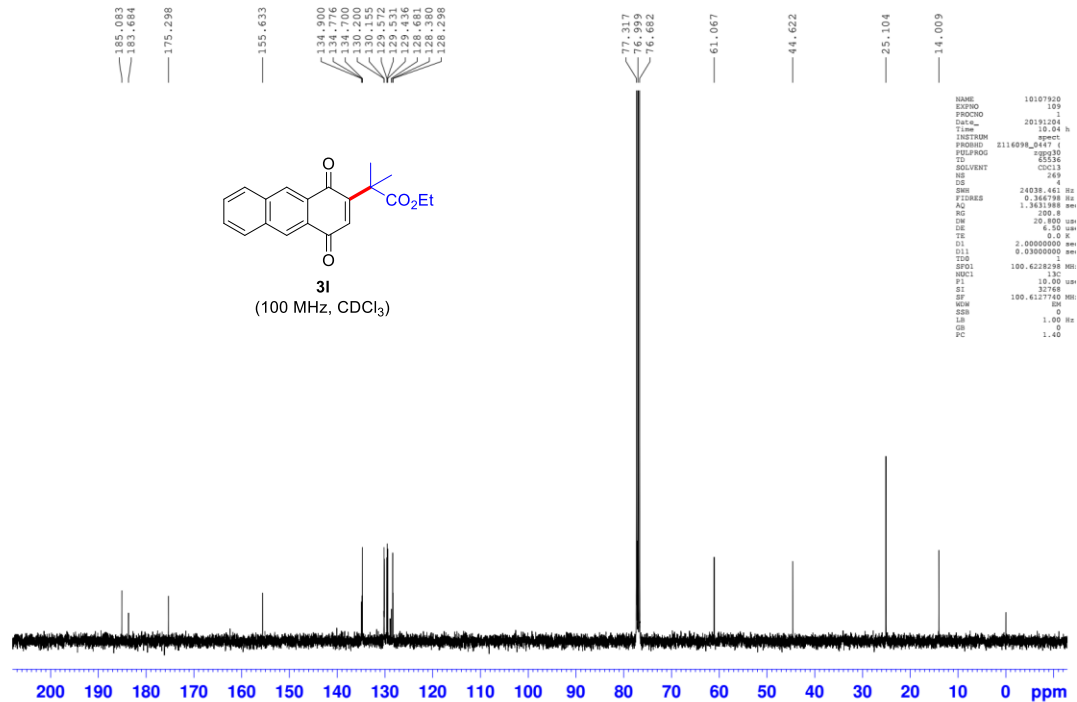
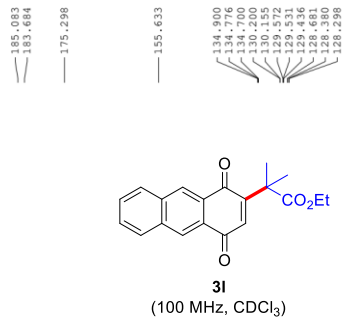
NAME 10107920
EXPNO 30
PROCNO 1
DATE_ 20191130
TIME 17.38 h
INSTRUM spect
PROBHD z116099_0447 f
PULPROG zgpg30
TD 65516
SOLVENT CDCl3
NS 14
DS 14
SWH 24819.44 Hz
FIDRES 0.366799 Hz
AQ 1.3611988 sec
RG 200.8
DW 20.500 usec
DE 6.50 usec
TE 0.0 K
D1 2.00000000 sec
D11 0.01000000 sec
TD0
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 12768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

ldk-2020-100 naBQ-di-Me 100h



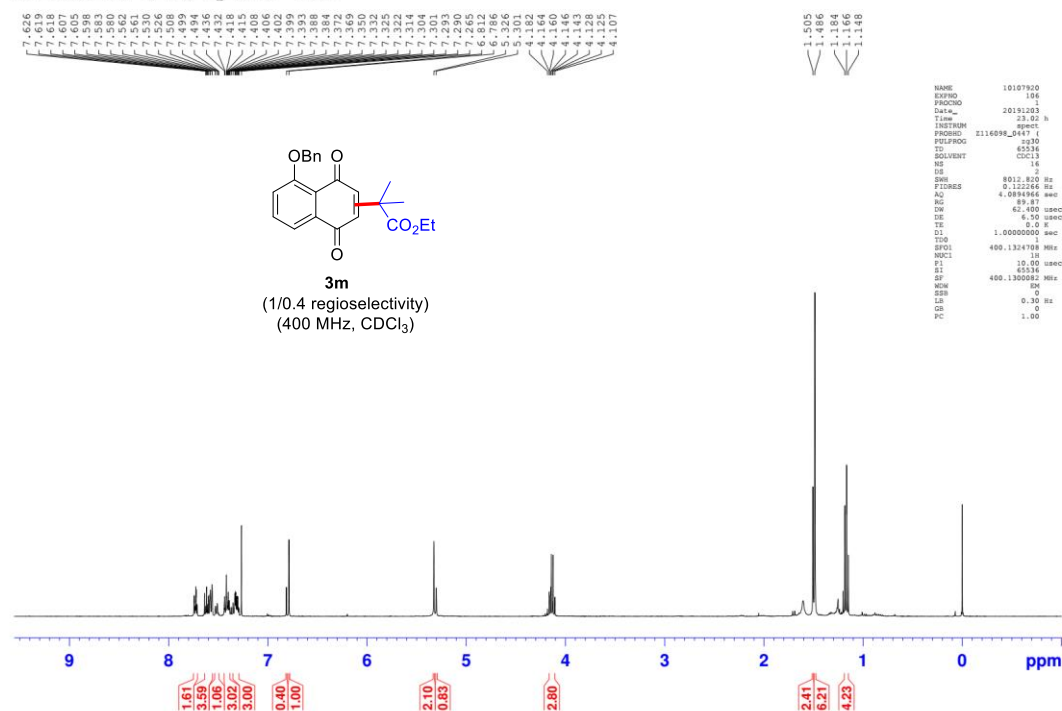
NAME	10107920
EXPNO	100
PROCNO	1
DATA_	20191203
Time	21.40 h
INSTRUM	spmt
PROBHD	2116098_0417 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122466 Hz
AQ	4.0894866 sec
RG	79.46
DM	63.400 usec
DE	6.50 usec
TE	300.2 K
D1	1.00000000 sec
TDO	4
SFO1	400.1324708 MHz
NUC1	13C
FI	10.00 usec
SI	65536
SF	400.1300103 MHz
WDW	RM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

ldk-2020-100 naBQ-di-Me 109c

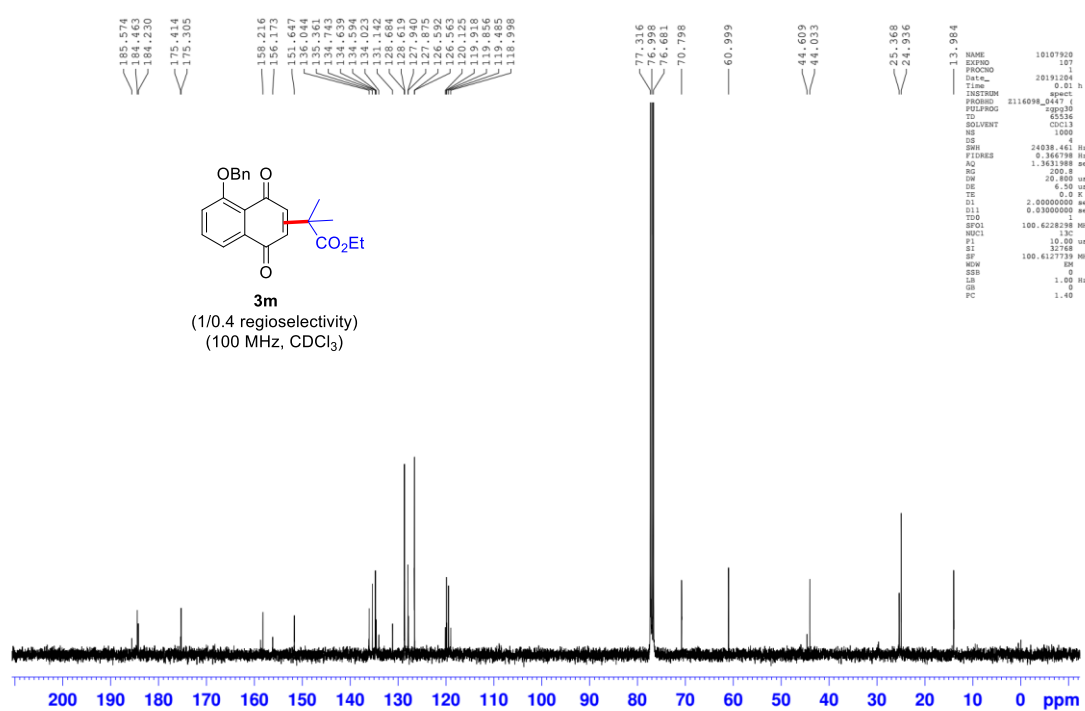


NAME	10107920
EXPNO	109
PROCNO	1
DATA_	20191204
Time	18.04 h
INSTRUM	spmt
PROBHD	2116098_0417 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	249
DS	4
SWH	24030.441 Hz
FIDRES	0.260708 Hz
AQ	1.3431398 sec
RG	200.8
DM	28.800 usec
DE	6.50 usec
TE	300.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	100.6228298 MHz
SFO1	100.6228298 MHz
NUC1	13C
FI	10.00 usec
SI	32768
SF	100.6217750 MHz
WDW	RM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

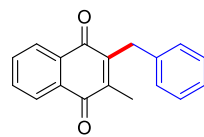
1dk-2020-104 5-BnO-BQ-diMe 106h



1dk-2020-104 5-BnO-BQ-diMe 107c



ldk-2019-29 naph-BnBr h55

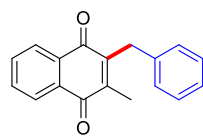


(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Data_     20190620
Time      18.52 h
INSTRUM   spect
PROBHD    B116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         146
DS         4
SWH        8012.820 Hz
F2FRES     0.122268 Hz
AQ         4.0984944 sec
RG         62.400 usec
DE         6.50 usec
TE         291.2 K
D1         1.00000000 sec
TDS
SFO1      400.1324700 MHz
NUC1       13C
P1         10.00 usec
PL         0.00 dB
SF         400.1300100 MHz
WDW        EM
GB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```

ldk-2019-29 naph-BnBr c56

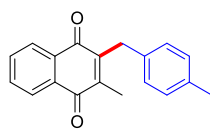
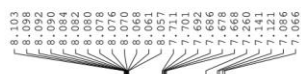


(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Data_     20190620
Time      19.02 h
INSTRUM   spect
PROBHD    B116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         146
DS         4
SWH        24038.461 Hz
F2FRES     0.364798 Hz
AQ         1.3431988 sec
RG         200.0
DE         6.50 usec
TE         291.2 K
D1         2.00000000 sec
TDS
SFO1      100.6228298 MHz
NUC1       13C
P1         10.00 usec
PL         0.00 dB
SF         100.6127791 MHz
WDW        EM
GB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```

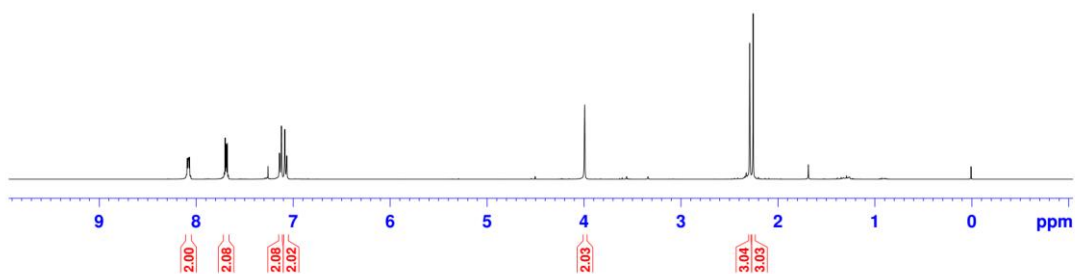
ldk-2019-38 naBQ-p-Me Bn new 79 h



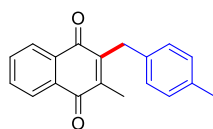
4b
(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190701
Time      23.03 h
INSTRUM   spect
PROBHD    E116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.810 Hz
FIDRES     0.122246 Hz
AQ         4.0894966 sec
RG         31
DW         62.400 usec
DE         6.50 usec
TE         290.2 K
D1         1.0000000 sec
TDO        1
SFO1       400.1324708 MHz
NUC1       13
P1         10.00 usec
SI         65536
SF         400.1300102 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



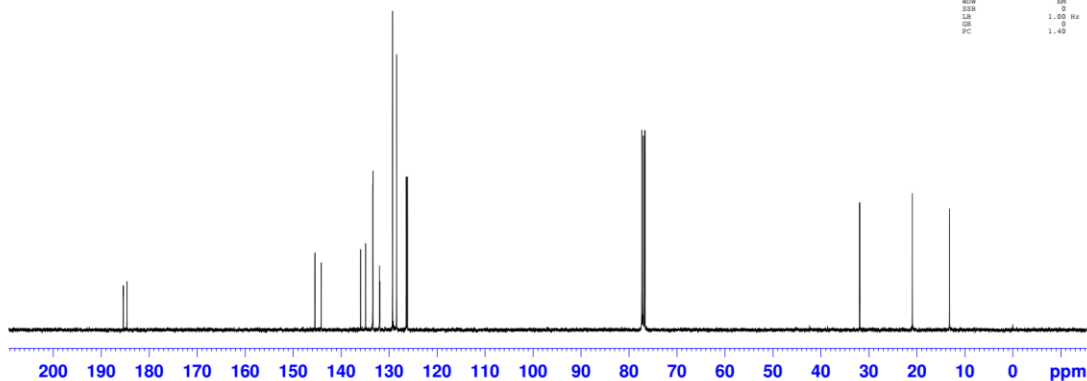
ldk-2019-38 naBQ-p-Me Bn new 80 c



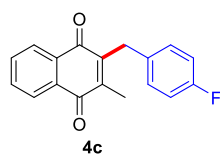
4b
(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190701
Time      23.13 h
INSTRUM   spect
PROBHD    E116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         330
DS         2
SWH        24039.461 Hz
FIDRES     0.364789 Hz
AQ         1.3631988 sec
RG         200.0
DW         20.800 usec
DE         6.50 usec
TE         290.2 K
D1         2.0000000 sec
TDO        0.0300000 sec
SFO1       100.628296 MHz
NUC1       13
P1         10.00 usec
SI         32768
SF         100.6127777 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



ldk-2019-34 naBQ-p-F-Bn 68 h

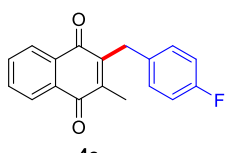


(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190731
Time      17.35 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         1
SWH        801.240 MHz
FIDRES     0.122244 Hz
AQ         4.084936 sec
RG         62.400 usec
DE         290.8 K
TE         1.0000000 sec
D1         1.0000000 sec
TDO        400.1324768 MHz
NUC1       13C
P1         10.00 usec
SI         65536
SF         400.1300100 MHz
WDW        EM
SSB        0
GB         0.30 Hz
PC         1.40
  
```

ldk-2019-34 naBQ-p-F-Bn 69 c

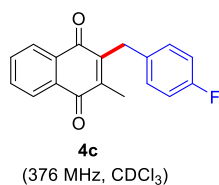


(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190731
Time      17.53 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         1
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.363188 sec
RG         200.8
DE         290.8 K
TE         1.0000000 sec
D1         2.00000000 sec
D11        0.03000000 sec
TDO        100.6228258 MHz
NUC1       13C
P1         10.00 usec
SI         32768
SF         100.6127764 MHz
WDW        EM
SSB        0
GB         1.00 Hz
PC         1.40
  
```

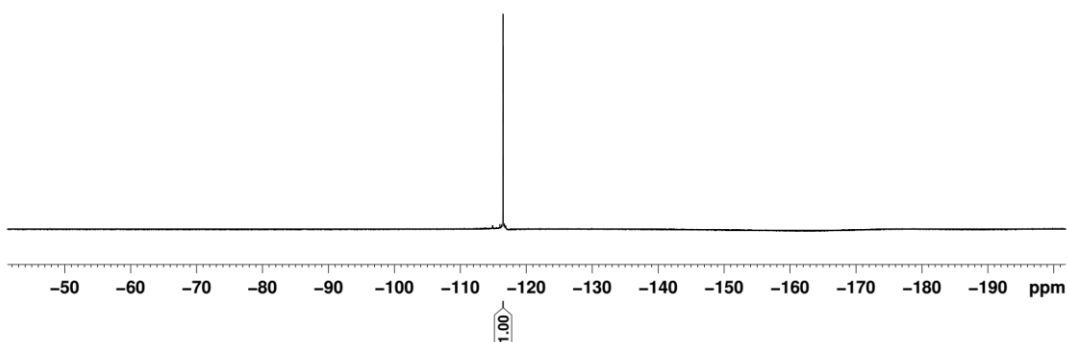
ldk-2019-34 naBQ-p-F-Bn 70 f



-116.44
-116.45
-116.46
-116.47
-116.48
-116.49
-116.51

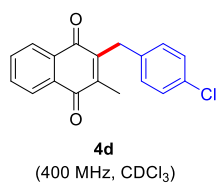
```

NAME      10107919
EXPNO     70
PROCNO    1
Date_     20190701
Time      17.55 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        89285.711 Hz
FIDRES     0.681196 Hz
AQ         0.7348532 sec
RG          200.8
DW          5.600 usec
DE          6.50 usec
TE         290.1 K
D1         1.00000000 sec
SFO1       376.4607164 MHz
NUC1       19F
P1         18.00 usec
SI         65536
SF         376.4983662 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
  
```



ldk-2019-59 naBQ p-Cl Bn 117 h

8.102
8.098
8.093
8.076
8.069
8.064
8.054
8.050
7.721
7.721
7.721
7.711
7.703
7.697
7.693
7.688
7.260
7.243
7.233
7.232
7.221
7.215
7.210
7.205
7.169
7.164
7.153
7.148

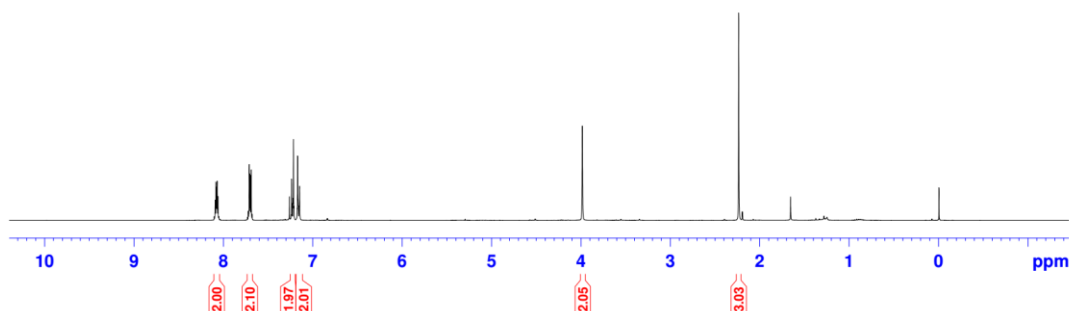


— 3.985

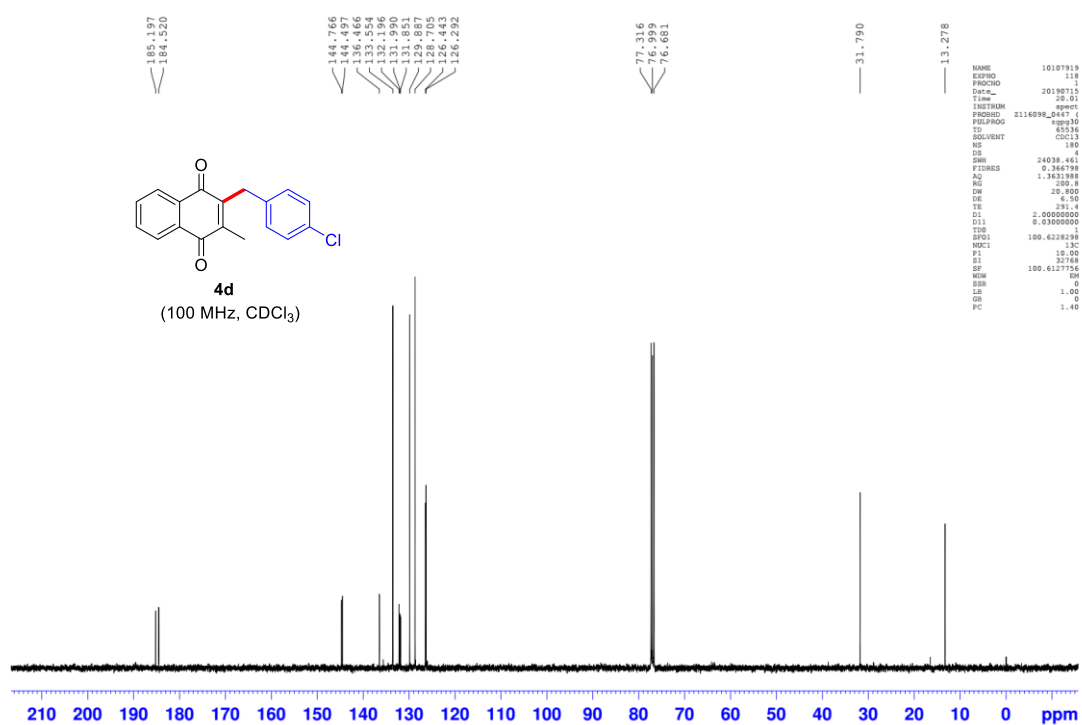
— 2.235

```

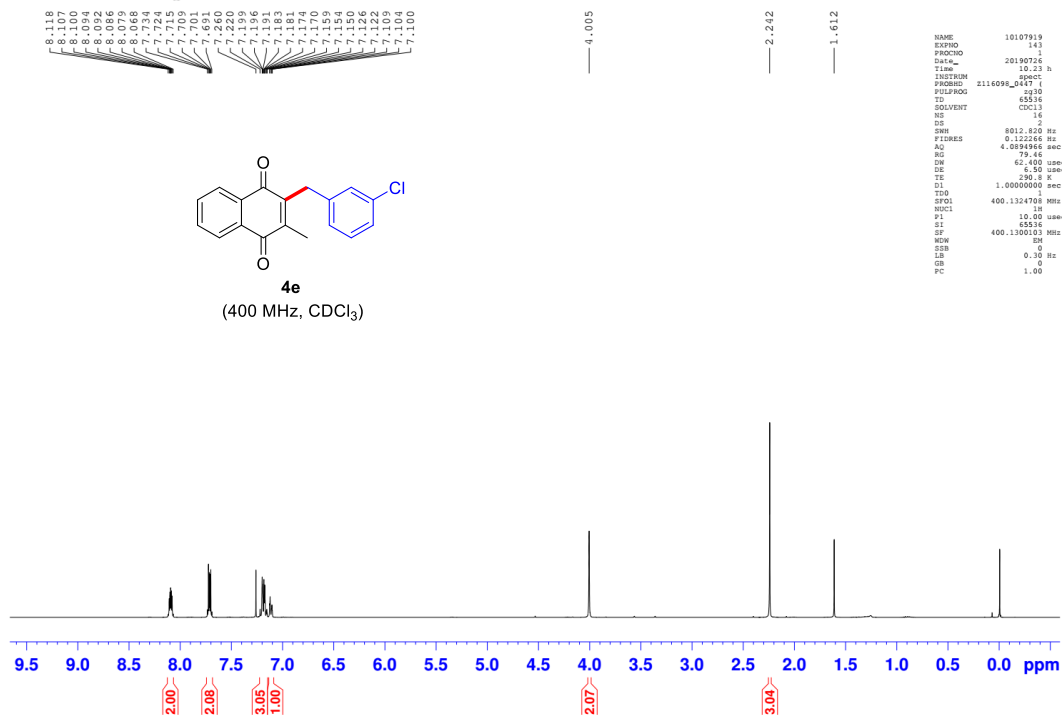
NAME      10107919
EXPNO     117
PROCNO    1
Date_     20190715
Time      15.49 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        8912.820 Hz
FIDRES     8.122266 Hz
AQ         4.8894966 sec
RG          96.68
DW          62.600 usec
DE          6.50 usec
TE         290.1 K
D1         1.00000000 sec
SFO1       400.1324708 MHz
NUC1       1H
P1         10.00 usec
SI         65536
SF         400.1300162 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00
  
```



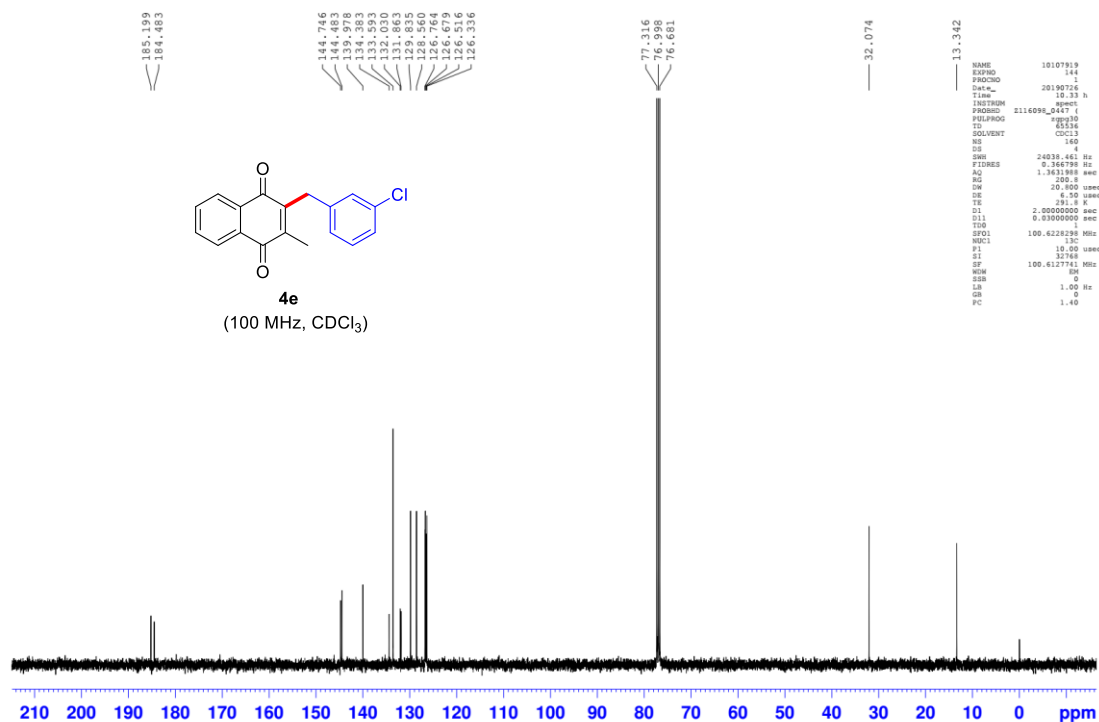
ldk-2019-59 naBQ p-Cl Bn 118 c



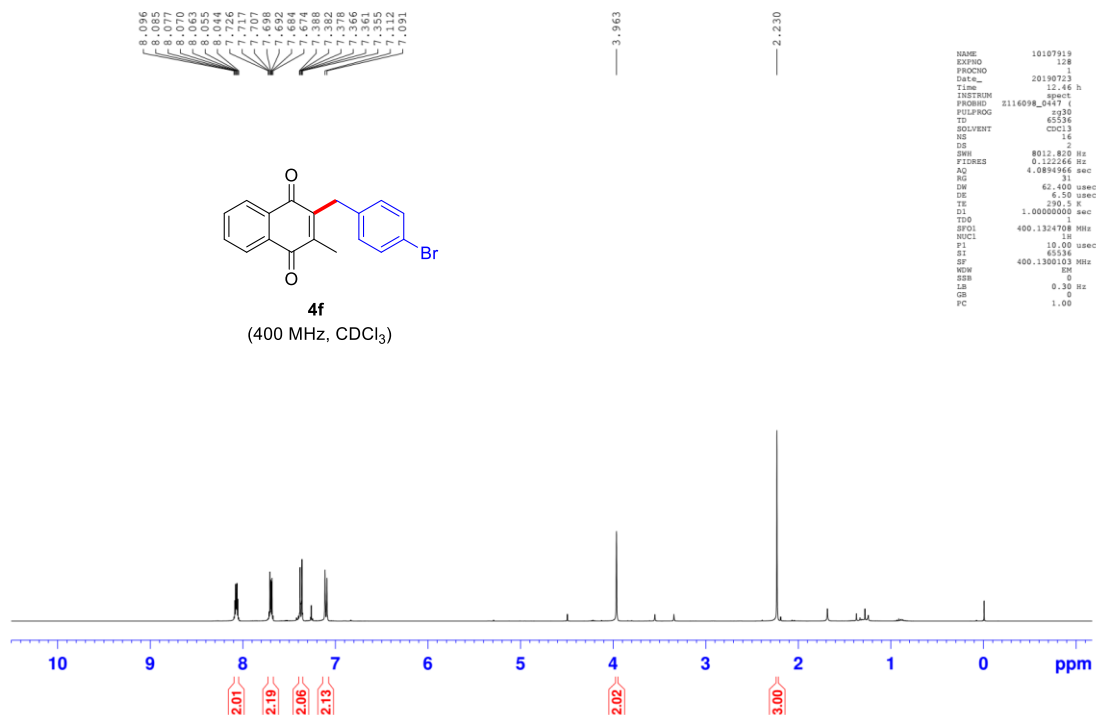
ldk-2019-69 naBQ 3-Cl Bn 143 h



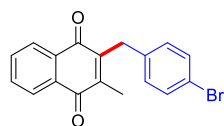
ldk-2019-69 naBQ 3-Cl Bn 144 c



ldk-2019-64 BQ-p-Br Bn 128 h

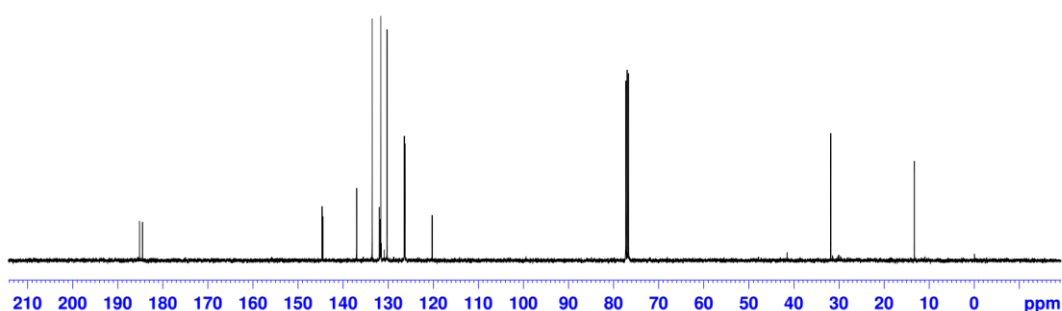


ldk-2019-64 BQ-p-Br Bn 129 c

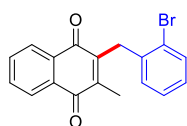


4f
(100 MHz, CDCl₃)

NAME	10107919
EXPNO	129
PROCNO	1
DATA_	20190723
Time	12.58 h
INSTRUM	agrest
PROBHD	z116098_0447 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	200
DS	4
SWH	24038.461 Hz
FIDRES	0.164798 Hz
AQ	1.3631988 sec
RG	200.0
DM	20.800 usec
DE	6.50 usec
TE	291.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	
SFO1	100.6228298 MHz
HUCL	13C
P1	10.00 usec
ST	32768
SF	100.6127775 MHz
WDW	EM
SBS	1.00 Hz
LB	
GB	
PC	1.40

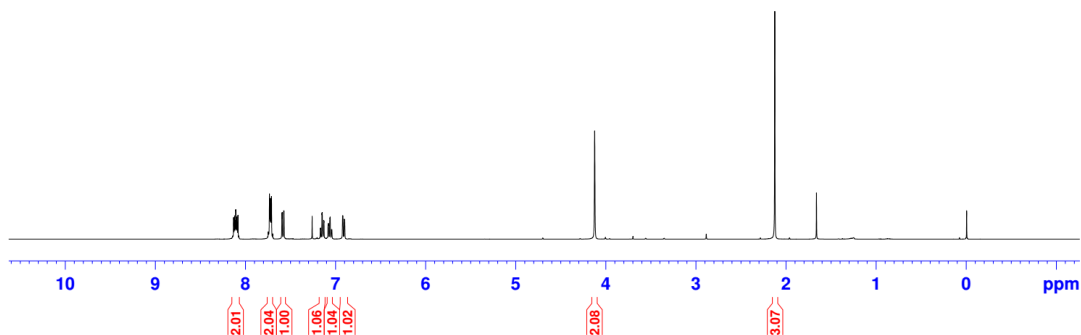


ldk-2019-81 naBQ-2-Br Bn 162 h

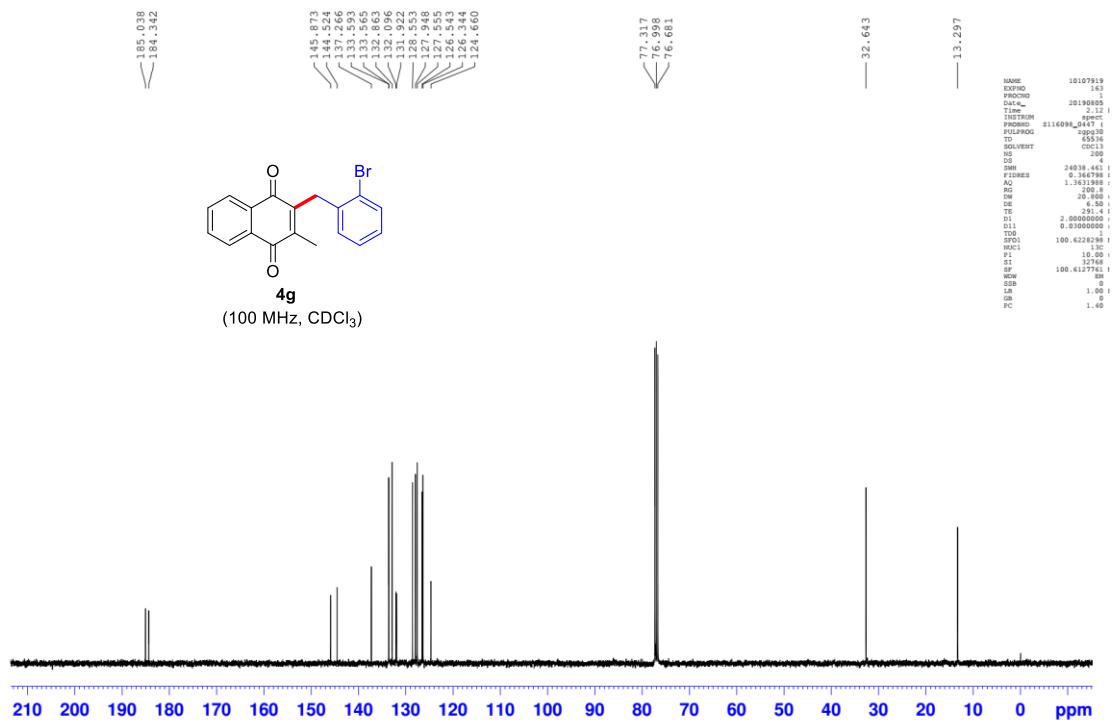


4g
(400 MHz, CDCl₃)

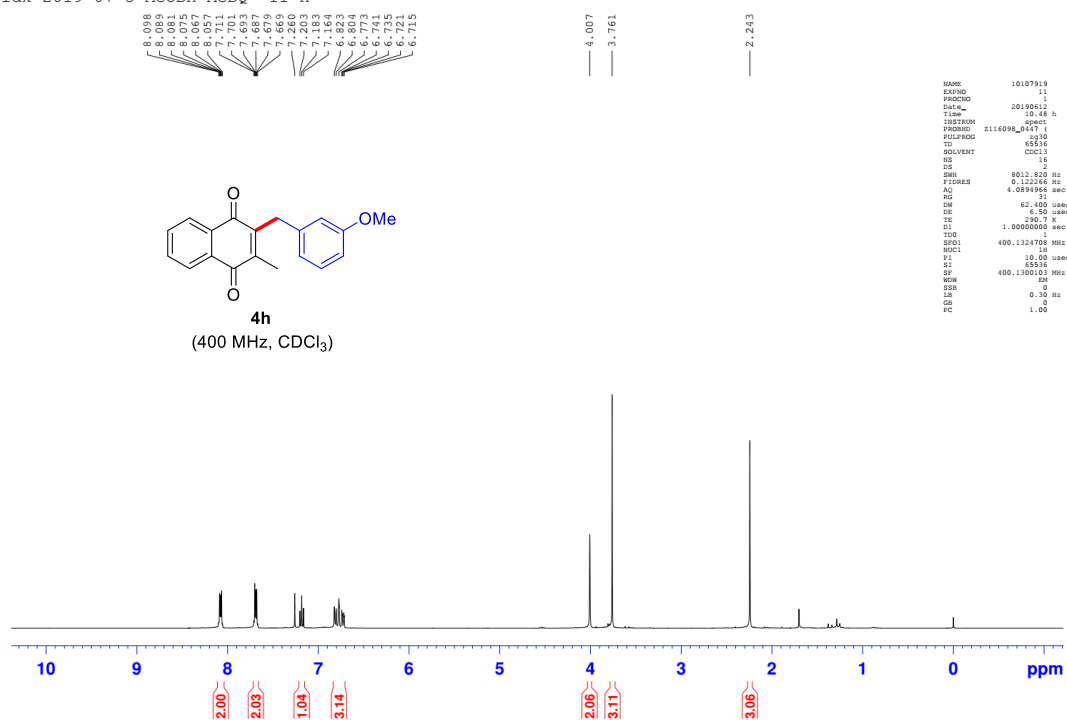
NAME	10107919
EXPNO	162
PROCNO	1
DATA_	20190805
Time	2.00 h
INSTRUM	agrest
PROBHD	z116098_0447 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	14
DS	2
SWH	8812.820 Hz
FIDRES	0.1222566 Hz
AQ	4.0899986 sec
RG	54.68
DM	62.160 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	
SFO1	400.1324708 MHz
HUCL	13C
P1	10.00 usec
ST	65536
SF	400.1300103 MHz
WDW	EM
SBS	0.30 Hz
LB	
GB	
PC	1.00



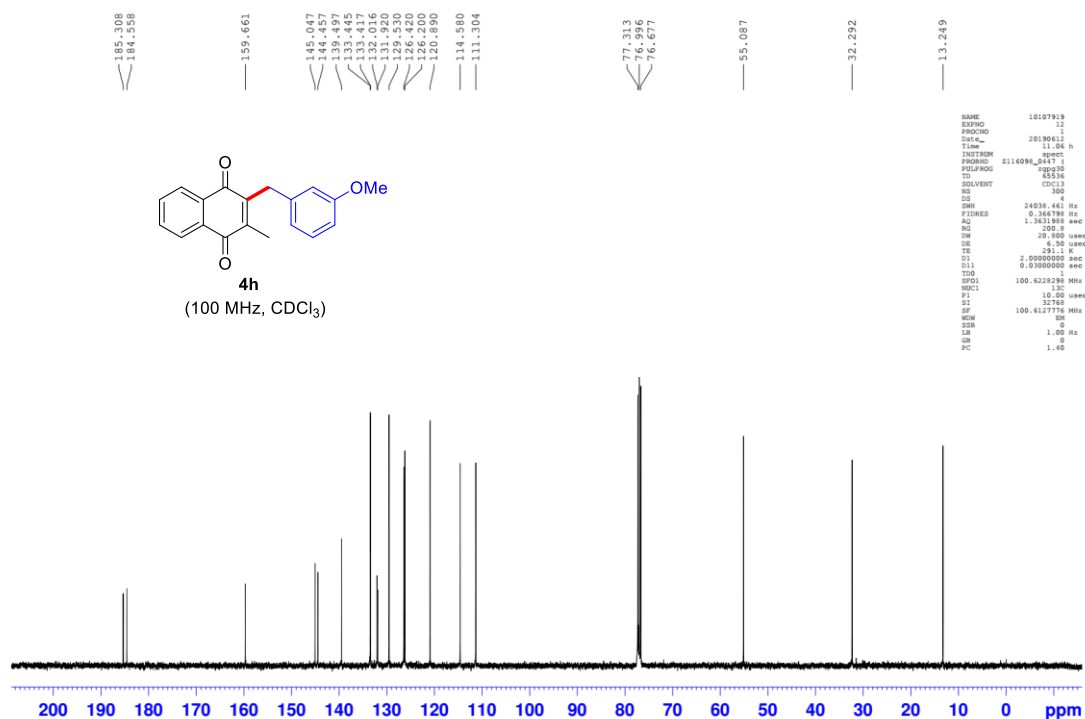
ldk-2019-81 naBQ-2-Br Bn 163 c



ldk-2019-07 3-MeOBn-MeBQ 11 h



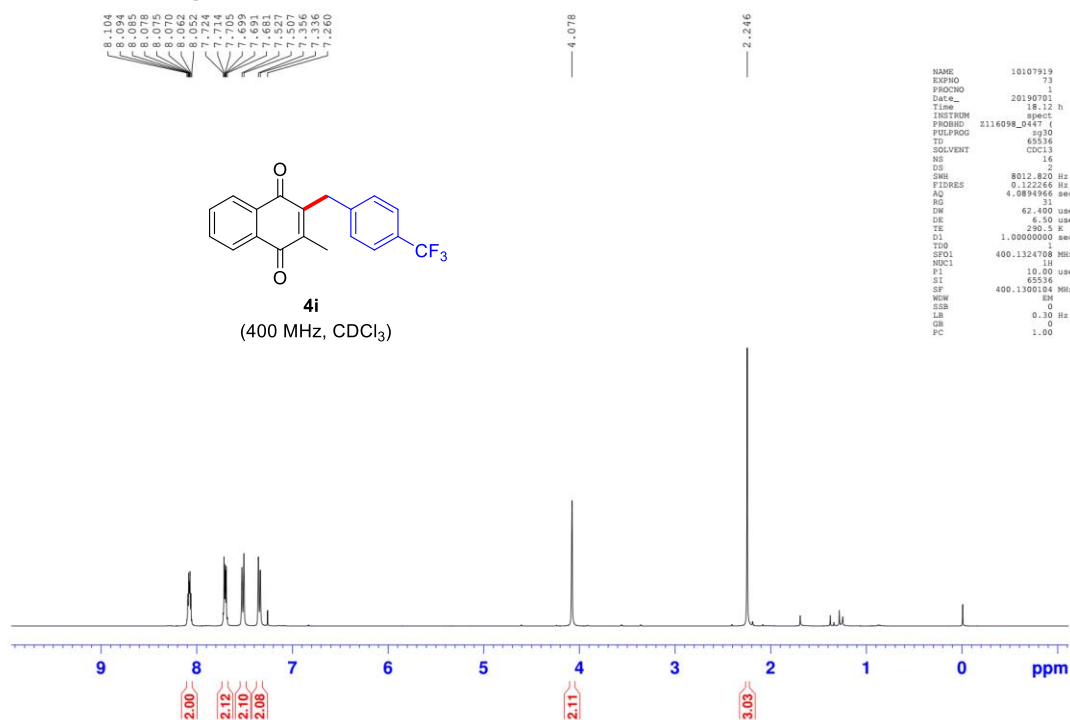
ldk-2019-07 3-MeOBn-MeBQ 12 c



```

NAME      10107919
EXPNO     12
PROCNO    1
Date_     20190612
Time      11.06 h
INSTRUM   spect
PROBHD    5116098_0447
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         24038.461 Hz
SWH        0.365798 Hz
AQ         1.3631988 sec
RG         200.0
DM         20.000 usec
DE         291.1 K
TE         2.0000000 sec
D1         0.0300000 sec
D11        1
TD0        100.4228298 MHz
SFO1       100.628298 MHz
NUC1       13C
P1         10.00 usec
SI         32768
SF         100.6177716 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

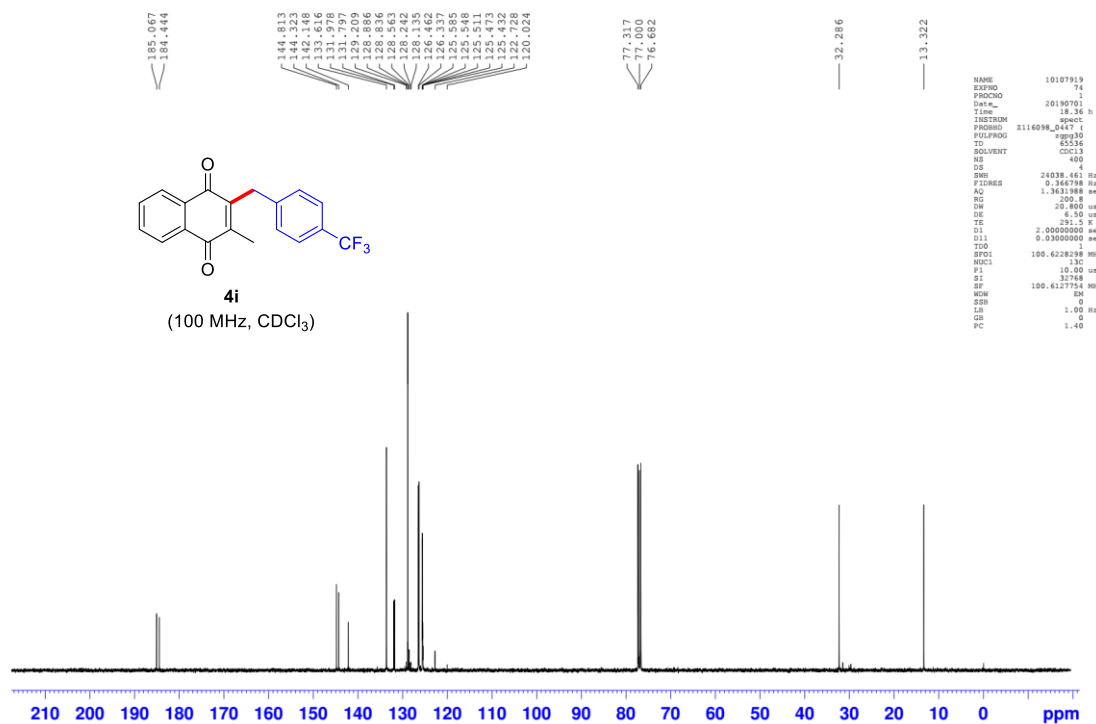
ldk-2019-36 naBQ-p-CF3 Bn 73 h



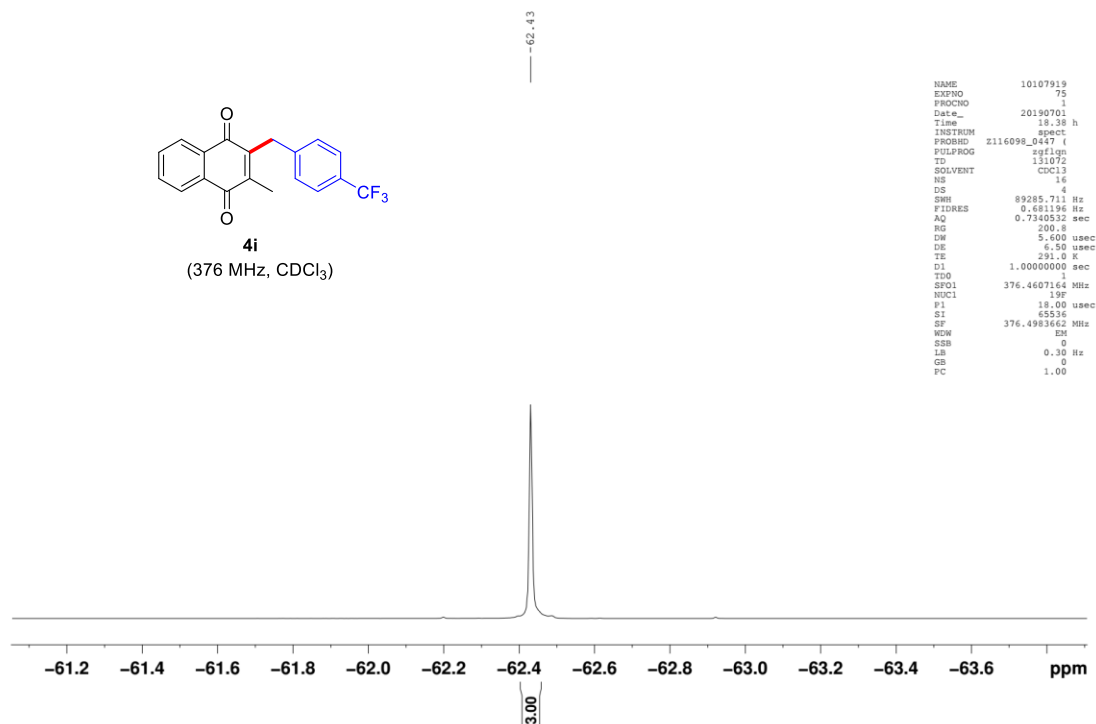
```

NAME      10107919
EXPNO     73
PROCNO    1
Date_     20190701
Time      18.12 h
INSTRUM   spect
PROBHD    5116098_0447
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         31
DM         62.400 usec
DE         6.50 usec
TE         296.5 K
D1         1.0000000 sec
D11        1
TD0        400.1324708 MHz
SFO1       400.1324708 MHz
NUC1       1H
P1         10.00 usec
SI         65536
SF         400.1300104 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

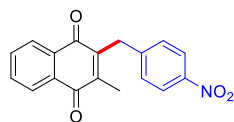
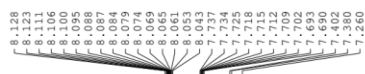
ldk-2019-36 naBQ-p-CF₃ Bn 74 c



ldk-2019-36 naBQ-p-CF₃ Bn 75 f



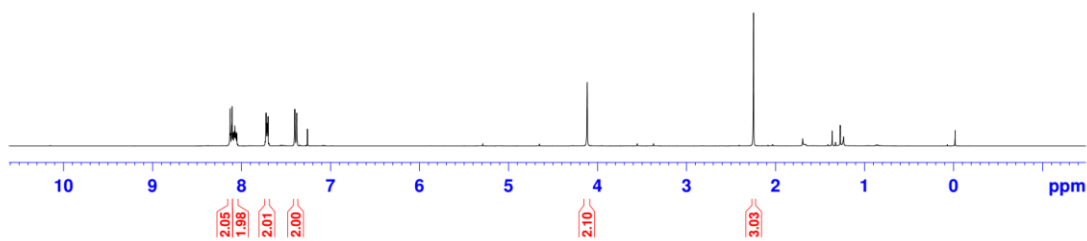
ldk-2019-56 naBQ-p-NO2Bn 111 h



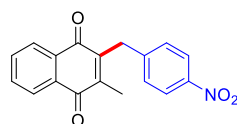
4j
(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     111
PROCNO    20190714
Date_     18.10.18
INSTRUM   spect
PROBHD    5mmBBO
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SHE        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.089361 sec
RG          62.400 usec
DM          280.19 s
DE          6.50 usec
TE         300.2 K
D1         1.0000000 sec
D11        0.0000000 sec
SFO1       400.1324705 MHz
NUC1       13C
P1         12.00 usec
SI         65536 usec
SF         400.1300103 MHz
WDW        EM
GB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



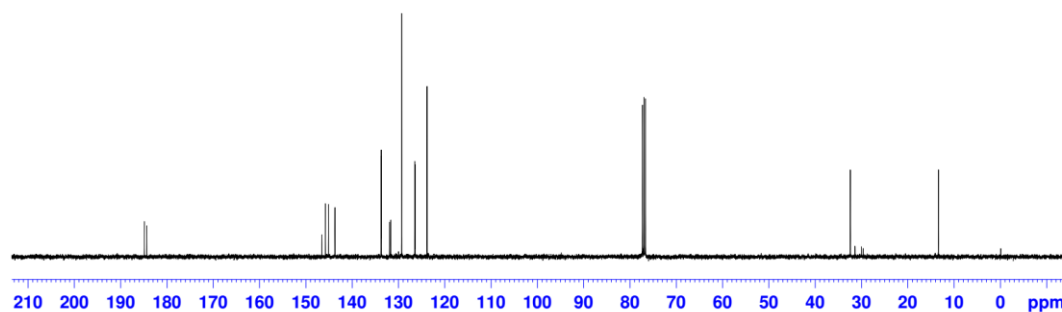
ldk-2019-56 naBQ-p-NO2Bn 112 c



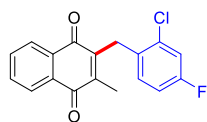
4j
(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     112
PROCNO    20190714
Date_     18.10.18
INSTRUM   spect
PROBHD    5mmBBO
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         114
DS         4
SHE        24819.440 Hz
FIDRES     0.364790 Hz
AQ         1.361210 sec
RG          200.00 usec
DM          28.000 usec
DE          28.50 usec
TE         301.5 K
D1         2.0000000 sec
D11        0.0000000 sec
SFO1       100.6220290 MHz
NUC1       13C
P1         10.00 usec
SI         32768 usec
SF         100.6127777 MHz
WDW        EM
GB         0
LB         1.00 Hz
GB         0
PC         1.00
  
```



1dk-2019-37 naBQ 2Cl-4F Bn 76h



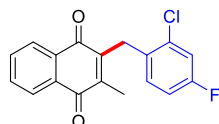
4k

(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     76
PROCNO    1
Date_     20190701
Time      18.42 h
INSTRUM   spect
PROBHD    z116098_0447
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         1
SFO1      8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         48.69
DM         62.400 usec
DE         6.50 usec
TE         290.2 K
D1         1.00000000 sec
TSD        1
SFO1      400.1324708 MHz
NUC1       1H
P1         10.00 usec
SI         65536
SF         400.1300102 MHz
WDM        0
SBB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

1dk-2019-37 naBQ 2Cl-4F Bn 77 c

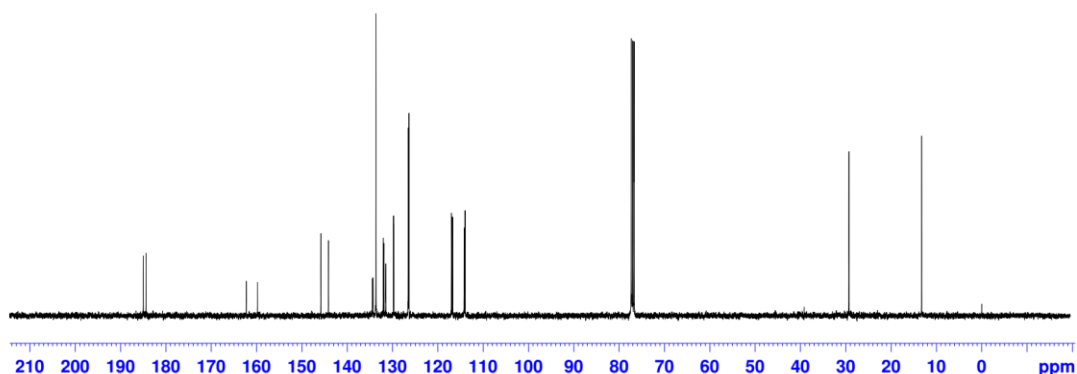


4k

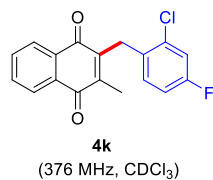
(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     77
PROCNO    1
Date_     20190701
Time      19.00 h
INSTRUM   spect
PROBHD    z116098_0447
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         300
DS         1
SFO1      24038.461 Hz
FIDRES    0.364798 Hz
AQ         1.3631388 sec
RG         200.8
DM         20.800 usec
DE         6.50 usec
TE         290.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TSD        1
SFO1      100.6228238 MHz
NUC1       13C
P1         10.00 usec
SI         32768
SF         100.6127755 MHz
WDM        0
SBB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



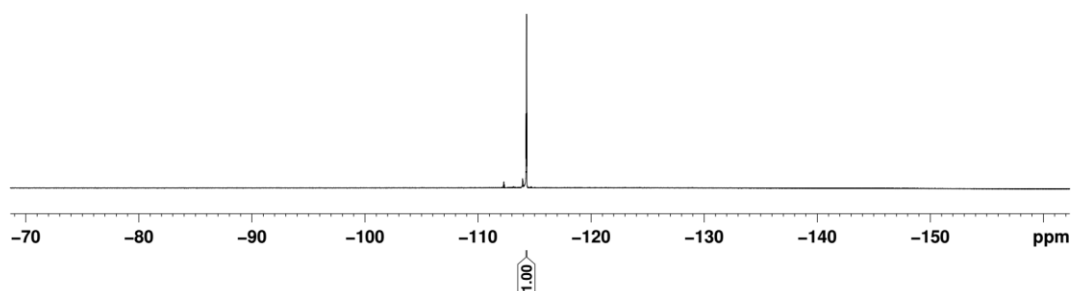
ldk-2019-37 naBQ 2Cl-4F Bn 78 f



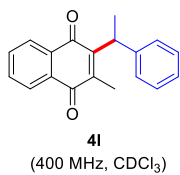
-114.36
-114.28
-114.30
-114.32

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190701
Time      19.04 h
INSTRUM   spect
PROBHD    Z116098_0447 f
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         16
DS         4
SWH        89285.111 Hz
FIDRES     0.681196 Hz
AQ         0.7340532 sec
RG         200.8
DW         5.600 usec
DE         6.50 usec
TE         290.5 K
D1         1.00000000 sec
TD0        1
SFO1       376.4607164 MHz
NUC1       13C
P1         18.00 usec
SI         65536
SF         376.4983662 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



ldk-2019-82 naBQ ethyl-Bn 164 h

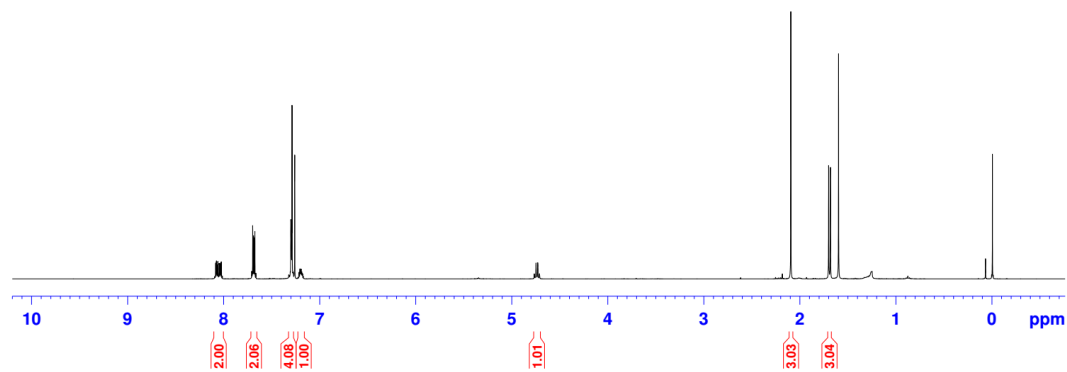


8.070
8.068
8.061
8.060
8.047
8.046
8.039
8.038
8.032
8.024
8.024
7.708
7.697
7.689
7.685
7.675
7.665
7.322
7.320
7.300
7.298
7.296
7.287
7.279
7.270
7.260
7.227
7.215
7.214
7.206
7.201
7.199
7.198
7.192
7.187
7.183
7.178
7.172
7.171
4.765
4.747
4.729
4.711

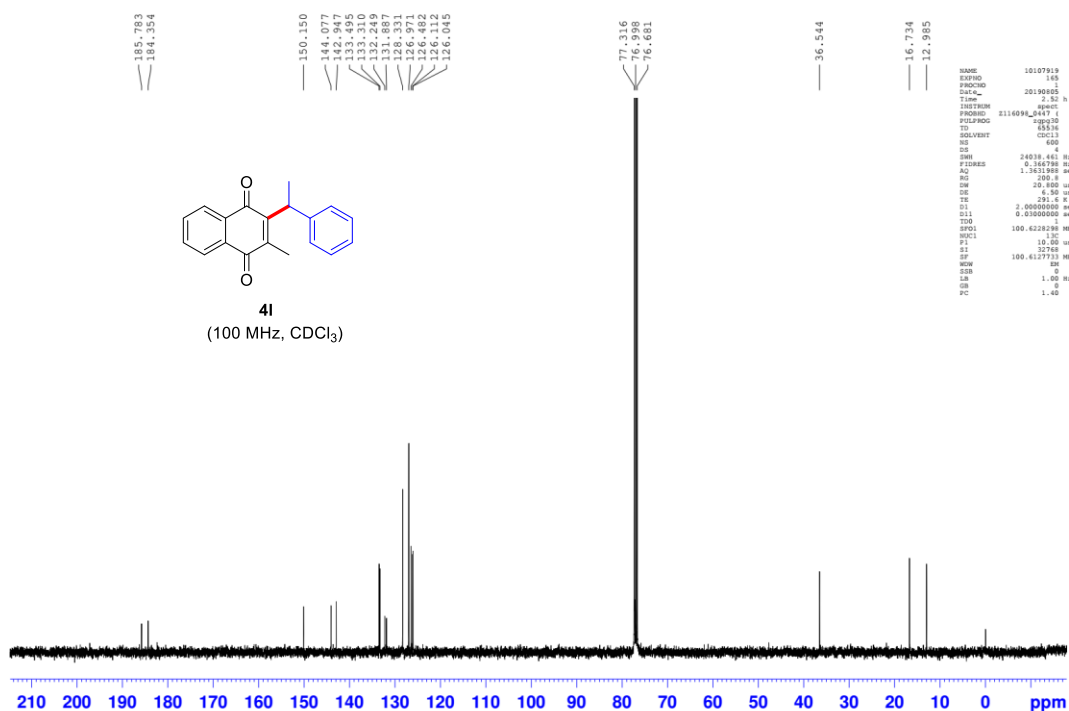
2.095
1.701
1.683

```

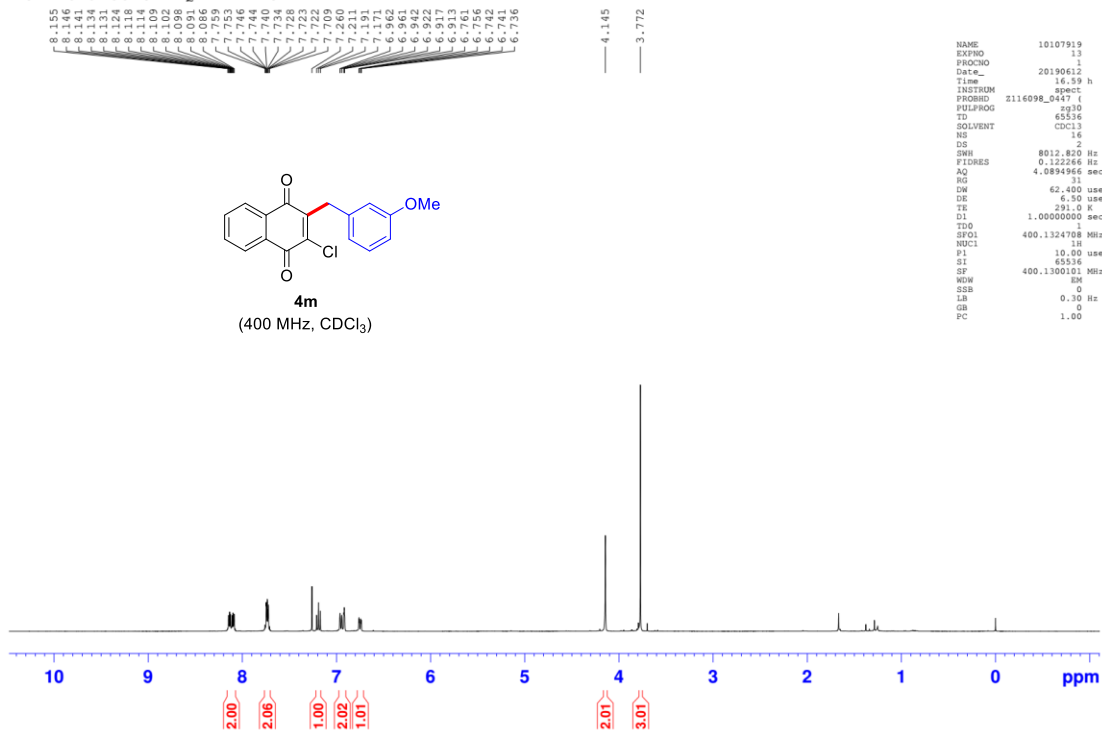
NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190805
Time      2.17 h
INSTRUM   spect
PROBHD    Z116098_0447 f
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        8012.402 Hz
FIDRES     0.122566 Hz
AQ         4.089486 sec
RG         99.96
DW         67.600 usec
DE         6.50 usec
TE         290.9 K
D1         1.00000000 sec
TD0        1
SFO1       400.1324708 MHz
NUC1       13C
P1         10.00 usec
SI         65536
SF         400.1300124 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```



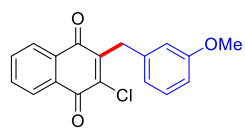
ldk-2019-82 naBQ ethyl-Bn 165 c



ldk-2019-08 Cl-BQ-Bn h 13



ldk-2019-08 Cl-BQ-Bn c 14

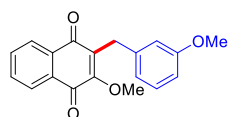
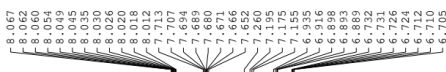


(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
Date_     20190812
Time      17.18 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         300
DS         4
SWH        24038.461 Hz
FIDRES     0.364798 Hz
AQ         1.3631988 sec
RG         200.0
DM         20.800 usec
DE         6.50 usec
TE         298.16 K
D1         2.00000000 sec
D11        0.03000000 sec
TDS        5
SFO1       100.628298 MHz
HDC1       135
P1         10.00 usec
S1         32768
SF         100.6127769 MHz
RG         80
WDR        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

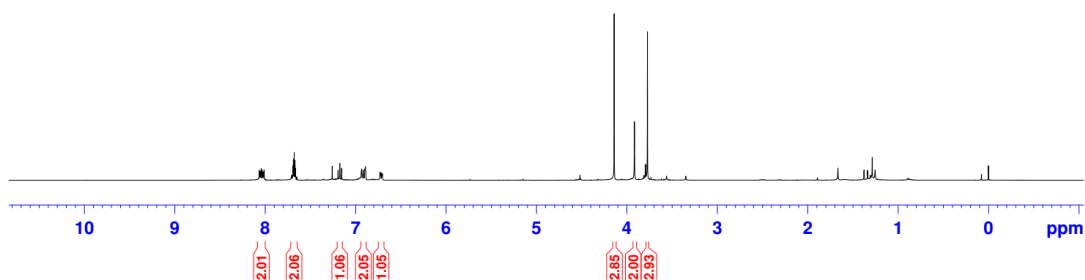
ldk-2019-83 MeO BQ 3-MeO Bn 166 h



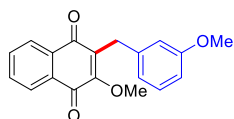
(400 MHz, CDCl₃)

```

NAME      10107919
EXPNO     166
PROCNO    1
Date_     20190805
Time      2.58 h
INSTRUM   spect
PROBHD    Z116098_0447 (
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         4
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0891966 sec
RG         31
DM         62.400 usec
DE         6.50 usec
TE         298.16 K
D1         1.00000000 sec
TDS        10
SFO1       400.1324708 MHz
HDC1       15
P1         10.00 usec
S1         65536
SF         400.1300103 MHz
WDR        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



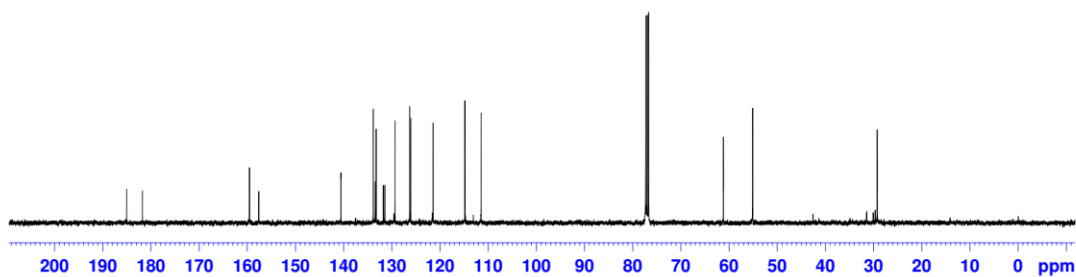
ldk-2019-83 MeO BQ 3-MeO Bn 167c



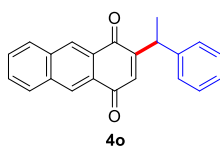
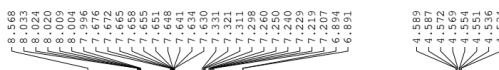
(100 MHz, CDCl₃)

```

NAME      10107919
EXPNO     1
PROCNO    1
DATE_     20190803
Time      3.16 h
INSTRUM   spect
PROBHD    z116098_0447 f
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         300
DS         24038.461 Hz
FIDRES    0.364798 Hz
AQ         1.3631988 sec
RG          200.0
OW         29.800 usec
DE         29.50 usec
TE         295.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        100.6228298 MHz
NUC1       13C
P1         15.00 usec
SF         100.6127768 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



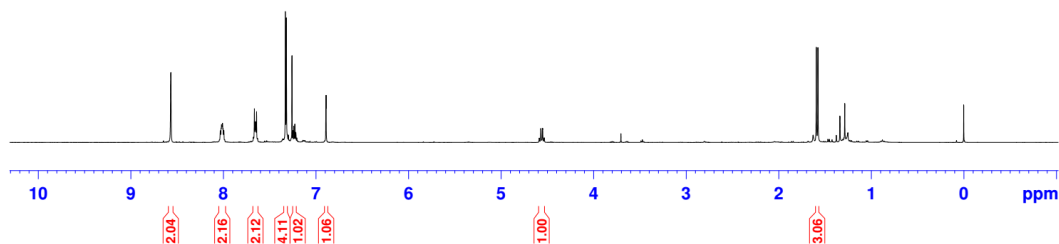
ldk-2020-19 enBQ-ethyl-bn h31



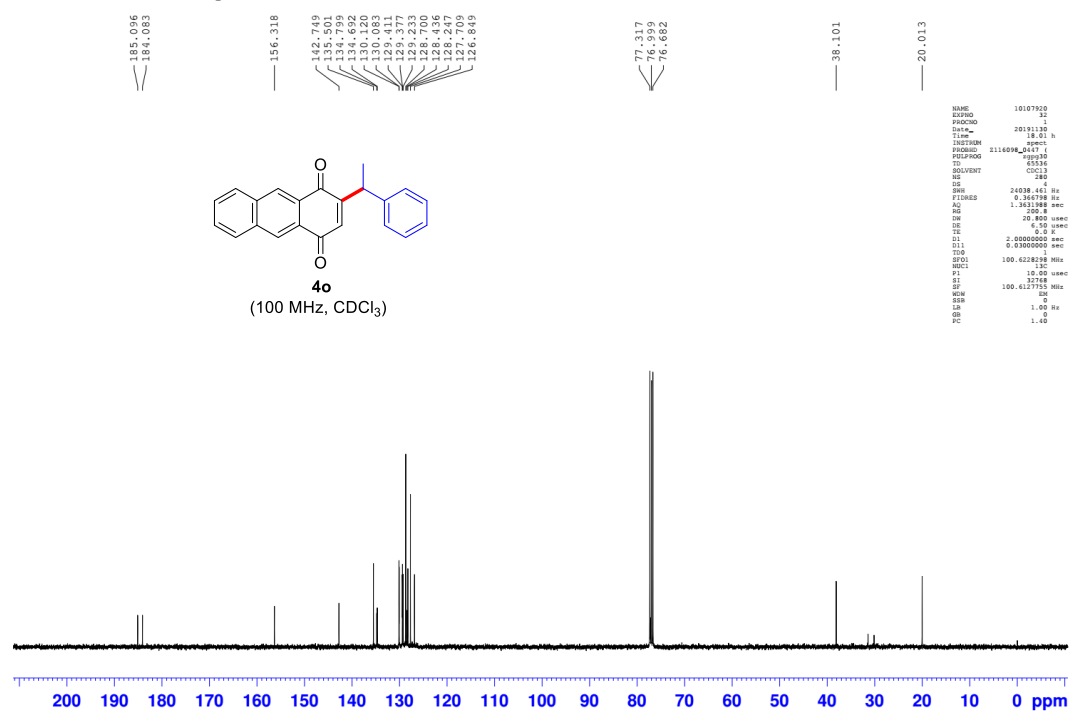
(400 MHz, CDCl₃)

```

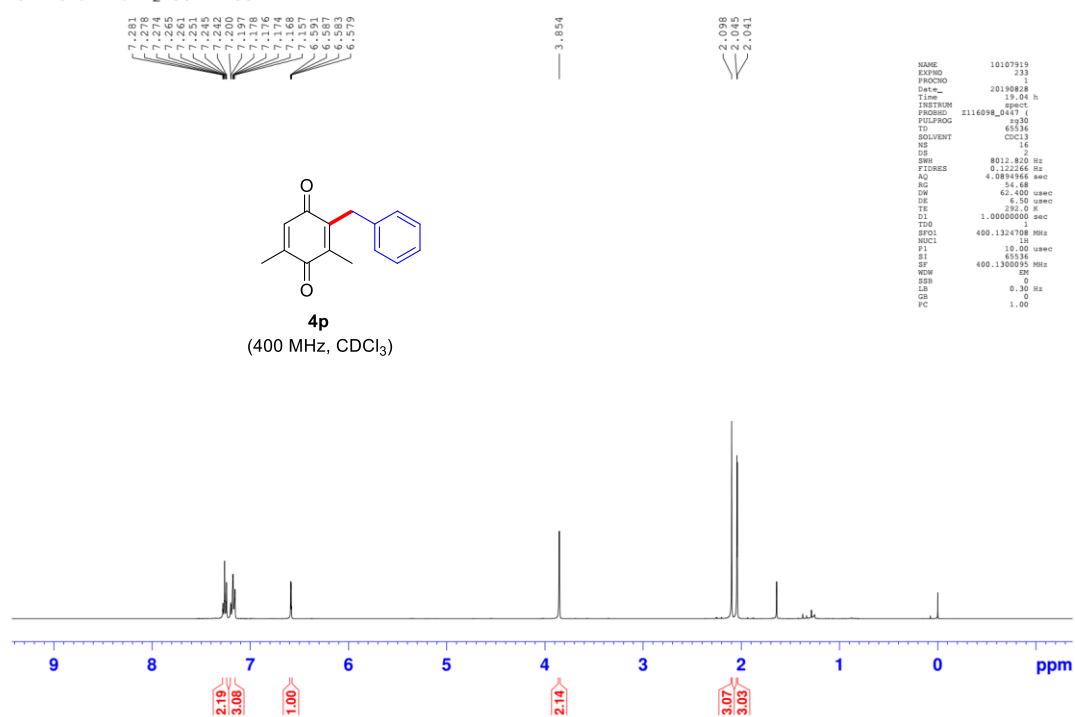
NAME      10107920
EXPNO     1
PROCNO    1
DATE_     20191113
Time      17.44 h
INSTRUM   spect
PROBHD    z116098_0447 f
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         8012.820 Hz
FIDRES    0.122246 Hz
AQ         4.084966 sec
RG          51.00
OW         61.450 usec
DE         6.50 usec
TE         300.2 K
D1         1.00000000 sec
TDO        400.1324708 MHz
NUC1       1H
P1         15.00 usec
SF         400.1300102 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



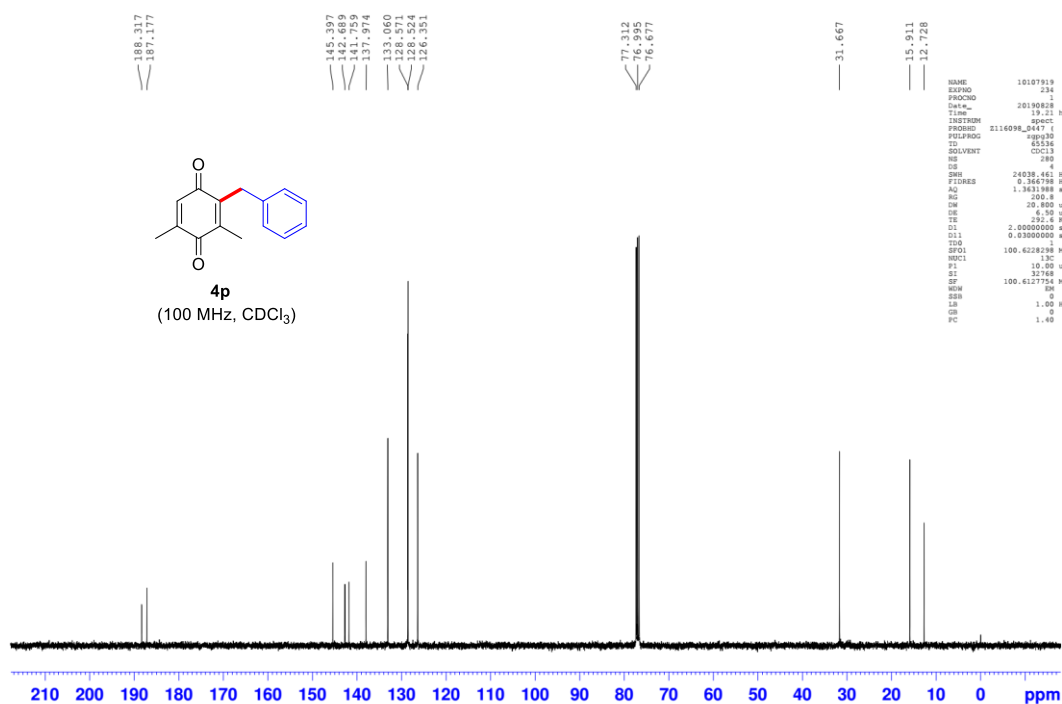
ldk-2020-19 enBQ-ethyl-bn c32



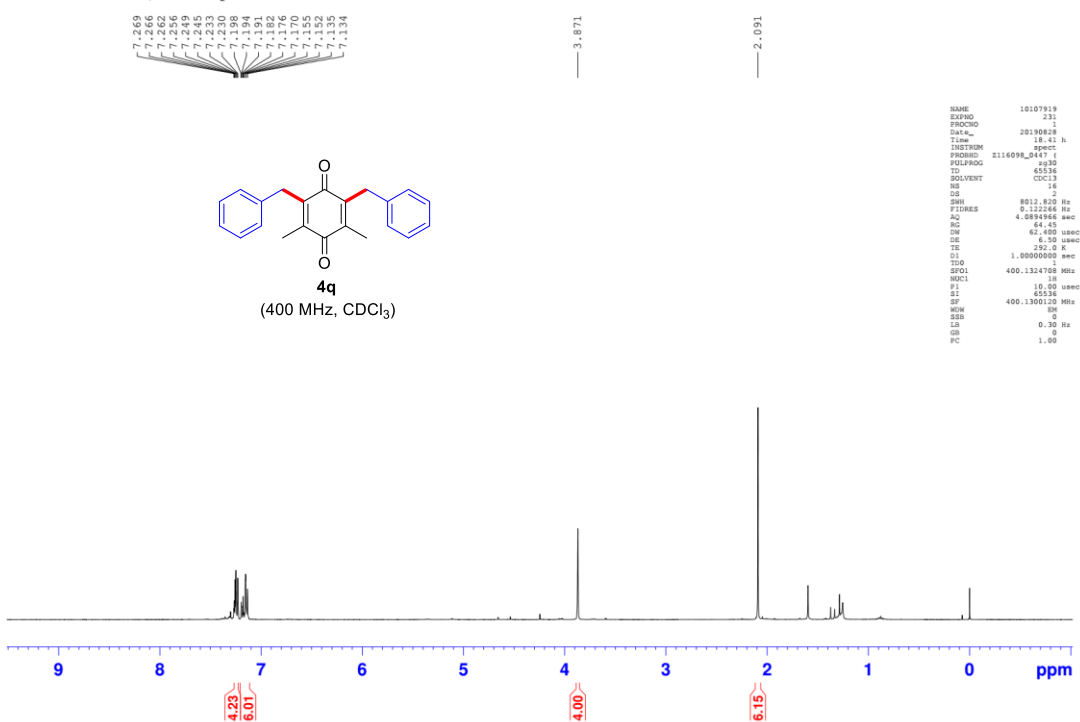
ldk-2019-118 BQ-down 233h



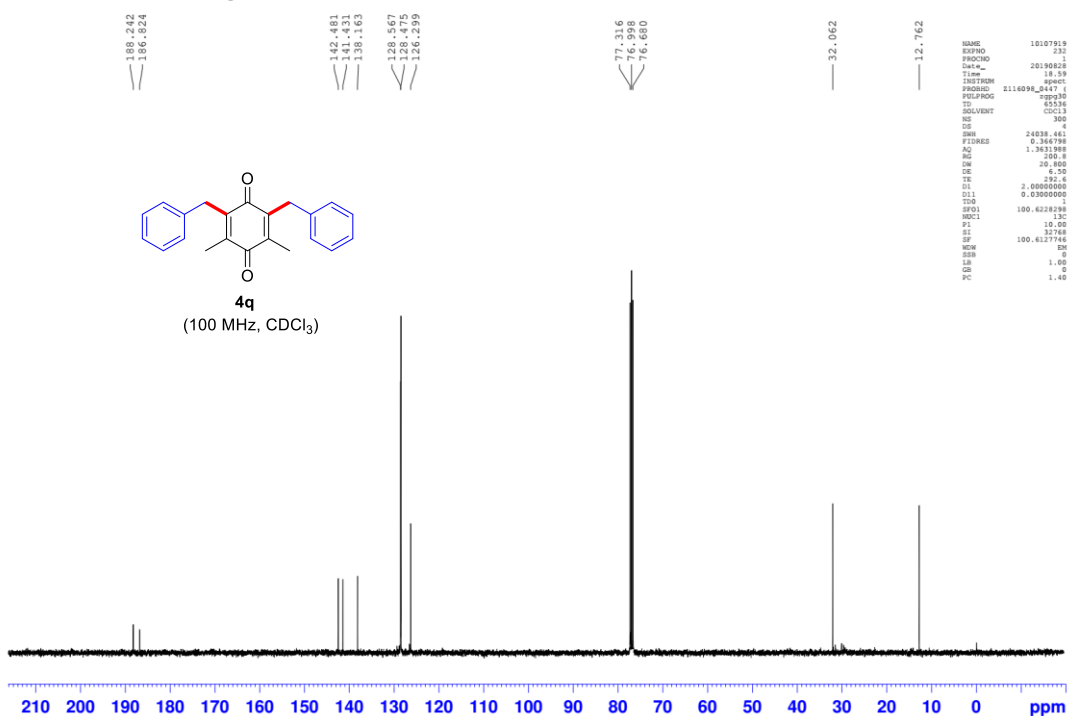
ldk-2019-118 BQ-down 234 c



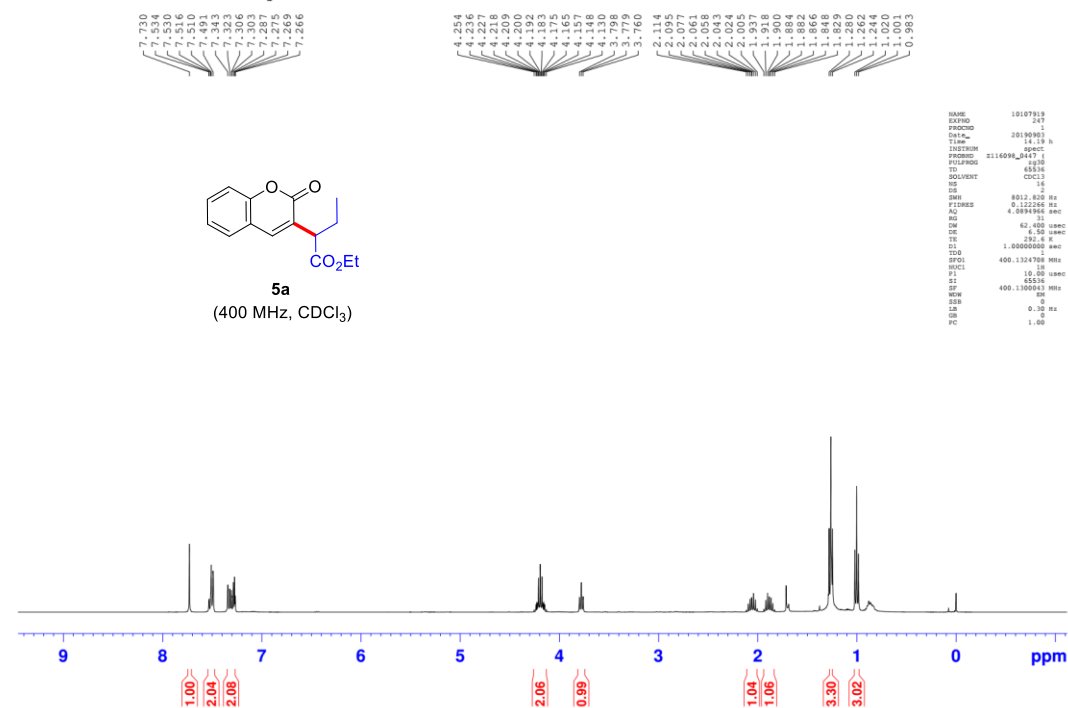
ldk-2019-117 2,6-BQ up TM 231 h



ldk-2019-117 2,6-BQ up TM 232c

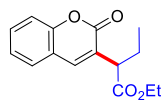


ldk-2019-124 coumarin Butyl-ester 247 h



ldk-2019-124 coumarin Butyl-ester 248 c

172.906
161.095
153.057
139.531
131.257
127.779
124.813
124.411
119.104
116.447



5a
(100 MHz, CDCl₃)

77.316
76.588
76.681

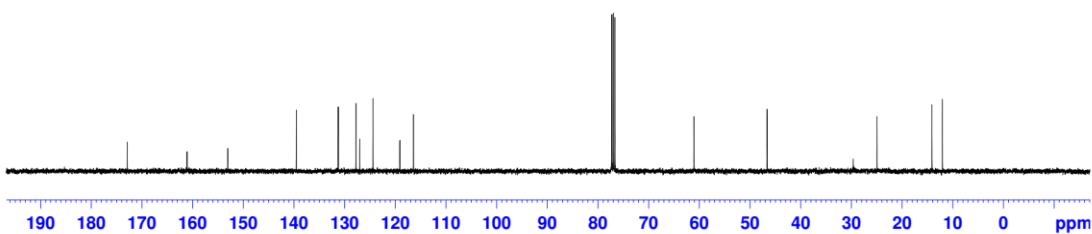
61.084

46.630

24.949

14.124
12.052

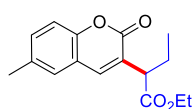
```
NAME      10107919
EXPNO     248
PROCNO    1
Date_     20190903
Time      14.24 h
INSTRUM    spect
PROBHD     E116099_0447 f
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         64
DS         4
SWH         24018.461 Hz
F2RES      0.165798 Hz
AQ         1.3811888 sec
RG         200.0
DM         20.000000 sec
DE         6.50 usec
TE         299.9 K
D1         2.00000000 sec
d11        0.03000000 sec
TSD        100.6228293 MHz
SFO1       100.6228293 MHz
NUC1       13C
P1         10.000 usec
SI         32768
SF         100.6127755 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
CB         1.40
PC         1.40
```



ldk-2019-142 6-Me coumarin 1-butyl ester 280 h

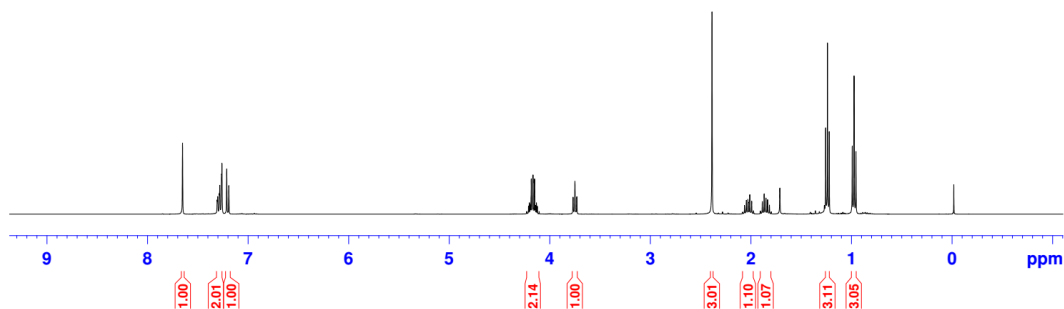
7.652
7.307
7.286
7.281
7.264
7.219
7.192

4.229
4.211
4.202
4.183
4.175
4.169
4.160
4.152
4.142
4.134
4.124
4.107
3.769
3.751
3.732
2.388
2.083
2.065
2.056
2.036
2.027
2.012
1.973
1.974
1.906
1.888
1.869
1.851
1.835
1.817
1.799
1.780
1.740
1.222
0.993
0.975
0.956

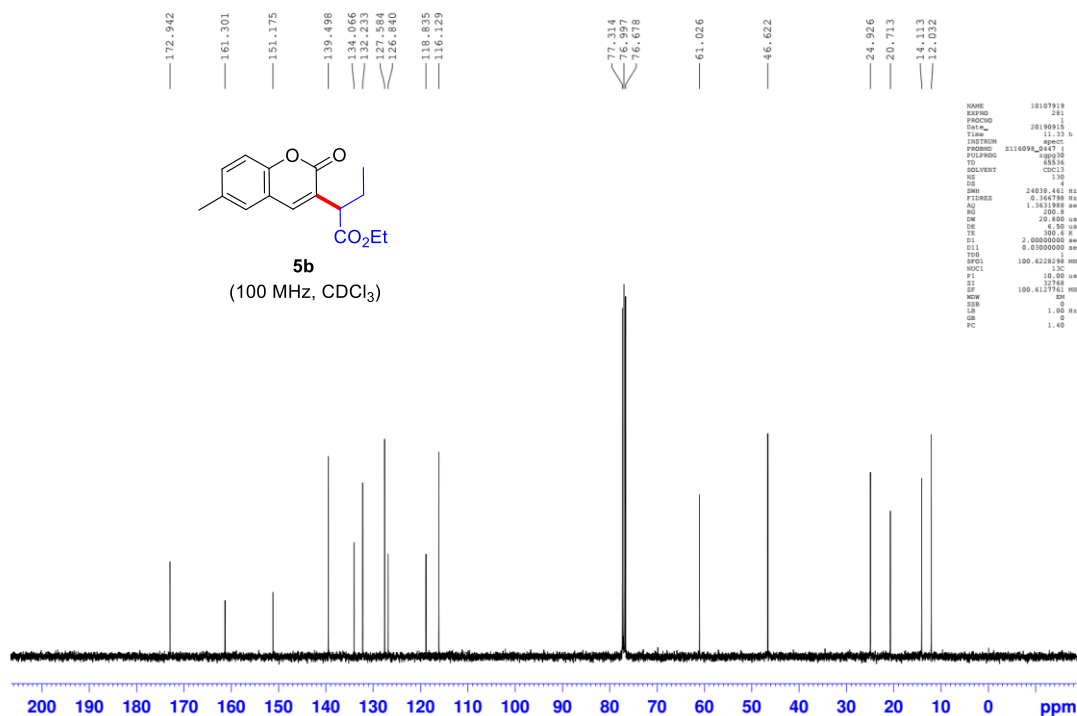


5b
(400 MHz, CDCl₃)

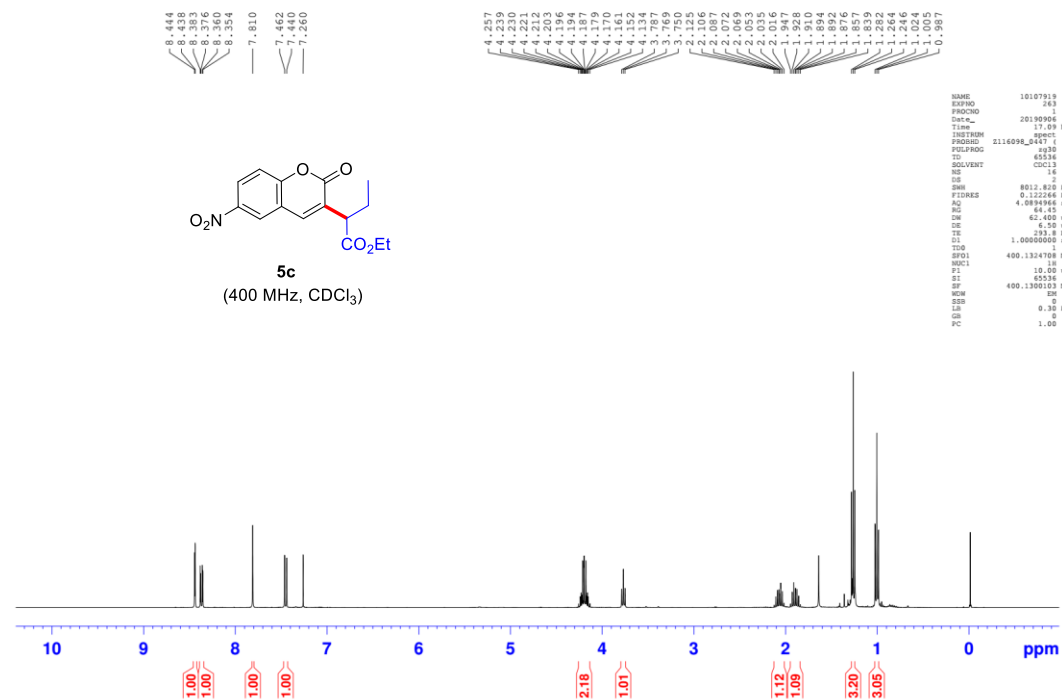
```
NAME      10107919
EXPNO     280
PROCNO    1
Date_     20190915
Time      11.25 h
INSTRUM    spect
PROBHD     E116099_0447 f
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         16
DS         4
SWH         8012.820 Hz
F2RES      0.122564 Hz
AQ         4.0894966 sec
RG         32
DM         62.400 usec
DE         6.50 usec
TE         299.9 K
D1         1.00000000 sec
TSD        400.1324703 MHz
SFO1       400.1324703 MHz
NUC1       13C
P1         10.000 usec
SI         65536
SF         400.1300163 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
CB         1.00
PC         1.00
```



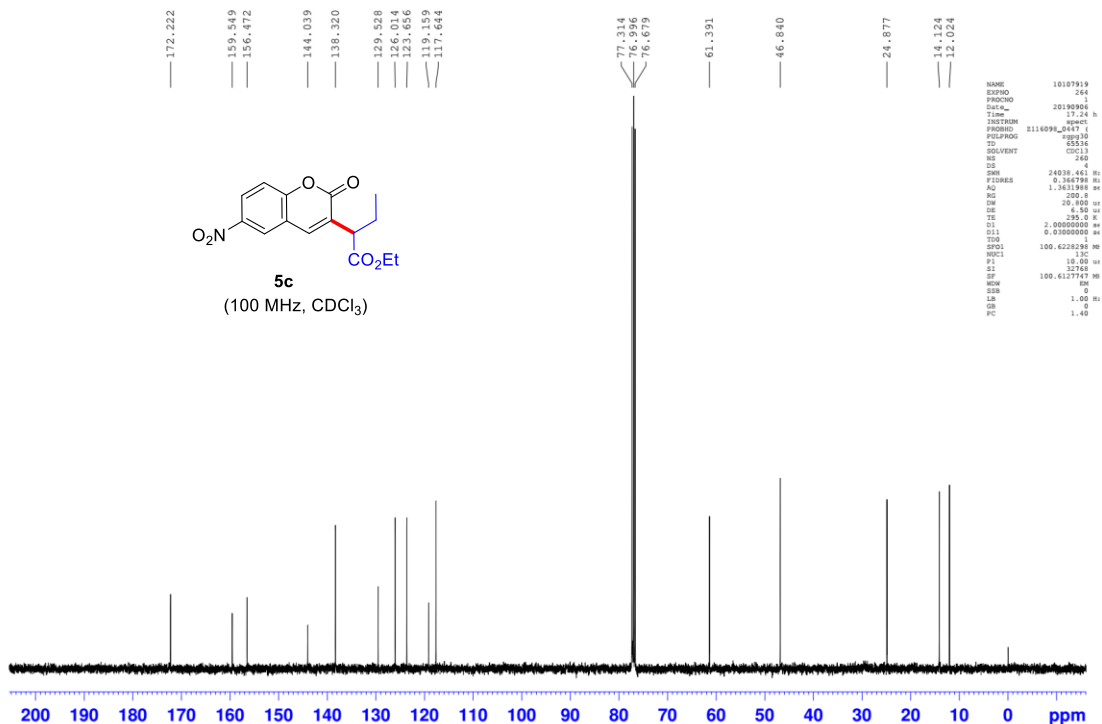
ldk-2019-142 6-Me coumarin 1-butyl ester 281c



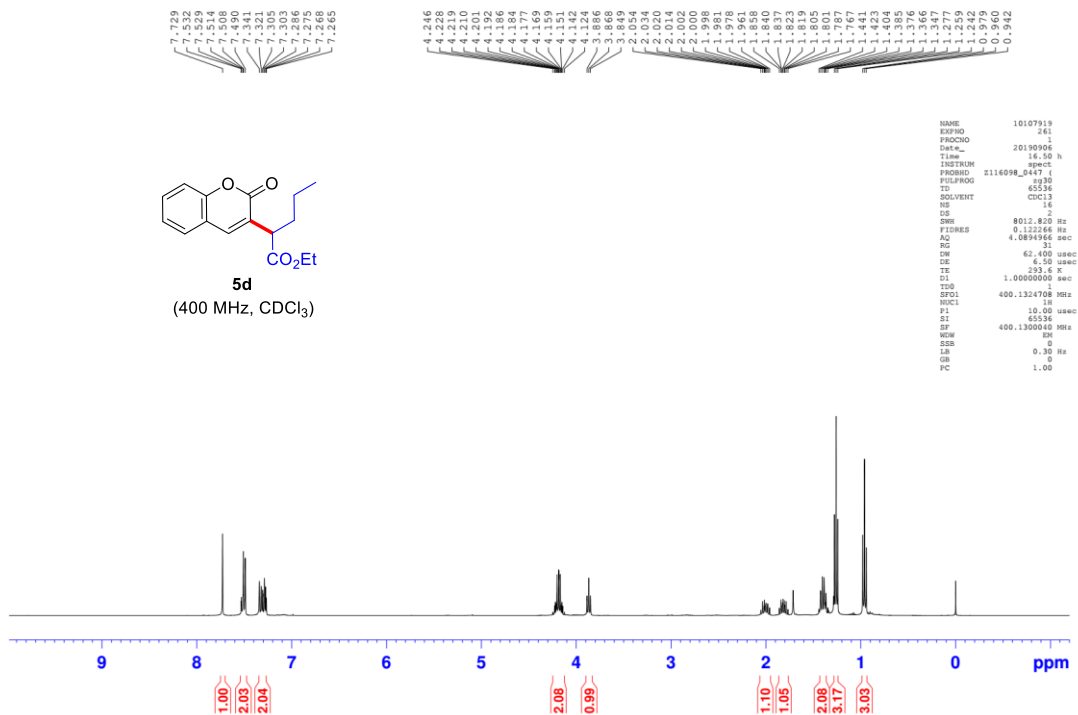
ldk-2019-131 6-NO2 1-butyl ester 263 h



ldk-2019-131 6-NO₂ 1-butyl ester 264 c



ldk-2019-130 coumarin 1-wu ester 261 h



ldk-2019-130 coumarin 1-wu ester 262 c

173.045
161.073
153.037
139.461
131.231
127.759
126.267
124.397
119.113
116.433

77.312
76.995
76.677

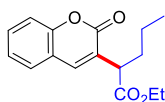
61.092

44.836

33.788

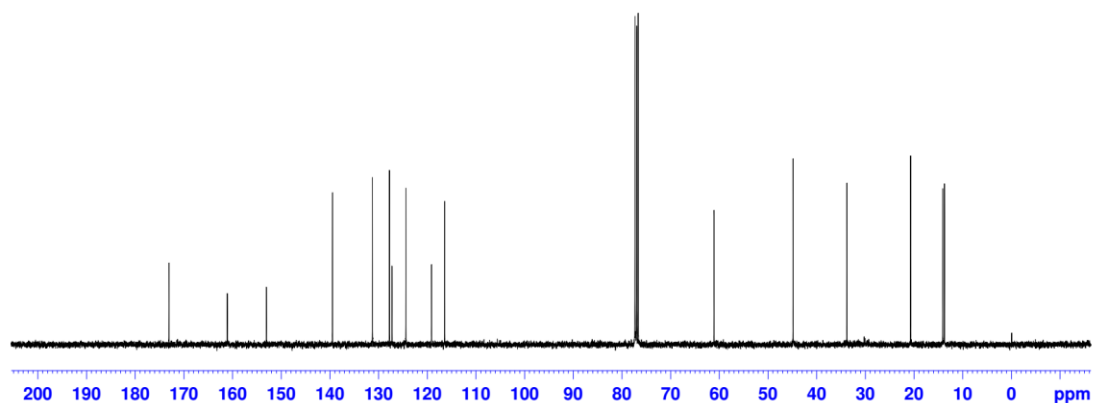
20.709

14.189
13.159



5d
(100 MHz, CDCl₃)

```
NAME      1007919
EXPNO     2
PROCNO    1
Date_     20190906
Time      17.51 h
INSTRUM   spect
PROBHD    5mmBBO
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         1
SWH        24000.00 Hz
FIDRES     0.126788 Hz
AQ         1.3611846 sec
RG          320
OW         62.400 us
DE         6.50 us
TE         300.2 K
D1         0.0000000 sec
TD0         1
SFO1       100.6228238 MHz
NUC1       13C
P1         18.00 us
Z1         65536
SF         400.1300105 MHz
WOW        0
SSB        0
LB         0.30 Hz
GB         0
PC         1.40
```

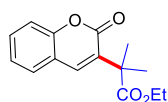


ldk-2020-101 coumarin-di-Me 102h

7.597
7.593
7.551
7.517
7.513
7.507
7.498
7.494
7.485
7.481
7.332
7.332
7.320
7.307
7.284
7.287
7.285
7.269
7.266
7.260

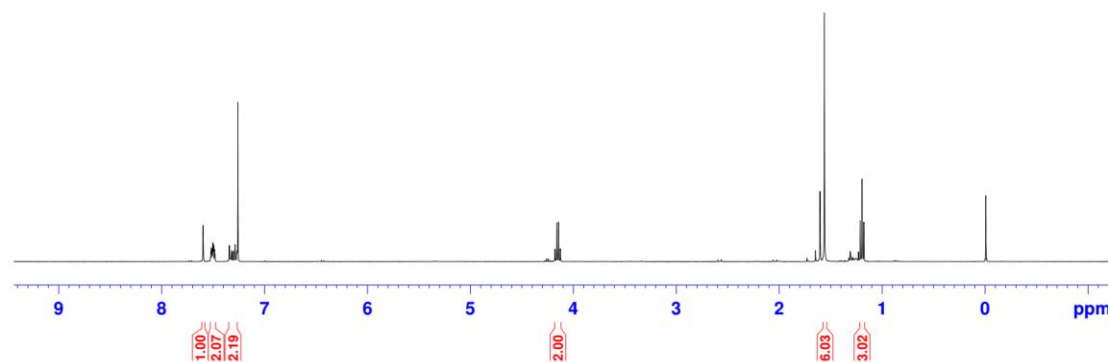
4.139
4.161
4.143
4.125

1.561
1.213
1.195
1.178

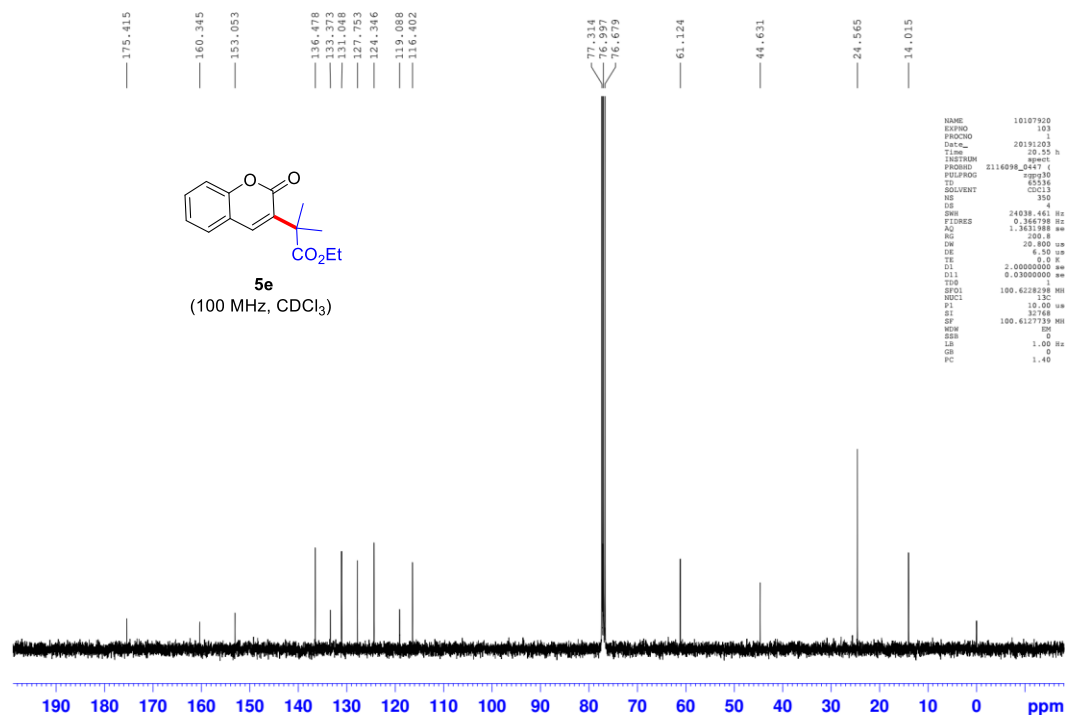


5e
(400 MHz, CDCl₃)

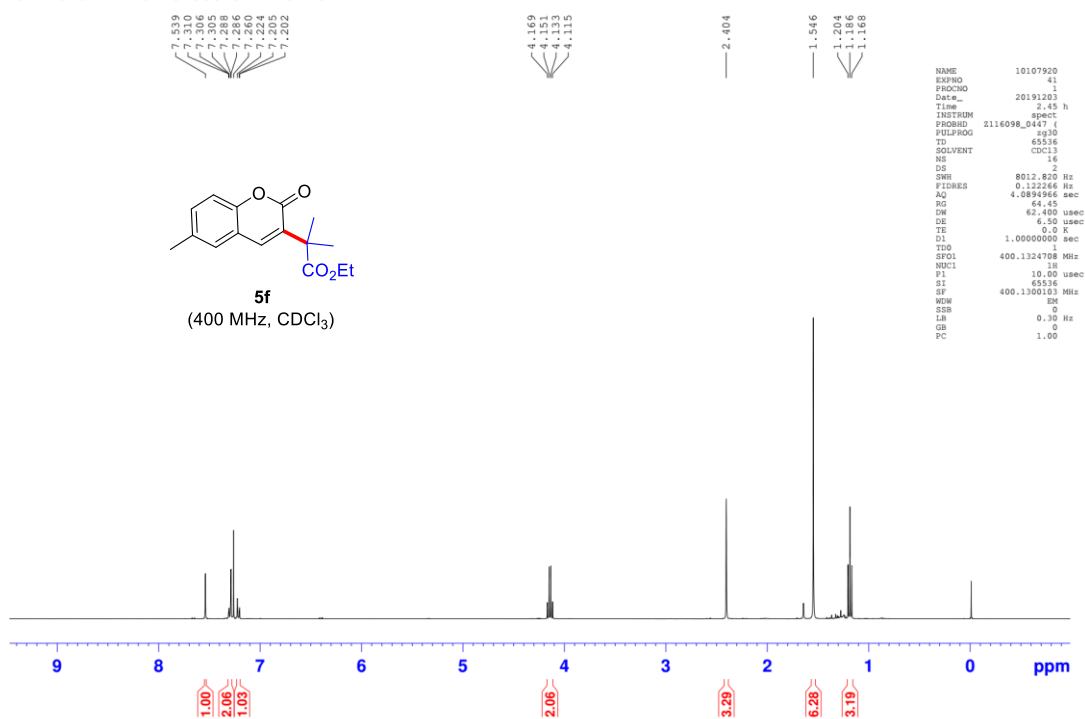
```
NAME      10107920
EXPNO     102
PROCNO    1
Date_     20191203
Time      20.34 h
INSTRUM   spect
PROBHD    5mmBBO
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         2
DS         1
SWH        8012.820 Hz
FIDRES     0.122566 Hz
AQ         4.0894966 sec
RG          320
OW         62.400 us
DE         6.50 us
TE         300.2 K
D1         0.0000000 sec
TD0         1
SFO1       400.1324708 MHz
NUC1       1H
P1         13.00 us
Z1         65536
SF         400.1300105 MHz
WOW        0
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```



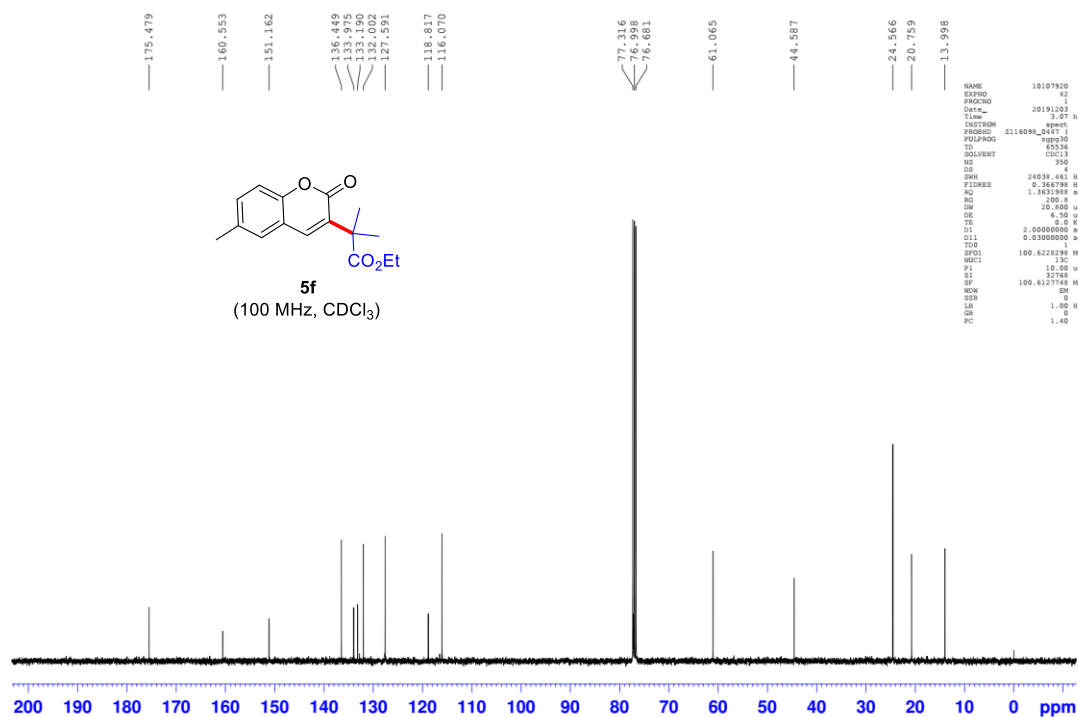
ldk-2020-101 coumarin-di-Me 103c



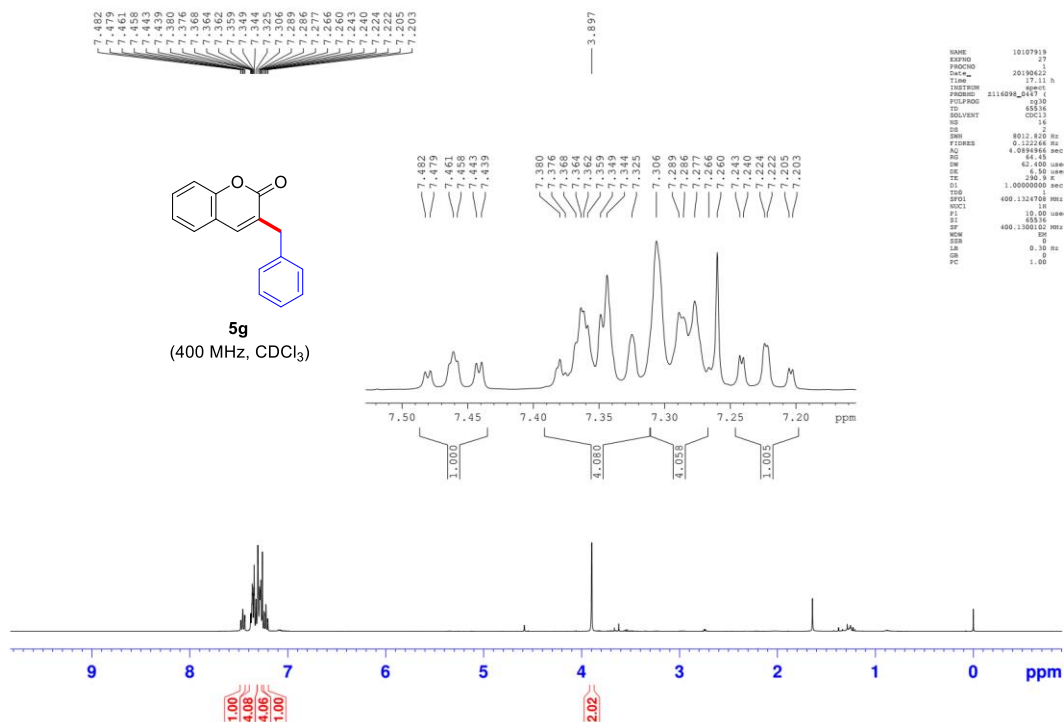
ldk-2020-24 6-Me coumarin diMe 41h



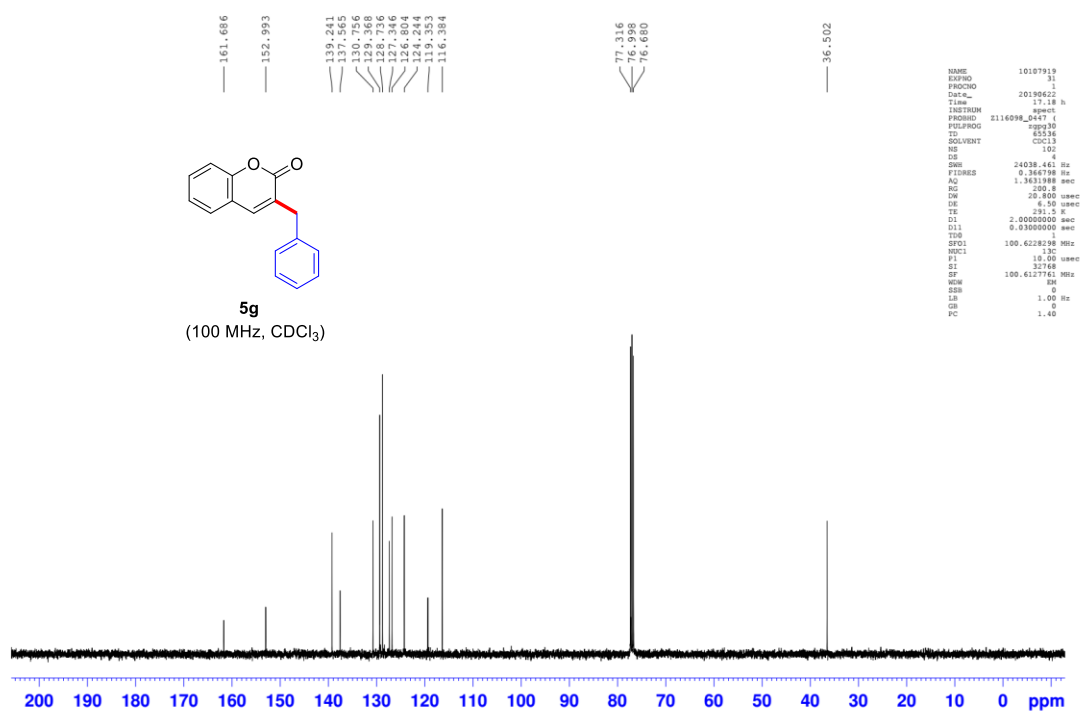
ldk-2020-24 6-Me coumarin diMe 42c



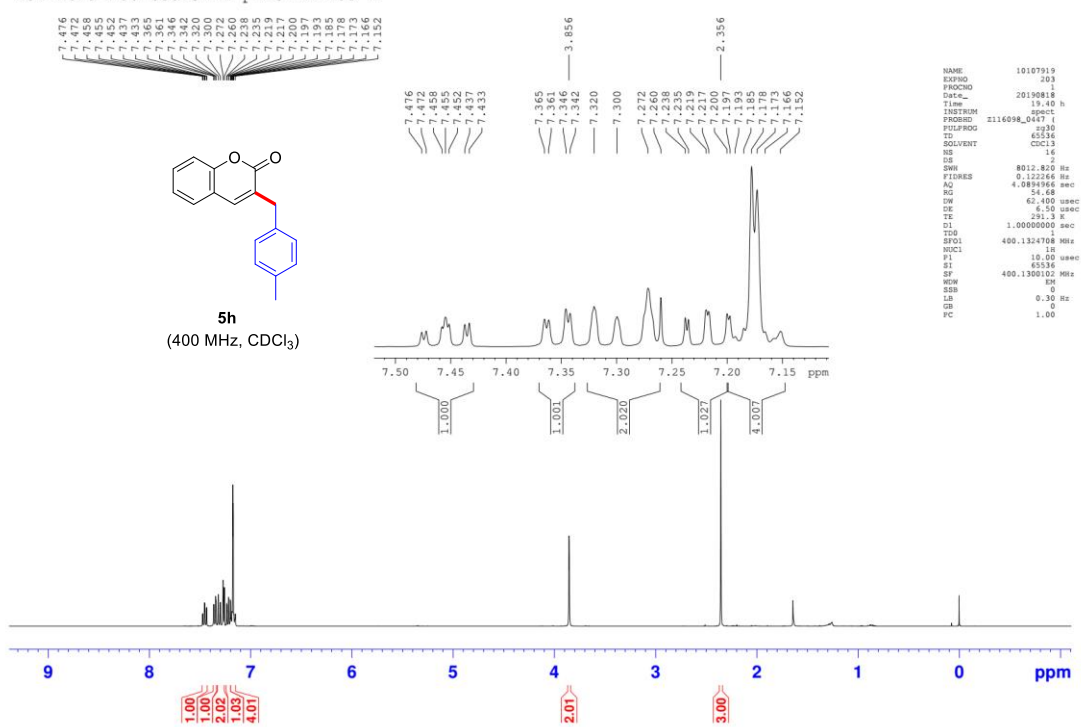
ldk-2019-17 new Fe-coumarin-BnBr h27



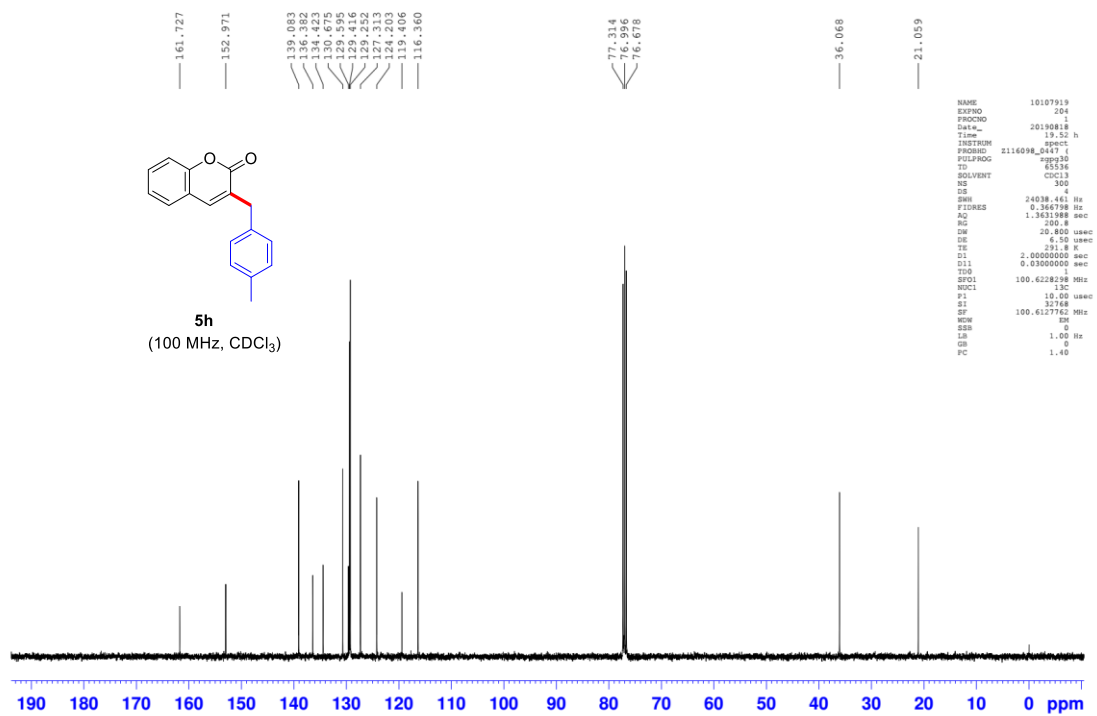
ldk-2019-17 new Fe-coumarin-BnBr c31



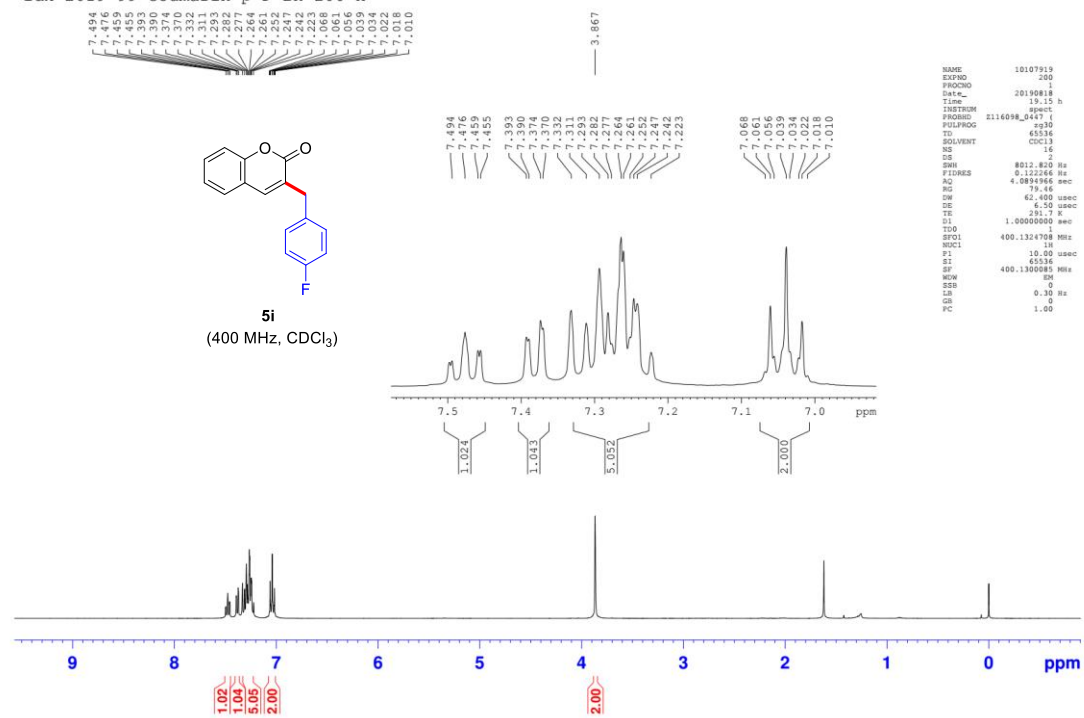
ldk-2019-100 coumarin p-Me Bn 203 h



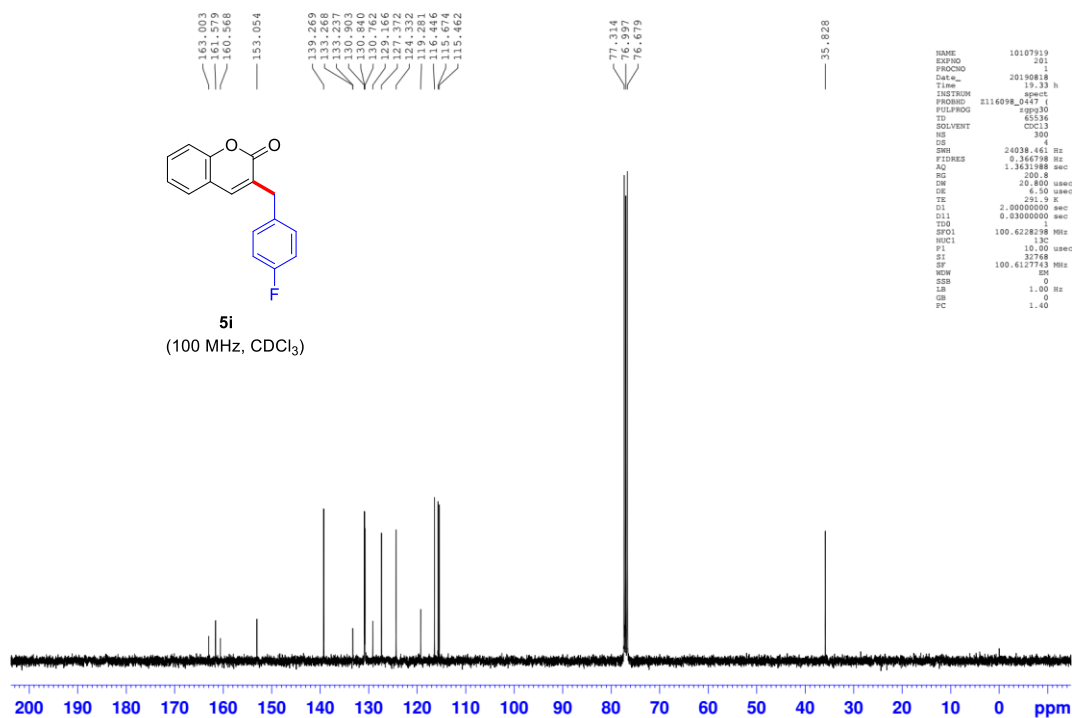
ldk-2019-100 coumarin p-Me Bn 204c



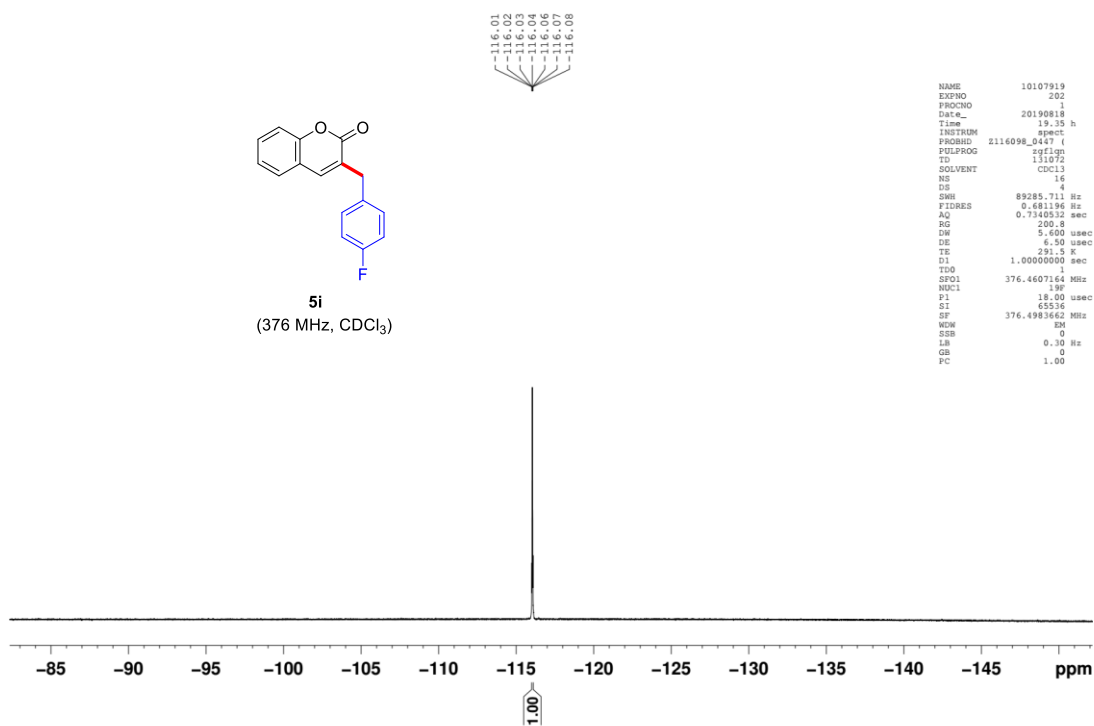
ldk-2019-99 coumarin p-F Bn 200 h



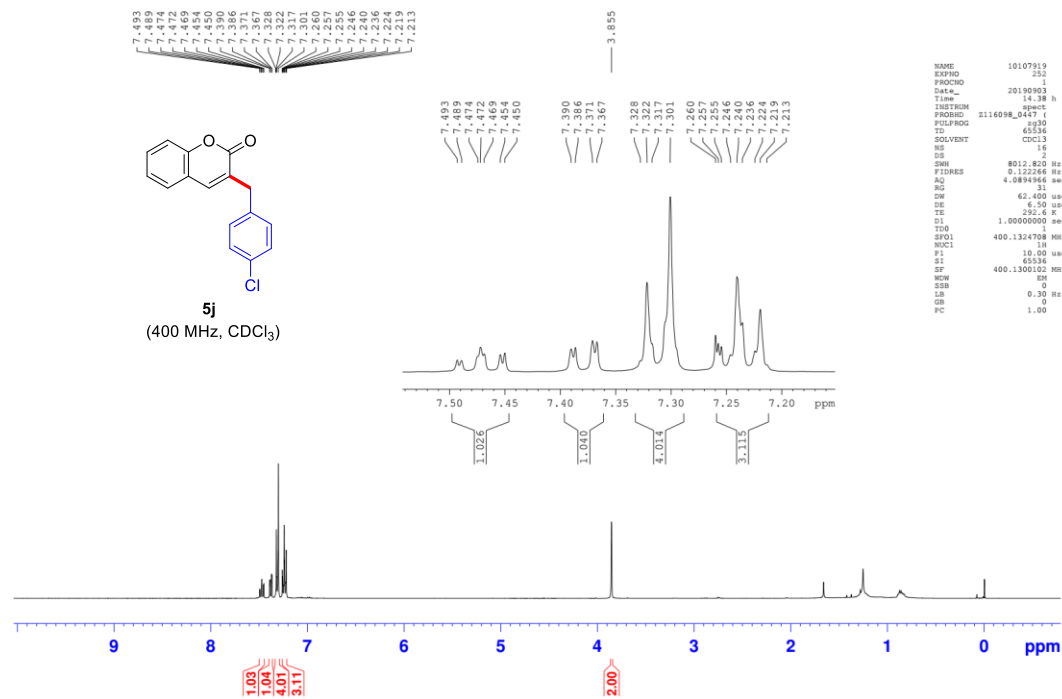
ldk-2019-99 coumarin p-F Bn 201c



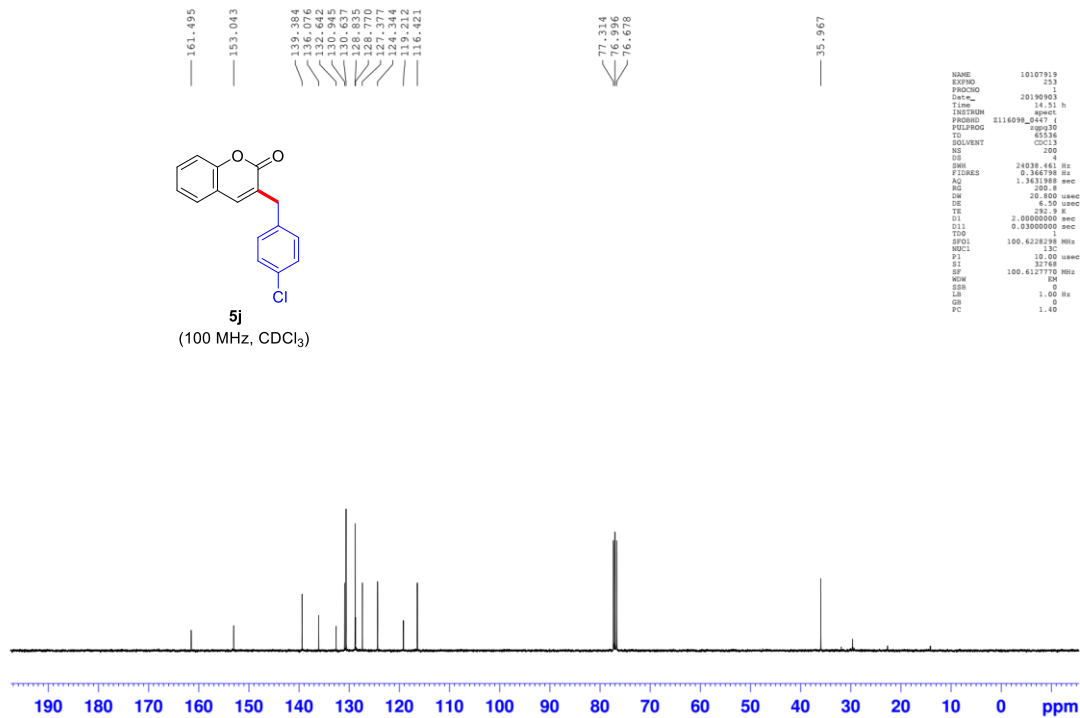
ldk-2019-99 coumarin p-F Bn 202 f



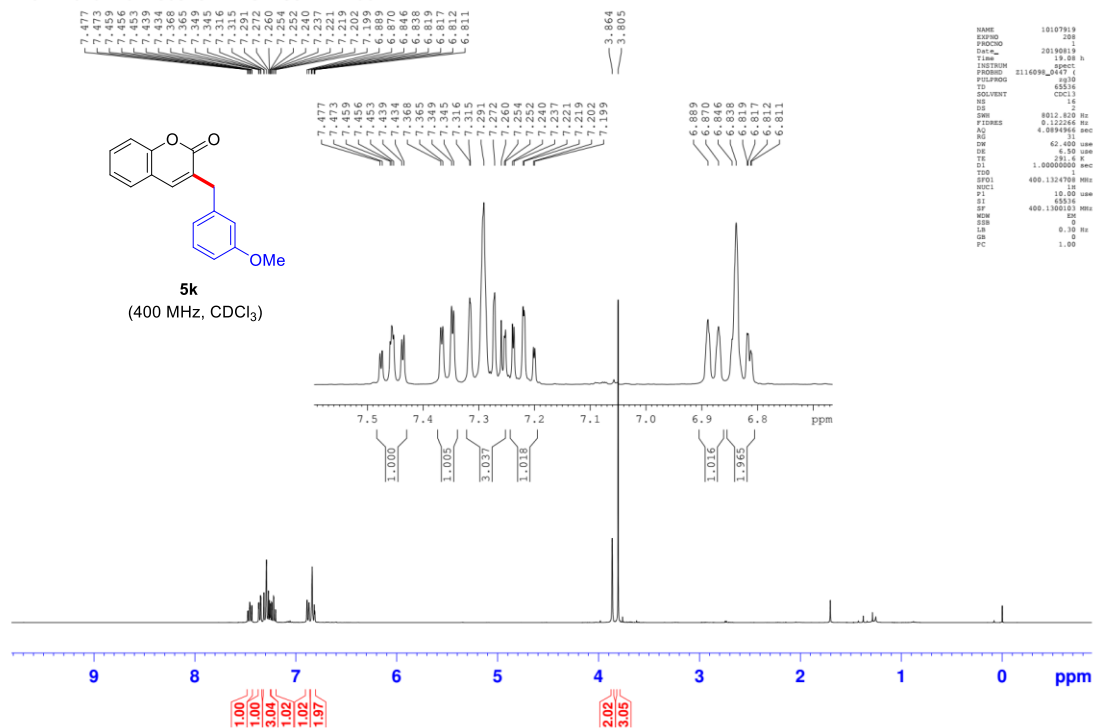
ldk-2019-126 coumarin p-Cl Bn 252 h



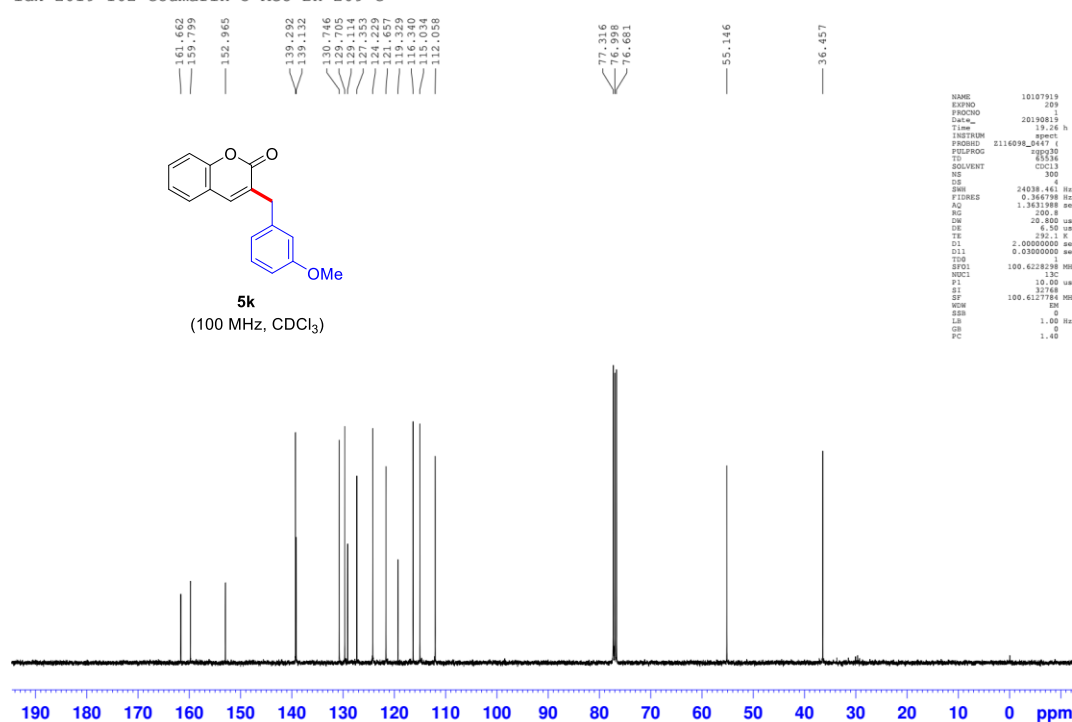
ldk-2019-126 coumarin p-Cl Bn 253 c



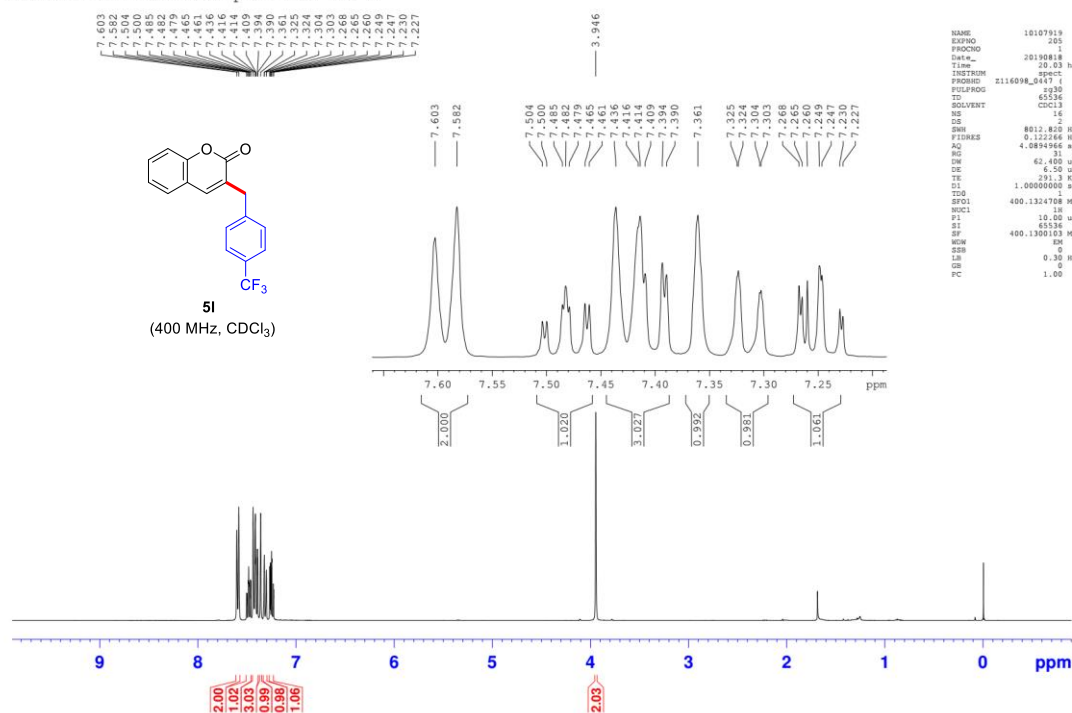
ldk-2019-102 coumarin 3-MeO Bn 208 h



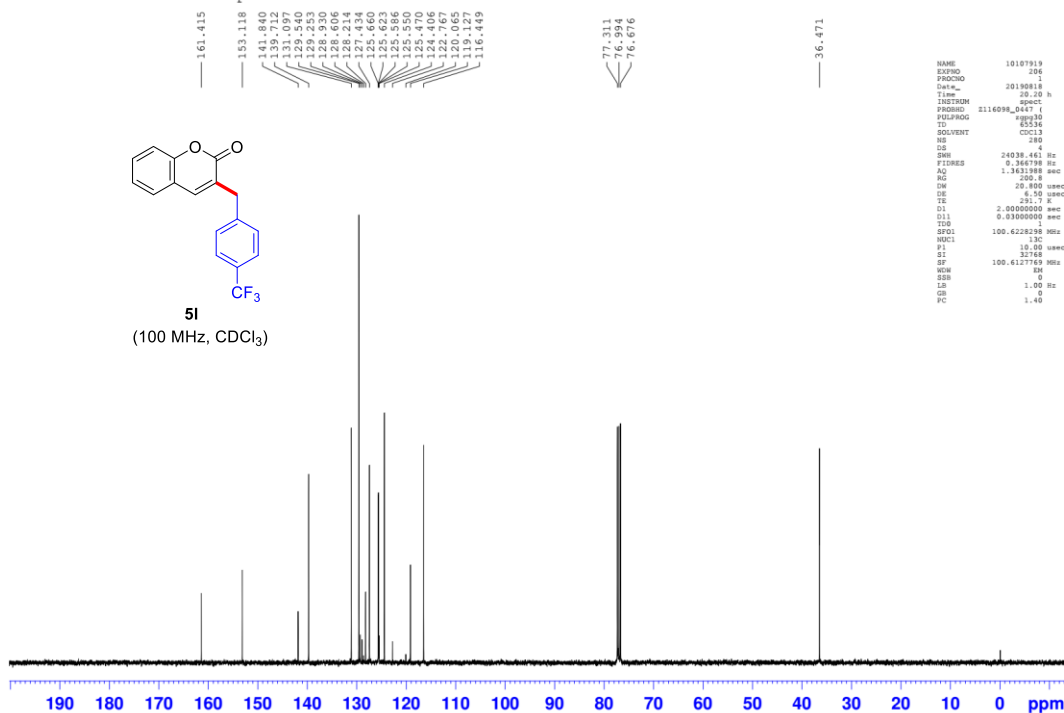
ldk-2019-102 coumarin 3-MeO Bn 209 c



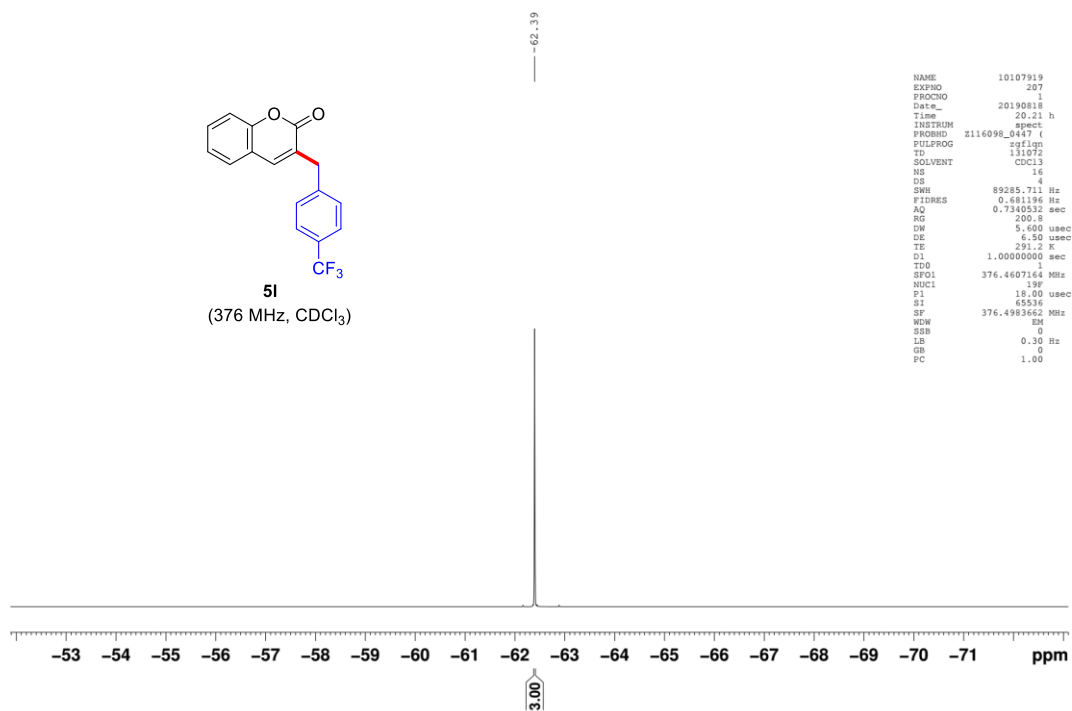
ldk-2019-101 coumarin p-CF₃ Bn 205 h



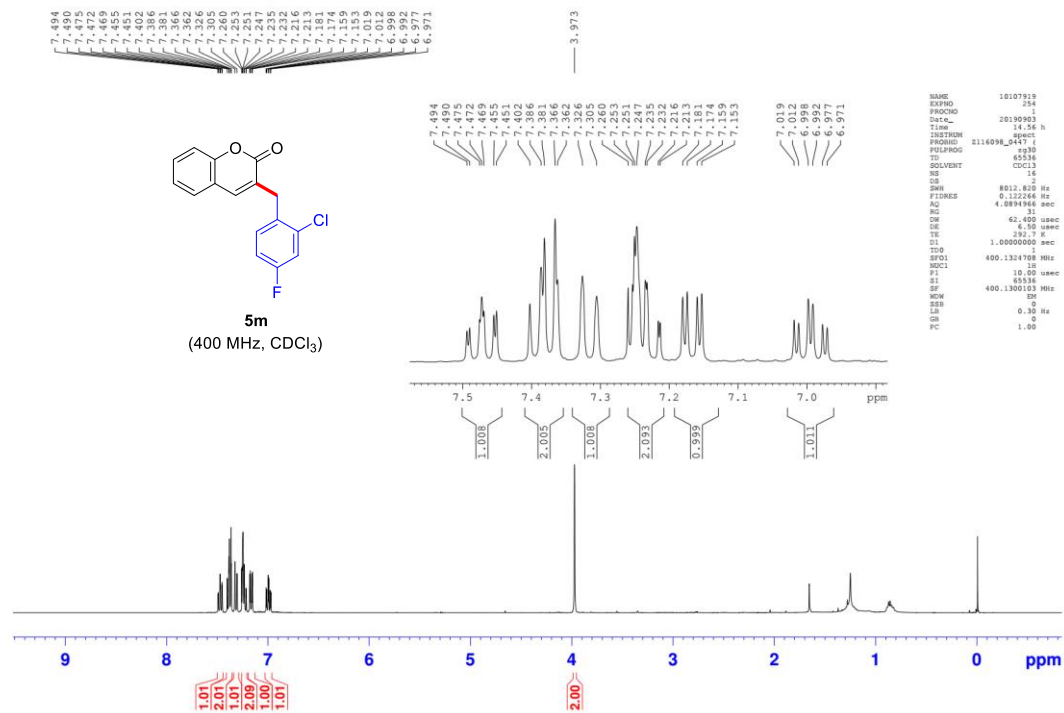
ldk-2019-101 coumarin p-CF₃ Bn 206c



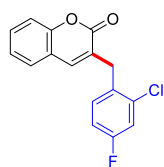
ldk-2019-101 coumarin p-CF₃ Bn 207f



ldk-2019-127 coumarin 2Cl,4F Bn 254 h

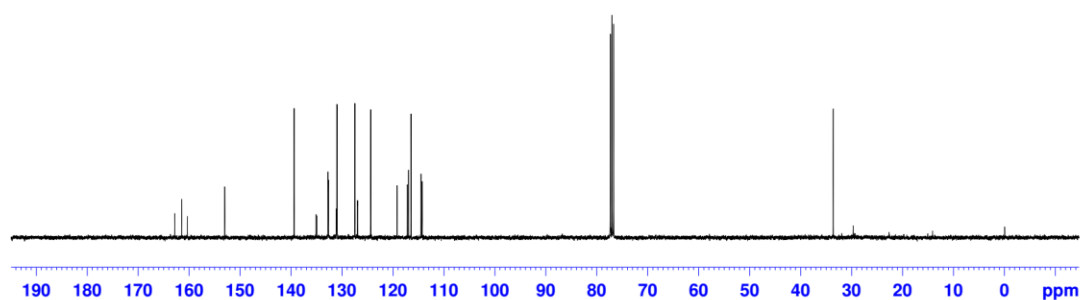


ldk-2019-127 coumarin 2Cl,4F Bn 255 c

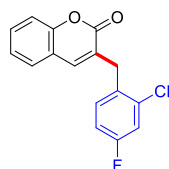


(100 MHz, CDCl₃)

NAME	10107919
EXPNO	255
PROCNO	1
Date_	20190903
Time	15.09 h
INSTRUM	spect
PROBHD	z116098_0447 f
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	4
SWH	24038.461 Hz
FIDRES	0.346798 Hz
AQ	1.363188 sec
RG	200.8
DM	20.800 usec
DE	4.50 usec
TE	293.2 K
D1	2.00000000 sec
D11	0.00000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P1	10.00 usec
SI	32768
SF	100.617762 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

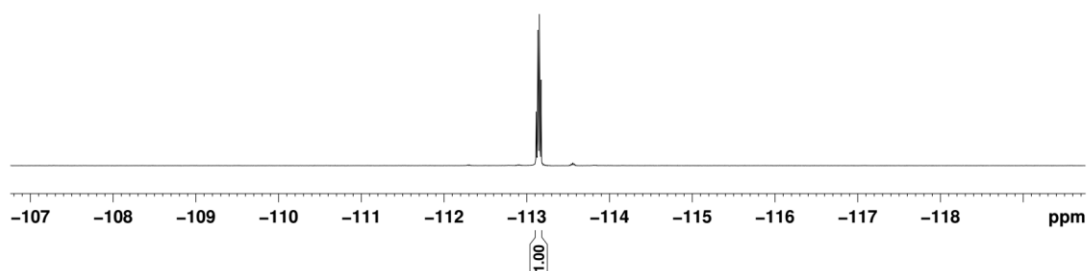


ldk-2019-127 coumarin 2Cl,4F Bn 256 f

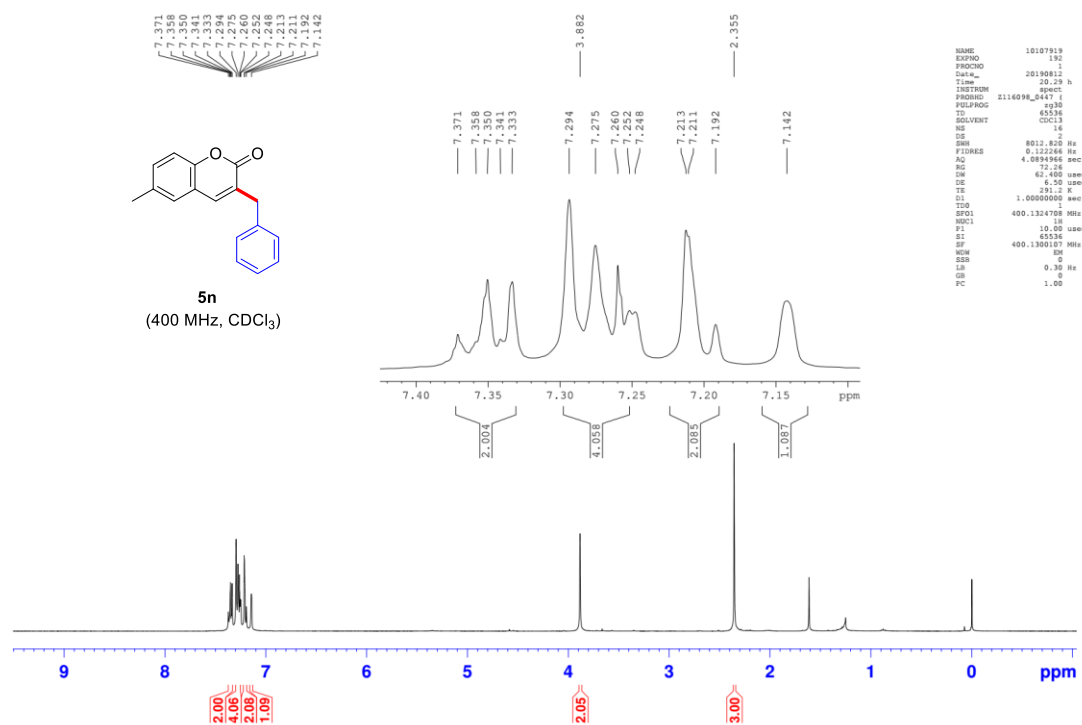


(376 MHz, CDCl₃)

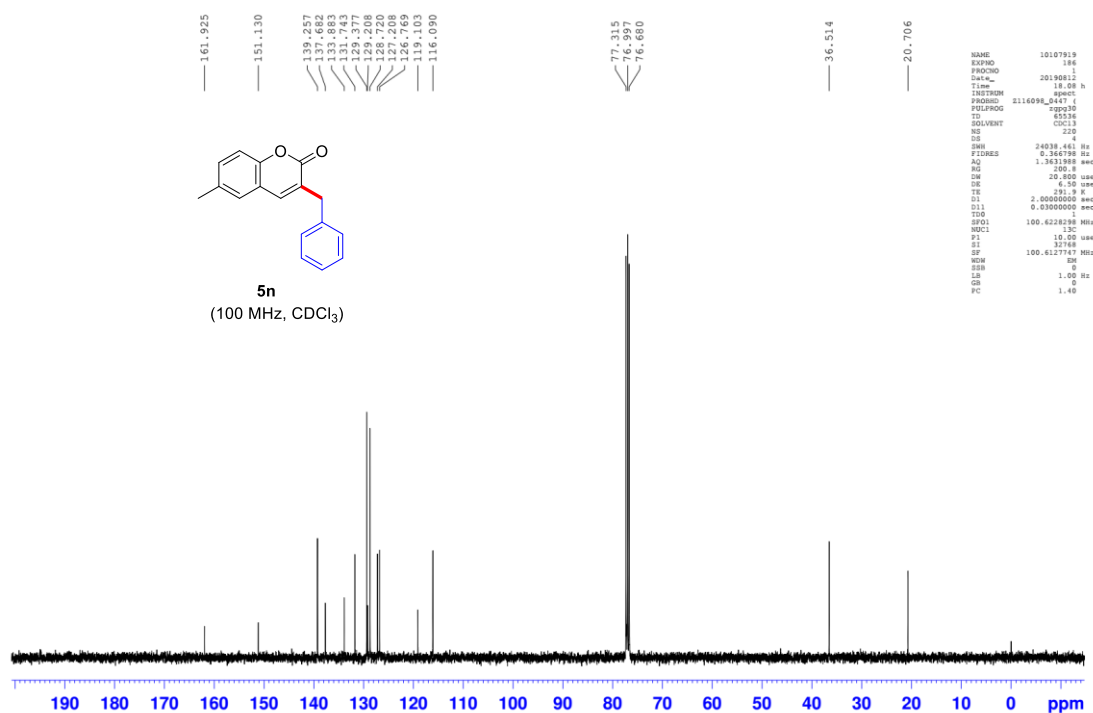
NAME	10107919
EXPNO	256
PROCNO	1
Date_	20190903
Time	19.12 h
INSTRUM	spect
PROBHD	z116098_0447 f
PULPROG	zgpg30
TD	131072
SOLVENT	CDCl3
NS	16
DS	4
SWH	89285.711 Hz
FIDRES	0.681194 Hz
AQ	0.7340532 sec
RG	200.8
DM	5.600 usec
DE	6.50 usec
TE	293.2 K
D1	1.00000000 sec
SFO1	376.4607164 MHz
NUC1	13C
P1	18.00 usec
SI	65536
SF	376.4983462 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



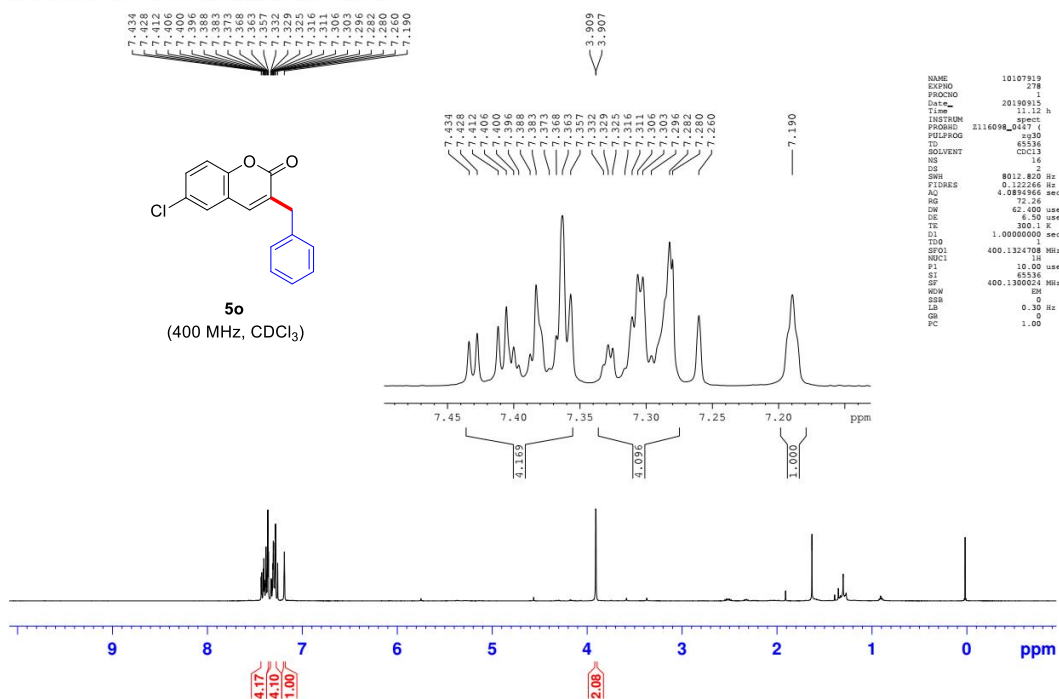
ldk-2019-91 new 6-Me coumarin 192 h



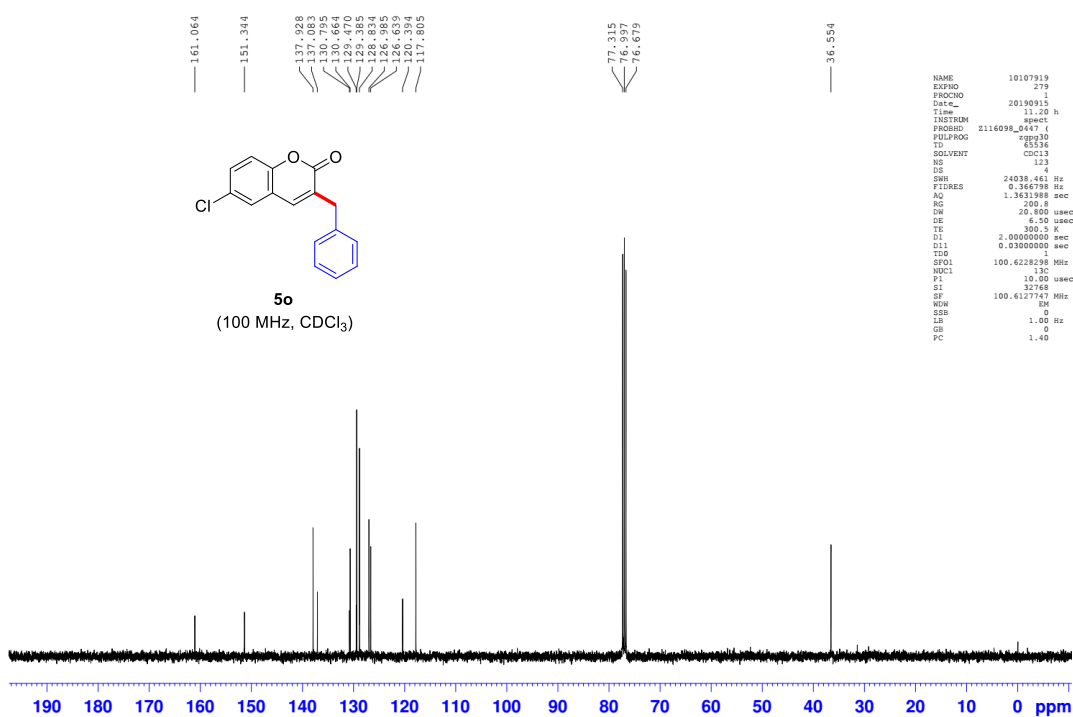
ldk-2019-91 new 6-Me coumarin Bn 186 c



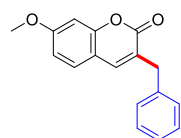
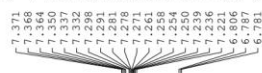
ldk-2019-141 6-Cl coumarin Bn 278 h



ldk-2019-141 6-Cl coumarin Bn 279 c



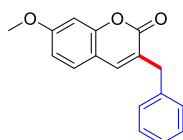
ldk-2019-90 7-MeO coumarin Bn 183 h



5p
(400 MHz, CDCl₃)

```
NAME      10107919
EXPNO     183
PROCNO    1
Date_     20190808
Time      18.42 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        8012.825 Hz
FIDRES     0.122264 Hz
AQ         4.0894966 sec
RG         641.45
DW         62.400 usec
DE         6.50 usec
TE         298.0 K
D1         1.00000000 sec
D11        0
D12        0
D13        0
SFO1       400.1324708 MHz
NUC1       13C
P1         10.00 usec
SI         65536
SF         400.1300098 MHz
WDM        0
EN         0
LB         0.30 Hz
GB         0
PC         1.00
```

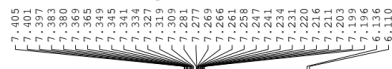
ldk-2019-90 7-MeO coumarin Bn 184 c



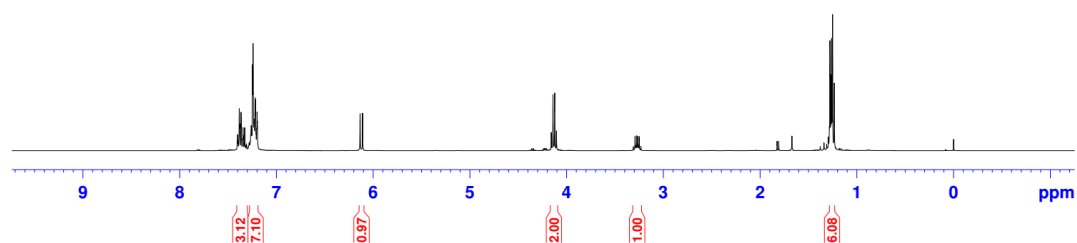
5p
(100 MHz, CDCl₃)

```
NAME      10107919
EXPNO     184
PROCNO    1
Date_     20190808
Time      19.19 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         400
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3613918 sec
RG         200.0
DW         20.000 usec
DE         6.50 usec
TE         298.0 K
D1         2.00000000 sec
D11        0
D12        0
D13        0
SFO1       100.6228255 MHz
NUC1       13C
P1         10.00 usec
SI         65536
SF         100.6127726 MHz
WDM        0
EN         0
LB         1.00 Hz
GB         0
PC         1.00
```


ldk-2019-95 new Ph jili 193 h



NAME	10107919
EXPNO	193
PROCNO	1
DATA_	20190812
Time	20.34 h
INSTRUM	cpoct
PROBHD	1116098_6447 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	4
SWH	8012.820 Hz
FIDRES	0.122264 Hz
AQ	4.0894966 sec
RG	32
DM	62.400 usec
DE	4.50 usec
TE	291.1 K
TD	1.00000000 sec
TD0	400.1324708 MHz
NUC1	13C
P1	10.00 usec
PT	45536
RF	400.1305204 MHz
RGW	DM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



ldk-2019-93 jili diPh-ene TM 189 c



NAME	10107919
EXPNO	189
PROCNO	1
DATA_	20190812
Time	18.36 h
INSTRUM	cpoct
PROBHD	1116098_6447 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	300
DS	4
SWH	24038.461 Hz
FIDRES	0.364798 Hz
AQ	1.3631988 sec
RG	320.8
DM	20.800 usec
DE	4.50 usec
TE	291.1 K
TD	2.00000000 sec
TD0	0.03000000 sec
TD1	100.6228298 MHz
NUC1	13C
P1	10.00 usec
PT	32768
RF	100.6127739 MHz
RGW	DM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

