*Electronic Supporting Information (**ESI**) for*

Highly efficient α-arylation of aryl ketones with aryl chlorides by using bulky imidazolylidene-ligated oxazoline palladacycle

Xian Wei, Kun Wang and Weiwei Fang*

Jiangsu Co-Innovation Center of Efficient Processing and Utilization of Forest Resources, International Innovation Center for Forest Chemicals and Materials, College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037 (China)

E-mail: wwfang2020@njfu.edu.cn

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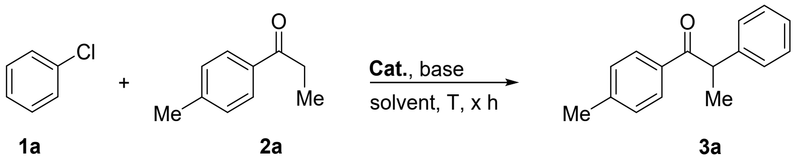
1. General experimental details

All reagents were commercially available unless otherwise noted. Precatalysts **Cat.1**-**Cat.12** were synthesized according to previously reported literatures.[1] All reactions were carried out under argon atmosphere in dried glassware. Air and moisture sensitive liquids and solutions were transferred *via* syringe. All solvents were dried and distilled by standard procedures. Solutions were concentrated under reduced pressure by rotary evaporation. Chromatographic purification of products was accomplished on silica gel Si 60® (300-400 mesh).

Nuclear magnetic resonance spectra were acquired on a Bruker AMX 400 (400 MHz, and 100 MHz for ^{1}H, and ^{13}C respectively) and a Bruker DRX 600 (500 MHz, and 150 MHz for ^{1}H, and ^{13}C respectively). All ^{1}H NMR spectra are reported in parts per million (ppm) downfield of TMS and were measured relative to the signals at 7.26 ppm ($CDCl_3$). All ^{13}C NMR spectra were reported in ppm relative to $CDCl_3$ (77.16 ppm) were obtained with ^{1}H -decoupling. Data for ^{1}H-NMR are reported as follows: chemical shift (δ in ppm), multiplicity (s = singlet; brs = broad singlet; vbs = vary broad singlet; d = doublet; t= triplet; q = quartet; quint = quintet; sext = sextet; m = multiplet), coupling constant (Hz), integration. Data for ^{13}C-NMR are reported in terms of chemical shift (δ in ppm), multiplicity, coupling constant (Hz). High-resolution mass spectra were obtained on a Finnigan MAT 8200 instrument.

2. Optimization of reaction conditions

2.1 α-Arylation of *p*-methylpropiophenone 2a with chlorobenzene 1a



Scheme S1 *α*-Arylation of chlorobenzene **1a** and *p*-methylpropiophenone **2a**

Table S1[a] Screening the amount of H_2O

Entry	H_2O/ μL	Yield/%
1	0	26
2	5	30
3	8	58
4	10	73
5	12	76
6	13	87
7	14	72
8	15	71
9	20	70
10	40	26
11	60	trace

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (x μL), 12 h, 100 °C. Isolated yield.

Table S2[a] Screening solvents

Entry	Solvent	Yield/%
1	dioxane	87
2	DME	83
3	THF	72
4	MTBE	77

5	toluene	trace
6	ACN	51
7	EtOH	NR
8	CPME	62
9	DMF	32
10	DMSO	8

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), solvent (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, 100 °C. Isolated yield. THF= terahydrofuran; MTBE =methyl *tert*-butyl ether; ACN = acetonitrile; DMF = dimethyl formamide; DMSO = dimethyl sulfoxide.

Table S3[a] Screening bases

Entry	Base	Yield/%
1	*t*BuONa	87
2	*t*BuOK	28
3	*t*BuOLi	9
4	Cs_2CO_3	NR
5	Na_2CO_3	NR
6	K_3PO_4	NR
7	KOH	55
8	Et_3N	NR

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), base (2.0 mmol), H_2O (13 μL), 12 h, 100 °C. Isolated yield.

Table S4[a] Screening equiv. of *t*BuONa

Entry	n equiv.	Yield/%
1	1.0	34
2	1.2	31
3	1.5	66
4	1.8	64

5	2.0	87
6	2.2	65
7	2.5	18

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (x mmol), H_2O (13 μL), 12 h, 100 °C. Isolated yield.

Table S5[a] Screening catalyst-loading

Entry	**Cat.**/mol%	Yield/%
1	0.25	63
2	0.5	87

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), dioxane (3 mL), **Cat.1** (x mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, 100 °C. Isolated yield.

Table S6[a] Screening temperature

Entry	T/°C	Yield/%
1	60	78
2	70	84
3	80	81
4	90	88
5	100	87
6	110	56

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.2 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, T °C. Isolated yield.

Table S7[a] Screening equiv. of *p*-methylphenylacetone **2a**

Entry	n equiv.	Yield/%
1	1.0	83
2	1.2	88
3	1.3	88
4	1.4	91

5	1.5	93
6	1.6	83

[a] Standard condition: **1a** (1.0 mmol), **2a** (x mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, 90 °C. Isolated yield.

Table S8[a] Screening the volume of solvent

Entry	Volume/mL	Yield/%
1	2	87
2	3	93
3	4	86

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.5 mmol), dioxane (x mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, 90 °C. Isolated yield.

Table S9[a] Screening reaction time

Entry	Time/h	Yield/%
1	6	90
2	12	93
3	18	91
4	24	90

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.5 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), x h, 90 °C. Isolated yield.

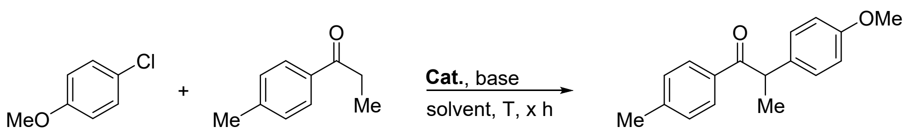
Table S10[a] Screening catalysts

Entry	**Cat.**	Yield/%
1	**Cat.1**	93
2	**Cat.2**	85
3	**Cat.3**	87
4	**Cat.4**	91
5	**Cat.5**	89
6	**Cat.6**	91

7	**Cat.7**	92
8	**Cat.8**	85
9	**Cat.9**	92

[a] Standard condition: **1a** (1.0 mmol), **2a** (1.5 mmol), dioxane (3 mL), **Cat.** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), 12 h, 90 °C. Isolated yield.

2.2 α-Arylation of *p*-methylpropiophenone 2a with *p*-chloroanisole 1e



1e 2a 3e

Scheme S2 *α*-Arylation of *p*-chloroanisole **1e** and *p*-methylpropiophenone **2a**

Table S11[a] Screening the amount of H_2O

Entry	H_2O/ μL	Yield/%
1	0	NR
2	8	63
3	10	64
4	13	61
5	15	44
6	18	44
7	20	NR

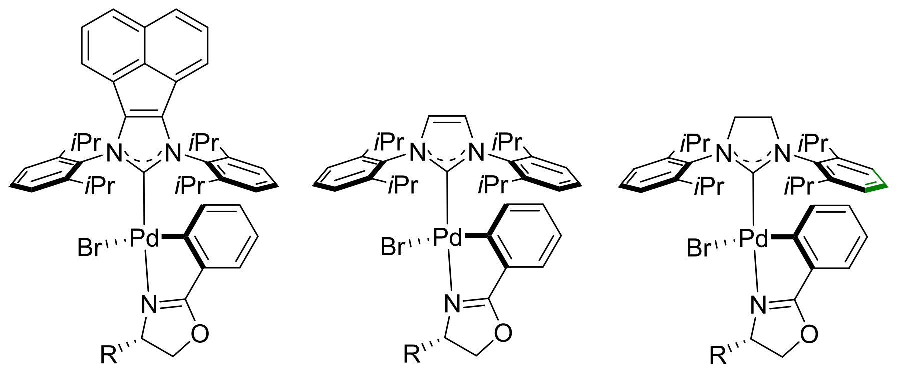
[a] Standard condition: **1e** (1.0 mmol), **2a** (1.5 mmol), dioxane (3 mL), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (x μL), 12 h, 90 °C. Isolated yield.

Table S12[a] Screening catalysts

Entry	**Cat.**	Yield/%
1	**Cat.1**	64
2	**Cat.2**	81

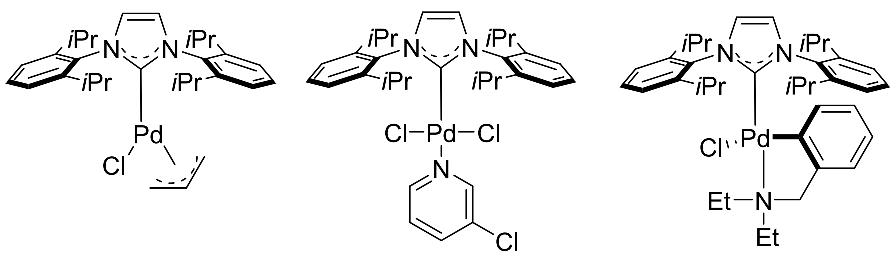
3	**Cat.3**	15
4	**Cat.4**	94/93[b]
5	**Cat.5**	89
6	**Cat.6**	55
7	**Cat.7**	68
8	**Cat.8**	67
9	**Cat.9**	58
10	**Cat.10**	79
11	**Cat.11**	93
12	**Cat.12**	82

[a] Standard condition: **1e** (1.0 mmol), **2a** (1.5 mmol), dioxane (3 mL), **Cat.** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (10 μL), 12 h, 90 °C. Isolated yield. [b] D_2O (10 μL).



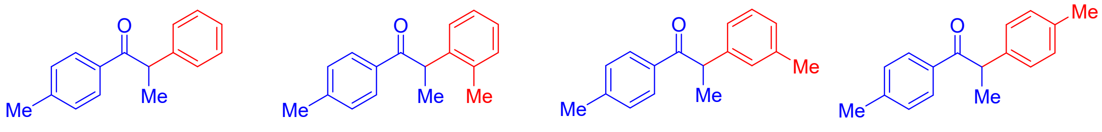
R = *i*Pr, *t*Bu, Ph R = *i*Pr, *t*Bu, Ph R = *i*Pr, *t*Bu, Ph

Cat.1-3 **Cat.4-6** **Cat.7-9**

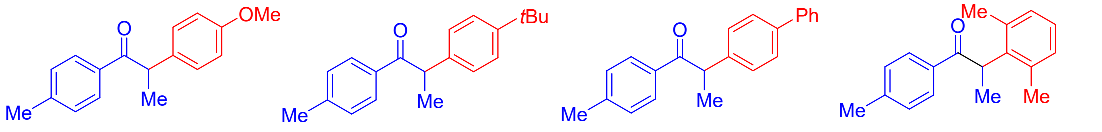


Cat.10 **Cat.11** **Cat.12**

3. Substrate scopes

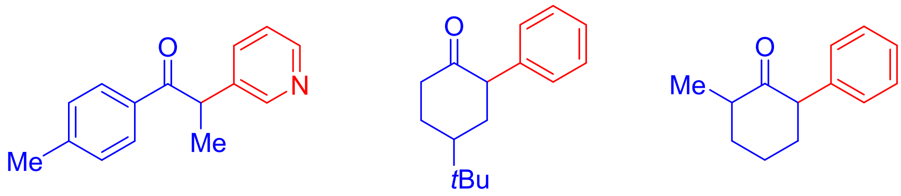


3a, 93% **3b**, 81% **3c**, 78% **3d**, 88%



3e, 61% **3f**, 49% **3g**, 77% **3h**, 65%

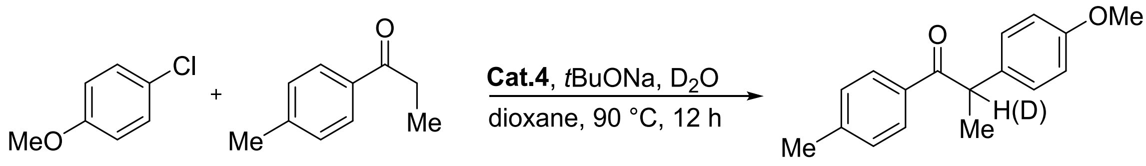
Scheme S3 Substrate scopes catalyzed by using **Cat.1** according to standard condition A: Standard condition (Method A): **1** (1.0 mmol), **2** (1.5 mmol), **Cat.1** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (13 μL), dioxane (3 mL), 12 h, 90 °C. Isolated yield.



15% complex trace

Scheme S4 Substrates tested with poor reactivity by using **Cat.4** according to standard condition (Method B): **1** (1.0 mmol), **2** (1.5 mmol), **Cat.4** (0.5 mol%), *t*BuONa (2.0 mmol), H_2O (10 μL), dioxane (3 mL), 12 h, 90 °C. Isolated yield.

4. Control experiments and proposal mechanism



Scheme S5 *α*-Arylation of *p*-chloroanisole **1e** and *p*-methylpropiophenone **2a** in the presence of D_2O

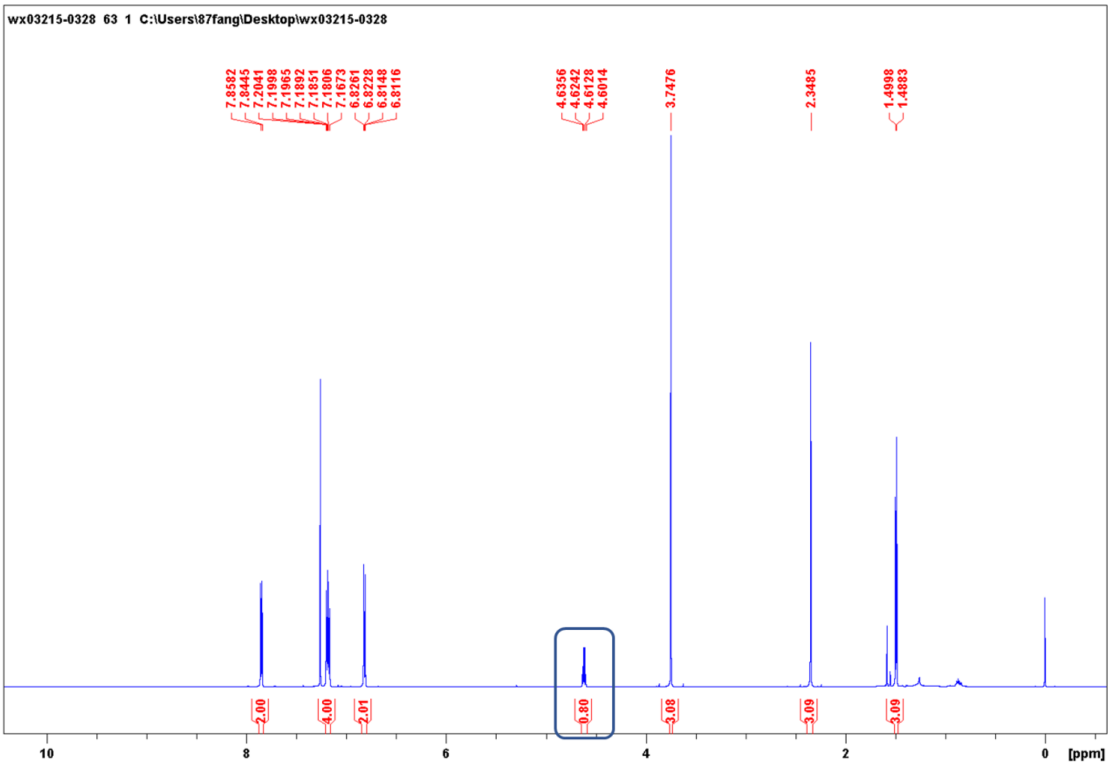


Fig. S1 ¹H NMR (600 MHz, $CDCl_3$) spectrum of 3e' in the presence of D_2O

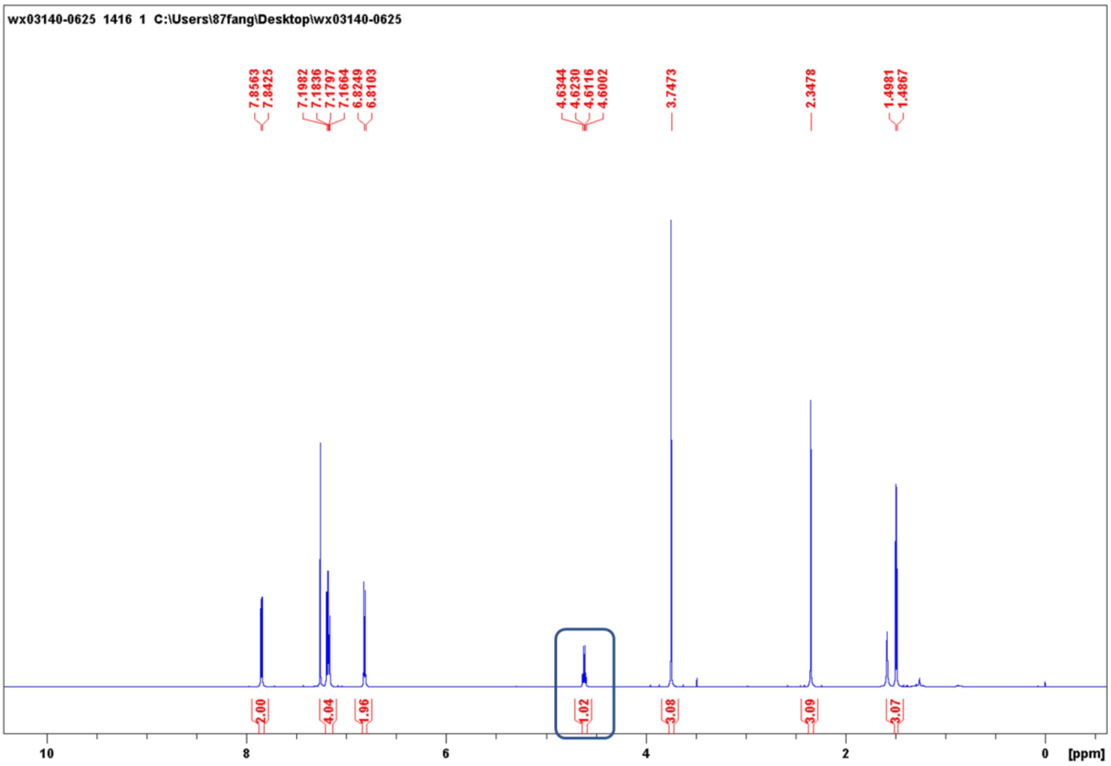
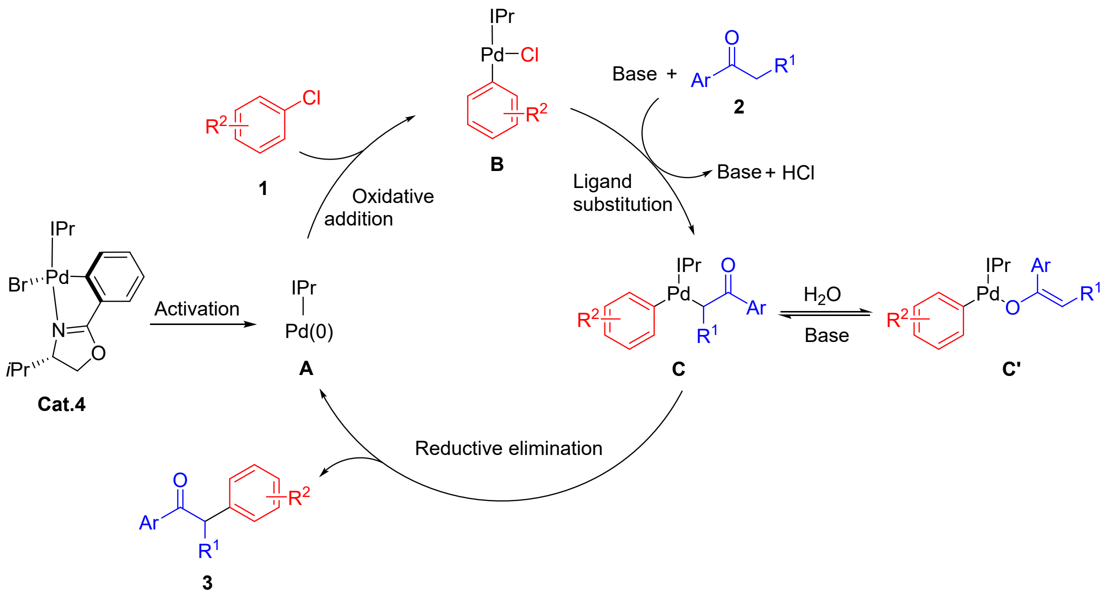


Fig. S2 ¹H NMR (600 MHz, $CDCl_3$) spectrum of **3e** in the presence of H_2O

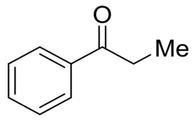


Scheme S6 Proposed reaction mechanism of *α*-arylation catalyzed by **Cat.4**

At the current stage, we suggested the presence of H_2O effected the keto-enol tautomerism equilibrium, however, its role in the activation of the precatalyst[2] could be excluded. We will carry out the DFT calculations with other groups to get a deep insight.

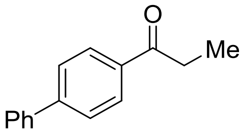
5. General procedure for synthesis of substrates

To a flame dried round bottom flask equipped with a magnetic stir bar, diisopropylamine (0.92 mL, 6.6 mmol) in dry THF (15 mL) was added at -78 °C. Then, *n*BuLi (2.64 mL, 6.6 mmol, 2.5 M in Hexane) was added dropwise, and the reaction mixture was stirred for 30 minutes. Then, acetophenone (0.70 mL, 6 mmol) was added and reacted for 30 minutes. Then, methyl iodide (0.45 mL, 7.2 mmol) in dry THF (15 mL) was added. After 4 h, the reaction was quenched with saturated ammonium chloride. The organic phase was separated, and the aqueous phase was washed with hexane (1×5 mL). The combined organic phases were washed with 1 M HCl (1×10 mL), dried over anhydrous sodium sulfate, filtered, and evaporated under reduced pressure. The crude products were further purified by column chromatography leading to desired products.



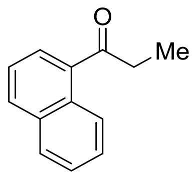
2q: Following the **General procedure**, **2q** was obtained as a yellow oil, 645.7 mg, yield = 27%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.98-7.95 (m, 2H), 7.57-7.54 (m, 1H), 7.48-7.44 (m, 2H), 3.01 (q, J = 7.2 Hz ,2H), 1.23 (t, J = 7.2 Hz, 3H). The data was the same to previous literature.[3]



2u: Following the **General procedure**, **2u** was obtained as a white solid, 359.3 mg, yield = 28%.

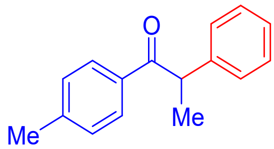
^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.06-8.03 (m, 2H), 7.70-7.67 (m, 2H), 7.64-7.62 (m, 2H), 7.49-7.46 (m, 2H), 7.46-7.38 (m, 1H), 3.04 (q, J = 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H). The data was the same to previous literature.[4]



2y: Following the **General procedure**, **2y** was obtained as a yellow oil, 325.8 mg, yield = 15%.

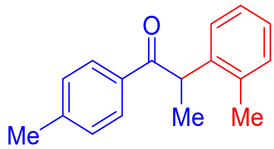
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (J = 8.5 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.98 (d, J = 8.0 Hz, 1H), 7.90-7.83 (dd, J = 7.5, 1.0 Hz, 2H), 7.62-7.47 (m, 3H), 3.08 (q, J = 7.0 Hz, 2H), 1.29 (t, J = 7.0 Hz, 3H). The data was the same to previous literature.[5]

6. Date for arylation products



3a: Pale yellow oil, 203.1 mg, yield: 91%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.86 (d, J = 8.2 Hz, 2H), 7.28-7.29 (d, J = 4.4 Hz, 4H), 7.22-7.16 (m, 3H), 4.67 (q, J = 6.8 Hz, 1H), 2.35 (s, 3H), 1.53 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[6]



new compound

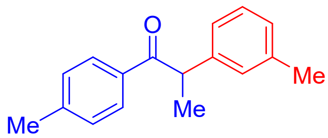
3b: Pale yellow solid, 206.0 mg, yield: 86%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.74 (d, J = 8.2 Hz, 2H), 7.20 (d, J = 7.1 Hz, 1H), 7.15 (d, J = 8.0 Hz, 2H),7.12-7.06 (m, 2H), 7.04-7.02 (d, J = 7.4 Hz, 1H), 4.74 (q, J = 6.8 Hz, 1H), 2.49 (s, 3H), 2.34 (s, 3H), 1.47 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.6, 143.4, 140.4, 134.5, 134.1, 130.9, 129.2, 128.6, 127.0, 126.8, 126.7, 44.5, 21.5, 19.6, 18.0.

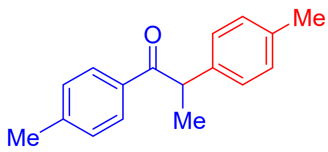
HR-MS (ESI, m/z): calcd for $C_{17}H_{18}O$ $[M+H]^{+}$: 239.1430. found: 239.1426.

m.p.: 63.4-66.7 °C.



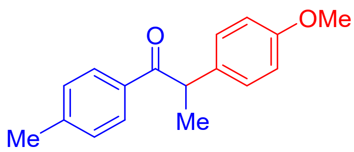
3c: Pale yellow oil, 215.8 mg, yield: 91%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.86 (d, J = 8.2 Hz, 2H), 7.20-7.15 (m, 3H), 7.08 (d, J = 1.8 Hz, 2H), 6.98 (d, J = 7.5 Hz, 1H), 4.62 (q, J = 6.8 Hz, 1H), 2.35 (s, 3H), 2.30 (s, 3H), 1.50 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[7]



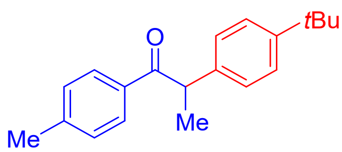
3d: Pale yellow oil, 219.0 mg, yield: 92%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.86 (d, J = 8.2 Hz, 2H), 7.17 (d, J = 8.1 Hz, 4H), 7.08 (d, J = 7.9 Hz, 2H), 4.63 (q, J = 6.8 Hz, 1H), 2.35 (s, 3H), 2.28 (s, 3H), 1.50 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[7]



3e: Pale yellow oil, 239.6 mg, yield: 94%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.85 (d, J = 8.2 Hz, 2H), 7.21-7.16 (m, 4H), 6.83-6.81 (dt, J = 8.2, 2.6 Hz, 2H), 4.62 (q, J = 6.8 Hz, 1H), 3.75 (s, 3H), 2.35 (s, 3H), 1.49 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[8]



new compound

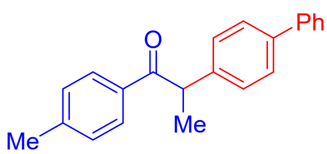
3f: Pale yellow solid, 253.8 mg, yield: 91%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.88 (d, J = 8.2 Hz, 2H), 7.29 (td, J = 8.4, 2.0 Hz, 2H), 7.22-7.18 (m, 4H), 4.66 (q, J = 6.8 Hz, 1H), 2.35 (s, 3H), 1.51 (d, J = 6.6 Hz, 3H), 1.27 (s, 9H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.2, 149.6, 143.5, 138.5, 134.1, 129.2, 129.0, 127.4, 125.8, 47.1, 34.4, 31.3, 21.6, 19.5.

HR-MS (ESI, m/z): calcd for $C_{20}H_{24}O$ $[M+H]^{+}$: 281.1900. found: 281.1894.

m.p.: 73.8-75.9 °C.



new compound

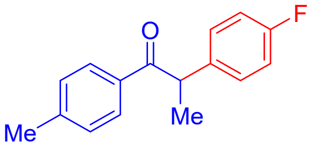
3g: White solid, 270.4 mg, yield: 90%.

^{1}H NMR (600 MHz, CDCl$_3$): δ = 7.90 (dt, J = 8.2 Hz, 2H), 7.55-7.51 (dd, J = 7.4, 8.2 Hz, 4H), 7.41 (t, J = 7.7 Hz, 2H), 7.35 (d, J = 8.2 Hz, 2H), 7.33-7.30 (t, J = 7.4 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 4.72 (q, J = 6.8 Hz, 1H), 2.36 (s, 3H), 1.56 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, CDCl$_3$): δ = 200.0, 143.7, 140.8, 140.7, 139.8, 134.0, 129.3, 129.0, 128.8, 128.2, 127.7, 127.3, 127.0, 47.4, 21.6, 19.5.

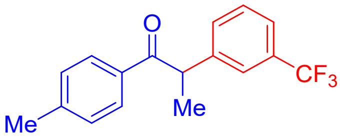
HR-MS (ESI, m/z): calcd for $C_{22}H_{20}O$ $[M+H]^+$: 301.1587. found: 301.1583.

m.p.: 140.8-143.2 °C.



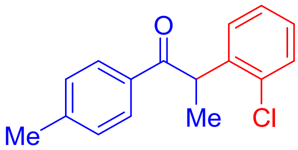
3h: Pale yellow oil, 234.0 mg, yield: 96%.

^{1}H NMR (600 MHz, CDCl$_3$): δ = 7.84 (d, J = 8.2 Hz, 2H), 7.25-7.23 (m, 2H), 7.19 (d, J = 8.0 Hz, 2H), 6.99-6.95 (tt, J = 8.7, 1.83 Hz, 2H), 4.66 (q, J = 6.9 Hz, 1H), 2.36 (s, 3H), 1.50 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[8]



3i: Pale yellow oil, 160.8 mg, yield: 55%.

^{1}H NMR (600 MHz, CDCl$_3$): δ = 7.85 (d, J = 8.2 Hz, 2H), 7.56 (s, 1H), 7.47 (t, J = 7.4 Hz, 2H), 7.40 (t, J = 7.7 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 4.75 (q, J = 6.9 Hz, 1H), 2.37 (s, 3H), 1.55 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[8]



new compound

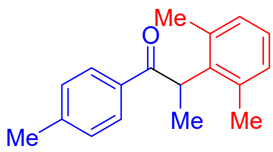
3j: Pale yellow oil, 113.5 mg, yield: 44%.

^{1}H NMR (600 MHz, CDCl$_3$): δ = 7.83 (d, J = 8.2 Hz, 2H), 7.41-7.39 (m, 1H), 7.18 (d,

J = 8.0 Hz, 2H), 7.15-7.13 (m, 3H), 5.12 (q, J = 6.8 Hz, 1H), 2.35 (s, 3H), 1.48 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 199.7, 143.8, 139.5, 133.6, 132.9, 129.8, 129.3, 128.7, 128.6, 128.2,127.5, 44.1, 21.6, 17.8.

HR-MS (ESI, m/z): calcd for $C_{16}H_{15}ONaCl$ [M+Na] $^{+}$: 287.0704. found: 287.0711.



new compound

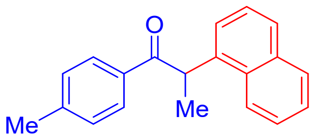
3k: Pale yellow solid, 194.6 mg, yield: 77%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.60 (d, J = 8.2 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 7.02-6.95 (m, 3H), 4.50 (q, J = 6.8 Hz, 1H), 2.30 (s, 9H), 1.50 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 201.9, 143.2, 140.1, 135.6, 134.3, 129.5, 129.0, 128.3, 126.6, 46.1, 21.5, 20.6, 14.9.

HR-MS (ESI, m/z): calcd for $C_{18}H_{20}O$ [M+H] $^{+}$: 253.1587. found: 253.1584.

m.p.: 74.8-78.9 °C.



new compound

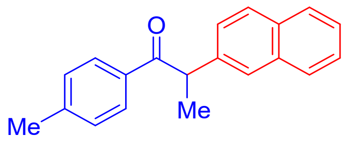
3l: Pale yellow solid, 247.3 mg, yield: 90%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.25 (d, J = 8.5 Hz, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.77 (d, J = 8.2 Hz, 2H), 7.72 (d, J = 8.2 Hz, 1H), 7.64-7.61 (m, 1H), 7.55-7.52 (m, 1H), 7.33 (t, J = 7.9 Hz, 1H), 7.21 (dd, J = 6.6 Hz, 0.6 Hz, 1H), 7.07 (t, J = 8.1 Hz, 2H), 5.36 (q, J = 6.8 Hz, 1H), 2.29 (s, 3H), 1.63 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.4, 143.5, 138.3, 134.4, 133.9, 130.7, 129.3, 129.2, 128.7, 127.5, 126.7, 125.9, 125.8, 125.0, 122.6, 43.6, 21.5, 18.6.

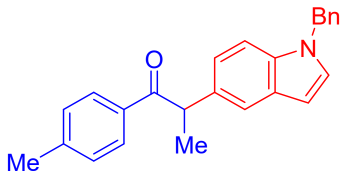
HR-MS (ESI, m/z): calcd for $C_{20}H_{18}O$ [M+H] $^{+}$: 275.1430. found: 275.1427.

m.p.: 116.8-120.8 ℃.



3m: Pale yellow oil, 257.7 mg, yield: 94%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.90 (d, J = 8.3 Hz, 2H), 7.78 (t, J = 8.2 Hz, 3H), 7.72 (t, J = 1.2 Hz, 1H), 7.46-7.40 (m, 3H), 7.16 (d, J = 8.0 Hz, 2H), 4.83 (q, J = 6.8 Hz, 1H), 2.33 (s, 3H), 1.61 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[8]



new compound

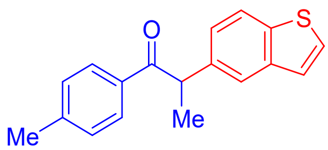
3n: Pale yellow solid, 287.6 mg, yield: 81%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.82 (d, J = 8.3 Hz, 2H), 7.56 (d, J = 8.1 Hz, 1H), 7.28-7.26 (m, 3H), 7.16 (s, 1H), 7.10 (d, J = 8.1 Hz, 2H), 7.08-7.05 (m, 4H), 6.47 (d, J = 3.0 Hz, 1H), 5.26 (d, J = 3.4 Hz, 2H), 4.71 (q, J = 6.8 Hz, 1H), 2.32 (s, 3H), 1.54 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.0, 143.6, 140.2, 138.3, 138.0, 127.0, 124.4, 123.8, 123.0, 122.6, 47.6, 29.8, 21.6, 19.9.

HR-MS (ESI, m/z): calcd for $C_{25}H_{23}NO$ $[M+H]^+$: 354.1852. found: 354.1845.

m.p.: 97.2-99.3 °C.



new compound

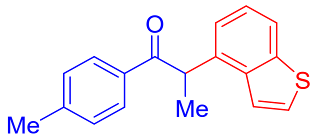
3o: Pale yellow solid, 266.9 mg, yield: 95%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.88 (d, J = 8.3 Hz, 2H), 7.80 (d, J = 8.3 Hz, 1H), 7.72 (d, J = 1.5 Hz, 1H), 7.41-7.40 (d, J = 5.4 Hz, 1H), 7.30-7.28 (dd, J = 1.6, 6.7 Hz, 1H), 7.27 (s, 1H), 7.16 (d, J = 8.1 Hz, 2H), 4.79 (d, J = 6.8 Hz, 1H), 2.33 (s, 3H), 1.58 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.0, 143.6, 140.7, 137.7, 136.8, 133.9, 129.2, 128.8, 127.0, 124.8, 123.0, 121.3, 121.2, 46.0, 21.6, 18.5.

HR-MS (ESI, m/z): calcd for $C_{18}H_{16}SO$ $[M+H]^+$: 281.0995. found: 281.0985.

m.p.: 71.4-74.8 °C.



new compound

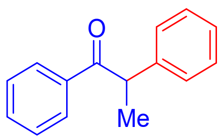
3p: Pale yellow solid, 257.8.9 mg, yield: 92%.

^1H NMR (600 MHz, $CDCl_3$): δ = 7.80 (d, J = 8.3 Hz, 2H), 7.74 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 5.5 Hz, 1H), 7.53 (d, J = 5.5 Hz, 1H), 7.25-7.22 (t, J = 7.7 Hz, 1H), 7.15 (d, J = 7.3 Hz, 1H), 7.11 (d, J = 8.0 Hz, 2H), 5.10 (d, J = 6.8 Hz, 1H), 2.30 (s, 3H), 1.62 (d, J = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$): δ = 200.4, 143.5, 138.3, 134.4, 133.8, 130.6, 129.3, 129.2, 128.7, 127.5, 126.7, 125.9, 125.8, 125.0, 122.6, 43.6, 21.6, 18.6.

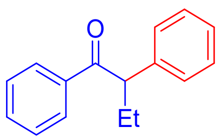
HR-MS (ESI, m/z): calcd for $C_{18}H_{16}SO$ $[M+H]^+$: 281.0995. found: 281.0984.

m.p.: 84.0-86.4 °C.



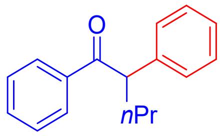
3q: Pale yellow oil, 196.6 mg, yield: 93%.

^1H NMR (600 MHz, $CDCl_3$): δ = 7.95 (d, J = 7.3 Hz, 2H), 7.47 (t, J = 6.8 Hz, 1H), 7.38 (t, J = 7.4 Hz, 2H), 7.30-7.25 (m, 4H), 7.20 (m, 1H), 4.69 (q, J = 6.7 Hz, 1H), 1.53 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[6]



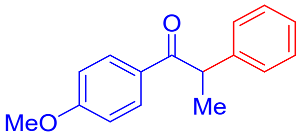
3r: Pale yellow oil, 215.6 mg, yield: 96%.

^1H NMR (600 MHz, $CDCl_3$): δ = 7.97-7.95 (m, 2H), 7.49-7.46 (m, 1H), 7.40-7.37 (m, 2H), 7.32-7.27 (m, 4H), 7.22-7.19 (m, 1H), 4.45 (t, J = 7.3 Hz, 1H), 2.24-2.17 (m, 1H), 1.90-1.83 (m, 1H), 0.91 (t, J = 7.4 Hz, 3H). Data is consistent with that reported in the literature.[6]



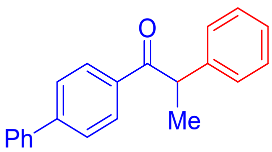
3s: Pale yellow oil, 217.0mg, yield: 91%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.97-7.95 (m, 2H), 7.49-7.46 (m, 1H), 7.40-7.38 (t, J = 7.7 Hz, 2H), 7.32-7.27 (m, 4H), 7.21-7.18 (m, 1H), 4.56 (t, J = 7.3 Hz, 1H), 2.19-2.13 (m, 1H), 1.85-1.79 (m, 1H), 1.38-1.25 (m, 2H), 0.92 (t, J = 7.5 Hz, 3H). Data is consistent with that reported in the literature.[9]



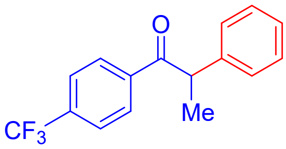
3t: Pale yellow oil, 237.0 mg, yield: 96%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.95 (d, J = 8.8 Hz, 2H), 7.30-7.28 (m, 4H), 7.22-7.18 (m, 1H), 6.85 (d, J = 8.8 Hz, 2H), 4.64 (q, J = 6.8 Hz, 1H), 3.81 (s, 3H), 1.51 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[8]



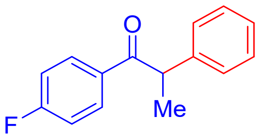
3u: Pale yellow oil, 218.7 mg, yield: 76%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.02 (d, J = 7.8 Hz, 2H), 7.60 (dd, J = 11.7, 8.0 Hz, 4H), 7.44 (d, J = 7.3 Hz, 2H), 7.38 (d, J = 6.9 Hz, 1H), 7.32-7.31 (m, 4H), 7.24-7.20 (m, 1H), 4.72 (q, J = 6.8 Hz, 1H), 1.56 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[6]



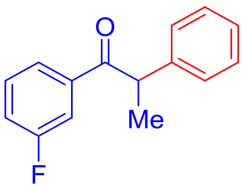
3v: Pale yellow oil, 225.2 mg, yield: 80%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.02 (d, J = 8.1 Hz, 2H), 7.63 (d, J = 7.2, 8.2 Hz, 2H), 7.32-7.29 (m, 2H), 7.26-7.24 (m, 2H), 7.23-7.20 (m, 1H), 4.65 (q, J = 6.8 Hz, 1H), 1.55 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[8]



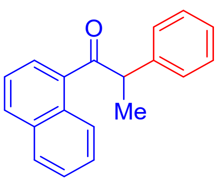
3w: Pale yellow oil, 190.4 mg, yield: 83%.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.98-7.95 (m, 2H), 7.32-7.26 (m, 4H), 7.22-7.20(m, 1H), 7.06-7.02 (m, 2H), 4.62 (q, J = 6.8 Hz, 1H), 1.52 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[10]



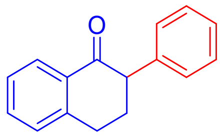
3w: Pale yellow oil, 164.7 mg, yield: 72%.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.71 (d, J = 7.8 Hz, 1H), 7.62 (dt, J = 9.6, 4.2 Hz, 1H), 7.37-7.26(m, 5H), 7.24-7.14 (m, 2H), 4.62 (q, J = 6.8 Hz, 1H), 1.53 (d, J = 6.8 Hz, 3H). Data is consistent with that reported in the literature.[7]



3y: Pale yellow oil, 85.0 mg, yield: 32%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.90 (d, J = 8.2 Hz, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.75 (d, J = 7.1 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.54-7.48 (m, 2H), 7.43-7.40 (m, 1H), 7.31-7.29 (m, 2H), 7.27-7.24 (m, 2H), 7.17 (t, J = 7.1 Hz, 1H), 4.70 (q, J = 6.8 Hz, 1H), 1.64 (d, J = 6.9 Hz, 3H). Data is consistent with that reported in the literature.[11]



3z: Pale yellow oil, 39.3 mg, yield: 18%.

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.10 (dd, J = 0.9, 7.8 Hz, 1H), 7.50 (td, J = 1.4, 7.5 Hz, 1H), 7.36-7.33 (m, 3H), 7.30-7.27 (m, 2H), 7.21-7.19 (m, 2H), 3.81 (dd, J = 2.8, 6.5 Hz, 1H), 3.15-3.04 (m, 2H), 2.46-2.42 (m, 2H). Data is consistent with that reported in the literature.[12]

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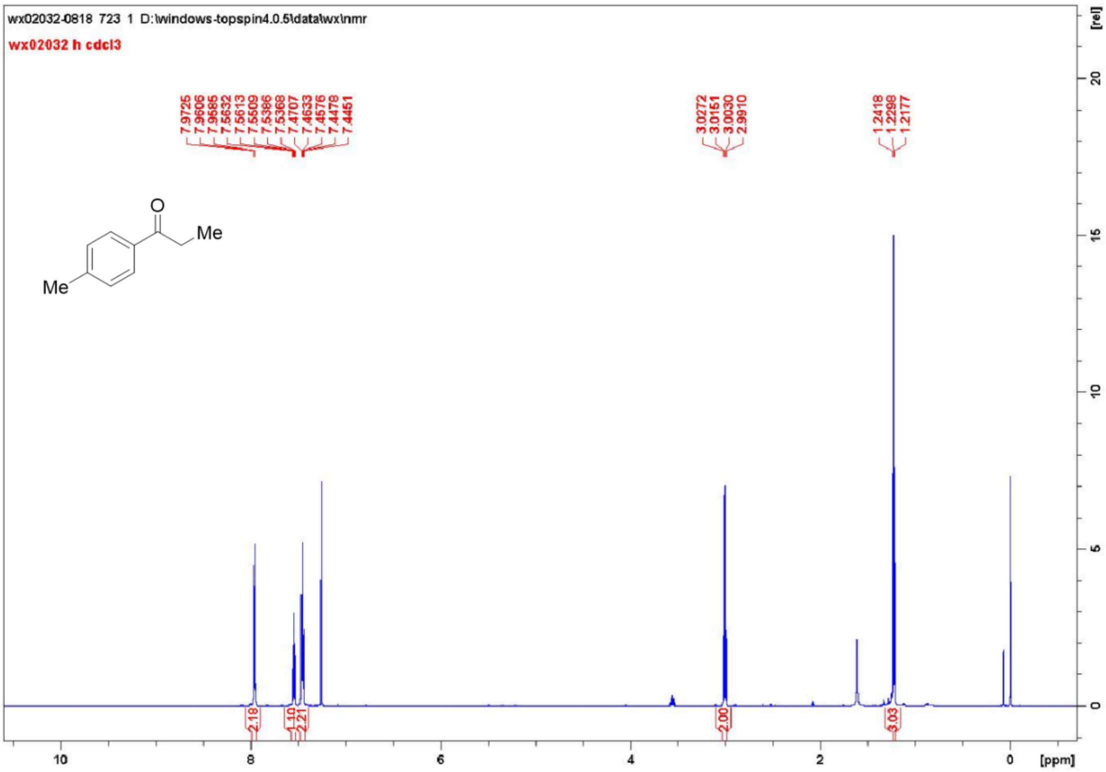
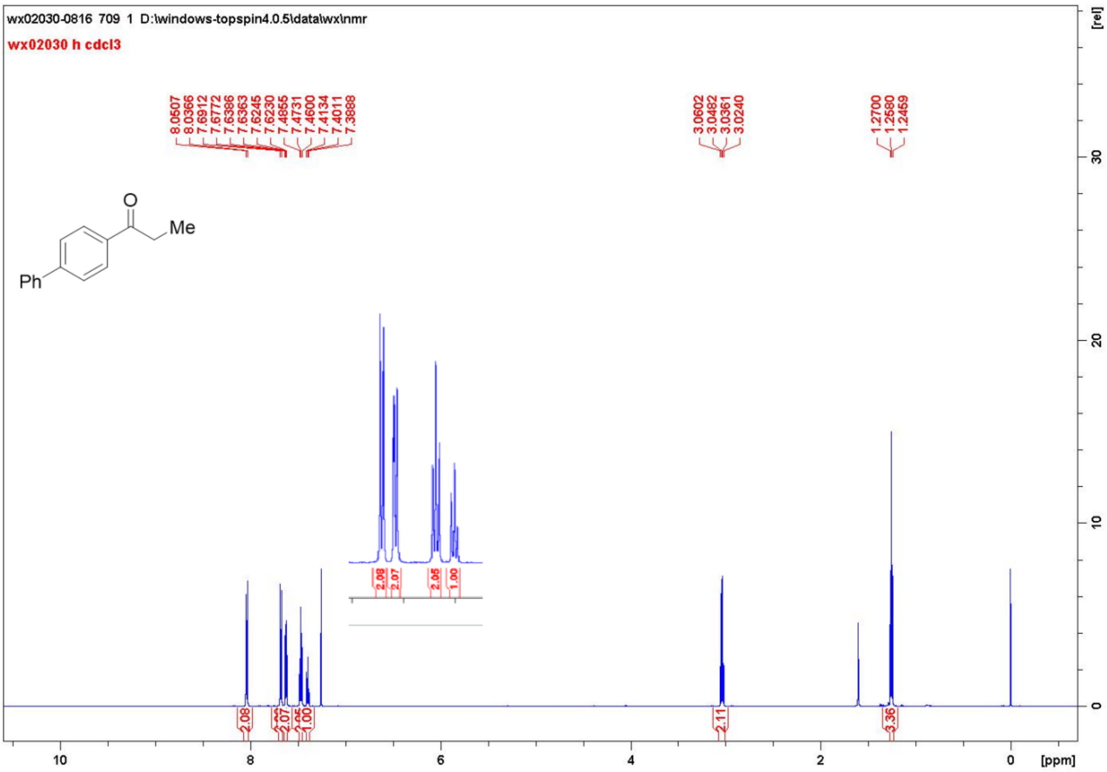
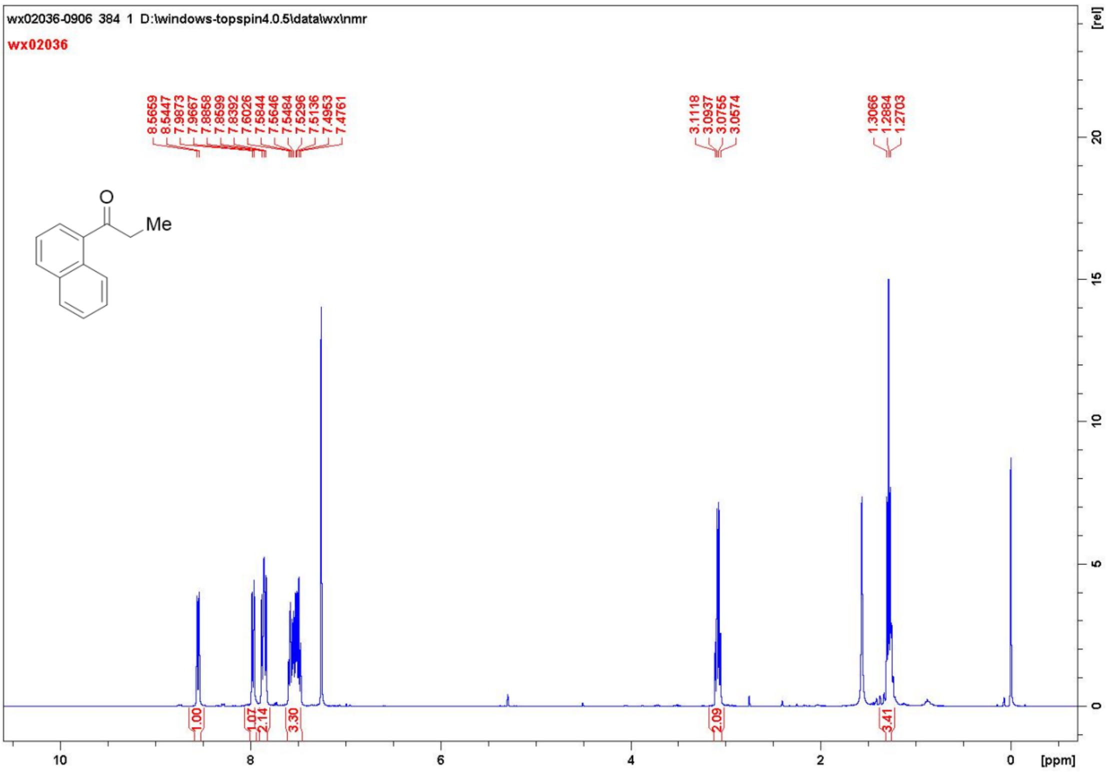
7. NMR and HR-MS (ESI) spectra



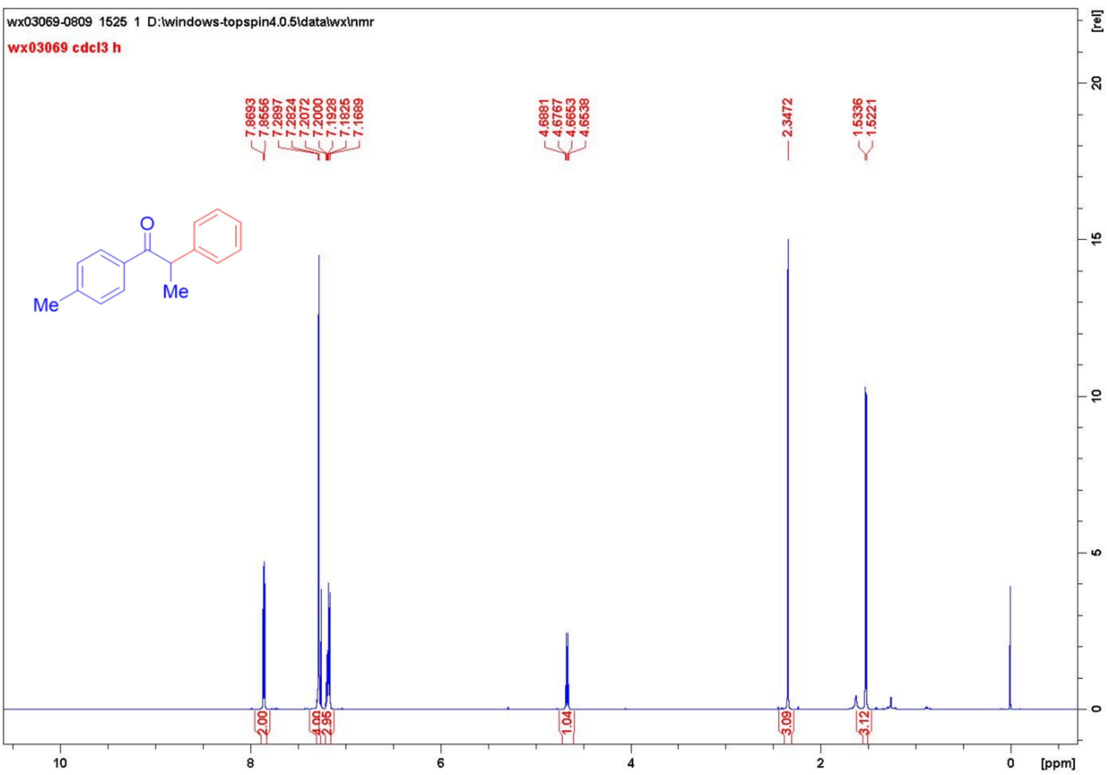
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2q**.



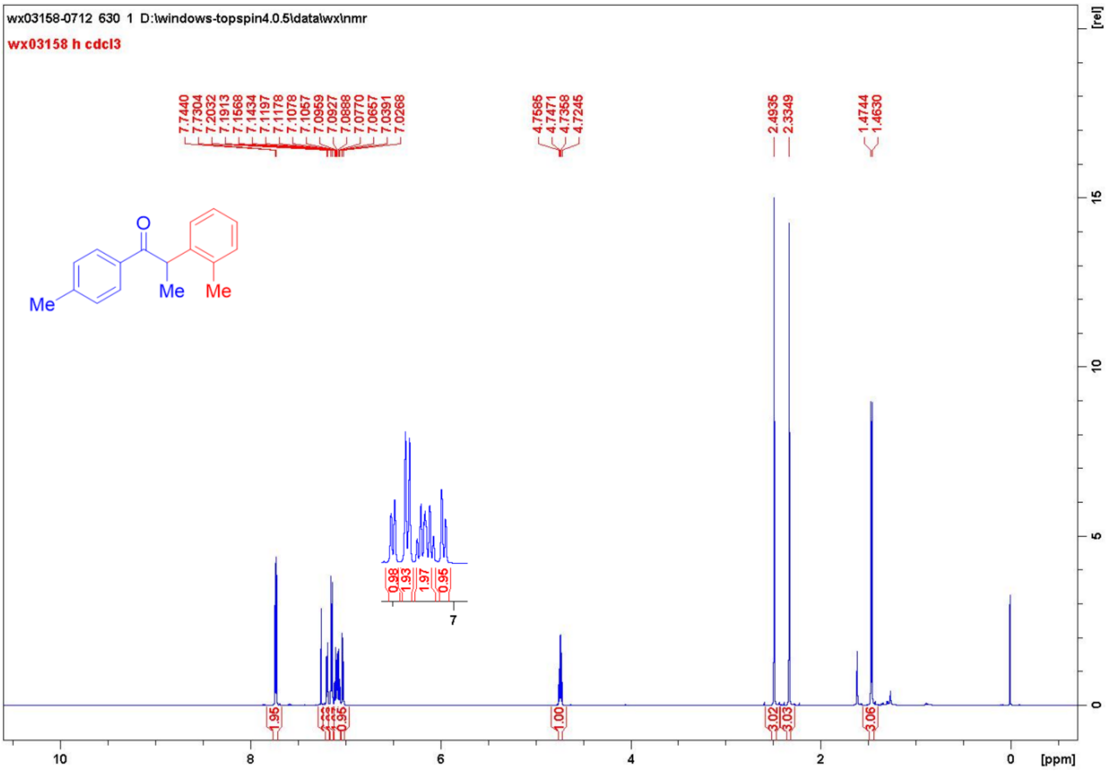
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **2u**.



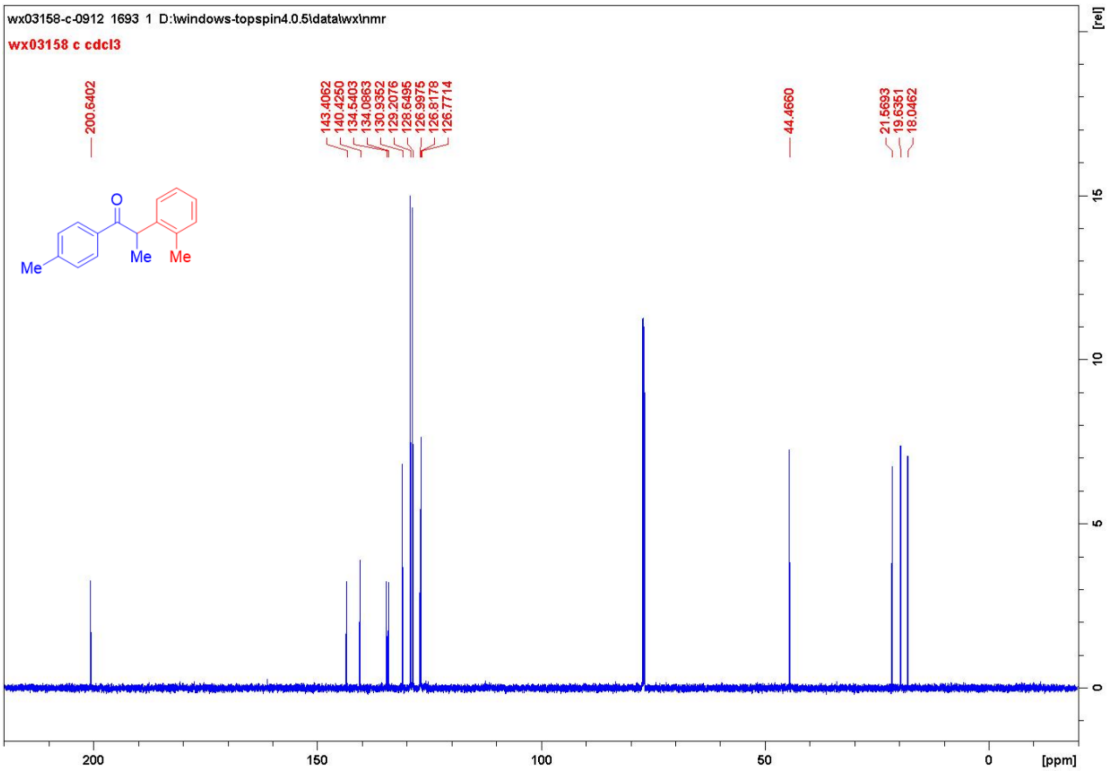
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **2y**.



^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3a**.

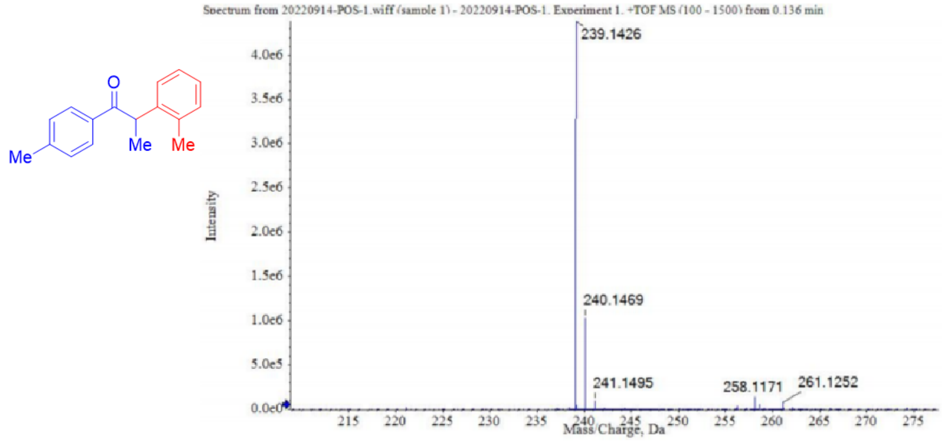


[1]H NMR (600 MHz, $CDCl_3$) spectrum of **3b**.



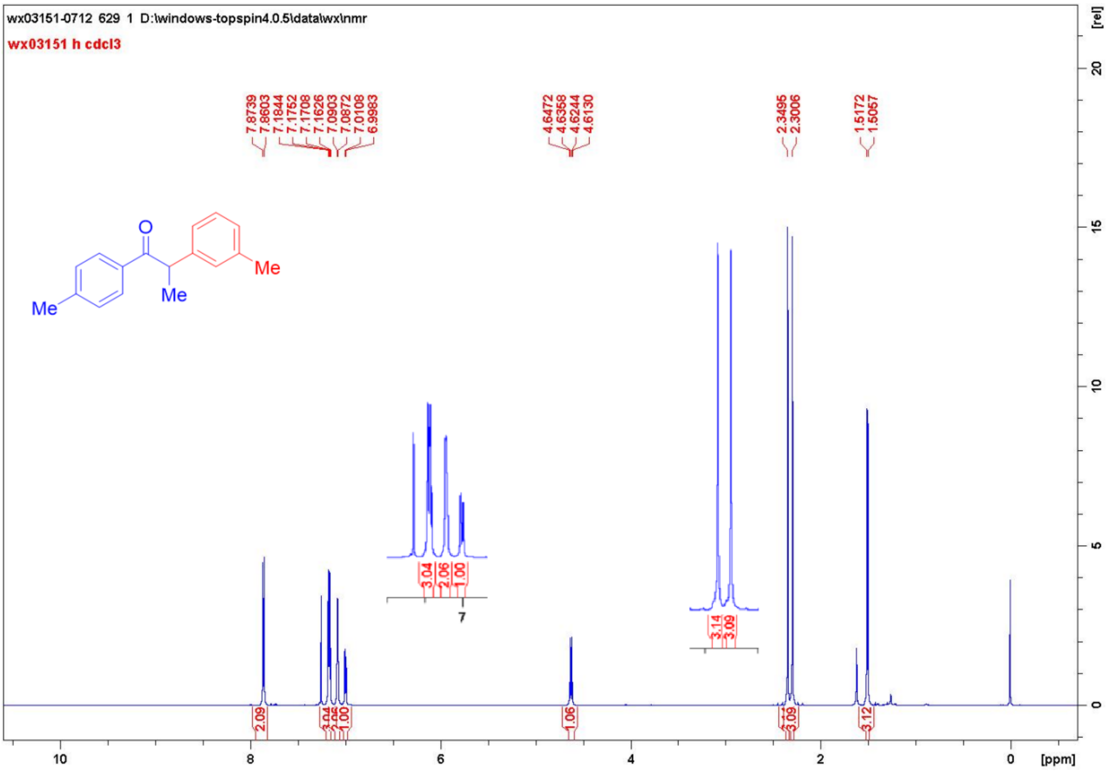
[13]C NMR ($CDCl_3$, 150 MHz) spectrum of **3b**.

样品 1：C17H18O
离子源：ESI Positive
仪器：AB Sciex Triple TOF 5600+
离子模式：正离子模式

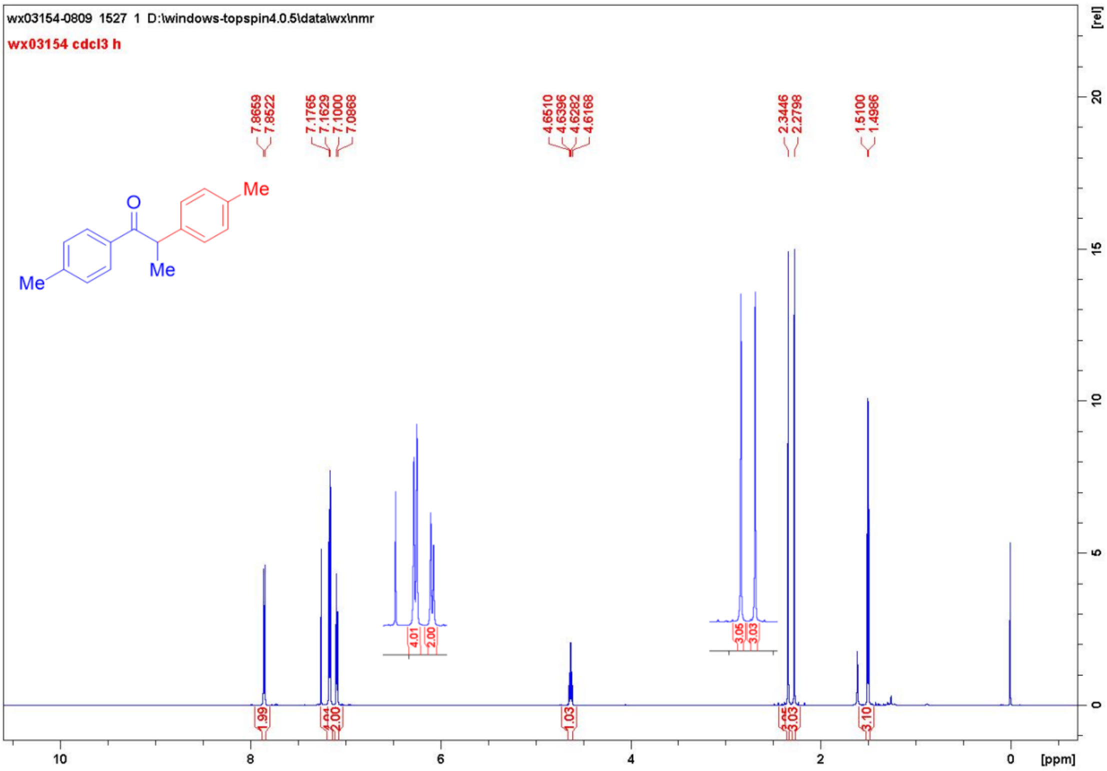


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
1	C17H18O	+H	239.1430	239.1426	-1.5

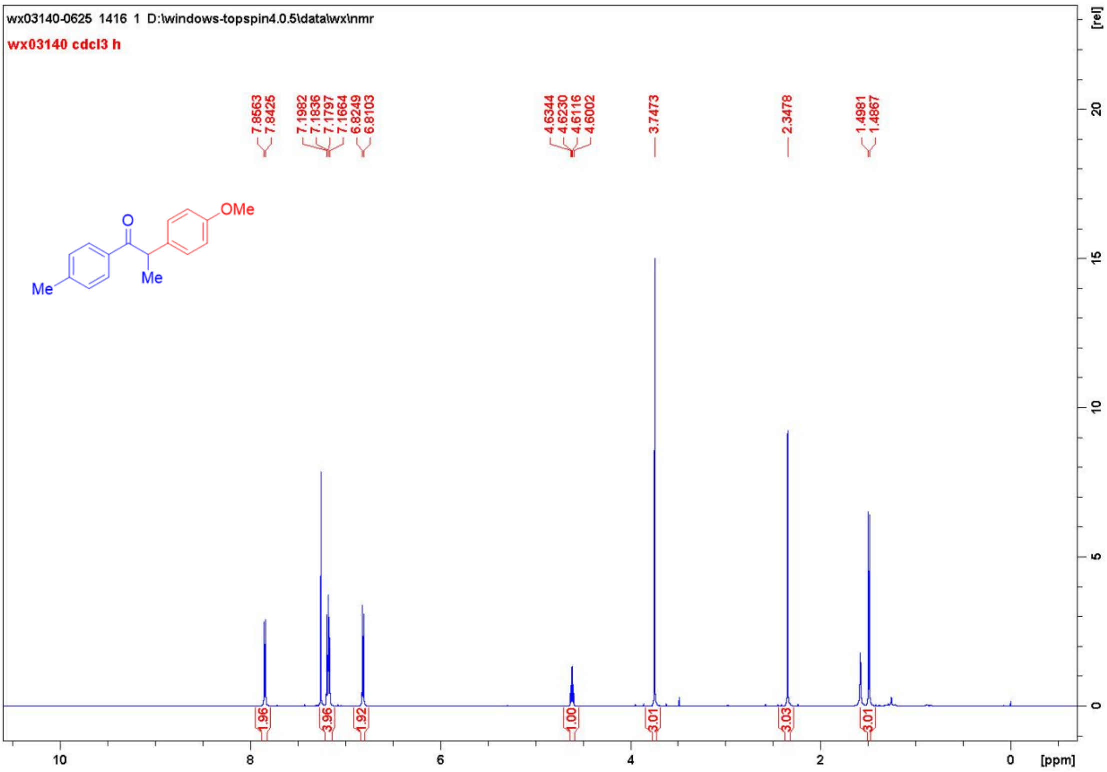
HR-MS (ESI) spectra of **3b**.



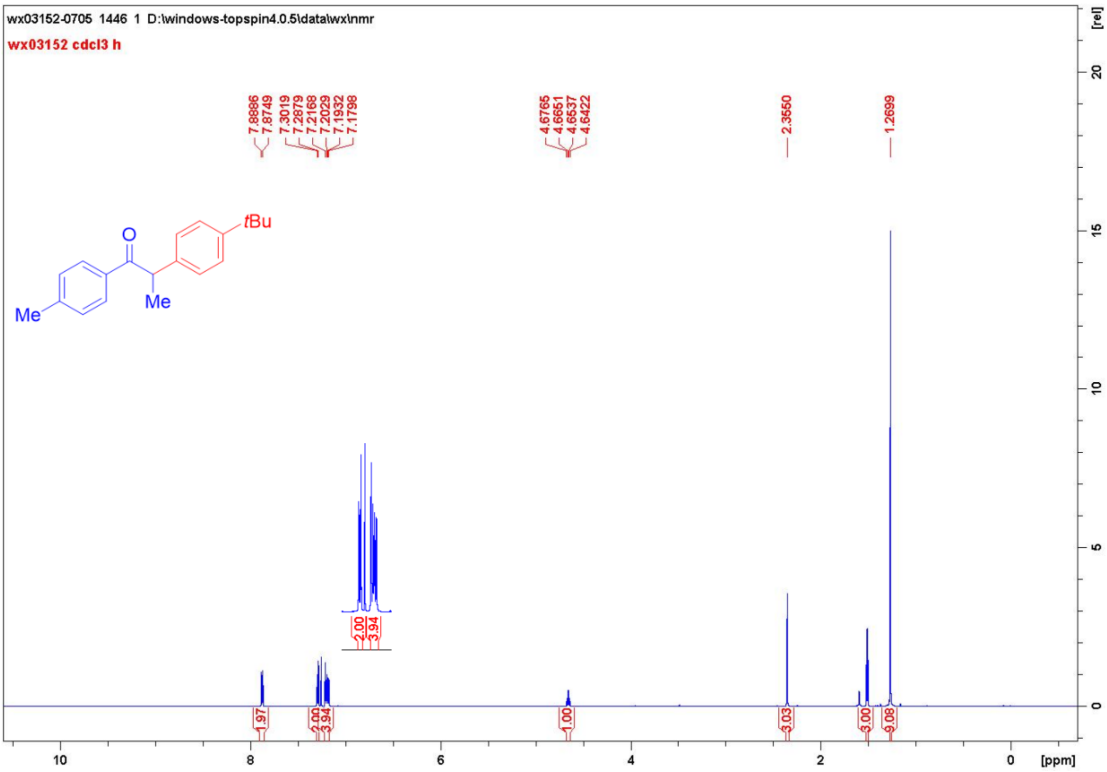
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3c**.



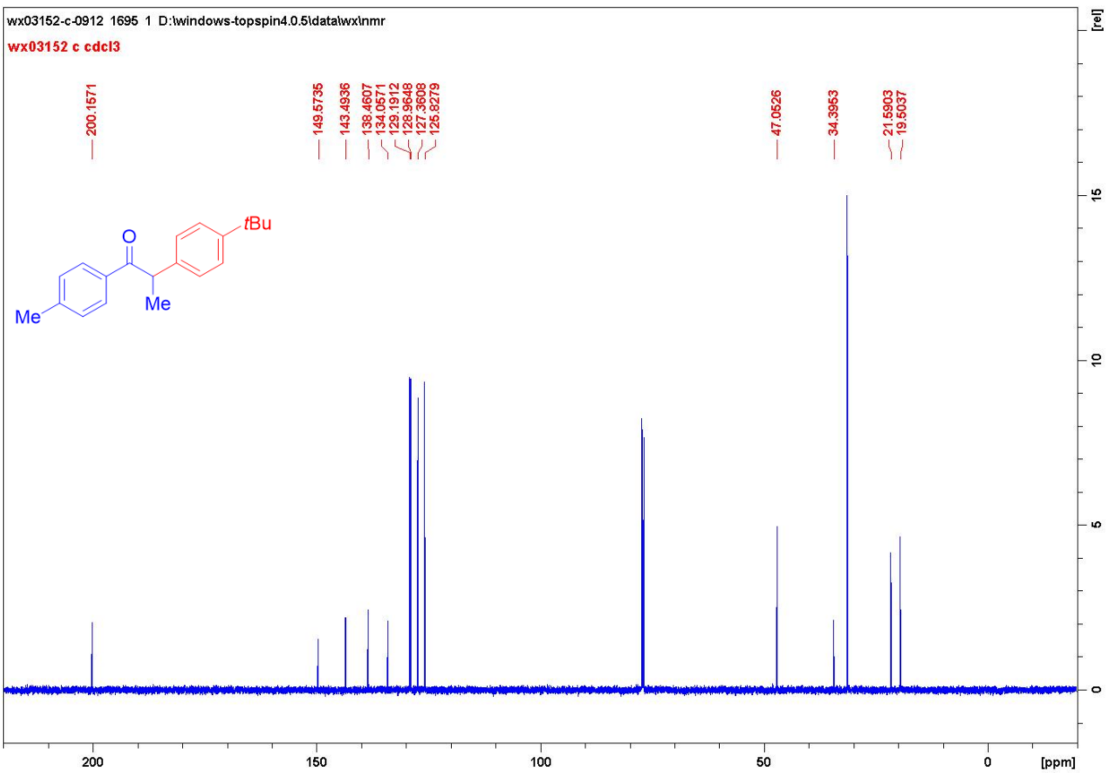
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3d**.



^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3e**.

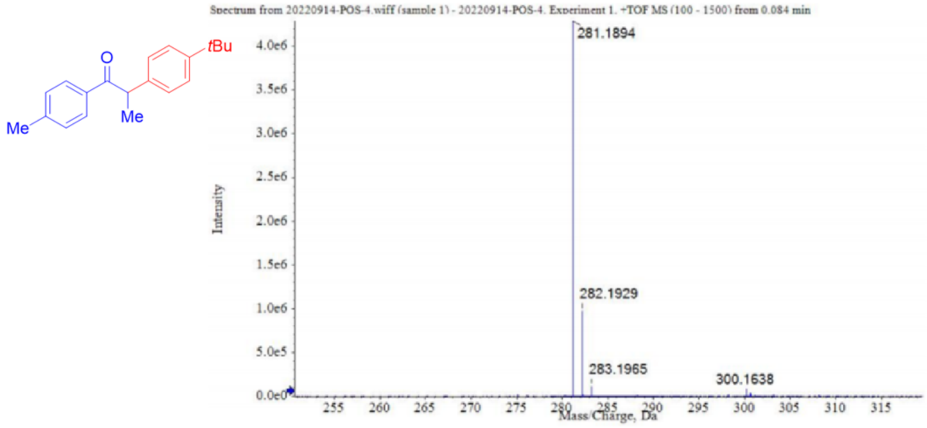


^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3f**.



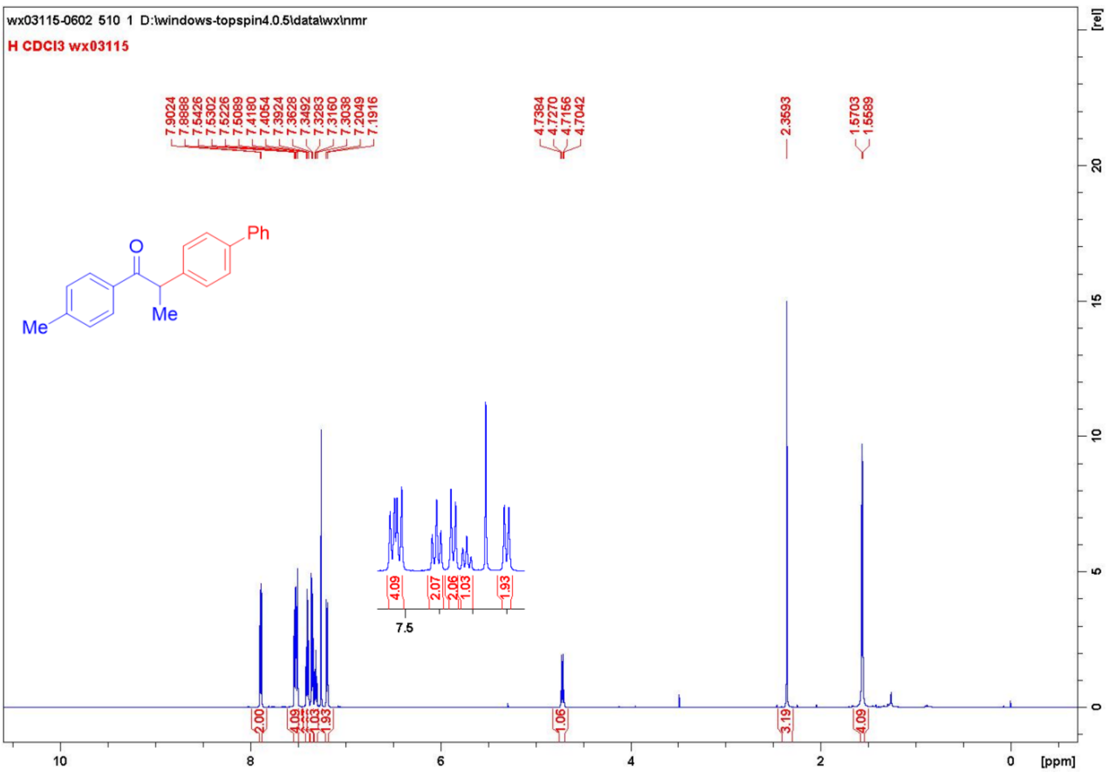
^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3f**.

样品 4：C20H24O
离子源：ESI Positive
仪器：AB Sciex Triple TOF 5600+
离子模式：正离子模式

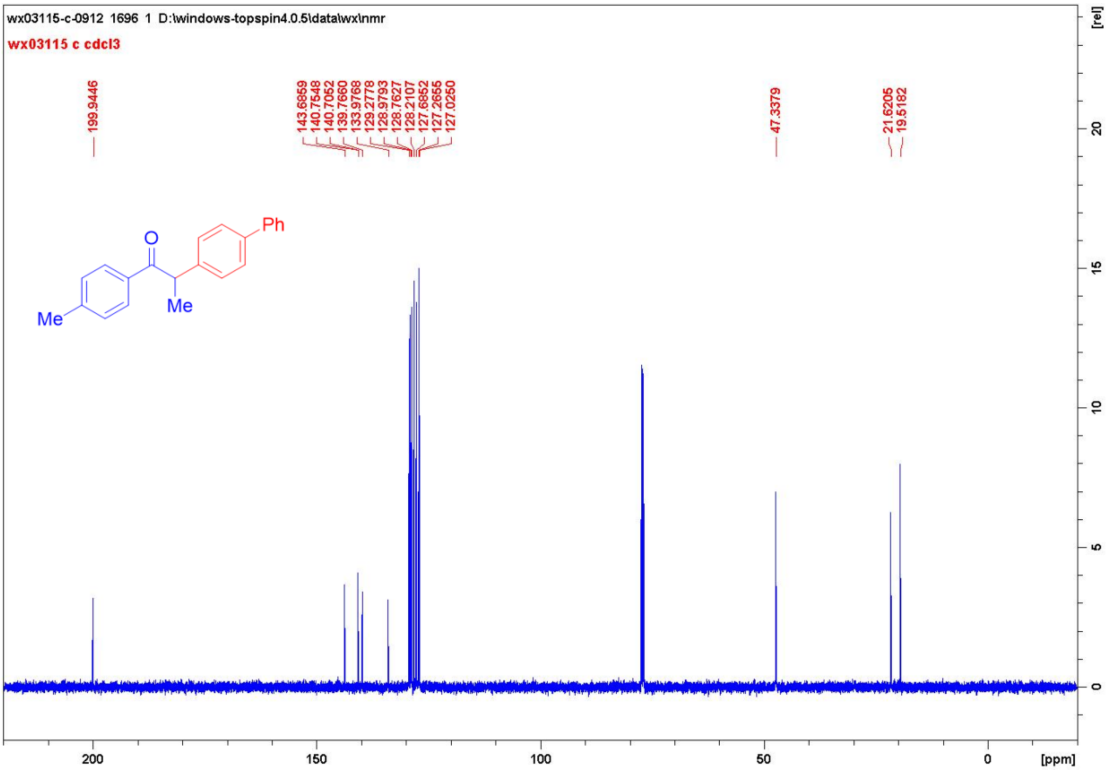


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
4	C20H24O	+H	281.1900	281.1894	-2.4

HR-MS (ESI) spectra of **3f**.

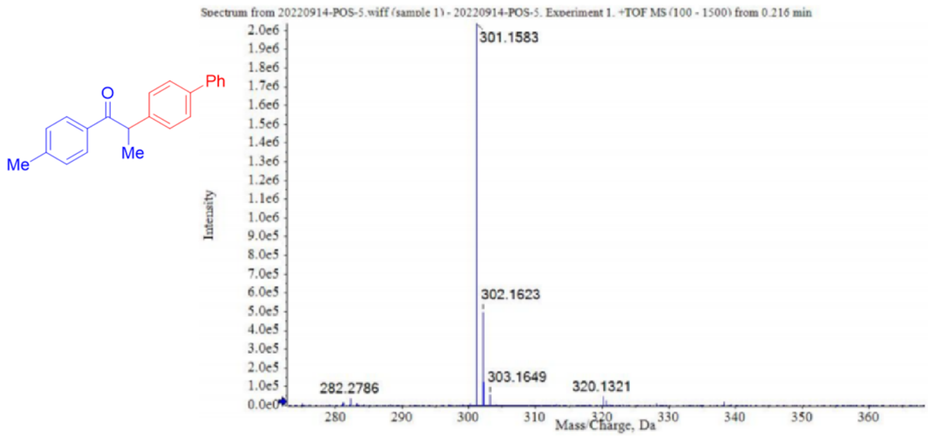


^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3g**.



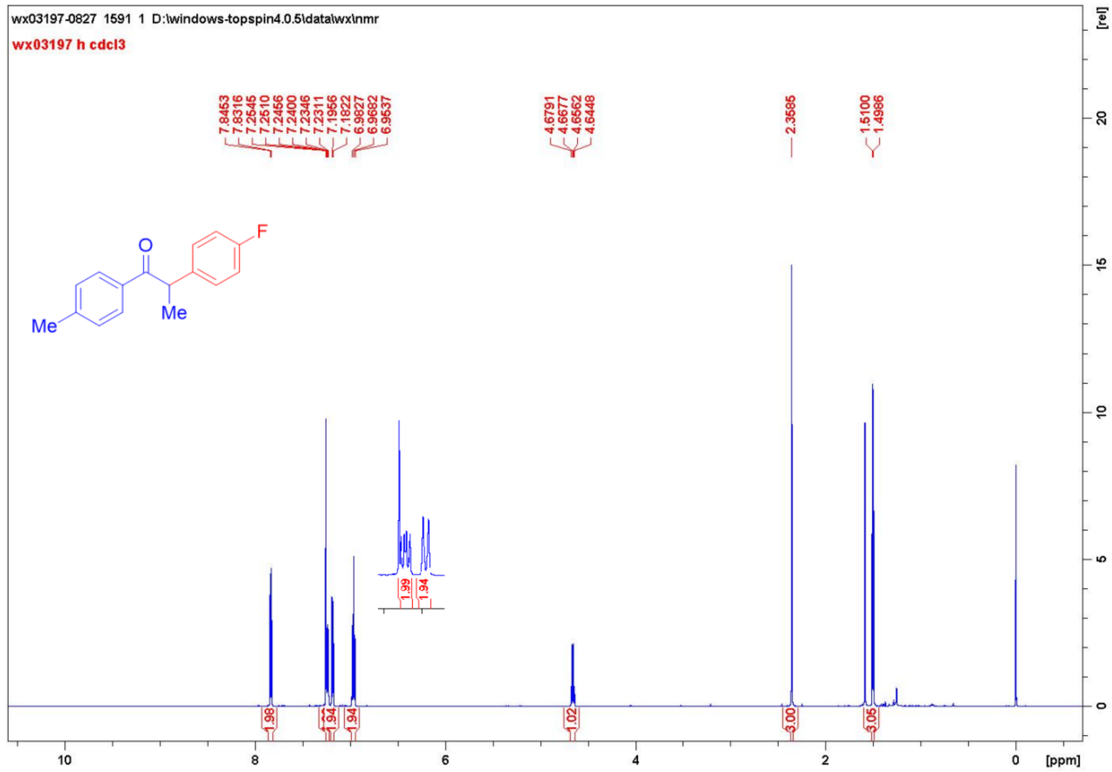
^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3g**.

样品 5：C22H20O
离子源：ESI Positive
仪器：AB Sciex Triple TOF 5600+
离子模式：正离子模式

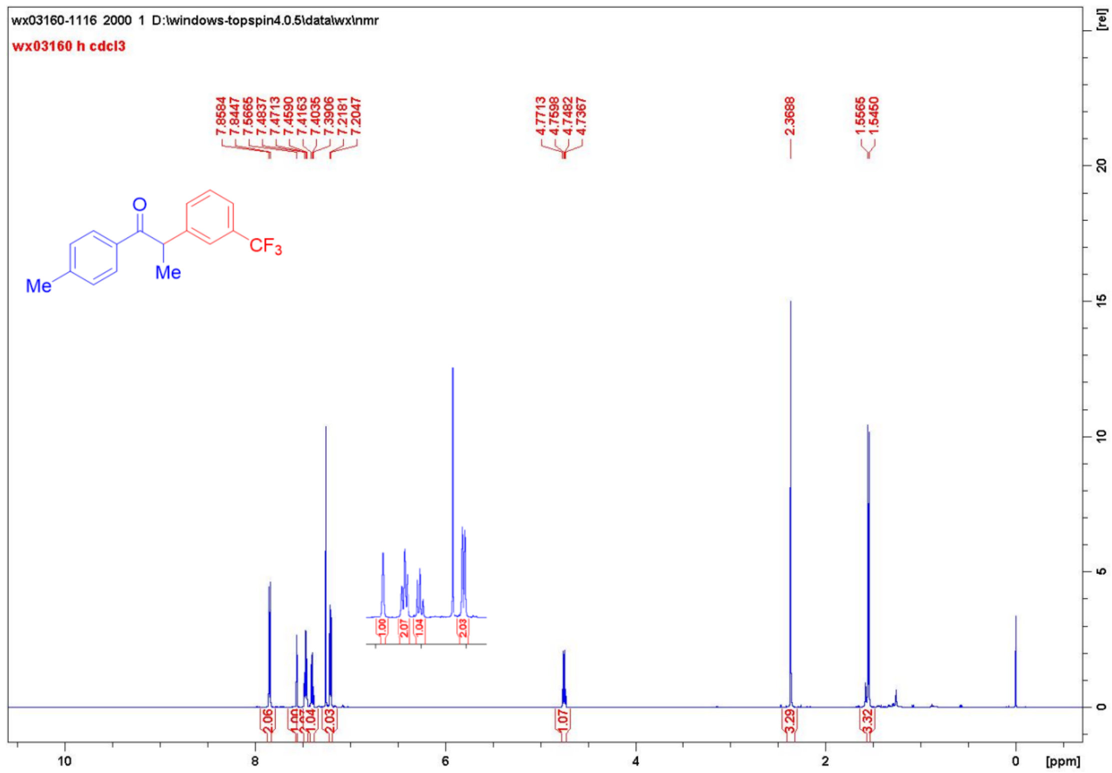


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
5	C22H20O	+H	301.1587	301.1583	-0.9

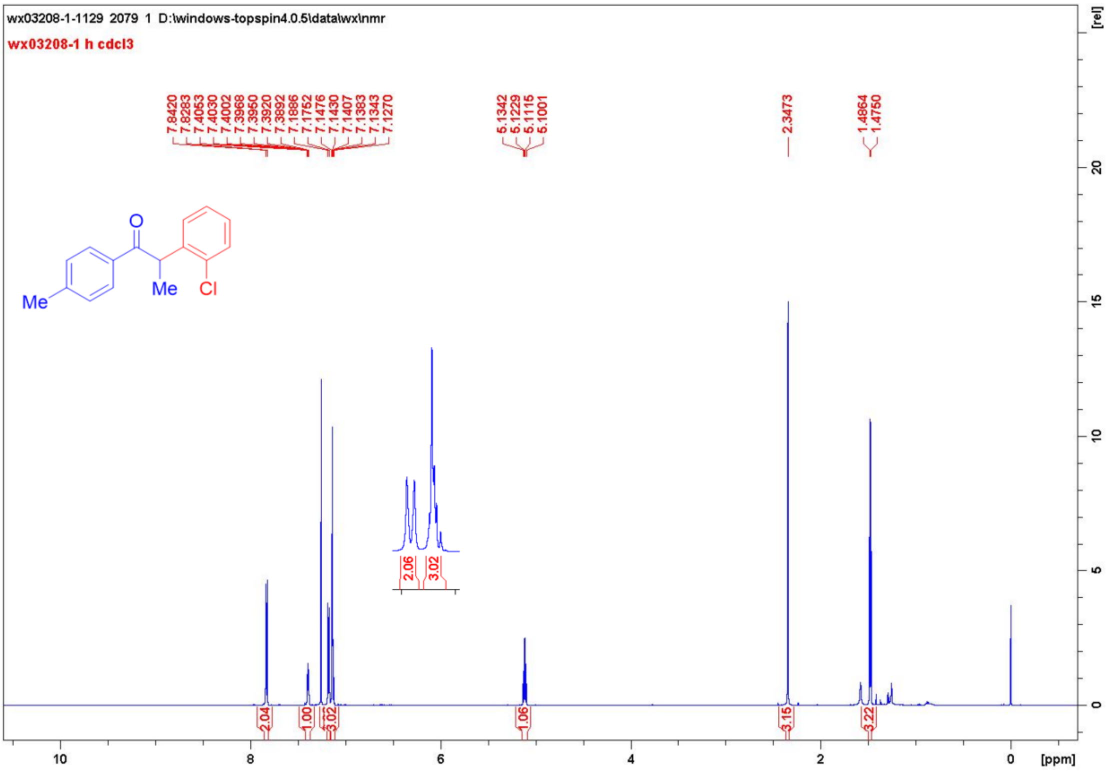
HR-MS (ESI) spectra of **3g**.



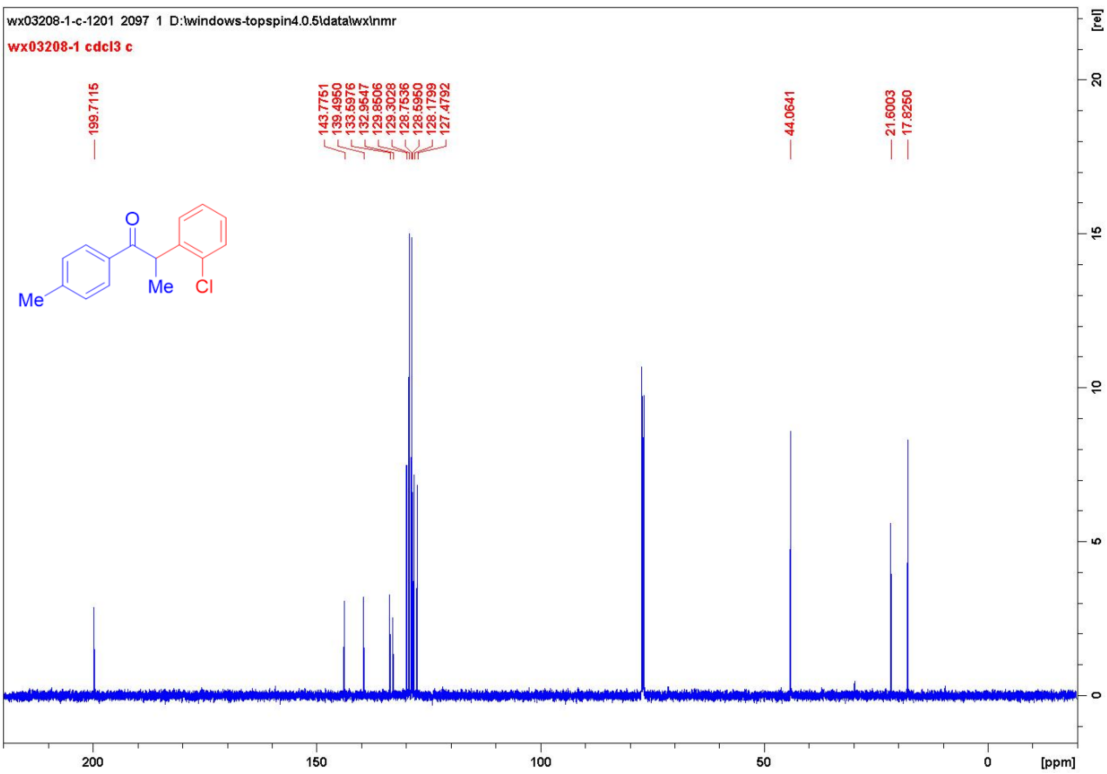
^1H NMR (400 MHz, $CDCl_3$) spectrum of **3h**.



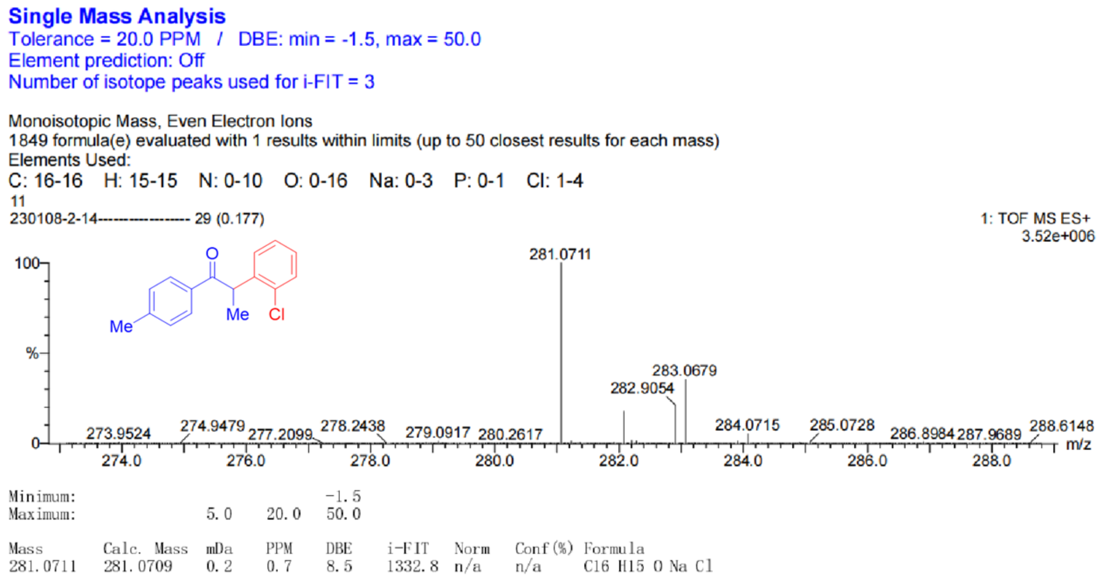
^1H NMR (600 MHz, $CDCl_3$) spectrum of **3i**.



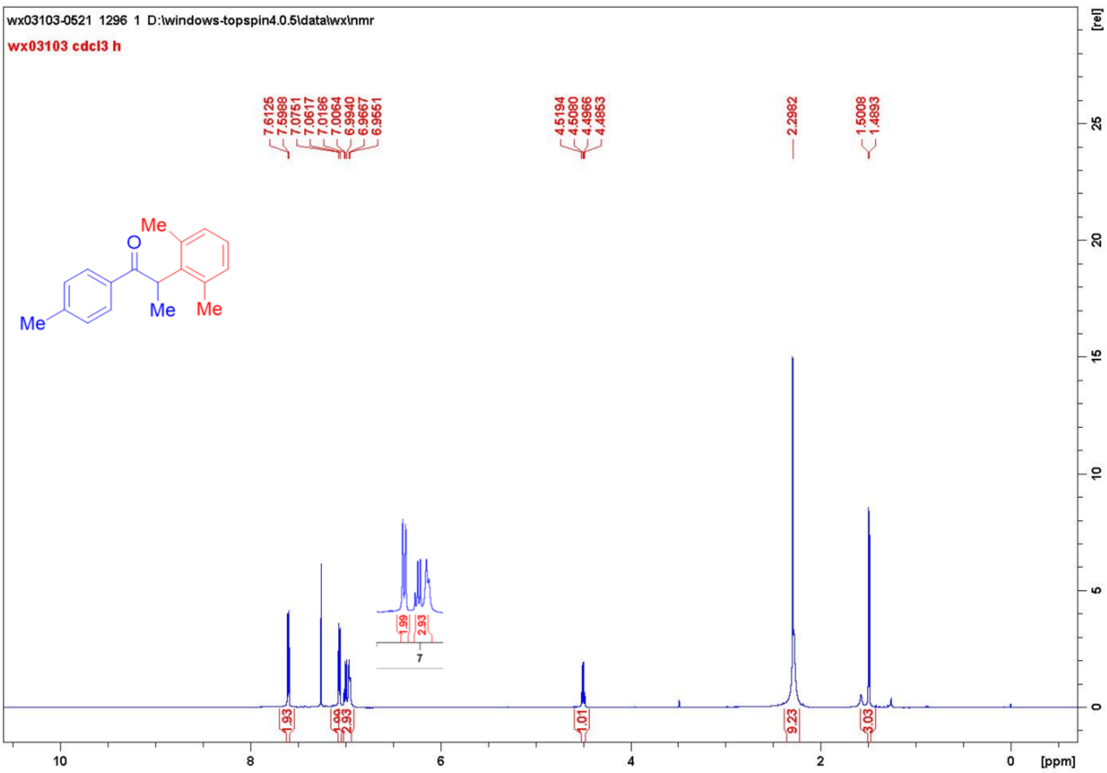
^1H NMR (600 MHz, $CDCl_3$) spectrum of **3j**.



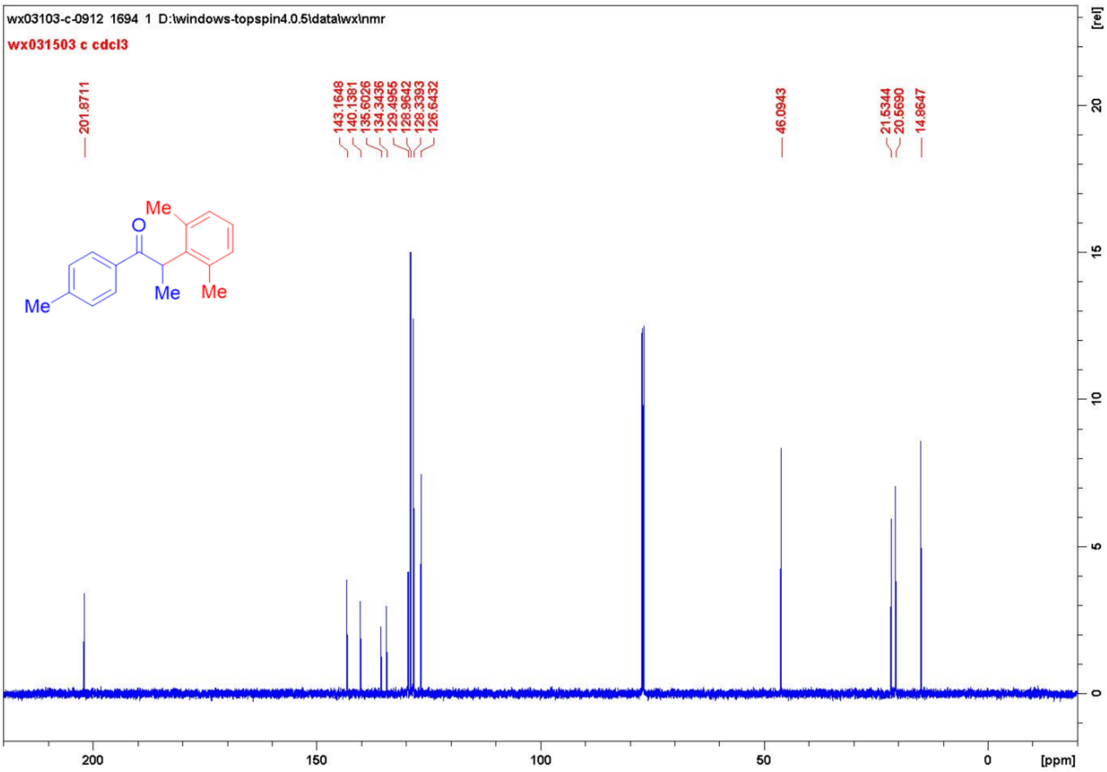
^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3j**.



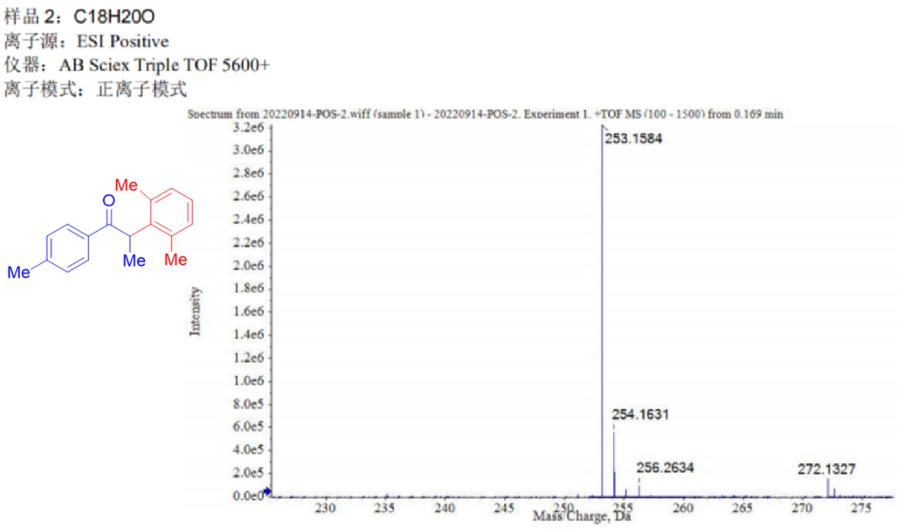
HR-MS (ESI) spectra of **3j**.



^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3k**.

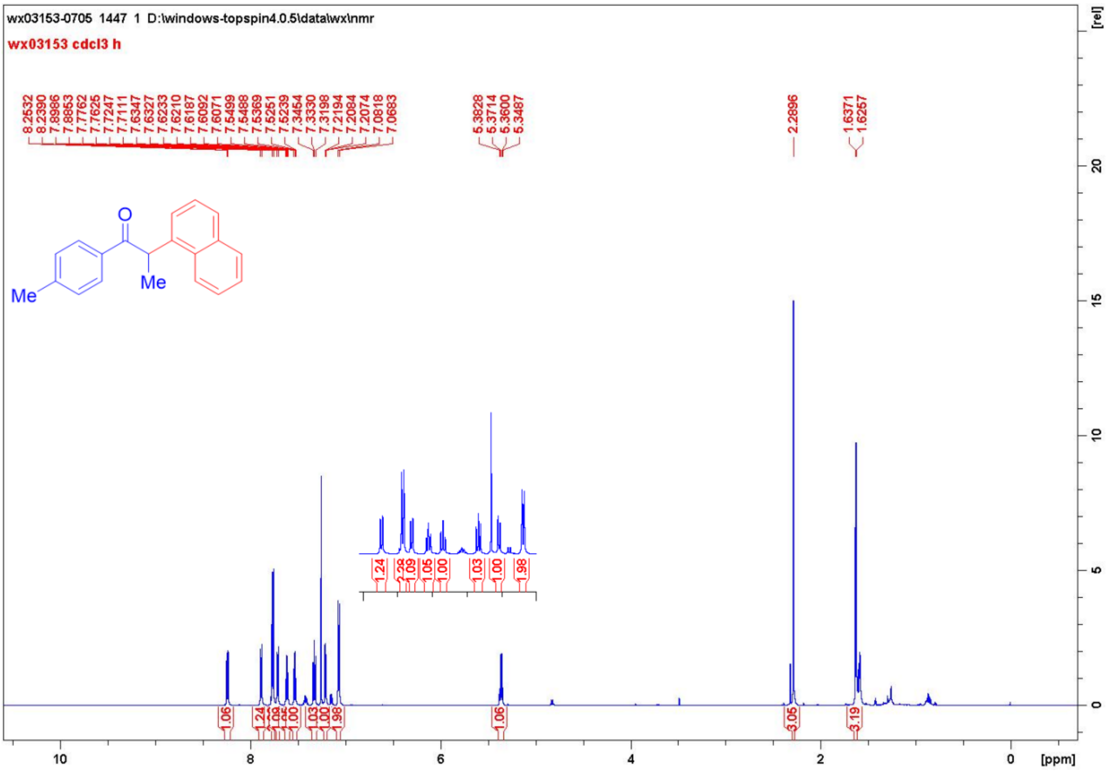


^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3k**.

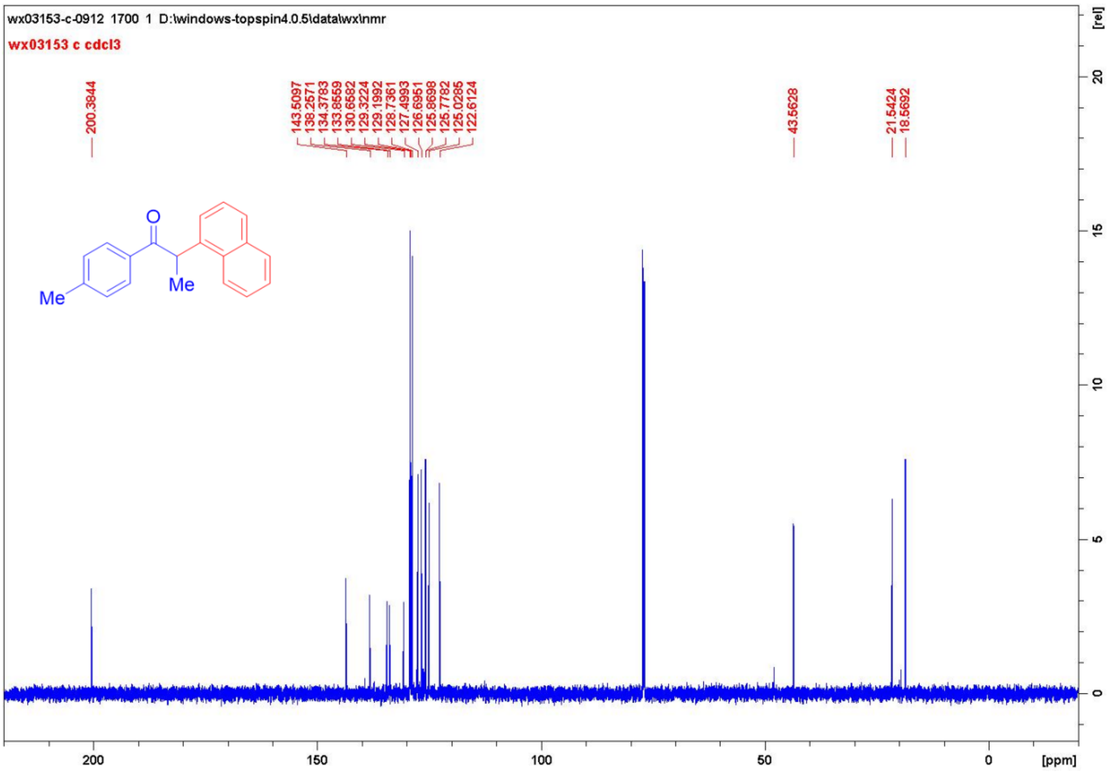


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
2	C18H20O	+H	253.1587	253.1584	-0.9

HR-MS (ESI) spectra of **3k**.

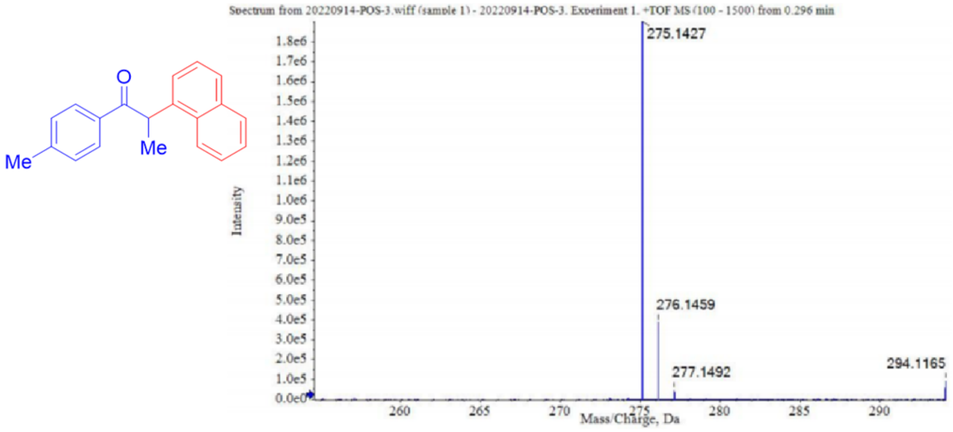


^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3l**.



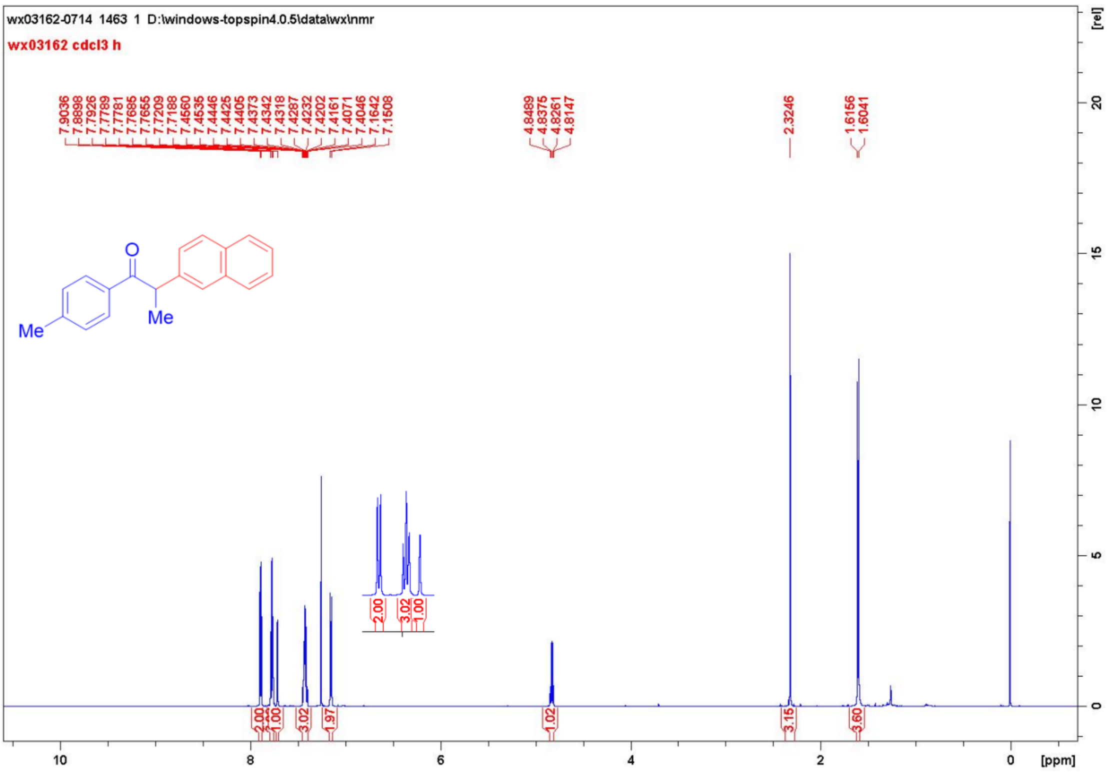
^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3l**.

样品 3：C20H18O
离子源：ESI Positive
仪器：AB Sciex Triple TOF 5600+
离子模式：正离子模式

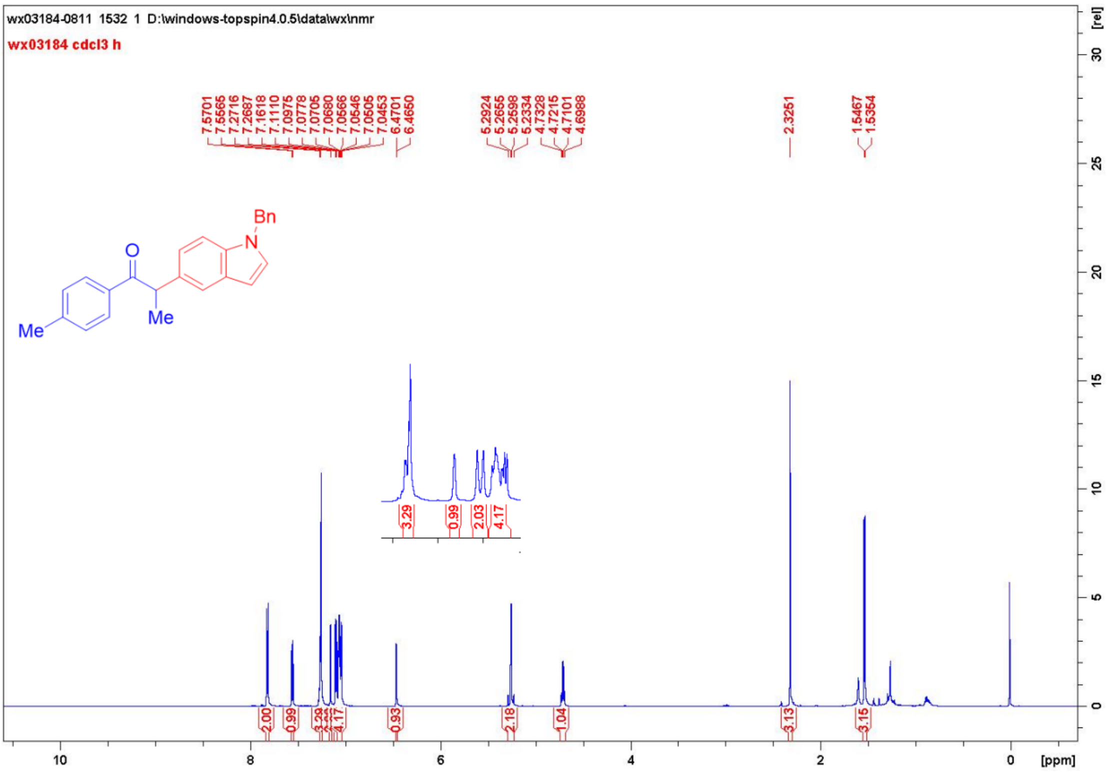


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
3	C20H18O	+H	275.1430	275.1427	-1.4

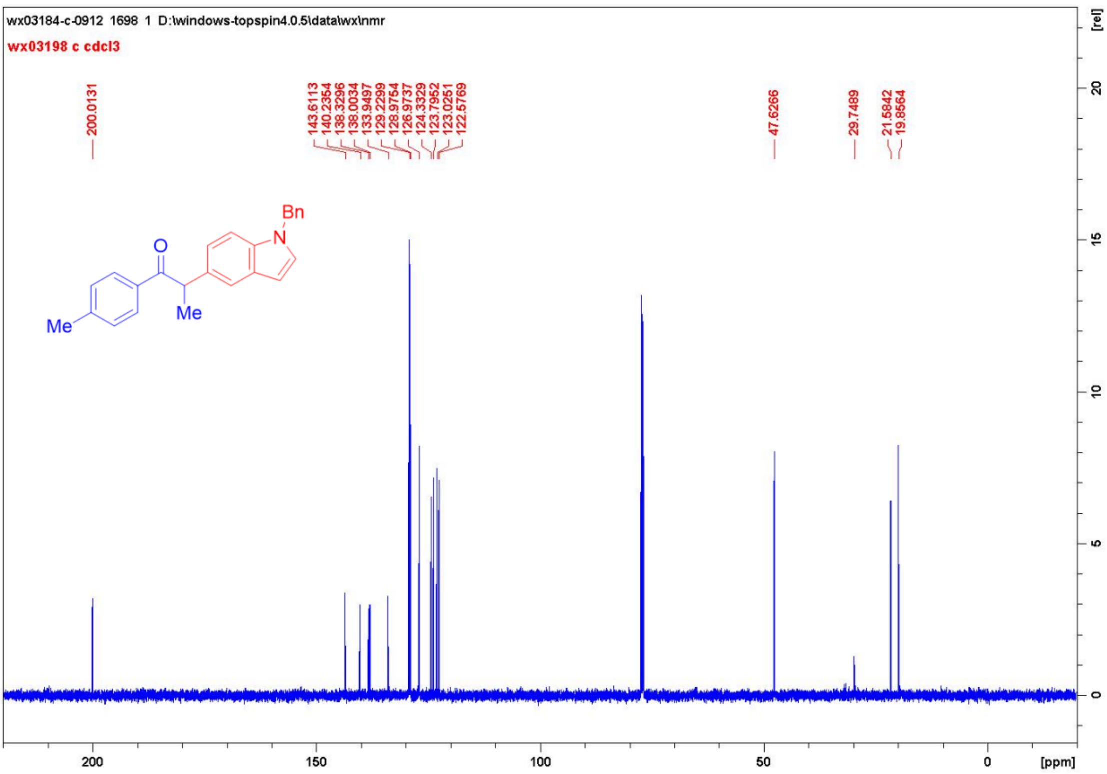
HR-MS (ESI) spectra of **3l**.



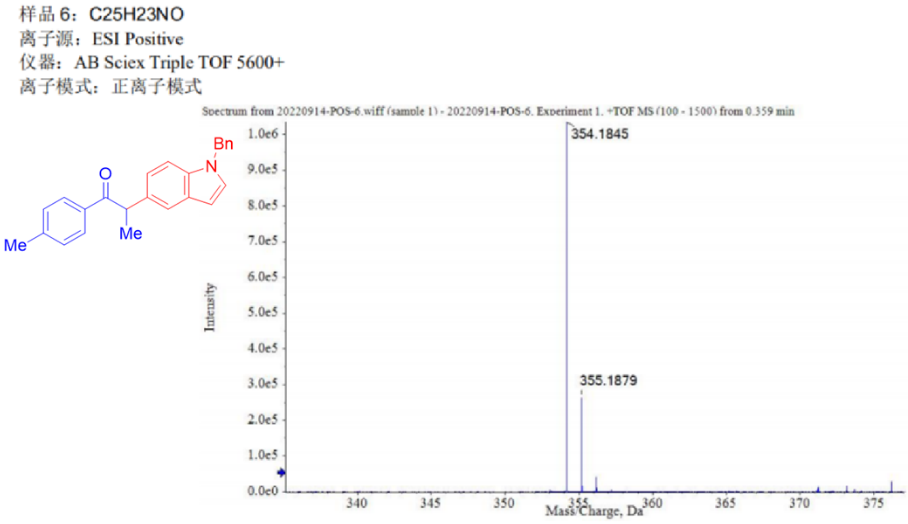
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3m**.



^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3n**.

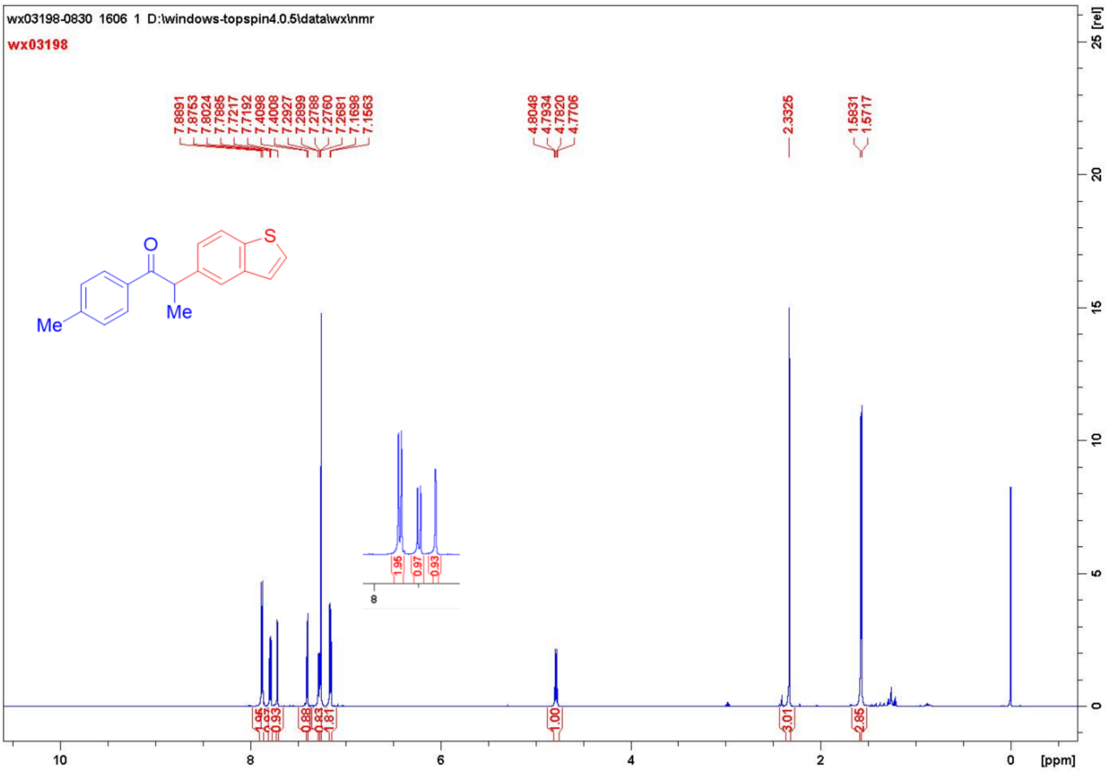


^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3n**.

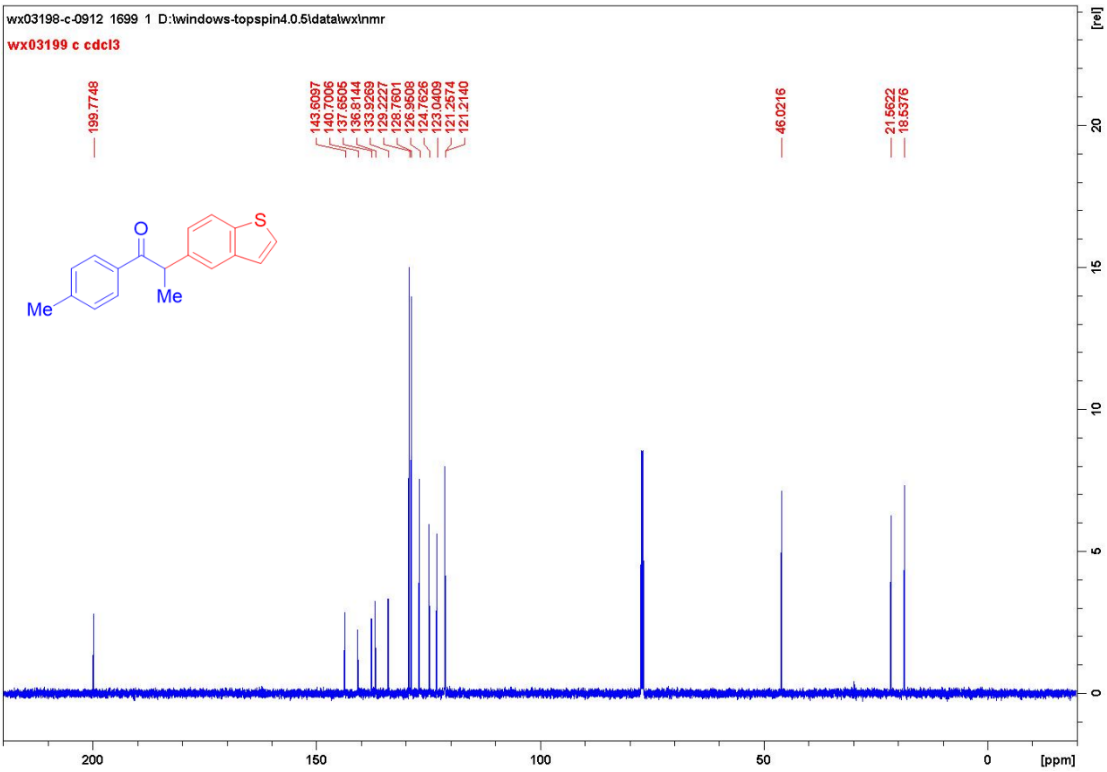


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
6	C25H23NO	+H	354.1852	354.1845	-2.5

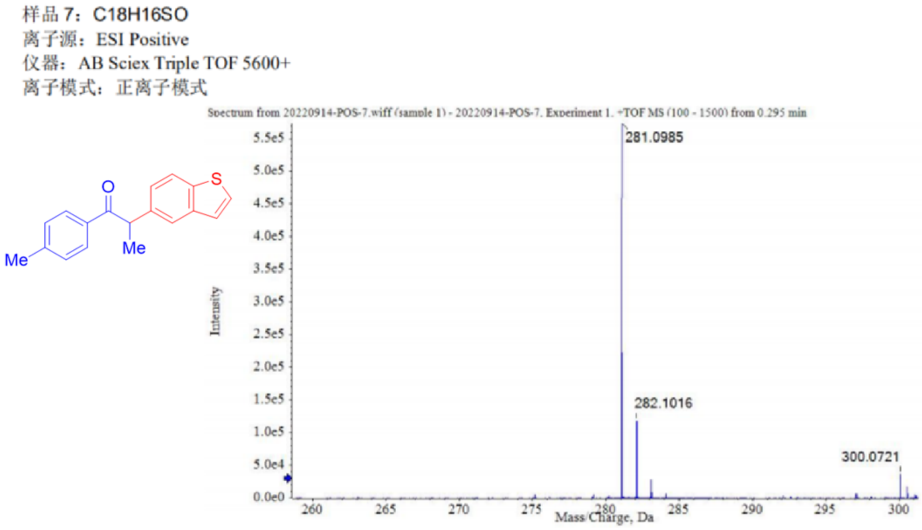
HR-MS (ESI) spectra of **3n**.



^1H NMR (600 MHz, $CDCl_3$) spectrum of **3o**.

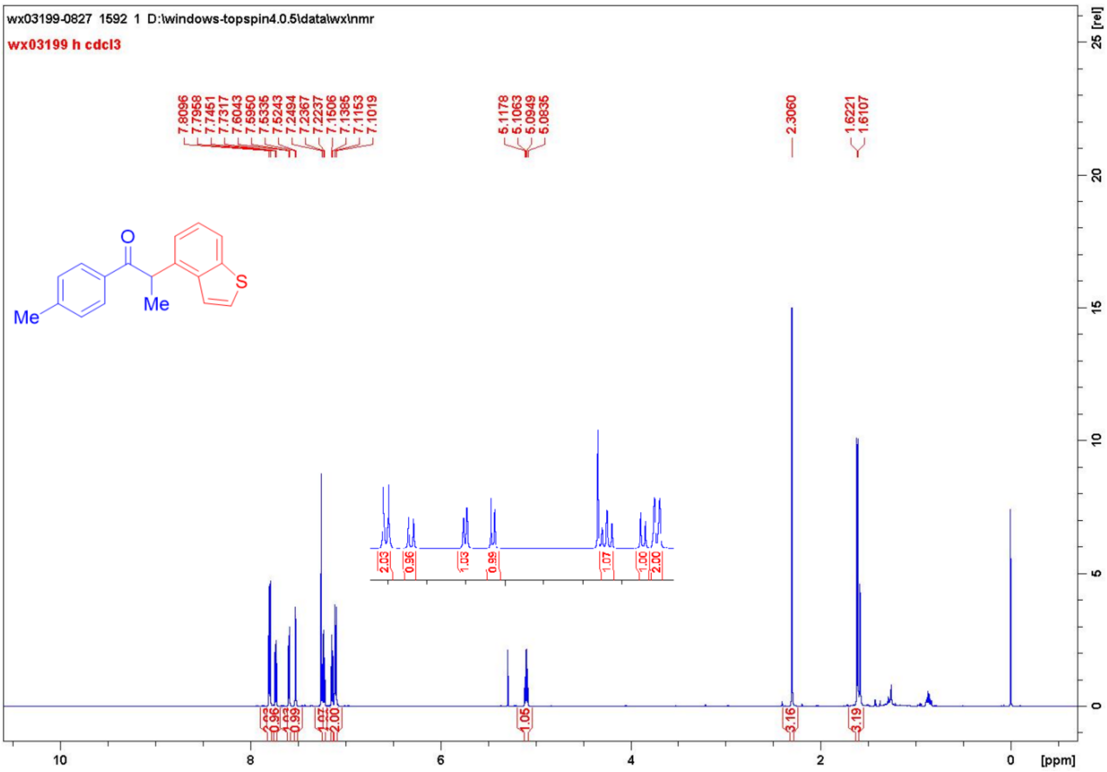


^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3o**.

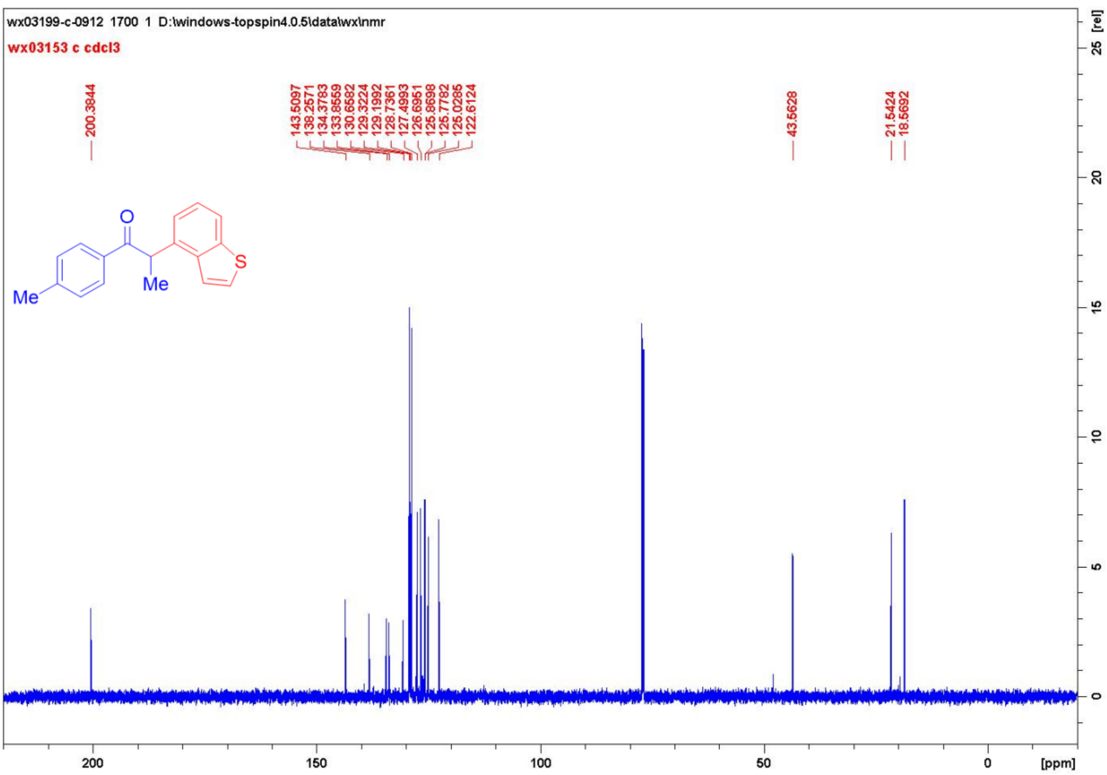


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
7	C18H16SO	+H	281.0995	281.0985	-3.6

HR-MS (ESI) spectra of **3o**.

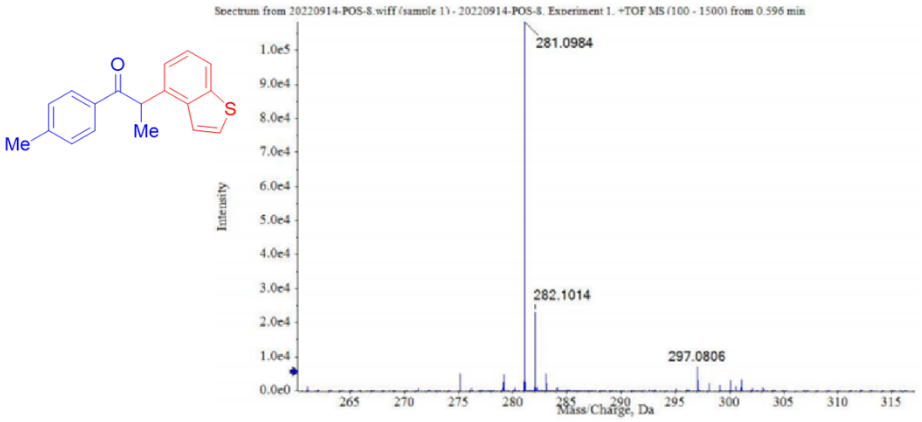


^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3p**.



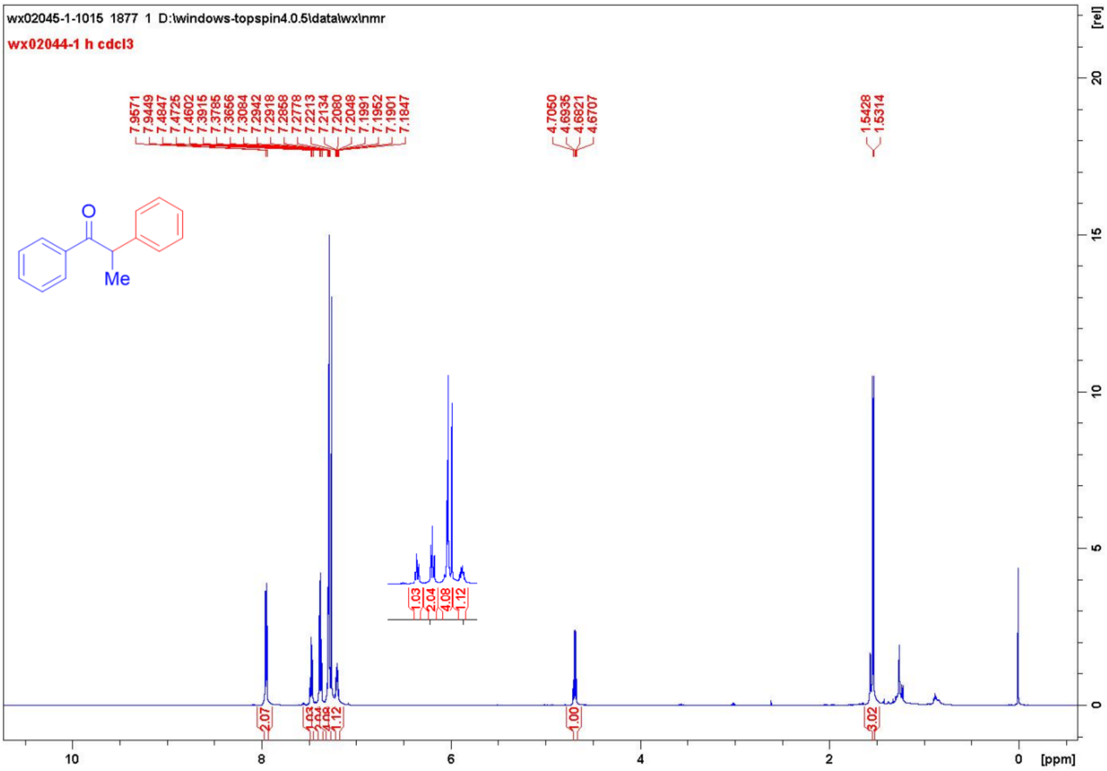
^{13}C NMR ($CDCl_3$, 150 MHz) spectrum of **3p**.

样品 8：C18H16SO
离子源：ESI Positive
仪器：AB Sciex Triple TOF 5600+
离子模式：正离子模式

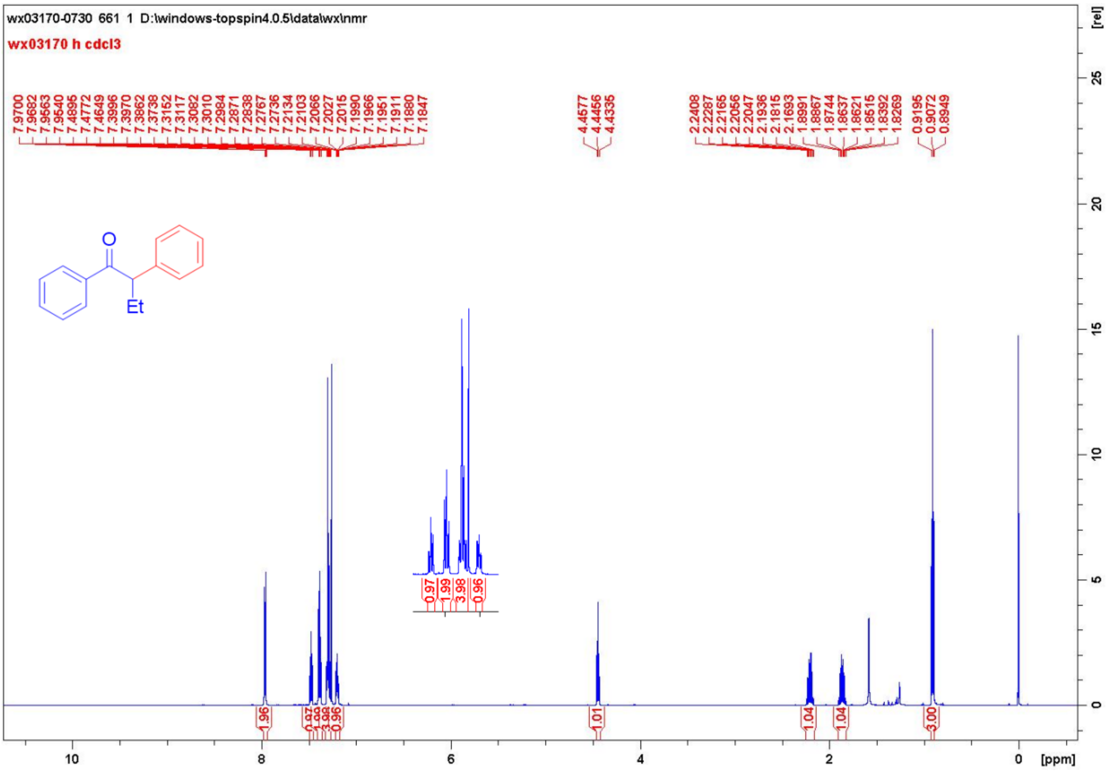


Name	Formula	Adduct	Extraction Mass	Found At Mass	Error (ppm)
8	C18H16SO	+H	281.0995	281.0984	-3.3

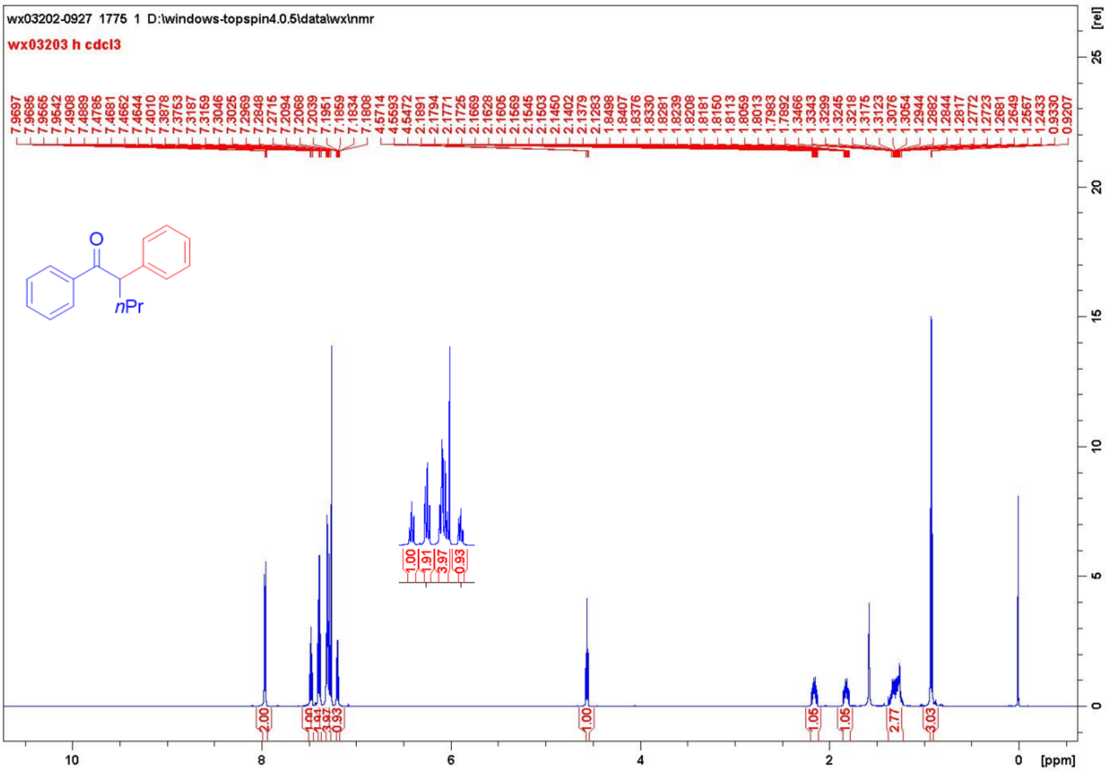
HR-MS (ESI) spectra of **3p**.



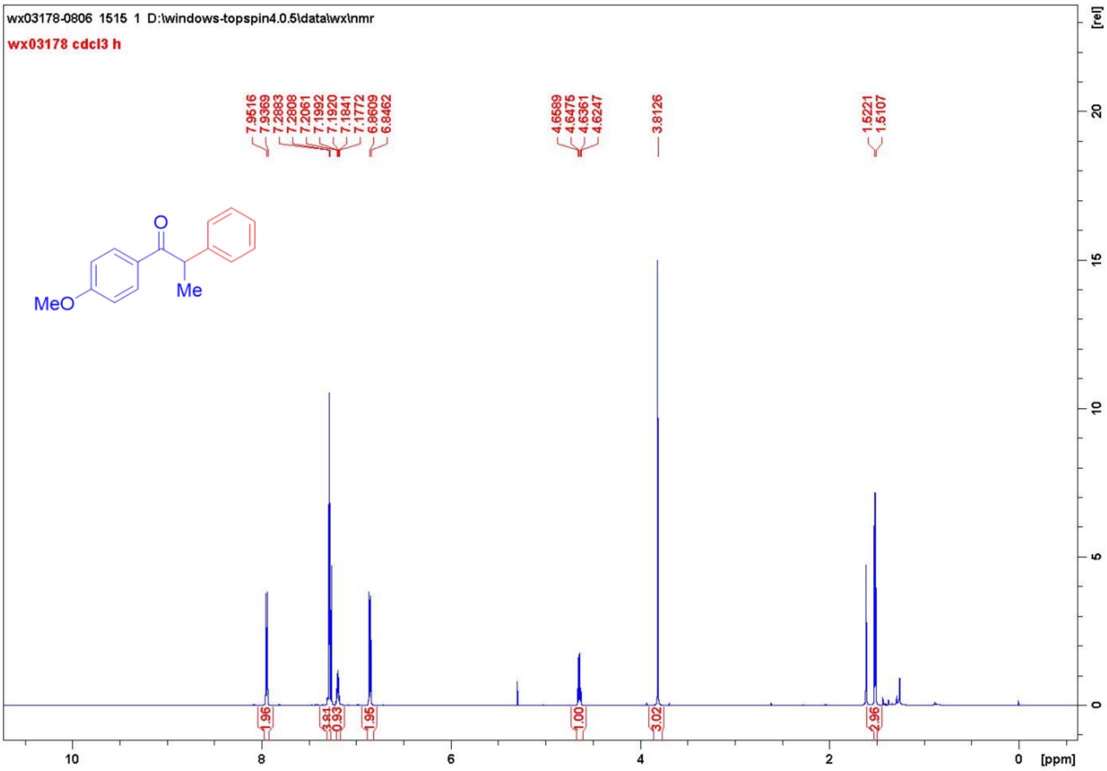
[1]H NMR (400 MHz, $CDCl_3$) spectrum of **3q**.



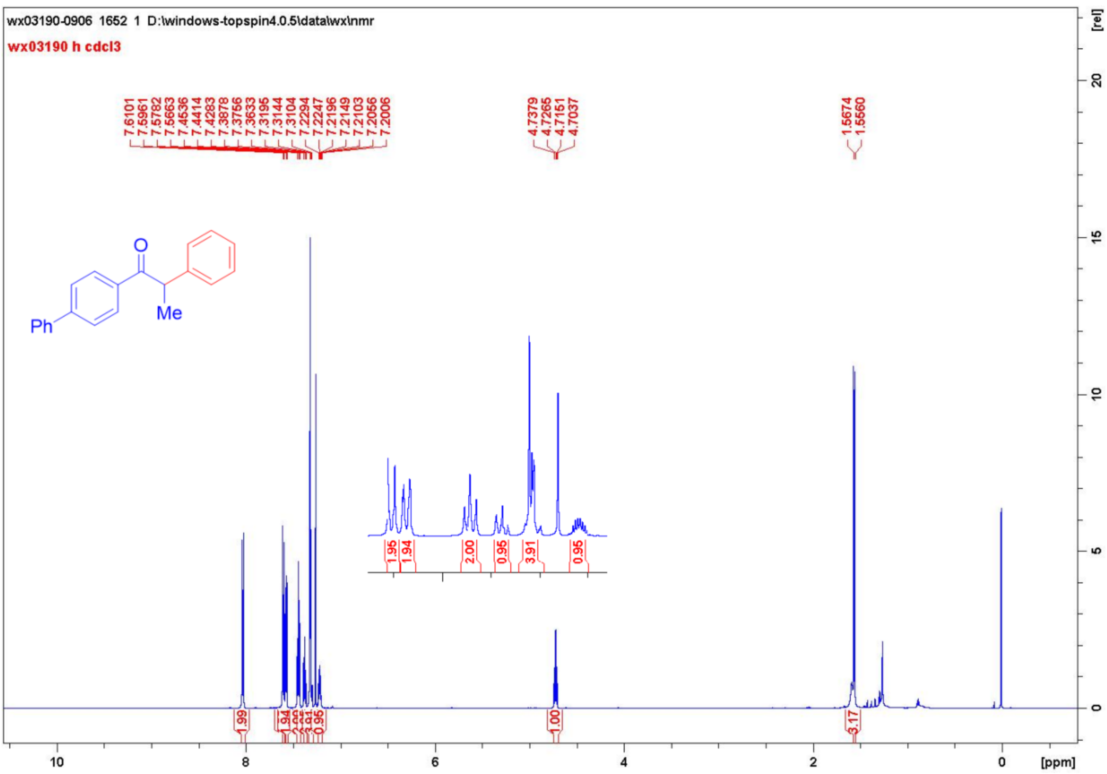
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3r**.



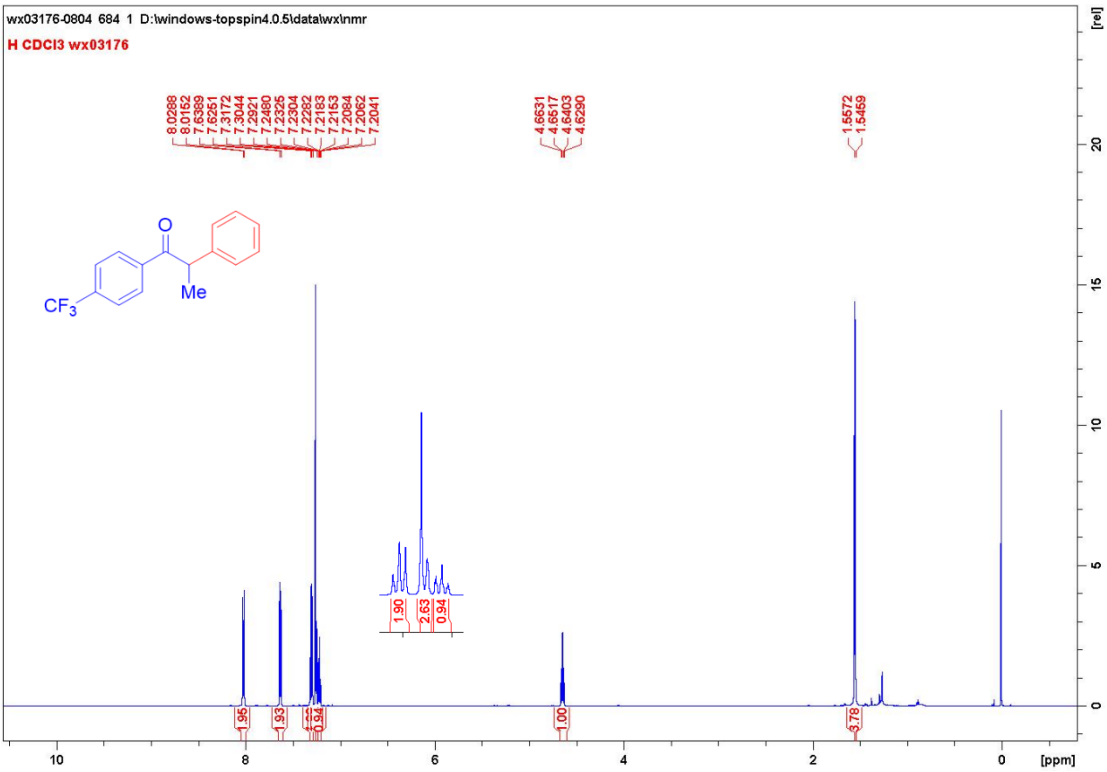
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3s**.



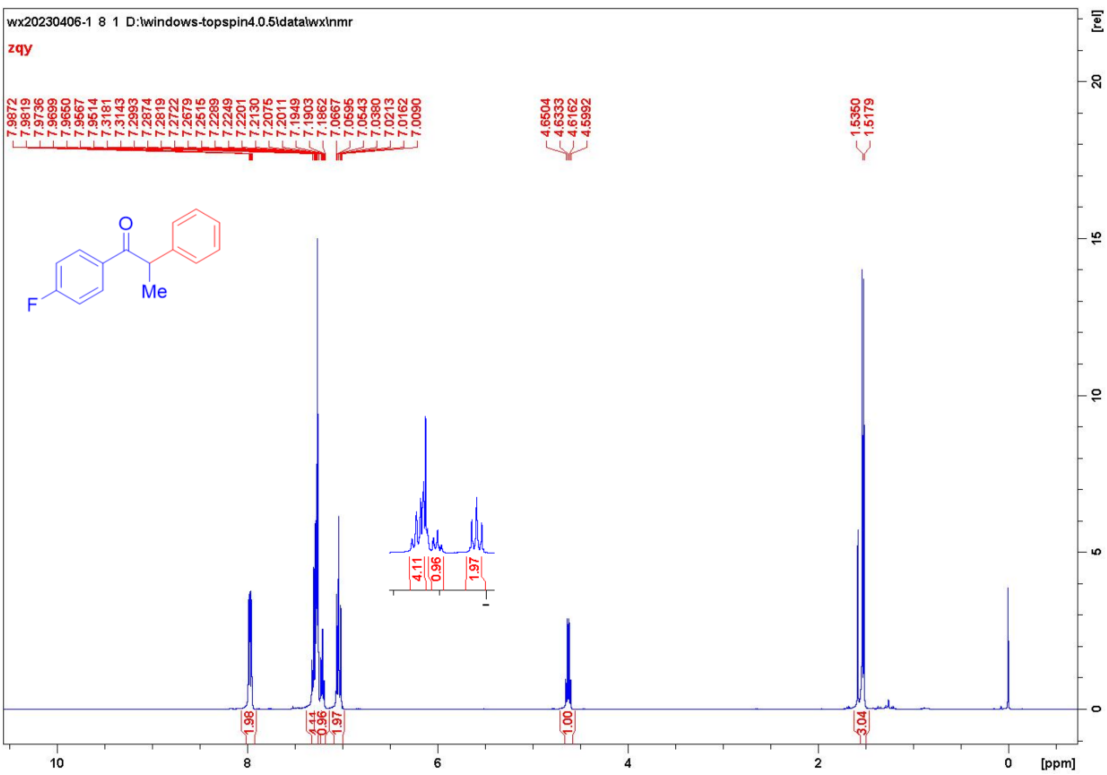
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3t**.



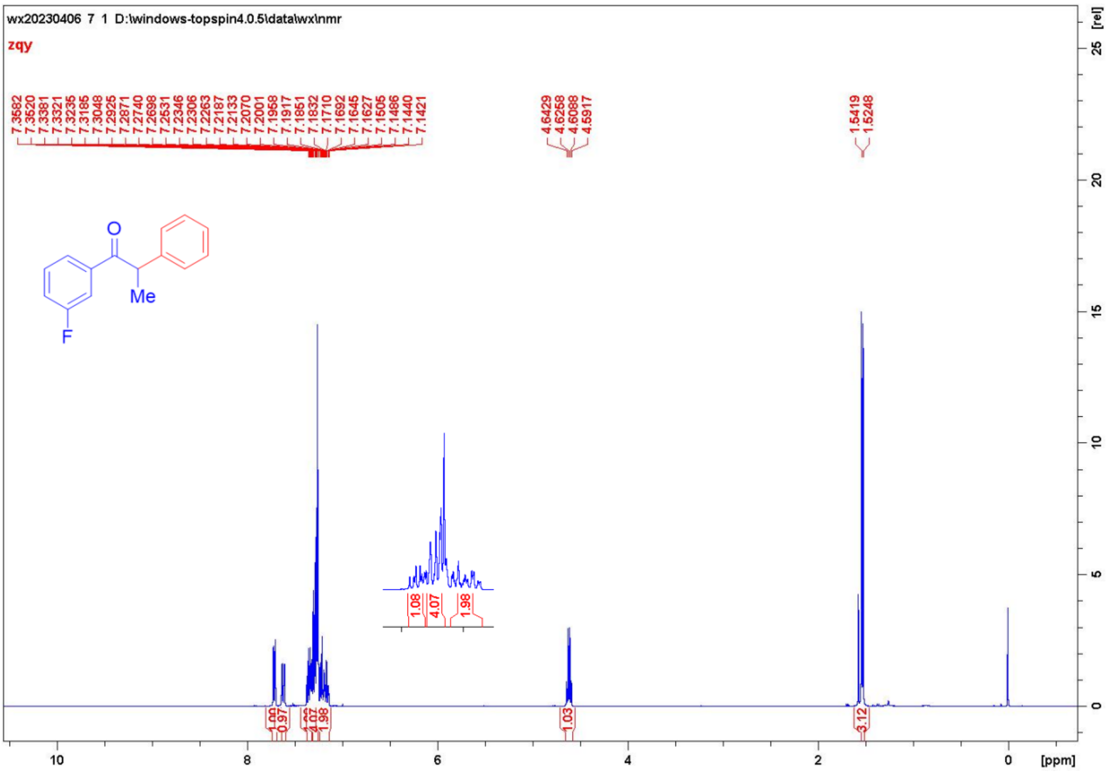
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3u**.



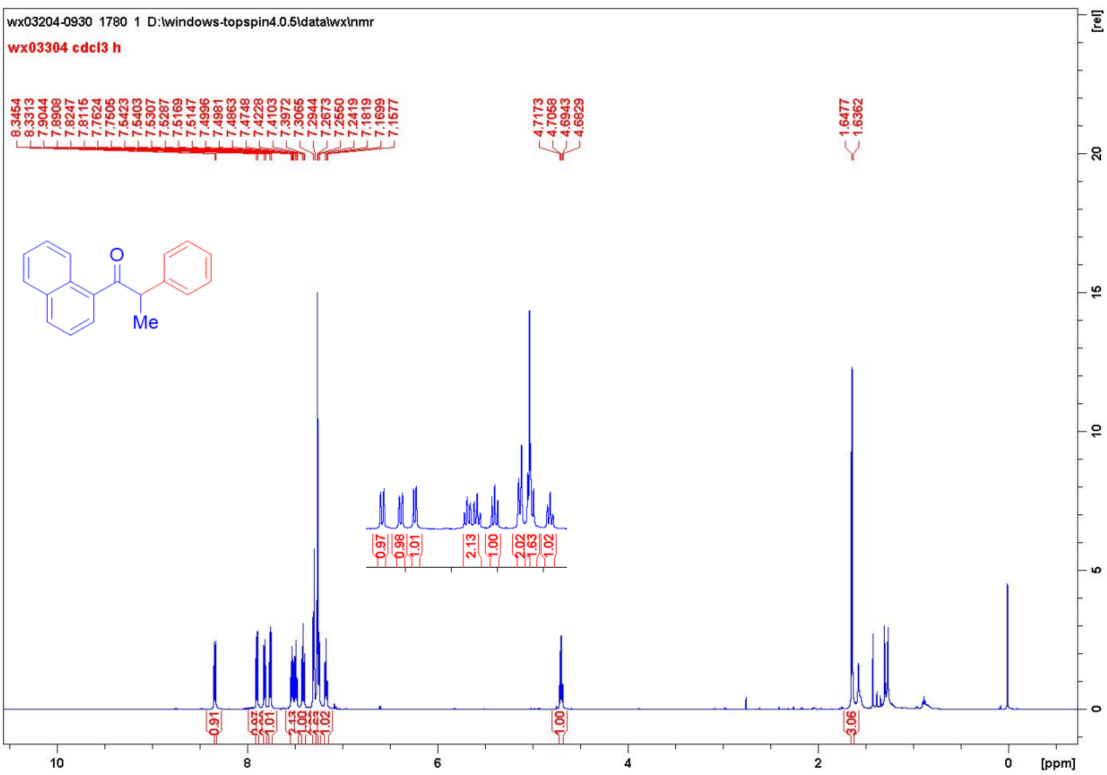
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3v**.



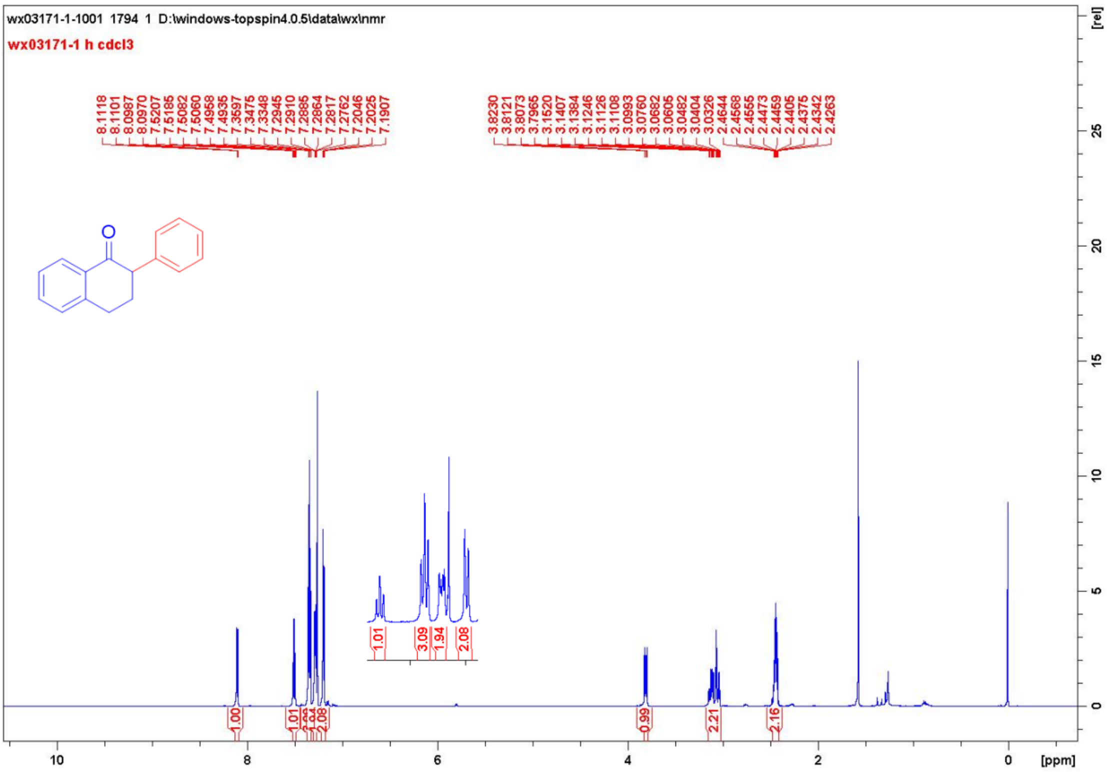
^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3w**.



^1H NMR (600 MHz, $CDCl_3$) spectrum of **3x**.



^1H NMR (600 MHz, $CDCl_3$) spectrum of **3y**.



^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3z**.