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Supporting Information

Brønsted acid-catalyzed selective C-C bond cleavage of 1,3-diketones: a facile synthesis of 4(*3H*)-quinazolinones in aqueous ethyl lactate

Guanshuo Shen,[a] Haifeng Zhou,*[a] Peng Du,[a] Sensheng Liu,[a] Kun Zou,[a] and Yasuhiro Uozumi*[a,b]

[a] Hubei Key Laboratory of Natural Products Research and Development, College of Biological and Pharmaceutical Sciences, China Three Gorges University, Yichang 443002, People's Republic of China.

[b] Institute for Molecular Science (IMS), Higashiyama 5-1, Myodaiji, Okazaki 444-8787, Japan

1. General Information

All reagents and solvents were purchased from commercial suppliers and used without further purification unless otherwise stated. Analytic thin-layer chromatography (TLC) was carried out with silica gel GF 254-coated plates. All products were isolated by column chromatography on silica gel (300-400 mesh) using petroleum ether (PE; bp 60-90 ^{o}C) and ethyl acetate. All compounds were characterized by ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz), and ESI-MS. All ^{1}H NMR shifts are reported in δ units (ppm) relative to the signals for residual $CHCl_3$ (δ = 7.26 ppm) or DMSO (δ = 2.50 ppm) in the corresponding deuterated solvent. All ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (δ = 77.23 ppm) or DMSO-d_6 (δ = 39.60 ppm). NMR data were recorded by Bruker 400 MHz instrument. HRMS data were recorded with ESI ionization sources on a Bruker Apex II instrument. Melting points were determined on an X-4 apparatus.

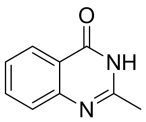
2. Typical procedure for the synthesis of 4(*3H*)-quinazolinones

A flask was charged with 2-aminobenzamide (**1a;** 27.2 mg, 0.2 mmol), pentane-2,4-dione (2**A**; 30.0 mg, 0.3 mmol), CSA (4.6 mg, 0.02 mmol), and 1:9 (v/v) ethyl lactate-H_2O (1.0 mL). The flask was sealed and the mixture was stirred at 100 ^{o}C for 16 h. When the reaction was complete (TLC), the mixture was cooled to r.t., extracted with EtOAc (3×20 mL), and washed with H_2O. The organic phase was dried (Na_2SO_4), filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (silica gel) to give the product **3aA** (31.7 mg, 98%) as white solid.

3. Analytical Data of the Products

2-methylquinazolin-4(*3H*)-one (3aA)

CAS: 1769-24-0



White solid, mp 176-177 °C;

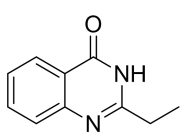
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.61 (s, 3H), 7.47 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.76 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.28 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 12.19 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 22.1, 120.2, 126.2, 126.4, 127.0, 134.9, 149.4, 153.3, 164.4;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_9H_8N_2O$ 161.0709; found 161.0714.

2-ethylquinazolin-4(*3H*)-one (3aB)

CAS: 3137-64-2



White solid, mp 232-233 °C;

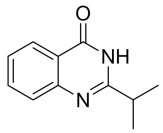
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.45 (t, J = 7.6 Hz, 3H), 2.84 (q, J = 7.6 Hz, 2H), 7.47 (t, J = 7.2 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.78 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 8.29 (d, J = 7.6 Hz, 1H), 11.80 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 11.5, 29.2, 120.5, 126.2, 126.4, 127.2, 134.8, 149.4, 157.5, 164.2 ;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{10}H_{10}N_2O$ 175.0866; found 175.0871.

2-isopropylquinazolin-4(*3H*)-one (3aC)

CAS: 13182-64-4



White solid, mp 232-233 °C;

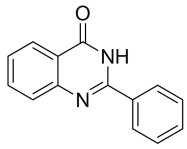
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.44 (d, *J* = 6.8 Hz, 6H), 2.97-3.08 (m, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.70-7.79 (m, 2H), 8.29 (d, *J* = 7.6Hz, 1H), 10.95 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.5, 35.0, 120.8, 126.3, 126.4, 127.4, 134.7, 149.4, 160.5, 163.7;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{11}H_{12}N_2O$ 189.1022; found 189.1027.

2-phenylquinazolin-4(*3H*)-one (3aE)

CAS: 1022-45-3



White solid, mp 122-123 °C;

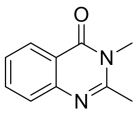
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.52 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.59-7.60 (m, 3H), 7.79-7.86 (m, 2H), 8.15 -8.17 (m, 2H), 8.33 (d, *J*=7.6 Hz, 1H), 10.67 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 126.5, 126.9, 127.1, 128.1, 129.2, 131.8, 132.8, 134.9, 149.4, 151.4, 163.1;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{14}H_{10}N_2O$ 223.0866; found 223.0871.

2,3-dimethylquinazolin-4(*3H*)-one (3bA)

CAS: 1769-25-1



White solid, mp 110-111 °C;

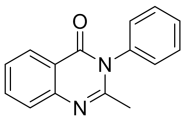
^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.63 (s, 3H), 3.63 (s, 3H), 7.44 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.71 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 8.25 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H) ppm;

^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.6, 31.1, 120.2, 126.5, 126.5, 126.8, 134.3, 147.1, 154.6, 162.3, ppm;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{10}H_{10}N_2O$ 175.0866; found 175.0870.

2-methyl-3-phenylquinazolin-4(*3H*)-one (3cA)

CAS: 2385-23-1



White solid, mp 147-148 °C;

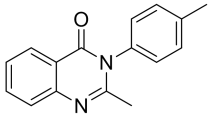
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.25 (s, 3H), 7.27-7.28 (m, 2H), 7.45-7.59 (m, 4H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.77 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.28 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ 24.4, 120.8, 126.7, 126.8, 127.1, 128.0, 129.3, 130.0, 134.6, 137.8, 147.5, 154.2, 162.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{12}N_2O$ 237.1022; found 237.1028.

2-methyl-3-(p-tolyl)quinazolin-4(*3H*)-one (3dA)

CAS: 22316-59-2



White solid, mp 150-151 °C;

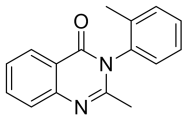
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.25 (s, 3H), 2.45 (s, 3H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.76 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 8.27 (d, *J* = 8.0 Hz, 1H) ppm;

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 21.3, 24.4, 120.8, 126.5, 126.7, 127.1, 127.7, 130.6, 134.5, 135.1, 139.3, 147.5, 154.5, 162.4;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{16}H_{14}N_2O$ 251.1179; found 251.1185.

2-methyl-3-(*o*-tolyl)quinazolin-4(*3H*)-one (3eA)

CAS: 72-44-6



White solid, mp 119-121 °C;

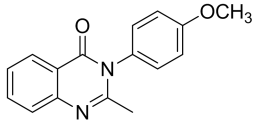
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.13 (s, 3H), 2.19 (s, 3H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.35-7.42 (m, 3H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.78 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.29 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 17.4, 23.9, 120.7, 126.6, 126.8, 127.1, 127.6, 127.9, 129.6, 131.5, 134.6, 135.3, 136.8, 147.6, 154.3, 161.7;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{16}H_{14}N_2O$ 251.1179; found 251.1186.

3-(4-methoxyphenyl)-2-methylquinazolin-4(*3H*)-one (3fA)

CAS: 53574-77-9



White solid, mp 169-171 °C;

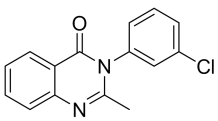
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.26 (s, 3H), 3.88 (s, 3H), 7.05 (d, *J* = 8.8 Hz, 2H), 7.17 (d, *J* = 8.8 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.76 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.26 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 24.4, 55.5, 115.2, 120.8, 126.6, 126.7, 127.1, 129.0, 130.2, 134.5, 147.5, 154.8, 159.9, 162.5;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{16}H_{14}N_2O_2$ 267.1128; found 267.1135.

3-(3-chlorophenyl)-2-methylquinazolin-4(*3H*)-one (3gA)

CAS: 340-94-3



White solid, mp 130-131 °C;

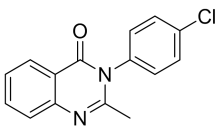
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.27 (s, 3H), 7.18-7.20 (m, 1H), 7.31 (s, 1H), 7.46-7.51 (m, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.79 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 8.26 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 24.4, 120.6, 126.5, 126.9, 126.9, 127.1, 128.6, 129.7, 131.0, 134.8, 135.6, 138.8, 147.4, 153.5, 162.1;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{11}ClN_2O$ 271.0633; found 271.0641.

3-(4-chlorophenyl)-2-methylquinazolin-4(*3H*)-one (3hA)

CAS: 1788-93-8



White solid, mp 157-158 °C;

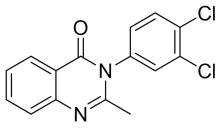
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.25 (s, 3H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.48 (t, d = 8.4 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.78 (t, *J* = 7.2 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 24.4, 120.6, 126.8, 127.1, 129.5, 130.3, 134.8, 135.4, 136.2, 147.4, 153.7, 162.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{11}ClN_2O$ 271.0633; found 271.0639.

3-(3,4-dichlorophenyl)-2-methylquinazolin-4(*3H*)-one (3iA)

CAS: 4285-67-0



White solid, mp 164-165 °C;

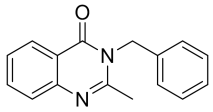
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.26 (s, 3H), 7.13 (d, *J* = 8.8 Hz, 1H), 7.41 (s, 1H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.61-7.67 (m, 2H), 7.77 (t, *J* = 7.6 Hz, 1H), 8.21 (d, *J* = 7.6 Hz, 1H) ppm;

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 24.3, 120.3, 126.9, 126.9, 126.9, 127.6, 130.2, 131.6, 133.9, 134.0, 134.9, 136.8, 147.2, 153.1, 161.9 ppm;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{10}Cl_2N_2O$ 305.0243; found 305.0252.

3-benzyl-2-methylquinazolin-4(*3H*)-one (3jA)

CAS: 4260-34-8



White solid, mp 123-124 °C;

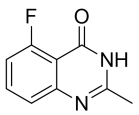
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.59 (s, 3H), 5.44 (s, 2H), 7.24 (d, *J* = 7.2 Hz, 2H), 7.31-7.38 (m, 3H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.79 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.35 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 23.4, 47.1, 120.3, 126.5, 126.5, 126.7, 127.1, 127.7, 128.9, 134.4, 135.8, 147.3, 154.6, 162.4;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{16}H_{14}N_2O$ 251.1179; found 251.1185.

5-fluoro-2-methylquinazolin-4(*3H*)-one (3kA)

CAS: 143745-24-8



White solid, mp 252-253 °C;

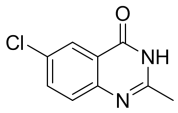
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.56 (s, 3H), 7.10 (t, *J* = 9.2 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.67-7.72 (m, 1H), 11.22 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 22.0, 110.2, 113.0, 123.0, 135.2, 151.3, 154.2, 160.1, 162.6;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_9H_7FN_2O$ 179.0615; found 179.0621.

6-chloro-2-methylquinazolin-4(*3H*)-one (3mA)

CAS: 7142-09-8



White solid, mp 286-287 °C;

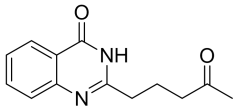
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.34 (s, 3H), 7.59 (d, J = 8.8 Hz, 1H), 7.79 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.80 (d, J = 2.4 Hz, 1H), 12.40 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 21.9, 122.3, 125.1, 129.3, 130.5, 134.8, 148.1, 155.4, 161.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_9H_7ClN_2O$ 195.0320; found 195.0325.

2-(4-oxopentyl)quinazolin-4(*3H*)-one (5aA)

CAS: 86663-60-7



White solid, mp 145-146 °C;

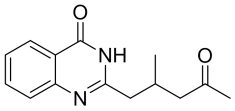
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.13-2.20 (m, 2H), 2.18 (s, 3H), 2.64 (t, J = 7.2 Hz, 2H), 2.80 (t, J = 7.2 Hz, 2H), 7.48 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.77 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 8.29 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 11.52 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 21.1, 30.0, 34.7, 42.3, 120.6, 126.3, 126.5, 127.2, 134.8, 149.2, 155.8, 163.8, 208.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{13}H_{14}N_2O_2$ 231.1128; found 231.1134.

2-(2-methyl-4-oxopentyl)quinazolin-4(*3H*)-one (5aB)

CAS: none



White solid, mp 154-157 °C;

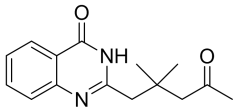
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.13 (d, J = 6.0 Hz, 1H), 2.19 (s, 3H), 2.47-2.53 (m, 1H), 2.68-2.83 (m, 4H), 7.51 (t, J = 7.2 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.81 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 8.33 (dd, J_1 = 7.6 Hz, J_2 = 0.4 Hz, 1H), 11.86 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.1, 28.6, 30.5, 42.4, 50.0, 120.7, 126.3, 126.5, 127.3, 134.8, 149.2, 155.3, 163.9, 208.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{14}H_{16}N_2O_2$ 245.1285; found 245.1284.

2-(2,2-dimethyl-4-oxopentyl)quinazolin-4(*3H*)-one (5aC)

CAS: 86663-57-2



White solid, mp 159-160 °C;

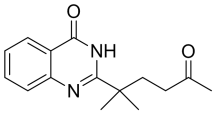
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.16 (s, 6H), 2.30 (s, 3H), 2.46 (s, 2H), 2.73 (s, 2H), 7.45(t, J = 7.2 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.74 (dt, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 8.28 (d, J = 8.0 Hz, 1H), 10.79 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 29.0, 33.6, 35.5, 45.4, 51.5, 121.1, 126.4, 126.4, 127.2, 134.4, 149.0, 154.0, 162.1, 212.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{18}N_2O_2$ 259.1441; found 259.1447.

2-(3,3-dimethyl-4-oxopentyl)quinazolin-4(*3H*)-one (5aD)

CAS: none



White solid, mp 137-139 °C;

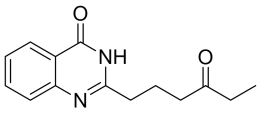
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.32 (s, 6H), 2.11-2.16 (m, 2H), 2.28 (s, 3H), 2.70-2.74 (m, 2H), 7.52 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.81 (dt, J_1 = 7.2 Hz, J_2 = 1.6 Hz, 1H), 8.30 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 11.63 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 24.4, 25.2, 31.6, 36.8, 47.6, 120.7, 126.3, 126.6, 127.2, 134.8, 149.3, 156.3, 163.9, 213.5;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{15}H_{18}N_2O_2$ 259.1441; found 259.1440.

2-(4-oxopentyl)quinazolin-4(*3H*)-one (5aE)

CAS: none



White solid, mp 149-151 °C;

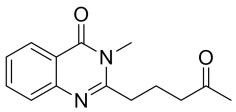
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.04 (t, J = 7.2 Hz, 3H), 2.14-2.21 (m, 2H), 2.45 (q, J = 7.2 Hz, 2H), 2.60 (t, J = 7.2 Hz, 2H), 2.80 (t, J = 7.2 Hz, 2H), 7.47 (dt, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.77 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 8.28 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 11.58 (s, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 7.7, 21.2, 34.8, 36.0, 41.0, 120.6, 126.3, 126.5, 127.2, 134.8, 149.2, 155.9, 163.8, 211.0;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{14}H_{16}N_2O_2$ 245.1285; found 245.1292.

3-methyl-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5bA)

CAS: 1616629-16-3



Pale yellow oily liquid;

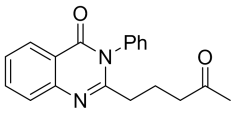
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.08-2.15 (m, 2H), 2.17 (s, 3H), 2.68 (t, J = 6.8 Hz, 2H), 2.84 (t, J = 7.2 Hz, 2H), 3.66 (s, 3H), 7.43 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.71 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.25 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.4, 30.2, 30.6, 34.6, 42.3, 120.3, 126.5, 126.8, 126.8, 134.1, 147.1, 156.4, 162.6, 208.4;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{14}H_{16}N_2O_2$ 245.1285; found 245.1292.

2-(4-oxopentyl)-3-phenylquinazolin-4(*3H*)-one (5cA)

CAS: none



Pale yellow solid, mp 131-134 °C;

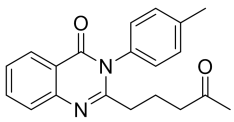
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.96-2.02 (m, 2H), 2.07 (s, 3H), 2.43 (t, J = 7.2 Hz, 2H), 2.50 (t, J = 7.2 Hz, 2H), 7.25-7.28 (m, 3H), 7.45-7.58 (m, 4H), 7.69 (dd, J_1 = 8.0 Hz, J_2 = 0.4 Hz, 1H), 7.76 (dt, J_1 = 6.8 Hz, J_2 = 1.6 Hz, 1H), 8.27 (q, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.6, 29.9, 34.8, 42.5, 120.9, 126.7, 127.1, 128.3, 129.3, 130.0, 134.5, 137.2, 147.4, 156.0, 162.5, 208.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{19}H_{18}N_2O_2$ 307.1441; found 307.1449.

2-(4-oxopentyl)-3-(p-tolyl)quinazolin-4(*3H*)-one (5dA)

CAS: none



Pale yellow solid, mp 97-99 °C;

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.94-2.02 (m, 2H), 2.08 (s, 3H), 2.42-2.46 (m, 3H), 2.42 (s, 3H), 2.50 (t, *J* = 7.2 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.45 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.75 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.26 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

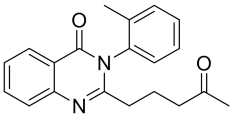
^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.6, 21.3, 29.9, 34.7, 42.6, 120.9, 127.0, 127.1, 128.0, 130.6, 134.5, 134.5, 139.4, 147.4, 156.2, 162.6, 208.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{20}H_{20}N_2O_2$ 321.1598; found 321.1602.

2-(4-oxopentyl)-3-(o-tolyl)quinazolin-4(*3H*)-one (5eA)

CAS: none

White solid, mp 113-115 °C;



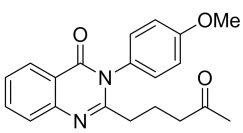
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.98-2.04 (m, 2H), 2.08 (s, 3H), 2.10 (s, 3H), 2.27-2.41 (m, 2H), 2.47-2.53 (m, 2H), 7.16 (d, *J* = 7.2 Hz, 1H), 7.34-7.41 (m, 3H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.64-7.72 (m, 1H), 7.77 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.28 (q, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 17.5, 20.3, 30.0, 34.3, 42.6, 120.8, 126.7, 127.1, 127.6, 128.3, 129.6, 131.6, 134.5, 135.5, 136.2, 147.6, 156.0, 161.8, 208.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{20}H_{20}N_2O_2$ 321.1598; found 321.1603.

3-(4-methoxyphenyl)-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5fA)

CAS: none



Pale yellow solid, mp 125-127 °C;

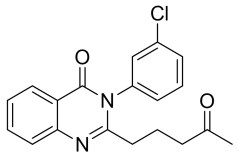
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.94-2.01 (m, 2H), 2.08 (s, 3H), 2.44 (t, *J* = 7.2 Hz, 2H), 2.49 (t, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 7.03-7.06 (m, 2H), 7.14-7.17 (m, 2H), 7.45 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.75 (dt, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 8.24 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.6, 29.9, 34.8, 42.5, 55.6, 115.2, 120.8, 126.6, 127.0, 127.1, 129.3, 129.6, 134.5, 147.4, 156.5, 160.0, 162.7, 208.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{20}H_{20}N_2O_3$ 337.1547; found 337.1554.

3-(3-chlorophenyl)-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5gA)

CAS: none



Pale yellow oily liquid .

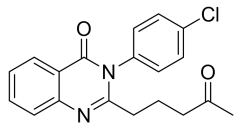
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.98-2.01 (m, 2H), 2.08 (s, 3H), δ = 2.42 (t, *J* = 7.2 Hz, 2H), 2.51-2.56 (m, 2H), 7.18-7.21 (m, 1H), 7.30 (s, 1H), 7.45-7.50 (m, 3H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.77 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 8.24 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.4, 29.9, 34.7, 42.4, 120.7, 126.8, 126.9, 127.1, 127.2, 128.8, 129.7, 130.9, 134.7, 135.6, 138.3, 147.3, 155.4, 162.3, 208.1;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{19}H_{17}ClN_2O_2$ 341.1051; found 341.1060.

3-(4-chlorophenyl)-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5hA)

CAS: none



Pale yellow oily liquid;

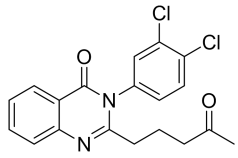
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.94-2.02 (m, 2H), 2.08 (s, 3H), 2.41 (t, *J* = 7.6 Hz, 2H), 2.52 (t, *J* = 6.8 Hz, 2H), 7.21-7.24 (m, 2H), 7.47 (dt, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.51-7.56 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.77 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.25 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.4, 29.9, 34.8, 42.4, 120.7, 122.1, 126.9, 127.1, 127.2, 129.2, 129.8, 130.3, 134.7, 135.4, 135.7, 147.3, 155.5, 162.4, 208.2;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{19}H_{17}ClN_2O_2$ 341.1051; found 341.1058.

3-(3,4-dichlorophenyl)-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5iA)

CAS: none



Pale yellow oily liquid;

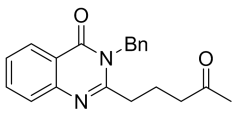
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 1.97-2.04 (m, 2H), 2.09 (s, 3H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.54-2.57 (m, 2H), 7.15 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 7.42-7.50 (m, 2H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.77 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.25 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.3, 30.0, 34.7, 42.3, 120.5, 127.0, 127.1, 127.2, 128.0, 130.6, 131.7, 134.0, 134.9, 136.4, 147.2, 155.0, 162.2, 208.1;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{19}H_{16}Cl_2N_2O_2$ 375.0662; found 375.0671.

3-benzyl-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5jA)

CAS: 161629-15-2



Pale yellow solid, mp 122-124 °C;

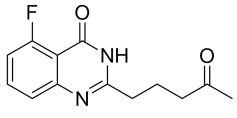
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.04-2.08 (m, 2H), 2.11 (s, 3H), 2.56 (t, *J* = 6.8 Hz, 2H), 2.74 (t, *J* = 7.6 Hz, 2H), 5.48 (s, 2H), 7.19 (d, *J* = 6.8 Hz, 2H), 7.27-7.35 (m, 3H), 7.47 (dt, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.75 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 1H), 8.32 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 20.9, 30.0, 34.1, 42.3, 46.3, 120.4, 126.4, 126.6, 127.0, 127.2, 127.6, 128.9, 134.4, 136.3, 147.3, 156.6, 162.6, 208.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{20}H_{20}N_2O_2$ 321.1598; found 321.1605.

5-fluoro-2-(4-oxopentyl)quinazolin-4(*3H*)-one (5kA)

CAS: none



White solid, mp 156-157 °C;

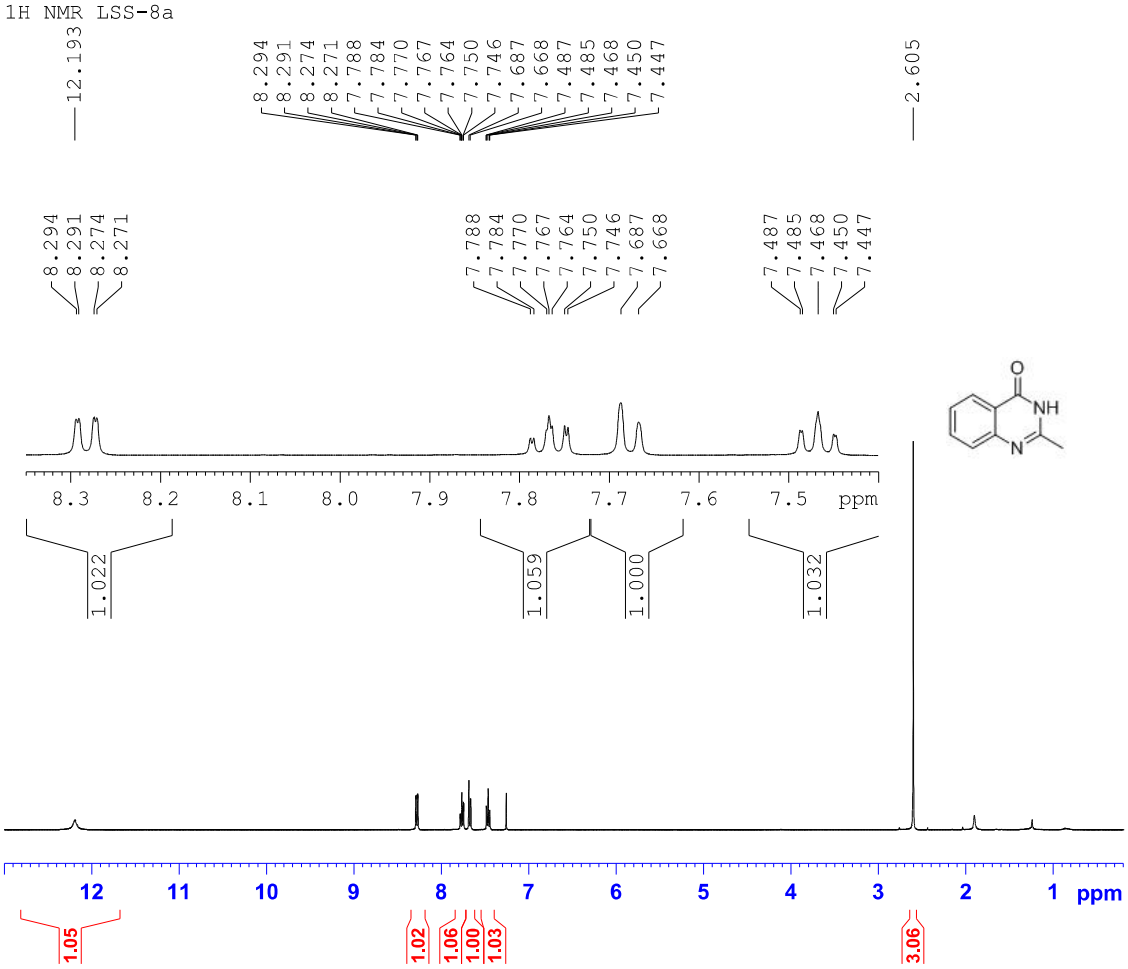
^{1}H NMR ($CDCl_3$, 400 MHz): δ = 2.10-2.16 (m, 2H), 2.17 (s, 3H), 2.64 (t, *J* = 6.8 Hz, 2H), 2.76 (t, *J* = 7.6 Hz, 2H), 7.09 (dt, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.65-7.71 (m, 1H);

^{13}C NMR ($CDCl_3$, 100 MHz): δ = 21.0, 30.0, 34.6, 42.5, 113.1, 123.2, 135.2, 151.3, 157.0, 160.0, 161.3, 162.7, 208.3;

HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{13}H_{13}FN_2O_2$ 249.1034; found 249.1039.

4. ^{1}H NMR & ^{13}C NMR Spectra of the Products

1H NMR LSS-8a



BRUKER

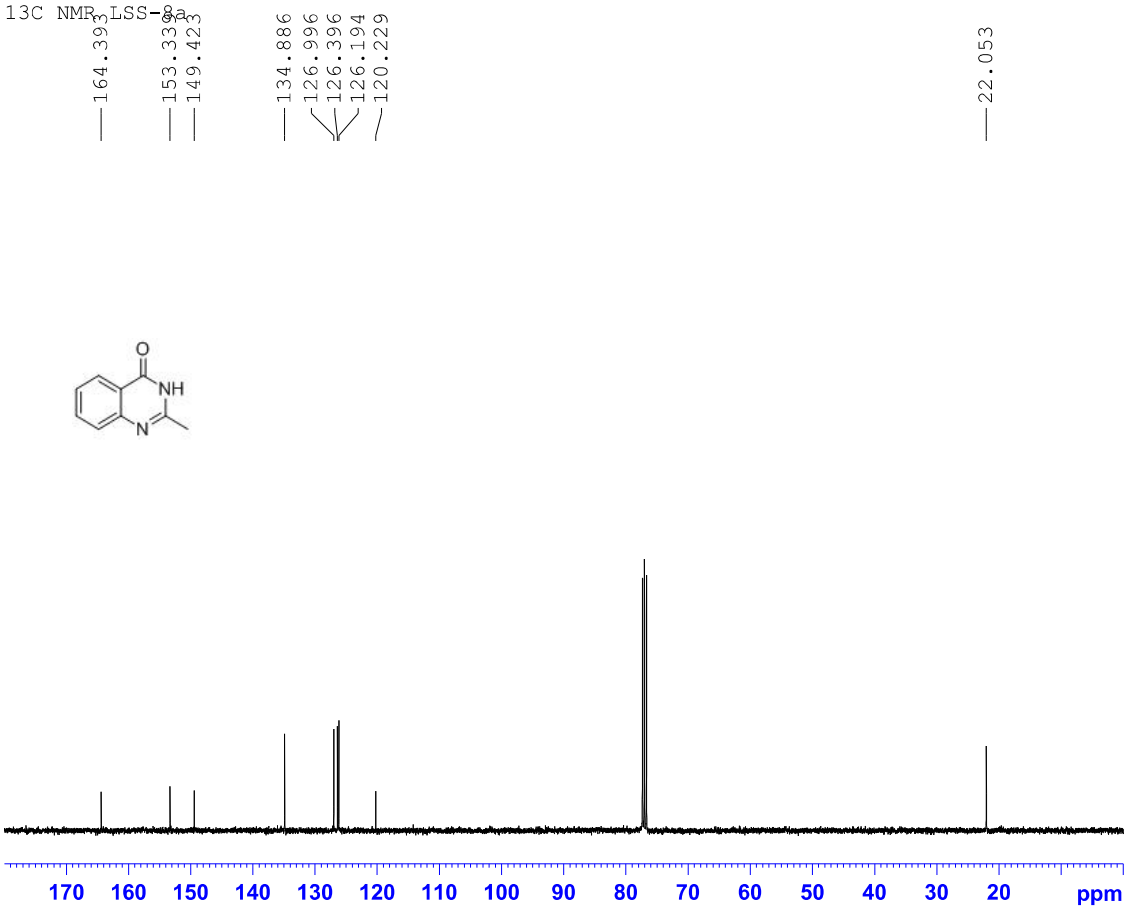
Current Data Parameters
NAME LSS-8a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140407
Time 11.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300178 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C NMR LSS-8a



BRUKER

Current Data Parameters
NAME LSS-8a
EXPNO 2
PROCNO 1

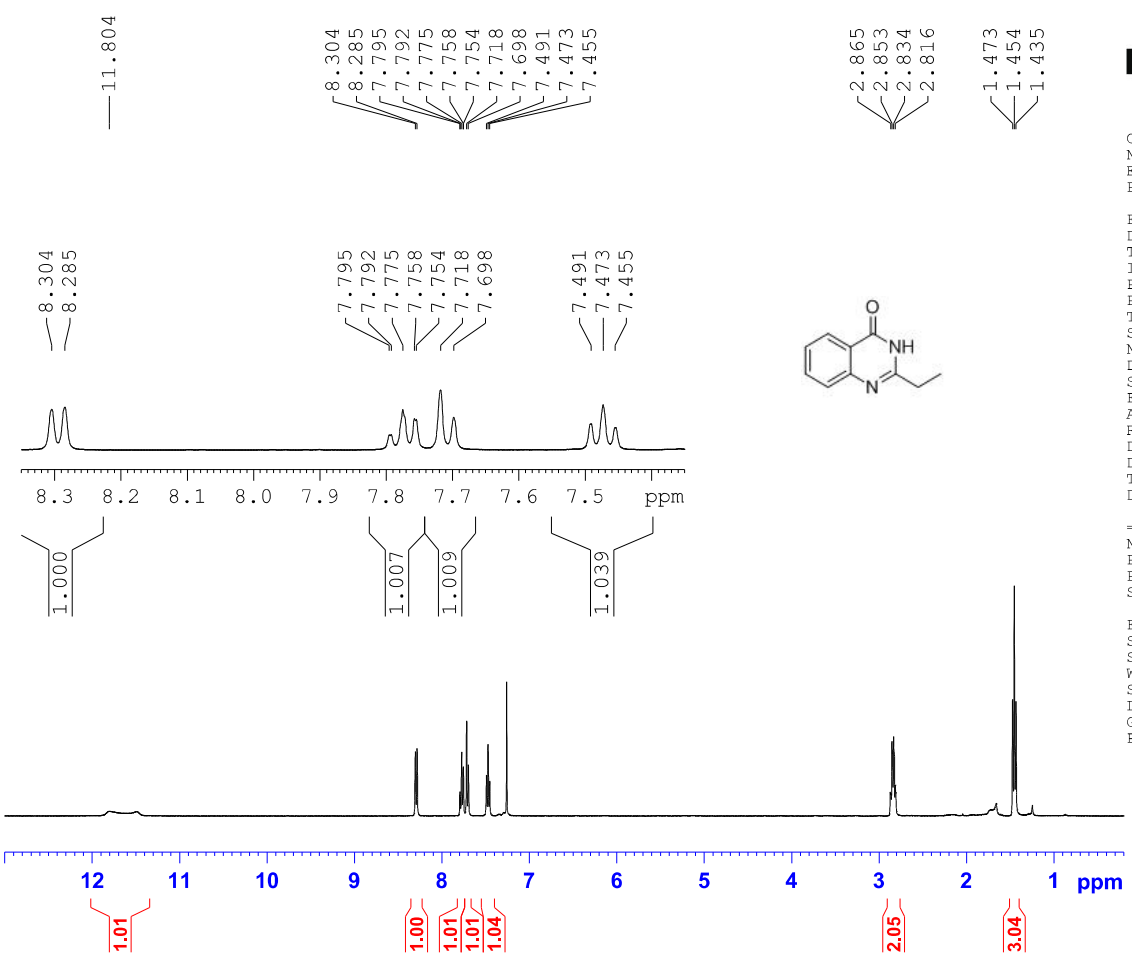
F2 - Acquisition Parameters
Date_ 20140407
Time 11.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 458
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 80.6
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-11-11



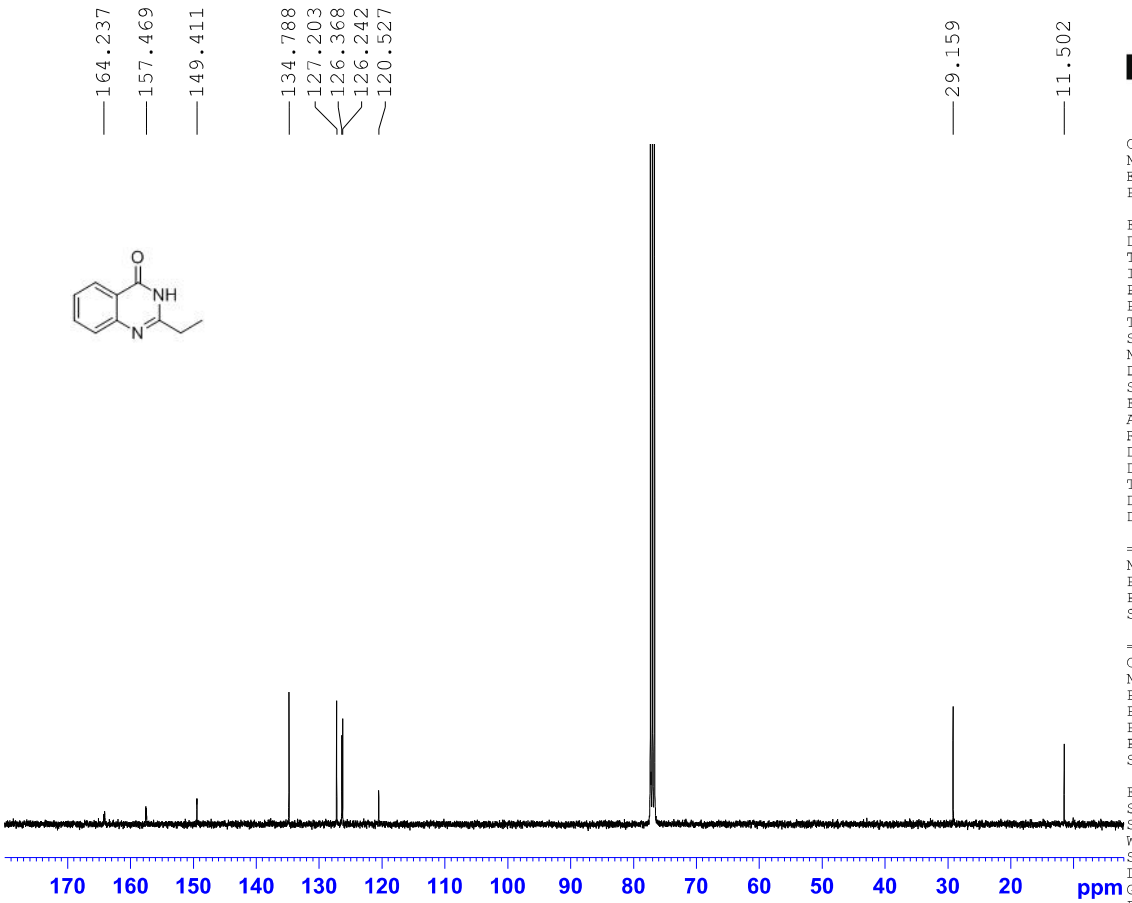
Current Data Parameters
NAME S-11-11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141127
Time 18.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300180 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H of S-11-11



Current Data Parameters
NAME S-11-11
EXPNO 2
PROCNO 1

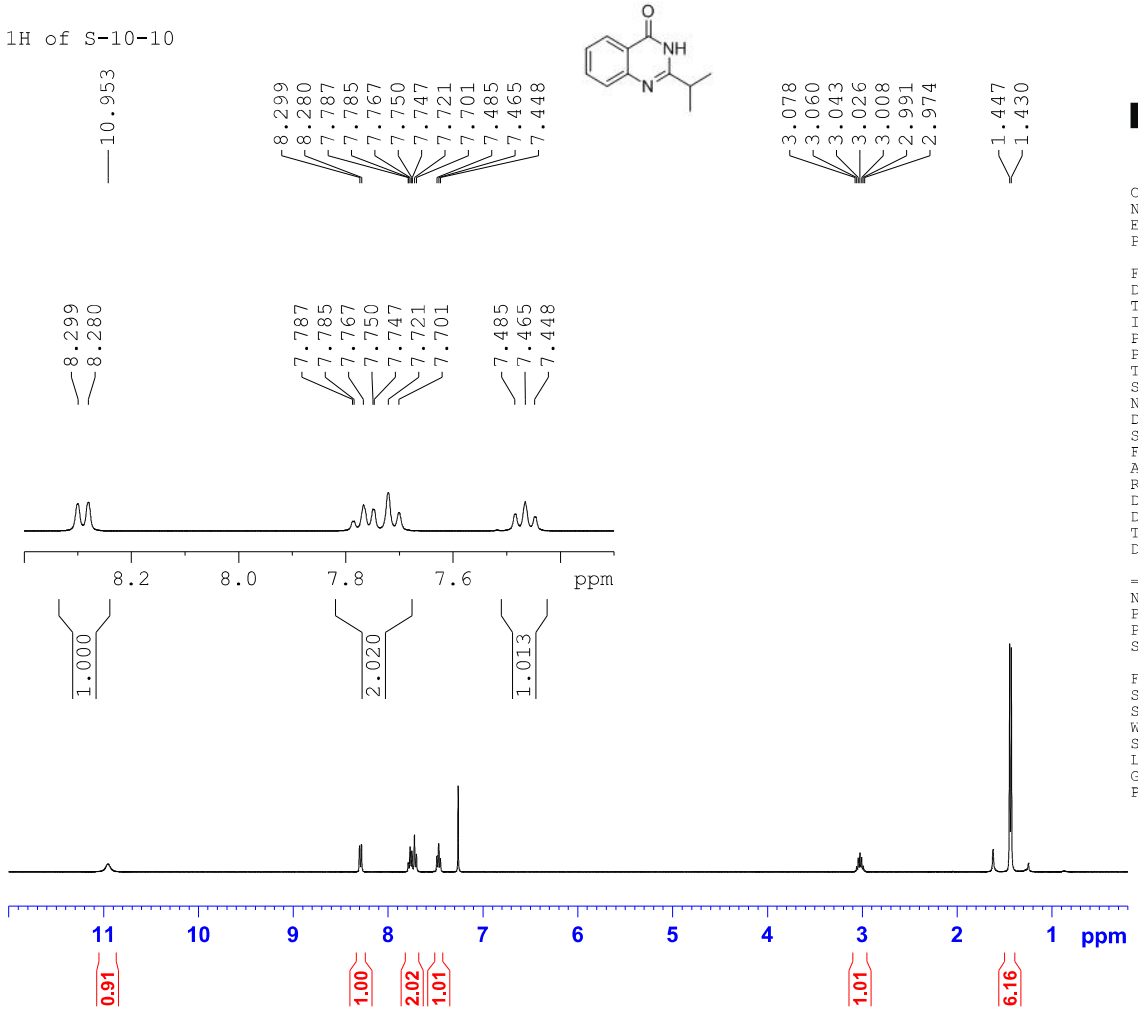
F2 - Acquisition Parameters
Date_ 20141127
Time 18.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2113
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 80.6
DW 20.800 usec
DE 6.50 usec
TE 293.5 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127748 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-10-10



BRUKER

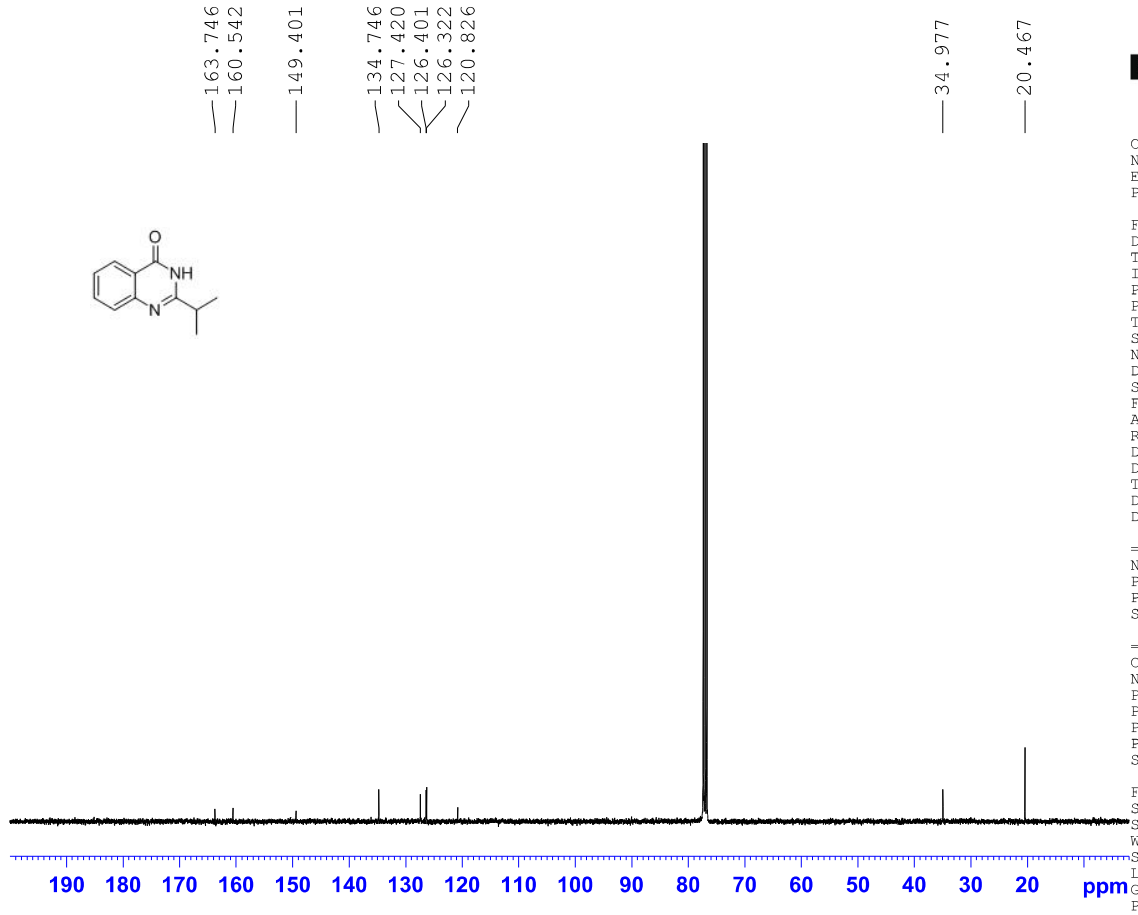
Current Data Parameters
NAME S-10-10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141125
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300178 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of S-10-10



BRUKER

Current Data Parameters
NAME S-10-10
EXPNO 2
PROCNO 1

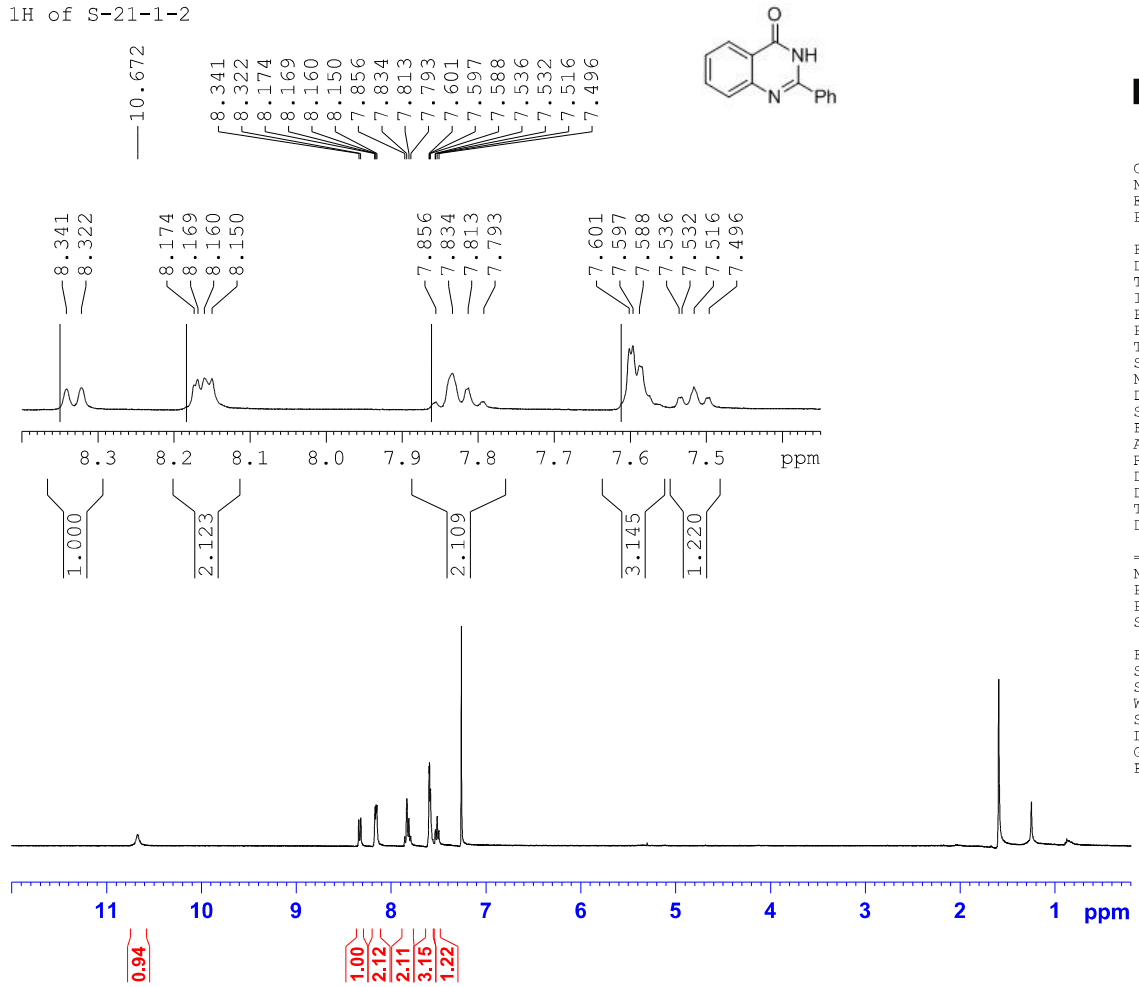
F2 - Acquisition Parameters
Date_ 20141125
Time 10.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 780
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 101
DW 20.800 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-21-1-2



BRUKER

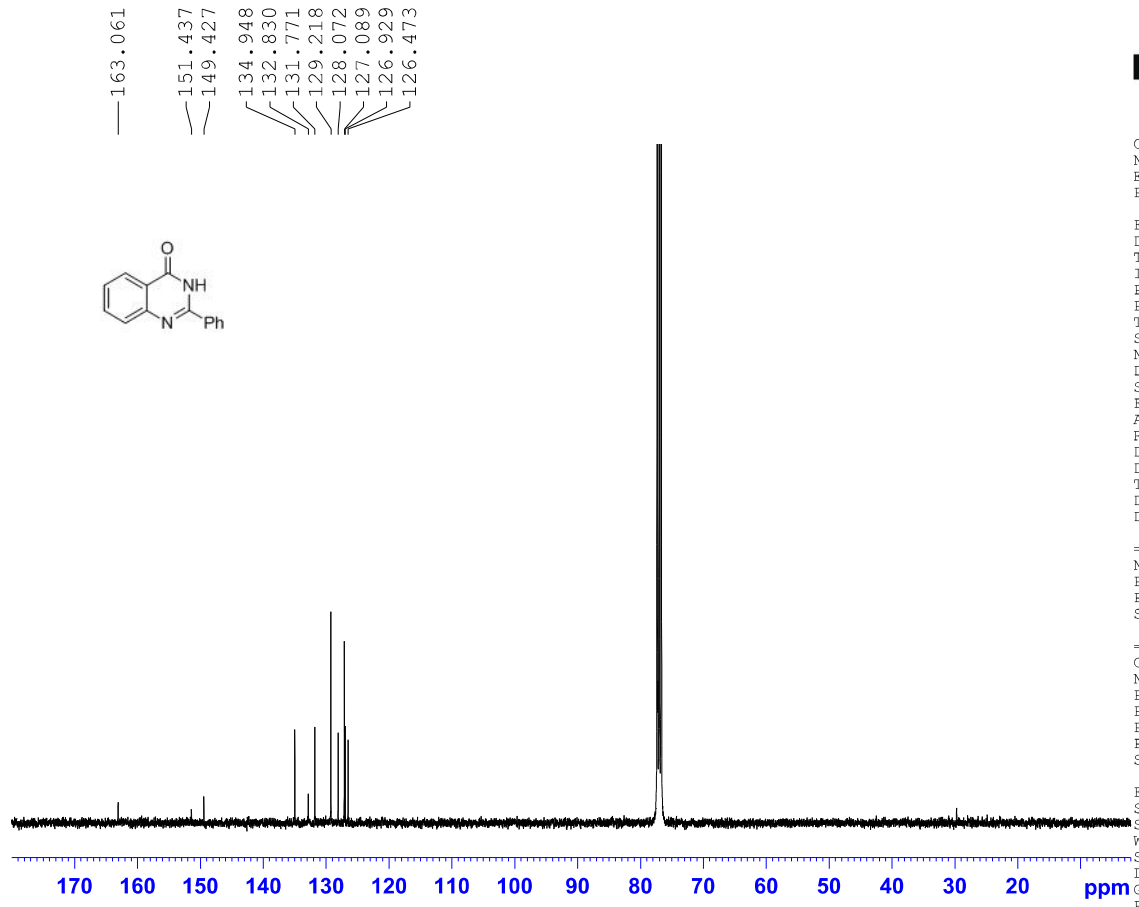
Current Data Parameters
NAME S-21-1-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141127
Time 20.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of S-21-1-2



BRUKER

Current Data Parameters
NAME S-21-1-2
EXPNO 1
PROCNO 1

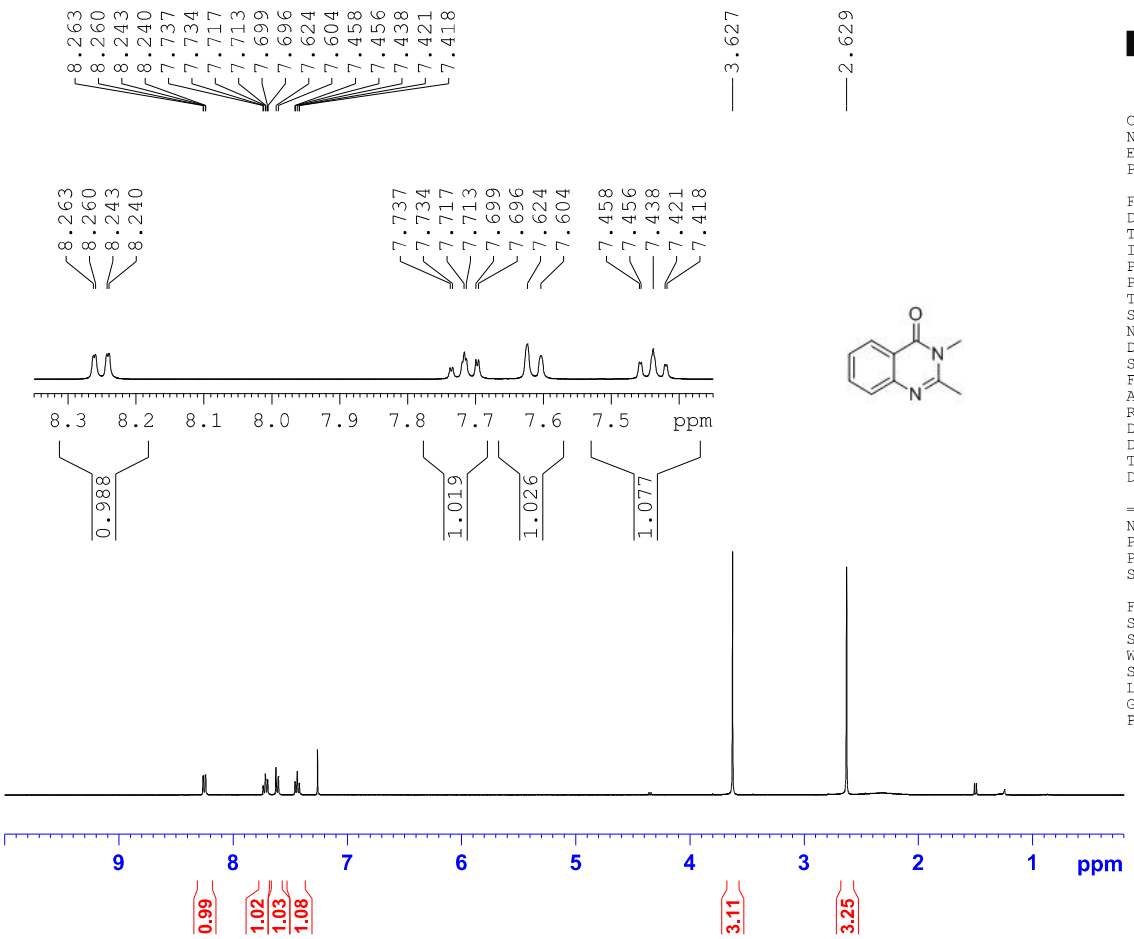
F2 - Acquisition Parameters
Date_ 20141127
Time 20.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.50 usec
TE 293.7 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

H NMR LSS-8-41



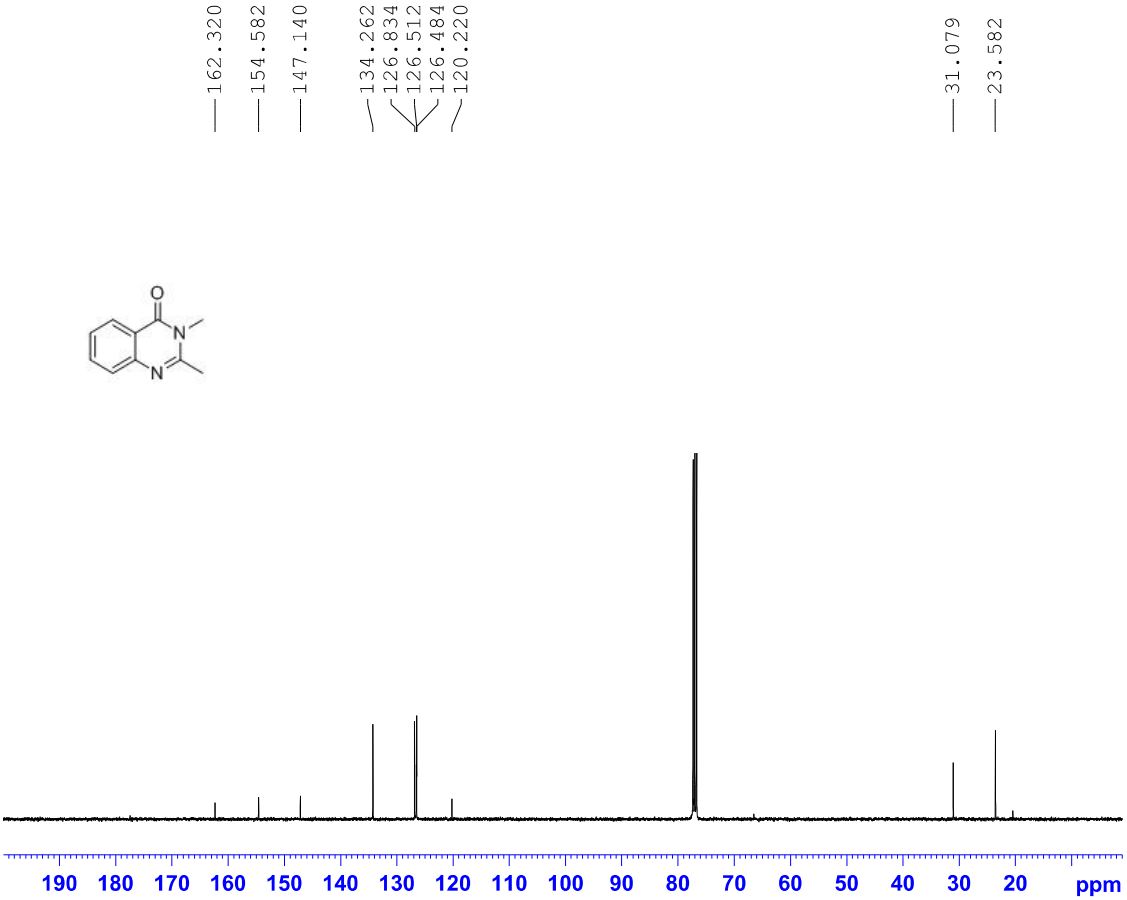
Current Data Parameters
NAME LSS-8-41
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140621
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300176 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

H NMR LSS-8-41



Current Data Parameters
NAME LSS-8-41
EXPNO 2
PROCNO 1

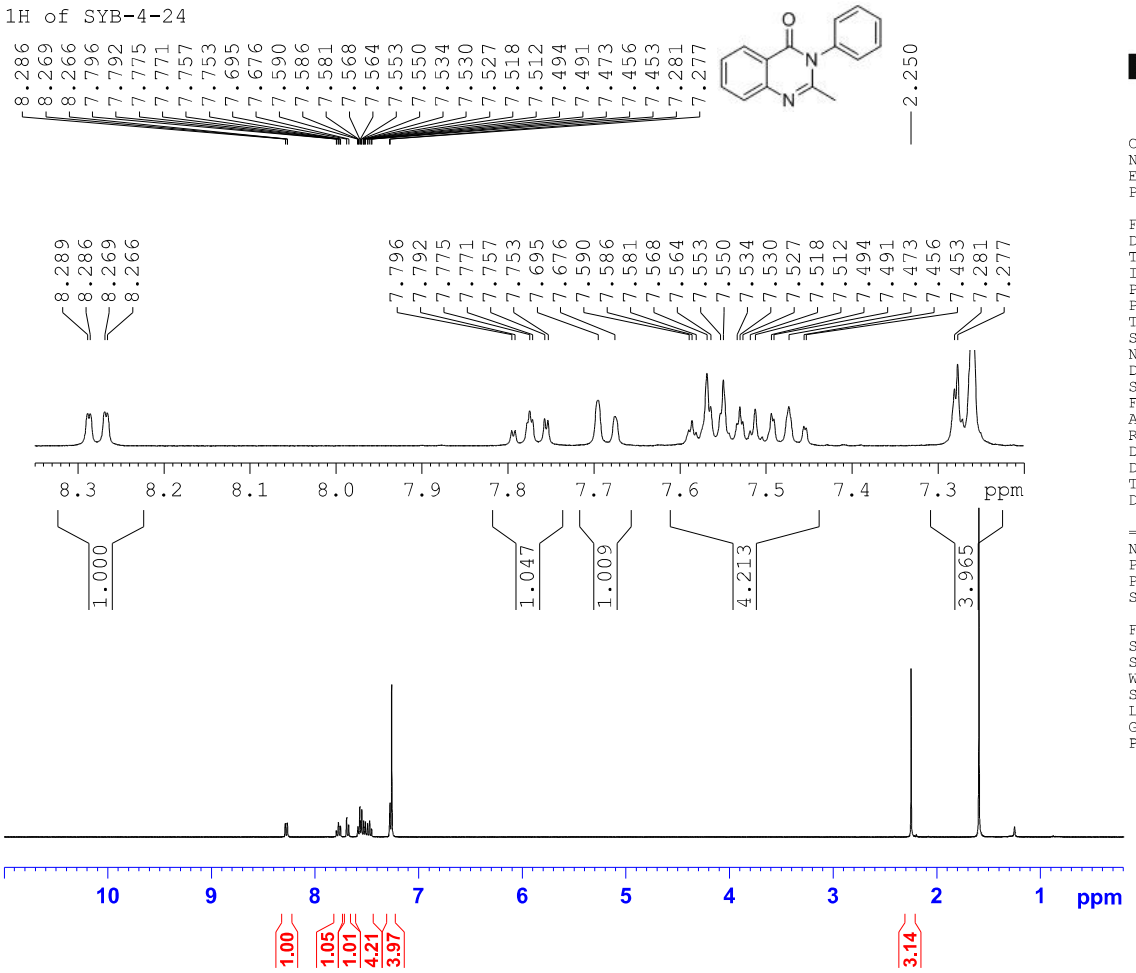
F2 - Acquisition Parameters
Date_ 20140621
Time 11.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3784
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SYB-4-24



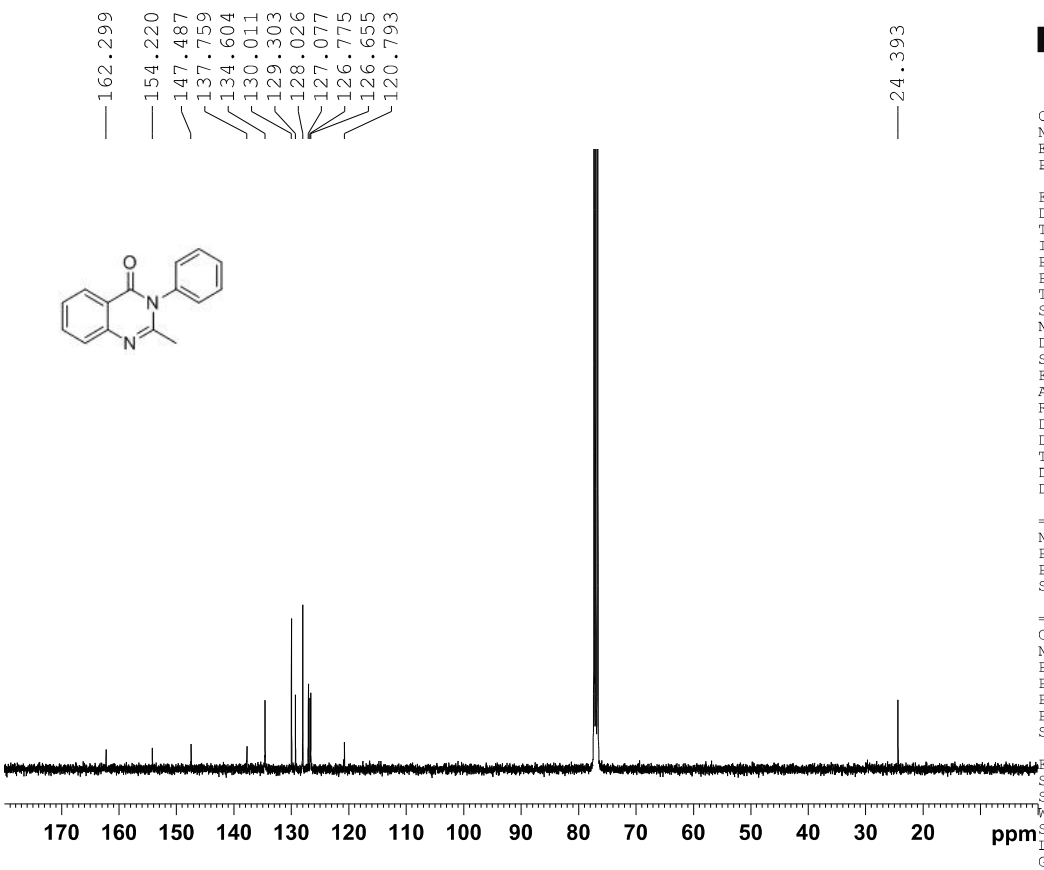
Current Data Parameters
NAME SYB-4-24
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140523
Time 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300177 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1H of SYB-4-24



Current Data Parameters
NAME SYB-4-24
EXPNO 2
PROCNO 1

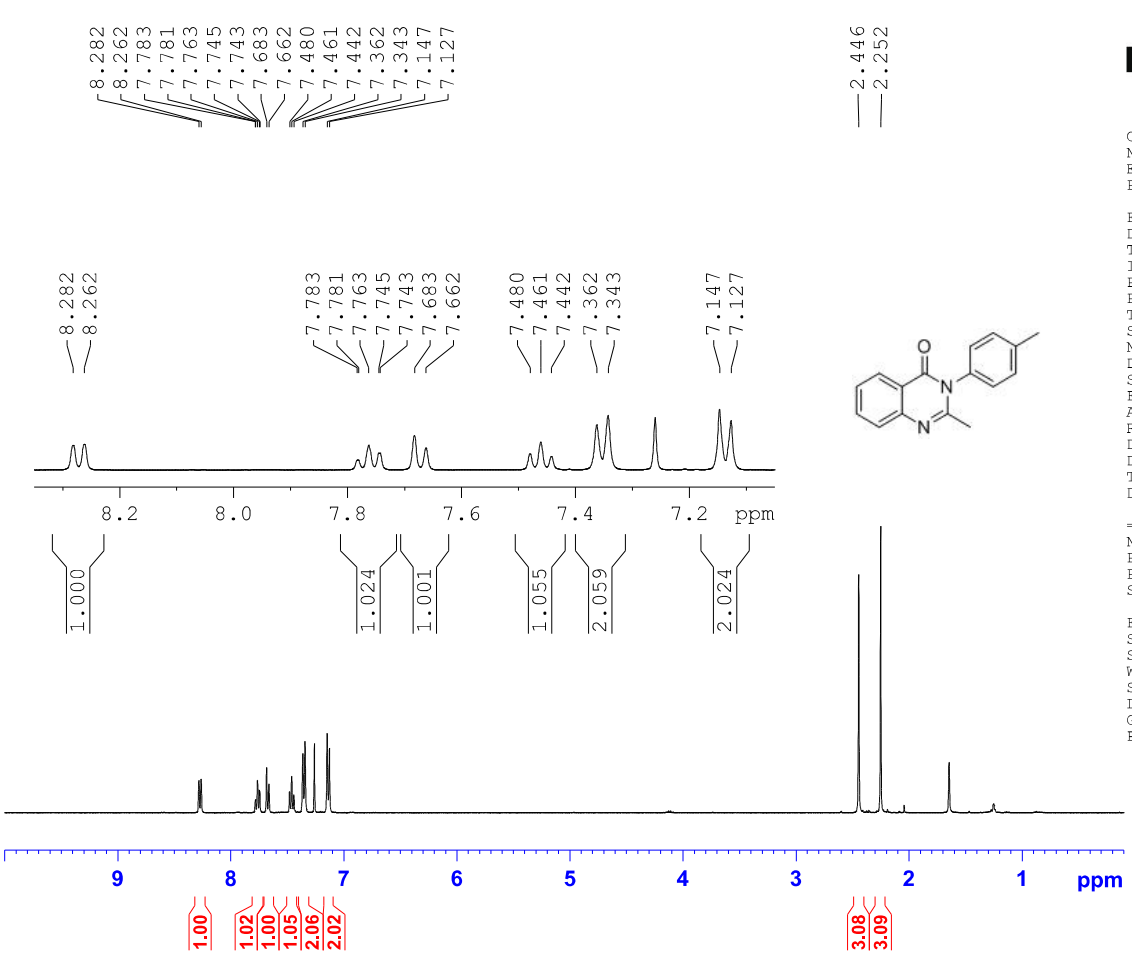
F2 - Acquisition Parameters
Date_ 20140523
Time 10.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9818
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 90.5
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-22-5



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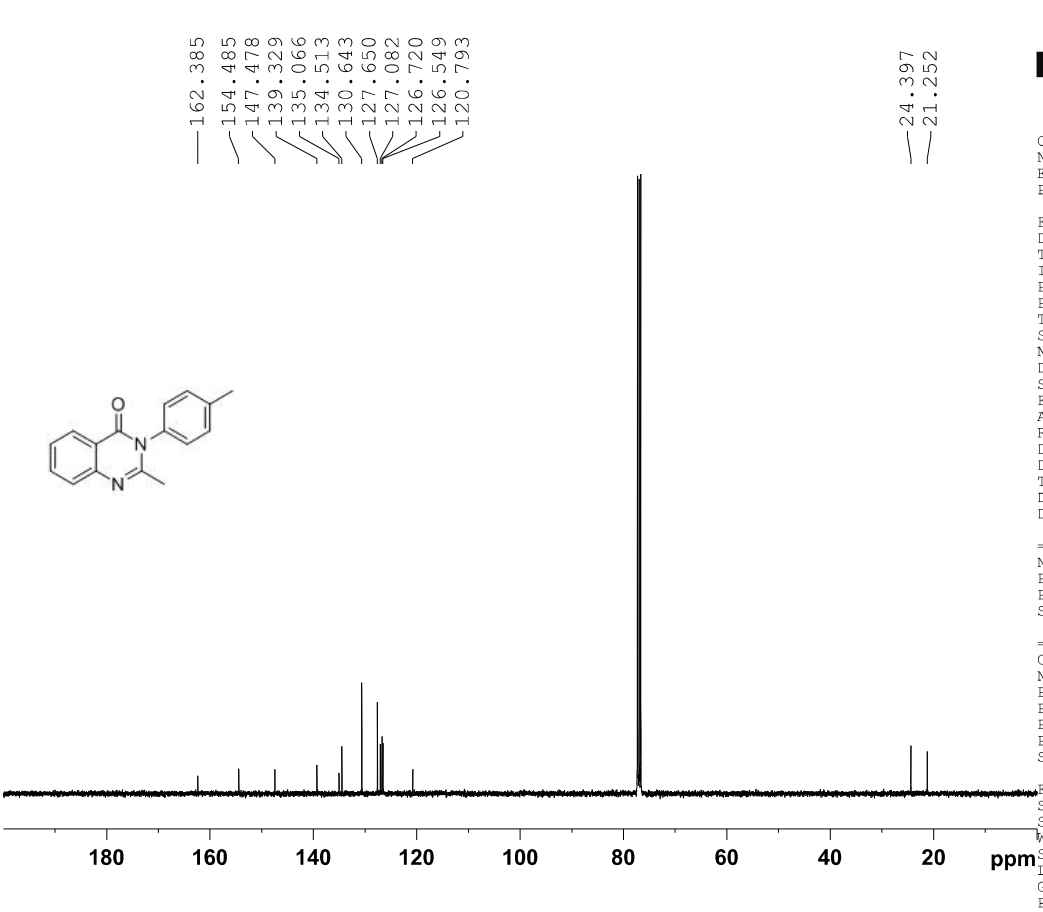
```
Current Data Parameters
NAME                  S-22-5
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141114
Time                   17.31
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      144
DW                   60.800 usec
DE                    6.50 usec
TE                   294.8 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.70 usec
PLW1            14.30000019 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300179 MHz
WDW                          EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

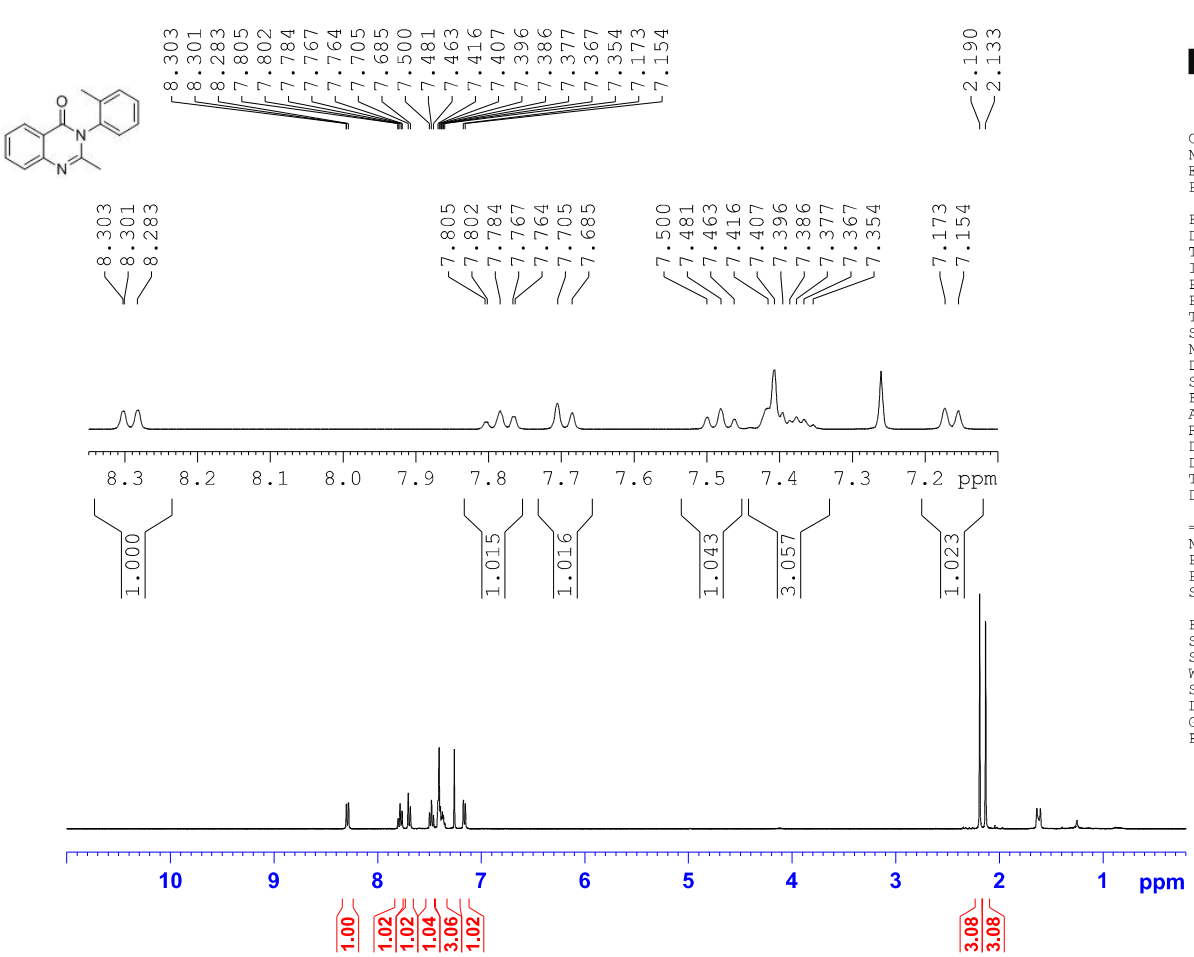
13C of S-22-5



BRUKER

```
Current Data Parameters
NAME                  S-22-5
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141114
Time                   17.44
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      516
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      114
DW                   20.800 usec
DE                    6.50 usec
TE                   295.4 K
D1                2.00000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.65 usec
PLW1           34.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2            14.30000019 W
PLW12            0.33135000 W
PLW13            0.26840001 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127746 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

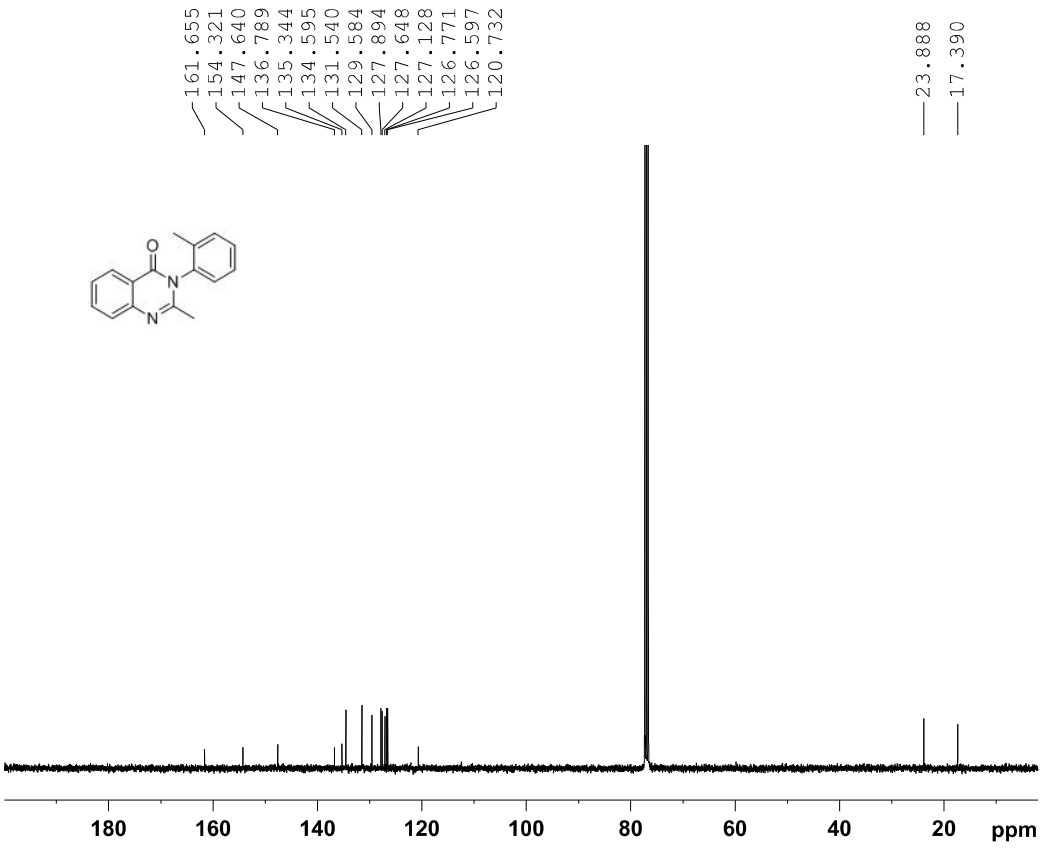
1H of S-7-7



BRUKER

```
Current Data Parameters
NAME                  S-7-7
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  11.20
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES                0.125483 Hz
AQ                 3.9846387 sec
RG                      144
DW                    60.800 usec
DE                     6.50 usec
TE                    294.2 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.70 usec
PLW1             14.30000019 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300176 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

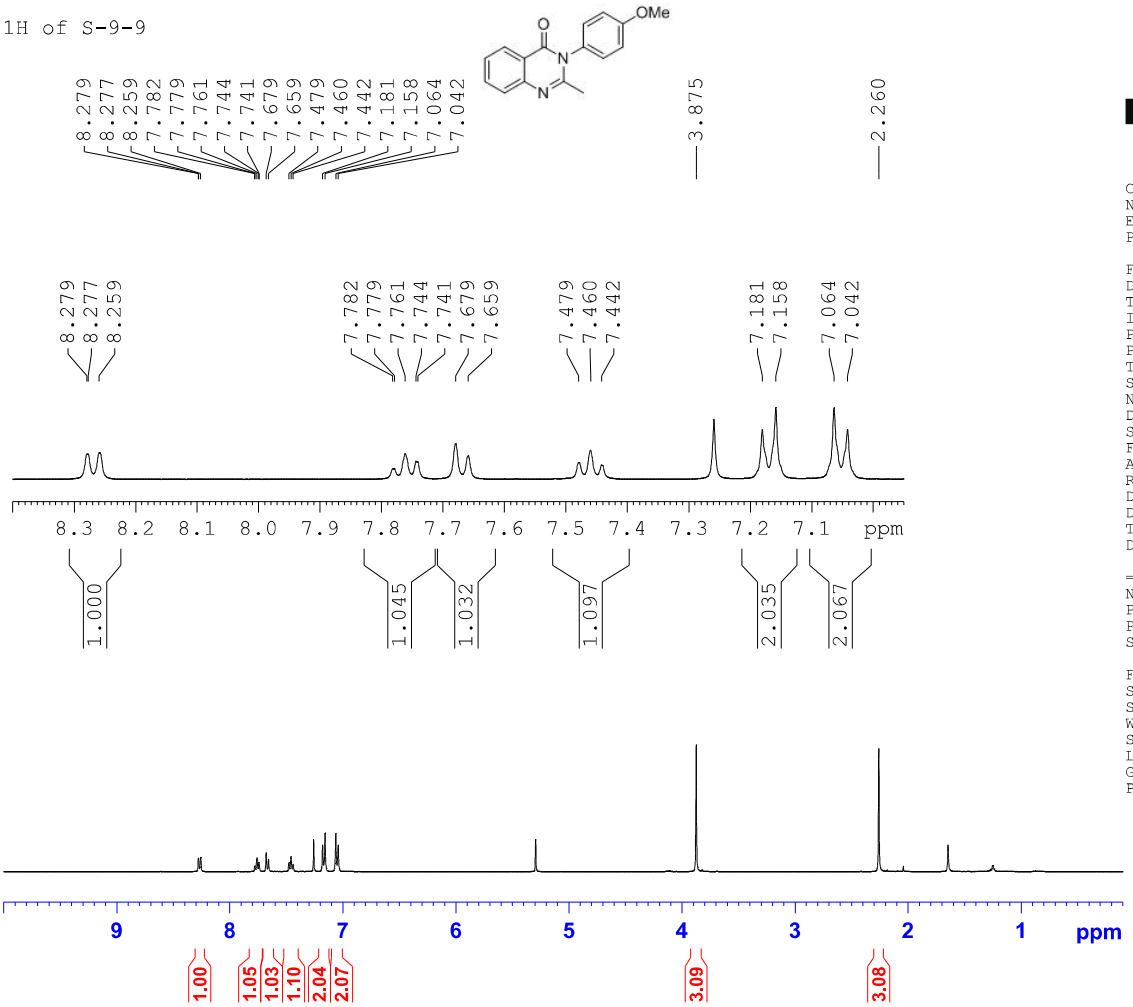
13C of S-7-7



BRUKER

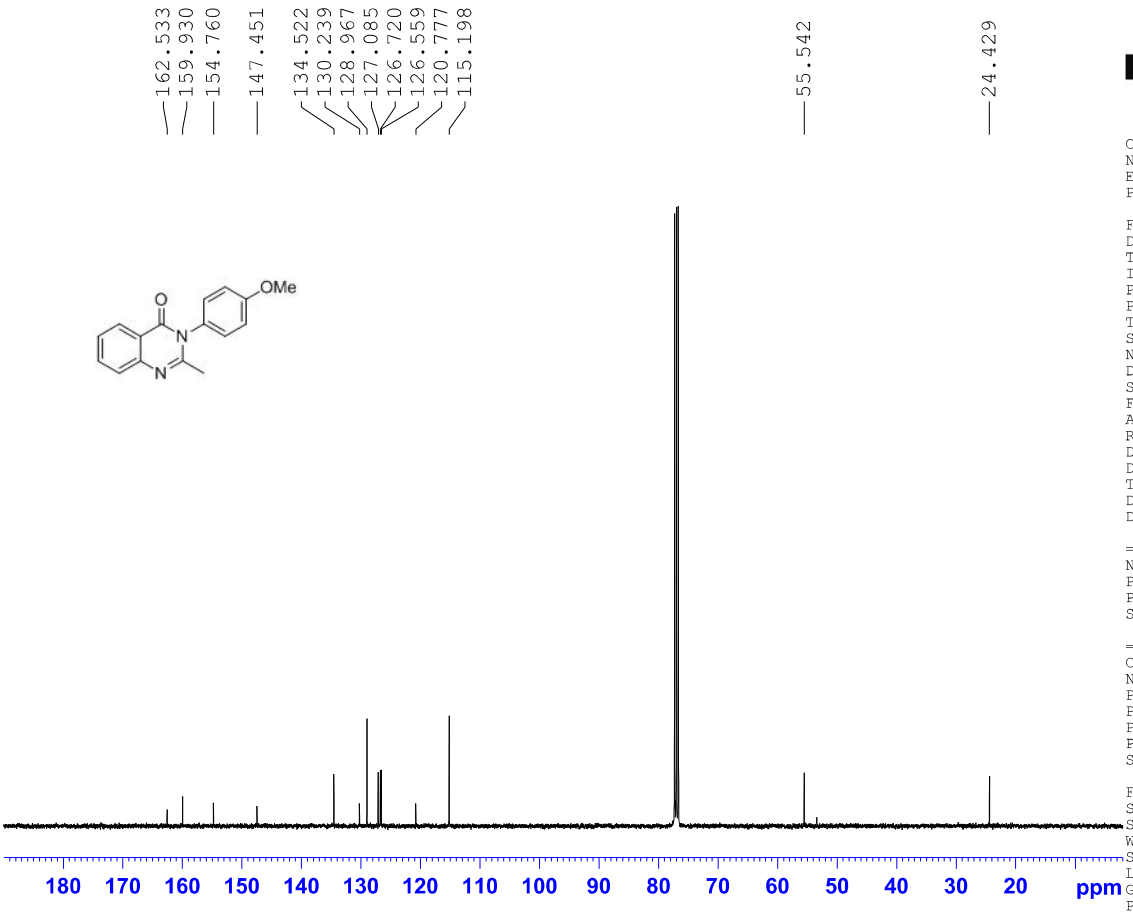
```
Current Data Parameters
NAME                  S-7-7
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  11.27
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      654
DS                        4
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631988 sec
RG                      128
DW                    20.800 usec
DE                     6.50 usec
TE                    294.3 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.65 usec
PLW1             34.00000000 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2             14.30000019 W
PLW12             0.33135000 W
PLW13             0.26840001 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127745 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

1H of S-9-9



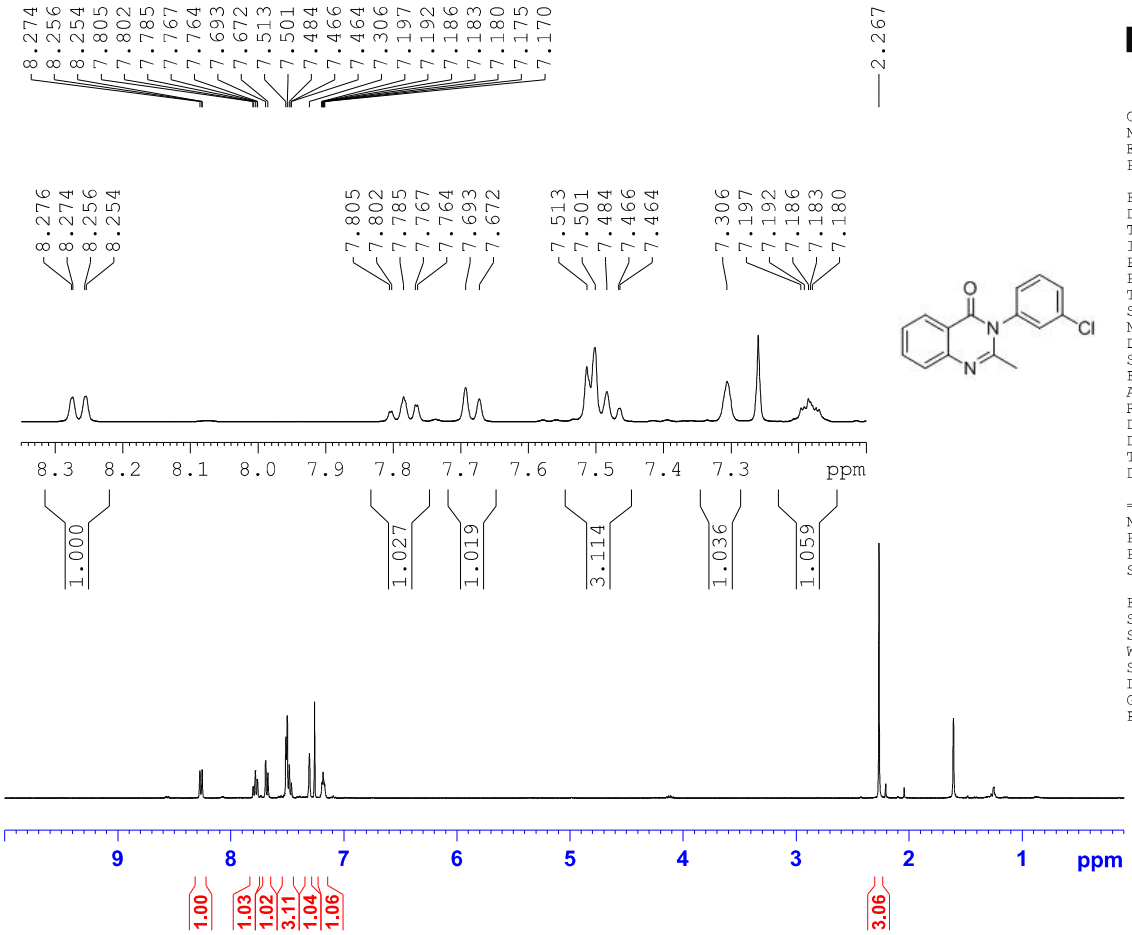

```
Current Data Parameters
NAME                  S-9-9
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  18.42
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              8223.685 Hz
FIDRES              0.125483 Hz
AQ               3.9846387 sec
RG                     144
DW                  60.800 usec
DE                   6.50 usec
TE                  294.7 K
D1               1.00000000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                   13.70 usec
PLW1           14.30000019 W
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300181 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

13C of S-9-9



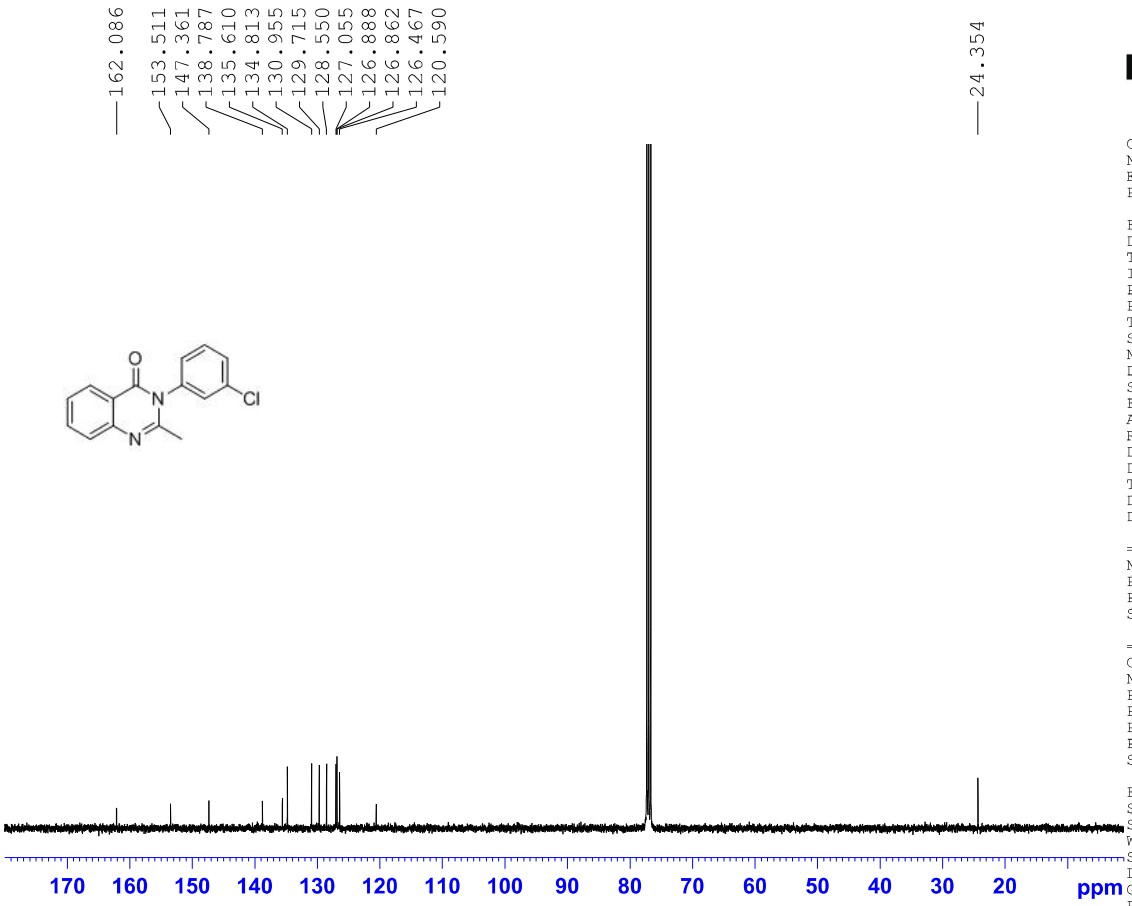

```
Current Data Parameters
NAME                  S-9-9
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  18.50
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     992
DS                       0
SWH             24038.461 Hz
FIDRES              0.366798 Hz
AQ               1.3631988 sec
RG                    80.6
DW                  20.800 usec
DE                   6.50 usec
TE                  295.3 K
D1               2.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   11.65 usec
PLW1           34.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                90.00 usec
PLW2           14.30000019 W
PLW12           0.33135000 W
PLW13           0.26840001 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127746 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

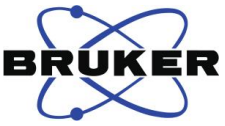
1H of S-22-4




```
Current Data Parameters
NAME                  S-22-4
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141114
Time                  18.16
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      161
DW                   60.800 usec
DE                    6.50 usec
TE                   294.8 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.70 usec
PLW1             14.30000019 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300180 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

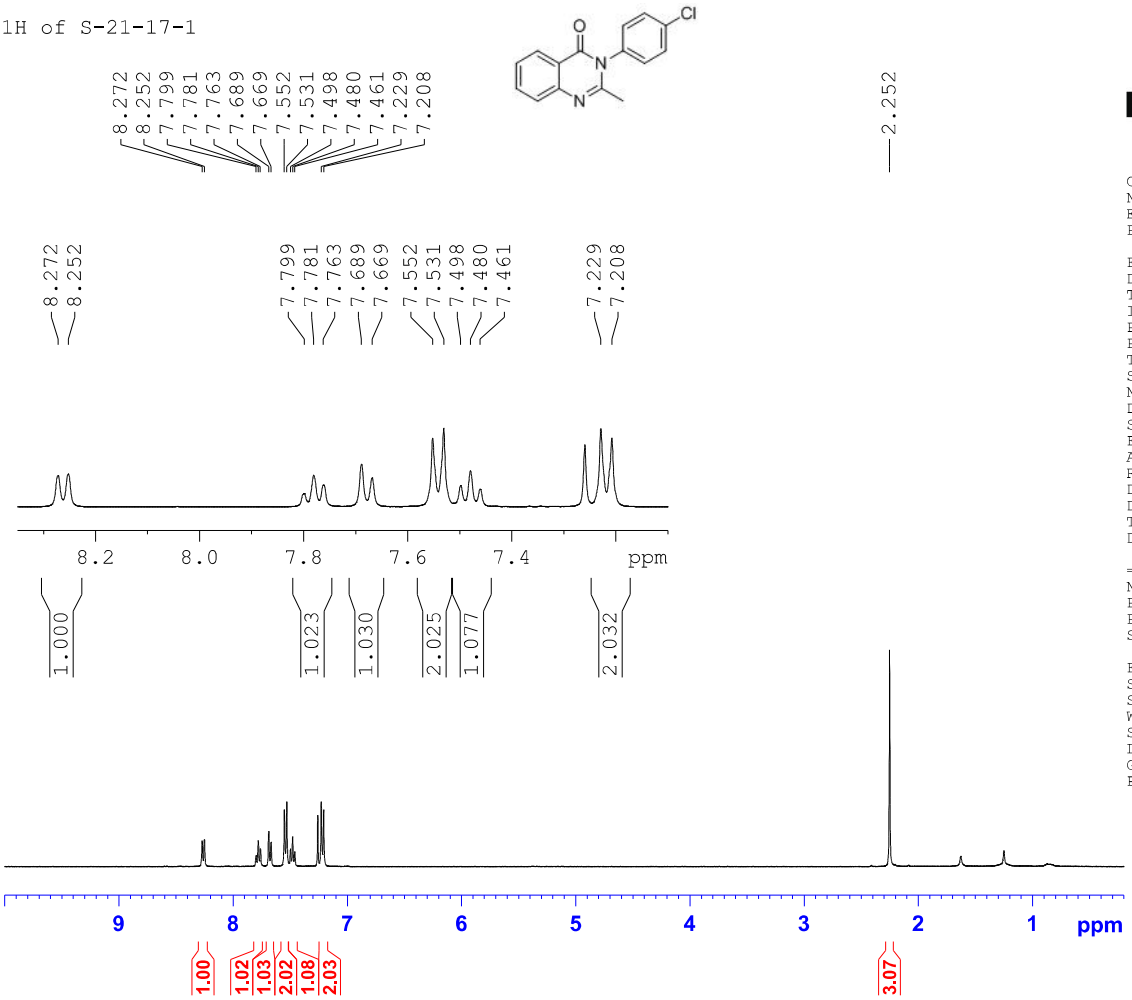
13C of S-22-4






```
Current Data Parameters
NAME                  S-22-4
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141114
Time                  18.24
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      792
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                      128
DW                   20.800 usec
DE                    6.50 usec
TE                   295.3 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.65 usec
PLW1             34.00000000 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  90.00 usec
PLW2             14.30000019 W
PLW12             0.33135000 W
PLW13             0.26840001 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127738 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

1H of S-21-17-1



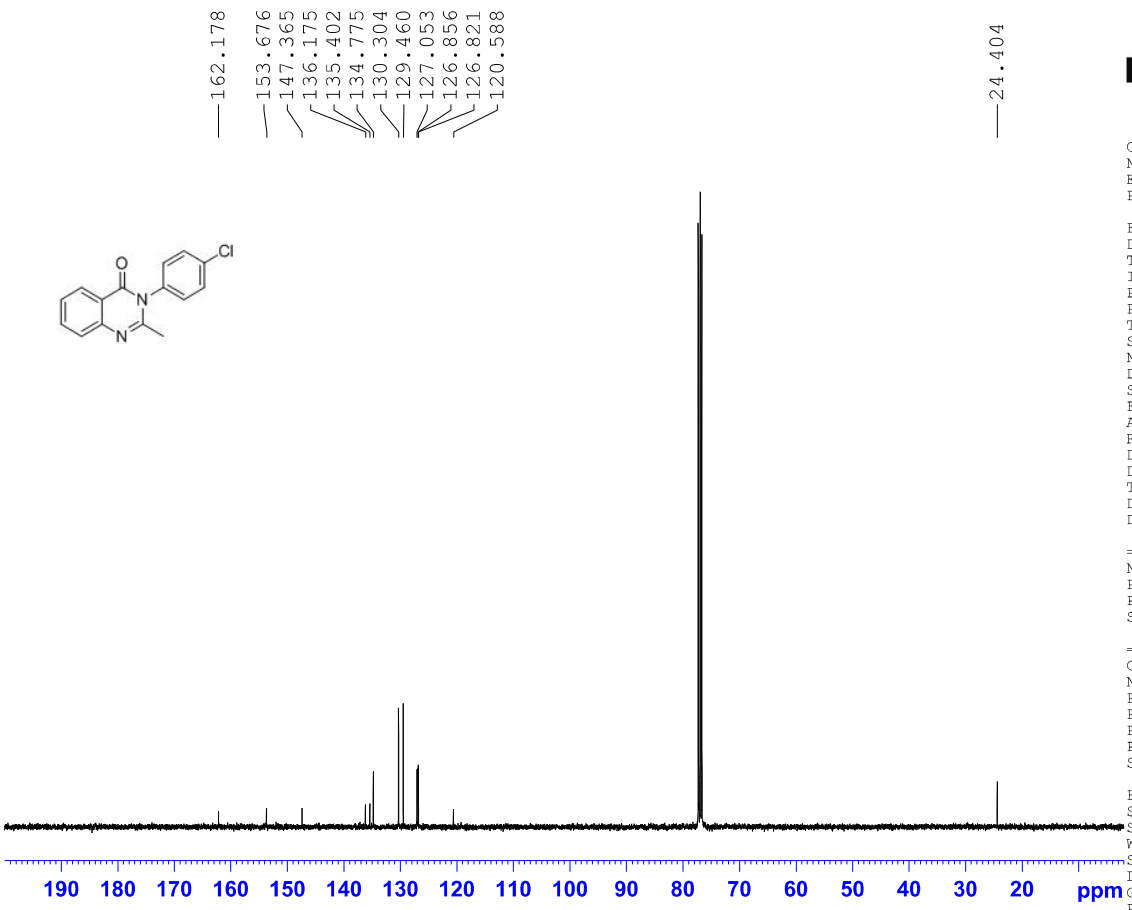
Current Data Parameters
NAME S-21-17-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141125
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of S-21-17-1



Current Data Parameters
NAME S-21-17-1
EXPNO 2
PROCNO 1

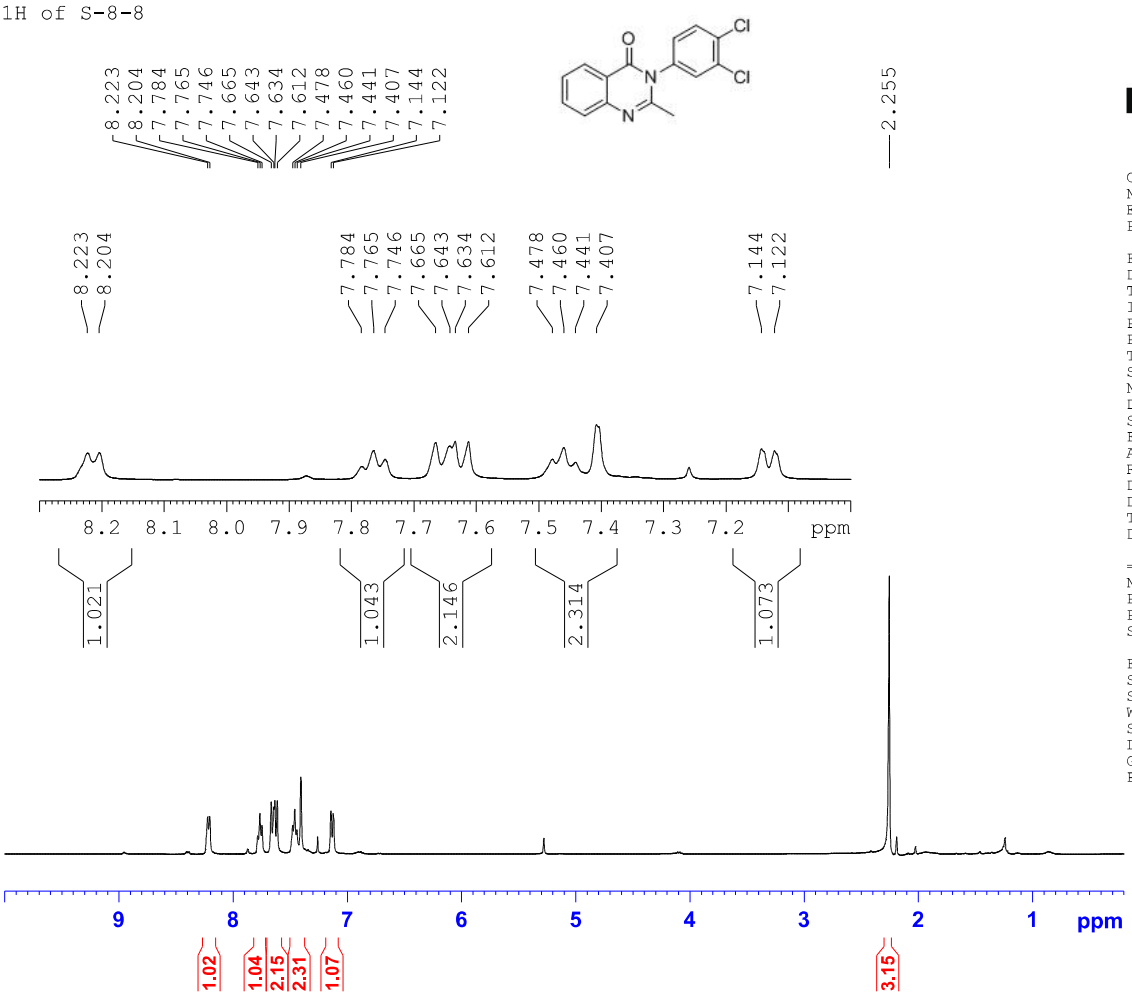
F2 - Acquisition Parameters
Date_ 20141125
Time 9.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 741
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 101
DW 20.800 usec
DE 6.50 usec
TE 293.8 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

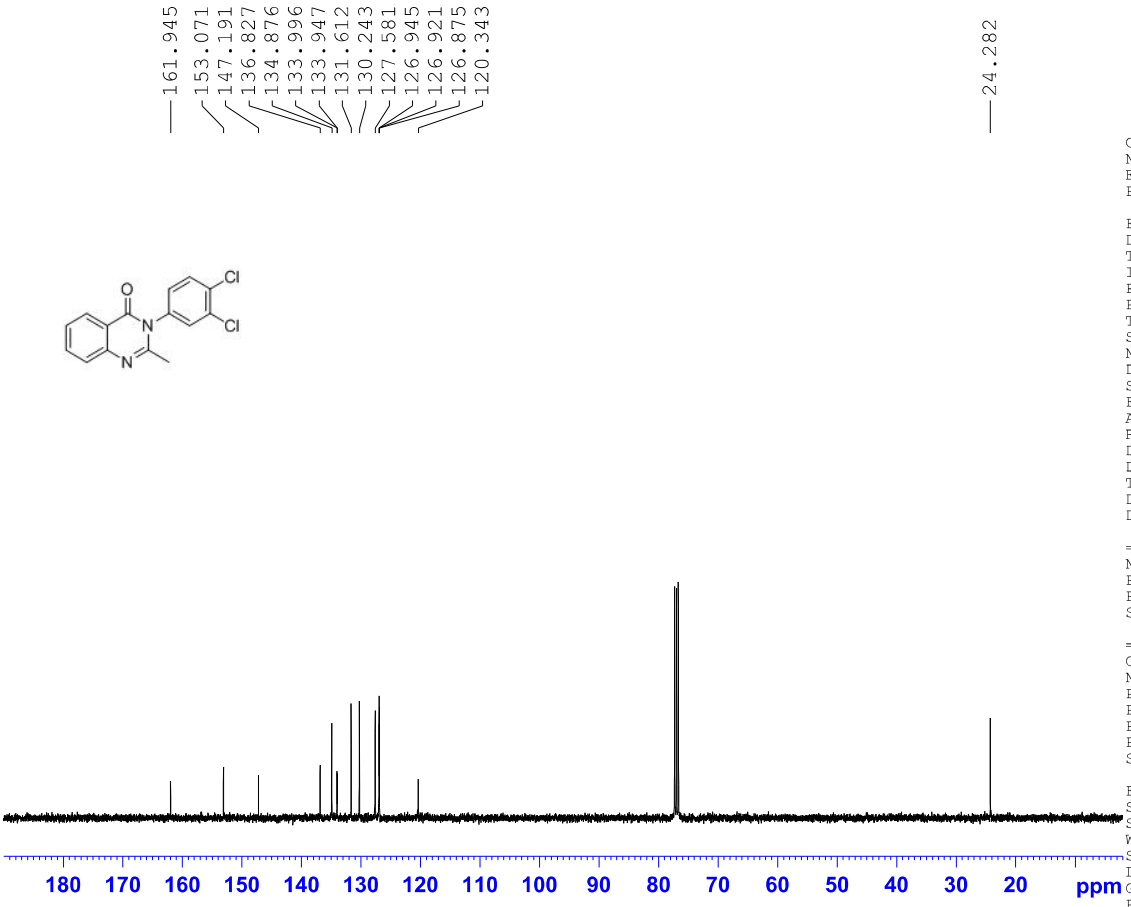
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-8-8



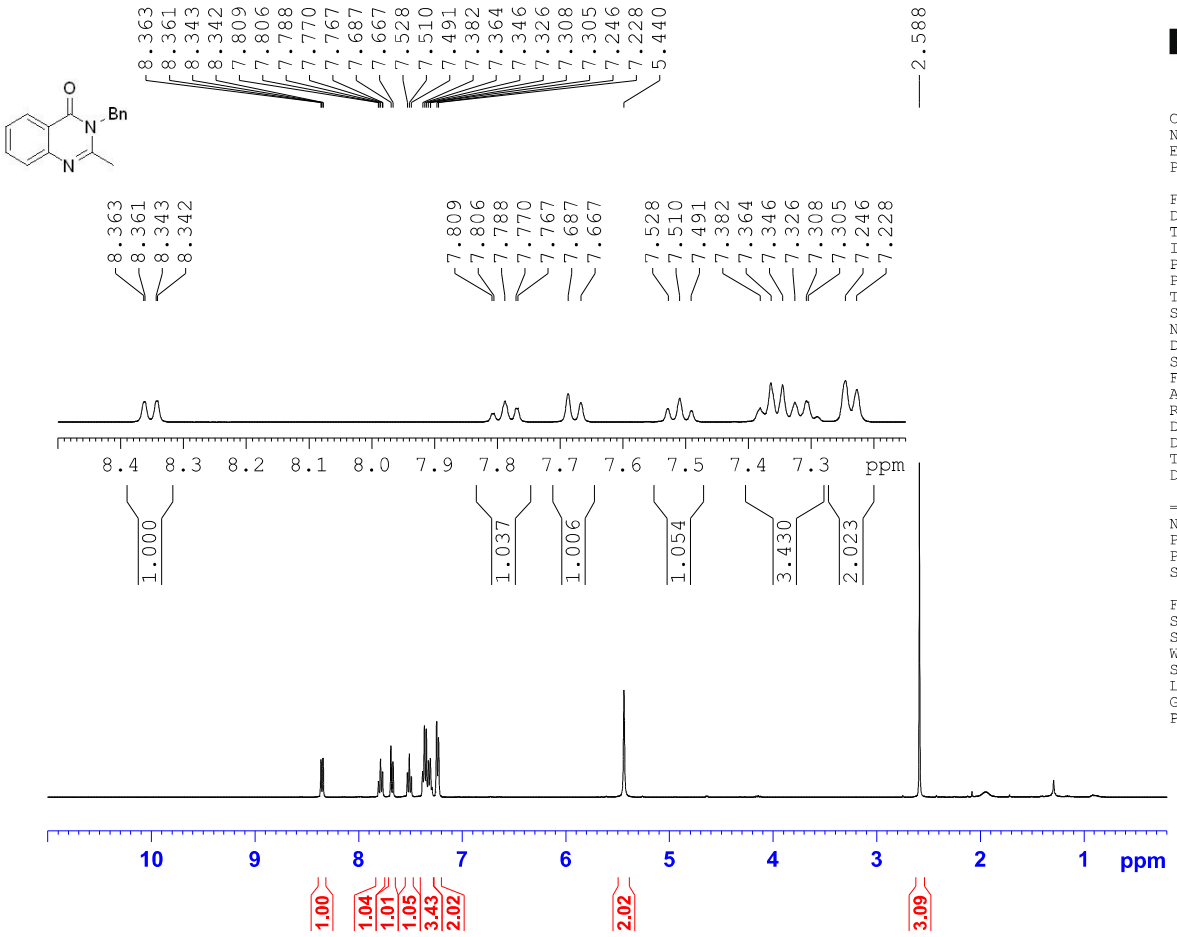

```
Current Data Parameters
NAME                  S-8-8
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  18.23
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES                0.125483 Hz
AQ                 3.9846387 sec
RG                     80.6
DW                    60.800 usec
DE                     6.50 usec
TE                    294.6 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.70 usec
PLW1              14.30000019 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300181 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

13C of S-8-8




```
Current Data Parameters
NAME                  S-8-8
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20141118
Time                  18.32
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       72
DS                        0
SWH               24038.461 Hz
FIDRES                0.366798 Hz
AQ                 1.3631988 sec
RG                      144
DW                    20.800 usec
DE                     6.50 usec
TE                    295.2 K
D1                 2.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.65 usec
PLW1              34.00000000 W
SFO1             100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2              14.30000019 W
PLW12              0.33135000 W
PLW13              0.26840001 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF               100.6127797 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

1H of S-6-6



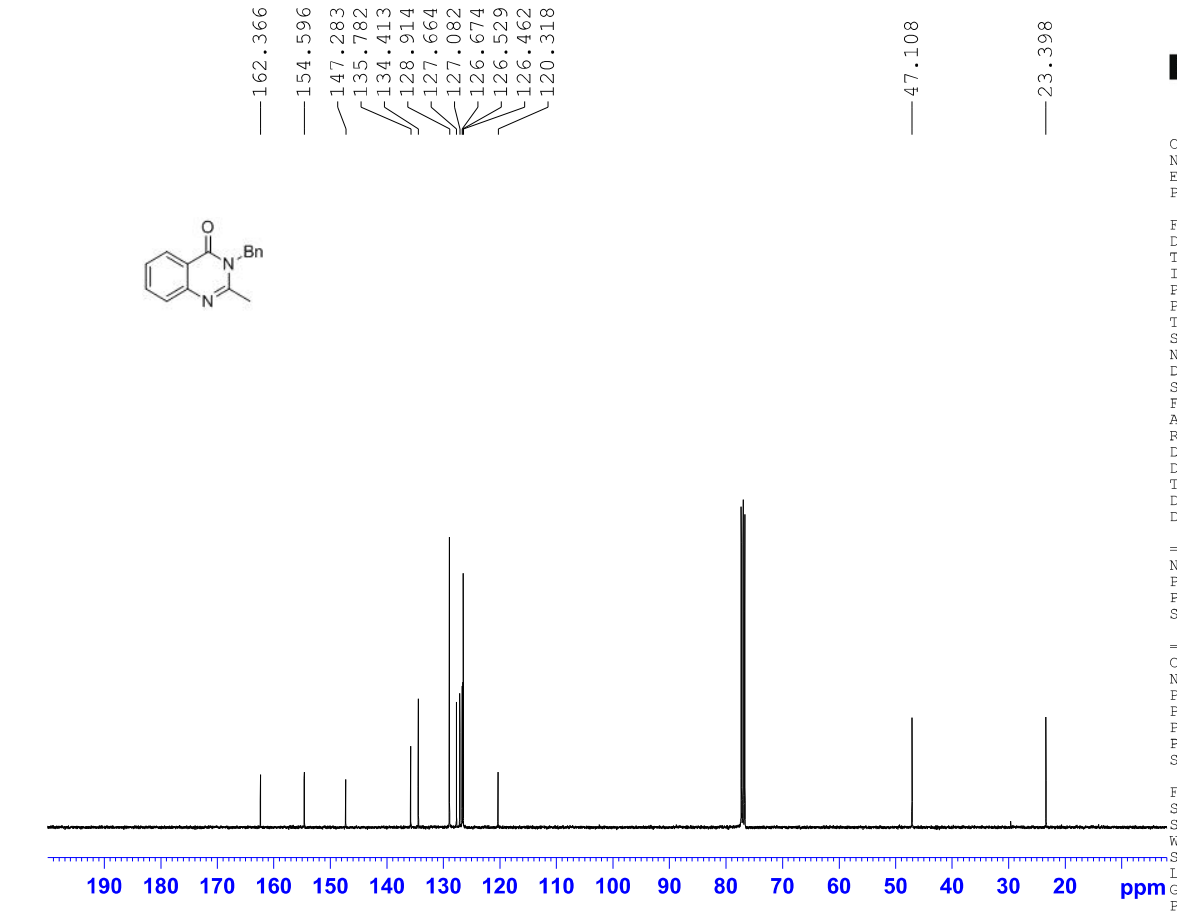
Current Data Parameters
NAME S-6-6
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141118
Time 10.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 71.8
DW 60.800 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of S-6-6



Current Data Parameters
NAME S-6-6
EXPNO 2
PROCNO 1

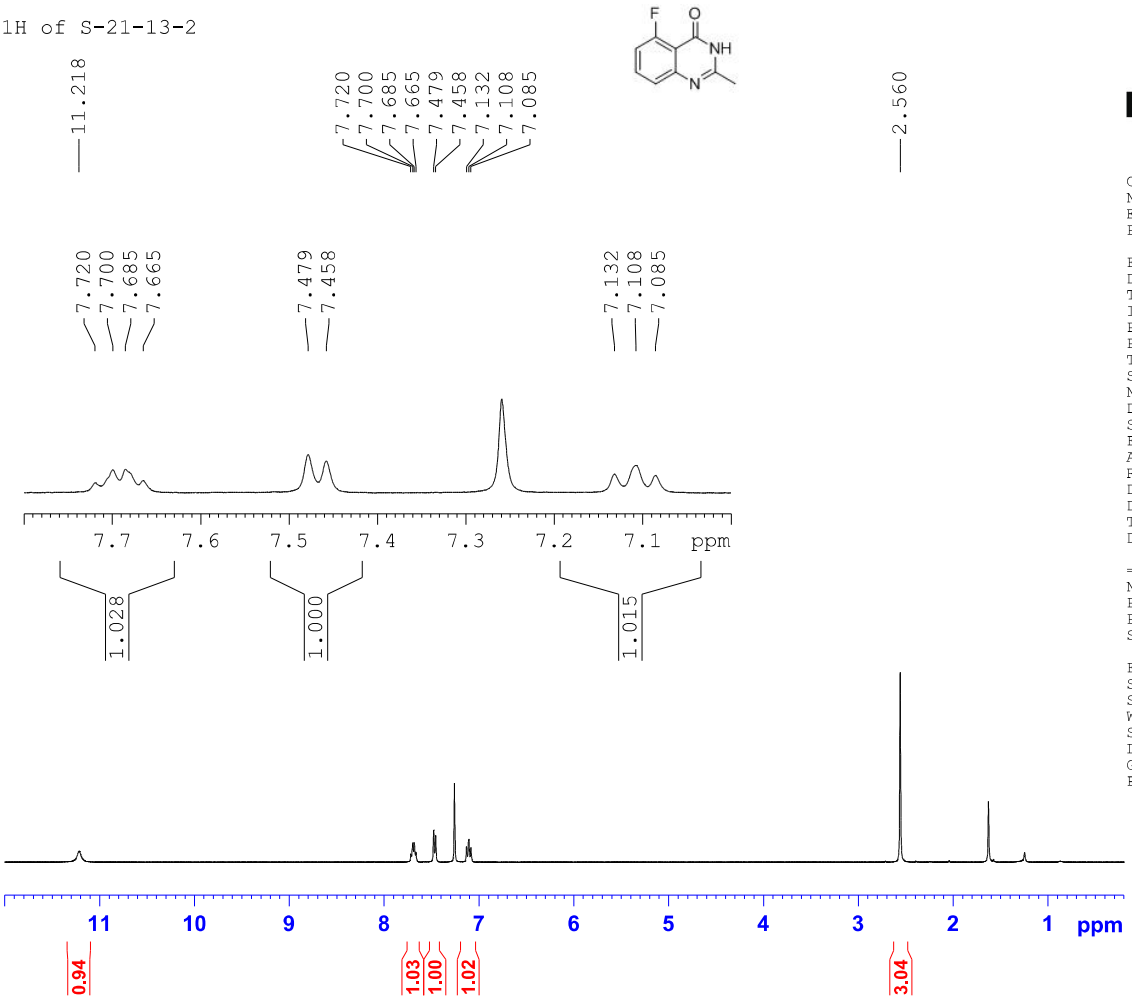
F2 - Acquisition Parameters
Date_ 20141118
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 921
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

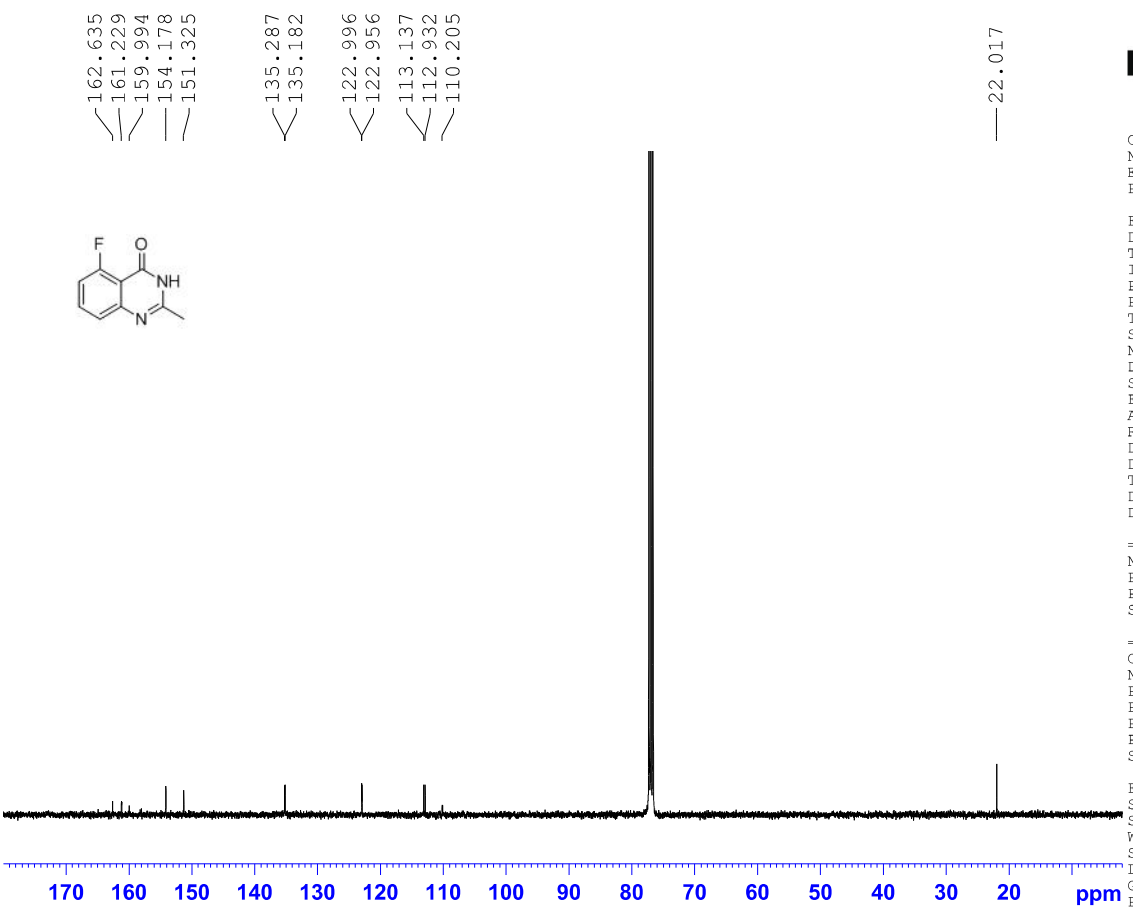
F2 - Processing parameters
SI 32768
SF 100.6127776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-21-13-2



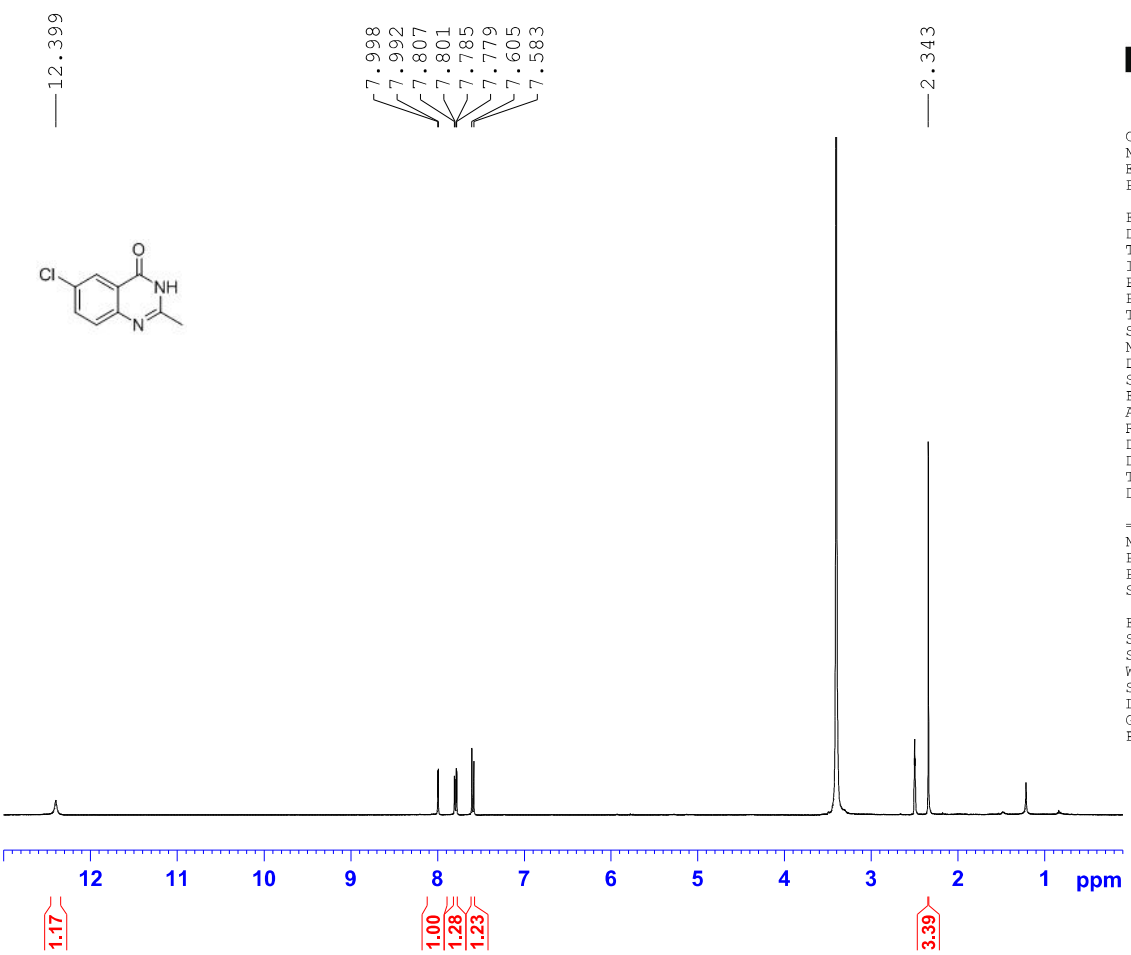

```
Current Data Parameters
NAME                  S-21-13-2
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20141125
Time                      11.24
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8223.685 Hz
FIDRES                0.125483 Hz
AQ                    3.9846387 sec
RG                         161
DW                      60.800 usec
DE                       6.50 usec
TE                      293.1 K
D1                    1.00000000 sec

======== CHANNEL f1 ========
NUC1                         1H
P1                       13.70 usec
PLW1                14.30000019 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                       65536
SF                 400.1300182 MHz
WDW                         EM
SSB                0
LB                       0.30 Hz
GB                 0
PC                       1.00
```

13C of S-21-13-2



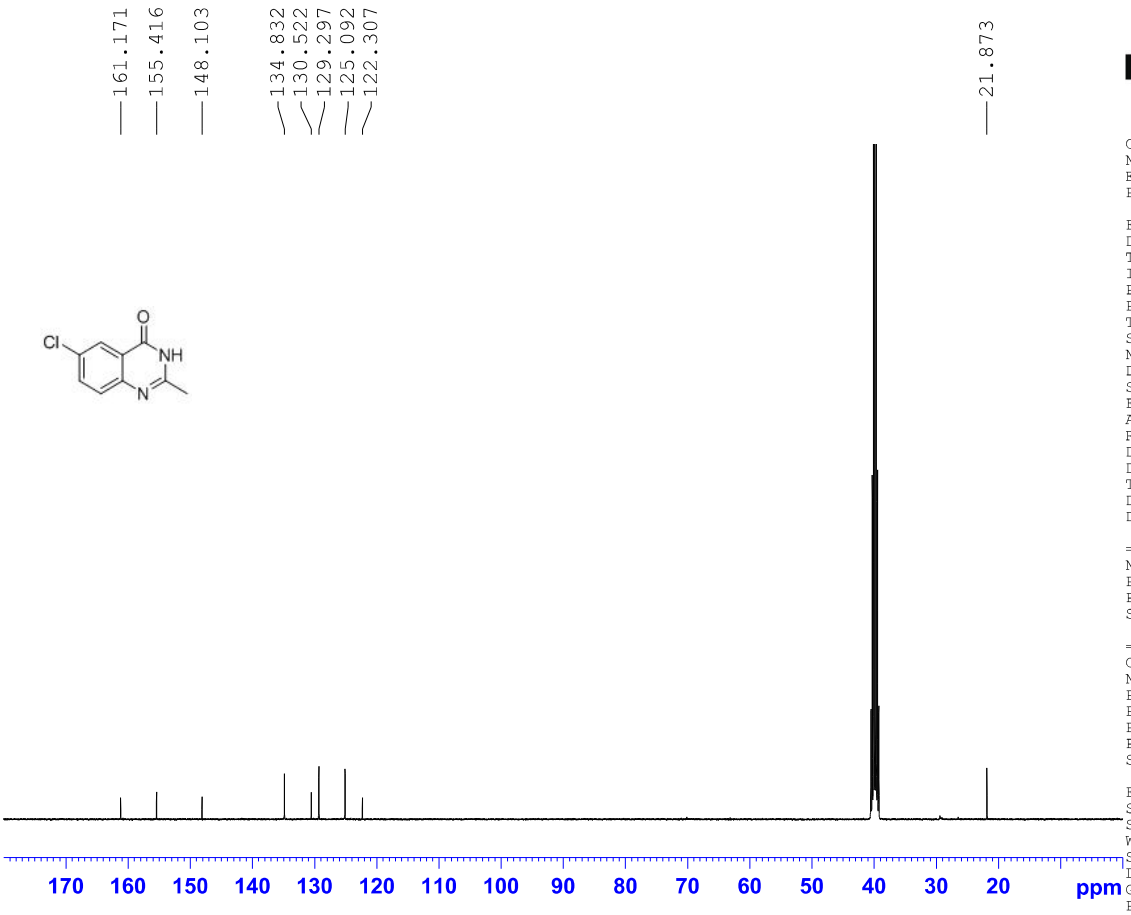

```
Current Data Parameters
NAME                  S-21-13-2
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20141125
Time                      11.35
INSTRUM                   spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        3134
DS                           0
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                        71.8
DW                      20.800 usec
DE                       6.50 usec
TE                      293.5 K
D1                    2.00000000 sec
D11                   0.03000000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                       11.65 usec
PLW1                34.00000000 W
SFO1               100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                    90.00 usec
PLW2                14.30000019 W
PLW12                0.33135000 W
PLW13                0.26840001 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6127738 MHz
WDW                         EM
SSB                0
LB                       1.00 Hz
GB                 0
PC                       1.40
```

1H of S-27-27



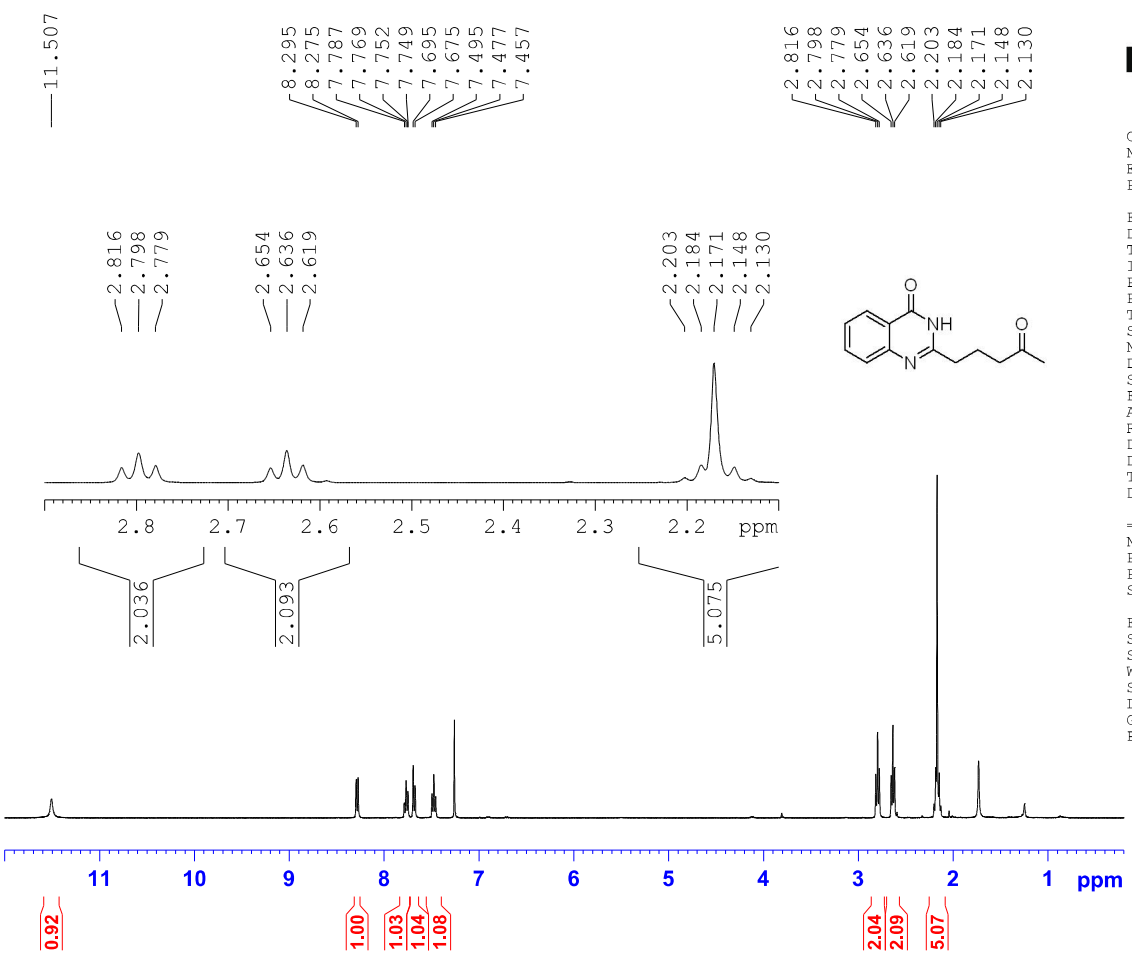

```
Current Data Parameters
NAME                  S-27-27
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150110
Time                 18.35
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                   80.6
DW                60.800 usec
DE                 6.50 usec
TE                292.9 K
D1             1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.73 usec
PLW1          14.30000019 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300074 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

13C of S-27-27




```
Current Data Parameters
NAME                  S-27-27
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150111
Time                  2.54
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                  15360
DS                      4
SWH              26785.715 Hz
FIDRES           0.408718 Hz
AQ               1.2233887 sec
RG                    203
DW                18.667 usec
DE                 6.50 usec
TE                296.8 K
D1             0.20000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 12.08 usec
PLW1          34.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2          14.30000019 W
PLW12          0.38304999 W
PLW13          0.31027001 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127736 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

1H NMR LSS-25



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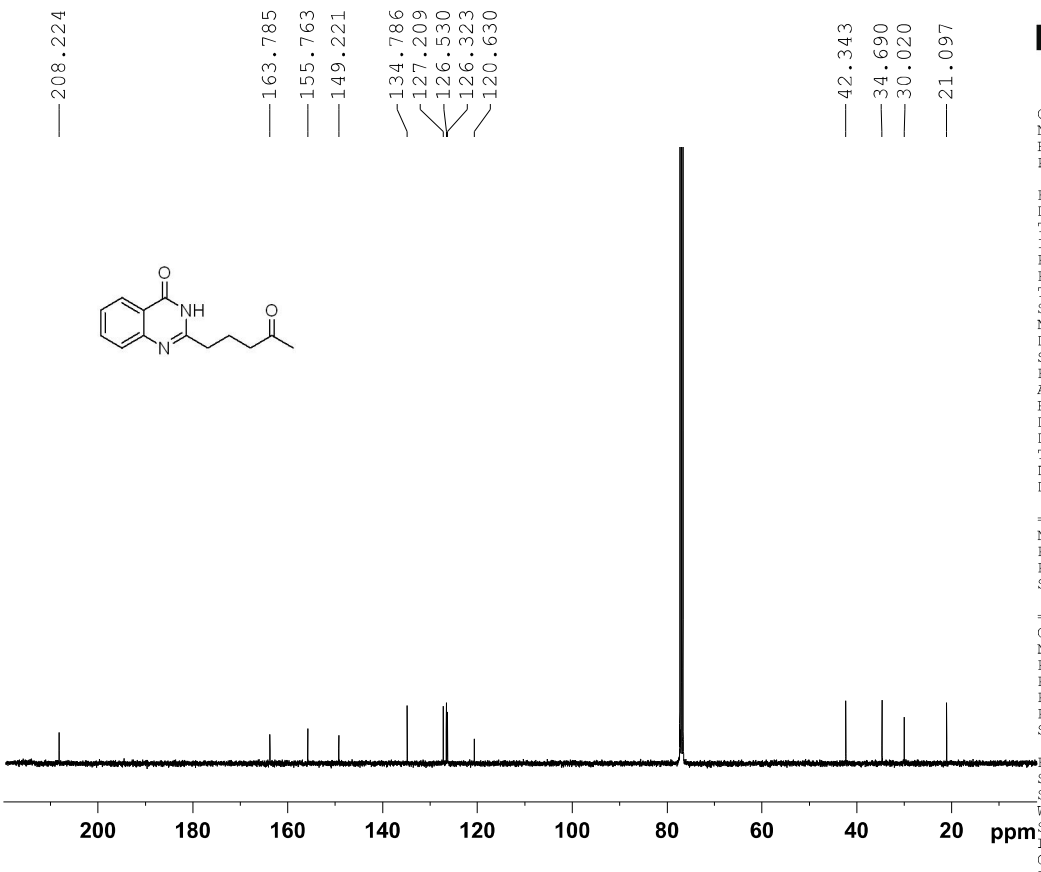
```
Current Data Parameters
NAME                  LSS-25
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141113
Time                  15.35
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      144
DW                   60.800 usec
DE                    6.50 usec
TE                   294.9 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.70 usec
PLW1            14.30000019 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300176 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

13C NMR LSS-25



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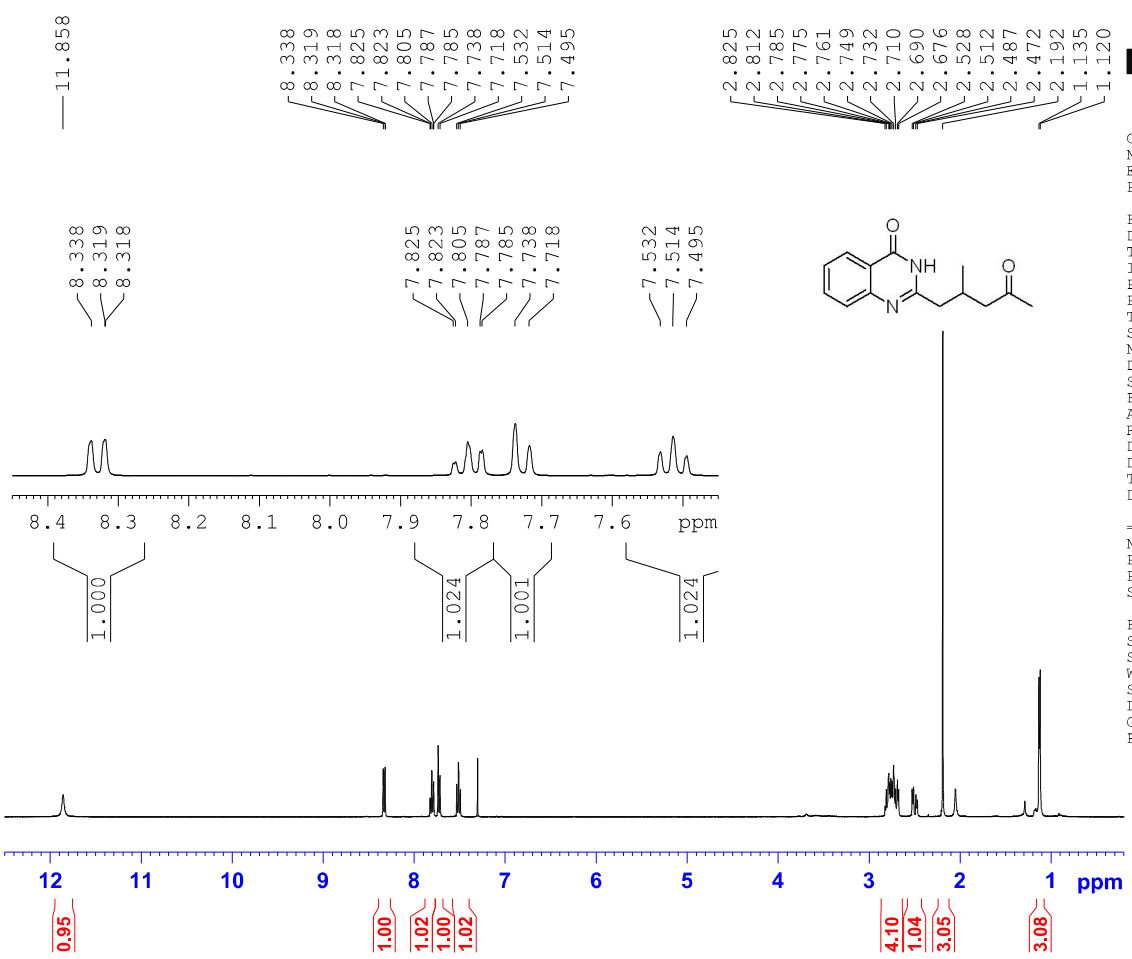
```
Current Data Parameters
NAME                  LSS-25
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20141113
Time                  15.45
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1075
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      128
DW                   20.800 usec
DE                    6.50 usec
TE                   295.4 K
D1                2.00000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.65 usec
PLW1           34.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2            14.30000019 W
PLW12            0.33135000 W
PLW13            0.26840001 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF              100.6127737 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

1H of SGS-65



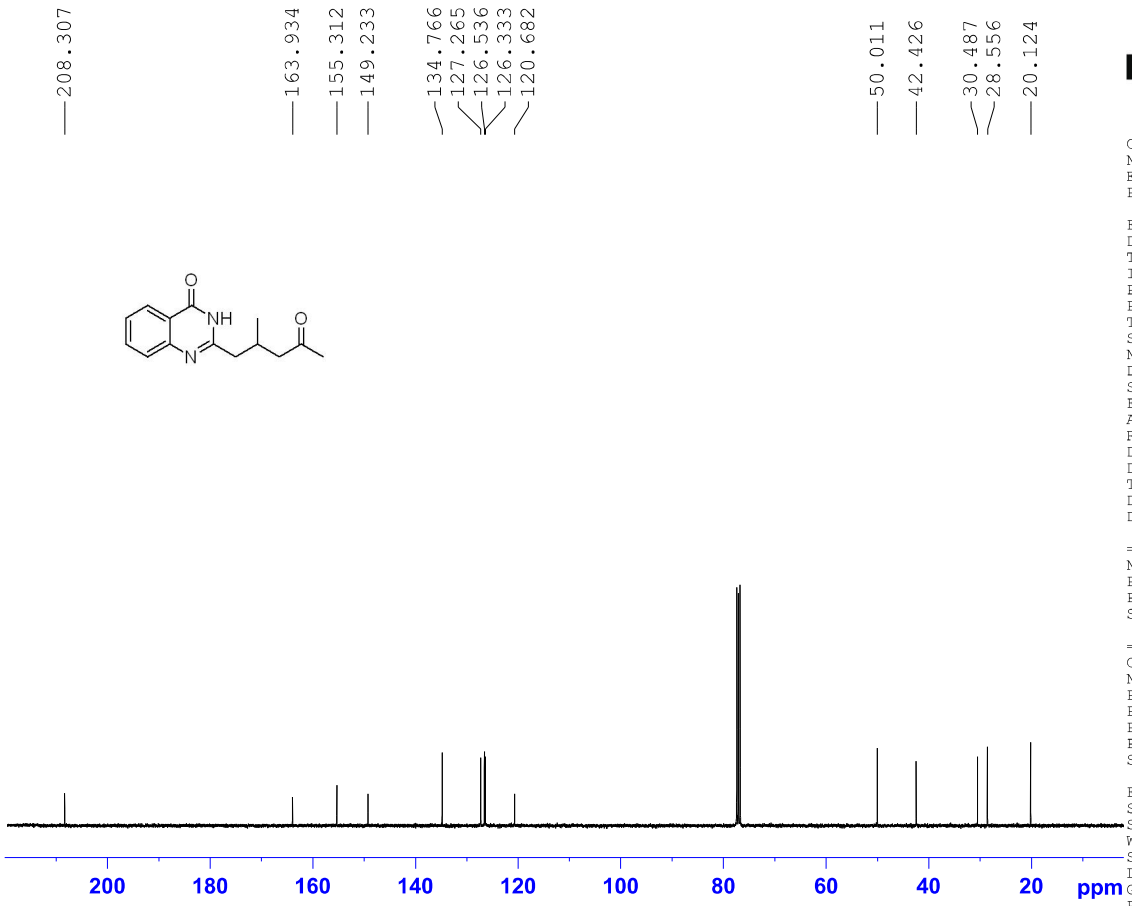
Current Data Parameters
NAME SGS-65
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150425
Time 12.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-65



Current Data Parameters
NAME SGS-65
EXPNO 2
PROCNO 1

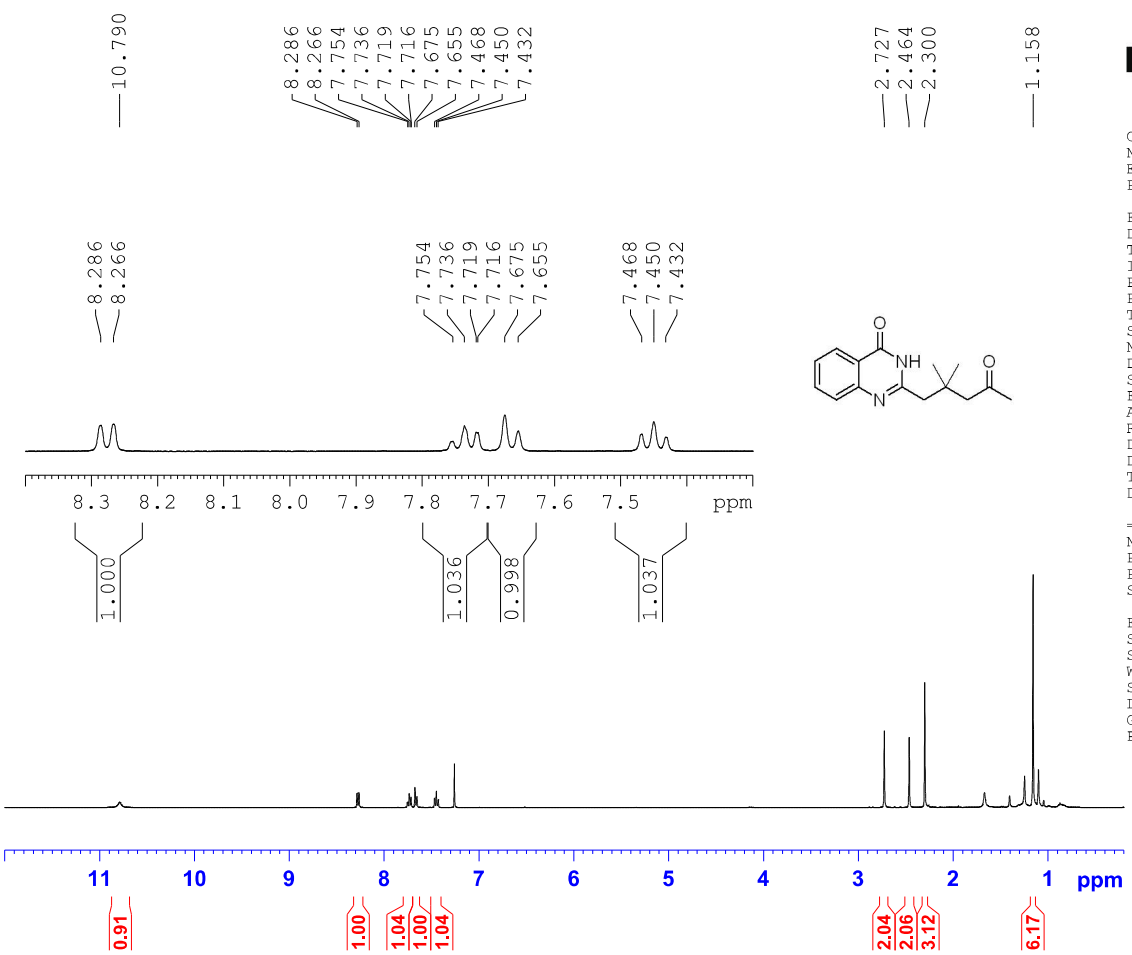
F2 - Acquisition Parameters
Date_ 20150425
Time 12.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 838
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H NMR LSS-26-1



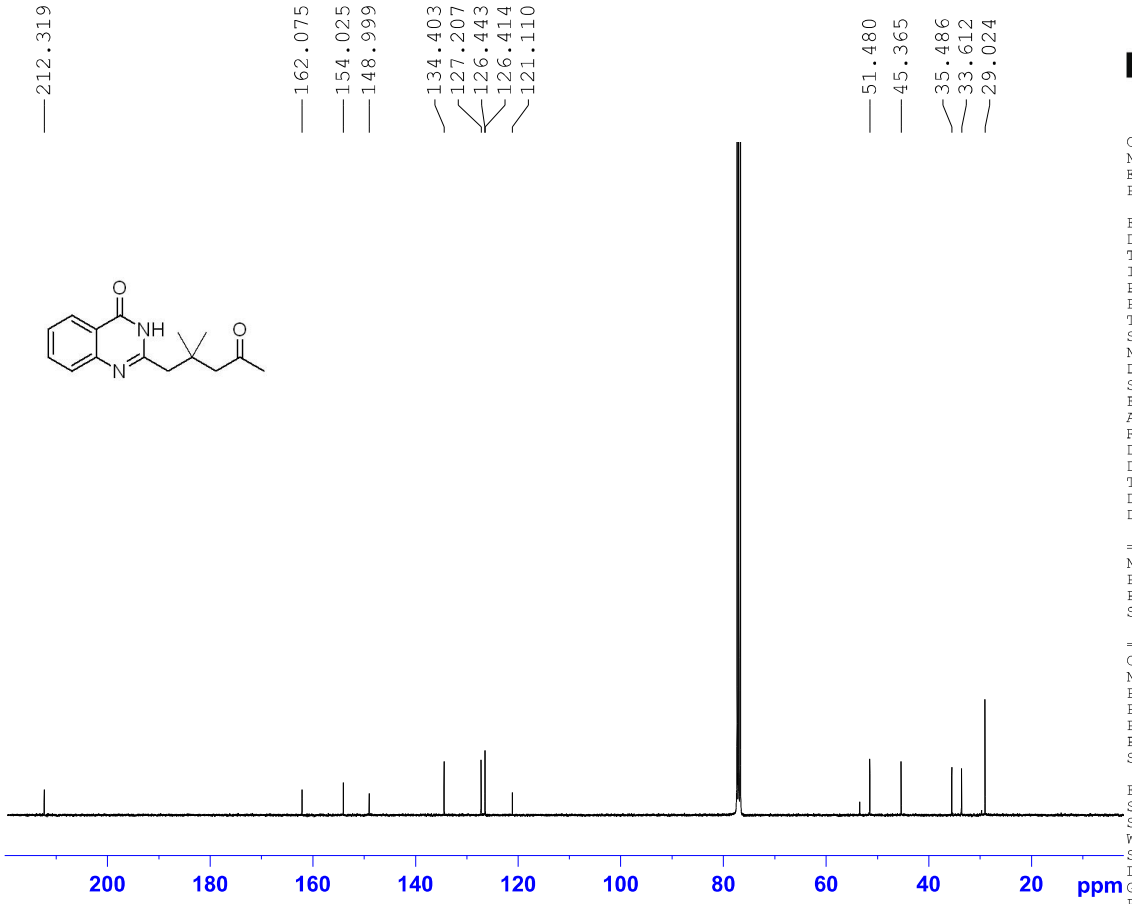
Current Data Parameters
NAME LSS-26-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141125
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C NMR LSS-26



Current Data Parameters
NAME LSS-26
EXPNO 2
PROCNO 1

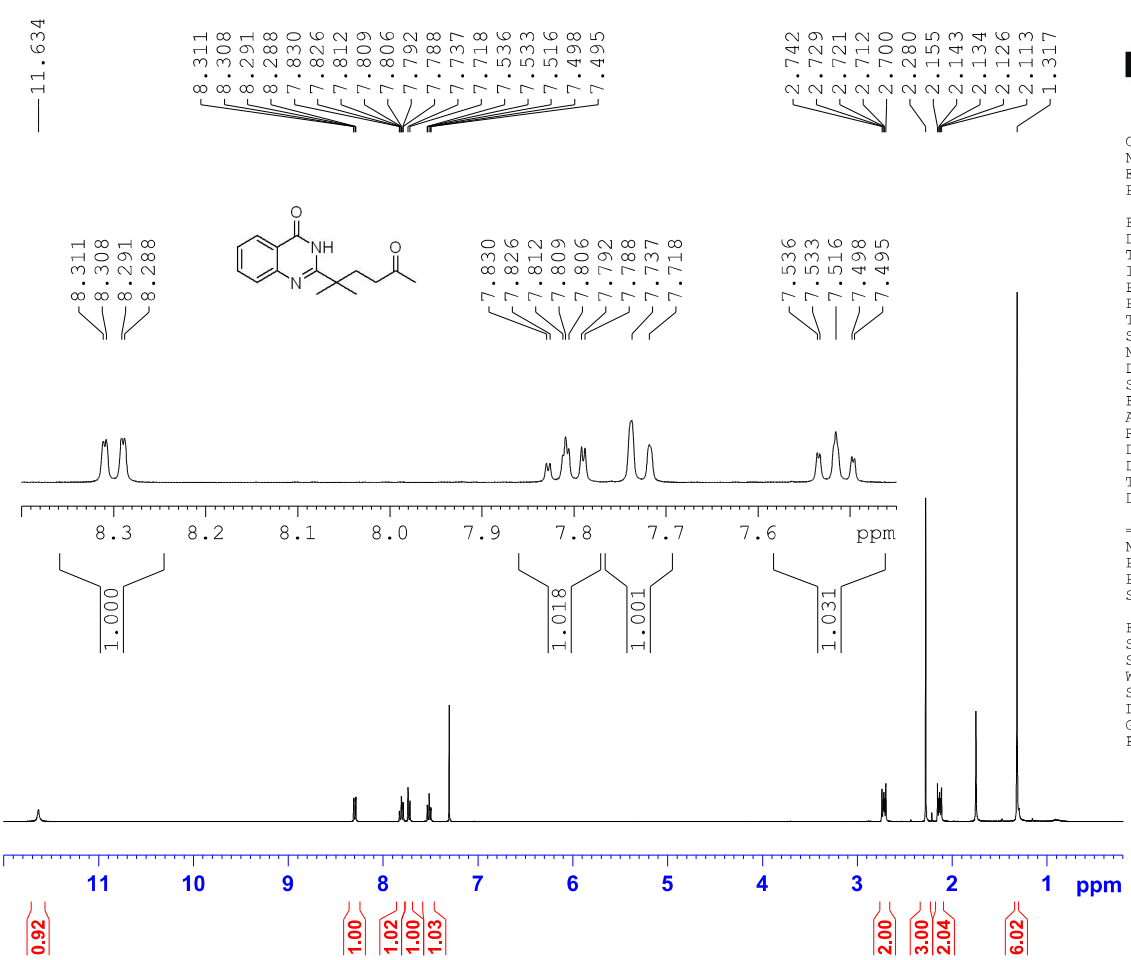
F2 - Acquisition Parameters
Date_ 20141124
Time 22.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SGS-66



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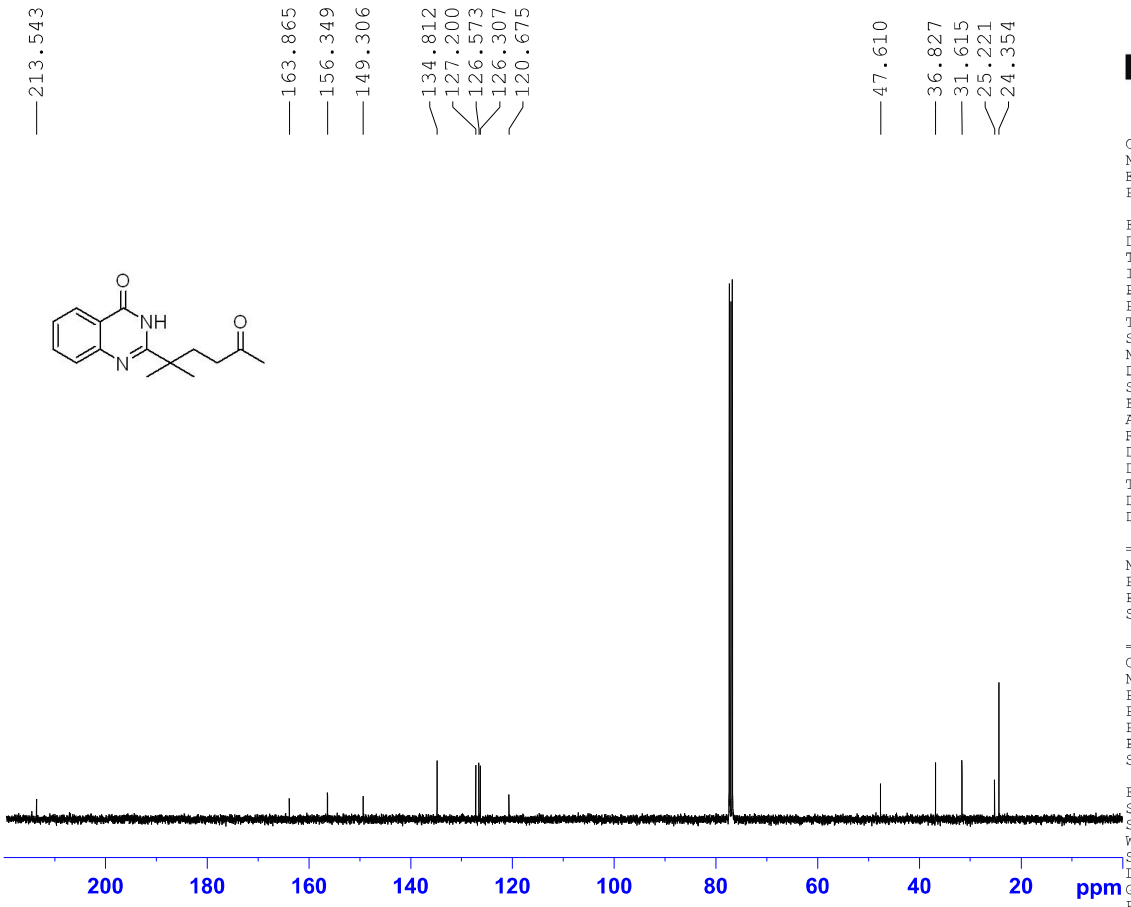
Current Data Parameters
NAME SGS-66
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150425
Time 11.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-66



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Current Data Parameters
NAME SGS-66
EXPNO 2
PROCNO 1

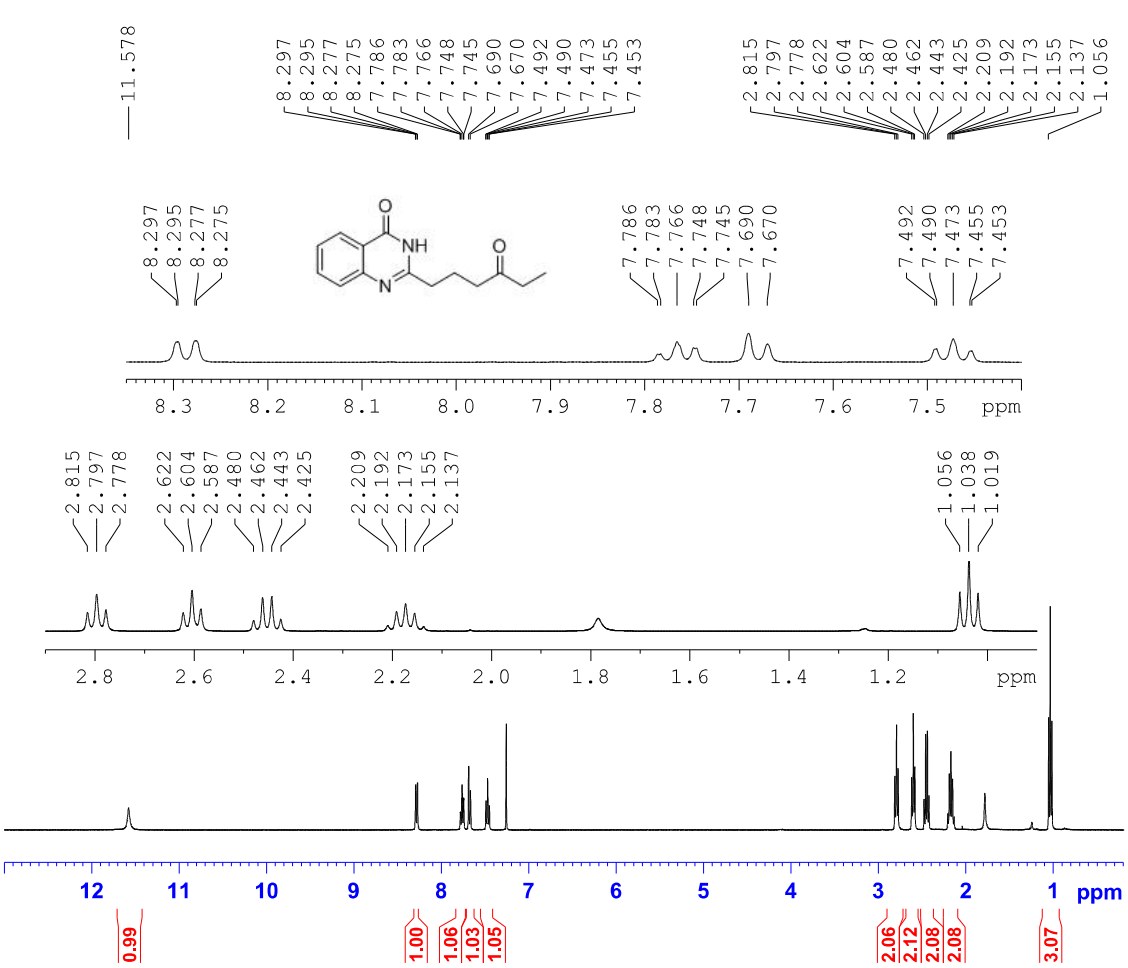
F2 - Acquisition Parameters
Date_ 20150425
Time 11.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 537
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H NMR LSS-28



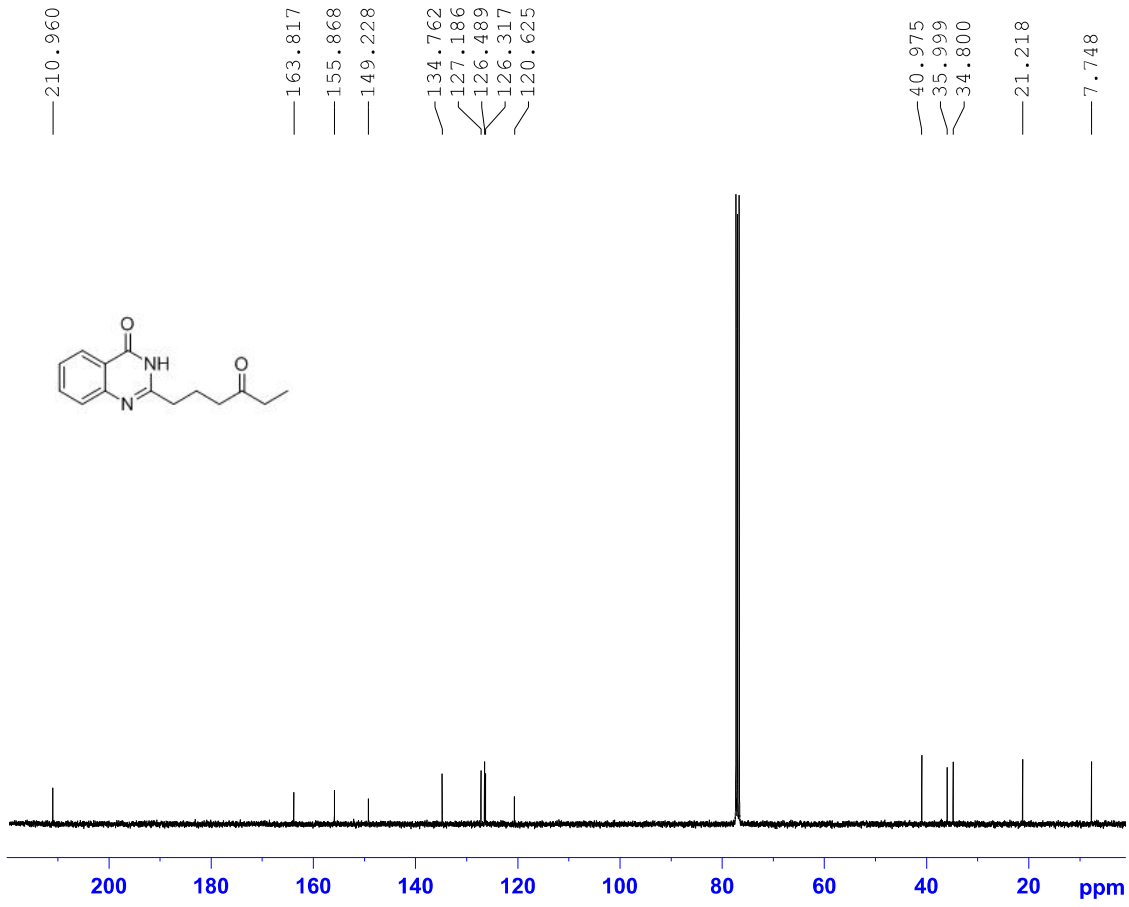
Current Data Parameters
NAME LSS-28
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141118
Time 17.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.70 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C NMR LSS-28



Current Data Parameters
NAME LSS-28
EXPNO 2
PROCNO 1

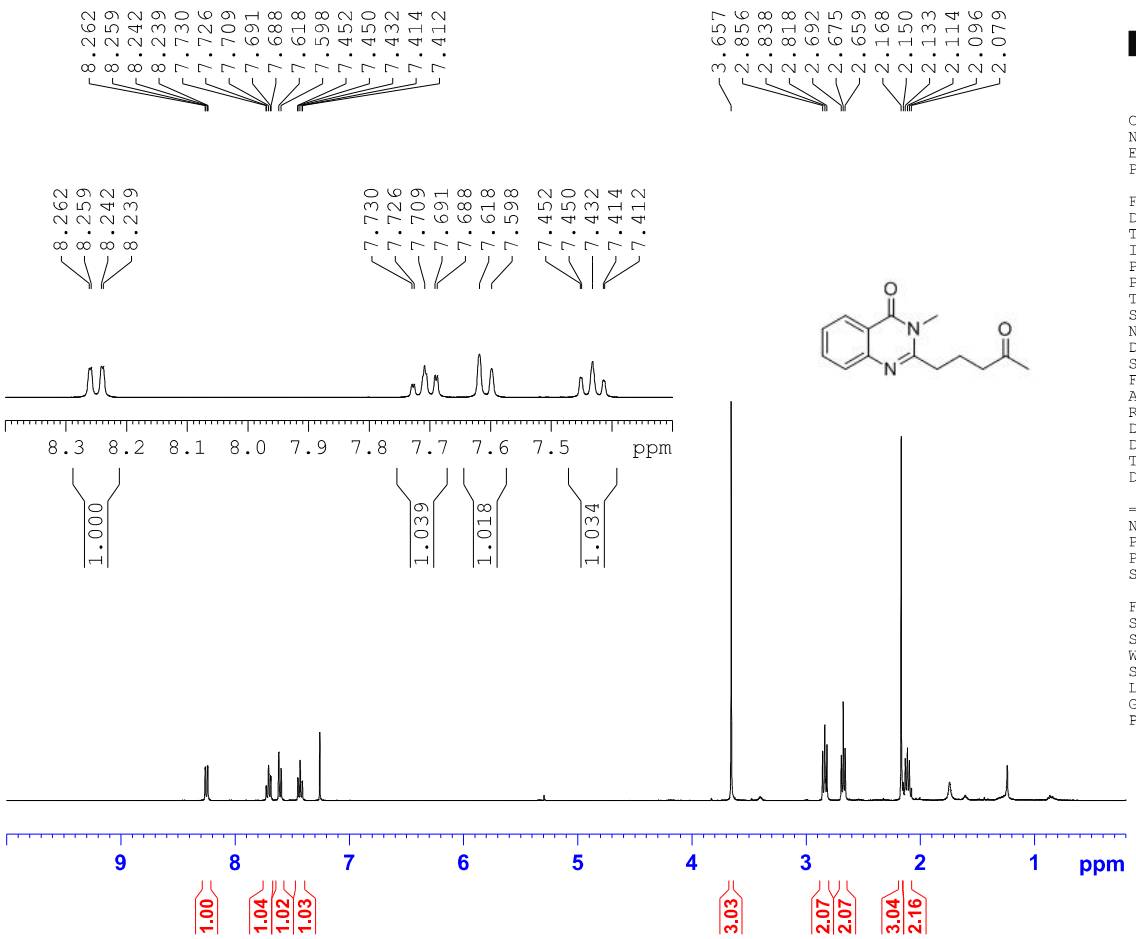
F2 - Acquisition Parameters
Date_ 20141118
Time 17.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 706
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 11.65 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.33135000 W
PLW13 0.26840001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127745 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of S-52



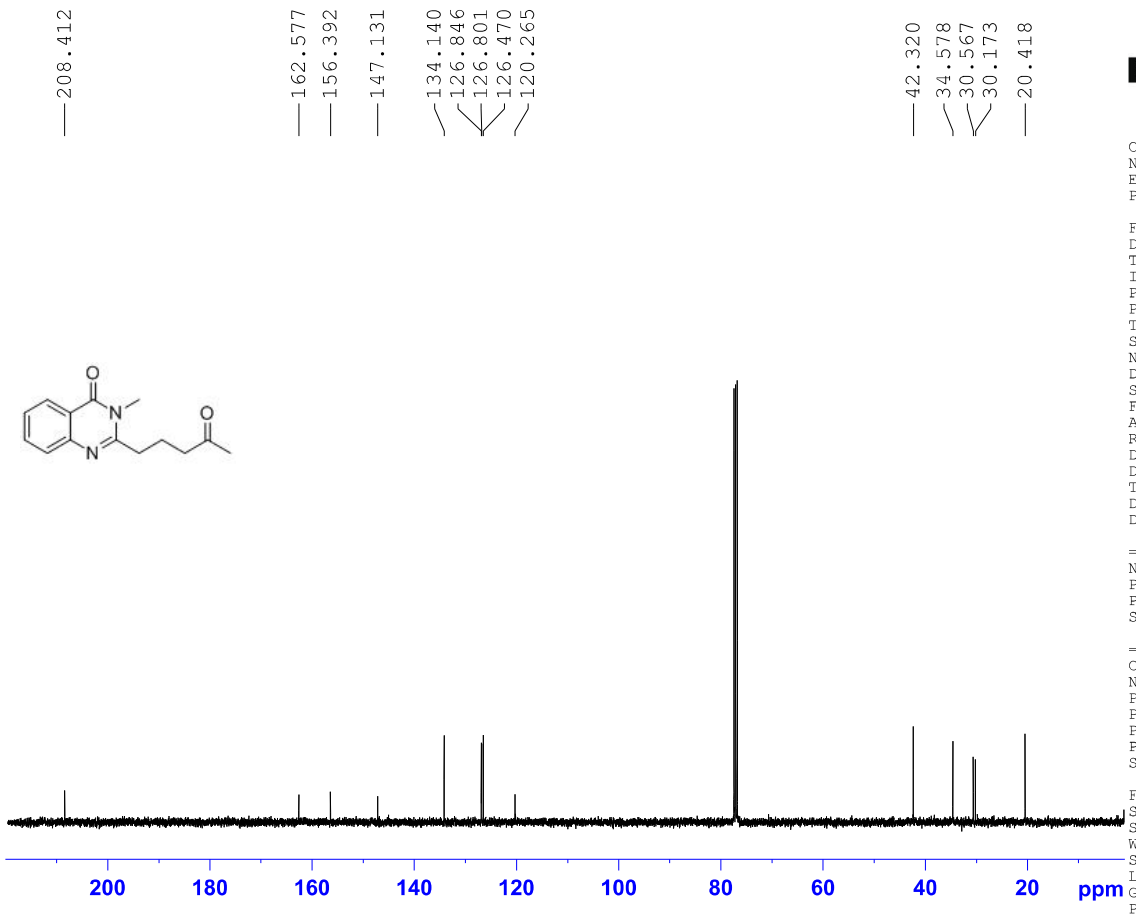
Current Data Parameters
NAME S-52
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150129
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 101
DW 60.800 usec
DE 6.50 usec
TE 288.1 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300181 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of S-52



Current Data Parameters
NAME S-52
EXPNO 2
PROCNO 1

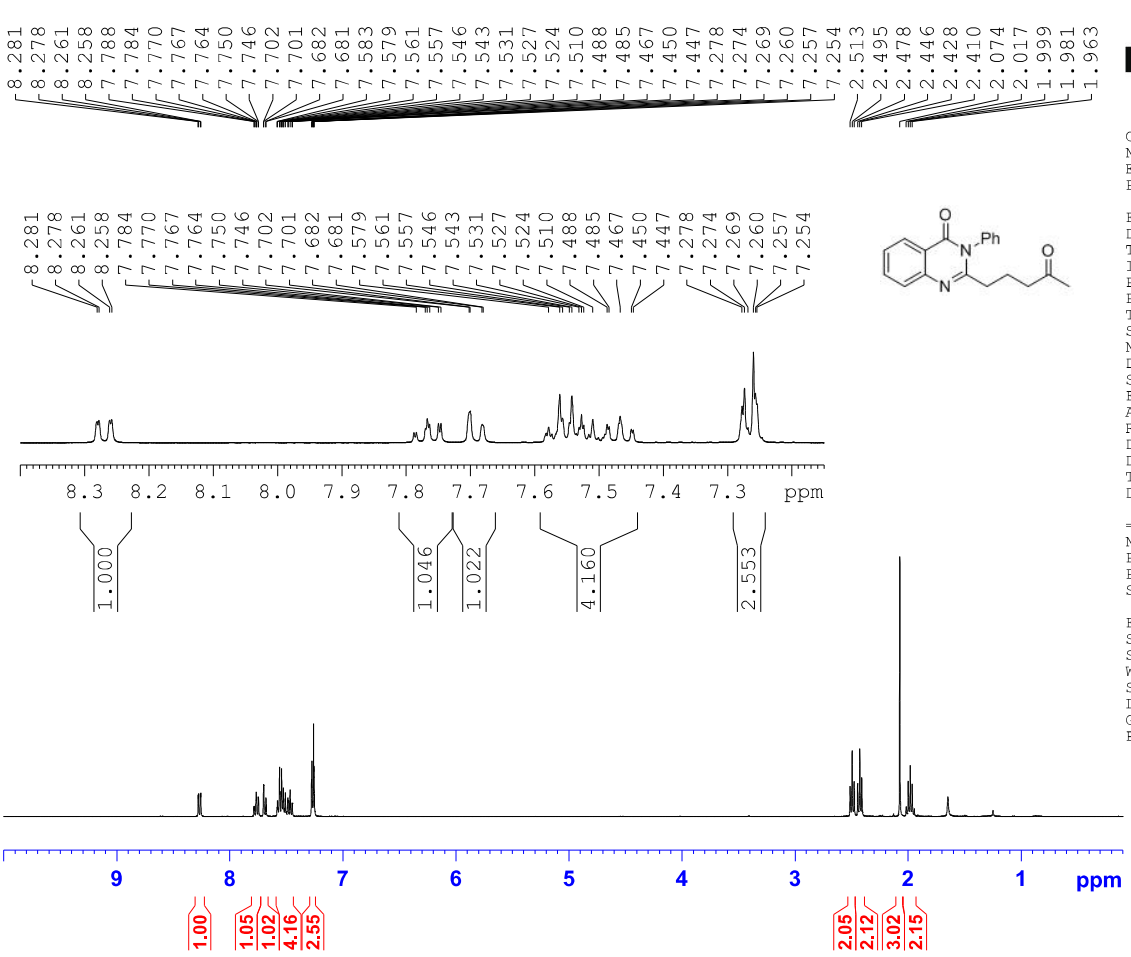
F2 - Acquisition Parameters
Date_ 20150129
Time 14.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 278
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 80.6
DW 20.800 usec
DE 6.50 usec
TE 288.8 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SGS-41



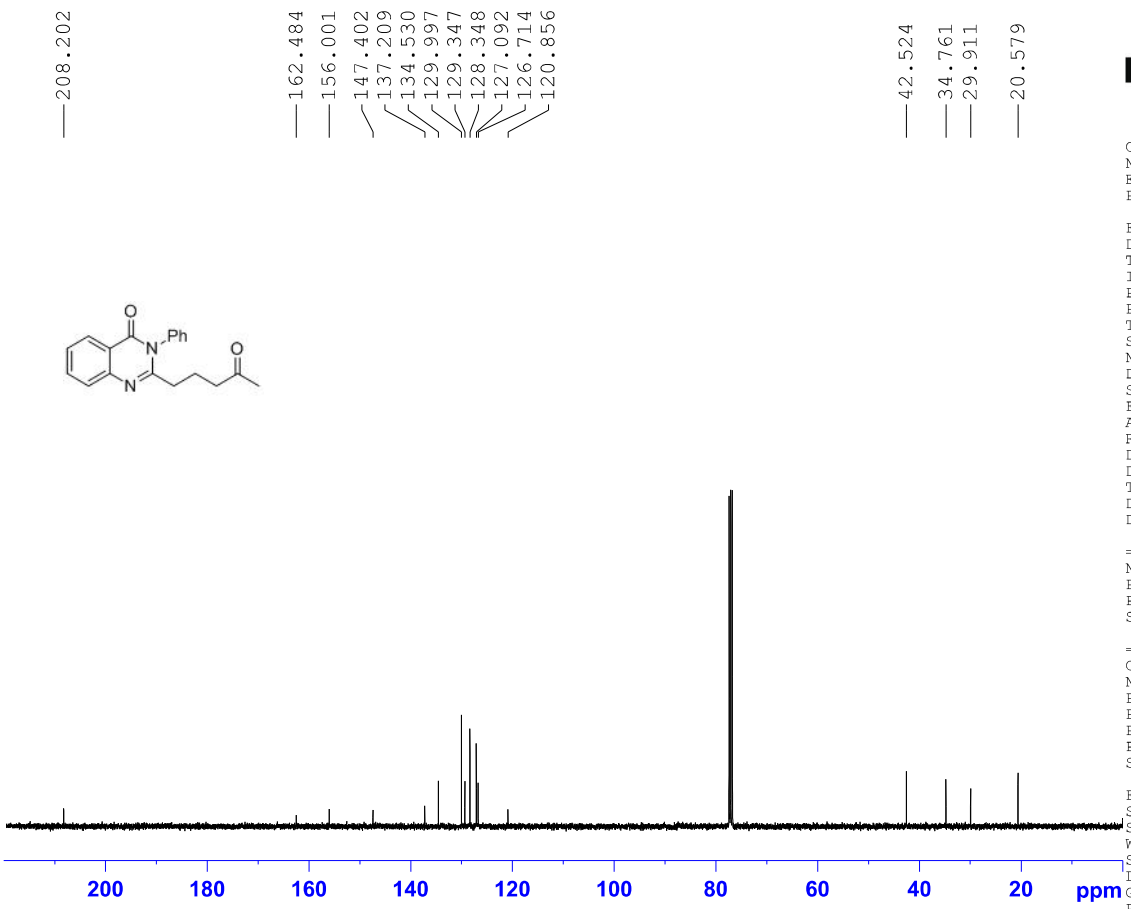
Current Data Parameters
NAME SGS-41
EXPNO 1
PROCNO 1

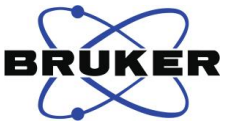
F2 - Acquisition Parameters
Date_ 20150121
Time 14.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-41





Current Data Parameters
NAME SGS-41
EXPNO 2
PROCNO 1

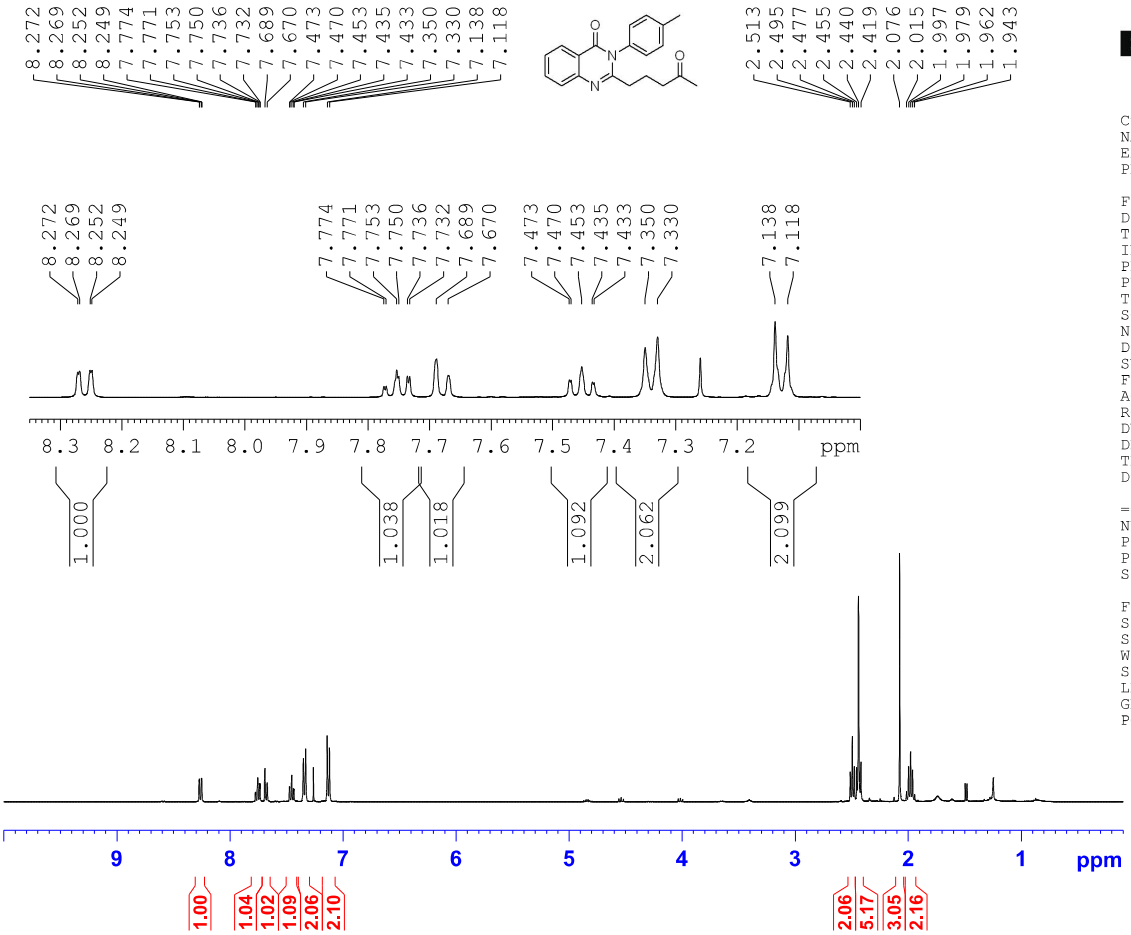
F2 - Acquisition Parameters
Date_ 20150121
Time 14.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 302
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SGS-45



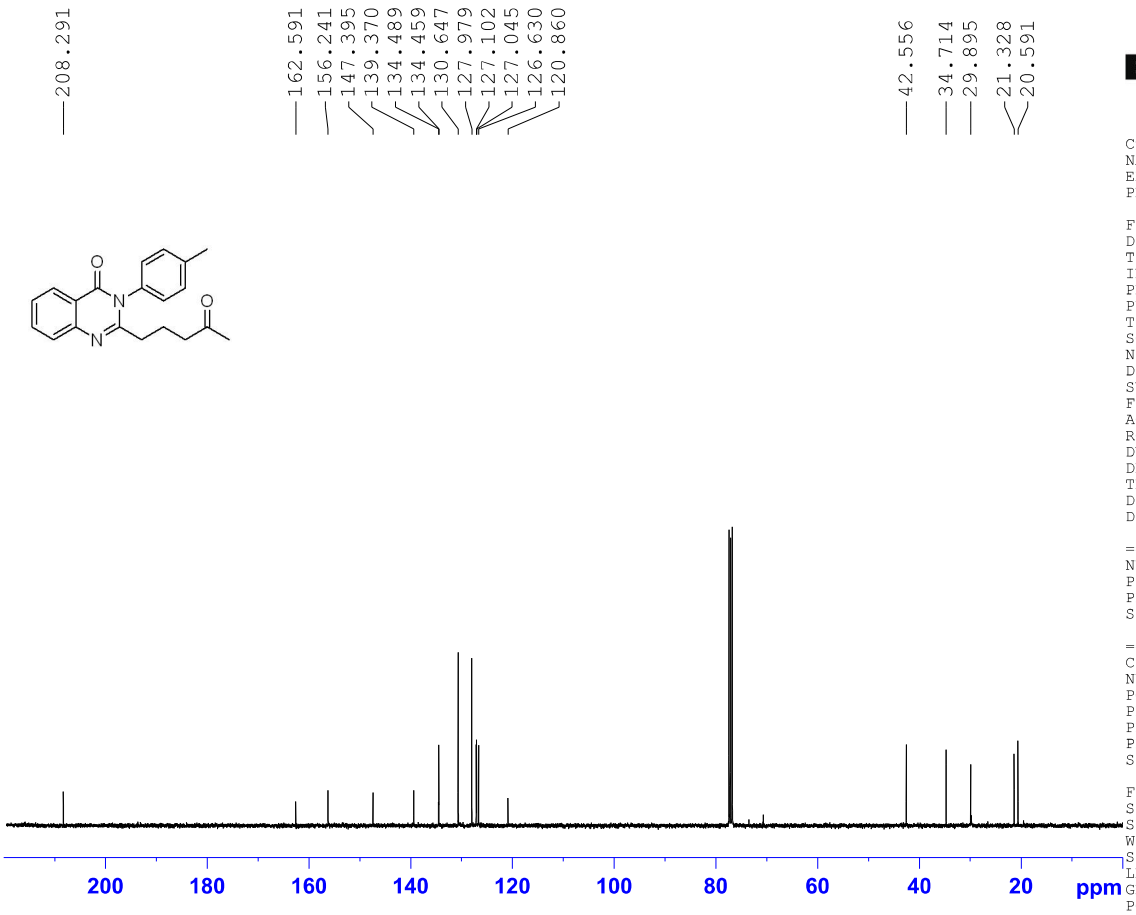
Current Data Parameters
NAME SGS-45
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 12.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-45



Current Data Parameters
NAME SGS-45
EXPNO 2
PROCNO 1

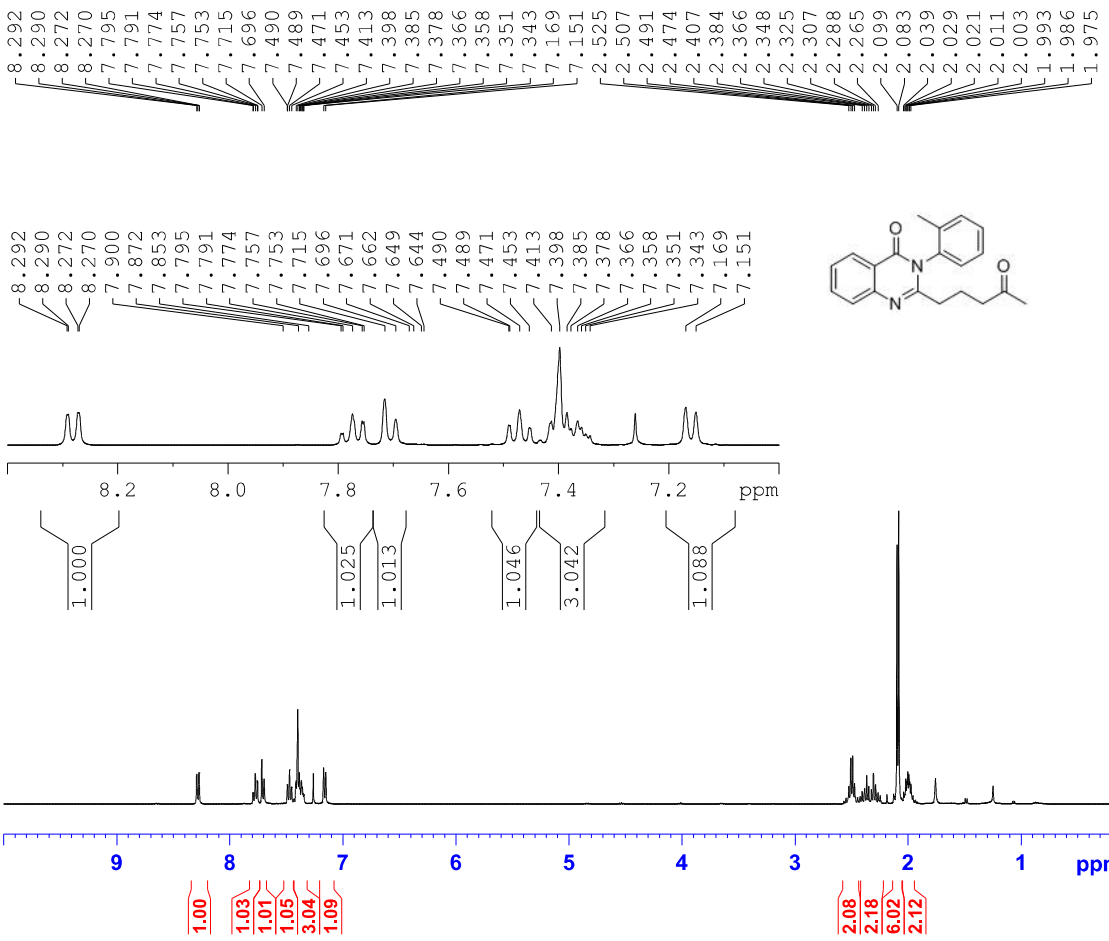
F2 - Acquisition Parameters
Date_ 20150121
Time 12.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 616
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SGS-47



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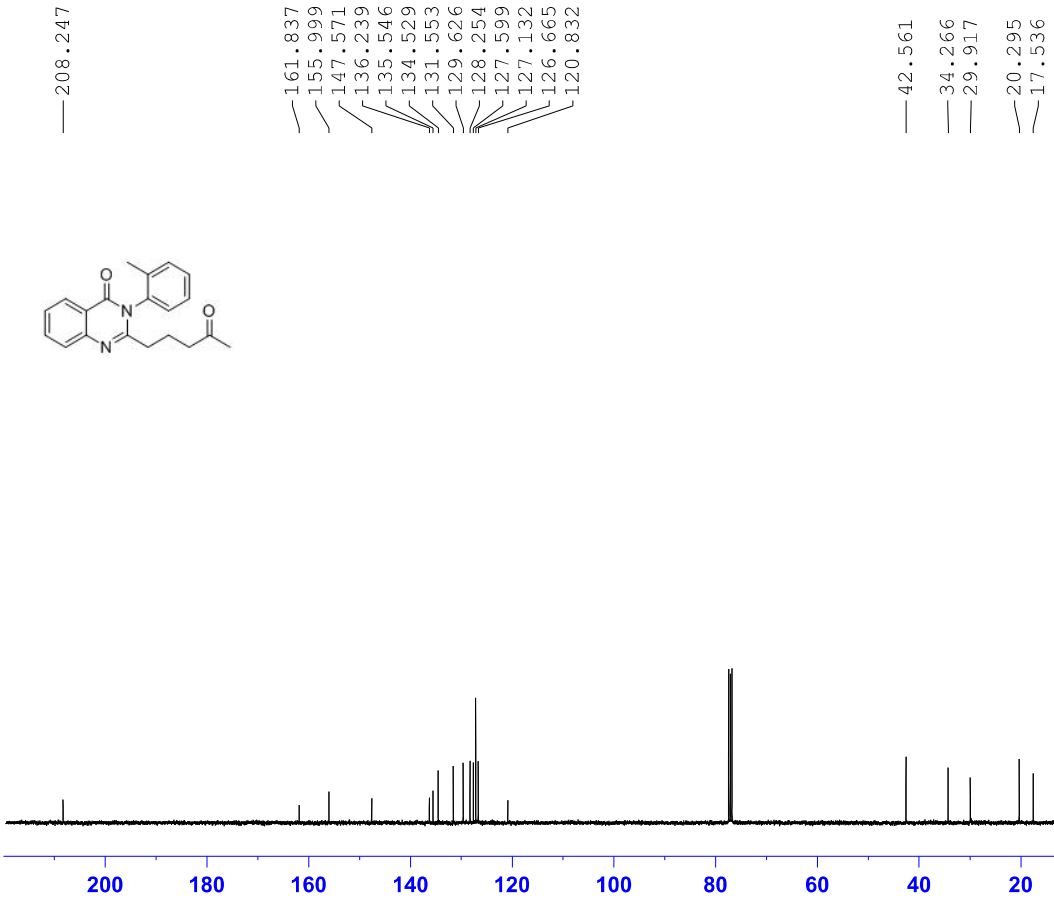
Current Data Parameters
NAME SGS-47
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 13.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 90.5
DW 60.800 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300174 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-47



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Current Data Parameters
NAME SGS-47
EXPNO 2
PROCNO 1

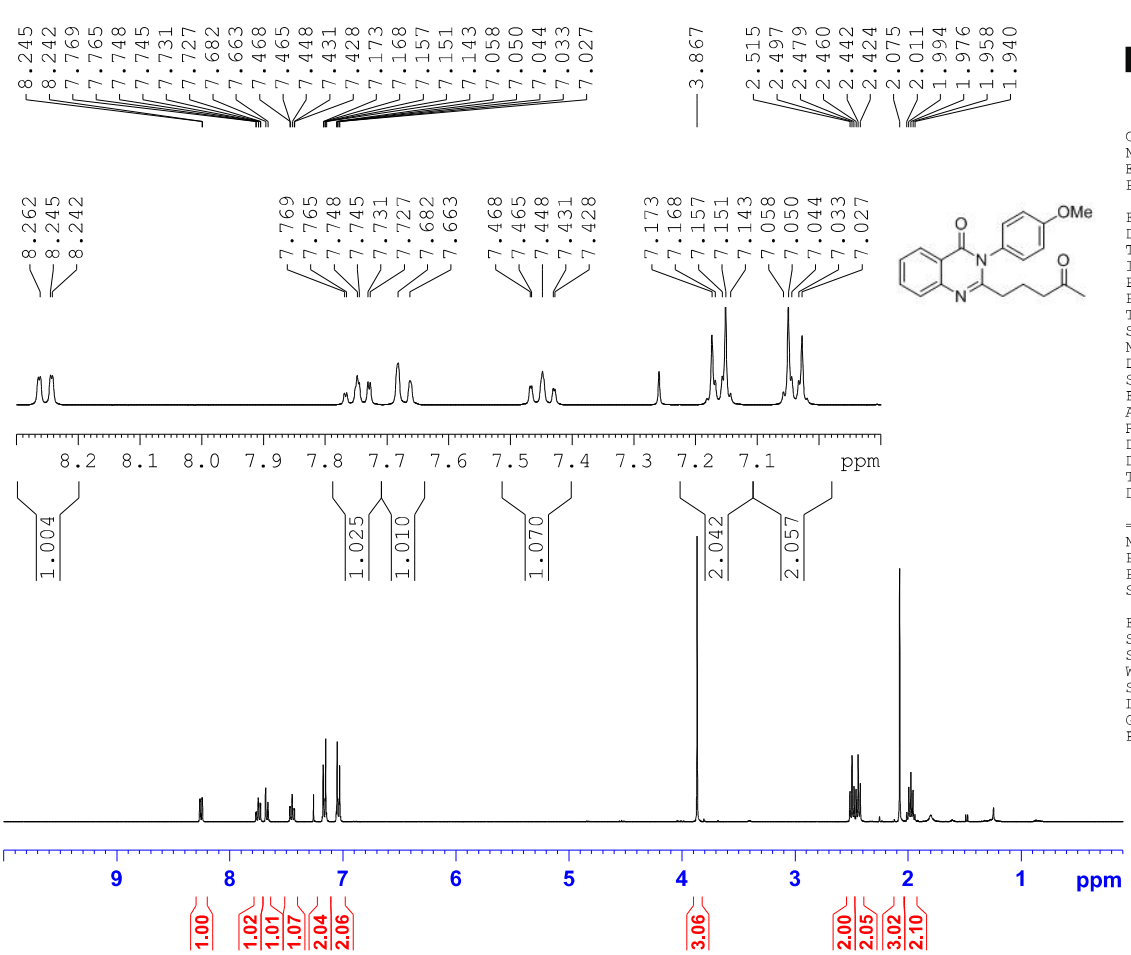
F2 - Acquisition Parameters
Date_ 20150121
Time 13.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 273
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

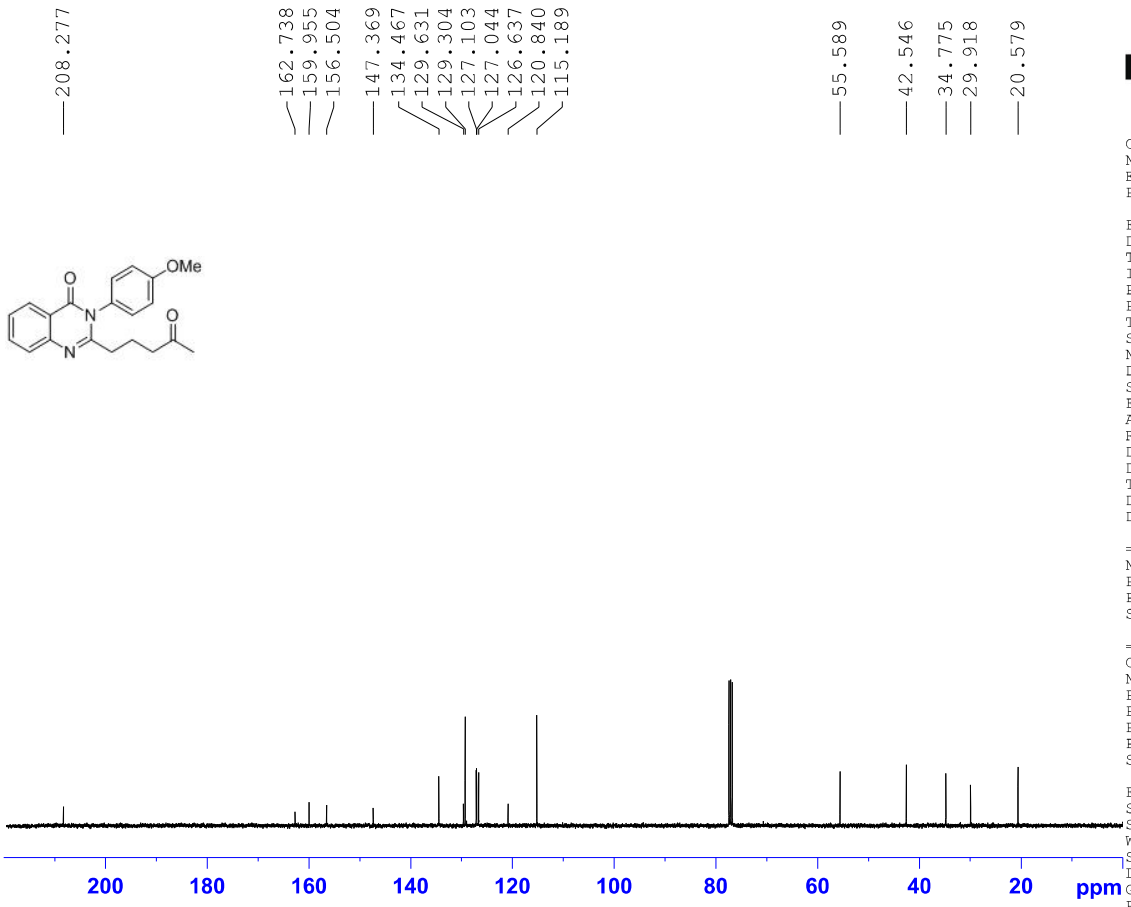
1H of SGS-44



BRUKER

```
Current Data Parameters
NAME                  SGS-44
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  13.32
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     80.6
DW                  60.800 usec
DE                   6.50 usec
TE                  293.7 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.73 usec
PLW1            14.30000019 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300181 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

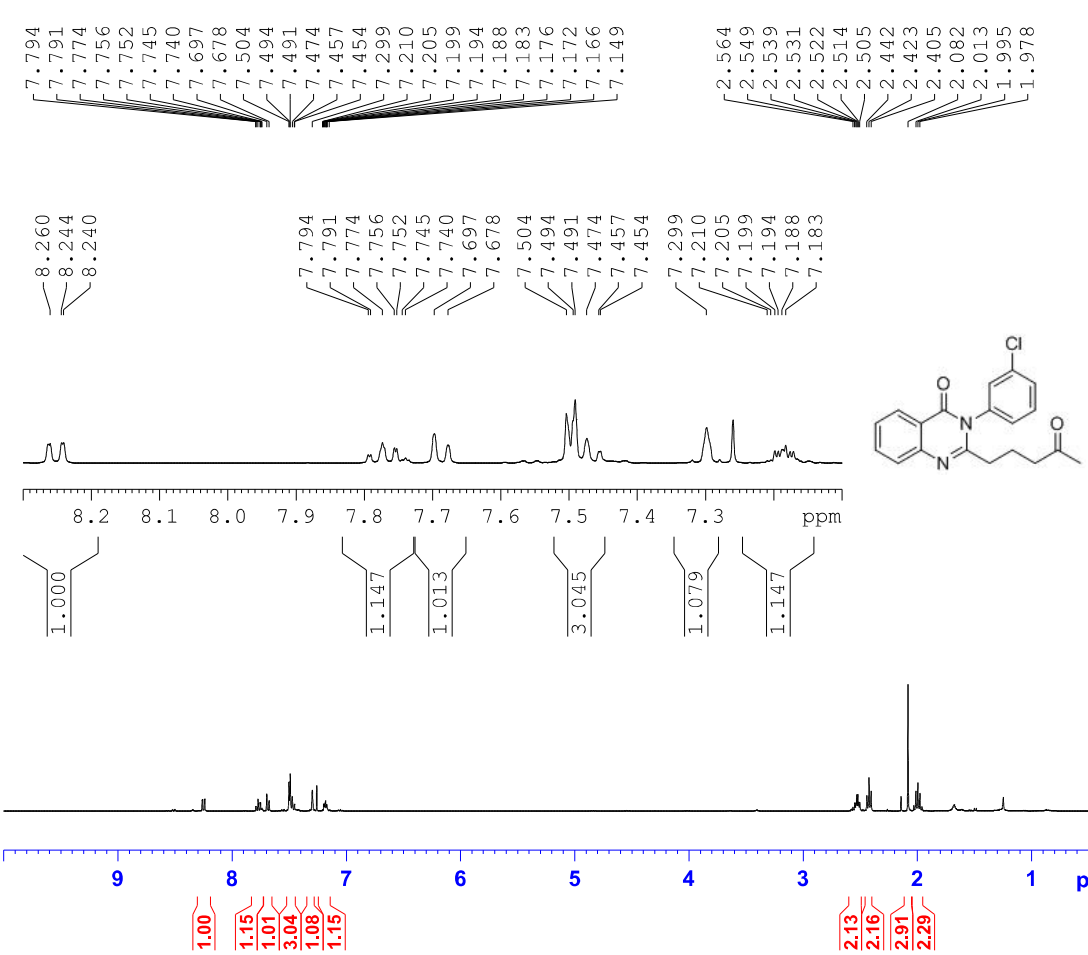
13C of SGS-44



BRUKER

```
Current Data Parameters
NAME                  SGS-44
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  13.37
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      176
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      144
DW                  20.800 usec
DE                   6.50 usec
TE                  294.4 K
D1                0.20000000 sec
D11               0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                     12.08 usec
PLW1            34.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2            14.30000019 W
PLW12            0.38304999 W
PLW13            0.31027001 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF               100.6127690 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

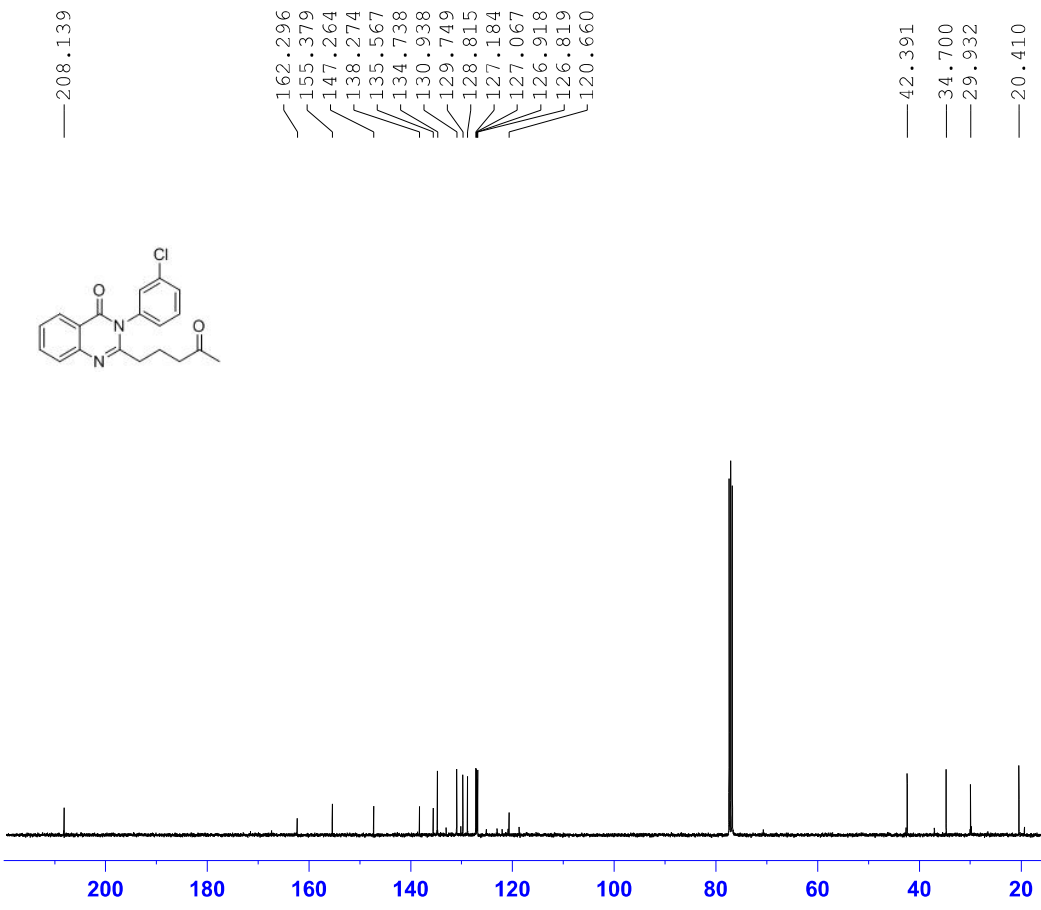
1H of SGS-43



BRUKER

```
Current Data Parameters
NAME                  SGS-43
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  12.35
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                     114
DW                60.800 usec
DE                 6.50 usec
TE                293.9 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.73 usec
PLW1          14.30000019 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300179 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

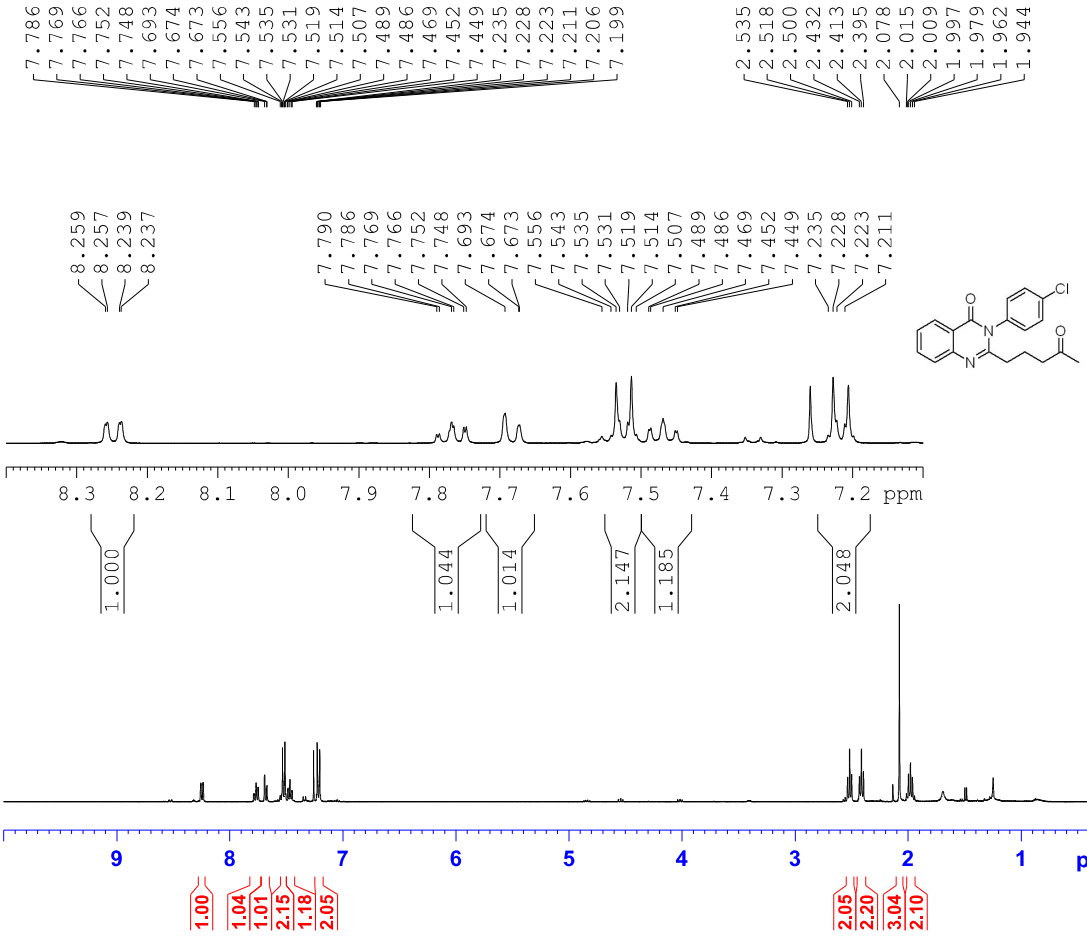
13C of SGS-43



BRUKER

```
Current Data Parameters
NAME                  SGS-43
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  13.08
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1293
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                     144
DW                20.800 usec
DE                 6.50 usec
TE                294.6 K
D1              0.20000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 12.08 usec
PLW1          34.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2          14.30000019 W
PLW12          0.38304999 W
PLW13          0.31027001 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127690 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

1H of SGS-48



BRUKER

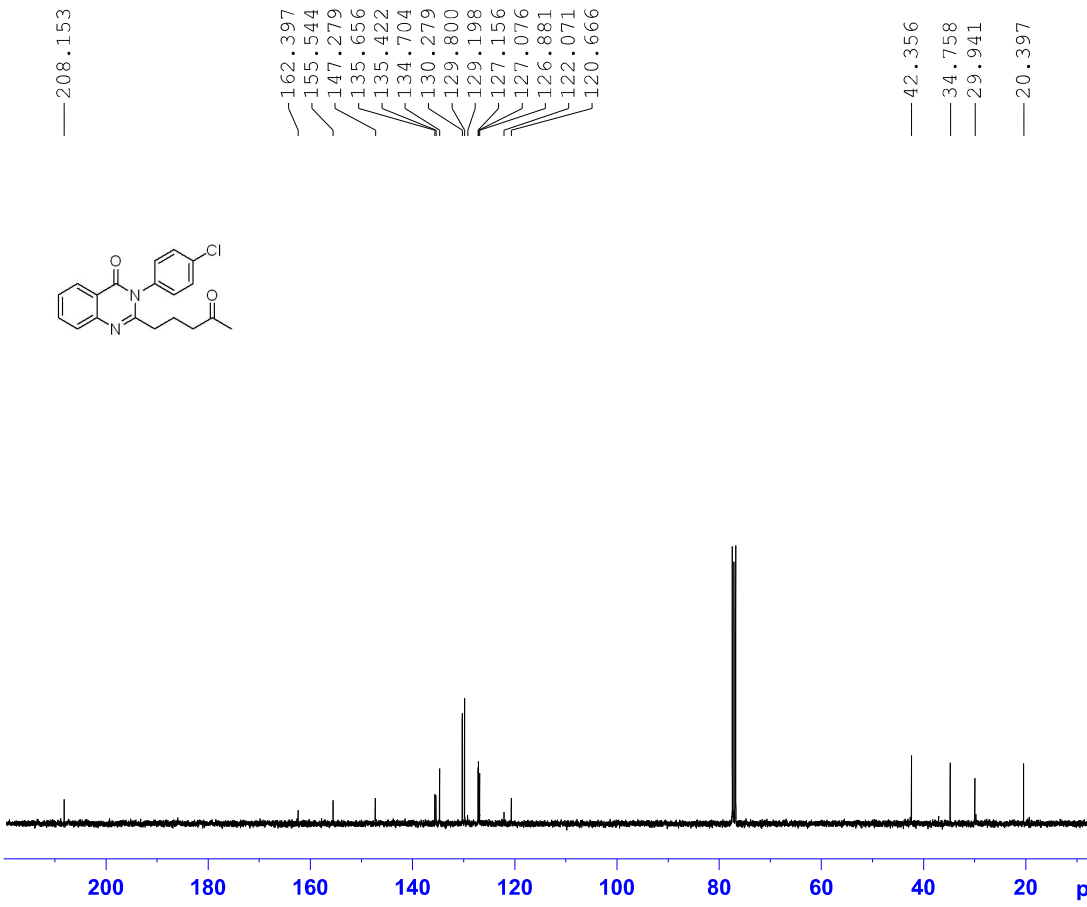
Current Data Parameters
NAME SGS-48
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300180 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-48



BRUKER

Current Data Parameters
NAME SGS-48
EXPNO 2
PROCNO 1

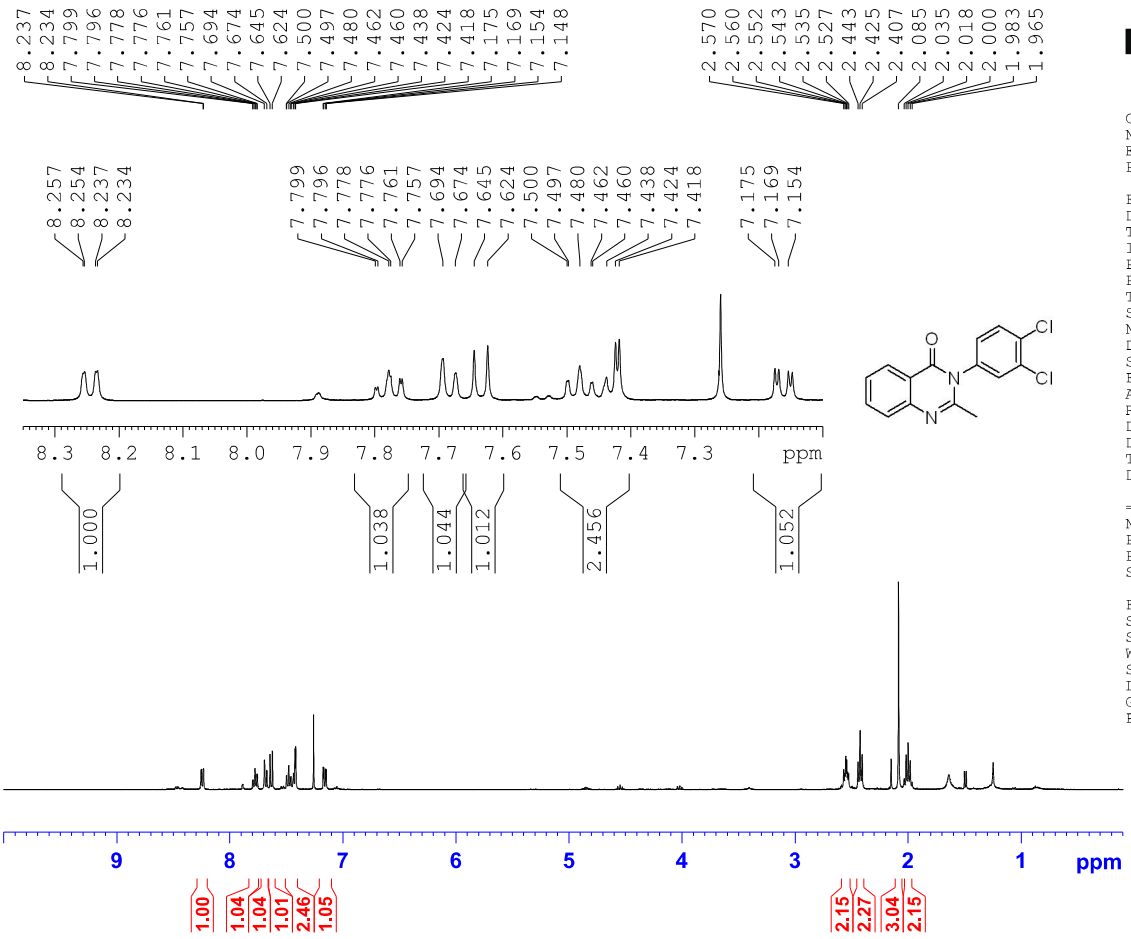
F2 - Acquisition Parameters
Date_ 20150121
Time 11.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 272
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1H of SGS-49



BRUKER

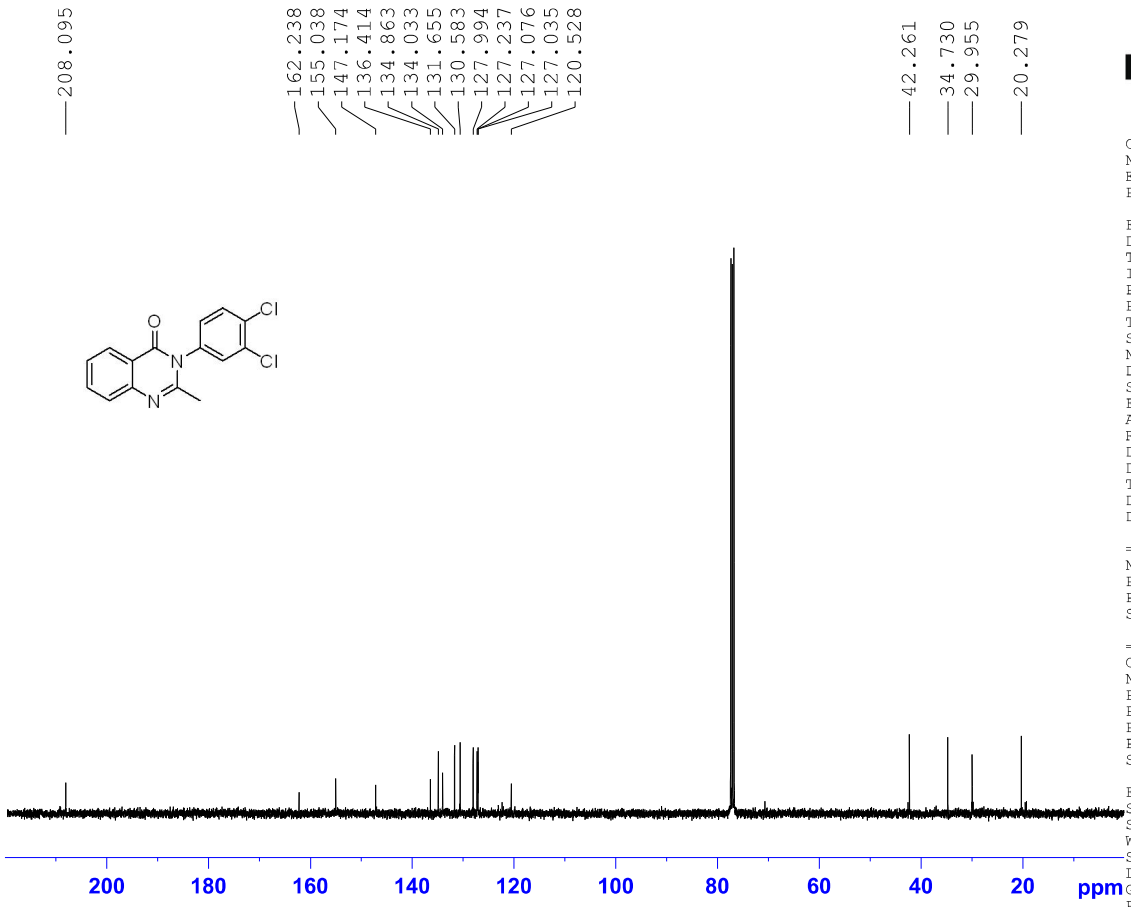
Current Data Parameters
NAME SGS-49
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 14.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-49



BRUKER

Current Data Parameters
NAME SGS-49
EXPNO 2
PROCNO 1

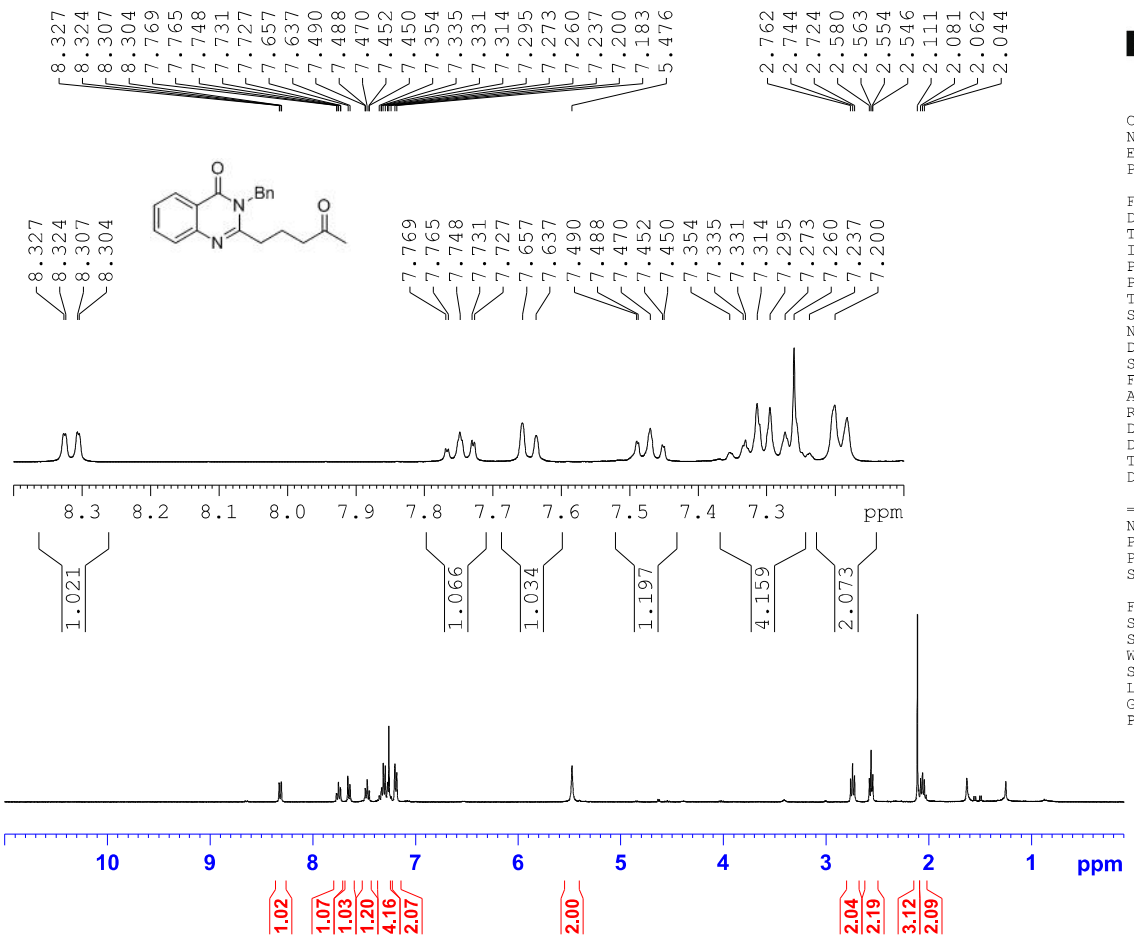
F2 - Acquisition Parameters
Date_ 20150121
Time 14.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 515
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 0.20000000 sec
D11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

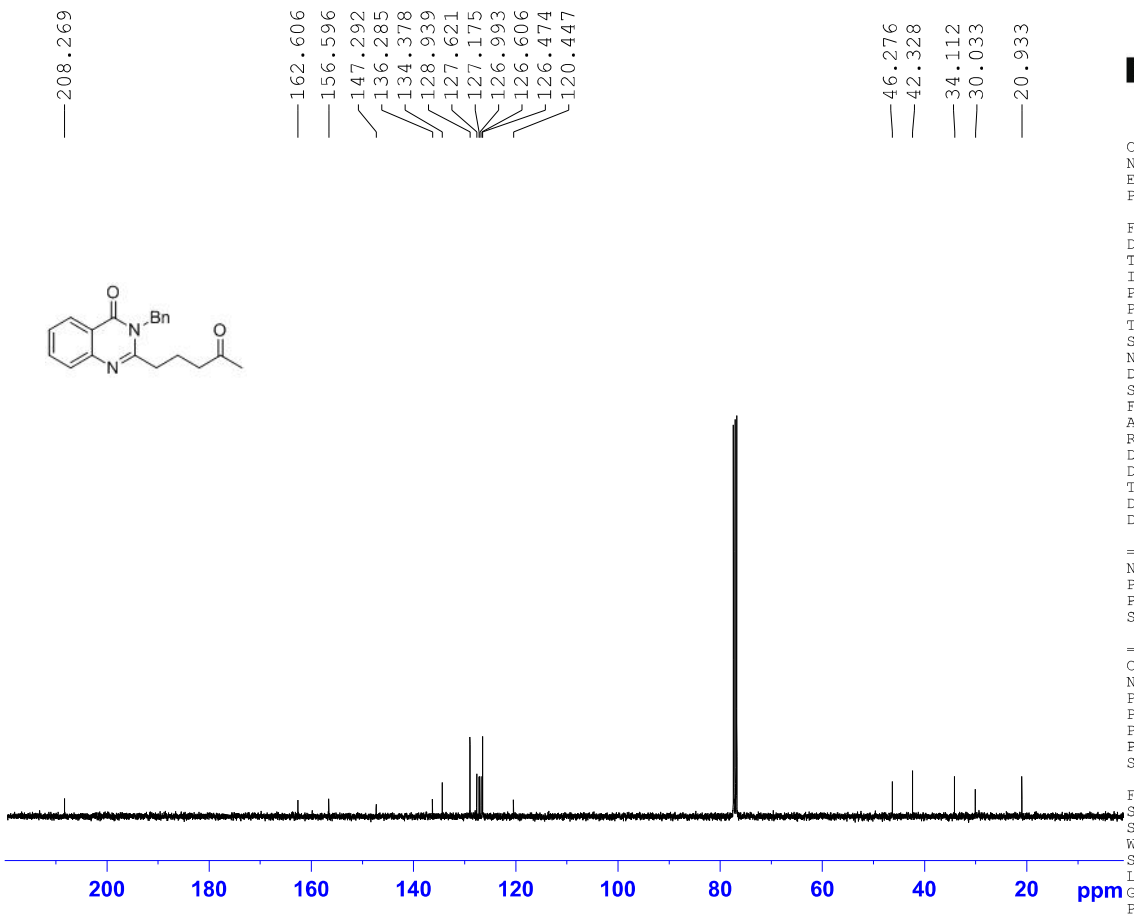
1H of SGS-46



BRUKER

```
Current Data Parameters
NAME                  SGS-46
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  11.28
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      128
DW                 60.800 usec
DE                  6.50 usec
TE                  294.1 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.73 usec
PLW1           14.30000019 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF             400.1300177 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

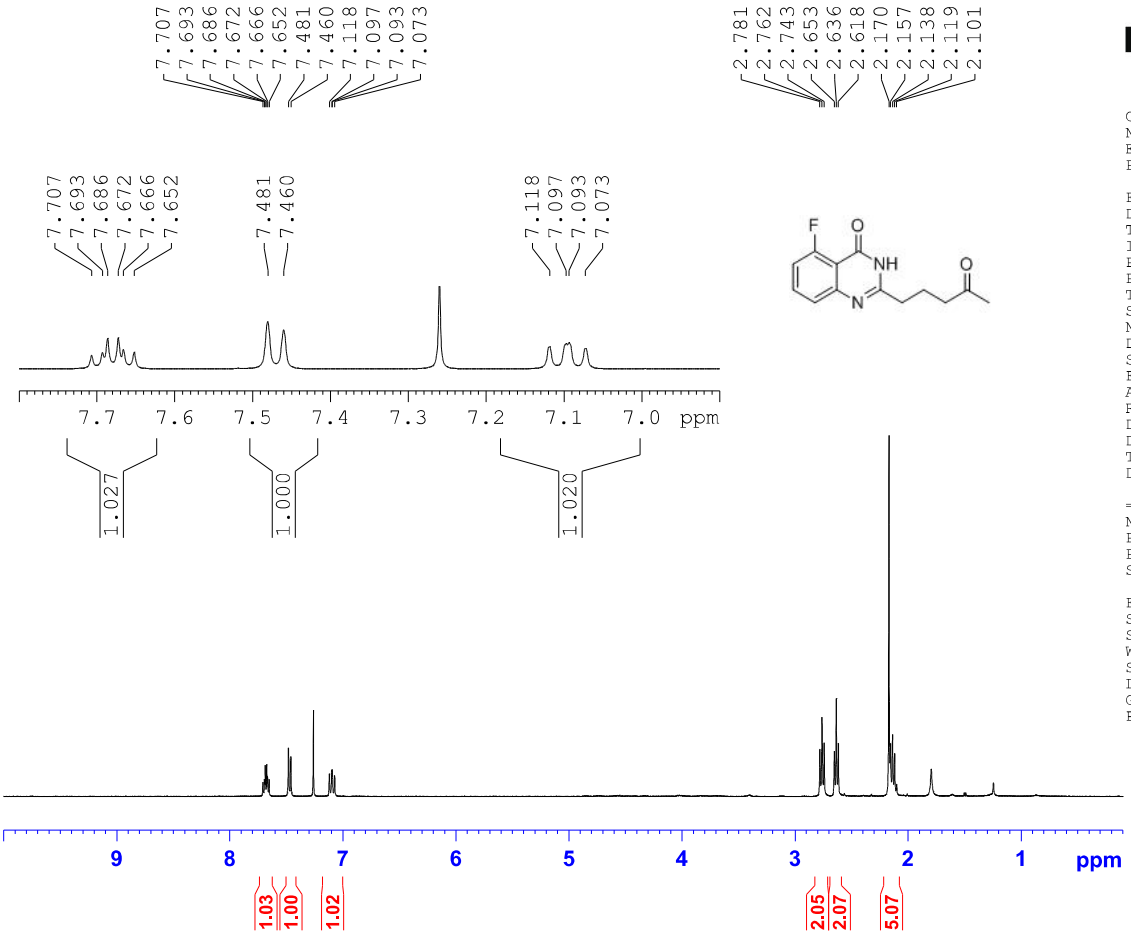
13C of SGS-46



BRUKER

```
Current Data Parameters
NAME                  SGS-46
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150121
Time                  11.36
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      436
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      144
DW                 20.800 usec
DE                  6.50 usec
TE                  294.8 K
D1              0.20000000 sec
D11             0.03000000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                    12.08 usec
PLW1           34.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2           14.30000019 W
PLW12           0.38304999 W
PLW13           0.31027001 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF             100.6127690 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

1H of SGS-50



BRUKER

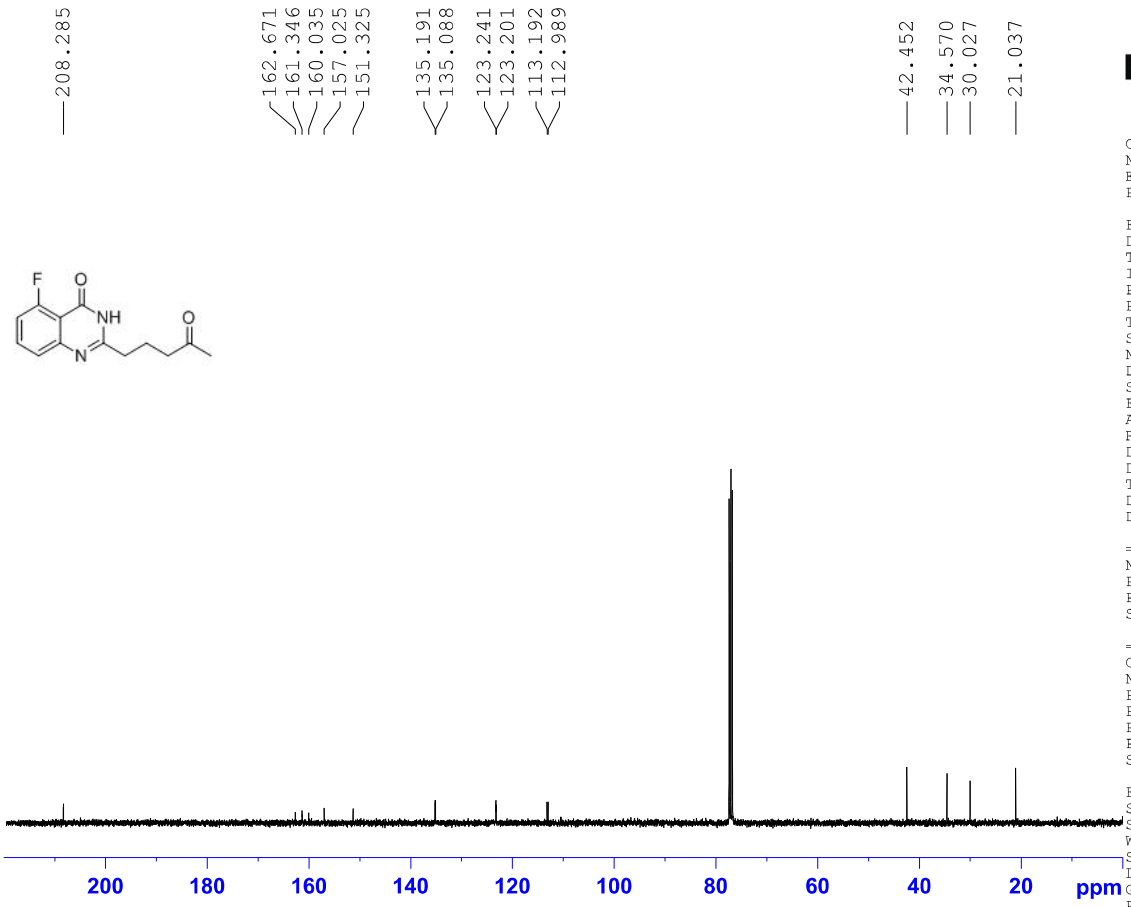
Current Data Parameters
NAME SGS-50
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 13.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 14.73 usec
PLW1 14.30000019 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13C of SGS-50



BRUKER

Current Data Parameters
NAME SGS-50
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 331
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 0.20000000 sec
D11 0.03000000 sec

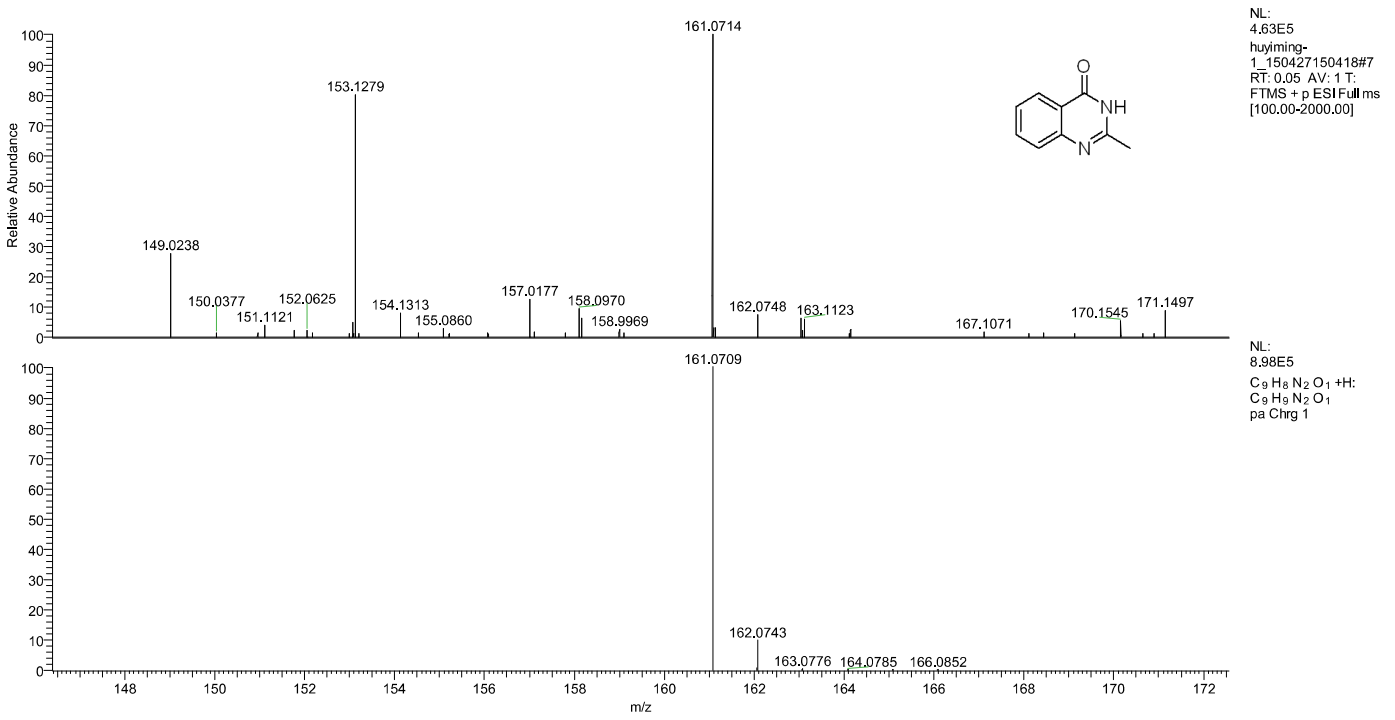
======== CHANNEL f1 ========
NUC1 13C
P1 12.08 usec
PLW1 34.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.30000019 W
PLW12 0.38304999 W
PLW13 0.31027001 W
SFO2 400.1316005 MHz

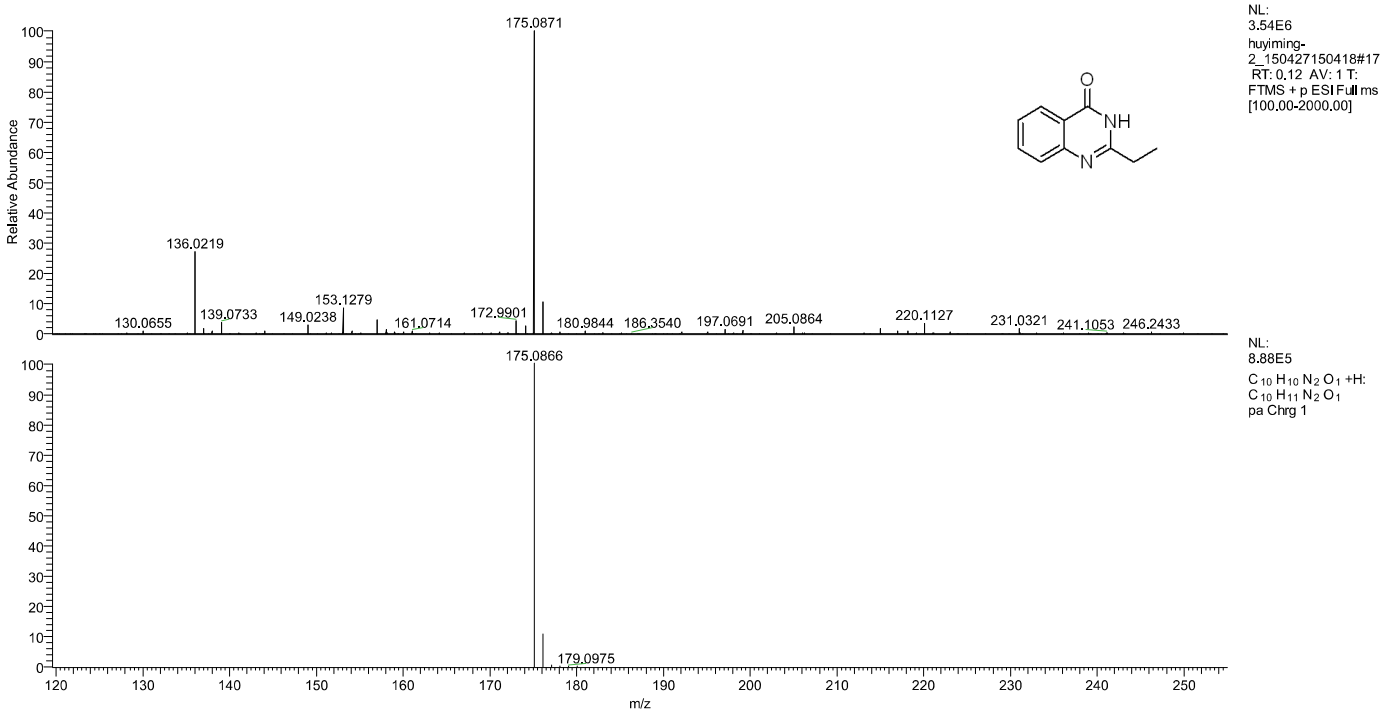
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5. HRMS of the Products

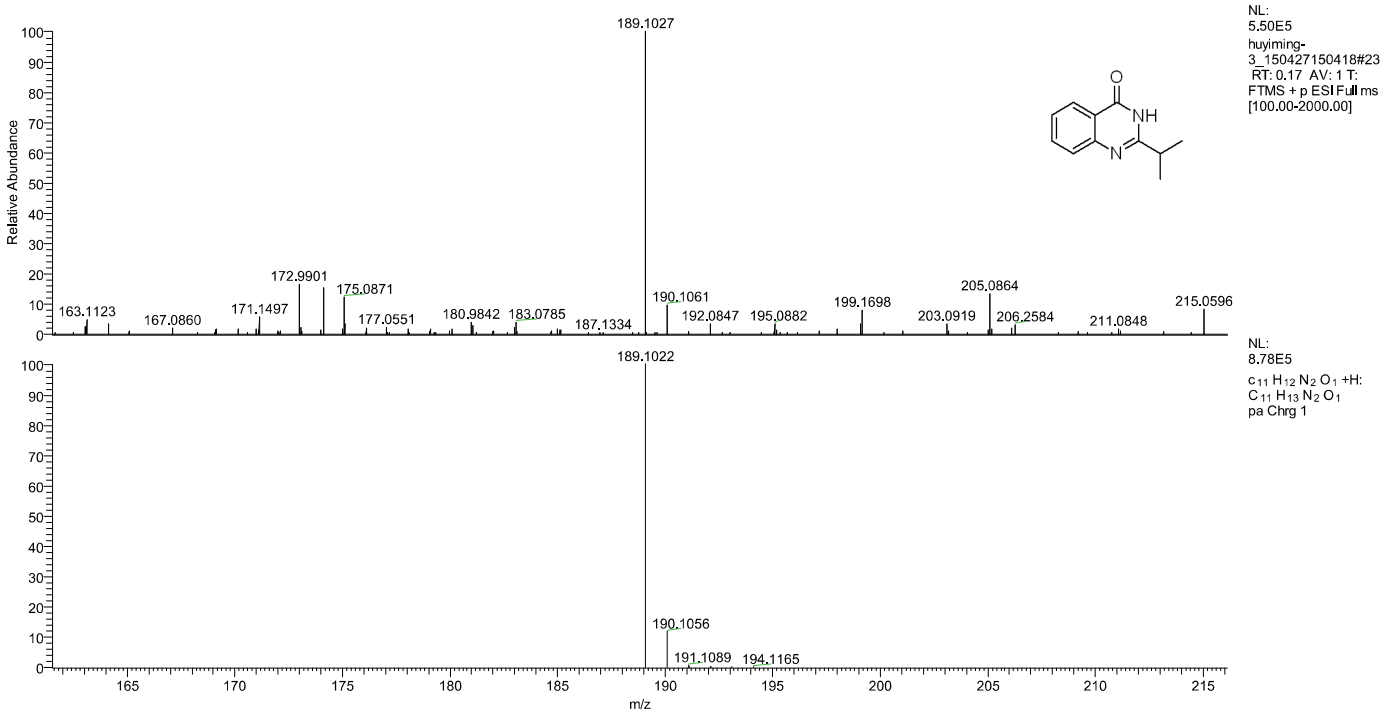
F:\Users\...\huyiming-1_150427150418 4/28/2015 10:03:30 AM 3aa
Error=3.1 ppm



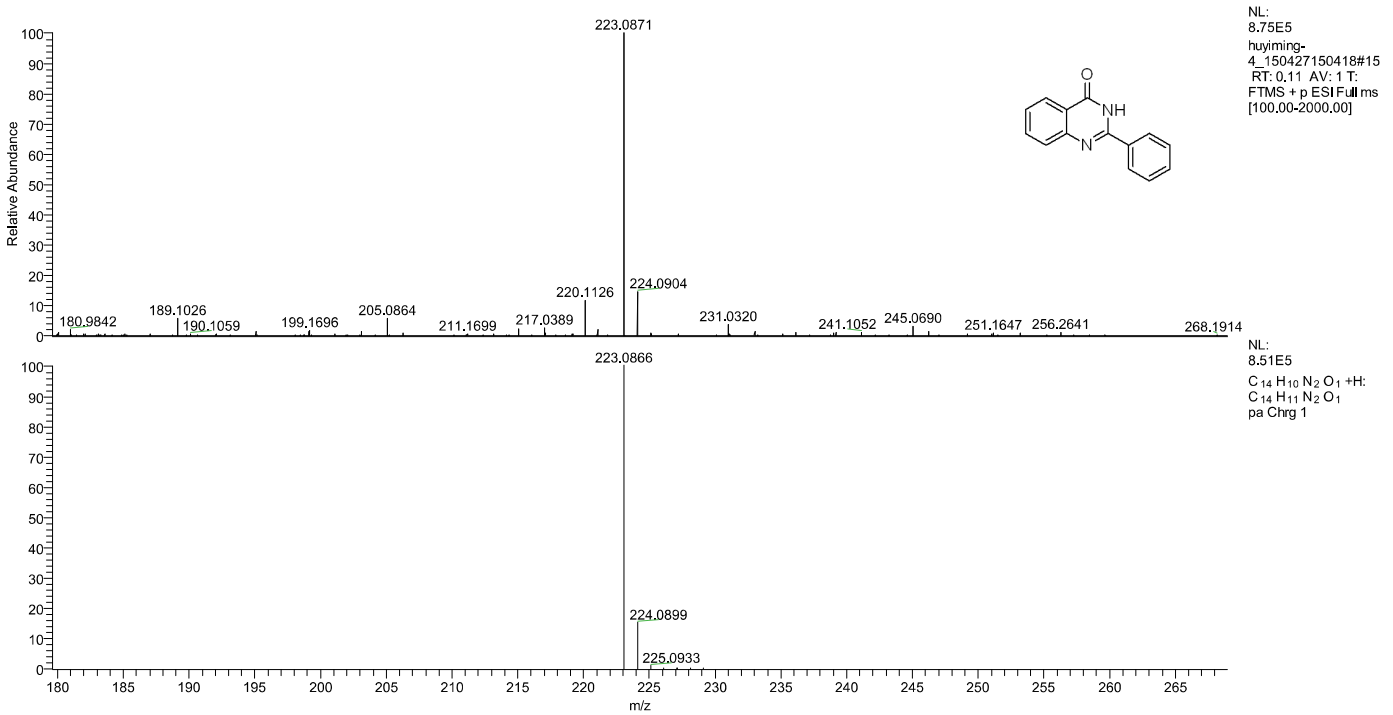
F:\Users\...\huyiming-2_150427150418 4/28/2015 10:08:57 AM 3ab
Error=2.9 ppm



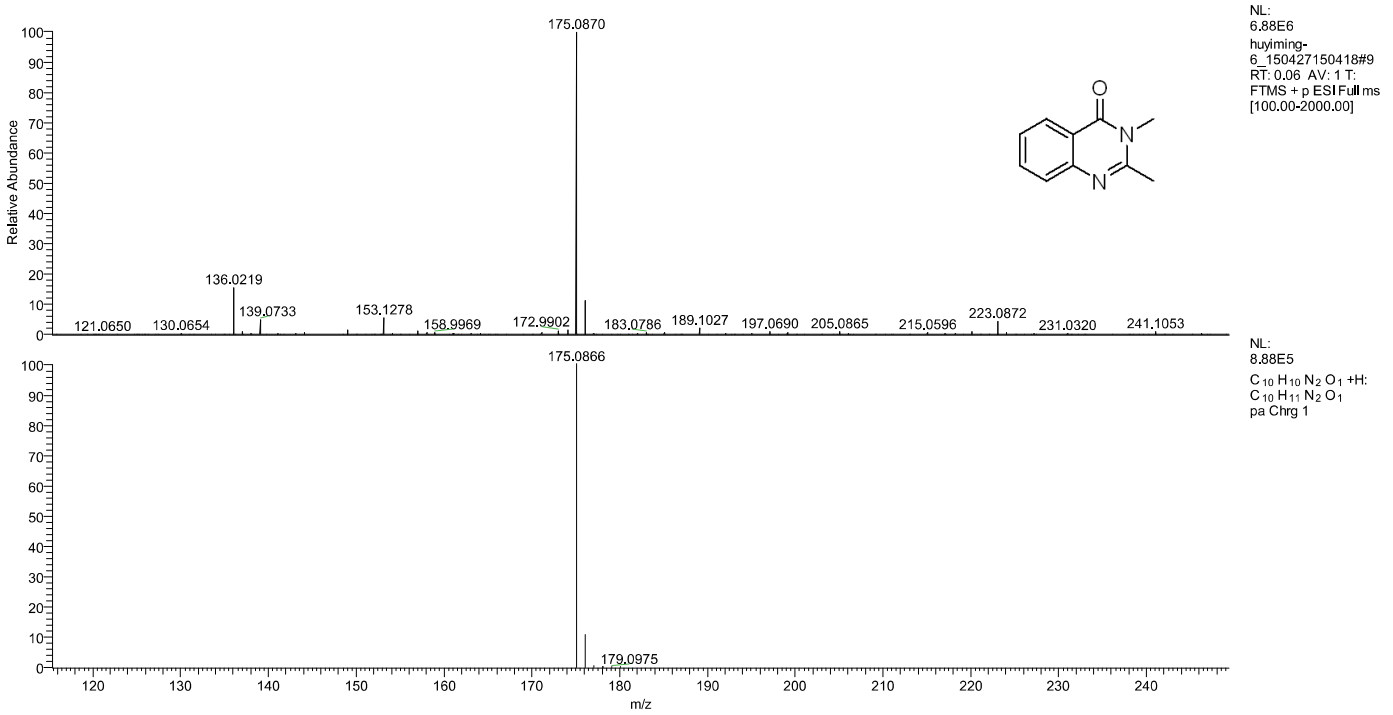
F:\Users\...\huyiming-3_150427150418 4/28/2015 10:16:01 AM 3ac
Error=2.6 ppm



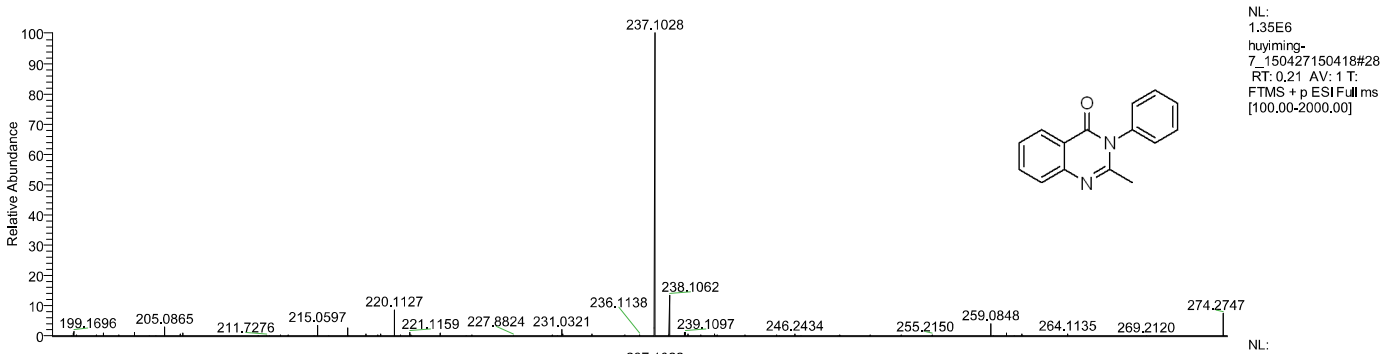
F:\Users\...\huyiming-4_150427150418 4/28/2015 10:22:01 AM 3ad
Error=2.2 ppm

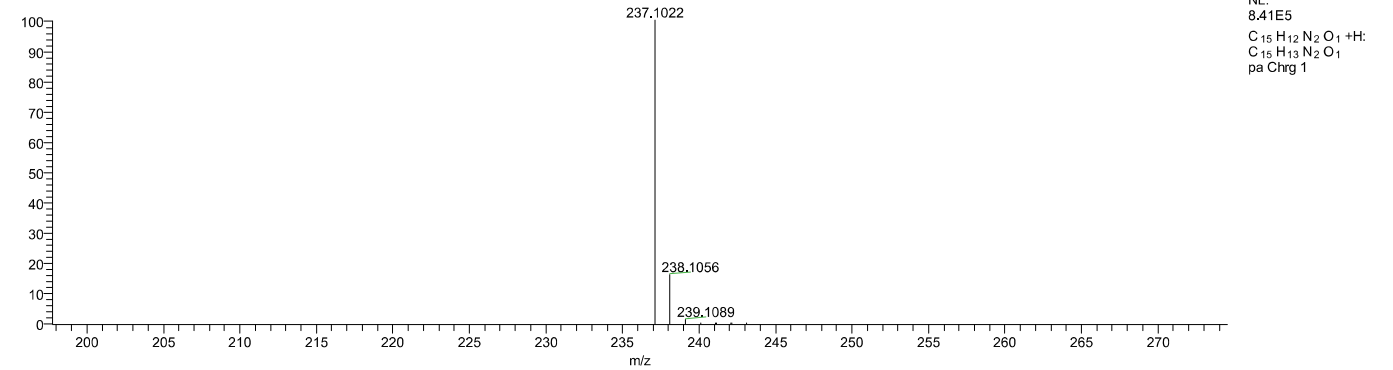


F:\Users\...\huyiming-6_150427150418 4/28/2015 10:27:40 AM 3ba
Error=2.3 ppm

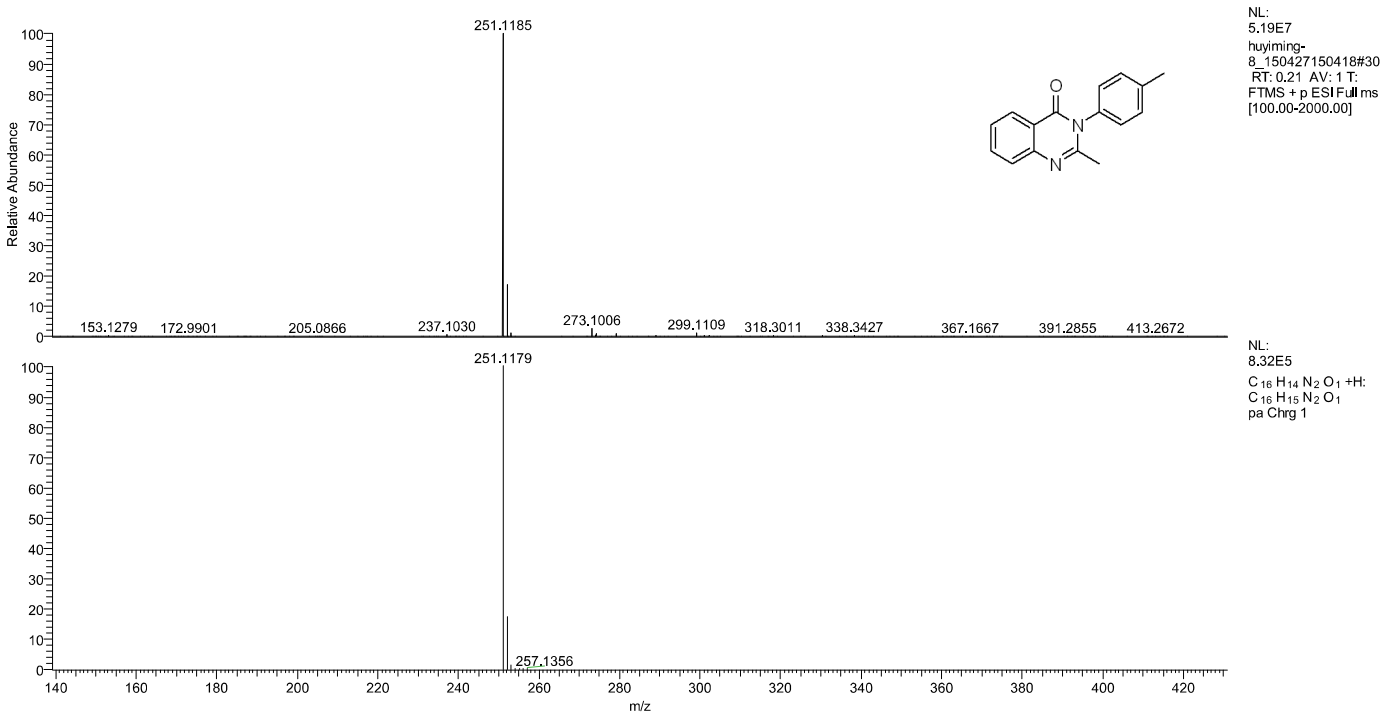


F:\Users\...\huyiming-7_150427150418 4/28/2015 10:33:33 AM 3ca
Error=2.5 ppm

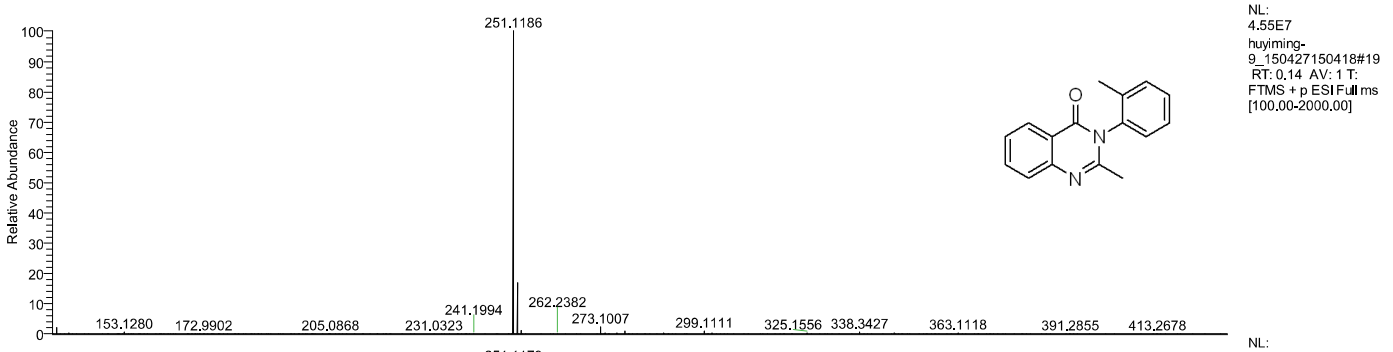


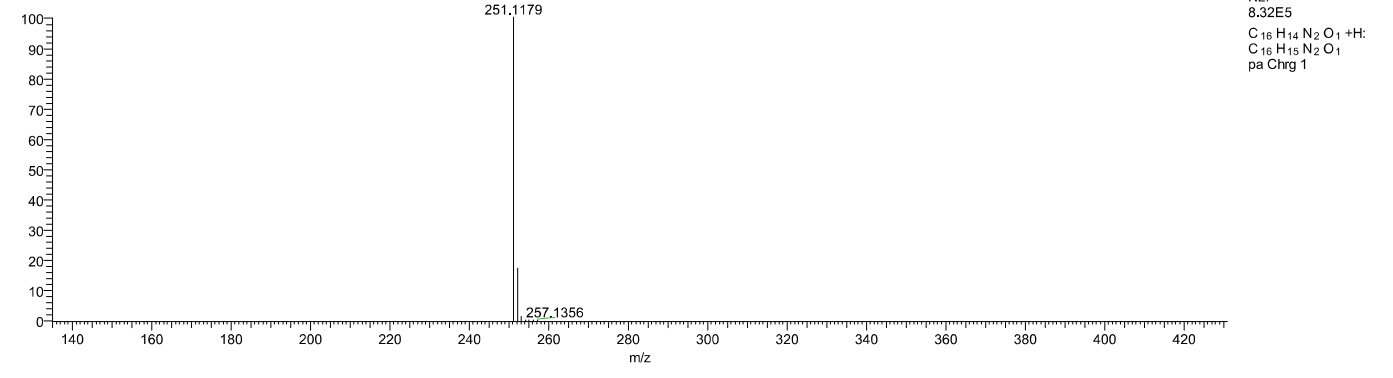


F:\Users\...\huyiming-8_150427150418 4/28/2015 10:39:26 AM 3da
Error=2.4 ppm

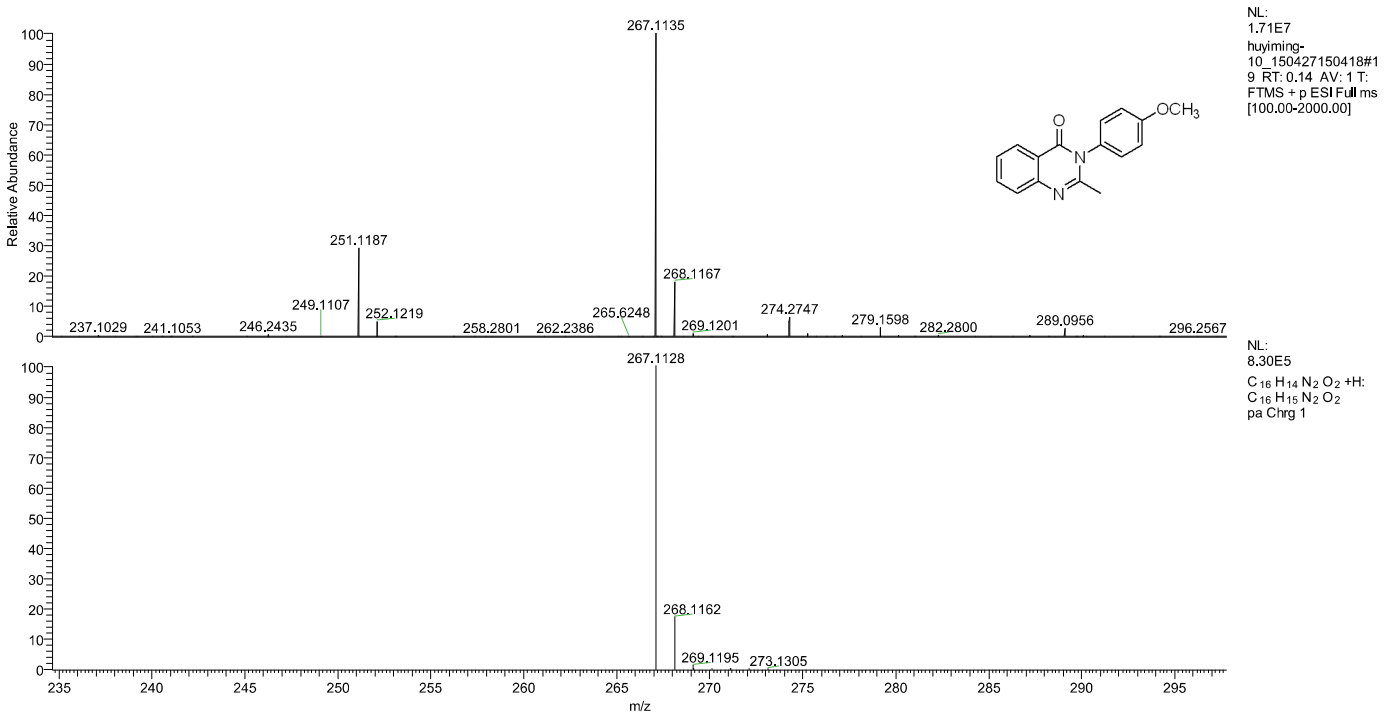


F:\Users\...\huyiming-9_150427150418 4/28/2015 10:44:22 AM 3ea
Error=2.9 ppm

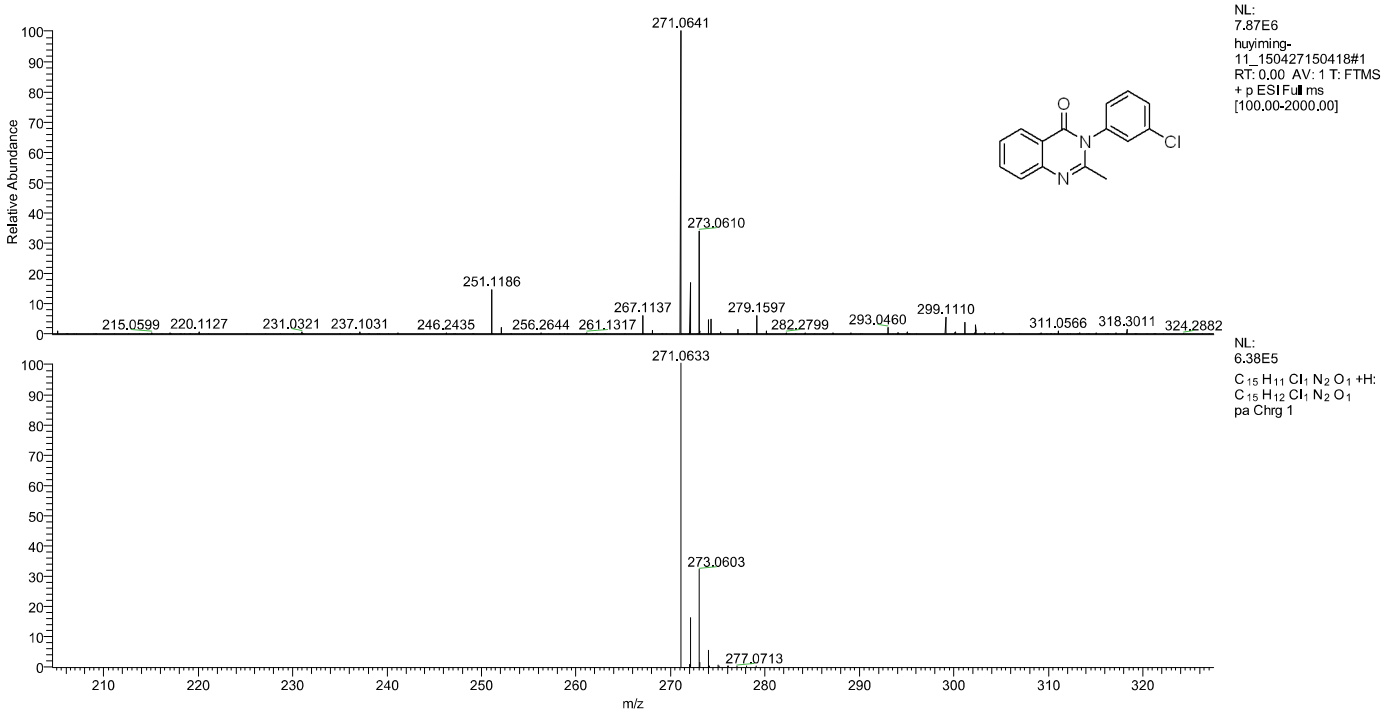




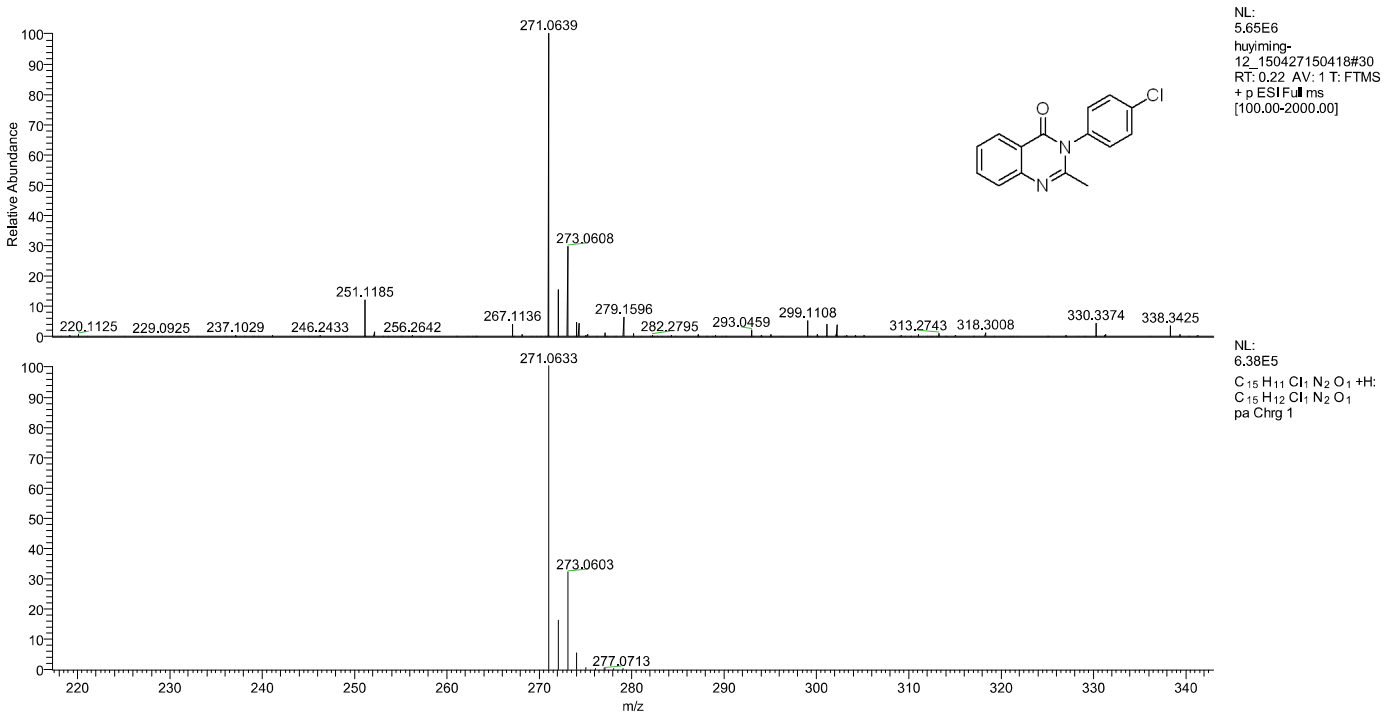
F:\Users\...\huyiming-10_150427150418 4/28/2015 10:49:31 AM 3fa
Error=2.6 ppm



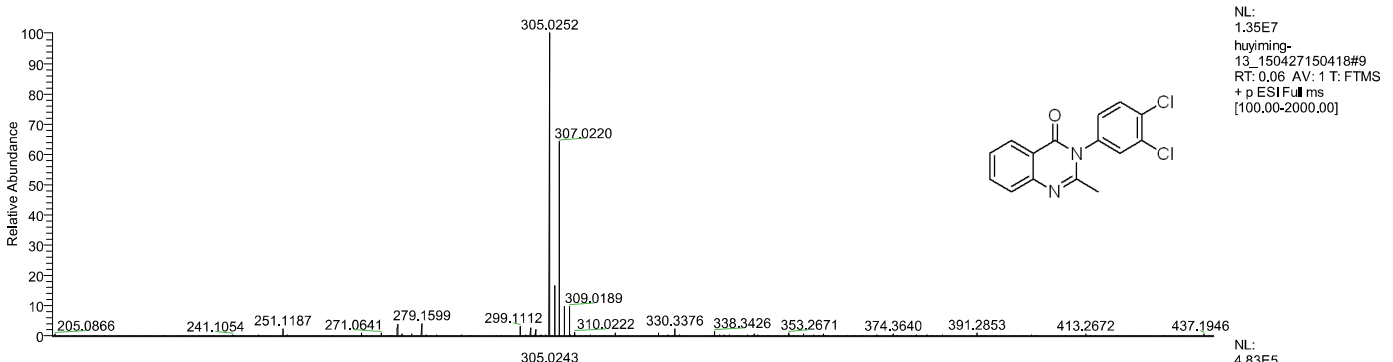
F:\Users\...\huyiming-11_150427150418 4/28/2015 10:54:30 AM 3ga
Error=3.0 ppm

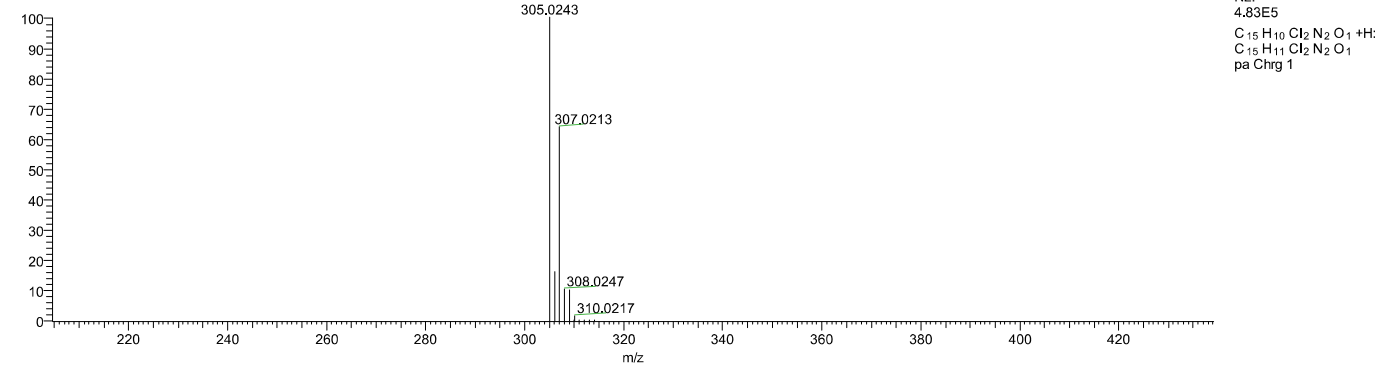


F:\Users\...\huyiming-12_150427150418 4/28/2015 10:56:35 AM 3ha
Error=2.2 ppm

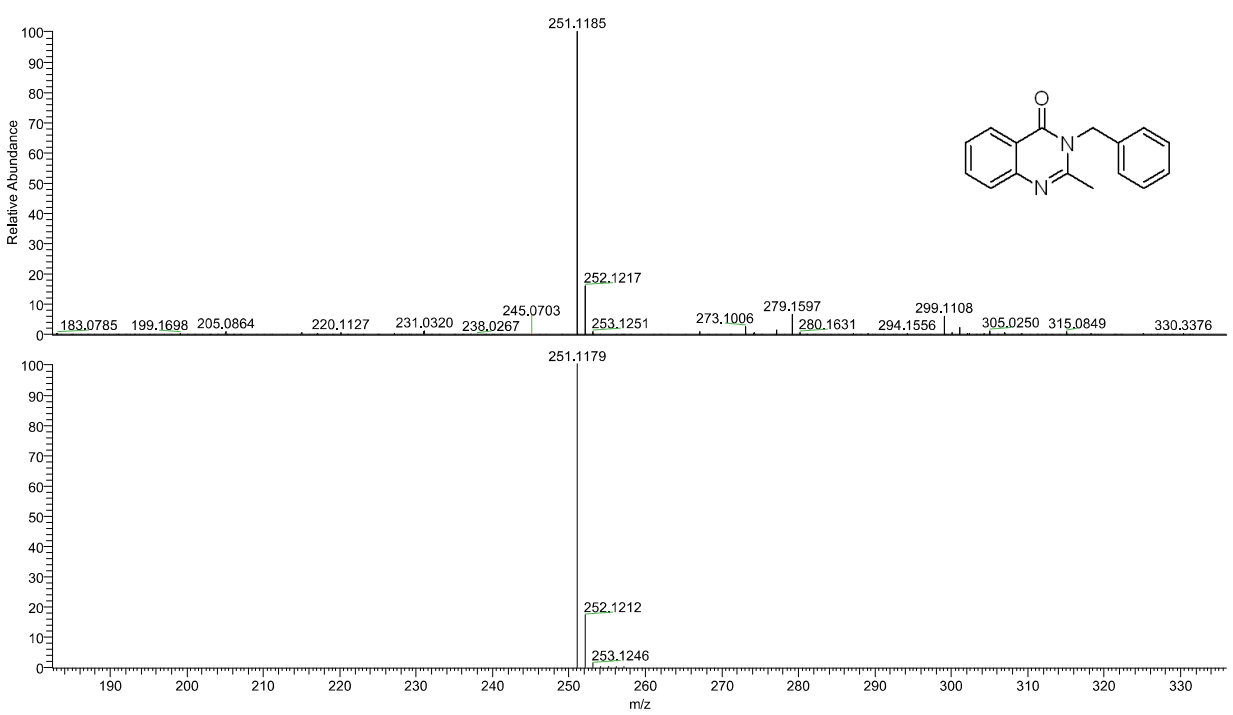


F:\Users\...\huyiming-13_150427150418 4/28/2015 11:01:10 AM 3ia
Error=3.0 ppm





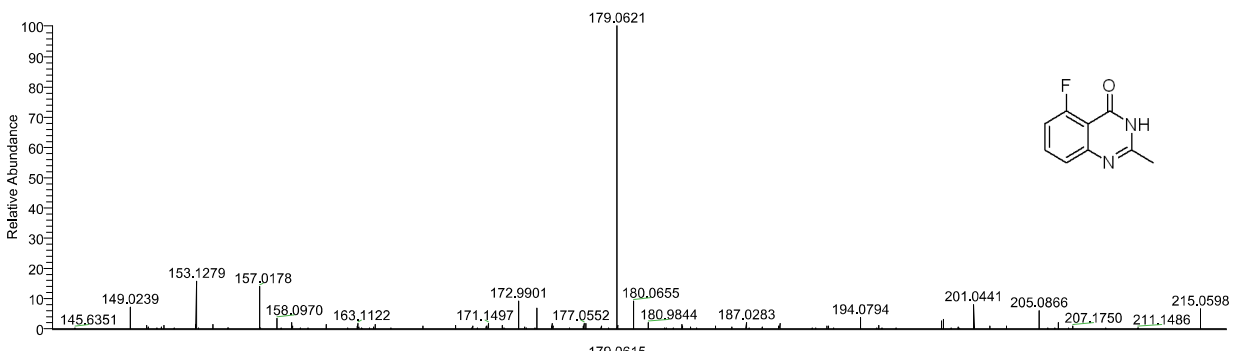
F:\Users\...\huyiming-14_150427150418 4/28/2015 11:07:45 AM 3ja
Error=2.4 ppm



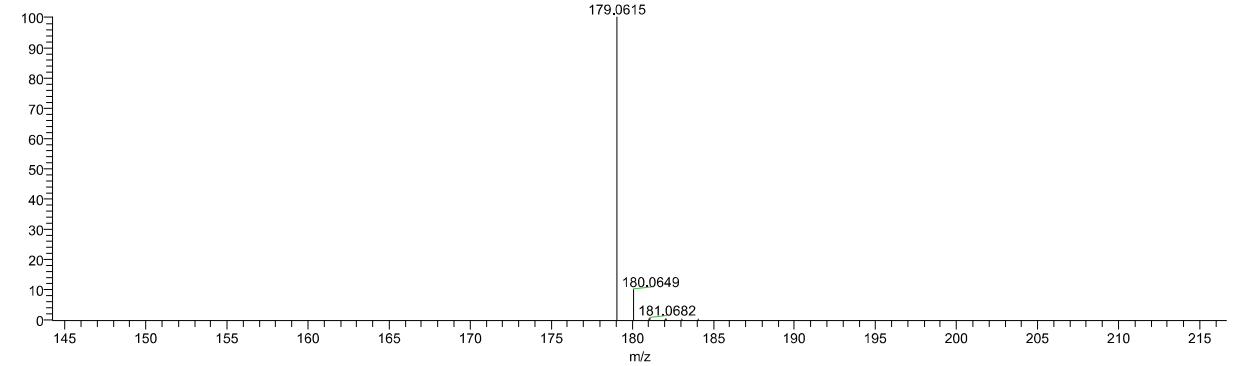
NL:
8.13E6
huyiming-14_150427150418#27 RT: 0.20 AV: 1 T: FTMS + p ESI Full ms [100.00-2000.00]

NL:
8.32E5
$C_{16}H_{14}N_2O_1$ +H:
$C_{16}H_{15}N_2O_1$
pa Chrg 1

F:\Users\...\huyiming-15_150427150418 4/28/2015 3:01:51 PM 3ka
Error=3.4 ppm

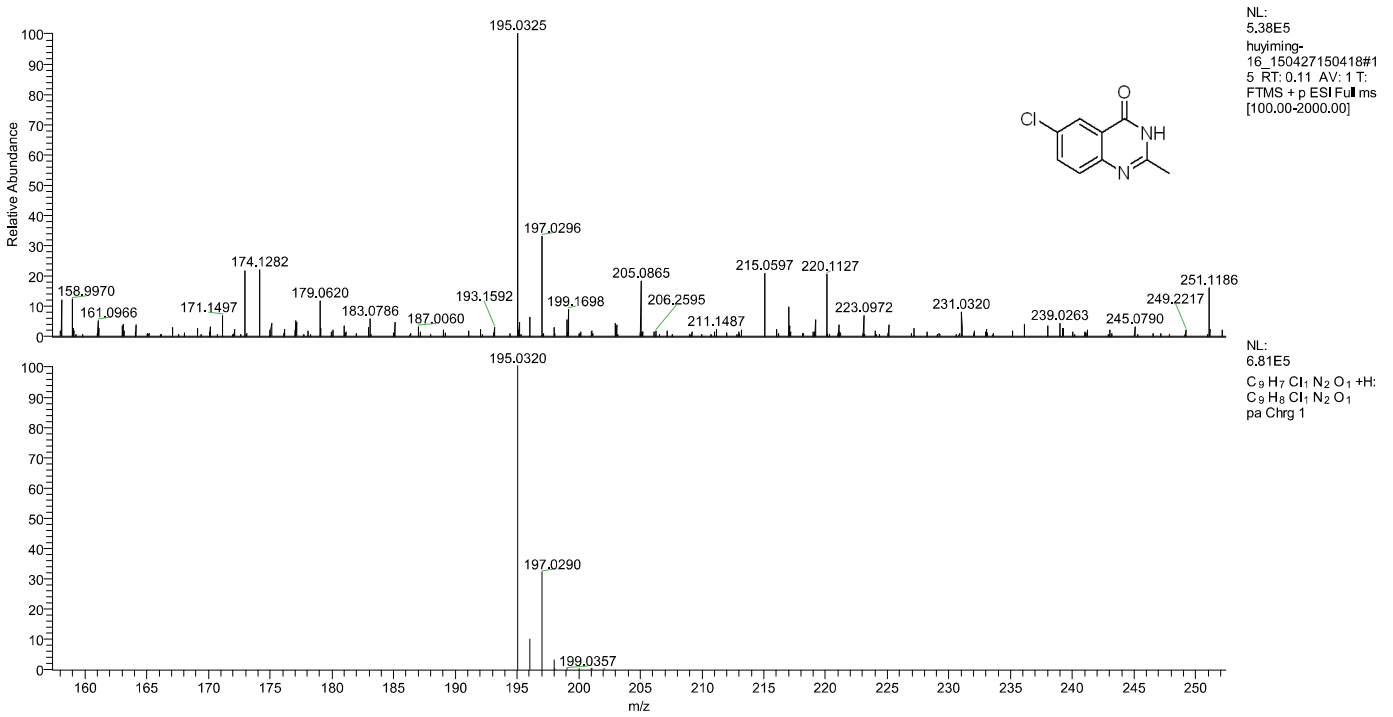


NL:
9.64E5
huyiming-15_150427150418#19 RT: 0.13 AV: 1 T: FTMS + p ESI Full ms [100.00-2000.00]

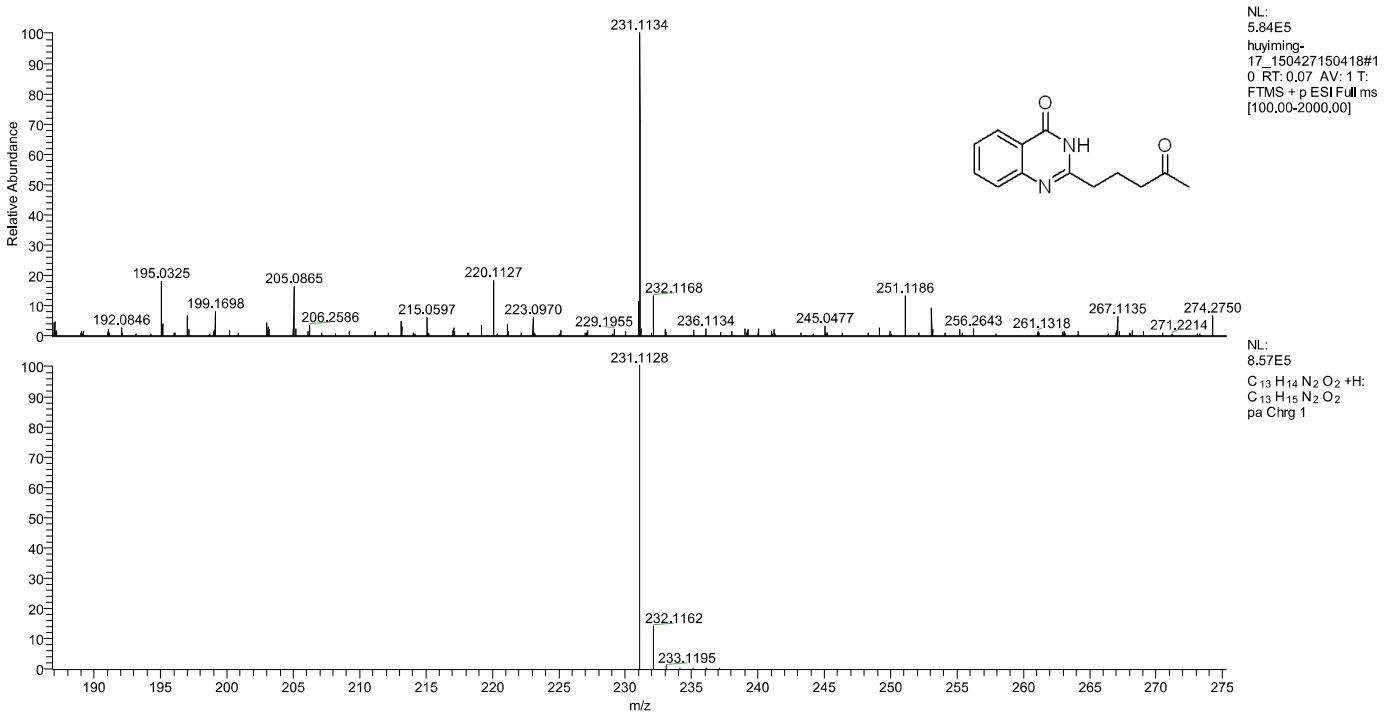


NL:
8.98E5
$C_9H_7F_1N_2O_1$ +H:
$C_9H_8F_1N_2O_1$
pa Chrg 1

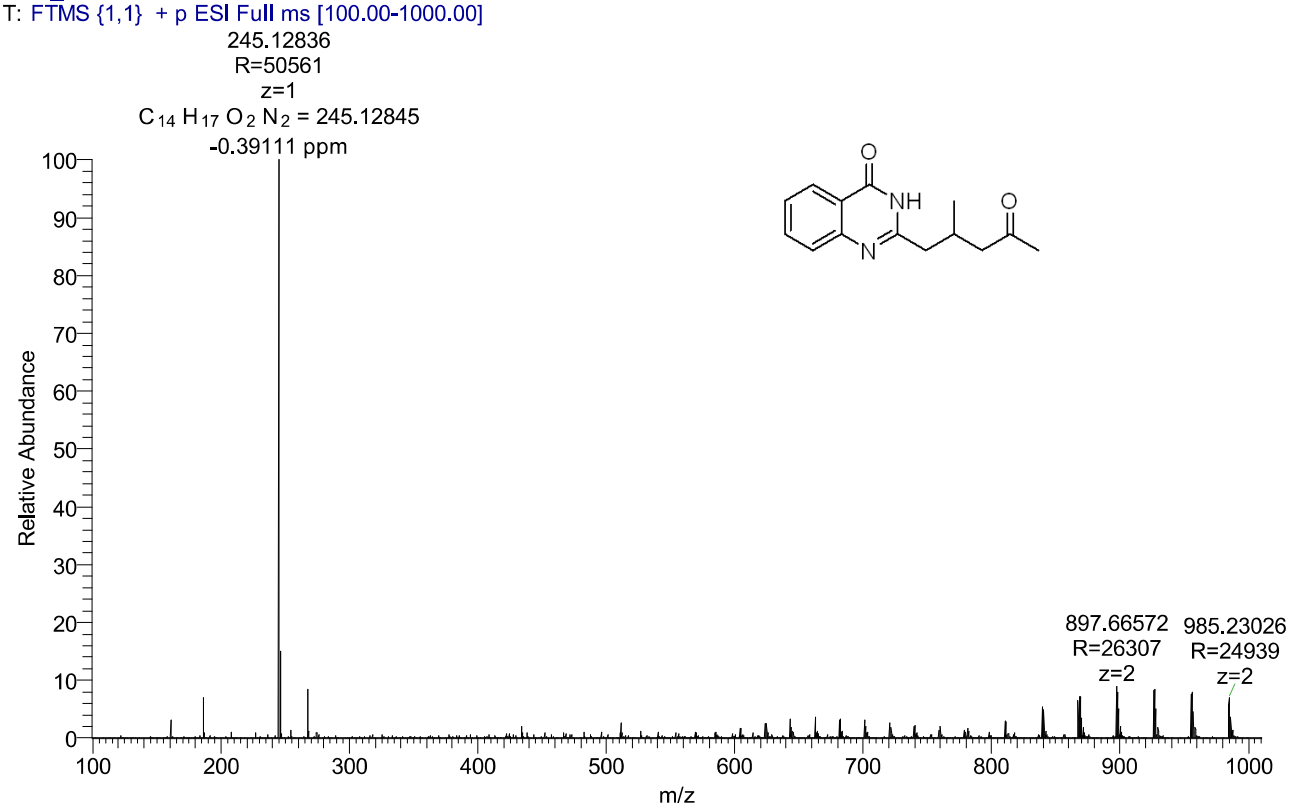
F:\Users\...\huyiming-16_150427150418 4/28/2015 3:07:01 PM 3la
Error=2.6 ppm



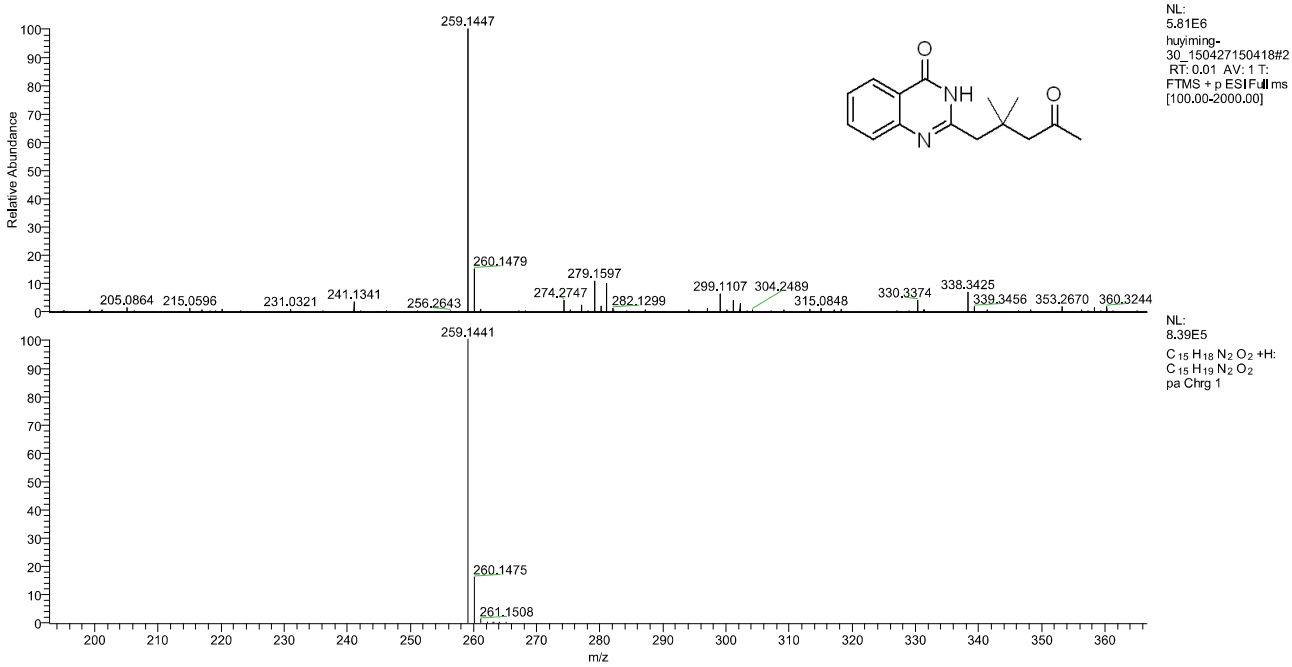
F:\Users\...\huyiming-17_150427150418 4/28/2015 3:12:29 PM 4ac
Error=2.6 ppm

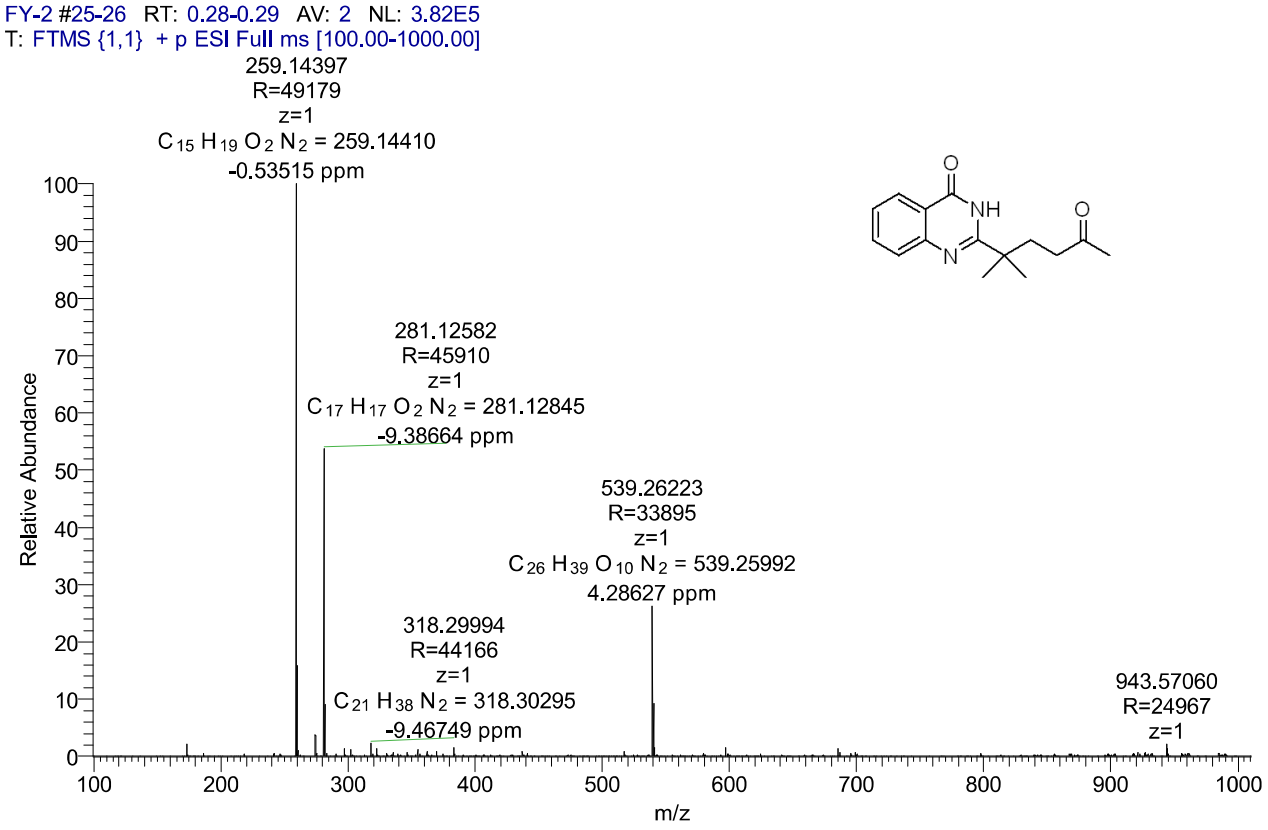


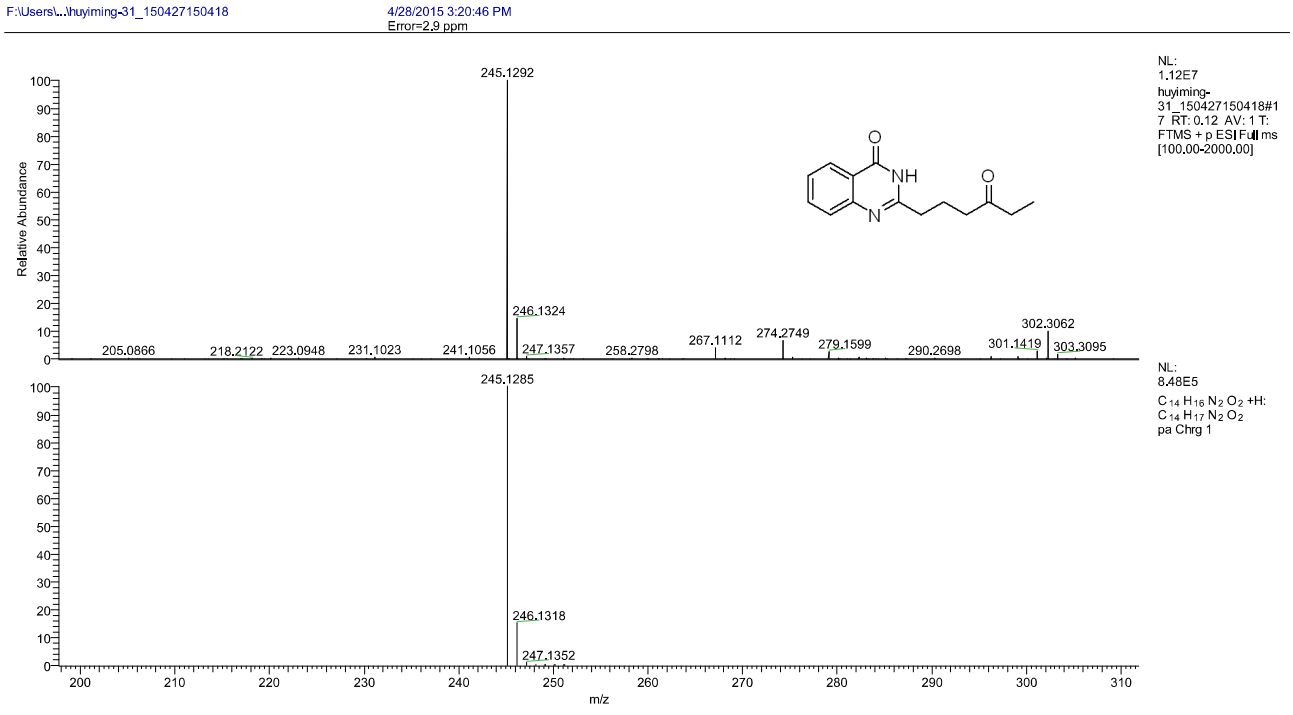
FY-1_150925171012 #37-38 RT: 0.41-0.42 AV: 2 NL: 3.21E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



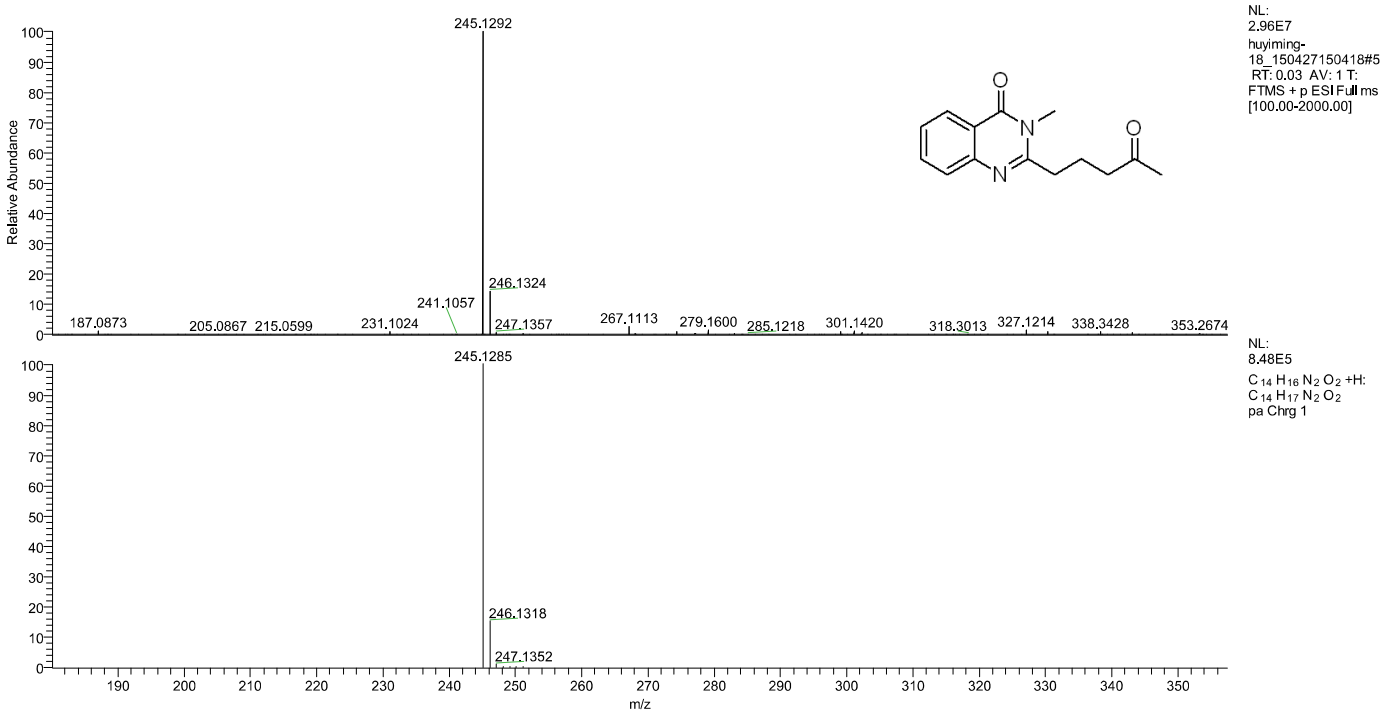
F:\Users\...\huyiming-30_150427150418 4/28/2015 4:22:06 PM
Error=2.3 ppm



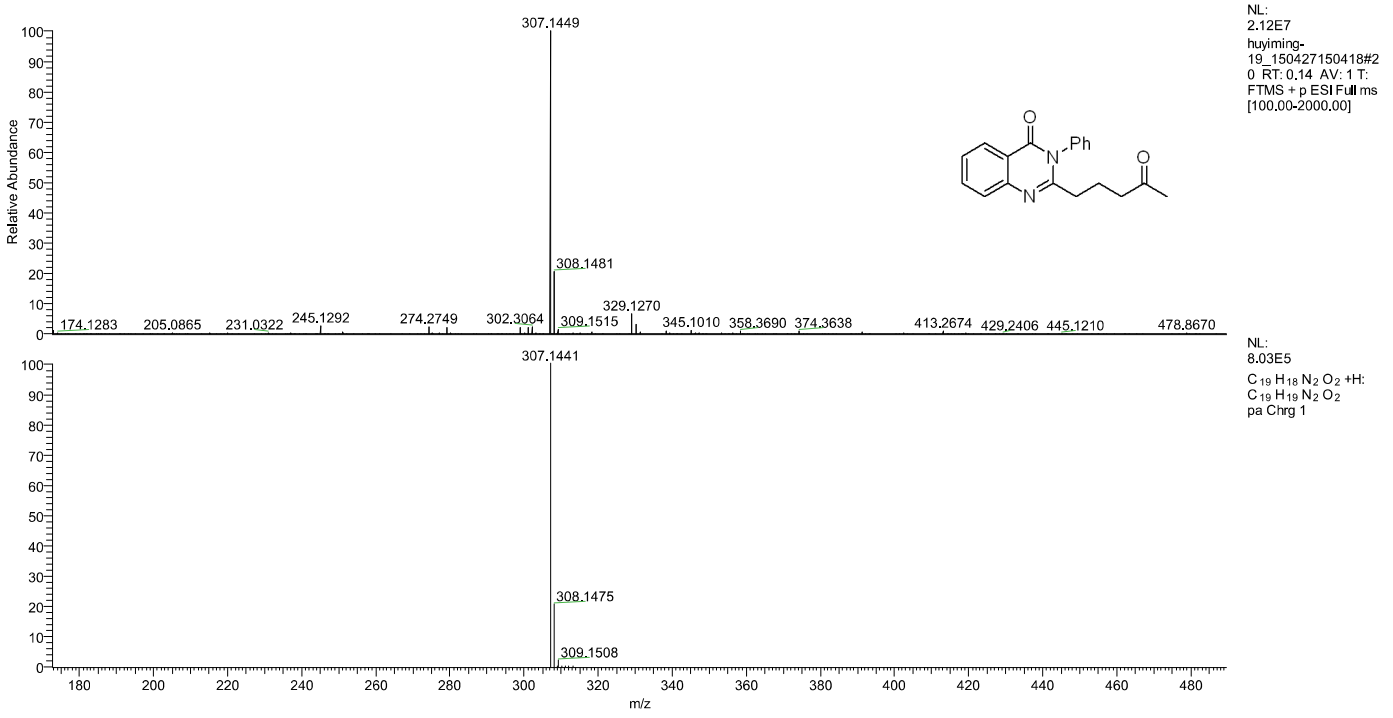

FY-2 #25-26 RT: 0.28-0.29 AV: 2 NL: 3.82E5
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]
259.14397
R=49179
z=1
C15 H19 O2 N2 = 259.14410
-0.53515 ppm
281.12582
R=45910
z=1
C17 H17 O2 N2 = 281.12845
-9.38664 ppm
539.26223
R=33895
z=1
C26 H39 O10 N2 = 539.25992
4.28627 ppm
318.29994
R=44166
z=1
C21 H38 N2 = 318.30295
-9.46749 ppm
943.57060
R=24967
z=1
Relative Abundance
m/z


F:\Users\...\huyiming-31_150427150418
4/28/2015 3:20:46 PM
Error=2.9 ppm
245.1292
246.1324
205.0866
218.2122
223.0948
231.1023
241.1056
247.1357
258.2798
267.1112
274.2749
279.1599
290.2698
301.1419
302.3062
303.3095
NL:
1.12E7
huyiming-31_150427150418#17 RT: 0.12 AV: 1 T: FTMS + p ESI Full ms [100.00-2000.00]
245.1285
246.1318
247.1352
NL:
8.48E5
C14 H16 N2 O2 +H:
C14 H17 N2 O2
pa Chrg 1
Relative Abundance
m/z

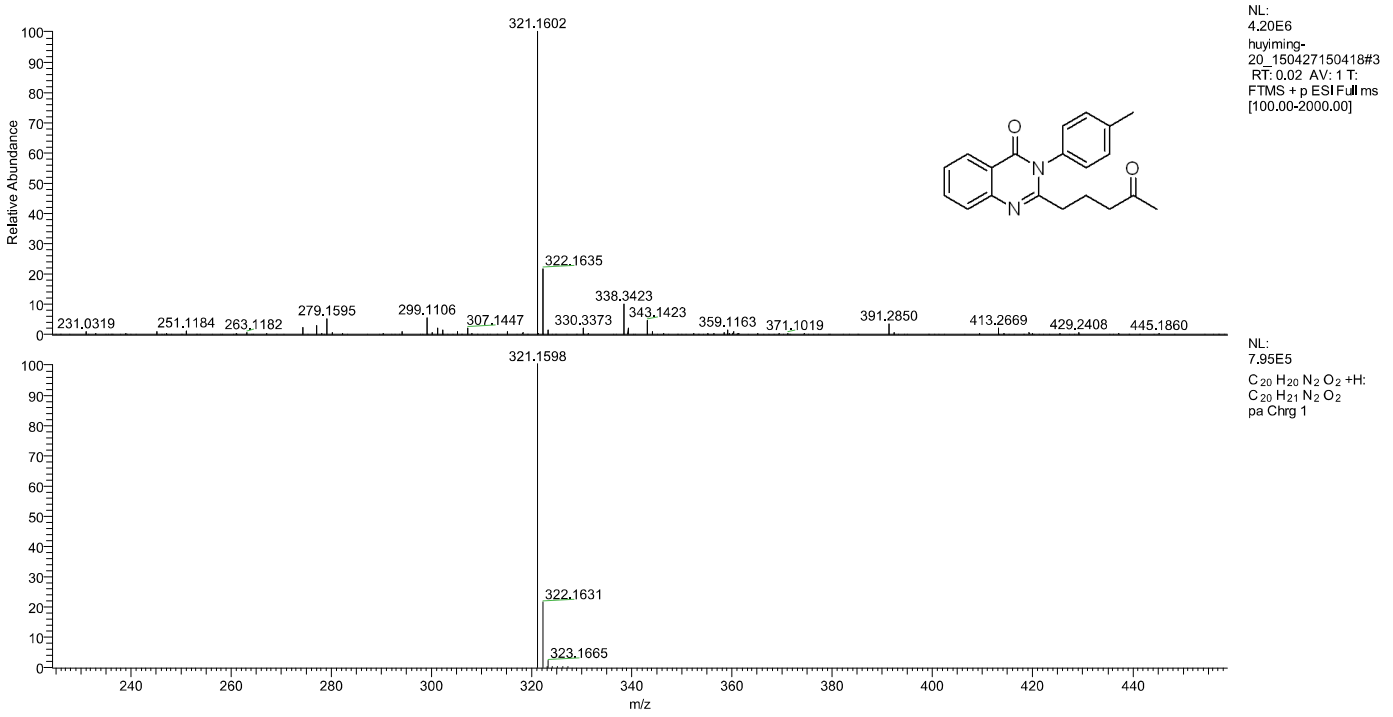
F:\Users\...\huyiming-18_150427150418 4/28/2015 3:17:39 PM 4bc
Error=2.9 ppm



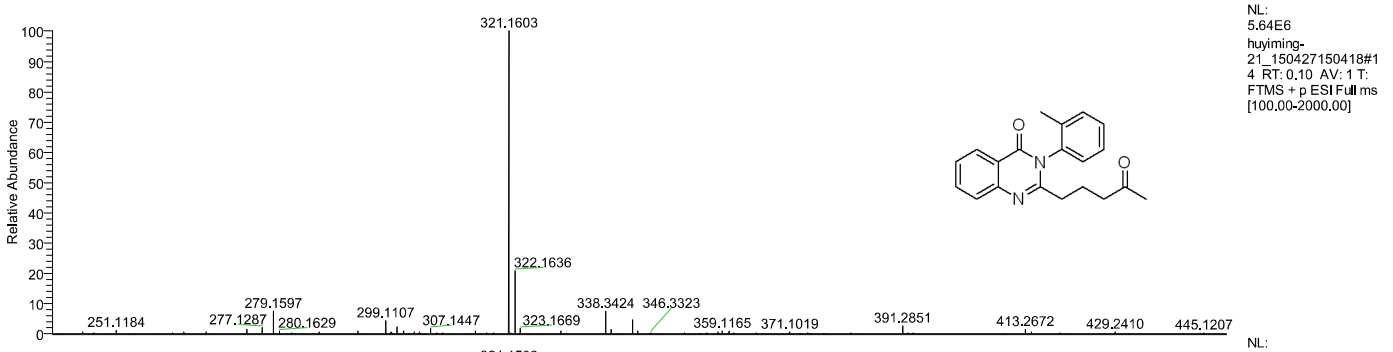
F:\Users\...\huyiming-19_150427150418 4/28/2015 3:25:59 PM 4cc
Error=2.6 ppm

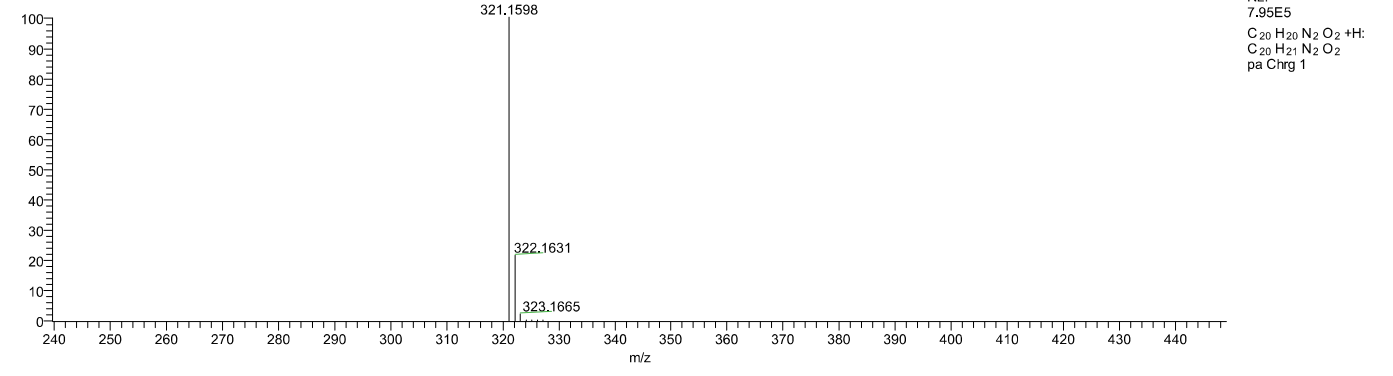


F:\Users\...\huyiming-20_150427150418 4/28/2015 3:33:14 PM 4dc
Error=1.2 ppm

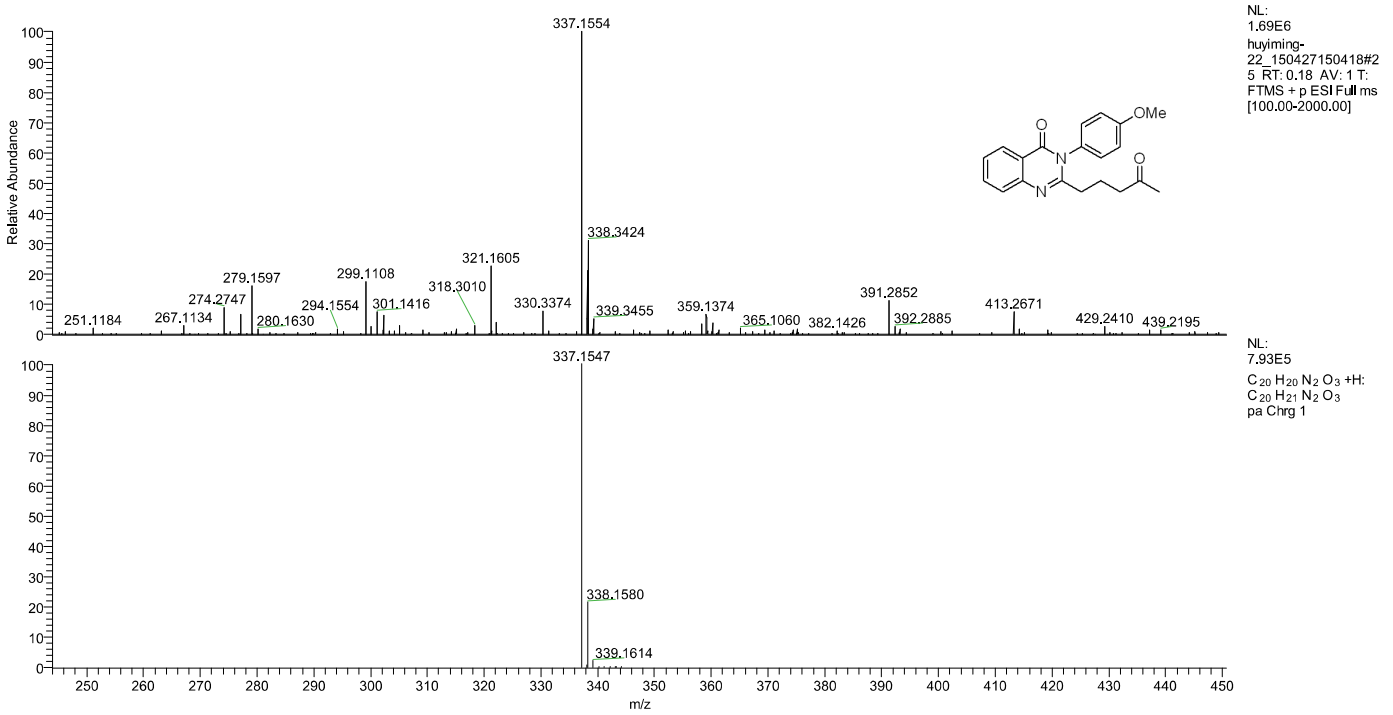


F:\Users\...\huyiming-21_150427150418 4/28/2015 3:35:23 PM 4ec
Error=1.6 ppm

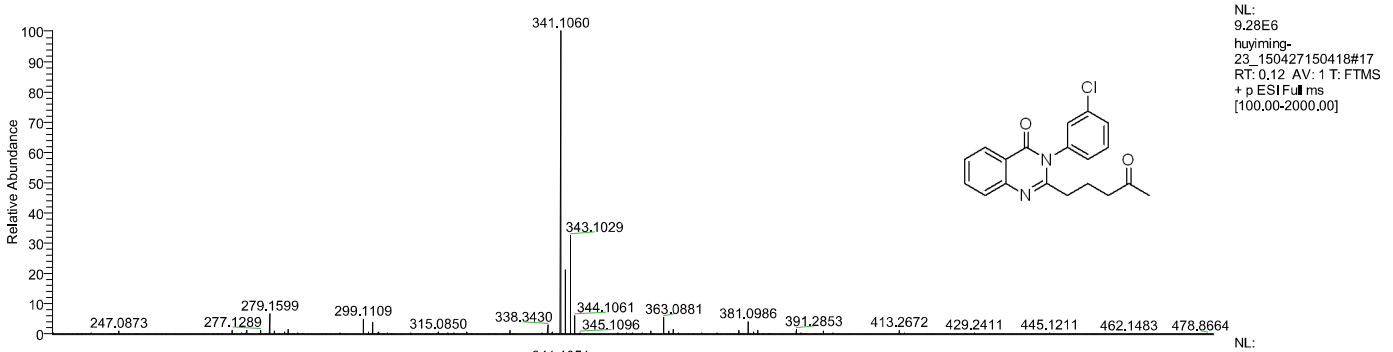


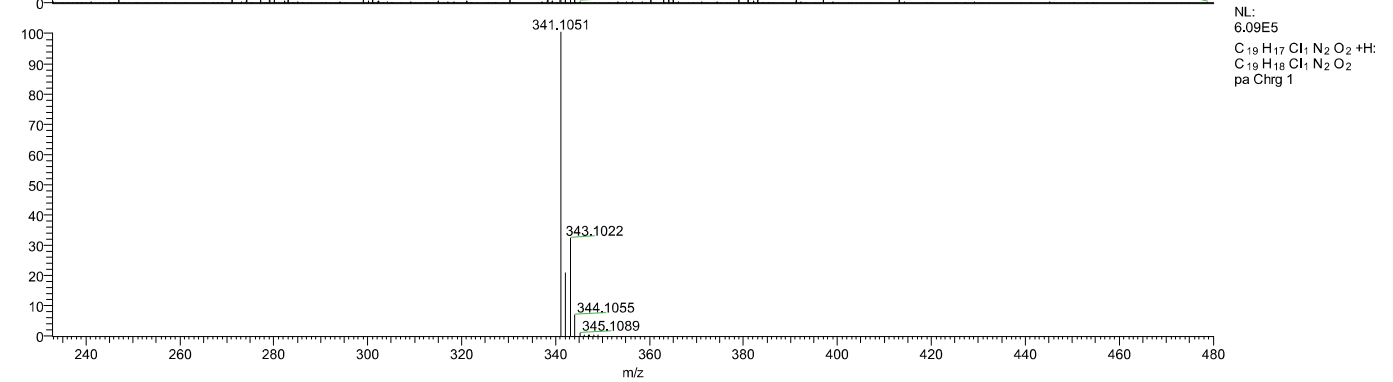


F:\Users\...\huyiming-22_150427150418 4/28/2015 3:45:50 PM 4fc
Error=2.1 ppm

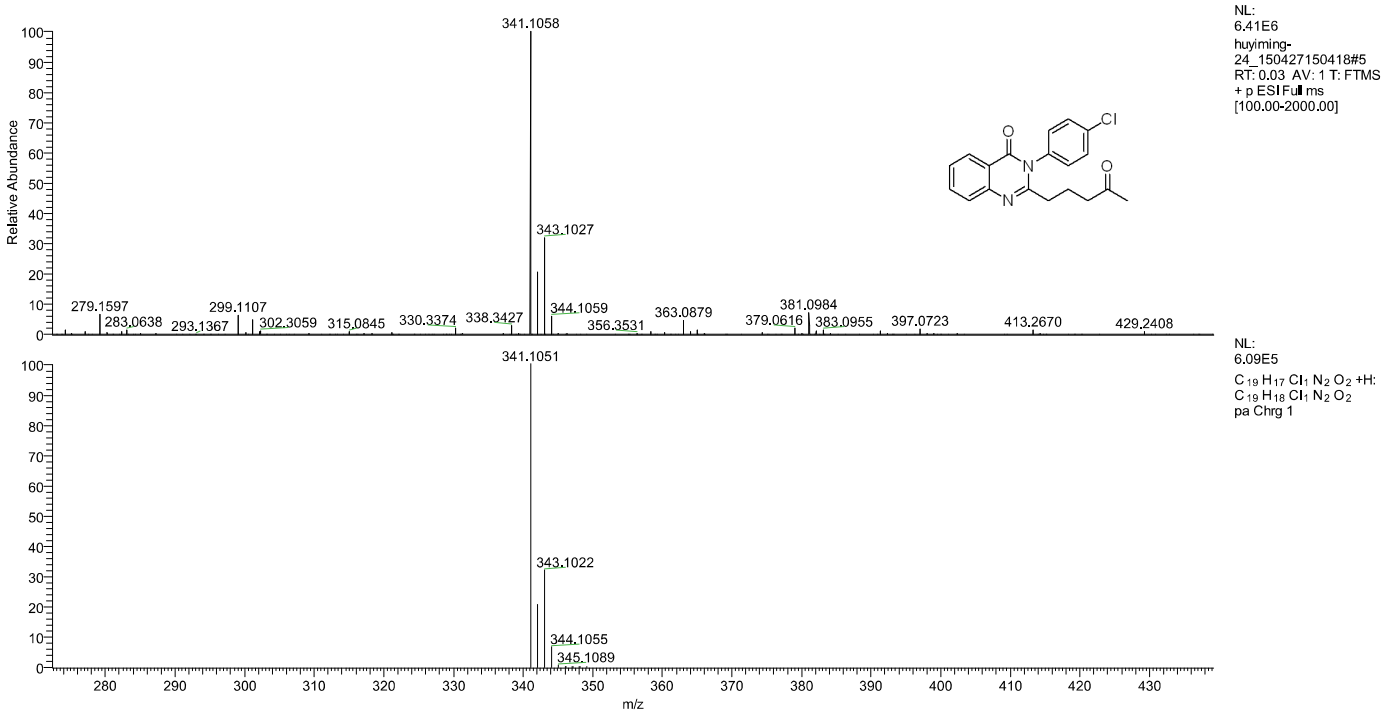


F:\Users\...\huyiming-23_150427150418 4/28/2015 3:51:02 PM 4gc
Error=2.6 ppm

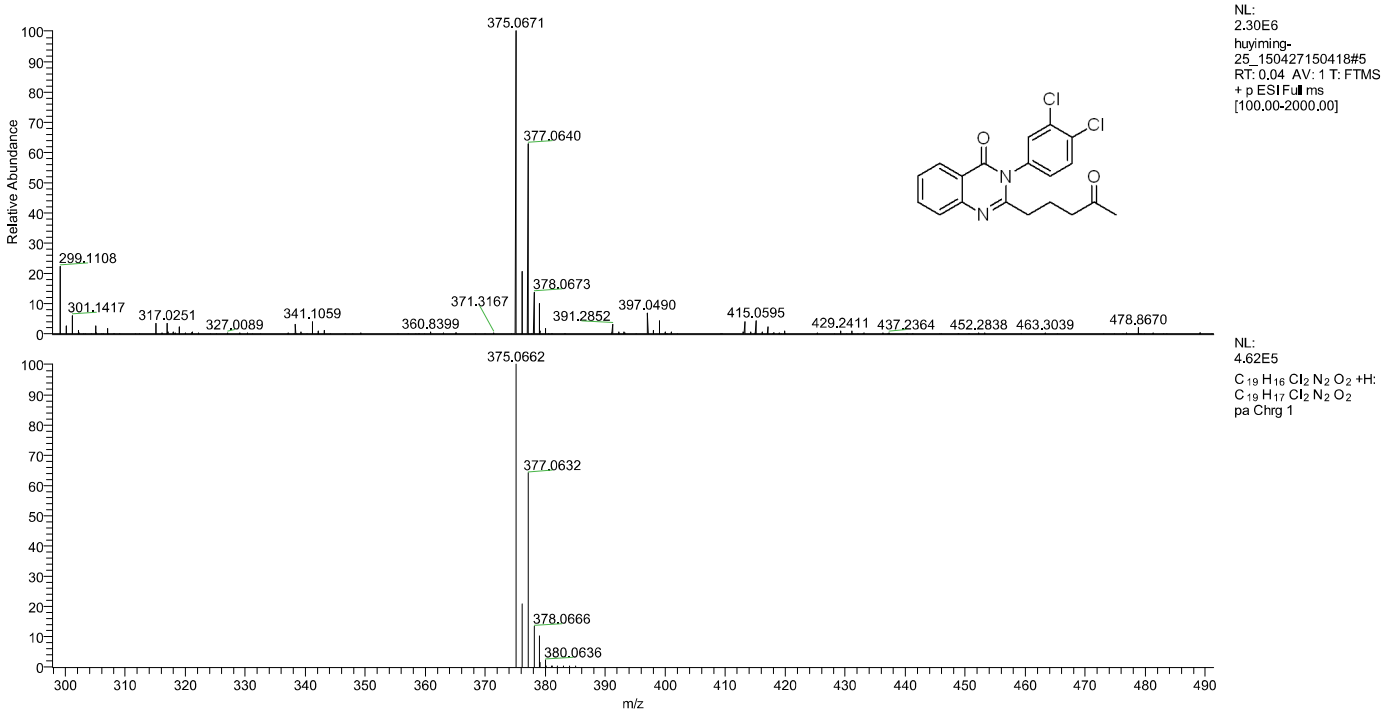




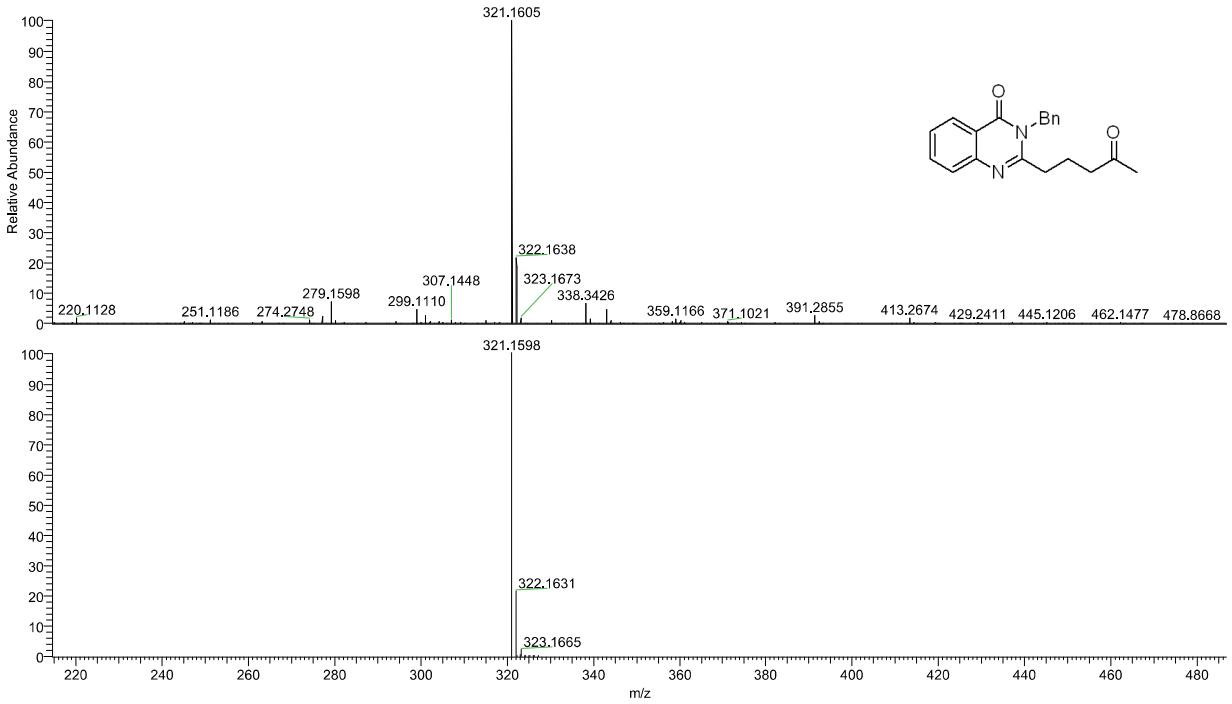
F:\Users\...\huyiming-24_150427150418 4/28/2015 3:53:38 PM 4hc
Error=2.1 ppm



F:\Users\...\huyiming-25_150427150418 4/28/2015 3:59:14 PM 4ic
Error=2.4 ppm



F:\Users\...\huyiming-26_150427150418 4/28/2015 3:38:57 PM 4jc
Error=2.2 ppm



F:\Users\...\huyiming-27_150427150418 4/28/2015 4:05:12 PM 4kc
Error=2.0 ppm