Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Cross-coupling reactions catalyzed by an *N*-heterocyclic carbene-Pd(II) complex under aerobic and CuI-free conditions

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Contents

Experimental Section

General information

^{1}H NMR spectra were recorded on Bruker Avance II (400 MHz) instruments. All aryl derivatives are known and identified by ^{1}H NMR.

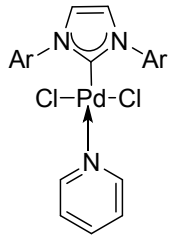
Typical Procedure for the Sonogashira Cross-Coupling Reactions

To a stirred mixture of aryl bromides **3** or aryl sulfonates **5** (0.80 mmol) and terminal acetylenes **2** (1.2 mmol) in DMSO (2 mL), was added Cat. 3 (1 mol%), and TEA (2 equiv.). The reaction mixture was stirred under aerobic condition at 80-85^{o}C for desired time until complete consumption of starting material as monitored by TLC. After the reaction was quenched by water, the mixture was then extracted with EtOAc three times. The organic fractions were combined and washed by brine twice, after that, the organic fractions were dried over Na_2SO_4, and filtered through celite; the filtrate was evaporated to dryness and the crude product was purified by column chromatography (**4a-u**).

Typical Procedure for the Heck Cross-Coupling Reactions

To a stirred mixture of aryl bromides **3** (0.80 mmol) and terminal olefins **6** (1.2 mmol) in Dioxane or DMF (2 mL), was added Cat. 3 (1 mol%), and TEA (2 equiv.). The reaction mixture was stirred under aerobic condition at 80^{o}C for desired time until complete consumption of starting material as monitored by TLC. After the reaction was quenched by water, the mixture was then extracted with EtOAc three times. The organic fractions were combined and washed by brine twice, after that, the organic fractions were dried over Na_2SO_4, and filtered through celite; the filtrate was evaporated to dryness and the crude product was purified by column chromatography (**7a-n**).

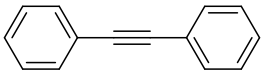
The characterization data of compounds Cat. 3



Cat. 3

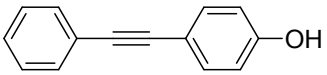
Cat. 3: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 – 9.09 (m, 2H), 7.85 – 7.77 (m, 1H), 7.49 – 7.41 (m, 8H), 7.37 (ddd, *J* = 7.6, 5.1, 1.4 Hz, 2H), 7.25 – 7.15 (m, 12H), 7.12 – 6.98 (m, 12H), 6.82 – 6.71 (m, 12H), 6.39 (s, 4H), 4.90 (s, 2H), 2.20 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.96 (CH, Py), 144.66 (C_{Ar}), 143.99 (C_{Ar}), 141.62 (C_{Ar}), 138.23 (C_{Ar}), 135.47 (CH, Py), 130.94 (CH_{Ar}), 130.56 (CH_{Ar}), 128.16 (CH_{Ar}), 127.80 (CH_{Ar}), 126.05 (d, *J* = 3.4 Hz, C-Pd), 124.16 (d, *J* = 17.9 Hz, CH, Im), 50.89 ($CHPh_2$), 21.83 (CH_3). Anal. Calcd for $C_{74}H_{61}Cl_2N_3Pd$: C, 75.99; H, 5.26; N, 3.59: found C, 76.29; H, 5.11; N, 3.79.

The characterization data of compounds 4a-u



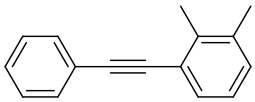
4a

1,2-diphenylethyne(4a): Yellow solid (0.12 g, 86% yield); m.p: 59-60°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (ddd, *J* = 6.4, 4.0, 2.8 Hz, 4H), 7.39 – 7.30 (m, 6H).



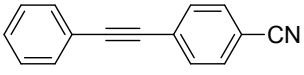
4b

4-(phenylethynyl)phenol(4b): White solid (0.10 g, 65% yield); m.p: 121-122°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.48 (m, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 7.37 – 7.28 (m, 3H), 6.82 (d, *J* = 8.6 Hz, 2H), 5.11 (s, 1H).



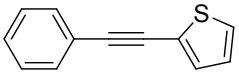
4c

1,2-dimethyl-3-(phenylethynyl)benzene(4c): Colorless oil (0.12 g, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.7, 1.7 Hz, 2H), 7.39 – 7.31 (m, 4H), 7.09 (dt, *J* = 15.0, 7.4 Hz, 2H), 2.47 (s, 3H), 2.30 (s, 3H).



4d

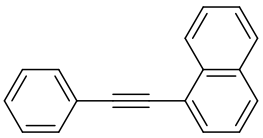
4-(phenylethynyl)benzonitrile(4d): Yellow solid (0.14 g, 89% yield); m.p: 107-108°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 4H), 7.60 – 7.54 (m, 2H), 7.44 – 7.38 (m, 3H).



4e

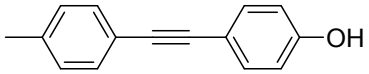
2-(phenylethynyl)thiophene(4e): Light yellow solid (0.13 g, 85% yield); m.p: 48-49°C; ^{1}H NMR

(400 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.41 – 7.36 (m, 3H), 7.35 – 7.30 (m, 2H), 7.07 – 7.02 (m, 1H).



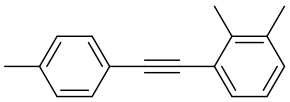
4f

1-(phenylethynyl)naphthalene(4f): Viscose yellow oil (0.14 g, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.3 Hz, 1H), 7.90 (t, *J* = 9.0 Hz, 2H), 7.81 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.74 – 7.68 (m, 2H), 7.65 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.58 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 7.50 (dd, *J* = 8.2, 7.2 Hz, 1H), 7.47 – 7.39 (m, 3H).



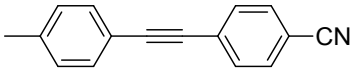
4g

4-(p-tolylethynyl)phenol(4g): Yellow solid (0,10 g, 60% yield); m.p: 120-121^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, *J* = 7.9, 6.3 Hz, 4H), 7.14 (d, *J* = 7.9 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 4.89 (s, 1H), 2.36 (s, 3H).



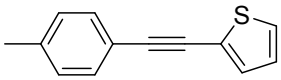
4h

1,2-dimethyl-3-(p-tolylethynyl)benzene(4h): Colorless oil (0,11 g, 63% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 7.3 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.08 (dt, *J* = 14.9, 7.4 Hz, 2H), 2.46 (s, 3H), 2.37 (s, 3H), 2.29 (s, 3H).



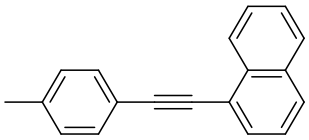
4i

4-(p-tolylethynyl)benzonitrile(4i): Yellow solid (0.14 g, 83% yield); m.p: 161-162^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (q, *J* = 8.3 Hz, 4H), 7.44 (d, *J* = 7.9 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 2.39 (s, 3H).



4j

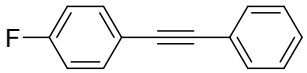
2-(p-tolylethynyl)thiophene(4j): Light yellow solid (0.12 g, 76% yield); m.p: 64-65^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.30 (qd, *J* = 3.4, 1.6 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.03 (dd, *J* = 5.1, 3.7 Hz, 1H), 2.40 (s, 3H).



4k

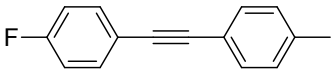
1-(p-tolylethynyl)naphthalene(4k): Light yellow solid (0.13 g, 65% yield); m.p: 54-55^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.3 Hz, 1H), 7.88 (dd, *J* = 12.8, 8.2 Hz, 2H), 7.79 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.66 – 7.55 (m, 4H), 7.49 (dd, *J* = 8.2, 7.2 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 2H), 2.43

(s, 3H).



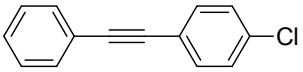
4l

1-fluoro-4-(phenylethynyl)benzene(4l): White solid (0.14 g, 88% yield); m.p: 108-109°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.51 (m, 4H), 7.42 – 7.34 (m, 3H), 7.08 (ddd, *J* = 8.8, 5.9, 2.5 Hz, 2H).



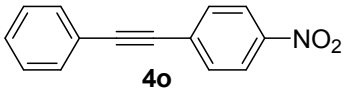
4m

1-fluoro-4-(p-tolylethynyl)benzene(4m): White solid (0.12 g, 74% yield); m.p: 96-97°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.50 (m, 2H), 7.48 – 7.41 (m, 2H), 7.19 (d, *J* = 7.9 Hz,2H), 7.11 – 7.03 (m, 2H), 2.40 (s, 3H).



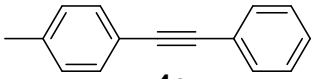
4n

1-chloro-4-(phenylethynyl)benzene(4n): White solid (0.14 g, 83% yield); m.p: 81-82°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.54 (m, 2H), 7.51 – 7.47 (m, 2H), 7.42 – 7.33 (m, 5H).



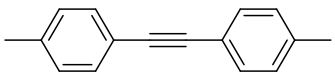
4o

1-nitro-4-(phenylethynyl)benzene(4o): Yellow solid (0.15 g, 86% yield); m.p: 121-122°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.20 (m, 2H), 7.73 – 7.65 (m, 2H), 7.58 (dt, *J* = 5.5, 2.1 Hz, 2H), 7.47 – 7.37 (m, 3H).



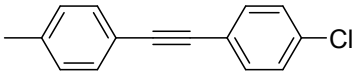
4p

1-methyl-4-(phenylethynyl)benzene(4p): White solid (0.11 g, 72% yield); m.p: 67-68°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.53 (m, 2H), 7.51 – 7.44 (m, 2H), 7.41 – 7.32 (m, 3H), 7.19 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H).



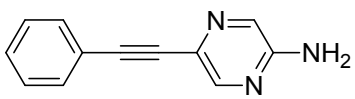
4q

1,2-di-p-tolylethyne(4q): White solid (0.10 g, 61% yield); m.p: 138-139°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.0 Hz, 4H), 7.15 (d, *J* = 7.9 Hz, 4H), 2.36 (s, 6H).



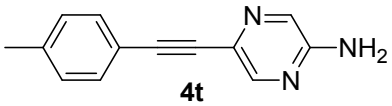
4r

1-chloro-4-(p-tolylethynyl)benzene(4r): White solid (0.14 g, 76% yield); m.p: 149-150°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (ddd, *J* = 10.8, 6.3, 2.0 Hz, 4H), 7.38 – 7.31 (m, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 2.40 (s, 3H).



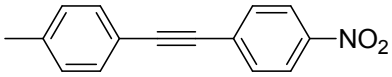
4s

5-(phenylethynyl)pyrazin-2-amine(4s): Yellow solid (0.11 g, 72% yield); m.p: 182-184°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 8.02 (s, 1H), 7.63 – 7.51 (m, 2H), 7.41 – 7.32 (m, 3H), 4.84 (s, 2H). ^{13}C NMR (125 MHz, DMSO-d6): δ 154.65 (C_{Py}), 145.71 (C_{Py}), 132.58 (C_{Py}), 131.18 (C_{Ph}), 128.75 (d, J = 11.7 Hz, C_{Ph}), 125.00 (C_{Py}), 122.23 (C_{Ph}), 88.55 (C-), 87.71 (-C). Anal. Calcd for $C_{12}H_9N_3$: C, 73.83; H, 4.65; N, 21.52: found C, 74.13; H, 4.72; N, 21.15.



4t

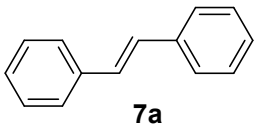
5-(*p*-tolylethynyl)pyrazin-2-amine(4t): Yellow solid (0.10 g, 67% yield); m.p: 205-208°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 8.00 (s, 1H), 7.47 (d, J = 8.1 Hz, 2H), 7.18 (d, J = 7.9 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, DMSO-d6): δ 154.56 (C_{Py}), 145.53 (C_{Py}), 138.45 (C_{Ph}), 132.51 (C_{Py}), 131.09 (C_{Ph}), 129.38 (C_{Ph}), 125.21 (C_{Py}), 119.20 (C_{Ph}), 88.70 (C-), 87.07 (-C), 21.03 (CH_3). Anal. Calcd for $C_{13}H_{11}N_3$: C, 74.62; H, 5.30; N, 20.08: found C, 74.37; H, 5.45; N, 20.18.



4u

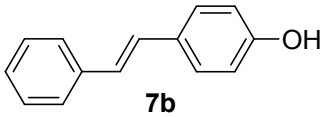
1-methyl-4-((4-nitrophenyl)ethynyl)benzene(4u): Yellow solid (0.15 g, 77% yield); m.p: 155-156°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.18 (m, 2H), 7.72 – 7.61 (m, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.22 (d, J = 7.9 Hz, 2H), 2.41 (s, 3H).

The characterization data of compounds 7a-n



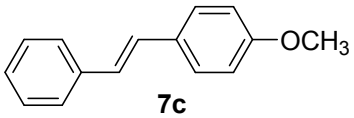
7a

(E)-1,2-diphenylethene(7a): White solid (0.11 g, 75% yield); m.p: 121-122°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (dd, J = 5.1, 3.4 Hz, 4H), 7.39 – 7.32 (m, 4H), 7.29 – 7.22 (m, 2H), 7.11 (s, 2H).



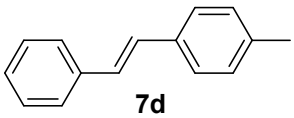
7b

(E)-4-styrylphenol(7b): White solid (0.097 g, 62% yield); m.p: 183-184°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 7.6 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.25 (d, J = 9.4 Hz, 2H), 7.05 (d, J = 16.3 Hz, 1H), 6.96 (d, J = 16.3 Hz, 1H), 6.83 (d, J = 8.3 Hz, 2H).



7c

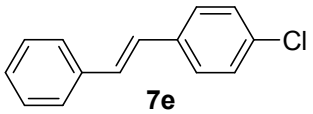
(E)-1-methoxy-4-styrylbenzene(7c): White solid (0.10 g, 60% yield); m.p: 135-136°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, J = 13.6, 8.0 Hz, 4H), 7.38 (t, J = 7.6 Hz, 2H), 7.30 – 7.22 (m, 1H), 7.05 (dd, J = 38.1, 16.3 Hz, 2H), 6.93 (d, J = 8.7 Hz, 2H), 3.86 (s, 3H).



7d

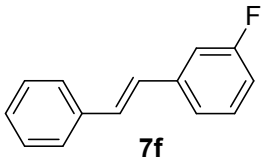
(E)-1-methyl-4-styrylbenzene(7d): White solid (0.10 g, 67% yield); m.p: 119-120°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.48 (m, 2H), 7.42 (d, J = 8.1 Hz, 2H), 7.36 (dd, J = 10.4, 4.8 Hz, 2H),

7.25 (dt, *J* = 9.1, 4.1 Hz, 1H), 7.17 (d, *J* = 7.9 Hz, 2H), 7.08 (d, *J* = 2.5 Hz, 2H), 2.36 (s, 3H).



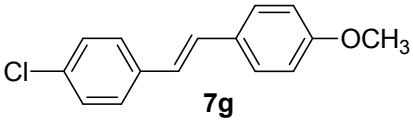
7e

(E)-1-chloro-4-styrylbenzene(7e): White solid (0.14 g, 79% yield); m.p: 127-128°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.3 Hz, 2H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.39 – 7.30 (m, 4H), 7.26 (d, *J* = 6.3 Hz, 1H), 7.06 (d, *J* = 2.7 Hz, 2H).



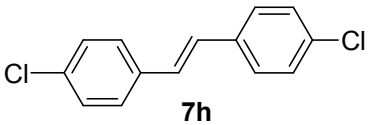
7f

(E)-1-fluoro-3-styrylbenzene(7f): White solid (0.12 g, 77% yield); m.p: 70-71°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.26 – 7.19 (m, 2H), 7.08 (d, *J* = 7.0 Hz, 2H), 6.95 (t, *J* = 8.3 Hz, 1H).



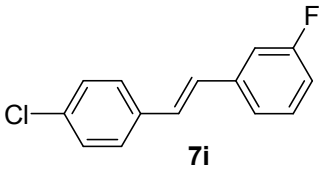
7g

(E)-1-chloro-4-(4-methoxystyryl)benzene(7g): White solid (0.11 g, 57% yield); m.p:178-179°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 12.9, 8.5 Hz, 4H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 16.3 Hz, 1H), 6.95 – 6.87 (m, 3H), 3.83 (s, 3H).



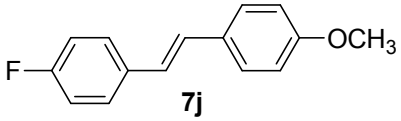
7h

(E)-1,2-bis(4-chlorophenyl)ethane(7h): White solid (0.16 g, 80% yield); m.p: 70-71°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 4H), 7.33 (d, *J* = 8.4 Hz, 4H), 7.02 (s, 2H).



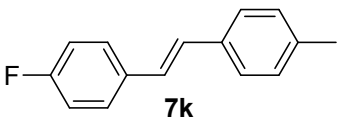
7i

(E)-1-(4-chlorostyryl)-3-fluorobenzene(7i): White solid (0.15 g, 80% yield); m.p: 83-84°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.5 Hz, 2H), 7.36 – 7.30 (m, 3H), 7.25 (d, *J* = 6.1 Hz, 2H), 7.20 (d, *J* = 10.2 Hz, 1H), 7.04 (s, 2H).



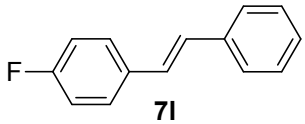
7j

(E)-1-fluoro-4-(4-methoxystyryl)benzene(7j): White solid (0.11 g, 62% yield); m.p:136-137°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (t, *J* = 7.1 Hz, 4H), 7.03 (dd, *J* = 14.8, 6.3 Hz, 2H), 6.95 (d, *J* = 6.0 Hz, 2H), 6.90 (d, *J* = 8.3 Hz, 2H), 3.83 (s, 3H).



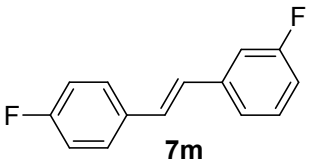
7k

(E)-1-fluoro-4-(4-methylstyryl)benzene(7k): White solid (0.12 g, 73% yield); m.p: 125-126°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.08 – 6.94 (m, 4H), 2.36 (s, 3H).



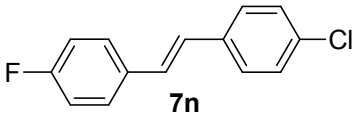
7l

(E)-1-fluoro-4-styrylbenzene(7l): White solid (0.12 g, 78% yield); m.p: 123-124°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (t, *J* = 9.4 Hz, 4H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.25 (d, *J* = 5.0 Hz, 1H), 7.10 – 6.98 (m, 4H).



7m

(E)-1-fluoro-3-(4-fluorostyryl)benzene(7m): White solid (0.14 g, 81% yield); m.p: 92-93°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 8.1, 5.7 Hz, 2H), 7.35 – 7.29 (m, 1H), 7.25 (s, 1H), 7.24 – 7.17 (m, 1H), 7.10 – 7.02 (m, 3H), 6.96 (dd, *J* = 16.1, 4.9 Hz, 2H).



7n

(E)-1-chloro-4-(4-fluorostyryl)benzene(7n): White solid (0.16 g, 85% yield); m.p: 130-131°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.39 (m, 4H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.04 (dd, *J* = 15.5, 6.8 Hz, 3H), 6.95 (d, *J* = 16.4 Hz, 1H).

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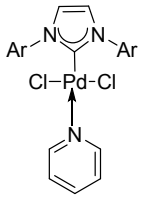
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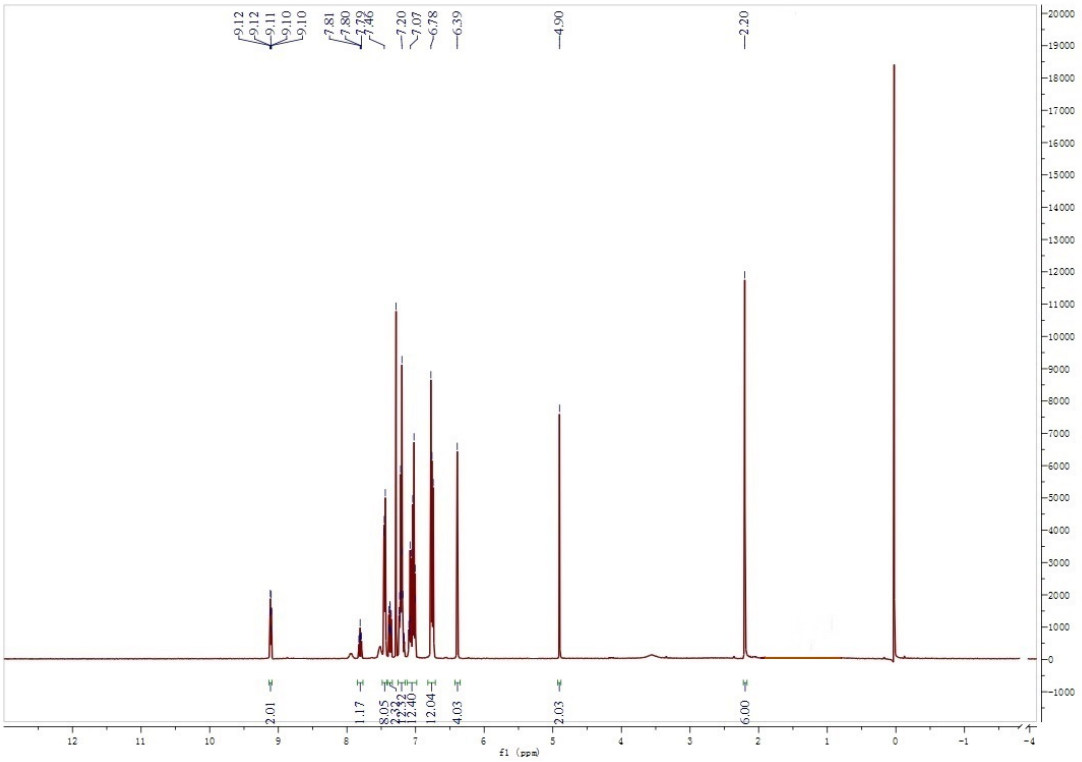
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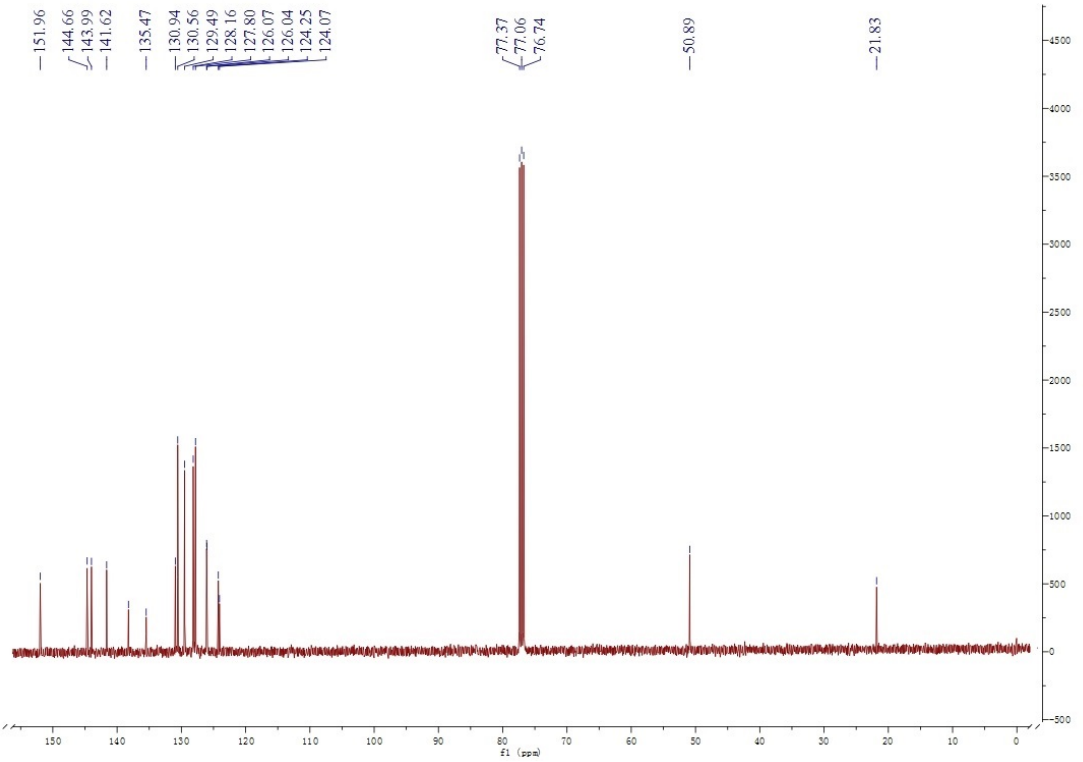
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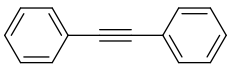

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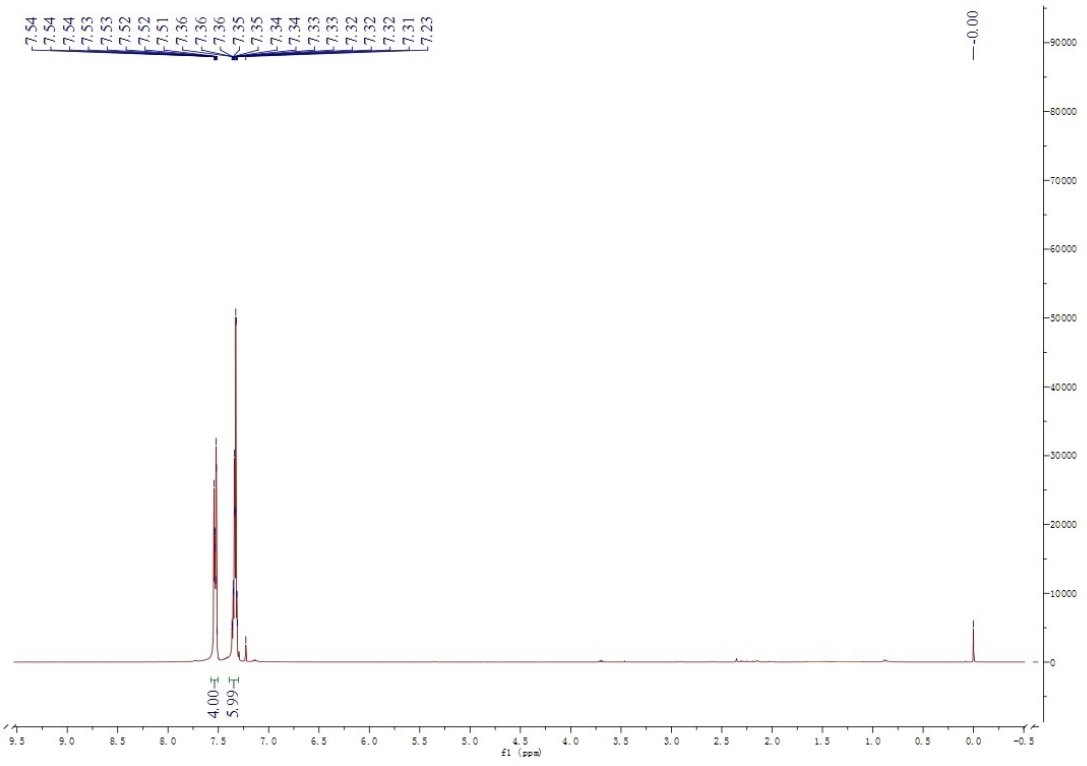
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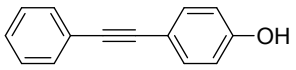
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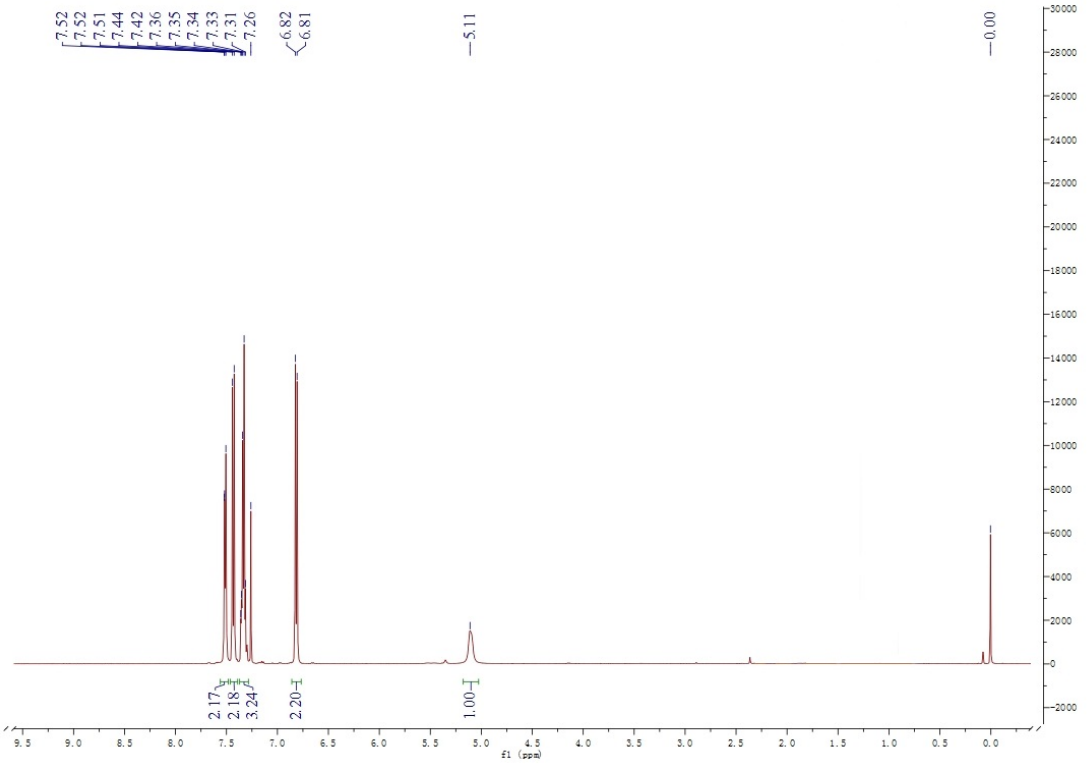
4b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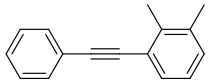

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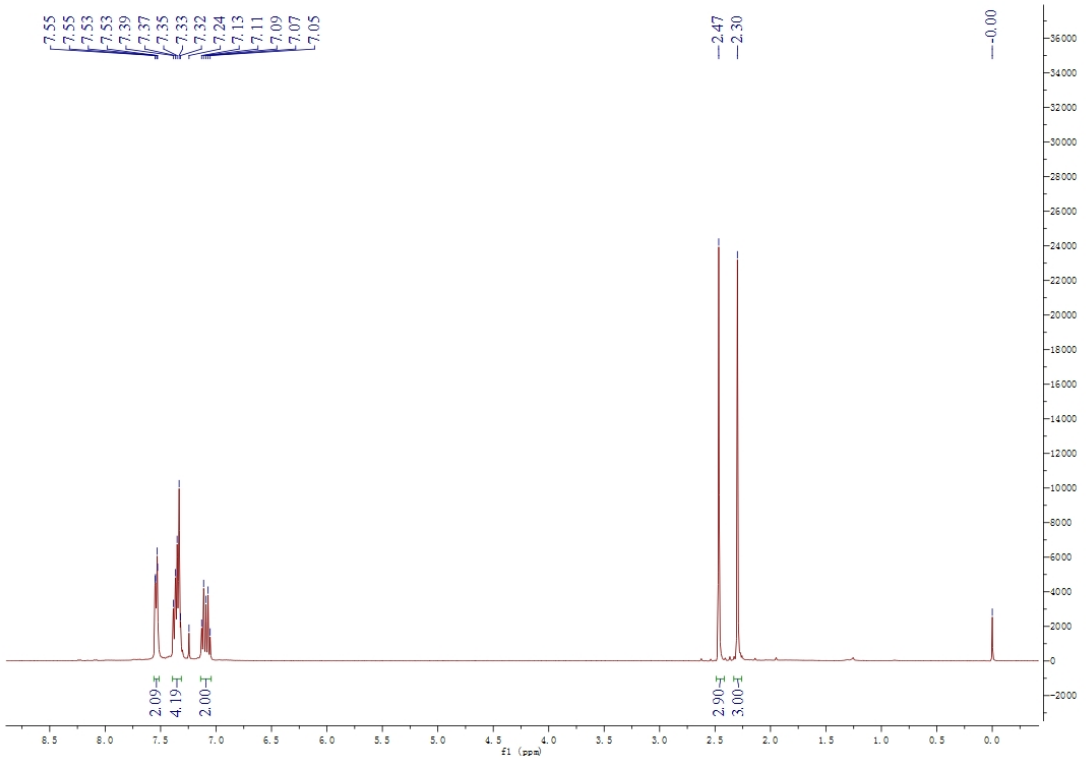
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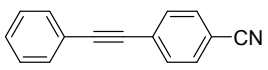
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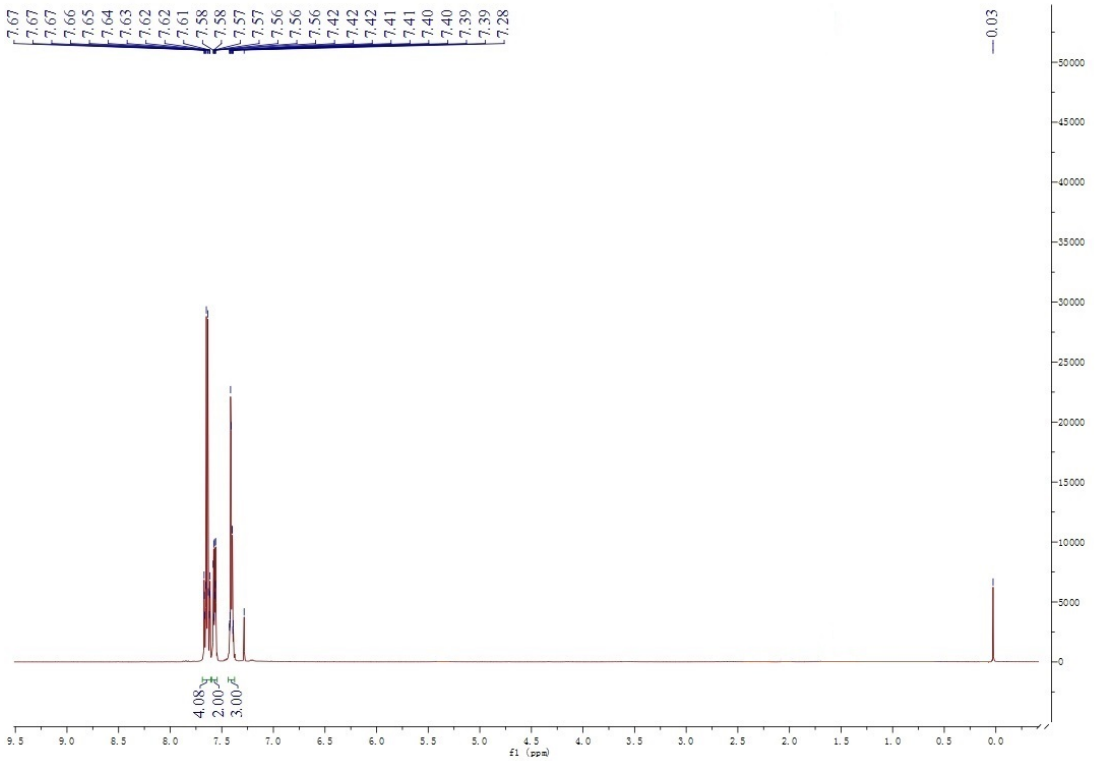
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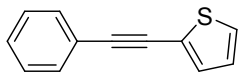
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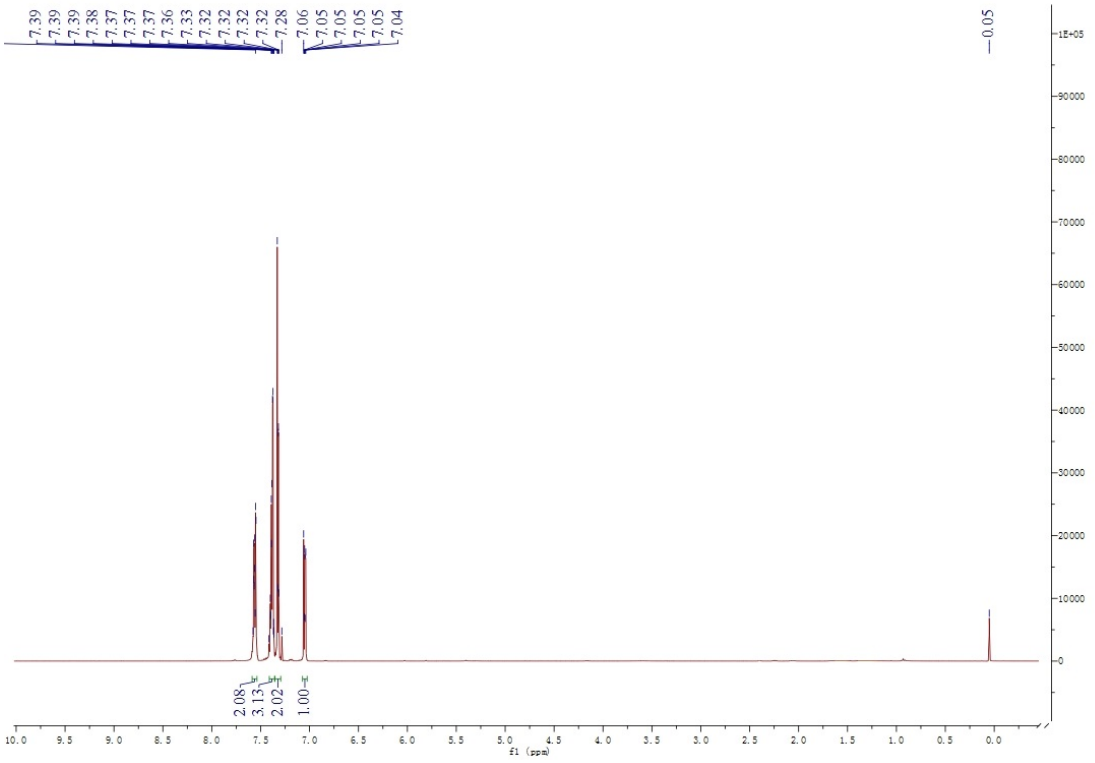
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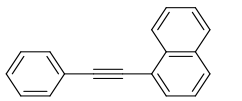

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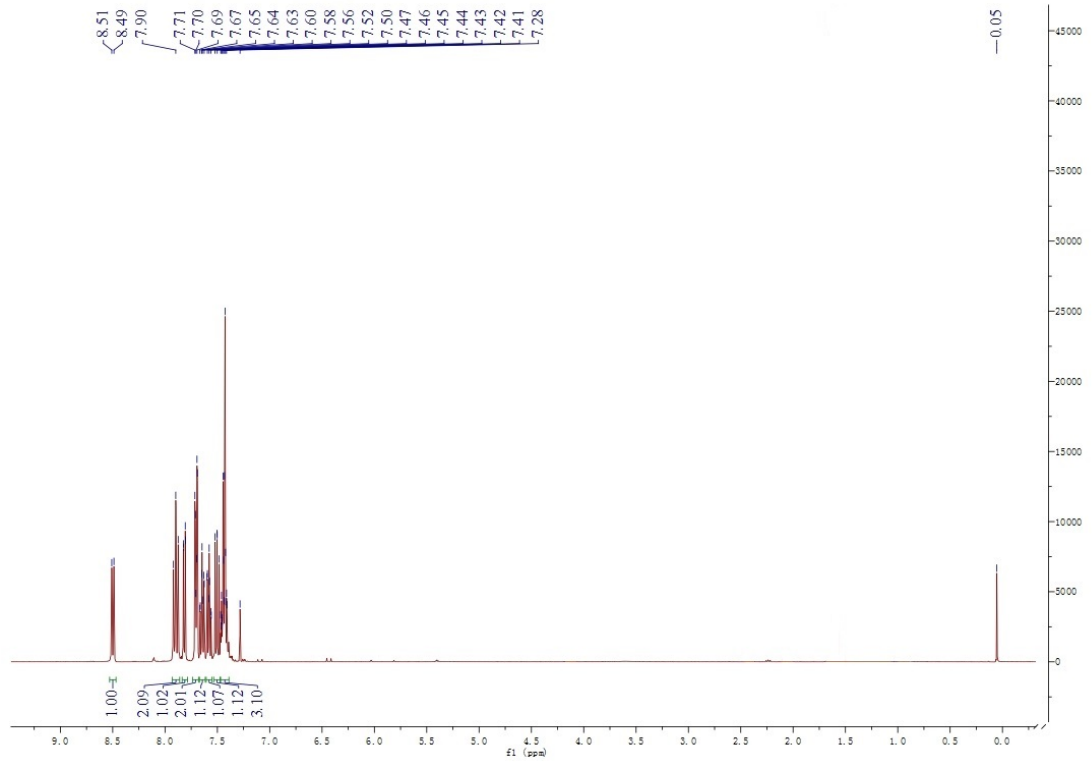
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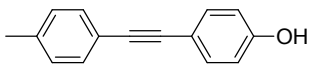
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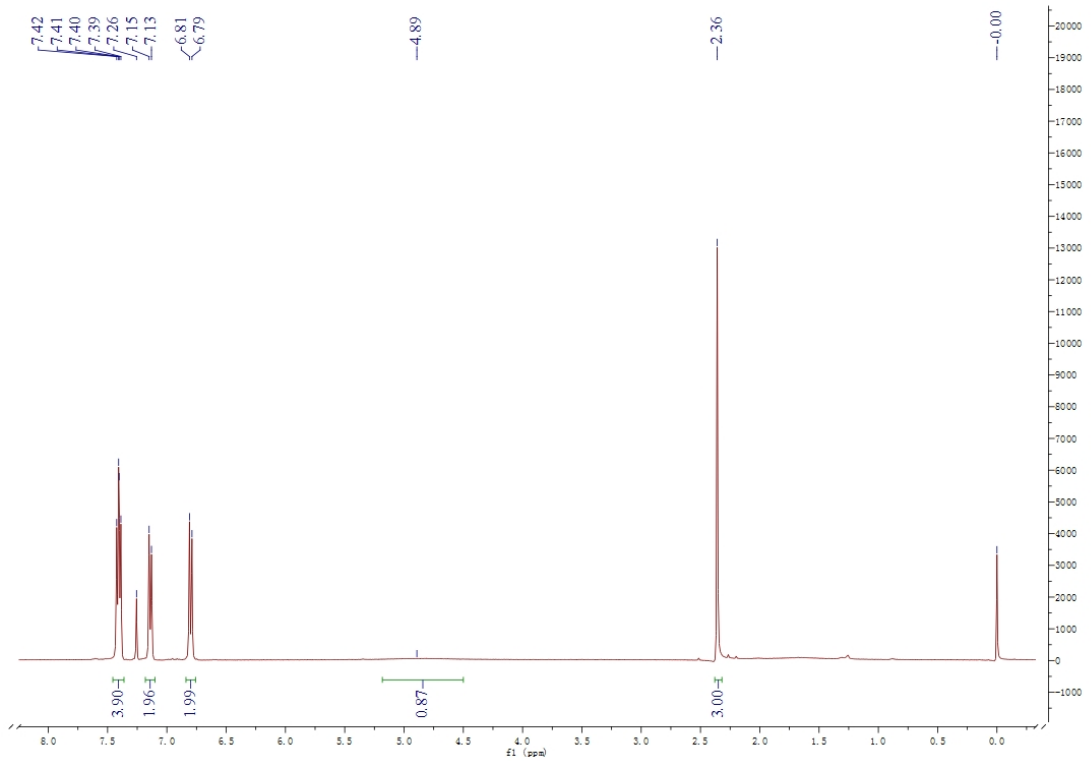
4g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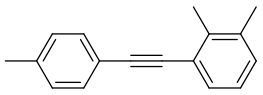

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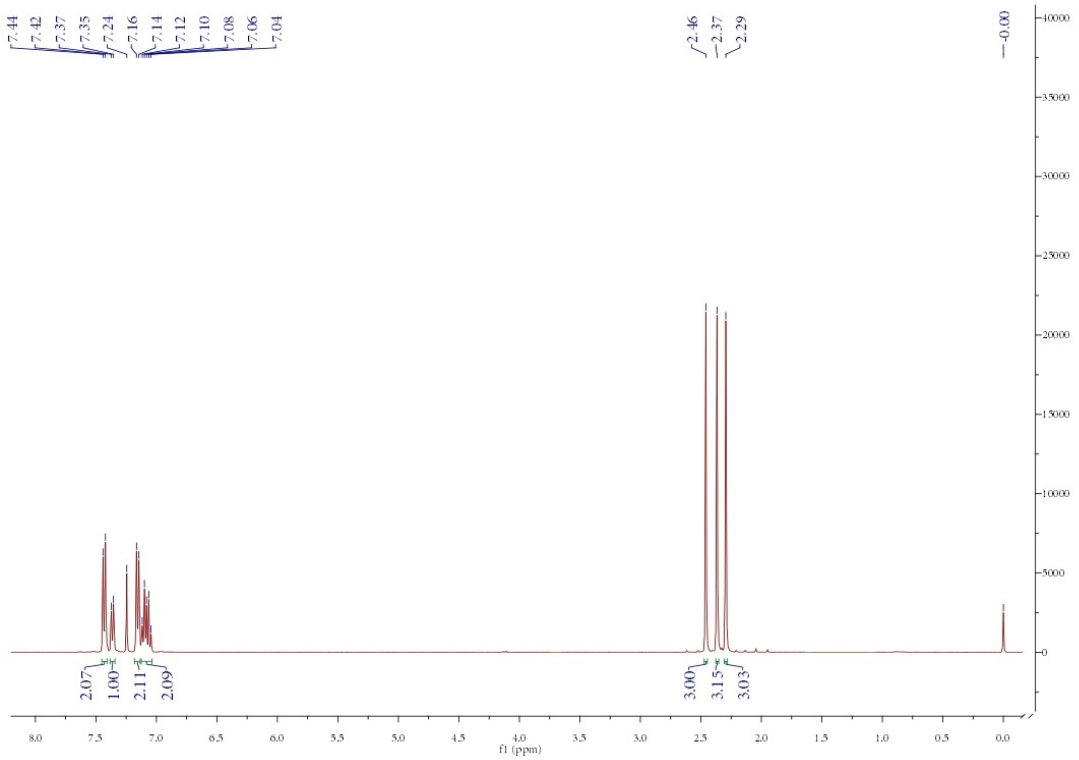
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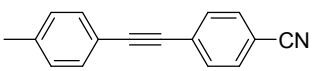
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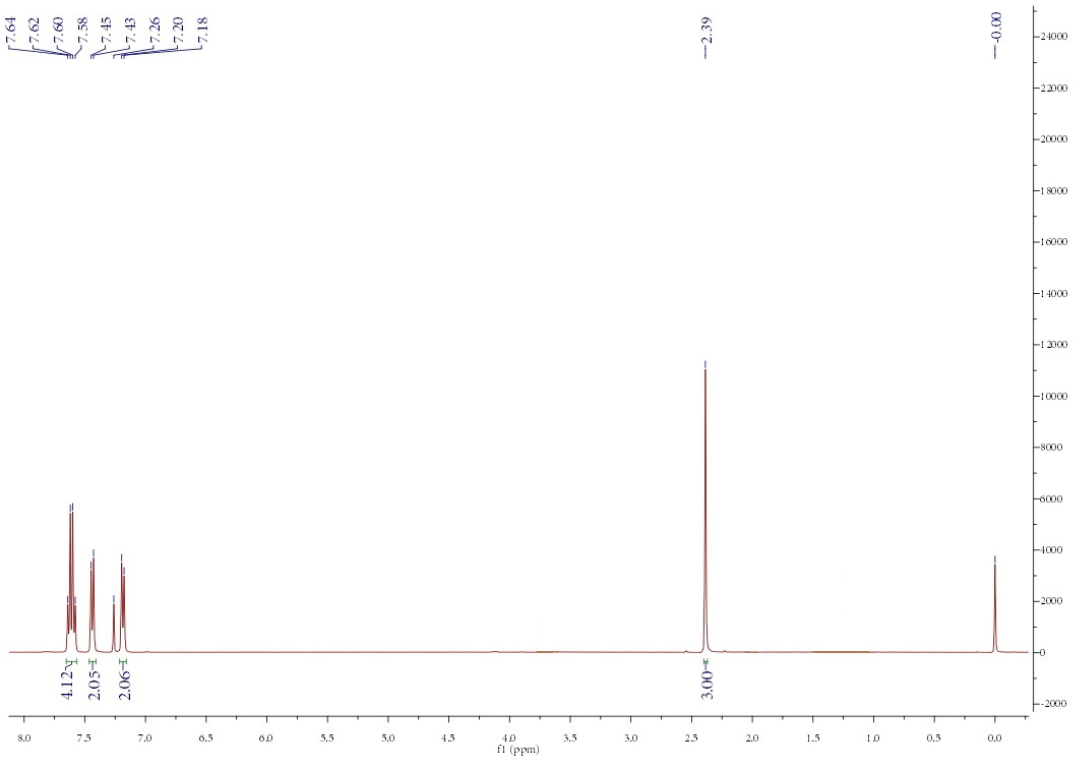
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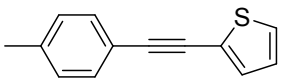
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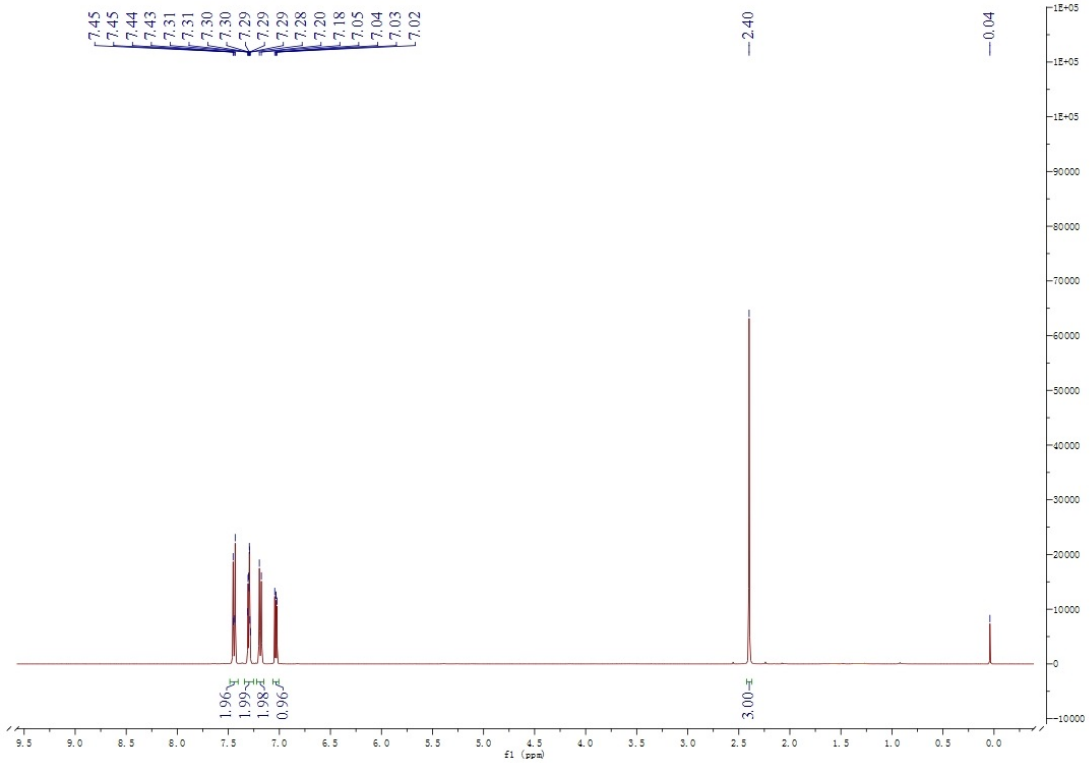
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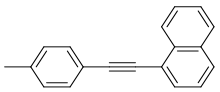
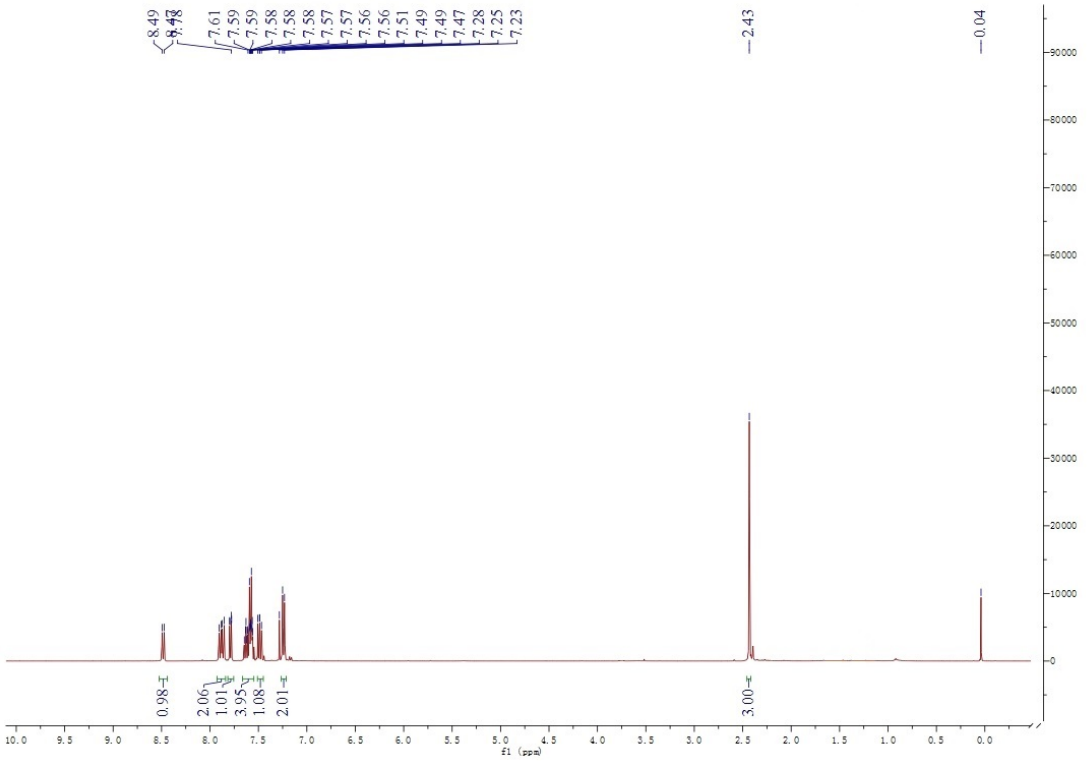
f1 (ppm)



4k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8.48
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7.59
7.58
7.58
7.58
7.57
7.57
7.56
7.56
7.51
7.49
7.49
7.47
7.28
7.25
7.23
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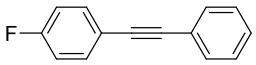
0.04
0.98
2.06
1.01
3.95
1.08
2.01
3.00
f1 (ppm)



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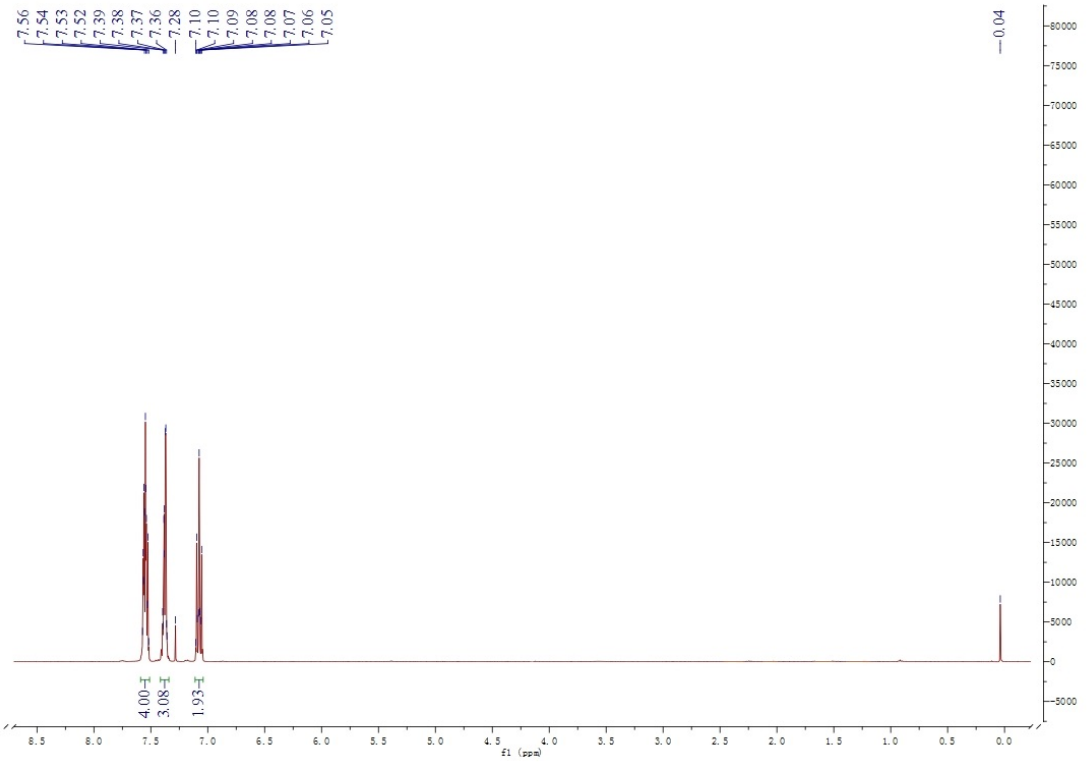
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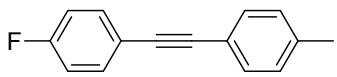
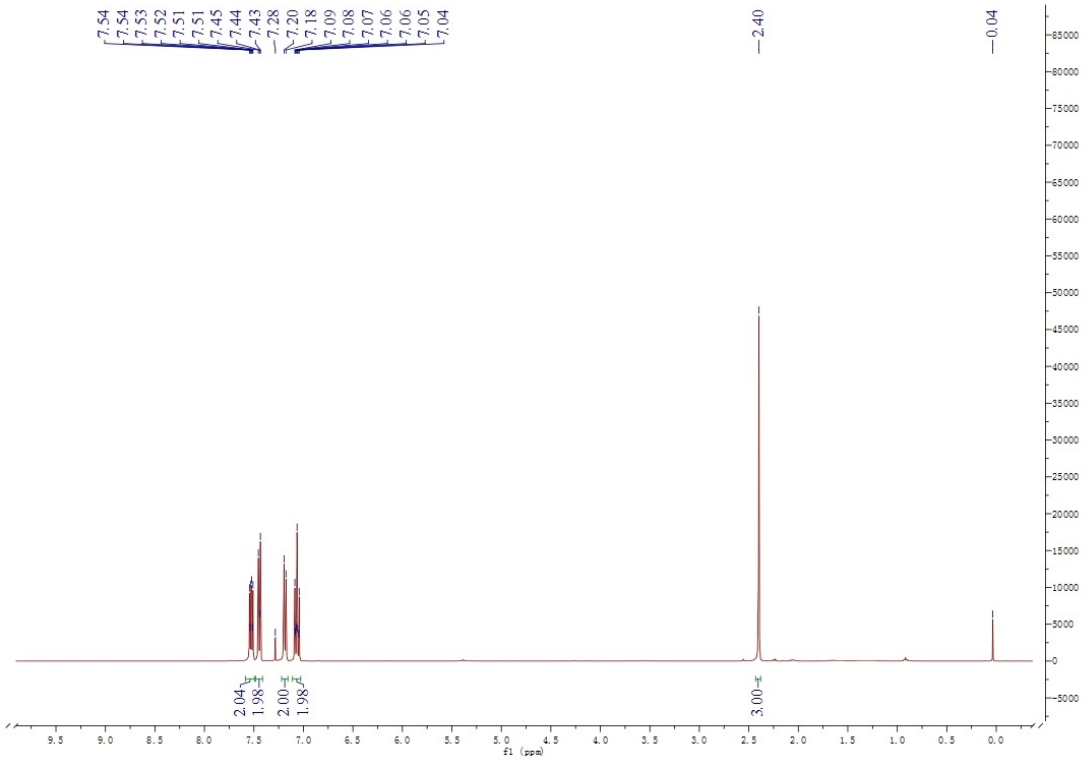
7.52
7.39
7.38
7.37
7.36
7.28
7.10
7.10
7.09
7.08
7.08
7.07
7.06
7.05
0.04
4.00
3.08
1.93
f1 (ppm)


F

4m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7.53
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7.51
7.45
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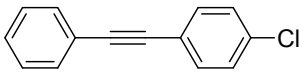
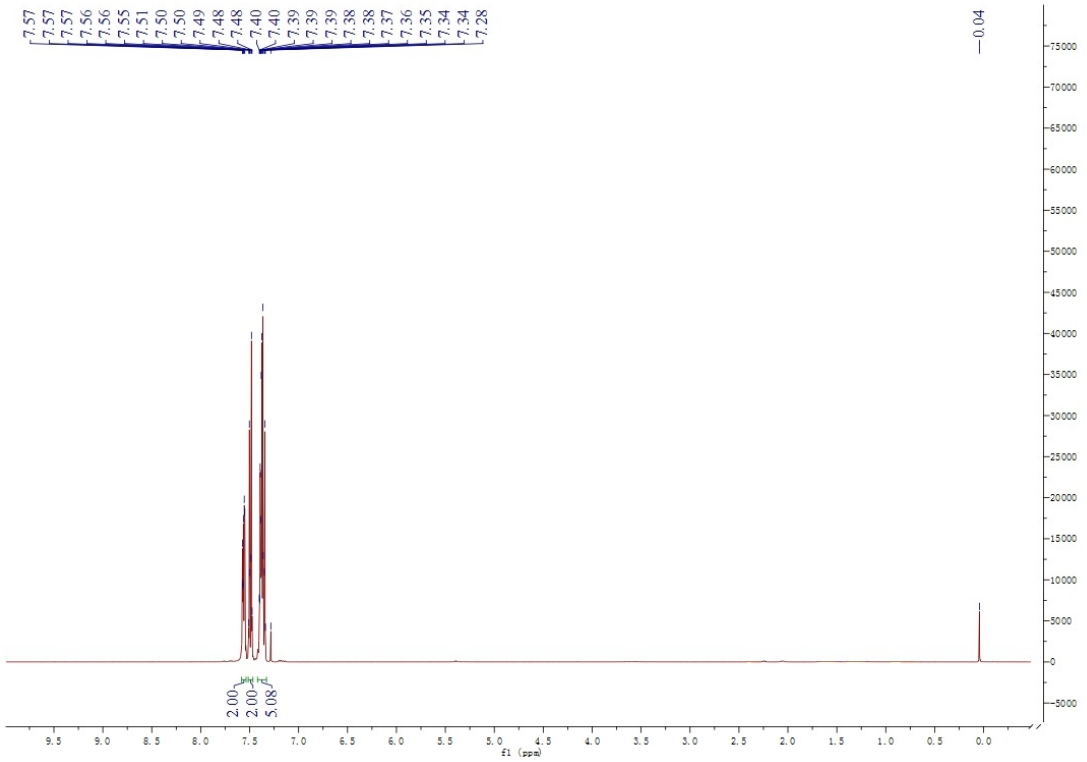
7.43
7.28
7.20
7.18
7.09
7.08
7.07
7.06
7.06
7.05
7.04
2.40
0.04
2.04
1.98
2.00
1.98
3.00
f1 (ppm)


Cl

4n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7.56
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7.50
7.50
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7.48
7.48
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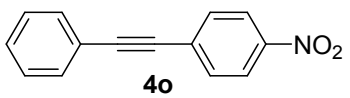
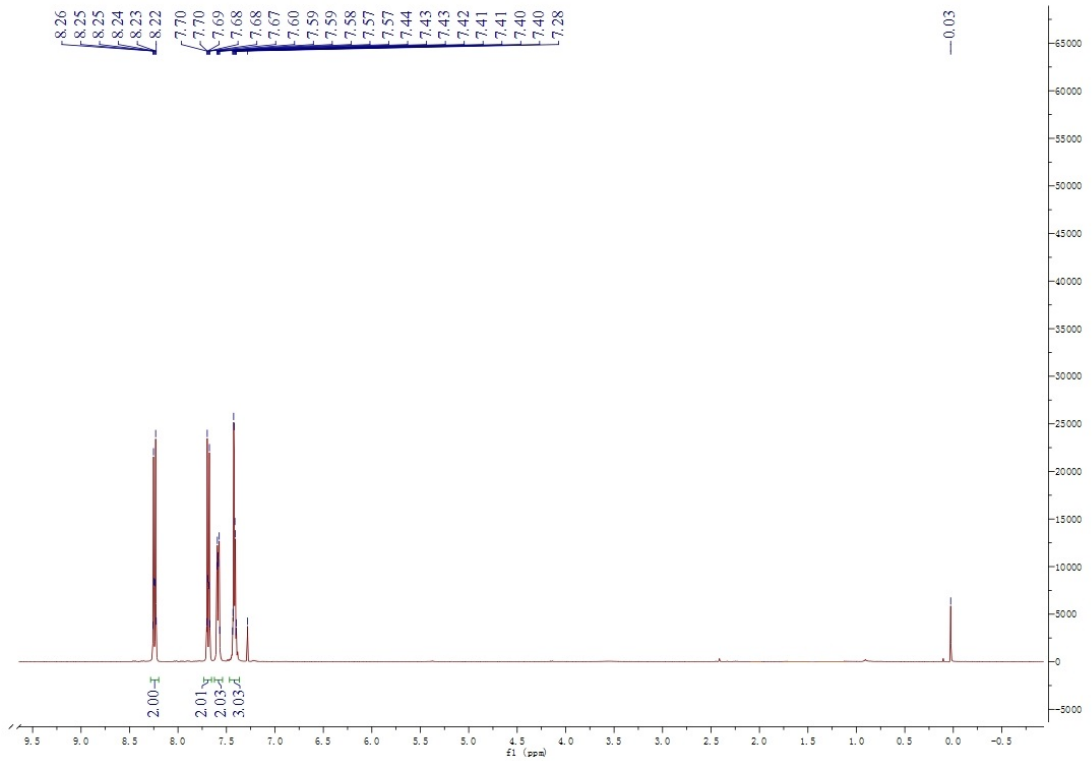
7.40
7.39
7.39
7.39
7.38
7.38
7.37
7.36
7.35
7.34
7.34
7.28
0.04
2.00
2.00
5.08
f1 (ppm)


NO2

4o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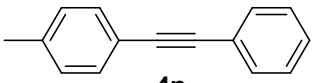
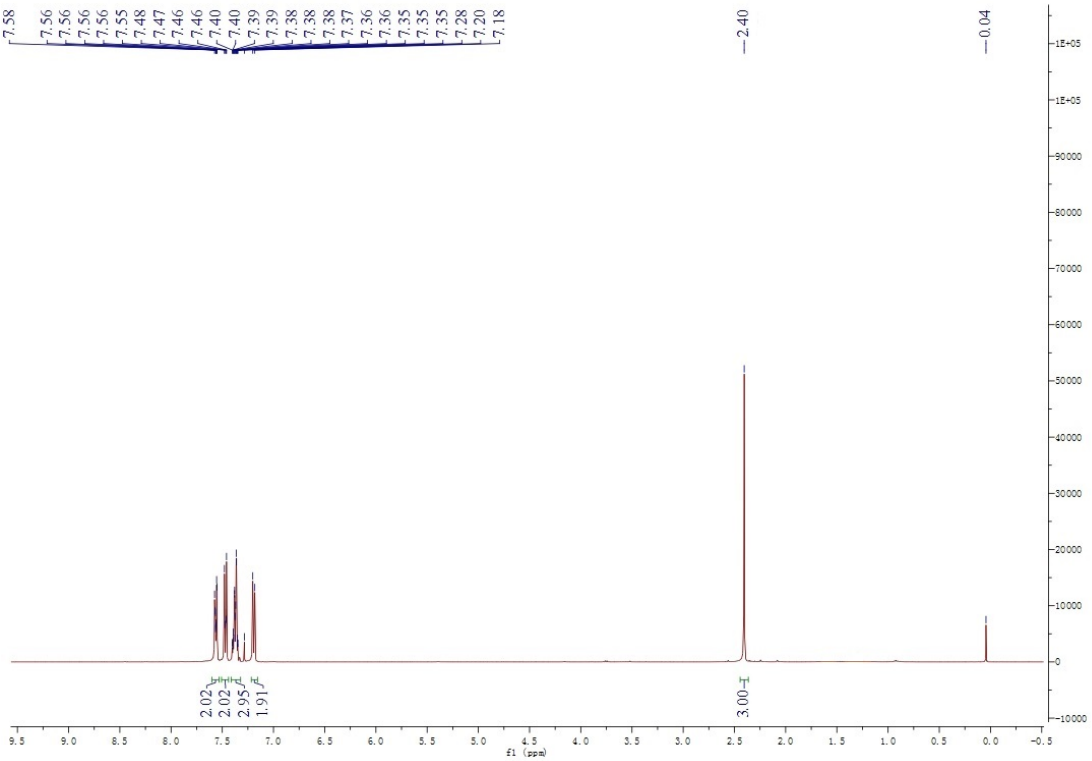
8.25
8.25
8.24
8.23
8.22
7.70
7.70
7.69
7.68
7.68
7.67
7.60
7.59
7.59
7.58
7.57
7.57
7.44
7.43
7.43
7.42
7.41
7.41
7.40
7.40
7.28
0.03
2.00
2.01
2.03
3.03
f1 (ppm)



4p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7.56
7.56
7.56
7.55
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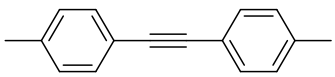
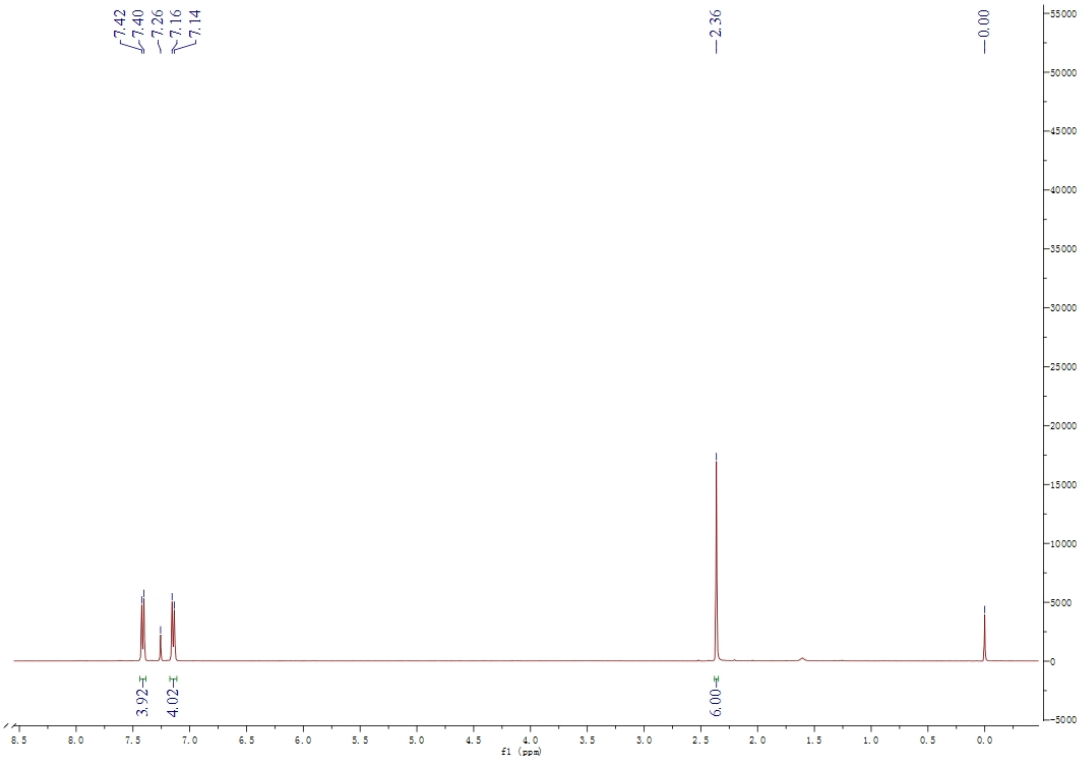
7.47
7.46
7.46
7.40
7.40
7.39
7.38
7.38
7.38
7.37
7.36
7.35
7.35
7.35
7.28
7.20
7.18
2.40
0.04
2.02
2.02
2.95
1.91
3.00
f1 (ppm)



4q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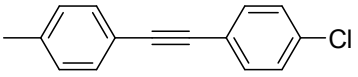
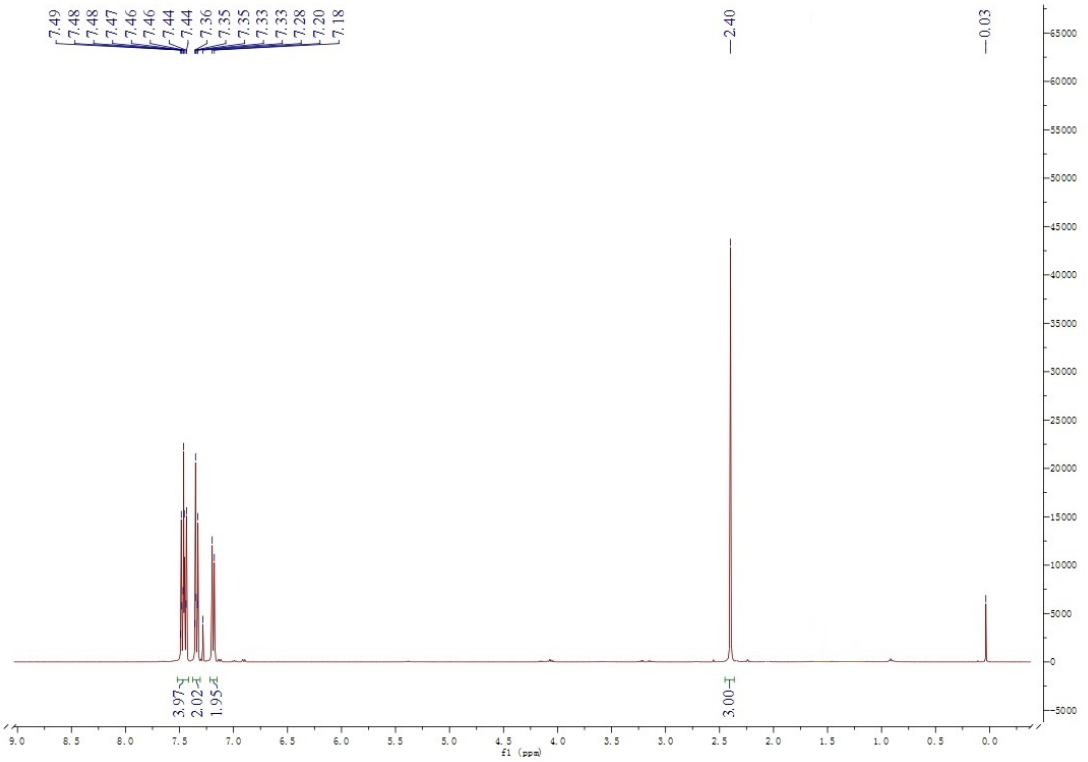
7.40
7.26
7.16
7.14
2.36
0.00
3.92
4.02
6.00
f1 (ppm)


Cl

4r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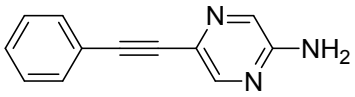
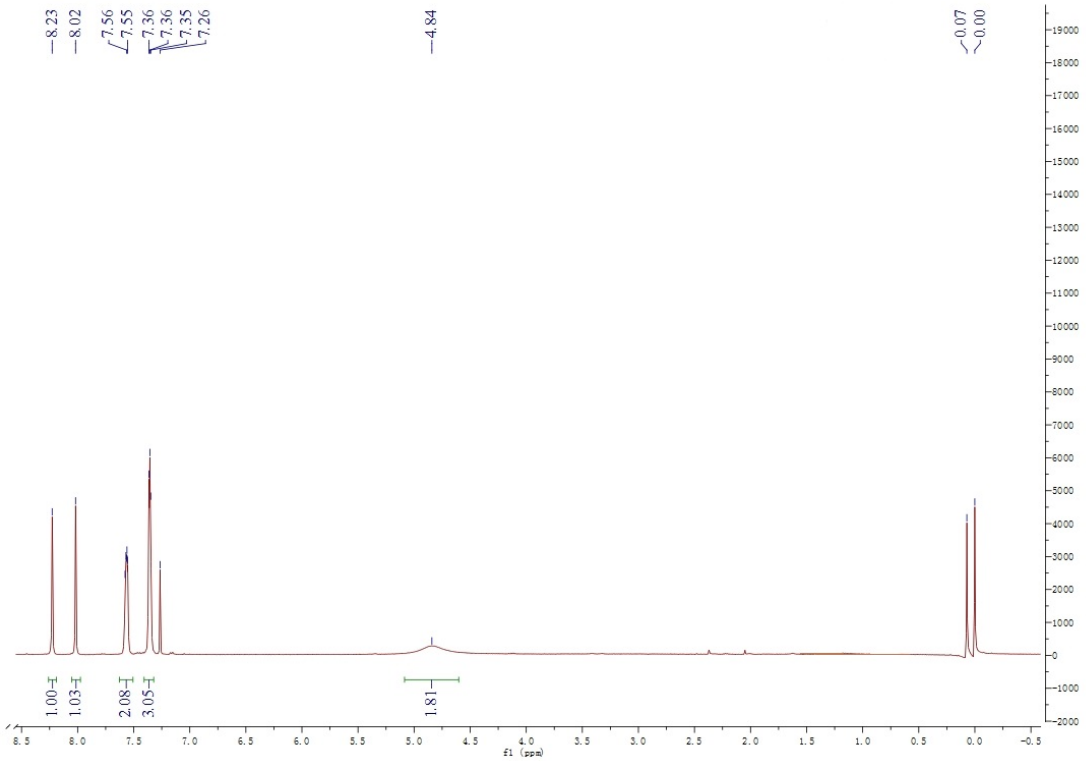
7.48
7.48
7.47
7.46
7.46
7.44
7.44
7.36
7.35
7.35
7.33
7.33
7.28
7.20
7.18
2.40
0.03
3.97
2.02
1.95
3.00
f1 (ppm)


N
NH2
N

4s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8.02
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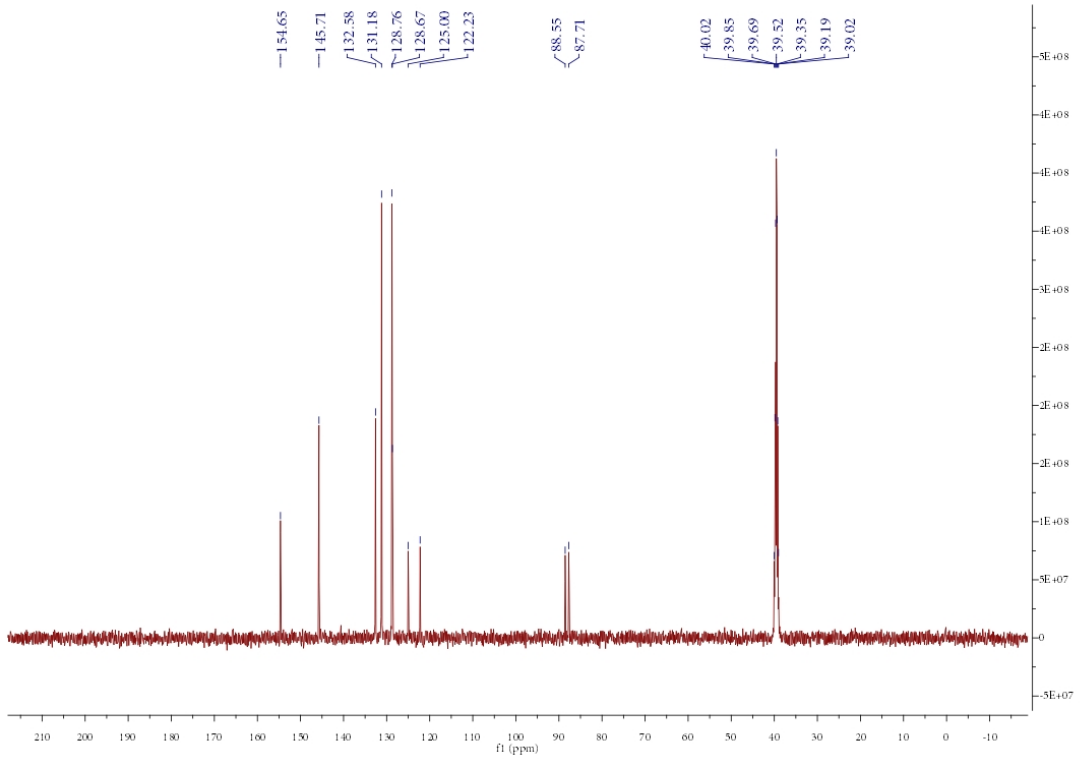
7.55
7.36
7.36
7.35
7.26
4.84
0.07
0.00
1.00
1.03
2.08
3.05
1.81
f1 (ppm)


154.65
145.71
132.58
131.18
128.76
128.67
125.00
122.23
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87.71
40.02
39.85
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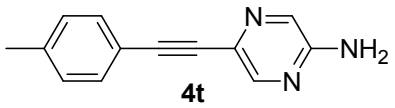
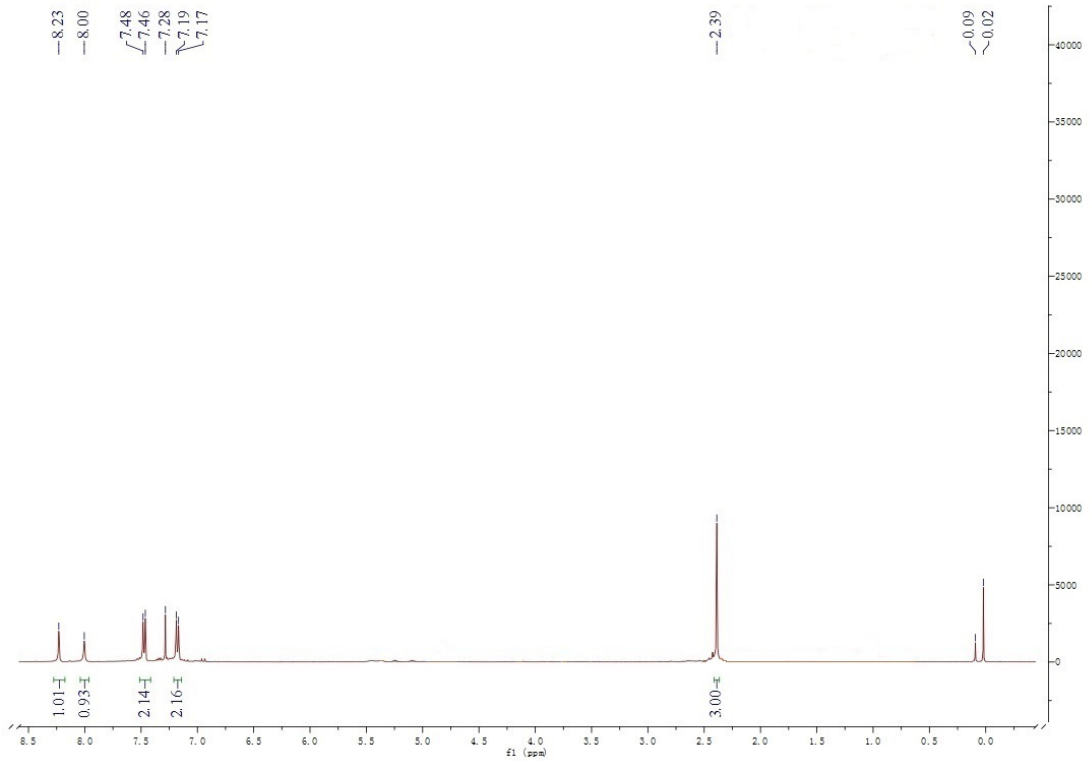
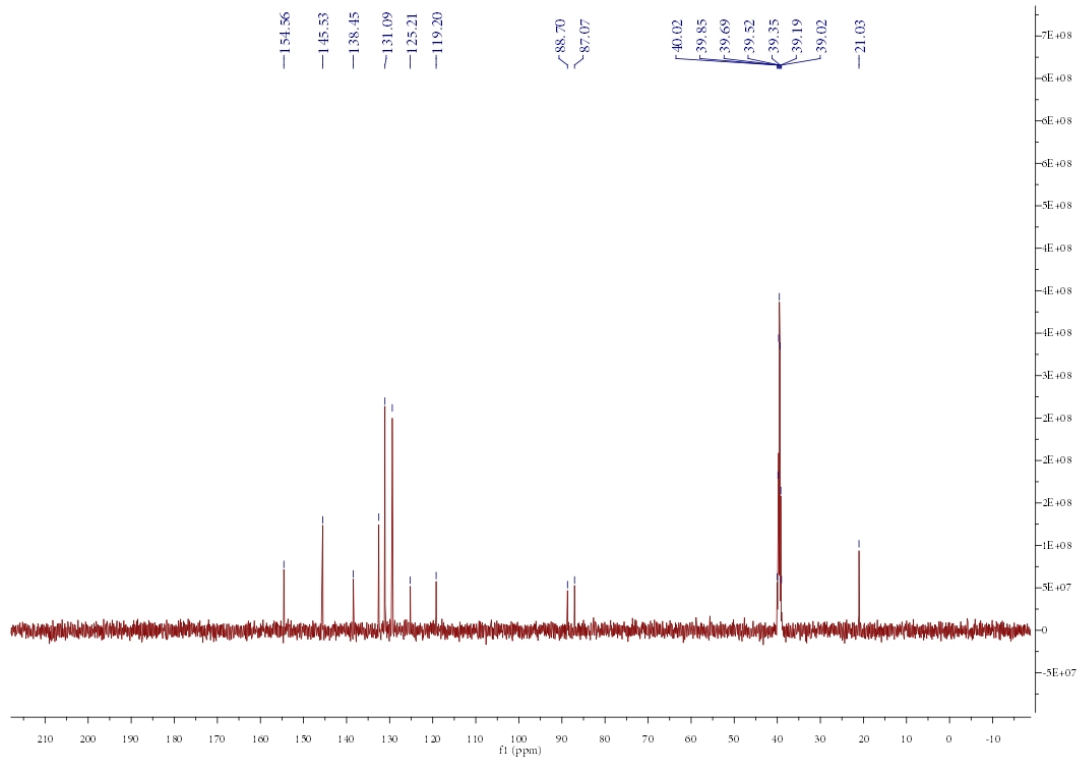
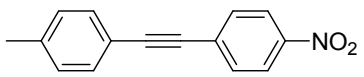
39.52
39.35
39.19
39.02
f1 (ppm)


N
NH2
N

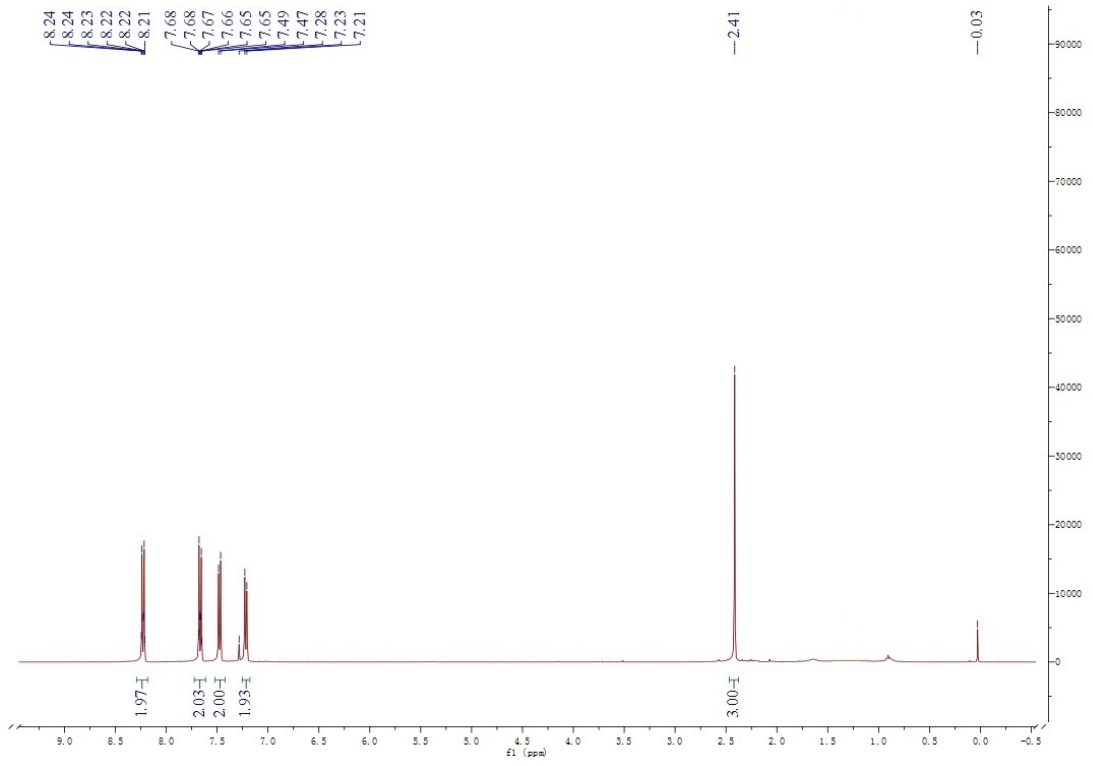
4t


8.23
8.00
7.48
7.46
7.28
7.19
7.17
2.39
0.09
0.02
1.01
0.93
2.14
2.16
3.00
f1 (ppm)


154.56
145.53
138.45
131.09
125.21
119.20
88.70
87.07
40.02
39.85
39.69
39.52
39.35
39.19
39.02
21.03
f1 (ppm)


NO2

4u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8.24
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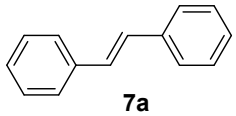
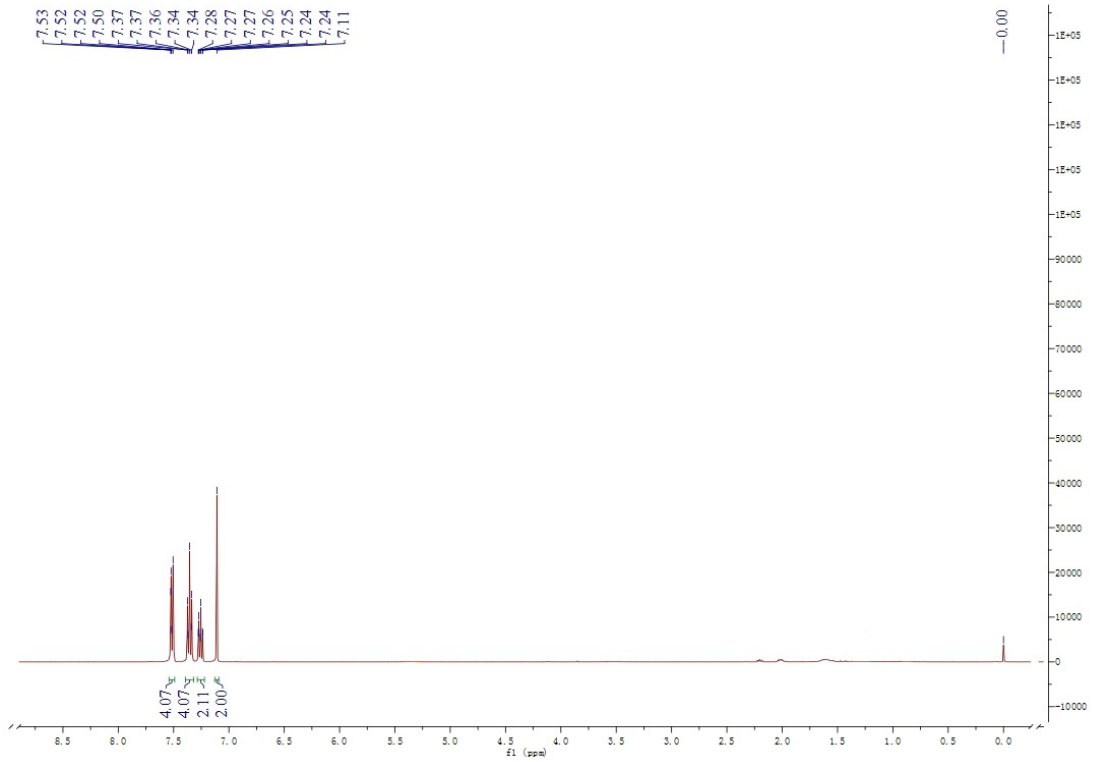
8.22
8.22
8.21
7.68
7.68
7.67
7.66
7.65
7.65
7.49
7.47
7.28
7.23
7.21
2.41
0.03
1.97
2.03
2.00
1.93
3.00
f1 (ppm)



7a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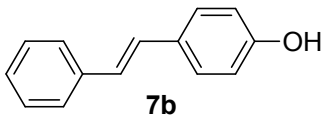
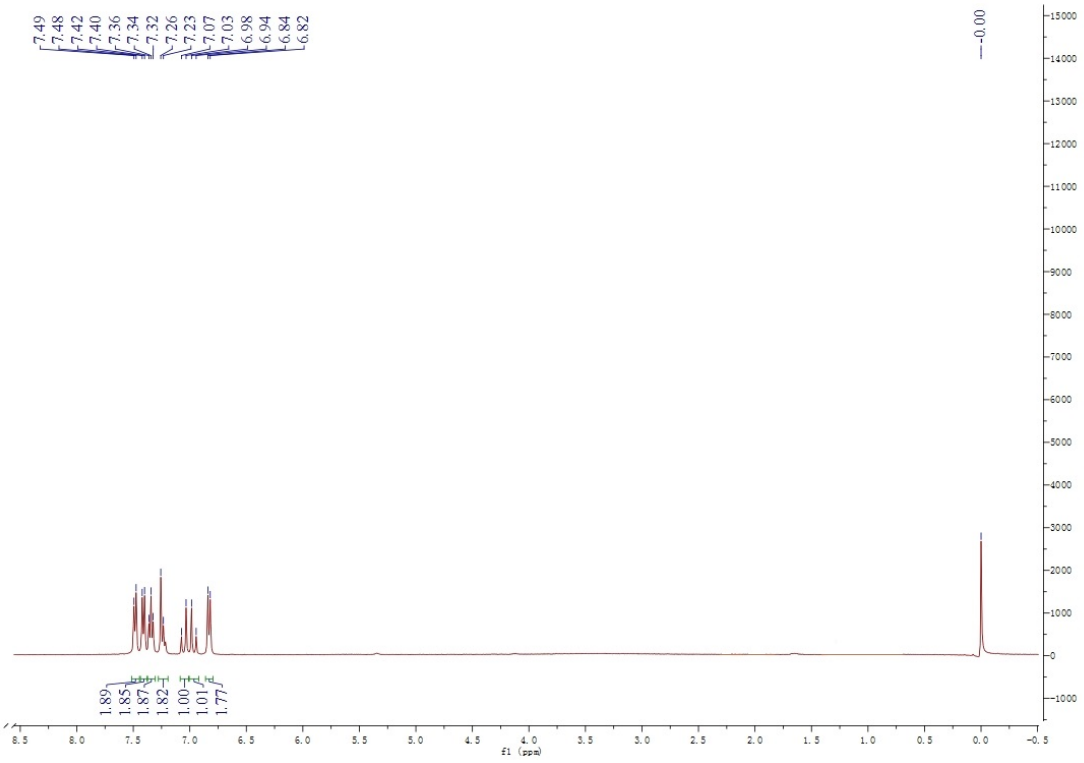
7.52
7.52
7.50
7.37
7.37
7.36
7.34
7.34
7.28
7.27
7.27
7.26
7.25
7.24
7.24
7.11
0.00
4.07
4.07
2.11
2.00
f1 (ppm)


OH

7b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7.48
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7.40
7.36
7.34
7.32
7.26
7.23
7.07
7.03
6.98
6.94
6.84
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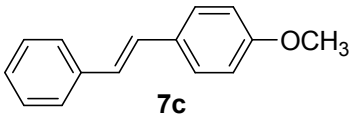
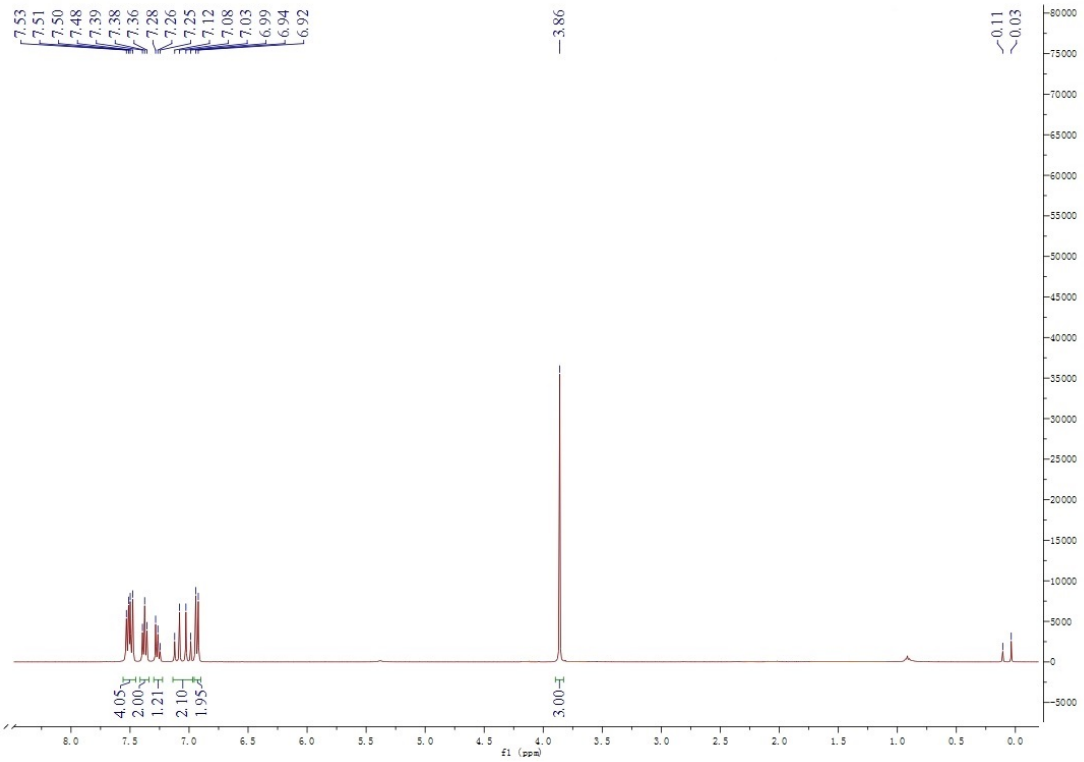
0.00
1.89
1.85
1.87
1.82
1.00
1.01
1.77
f1 (ppm)


OCH3

7c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7.39
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7.36
7.28
7.26
7.25
7.12
7.08
7.03
6.99
6.94
6.92
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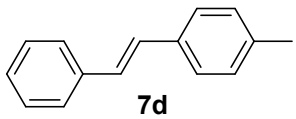
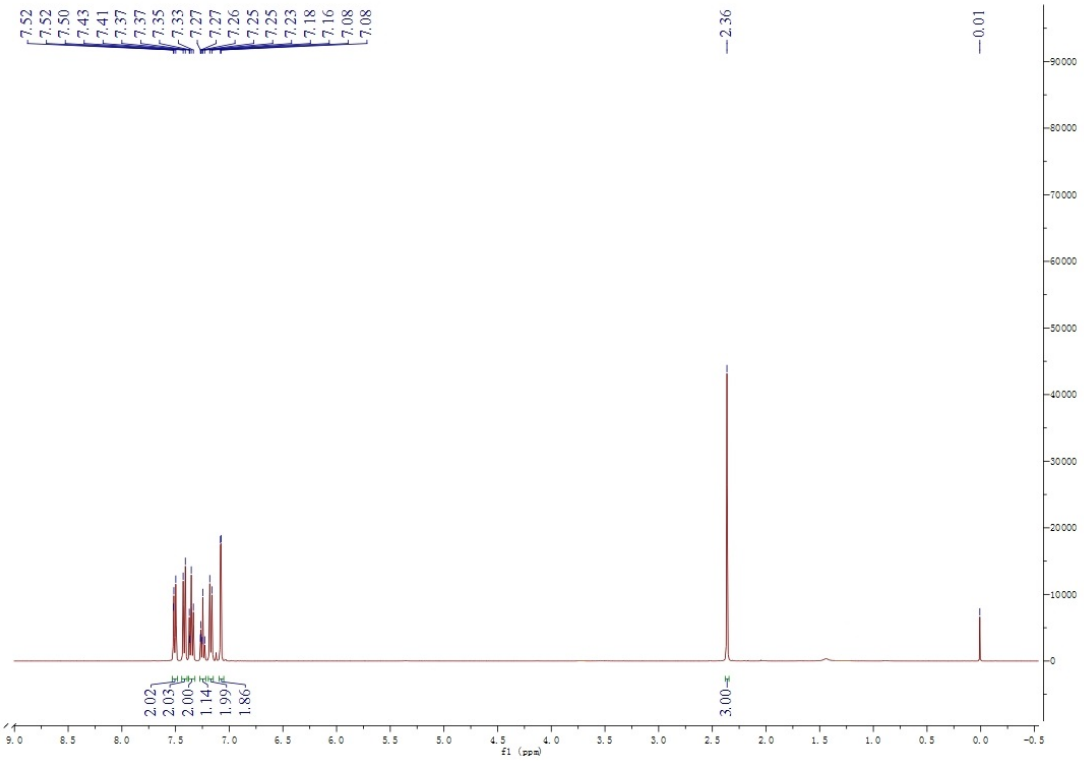
0.11
0.03
4.05
2.00
1.21
2.10
1.95
3.00
f1 (ppm)



7d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7.52
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7.37
7.37
7.35
7.33
7.27
7.27
7.26
7.25
7.25
7.23
7.18
7.16
7.08
7.08
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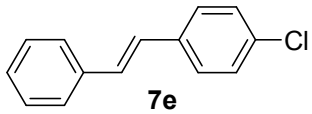
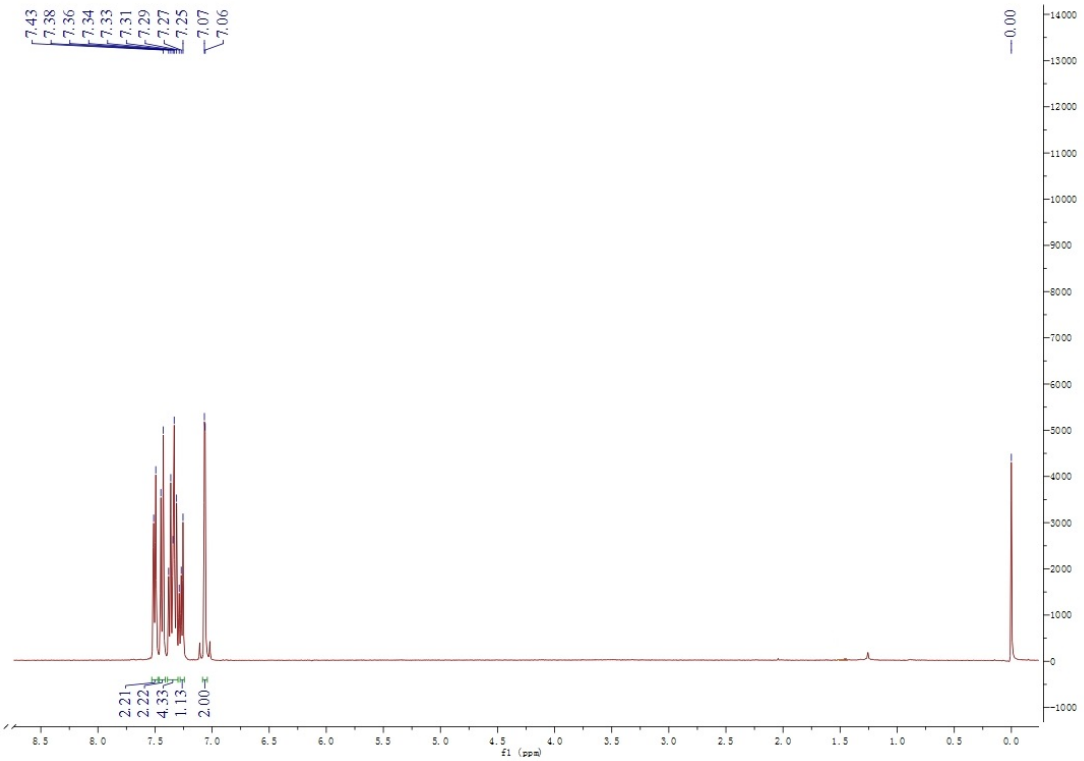
0.01
2.02
2.03
2.00
1.14
1.99
1.86
3.00
f1 (ppm)


Cl

7e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7.38
7.36
7.34
7.33
7.31
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7.27
7.25
7.07
7.06
0.00
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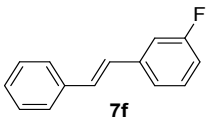
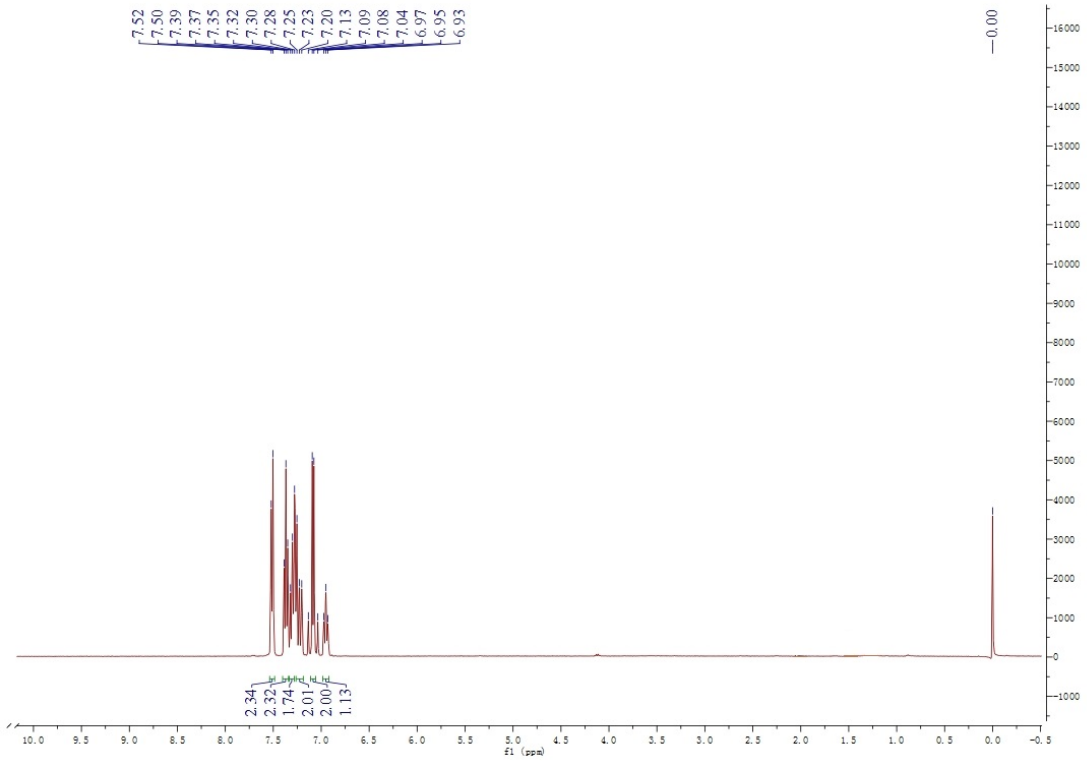
2.22
4.33
1.13
2.00
f1 (ppm)


F

7f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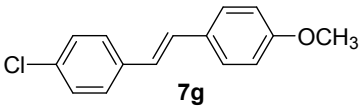
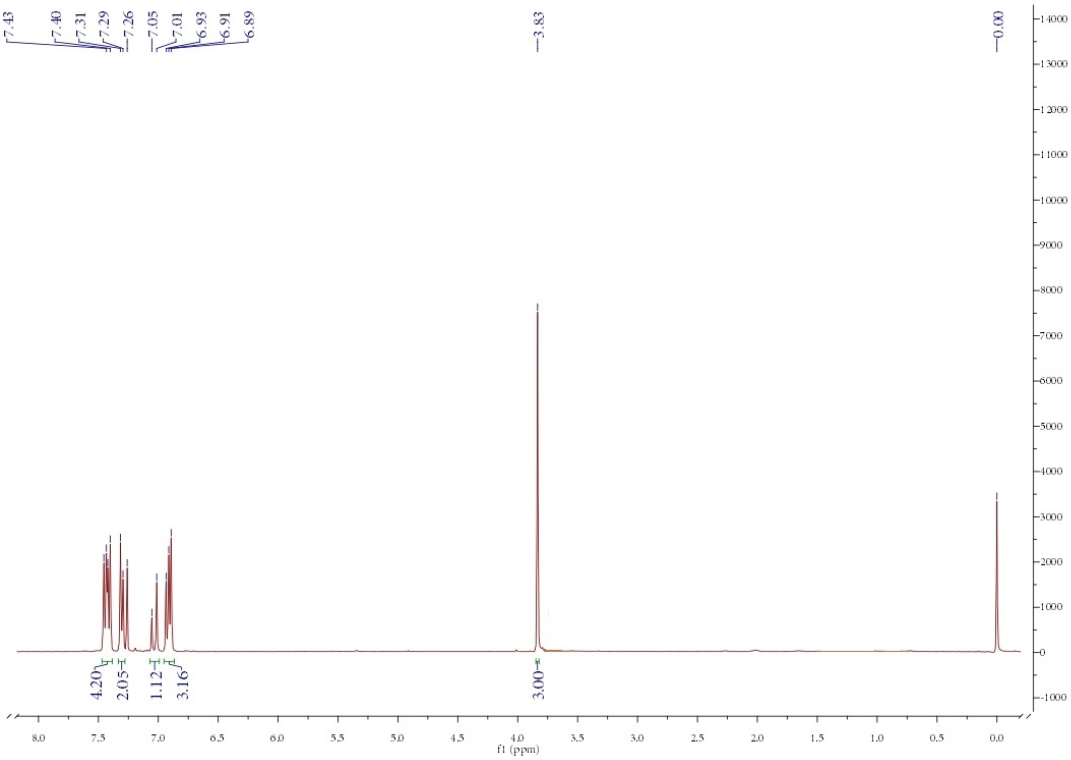
7.50
7.39
7.37
7.35
7.32
7.30
7.28
7.25
7.23
7.20
7.13
7.09
7.08
7.04
6.97
6.95
6.93
0.00
2.34
2.32
1.74
2.01
2.00
1.13
f1 (ppm)


Cl
OCH3

7g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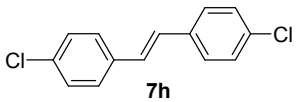
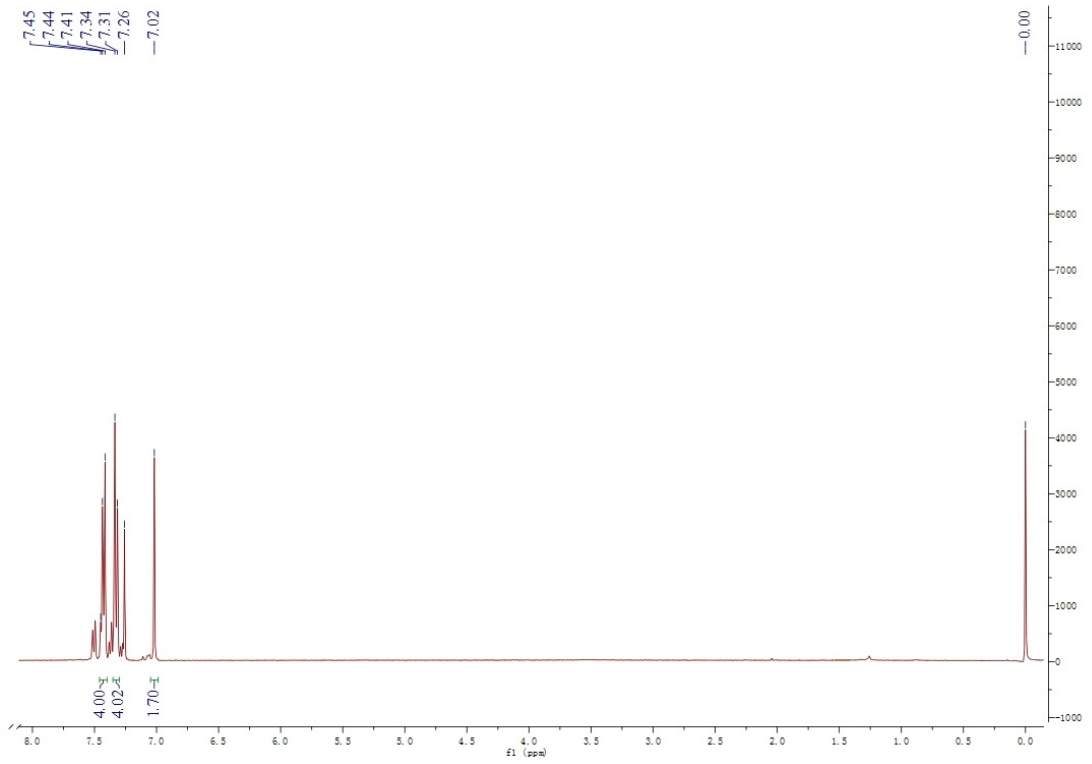
7.40
7.31
7.29
7.26
7.05
7.01
6.93
6.91
6.89
3.83
0.00
4.20
2.05
1.12
3.16
3.00
f1 (ppm)


Cl
Cl

7h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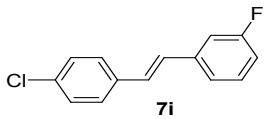
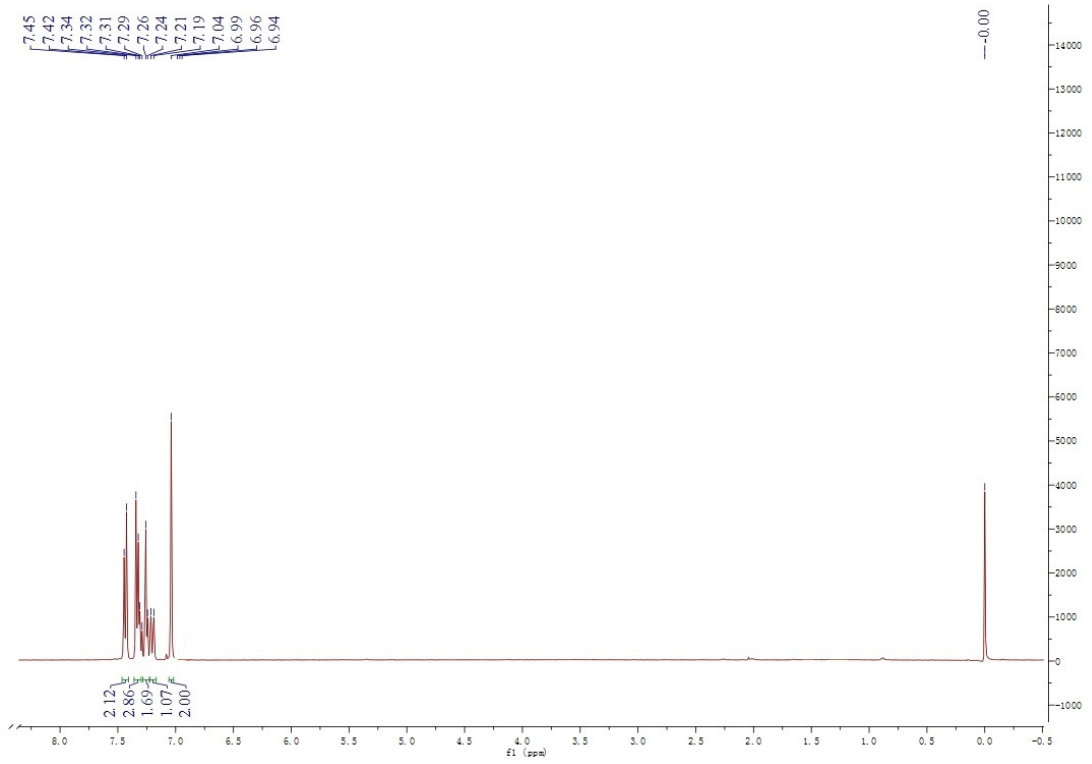
7.31
7.26
7.02
0.00
4.00
4.02
1.70
f1 (ppm)


F
Cl

7i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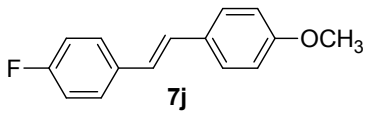
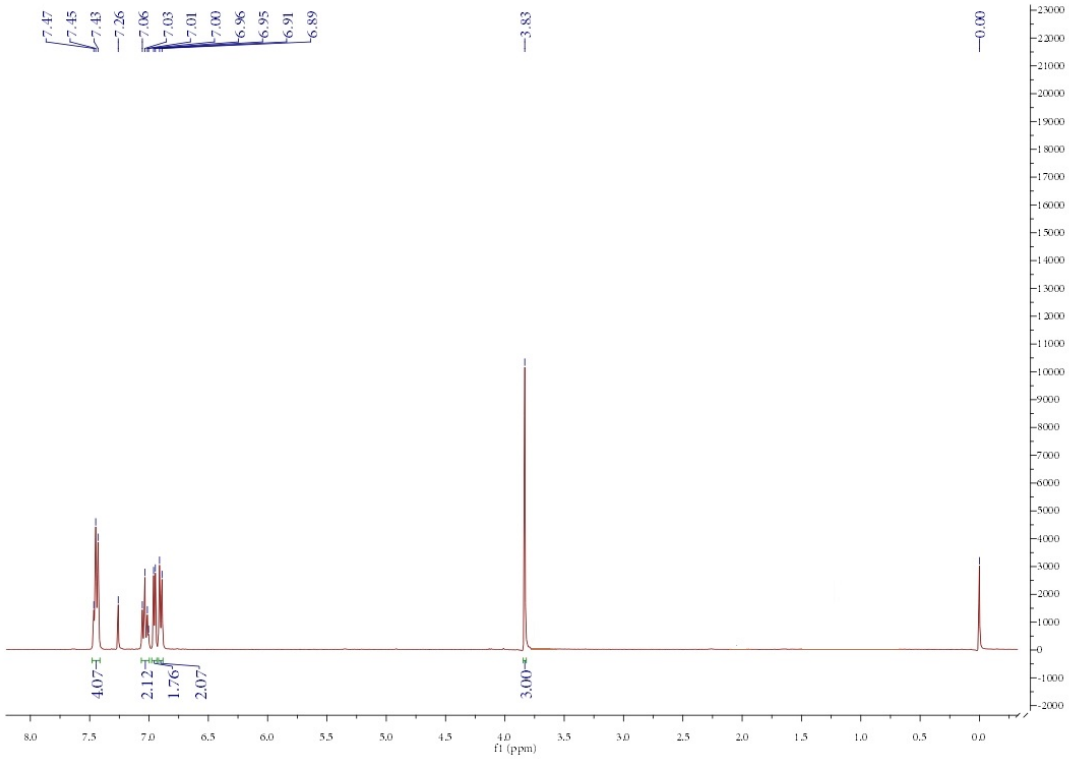
7.42
7.34
7.32
7.31
7.29
7.26
7.24
7.21
7.19
7.04
6.99
6.96
6.94
0.00
2.12
2.86
1.69
1.07
2.00
f1 (ppm)


F
OCH3

7j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7.45
7.43
7.26
7.06
7.03
7.01
7.00
6.96
6.95
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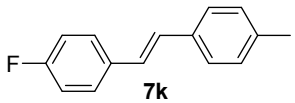
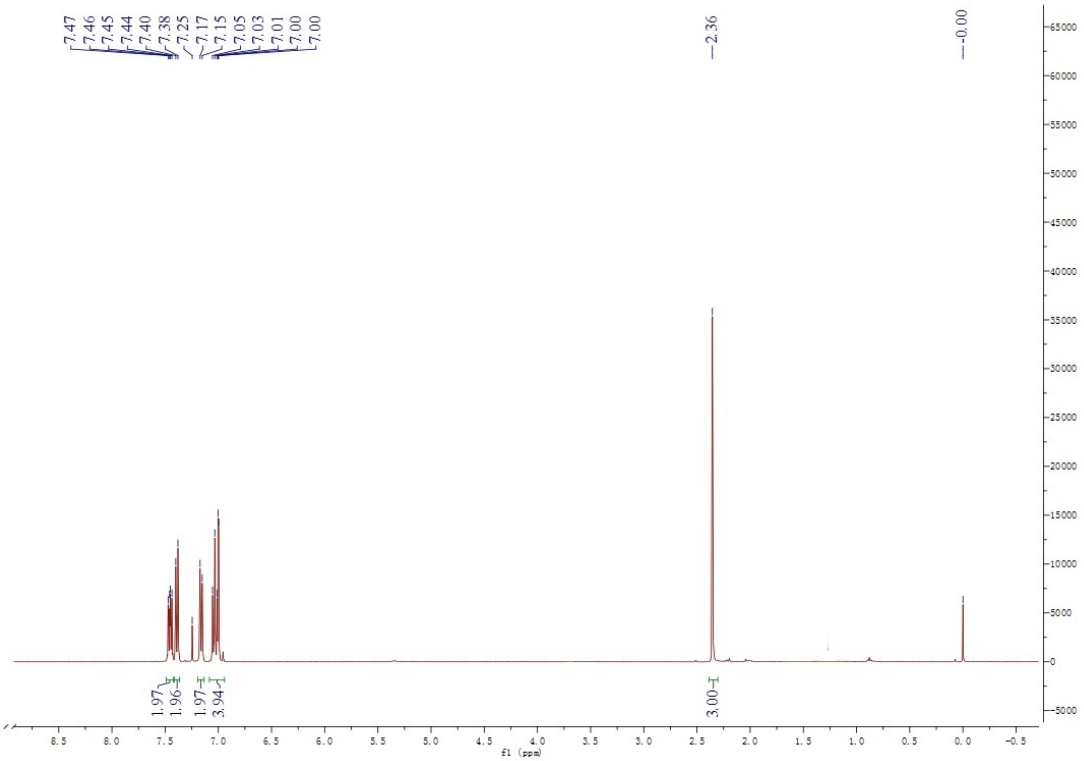
6.89
3.83
0.00
4.07
2.12
1.76
2.07
3.00
f1 (ppm)


F

7k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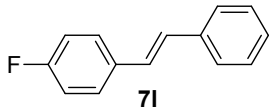
7.46
7.45
7.44
7.40
7.38
7.25
7.17
7.15
7.05
7.03
7.01
7.00
7.00
2.36
0.00
1.97
1.96
1.97
3.94
3.00
f1 (ppm)



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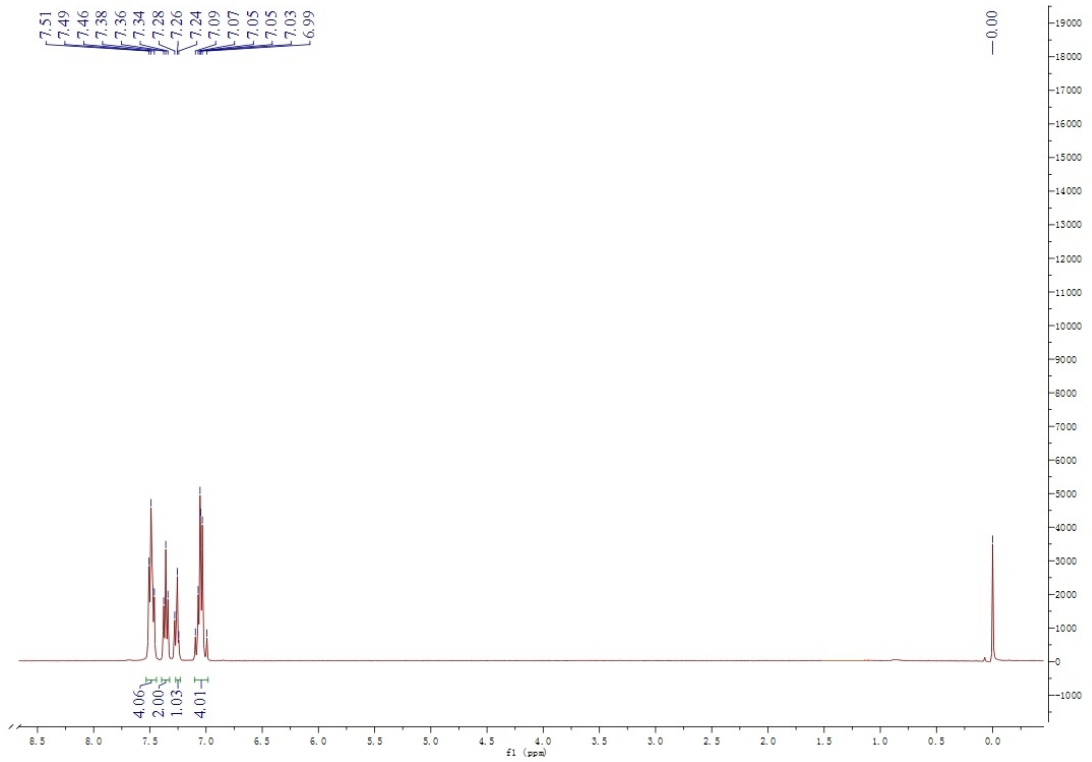
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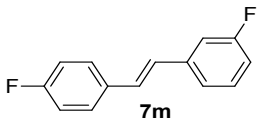
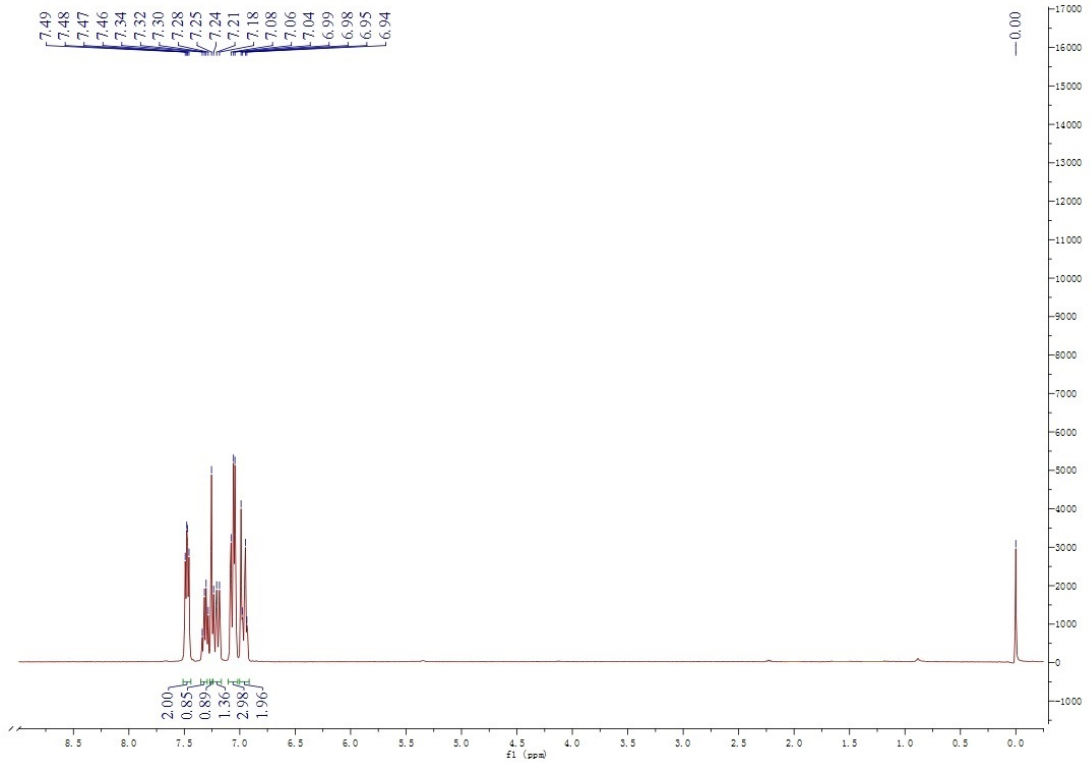
7.49
7.46
7.38
7.36
7.34
7.28
7.26
7.24
7.09
7.07
7.05
7.03
6.99
0.00
4.06
2.00
1.03
4.01
f1 (ppm)



7m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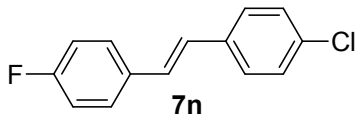
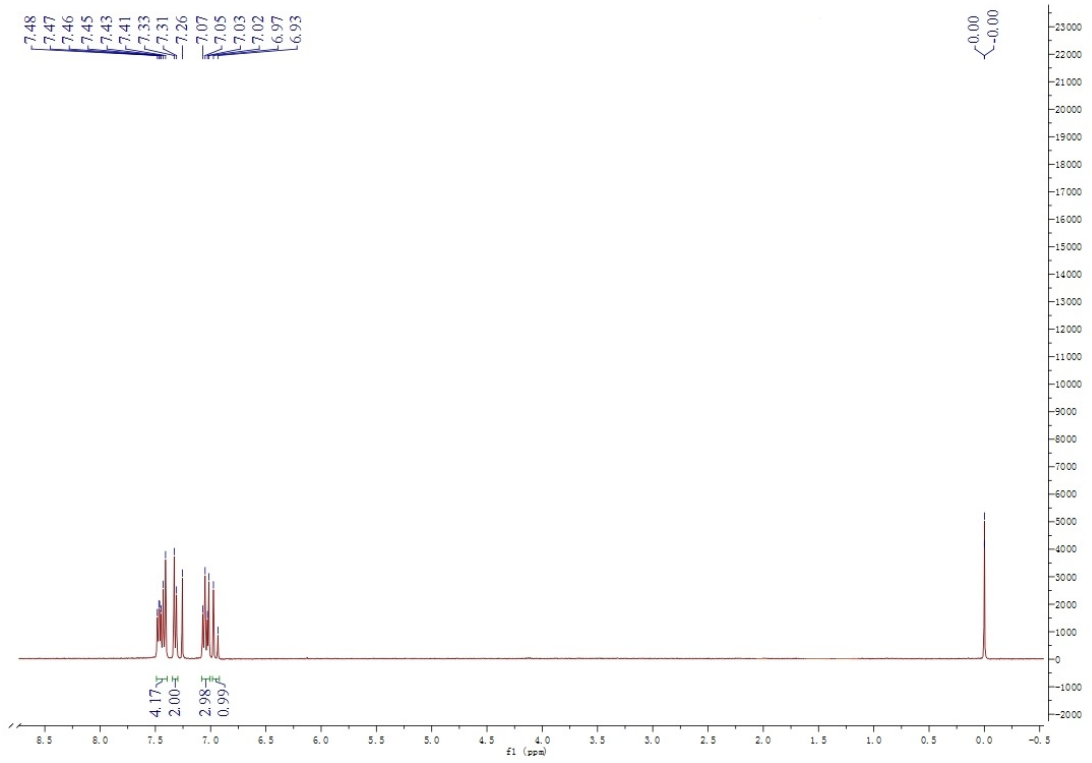
7.48
7.47
7.46
7.34
7.32
7.30
7.28
7.25
7.24
7.21
7.18
7.08
7.06
7.04
6.99
6.98
6.95
6.94
0.00
2.00
0.85
0.89
1.36
2.98
1.96
f1 (ppm)


F
Cl

7n


7.48
7.47
7.46
7.45
7.43
7.41
7.33
7.31
7.26
7.07
7.05
7.03
7.02
6.97
6.93
0.00
-0.00
4.17
2.00
2.98
0.99
f1 (ppm)