# Supporting Information

# Lewis-Acid-Promoted Cyclization Reaction: Synthesis of N3-Chloroethyl and N3-Thiocyanatoethyl Quinazolinones

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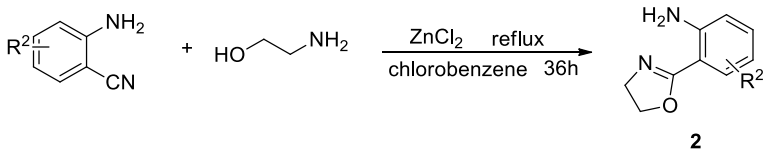
## Table of contents

## 1. General information

$^{1}H$ NMR, and $^{13}C$ NMR spectra were recorded on Mercury 400M or 600M in $CDCl_3$. All $^{1}H$ NMR and $^{13}C$ NMR chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. Copies of their $^{1}H$ NMR and $^{13}C$ NMR spectra were provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. All reactions were carried out in oven-dried glassware, unless otherwise noted. Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification.

## 2. Experimental section

### 2.1 General procedure for the synthesis of 2-(4,5-dihydrooxazol-2-yl)anilines.[1]



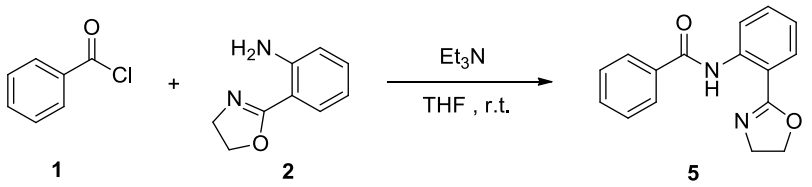

**2**

2-aminobenzonitrile (250.0 mmol) and $ZnCl_2$ (25.0 mmol) was added to a 500 mL three-necked flask, and then suspended in chlorobenzene (350 mL) under nitrogen. 2-aminoethanol (45 mL, 750.0 mmol) was added to the suspension via a syringe. The mixture was slowly heated to reflux until no gas was produced. After refluxing for 36 hours, the reaction mixture was cooled down to room temperature and the solvent was removed in a rotary

evaporator. $CH_2Cl_2$ (250 mL) was added to the residue and washed with saturated $NaHCO_3$ (150 mL) and $H_2O$ (150 mL). The aqueous fraction was extracted with $CH_2Cl_2$ (250 mL × 3). The combined organic phase was dried over $Na_2SO_4$, filtered and the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the compound **2** (72%).

## 2.2 General procedure for the synthesis of intermediates.

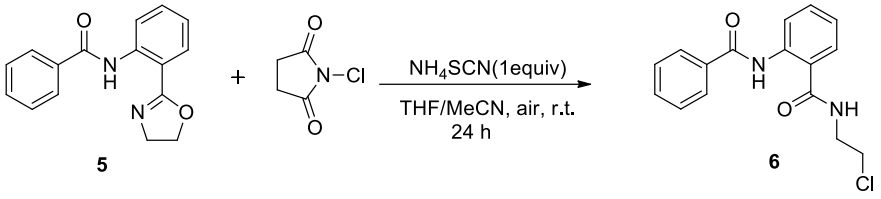
### 2.2.1 Synthesis of intermediate 5. [1]




1 2 5

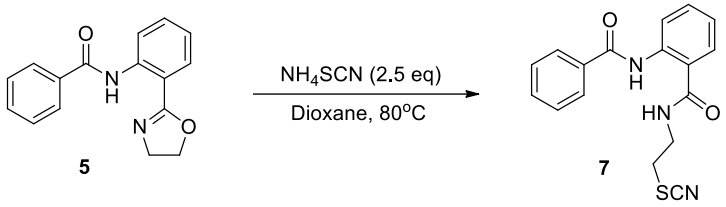
An acid chloride (5.0 mmol), prepared from the corresponding carboxylic acid and oxalyl chloride and 2-(4,5-dihydrooxazol-2-yl)aniline (5.0 mmol) were added to a 50 mL flask and then dissolved with THF (10 mL). $Et_3N$ (7.5 mmol) was taken to the vigorously stirred solution via a syringe. The reaction mixture was stirred at room temperature for 6 h and quenched with saturated $NaHCO_3 \cdot H_2O$ (100 mL) was added to the mixture and extracted with EtOAc (150 mL × 3). Combined organic phase was washed with saturated NaCl (aq) and dried over $Na_2SO_4$, and then filtered, the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the product **5** (82%).

### 2.2.2 Synthesis of intermediate 6. [2]




In a Schlenk tube, the corresponding aryl oxazolines **5** (0.2 mmol, 1.0 equiv), NCS (0.4 mmol, 2.0 equiv), $NH_4SCN$ (0.2 mmol, 1.0 equiv) and 2 mL THF/MeCN were added under air atmosphere. The resulting solution was stirred 24h at room temperature. Then the mixture was poured into water (10 mL) and extracted with ethyl acetate (20 mL × 3), the combined organic layers were dried over anhydrous $Na_2SO_4$, filtered and the solvent was evaporated under vacuum. The residue was purified by flash chromatography using EtOAc/hexanes (1:4) as eluent to afford the product **6** (96%).

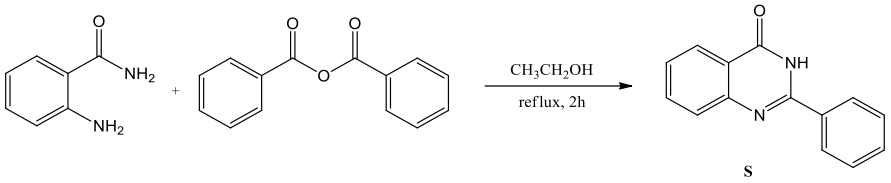
### 2.2.3 Synthesis of intermediate 7.




A mixture of **5** (1.0 equiv, 0.10 mmol), $NH_4SCN$ (0.25 mmol), Dioxane (1.0 mL), were stirred at 80 ℃ under air for 6h (TLC monitored). Upon completion of the reaction, the solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum *n*-hexane/ethyl acetate (4:1) to afford the desired **7** (97%). Liquid in 97% yield; $^1H$ NMR (600 MHz,$CDCl_3$) δ 11.97 (s, 1H), 8.67 (d,

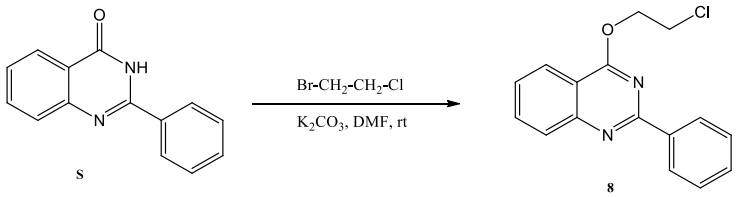
*J* = 8.3 Hz, 1H), 7.99 (d, *J* = 7.3 Hz, 2H), 7.56 (d, *J* = 7.0 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 21H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.44 (s, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 3.90 – 3.71 (m, 2H), 3.23 (t, *J* = 6.1 Hz, 2H). $^{13}$C NMR (151 MHz,$CDCl_3$) δ 169.7, 165.8, 139.7, 134.6, 132.8, 132.0, 128.8, 127.3, 127.1, 123.0, 121.6, 119.8, 111.8, 39.7, 33.1.

### 2.2.4 Synthesis of intermediate 8. [3]




S

Anthranilamide (36.7 mmol) was coupled with benzoic anhydride (41.1 mmol) in absolute ethanol (30 mL) at reflux for 2h. The reaction mixture was filtered to give a white solid, which was purified from 1 N aqueous NaOH and followed by 2 N aqueous HCl to afford **S** (83%) as white crystals.



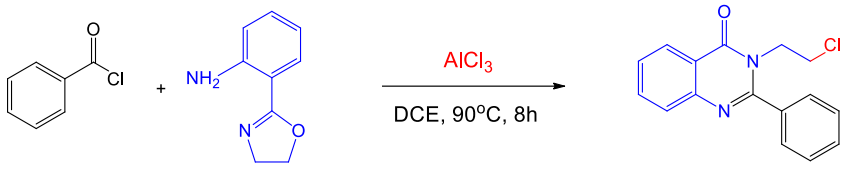

S 8

To a stirred mixture of **S** (4.5 mmol) and potassium carbonate (4.5 mmol) in DMF (10 mL) was added dropwise the appropriate bromochloroalkane (6.7 mmol) at room temperature for 24-48 h. The reaction was quenched by water (25 mL) and extracted with ethyl acetate (25 mL × 2). The combined organic extracts were washed with brine (25 mL × 3), dried by $Na_2SO_4$, and evaporated under reduced pressure. The residue was then

purified by column chromatograph over silica gel eluting with ethyl acetate/*n*-hexane = 1/4 to afford the desired **8** (70%).

## 2.3 Optimization of reaction conditions.

### 2.3.1 The reaction for the synthesis of N3-chloroethyl quinazolinones.[a]

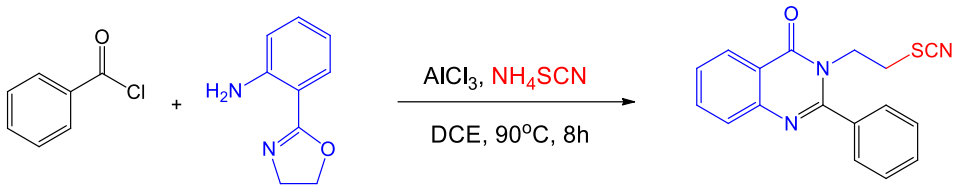



**1a** **2a** **3a**

| Entry | T (°C) | Acid (equiv) | Solvent | Yield(%)[b] |
|---|---|---|---|---|
| 1 | 120 | $AlCl_3$ (2.0) | DCE | 62 |
| 2 | 110 | $AlCl_3$ (2.0) | DCE | 71 |
| 3 | 100 | $AlCl_3$ (2.0) | DCE | 80 |
| **4** | **90** | **$AlCl_3$ (2.0)** | **DCE** | **86** |
| 5 | 80 | $AlCl_3$ (2.0) | DCE | 65 |
| 6 | 90 | $AlCl_3$ (2.5) | DCE | 82 |
| 7 | 90 | $AlCl_3$ (2.0) | DCE | 82[c] |
| 8 | 90 | $AlCl_3$ (2.0) | DCE | 84[d] |
| 9 | 90 | $AlCl_3$ (1.5) | DCE | 74 |
| 10 | 90 | $FeCl_3$ (2.0) | DCE | 49 |
| 11 | 90 | $BF_3{\cdot}O(C_2H_5)_2$ (2.0) | DCE | 0 |
| 12 | 90 | $BiCl_3$ (2.0) | DCE | Trace |
| 13 | 90 | $CoCl_2$ (2.0) | DCE | Trace |
| 14 | 90 | $NiCl_2$ (2.0) | DCE | 0 |
| 15 | 90 | HCl (2.0) | DCE | 0 |
| 16 | 90 | $H_2SO_4$ (2.0) | DCE | 0 |
| 17 | 90 | TfOH (2.0) | DCE | 0 |
| 18 | 90 | $AlCl_3$ (2.0) | Toluene | 49 |
| 19 | 90 | $AlCl_3$ (2.0) | Hexane | Trace |
| 20 | 90 | $AlCl_3$ (2.0) | Dioxane | 68 |
| 21 | 90 | $AlCl_3$ (2.0) | THF | 39 |
| 22 | 90 | $AlCl_3$ (2.0) | $CF_3CH_2OH$ | 47 |
| 23 | 90 | $AlCl_3$ (2.0) | DMA | Trace |
| 24 | 90 | $AlCl_3$ (2.0) | DMF | Trace |
| 25 | 90 | $AlCl_3$ (2.0) | $CH_3CN$ | 56 |
| 26 | 90 | $AlCl_3$ (2.0) | DMSO | Trace |

[a] Reaction conditions: benzoyl chloride **1a** (0.1 mmol), 2-(4,5-dihydrooxazol-2-yl)aniline **2a** (0.14 mmol) and acid in 1.0 mL solvent at 90 °C for 8 h. [b] isolated yield. [c] 6 h. [d] 10 h.

## 2.3.2 The reaction for the synthesis of N3-thiocyanatoethyl quinazolinones.[a]

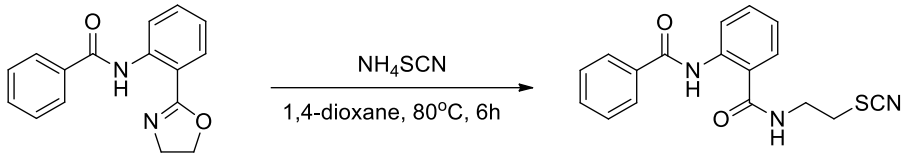



1a 2a 4a

| Entry | T (°C) | Acid (equiv) | Solvent | [SCN$^-$]( equiv) | Yield(%)[b] |
|---|---|---|---|---|---|
| 1 | 120 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 60 |
| 2 | 110 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 69 |
| 3 | 100 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 76 |
| **4** | **90** | **$AlCl_3$ (2.0)** | **DCE** | **$NH_4SCN$**(4.0) | **83** |
| 5 | 80 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 75 |
| 6 | 90 | $AlCl_3$ (1.5) | DCE | $NH_4SCN$(4.0) | 76 |
| 7 | 90 | $AlCl_3$ (2.5) | DCE | $NH_4SCN$(4.0) | 67 |
| 8 | 90 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 39[c] |
| 9 | 90 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 82[d] |
| 10 | 90 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(2.0) | 29 |
| 11 | 90 | $AlCl_3$ (2.0) | DCE | $NH_4SCN$(3.0) | 65 |
| 12 | 90 | $FeCl_3$ (2.0) | DCE | $NH_4SCN$(4.0) | 39 |
| 13 | 90 | $BF_3{\cdot}O(C_2H_5)_2$ (2.0) | DCE | $NH_4SCN$(4.0) | Trace |
| 14 | 90 | $CH_3COOH$ (2.0) | DCE | $NH_4SCN$(4.0) | 0 |
| 15 | 90 | PivOH (2.0) | DCE | $NH_4SCN$(4.0) | 0 |
| 16 | 90 | HCl (2.0) | DCE | $NH_4SCN$(4.0) | 19 |
| 17 | 90 | $H_2SO_4$ (2.0) | DCE | $NH_4SCN$(4.0) | 28 |
| 18 | 90 | - | DCE | $NH_4SCN$(4.0) | 0 |
| 19 | 90 | $AlCl_3$ (2.0) | THF | $NH_4SCN$(4.0) | 29 |
| 20 | 90 | $AlCl_3$ (2.0) | Toluene | $NH_4SCN$(4.0) | 32 |
| 21 | 90 | $AlCl_3$ (2.0) | $CH_3CN$ | $NH_4SCN$(4.0) | 19 |
| 22 | 90 | $AlCl_3$ (2.0) | Dioxane | $NH_4SCN$(4.0) | 45 |
| 23 | 90 | $AlCl_3$ (2.0) | DMSO | $NH_4SCN$(4.0) | 0 |
| 24 | 90 | $AlCl_3$ (2.0) | DME | $NH_4SCN$(4.0) | 17 |
| 25 | 90 | $AlCl_3$ (2.0) | DMF | $NH_4SCN$(4.0) | 0 |
| 26 | 90 | $AlCl_3$ (2.0) | DCE | KSCN(4.0) | 19 |
| 27 | 90 | $AlCl_3$ (2.0) | DCE | NaSCN(4.0) | 35 |

[a] Reaction conditions: benzoyl chloride **1a** (0.1 mmol), 2-(4,5-dihydrooxazol-2-yl)aniline **2a** (0.14 mmol), acid and [SCN$^-$] in 1.0 mL solvent at 90 °C for 8 h. [b] isolated yield. [c] 6 h. [d] 10 h.

### 2.3.3 The ring-opening reaction of amide-oxazoline 5. [a]




5 7

| Entry | Solvent | T (℃) | [$SCN^-$] (equiv) | Yield(%)[b] |
|---|---|---|---|---|
| 1 | Dioxane | 80 | $NH_4SCN$ (2.0) | 89 |
| **2** | **Dioxane** | **80** | **$NH_4SCN$ (2.5)** | **97** |
| 3 | Dioxane | 80 | $NH_4SCN$ (3.0) | 92 |
| 4 | DMSO | 80 | $NH_4SCN$ (2.5) | 0 |
| 5 | DMF | 80 | $NH_4SCN$ (2.5) | 0 |
| 6 | $CH_3CN$ | 80 | $NH_4SCN$ (2.5) | 80 |
| 7 | DCE | 80 | $NH_4SCN$ (2.5) | 65 |
| 8 | Toluene | 80 | $NH_4SCN$ (2.5) | 29 |
| 9 | Dioxane | 60 | $NH_4SCN$ (2.5) | 82 |
| 10 | Dioxane | 100 | $NH_4SCN$ (2.5) | 91 |

[a] Reaction conditions: amide-oxazoline **5** (0.1 mmol) and $NH_4SCN$ (0.25 mmol) in 1.0 mL solvent at 80 °C for 6 h. [b] isolated yield.

## 2.4 General procedure for synthesis of N3-chloroethyl quinazolinones.

To a 15 mL sealed tube containing a magnetic stir bar were added benzoyl chlorides **1** (1.0 equiv, 0.1 mmol), 2-(4,5-dihydrooxazol-2-yl)anilines **2** (1.4 equiv, 0.14 mmol) and $AlCl_3$ (2.0 equiv, 0.2 mmol) in DCE (1.0 mL). After stirred for 8 h at 90 °C, the mixture was concentrated under reduced pressure and purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate (v/v) = 4:1) to afford N3-chloroethyl quinazolinones **3**.

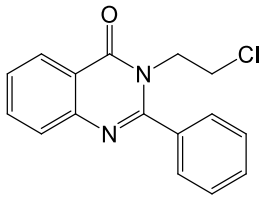
## 2.5 General procedure for synthesis of N3-thiocyanatoethyl quinazolinones.

To a 15 mL sealed tube containing a magnetic stir bar were added benzoyl chlorides **1** (1.0 equiv, 0.1 mmol), 2-(4,5-dihydrooxazol-2-yl)anilines **2** (1.4 equiv, 0.14 mmol) $NH_4SCN$ (4.0 equiv, 0.4 mmol), and $AlCl_3$ (2.0 equiv, 0.2 mmol) in DCE (1.0 mL). After stirred for 8 h at 90 °C, the mixture was concentrated under reduced pressure and purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate (v/v) = 2:1) to afford N3-thiocyanatoethyl quinazolinones **4**.

[1] M. Shang, S. Z. Sun, H. X. Dai, J. Q. Yu, *J Am Chem Soc.,* **2014**, *136*, 3354-3357.
[2] D. Guan, H. X. Luan, M. Patiguli, Q. J. Jiao, Q. Q. Yun, Q. S. Chen, C. J. Xu, X. B. Nie, F. P. Hu, G. S. Huang, *ChemistrySelect.,* **2019**, *4*, 6668-6671.
[3] G. S. Chen, S. Kalchar, C. W. Kuo, C. S. Chang, C. O. Usifoh, J. W. Chern, *J Org Chem.,* **2003**, *68*, 2502-2505.

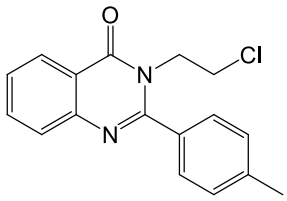
## 3 Characterization data of products.

### 3-(2-chloroethyl)-2-phenylquinazolin-4(3*H*)-one (3a)



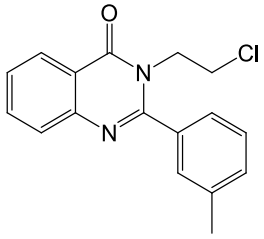

White solid in 86% yield; M.p. =125-128℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.90 – 7.69 (m, 2H), 7.66 – 7.45 (m, 6H), 4.36 (t, *J* = 6.6 Hz, 2H), 3.74 (t, *J* = 6.6 Hz, 2H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 156.0, 147.2, 135.1, 134.8, 130.1, 129.0, 128.2, 127.7, 127.3, 126.8, 120.73, 47.2, 40.4; HRMS (ESI) calcd for $C_{16}H_{13}ClN_2OH$: $[M+H]^+$ 285.0789, found:. 285.0792.

### 3-(2-chloroethyl)-2-(*p*-tolyl)quinazolin-4(3*H*)-one (3b)



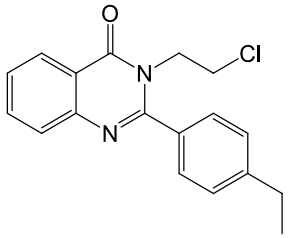

White solid in 82% yield; M.p. =100-103℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.7 Hz, 1H), 7.86 – 7.69 (m, 2H), 7.51 (m, *J* = 8.2, 6.6, 1.7 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 4.38 (t, *J* = 6.6 Hz, 2H), 3.73 (t, *J* = 6.6 Hz, 2H), 2.44 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.1, 147.2, 140.3, 134.7, 132.2, 129.6, 128.1, 127.7, 127.2, 126.8, 120.6, 47.1, 40.4, 21.5; HRMS (ESI) calcd for $C_{17}H_{15}ClN_2OH$: $[M+H]^+$ 299.0946, found:299.0949.

**3-(2-chloroethyl)-2-(*m*-tolyl)quinazolin-4(3*H*)-one (3c)**



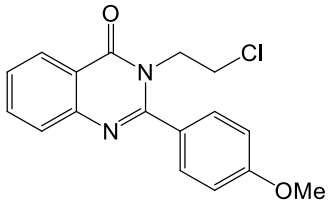

White solid in 85% yield; M.p. =127-129℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.25 (m, 1H), 7.84 – 7.71 (m, 2H), 7.57 – 7.48 (m, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.33 (dd, *J* = 16.3, 4.5 Hz, 3H), 4.36 (t, *J* = 6.6 Hz, 2H), 3.74 (t, *J* = 6.6 Hz, 2H), 2.44 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 156.2, 147.2, 139.0, 135.0, 134.7, 130.9, 128.8, 128.8, 127.7, 127.2, 126.8, 125.1, 120.7, 47.2, 40.4, 21.5; HRMS (ESI) calcd for $C_{17}H_{15}ClN_2OH$: $[M+H]^+$ 299.0946, found:299.0944.

**3-(2-chloroethyl)-2-(4-ethylphenyl)quinazolin-4(3*H*)-one (3d)**



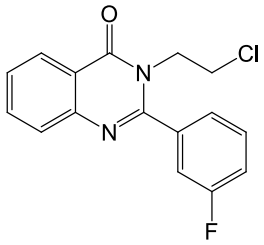

White solid in 80% yield; M.p. =105-107℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.2 Hz, 1H), 7.83 – 7.70 (m, 2H), 7.51 (m, *J* = 8.0, 1.7, 1.0 Hz, 1H), 7.45 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.39 (t, *J* = 6.6 Hz, 2H), 3.74 (t, *J* = 6.6 Hz, 2H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.42 – 1.19 (m, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.2, 147.2, 146.6, 134.7, 132.4, 128.5, 128.2, 127.7, 127.2, 126.8, 120.6, 47.2, 40.4, 28.8, 15.4; HRMS (ESI) calcd for $C_{18}H_{17}ClN_2OH$: $[M+H]^+$ 313.1102, found:313.1103.

**3-(2-chloroethyl)-2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (3e)**



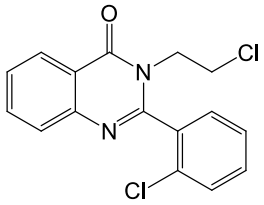

White solid in 84% yield; M.p. =105-108℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.45 – 8.19 (m, 1H), 7.92 – 7.67 (m, 2H), 7.61 – 7.42 (m, 3H), 7.15 – 6.96 (m, 2H), 4.41 (t, *J* = 6.6 Hz, 2H), 3.88 (s, 3H), 3.74 (t, *J* = 6.6 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.4, 160.9, 155.9, 147.2, 134.7, 129.8, 127.6, 127.5, 127.1, 126.8, 120.6, 114.4, 55.5, 47.2, 40.5; HRMS (ESI) calcd for $C_{17}H_{15}ClN_2O_2H$: $[M+H]^+$ 315.0895, found: 315.0890.

**3-(2-chloroethyl)-2-(3-fluorophenyl)quinazolin-4(3*H*)-one (3f)**



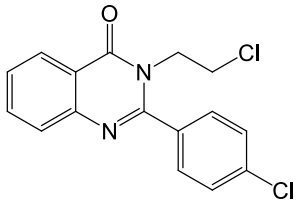

White liquid in 76% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.84 – 7.76 (m, 1H), 7.76 – 7.71 (m, 1H), 7.58 – 7.45 (m, 2H), 7.38 – 7.28 (m, 2H), 7.27 – 7.20 (m, 1H), 4.36 (t, *J* = 6.4 Hz, 2H), 3.76 (t, *J* = 6.4 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.9, 162.0, 161.4, 154.6, 147.0, 136.9 (d, *J* = 7.7 Hz), 134.9, 130.8 (d, *J* = 8.1 Hz), 127.6 (d, *J* = 13.9 Hz), 126.8, 124.1 (d, *J* = 3.2 Hz), 120.7, 117.3 (d, *J* = 21.0 Hz), 116.0 (d, *J* = 23.4 Hz), 47.3, 40.4; HRMS (ESI) calcd for $C_{16}H_{12}ClFN_2OH$: $[M+H]^+$ 303.0695, found:303.0695.

**3-(2-chloroethyl)-2-(2-chlorophenyl)quinazolin-4(3*H*)-one (3g)**



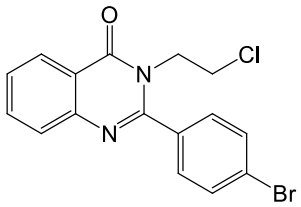

White liquid in 73% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.85 – 7.73 (m, 2H), 7.63 – 7.58 (m, 1H), 7.55 (m, *J* = 8.6, 5.3, 1.5 Hz, 1H), 7.53 – 7.43 (m, 3H), 4.97 – 4.29 (m, 1H), 3.87 (m, *J* = 17.5, 11.7, 5.8 Hz, 2H), 3.77 – 3.53 (m, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.8, 153.3, 147.2, 134.8, 134.0, 132.4, 131.5, 131.0, 129.8, 127.8, 127.6, 127.5, 126.8, 121.0, 47.0, 40.4; HRMS (ESI) calcd for $C_{16}H_{12}Cl_2N_2OH$: $[M+H]^+$ 319.0400, found: 319.0397.

**3-(2-chloroethyl)-2-(4-chlorophenyl)quinazolin-4(3*H*)-one (3h)**



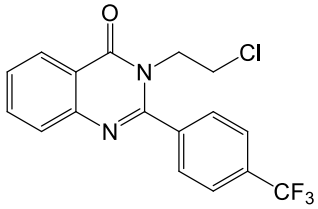

White solid in 77% yield; M.p. =127-129℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.85 – 7.76 (m, 1H), 7.76 – 7.72 (m, 1H), 7.62 – 7.44 (m, 5H), 4.36 (t, *J* = 6.3 Hz, 2H), 3.76 (t, *J* = 6.3 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.1, 155.0, 147.0, 136.4, 134.9, 133.5, 129.9, 129.3, 127.7, 127.5, 126.8, 120.7, 47.3, 40.5; HRMS (ESI) calcd for $C_{16}H_{12}Cl_2N_2OH$: $[M+H]^+$ 319.0400, found:319.0400.

**2-(4-bromophenyl)-3-(2-chloroethyl)quinazolin-4(3*H*)-one (3i)**



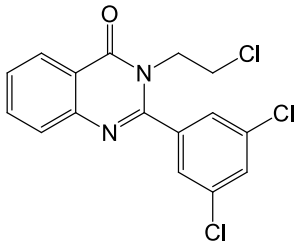

White solid in 71% yield; M.p. =107-109℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.33 (t, *J* = 7.4 Hz, 1H), 7.88 – 7.62 (m, 4H), 7.54 (dd, *J* = 14.7, 7.2 Hz, 1H), 7.44 (dd, *J* = 10.9, 4.4 Hz, 2H), 4.37 (q, *J* = 6.5 Hz, 2H), 3.77 (q, *J* = 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.1, 155.0, 147.0, 134.9, 134.0, 132.2, 130.1, 127.7, 127.5, 126.8, 124.6, 120.7, 47.3, 40.5; HRMS (ESI) calcd for $C_{16}H_{12}BrClN_2OH$: $[M+H]^+$ 362.9895, found:362.9899.

**3-(2-chloroethyl)-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (3j)**



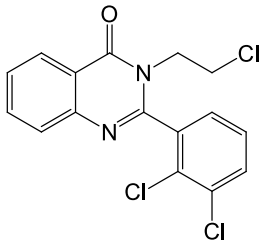

White solid in 60% yield; M.p. =127-129℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 7.9 Hz, 1H), 8.17 – 8.07 (m, 1H), 7.82 (dd, *J* = 8.1, 7.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.64 (dd, *J* = 3.4, 1.5 Hz, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 4.35 (t, *J* = 6.2 Hz, 1H), 3.81 (t, *J* = 6.2 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.1, 154.8, 147.0, 144.9, 135.4, 134.9, 130.3, 129.3, 127.7 (d, *J* = 7.3 Hz), 127.1, 126.3 (d, *J* = 103.4 Hz), 120.8, 96.7, 47.4, 40.5; HRMS (ESI) calcd for $C_{17}H_{12}ClF_3N_2OH$: $[M+H]^+$ 353.0663, found:353.0664.

**3-(2-chloroethyl)-2-(3,5-dichlorophenyl)quinazolin-4(3*H*)-one (3k)**




White solid in 68% yield; M.p. =130-132℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.87 – 7.77 (m, 1H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.54 (dt, *J* = 3.7, 1.4 Hz, 2H), 7.46 (d, *J* = 1.9 Hz, 2H), 4.36 (t, *J* = 6.1 Hz, 2H), 3.80 (t, *J* = 6.1 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.8, 153.3, 146.8, 137.6, 135.8, 135.0, 130.3, 127.8, 127.7, 127.1, 126.9, 120.7, 47.4, 40.7; HRMS (ESI) calcd for $C_{16}H_{11}Cl_3N_2OH$: $[M+H]^+$ 353.0010, found:353.0005.

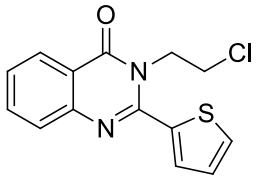
**3-(2-chloroethyl)-2-(2,3-dichlorophenyl)quinazolin-4(3*H*)-one (3l)**




White liquid in 60% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.81 (m, *J* = 8.3, 7.0, 1.4 Hz, 1H), 7.75 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.65 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.53 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 4.62 (m, *J* = 13.8, 5.8, 3.8 Hz, 1H), 3.92 (m, *J* = 10.9, 8.5, 5.8 Hz, 1H), 3.86 – 3.73 (m, 1H), 3.73 – 3.61 (m, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.7, 152.7, 147.1, 135.9, 134.9,

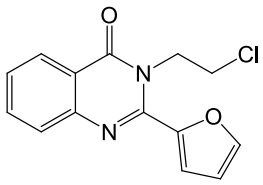
133.8, 132.1, 131.1, 129.3, 128.4, 128.1, 127.8, 126.9, 121.0, 47.3, 40.5; HRMS (ESI) calcd for $C_{16}H_{11}Cl_3N_2OH$: $[M+H]^+$ 353.0010, found:353.0011.

**3-(2-chloroethyl)-2-(thiophen-2-yl)quinazolin-4(3*H*)-one (3m)**




White solid in 85% yield; M.p. =121-124℃;$^1$H NMR (600 MHz, $CDCl_3$) δ 8.29 (d, *J* = 7.9 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 5.1 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 3.7 Hz, 1H), 7.18 (dd, *J* = 5.0, 3.7 Hz, 1H), 4.58 (t, *J* = 7.0 Hz, 2H), 3.85 (t, *J* = 7.0 Hz, 2H); $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.1, 149.6, 146.9, 136.1, 134.6, 129.4, 129.2, 127.6, 127.4, 127.3, 126.7, 120.3, 47.0, 40.1; HRMS (ESI) calcd for $C_{14}H_{11}ClN_2OSH$: $[M+H]^+$ 291.0354, found:. 291.0358.

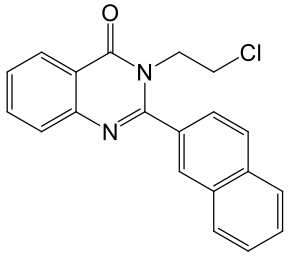
**3-(2-chloroethyl)-2-(furan-2-yl)quinazolin-4(3*H*)-one (3n)**




White solid in 90% yield; M.p. =135-137℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.82 – 7.69 (m, 2H), 7.66 (d, *J* = 0.8 Hz, 1H), 7.56 – 7.40 (m, 1H), 7.23 (d, *J* = 3.6 Hz, 1H), 6.63 (dd, *J* = 3.3, 1.8 Hz, 1H), 4.91 – 4.42 (m, 2H), 4.25 – 3.60 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 147.6, 147.3, 145.8, 144.8, 135.7, 127.7, 127.4, 126.9,

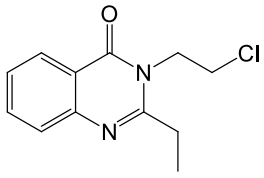
120.5, 116.0, 112.2, 46.7, 40.5; HRMS (ESI) calcd for $C_{14}H_{11}ClN_2O_2H$: $[M+H]^+$ 275.0582, found:. 275.0576.

**3-(2-chloroethyl)-2-(naphthalen-2-yl)quinazolin-4(3*H*)-one (3o)**




White solid in 85% yield; M.p. =109-111℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.31 (m, 1H), 8.07 (s, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.96 – 7.88 (m, 2H), 7.82 – 7.75 (m, 2H), 7.59 (m, *J* = 5.6, 4.1, 1.8 Hz, 3H), 7.53 m, *J* = 4.5, 4.0, 2.5 Hz, 1H), 4.42 (m, *J* = 6.4, 1.6 Hz, 2H), 3.75 (m, *J* = 6.4, 1.7 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.1, 147.2, 134.8, 133.7, 132.9, 132.4, 128.9, 128.6, 128.5, 127.9, 127.7, 127.6, 127.3, 127.2, 126.8, 124.9, 120.7, 47.3, 40.5; HRMS (ESI) calcd for $C_{20}H_{15}ClN_2OH$: $[M+H]^+$ 335.0946, found:335.0946.

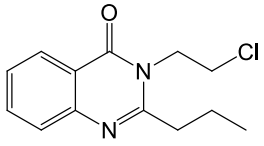
**3-(2-chloroethyl)-2-ethylquinazolin-4(3*H*)-one (3p)**




White solid in 67% yield; M.p. =120-122℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.73 (m, *J* = 8.4, 5.4, 1.5 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.50 – 7.39 (m, 1H), 4.44 (m, *J* = 6.4, 1.8 Hz, 2H), 4.04 – 3.68 (m, 2H), 2.97 (m, *J* = 7.3, 1.8 Hz, 2H), 1.41 (dd, *J* = 8.4, 6.4 Hz, 3H);

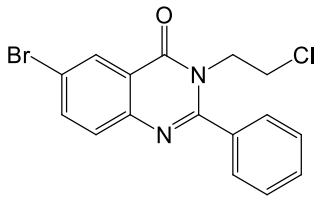
$^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 157.4, 147.3, 134.5, 127.2, 126.6, 126.6, 120.3, 45.2, 40.8, 28.7, 11.4; HRMS (ESI) calcd for $C_{12}H_{13}ClN_2OH$: $[M+H]^+$ 237.0789, found:. 237.0794.

**3-(2-chloroethyl)-2-propylquinazolin-4(3*H*)-one (3q)**



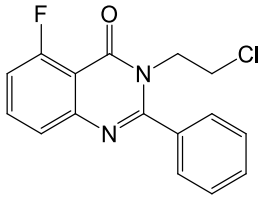

White solid in 59% yield; M.p. =129-131℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.31 – 8.16 (m, 1H), 7.73 (m, *J* = 8.2, 7.0, 1.3 Hz, 1H), 7.65 (d, *J* = 8.2 Hz, 1H), 7.53 – 7.38 (m, 1H), 4.44 (t, *J* = 6.5 Hz, 2H), 3.88 (t, *J* = 6.5 Hz, 2H), 3.05 – 2.73 (m, 2H), 1.88 (dd, *J* = 15.2, 7.6 Hz, 2H), 1.10 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.6, 147.3, 134.5, 127.1, 126.6, 126.6, 120.3, 45.4, 40.8, 37.3, 20.7, 13.9; HRMS (ESI) calcd for $C_{13}H_{15}ClN_2OH$: $[M+H]^+$ 251.0946, found: 251.0946.

**6-bromo-3-(2-chloroethyl)-2-phenylquinazolin-4(3*H*)-one (3r)**



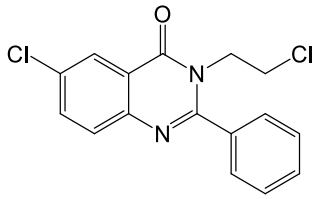

White solid in 85% yield; M.p. =170-172℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 2.3 Hz, 1H), 7.84 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.53 (d, *J* = 6.7 Hz, 5H), 4.37 (t, *J* = 6.5 Hz, 2H), 3.72 (t, *J* = 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.1, 156.4, 146.0, 137.9, 134.8, 130.3, 129.5, 129.3, 129.0, 128.2, 122.0, 120.8, 47.3, 40.3; HRMS (ESI) calcd for $C_{16}H_{12}BrClN_2OH$: $[M+H]^+$ 362.9895, found: 362.9899.

**3-(2-chloroethyl)-5-fluoro-2-phenylquinazolin-4(3*H*)-one (3s)**



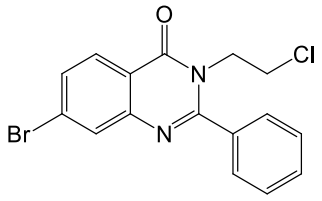

White liquid in 67% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.70 (m, *J* = 8.2, 5.5 Hz, 1H), 7.61 – 7.43 (m, 6H), 7.22 – 7.01 (m, 1H), 4.34 (t, *J* = 6.5 Hz, 2H), 3.76 (t, *J* = 6.4 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.6, 159.9, 159.3 (d, *J* = 3.9 Hz), 157.1, 149.1, 135.1 (d, *J* = 10.3 Hz), 134.8, 130.3, 129.0, 128.2, 123.6, 113.9 (d, *J* = 7.2 Hz), 113.7 (d, *J* = 7.3 Hz), 110.4 (d, *J* = 5.8 Hz), 47.1, 40.3 (d, *J* = 7.7 Hz); HRMS (ESI) calcd for $C_{16}H_{12}ClFN_2OH$: $[M+H]^+$ 303.0695, found: 303.0693.

**6-chloro-3-(2-chloroethyl)-2-phenylquinazolin-4(3*H*)-one (3t)**



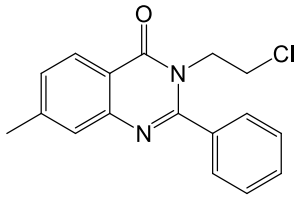

White solid in 84% yield; M.p. =147-149℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.33 – 8.21 (m, 1H), 7.77 – 7.63 (m, 2H), 7.55 (d, *J* = 15.2 Hz, 5H), 4.37 (t, *J* = 6.5 Hz, 2H), 3.72 (t, *J* = 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.2, 156.3, 145.6, 135.2, 134.8, 133.1, 130.3, 129.4, 129.0, 128.2, 126.1, 121.7, 47.2, 40.4; HRMS (ESI) calcd for $C_{16}H_{12}Cl_2N_2OH$: $[M+H]^+$ 319.0400, found: 319.0406.

**7-bromo-3-(2-chloroethyl)-2-phenylquinazolin-4(3*H*)-one (3u)**



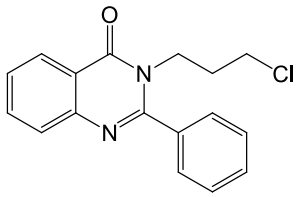

White solid in 81% yield; M.p. =166-168℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 1H), 7.92 (d, *J* = 1.8 Hz, 1H), 7.61 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.57 – 7.48 (m, 5H), 4.36 (t, *J* = 6.5 Hz, 2H), 3.72 (t, *J* = 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.8, 157.3, 148.1, 134.8, 130.7, 130.4, 130.3, 129.5, 129.0, 128.2, 128.2, 119.5, 47.2, 40.3; HRMS (ESI) calcd for $C_{16}H_{12}BrClN_2OH$: $[M+H]^+$ 362.9895, found: 362.9891.

**3-(2-chloroethyl)-7-methyl-2-phenylquinazolin-4(3*H*)-one (3v)**



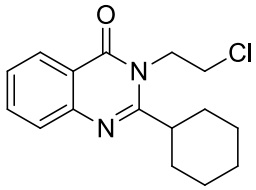

White solid in 79% yield; M.p. =145-147℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.50 (m, 6H), 7.34 (d, *J* = 8.1 Hz, 1H), 4.35 (t, *J* = 6.6 Hz, 2H), 3.73 (t, *J* = 6.6 Hz, 2H), 2.50 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.1, 156.0, 147.3, 145.8, 135.2, 130.0, 128.9, 128.9, 128.2, 127.4, 126.6, 118.3, 47.1, 40.4, 22.0; HRMS (ESI) calcd for $C_{17}H_{15}ClN_2OH$: $[M+H]^+$ 299.0946, found: 299.0946.

**3-(3-chloropropyl)-2-phenylquinazolin-4(3*H*)-one (3w)**



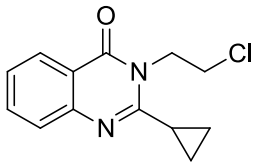
White solid in 87% yield; M.p. =133-135℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.84 – 7.71 (m, 2H), 7.56 – 7.47 (m, 6H), 4.40 – 3.98 (m, 2H), 3.44 (t, *J* = 6.3 Hz, 2H), 2.48 – 1.97 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.0, 147.2, 135.2, 134.5, 130.1, 129.0, 127.8, 127.6, 127.2, 126.7, 120.8, 44.0, 42.0, 31.4; HRMS (ESI) calcd for $C_{17}H_{15}ClN_2OH$: $[M+H]^+$ 299.0946, found:. 299.0940.

**3-(2-chloroethyl)-2-cyclohexylquinazolin-4(3*H*)-one (3x)**



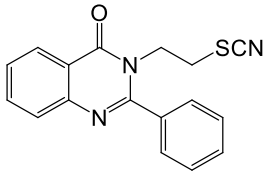
White solid in 71% yield; M.p. =130-131℃; $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.0 Hz, 1H), 7.77 – 7.68 (m, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.48 – 7.37 (m, 1H), 4.47 (t, *J* = 6.4 Hz, 2H), 3.87 (t, *J* = 6.4 Hz, 2H), 2.94 (m, *J* = 11.5, 7.3, 2.9 Hz, 1H), 1.91 (dd, *J* = 14.4, 7.1 Hz, 4H), 1.85 – 1.72 (m, 4H), 1.45 – 1.31 (m, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.4, 160.0, 147.4, 134.2, 127.2, 126.5, 126.3, 120.1, 44.4, 42.1, 41.1, 31.3, 26.0, 25.7. HRMS (ESI) calcd for $C_{16}H_{19}ClN_2OH$: $[M+H]^+$ 291.1259, found:. 291.1253.

**3-(2-chloroethyl)-2-cyclopropylquinazolin-4(3*H*)-one (3y)**



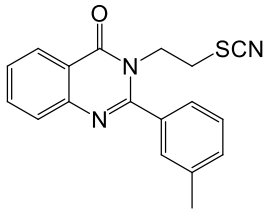

White solid in 54% yield; M.p. =120-121℃; $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 6.9 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 4.67 (t, *J* = 6.8 Hz, 2H), 3.92 (t, *J* = 6.8 Hz, 2H), 2.22 – 2.13 (m, 1H), 1.33 – 1.27 (m, 2H), 1.14 – 1.08 (m, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.2, 156.9, 147.3, 134.2, 126.9, 126.5, 126.2, 120.1, 45.0, 40.6, 14.2, 8.7. HRMS (ESI) calcd for $C_{13}H_{13}ClN_2OH$: $[M+H]^+$ 249.0789, found:. 249.0788.

**2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4a)**



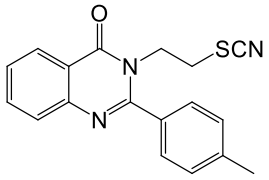

White solid in 83% yield; M.p. =188-190℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.9 Hz, 1H), 7.91 – 7.70 (m, 2H), 7.65 – 7.50 (m, 6H), 4.42 (dd, *J* = 7.6, 6.6 Hz, 2H), 3.21 (dd, *J* = 7.5, 6.7 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.4, 147.1, 135.0, 134.5, 130.6, 129.4, 127.9, 127.8, 127.5, 126.8, 120.5, 110.5, 45.5, 31.1; HRMS (ESI) calcd for $C_{17}H_{13}N_3OSH$: $[M+H]^+$ 308.0852, found:. 308.0855.

**3-(2-thiocyanatoethyl)-2-(m-tolyl)quinazolin-4(3*H*)-one (4b)**



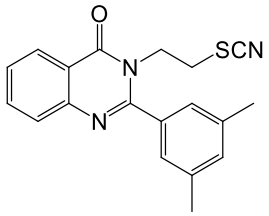

White solid in 72% yield; M.p. =153-156℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.35 – 8.27 (m, 1H), 7.86 – 7.71 (m, 2H), 7.53 (m, *J* = 8.1, 6.6, 1.5 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.41 – 7.34 (m, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 4.70 – 4.24 (m, 2H), 3.36 – 3.12 (m, 2H), 2.46 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.6, 147.1, 139.5, 135.0, 134.4, 131.3, 129.2, 128.4, 127.8, 127.5, 126.7, 124.8, 120.5, 110.5, 45.5, 31.1, 21.6; HRMS (ESI) calcd for $C_{18}H_{15}N_3OSH$: $[M+H]^+$ 322.1009, found:. 322.1009.

**3-(2-thiocyanatoethyl)-2-(p-tolyl)quinazolin-4(3*H*)-one (4c)**



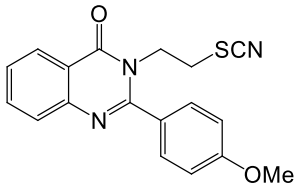

White solid in 75% yield; M.p. =120-123℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.25 (m, 1H), 7.89 – 7.71 (m, 2H), 7.52 (m, *J* = 6.9, 2.4 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 7.8 Hz, 2H), 4.92 – 4.25 (m, 2H), 3.34 – 3.07 (m, 2H), 2.45 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.6, 147.2, 140.9, 134.9, 131.6, 130.0, 129.9, 128.2, 127.3, 126.7, 120.5, 110.6, 45.5, 31.1, 21.5; HRMS (ESI) calcd for $C_{18}H_{15}N_3OSH$: $[M+H]^+$ 322.1009, found:. 322.1014.

**2-(3,5-dimethylphenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4d)**



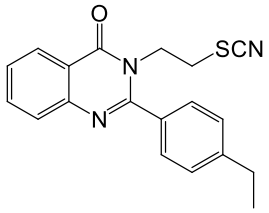

White solid in 73% yield; M.p. =143-147℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.85 – 7.72 (m, 2H), 7.62 – 7.48 (m, 1H), 7.19 (s, 1H), 7.12 (s, 2H), 4.75 – 4.18 (m, 2H), 3.42 – 3.07 (m, 2H), 2.41 (s, 6H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.9, 147.1, 139.3, 134.9, 134.3, 132.1, 127.8, 127.4, 126.7, 125.3, 120.5, 110.5, 45.5, 31.1, 21.4; HRMS (ESI) calcd for $C_{19}H_{17}N_3OSH$: $[M+H]^+$ 336.1165, found:. 336.1167.

**2-(4-methoxyphenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4e)**



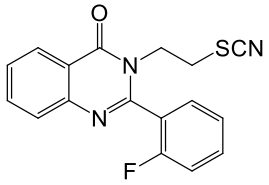

White solid in 76% yield; M.p. =151-153℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.93 – 7.67 (m, 2H), 7.63 – 7.38 (m, 3H), 7.18 – 6.99 (m, 2H), 4.46 (dd, *J* = 7.6, 6.6 Hz, 2H), 3.88 (s, 3H), 3.22 (dd, *J* = 7.7, 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.4, 161.3, 155.4, 147.2, 134.9, 129.6, 127.7, 127.3, 126.8, 126.7, 120.4, 114.8, 110.6, 55.6, 45.5, 31.2; HRMS (ESI) calcd for $C_{18}H_{15}N_3O_2SH$: $[M+H]^+$ 338.0958, found:. 338.0951.

**2-(4-ethylphenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4f)**



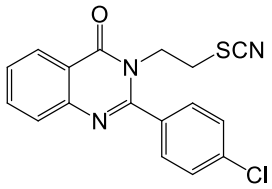

White solid in 82% yield; M.p. =107-109℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.90 – 7.68 (m, 2H), 7.60 – 7.49 (m, 1H), 7.46 (d, *J* = 8.1 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H), 4.70 – 4.24 (m, 2H), 3.35 – 3.11 (m, 2H), 2.74 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.6, 147.2, 147.1, 134.9, 131.8, 128.8, 127.9, 127.8, 127.4, 126.7, 120.5, 110.6, 45.5, 31.1, 28.9, 15.4; HRMS (ESI) calcd for $C_{19}H_{17}N_3OSH$: $[M+H]^+$ 336.1165, found:. 336.1164.

**2-(2-fluorophenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4g)**



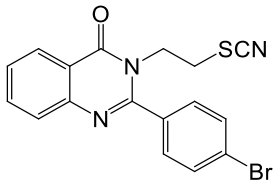

White solid in 63% yield; M.p. =130-132℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, *J* = 7.8, 0.8 Hz, 1H), 7.89 – 7.71 (m, 2H), 7.67 – 7.52 (m, 3H), 7.46 – 7.34 (m, 1H), 7.34 – 7.22 (m, 1H), 4.77 – 4.08 (m, 2H), 3.49 – 3.02 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.9, 160.3, 157.8, 150.9, 147.1, 135.0, 132.9, 130.5 (d, *J* = 16.7 Hz), 127.9, 126.8 (d, *J* = 26.3 Hz), 125.5 (d, *J* = 27.1 Hz), 122.6 (d, *J* = 15.9 Hz), 120.8, 117.1, 110.5, 45.7, 30.9; HRMS (ESI) calcd for $C_{17}H_{12}FN_3OSH$: $[M+H]^+$ 326.0758, found:. 326.0755.

**2-(4-chlorophenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3H)-one (4h)**



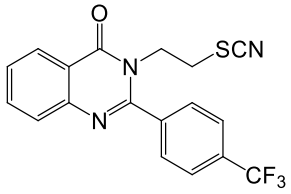

White solid in 61% yield; M.p. =161-164℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.27 (m, 1H), 7.89 – 7.78 (m, 1H), 7.74 (d, *J* = 7.7 Hz, 1H), 7.54 (m, *J* = 18.2, 6.2, 4.5 Hz, 5H), 4.95 – 4.18 (m, 2H), 3.76 – 2.92 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 154.3, 147.0, 136.9, 135.1, 132.9, 129.6, 129.4, 127.8, 126.9, 126.7, 120.5, 110.5, 45.6, 31.2; HRMS (ESI) calcd for $C_{17}H_{12}ClN_3OSH$: $[M+H]^+$ 342.0463, found:. 342.0463.

**2-(4-bromophenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4i)**



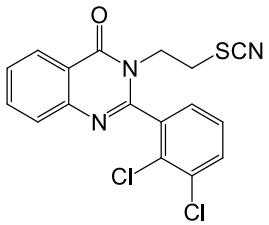

White solid in 61% yield; M.p. =168-170℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.85 – 7.77 (m, 1H), 7.77 – 7.68 (m, 3H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.37 (m, 2H), 4.64 – 4.09 (m, 2H), 3.50 – 2.91 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 154.4, 147.0, 135.1, 133.3, 132.6, 129.8, 129.6, 127.8, 126.9, 125.1, 120.5, 110.5, 45.6, 31.1; HRMS (ESI) calcd for $C_{17}H_{12}BrN_3OSH$: $[M+H]^+$ 385.9957, found:. 385.9950.

**3-(2-thiocyanatoethyl)-2-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (4j)**




White liquid in 55% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.89 – 7.80 (m, 3H), 7.76 (dd, *J* = 9.5, 5.9 Hz, 3H), 7.61 – 7.54 (m, 1H), 4.40 (t, *J* = 6.8 Hz, 2H), 3.25 (t, *J* = 6.8 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.1, 153.9, 146.9, 135.2, 132.0 (d, *J* = 33.3 Hz), 131.3, 130.0, 127.9 (d, *J* = 10.6 Hz), 127.4, 126.8, 125.3, 123.5 (d, *J* = 272.6 Hz), 120.6, 110.2, 45.6, 31.2; HRMS (ESI) calcd for $C_{18}H_{12}F_3N_3OSH$: $[M+H]^+$ 376.0726, found:. 376.0727.

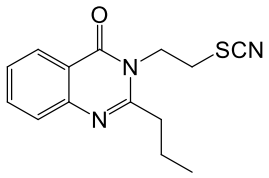
**2-(2,3-dichlorophenyl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4k)**




White liquid in 53% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.89 – 7.79 (m, 1H), 7.76 (d, *J* = 7.4 Hz, 1H), 7.69 (dd, *J* = 7.6, 2.1 Hz, 1H), 7.63 – 7.55 (m, 1H), 7.53 – 7.43 (m, 2H), 4.55 (m, *J* = 13.8, 7.9, 4.9 Hz, 1H), 4.09 – 3.82 (m, 1H), 3.44 – 3.09 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.8, 152.1, 147.0, 135.4, 135.1, 134.4, 132.6, 131.0, 128.8, 128.3, 128.1, 127.9, 126.9, 120.9, 110.5, 45.4, 30.9; HRMS (ESI)

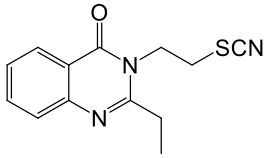
calcd for $C_{17}H_{11}Cl_2N_3OSH$: $[M+H]^+$ 376.0073, found:. 376.0070.

**2-propyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4l)**



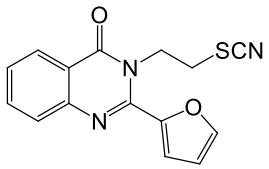

White solid in 82% yield; M.p. =127-129℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.32 – 8.17 (m, 1H), 7.87 – 7.71 (m, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 4.60 – 4.42 (m, 2H), 3.34 (dd, *J* = 8.1, 6.5 Hz, 2H), 2.87 (dd, *J* = 9.2, 6.2 Hz, 2H), 1.92 (dd, *J* = 15.2, 7.5 Hz, 2H), 1.13 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 155.9, 147.2, 134.7, 127.2, 126.8, 126.6, 120.1, 111.3, 43.7, 37.2, 31.0, 20.9, 13.8; HRMS (ESI) calcd for $C_{14}H_{15}N_3OSH$: $[M+H]^+$ 274.1009, found:. 274.1014.

**2-ethyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4m)**



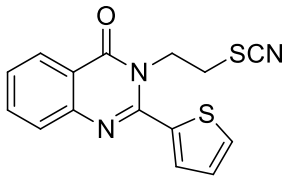

White solid in 83% yield; M.p. =138-141℃; $^1$H NMR (400 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.81 – 7.72 (m, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.50 – 7.40 (m, 1H), 4.49 (dd, *J* = 8.0, 6.5 Hz, 2H), 3.62 – 3.18 (m, 2H), 2.93 (q, *J* = 7.3 Hz, 2H), 1.45 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.3, 156.6, 147.2, 134.7, 127.3, 126.8, 126.6, 120.2, 111.3, 43.5, 31.0, 28.5, 11.4; HRMS (ESI) calcd for $C_{13}H_{13}N_3OSH$: $[M+H]^+$ 260.0852, found:. 260.0852.

**2-(furan-2-yl)-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4n)**



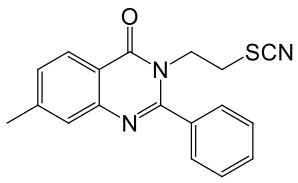

White solid in 80% yield; M.p. =134-136℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.76 (m, *J* = 16.6, 15.7, 4.7 Hz, 3H), 7.50 (m, *J* = 8.1, 7.0, 1.2 Hz, 1H), 7.37 – 7.30 (m, 1H), 6.64 (dd, *J* = 3.3, 1.8 Hz, 1H), 4.68 – 4.57 (m, 2H), 3.65 – 3.40 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.4, 147.4, 147.4, 145.5, 145.2, 134.9, 127.7, 127.4, 126.8, 120.3, 116.8, 112.3, 111.3, 45.9, 31.1; HRMS (ESI) calcd for $C_{15}H_{11}N_3O_2SH$: $[M+H]^+$ 298.0645, found:. 298.0646.

**3-(2-thiocyanatoethyl)-2-(thiophen-2-yl)quinazolin-4(3*H*)-one (4o)**



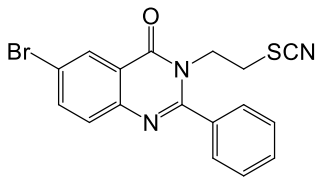

White solid in 57% yield; M.p. =131-133℃; $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.35 – 8.22 (m, 1H), 7.85 – 7.77 (m, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.63 – 7.58 (m, 1H), 7.52 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.21 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.84 – 4.33 (m, 2H), 3.92 – 3.05 (m, 2H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 161.2, 148.2, 145.9, 134.3, 133.9, 128.5, 128.4, 126.8, 126.7, 125.8, 119.2, 109.6, 44.6, 29.9. HRMS (ESI) calcd for $C_{15}H_{11}N_3OS_2H$: $[M+H]^+$ 314.0417, found:. 314.0411.

**7-methyl-2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4p)**



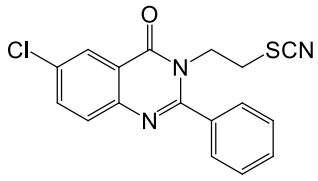

White solid in 65% yield; M.p. =140-143℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.1 Hz, 1H), 7.56 (m, *J* = 6.0, 4.0 Hz, 6H), 7.36 (d, *J* = 8.2 Hz, 1H), 4.40 (t, *J* = 7.1 Hz, 2H), 3.21 (dd, *J* = 7.5, 6.7 Hz, 2H), 2.51 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.2, 155.5, 147.2, 146.1, 134.6, 130.5, 129.4, 129.1, 127.9, 127.5, 126.6, 118.1, 110.5, 45.4, 31.1, 22.0; HRMS (ESI) calcd for $C_{18}H_{15}N_3OSH$: $[M+H]^+$ 322.1009, found:. 322.1004.

**6-bromo-2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4q)**



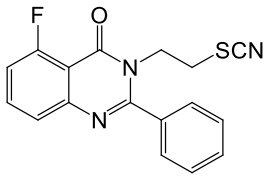

White solid in 84% yield; M.p. =140-143℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 2.3 Hz, 1H), 7.86 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.68 – 7.49 (m, 6H), 4.77 – 4.29 (m, 2H), 3.57 – 2.71 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.1, 155.8, 145.9, 138.2, 134.2, 130.7, 129.6, 129.4, 129.3, 127.9, 121.9, 121.1, 110.4, 45.7, 31.0; HRMS (ESI) calcd for $C_{17}H_{12}BrN_3OSH$: $[M+H]^+$ 385.9957, found:. 385.9959.

**6-chloro-2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4r)**



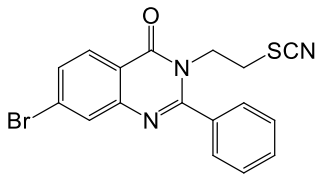

White solid in 83% yield; M.p. =185-188℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 2.3 Hz, 1H), 7.80 – 7.65 (m, 2H), 7.66 – 7.49 (m, 5H), 4.69 – 4.25 (m, 2H), 3.57 – 2.96 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.3, 155.6, 145.6, 135.4, 134.2, 133.4, 130.7, 129.5, 129.4, 127.9, 126.1, 121.5, 110.4, 45.7, 31.0; HRMS (ESI) calcd for $C_{17}H_{12}ClN_3OSH$: $[M+H]^+$ 342.0463, found:. 342.0457.

**5-fluoro-2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4s)**



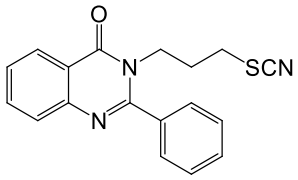

White liquid in 60% yield; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 7.72 (m, *J* = 8.2, 5.4 Hz, 1H), 7.64 – 7.51 (m, 6H), 7.23 – 7.12 (m, 1H), 4.79 – 4.31 (m, 2H), 3.80 – 3.09 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.5, 159.6 (d, *J* = 52.3 Hz), 156.5, 149.0, 135.4 (d, *J* = 10.4 Hz), 134.1, 130.8, 129.4, 127.8, 123.8 (d, *J* = 4.1 Hz), 114.0 (d, *J* = 20.8 Hz), 110.4, 110.3, 45.5, 30.9; HRMS (ESI) calcd for $C_{17}H_{12}FN_3OSH$: $[M+H]^+$ 326.0758, found:. 326.0759.

**7-bromo-2-phenyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4t)**



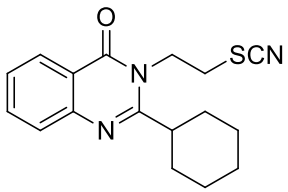

White solid in 75% yield; M.p. =145-148℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.6 Hz, 1H), 7.93 (d, *J* = 1.8 Hz, 1H), 7.77 – 7.46 (m, 6H), 4.71 – 4.14 (m, 2H), 3.20 (dd, *J* = 7.6, 6.5 Hz, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 161.8, 156.7, 148.0, 134.2, 130.9, 130.8, 130.6, 129.8, 129.4, 128.2, 127.8, 119.3, 110.4, 45.6, 31.0; HRMS (ESI) calcd for $C_{17}H_{12}BrN_3OSH$: $[M+H]^+$ 385.9957, found:. 385.9953.

**2-phenyl-3-(3-thiocyanatopropyl)quinazolin-4(3*H*)-one (4u)**

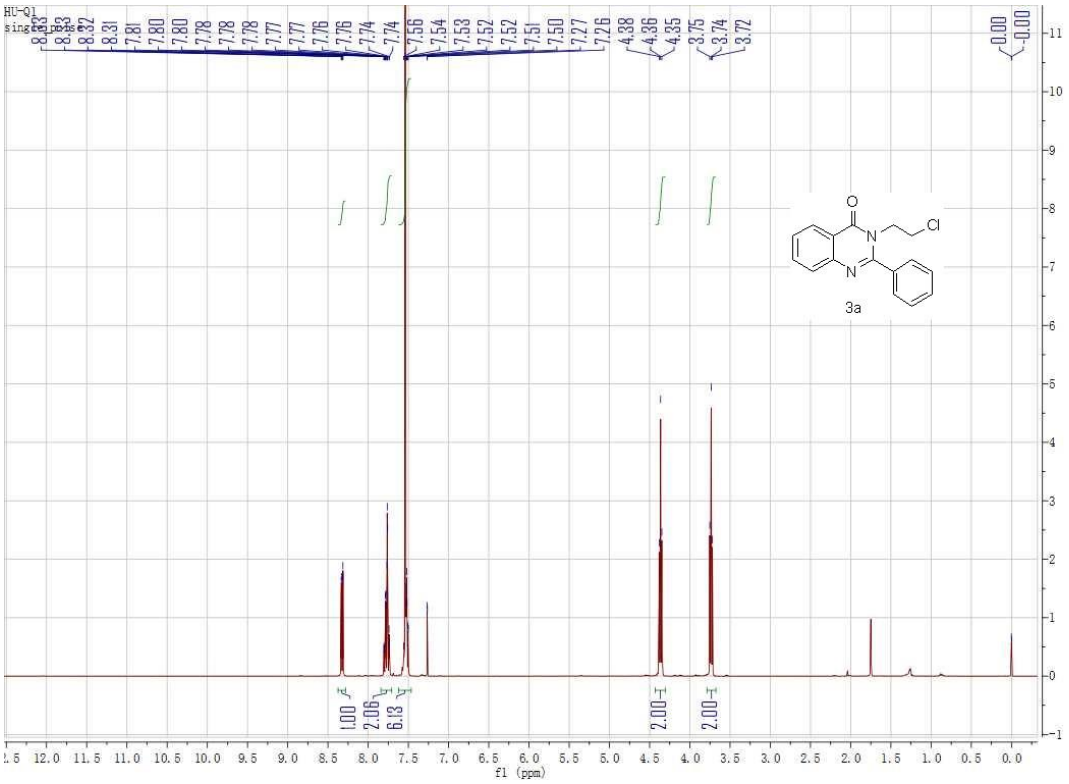


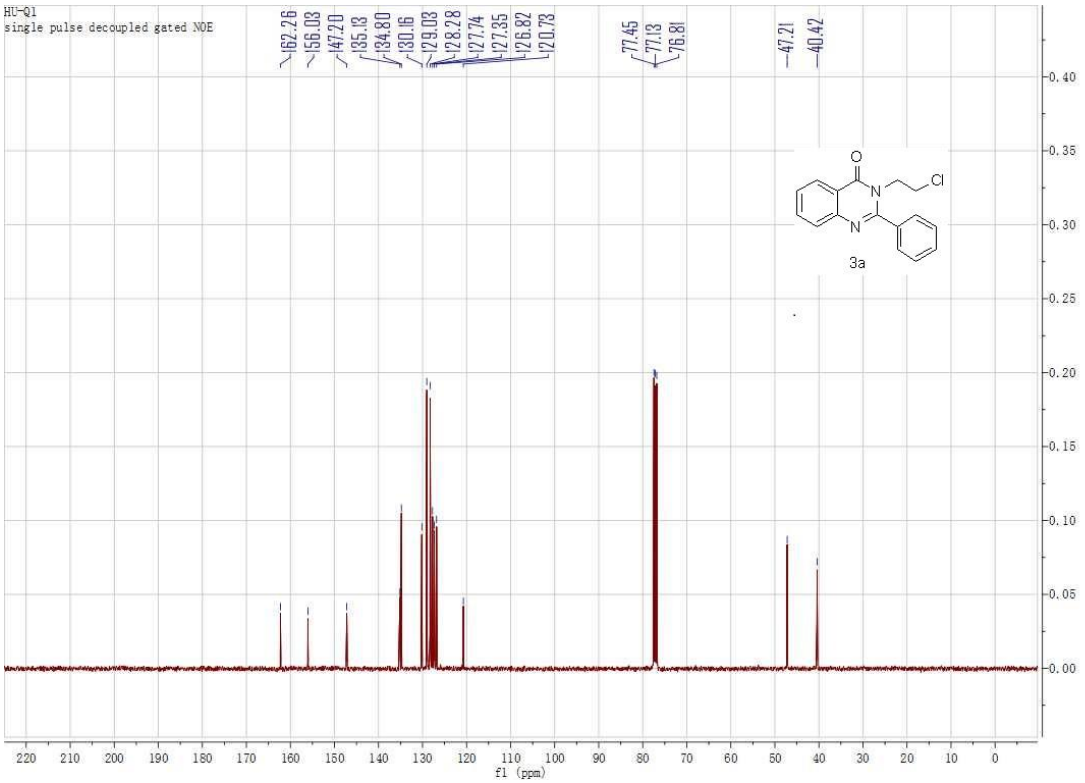

White solid in 85% yield; M.p. =153-155℃; $^{1}$H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.9 Hz, 1H), 7.89 – 7.68 (m, 2H), 7.62 – 7.39 (m, 6H), 4.56 – 3.72 (m, 2H), 2.88 (t, *J* = 6.9 Hz, 2H), 2.35 – 2.01 (m, 2H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.4, 155.7, 147.1, 135.0, 134.7, 130.3, 129.2, 127.7, 127.7, 127.4, 126.8, 120.7, 111.7, 43.8, 31.6, 29.2; HRMS (ESI) calcd for $C_{18}H_{15}N_3OSH$: $[M+H]^+$ 322.1009, found:. 322.1007.

**2-cyclohexyl-3-(2-thiocyanatoethyl)quinazolin-4(3*H*)-one (4v)**




White solid in 61% yield; M.p. =145-147℃; $^{1}$H NMR (600 MHz, $CDCl_3$) δ 8.27 – 8.17 (m, 1H), 7.80 – 7.70 (m, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 4.64 – 4.27 (m, 2H), 3.55 – 3.14 (m, 2H), 2.84 (tt, *J* = 11.4, 3.0 Hz, 1H), 2.00 – 1.87 (m, 4H), 1.87 – 1.75 (m, 3H), 1.51 (dtd, *J* = 13.2, 9.9, 3.1 Hz, 2H), 1.36 (ddt, *J* = 16.6, 13.1, 6.5 Hz, 1H). $^{13}$C NMR (151 MHz, $CDCl_3$) δ 162.4, 159.3, 147.3, 134.4, 127.3, 126.5, 126.4, 120.0, 111.2, 42.7, 42.1, 31.6, 31.4, 25.8, 25.6. HRMS (ESI) calcd for $C_{17}H_{19}N_3OSH$: $[M+H]^+$ 314.1322, found:. 314.1325.


HU-Q1
8.33
8.32
8.31
7.81
7.80
7.80
7.78
7.78
7.78
7.77
7.77
7.76
7.76
7.74
7.74
7.56
7.54
7.53
7.52
7.52
7.51
7.50
7.27
7.26
4.38
4.36
4.35
3.75
3.74
3.72
0.00
0.00
1.00
2.06
6.13
2.00
2.00
O
N
Cl
N
3a
fl (ppm)


HU-Q1
single pulse decoupled gated NOE
162.26
156.03
147.20
135.43
134.80
130.16
129.03
128.28
127.74
127.35
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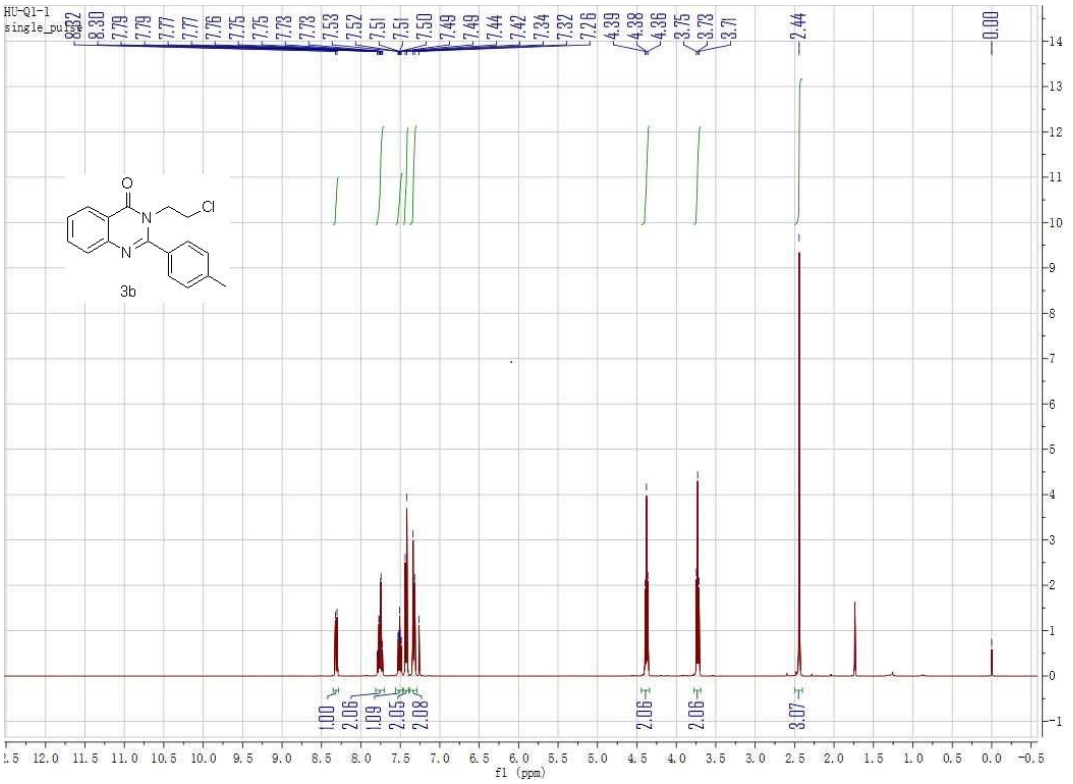
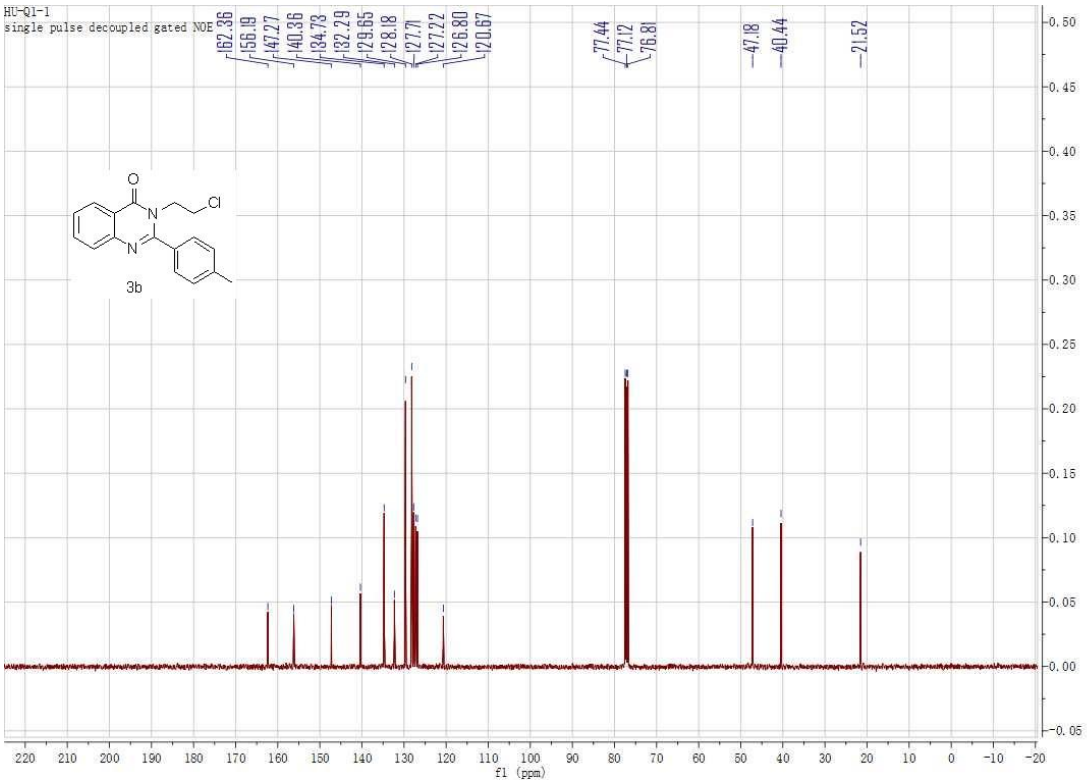
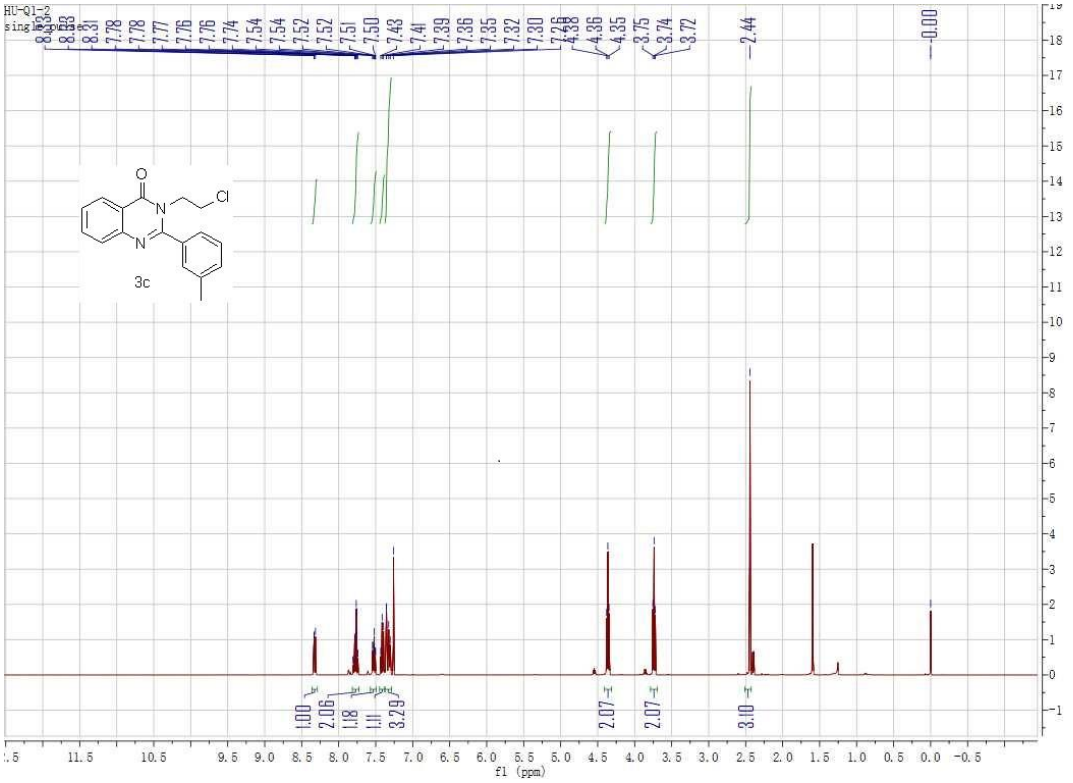
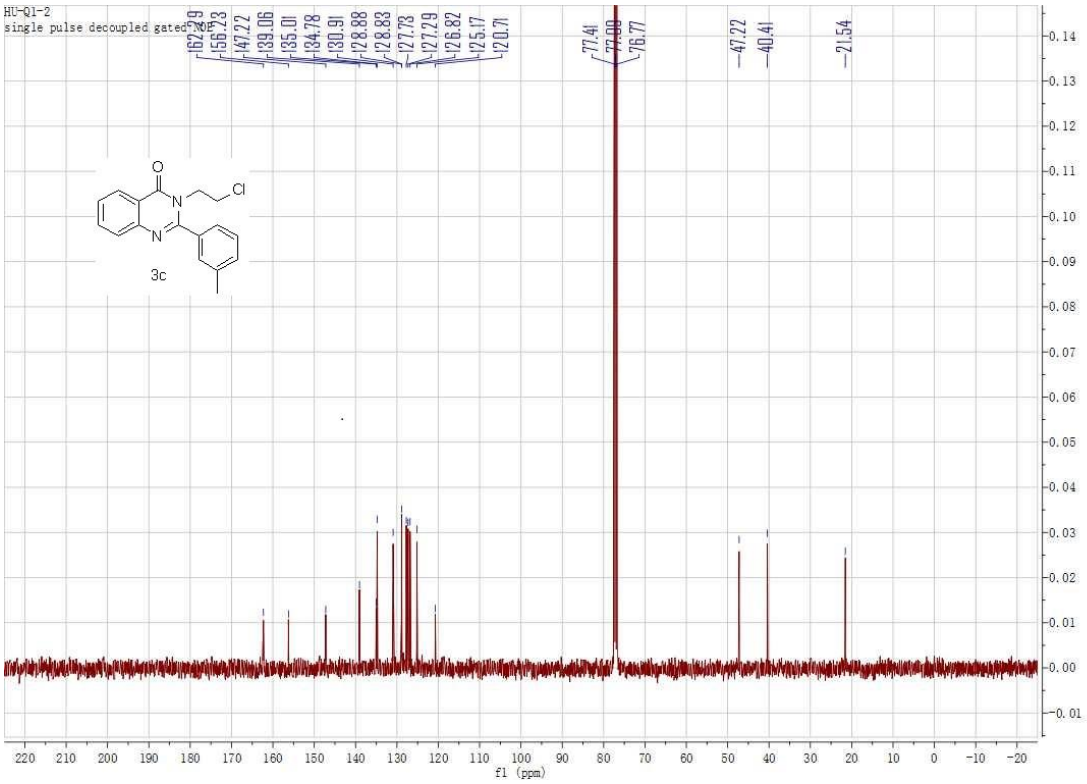
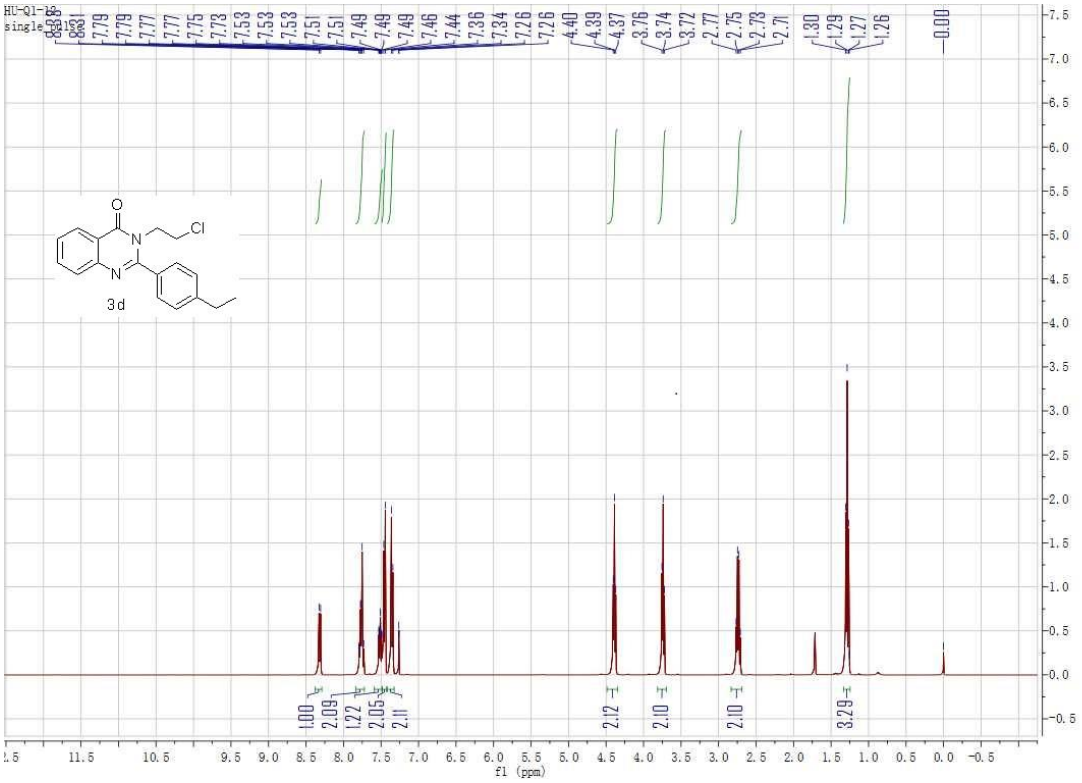
40.42
O
N
Cl
N
3a
fl (ppm)

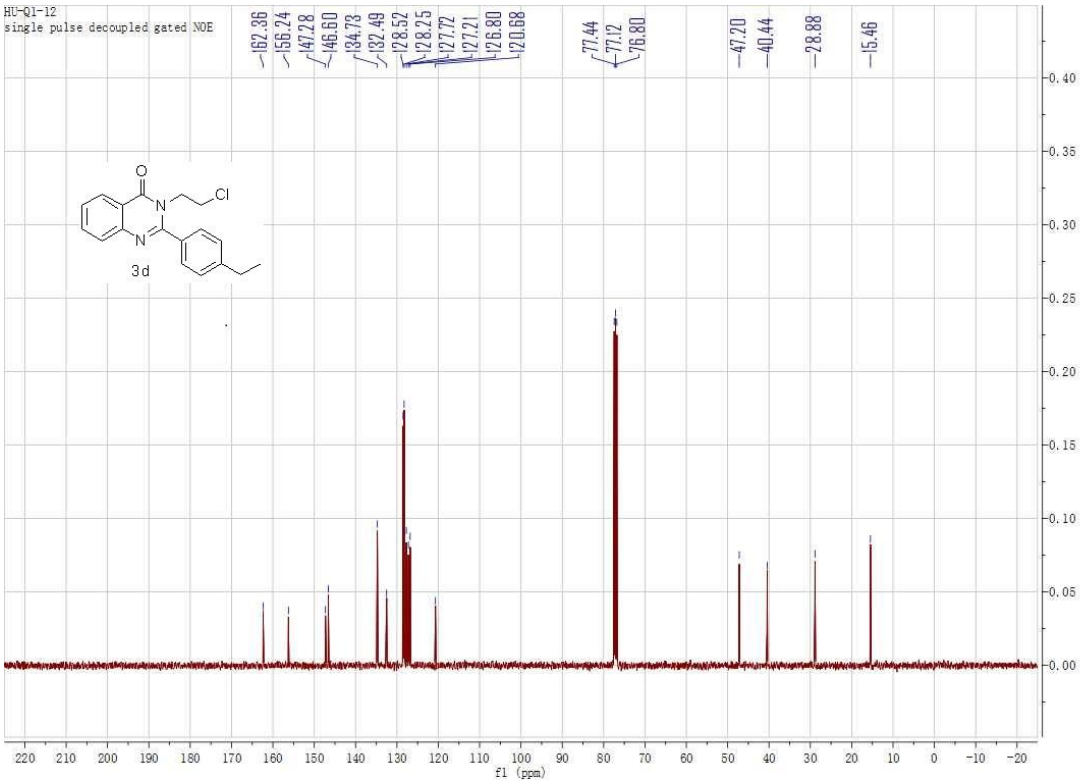

HU-Q1-1
single_pu
8.32
8.30
7.79
7.79
7.77
7.77
7.76
7.75
7.75
7.73
7.73
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.44
7.42
7.34
7.32
7.26
4.39
4.38
4.36
3.75
3.73
3.71
2.44
0.00
3b
1.00
2.06
1.09
2.05
2.08
2.06
2.06
8.07
f1 (ppm)

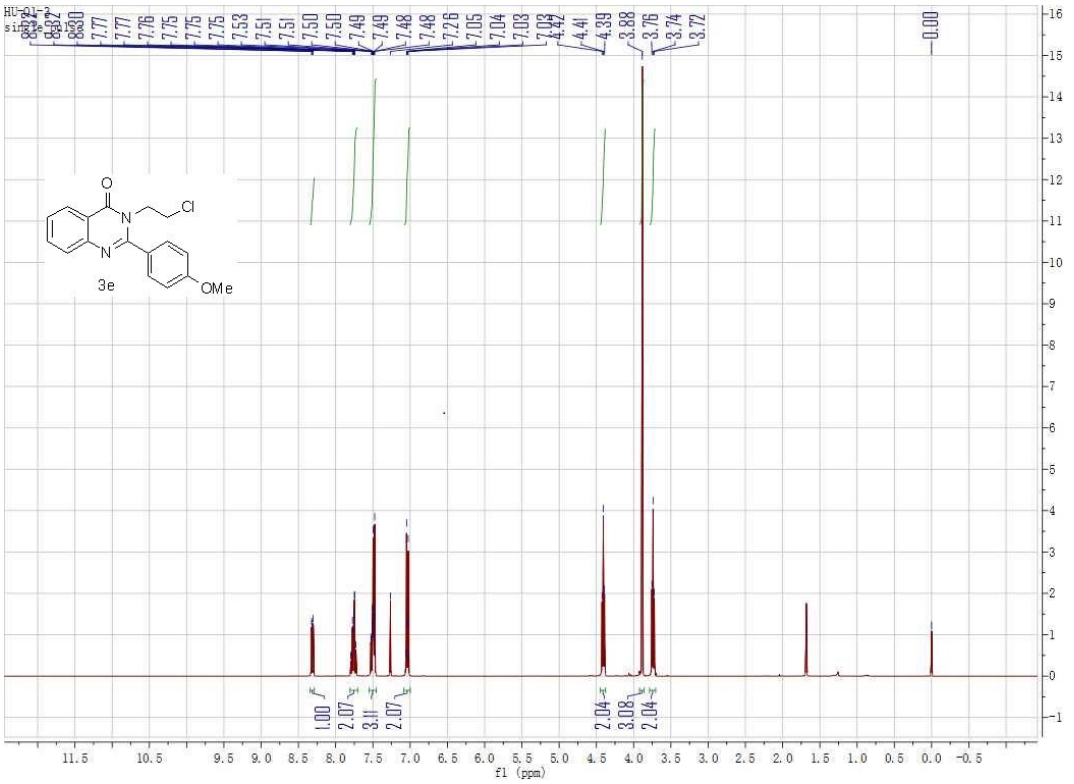

HU-Q1-1
single pulse decoupled gated NOE
162.36
156.19
147.27
140.36
134.73
132.29
129.65
128.18
127.71
127.22
126.80
120.67
77.44
77.12
76.81
47.18
40.44
21.52
3b
f1 (ppm)

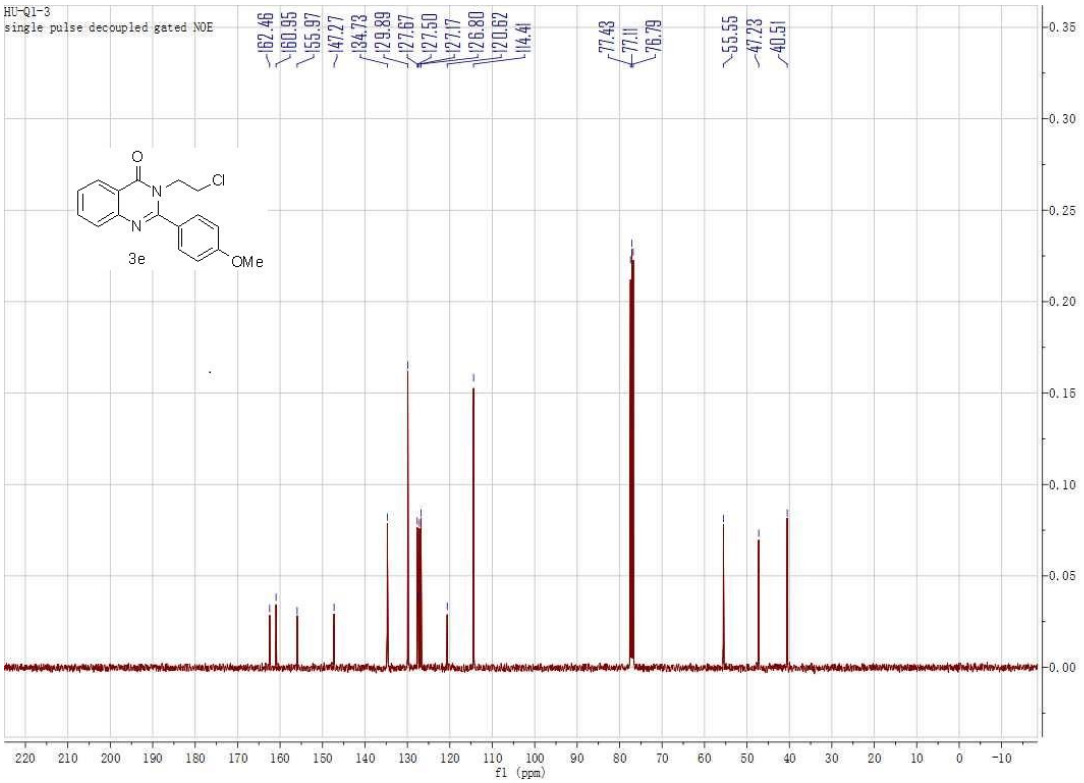

HU-Q1-2
8.33
8.31
7.78
7.78
7.77
7.76
7.76
7.74
7.54
7.54
7.52
7.52
7.51
7.50
7.43
7.41
7.39
7.36
7.35
7.32
7.30
4.36
4.35
3.75
3.74
3.72
2.44
0.00
3c
1.00
2.06
1.18
1.11
3.29
2.07
2.07
3.10
f1 (ppm)

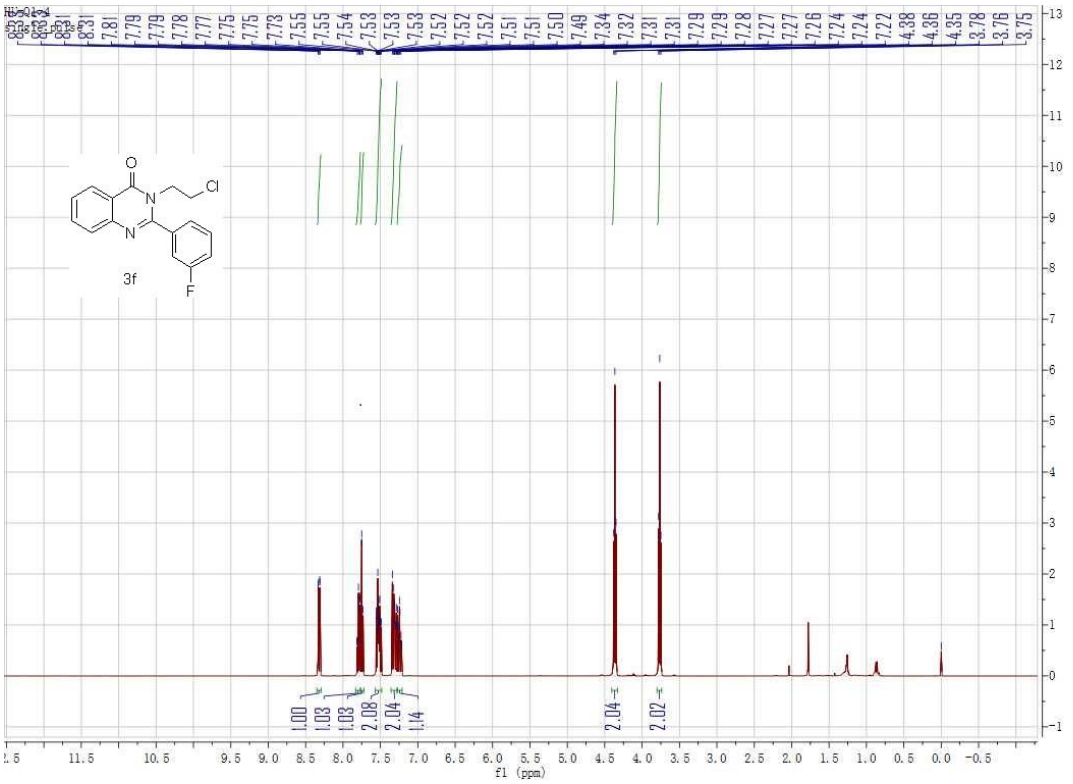

HU-Q1-2
single pulse decoupled gated 13C
162.39
156.73
147.22
139.06
135.01
134.78
130.91
128.88
128.83
127.73
127.29
126.82
125.17
120.71
77.41
77.00
76.77
47.22
40.41
21.54
3c
f1 (ppm)

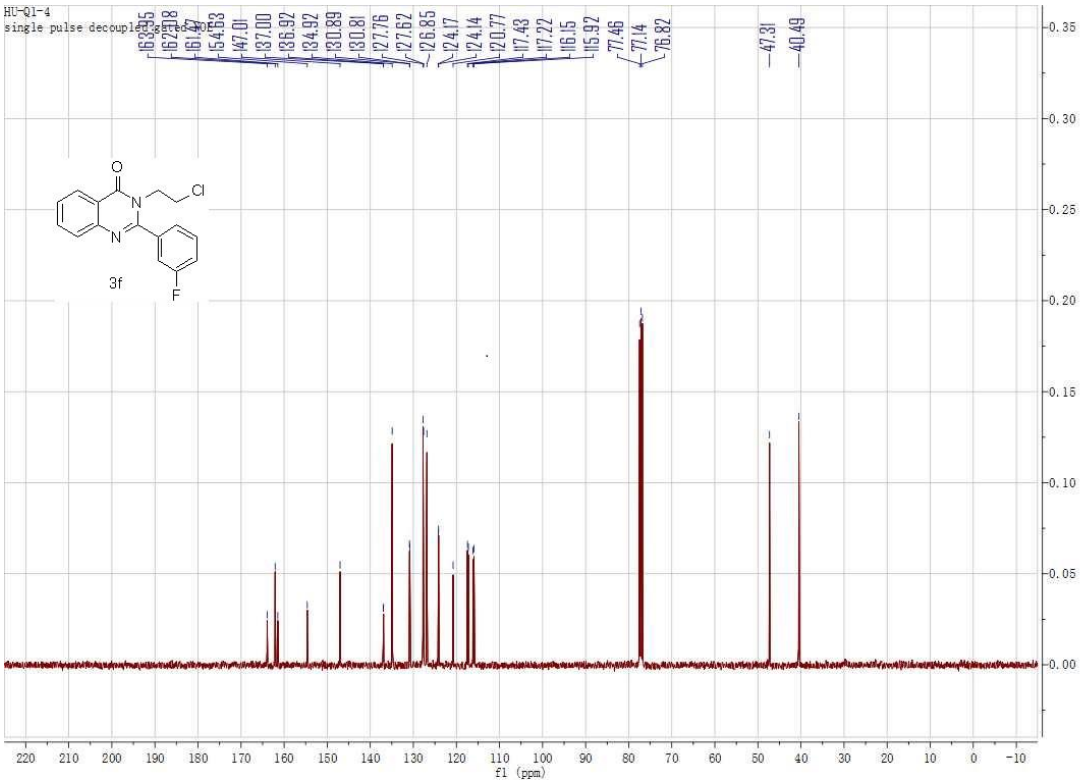

3d
fl (ppm)

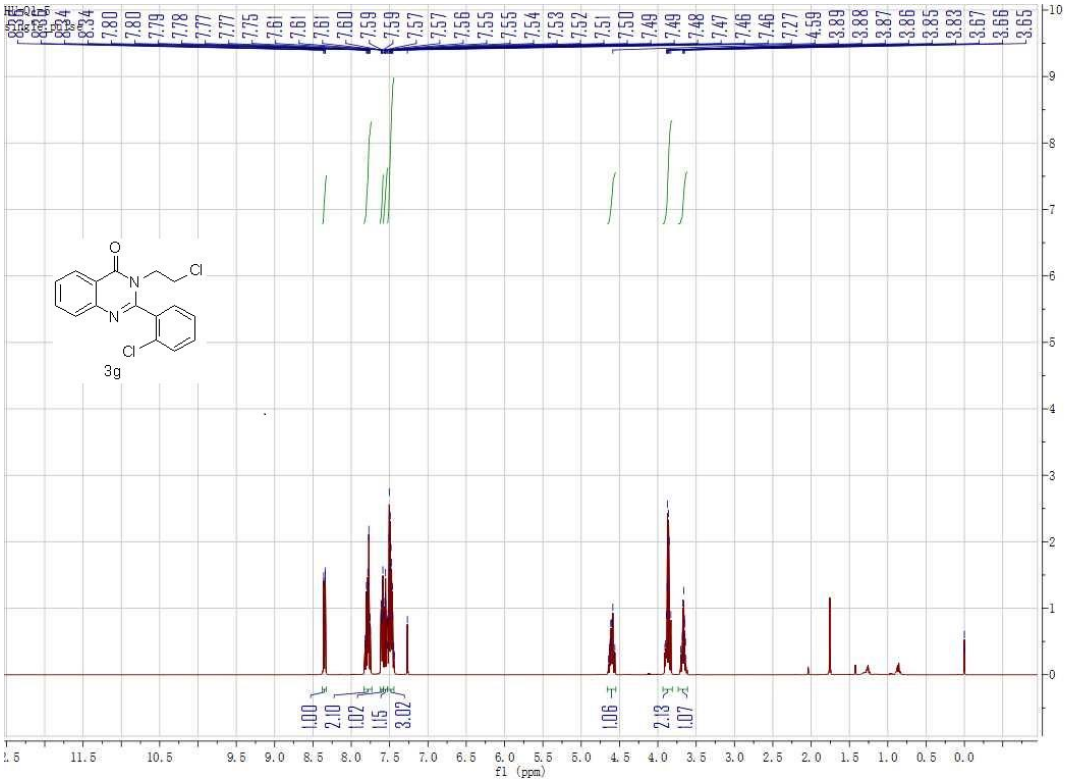

HU-Q1-12
single pulse decoupled gated NOE
3d
fl (ppm)


3e
OMe
fl (ppm)


HU-Q1-3
single pulse decoupled gated NOE
3e
OMe
fl (ppm)


3f
F
Cl
N
O
1.00
1.03
1.03
2.08
2.04
1.14
2.04
2.02
f1 (ppm)


HU-Q1-4
single pulse decoupled
3f
F
Cl
N
O
47.31
40.49
77.46
77.14
76.82
f1 (ppm)


8.34
7.80
7.79
7.78
7.77
7.77
7.75
7.61
7.61
7.61
7.60
7.59
7.59
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.52
7.51
7.50
7.49
7.49
7.48
7.47
7.46
7.46
7.27
4.59
3.89
3.88
3.87
3.86
3.85
3.83
3.67
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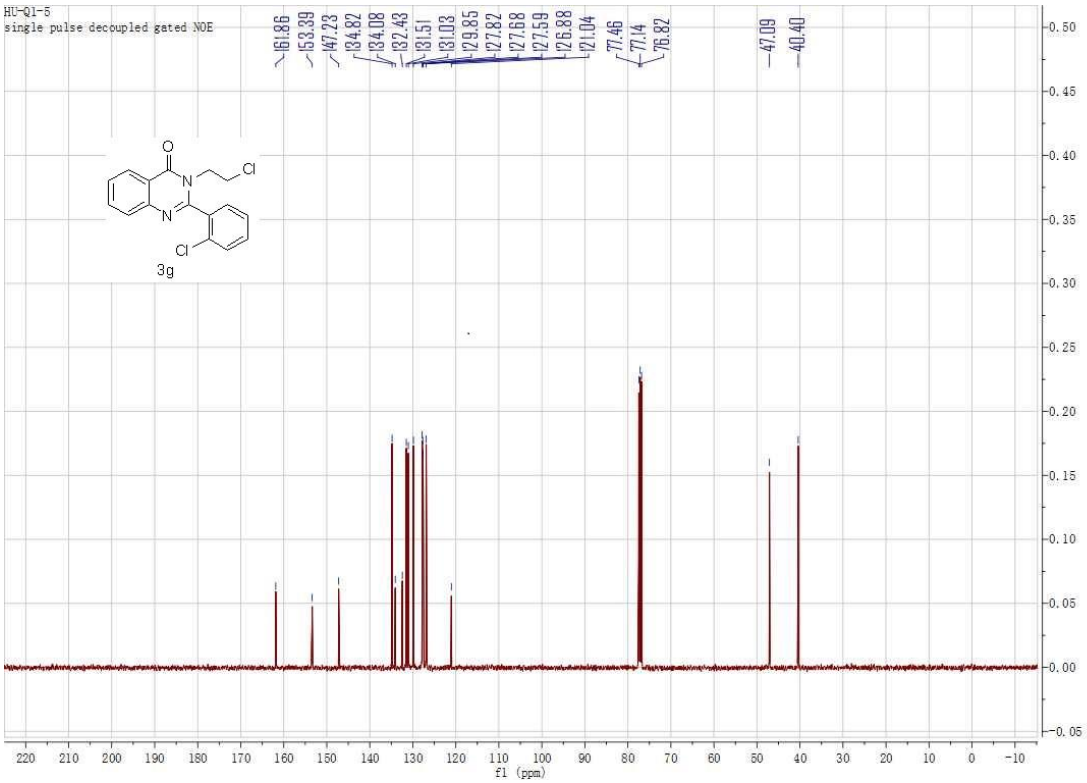
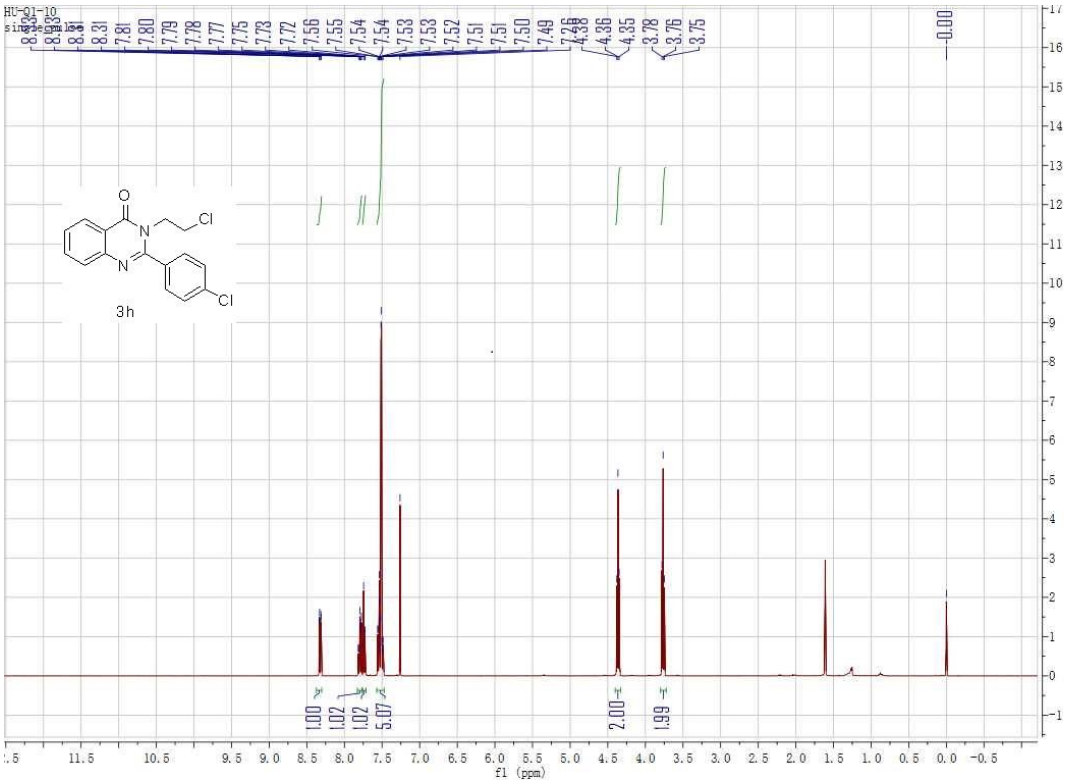
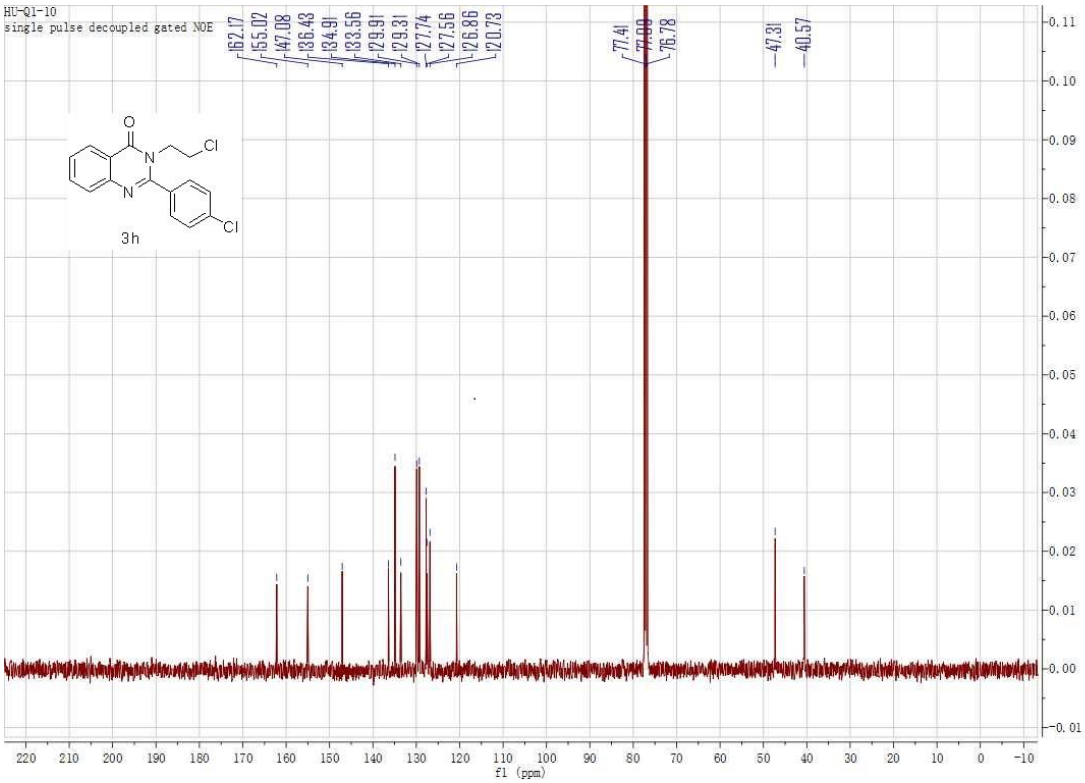
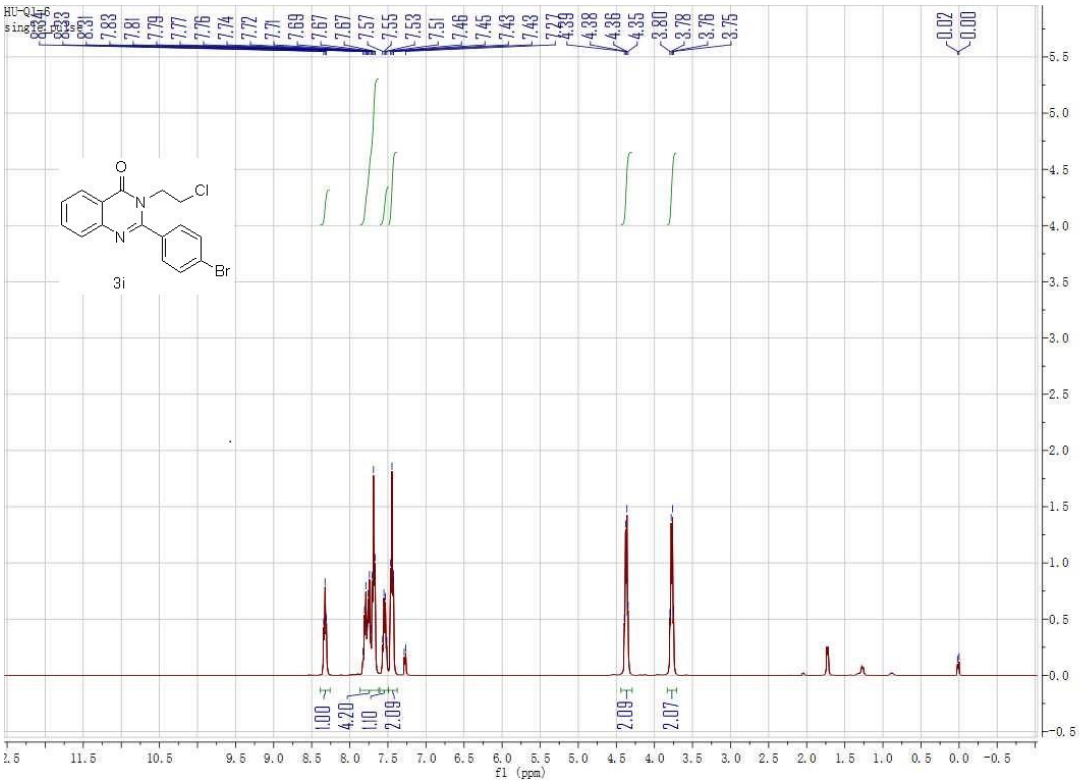
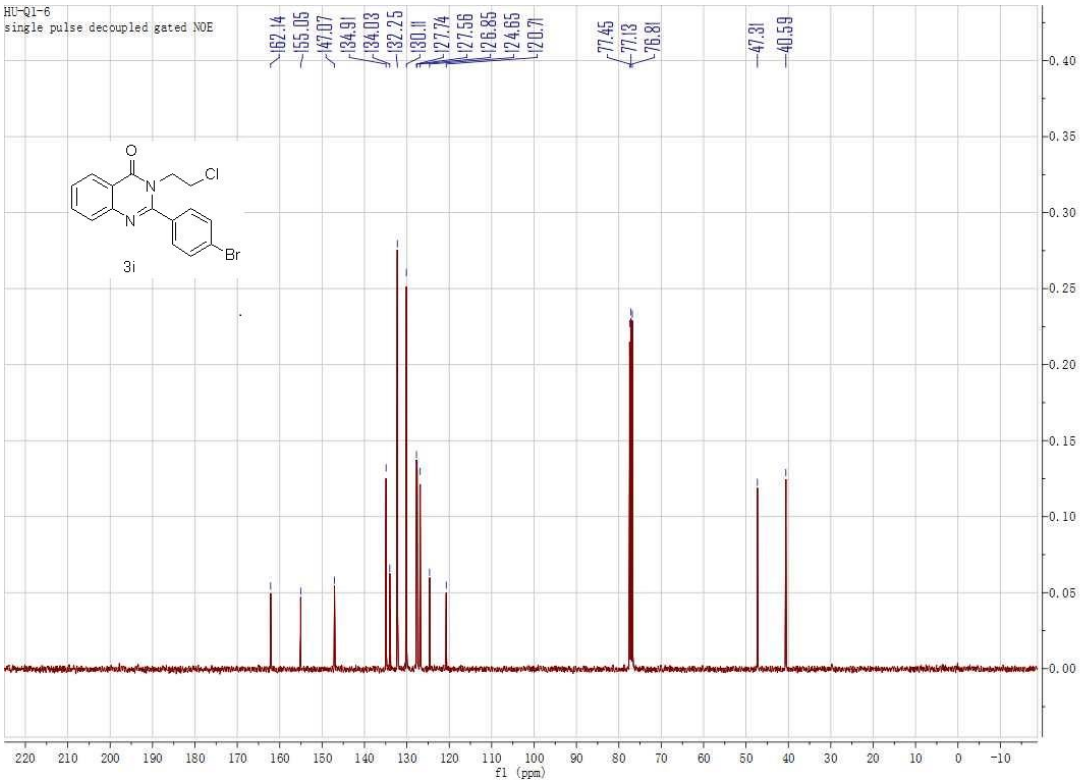
8.02
1.06
2.13
1.07
fl (ppm)
3g

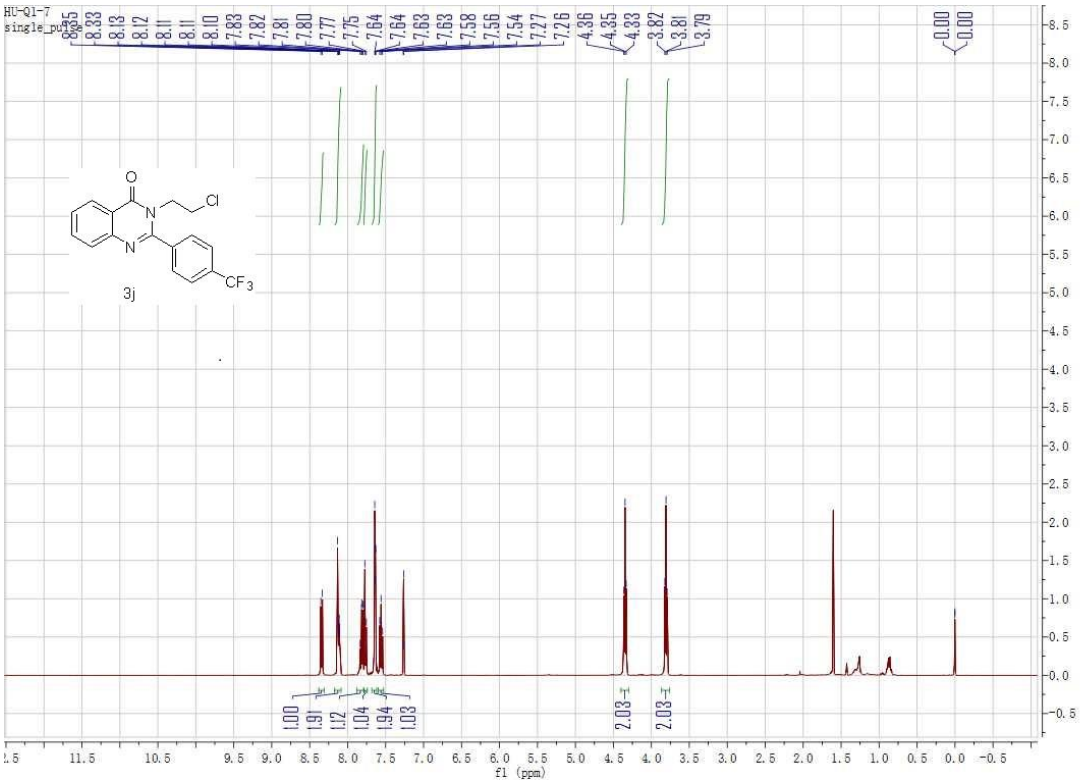

HU-Q1-5
single pulse decoupled gated NOE
161.86
153.39
147.23
134.82
134.08
132.43
131.51
131.03
129.85
127.82
127.68
127.59
126.88
121.04
77.46
77.14
76.82
47.09
40.40
fl (ppm)
3g

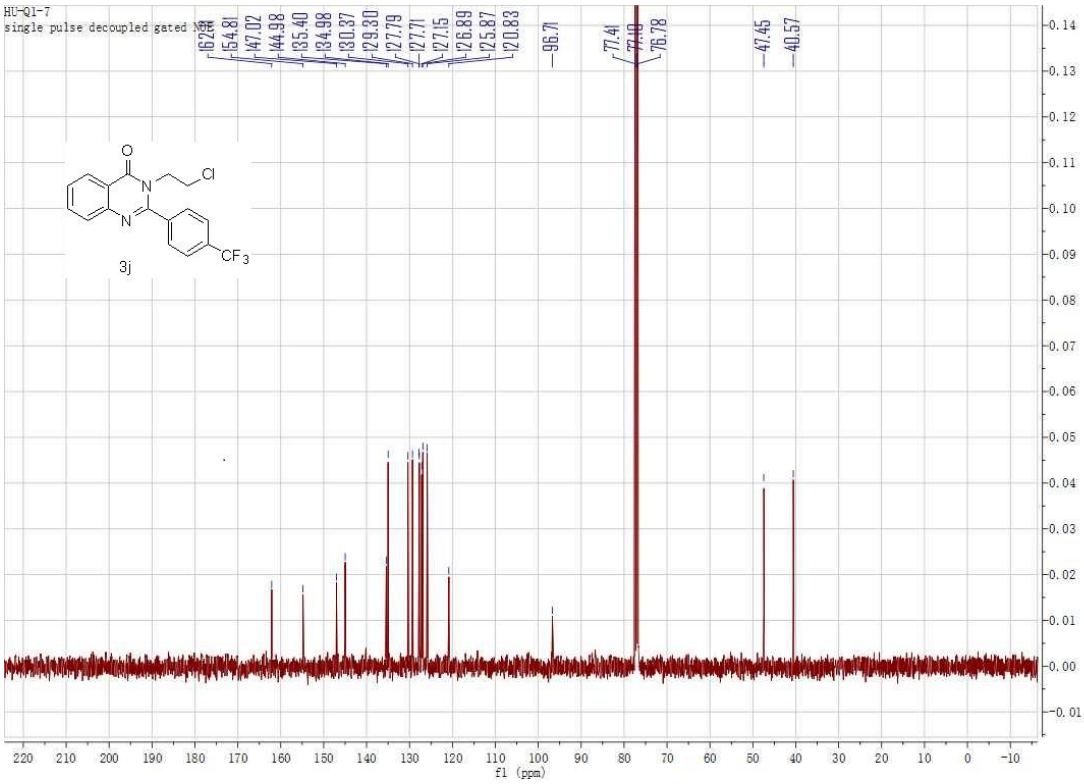

HU-Q1-10
3h
1.00
1.02
1.02
5.07
2.00
1.99
f1 (ppm)

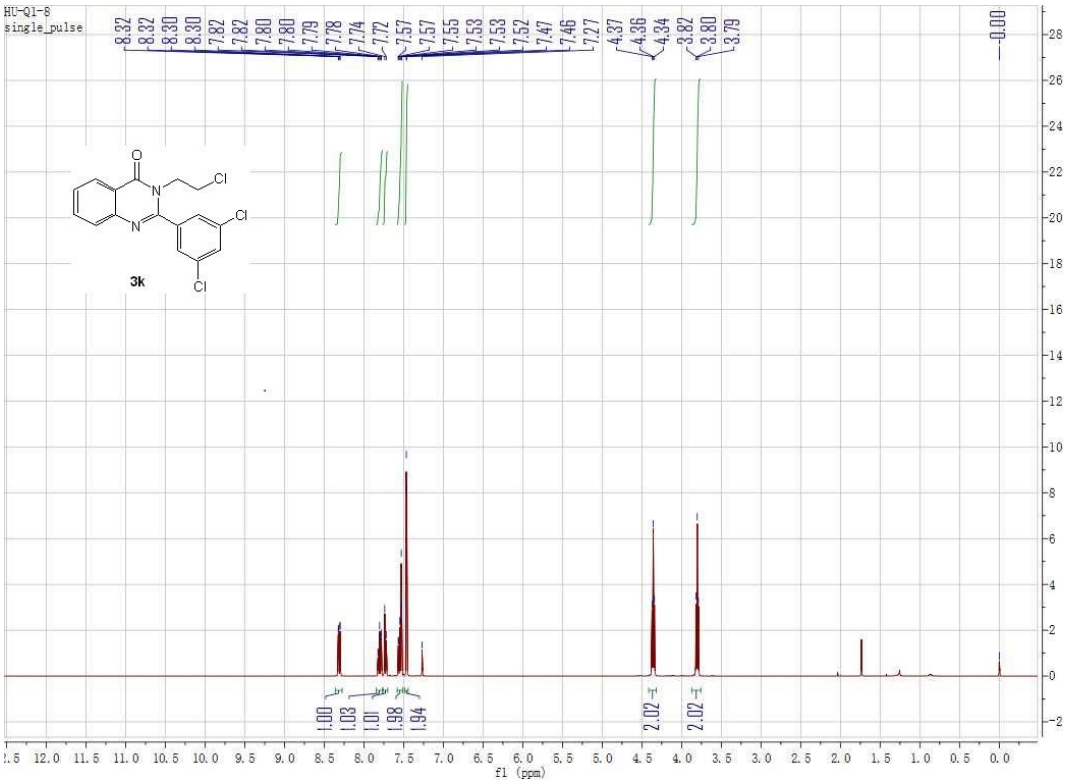

HU-Q1-10
single pulse decoupled gated NOE
162.17
155.02
147.08
136.43
134.91
133.56
129.91
129.31
127.74
127.56
126.86
120.73
77.41
77.00
76.78
47.31
40.57
3h
f1 (ppm)

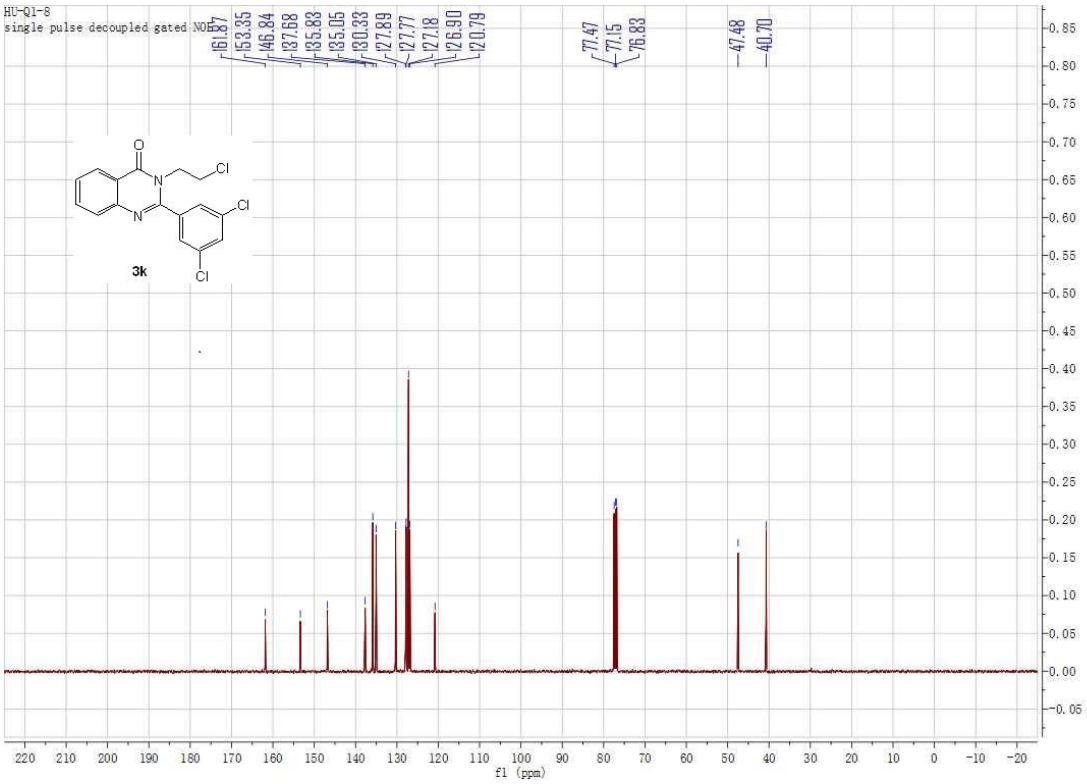

HU-Q1-6
8.34
8.33
8.31
7.83
7.81
7.79
7.77
7.76
7.74
7.72
7.71
7.69
7.67
7.67
7.57
7.55
7.53
7.51
7.46
7.45
7.43
7.43
7.27
4.39
4.38
4.36
4.35
3.80
3.78
3.76
3.75
0.02
0.00
O
N
N
Cl
Br
3i
1.00
4.20
1.10
2.09
2.09
2.07
f1 (ppm)

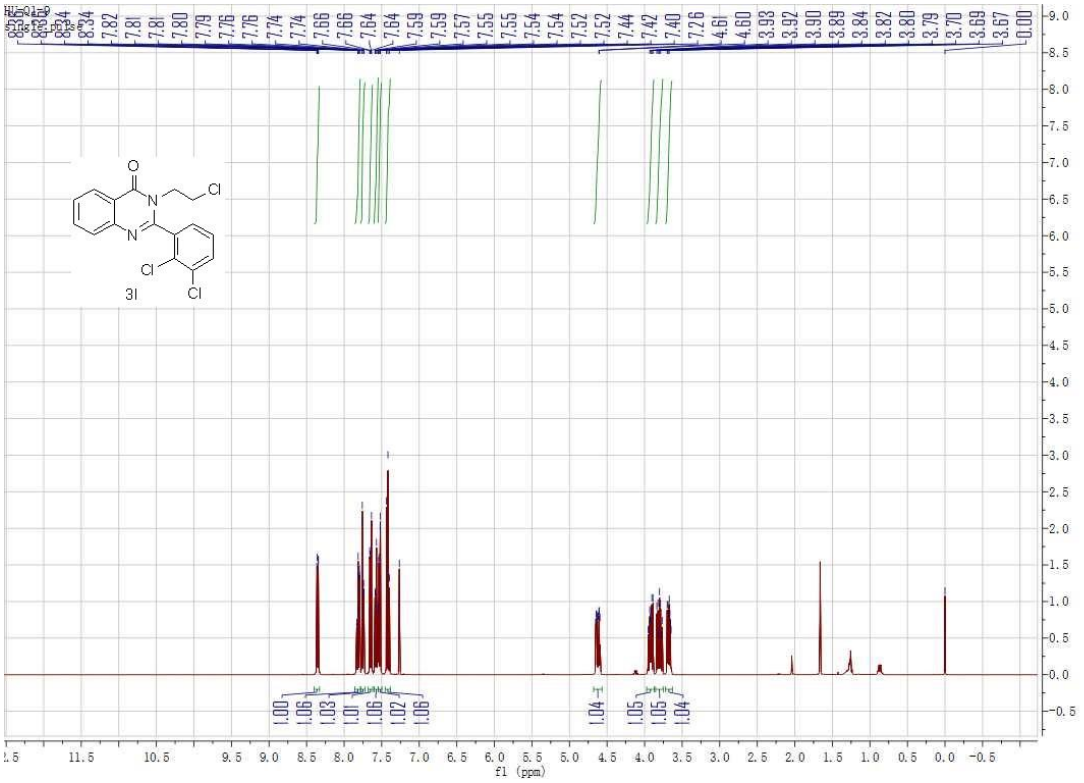

HU-Q1-6
single pulse decoupled gated NOE
162.14
155.05
147.07
134.91
134.03
132.25
130.11
127.74
127.56
126.85
124.65
120.71
77.45
77.13
76.81
47.31
40.59
O
N
N
Cl
Br
3i
f1 (ppm)

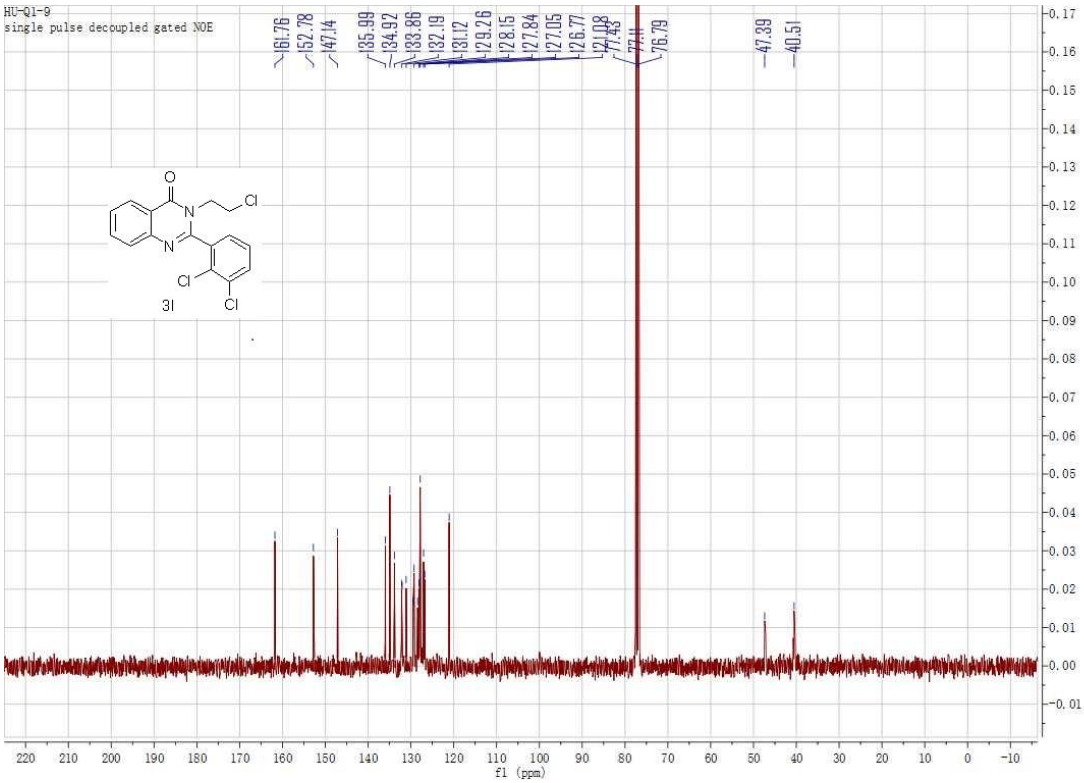

HU-Q1-7
single_pu
8.35
8.33
8.13
8.12
8.11
8.11
8.10
7.83
7.82
7.81
7.80
7.77
7.75
7.64
7.64
7.63
7.63
7.58
7.56
7.54
7.27
7.26
4.36
4.35
4.33
3.82
3.81
3.79
0.00
0.00
O
N
Cl
N
CF3
3j
1.00
1.91
1.12
1.04
1.94
1.03
2.03
2.03
f1 (ppm)

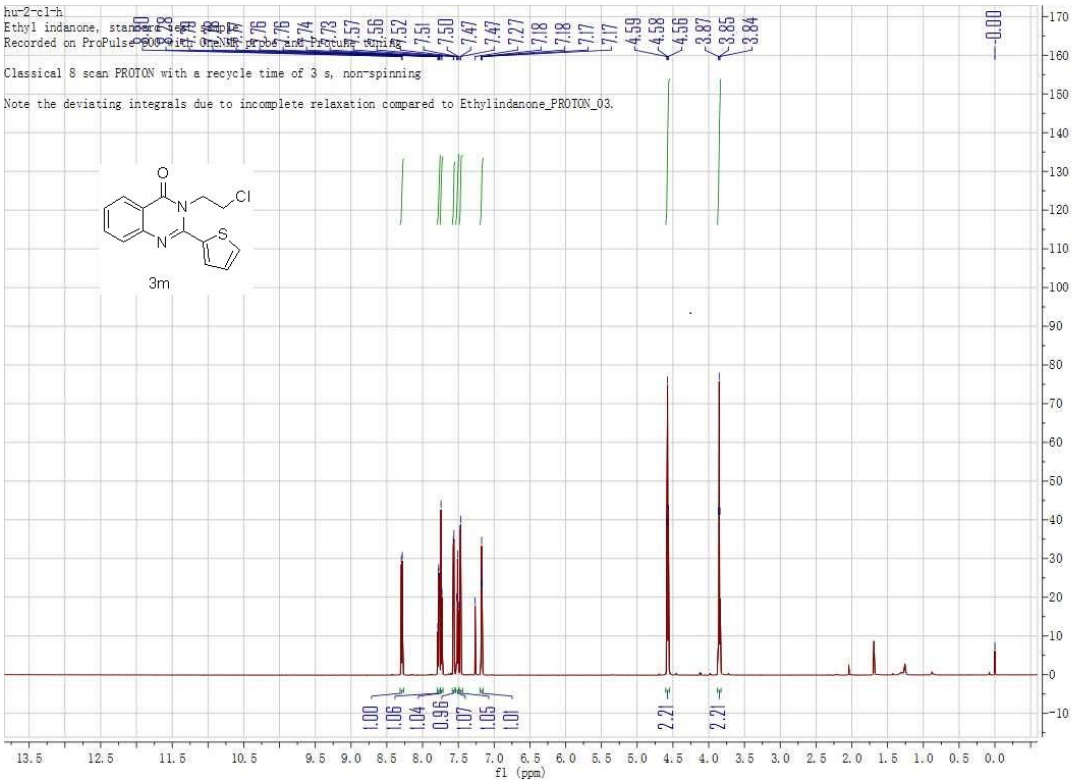

HU-Q1-7
single pulse decoupled gated
162.78
154.81
147.02
144.98
135.40
134.98
130.37
129.30
127.79
127.71
127.15
126.89
125.87
120.83
96.71
77.41
77.16
76.78
47.45
40.57
O
N
Cl
N
CF3
3j
f1 (ppm)

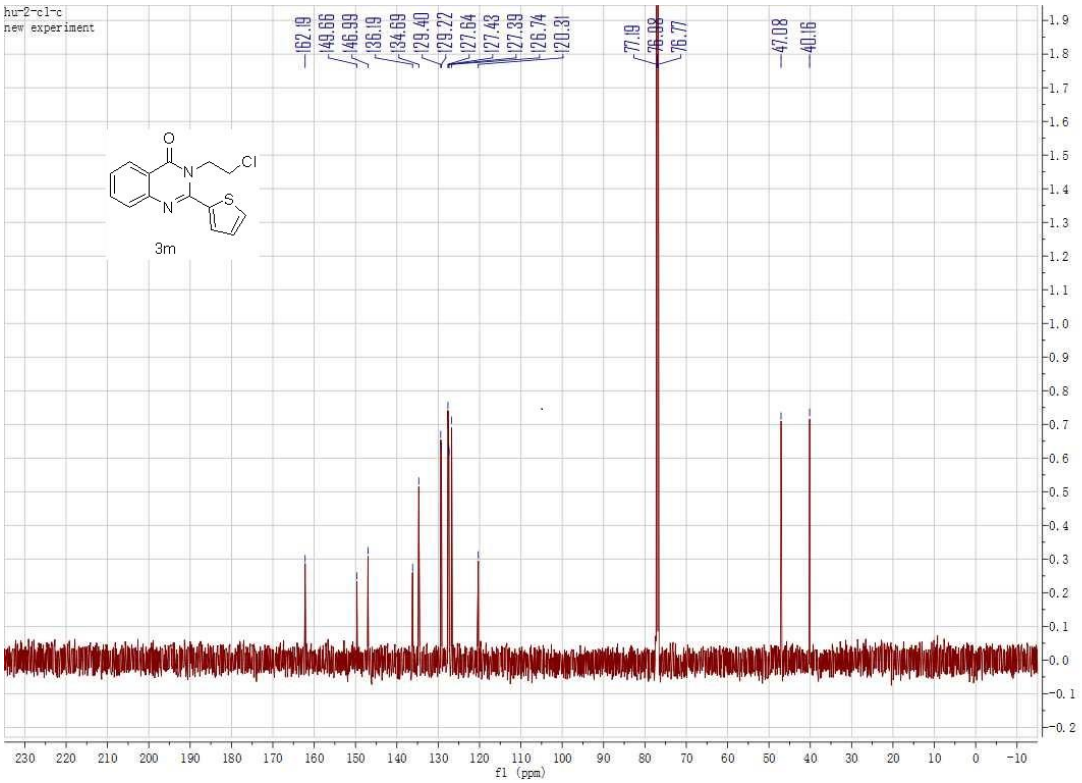

HU-Q1-8
single_pulse
8.32
8.32
8.30
8.30
7.82
7.82
7.80
7.80
7.79
7.78
7.74
7.72
7.57
7.57
7.55
7.53
7.52
7.47
7.46
7.27
4.37
4.36
4.34
3.82
3.80
3.79
0.00
3k
1.00
1.03
1.01
1.98
1.94
2.02
2.02
f1 (ppm)

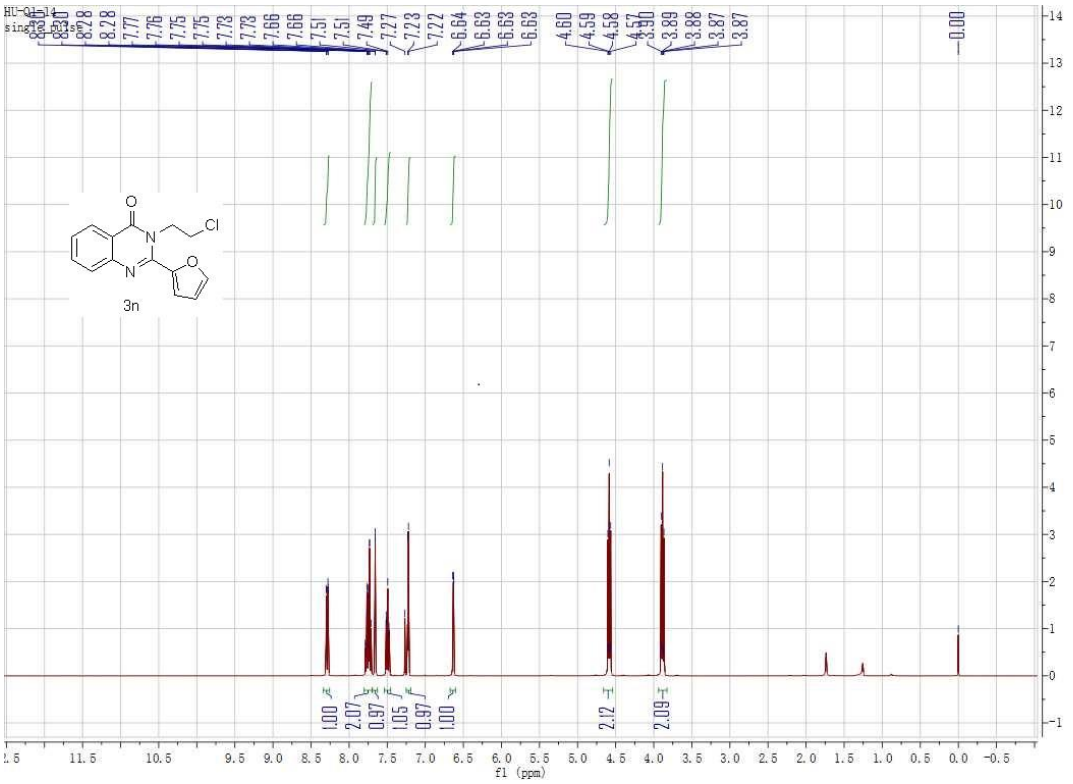

HU-Q1-8
single pulse decoupled gated NOE
161.87
153.35
146.84
137.68
135.83
135.05
130.33
127.89
127.77
127.18
126.90
120.79
77.47
77.15
76.83
47.48
40.70
3k
f1 (ppm)

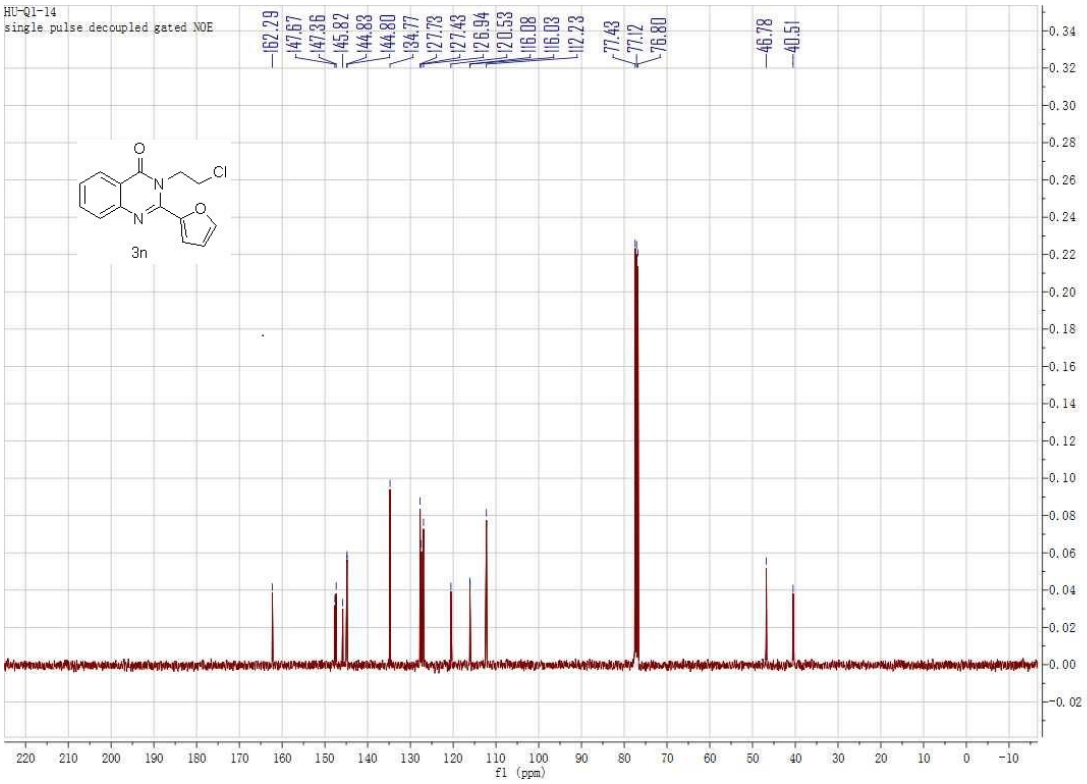

3l
f1 (ppm)

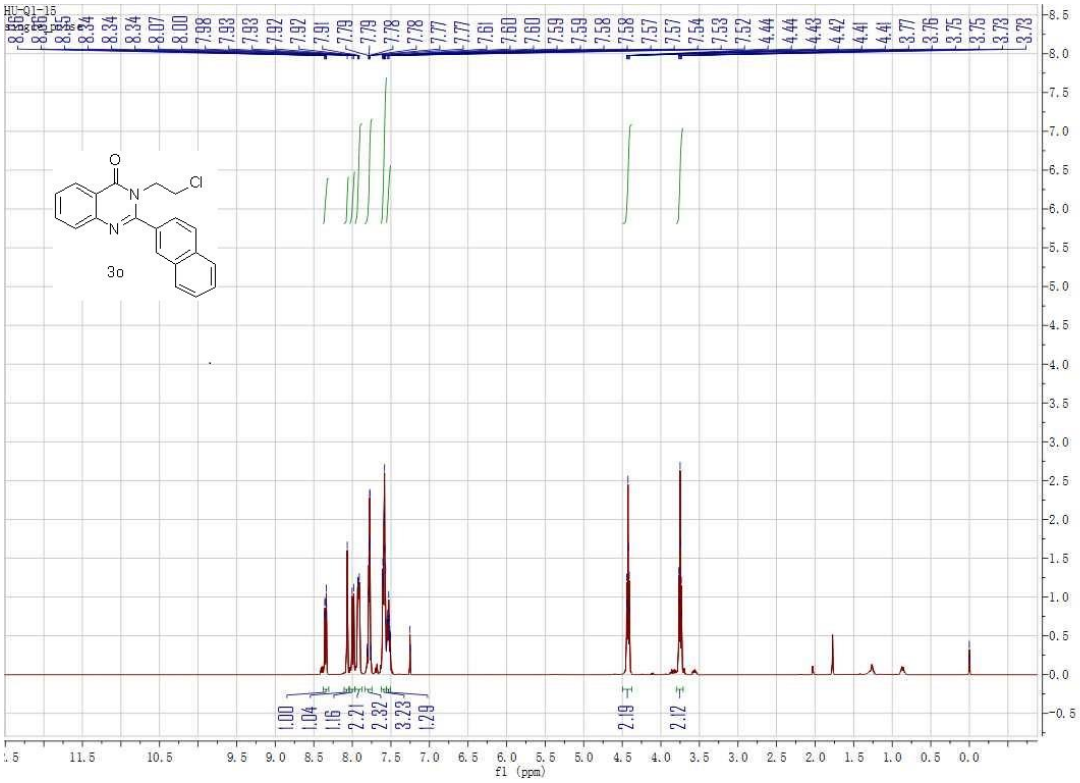

HU-Q1-9
single pulse decoupled gated NOE
3l
f1 (ppm)

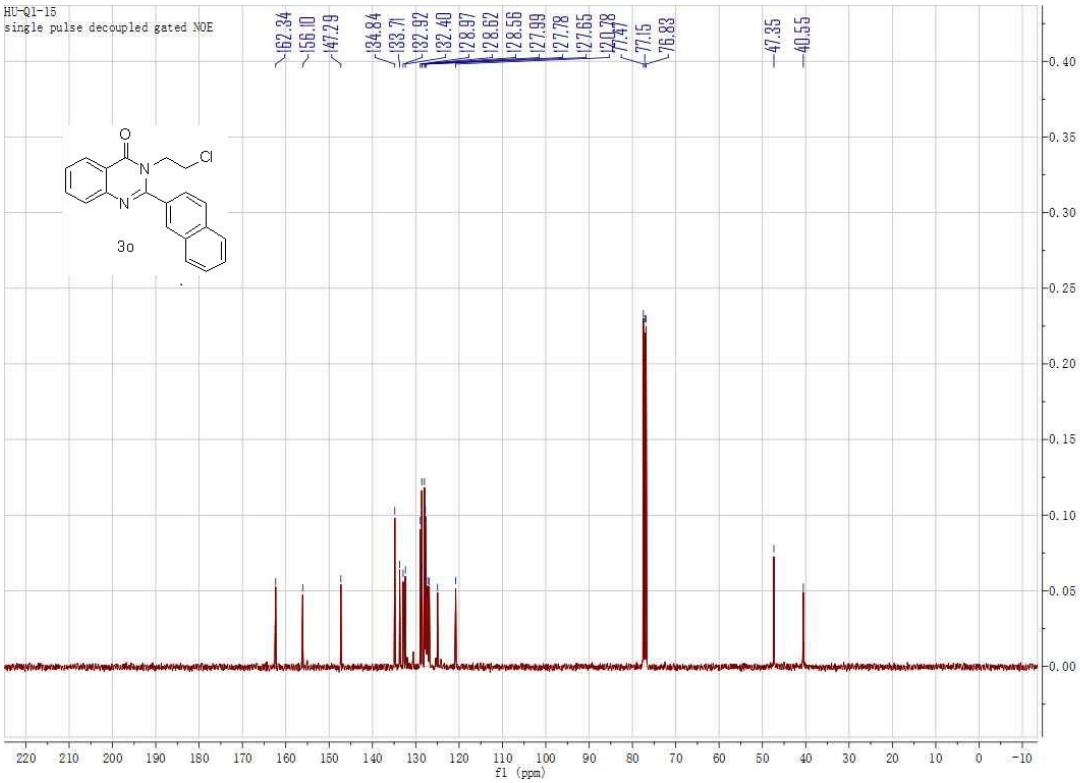

hu-2-c1-h
Ethyl indanone, standard single pulse
Recorded on ProPulse-500 with OneNMR probe and Protune tuning
Classical 8 scan PROTON with a recycle time of 3 s, non-spinning
Note the deviating integrals due to incomplete relaxation compared to Ethylindanone_PROTON_03.
3m
f1 (ppm)

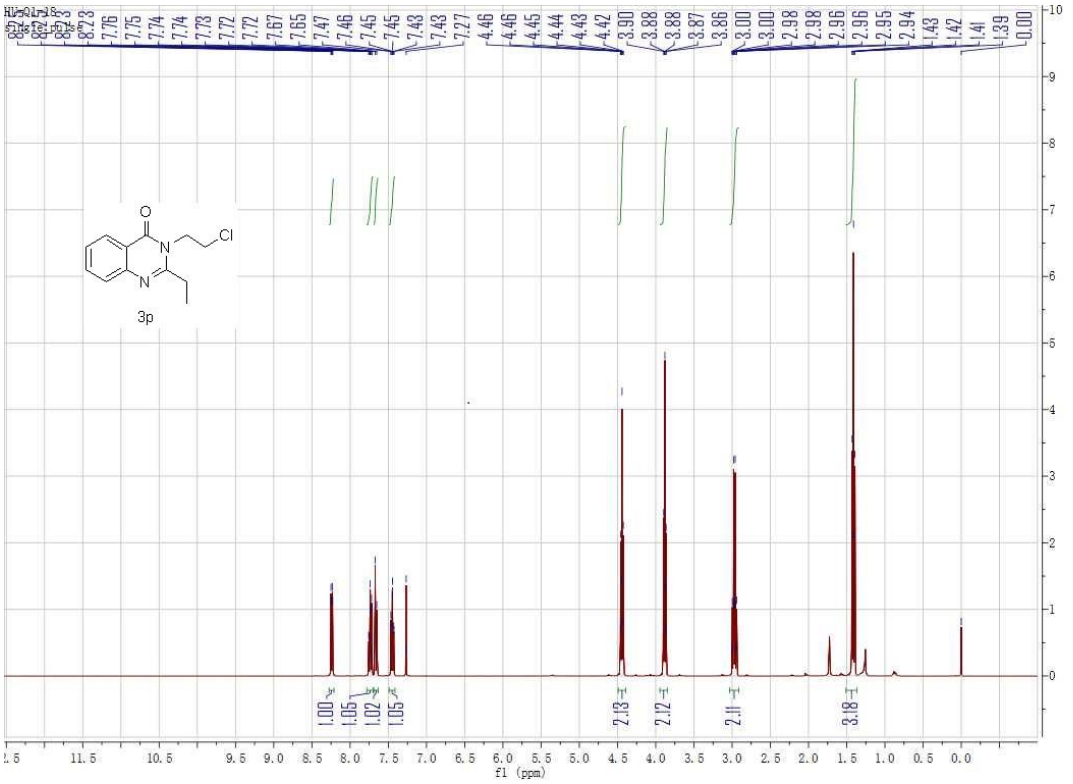

hu-2-c1-c
new experiment
3m
f1 (ppm)

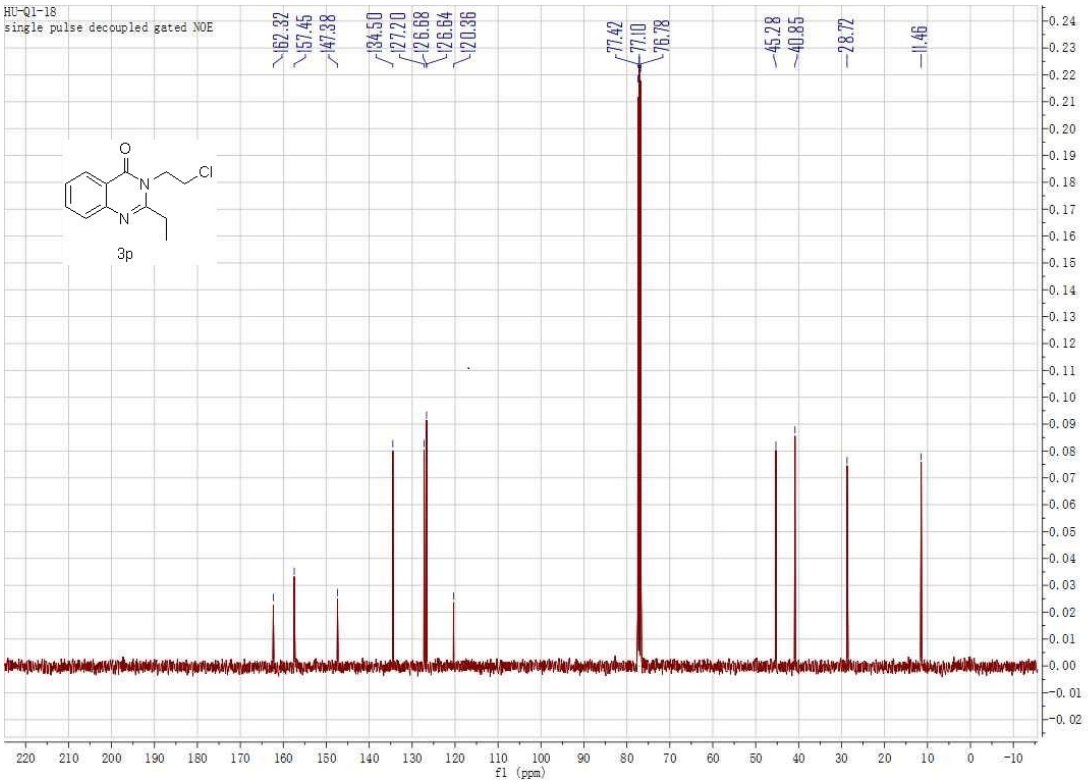

3n
fl (ppm)

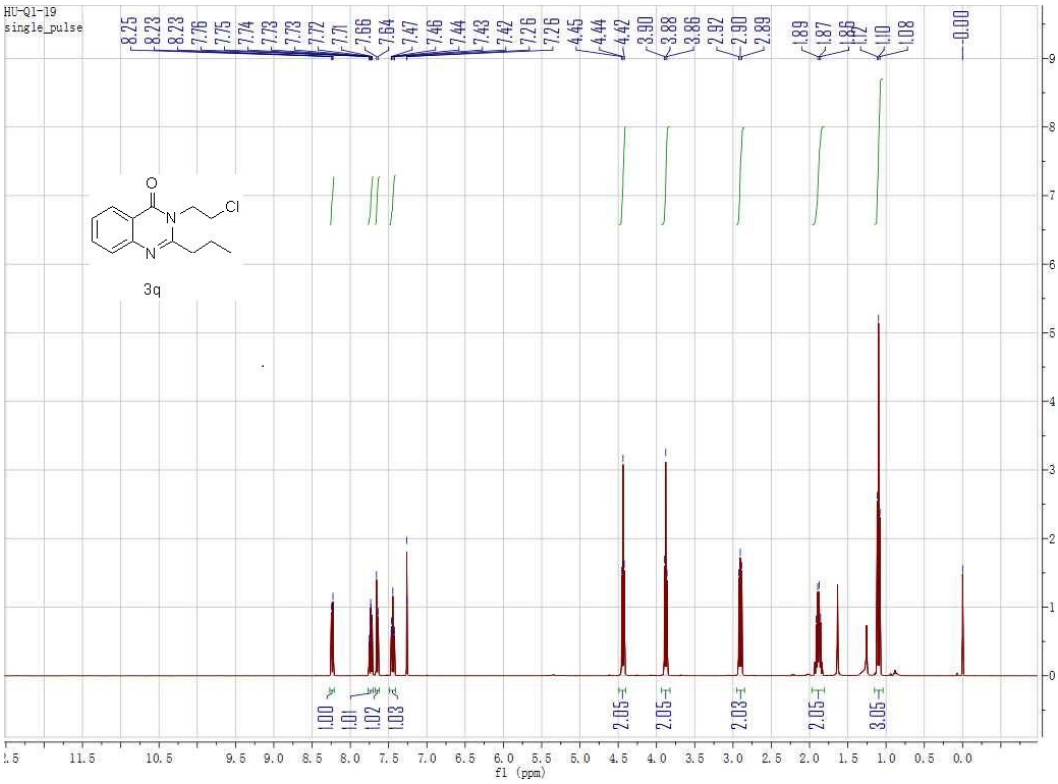

HU-Q1-14
single pulse decoupled gated NOE
3n
fl (ppm)

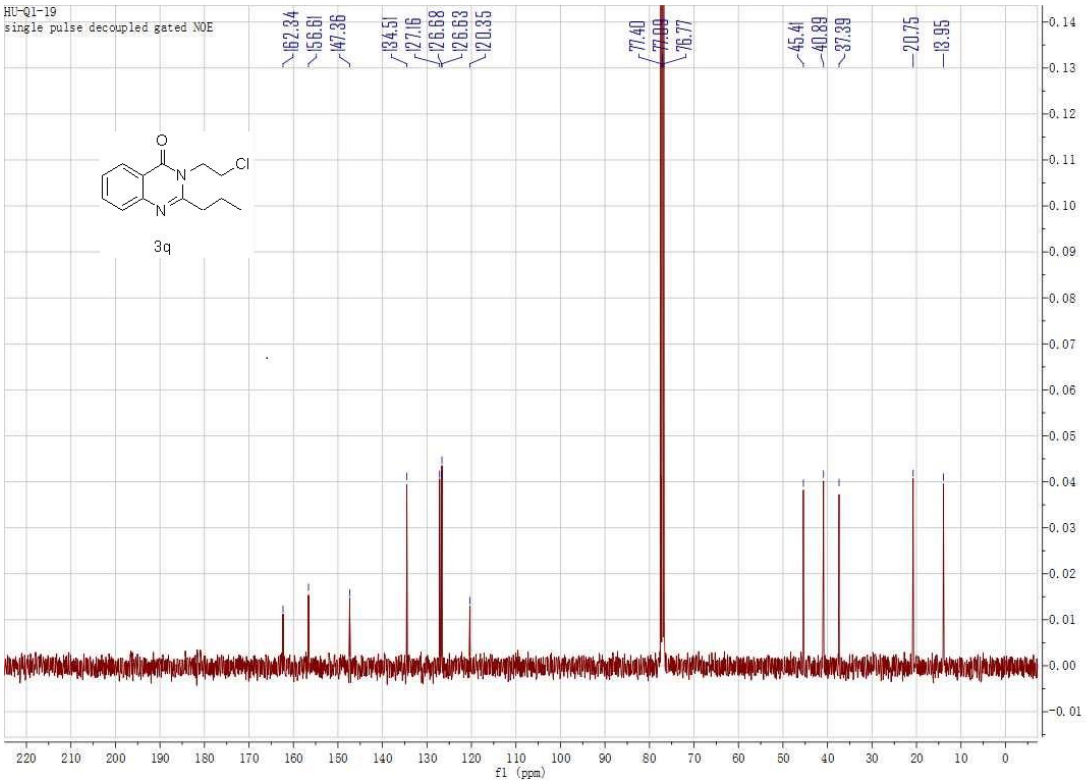

HU-Q1-15
3o
f1 (ppm)

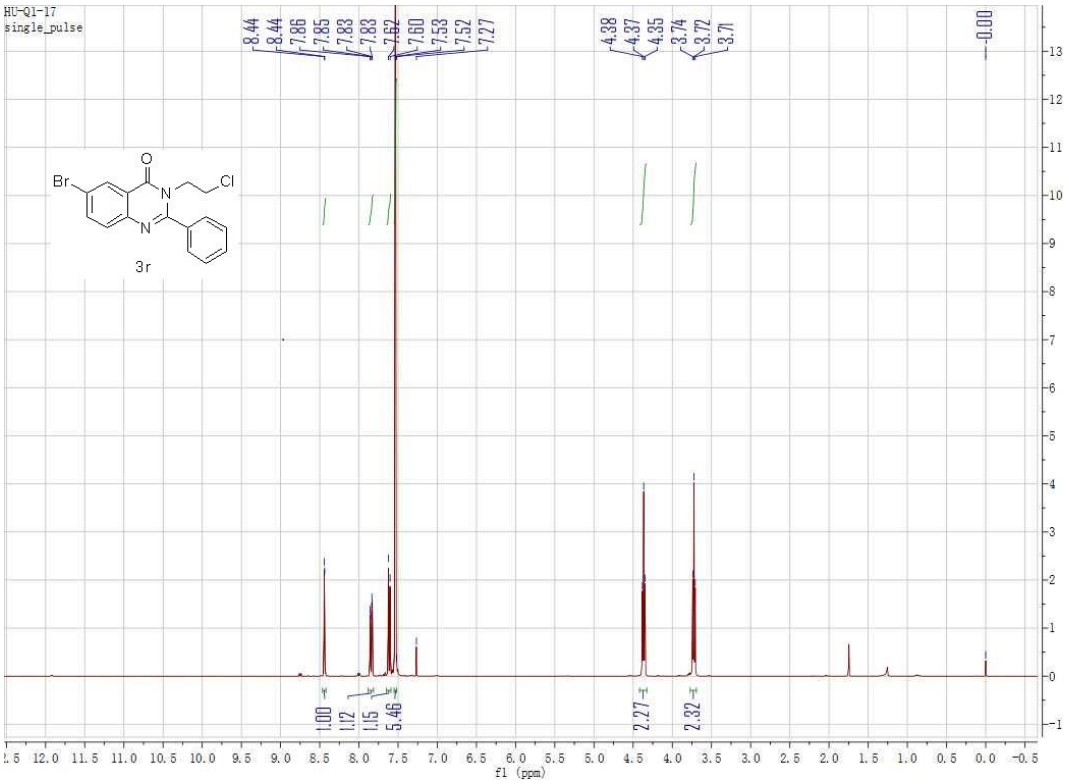

HU-Q1-15
single pulse decoupled gated NOE
3o
f1 (ppm)

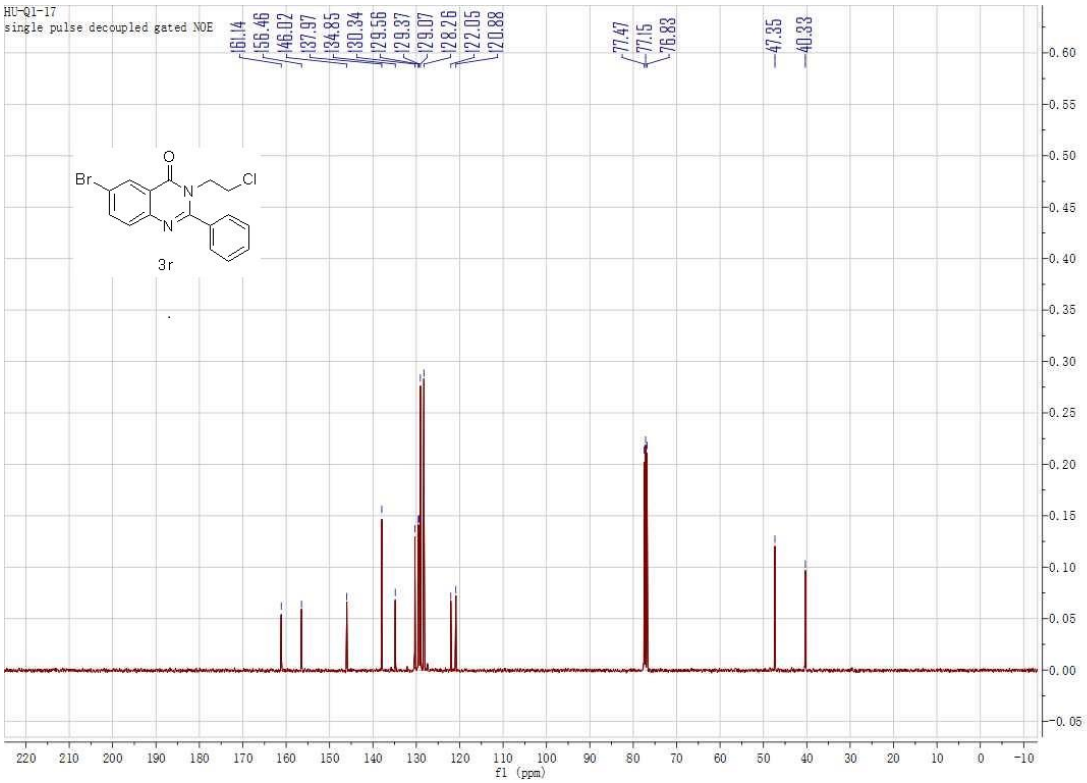

3p
fl (ppm)

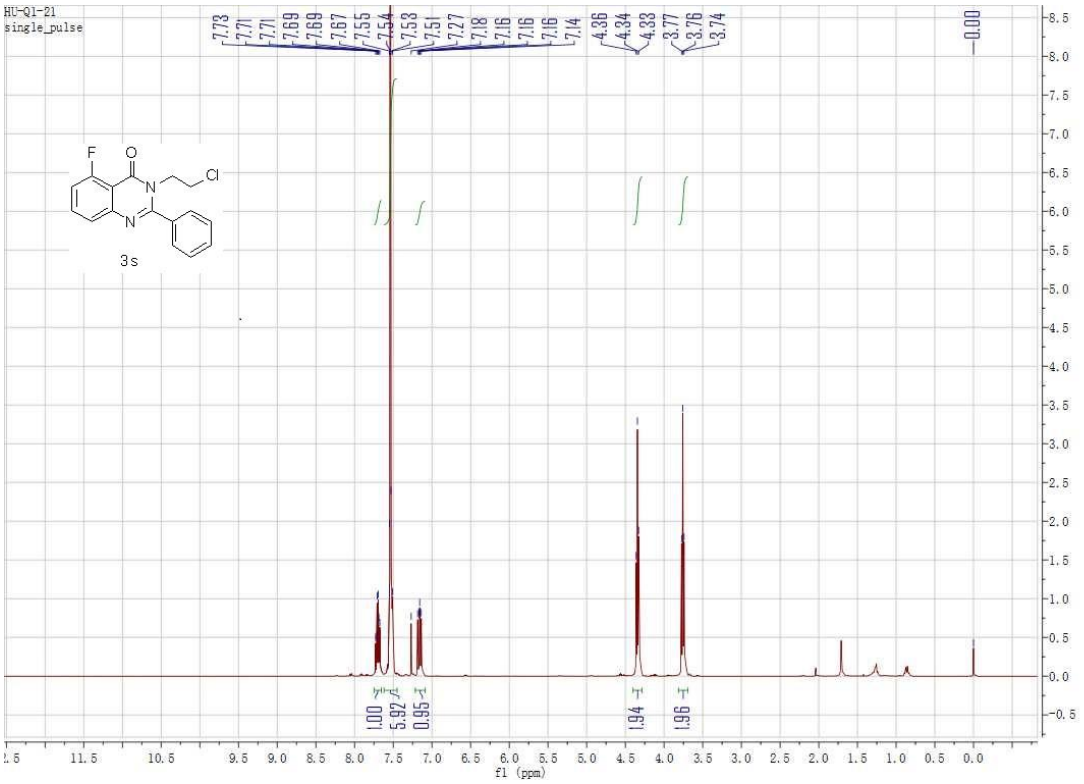

HU-Q1-18
single pulse decoupled gated NOE
162.32
157.45
147.38
134.50
127.20
126.68
126.64
120.36
77.42
77.10
76.78
45.28
40.85
28.72
11.46
3p
fl (ppm)

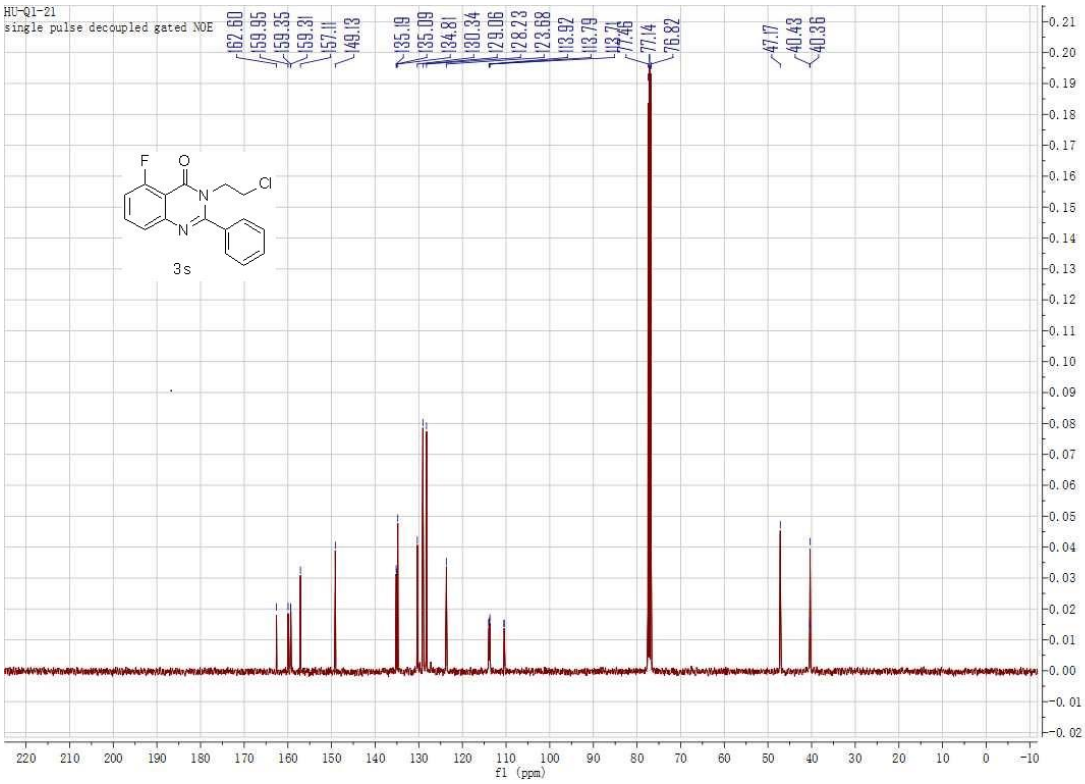

HU-Q1-19
single_pulse
3q
fl (ppm)

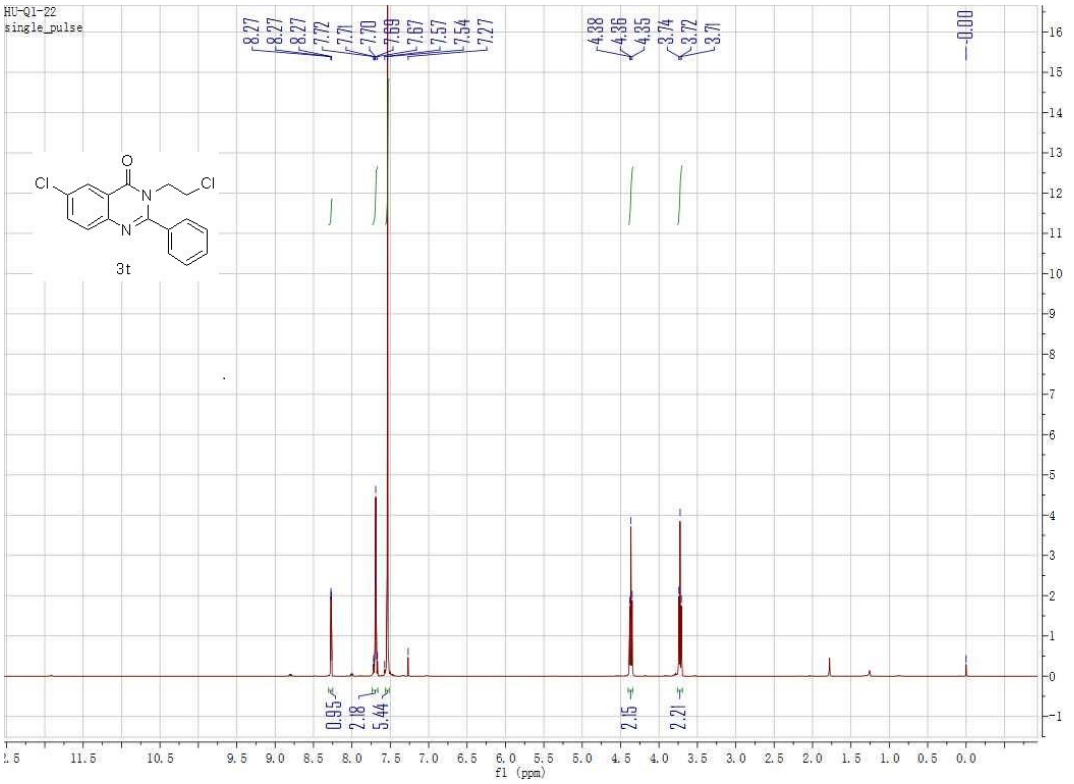

HU-Q1-19
single pulse decoupled gated NOE
3q
fl (ppm)

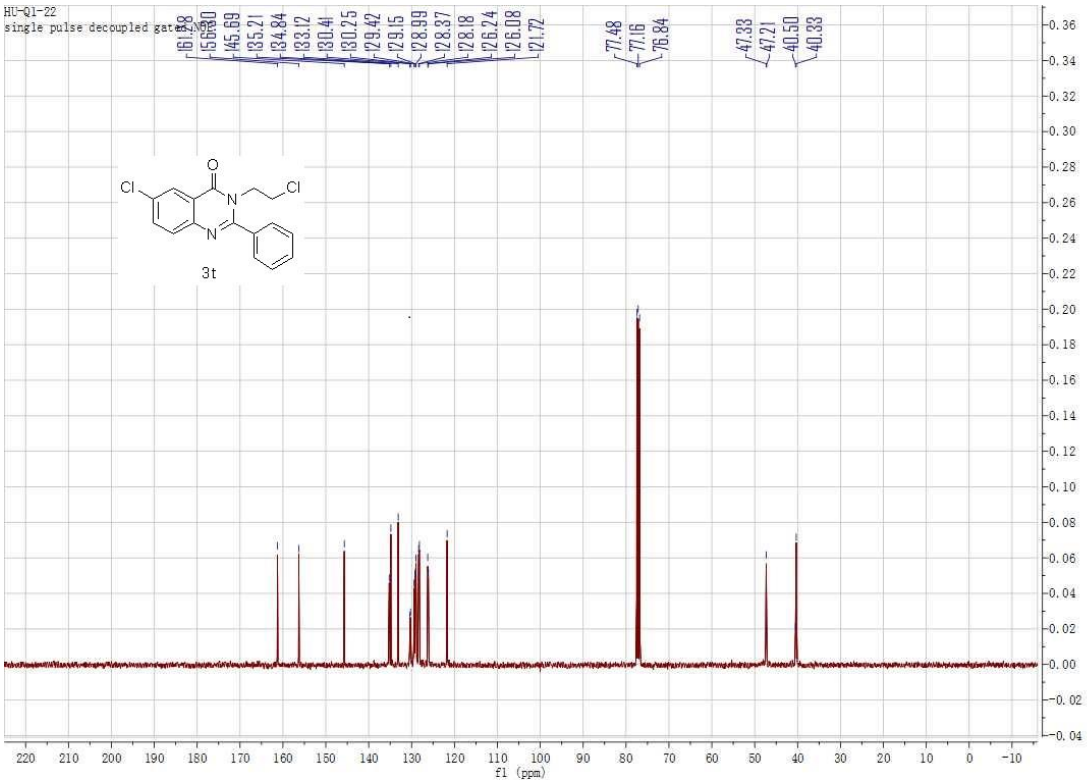

HU-Q1-17
single_pulse
8.44
8.44
7.86
7.85
7.83
7.83
7.82
7.60
7.53
7.52
7.27
4.38
4.37
4.35
3.74
3.72
3.71
0.00
Br
O
N
Cl
N
3r
1.00
1.12
1.15
5.46
2.27
2.32
f1 (ppm)

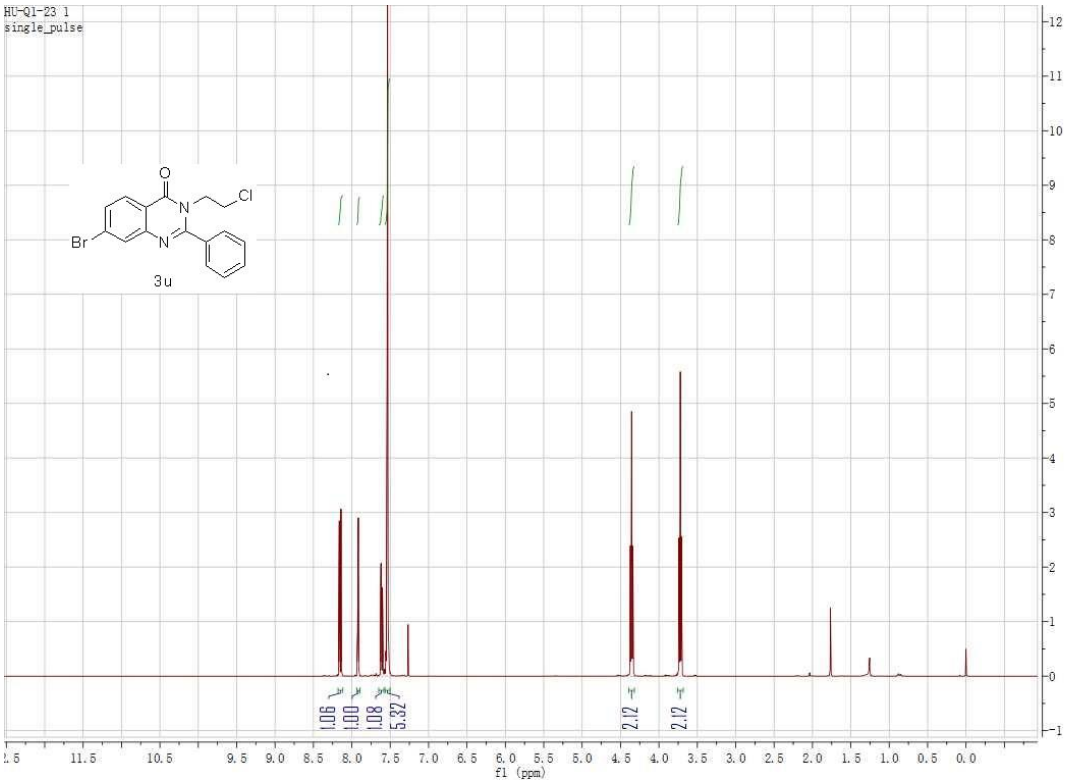

HU-Q1-17
single pulse decoupled gated NOE
161.14
156.46
146.02
137.97
134.85
130.34
129.56
129.37
129.07
128.28
122.05
120.88
77.47
77.15
76.83
47.35
40.33
Br
O
N
Cl
N
3r
f1 (ppm)

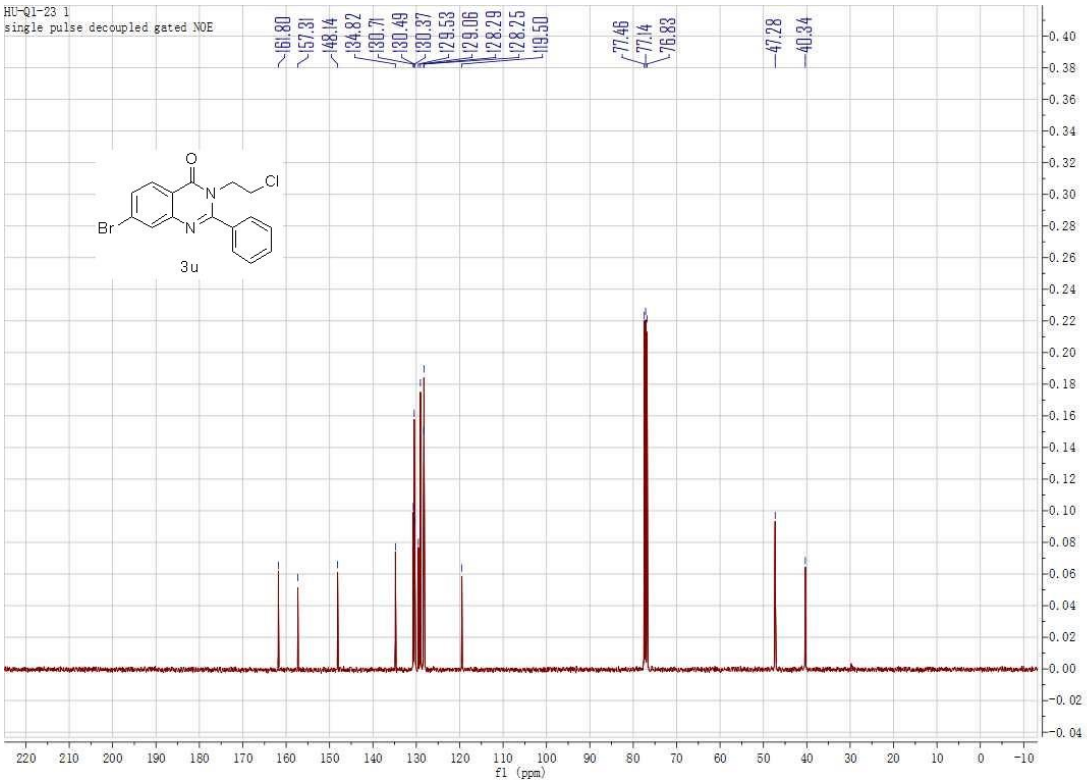

HU-Q1-21
single_pulse
7.73
7.71
7.71
7.69
7.69
7.67
7.55
7.54
7.53
7.51
7.27
7.18
7.16
7.16
7.16
7.14
4.36
4.34
4.33
3.77
3.76
3.74
0.00
F
O
N
Cl
N
3s
1.00
5.92
0.95
1.94
1.96
f1 (ppm)

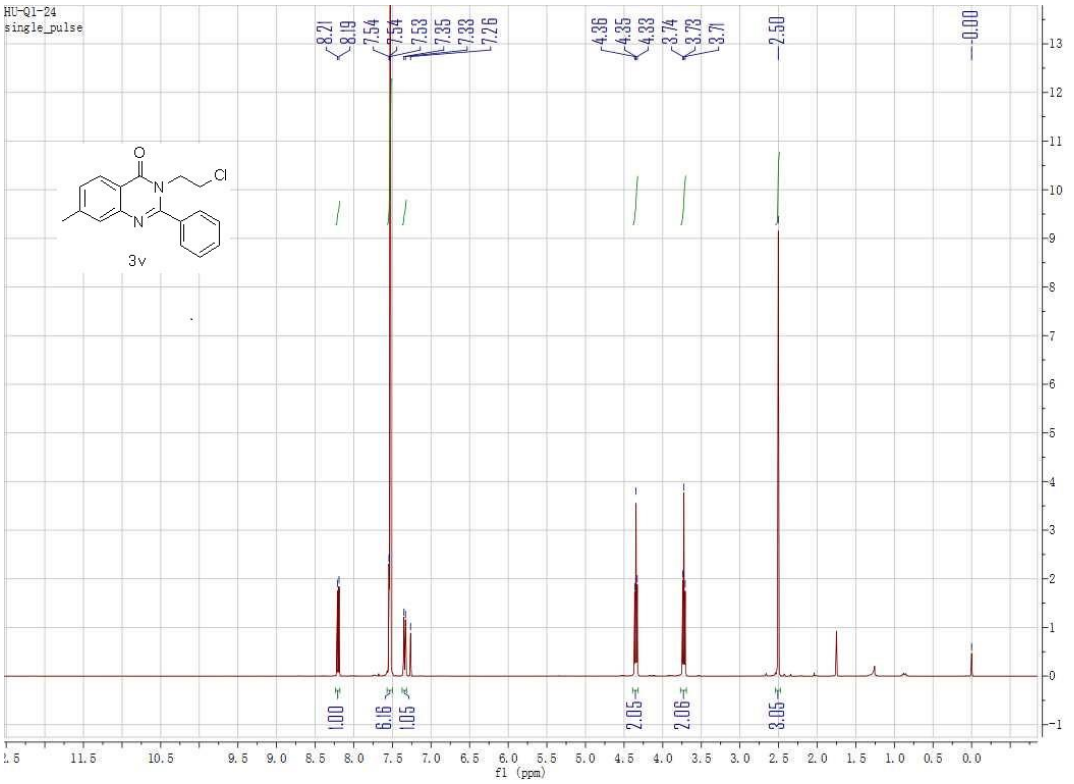

HU-Q1-21
single pulse decoupled gated NOE
162.60
159.95
159.35
159.31
157.11
149.13
135.19
135.09
134.81
130.34
129.06
128.23
123.68
113.92
113.79
113.71
77.46
77.14
76.82
47.17
40.43
40.36
F
O
N
Cl
N
3s
f1 (ppm)

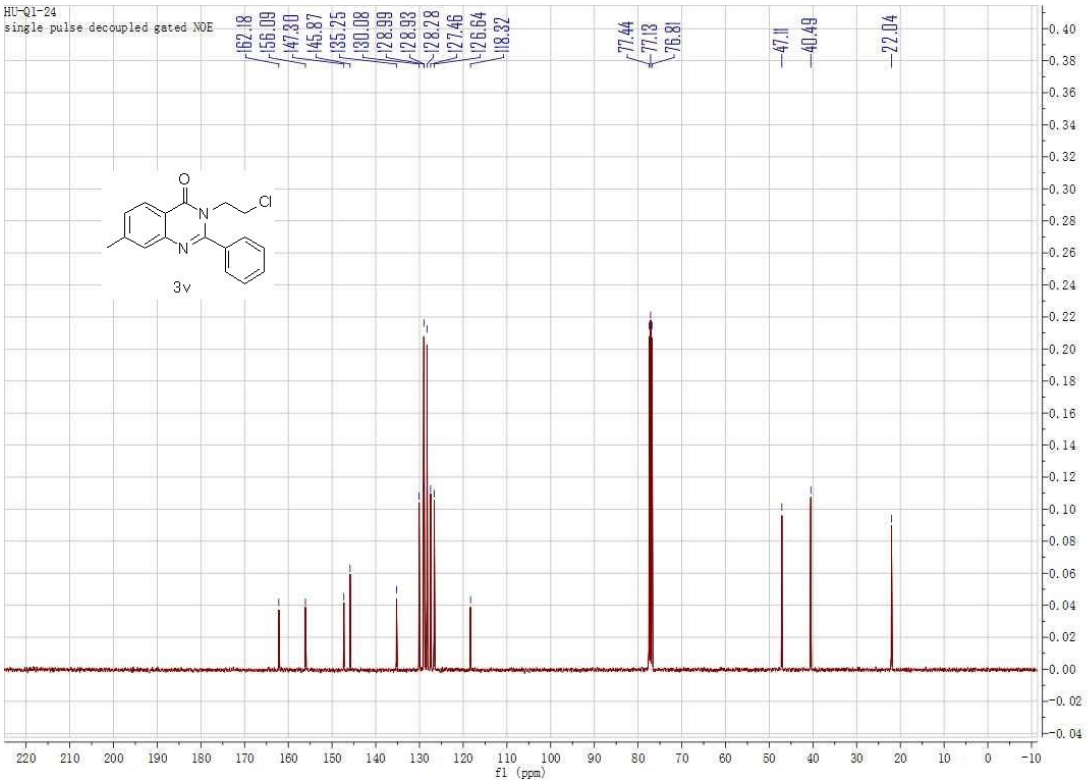

HU-Q1-22
single_pulse
8.27
8.27
8.27
7.72
7.71
7.70
7.69
7.67
7.57
7.54
7.27
4.38
4.36
4.35
3.74
3.72
3.71
0.00
Cl
O
N
Cl
N
3t
0.95
2.18
5.44
2.15
2.21
f1 (ppm)

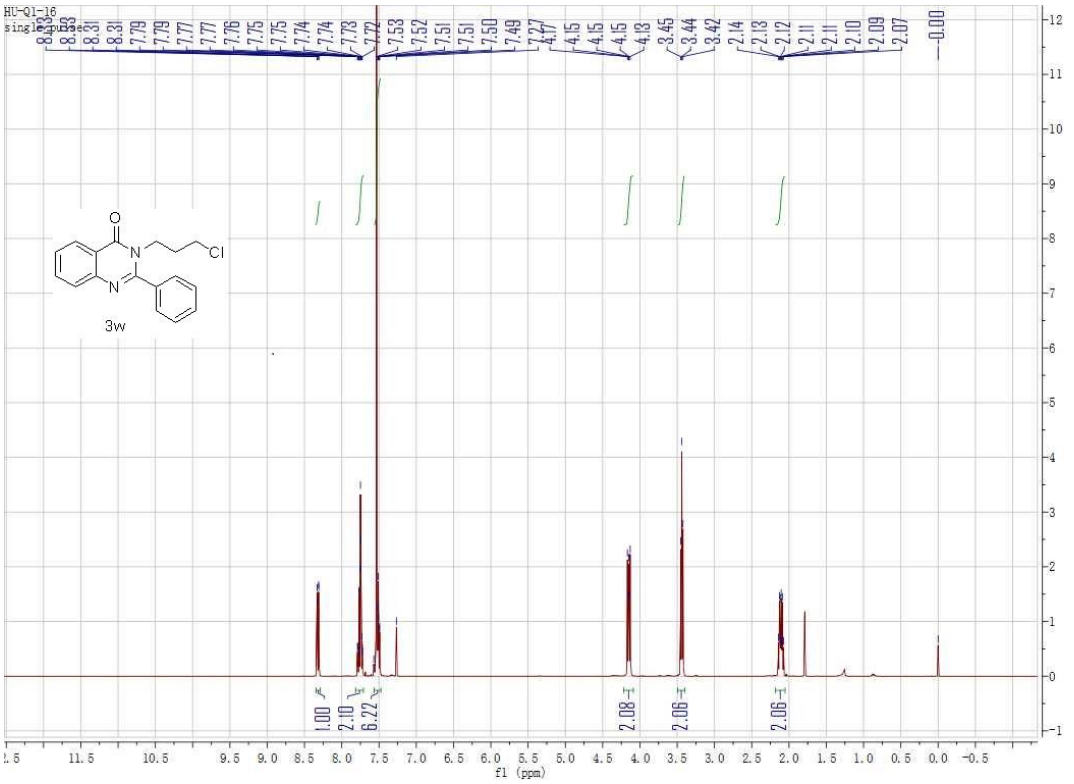

HU-Q1-22
single pulse decoupled gated
161.28
155.80
145.69
135.21
134.84
133.12
130.41
130.25
129.42
129.15
128.99
128.87
128.18
126.24
126.08
121.72
77.48
77.16
76.84
47.33
47.21
40.50
40.33
Cl
O
N
Cl
N
3t
f1 (ppm)

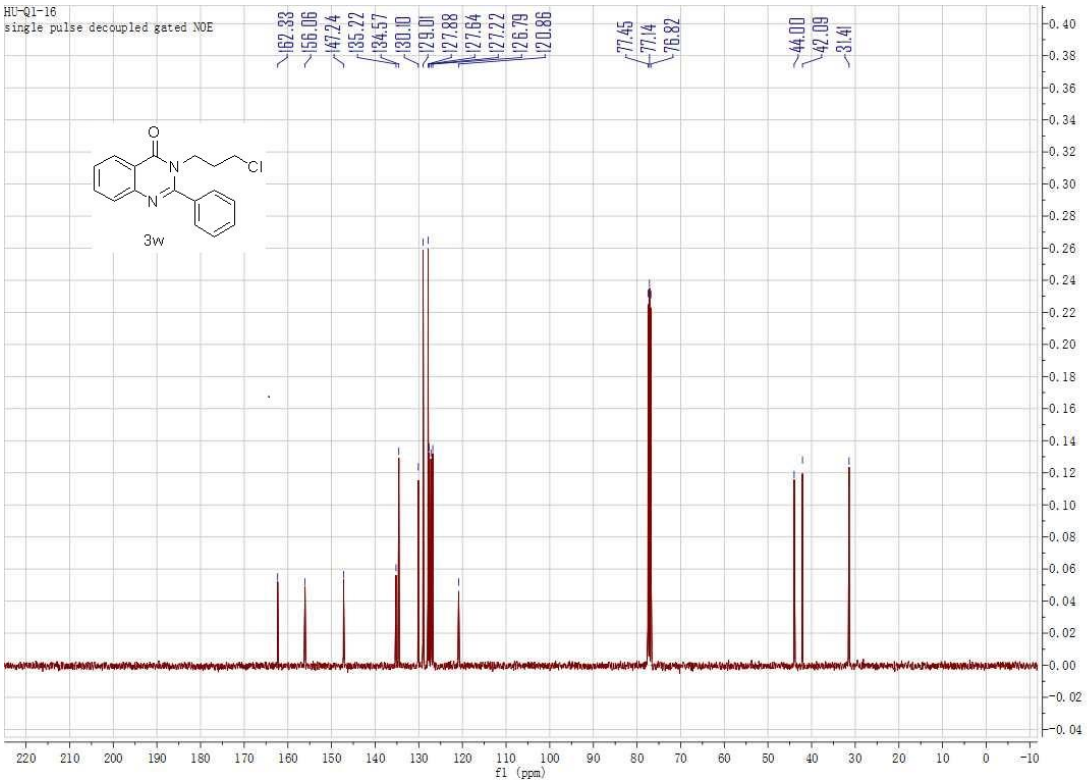

HU-Q1-23 1
single_pulse
O
N
Cl
Br
N
3u
1.06
1.00
1.08
5.32
2.12
2.12
f1 (ppm)

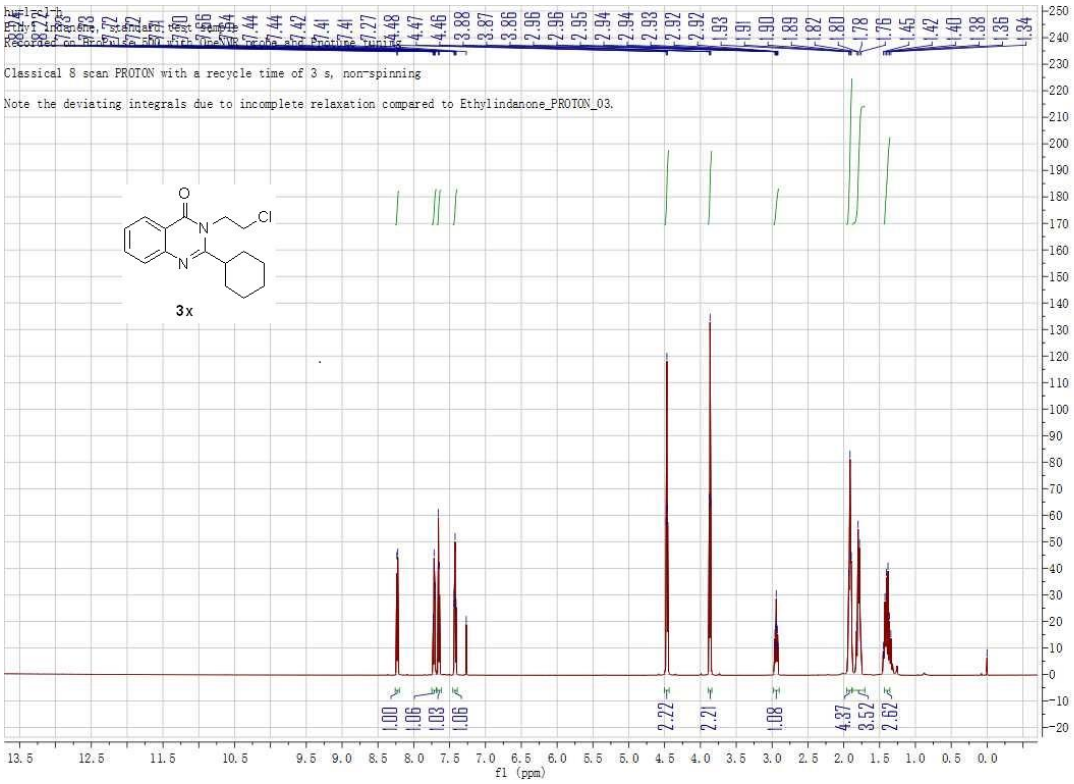

HU-Q1-23 1
single pulse decoupled gated NOE
161.80
157.31
148.14
134.82
130.71
130.49
130.37
129.53
129.06
128.29
128.25
119.50
77.46
77.14
76.83
47.28
40.34
O
N
Cl
Br
N
3u
f1 (ppm)

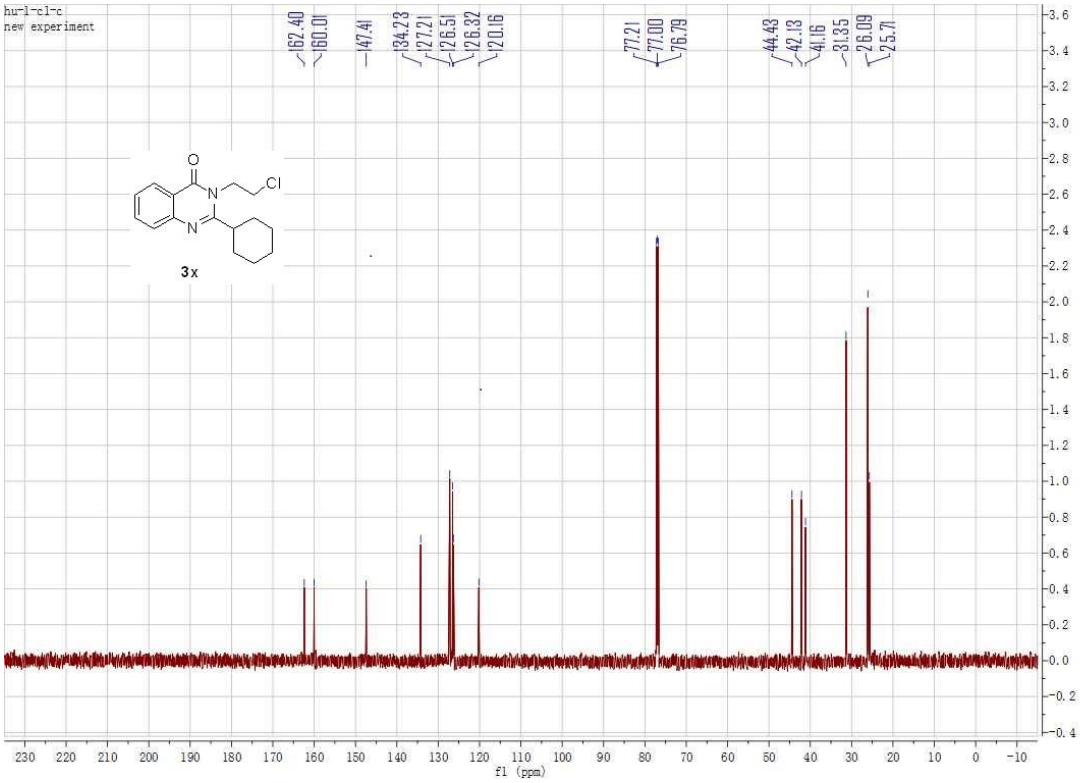

HU-Q1-24
single_pulse
8.21
8.19
7.54
7.54
7.53
7.35
7.33
7.26
4.36
4.35
4.33
3.74
3.73
3.71
2.50
0.00
3v
1.00
6.16
1.05
2.05
2.06
3.05
fl (ppm)

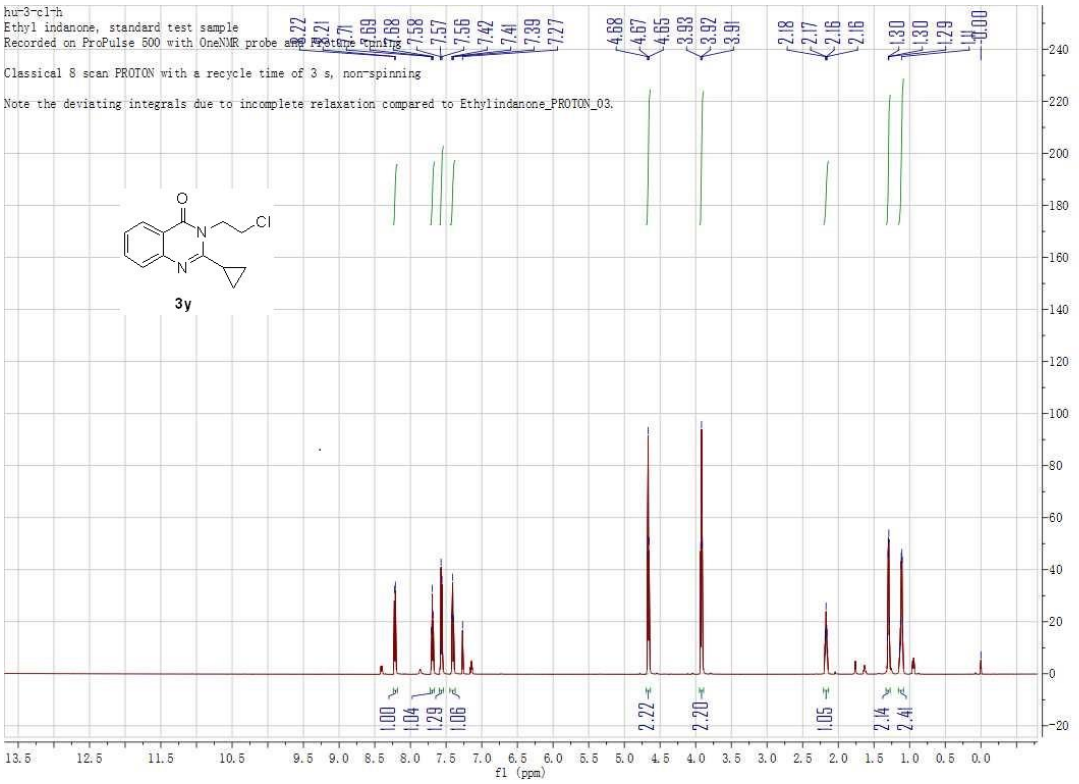

HU-Q1-24
single pulse decoupled gated NOE
162.18
156.09
147.30
145.87
135.25
130.08
128.99
128.93
128.28
127.46
126.64
118.32
77.44
77.13
76.81
47.11
40.49
22.04
3v
fl (ppm)

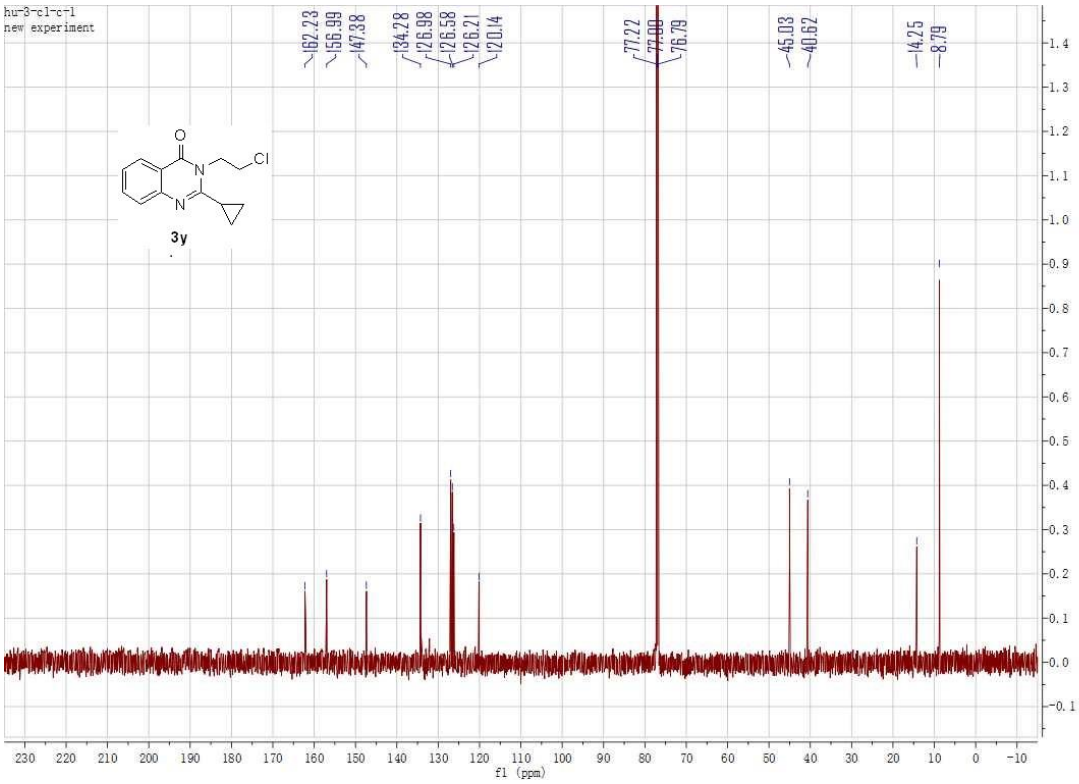

HU-Q1-16
3w
fl (ppm)

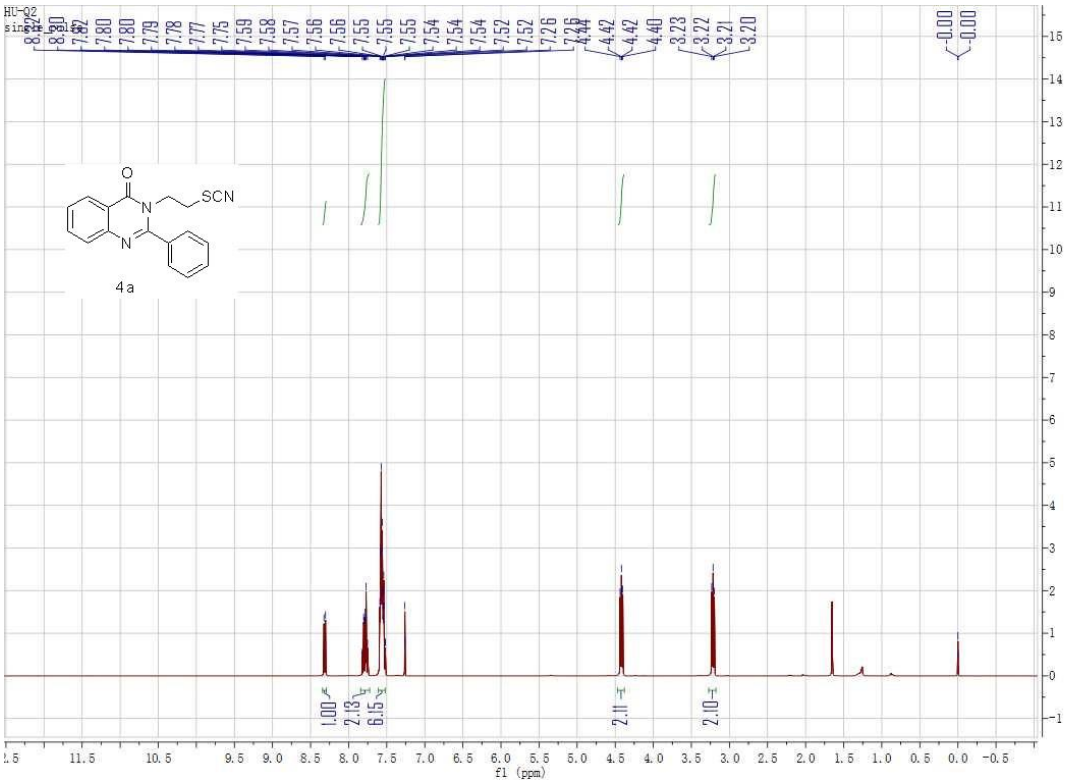

HU-Q1-16
single pulse decoupled gated NOE
3w
fl (ppm)

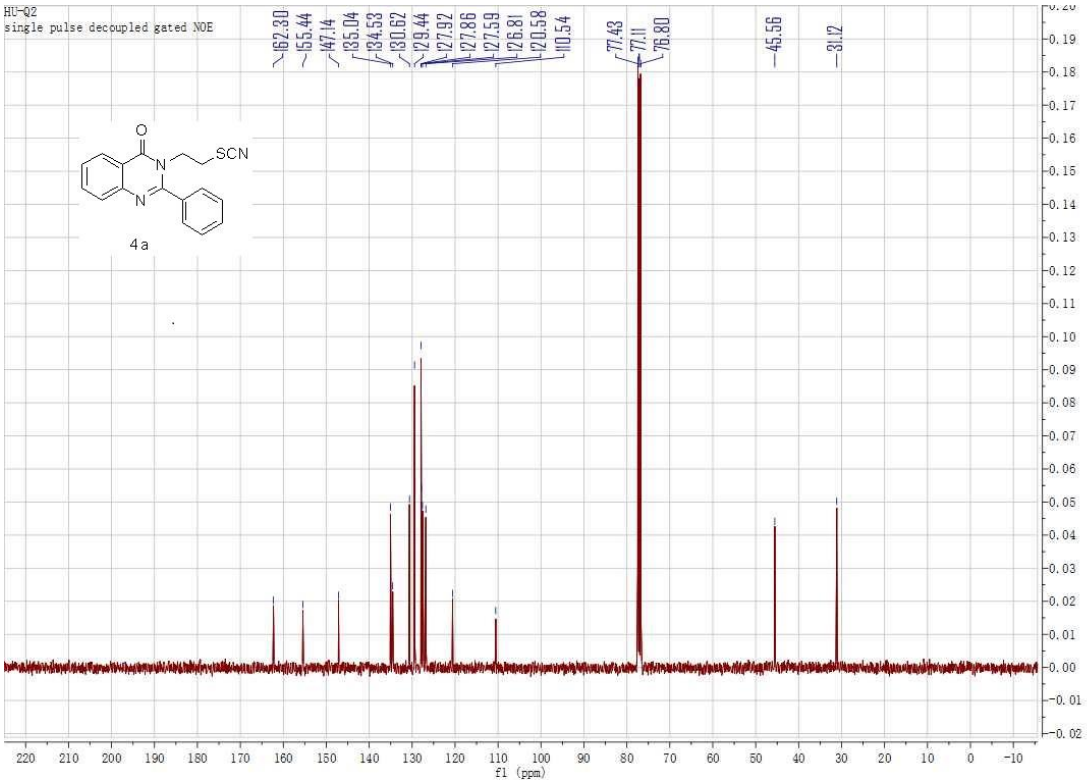

Classical 8 scan PROTON with a recycle time of 3 s, non-spinning
Note the deviating integrals due to incomplete relaxation compared to Ethylindanone_PROTON_03.
3x
f1 (ppm)

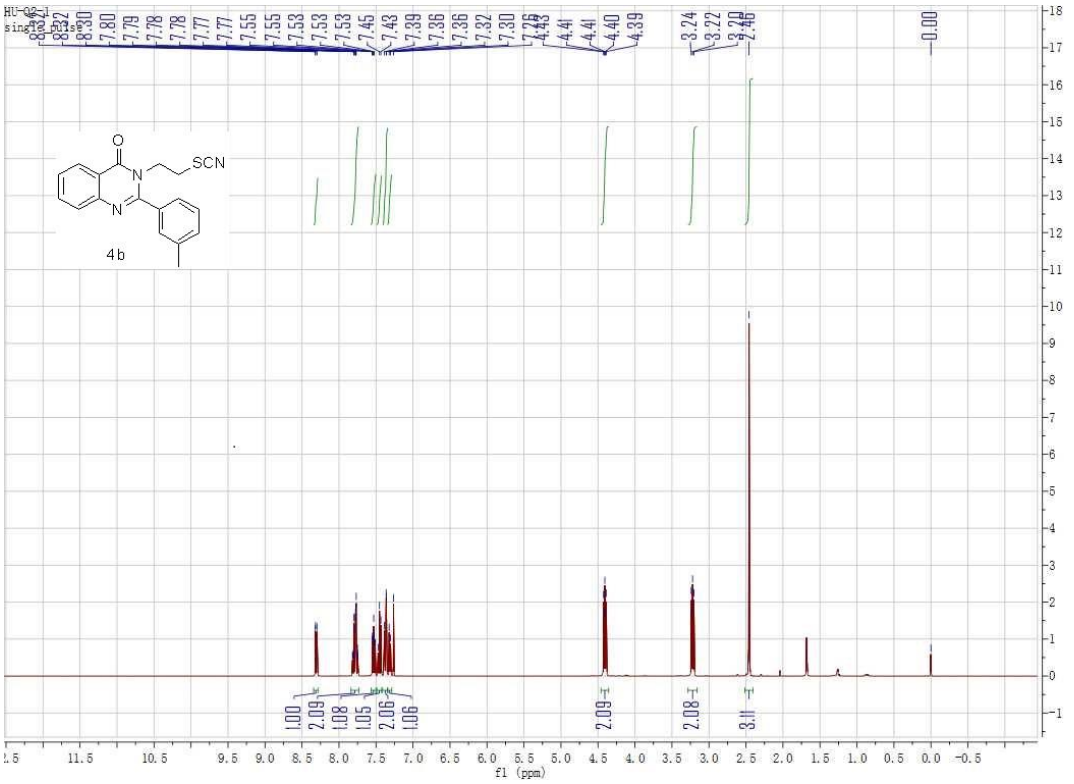

hu-1-c1-c
new experiment
3x
f1 (ppm)

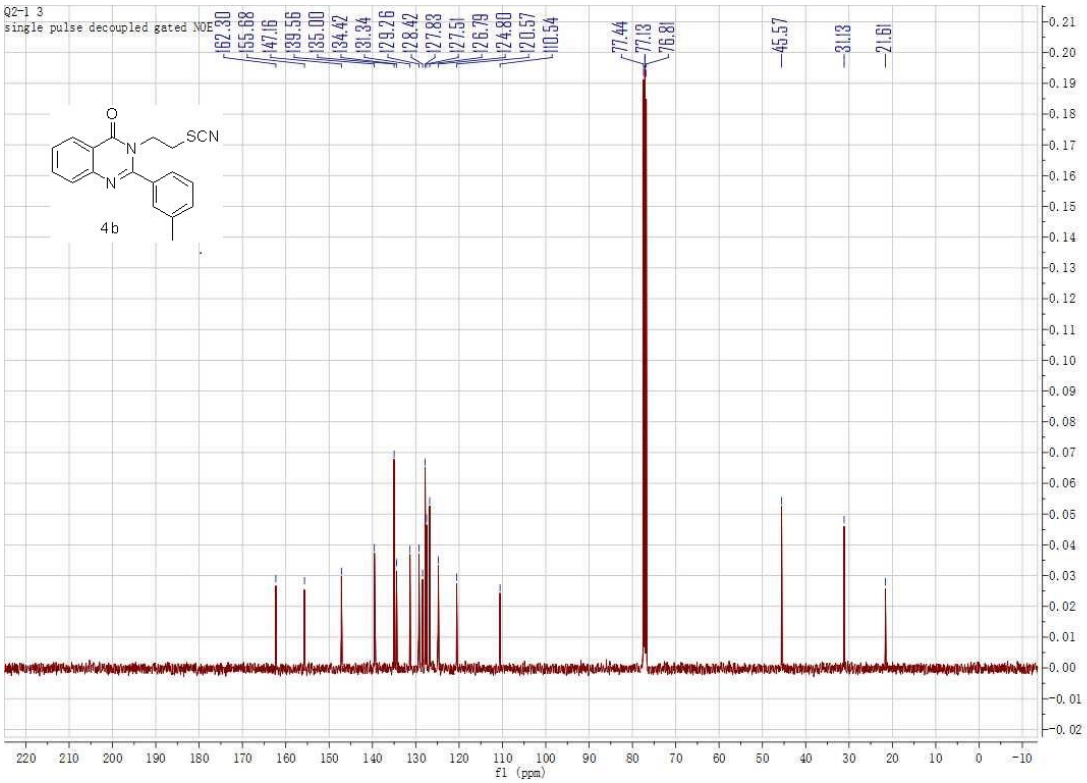

hu-3-cl-h
Ethyl indanone, standard test sample
Recorded on ProPulse 500 with OneNMR probe and Protune spinning
Classical 8 scan PROTON with a recycle time of 3 s, non-spinning
Note the deviating integrals due to incomplete relaxation compared to Ethylindanone_PROTON_03.
3y
f1 (ppm)

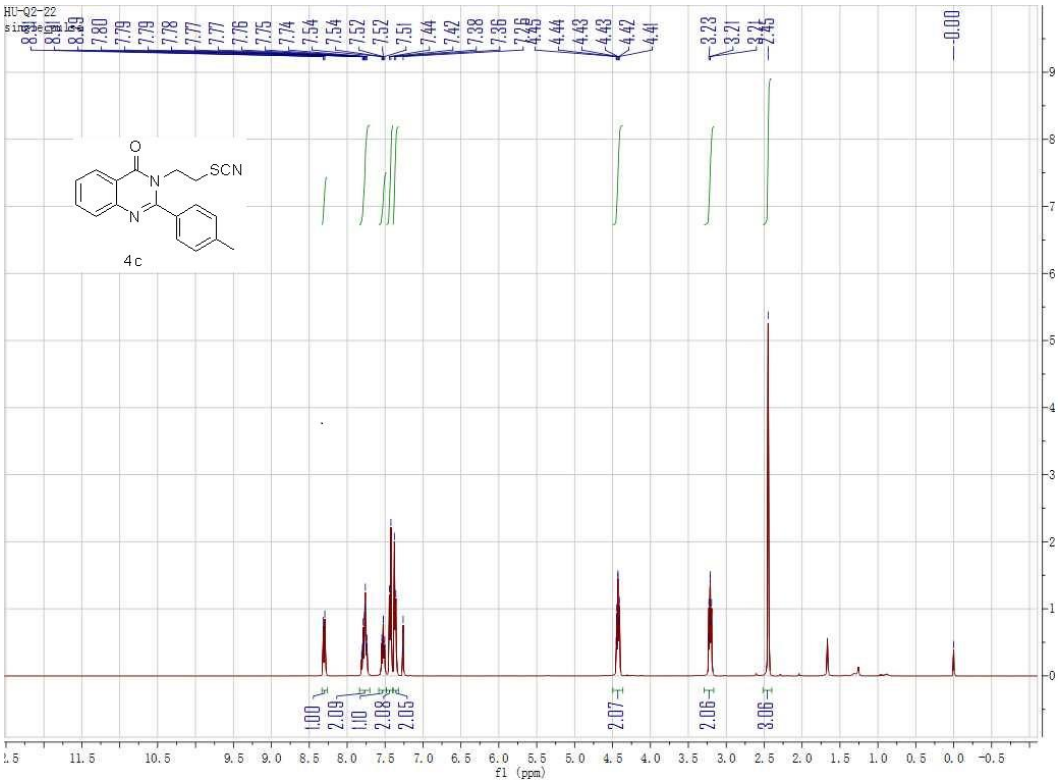

hu-3-cl-c-1
new experiment
3y
f1 (ppm)

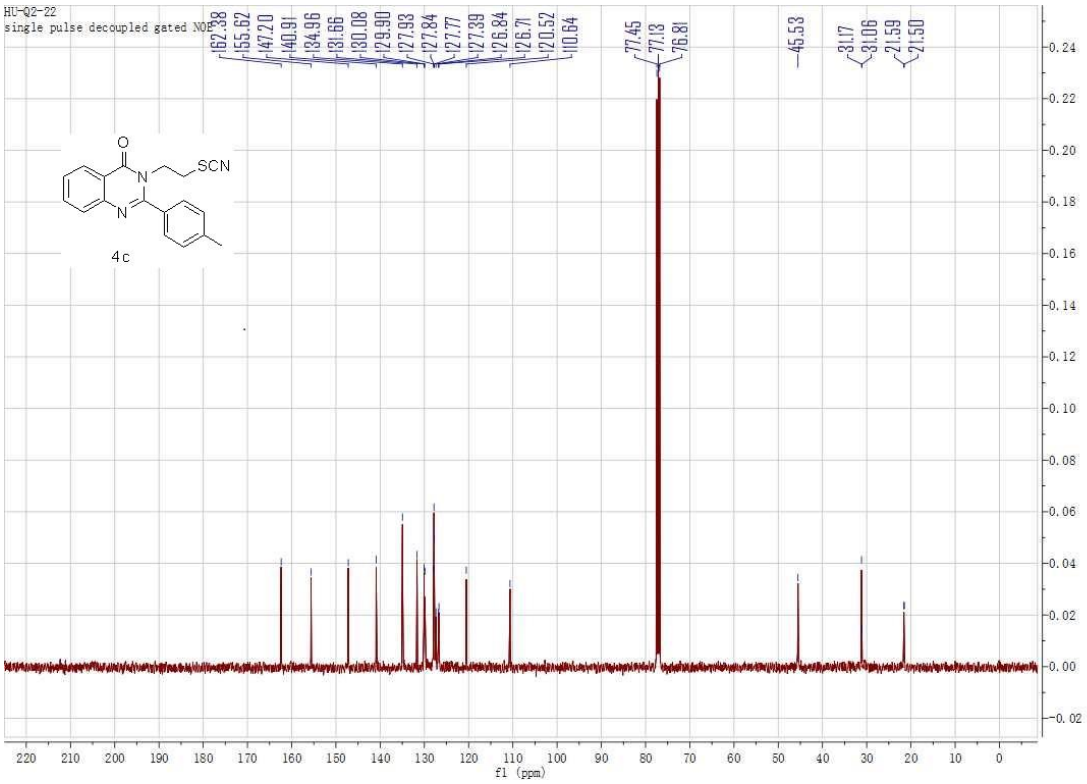

SCN
4a
fl (ppm)

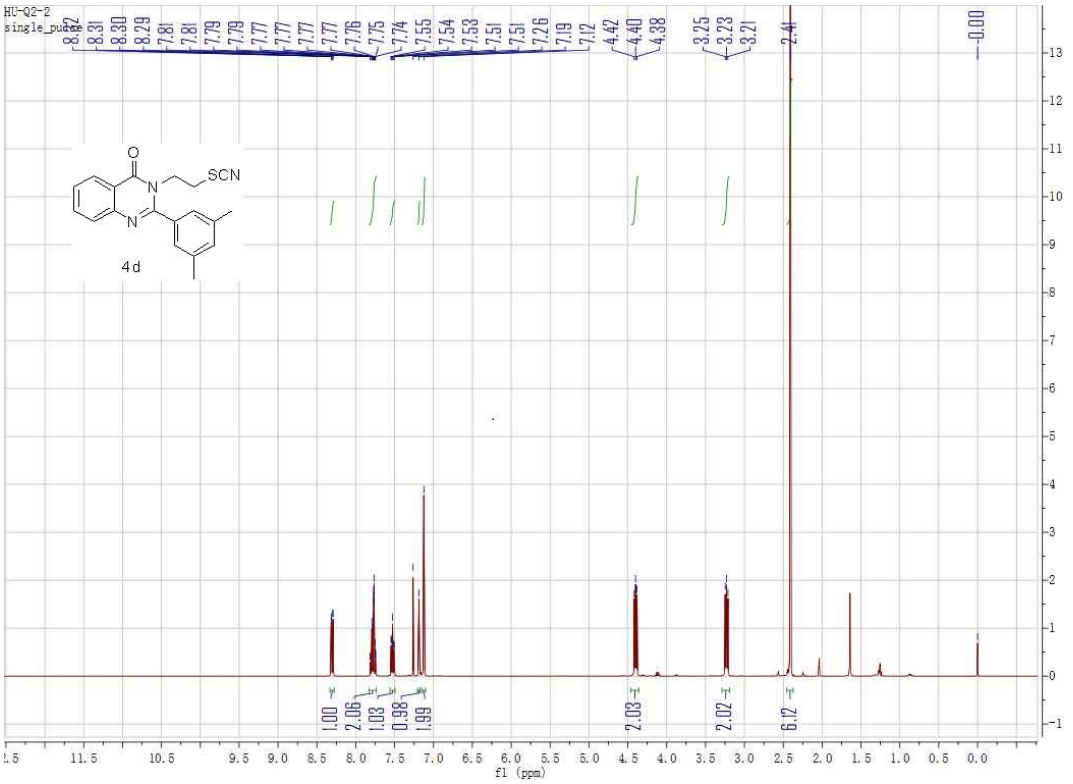

HU-Q2
single pulse decoupled gated NOE
SCN
4a
fl (ppm)

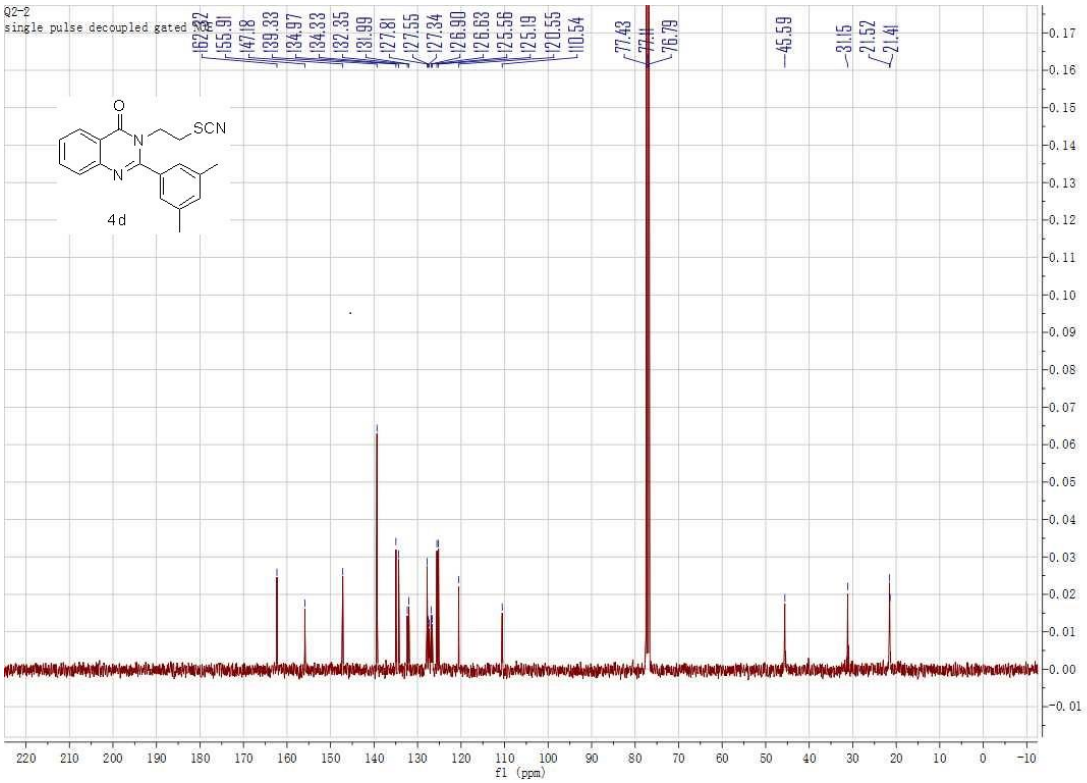

SCN
4b
fl (ppm)

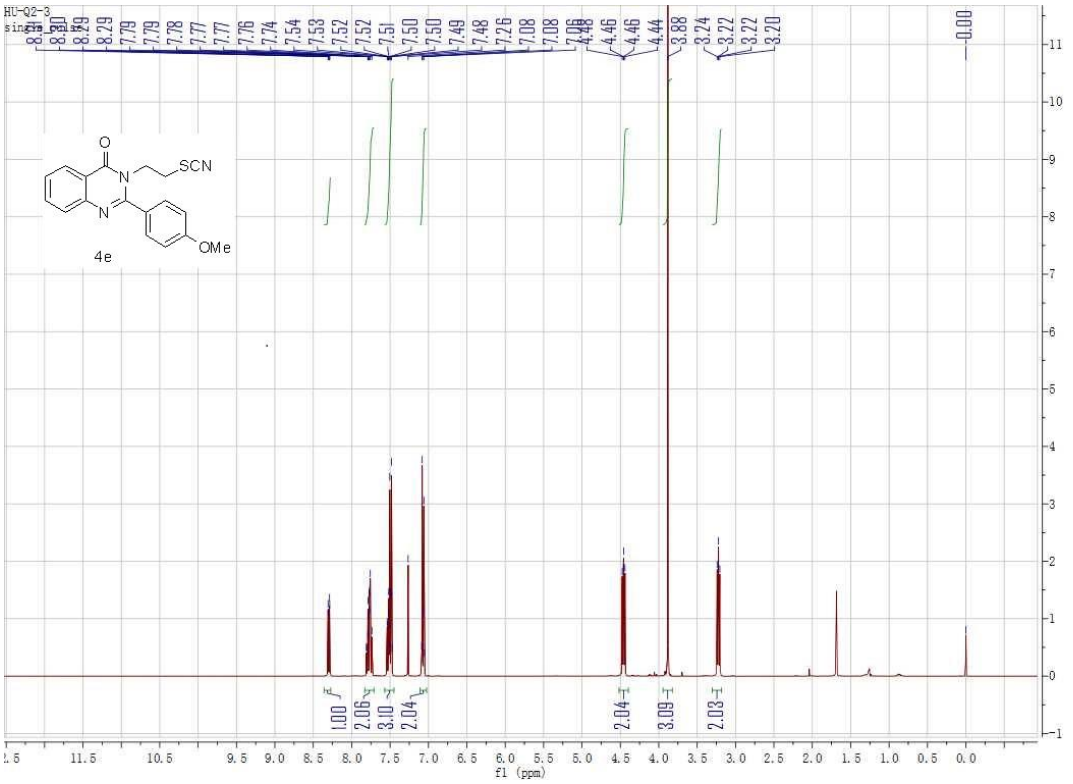

Q2-1 3
single pulse decoupled gated NOE
SCN
4b
fl (ppm)

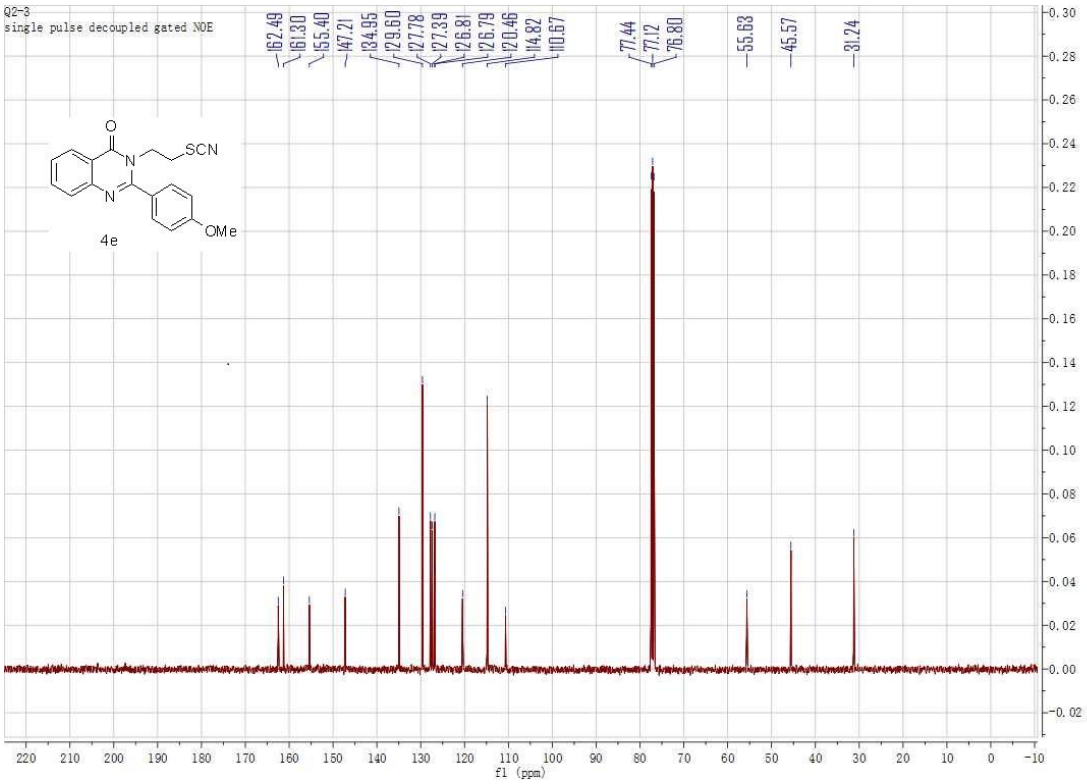

HU-Q2-22
SCN
4c
f1 (ppm)

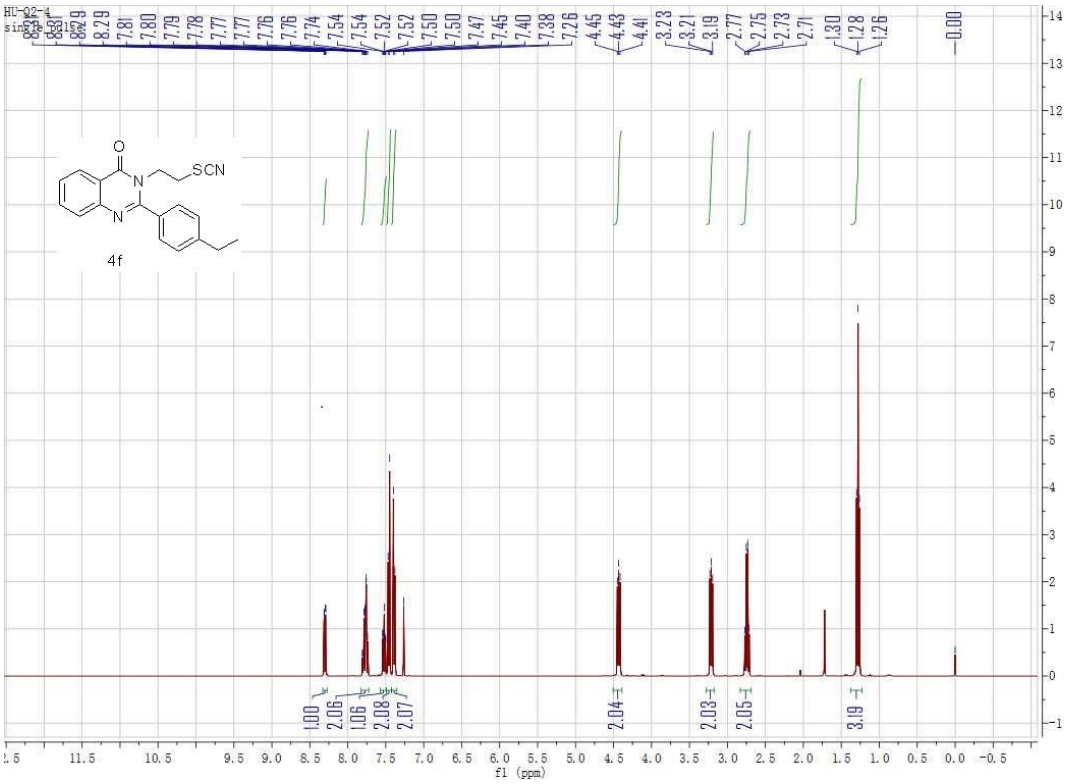

HU-Q2-22
single pulse decoupled gated NOE
SCN
4c
f1 (ppm)

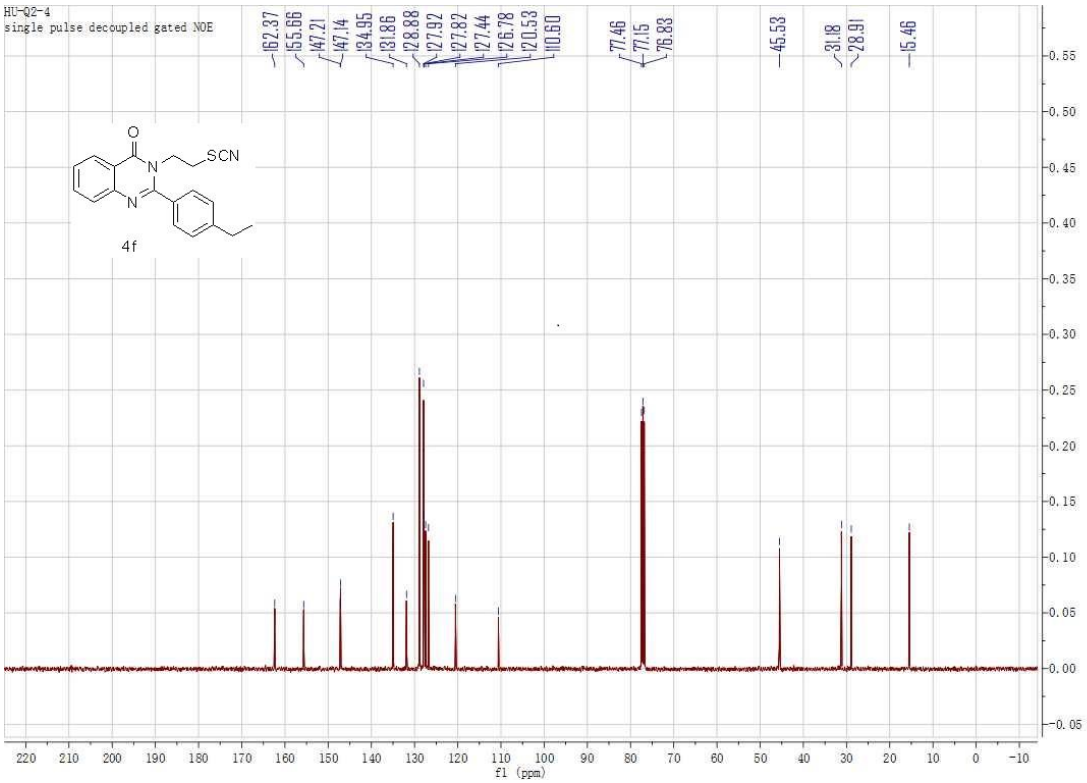

HU-Q2-2
single_pulse
8.32
8.31
8.30
8.29
7.81
7.81
7.79
7.79
7.77
7.77
7.77
7.77
7.76
7.75
7.74
7.55
7.54
7.53
7.51
7.51
7.26
7.19
7.12
4.42
4.40
4.38
3.25
3.23
3.21
2.41
0.00
SCN
4d
1.00
2.06
1.03
0.98
1.99
2.03
2.02
6.12
f1 (ppm)

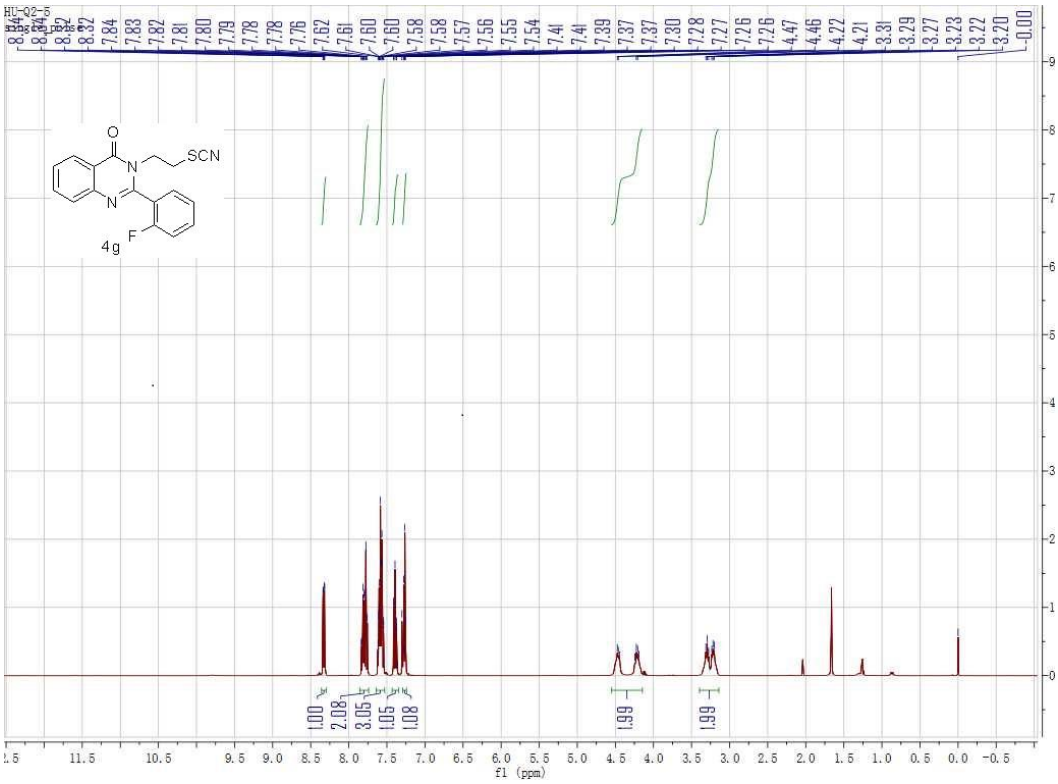

Q2-2
single pulse decoupled gated
162.82
155.91
147.18
139.33
134.97
134.33
132.35
131.99
127.81
127.55
127.34
126.90
126.63
125.56
125.19
120.55
110.54
77.43
77.11
76.79
45.59
31.15
21.52
21.41
SCN
4d
f1 (ppm)

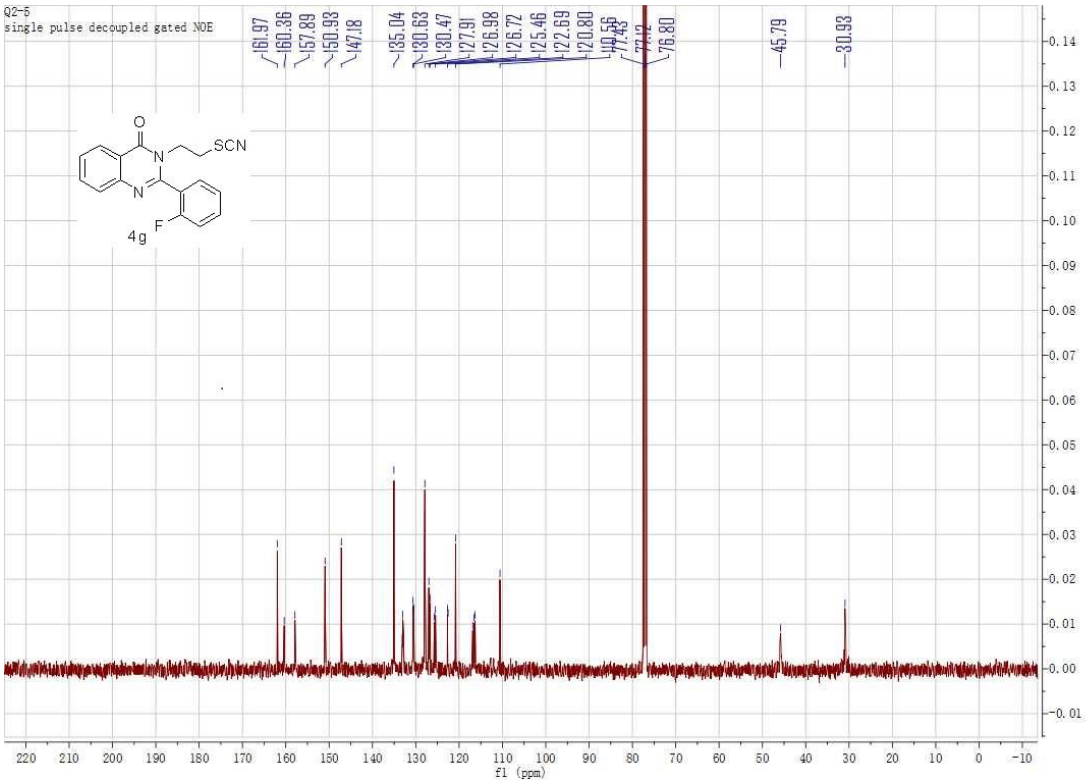

HU-Q2-3
SCN
OMe
4e
f1 (ppm)

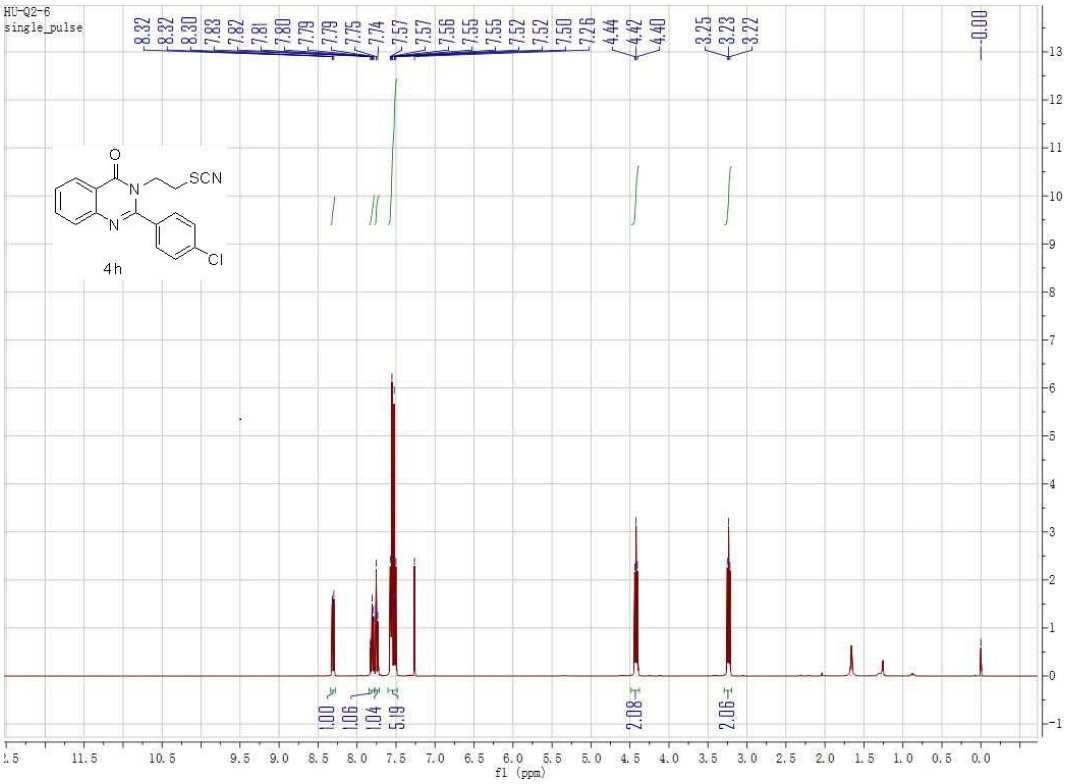

Q2-3
single pulse decoupled gated NOE
SCN
OMe
4e
f1 (ppm)

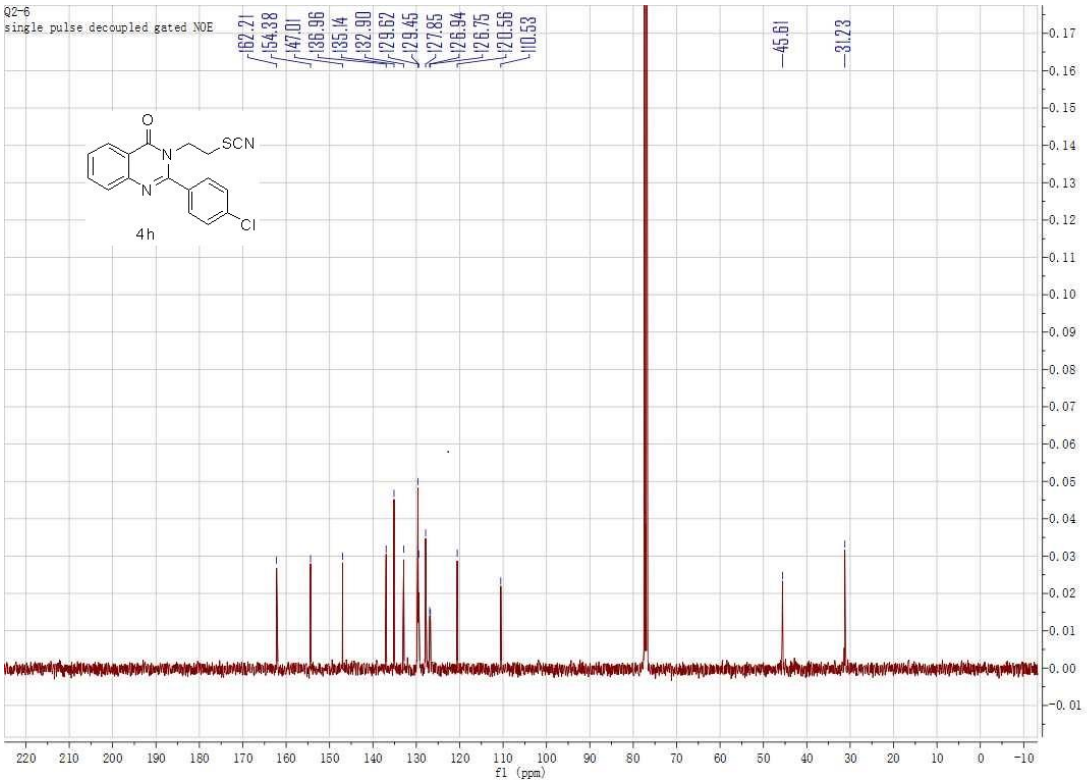

HU-Q2-4
8.29
7.81
7.80
7.79
7.78
7.77
7.77
7.76
7.76
7.74
7.54
7.54
7.52
7.52
7.50
7.50
7.47
7.45
7.40
7.38
7.26
4.45
4.43
4.41
3.23
3.21
3.19
2.77
2.75
2.73
2.71
1.30
1.28
1.26
0.00
SCN
4f
1.00
2.06
1.06
2.08
2.07
2.04
2.03
2.05
3.19
fl (ppm)

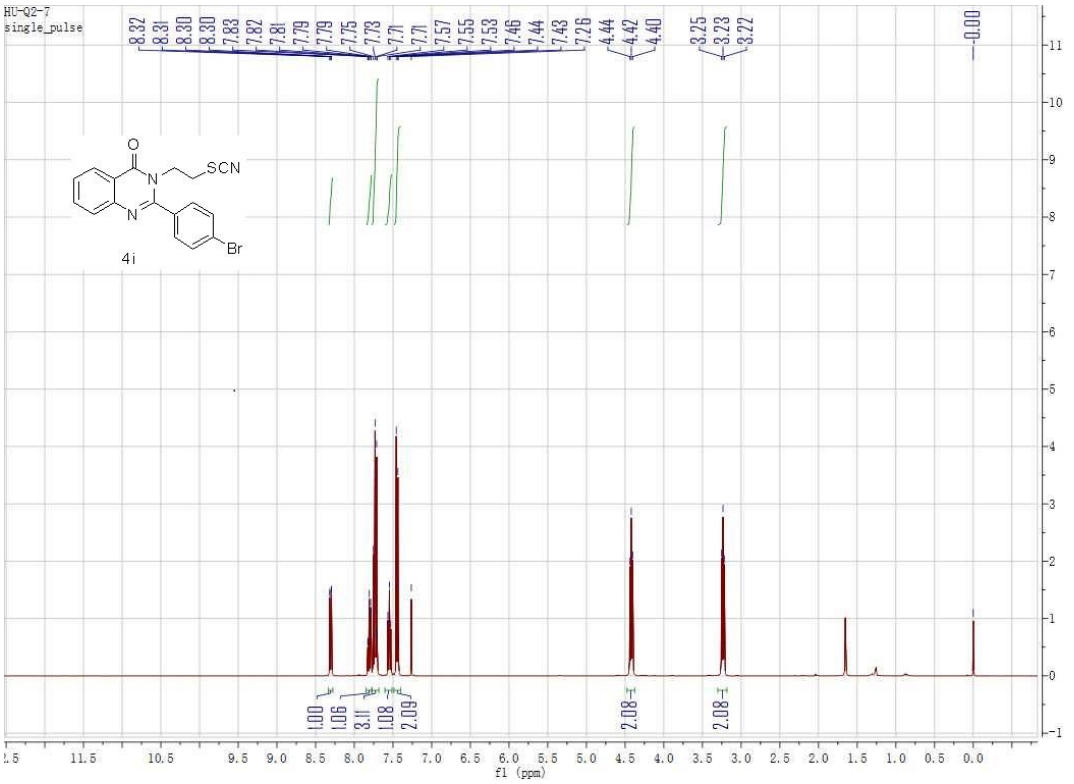

HU-Q2-4
single pulse decoupled gated NOE
162.37
155.66
147.21
147.14
134.95
131.86
128.88
127.92
127.82
127.44
126.78
120.53
110.60
77.46
77.15
76.83
45.53
31.18
28.91
15.46
SCN
4f
fl (ppm)

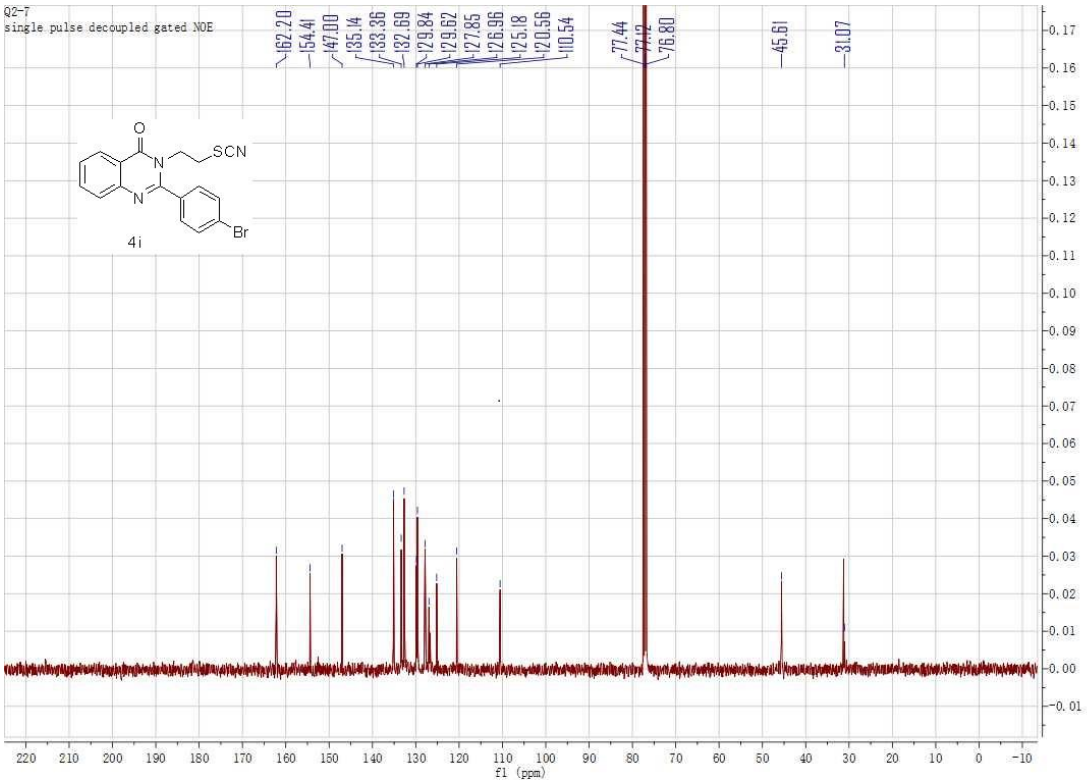

HL-Q2-5
SCN
4g
F
fl (ppm)

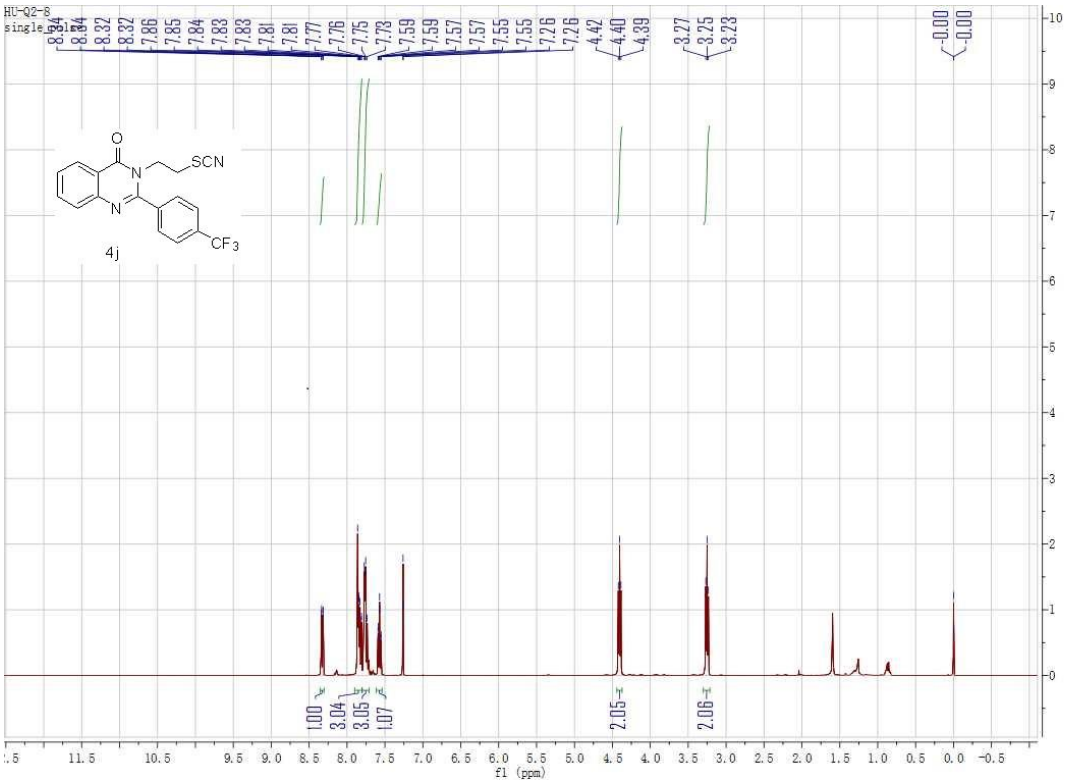

Q2-5
single pulse decoupled gated NOE
SCN
4g
F
fl (ppm)

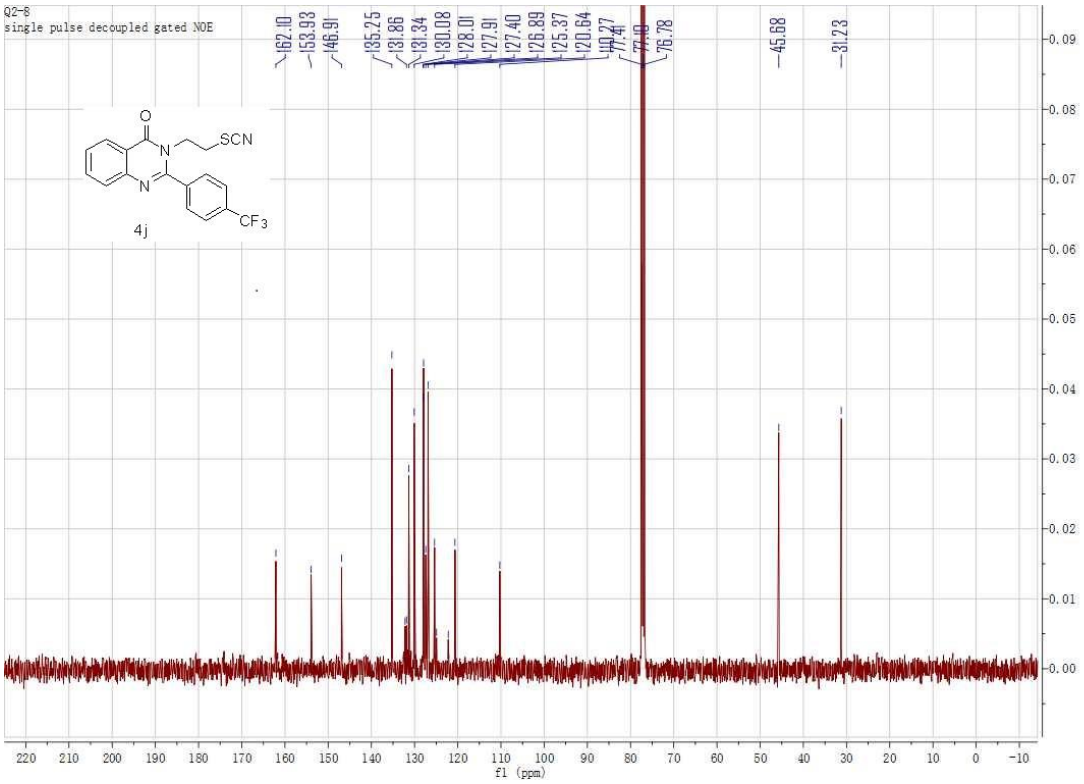

HU-Q2-6
single_pulse
8.32
8.32
8.30
7.83
7.82
7.81
7.80
7.79
7.79
7.75
7.74
7.57
7.57
7.56
7.55
7.55
7.52
7.52
7.50
7.26
4.44
4.42
4.40
3.25
3.23
3.22
0.00
SCN
Cl
4h
1.00
1.06
1.04
5.19
2.08
2.06
f1 (ppm)

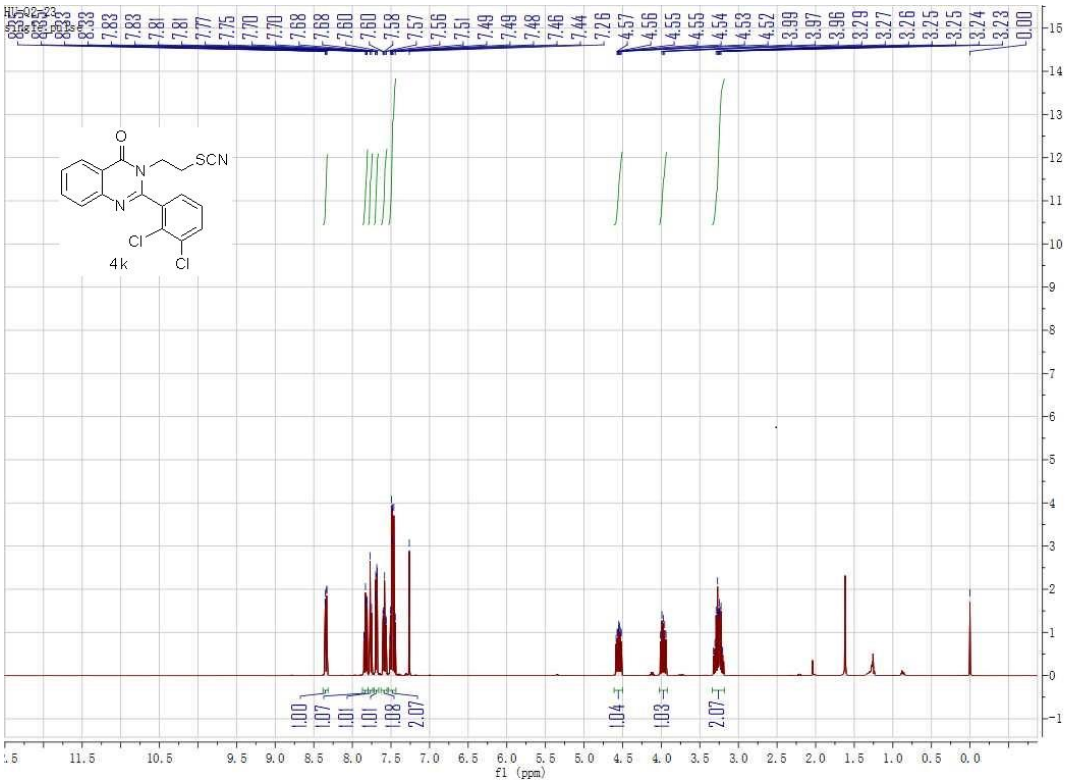

Q2-6
single pulse decoupled gated NOE
162.21
154.38
147.01
136.96
135.14
132.90
129.62
129.45
127.85
126.94
126.75
120.56
110.53
45.61
31.23
SCN
Cl
4h
f1 (ppm)

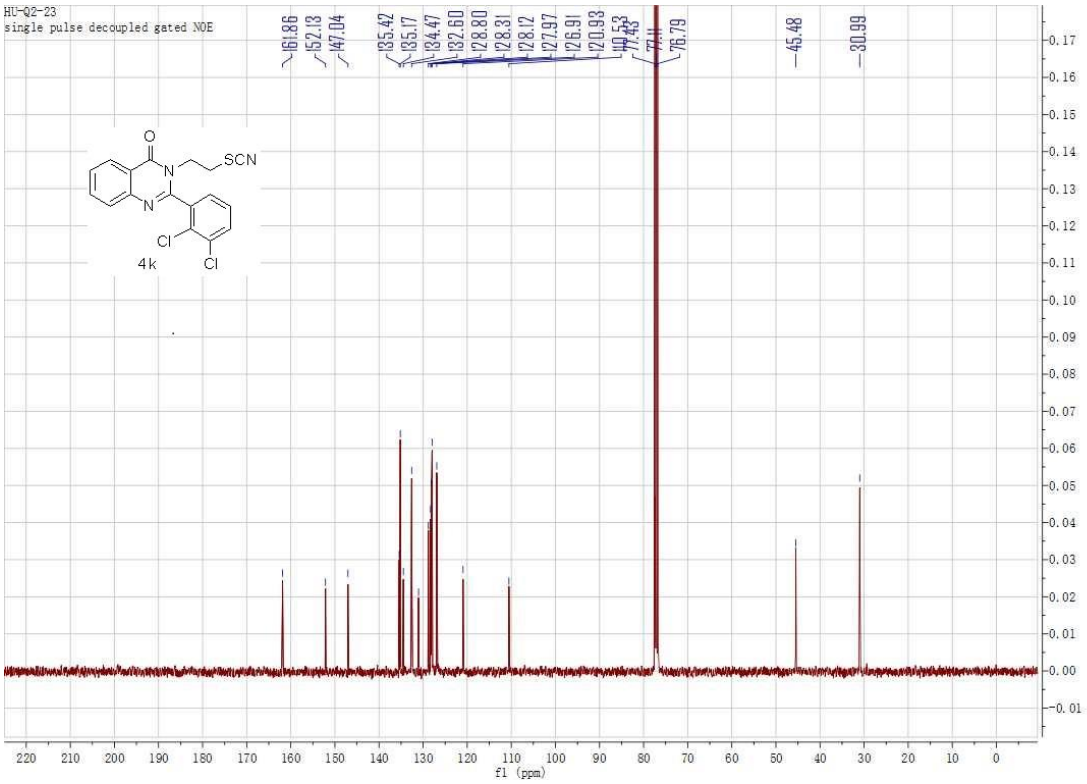

HU-Q2-7
single_pulse
8.32
8.31
8.30
8.30
7.83
7.82
7.81
7.79
7.79
7.75
7.73
7.71
7.71
7.57
7.55
7.53
7.46
7.44
7.43
7.26
4.44
4.42
4.40
3.25
3.23
3.22
0.00
SCN
Br
4i
1.00
1.06
8.11
1.08
2.09
2.08
2.08
f1 (ppm)

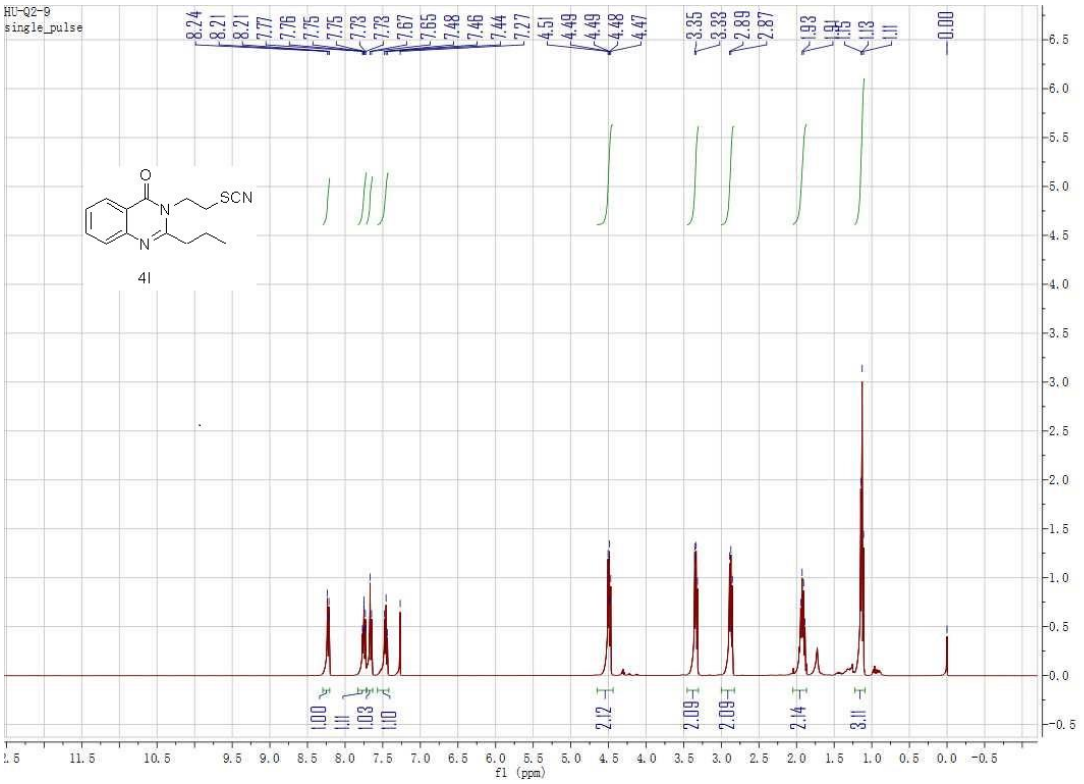

Q2-7
single pulse decoupled gated NOE
162.20
154.41
147.00
135.14
133.36
132.69
129.84
129.62
127.85
126.96
125.18
120.56
110.54
77.44
76.80
45.61
31.07
SCN
Br
4i
f1 (ppm)

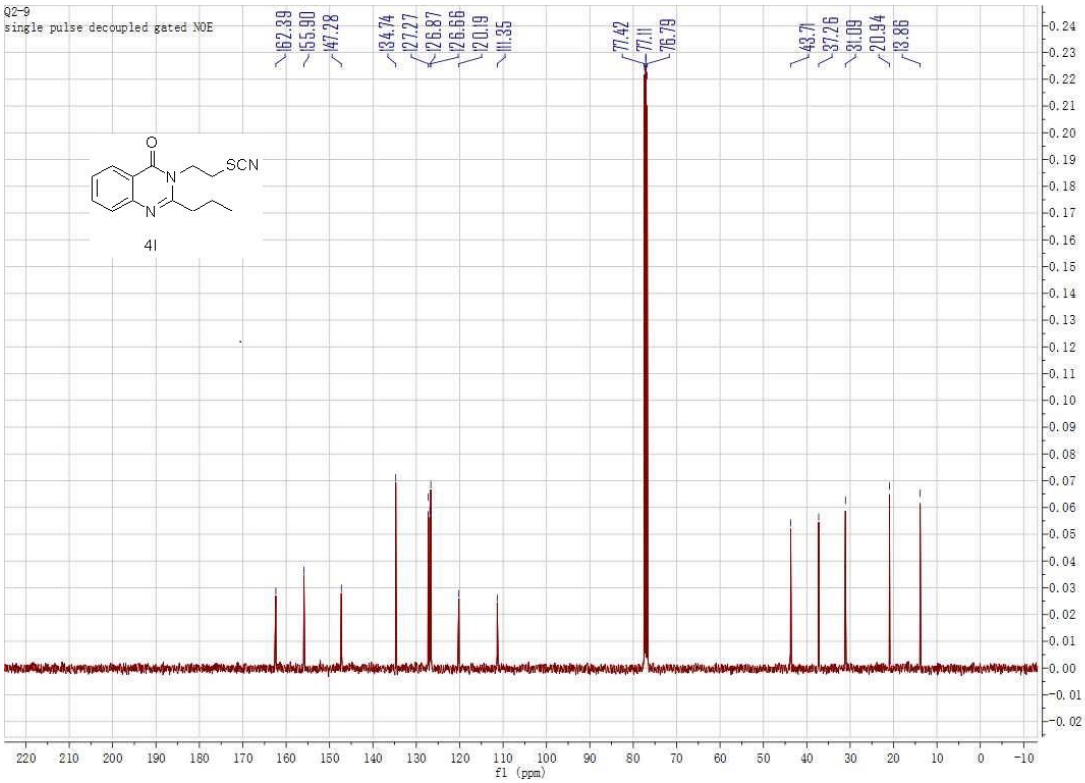

HU-Q2-8
single_pulse
8.34
8.32
7.86
7.85
7.84
7.83
7.81
7.77
7.76
7.75
7.73
7.59
7.57
7.55
7.26
4.42
4.40
4.39
3.27
3.25
3.23
0.00
1.00
3.04
8.05
1.07
2.05
2.06
f1 (ppm)
SCN
CF3
4j

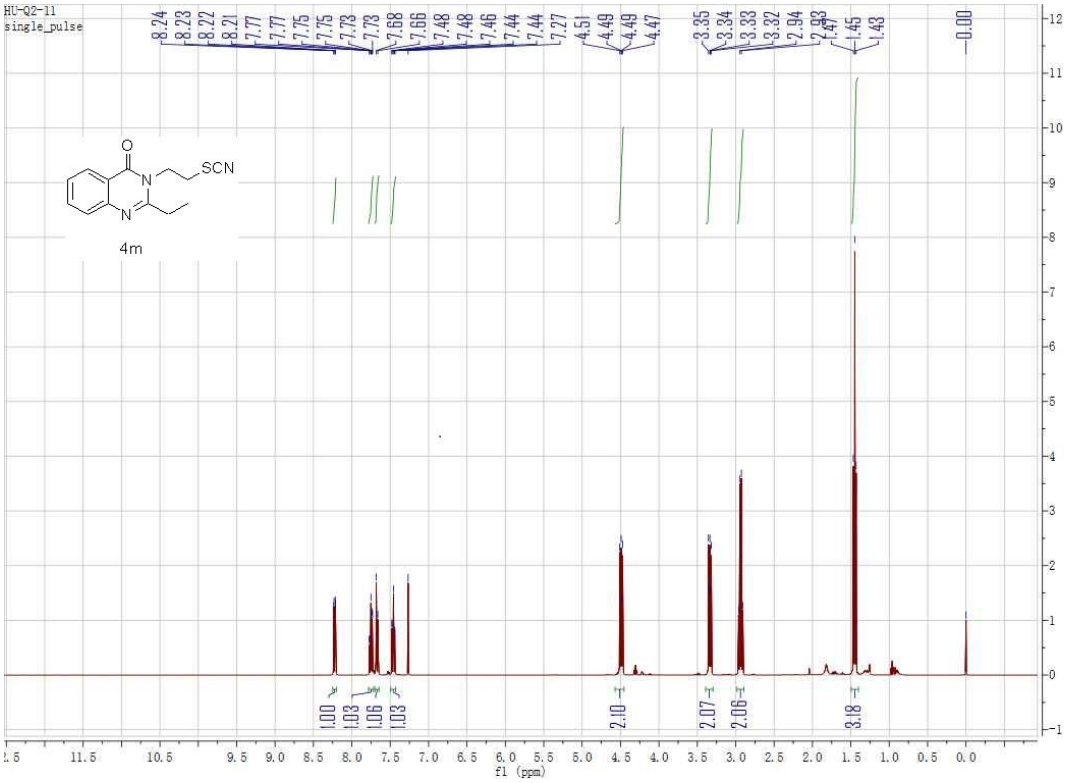

Q2-8
single pulse decoupled gated NOE
162.10
153.93
146.91
135.25
131.86
131.34
130.08
128.01
127.91
127.40
126.89
125.37
120.64
110.27
77.41
77.00
76.78
45.68
31.23
f1 (ppm)
SCN
CF3
4j

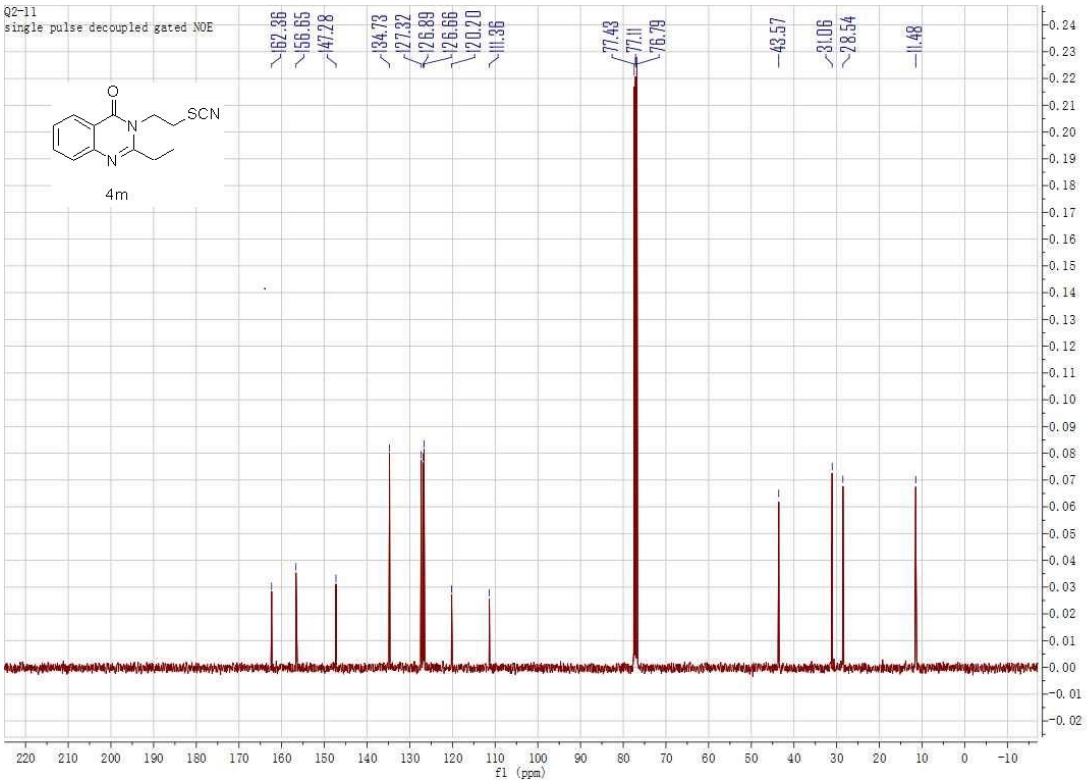

HU-Q2-23
O
N
N
SCN
Cl
Cl
4k
fl (ppm)

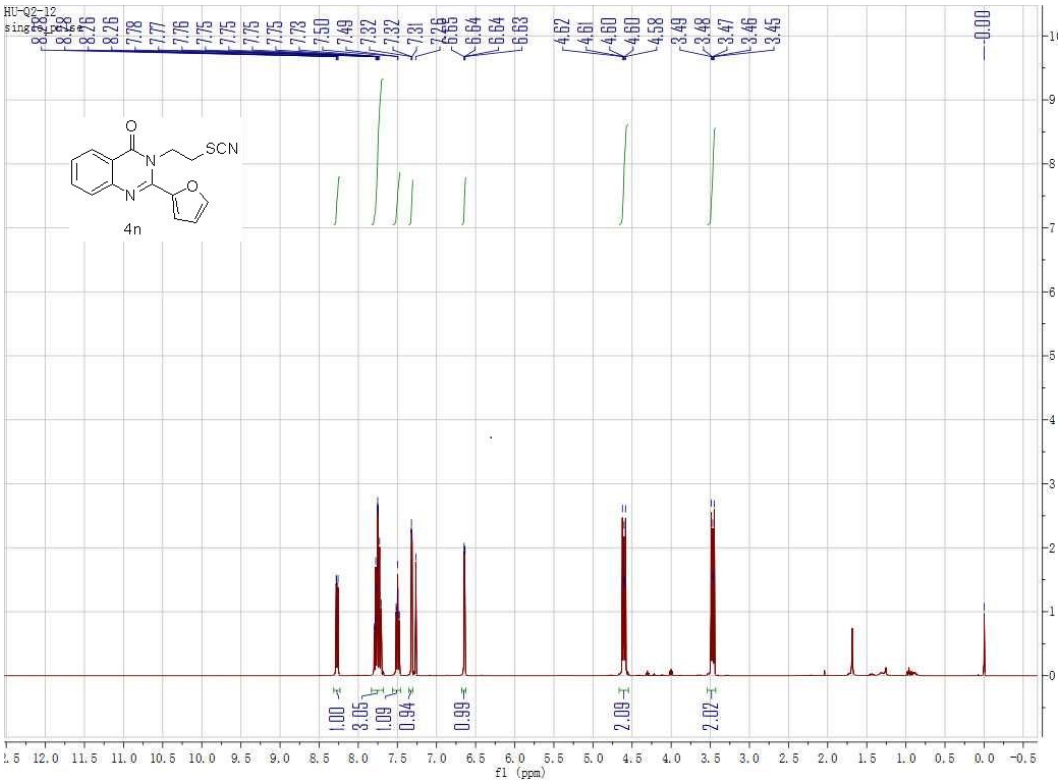

HU-Q2-23
single pulse decoupled gated NOE
161.86
152.13
147.04
135.42
135.17
134.47
132.60
128.80
128.31
128.12
127.97
126.91
120.93
77.11
76.79
45.48
30.99
O
N
N
SCN
Cl
Cl
4k
fl (ppm)

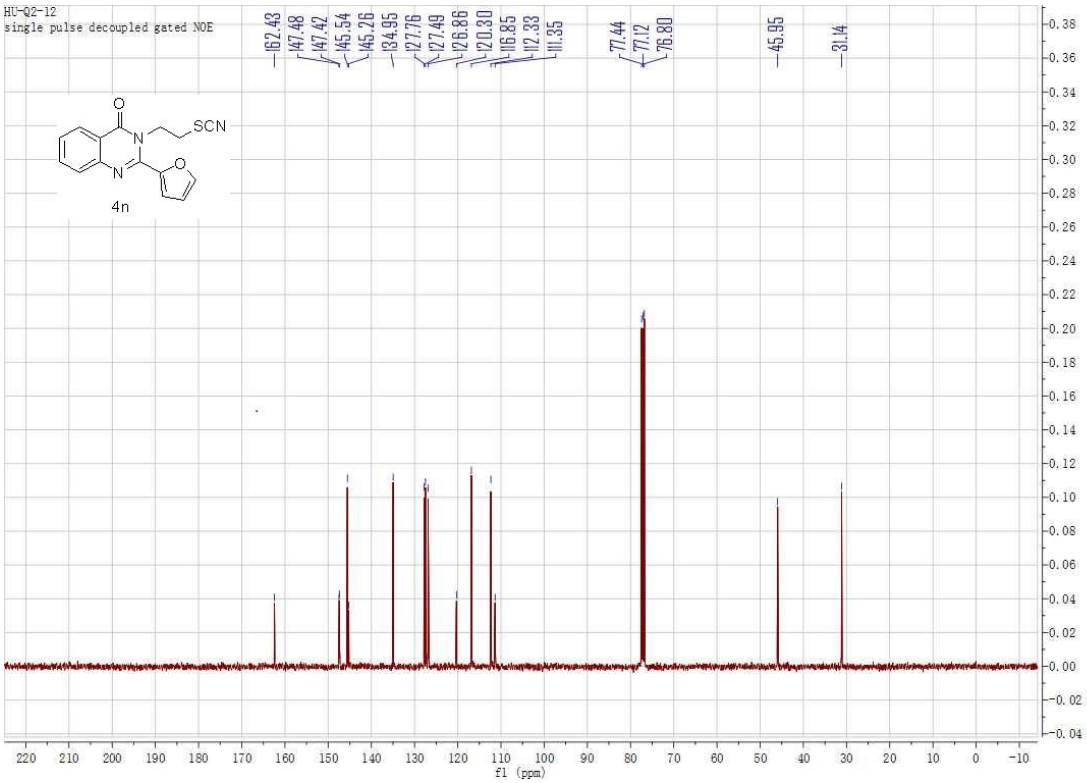

HU-Q2-9
single_pulse
8.24
8.21
8.21
7.77
7.76
7.75
7.75
7.73
7.73
7.67
7.65
7.48
7.46
7.44
7.27
4.51
4.49
4.49
4.48
4.47
3.35
3.33
2.89
2.87
1.93
1.91
1.15
1.13
1.11
0.00
SCN
4l
1.00
1.11
1.03
1.10
2.12
2.09
2.09
2.14
3.11
f1 (ppm)

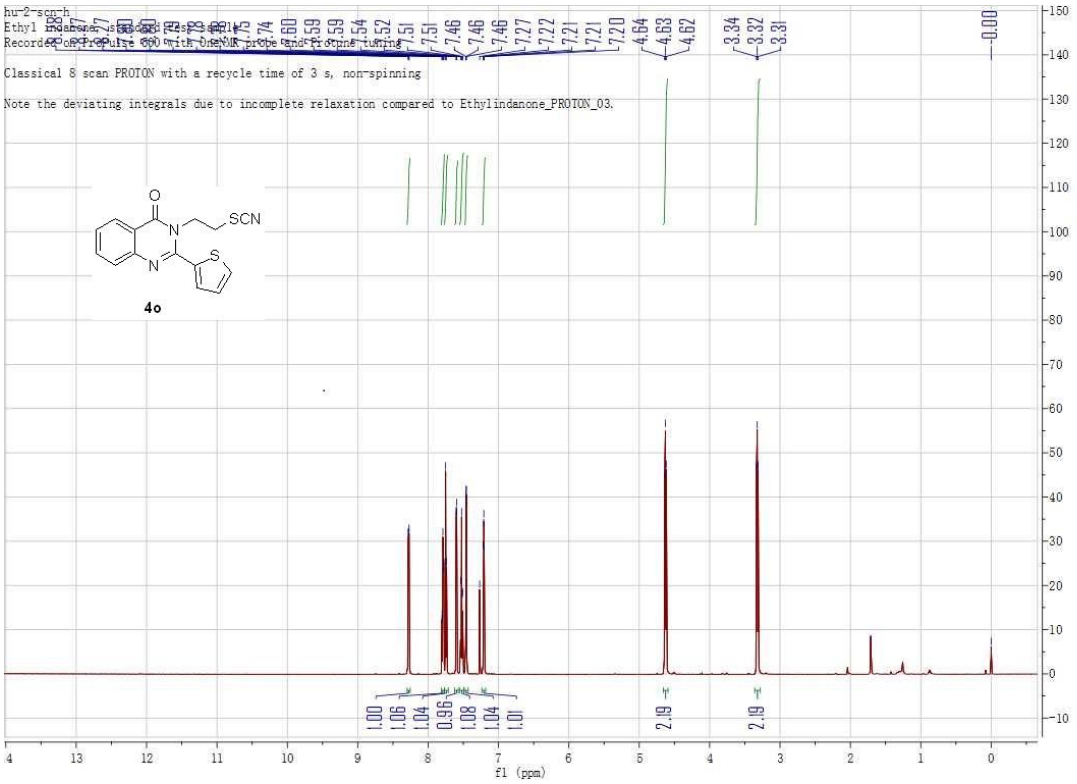

Q2-9
single pulse decoupled gated NOE
162.39
155.90
147.28
134.74
127.27
126.87
126.66
120.19
111.36
77.42
77.11
76.79
43.71
37.26
31.09
20.94
13.86
SCN
4l
f1 (ppm)

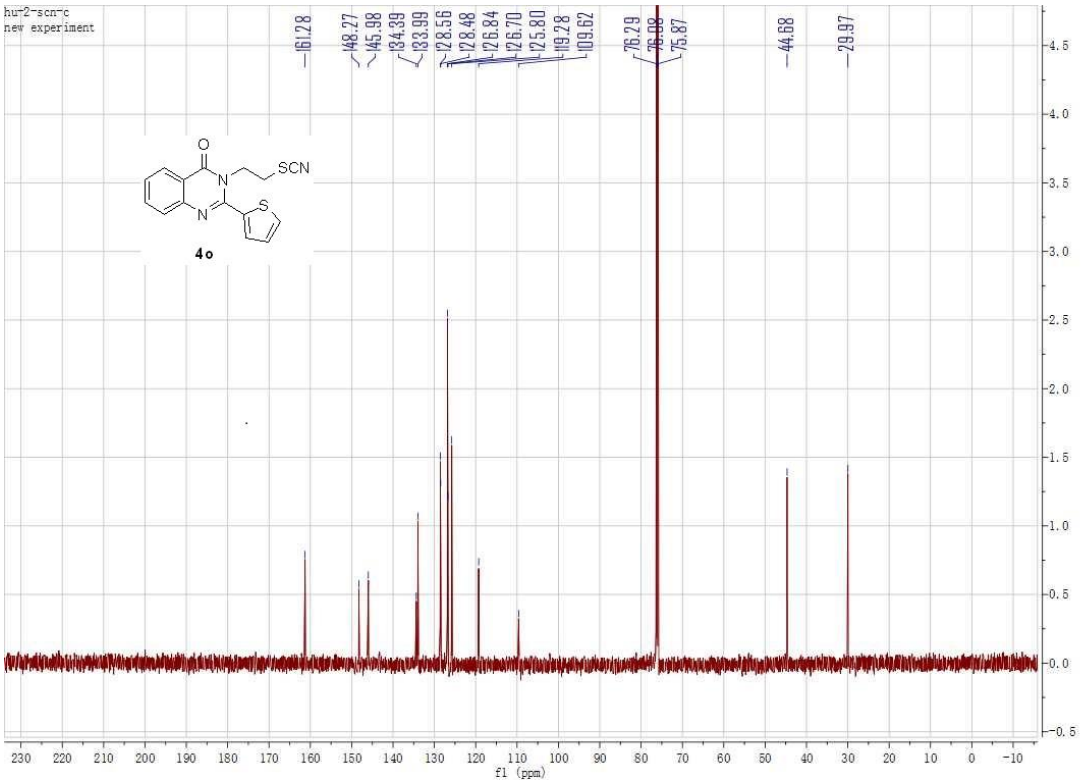

HU-Q2-11
single_pulse
8.24
8.23
8.22
8.21
7.77
7.77
7.75
7.75
7.73
7.73
7.68
7.66
7.48
7.48
7.46
7.44
7.44
7.27
4.51
4.49
4.49
4.47
3.35
3.34
3.33
3.32
2.94
2.93
2.47
1.45
1.43
0.00
SCN
4m
1.00
1.03
1.06
1.03
2.10
2.07
2.06
8.18
f1 (ppm)

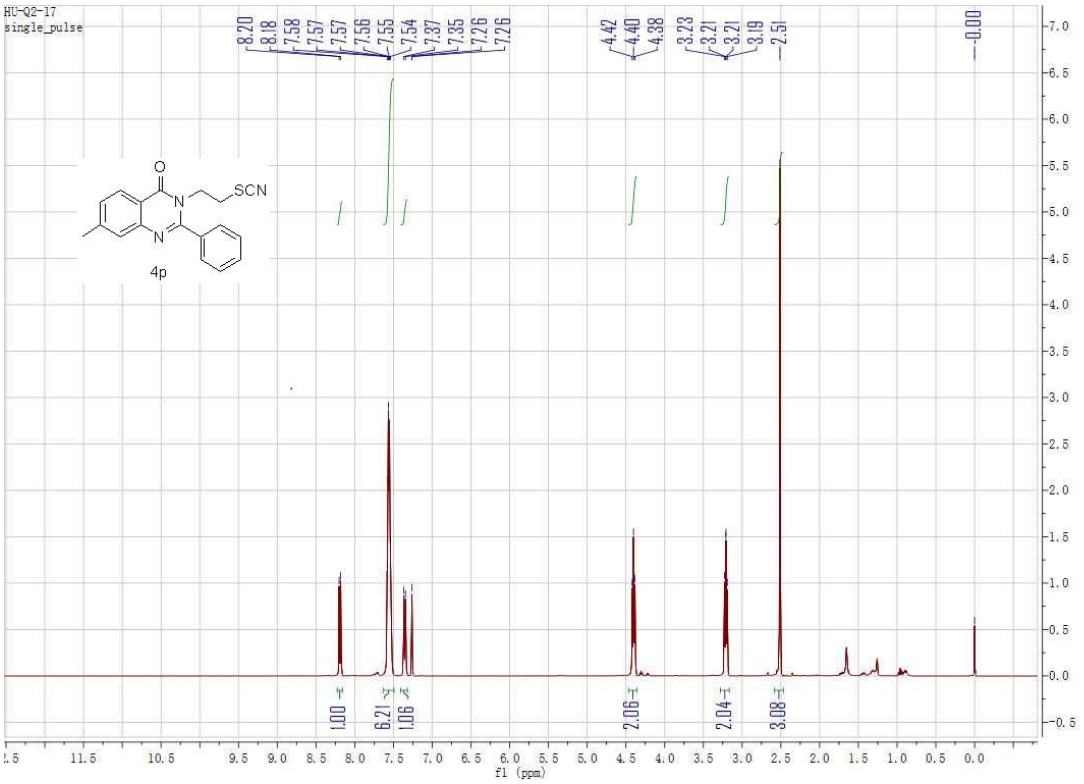

Q2-11
single pulse decoupled gated NOE
162.38
156.65
147.28
134.73
127.32
126.89
126.66
120.70
111.36
77.43
77.11
76.79
43.57
31.06
28.54
11.48
SCN
4m
f1 (ppm)

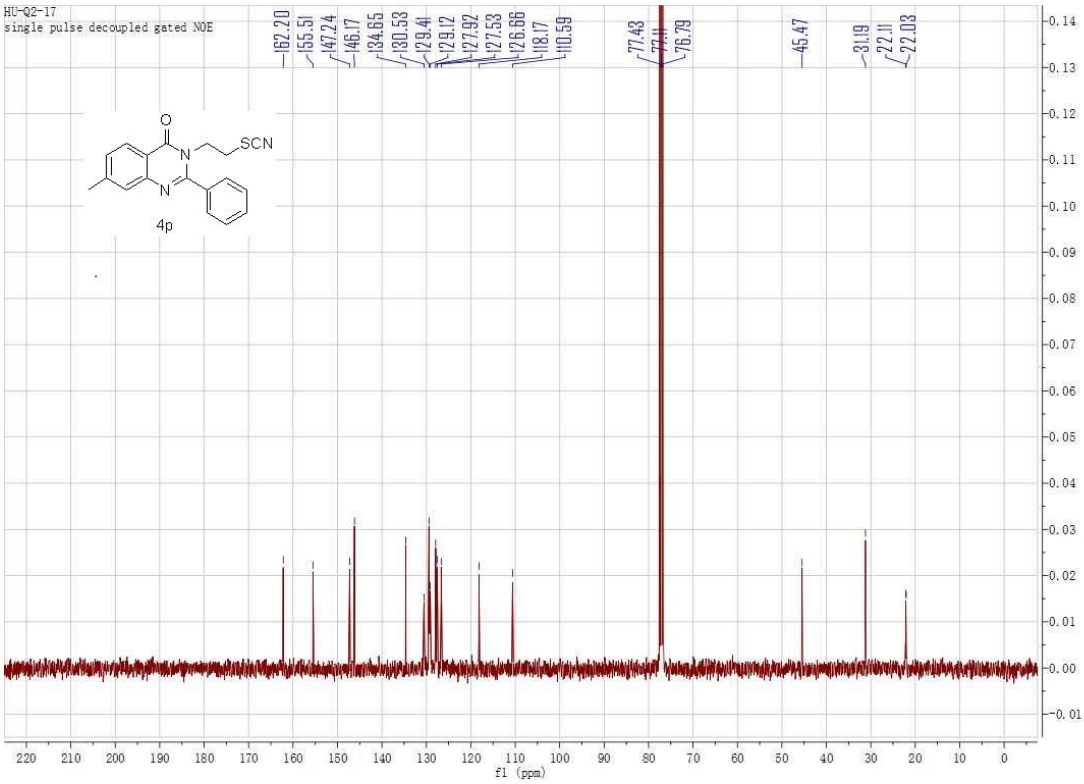

HU-Q2-12
SCN
4n
fl (ppm)

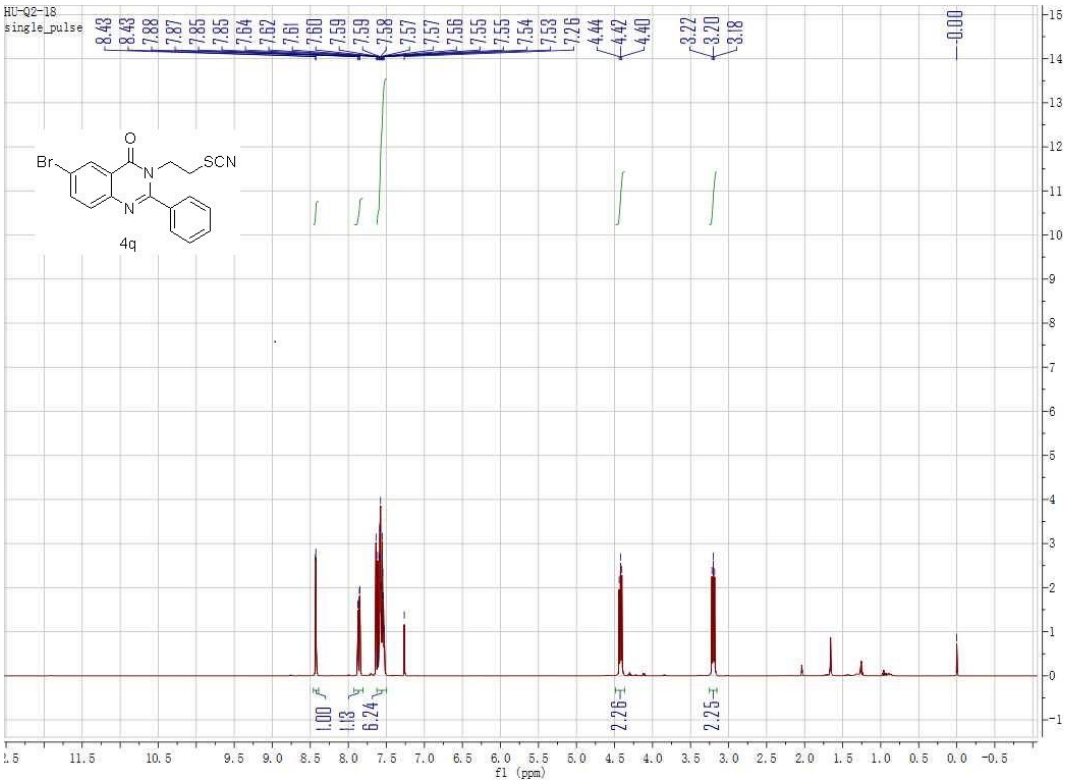

HU-Q2-12
single pulse decoupled gated NOE
SCN
4n
fl (ppm)

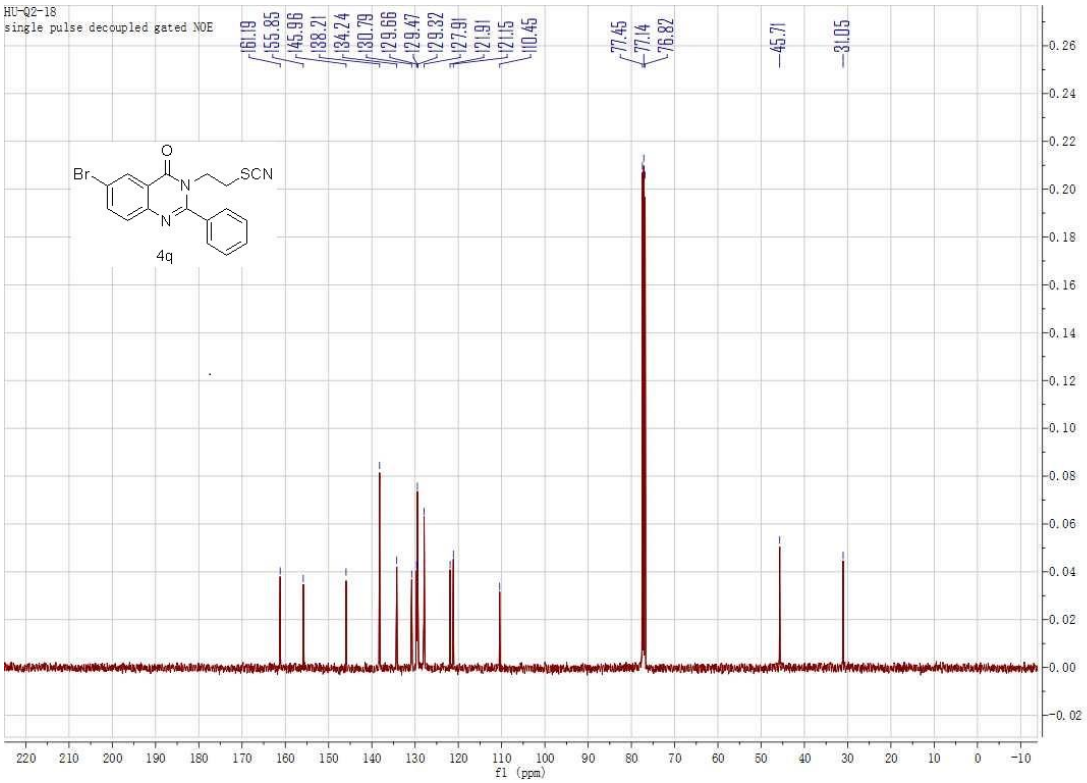

hu-2-scn-h
Classical 8 scan PROTON with a recycle time of 3 s, non-spinning
Note the deviating integrals due to incomplete relaxation compared to Ethylindanone_PROTON_03.
4o
f1 (ppm)

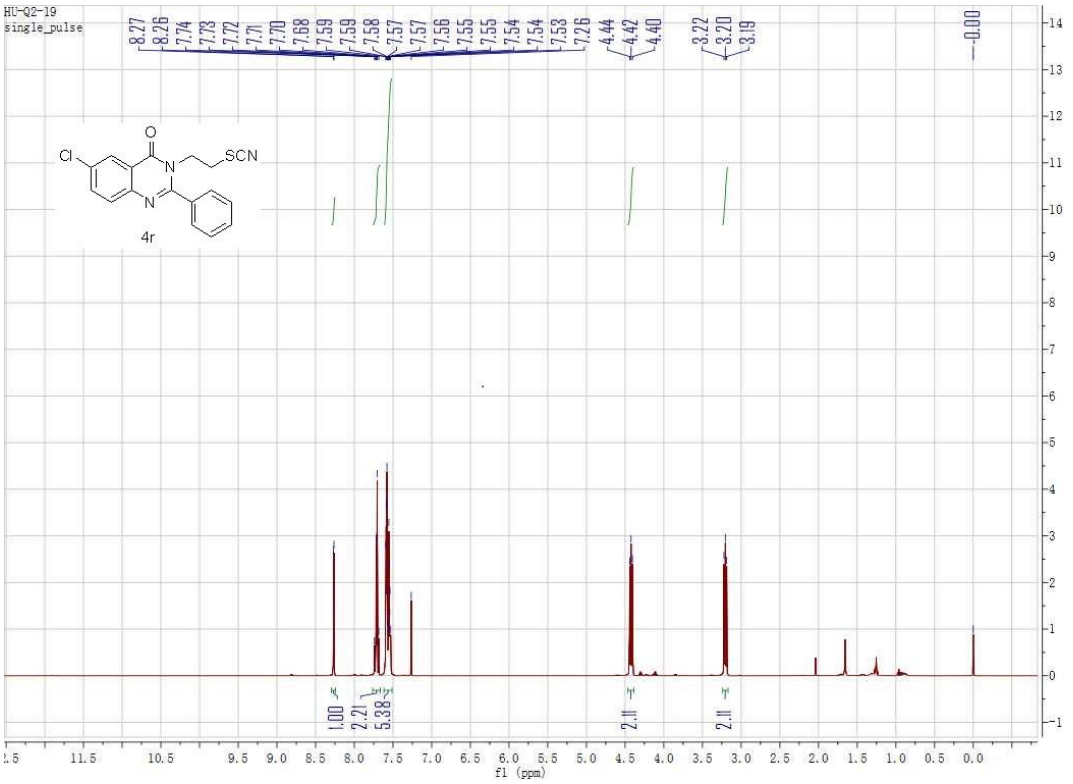

hu-2-scn-c
new experiment
4o
f1 (ppm)

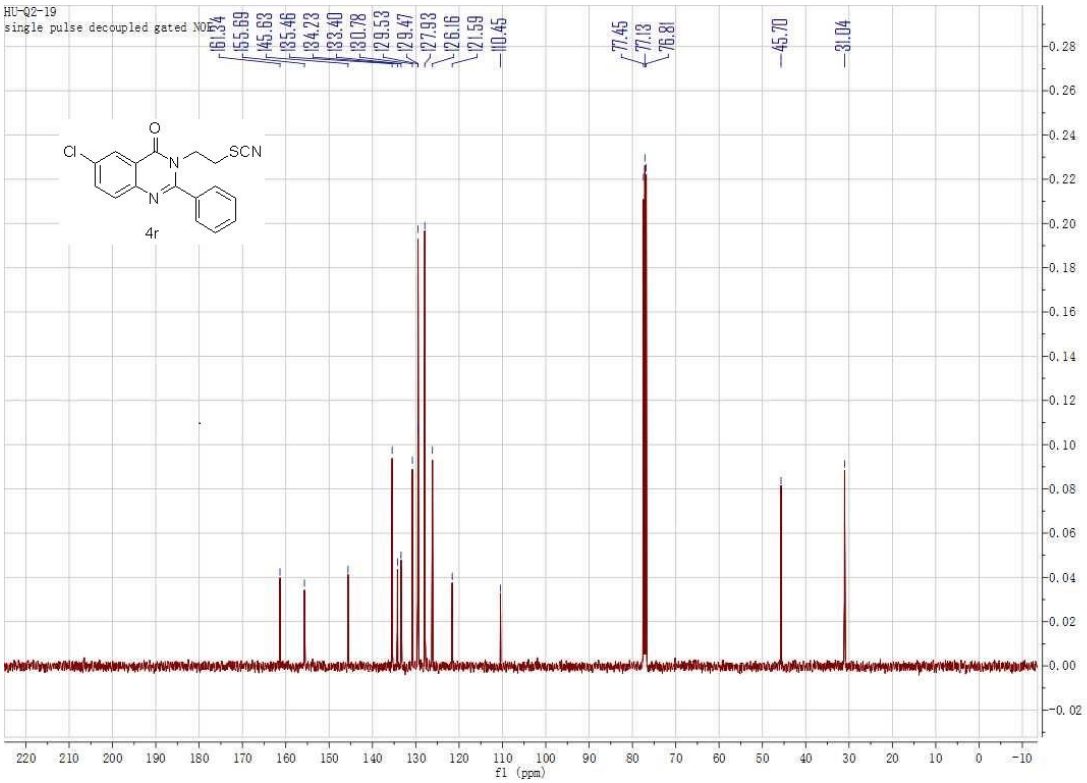

HU-Q2-17
single_pulse
8.20
8.18
7.58
7.57
7.57
7.56
7.55
7.54
7.37
7.35
7.26
7.26
4.42
4.40
4.38
3.23
3.21
3.21
3.19
2.51
0.00
SCN
4p
1.00
6.21
1.06
2.06
2.04
3.08
f1 (ppm)

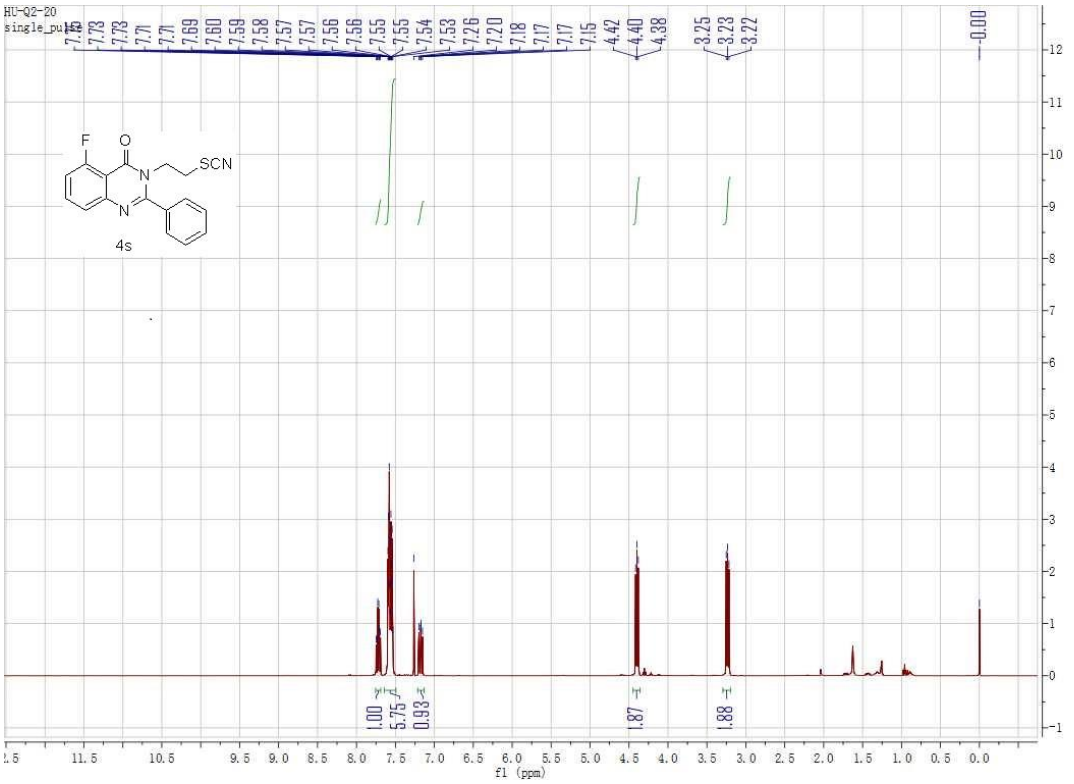

HU-Q2-17
single pulse decoupled gated NOE
162.20
155.51
147.24
146.17
134.65
130.53
129.41
129.12
127.92
127.53
126.66
118.17
110.59
77.43
77.11
76.79
45.47
31.19
22.11
22.03
SCN
4p
f1 (ppm)

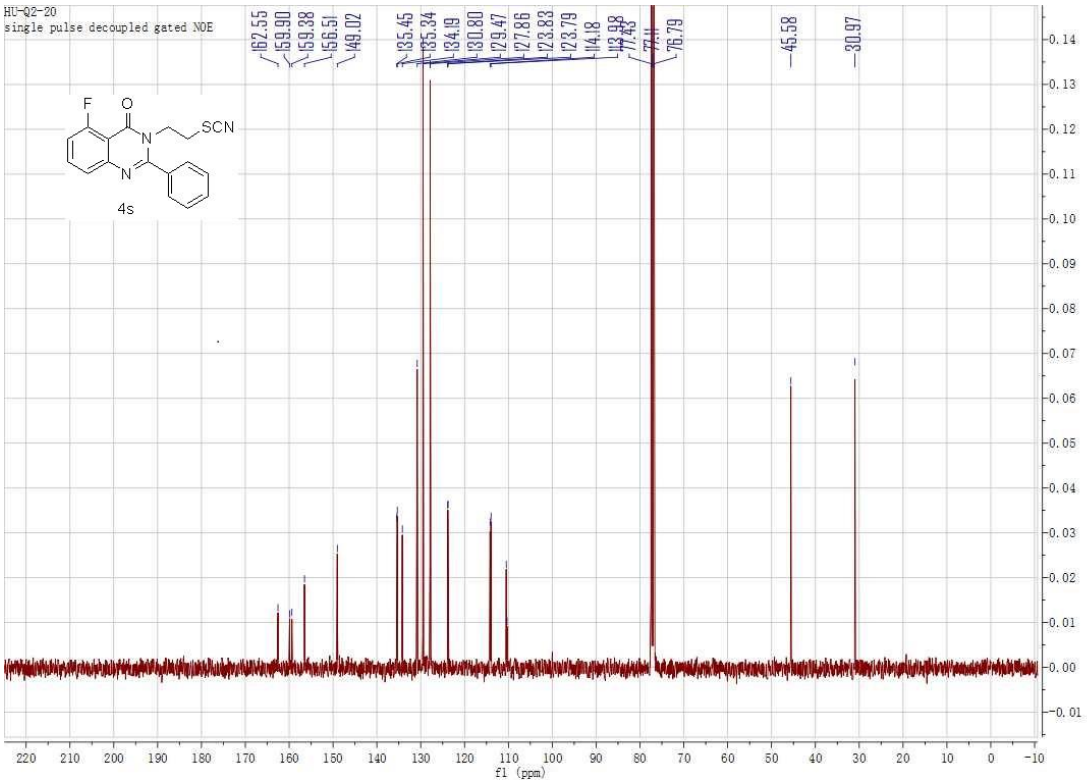

HU-Q2-18
single_pulse
8.43
8.43
7.88
7.87
7.85
7.85
7.64
7.62
7.61
7.60
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.26
4.44
4.42
4.40
3.22
3.20
3.18
0.00
Br
O
N
N
SCN
4q
1.00
1.13
6.24
2.26
2.25
f1 (ppm)

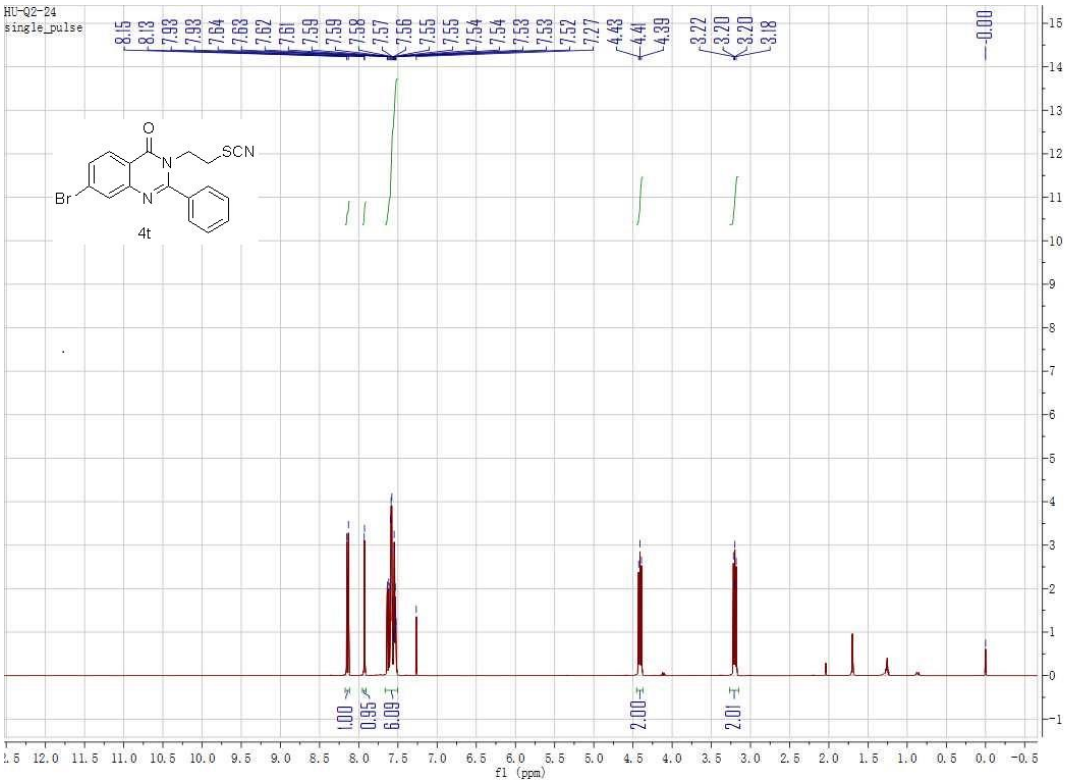

HU-Q2-18
single pulse decoupled gated NOE
161.19
155.85
145.96
138.21
134.24
130.79
129.66
129.47
129.32
127.91
121.91
121.15
110.45
77.45
77.14
76.82
45.71
31.05
Br
O
N
N
SCN
4q
f1 (ppm)

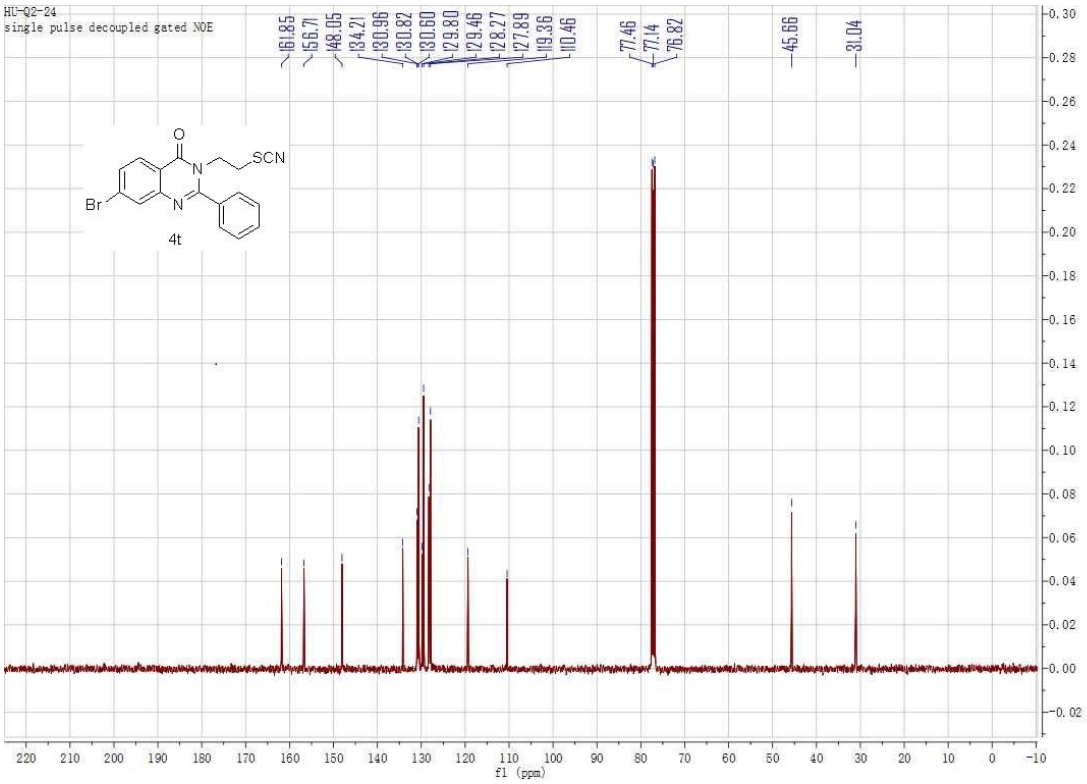

HU-Q2-19
single_pulse
8.27
8.26
7.74
7.73
7.72
7.71
7.70
7.68
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.55
7.54
7.54
7.53
7.26
4.44
4.42
4.40
3.22
3.20
3.19
0.00
Cl
O
N
N
SCN
4r
1.00
2.21
5.38
2.11
2.11
f1 (ppm)

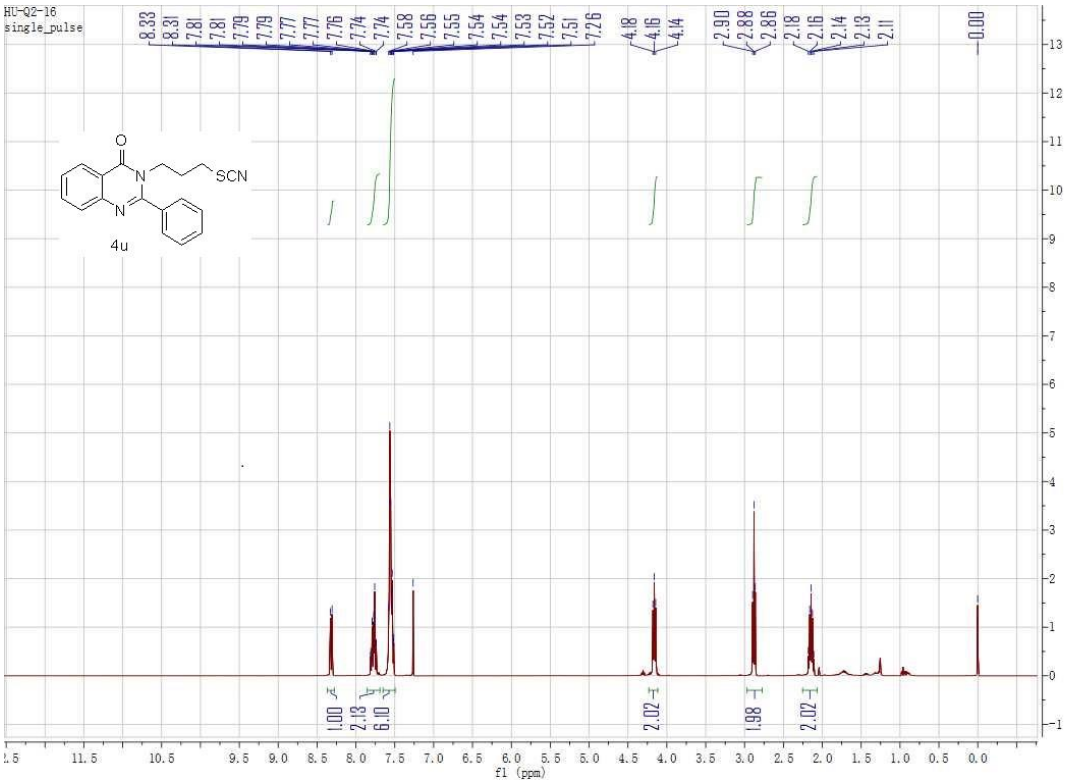

HU-Q2-19
single pulse decoupled gated NOE
161.34
155.69
145.63
135.46
134.23
133.40
130.78
129.53
129.47
127.93
126.16
121.59
110.45
77.45
77.13
76.81
45.70
31.04
Cl
O
N
N
SCN
4r
f1 (ppm)

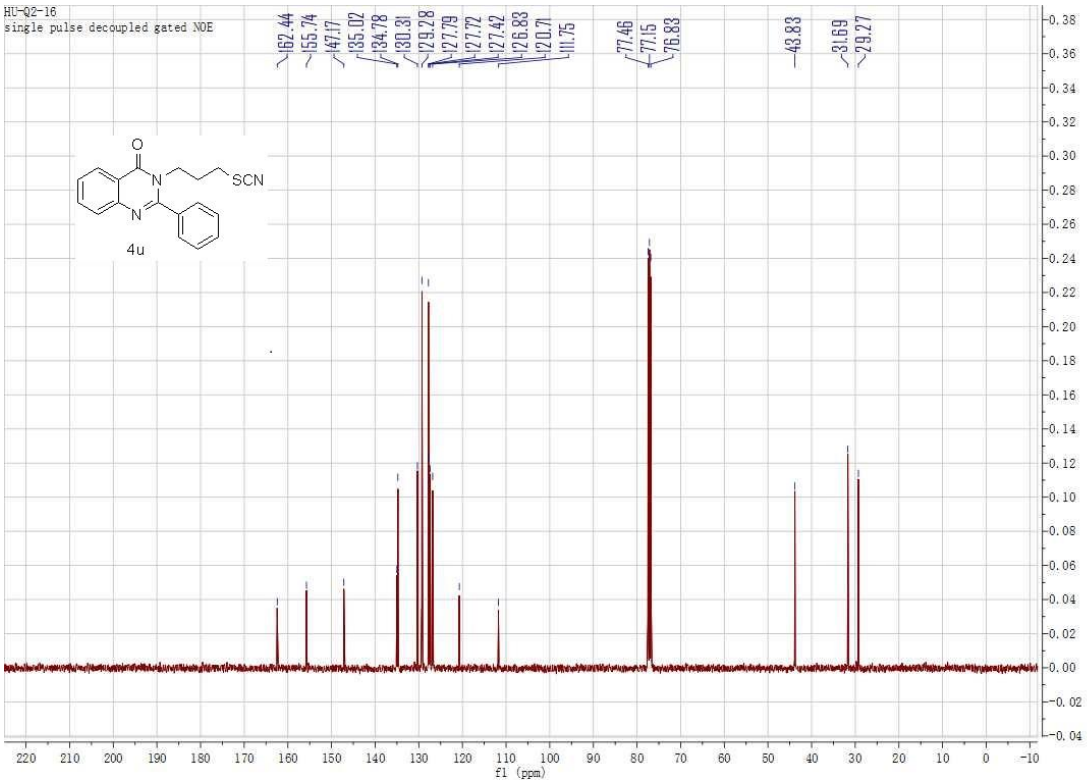

HU-Q2-20
single_pulse
F
O
N
N
SCN
4s
7.75
7.73
7.73
7.71
7.71
7.69
7.60
7.59
7.58
7.57
7.57
7.56
7.56
7.55
7.55
7.54
7.53
7.26
7.20
7.18
7.17
7.17
7.15
4.42
4.40
4.38
3.25
3.23
3.22
0.00
1.00
5.75
0.93
1.87
1.88
f1 (ppm)

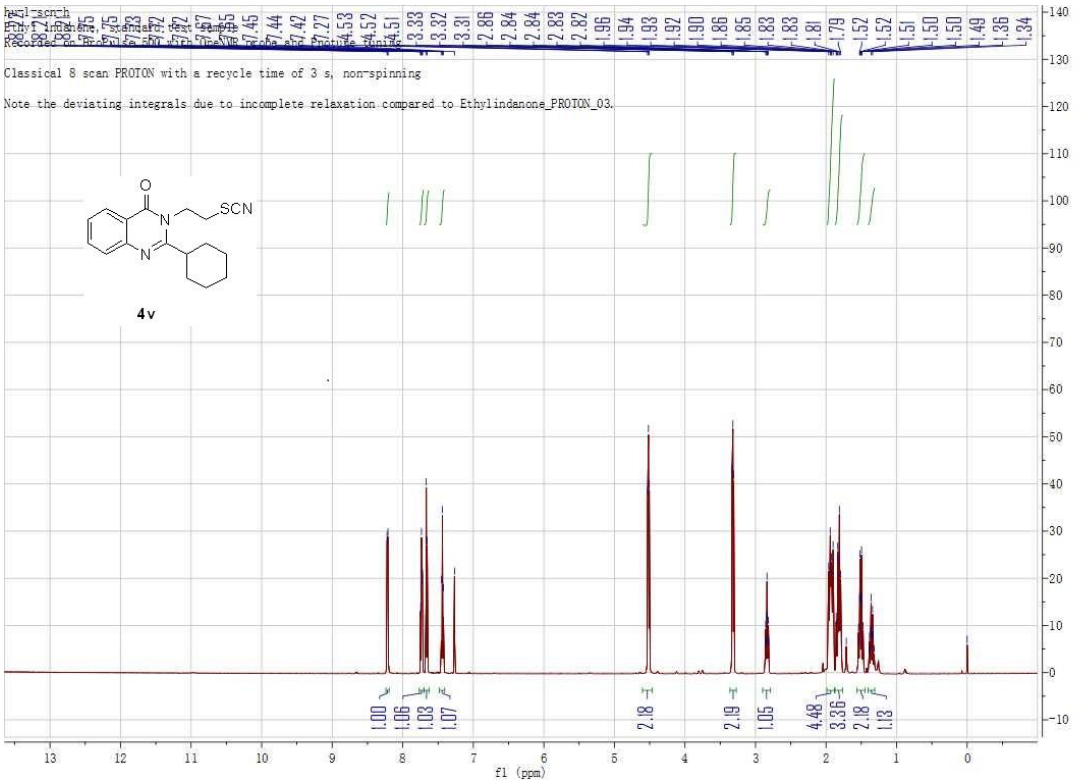

HU-Q2-20
single pulse decoupled gated NOE
F
O
N
N
SCN
4s
162.55
159.90
159.38
156.51
149.02
135.45
135.34
134.19
130.80
129.47
127.86
123.83
123.79
114.18
77.11
76.79
45.58
30.97
f1 (ppm)

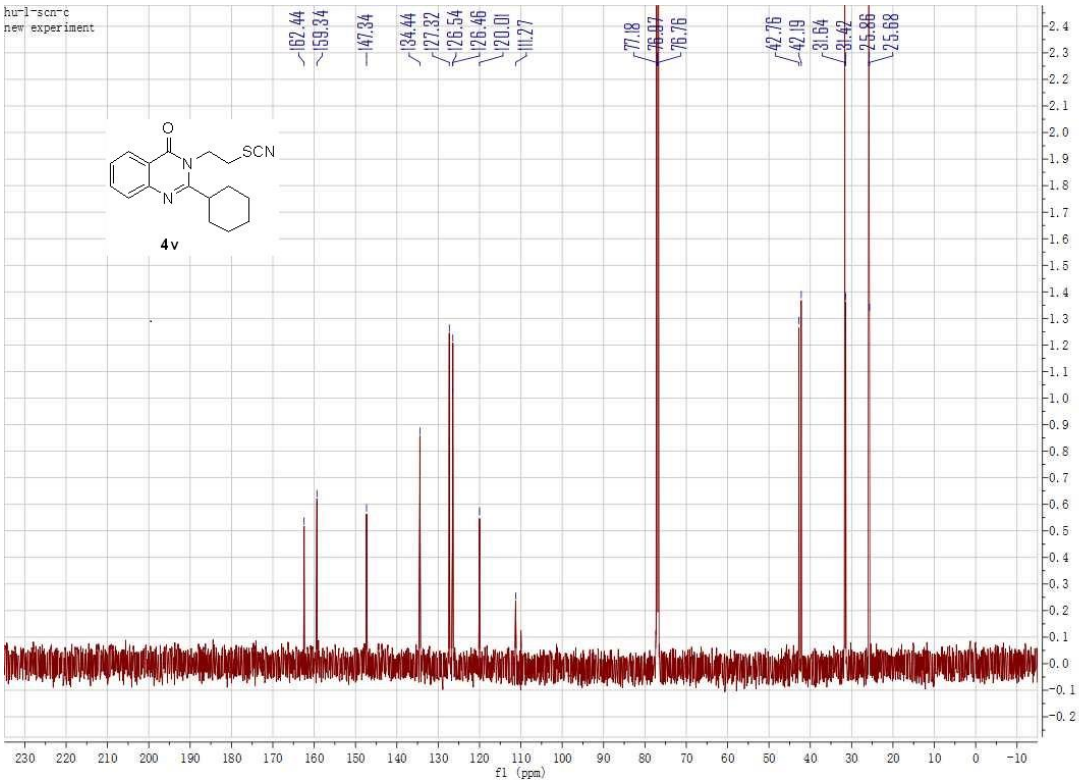

HU-Q2-24
single_pulse
8.15
8.13
7.93
7.93
7.64
7.63
7.62
7.61
7.59
7.59
7.58
7.57
7.56
7.55
7.55
7.54
7.54
7.53
7.53
7.52
7.27
4.43
4.41
4.39
3.22
3.20
3.20
3.18
0.00
O
N
SCN
Br
N
4t
1.00
0.95
6.09
2.00
2.01
f1 (ppm)


HU-Q2-24
single pulse decoupled gated NOE
161.85
156.71
148.05
134.21
130.96
130.82
130.60
129.80
129.46
128.27
127.89
119.36
110.46
77.46
77.14
76.82
45.66
31.04
O
N
SCN
Br
N
4t
f1 (ppm)


HU-Q2-16
single_pulse
8.33
8.31
7.81
7.81
7.79
7.79
7.77
7.77
7.76
7.74
7.74
7.58
7.56
7.55
7.54
7.54
7.53
7.52
7.51
7.26
4.18
4.16
4.14
2.90
2.88
2.86
2.18
2.16
2.14
2.13
2.11
0.00
SCN
4u
1.00
2.13
6.10
2.02
1.98
2.02
f1 (ppm)


HU-Q2-16
single pulse decoupled gated NOE
162.44
155.74
147.17
135.02
134.78
130.31
129.28
127.79
127.72
127.42
126.83
120.71
111.75
77.46
77.15
76.83
43.83
31.69
29.27
SCN
4u
f1 (ppm)


Classical 8 scan PROTON with a recycle time of 3 s, non-spinning
Note the deviating integrals due to incomplete relaxation compared to Ethylindanone_PROTON_03.
SCN
4v
f1 (ppm)


new experiment
162.44
159.34
147.84
134.44
127.32
126.54
126.46
120.01
111.27
77.18
76.97
76.76
42.76
42.19
31.64
31.42
25.86
25.68
SCN
4v
f1 (ppm)