Supporting Information

for

New simple synthesis of ring-fused 4-alkyl-4*H*-3,1-benzothiazine-2-thiones: direct formation from carbon disulfide and (*E*)-3-(2-aminoaryl)acrylates or (*E*)-3-(2-aminoaryl)acrylonitriles

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General procedure, characterization data and copies of spectra

General procedure for the synthesis of 2-(2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate, **2**:

A mixture of 3-(2-aminoaryl)acrylate **1** (0.3 mmol), CS_2 (1.2 mmol, 4.0 equiv, 91.2 mg), and DABCO (0.3 mmol, 1.0 equiv, 33.6 mg) was stirred in DMSO (2 mL) at room temperature. After completion of the reaction as indicated by TLC (about 2 d), the reaction was quenched by water and extracted with ethyl acetate. The organic layers were dried with anhydrous $MgSO_4$, the solvent was evaporated under vacuum, and the residue was isolated by column chromatography with EtOAc/petroleum ether (1/5, v/v) as eluent to yield the desired products **2**.

Butyl 2-(2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2a**): yellow oil (77.9 mg, 88%); R_f 0.33; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.90 (t, *J* = 7.6 Hz, 3H), 1.27-1.35 (m, 2H), 1.53-1.59 (m, 2H), 2.79 (dd, *J* = 7.2, 6.8 Hz, 1H), 2.95 (dd, *J* = 8.4, 8.0 Hz, 1H), 4.09 (t, *J* = 6.8 Hz, 2H), 4.47 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 1H), 7.18 (t, *J* = 7.2 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 10.75 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.6, 19.0, 29.7, 42.1, 42.5, 65.1, 117.5, 121.7, 126.0, 127.6, 129.2, 136.0, 169.8, 192.7; IR (KBr) ν/cm^{-1}: 3249 (m), 3163 (m), 2932 (m), 1731 (st), 1515 (st), 1487 (st), 1340 (m), 1024 (m), 757 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{14}H_{18}NO_2S_2$: 296.0779; found: 296.0783.

Butyl 2-(6-methyl-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2b**): yellow oil (69.5 mg, 75%); R_f 0.39; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 7.6 Hz, 3H), 1.24-1.35 (m, 2H), 1.53-1.60 (m, 2H), 2.33 (s, 3H), 2.76 (dd, *J* = 7.2, 6.8 Hz, 1H), 2.92 (dd, *J* = 8.4, 8.0 Hz, 1H), 4.09 (t, *J* = 6.8 Hz, 2H), 4.42 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 7.05 (s, 1H), 7.12 (d, *J* = 7.6 Hz, 1H), 10.45 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 19.0, 20.9, 30.5, 42.2,

42.6, 65.1, 117.3, 121.6, 128.0, 129.7, 133.9, 136.0, 169.8, 192.2; IR (KBr) ν/cm^{-1}: 3244 (m), 3159 (m), 2926 (st), 1731 (st), 1500 (st), 1337 (m), 1028 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{15}H_{20}NO_2S_2$: 310.0935; found: 310.0938.

Butyl 2-(6-chloro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2c**): yellow oil (72.0 mg, 73%); R_f 0.39; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.6 Hz, 3H), 1.25-1.35 (m, 2H), 1.53-1.60 (m, 2H), 2.80 (dd, *J* = 7.2, 7.2 Hz, 1H), 2.95 (dd, *J* = 8.0, 8.0 Hz, 1H), 4.09-4.13 (m, 2H), 4.44 (t, *J* = 7.6 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 7.26-7.30 (m, 2H), 10.92 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 19.0, 30.5, 41.8, 42.3, 65.3, 118.7, 123.3, 127.6, 129.2, 130.9, 134.7, 169.6, 192.4; IR (KBr) ν/ cm^{-1}: 3239 (m), 3161 (m), 2959 (st), 1731 (st), 1486 (st), 1325 (m), 1031 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{14}H_{17}ClNO_2S_2$: 330.0389; found: 330.0392.

Butyl 2-(6-fluoro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2d**): yellow oil (80.7 mg, 86%); R_f 0.36; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, *J* = 7.6 Hz, 3H), 1.26-1.35 (m, 2H), 1.55-1.60 (m, 2H), 2.81 (dd, *J* = 7.6, 7.6 Hz, 1H), 2.95 (dd, *J* = 8.0, 8.0 Hz, 1H), 4.11 (t, *J* = 6.8 Hz, 1H), 4.45 (t, *J* = 7.6 Hz, 1H), 6.99-7.07 (m, 2H), 7.15 (dd, *J* = 3.2, 8.0 Hz, 1H), 11.07 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 19.0, 30.5, 41.8, 42.1, 65.3, 114.6 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 116.2 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 119.1 (d, $^2J_{C\text{-}F}$ = 8.0 Hz), 123.8 (d, $^2J_{C\text{-}F}$ = 8.0 Hz), 132.5, 159.8 (d, $^1J_{C\text{-}F}$ = 247.0 Hz), 169.7, 192.0; IR (KBr) ν/ cm^{-1}: 3165 (m), 2960 (st), 1731 (st), 1494 (st), 1344 (m), 1027 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{14}H_{17}FNO_2S_2$: 314.0685; found: 314.0690.

Butyl 2-(6-nitro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2e**): yellow solid (36.7 mg, 36%); R_f 0.33; mp 98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 0.92 (t, *J* = 7.6 Hz, 3H), 1.27-1.36 (m, 2H), 1.56-1.62 (m, 2H), 2.86 (dd, *J* = 7.6, 7.2 Hz, 1H), 2.95 (dd, *J* = 7.6, 7.6 Hz, 1H), 4.10-4.13 (m, 2H), 4.60 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 9.6 Hz, 1H), 8.22-8.24 (m, 2H), 10.56 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.2, 18.5, 29.9, 41.2, 41.5, 65.0, 117.2, 122.0, 123.4, 124.5, 139.9, 143.8, 168.7, 193.1; IR (KBr) ν/ cm^{-1}: 3203 (m), 2959 (st), 1728 (st), 1337 (m), 1290 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{14}H_{17}N_2O_4S_2$: 341.0630; found: 341.0627.

tert-Butyl 2-(6-methyl-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2f**): yellow solid (80.6 mg, 87%); R_f 0.15; mp 115-116 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.43 (s, 9H), 2.30 (s, 3H), 2.67-2.73 (m, 1H), 2.79-2.84 (m, 1H), 4.39 (t, *J* = 7.6 Hz, 1H), 4.42 (t, *J* = 7.6 Hz, 1H), 7.03 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 11.08 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ20.9, 28.0, 42.3, 42.8, 81.8, 117.4, 121.6, 128.0, 129.6, 133.9, 135.7, 169.0, 191.7; IR (KBr) ν/ cm^{-1}: 3440 (m), 3149 (m), 2977 (st), 1603 (m), 1497 (st), 1348 (st), 1025 (st); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{15}H_{20}NO_2S_2$: 310.0935; found: 310.0932.

Ethyl 2-(2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2g**): yellow solid (64.1 mg, 80%); R_f 0.27; mp 96-97 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.11 (t, *J* = 7.6 Hz, 3H), 2.70 (dd, *J* = 8.0, 8.0 Hz, 1H), 2.84 (dd, *J* = 8.0, 8.0 Hz, 1H), 4.05 (t, *J* = 8.0 Hz, 2H), 4.42 (t, *J* = 8.0 Hz, 1H), 7.05-7.20 (m, 4H), 10.07 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.5, 42.4, 42.9, 65.6, 117.9, 121.9, 126.3, 127.9, 129.5, 136.4, 170.2, 192.6; IR (KBr) ν/ cm^{-1}: 3431 (m), 2980 (st), 1727 (st), 1486 (m), 1347 (m), 1021 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{12}H_{14}NO_2S_2$: 268.0466; found: 268.0470.

Methyl 2-(2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2h**): yellow solid (45.5 mg, 60%); R_f 0.27; mp 119-120 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 2.80 (dd, *J* = 6.4, 6.8 Hz, 1H), 2.96 (dd, *J* = 8.4, 8.4 Hz, 1H), 3.68 (s, 3H), 4.48 (t, *J* = 8.0 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 10.89 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ42.0, 42.3, 52.2, 117.6, 121.6, 126.0, 127.6, 129.2, 136.1, 170.2, 192.5; IR (KBr) ν/cm^{-1}: 3453 (w), 3160 (m), 2952 (st), 1731 (st), 1486 (st), 1245 (m), 1029 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{11}H_{12}NO_2S_2$: 254.0309; found: 254.0302.

Methyl 2-(6-chloro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2i**): yellow solid (62.0 mg, 72%); R_f 0.27; mp 120-121 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ2.80 (dd, *J* = 8.0, 8.0 Hz, 1H), 2.96 (dd, *J* = 8.0, 8.0 Hz, 1H), 3.69 (s, 3H), 4.44 (t, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.25 (s, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 11.00 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ42.1, 42.4, 52.6, 119.1, 123.7, 127.9, 129.6, 131.2, 135.1, 170.3, 192.6; IR (KBr) ν/cm^{-1}: 3434 (m), 3145 (m), 2967 (st), 1727 (st), 1517 (st), 1484 (m), 1347 (m), 1034 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{11}H_{11}ClNO_2S_2$: 287.9920; found: 287.9925.

Methyl 2-(6-methyl-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**2j**): yellow solid (56.9 mg, 71%); R_f 0.24; mp 83-84 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ2.23 (s, 3H), 2.69 (dd, *J* = 6.4, 6.4 Hz, 1H), 2.85 (dd, *J* = 8.4, 8.4 Hz, 1H), 3.60 (s, 3H), 4.33 (t, *J* = 8.0 Hz, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.96 (s, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 10.86 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ20.9, 42.1, 42.4, 52.1, 117.5, 121.5, 127.9, 129.7, 133.9, 136.0, 170.3, 191.6; IR (KBr) ν/cm^{-1}: 3164 (m), 2922 (st), 1731 (st), 1504 (st), 1025 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{12}H_{14}NO_2S_2$: 268.0466; found: 268.0468.

Methyl 2-(2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)propanoate (**2k**): yellow solid (59.3 mg, 74%); R_f 0.32; mp 105-106 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 1.02 (d, *J* = 6.8 Hz, 0.65H), 1.33 (d, *J* = 6.8 Hz, 2.35H), 2.83-2.87 (m, 1H), 3.55 (s, 2.35H), 3.76 (s, 0.65H), 4.13 (d, *J* = 7.2 Hz, 0.22H), 4.30 (d, *J* = 8.0 Hz, 0.78H), 7.05-7.10 (m, 1H), 7.12-7.18 (m, 2H), 7.30-7.34 (m, 1H), 10.45 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ13.5, 46.9, 48.9, 52.1, 117.3, 120.6, 125.7, 128.2, 129.2, 136.3, 173.4, 192.6; IR (KBr) ν/cm^{-1}: 3459 (w), 3162 (m), 2985 (st), 1733 (st), 1487 (st), 1347 (m), 1021 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{12}H_{14}NO_2S_2$: 268.0466; found: 268.0461.

Methyl 2-(6-chloro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)propanoate (**2l**): yellow solid (49.7 mg, 55%); R_f 0.48; mp 99-100 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 1.06 (d, *J* = 6.8 Hz, 0.6H), 1.33 (d, *J* = 6.8 Hz, 2.4H), 2.83-2.91 (m, 1H), 3.61 (s, 2.4H), 3.77 (s, 0.6H), 4.15 (d, *J* = 7.6 Hz, 0.2H), 4.27 (d, *J* = 7.6 Hz, 0.8H), 7.03 (d, *J* = 8.4 Hz, 1H), 7.17 (s, 1H), 7.29 (d, *J* = 8.8 Hz, 1H), 10.65 (br, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ13.4, 46.8, 48.5, 52.2, 118.5, 122.3, 128.1, 129.2, 130.6, 134.9, 173.2, 192.3; IR (KBr) ν/cm^{-1}: 3441 (m), 3243 (m), 2973 (st), 1732 (st), 1486 (st), 1333 (m), 1026 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{12}H_{13}ClNO_2S_2$: 302.0076; found: 302.0081.

Methyl 2-(6-fluoro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)propanoate (**2m**): yellow solid (46.2 mg, 54%); R_f 0.41; mp 142-143 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 0.99 (d, *J* = 7.2 Hz, 1.5H), 1.26 (d, *J* = 7.2 Hz, 1.5H), 2.84-2.95 (m, 1H), 3.61 (s, 1.5H), 3.77 (m, 1.5H), 4.18 (d, *J* = 9.6 Hz, 0.5H), 4.27 (d, *J* = 7.6 Hz, 0.5H), 6.92 (d, *J* = 8.0 Hz, 1H), 7.02-7.15 (m, 2H), 10.83 (br, 0.5H), 10.90 (br, 0.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 13.6, 46.6, 47.8, 52.4, 115.1 (d, $^2J_{C-F}$ = 23.0 Hz), 115.8 (d, $^2J_{C-F}$ = 23.0 Hz), 116.4 (d, $^2J_{C-F}$ = 8.0 Hz), 121.8 (d, $^2J_{C-F}$ = 8.0 Hz),

133.0, 159.5 (d, $^{1}J_{C\text{-}F}$ = 246.0 Hz), 173.3, 192.5; 15.5, 46.1, 48.6, 52.2, 115.1 (d, $^{2}J_{C\text{-}F}$ = 23.0 Hz), 115.8 (d, $^{2}J_{C\text{-}F}$ = 23.0 Hz), 116.2 (d, $^{2}J_{C\text{-}F}$ = 8.0 Hz), 122.7 (d, $^{2}J_{C\text{-}F}$ = 8.0 Hz), 132.8, 159.7 (d, $^{1}J_{C\text{-}F}$ = 246.0 Hz), 173.9, 191.7; IR (KBr) ν/cm^{-1}: 3161 (w), 2986 (w), 1731 (st), 1494 (st), 1337 (m), 1011 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{12}H_{13}FNO_2S_2$: 286.0372; found: 286.0375.

Methyl 2-(6-methyl-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)propanoate (**2n**): yellow solid (62.4 mg, 74%); R_f 0.41; mp 151-152 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (d, *J* = 7.2 Hz, 1.2H), 1.31 (d, *J* = 7.2 Hz, 1.8H), 2.32 (s, 1.8H), 2.34 (s, 1.2H), 2.83-2.91 (m, 1H), 3.57 (s, 1.8H), 3.76 (s, 1.2H), 4.14 (d, *J* = 7.6 Hz, 0.4H), 4.28 (d, *J* = 7.6 Hz, 0.6H), 6.92-7.00 (m, 2H), 7.10-7.15 (m, 1H), 10.41 (br, 0.6H), 10.49 (br, 0.4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ13.2, 20.9, 47.1, 48.9, 52.0, 117.3, 120.4, 128.6, 129.8, 134.1, 135.8, 173.4, 190.9; 15.6, 21.0, 46.3, 48.1, 52.2, 117.2, 119.6, 129.4, 129.9, 134.2, 135.5, 174.2, 192.2; IR (KBr) ν/cm^{-1}: 3450 (w), 3157 (m), 2977 (st), 1731 (st), 1455(st), 1024 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{13}H_{16}NO_2S_2$: 282.0622; found: 282.0618.

2-(2-Thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetonitrile (**2o**): yellow solid (59.4 mg, 90%); R_f 0.16; mp 174-175 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.05 (t, *J* = 7.6 Hz, 2H), 4.64 (d, *J* = 5.6 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.36-7.40 (m, 2H), 12.66 (br, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ26.6, 40.6, 117.4, 117.8, 120.1, 125.2, 128.2, 129.3, 136.3, 189.3; IR (KBr) ν/cm^{-1}: 3441 (m), 3156 (m), 2910 (st), 2247 (w), 1609 (m), 1525 (st), 1492 (st), 1363 (m), 1014 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{10}H_9N_2S_2$: 221.0207; found: 221.0205.

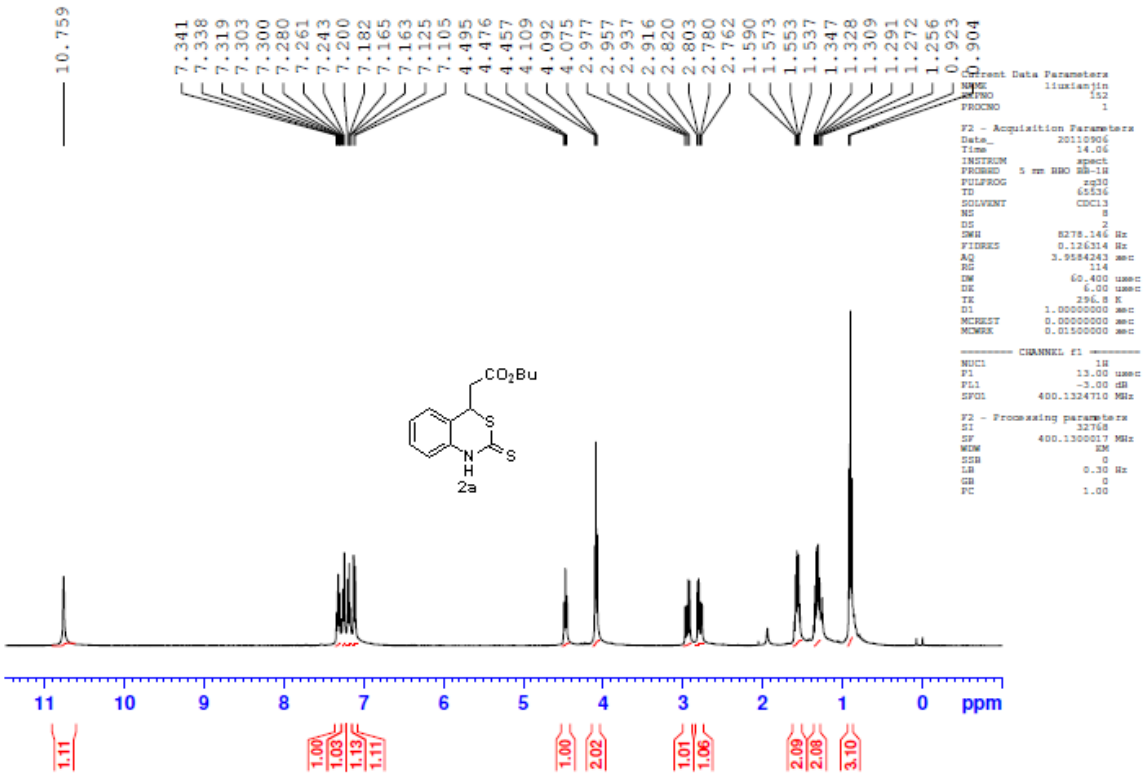
2-(6-Methyl-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetonitrile (**2p**): yellow solid (52.6 mg, 75%); R_f 0.18; mp 201-202 ^oC; ^1H NMR (400 MHz, DMSO-d_6) δ 2.29 (s, 3H), 3.05 (t, J = 6.2 Hz, 2H), 4.61 (t, J = 6.4 Hz, 1H), 7.19 (d, J = 6.8 Hz, 3H), 12.71 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 21.7, 28.0, 41.8, 118.8, 119.0, 121.0, 129.5, 131.0, 135.4, 135.9, 189.8; IR (KBr) ν/cm^{-1}: 3148 (m), 2957 (m), 2924 (m), 2250 (w), 1503 (st), 1027 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{11}H_{11}N_2S_2$: 235.0364; found: 235.0362.

2-(6-Chloro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetonitrile (**2q**): yellow solid (33.5 mg, 44%); R_f 0.21; mp 226-227 ^oC; ^{1}HNMR (400 MHz, DMSO-d_6) δ 3.13 (s, 2H), 4.70 (s, 1H), 7.32 (d, J = 8.0 Hz, 1H), 7.47-7.52 (m, 2H), 12.87 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 26.5, 40.2, 117.5, 119.5, 121.8, 127.8, 128.7, 129.3, 135.3, 189.3; IR (KBr) ν/cm^{-1}: 3438 (m), 3144 (m), 2962 (st), 2251 (w), 1508 (st), 1483 (st), 1341 (st), 1029 (st); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{10}H_8ClN_2S_2$: 254.9817; found: 254.9822.

2-(6-Fluoro-2-thioxo-2,4-dihydro-1*H*-benzo[*d*][1,3]thiazin-4-yl)acetonitrile (**2r**): yellow solid (37.8 mg, 53%); R_f 0.18; mp 210-212 ^oC; ^{1}HNMR (400 MHz, DMSO-d_6) δ 2.90-3.00 (m, 2H), 4.50 (t, 1H, J = 6.6 Hz, 1H), 7.08-7.19 (m, 3H), 12.66 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 26.3, 40.3, 114.7 (d, $^2J_{C\text{-}F}$ = 24.0 Hz), 116.3 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 117.6, 119.7 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 122.0 (d, $^3J_{C\text{-}F}$ = 8.0 Hz), 133.1, 158.6 (d, $^1J_{C\text{-}F}$ = 242.0 Hz), 188.8; IR (KBr) ν/cm^{-1}: 3455 (m), 3158 (m), 2977 (st), 2250 (w), 1698 (st), 1521 (st), 1493 (st), 1351 (m), 1028 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{10}H_8FN_2S_2$: 239.0113; found: 239.0118.

Ethyl 2-(2-(methylthio)-4*H*-benzo[*d*][1,3]thiazin-4-yl)acetate (**3**): yellow oil (59.0 mg, 70%); R_f 0.63; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.22 (t, *J* = 7.2 Hz, 3H), 2.60-2.66 (m, 3H), 2.69 (d, *J* = 8.4 Hz, 1H) 4.09-4.15 (m, 2H), 4.45 (t, *J* = 7.0 Hz, 1H), 7.15-7.22 (m, 2H), 7.31-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 14.4, 40.1, 41.4, 60.9, 123.0, 126.2, 126.7, 126.8, 128.8, 142.6, 158.9, 170.1; IR (KBr) ν/cm^{-1}: 3030 (m), 2980 (m), 1731 (st), 1537 (st), 1392 (m); HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{13}H_{16}NO_2S_2$: 282.0622; found: 282.0618.

LXJ-9-3-1



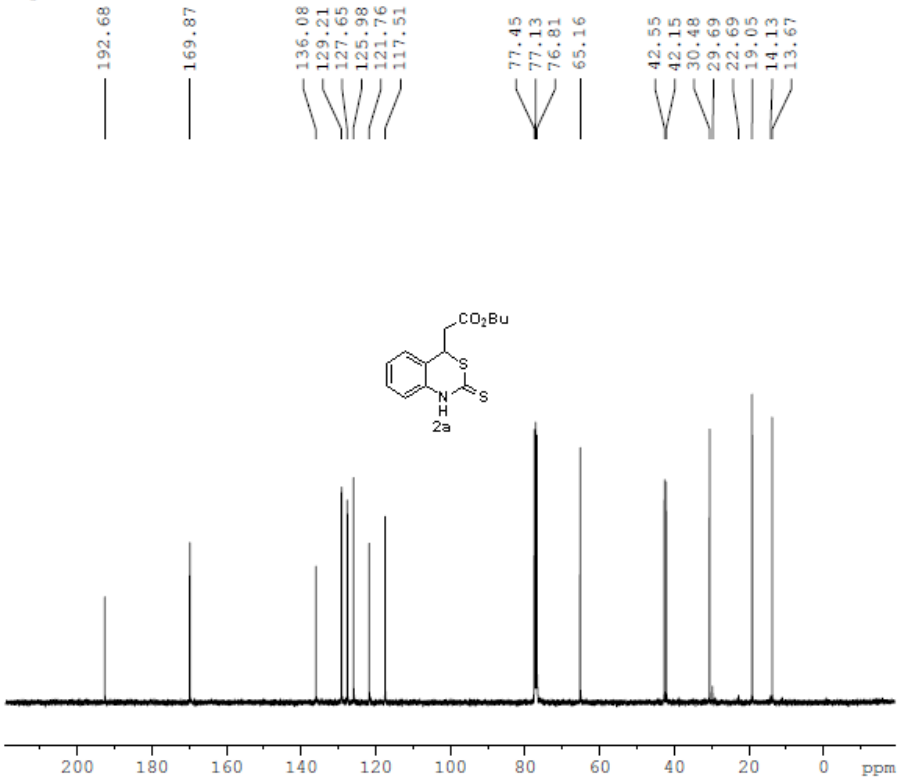
Current Data Parameters
NAME liuxianjin
EXPNO 152
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110906
Time 14.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 114
DW 60.400 usec
DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Lxj-9-3-1



Current Data Parameters
NAME liuxianjin
EXPNO 154
PROCNO 1

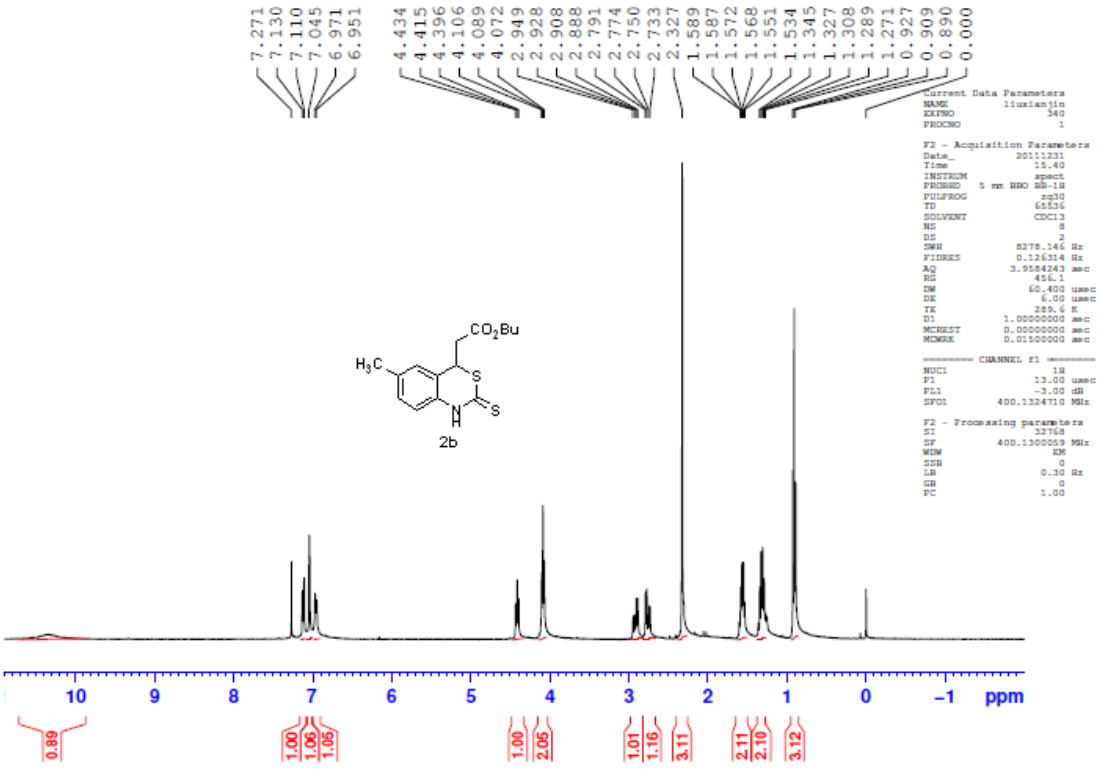
F2 - Acquisition Parameters
Date_ 20110908
Time 9.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 962
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 13c
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz

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

12-16-3



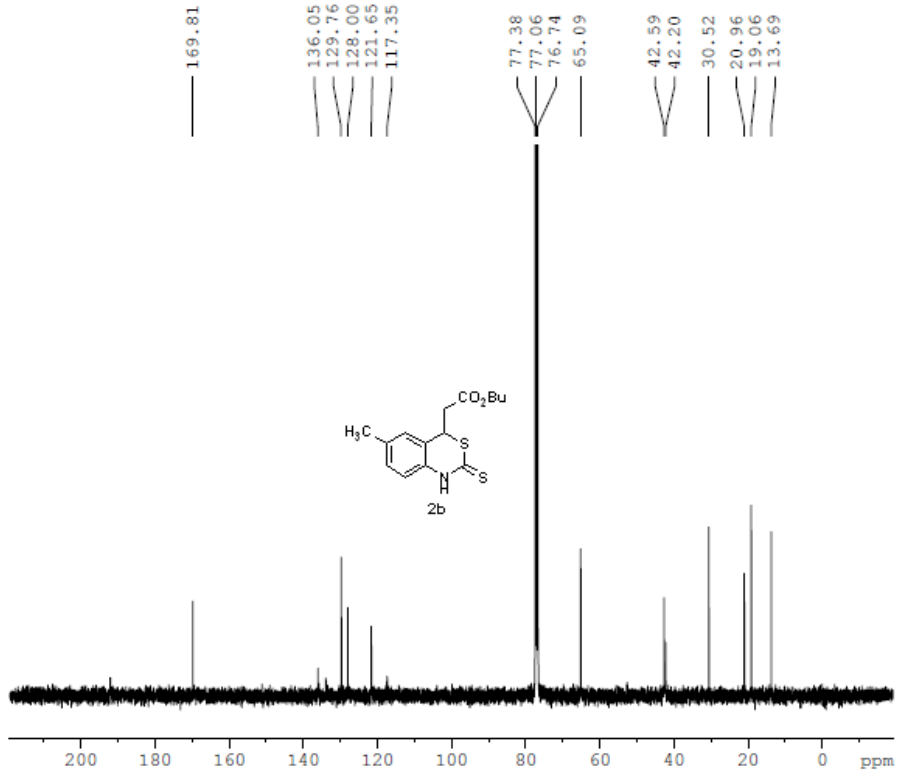
Current Data Parameters
NAME liuxianjin
EXPNO 340
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111231
Time 15.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DW 60.400 usec
DE 6.00 usec
TE 289.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300059 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

lxj-12-16-3



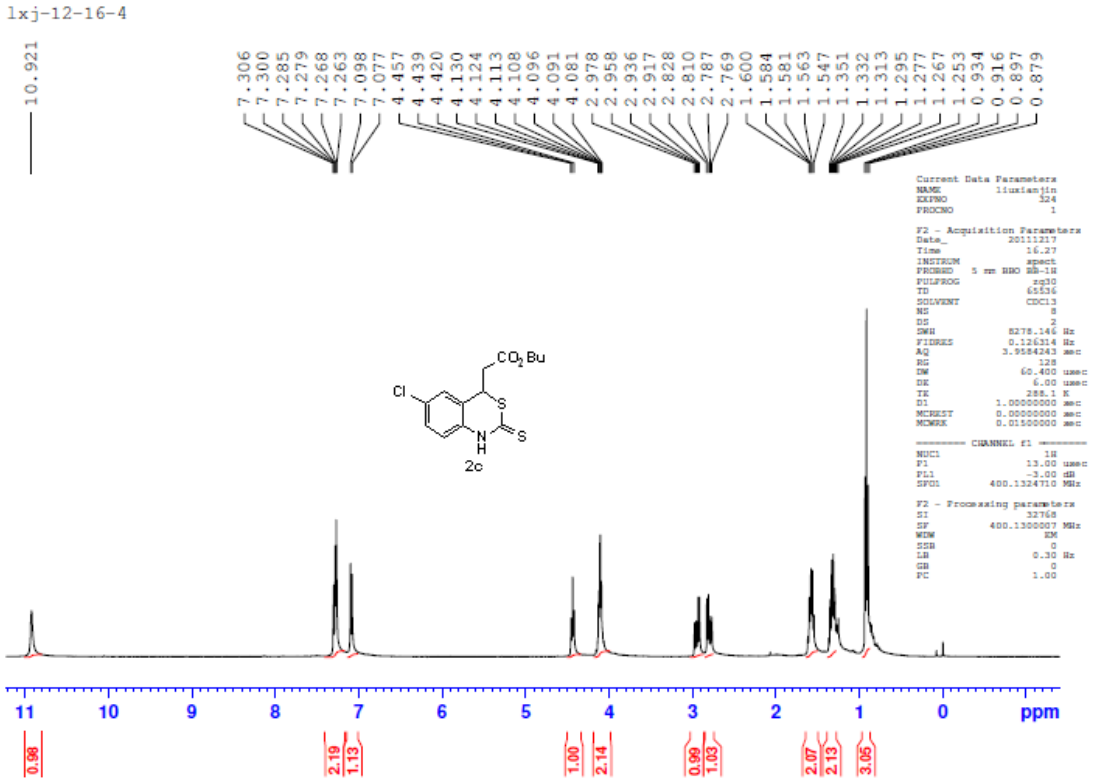
Current Data Parameters
NAME liuxianjin
EXPNO 341
PROCNO 1

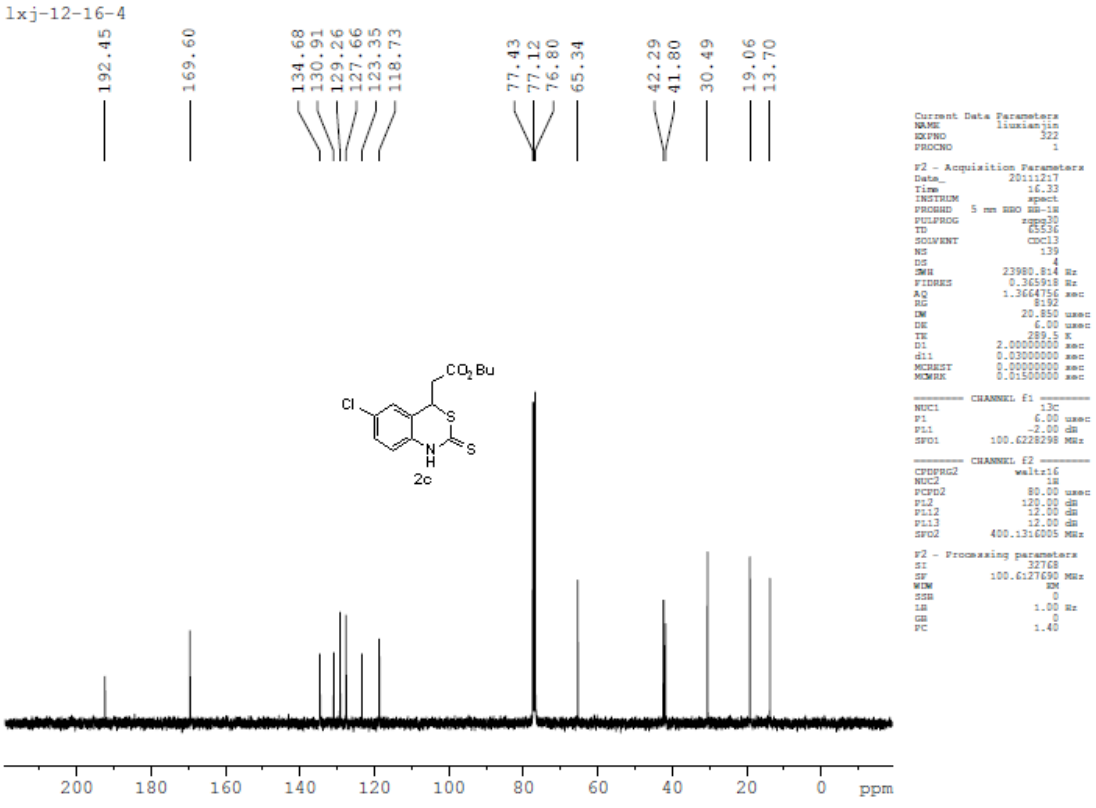
F2 - Acquisition Parameters
Date_ 20111231
Time 16.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 616
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 291.7 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

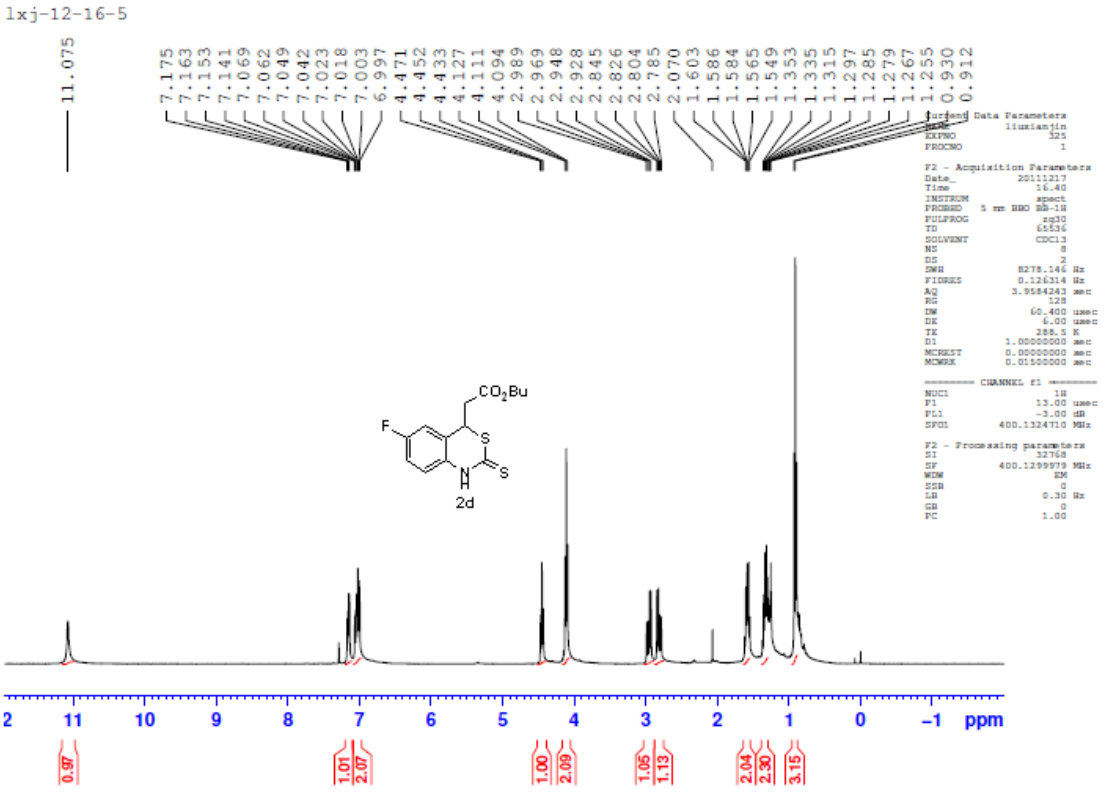
CHANNEL f1
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

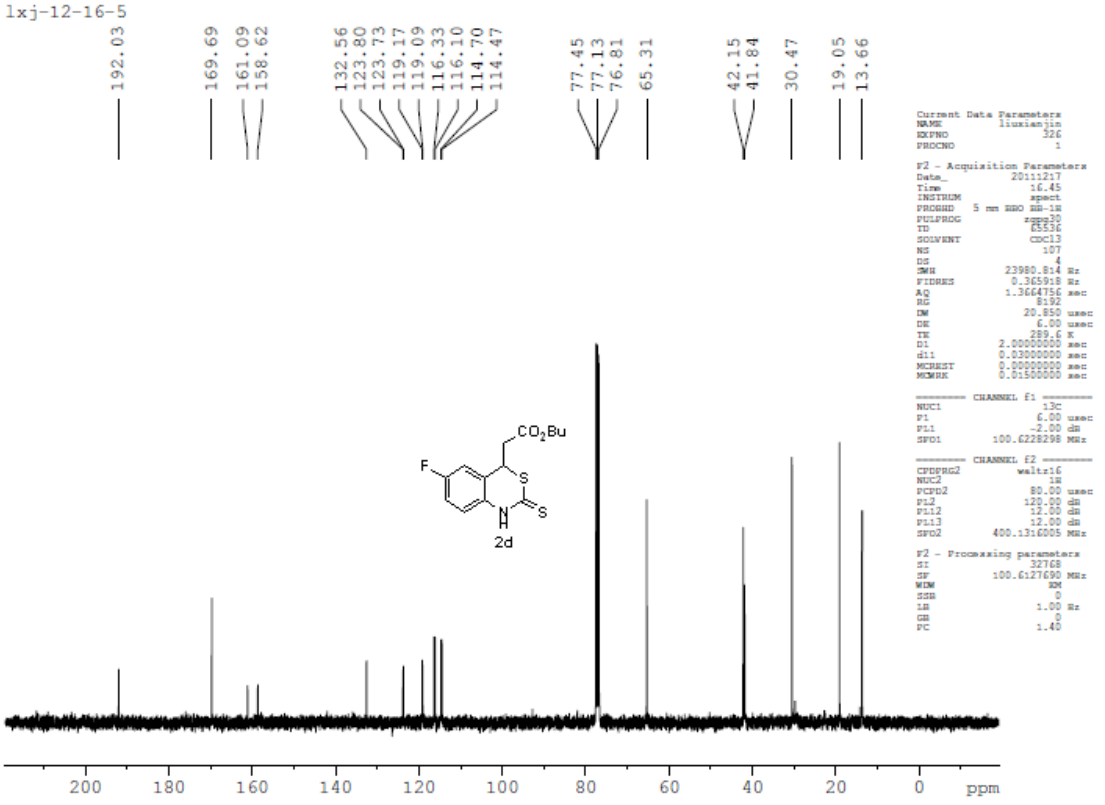
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz

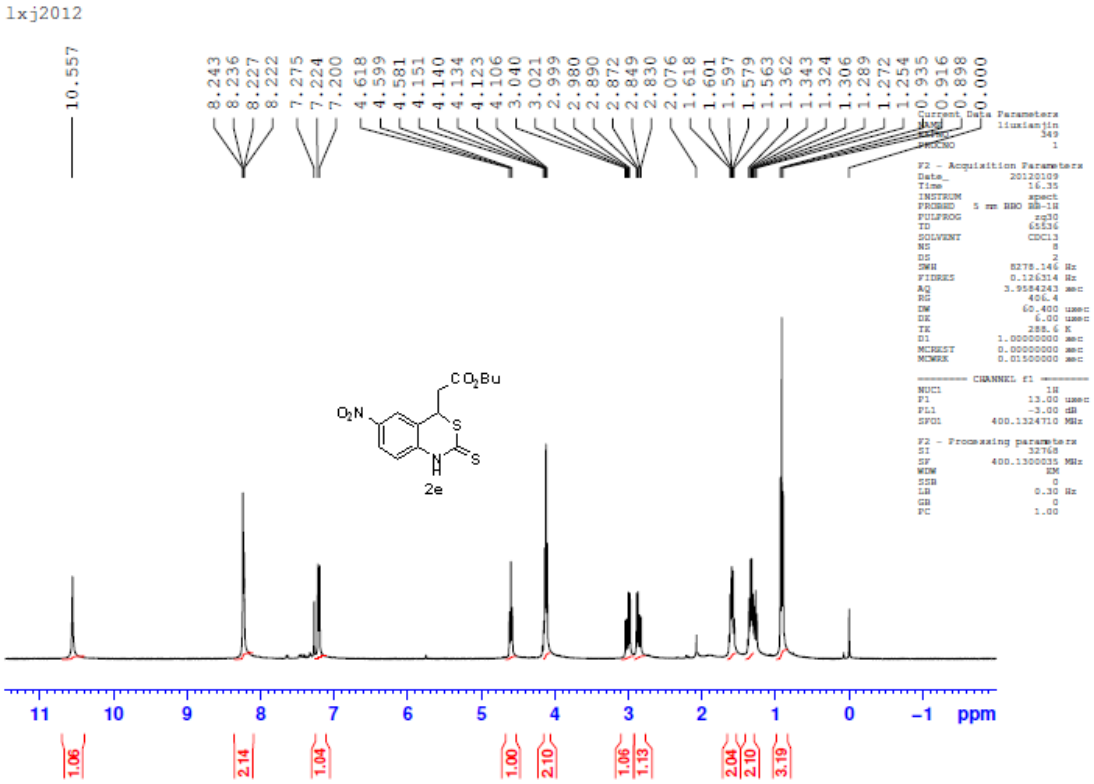
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

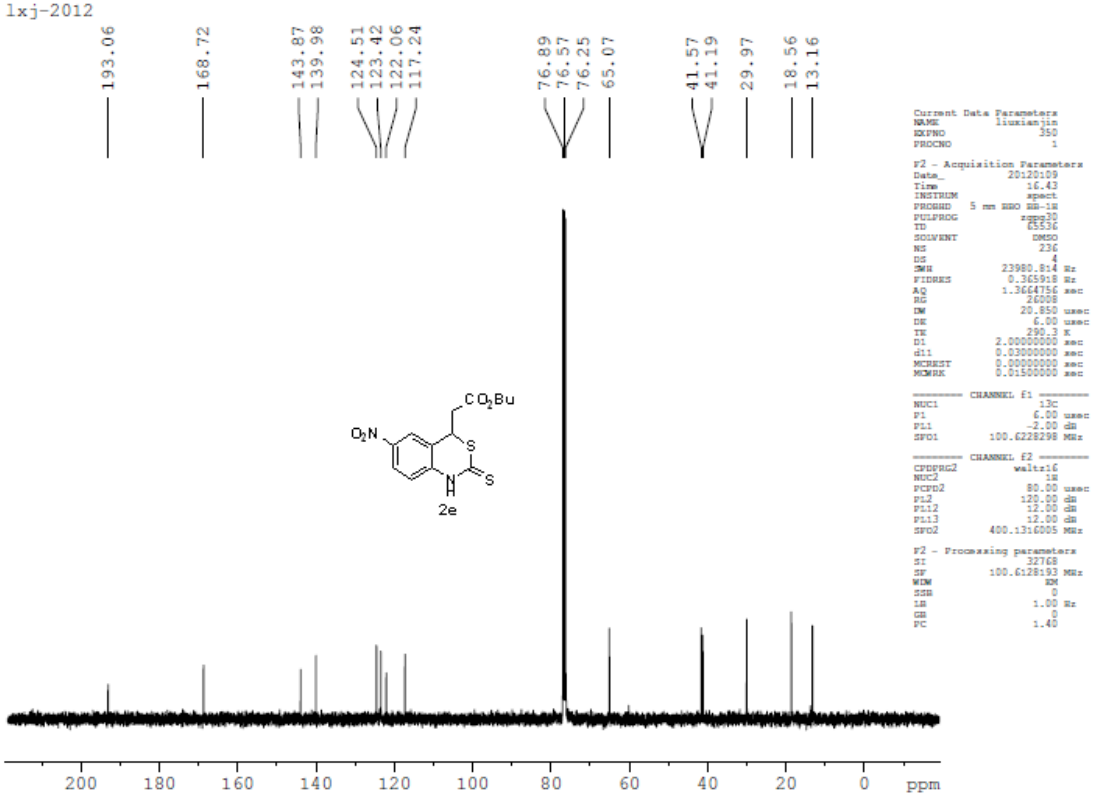

lxj-12-16-4
10.921
7.306
7.300
7.285
7.279
7.268
7.263
7.098
7.077
4.457
4.439
4.420
4.130
4.124
4.113
4.108
4.096
4.091
4.081
2.978
2.958
2.936
2.917
2.828
2.810
2.787
2.769
1.600
1.584
1.581
1.563
1.547
1.351
1.332
1.313
1.295
1.277
1.267
1.253
0.934
0.916
0.897
0.879
CO2 Bu
Cl
S
N
H
S
2c
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
2.19
1.13
1.00
2.14
0.99
1.03
2.07
2.13
3.05


lxj-12-16-4
192.45
169.60
134.68
130.91
129.26
127.66
123.35
118.73
77.43
77.12
76.80
65.34
42.29
41.80
30.49
19.06
13.70
CO2 Bu
Cl
S
N
H
S
2c
200
180
160
140
120
100
80
60
40
20
0
ppm

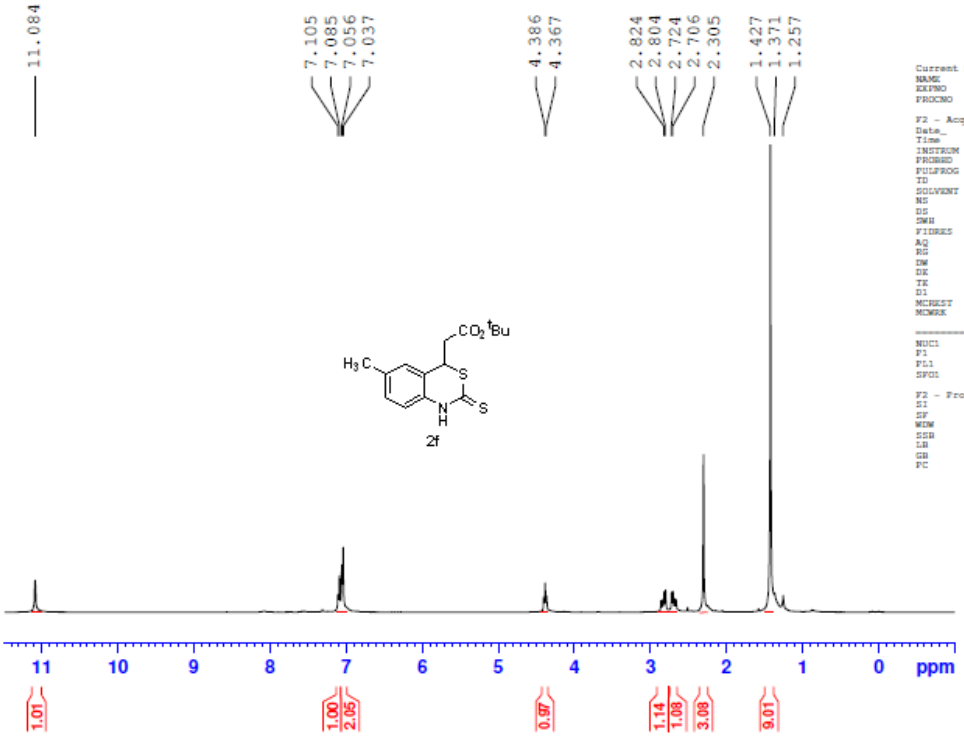

lxj-12-16-5
11.075
7.175
7.163
7.153
7.141
7.069
7.062
7.049
7.042
7.023
7.018
7.003
6.997
4.471
4.452
4.433
4.127
4.111
4.094
2.989
2.969
2.948
2.928
2.845
2.826
2.804
2.785
2.070
1.603
1.586
1.584
1.565
1.549
1.353
1.335
1.315
1.297
1.285
1.279
1.267
1.255
0.930
0.912
CO2Bu
F
S
N
H
S
2d
2 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
0.97
1.01
2.07
1.00
2.09
1.06
1.13
2.04
2.30
3.15


lxj-12-16-5
192.03
169.69
161.09
158.62
132.56
123.80
123.73
119.17
119.09
116.33
116.10
114.70
114.47
77.45
77.13
76.81
65.31
42.15
41.84
30.47
19.05
13.66
CO2Bu
F
S
N
H
S
2d
200 180 160 140 120 100 80 60 40 20 0 ppm


lxj2012
10.557
8.243
8.236
8.227
8.222
7.275
7.224
7.200
4.618
4.599
4.581
4.151
4.140
4.134
4.123
4.106
3.040
3.021
2.999
2.980
2.890
2.872
2.849
2.830
2.076
1.618
1.601
1.597
1.579
1.563
1.362
1.343
1.324
1.306
1.289
1.272
1.254
0.935
0.916
0.898
0.000
2e
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm
1.06
2.14
1.04
1.00
2.10
1.06
1.13
2.04
2.10
3.19

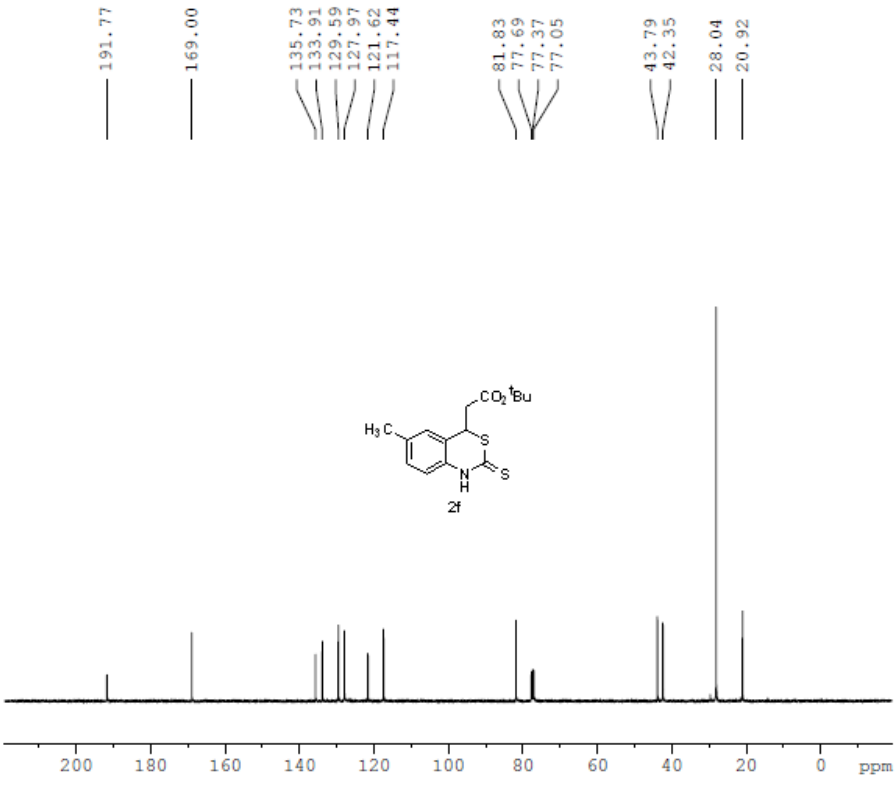

lxj-2012
193.06
168.72
143.87
139.98
124.51
123.42
122.06
117.24
76.89
76.57
76.25
65.07
41.57
41.19
29.97
18.56
13.16
2e
200
180
160
140
120
100
80
60
40
20
0
ppm

DGN3-27-1

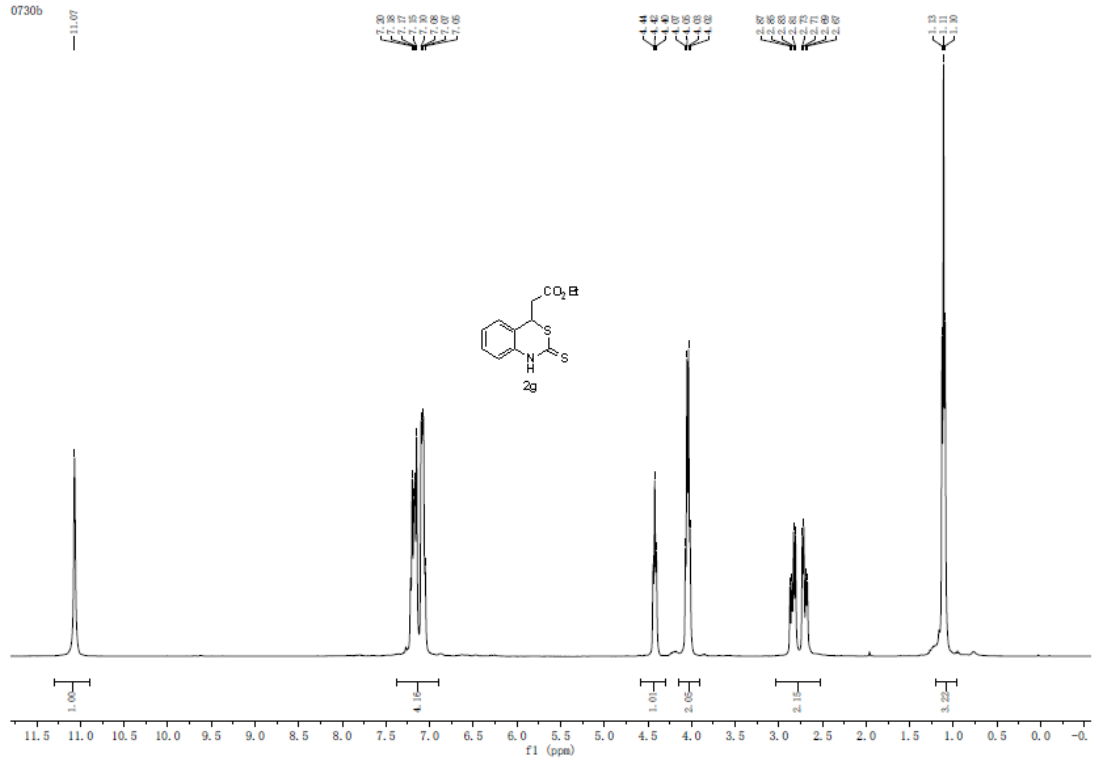


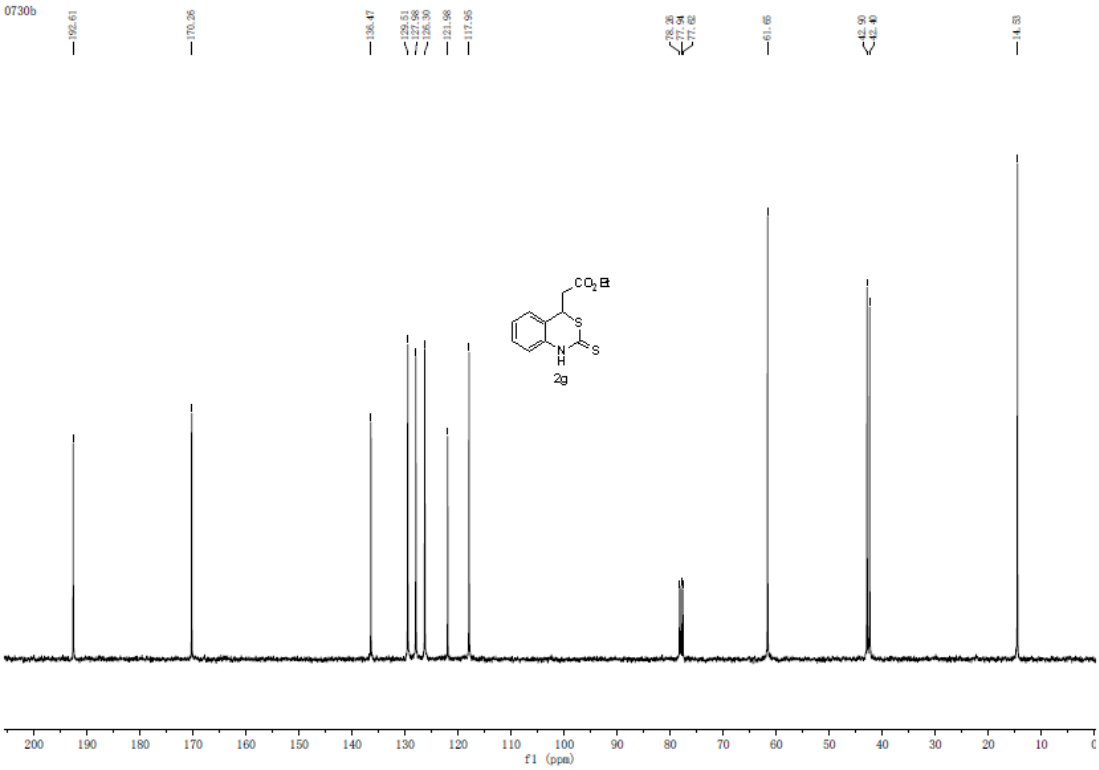

```
Current Data Parameters
NAME                 wangdan
EXPNO                    178
PROCNO                     1

F2 - Acquisition Parameters
Date_               20120415
Time                    9.14
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       31
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                 3.9584243 sec
RG                       57
DW                   60.400 usec
DE                    6.00 usec
TE                   295.8 K
D1                1.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    13.00 usec
PL1                   -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                       32768
SF                400.1299896 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

DGN-3-27-1

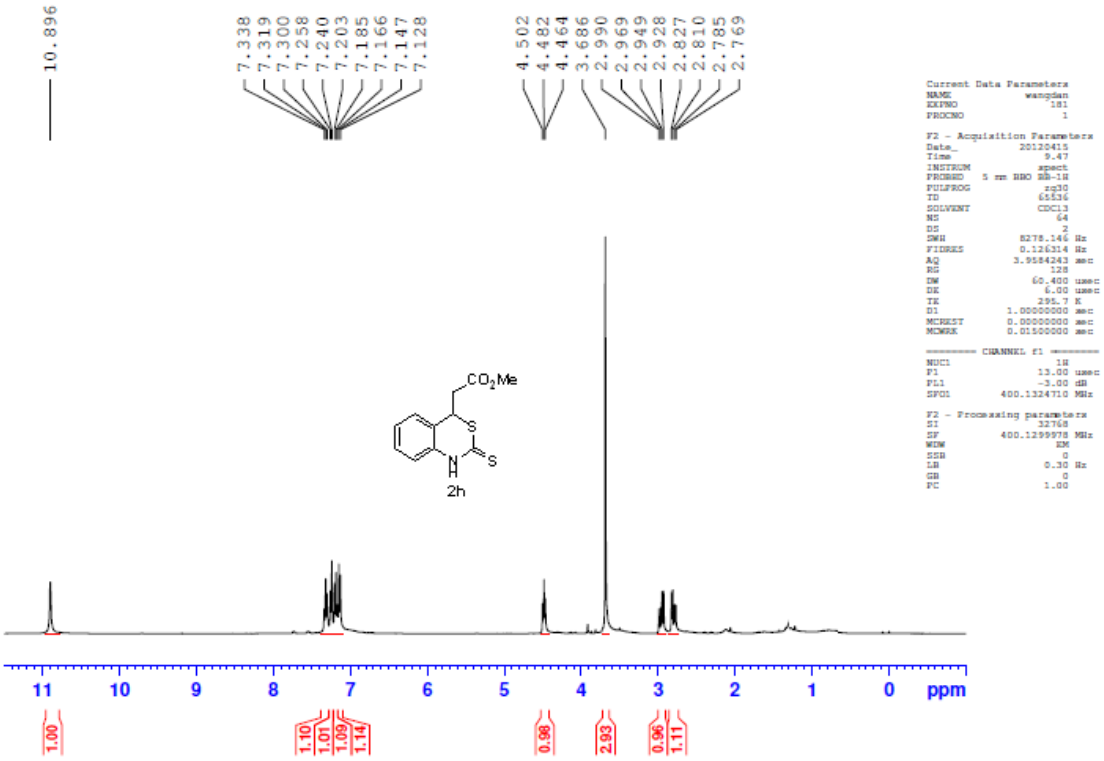



```
Current Data Parameters
NAME                 kaifanshiyan
EXPNO                           9
PROCNO                          1

F2 - Acquisition Parameters
Date_               20120426
Time                    19.51
INSTRUM                spect
PROBHD     5 mm BBO BB-1H
PULPROG                zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      137
DS                        4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                 1.3664756 sec
RG                   10321.3
DW                   20.850 usec
DE                    6.00 usec
TE                   297.9 K
D1                2.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                    6.00 usec
PL1                  -2.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                80.00 usec
PL2                  120.00 dB
PL12                  12.00 dB
PL13                  12.00 dB
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
```


0730b
11.07
7.20
7.18
7.17
7.15
7.08
7.07
7.05
4.44
4.43
4.42
4.40
4.07
4.06
4.05
4.03
4.02
2.87
2.86
2.83
2.82
2.73
2.71
2.69
2.67
1.13
1.11
1.10
CO2Et
S
N
H
S
2g
1.00
4.16
1.01
2.05
2.15
3.22
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


0730b
192.61
170.26
136.47
129.51
127.98
126.30
121.98
117.95
78.26
77.94
77.62
61.65
42.90
42.40
14.53
CO2Et
S
N
H
S
2g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

3-26-2



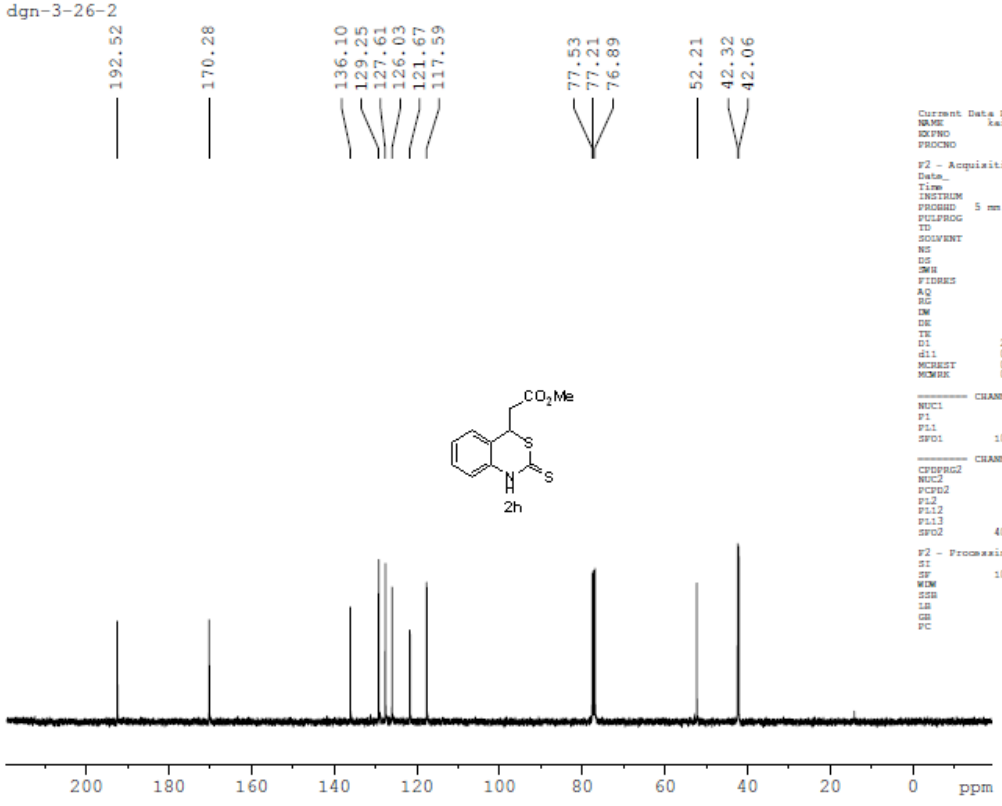
Current Data Parameters
NAME wangdan
EXPNO 181
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120415
Time 9.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.00 usec
TE 295.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299978 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

dgn-3-26-2



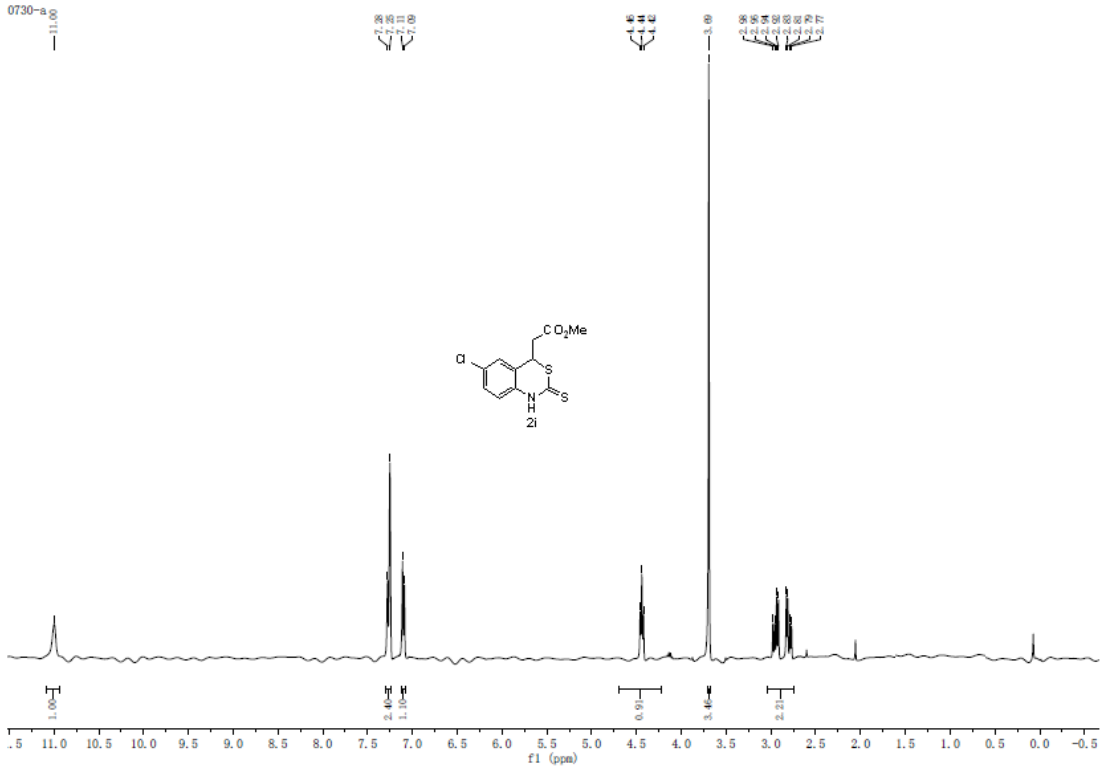
Current Data Parameters
NAME kaifanshiyan
EXPNO 13
PROCNO 1

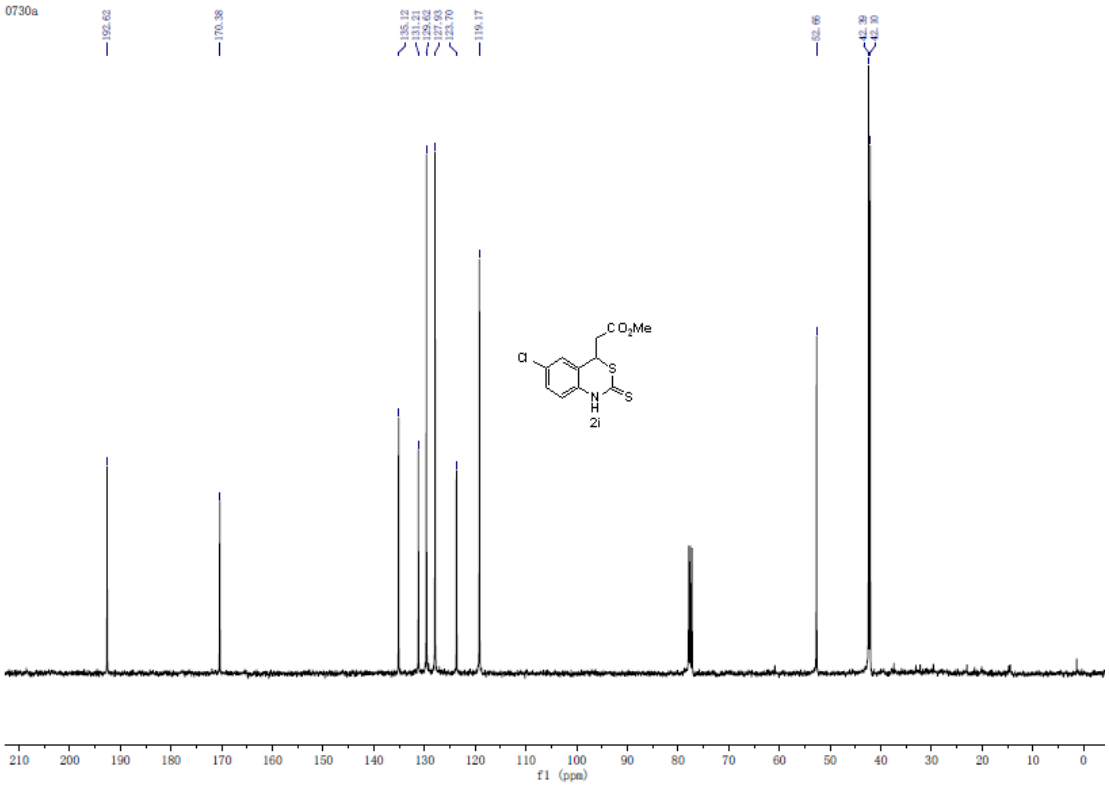
F2 - Acquisition Parameters
Date_ 20120426
Time 20.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 143
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

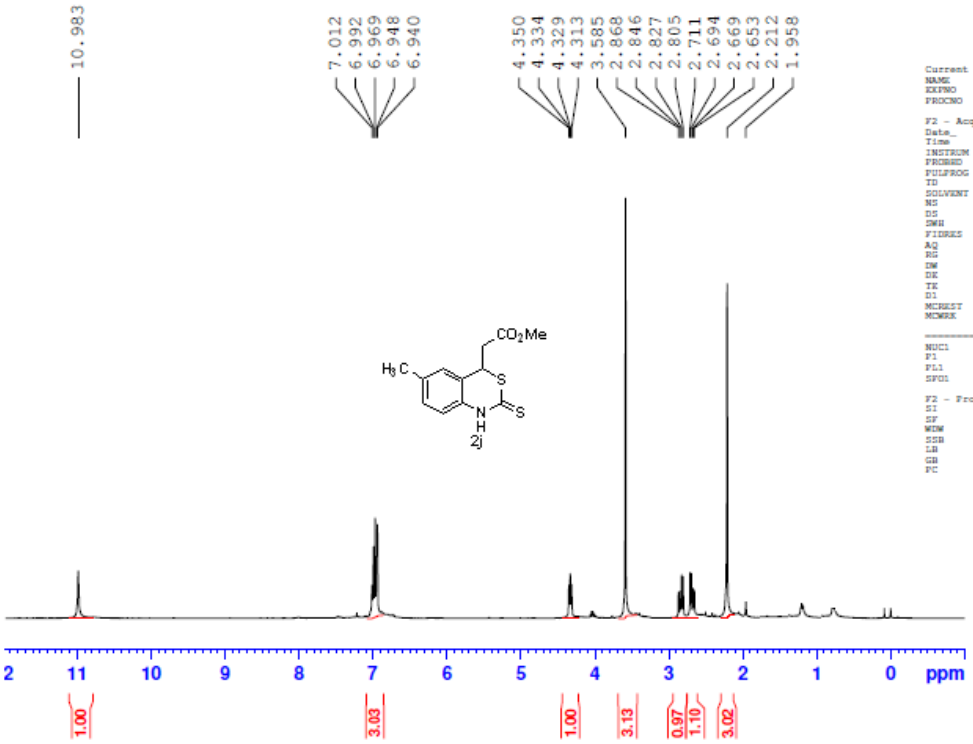
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz

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


0730-a
11.00
7.28
7.25
7.11
7.09
4.45
4.44
4.42
3.69
2.96
2.95
2.94
2.93
2.92
2.91
2.90
2.89
2.88
2.79
2.77
CO2Me
Cl
S
N
H
S
2i
1.00
2.40
1.10
0.91
3.46
2.21
f1 (ppm)


0730a
192.62
170.38
135.12
131.21
129.64
127.55
123.70
119.17
52.66
42.39
42.30
CO2Me
Cl
S
N
H
S
2i
f1 (ppm)

dgn-3-7



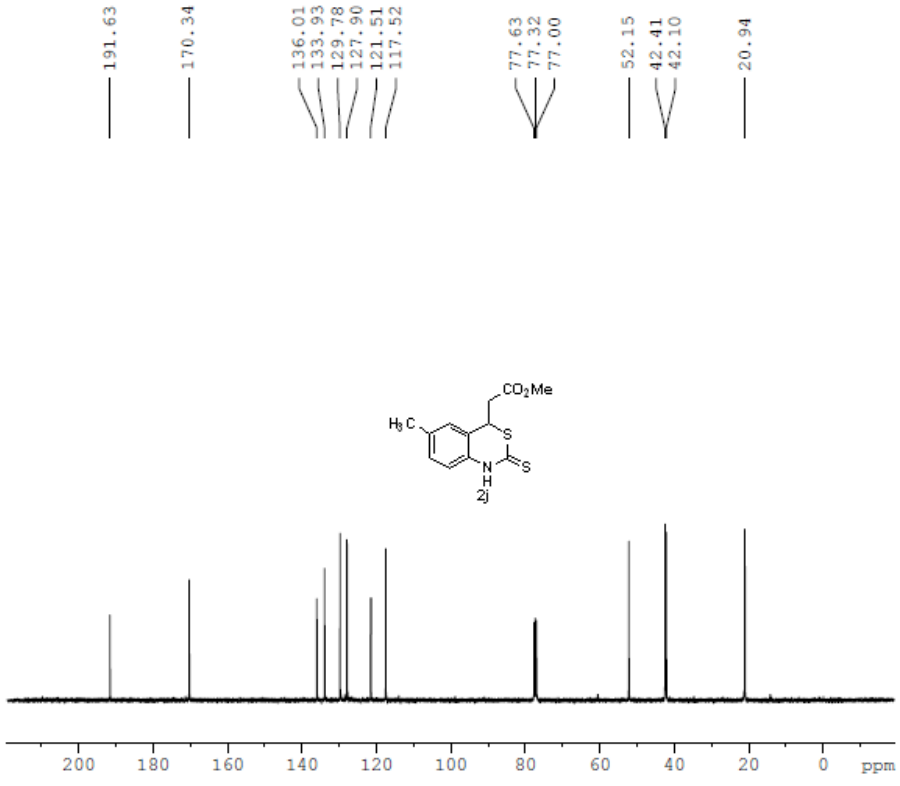
Current Data Parameters
NAME kaifanshiyan
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120426
Time 20.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 64
DW 60.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300280 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

dgn-3-7



Current Data Parameters
NAME kaifanshiyan
EXPNO 11
PROCNO 1

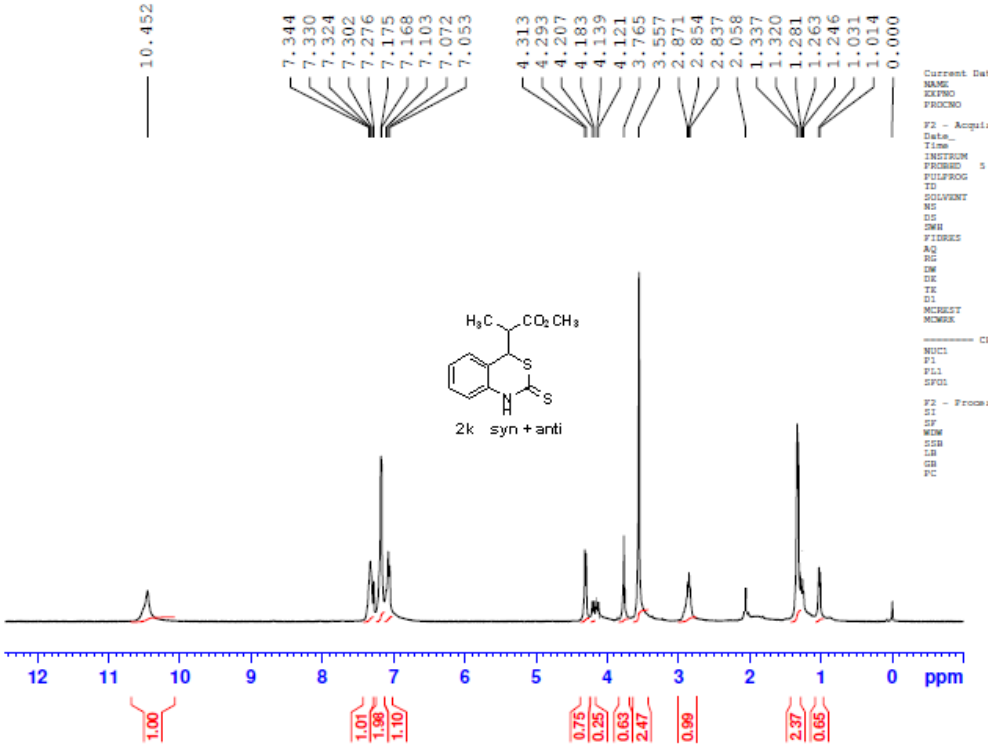
F2 - Acquisition Parameters
Date_ 20120426
Time 20.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DW 20.850 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
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

Lxj-12-17-1



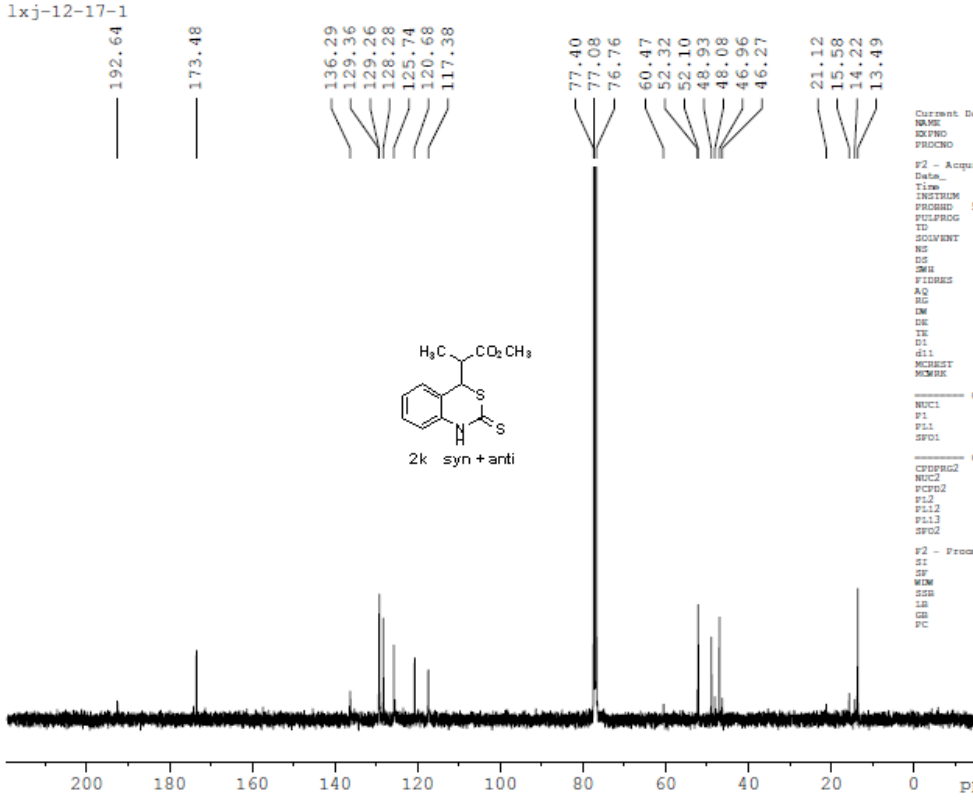
Current Data Parameters
NAME liuxianjin
EXPNO 537
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111230
Time 14.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 290.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

lxj-12-17-1



Current Data Parameters
NAME liuxianjin
EXPNO 544
PROCNO 1

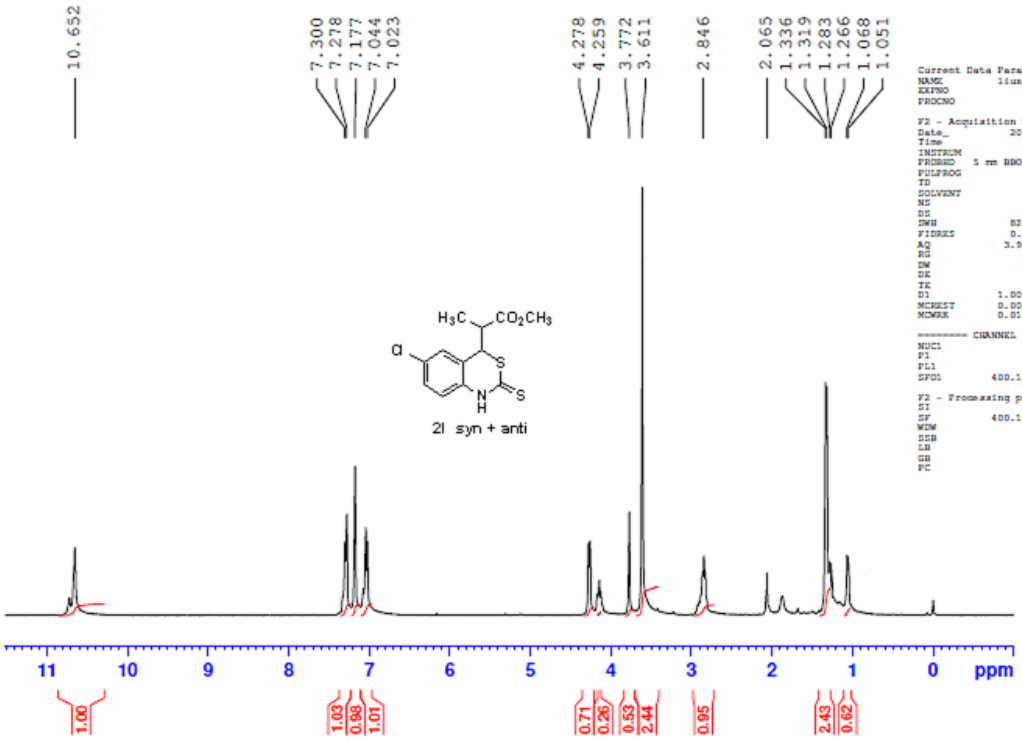
F2 - Acquisition Parameters
Date_ 20111231
Time 18.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 506
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 20642.5
DW 20.850 usec
DE 6.00 usec
TE 290.9 K
D1 2.00000000 sec
D11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

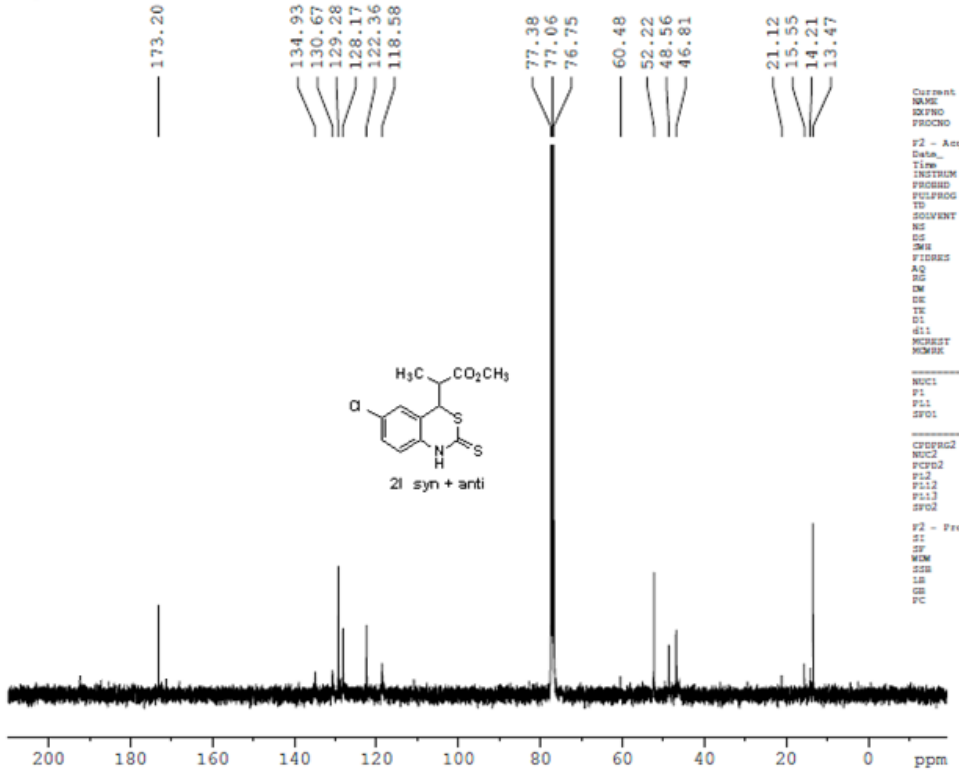
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz

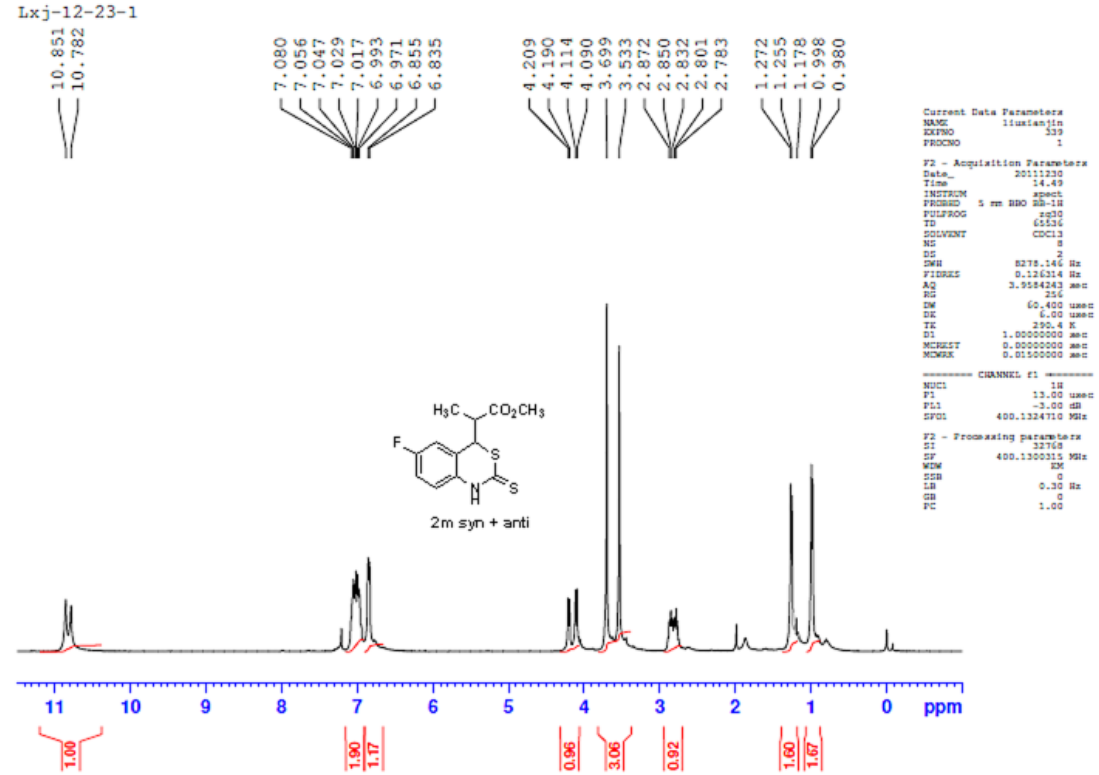
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

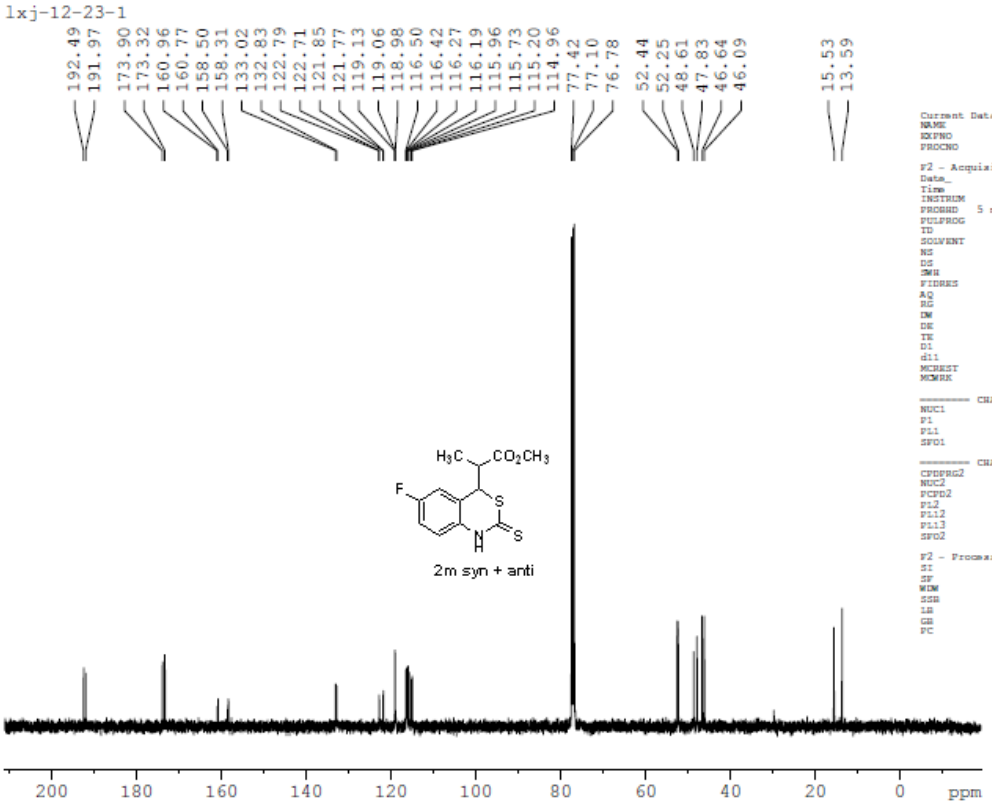
Lxj-12-17-2



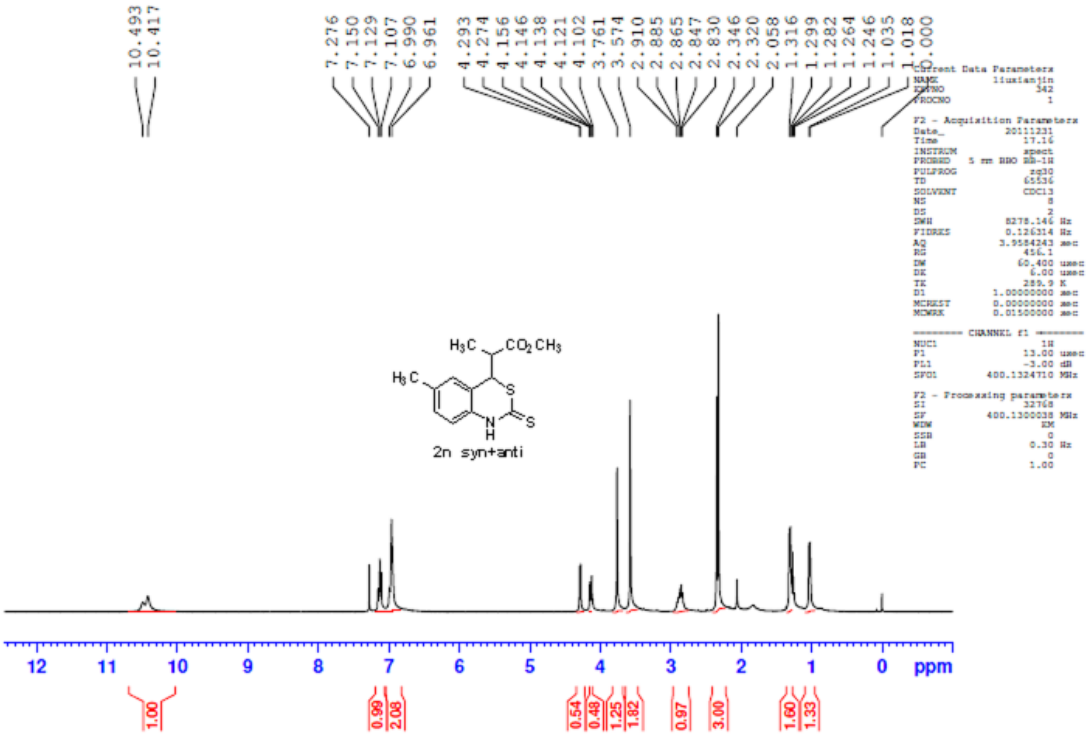
lxj-12-17-2



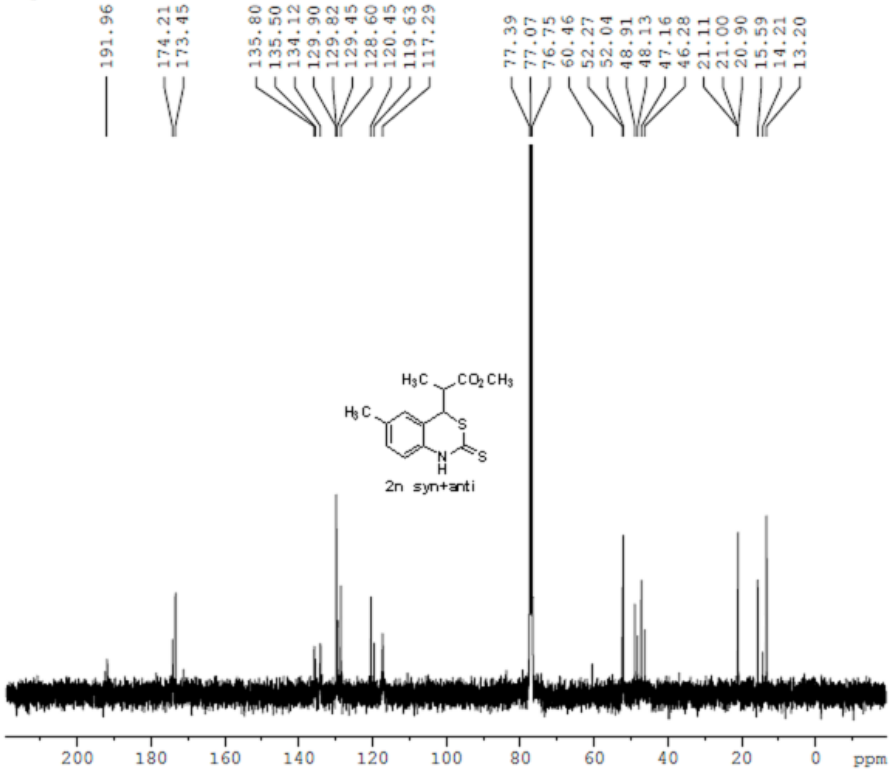

Lxj-12-23-1
10.851
10.782
7.080
7.056
7.047
7.029
7.017
6.993
6.971
6.855
6.835
4.209
4.190
4.114
4.090
3.699
3.533
2.872
2.850
2.832
2.801
2.783
1.272
1.255
1.178
0.998
0.980
2m syn + anti
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.90
1.17
0.96
3.06
0.92
1.60
1.67

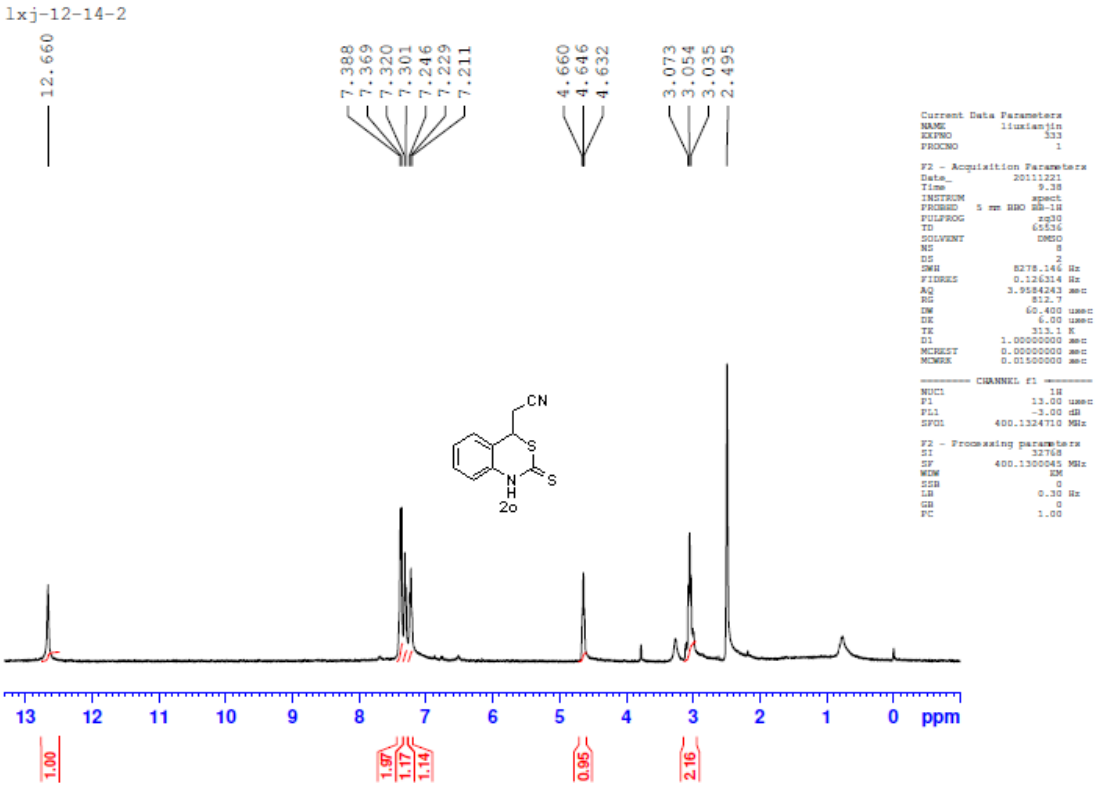

lxj-12-23-1
192.49
191.97
173.90
173.32
160.96
160.77
158.50
158.31
133.02
132.83
122.79
122.71
121.85
121.77
119.13
119.06
118.98
116.50
116.42
116.27
116.19
115.96
115.73
115.20
114.96
77.42
77.10
76.78
52.44
52.25
48.61
47.83
46.64
46.09
15.53
13.59
2m syn + anti
200
180
160
140
120
100
80
60
40
20
0
ppm

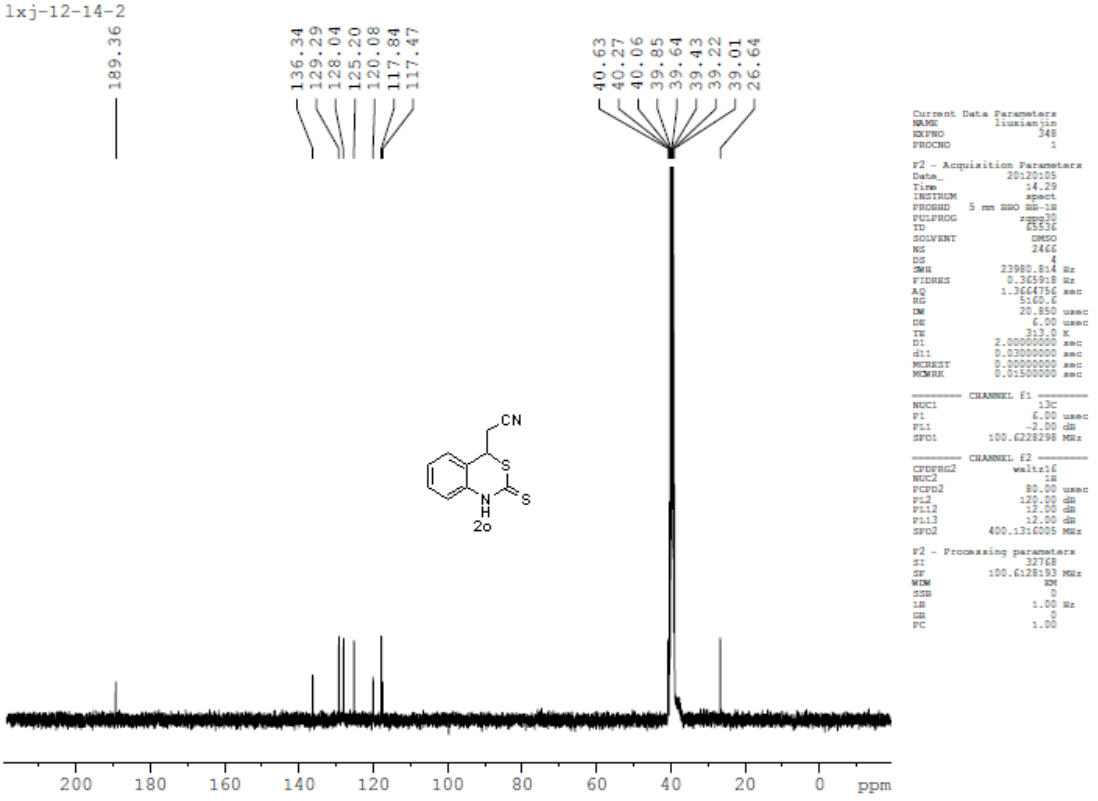
lxj-12-14-1

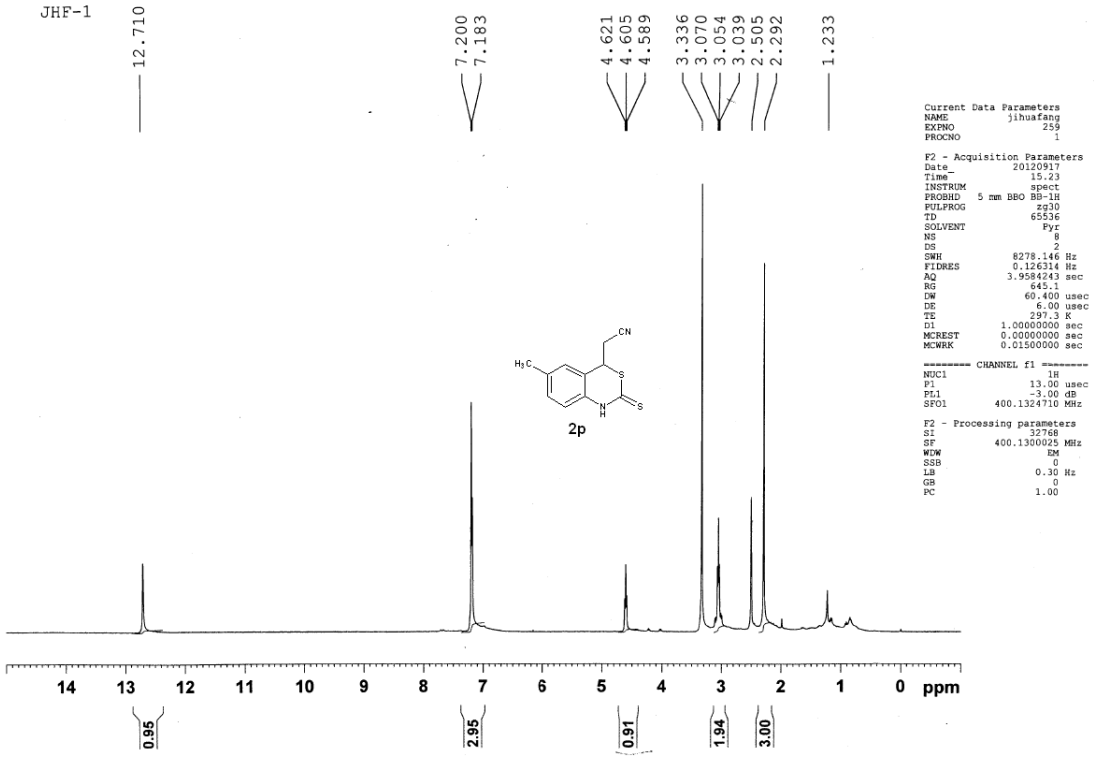


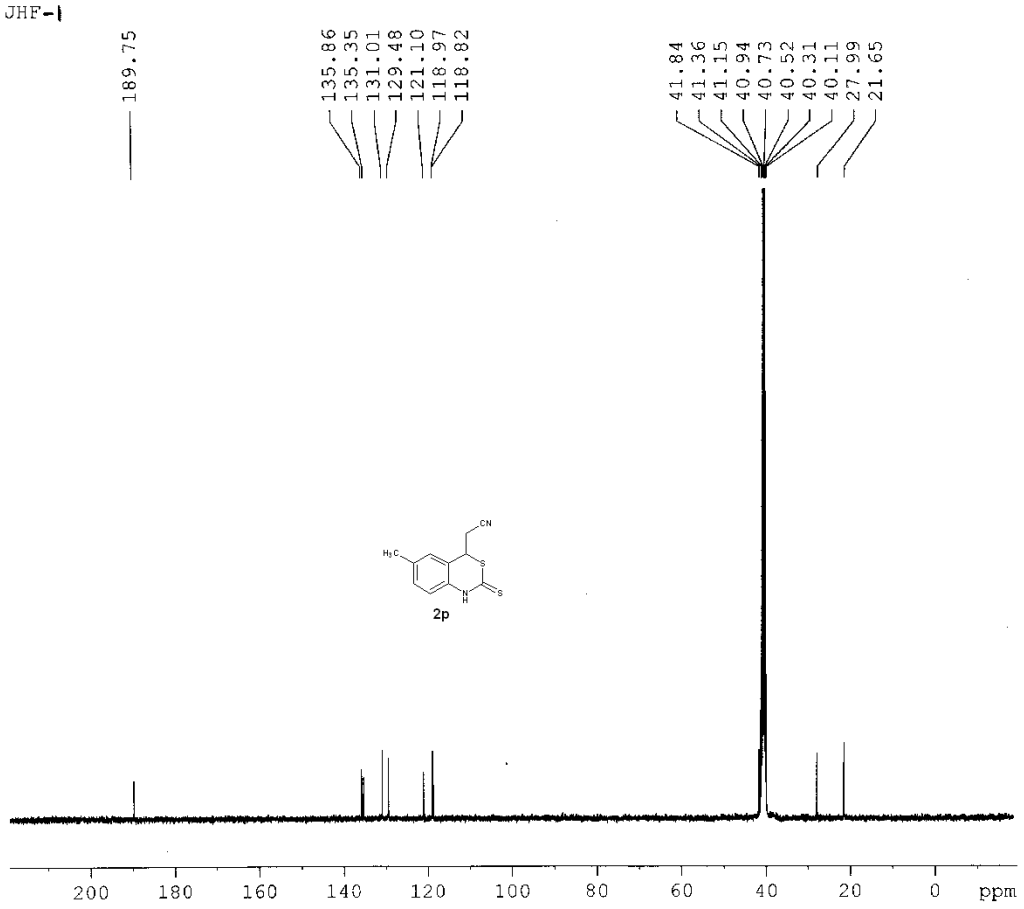
lxj-12-14-1

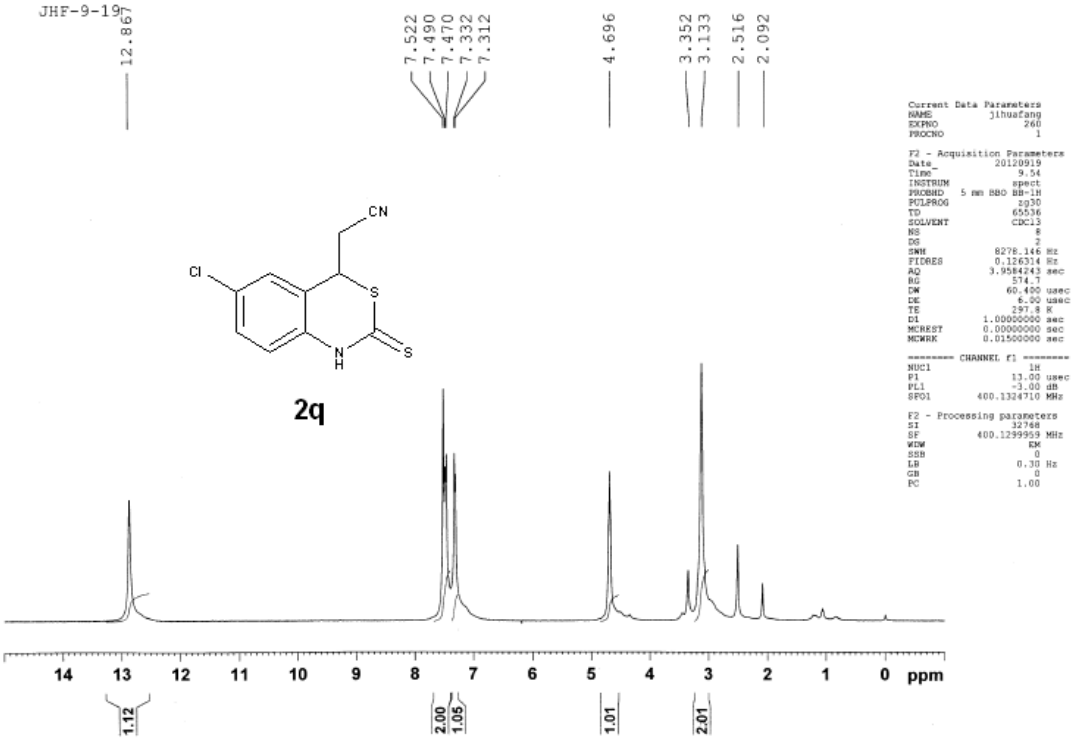



lxj-12-14-2
12.660
7.388
7.369
7.320
7.301
7.246
7.229
7.211
4.660
4.646
4.632
3.073
3.054
3.035
2.495
CN
S
N
H
S
2o
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.97
1.17
1.14
0.95
2.16

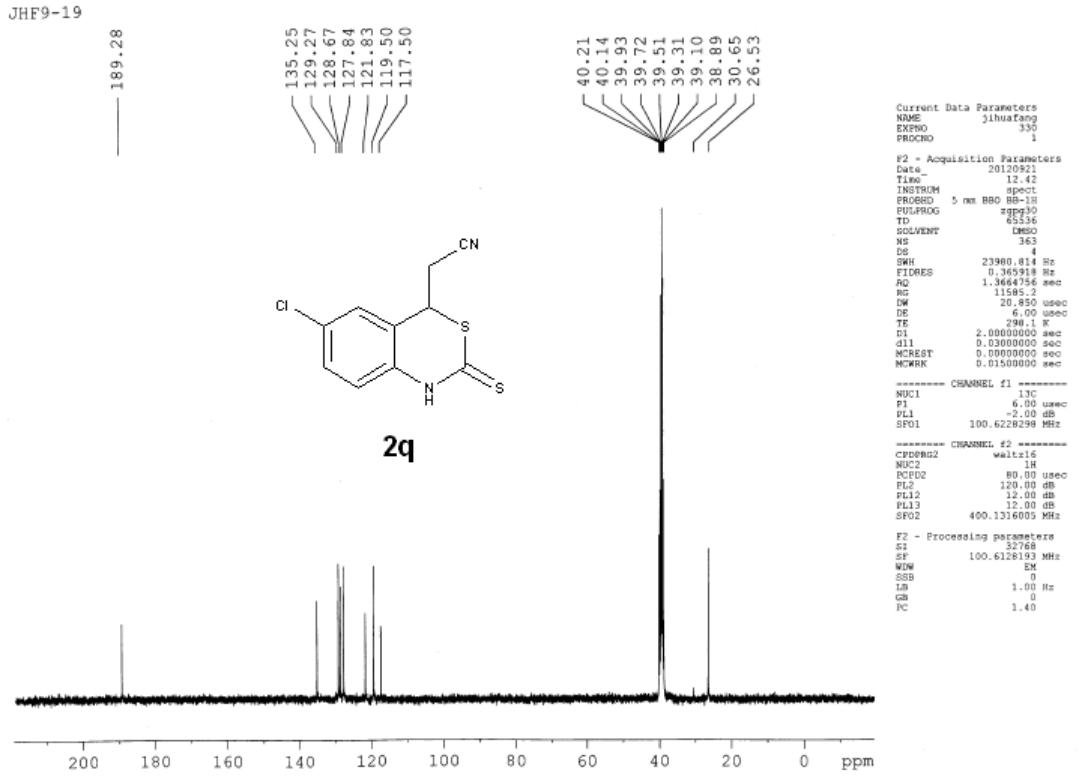

lxj-12-14-2
189.36
136.34
129.29
128.04
125.20
120.08
117.84
117.47
40.63
40.27
40.06
39.85
39.64
39.43
39.22
39.01
26.64
CN
S
N
H
S
2o
200
180
160
140
120
100
80
60
40
20
0
ppm


JHF-1
12.710
7.200
7.183
4.621
4.605
4.589
3.336
3.070
3.054
3.039
2.505
2.292
1.233
Current Data Parameters
NAME jihuafang
EXPNO 259
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120917
Time_ 15.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT Pyr
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 645.1
DW 60.400 usec
DE 6.00 usec
TE 297.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2p
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.95
2.95
0.91
1.94
3.00

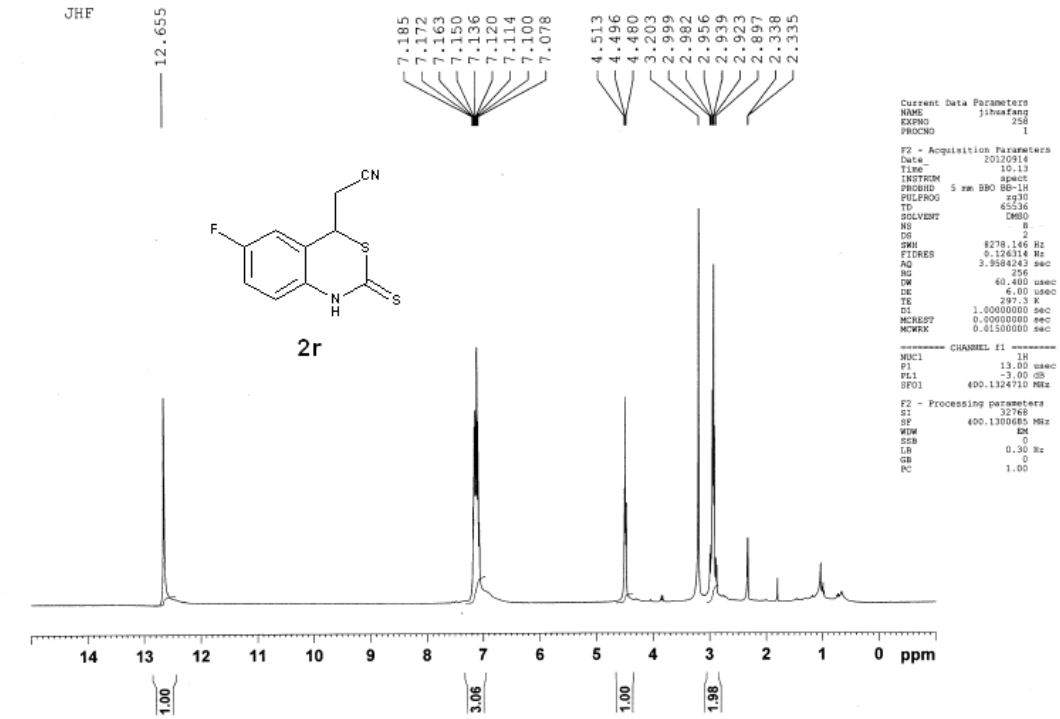

JHF-1
189.75
135.86
135.35
131.01
129.48
121.10
118.97
118.82
41.84
41.36
41.15
40.94
40.73
40.52
40.31
40.11
27.99
21.65
2p
200 180 160 140 120 100 80 60 40 20 0 ppm

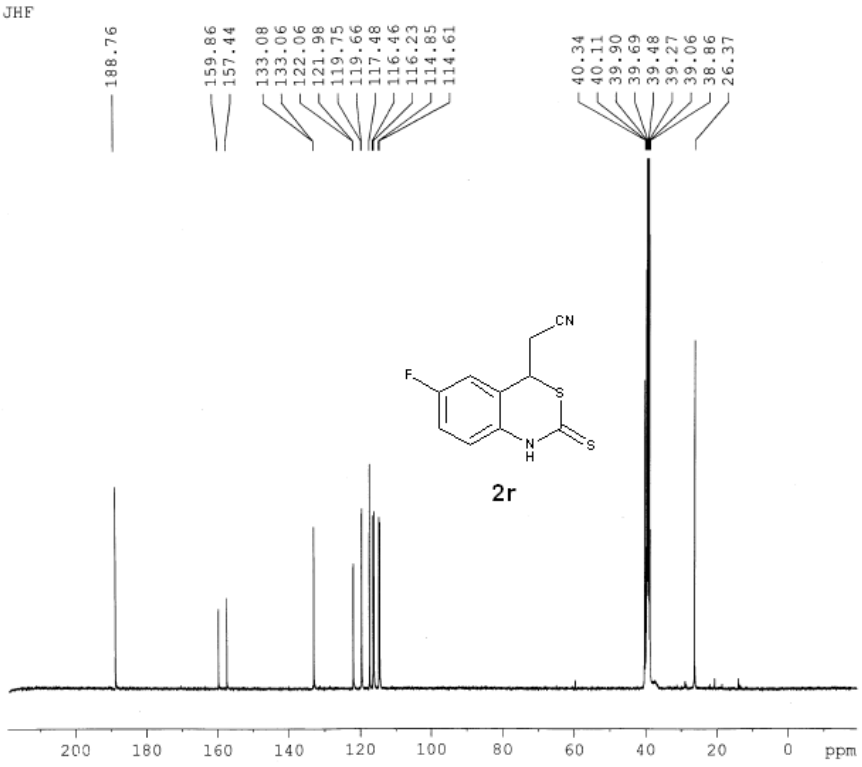


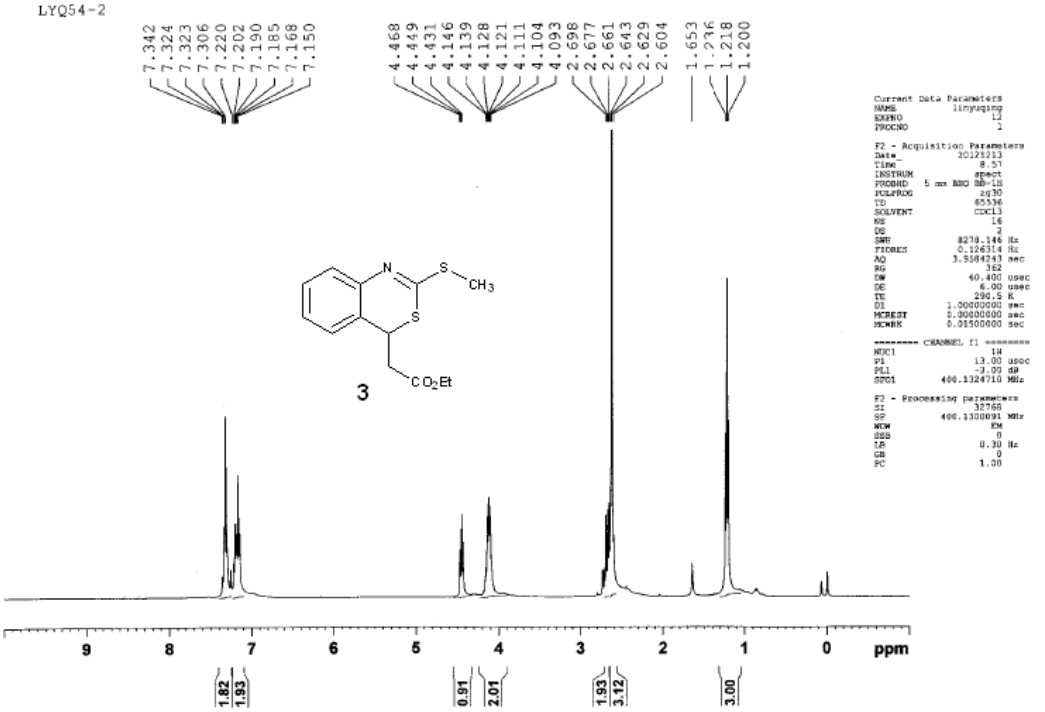

```
Current Data Parameters
NAME                  jihuafang
EXPNO                       260
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120919
Time                       9.54
INSTRUM                    spect
PROBHD   5 mm BBO BB-1H
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                            8
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                         574.7
DW                        60.400 usec
DE                         6.00 usec
TE                        297.8 K
D1                     1.00000000 sec
MCREST                 0.00000000 sec
MCWRK                  0.01500000 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                         13.00 usec
PL1                        -3.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                  400.1299959 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

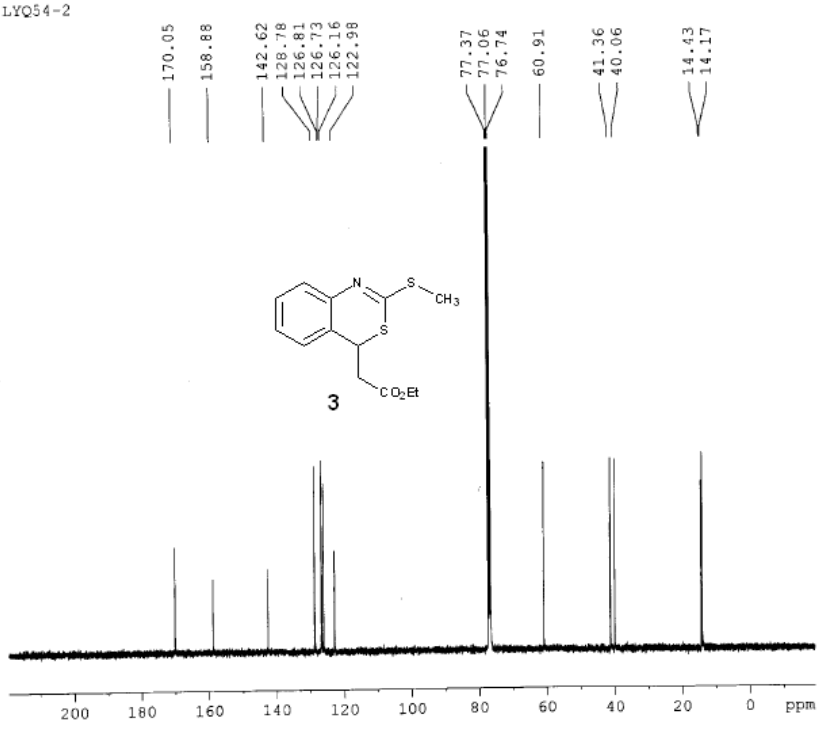



```
Current Data Parameters
NAME                  jihuafang
EXPNO                       330
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20120921
Time                      12.42
INSTRUM                    spect
PROBHD   5 mm BBO BB-1H
PULPROG                  zgpg30
TD                        65536
SOLVENT                    DMSO
NS                          363
DS                            4
SWH                   23980.814 Hz
FIDRES                 0.365918 Hz
AQ                     1.3664756 sec
RG                        11585.2
DW                        20.850 usec
DE                         6.00 usec
TE                        298.1 K
D1                     2.00000000 sec
d11                    0.03000000 sec
MCREST                 0.00000000 sec
MCWRK                  0.01500000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                         6.00 usec
PL1                        -2.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                     80.00 usec
PL2                       120.00 dB
PL12                       12.00 dB
PL13                       12.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                  100.6128193 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```


JHF
12.655
7.185
7.172
7.163
7.150
7.136
7.120
7.114
7.100
7.078
4.513
4.496
4.480
3.203
2.999
2.982
2.956
2.939
2.923
2.897
2.338
2.335
CN
F
S
N
H
S
2r
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
3.06
1.00
1.98


JHF
188.76
159.86
157.44
133.08
133.06
122.06
121.98
119.75
119.66
117.48
116.46
116.23
114.85
114.61
40.34
40.11
39.90
39.69
39.48
39.27
39.06
38.86
26.37
CN
F
S
N
H
S
2r
200 180 160 140 120 100 80 60 40 20 0 ppm


LYQ54-2
7.342
7.324
7.323
7.306
7.220
7.202
7.190
7.185
7.168
7.150
4.468
4.449
4.431
4.146
4.139
4.128
4.121
4.111
4.104
4.093
2.698
2.677
2.661
2.643
2.629
2.604
1.653
1.216
1.218
1.200
N
S
CH3
S
CO2Et
3
9
8
7
6
5
4
3
2
1
0
ppm
1.82
1.93
0.91
2.01
1.93
3.12
3.00


LYQ54-2
170.05
158.88
142.62
128.78
126.81
126.73
126.16
122.98
77.37
77.06
76.74
60.91
41.36
40.06
14.43
14.17
N
S
CH3
S
CO2Et
3
200
180
160
140
120
100
80
60
40
20
0
ppm