Supporting Information

Iron-Promoted Free Radical Cascade Difunctionalization of Unsaturated Benzamides with Silanes

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General Information

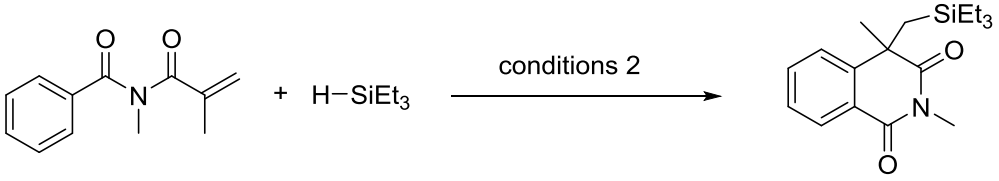
^{1}H and ^{13}C NMR spectra were recorded on a Bruker advance Ⅲ 400 or 500 spectrometer in $CDCl_3$ with TMS as internal standard. High-resolution mass spectral analysis (HRMS) data were measured on a Bruker Apex II. All products were identified by ^{1}H and ^{13}C NMR, HRMS. The starting materials were purchased from Energy, J&K Chemicals or Aldrich and used without further purification.

Typical procedure for the reaction

Reaction conditions 1: *N*-allylbenzamides (1 equiv., 0.2 mmol), silanes (10 equiv., 2 mmol), *tert*-butanol (2 mL), ferrous chloride (10 mmol %, 0.02 mmol), DTBP (3 equiv., 0.6 mmol), 120 ℃, 18 h. When the reaction was finished, the mixture was condensed under vacuum and purified by column chromatography to afford the final product.

Reaction conditions 2: *N*-methacryloyl-*N*-alkylbenzamides (1 equiv., 0.1 mmol), silanes (10 equiv., 1 mmol), benzotrifluoride (3 mL), ferrous chloride (10 mmol %, 0.01 mmol), TBPB (3 equiv., 0.3 mmol), 110 ℃, 24 h. When the reactions were finished, the final products were isolated via the same work-up procedure.

The modification of the cascade reaction conditions 2.



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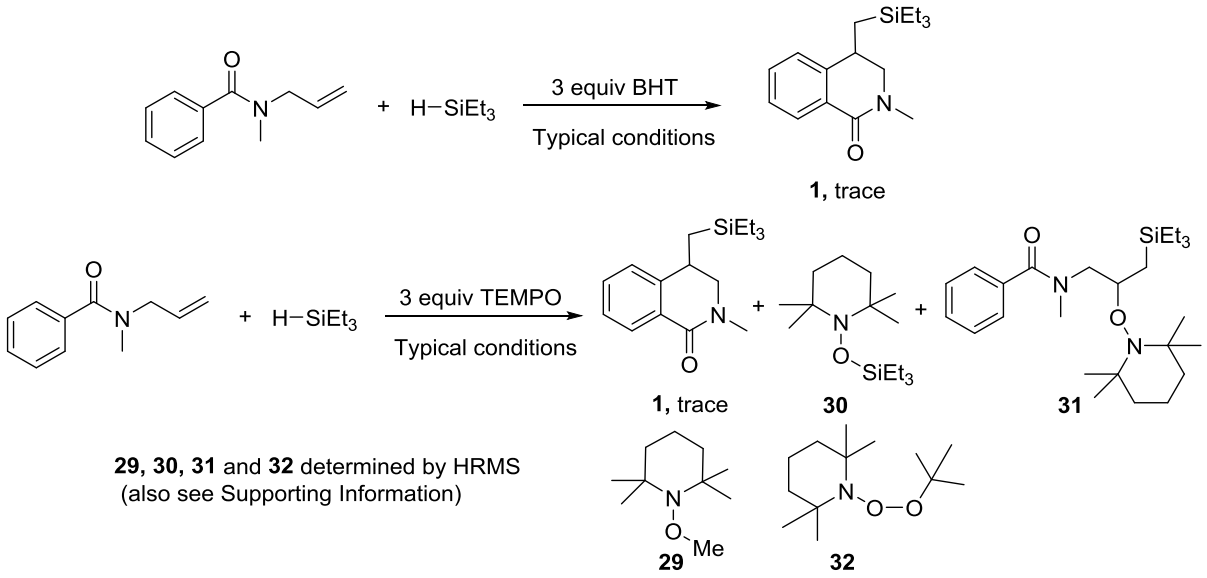
Entry	Silanes (equiv)	Catalyst (mol %)	Initiator (equiv)	Solvent (mL)	Yield (%)
1	5eq	$FeCl_2$(10)	DTBP(3eq)	t-BuOH	54
2	10eq	$FeCl_2$(10)	DTBP(3eq)	t-BuOH	72
3	10eq	$FeCl_2$(10)	TBPA(3eq)	t-BuOH	75
4	10eq	$FeCl_2$(10)	TBPB(3eq)	t-BuOH	77
5	10eq	$FeCl_2$(10)	TBHP(3eq)	t-BuOH	51
6	10eq	$FeCl_2$(10)	BPO(3eq)	t-BuOH	70
7	10eq	$FeCl_2$(10)	TBPB(3eq)	Benzotrifluoride	79

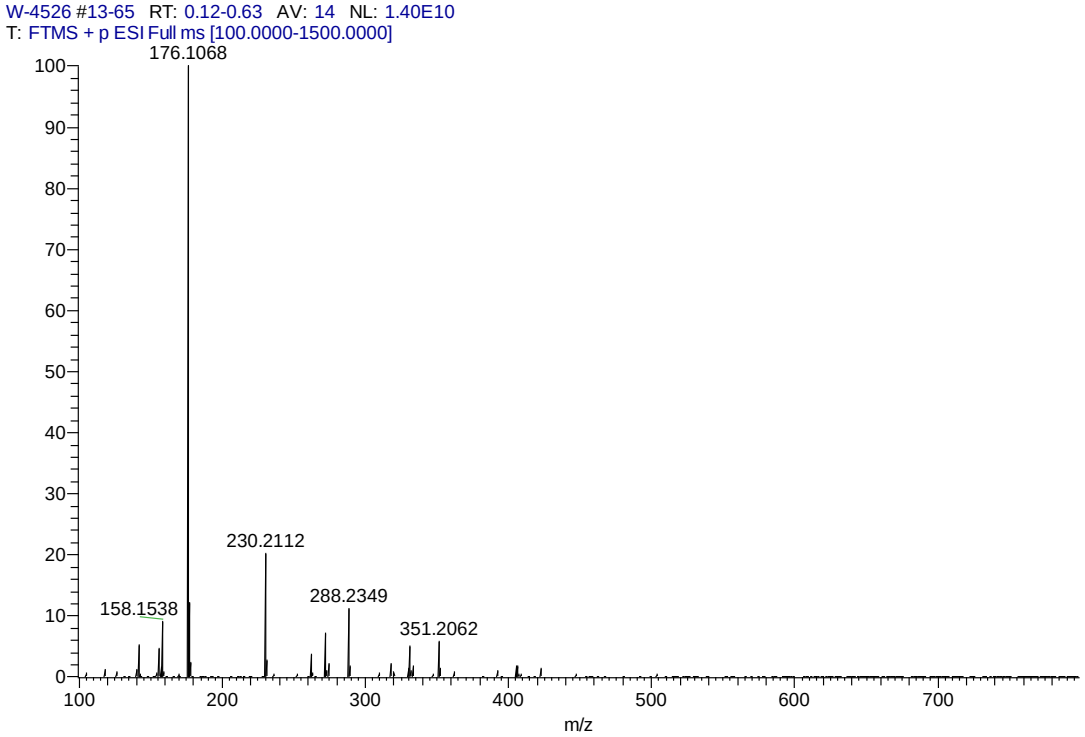
Reaction conditions 2: *N*-methacryloyl-*N*-alkylbenzamides (1 equiv., 0.1 mmol), silanes (10 equiv., 1 mmol), benzotrifluoride (3 mL), ferrous chloride (10 mmol %, 0.01 mmol), TBPB (3 equiv., 0.3 mmol), 110 ℃, 24 h, isolated yields.

Mechanistic study

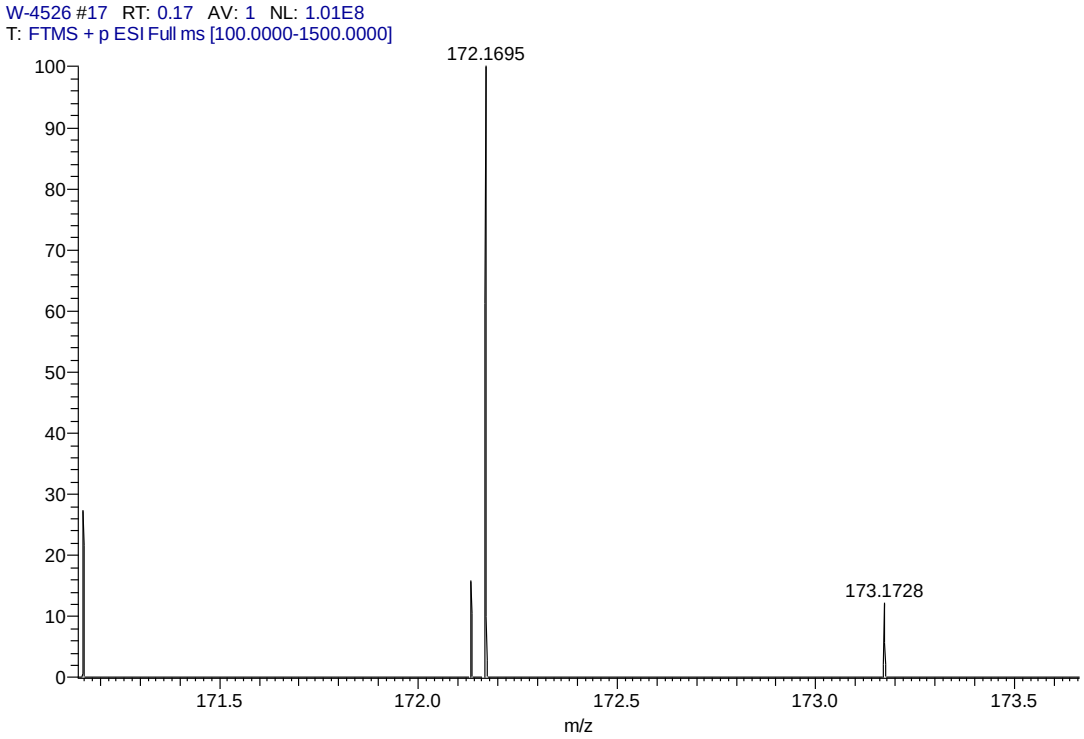


HRMS of reaction system

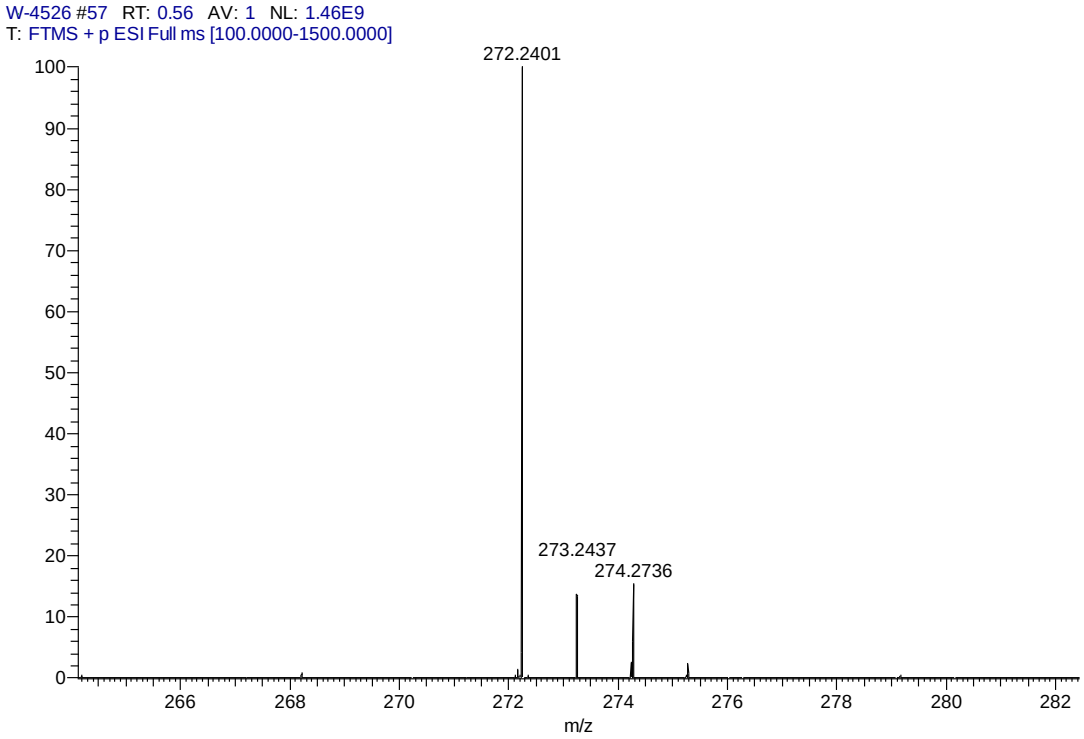
Sample No.	Formula (M)	Ion Formula	Measured m/z	Calc m/z	Diff (ppm)
29	$C_{10}H_{21}NO$	$[M+H]^+$	172.1695	172.1696	-0.58
30	$C_{15}H_{33}NOSi$	$[M+H]^+$	272.2401	272.2404	-1.10
31	$C_{26}H_{46}N_2O_2Si$	$[M+H]^+$	447.3397	447.3401	-0.89
32	$C_{13}H_{27}NO_2$	$[M+H]^+$	230.2112	230.2115	-1.30



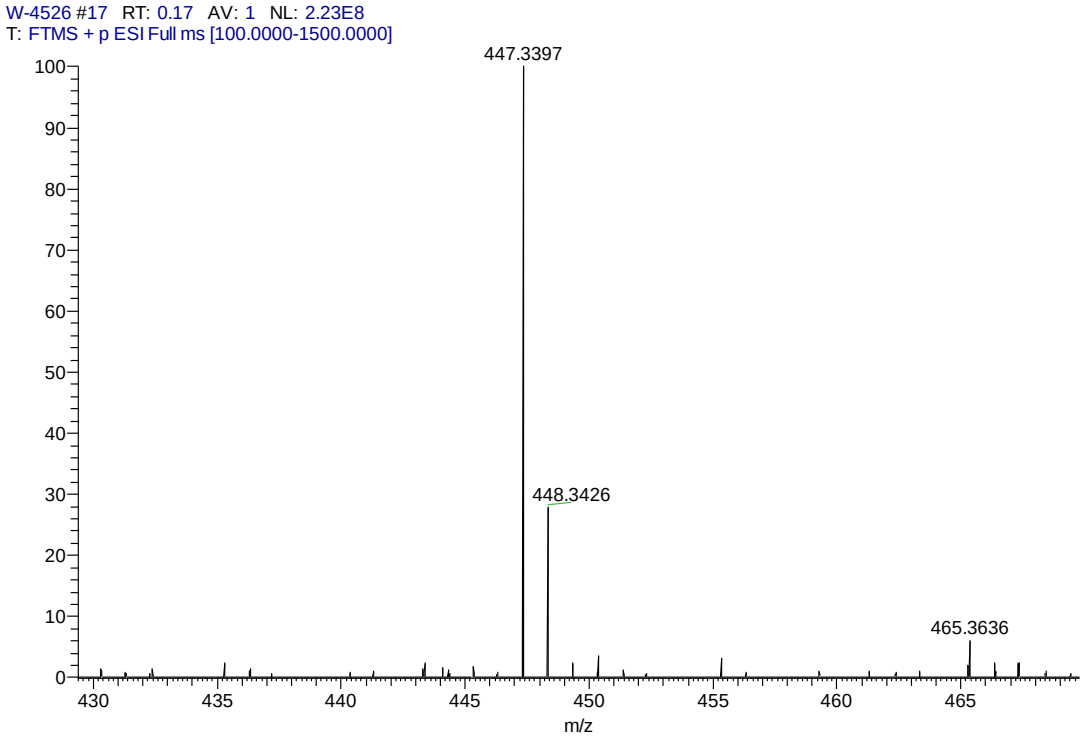
HRMS of product **29**



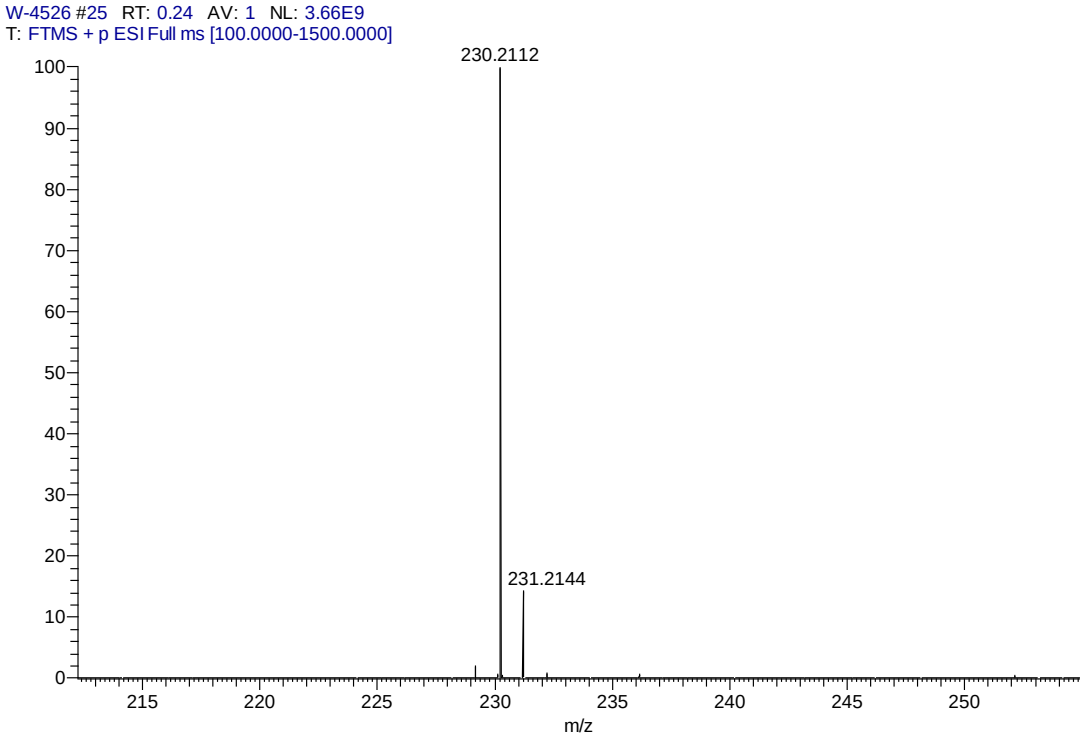
HRMS of product **30**



HRMS of product **31**



HRMS of product **32**



Physical data and references for the following products

References:

1 A. A. Toutov, W.-B. Liu, K. N. Betz, A. Fedorov, B. M. Stoltz and R. H. Grubbs, *Nature*, 2015, **518**, 80.

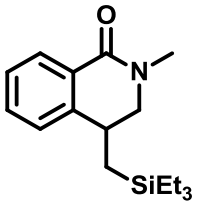
2 (*a*) L. Zhang, D. Liu and Z.-Q. Liu, *Org. Lett.*, 2015, **17**, 2534; (*b*) L. Zhang, Z. Hang and Z.-Q. Liu, *Angew. Chem., Int. Ed.*, 2016, **55**, 236.

3 W. Zhou, S. Ni, H. Mei, J. Han and Y. Pan, *Org. Lett.*, 2015, **17**, 2724.

Physical data for the following products:

1. 2-methyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



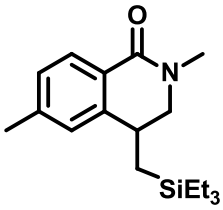
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.29 – 7.25 (m, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 3.74 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.20 (dd, *J* = 12.4, 3.6 Hz, 1H), 3.13 (s, 3H), 2.99 (td, *J* = 8.8, 4.4 Hz, 1H), 1.03 (dd, *J* = 15.2, 9.6 Hz, 1H), 0.90 (t, *J* = 8.0 Hz, 9H), 0.90 – 0.84 (m, 1H), 0.52 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.5, 144.8, 131.5, 128.1, 128.0, 126.6, 125.7, 54.6, 35.4, 33.9, 16.5, 7.3, 3.8.

HRMS (ESI, m/z): Calculated for $C_{17}H_{28}NOSi$ $(M+H)^+$ 290.1935, found 290.1931.

2. 2,6-dimethyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



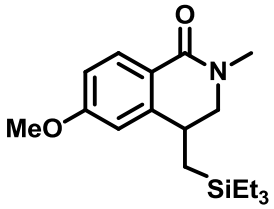
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.6 Hz, 1H), 7.11 (dd, *J* = 7.6, 0.8 Hz, 1H), 6.95 (s, 1H), 3.74 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.20 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.14 (s, 3H), 2.96 (td, *J* = 8.8, 4.0 Hz, 1H), 2.36 (s, 3H), 1.05 (dd, *J* = 15.2, 9.6 Hz, 1H), 0.93 (t, *J* = 8.0 Hz, 9H), 0.89 – 0.86 (m, 1H), 0.56 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.8, 144.9, 142.0, 128.3, 127.5, 126.3, 125.5, 54.7, 35.4, 34.0, 21.6, 16.6, 7.4, 3.9.

HRMS (ESI, m/z): Calculated for $C_{18}H_{30}NOSi$ $(M+H)^+$ 304.2091, found 304.2090.

3. 6-methoxy-2-methyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 15/1).



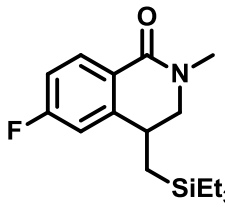
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, *J* = 8.8 Hz, 1H), 6.81 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.64 (d, *J* = 2.4 Hz, 1H), 3.83 (s, 3H), 3.73 (dd, *J* = 12.0, 4.4 Hz, 1H), 3.19 (dd, *J* = 12.0, 4.0 Hz, 1H), 3.13 (s, 3H), 2.96 (td, *J* = 8.8, 4.4 Hz, 1H), 1.05 (dd, *J* = 15.2, 10.0 Hz, 1H), 0.93 (t, *J* = 8.0, 9H), 0.87 (d, *J* = 4.4 Hz, 1H), 0.56 (q, *J* = 7.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 162.2, 147.0, 130.4, 121.1, 111.7, 111.2, 55.3, 54.6, 35.4, 34.3, 16.4, 7.4, 3.9.

HRMS (ESI, m/z): Calculated for $C_{18}H_{30}NO_2Si$ $(M+H)^+$ 320.2040, found 320.2045.

4. 6-fluoro-2-methyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 15/1).



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (dd, *J* = 8.8, 6.0 Hz, 1H), 6.96 (td, *J* = 8.4, 2.4 Hz, 1H), 6.84 (dd, *J* = 9.2, 2.4 Hz, 1H), 3.74 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.22 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.13 (s, 3H), 3.02 – 2.97 (m, 1H), 1.04 (dd, *J* = 15.2, 10.0 Hz, 1H), 0.93 (t, *J* = 8.0 Hz, 9H), 0.87 (dd, *J* = 19.2, 8.4 Hz, 1H), 0.56 (q, *J* = 7.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0, 163.6 (d, *J* = 37.1 Hz), 147.7 (d, *J* = 8.1 Hz), 131.1 (d, *J* = 9.2 Hz), 124.4 (d, *J* = 2.9 Hz), 113.8 (d, *J* = 21.6 Hz), 112.5 (d, *J* = 22.0 Hz), 54.4,

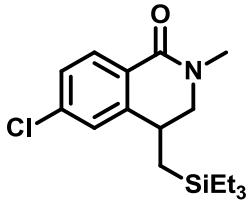
35.4, 34.1, 16.2, 7.3, 3.8.

^{19}F NMR (375 MHz, $CDCl_3$): δ -107.73(s, 1F).

HRMS (ESI, m/z): Calculated for $C_{17}H_{27}FNOSi$ $(M+H)^+$ 308.1840, found 308.1835.

5. 6-chloro-2-methyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 15/1).



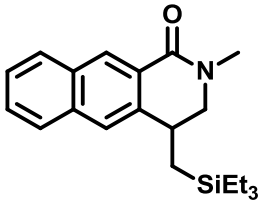
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.27 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.14 (d, *J* = 2.0 Hz, 1H), 3.74 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.22 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.14 (s, 3H), 3.00 (dt, *J* = 9.2, 4.4 Hz, 1H), 1.05 (dd, *J* = 15.2, 9.6 Hz, 1H), 0.93 (t, *J* = 8.0 Hz, 9H), 0.87 (dd, *J* = 18.0, 8.0 Hz, 1H), 0.57 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.8, 146.6, 137.6, 130.0, 127.0, 126.6, 125.8, 54.4, 35.5 34.0, 16.4, 7.3, 3.9.

HRMS (ESI, m/z): Calculated for $C_{17}H_{26}ClNOSiNa$ $(M+Na)^+$ 346.1364, found 346.1365.

6. 2-methyl-4-((triethylsilyl)methyl)-3,4-dihydrobenzo[g]isoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



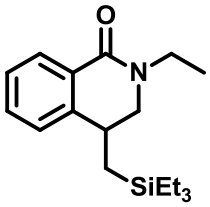
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.99 – 7.96 (m, 1H), 7.89 – 7.87 (m, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.59 – 7.54 (m, 2H), 3.96 – 3.92 (m, 1H), 3.72 – 3.67 (m, 1H), 3.39 (dd, *J* = 12.8, 1.6 Hz, 1H), 3.22 (s, 3H), 1.34 (dd, *J* = 15.2, 12.0 Hz, 1H), 1.01 (t, *J* = 8.0 Hz, 10H), 0.70 – 0.64 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 143.1, 135.4, 129.0, 128.8, 127.2, 126.8, 126.6, 124.8, 124.5, 123.6, 53.1, 35.5, 30.0, 15.9, 7.4, 4.0.

HRMS (ESI, m/z): Calculated for $C_{21}H_{29}NOSiNa$ $(M+Na)^+$ 362.1911, found 362.1919.

7. 2-ethyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



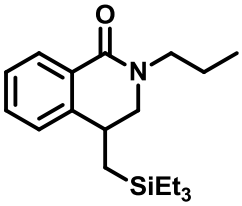
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.40 (td, *J* = 7.2, 1.2 Hz, 1H), 7.30 (td, *J* = 7.6, 1.2 Hz, 1H), 7.17 (d, *J* = 7.2 Hz, 1H), 3.77 – 3.67 (m, 2H), 3.56 – 3.47 (m, 1H), 3.20 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.05 – 2.99 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H), 1.04 – 0.95 (m, 2H), 0.91 (t, *J* = 8.0 Hz, 9H), 0.55 (q, *J* = 7.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.8, 144.5, 131.5, 128.5, 128.3, 126.7, 125.7, 52.4, 42.3, 33.8, 16.3, 12.5, 7.3, 3.8.

HRMS (ESI, m/z): Calculated for $C_{18}H_{30}NOSi$ $(M+H)^+$ 304.2091, found 304.2083.

8. 2-propyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.40 (td, *J* = 7.6, 1.6 Hz, 1H), 7.31 (td, *J* = 7.6, 1.6 Hz, 1H), 7.19 – 7.16 (m, 1H), 3.73 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.70 – 3.63 (m, 1H), 3.42 – 3.35 (m, 1H), 3.21 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.06 – 3.00 (m, 1H), 1.70 – 1.60 (m, 2H), 0.98 (dd, *J* = 8.0, 4.4 Hz, 5H), 0.91 (t, *J* = 8.0 Hz, 9H), 0.55 (q, *J* = 8.0 Hz, 6H).

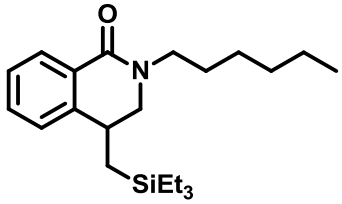
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 144.5, 131.5, 128.5, 128.3, 126.8, 125.7, 53.0, 49.3, 33.8, 20.7, 16.2, 11.4, 7.4, 3.8.

HRMS (ESI, m/z): Calculated for $C_{19}H_{33}NOSi$ $(M+2H)^+$ 319.2280, found 319.2278.

9. 2-hexyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate =

20/1).



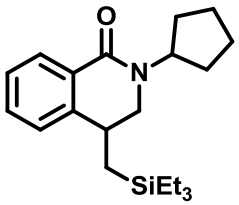
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 – 8.04 (m, 1H), 7.40 (td, *J* = 7.6, 1.6 Hz, 1H), 7.30 (td, *J* = 7.6, 1.2 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 3.73 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.69 – 3.64 (m, 1H), 3.46 – 3.39 (m, 1H), 3.21 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.05 – 3.00 (m, 1H), 1.64 – 1.58 (m, 2H), 1.38 – 1.28 (m, 7H), 0.97 (dd, *J* = 8.0, 4.8 Hz, 2H), 0.91 (t, *J* = 8.4 Hz, 9H), 0.87 (d, *J* = 7.2 Hz, 2H), 0.55 (q, *J* = 7.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.0, 144.5, 131.5, 128.5, 128.3, 126.8, 125.6, 53.0, 47.7, 33.8, 31.6, 27.5, 26.7, 22.5, 16.1, 14.0, 7.4, 3.9.

HRMS (ESI, m/z): Calculated for $C_{22}H_{37}NOSiK$ $(M+K)^+$ 398.2276, found 398.2279.

10. 2-cyclopentyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



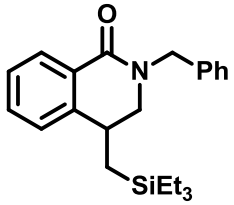
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.40 (td, *J* = 7.6, 1.6 Hz, 1H), 7.31 (td, *J* = 7.6, 1.2 Hz, 1H), 7.20 – 7.18 (m, 1H), 5.21 (p, *J* = 8.8 Hz, 1H), 3.54 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.14 (dd, *J* = 12.0, 5.2 Hz, 1H), 3.06 – 3.00 (m, 1H), 1.96 – 1.85 (m, 2H), 1.76 – 1.62 (m, 4H), 1.57 – 1.48 (m, 2H), 1.03 (dd, *J* = 14.8, 6.0 Hz, 1H), 0.90 (t, *J* = 8.4 Hz, 9H), 0.91 – 0.85 (m, 1H), 0.54 (q, *J* = 7.6 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1, 143.9, 131.4, 129.0, 128.5, 126.8, 125.5, 53.7, 47.4, 33.6, 28.4, 24.3, 15.3, 7.4, 3.9.

HRMS (ESI, m/z): Calculated for $C_{21}H_{33}NOSiNa$ $(M+Na)^+$ 366.2224, found 366.2224.

11. 2-benzyl-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



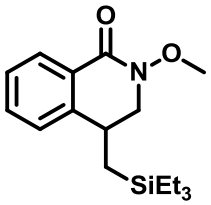
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.43 (td, *J* = 7.2, 1.2 Hz, 1H), 7.36 – 7.32 (m, 5H), 7.31 – 7.27 (m, 1H), 7.17 (dd, *J* = 7.6, 0.4 Hz, 1H), 4.78 (dd, *J* = 36.8, 14.4 Hz, 2H), 3.61 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.14 (dd, *J* = 12.4, 4.8 Hz, 1H), 2.98 – 2.92 (m, 1H), 0.83 (t, *J* = 8.0 Hz, 10H), 0.79 – 0.75 (m, 1H), 0.42 (dd, *J* = 7.6, 1.2 Hz, 3H), 0.38 (dd, *J* = 8.0, 2.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.3, 144.7, 137.1, 131.8, 128.6, 128.5, 128.3, 127.5, 126.8, 125.7, 51.8, 50.5, 33.6, 29.7, 16.1, 7.3, 3.7.

HRMS (ESI, m/z): Calculated for $C_{23}H_{32}NOSi$ $(M+H)^+$ 366.2248, found 366.2241.

12. 2-methoxy-4-((triethylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



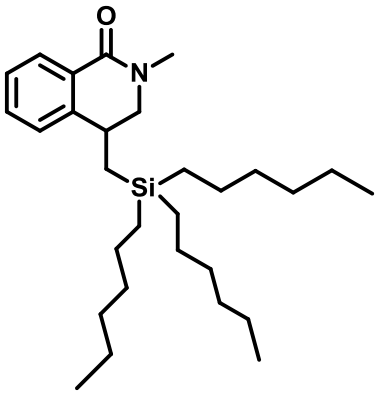
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 7.6 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.33 (td, *J* = 7.6, 1.2 Hz, 1H), 7.19 (dd, *J* = 7.6, 0.4 Hz, 1H), 4.01 (dd, *J* = 11.2, 4.4 Hz, 1H), 3.90 (d, *J* = 1.2 Hz, 3H), 3.53 (dd, *J* = 11.2, 4.0 Hz, 1H), 3.23 – 3.17 (m, 1H), 1.17 (dd, *J* = 15.2, 9.6 Hz, 1H), 0.99 (d, *J* = 5.2 Hz, 1H), 0.94 (t, *J* = 8.0 Hz, 9H), 0.59 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 162.8, 144.1, 132.3, 128.4, 127.5, 127.0, 126.1, 61.5, 54.5, 35.2, 16.9, 7.4, 3.8.

HRMS (ESI, m/z): Calculated for $C_{17}H_{28}NO_2Si$ $(M+H)^+$ 306.1884, found 306.1880.

13. 2-methyl-4-((trihexylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



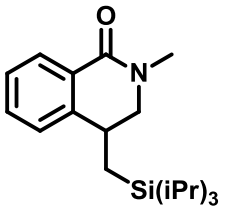
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.32 – 7.27 (m, 1H), 7.15 (dd, *J* = 7.6, 0.8 Hz, 1H), 3.76 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.21 (dd, *J* = 12.4, 3.6 Hz, 1H), 3.15 (s, 3H), 3.00 (td, *J* = 9.2, 4.4 Hz, 1H), 1.29 – 1.22 (m, 30H), 1.03 (dd, *J* = 15.2, 9.2 Hz, 1H), 0.92 – 0.88 (m, 7H), 0.52 (t, *J* = 8.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 144.8, 131.6, 128.2, 128.1, 126.7, 125.8, 54.8, 35.5, 34.1, 33.5, 31.5, 23.8, 22.6, 17.6, 14.1, 13.0.

HRMS (ESI, m/z): Calculated for $C_{29}H_{52}NOSi$ $(M+H)^+$ 458.3813, found 458.3819.

14. 2-methyl-4-((triisopropylsilyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.42 (td, *J* = 7.6, 1.6 Hz, 1H), 7.31 (td, *J* = 7.6, 1.6 Hz, 1H), 7.21 – 7.19 (m, 1H), 3.78 (dd, *J* = 12.0, 4.0 Hz, 1H), 3.29 (dd, *J* = 12.4, 3.6 Hz, 1H), 3.16 (s, 3H), 3.15 – 3.12 (m, 1H), 1.19 (dd, *J* = 15.2, 10.0 Hz, 1H), 1.10 – 1.07 (m, 10H), 1.06 – 1.03 (m, 10H), 0.98 – 0.96 (m, 1H), 0.92 – 0.87 (m, 1H).

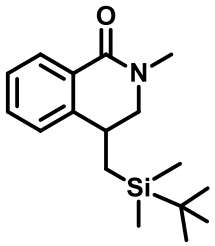
^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7, 145.3, 131.8, 128.2, 127.9, 126.8, 125.6, 54.5, 35.6, 33.9, 18.9, 14.5, 11.6.

HRMS (ESI, m/z): Calculated for $C_{20}H_{34}NOSi$ $(M+H)^+$ 332.2404, found 332.2395.

15. 4-((tert-butyldimethylsilyl)methyl)-2-methyl-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate =

20/1).



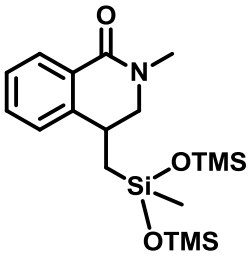
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.41 (td, *J* = 7.6, 1.6 Hz, 1H), 7.31 (td, *J* = 7.6, 1.2 Hz, 1H), 7.16 (dd, *J* = 7.6, 0.4 Hz, 1H), 3.76 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.24 (dd, *J* = 12.4, 4.0 Hz, 1H), 3.16 (s, 3H), 3.01 (dt, *J* = 9.2, 4.4 Hz, 1H), 1.03 (dd, *J* = 15.2, 9.6 Hz, 1H), 0.89 (dd, *J* = 15.2, 4.8 Hz, 1H), 0.86 (s, 9H), 0.06 (s, 3H), -0.03 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 144.9, 131.7, 128.3, 128.1, 126.8, 125.7, 54.4, 35.5, 34.2, 26.3, 17.2, 16.6, -4.8, -5.9.

HRMS (ESI, m/z): Calculated for $C_{17}H_{28}NOSi$ $(M+H)^+$ 290.1935, found 290.1941.

16. 4-((1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)methyl)-2-methyl-3,4-dihydroisoquinolin-1(2H)-one

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1).



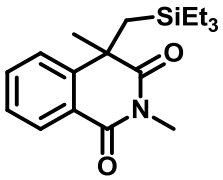
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.41 (td, *J* = 7.6, 1.6 Hz, 1H), 7.30 (td, *J* = 7.6, 1.6 Hz, 1H), 7.20 – 7.18 (m, 1H), 3.73 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.37 (dd, *J* = 12.4, 4.8 Hz, 1H), 3.16 (s, 3H), 3.12 – 3.06 (m, 1H), 0.96 (dd, *J* = 15.2, 10.0 Hz, 1H), 0.86 (dd, *J* = 15.2, 5.2 Hz, 1H), 0.11 (d, *J* = 2.4 Hz, 18H), 0.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 144.5, 131.6, 128.3, 128.2, 126.7, 125.7, 54.1, 35.4, 33.3, 22.0, 1.9, 0.7.

HRMS (ESI, m/z): Calculated for $C_{18}H_{33}NO_3Si_3Na$ $(M+Na)^+$ 418.1660, found 418.1655.

17. 2,4-dimethyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



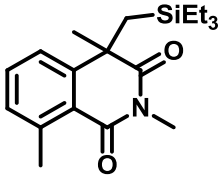
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.60 (td, *J* = 8.0, 1.2 Hz, 1H), 7.47 – 7.40 (m, 2H), 3.37 (s, 3H), 1.75 (d, *J* = 14.8 Hz, 1H), 1.66 (s, 3H), 1.35 (d, *J* = 14.8 Hz, 1H), 0.71 (t, *J* = 7.6 Hz, 9H), 0.19 – 0.03 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 177.0, 164.5, 145.2, 133.7, 128.8, 127.3, 125.9, 123.7, 45.1, 34.2, 27.3, 27.1, 7.0, 3.4.

HRMS (ESI, m/z): Calculated for $C_{18}H_{28}NO_2Si$ $(M+H)^+$ 318.1884, found 318.1888.

18. 2,4,8-trimethyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



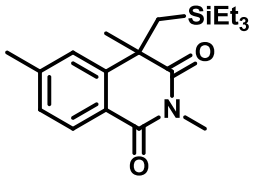
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 1H), 3.33 (s, 3H), 2.78 (s, 3H), 1.72 (d, *J* = 14.4 Hz, 1H), 1.66 (s, 3H), 1.33 (d, *J* = 14.4 Hz, 1H), 0.72 (t, *J* = 8.0 Hz, 9H), 0.22 – 0.03 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.8, 165.0, 146.7, 142.3, 132.5, 131.2, 124.2, 122.1, 45.2, 34.2, 27.7, 27.1, 24.0, 7.1, 3.5.

HRMS (ESI, m/z): Calculated for $C_{19}H_{30}NO_2Si$ $(M+H)^+$ 332.2040, found 332.2047.

19. 2,4,6-trimethyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



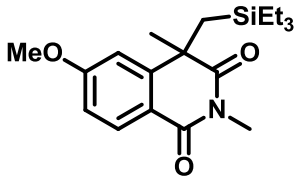
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.24 – 7.21 (m, 2H), 3.34 (s, 3H), 2.42 (s, 3H), 1.74 (d, *J* = 14.5 Hz, 1H), 1.64 (s, 3H), 1.34 (d, *J* = 14.5 Hz, 1H), 0.71 (t, *J* = 7.5 Hz, 9H), 0.19 – 0.11 (m, 3H), 0.04 – -0.03 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 177.2, 164.5, 145.2, 144.4, 128.8, 128.3, 126.4, 121.1, 45.0, 34.3, 27.0, 26.9, 21.8, 7.0, 3.4.

HRMS (ESI, m/z): Calculated for $C_{19}H_{30}NO_2Si$ $(M+H)^+$ 332.2040, found 332.2045.

20. 6-methoxy-2,4-dimethyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



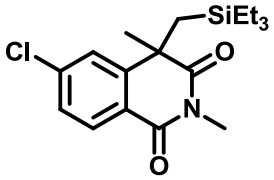
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.5 Hz, 1H), 6.93 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 3.88 (s, 3H), 3.34 (s, 3H), 1.74 (d, *J* = 14.5 Hz, 1H), 1.64 (s, 3H), 1.31 (d, *J* = 15.0 Hz, 1H), 0.73 (t, *J* = 8.0 Hz, 9H), 0.21 – 0.14 (m, 3H), 0.10 – 0.03 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 177.1, 164.1, 163.9, 147.5, 131.1, 116.8, 113.3, 110.9, 55.5, 45.4, 34.4, 27.1, 27.0, 7.1, 3.4.

HRMS (ESI, m/z): Calculated for $C_{19}H_{30}NO_3Si$ $(M+H)^+$ 348.1989, found348.1990.

21. 6-chloro-2,4-dimethyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



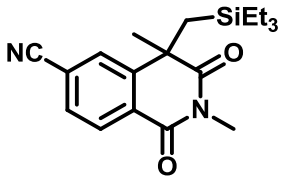
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (d, *J* = 8.5 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.39 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.35 (s, 3H), 1.75 (d, *J* = 15.0 Hz, 1H), 1.65 (s, 3H), 1.30 (d, *J* = 15.0 Hz, 1H), 0.73 (t, *J* = 8.0 Hz, 9H), 0.21 – 0.13 (m, 3H), 0.08 – 0.00 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 176.4, 163.6, 146.9, 140.3, 130.4, 127.8, 126.2, 122.1, 45.2, 34.1, 27.2, 27.1, 7.0, 3.4.

HRMS (ESI, m/z): Calculated for $C_{18}H_{27}ClNO_2Si$ $(M+H)^+$ 352.1494, found 352.1497.

22. 2,4-dimethyl-1,3-dioxo-4-((triethylsilyl)methyl)-1,2,3,4-tetrahydroisoquinoline-6-carbonitrile

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



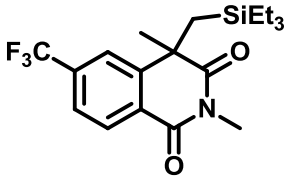
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.34 (d, *J* = 8.0 Hz, 1H), 7.78 (s, 1H), 7.70 (dd, *J* = 8.0, 1.0 Hz, 1H), 3.37 (s, 3H), 1.78 (d, *J* = 14.5 Hz, 1H), 1.68 (s, 3H), 1.30 (d, *J* = 15.0 Hz, 1H), 0.72 (t, *J* = 8.0 Hz, 9H), 0.19 – 0.11 (m, 3H), 0.07 – -0.01 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 175.7, 162.9, 146.3, 130.4, 130.2, 129.7, 127.0, 117.5, 117.2, 45.1, 33.8, 27.4, 7.0, 3.5.

HRMS (ESI, m/z): Calculated for $C_{19}H_{27}N_2O_2Si$ $(M+H)^+$ 343.1836, found 343.1840.

23. 2,4-dimethyl-4-((triethylsilyl)methyl)-6-(trifluoromethyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.72 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 3.38 (s, 3H), 1.80 (d, *J* = 15.0 Hz, 1H), 1.69 (s, 3H), 1.37 (d, *J* = 15.0 Hz, 1H), 0.71 (t, *J* = 7.9 Hz, 9H), 0.20 – 0.12 (m, 3H), 0.05 – 0.03 (m, 3H).

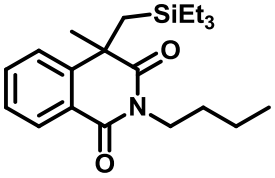
^{13}C NMR (125 MHz, $CDCl_3$): δ 176.2, 163.3, 146.0, 135.2 (d, *J* = 32.6 Hz), 129.7, 126.6, 124.0 (d, *J* = 3.5 Hz), 123.2 (d, *J* = 3.8 Hz), 122.3, 120.1, 45.4, 34.2, 27.3, 26.9, 6.9, 3.4.

^{19}F NMR (375 MHz, $CDCl_3$): δ -63.21(s, 3F).

HRMS (ESI, m/z): Calculated for $C_{19}H_{27}F_3NO_2Si$ $(M+H)^+$ 386.1758, found 386.1761.

24. 2-butyl-4-methyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.59 (td, *J* = 8.0, 1.6 Hz, 1H), 7.46 – 7.39 (m, 2H), 4.00 – 3.95 (m, 2H), 1.77 (d, *J* = 14.8 Hz, 1H), 1.63 (s, 3H), 1.66 – 1.57

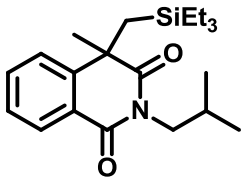
(m, 2H), 1.43 – 1.33 (m, 2H), 1.35 (d, *J* = 14.8 Hz, 1H), 0.95 (t, *J* = 7.3 Hz, 3H), 0.72 (t, *J* = 7.6 Hz, 9H), 0.23 – -0.02 (m, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 176.8, 164.1, 145.2, 133.5, 128.8, 127.2, 125.8, 123.9, 45.3, 40.4, 35.0, 30.0, 26.1, 20.3, 13.8, 7.1, 3.6.

HRMS (ESI, m/z): Calculated for $C_{21}H_{34}NO_2Si$ $(M+H)^+$ 360.2353, found 360.2360.

25. 2-isobutyl-4-methyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



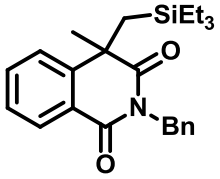
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 3.86 (d, *J* = 7.6 Hz, 2H), 2.12 (dt, *J* = 13.6, 6.8 Hz, 1H), 1.78 (d, *J* = 14.8 Hz, 1H), 1.65 (s, 3H), 1.35 (d, *J* = 14.8 Hz, 1H), 0.94 (d, *J* = 6.8 Hz, 3H), 0.90 (d, *J* = 6.8 Hz, 3H), 0.72 (t, *J* = 8.0 Hz, 9H), 0.23 – 0.14 (m, 3H), 0.11 – 0.02 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 177.2, 164.5, 145.2, 133.6, 129.0, 127.3, 125.8, 123.8, 47.1, 45.4, 35.3, 27.2, 25.8, 20.3, 20.1, 7.1, 3.6.

HRMS (ESI, m/z): Calculated for $C_{21}H_{34}NO_2Si$ $(M+H)^+$ 360.2353, found 360.2358.

26. 2-benzyl-4-methyl-4-((triethylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



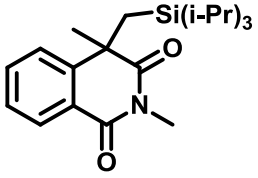
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.64 – 7.61 (m, 1H), 7.50 (d, *J* = 7.5 Hz, 2H), 7.45 (dd, *J* = 16.5, 8.5 Hz, 2H), 7.32 – 7.28 (m, 2H), 7.24 (d, *J* = 7.0 Hz, 1H), 5.28 (d, *J* = 13.5 Hz, 1H), 5.15 (d, *J* = 14.0 Hz, 1H), 1.79 (d, *J* = 14.5 Hz, 1H), 1.66 (s, 3H), 1.39 (d, *J* = 15.0 Hz, 1H), 0.70 (t, *J* = 8.0 Hz, 9H), 0.17 – 0.09 (m, 3H), 0.07 – -0.01 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 176.7, 164.2, 145.2, 137.0, 133.7, 129.1, 129.0, 128.3, 127.4, 127.3, 125.9, 123.8, 45.5, 43.7, 34.9, 26.2, 7.0, 3.6.

HRMS (ESI, m/z): Calculated for $C_{24}H_{32}NO_2Si$ $(M+H)^+$ 394.2197, found 394.2199.

27. 2,4-dimethyl-4-((triisopropylsilyl)methyl)isoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



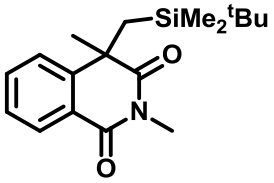
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 3.36 (s, 3H), 1.84 (d, *J* = 15.0 Hz, 1H), 1.67 (s, 3H), 1.45 – 1.43 (m, 1H), 0.86 (d, *J* = 7.5 Hz, 9H), 0.79 (d, *J* = 7.5 Hz, 9H), 0.74 – 0.67 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 177.0, 164.5, 145.5, 133.6, 128.8, 127.3, 126.0, 123.9, 45.3, 36.1, 27.1, 24.6, 18.6, 18.5, 11.4.

HRMS (ESI, m/z): Calculated for $C_{21}H_{34}NO_2Si$ $(M+H)^+$ 360.2353, found 360.2360.

28. 4-((tert-butyldimethylsilyl)methyl)-2,4-dimethylisoquinoline-1,3(2H,4H)-dione

A colorless liquid after purification by flash column chromatography (petroleum ether/ethyl acetate = 20/1)



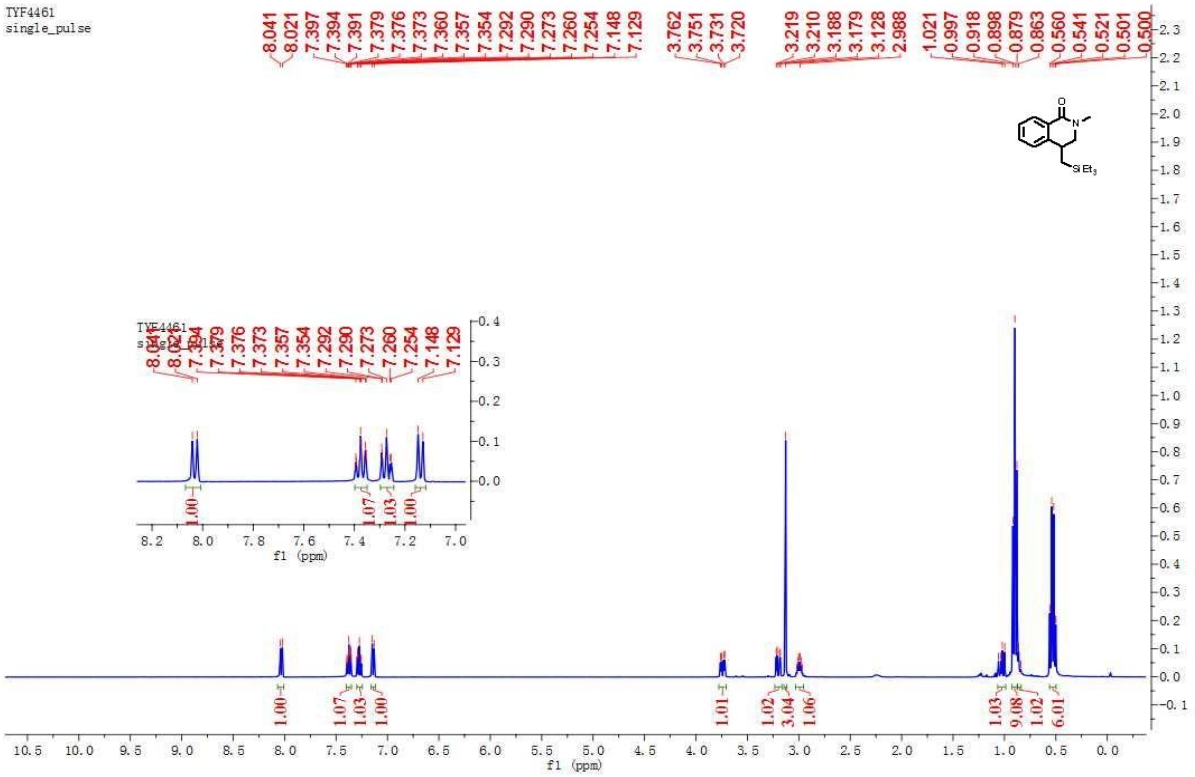
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.24 (d, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 7.0 Hz, 1H), 7.45 – 7.40 (m, 2H), 3.36 (s, 3H), 1.83 (d, *J* = 14.5 Hz, 1H), 1.66 (s, 3H), 1.34 (d, *J* = 14.5 Hz, 1H), 0.77 (s, 9H), -0.38 (s, 3H), -0.79 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ 177.0, 164.5, 144.9, 133.7, 128.8, 127.3, 126.2, 123.8, 45.2, 35.1, 27.1, 26.6, 26.1, 16.4, -5.7, -6.3.

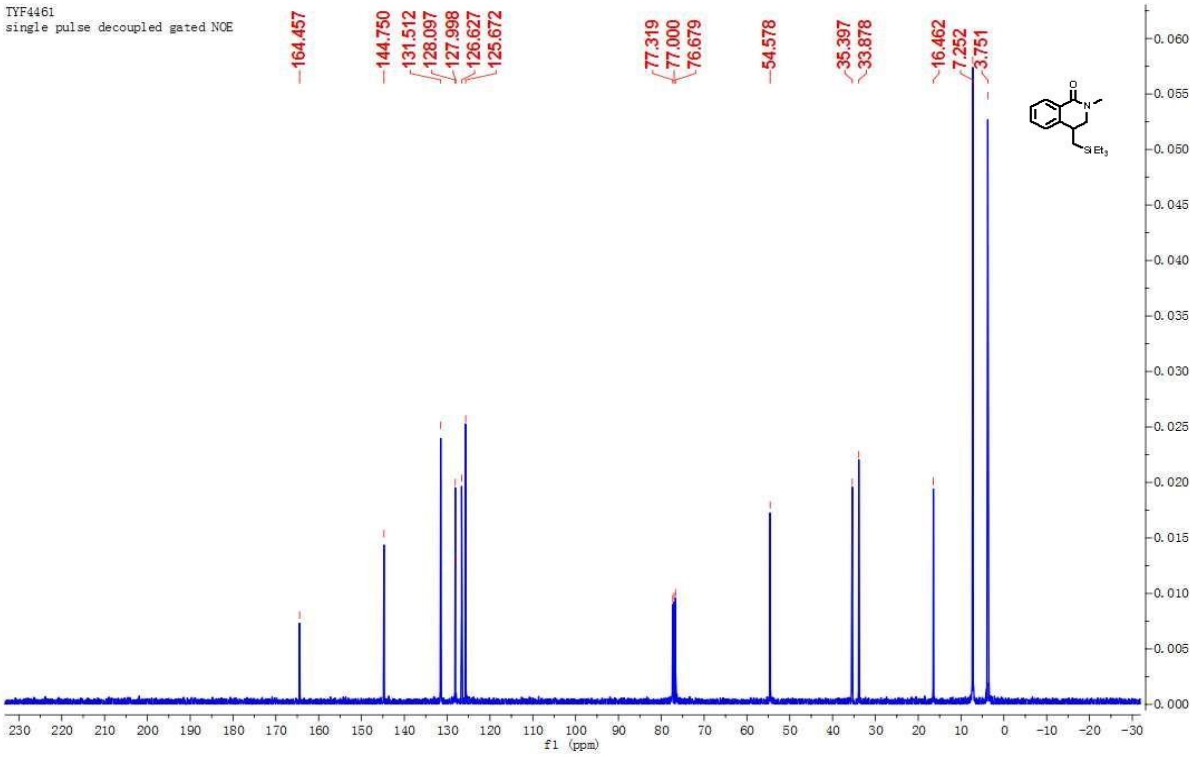
HRMS (ESI, m/z): Calculated for $C_{18}H_{28}NO_2Si$ $(M+H)^+$ 318.1884, found 318.1889.

Copies of the ^{1}H NMR, ^{13}C NMR, ^{19}F NMR

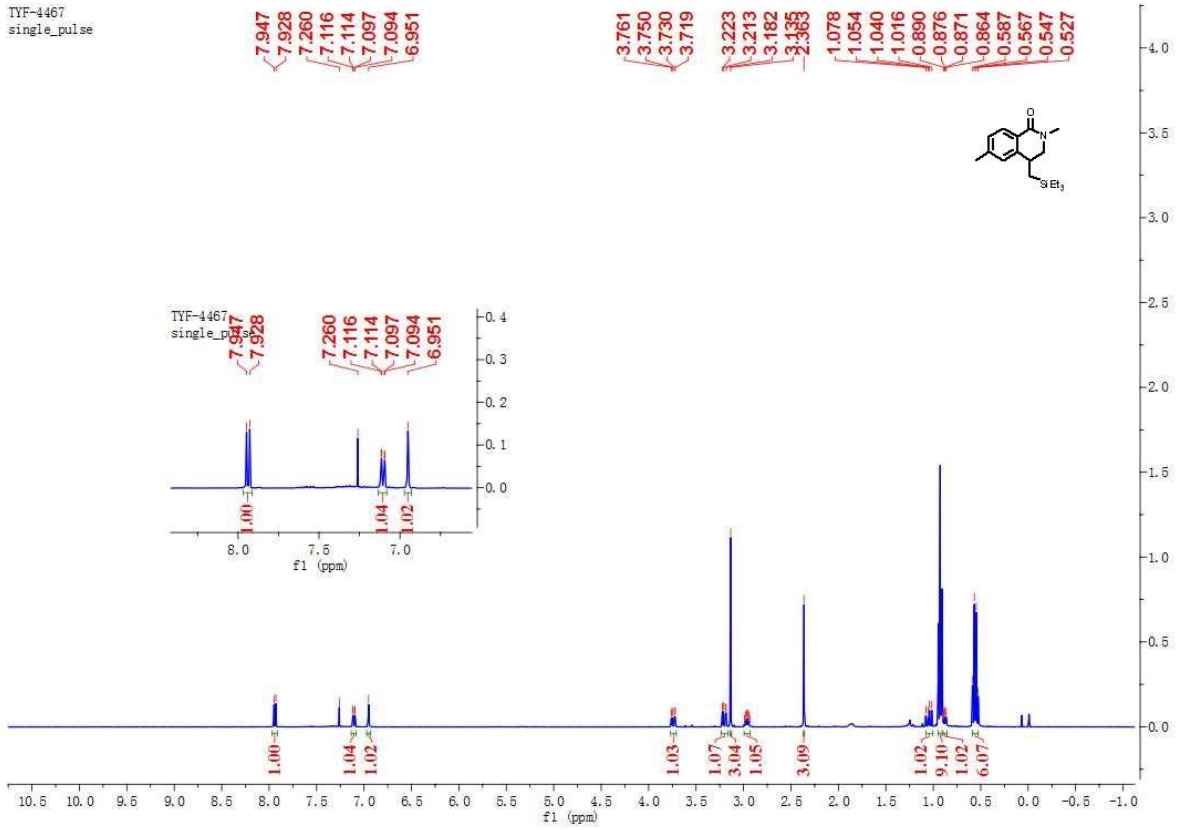
1-^{1}H NMR



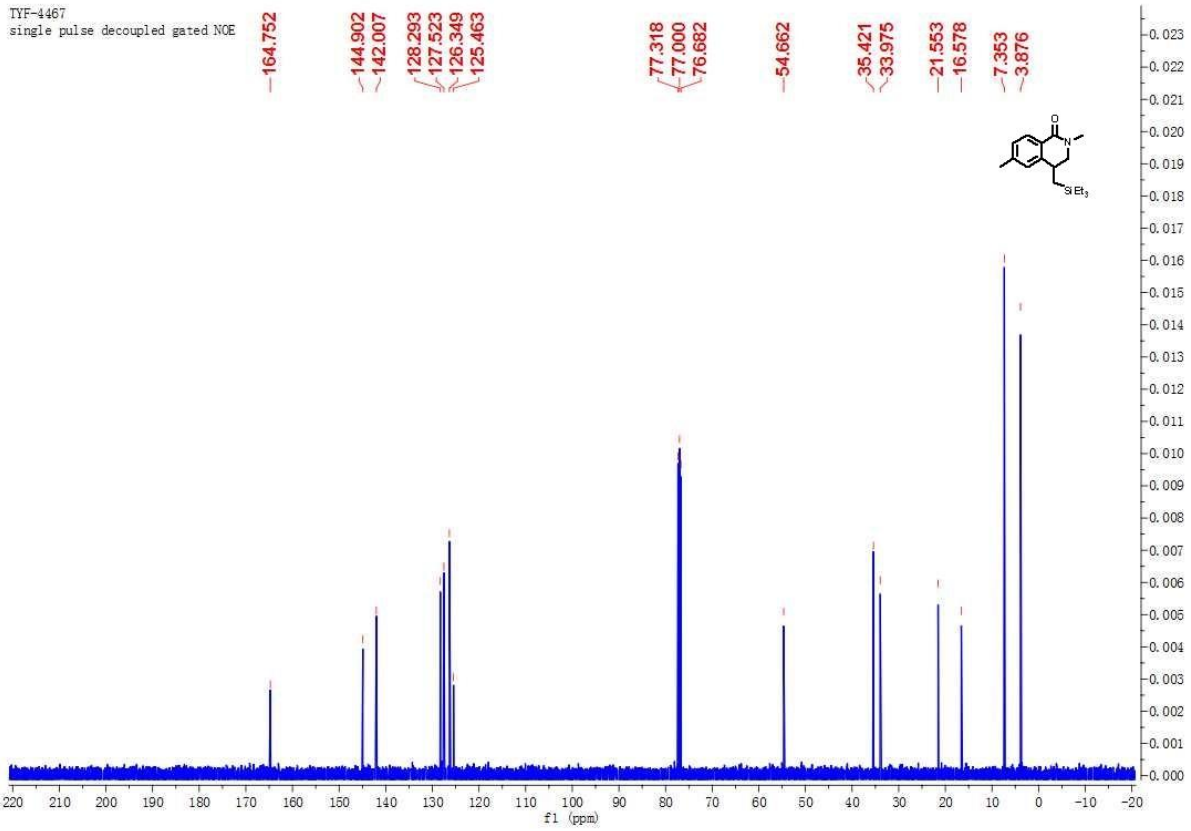
1-^{13}C NMR



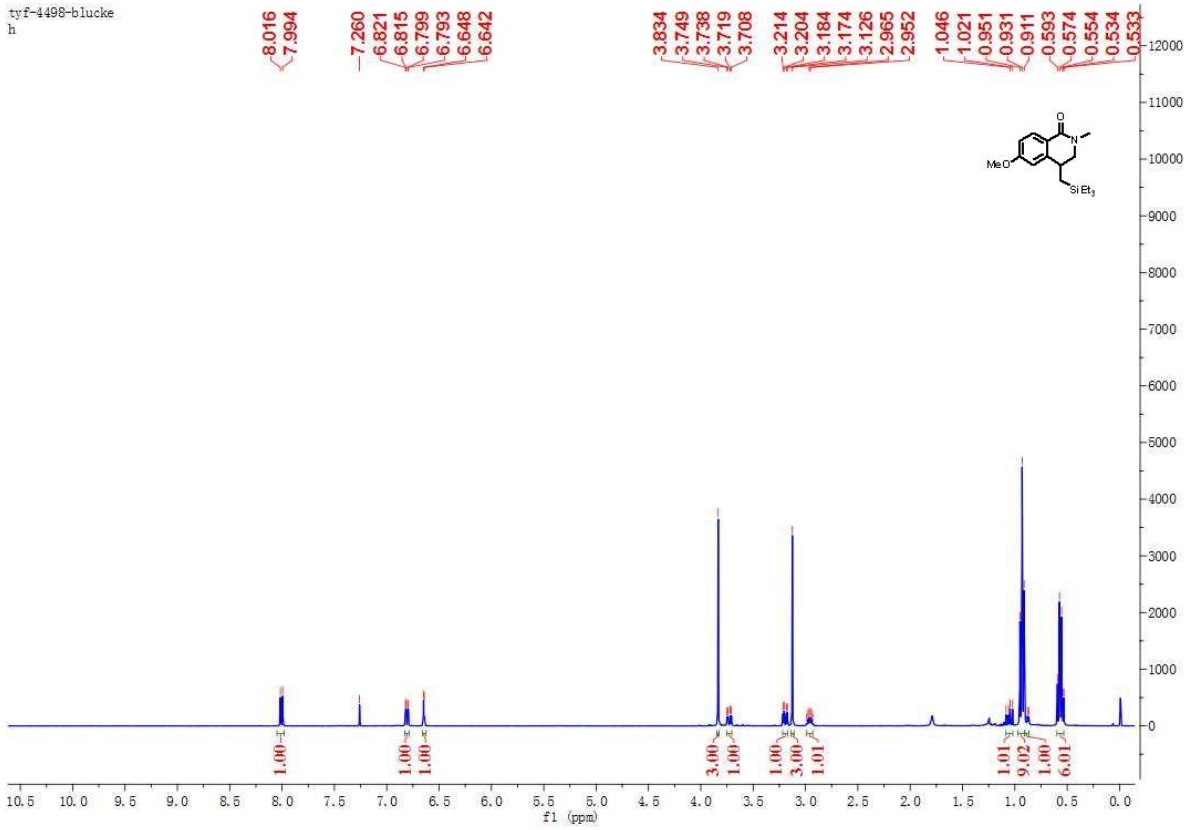
2-^{1}H NMR



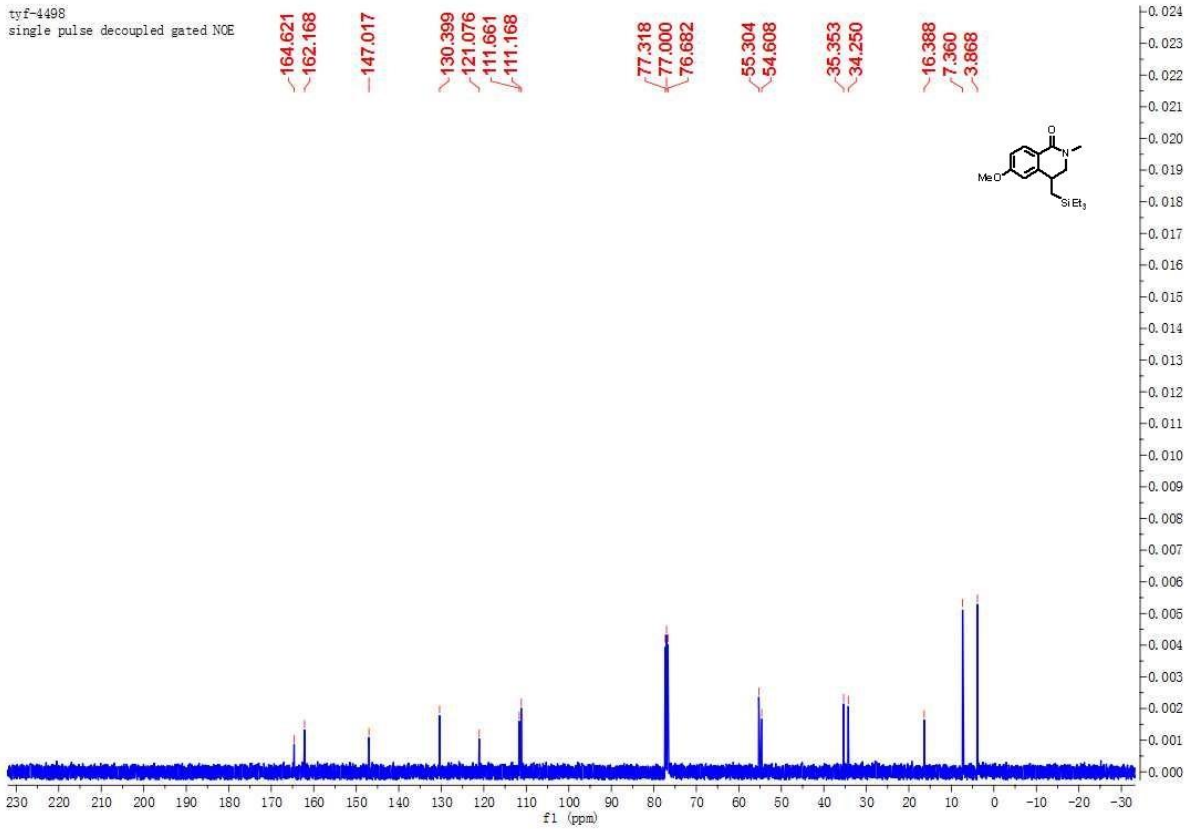
2-^{13}C NMR



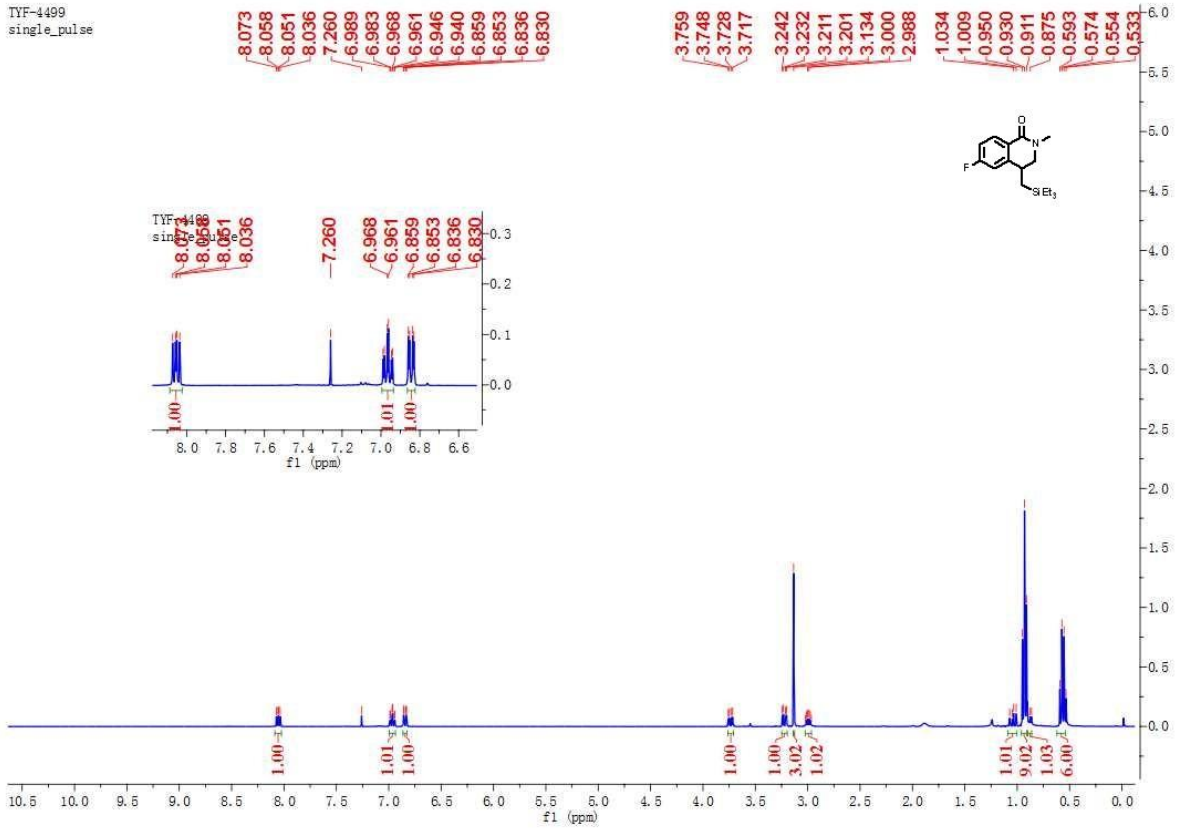
3-^{1}H NMR



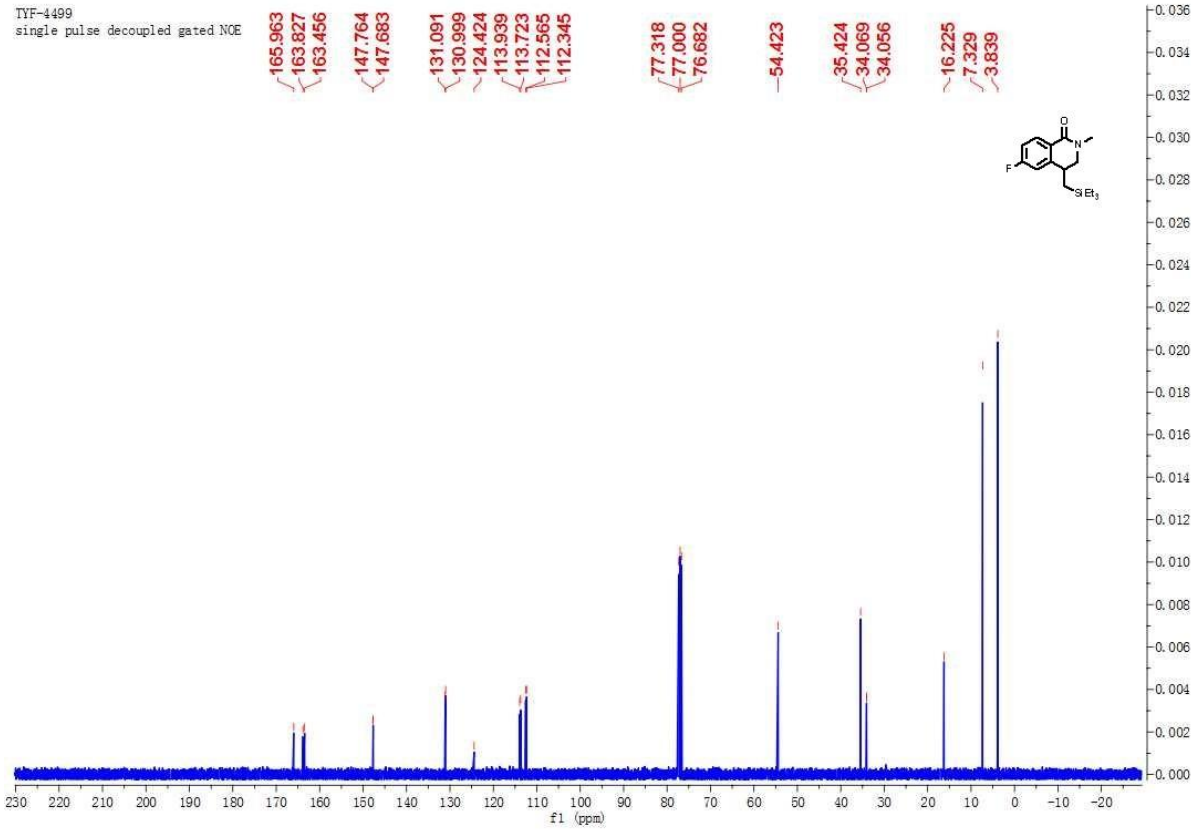
3-^{13}C NMR



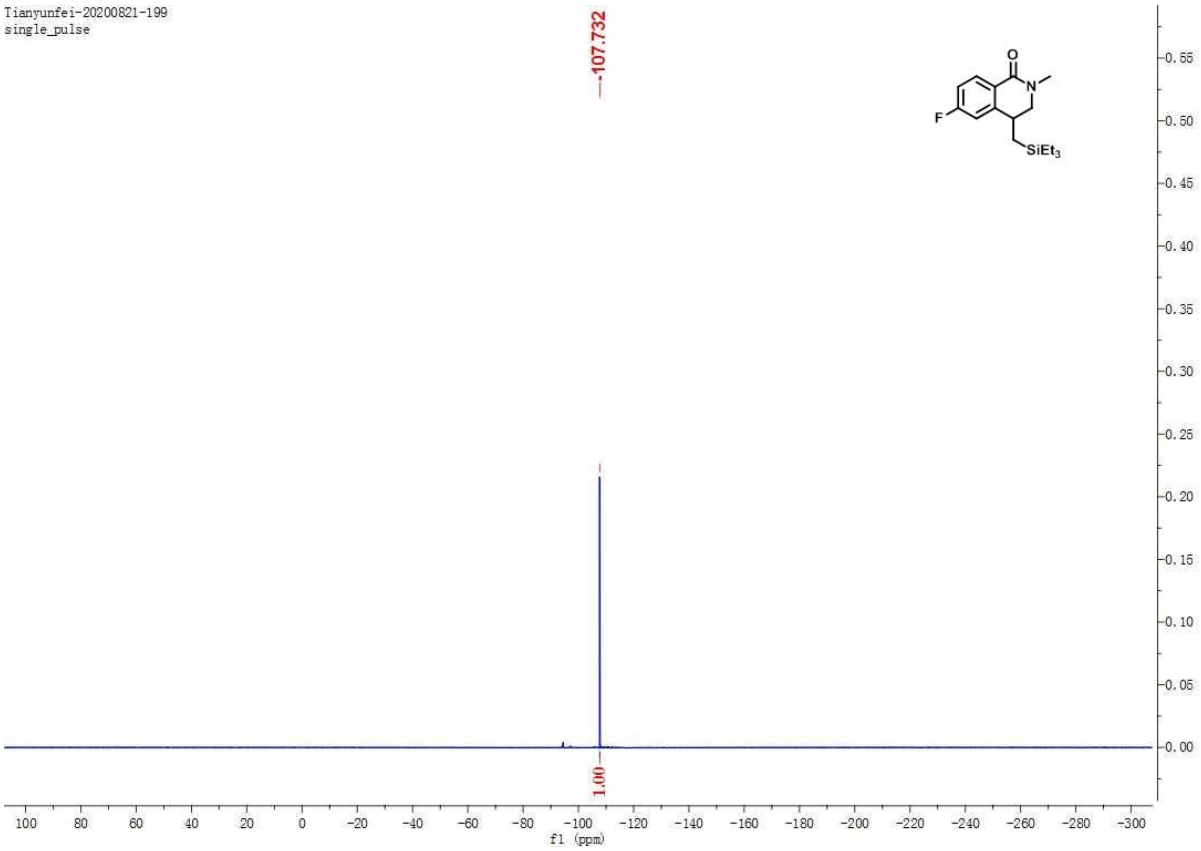
4-^{1}H NMR



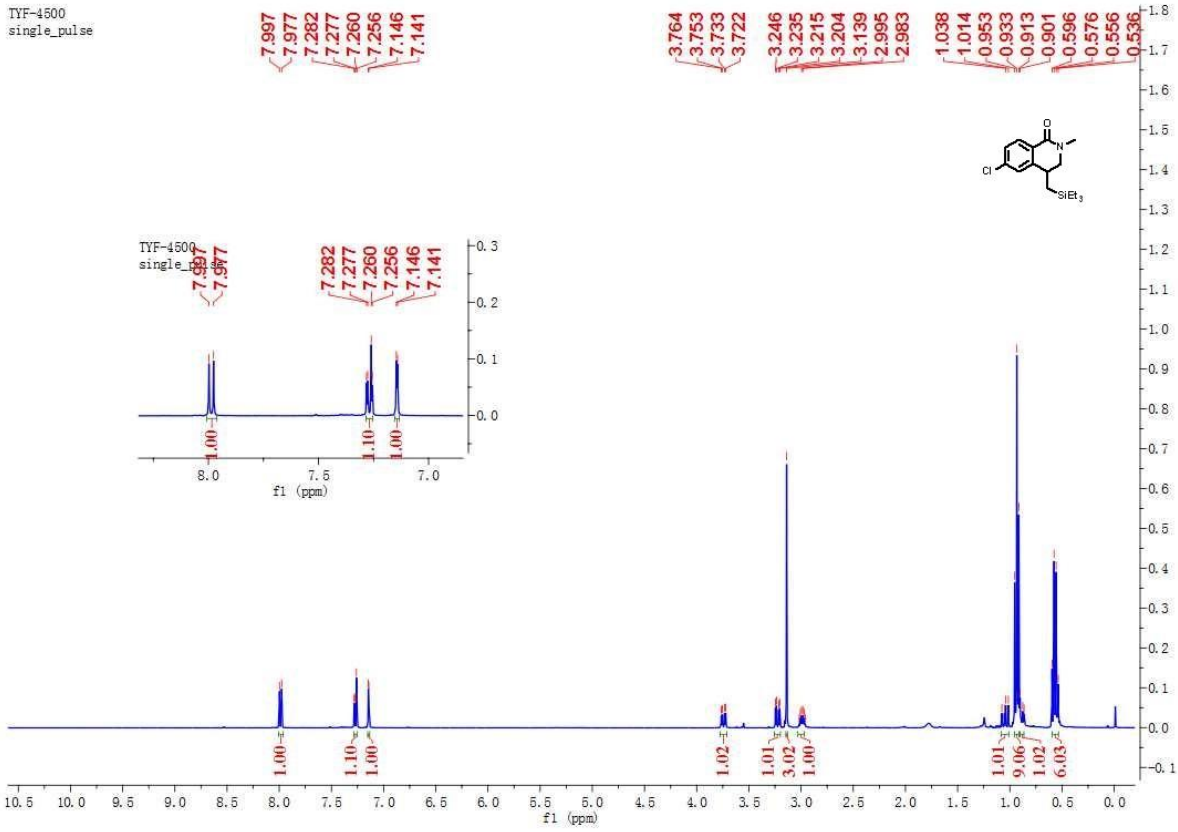
4-^{13}C NMR



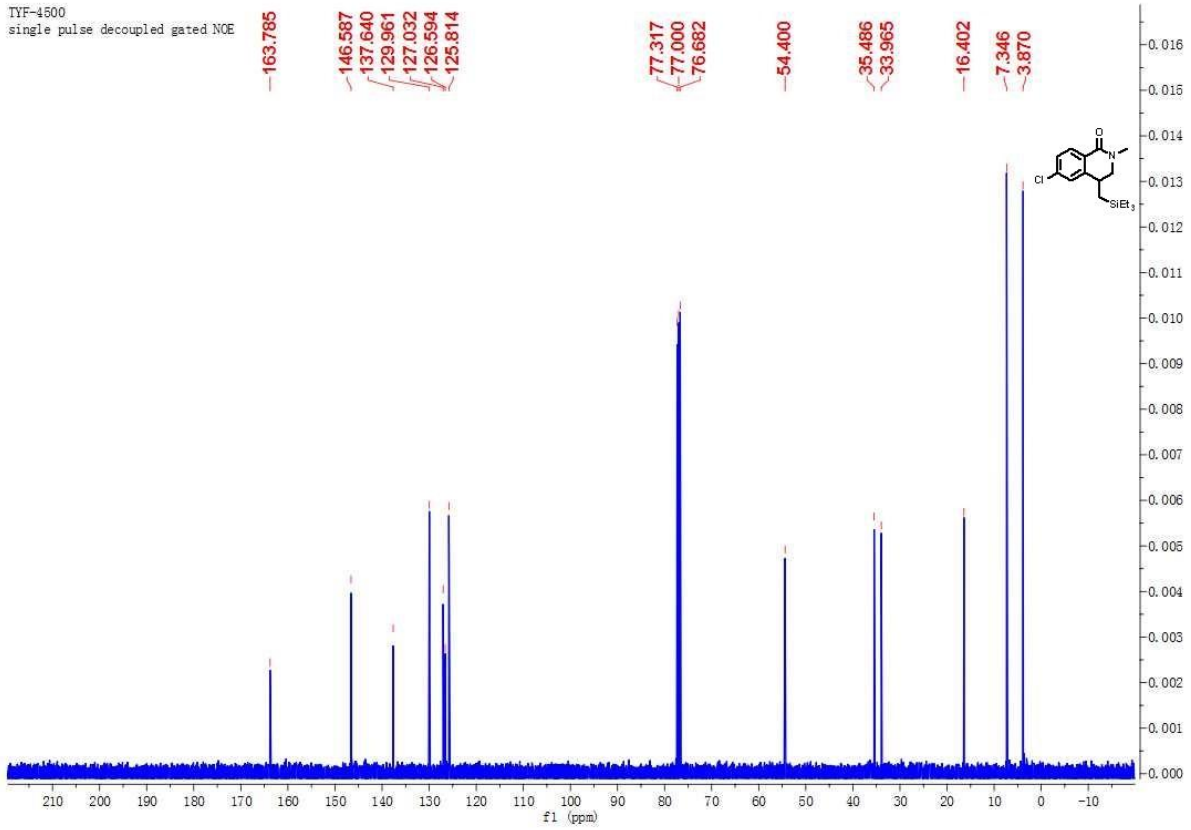
4-^{19}F NMR



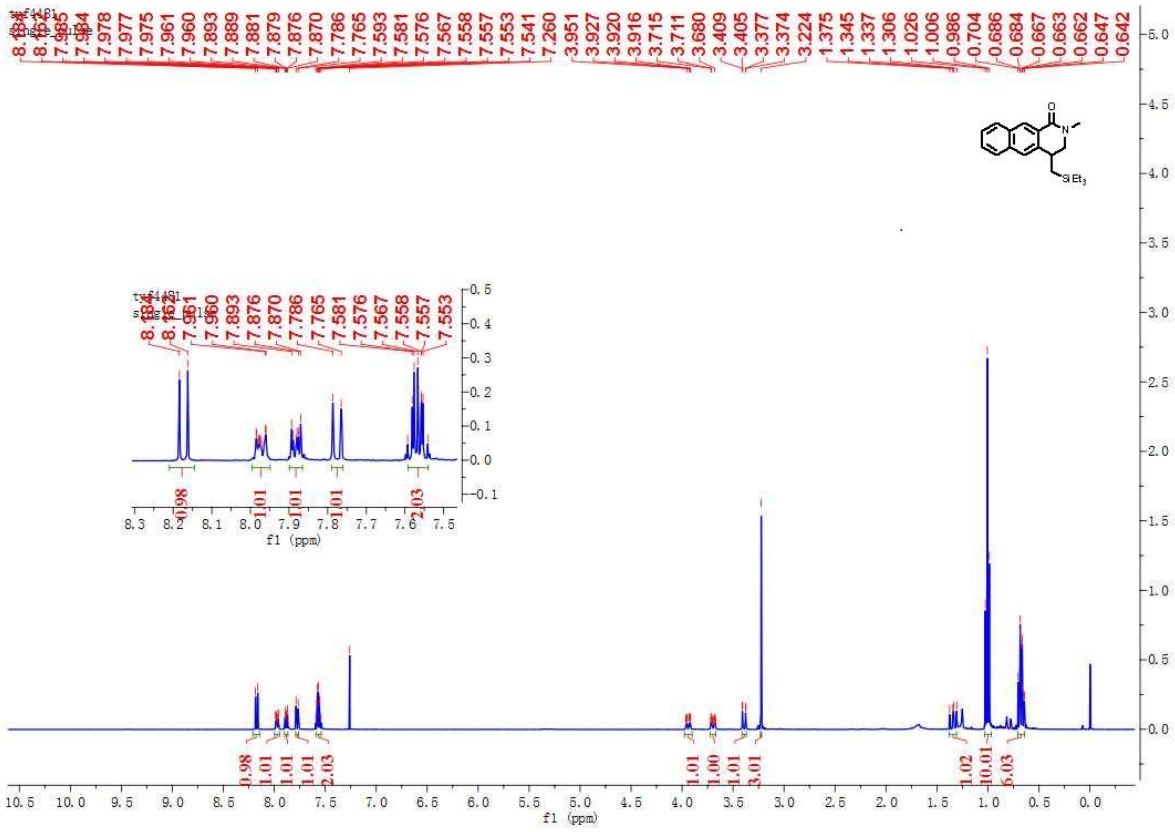
5-^{1}H NMR



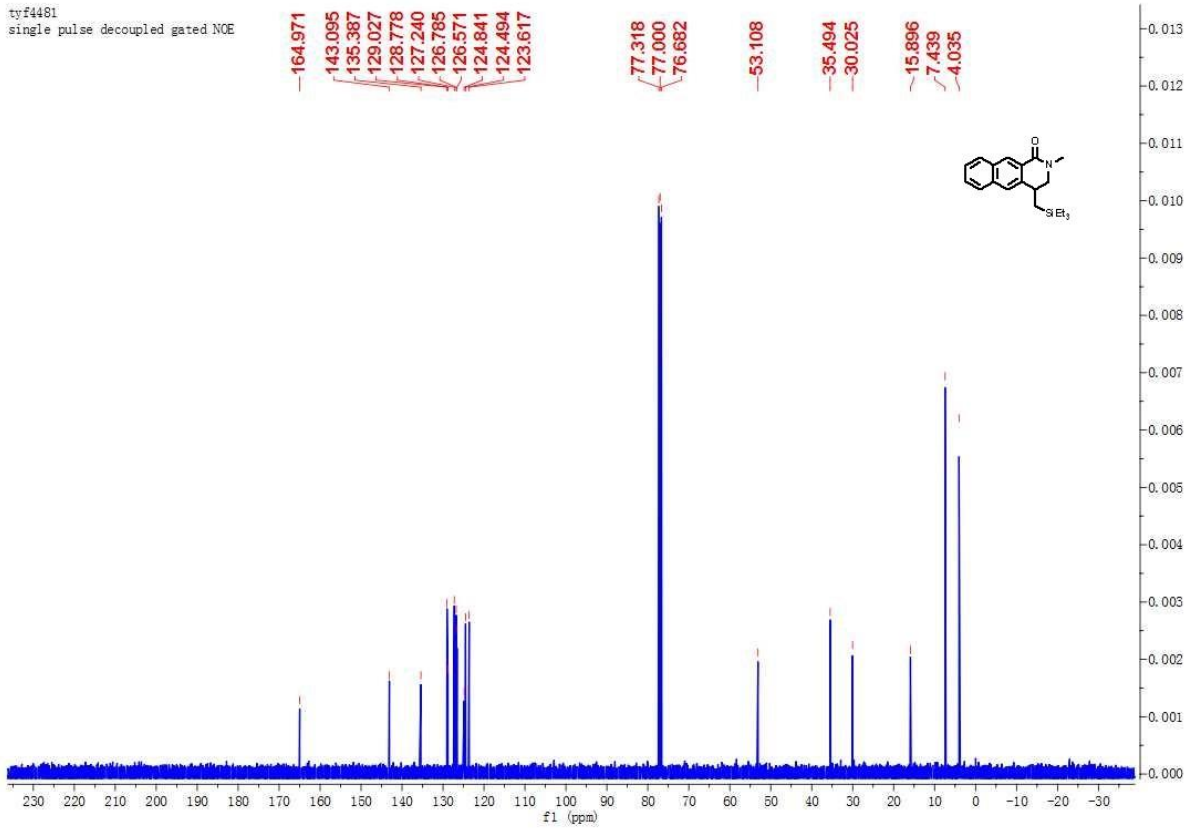
5-^{13}C NMR



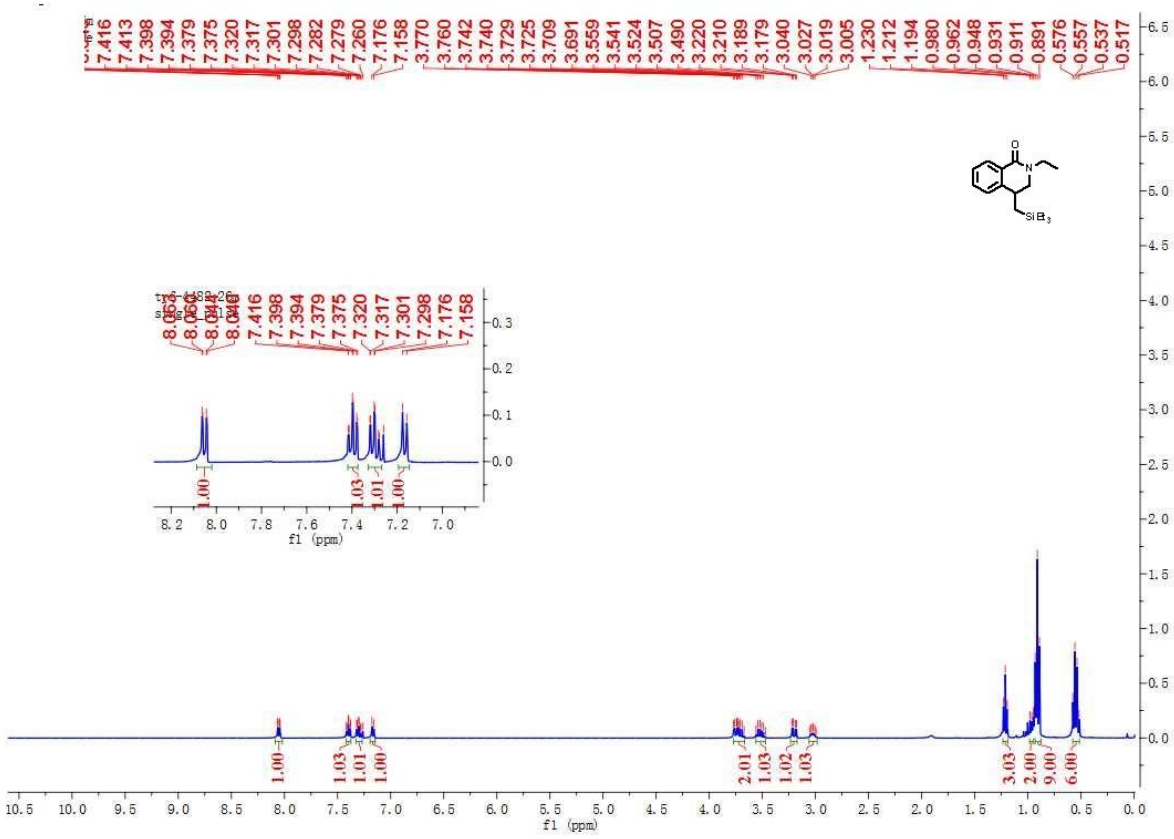
6-^{1}H NMR



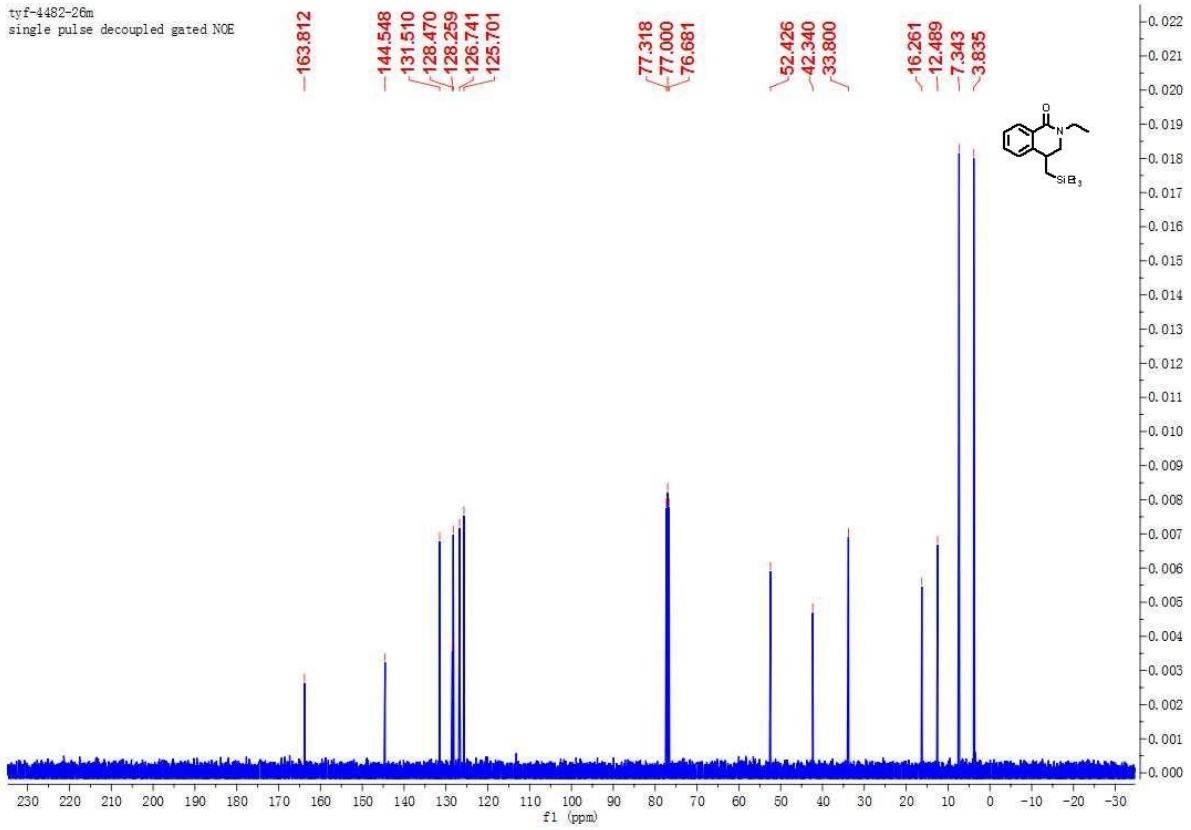
6-^{13}C NMR



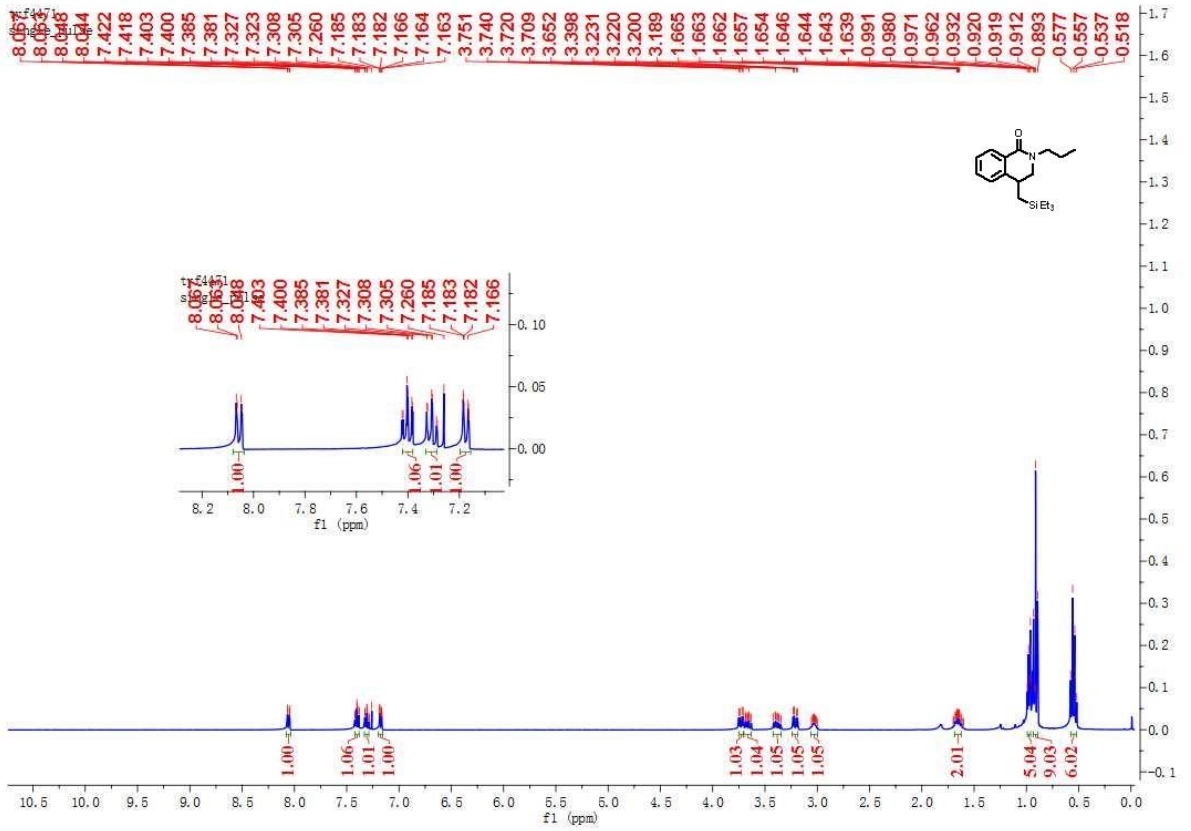
7-^{1}H NMR



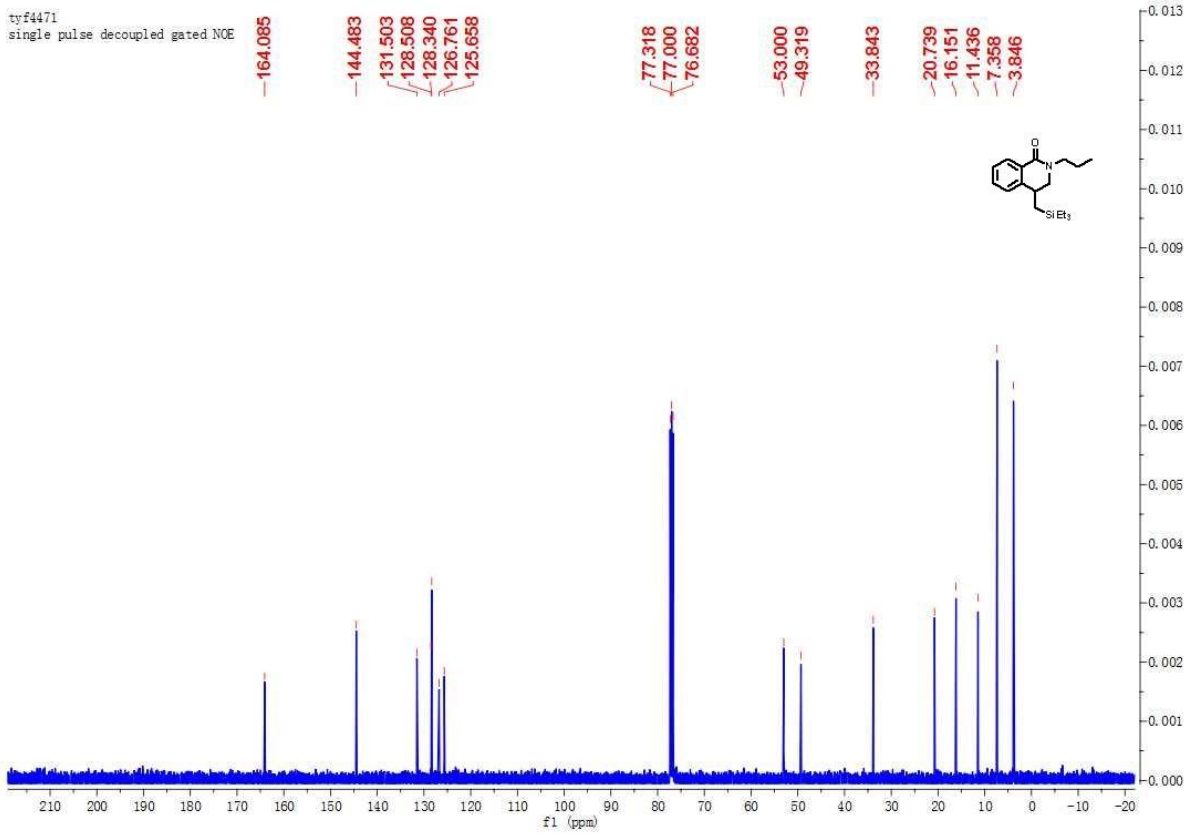
7-^{13}C NMR



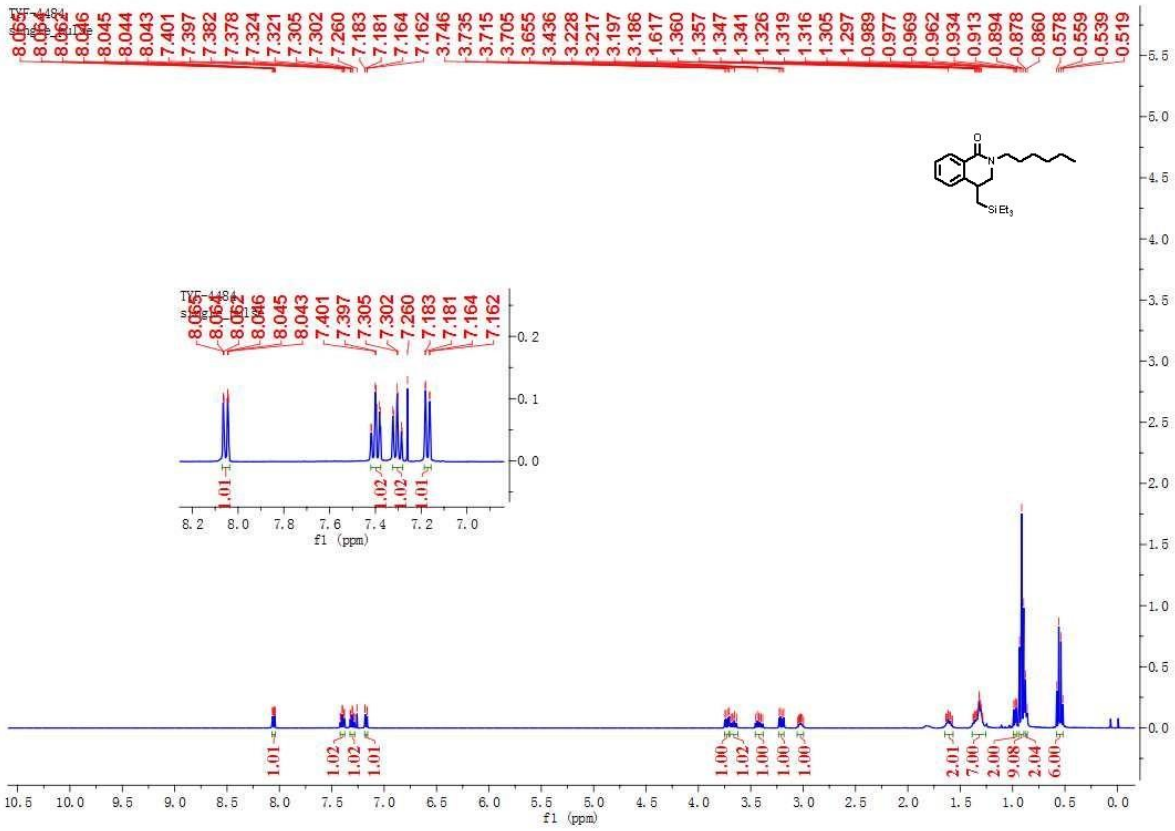
8-^{1}H NMR



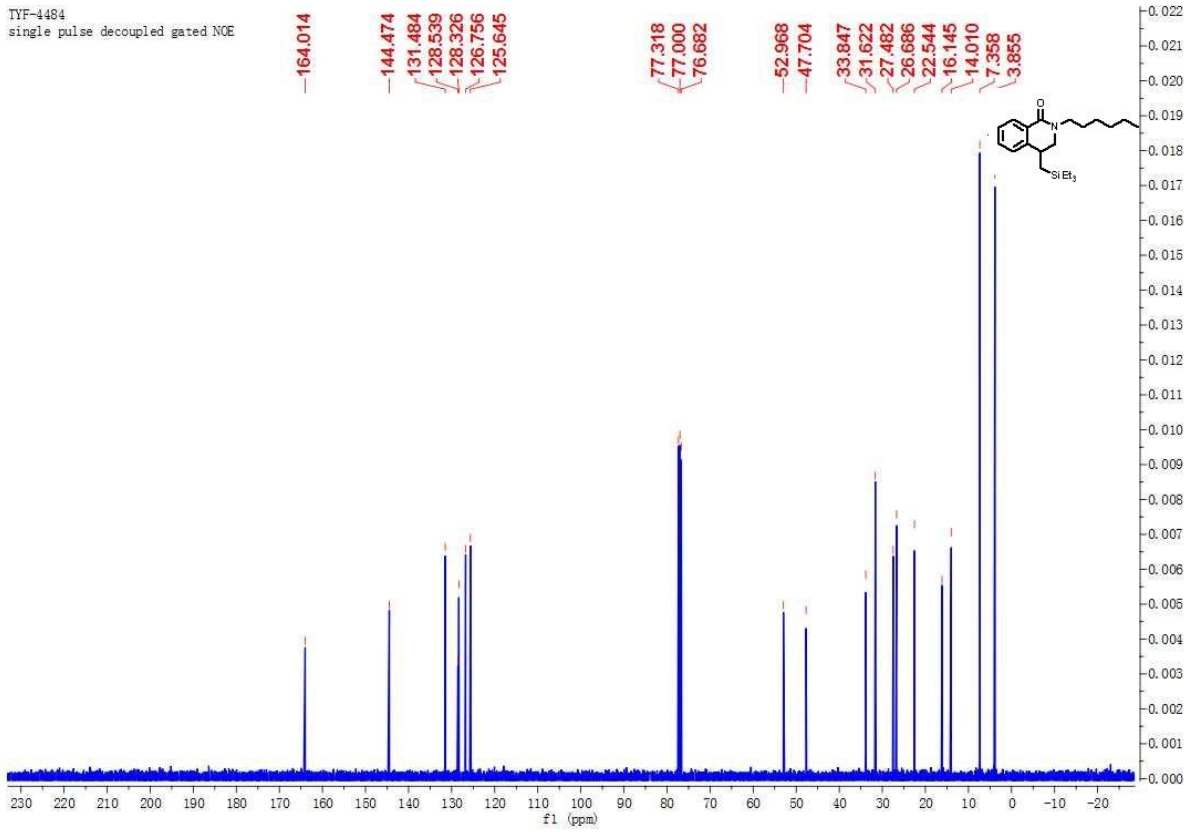
8-^{13}C NMR



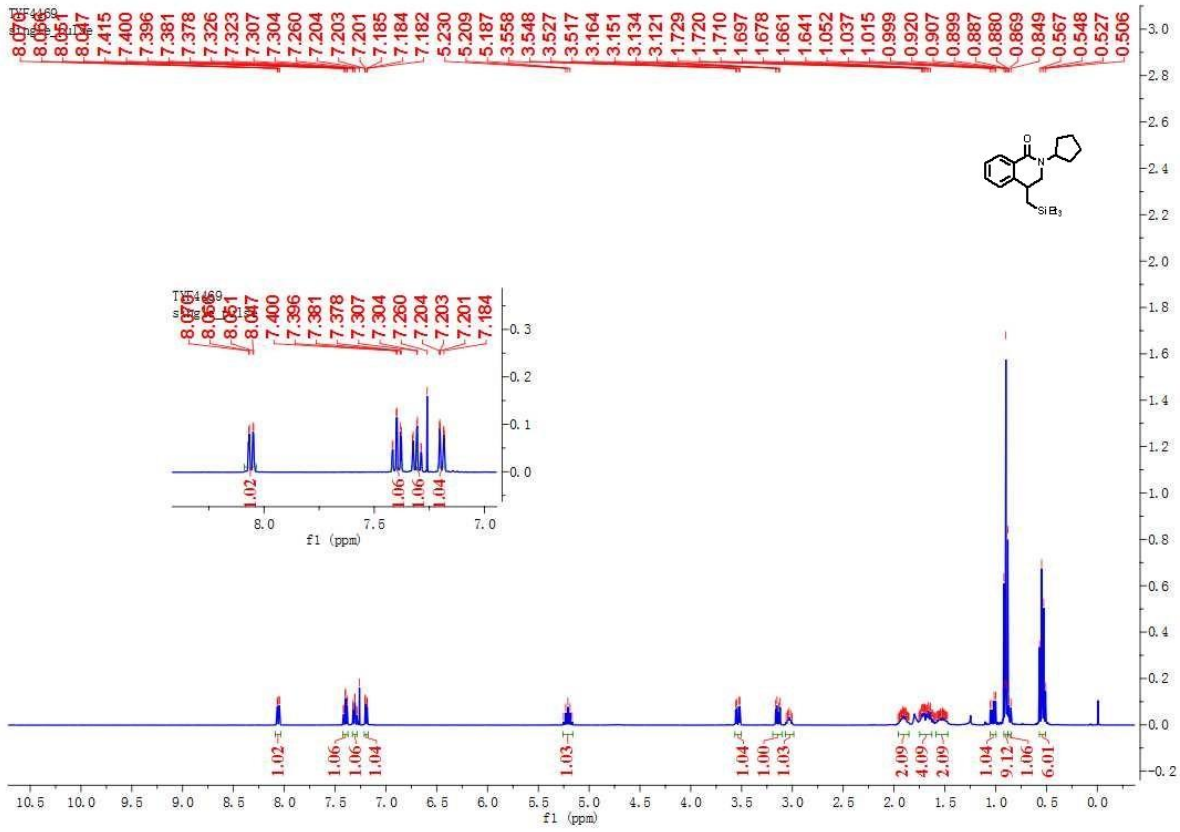
9-^{1}H NMR



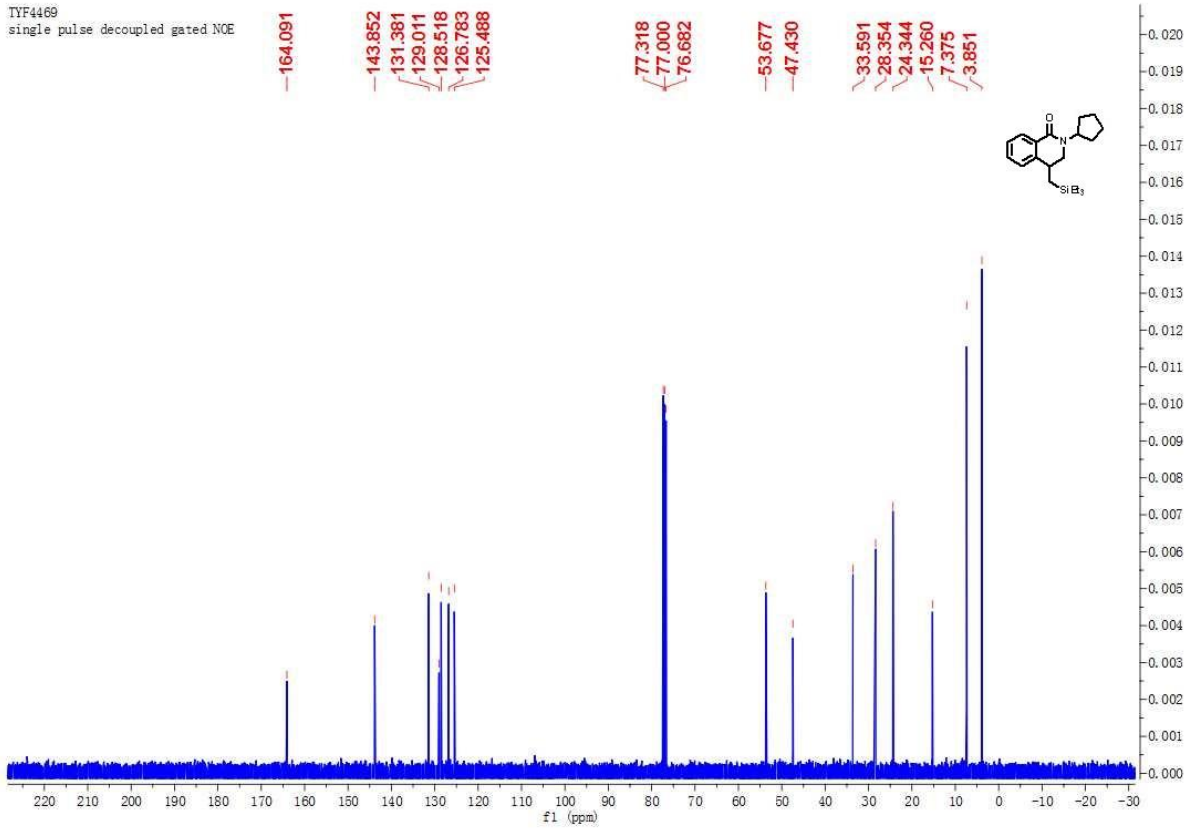
9-^{13}C NMR



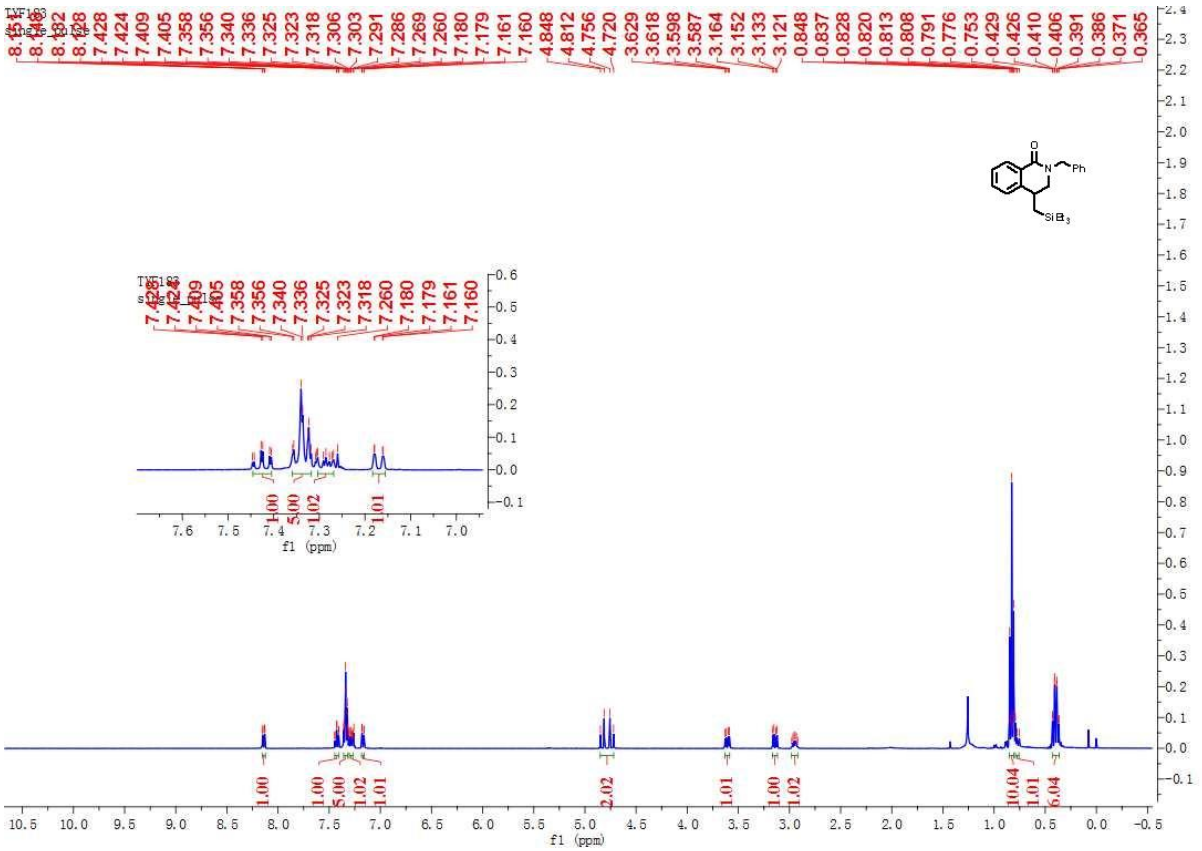
10-^{1}H NMR



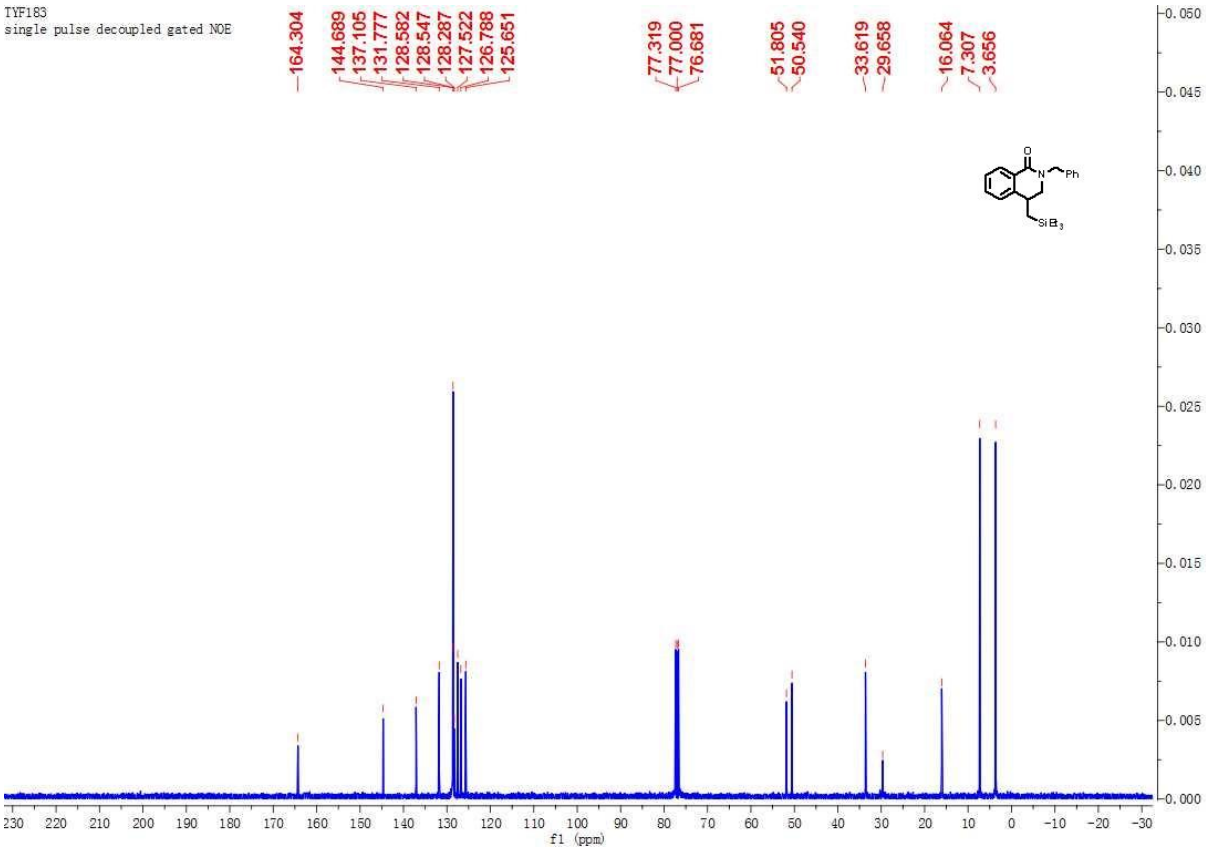
10-^{13}C NMR



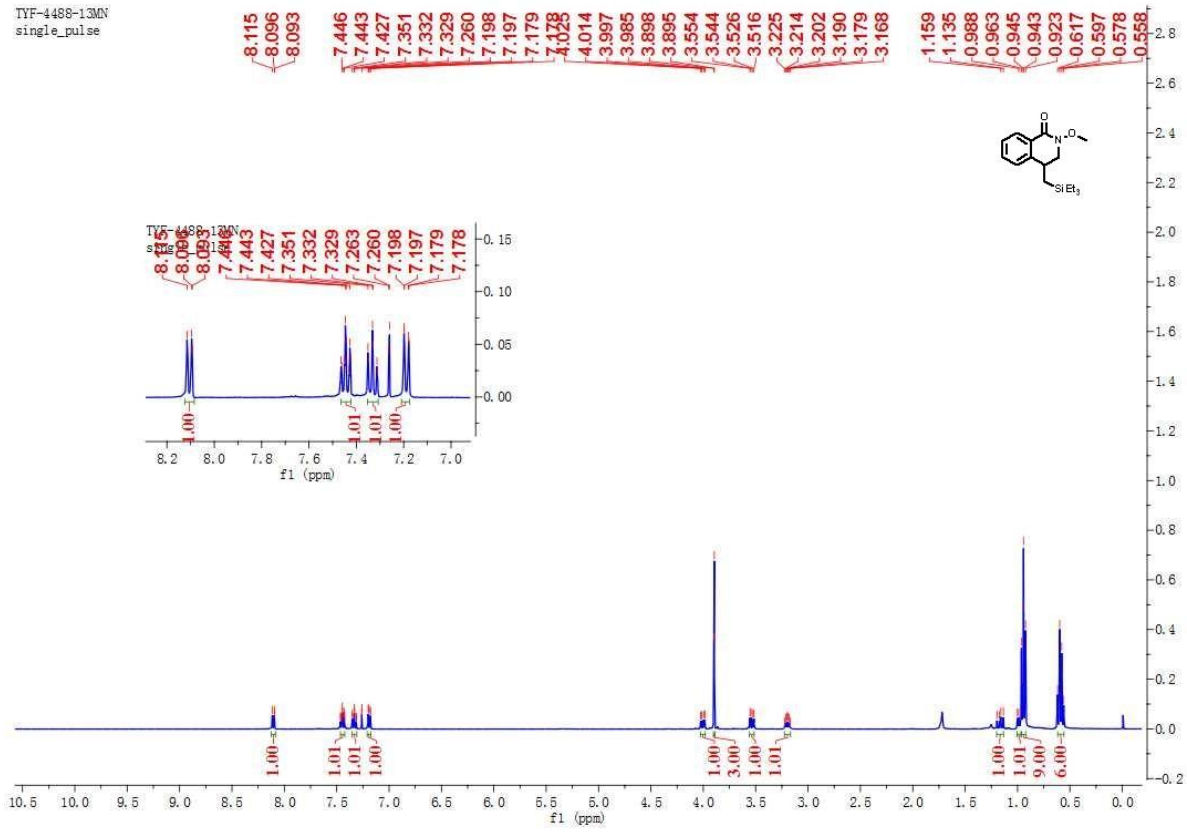
11-^{1}H NMR



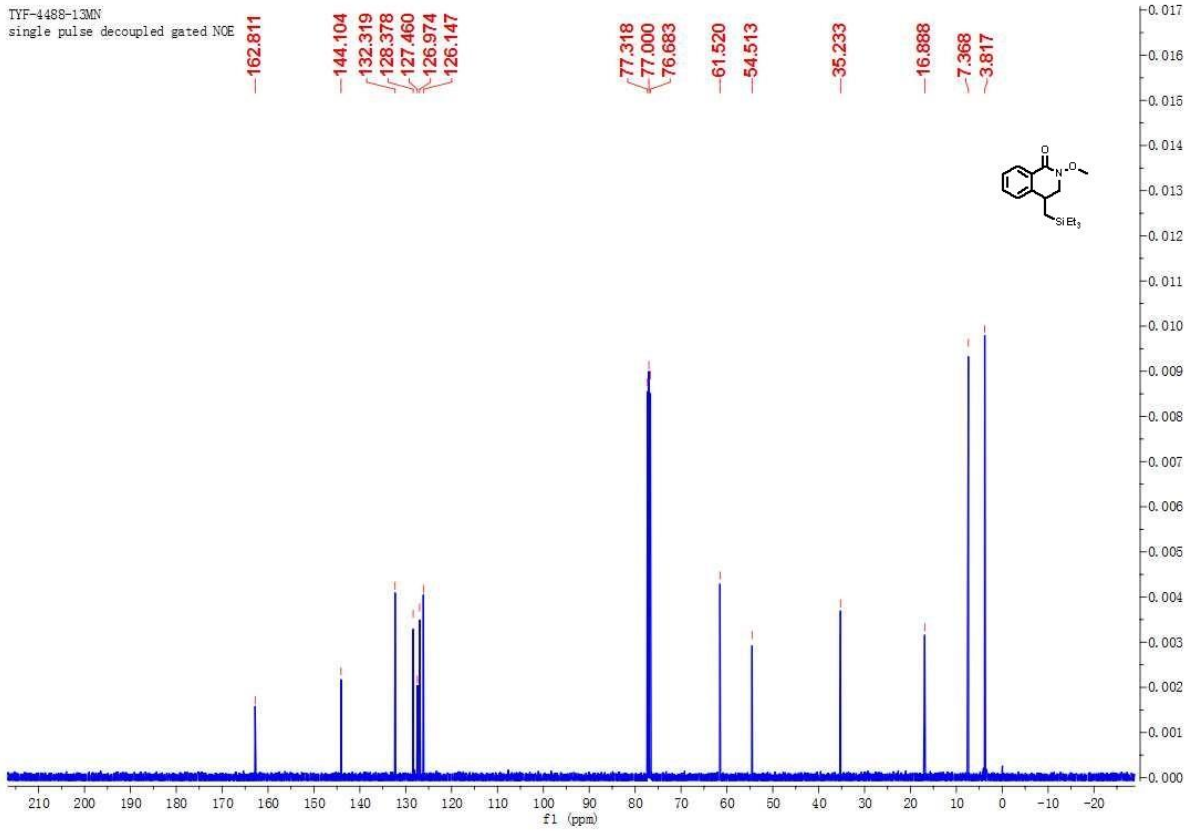
11-^{13}C NMR



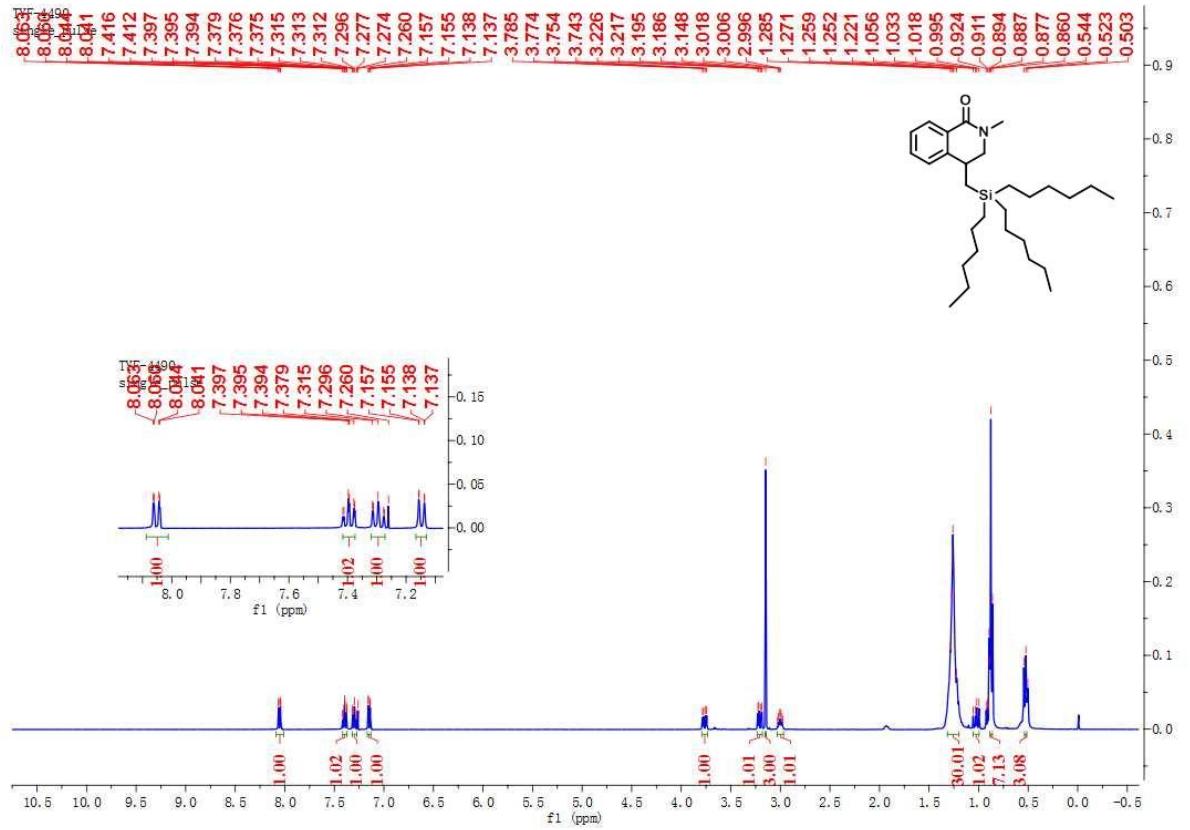
12-^{1}H NMR



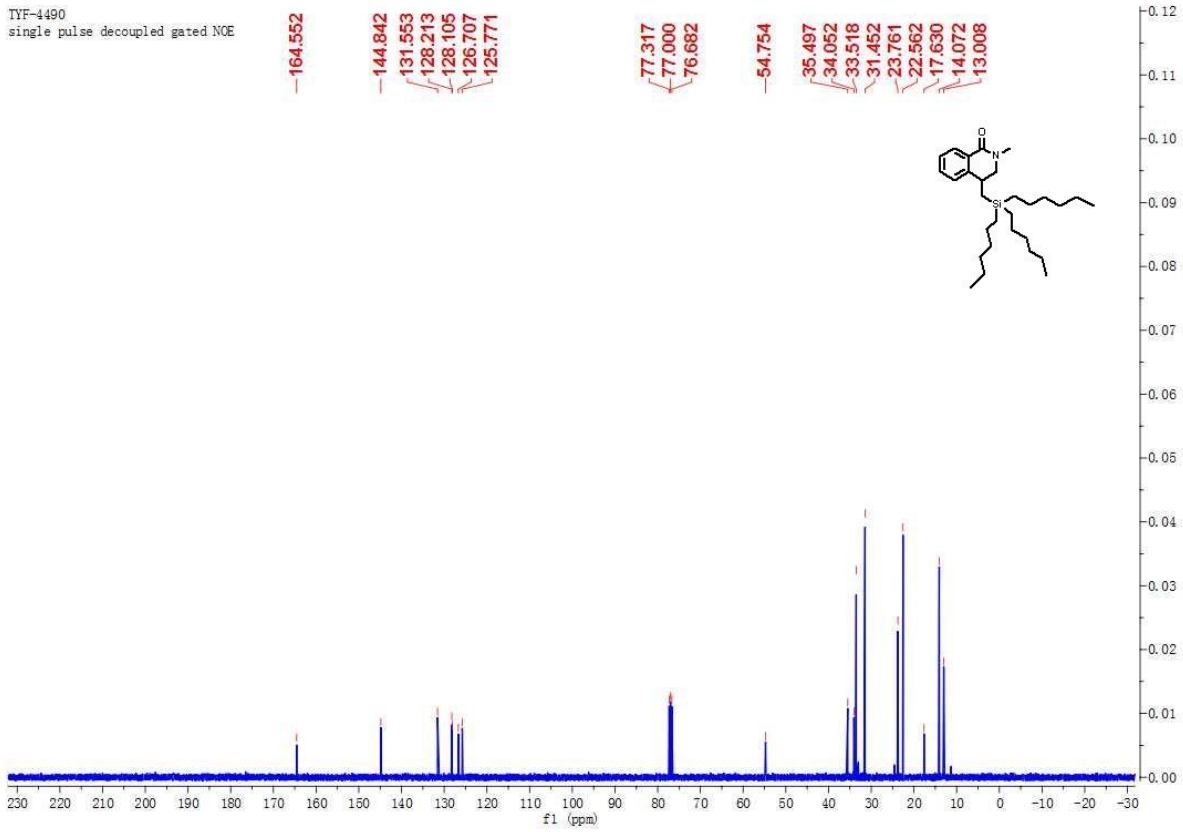
12-^{13}C NMR



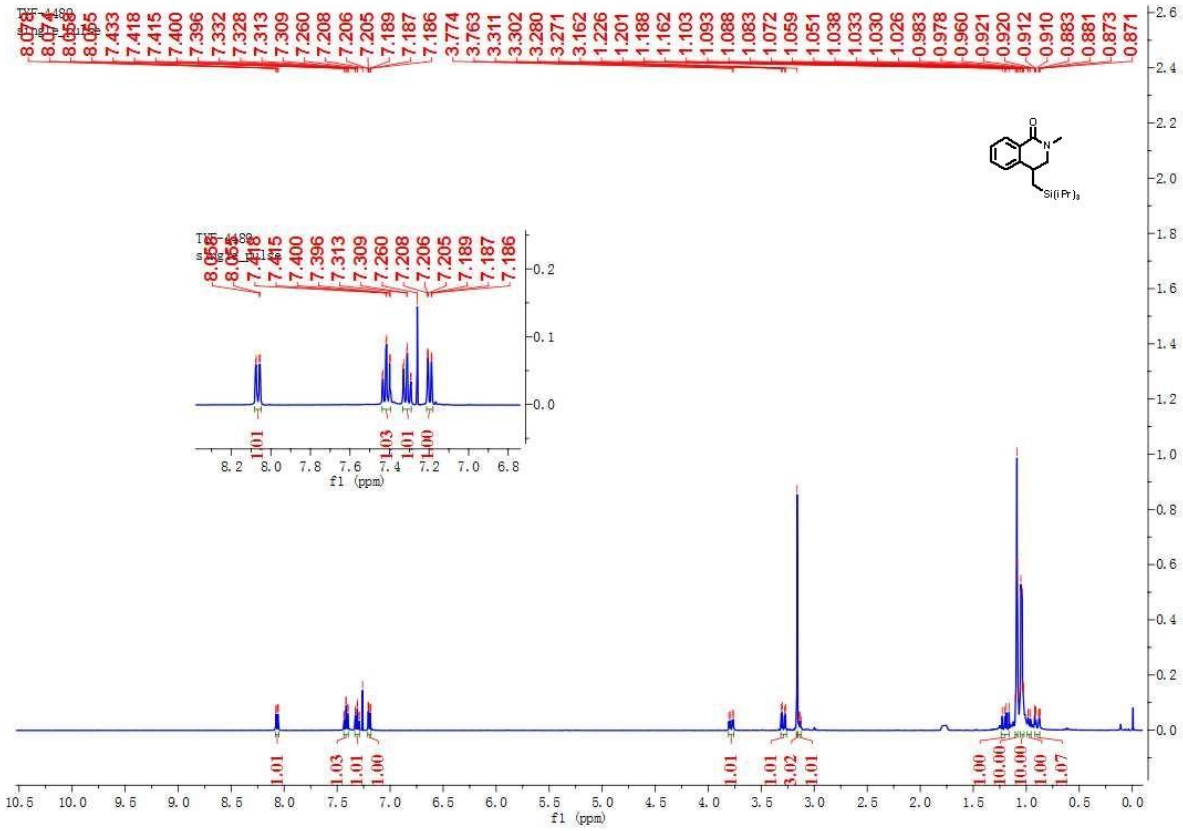
13-^{1}H NMR



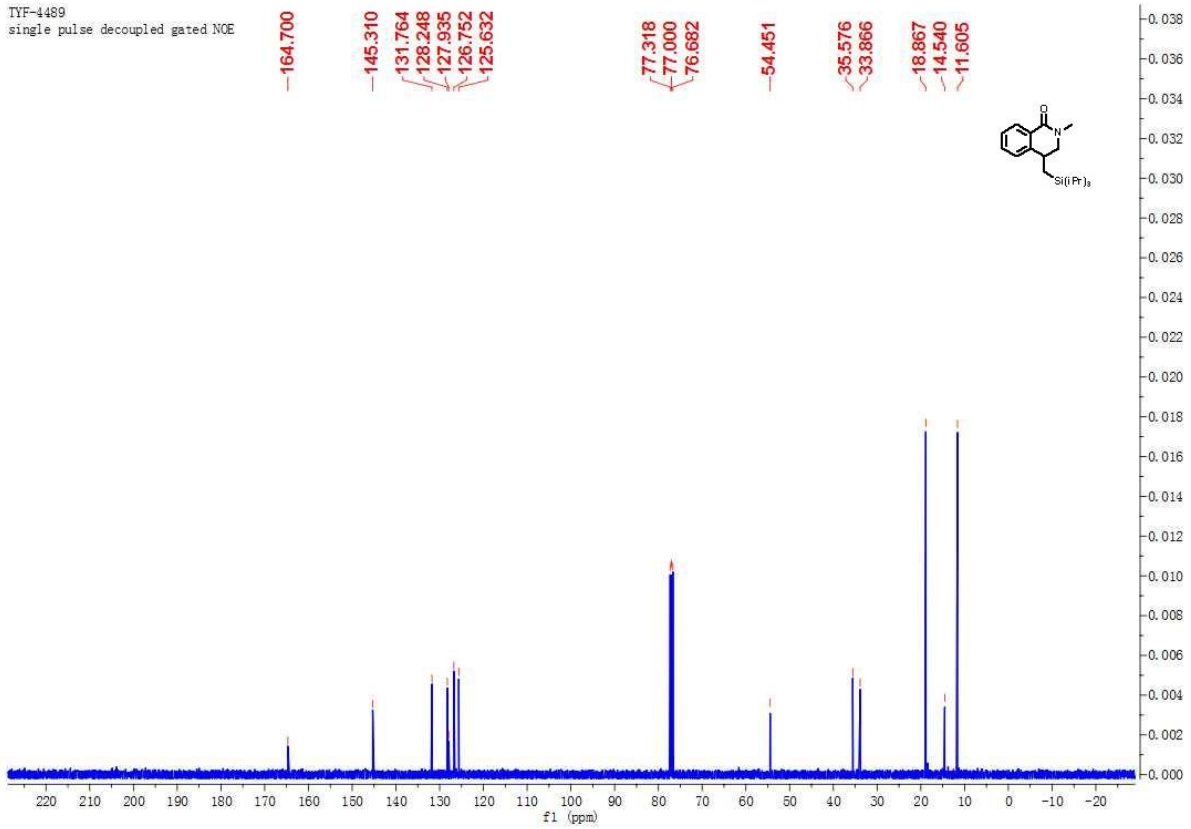
13-^{13}C NMR



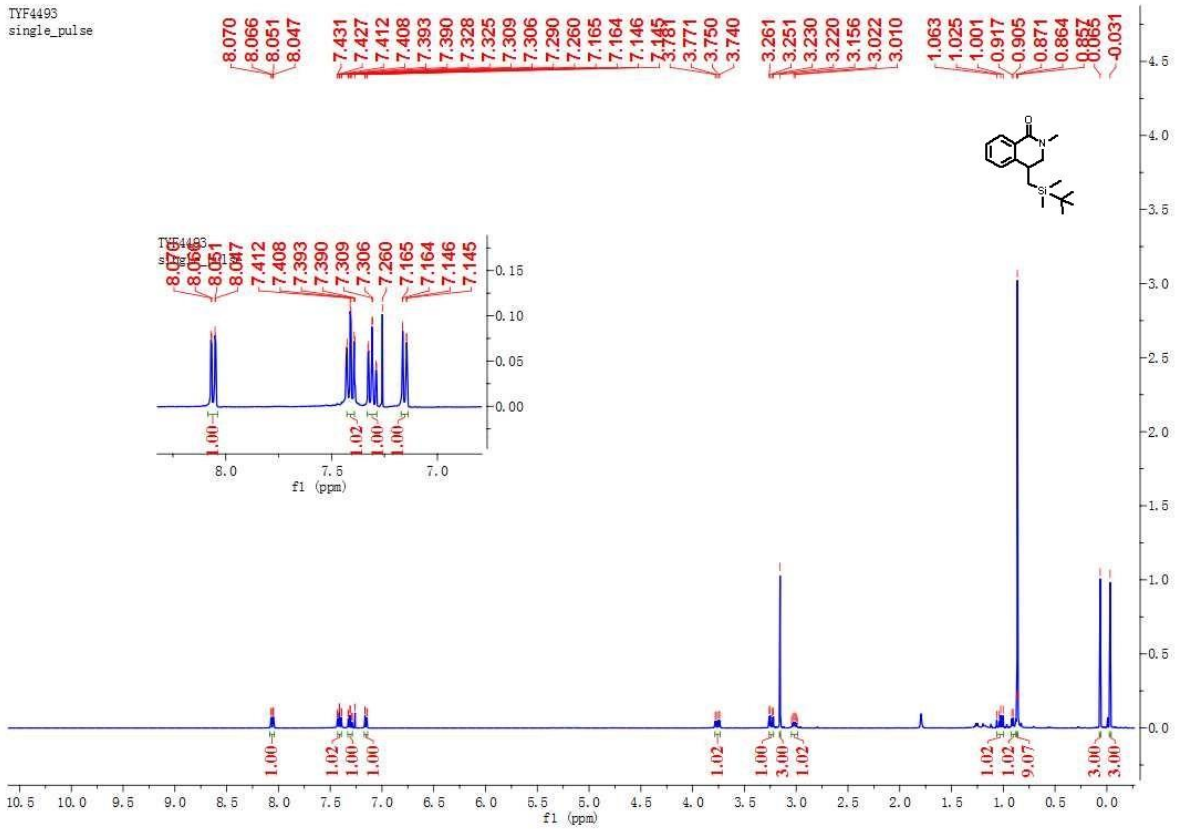
14-^{1}H NMR



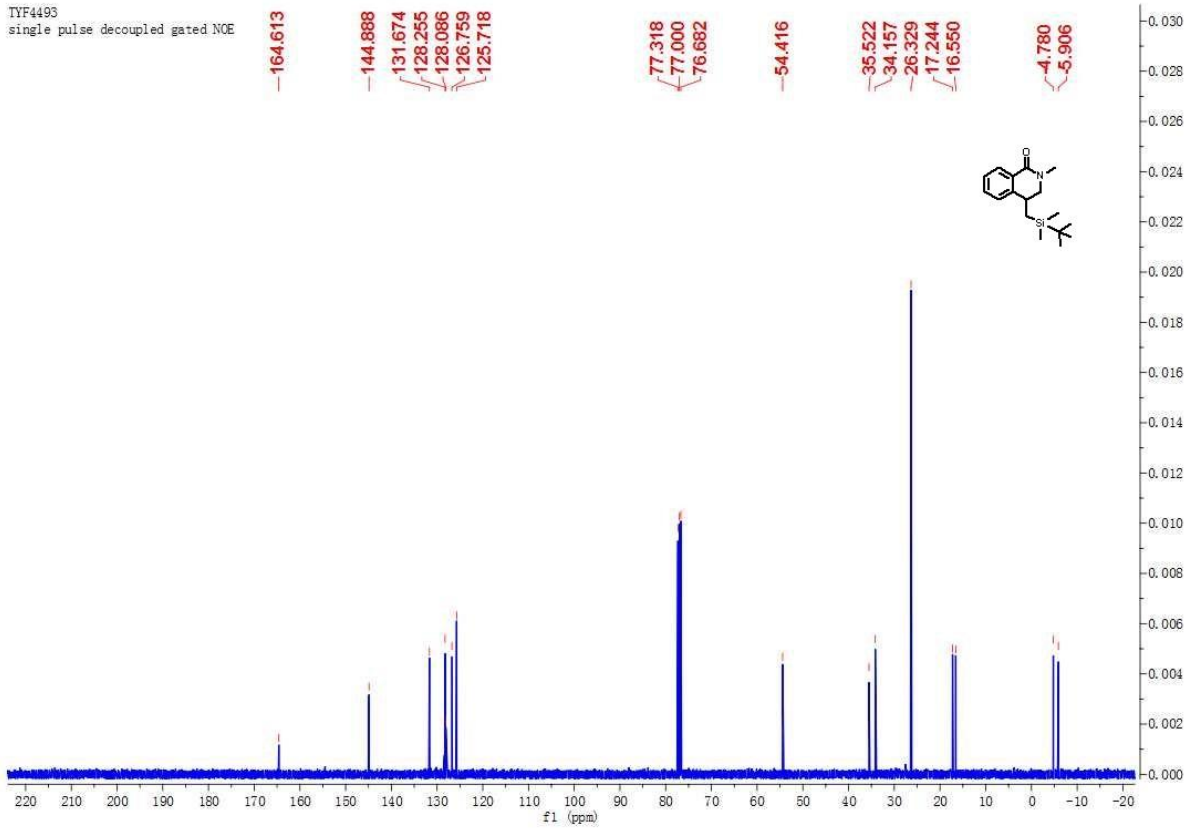
14-^{13}C NMR



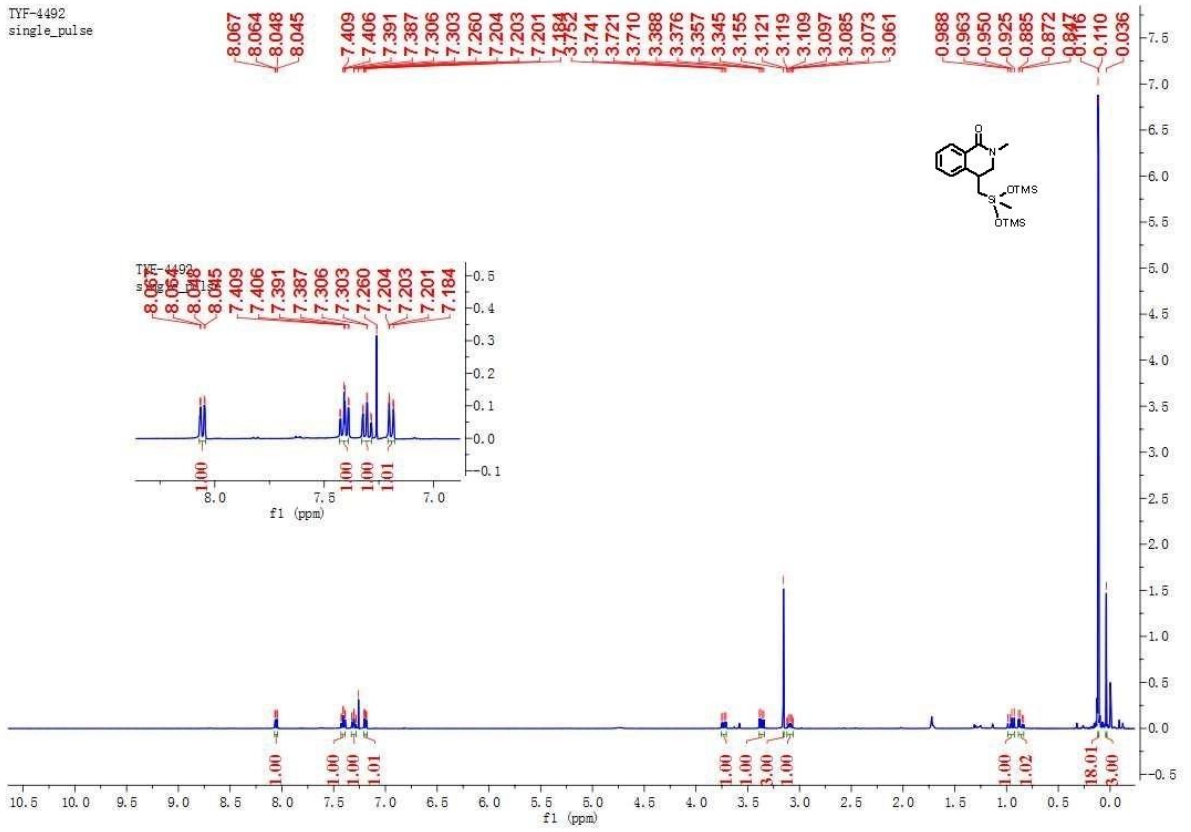
15-^{1}H NMR



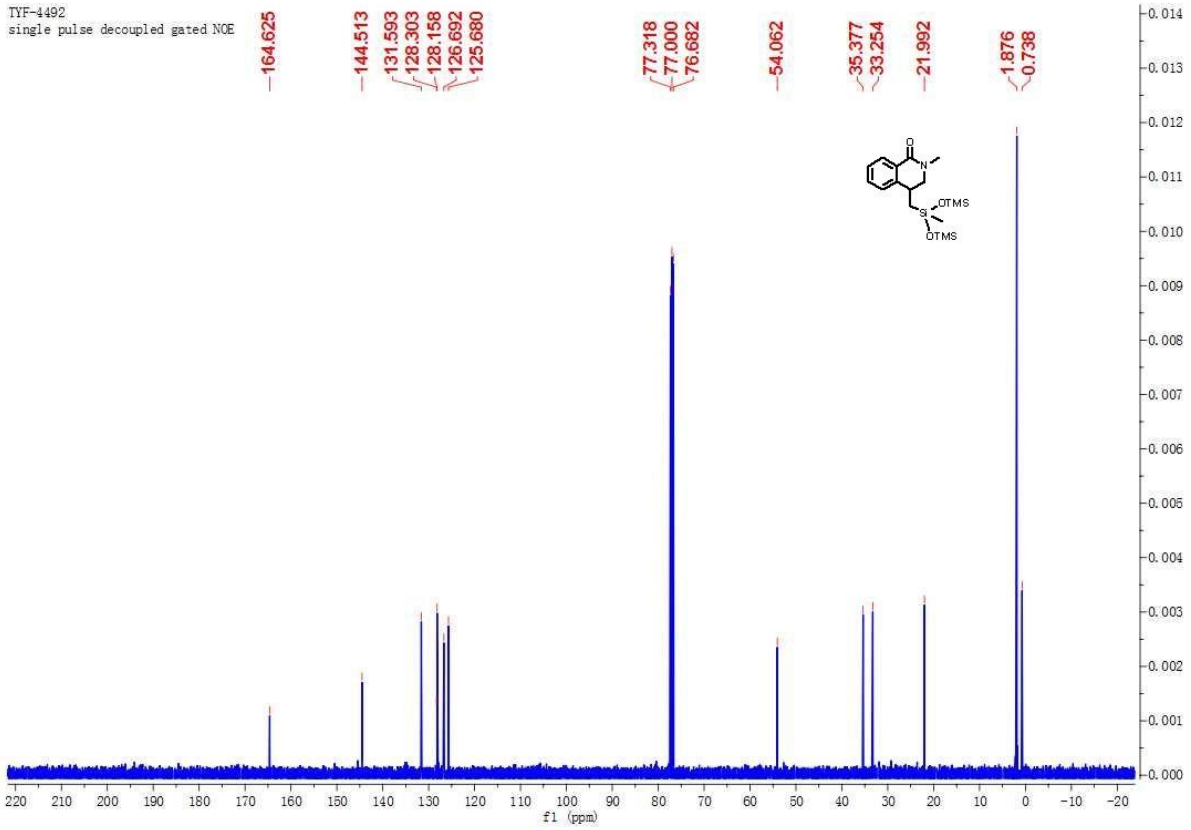
15-^{13}C NMR



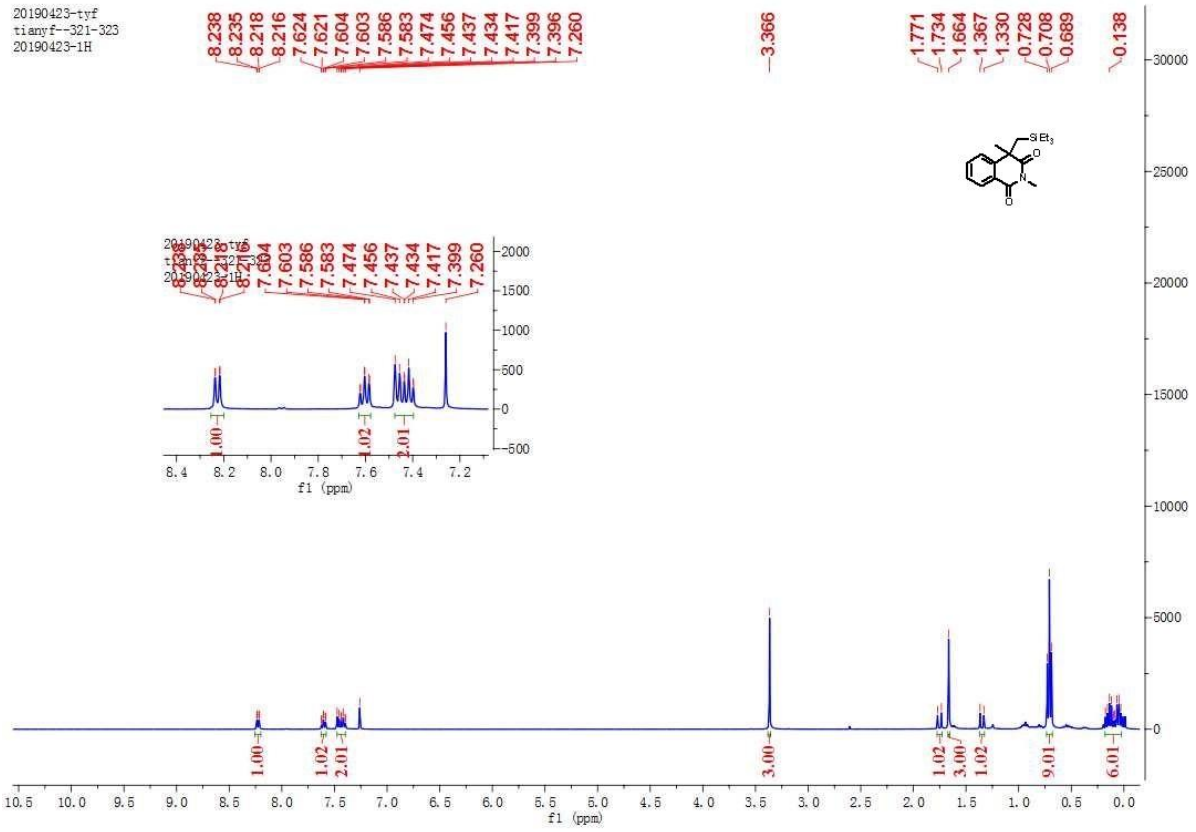
16-^{1}H NMR



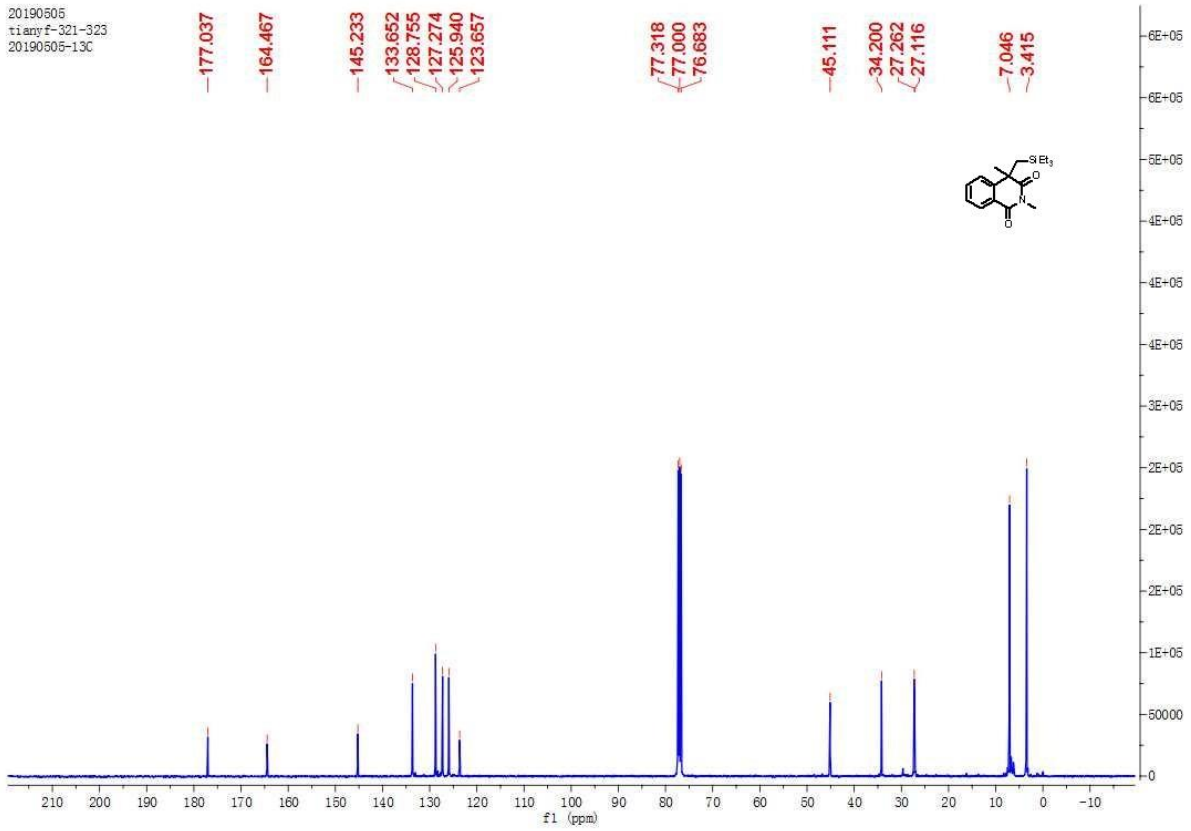
16-^{13}C NMR



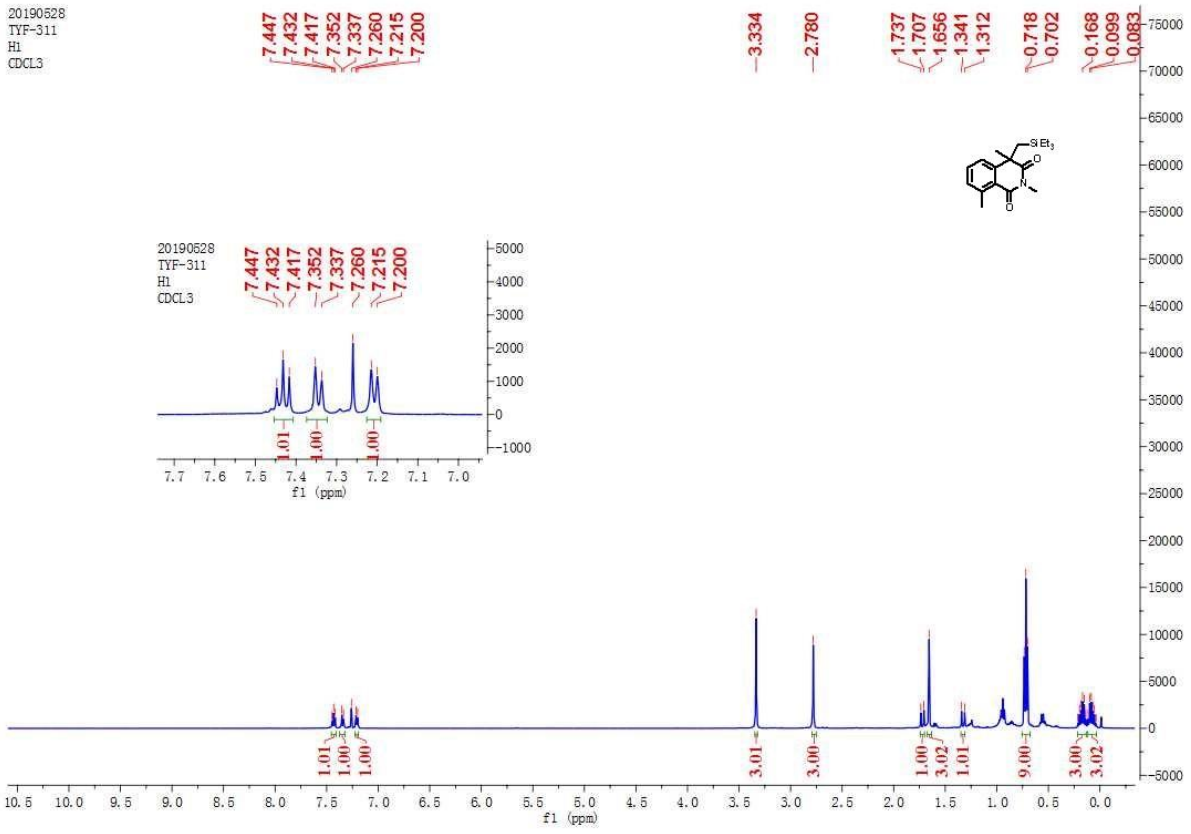
17-^{1}H NMR



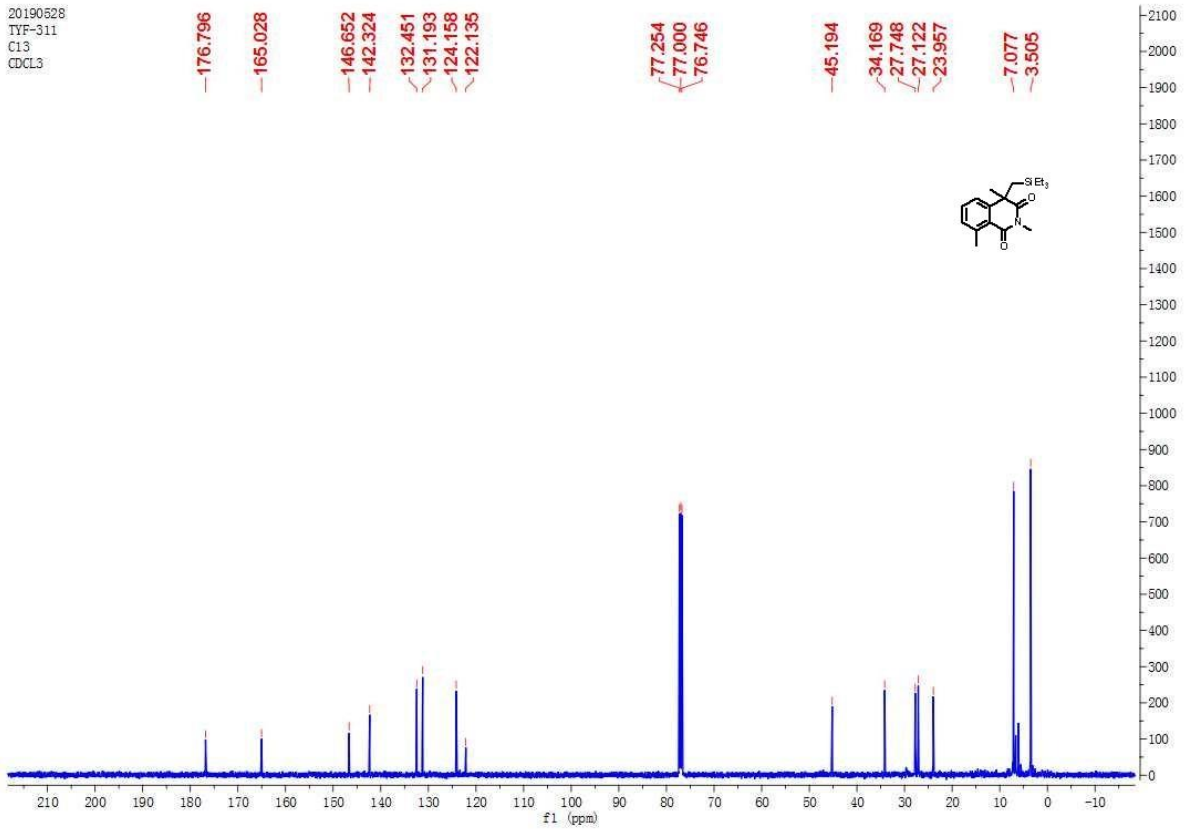
17-^{13}C NMR



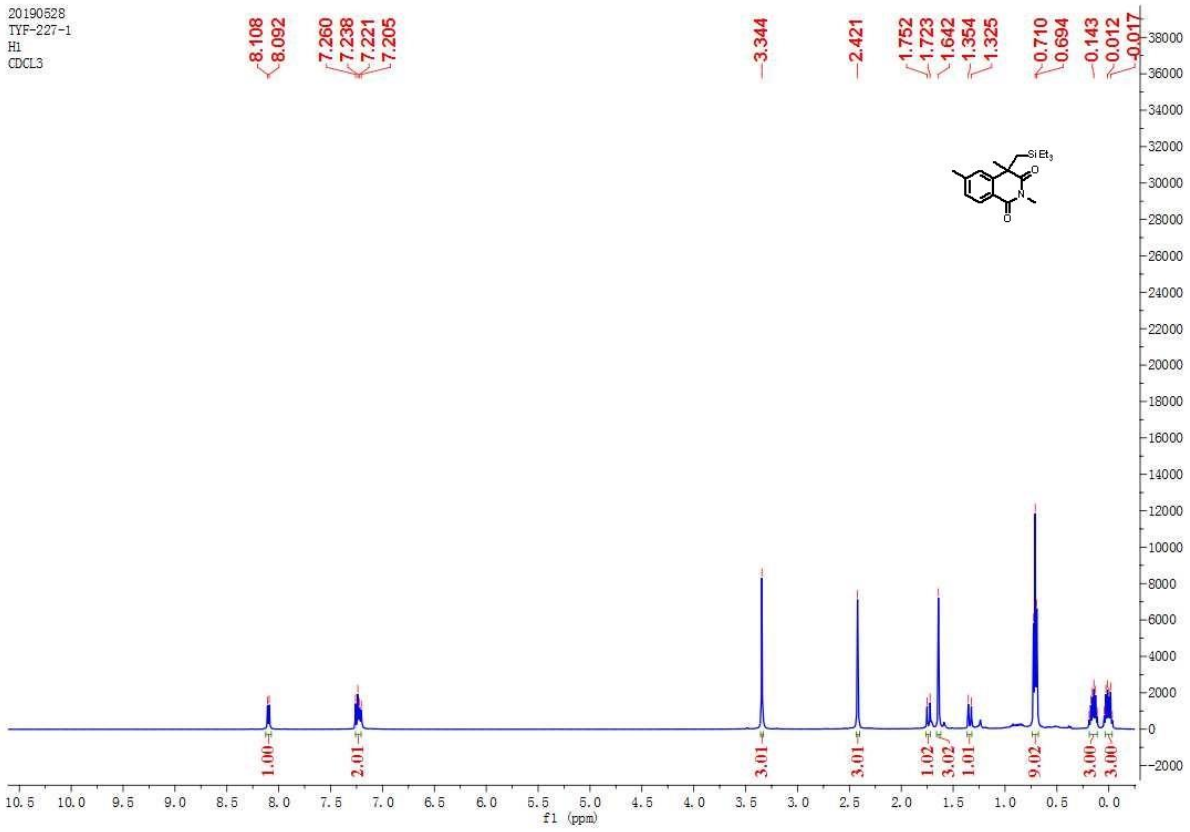
18-^{1}H NMR



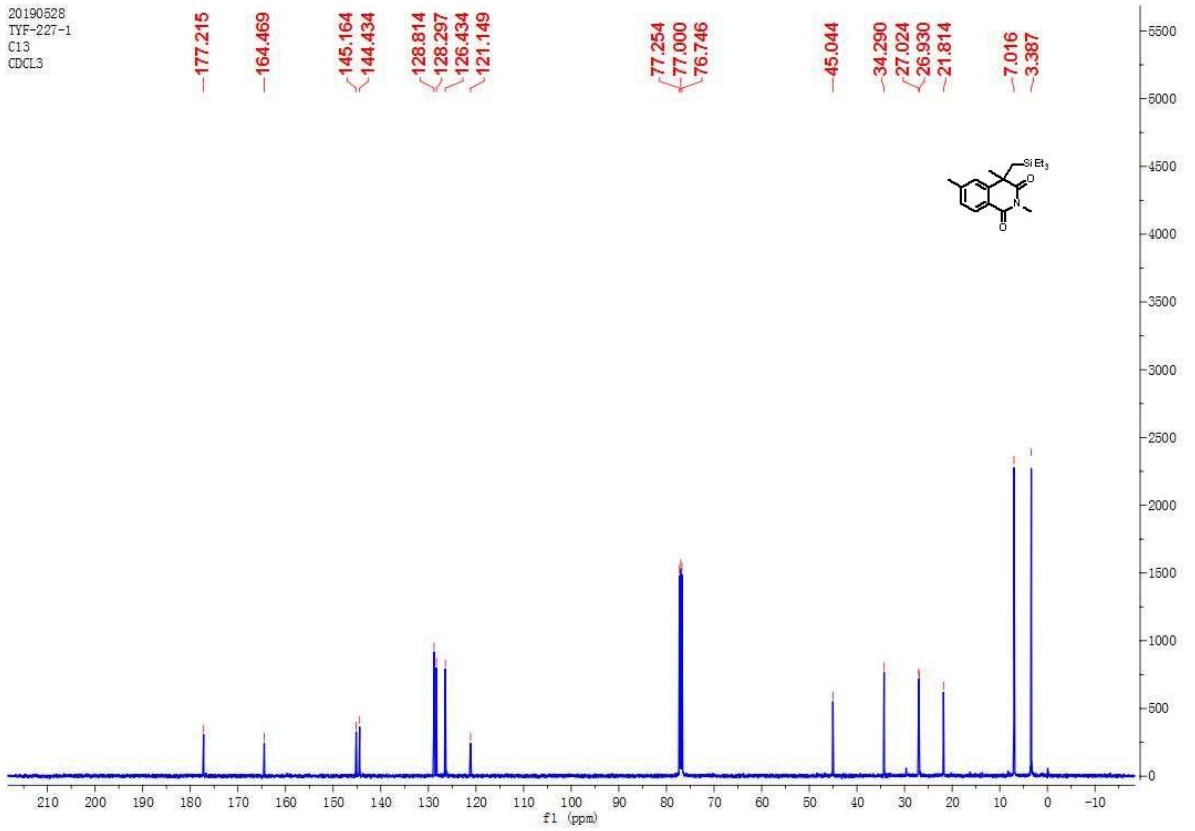
18-^{13}C NMR



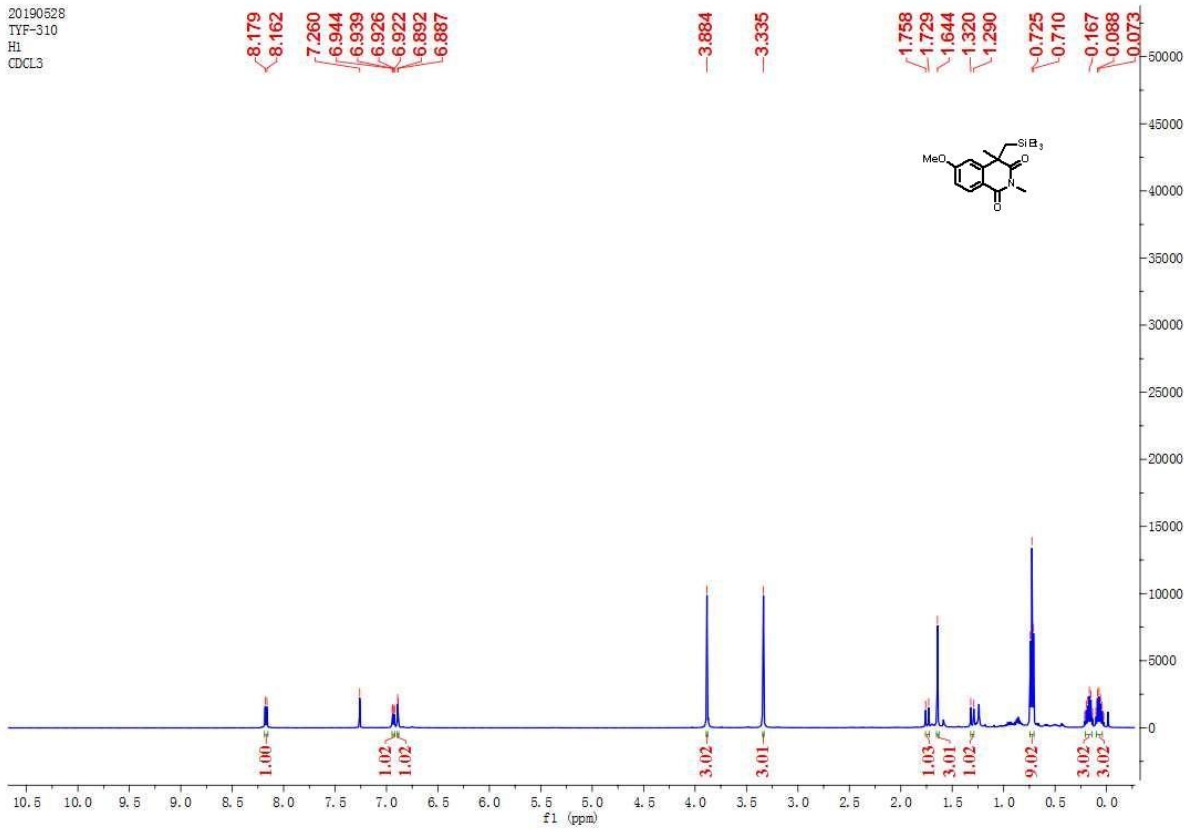
19-^{1}H NMR



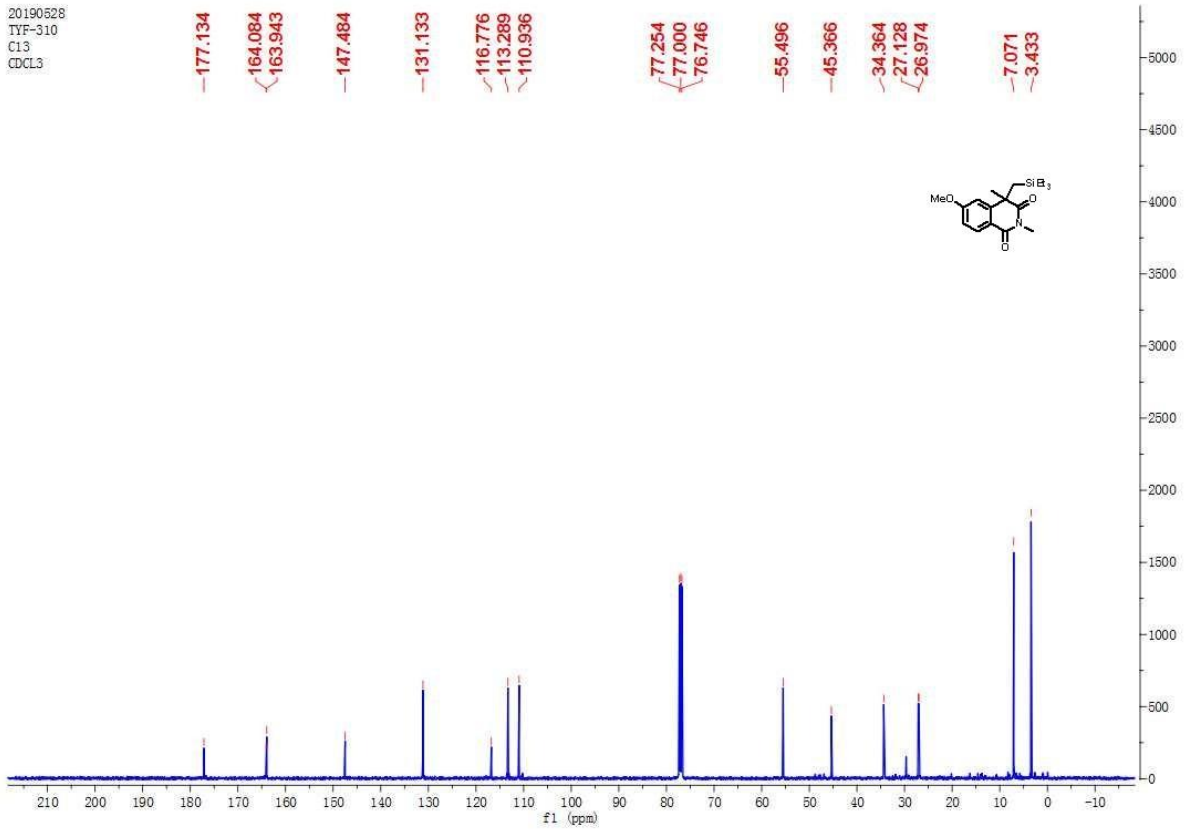
19-^{13}C NMR



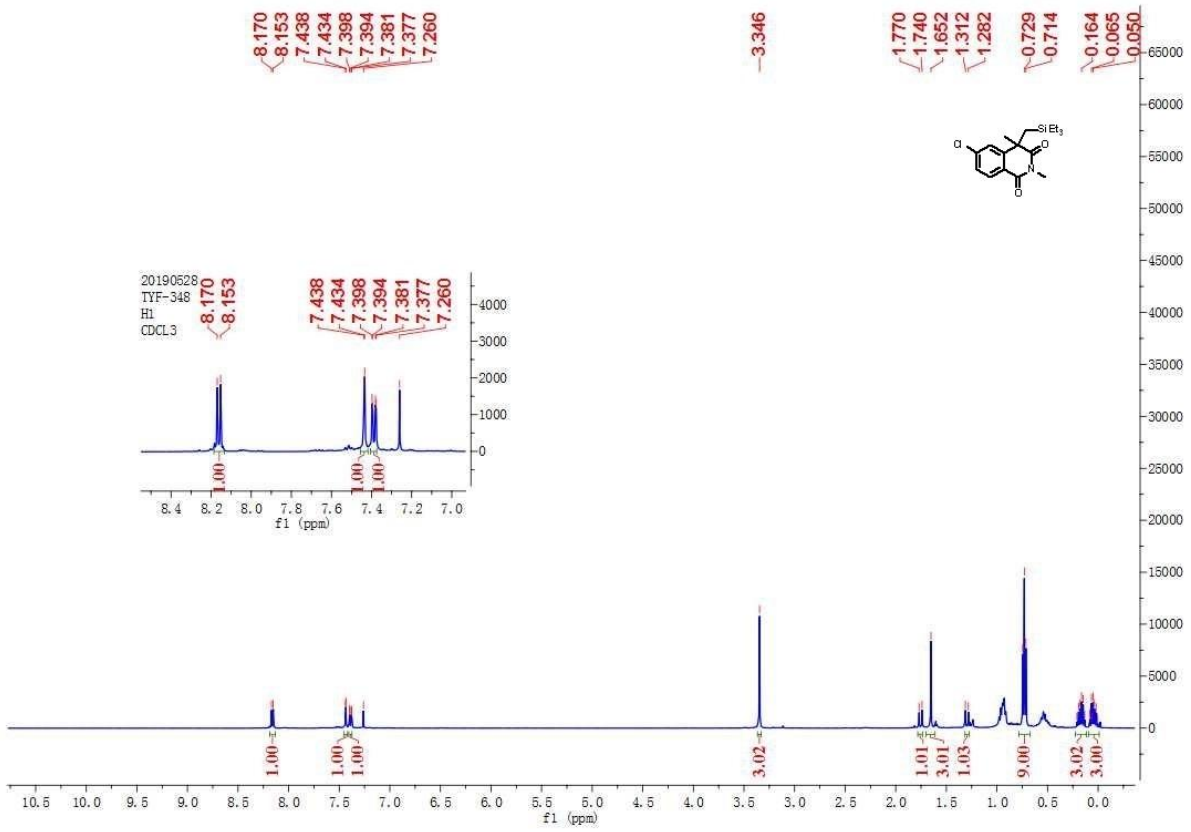
20-^{1}H NMR



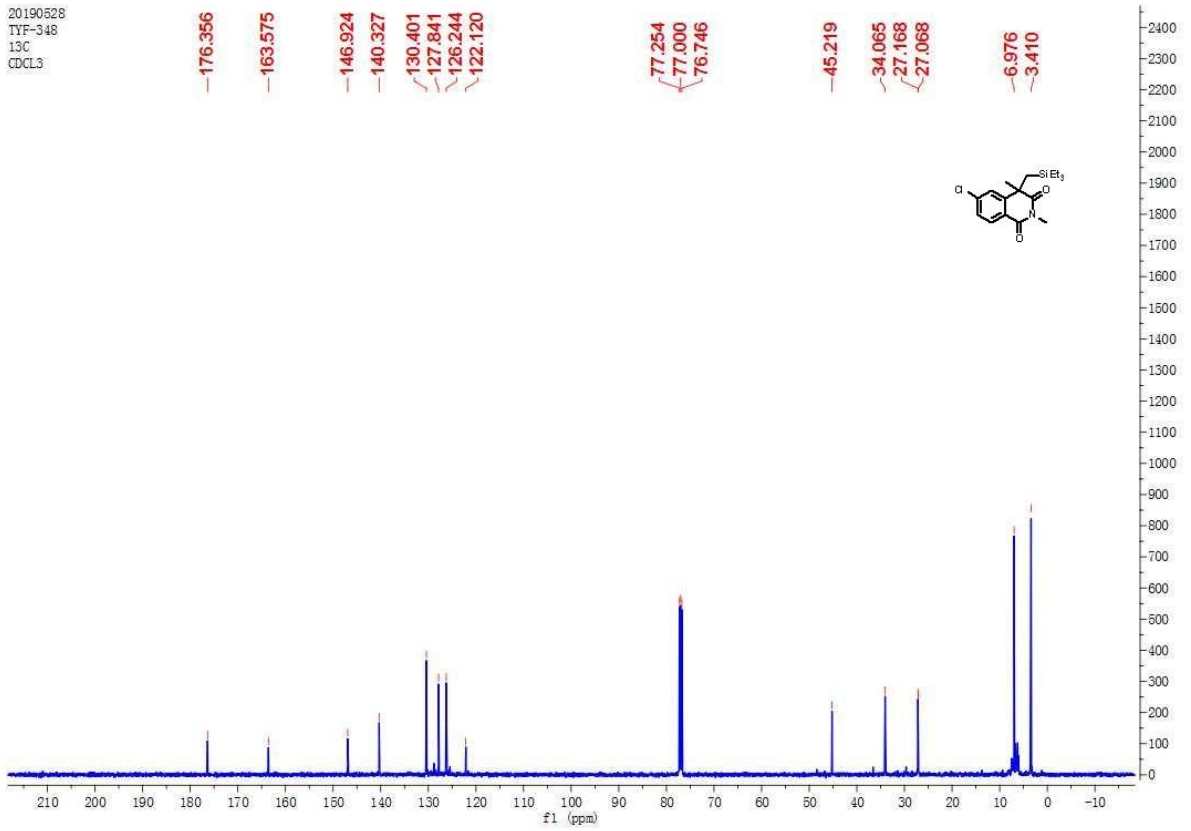
20-^{13}C NMR



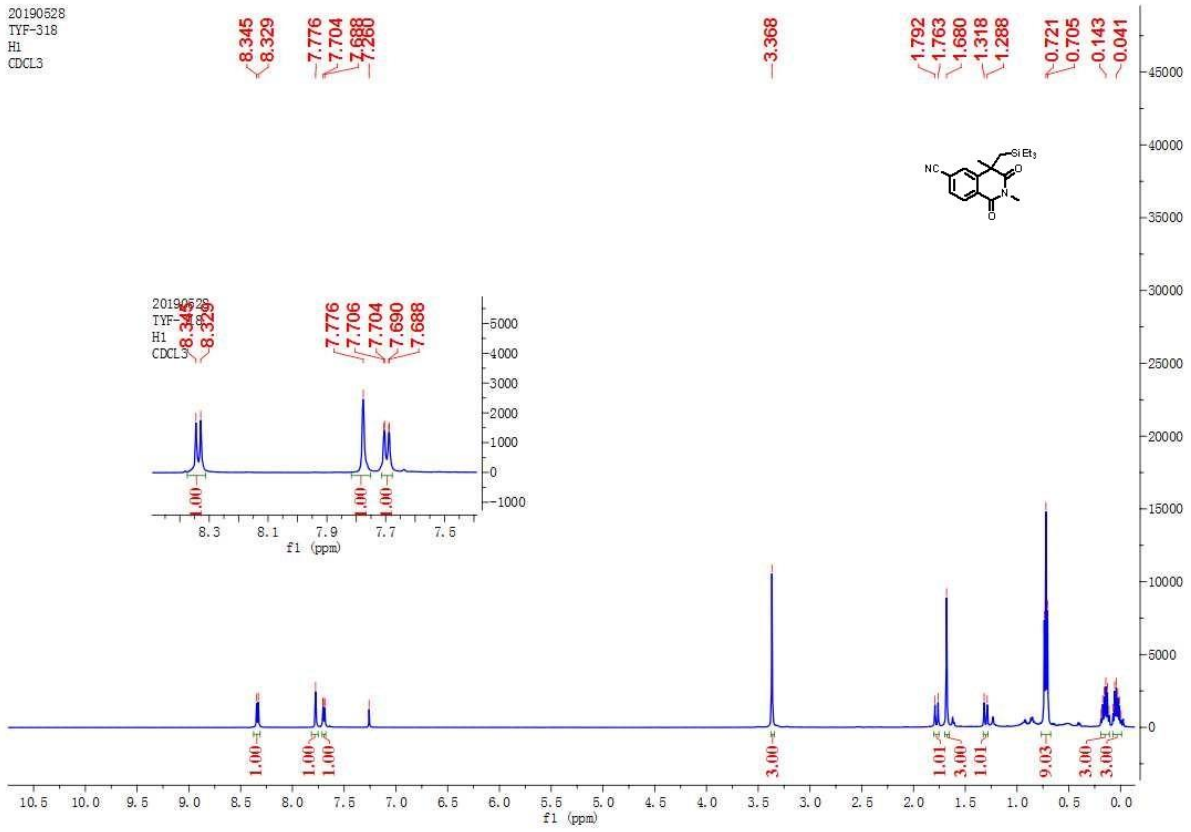
21-^{1}H NMR



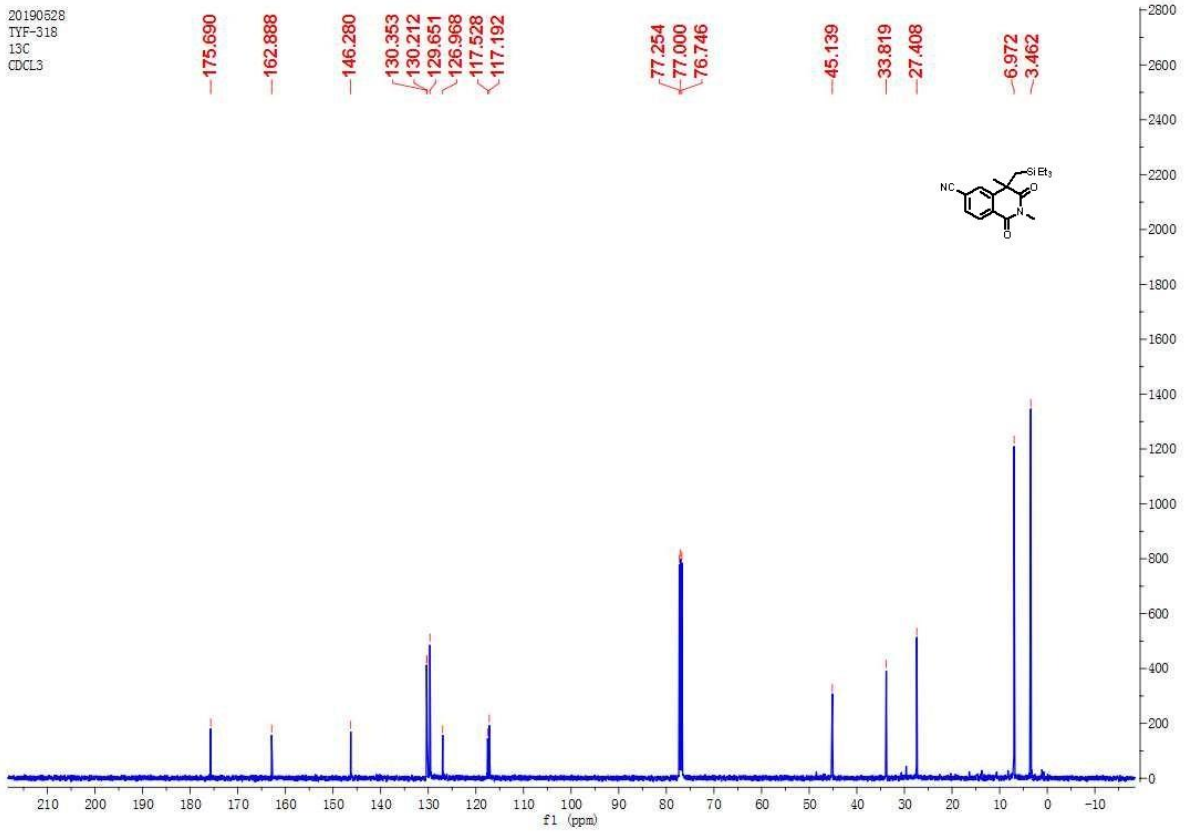
21-^{13}C NMR



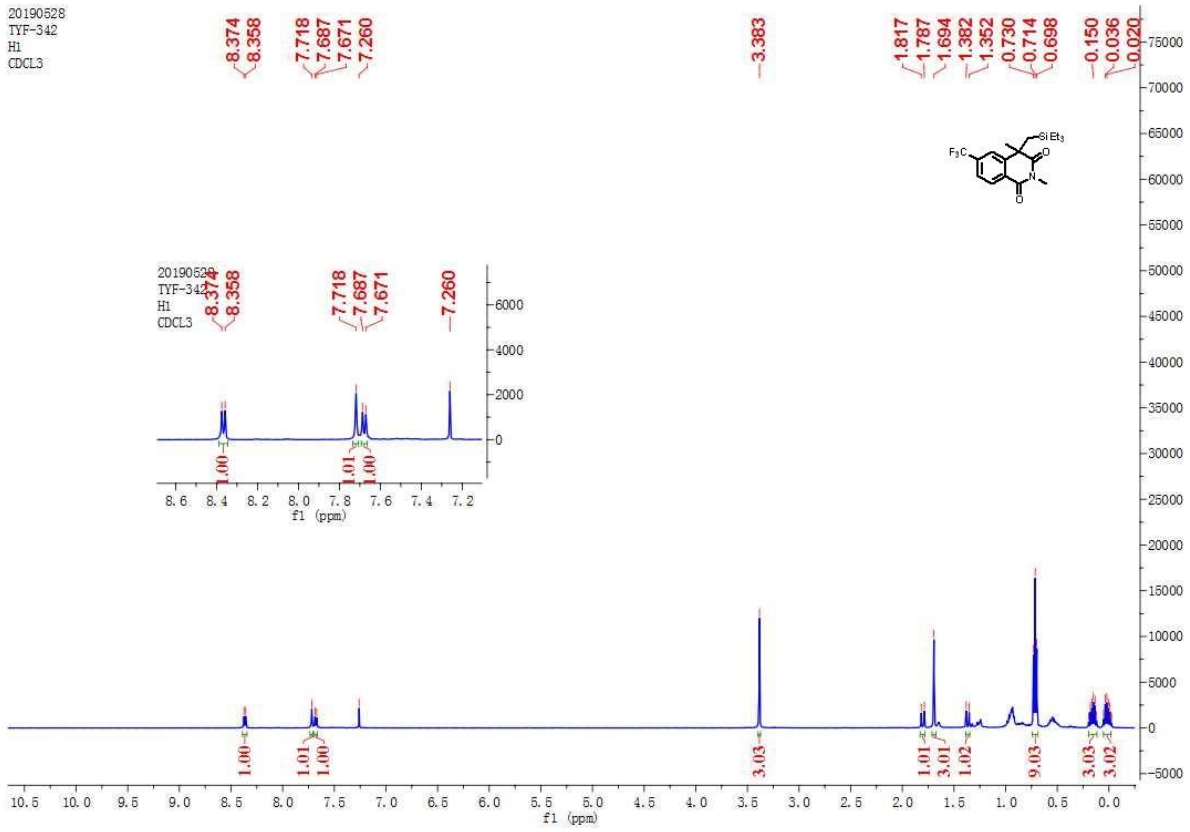
22-^{1}H NMR



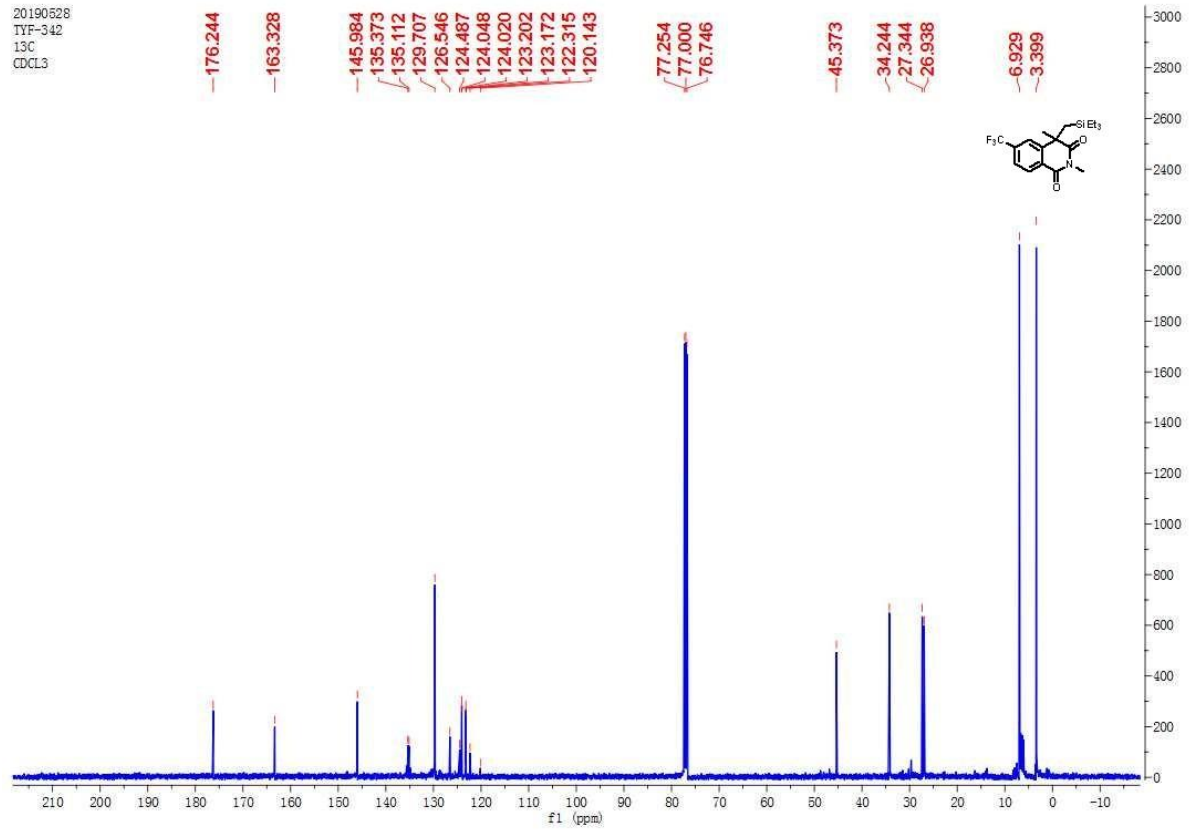
22-^{13}C NMR



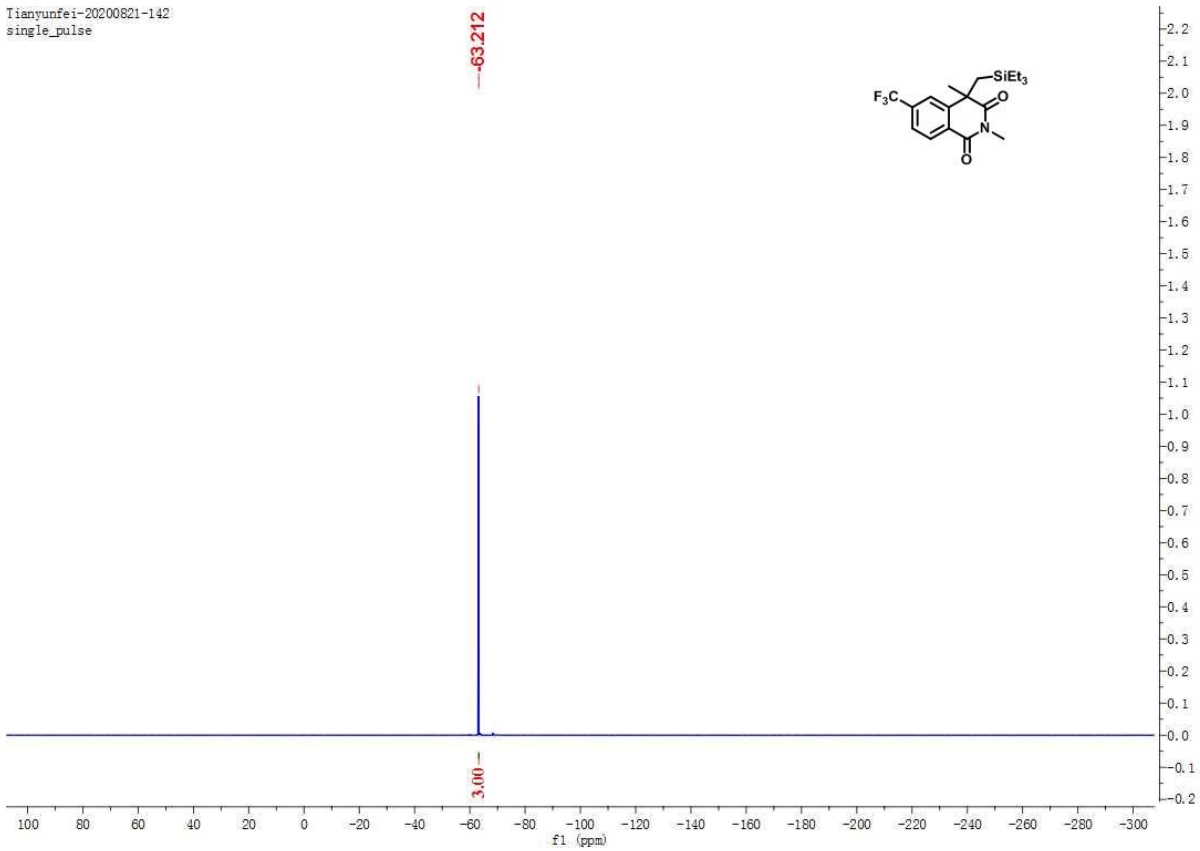
23-^{1}H NMR



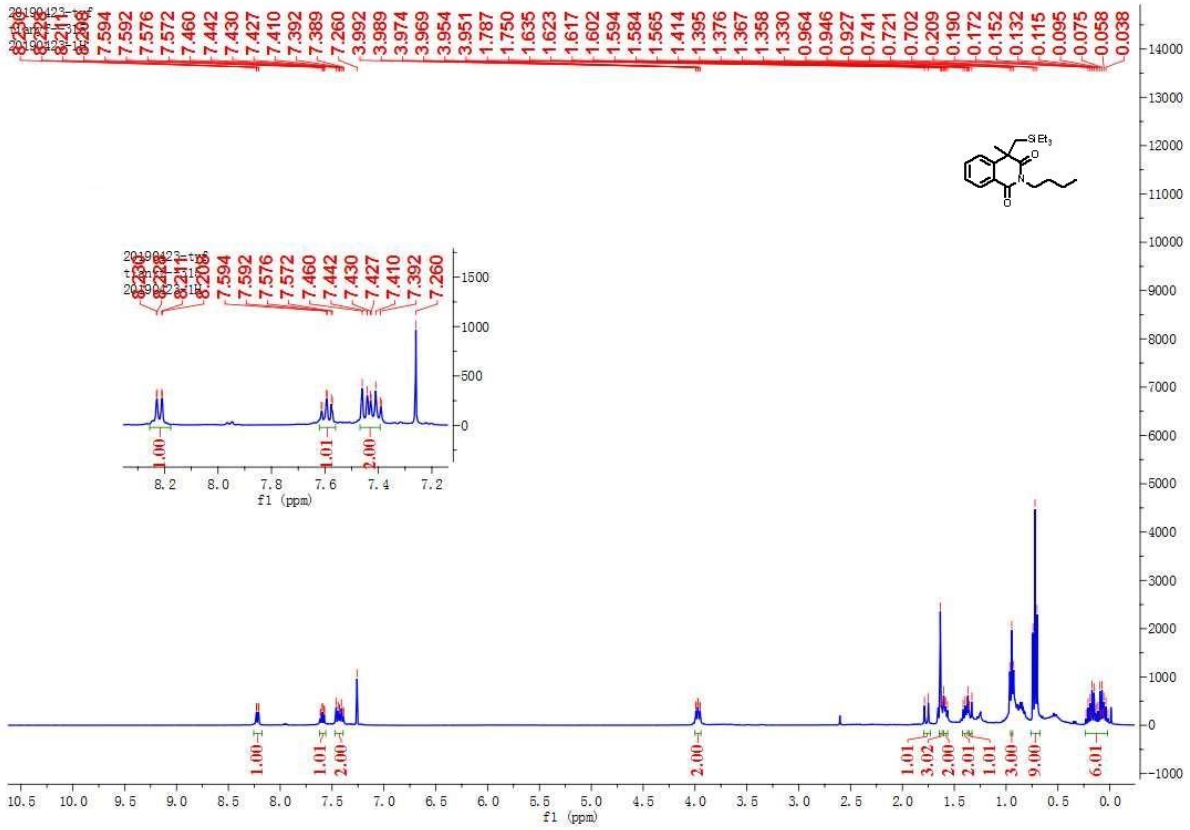
23-^{13}C NMR



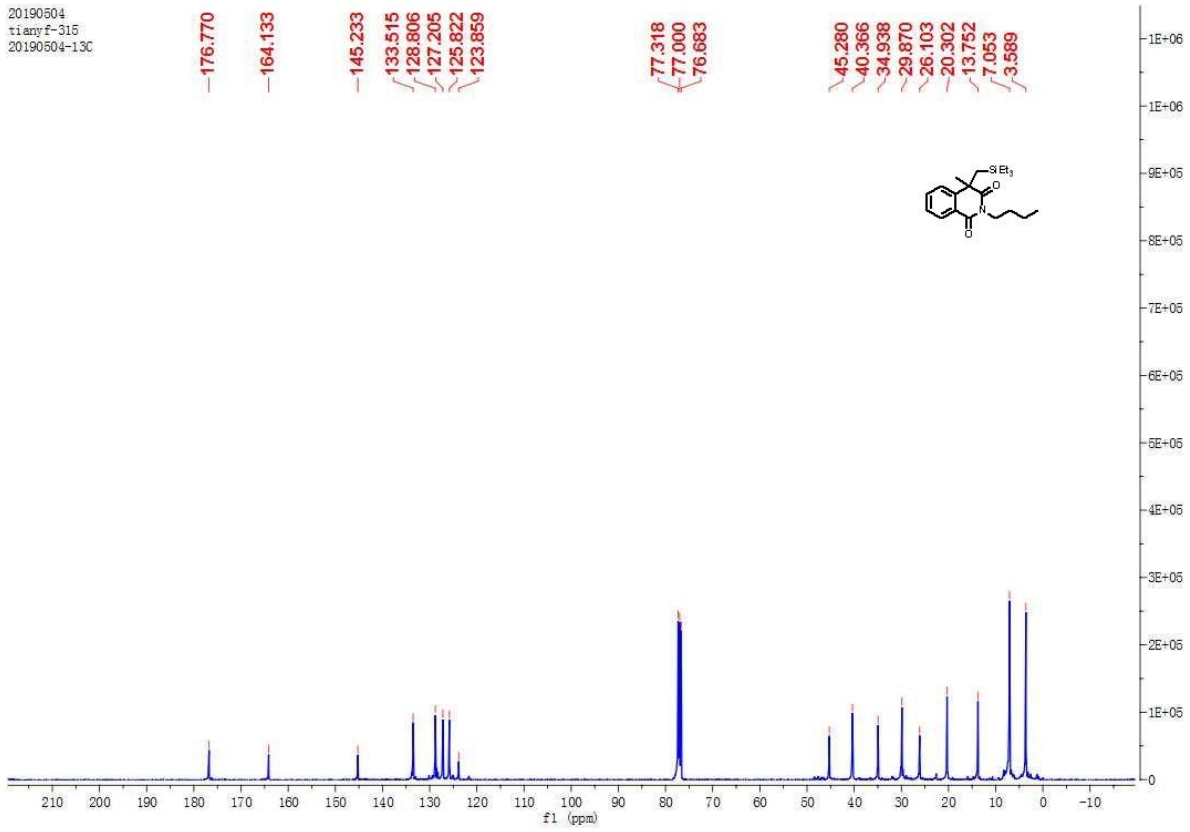
23-^{19}F NMR



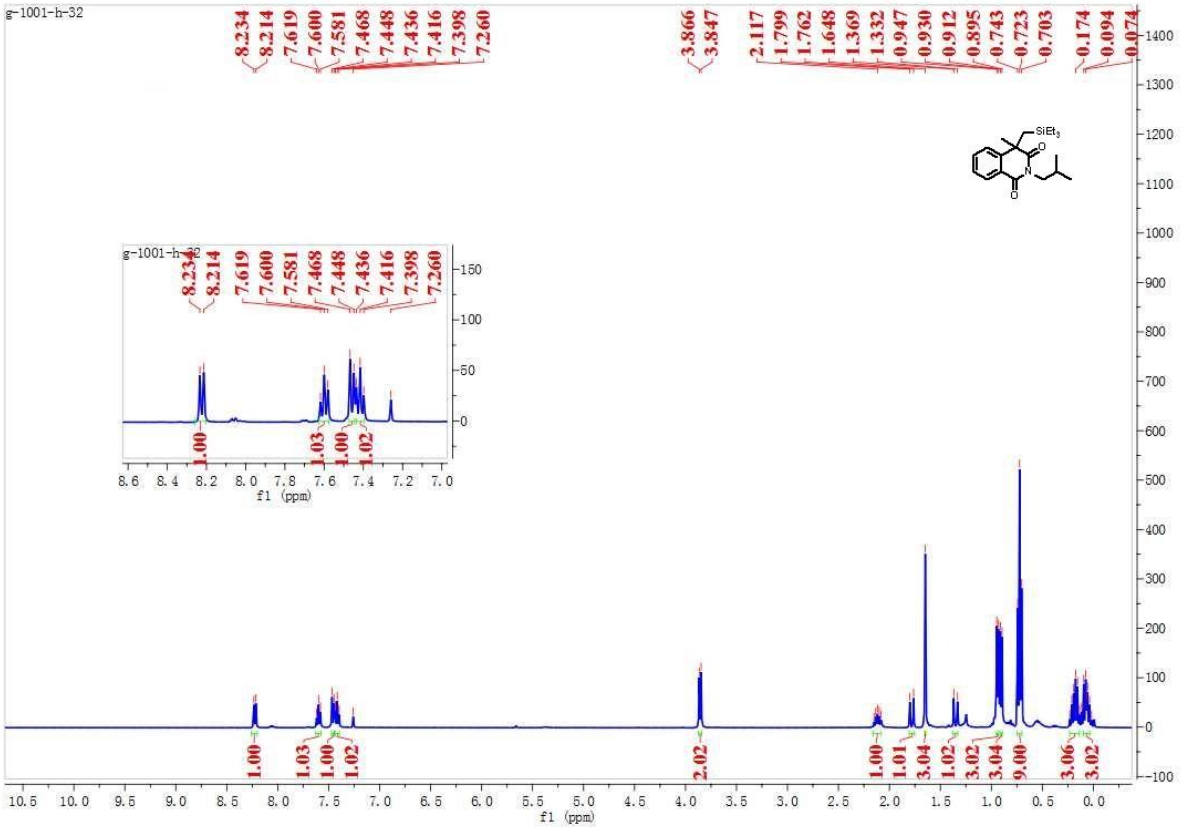
24-^{1}H NMR



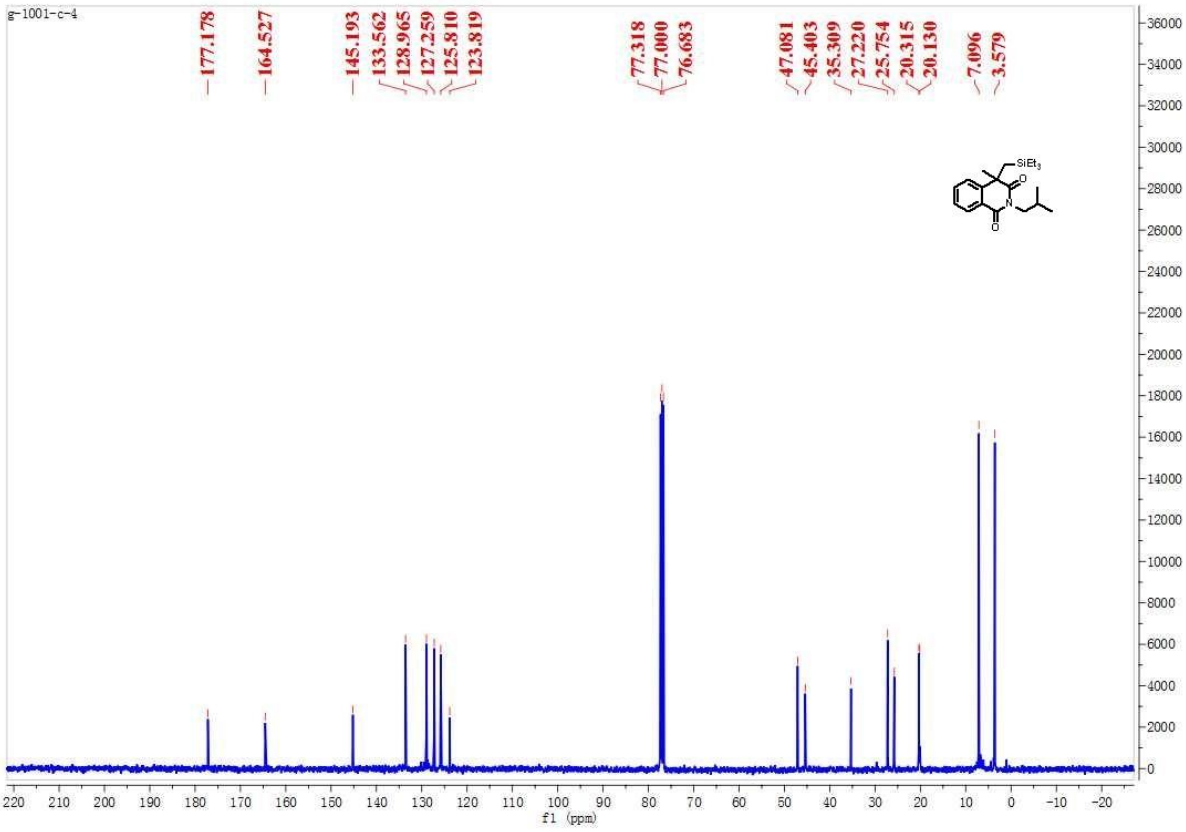
24-^{13}C NMR



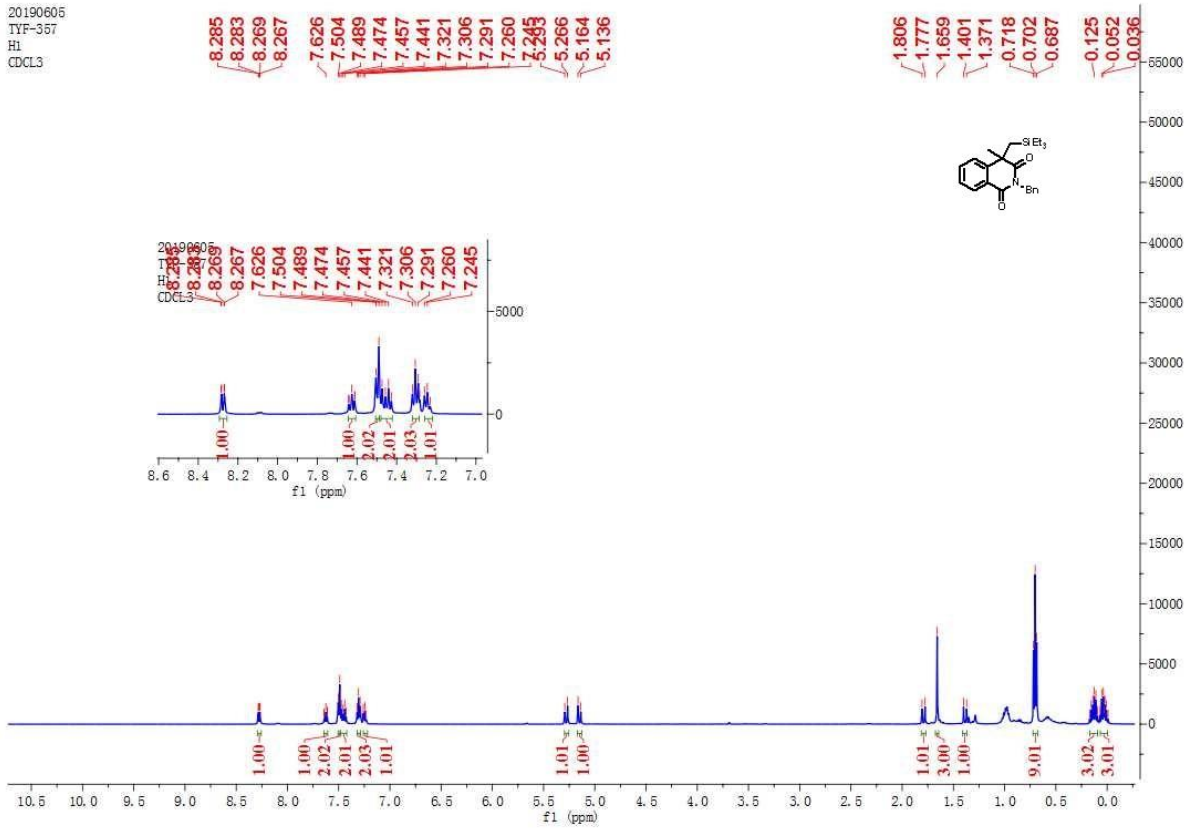
25-^{1}H NMR



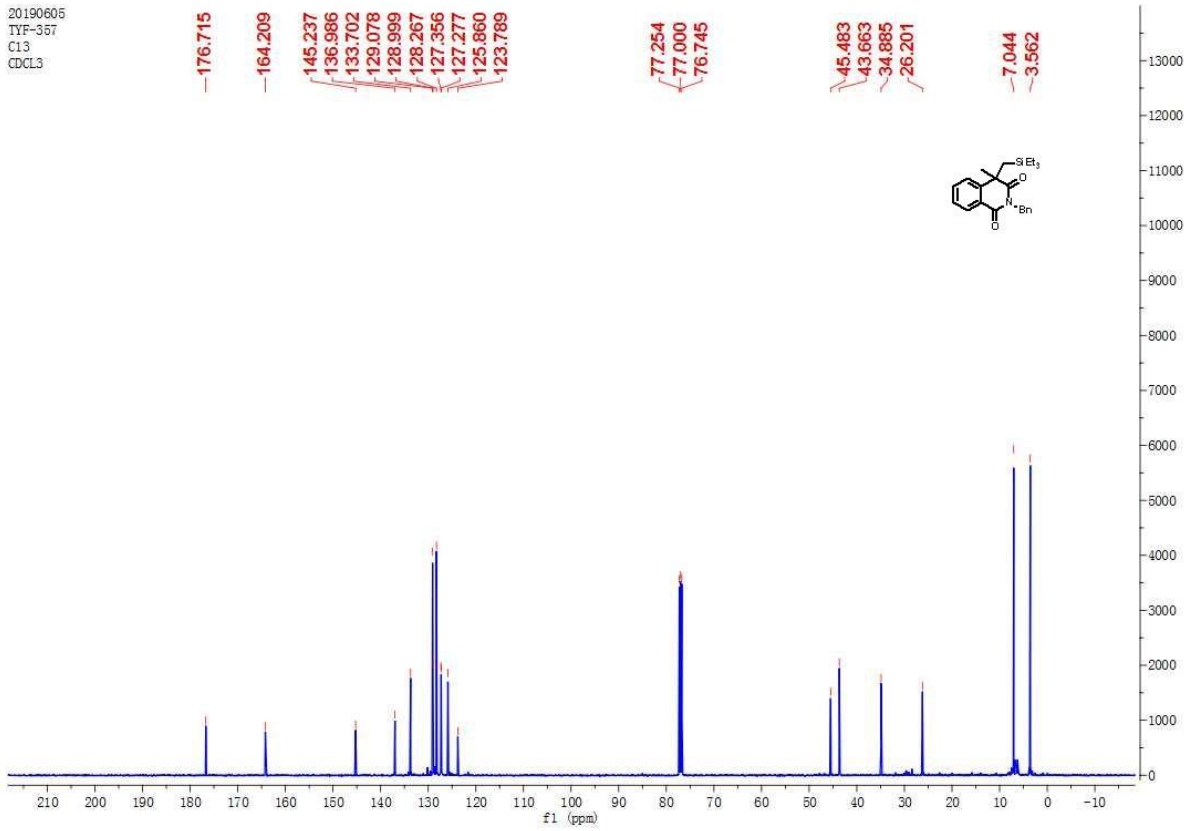
25-^{13}C NMR



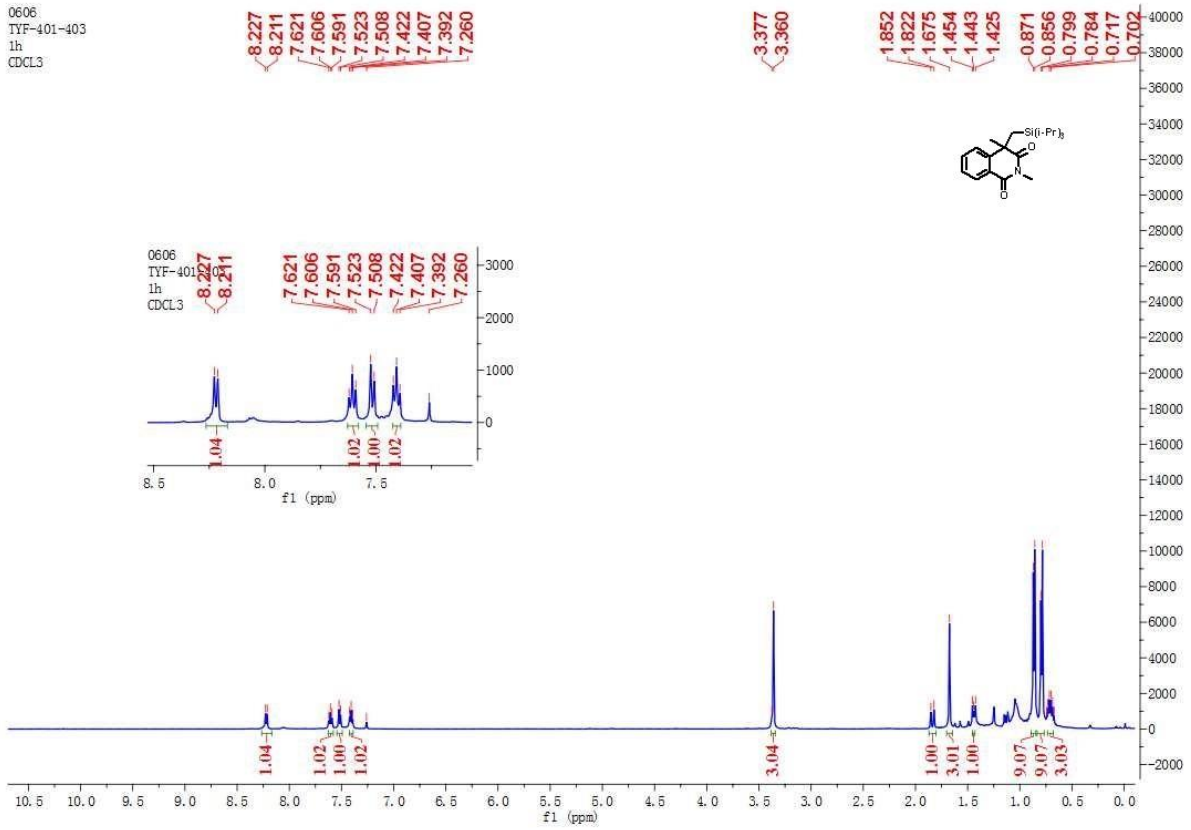
26-^{1}H NMR



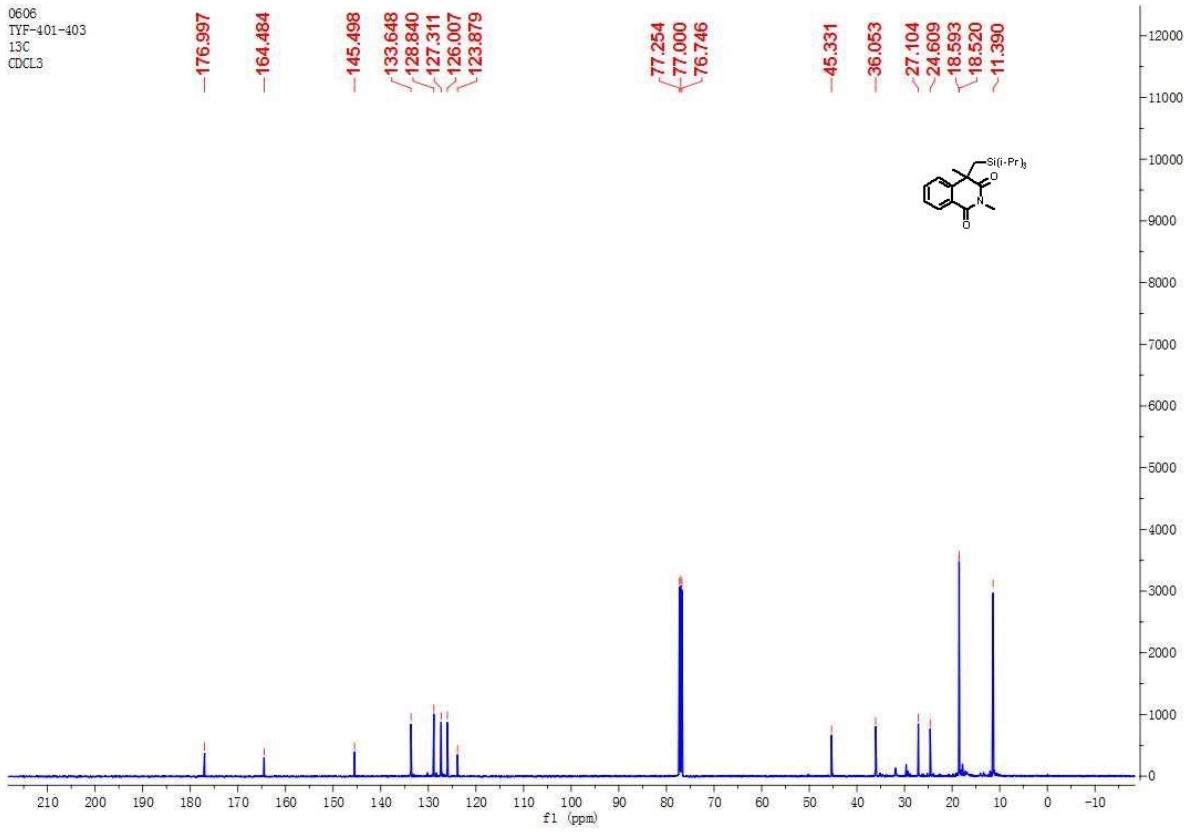
26-^{13}C NMR



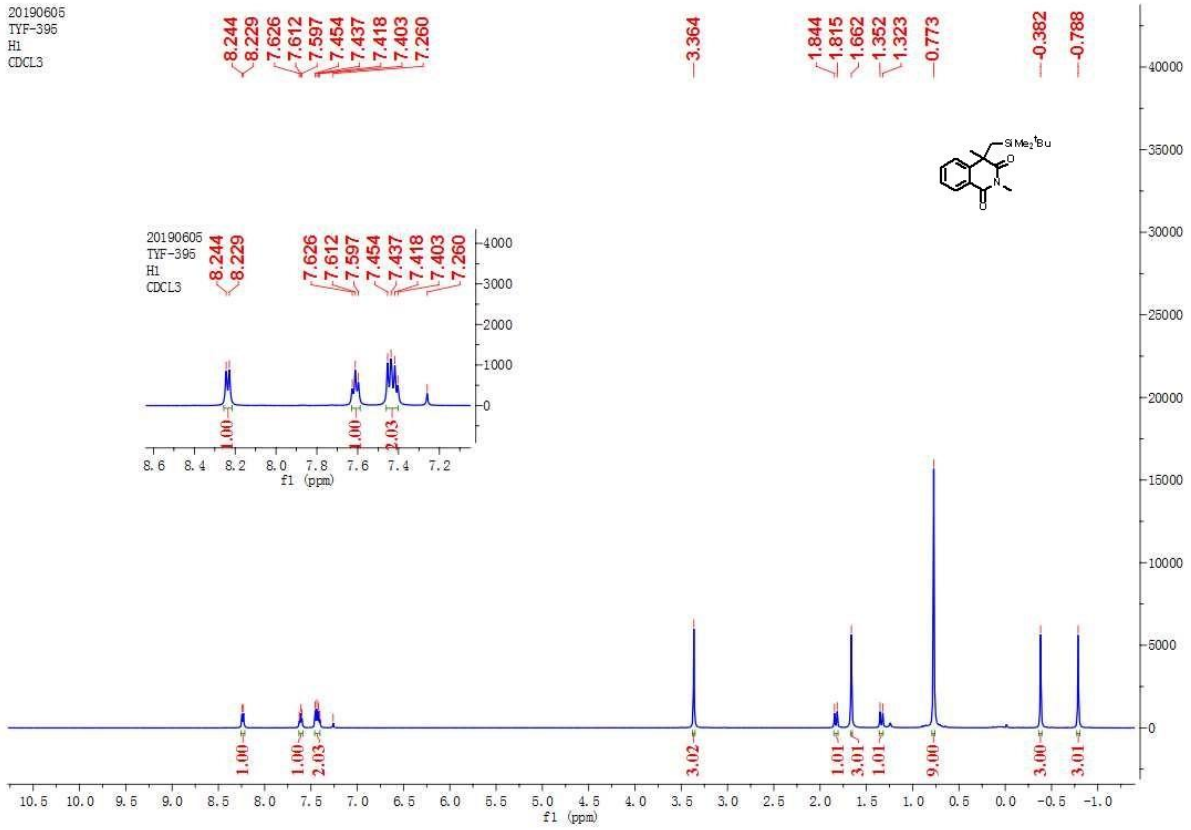
27-^{1}H NMR



27-^{13}C NMR



28-^{1}H NMR



28-^{13}C NMR