

Supporting Information

Copper-catalyzed direct C-3 oxidative amidation of quinoxalin- 2(1H)-ones with amidates under microwave irradiation

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1. Optimization of reaction conditions

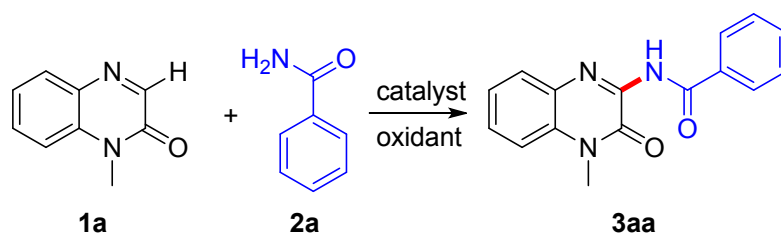


Table S1 Screening the loading amount of **1a** and **2a**^a

Entry	The molar ratio of 1a and 2a (equiv.)	Yields (%) ^b
1	2:1	35
2	1:1	63
3	1:1.5	68
4	1:2	73
5	1:2.5	75

^a Reaction conditions: 1-methylquinoxalin-2(1H)-one **1a** (0.2 mmol, 32.0 mg), benzamide **2a**, CuBr (0.04 mmol, 5.7 mg), K₂S₂O₈ (0.6 mmol, 162 mg) in CH₃CN (2.0 mL) at 100 °C for 0.5 h under microwave irradiation.

^b Isolated yield.

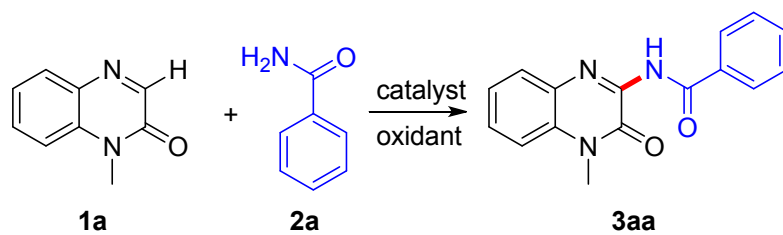


Table S2 Screening the reaction temperature^a

Entry	Temperature (°C)	Yields (%) ^b
1	20	0
2	60	58
3	70	65
4	80	78
5	90	78
6	100	78

^a Reaction conditions: 1-methylquinoxalin-2(1H)-one **1a** (0.2 mmol, 32.0 mg), benzamide **2a** (0.5 mmol, 60.5 mg), CuBr (0.04 mmol, 5.7 mg), K₂S₂O₈ (0.6 mmol, 162 mg) in CH₃CN (2.0 mL) for 0.5 h under microwave irradiation.

^b Isolated yield.

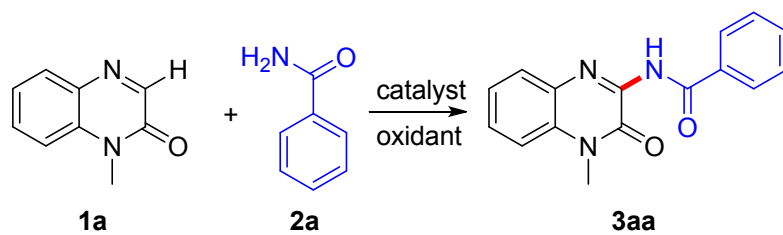


Table S3 Screening the reaction times^a

Entry	Times (min)	Yields (%) ^b
1	10	63
2	20	70
3	30	78
4	40	76

^a Reaction conditions: 1-methylquinoxalin-2(1H)-one **1a** (0.2 mmol, 32.0 mg), benzamide **2a** (0.5 mmol, 60.5 mg), CuBr (0.04 mmol, 5.7 mg), K₂S₂O₈ (0.6 mmol, 162 mg) in CH₃CN (2.0 mL) under microwave irradiation.

^b Isolated yield.

2. Copies of spectra of products

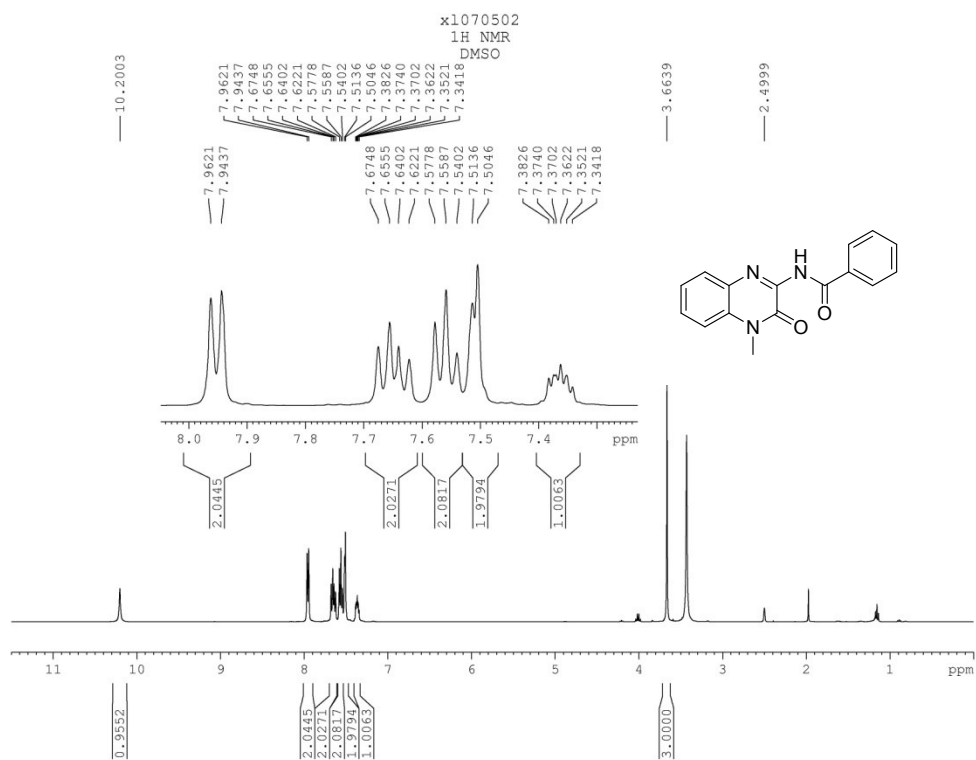


Fig. 1 ¹H NMR spectrum of compound 3aa

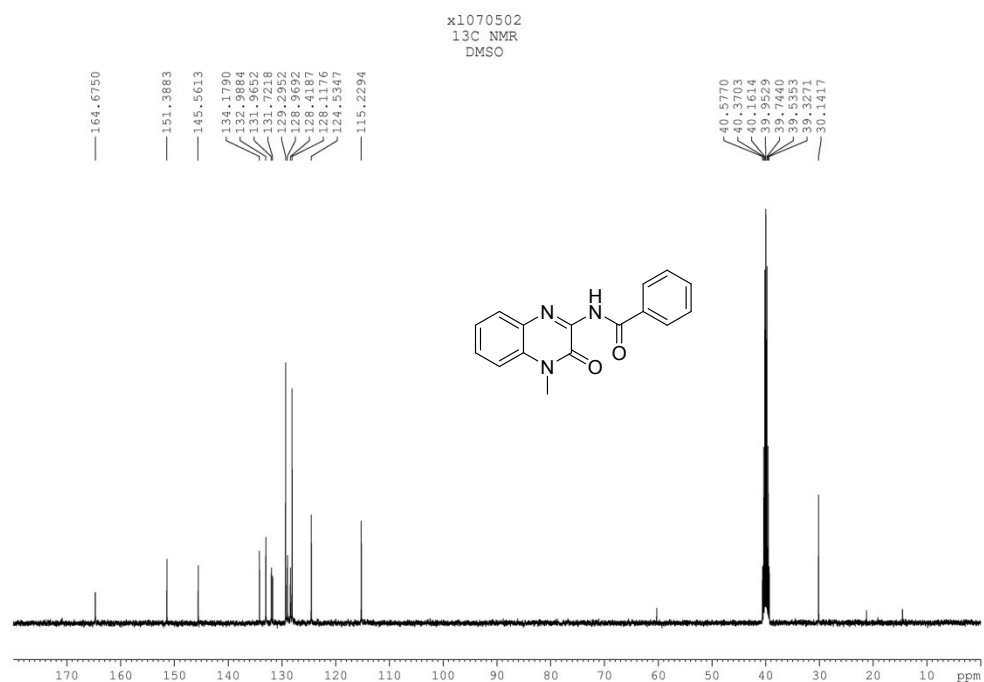


Fig. 2 ¹³C NMR spectrum of compound 3aa

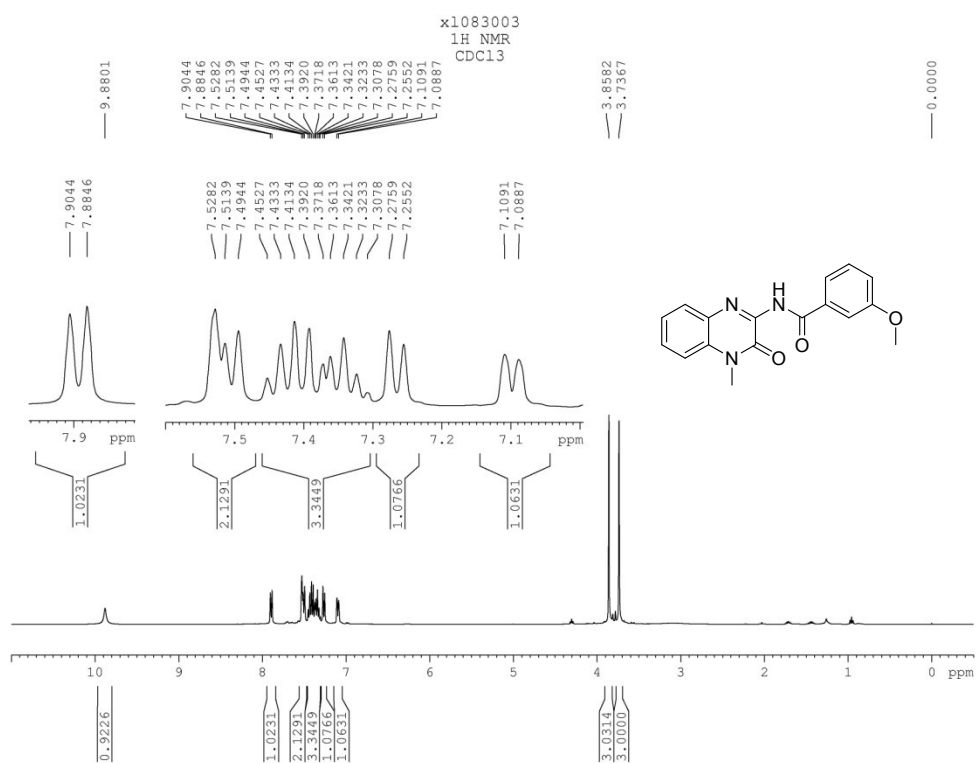


Fig. 3 ¹H NMR spectrum of compound **3ab**

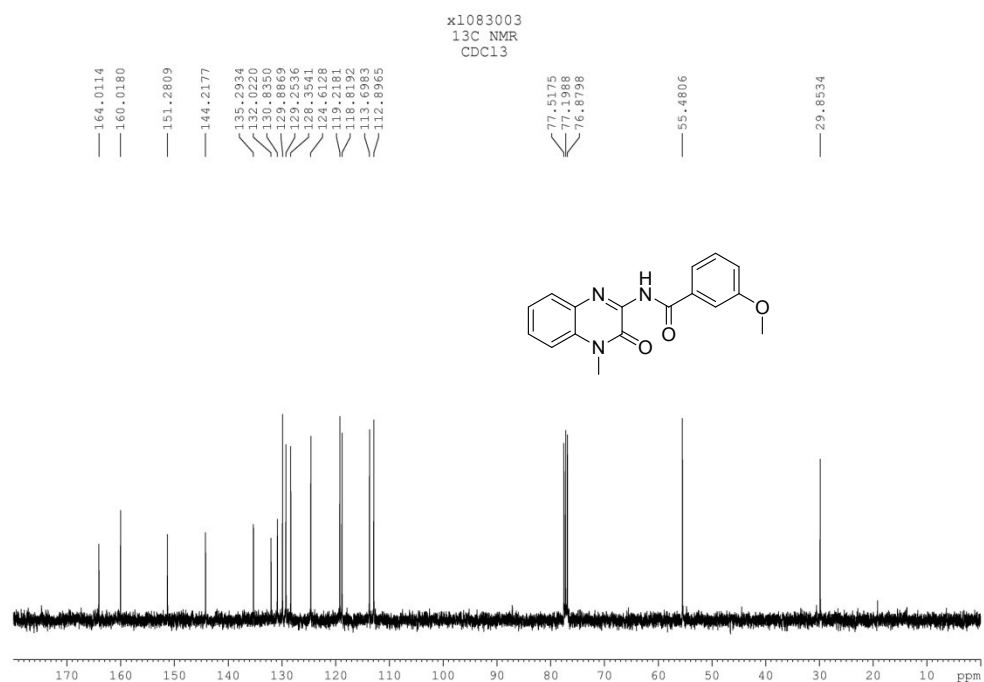


Fig. 4 ¹³C NMR spectrum of compound **3ab**

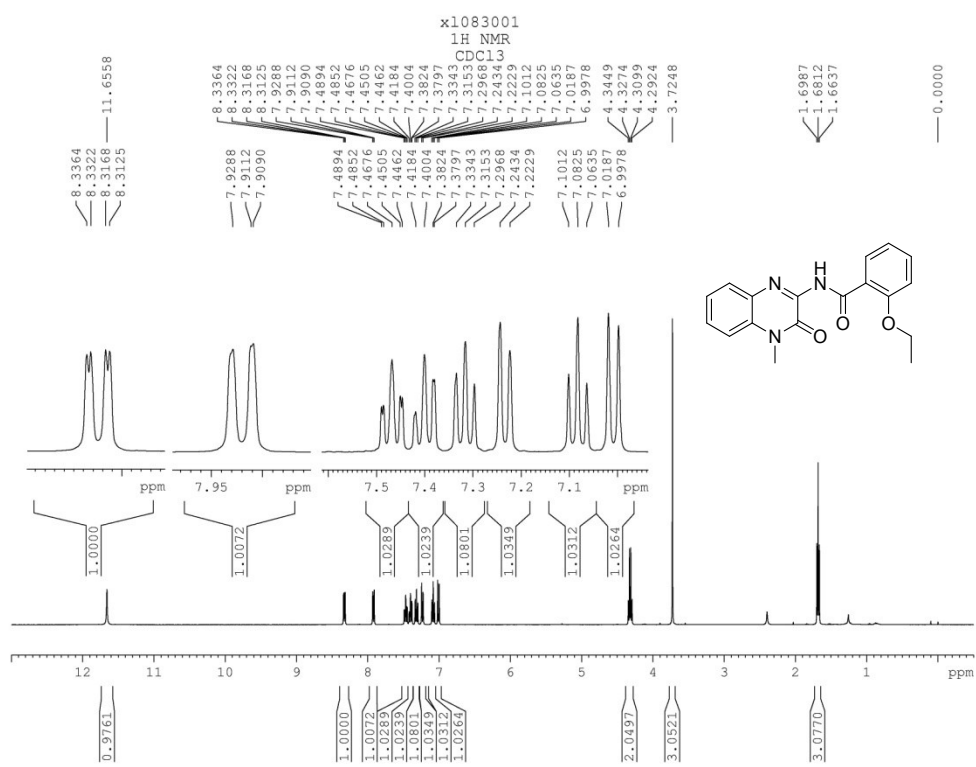


Fig. 5 ¹H NMR spectrum of compound 3ac

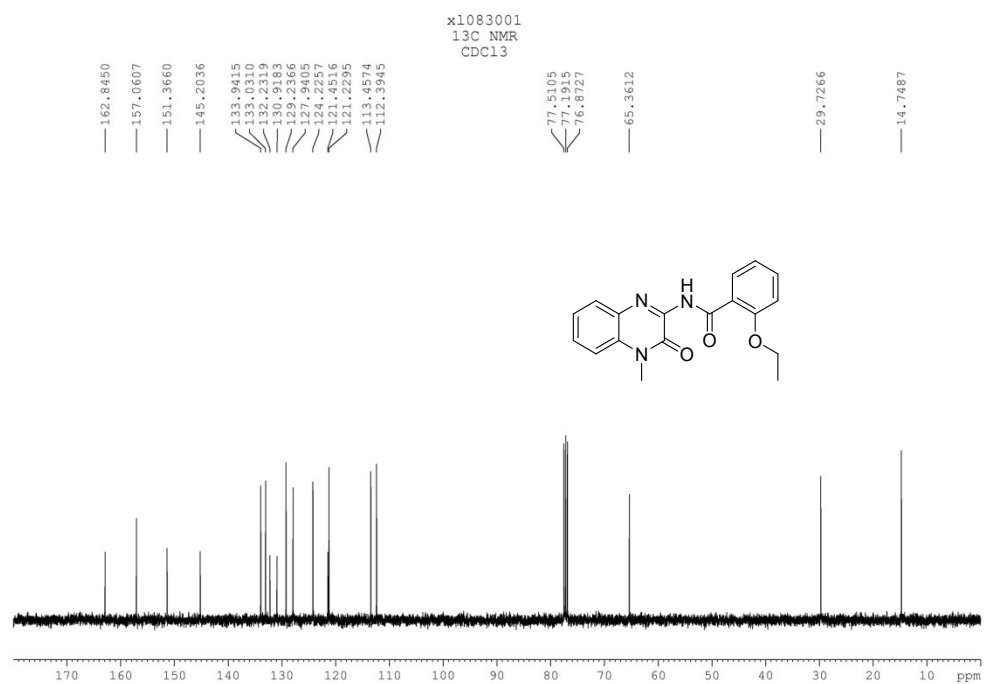


Fig. 6 ¹³C NMR spectrum of compound 3ac

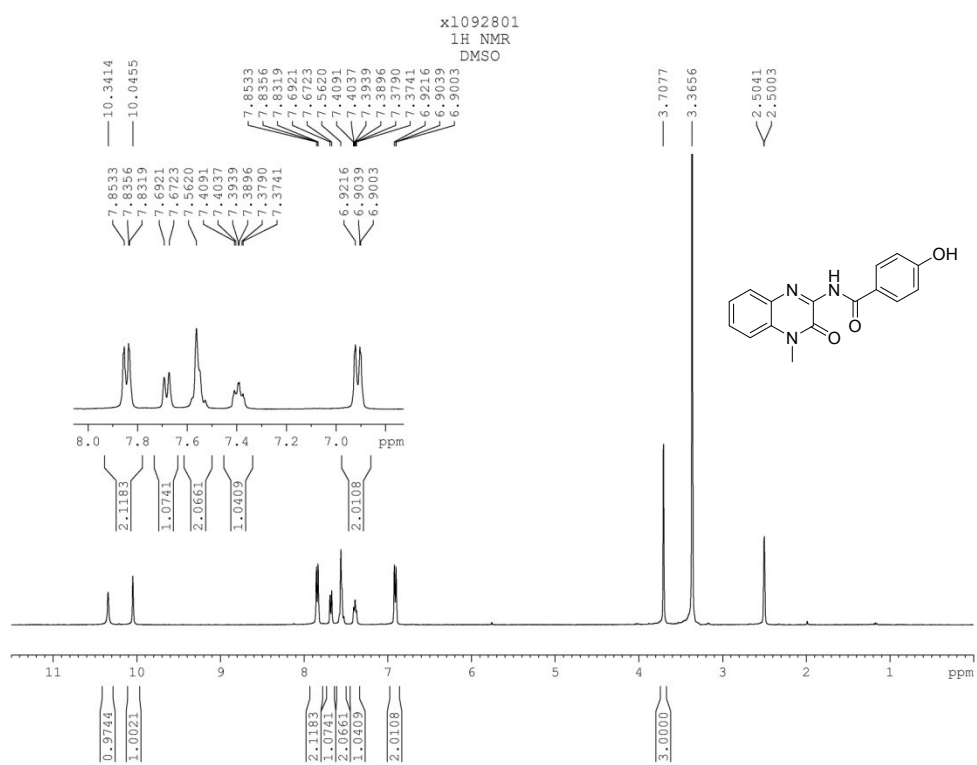


Fig. 7 ^1H NMR spectrum of compound 3ad

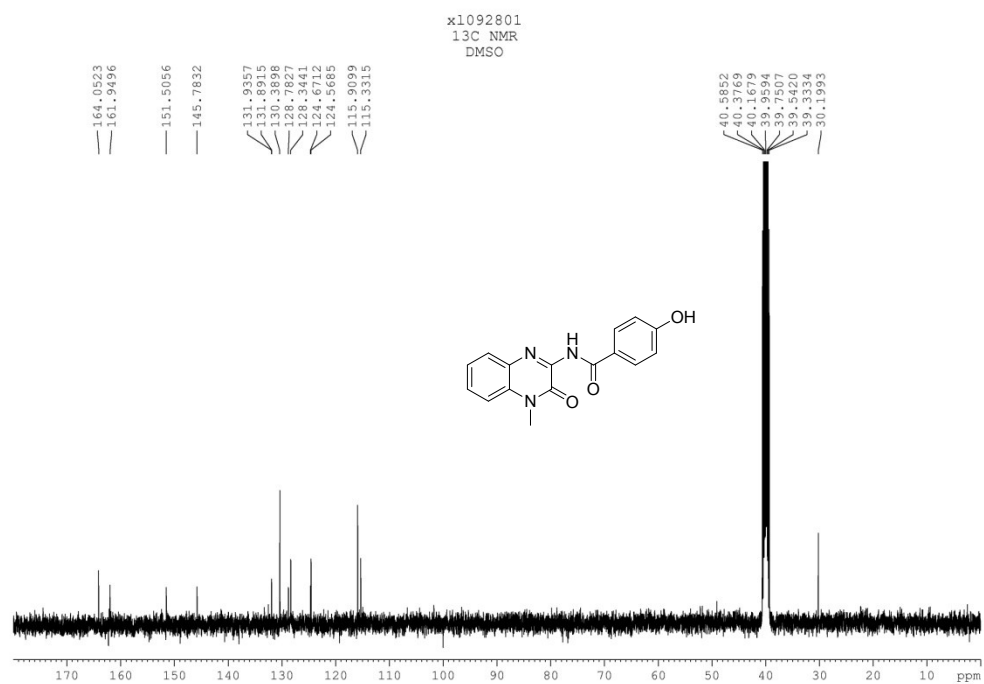


Fig. 8 ^{13}C NMR spectrum of compound 3ad

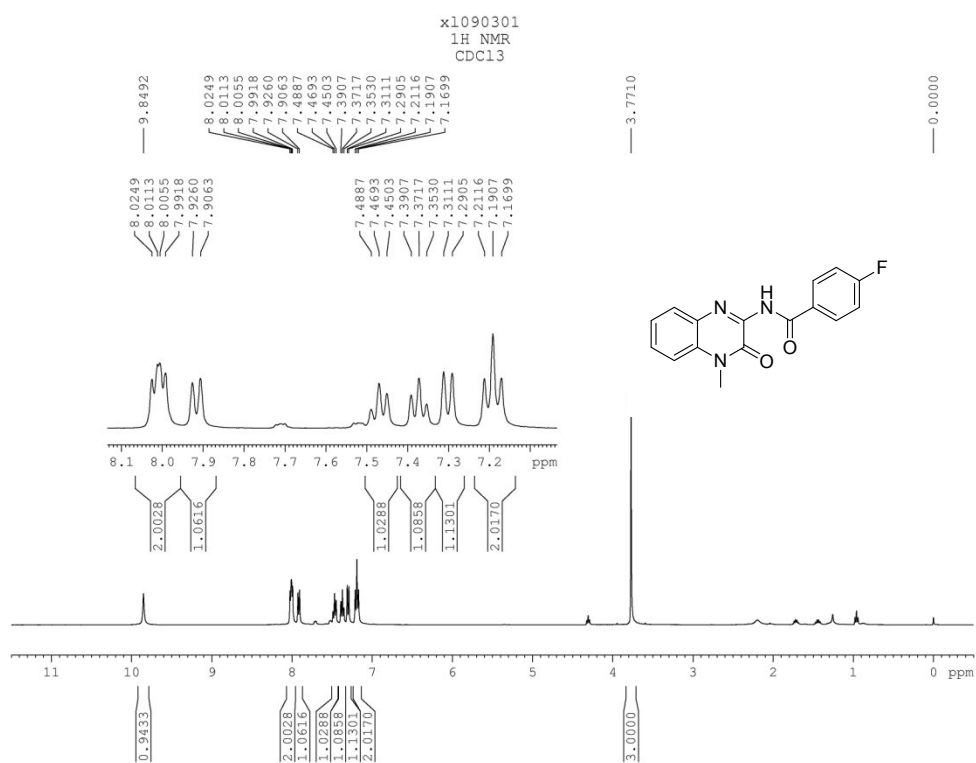


Fig. 9 ¹H NMR spectrum of compound 3ae

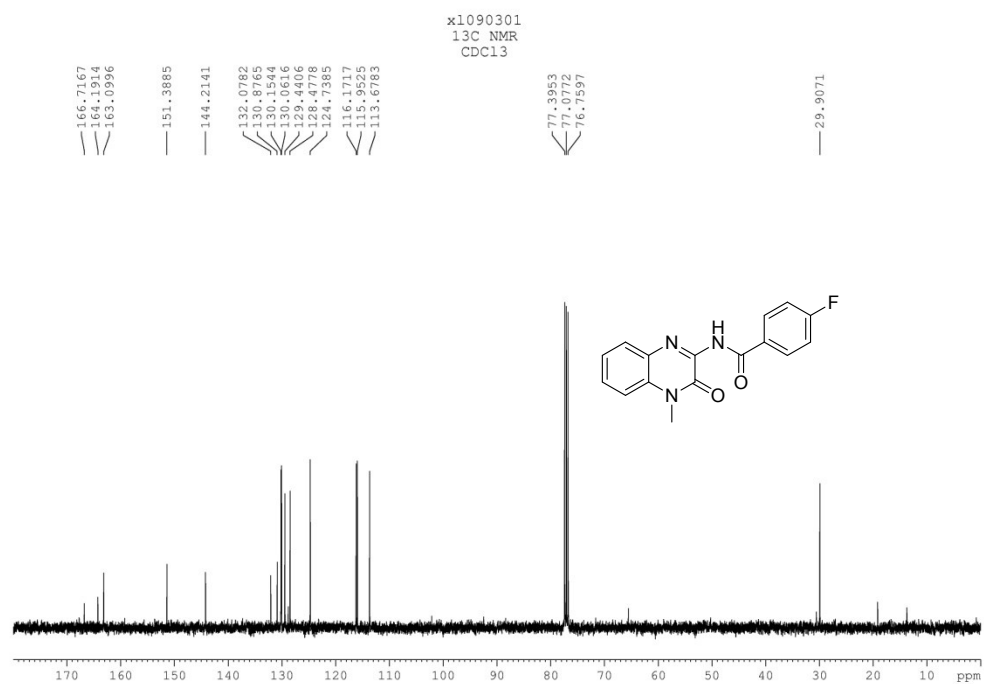


Fig. 10 ¹³C NMR spectrum of compound 3ae

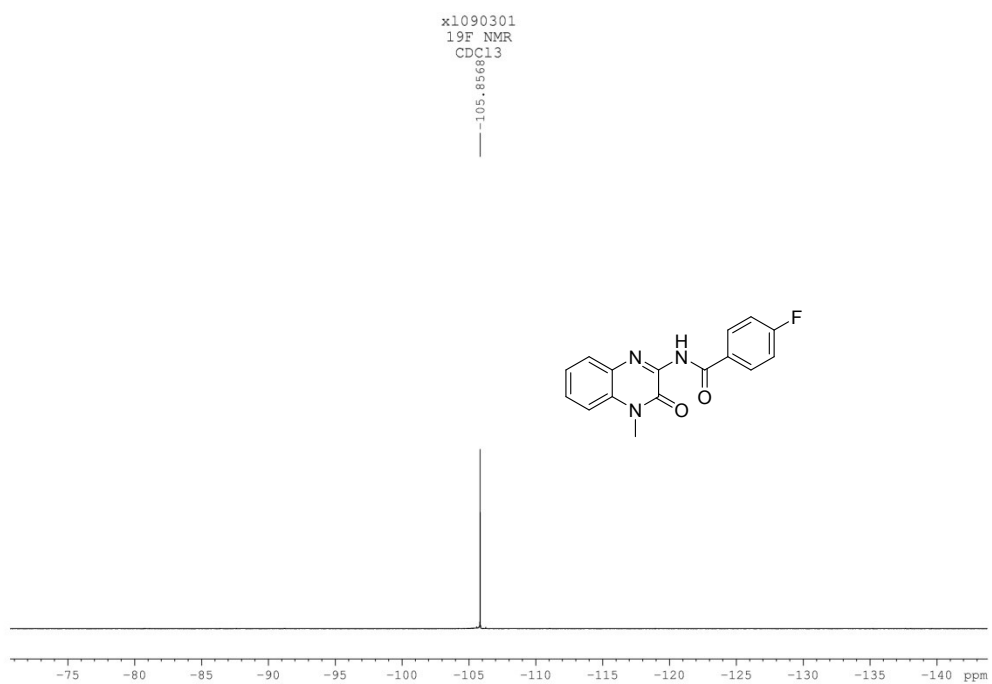


Fig. 11 ^{19}F NMR spectrum of compound **3ae**



Fig. 12 ^1H NMR spectrum of compound **3af**

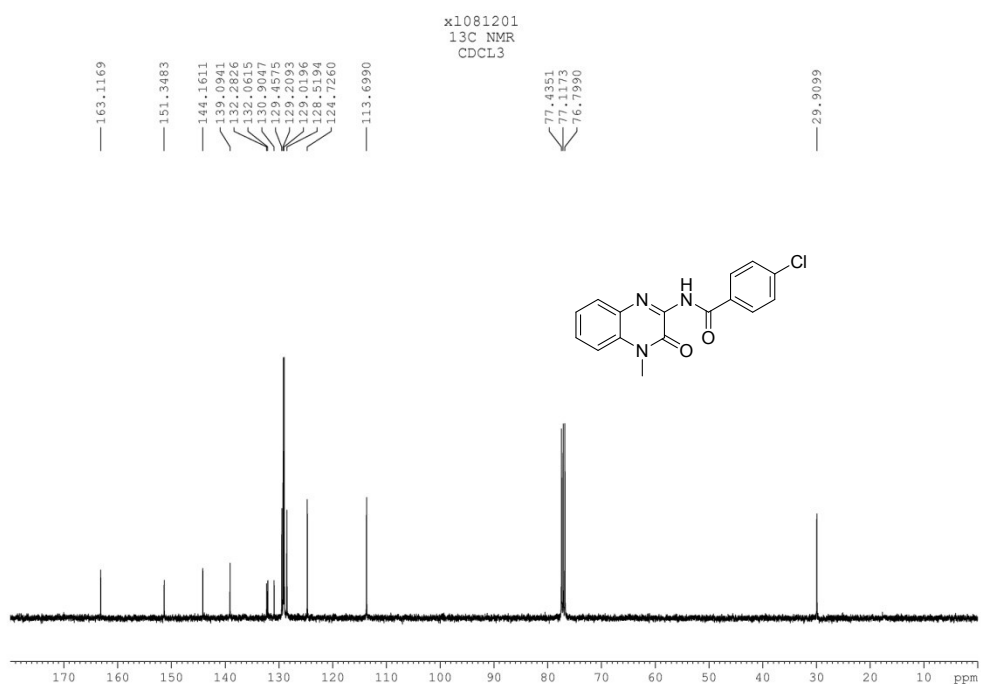


Fig. 13 ¹³C NMR spectrum of compound 3af

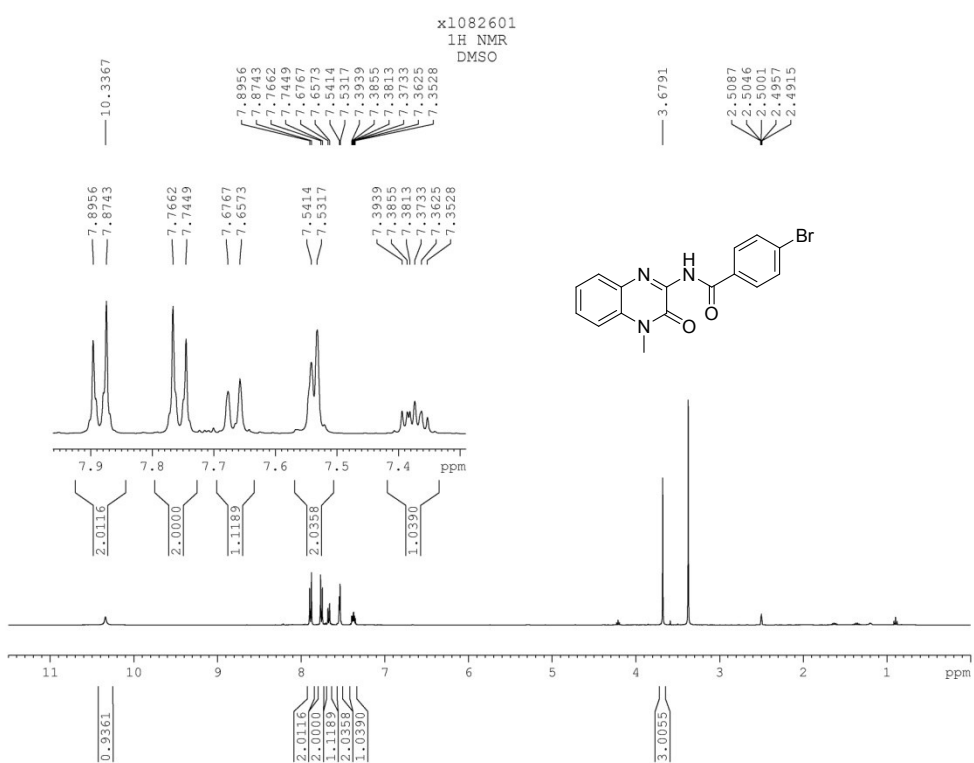


Fig. 14 ¹H NMR spectrum of compound 3ag

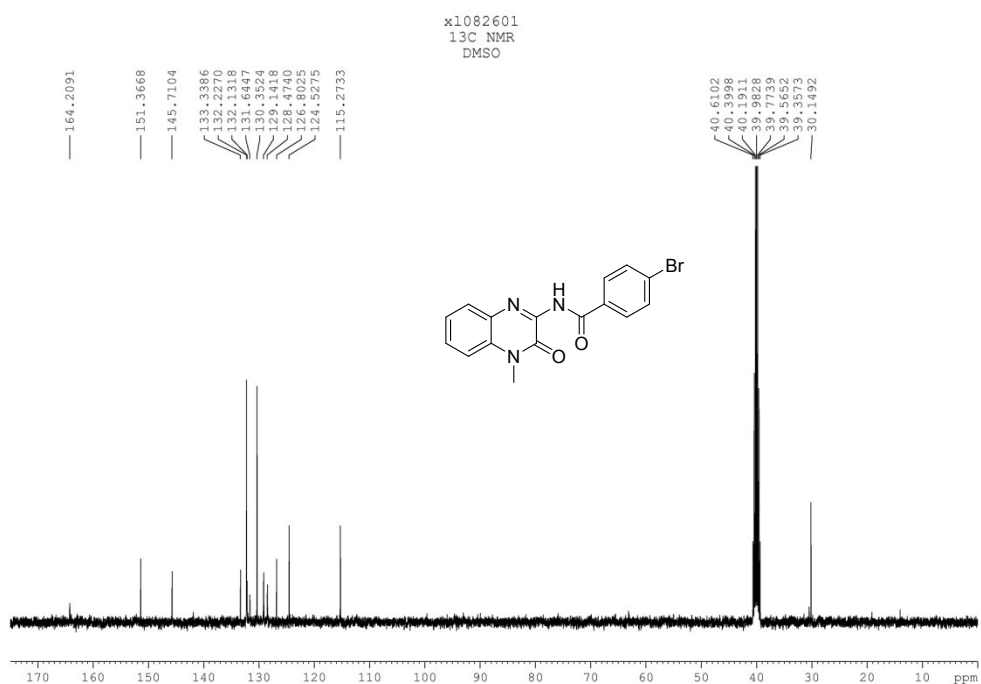


Fig. 15 ¹³C NMR spectrum of compound 3ag

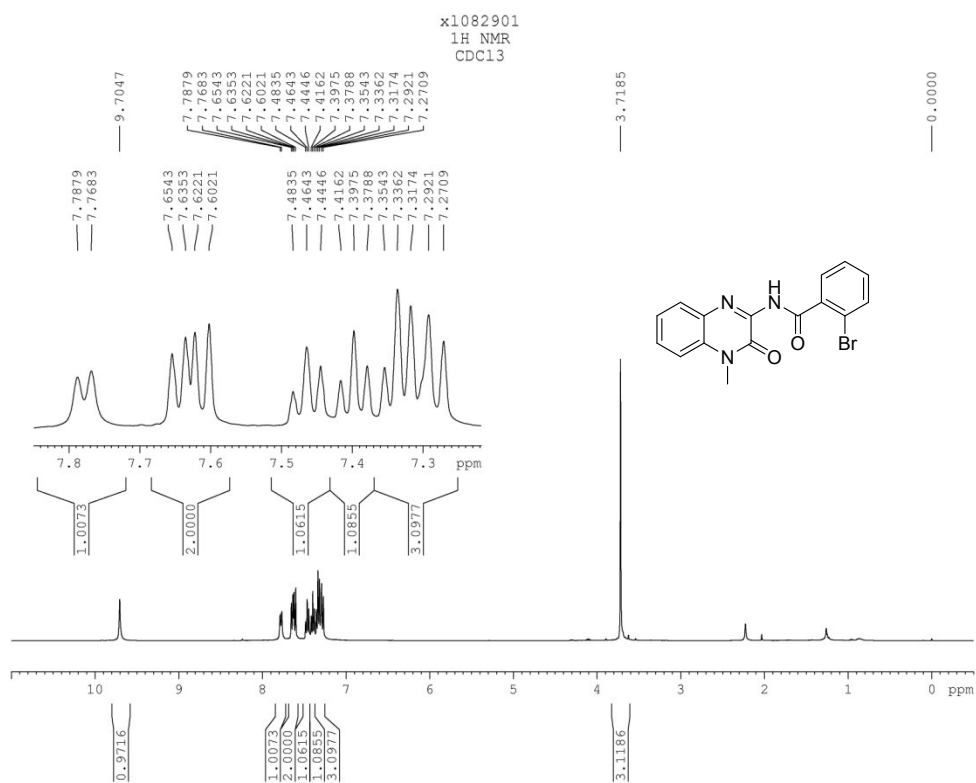


Fig. 16 ¹H NMR spectrum of compound 3ah

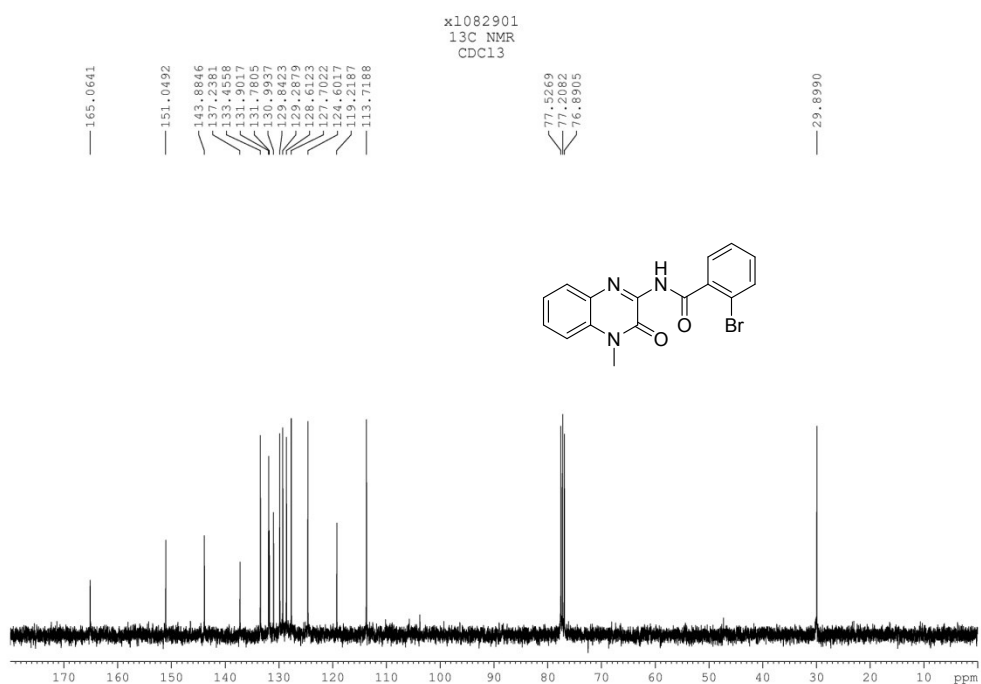


Fig. 17 ¹³C NMR spectrum of compound 3ah

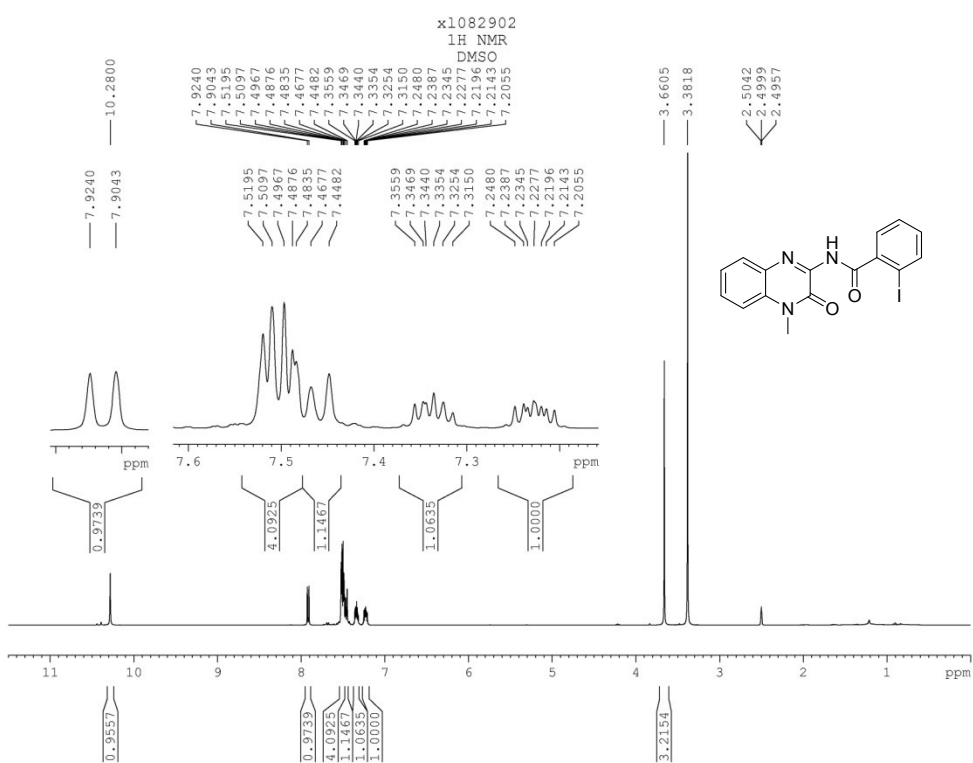


Fig. 18 ¹H NMR spectrum of compound 3ai

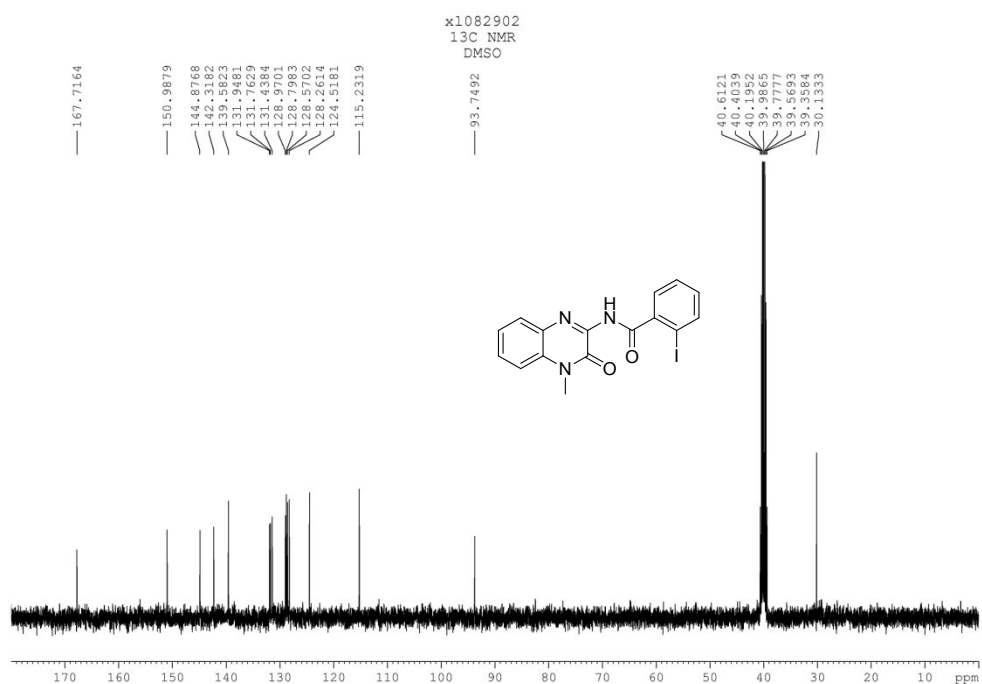


Fig. 19 ¹³C NMR spectrum of compound 3ai

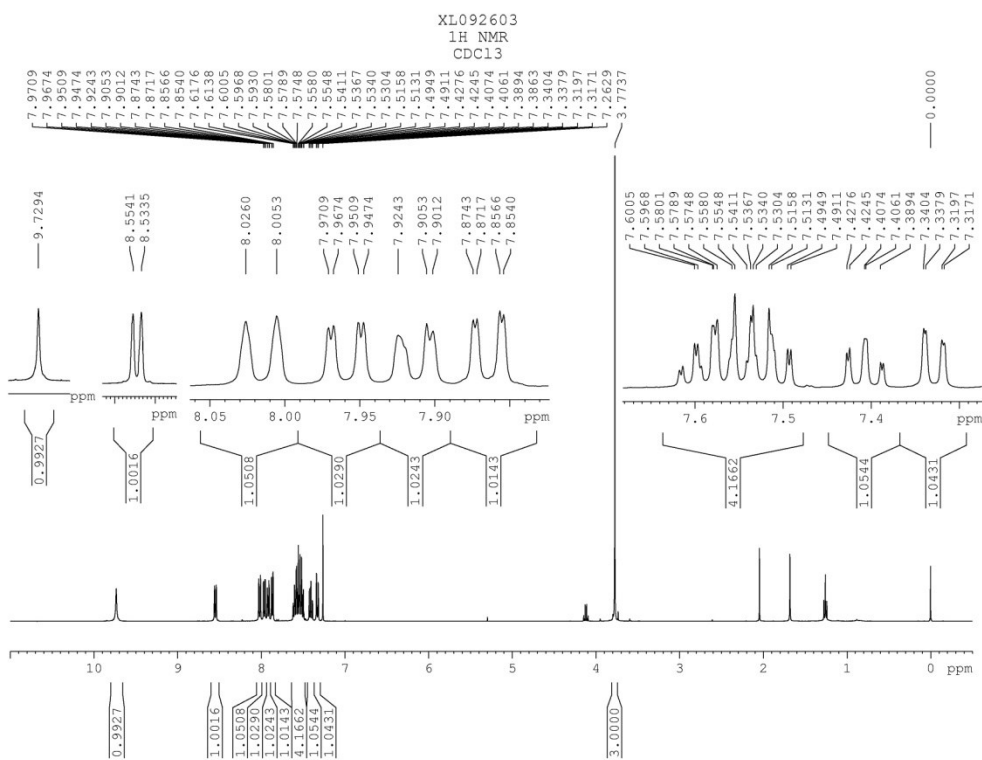


Fig. 20 ¹H NMR spectrum of compound 3ak

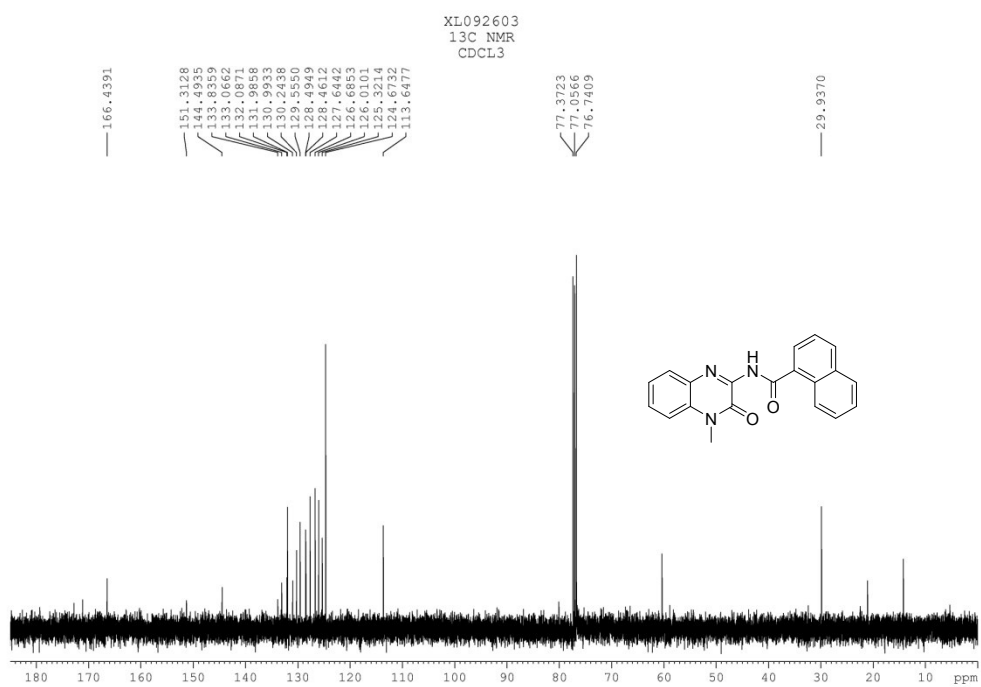


Fig. 21 ¹³C NMR spectrum of compound 3ak

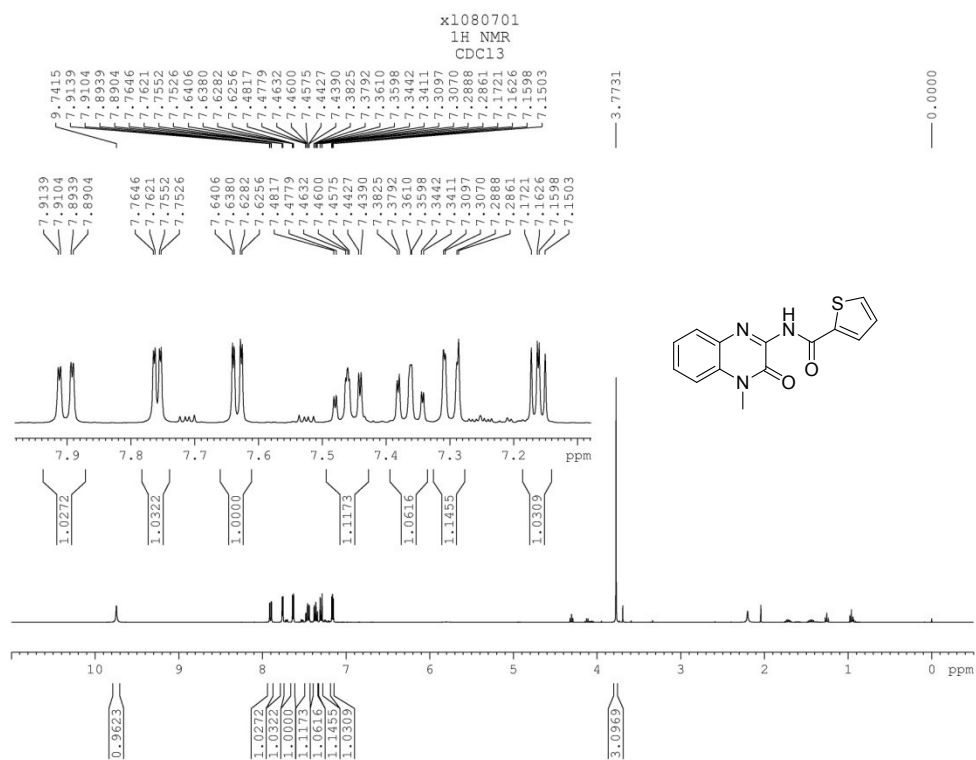


Fig. 22 ¹H NMR spectrum of compound 3al

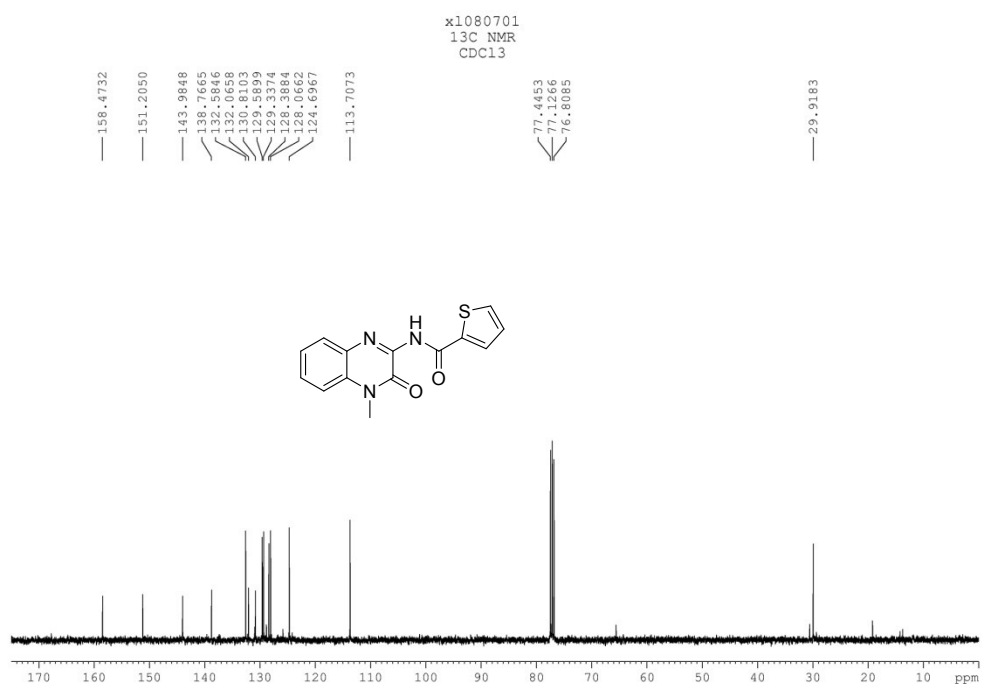


Fig. 23 ¹³C NMR spectrum of compound 3a

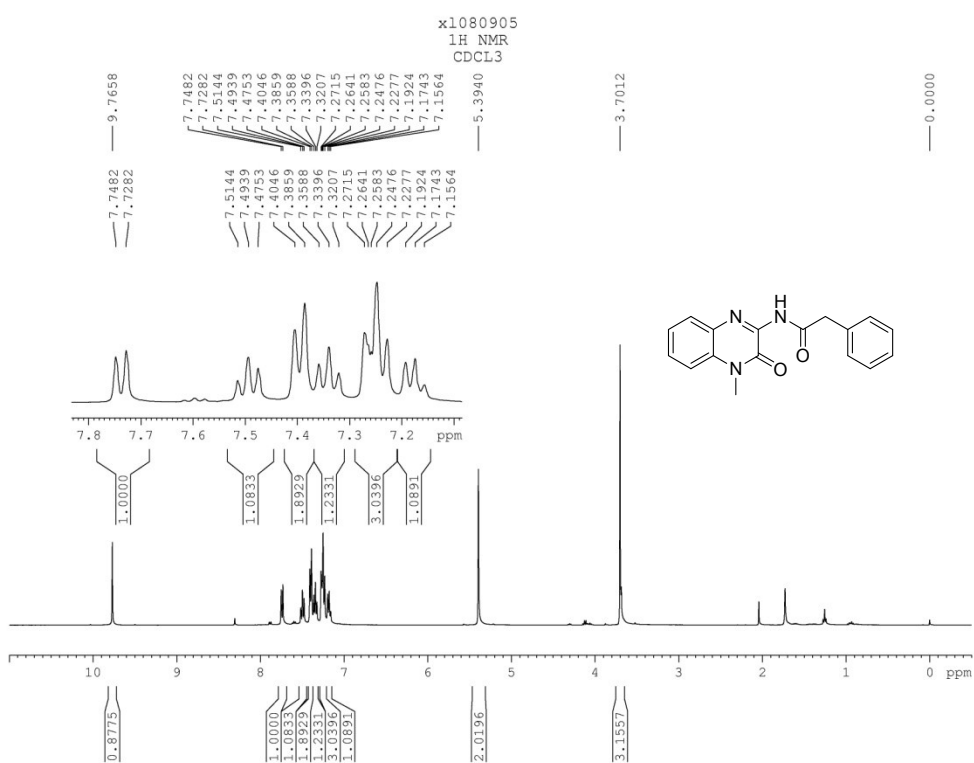


Fig. 24 ¹H NMR spectrum of compound 3a

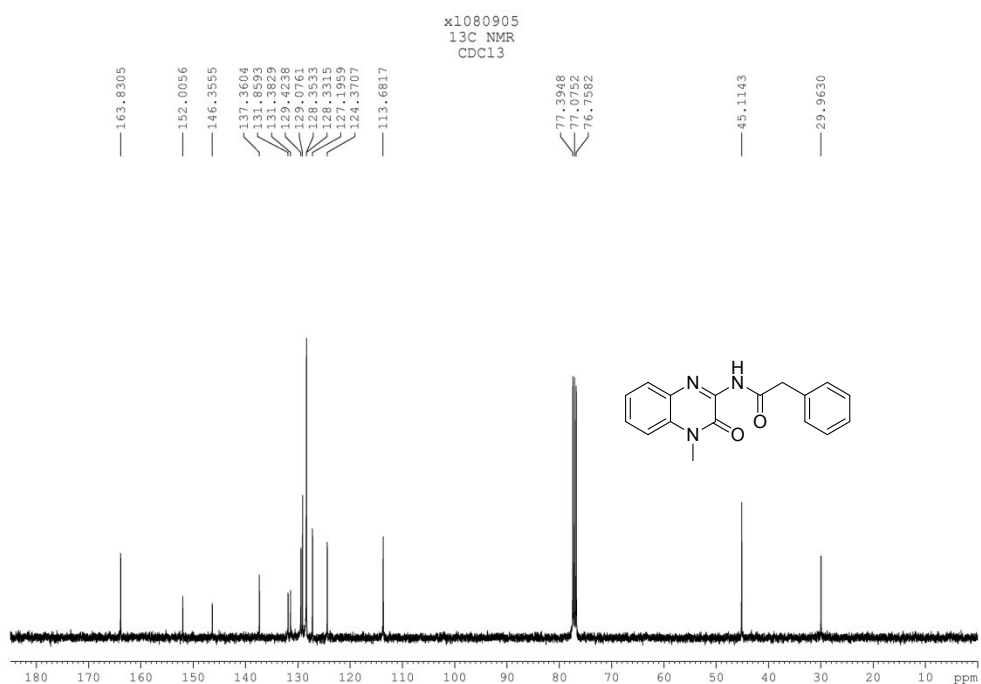


Fig. 25 ¹³C NMR spectrum of compound 3am

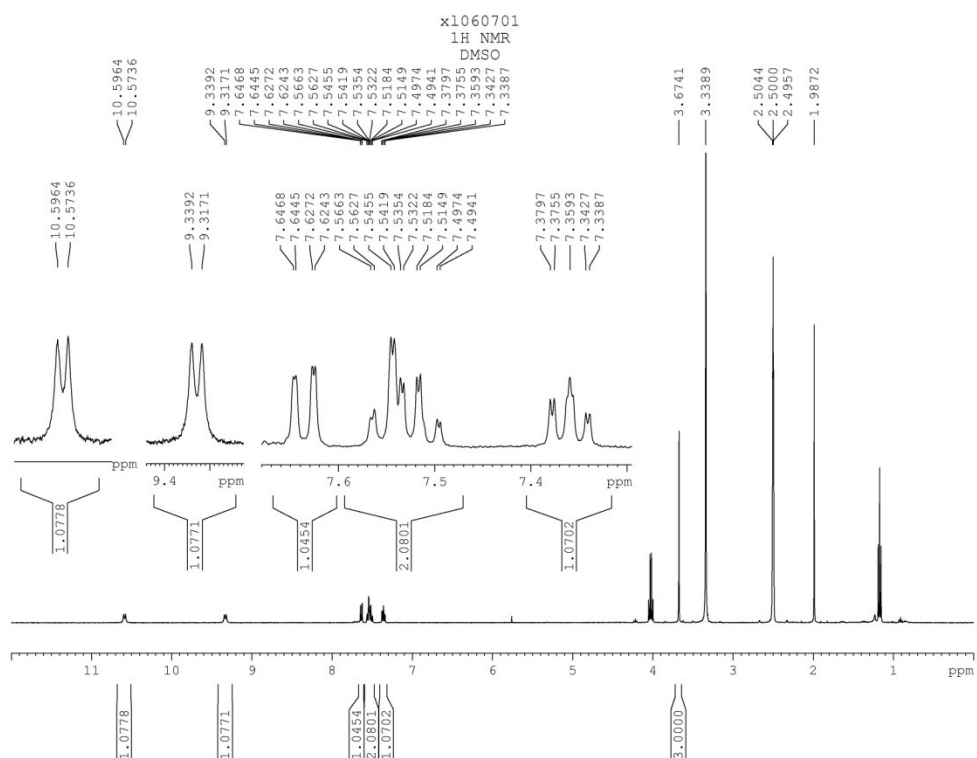


Fig. 26 ¹H NMR spectrum of compound 3am

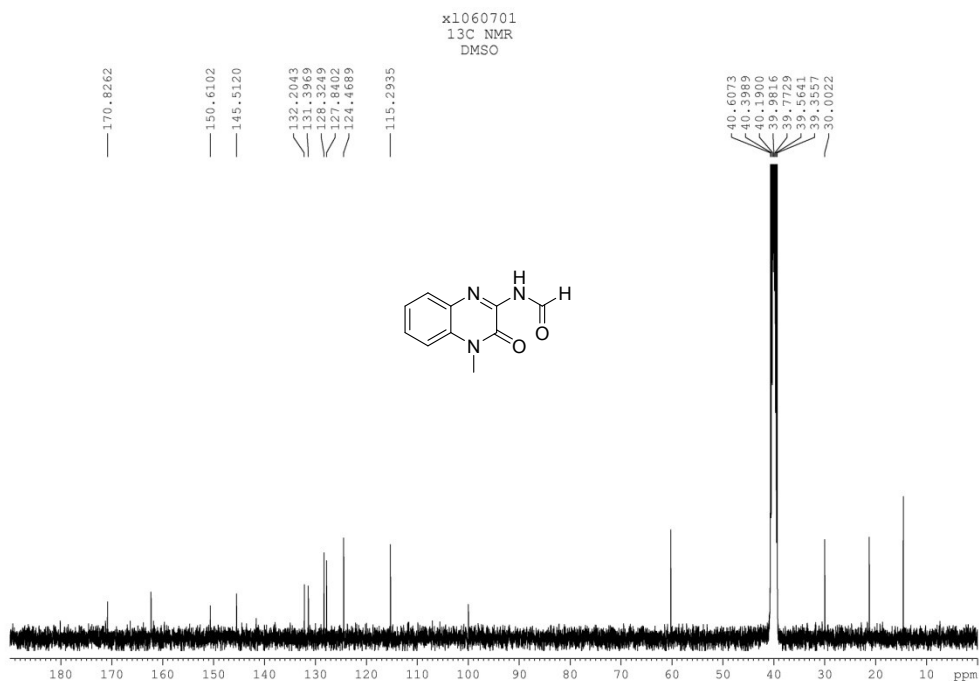


Fig. 27 ¹³C NMR spectrum of compound 3an

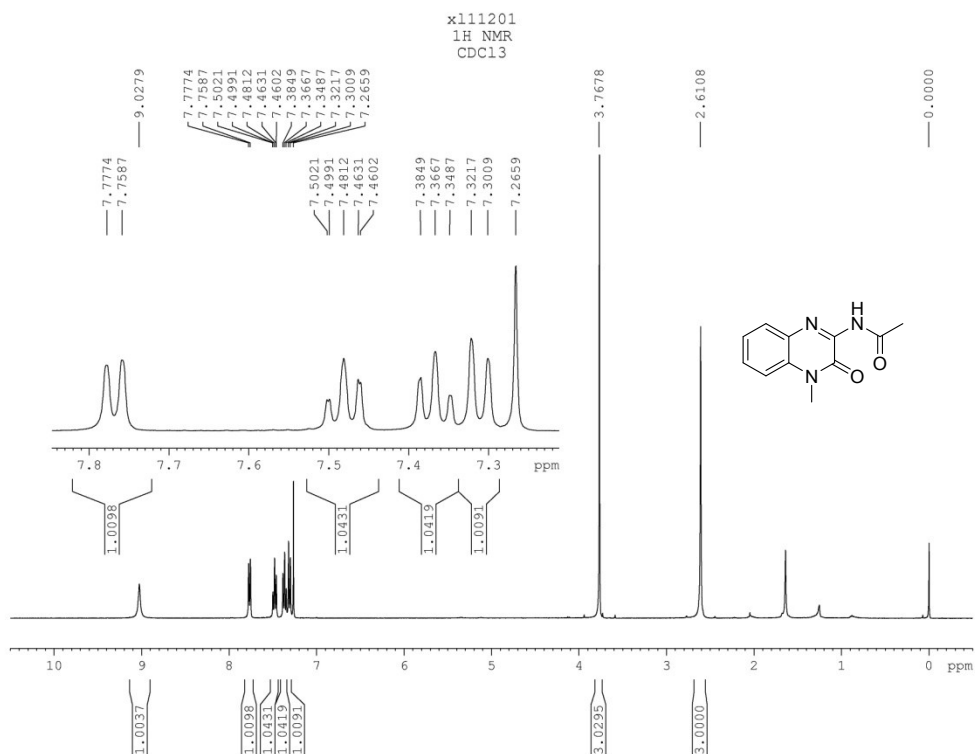


Fig. 28 ¹H NMR spectrum of compound 3ao

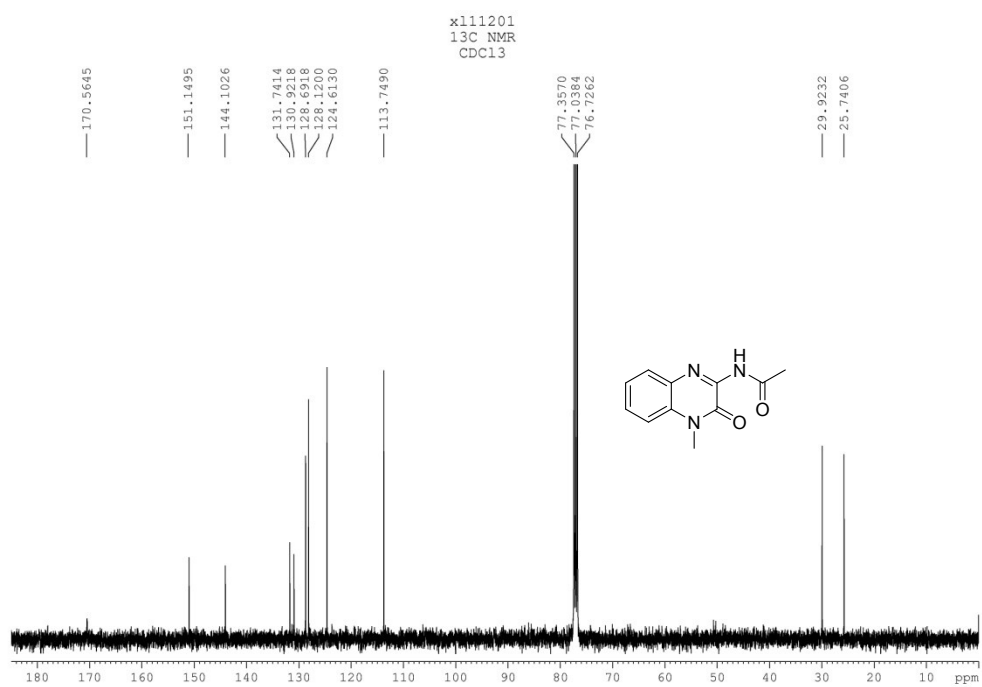


Fig. 29 ¹³C NMR spectrum of compound 3ao

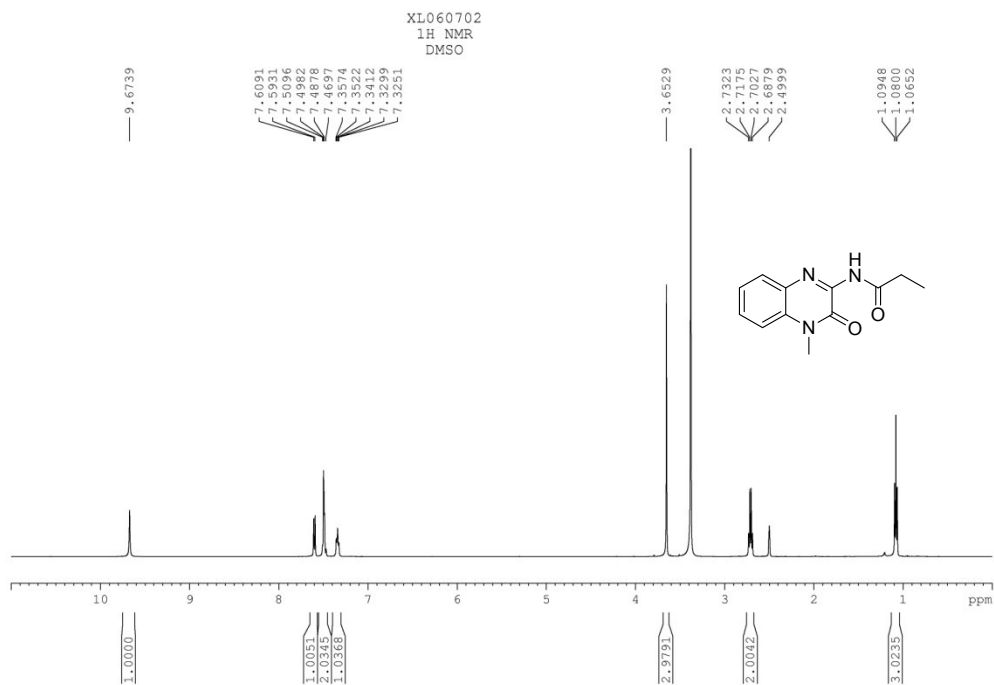


Fig. 30 ¹H NMR spectrum of compound 3ap

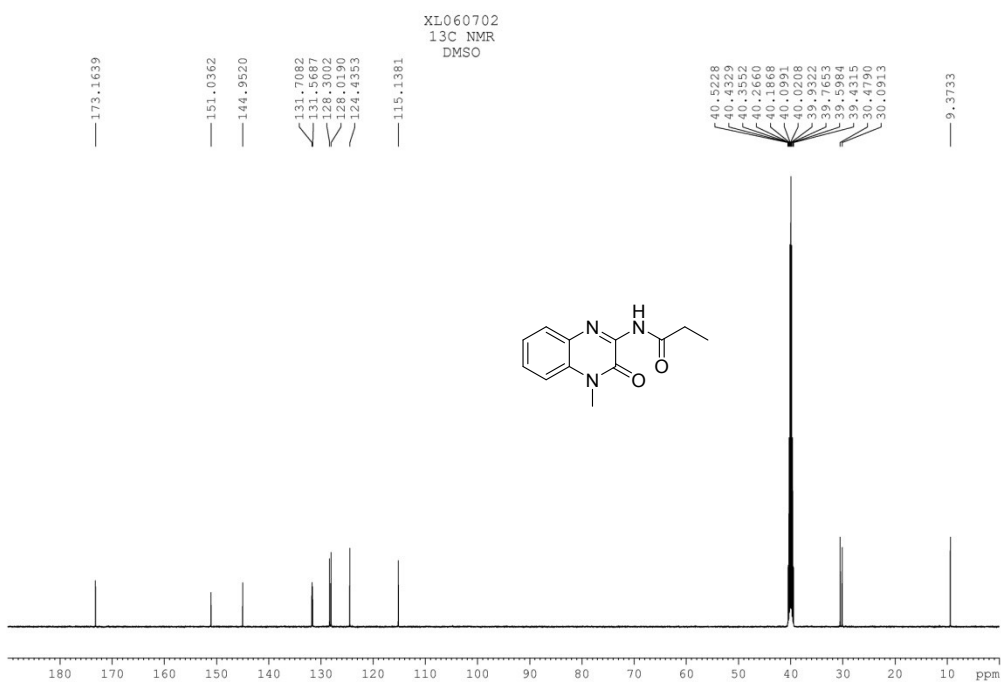


Fig. 31 ¹³C NMR spectrum of compound 3ap

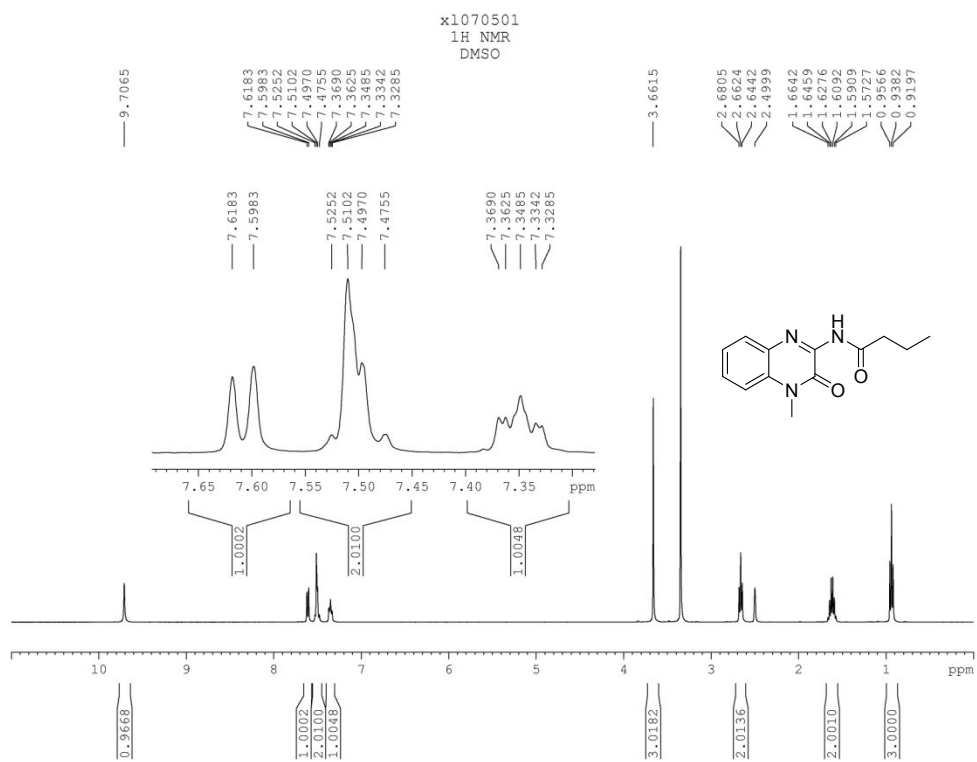


Fig. 32 ¹H NMR spectrum of compound 3aq

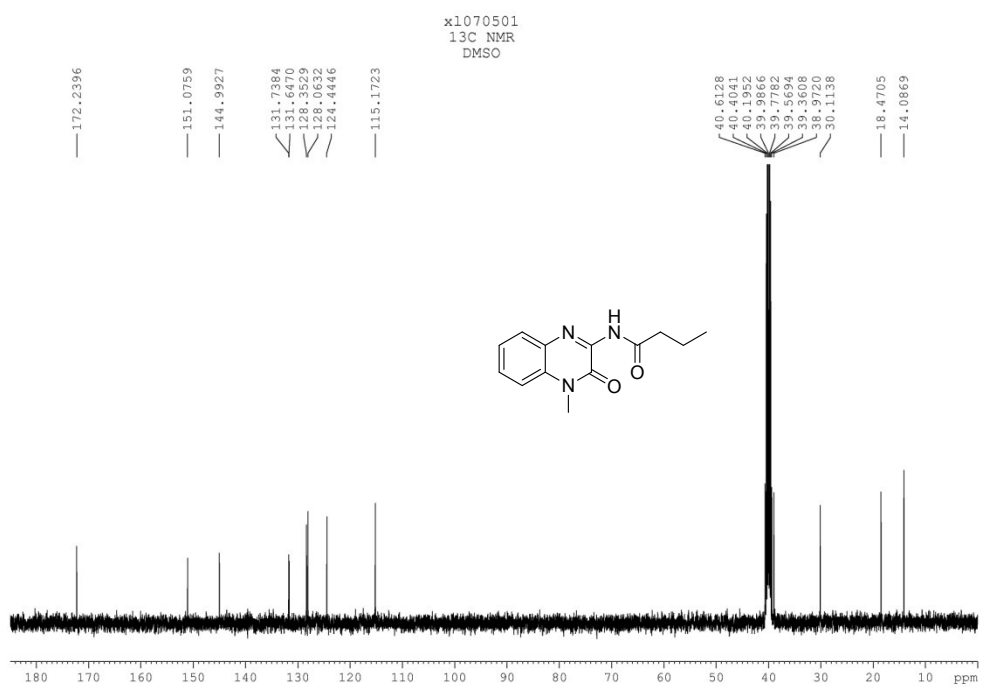


Fig. 33 ¹³C NMR spectrum of compound 3aq

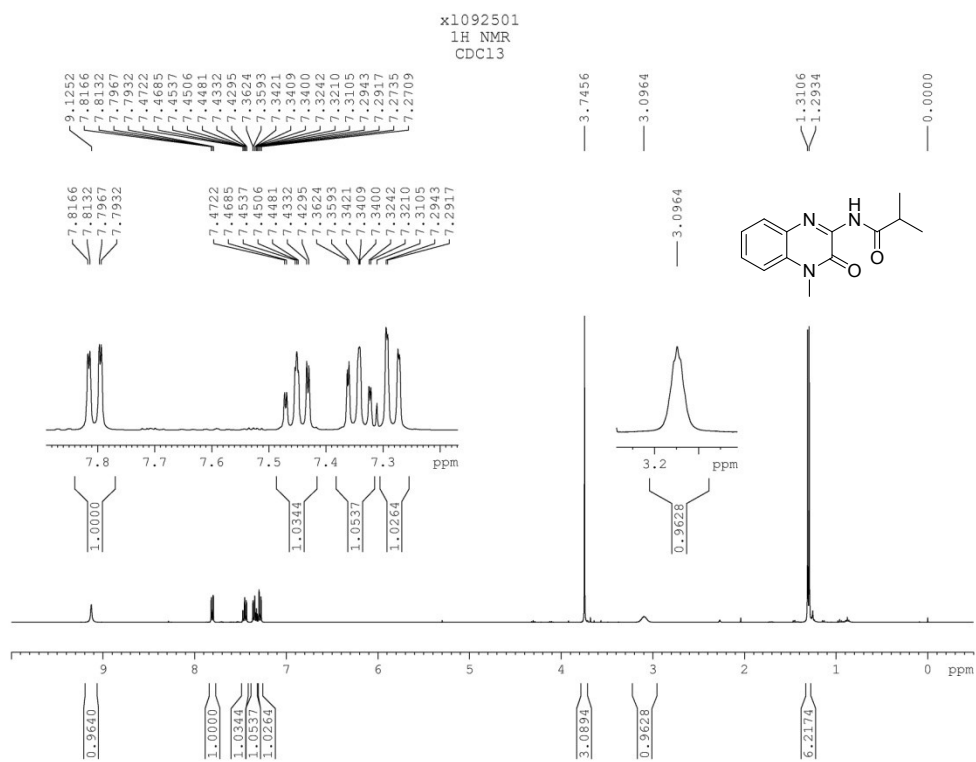


Fig. 34 ¹H NMR spectrum of compound 3ar

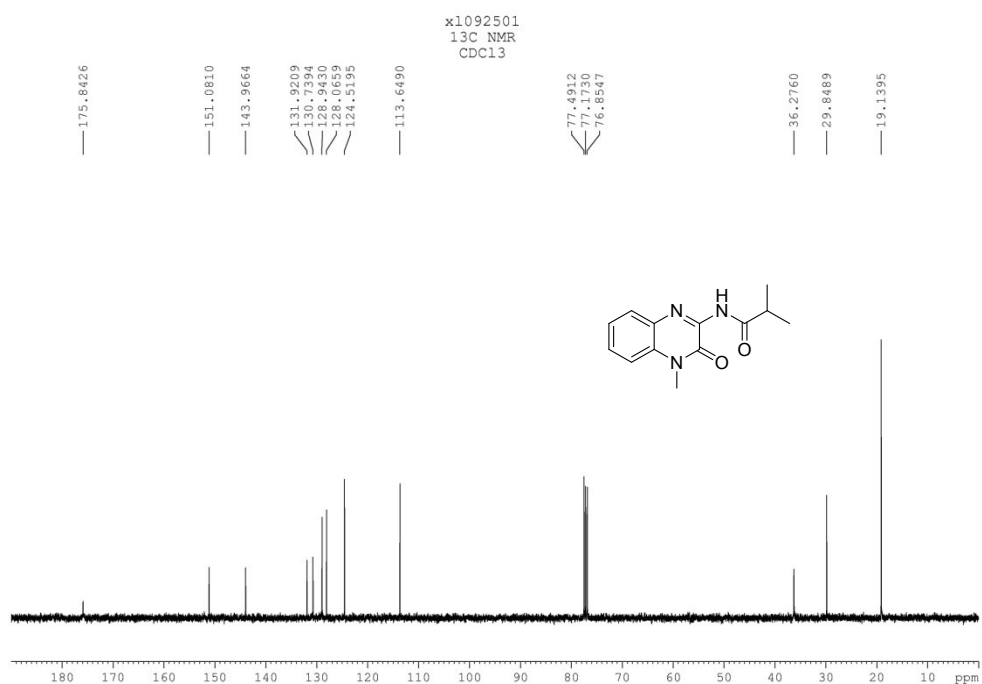


Fig. 35 ^{13}C NMR spectrum of compound **3ar**

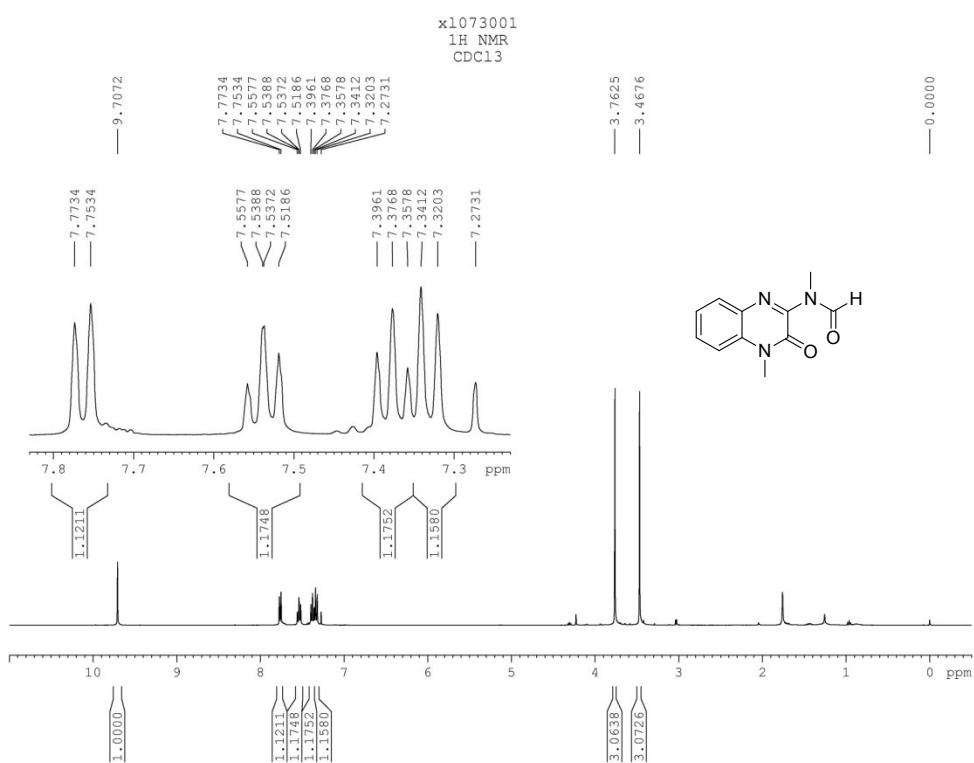


Fig. 36 ^1H NMR spectrum of compound **3as**

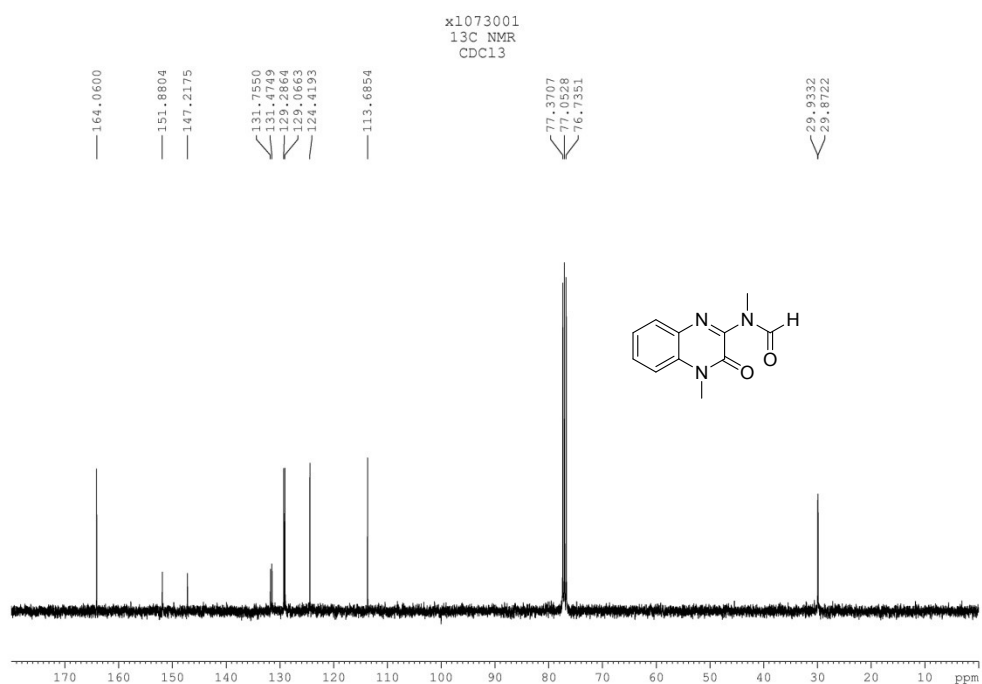


Fig. 37 ^{13}C NMR spectrum of compound 3as

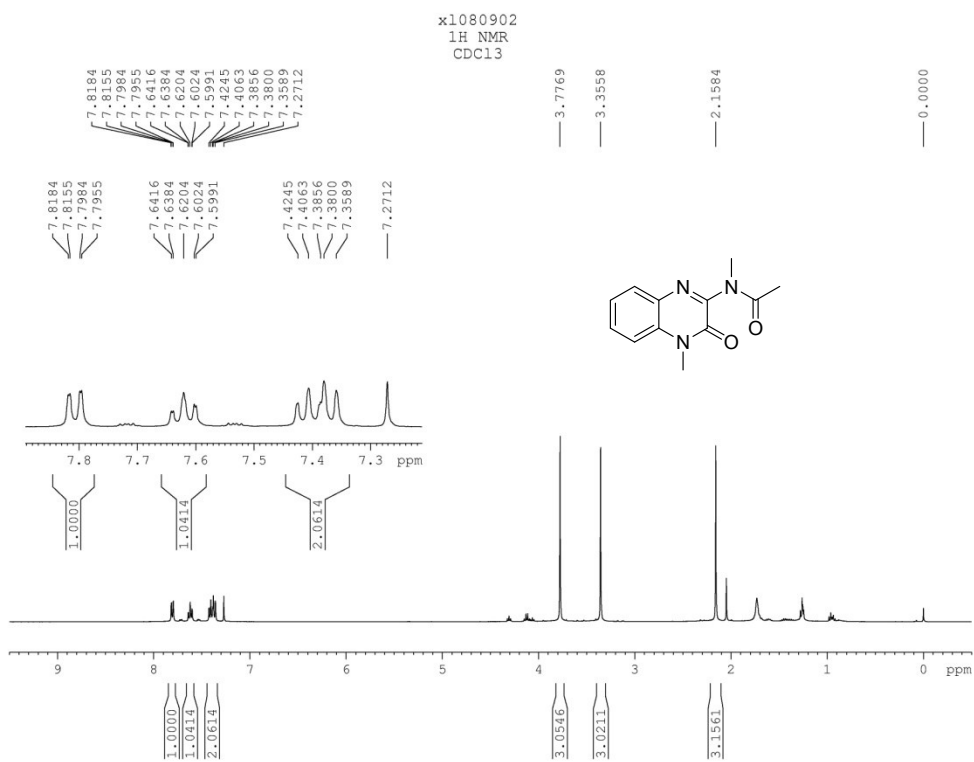


Fig. 38 ^1H NMR spectrum of compound 3at

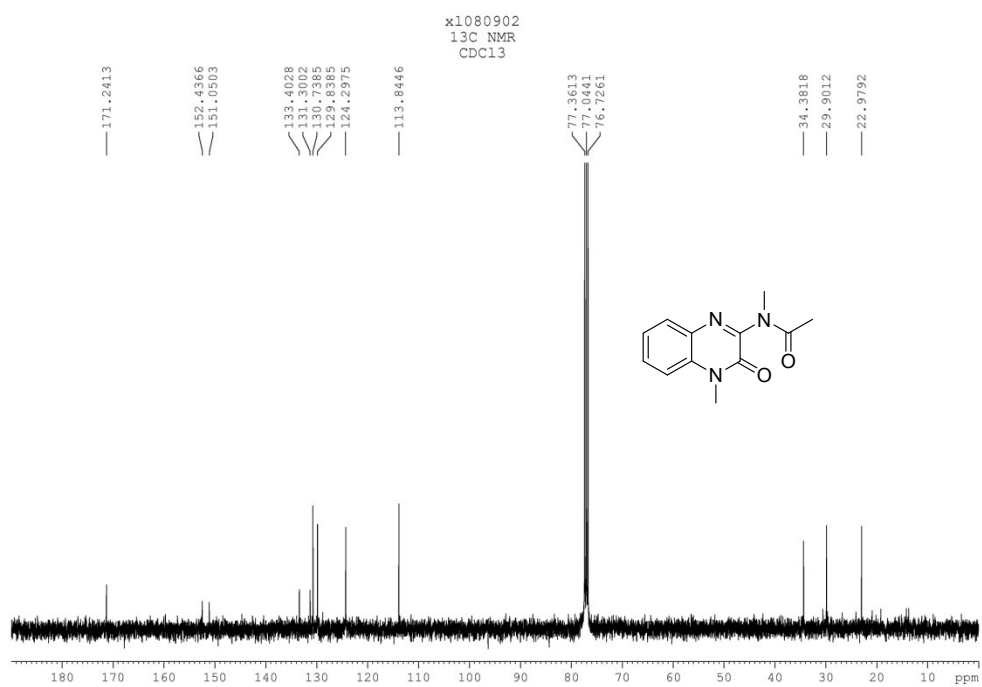


Fig. 39 ¹³C NMR spectrum of compound 3at

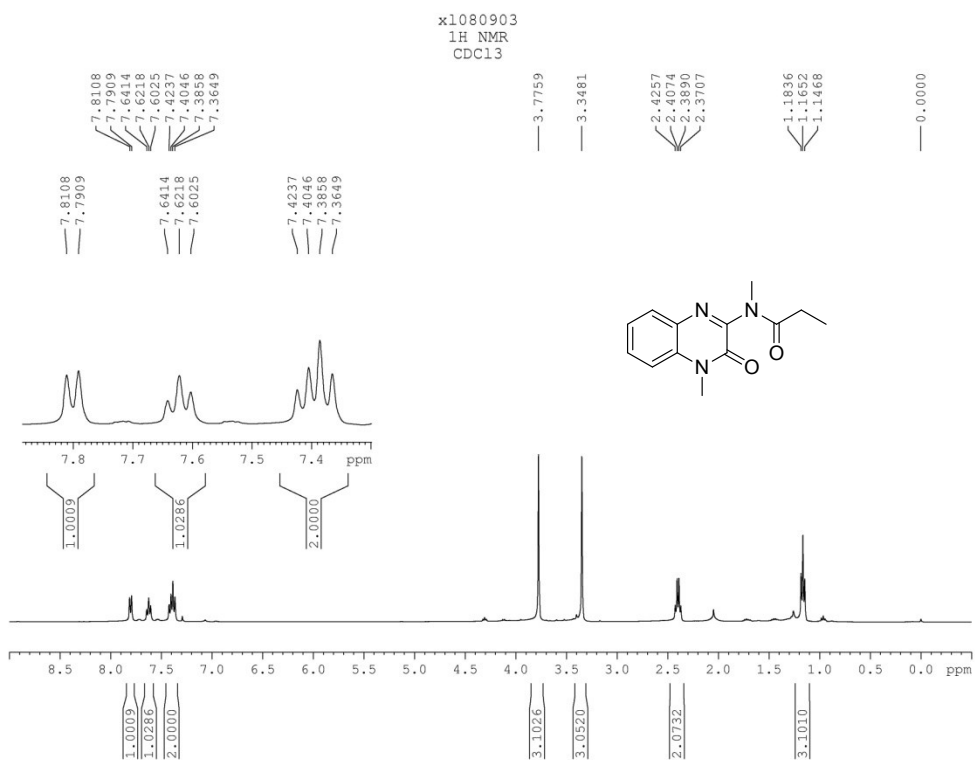


Fig. 40 ¹H NMR spectrum of compound 3au

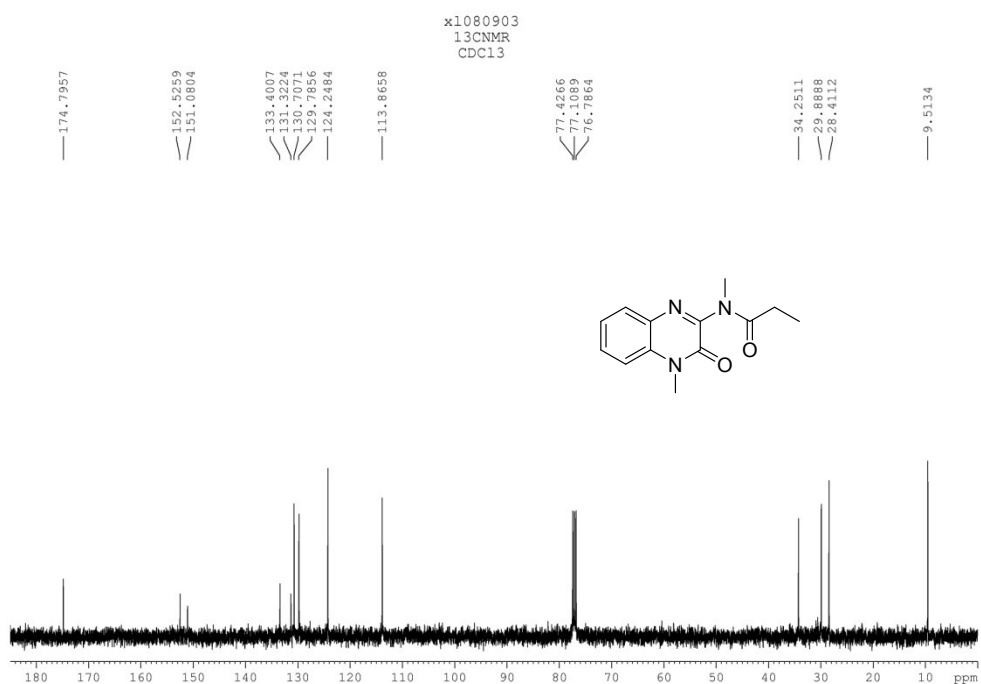


Fig. 41 ¹³C NMR spectrum of compound 3au

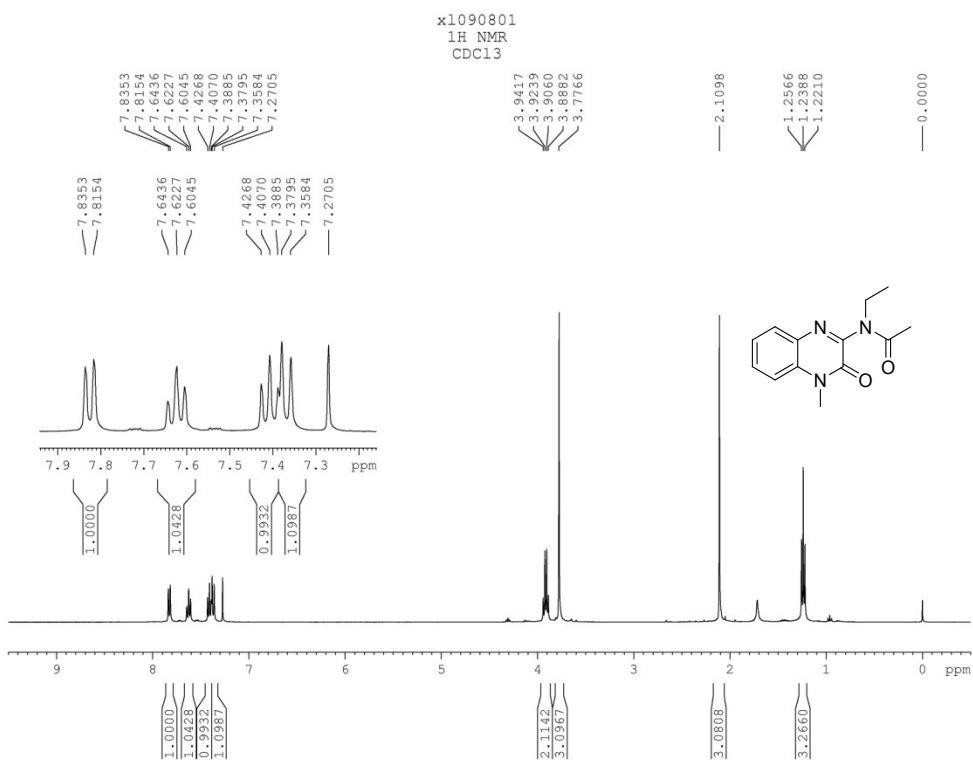


Fig. 42 ¹H NMR spectrum of compound 3av

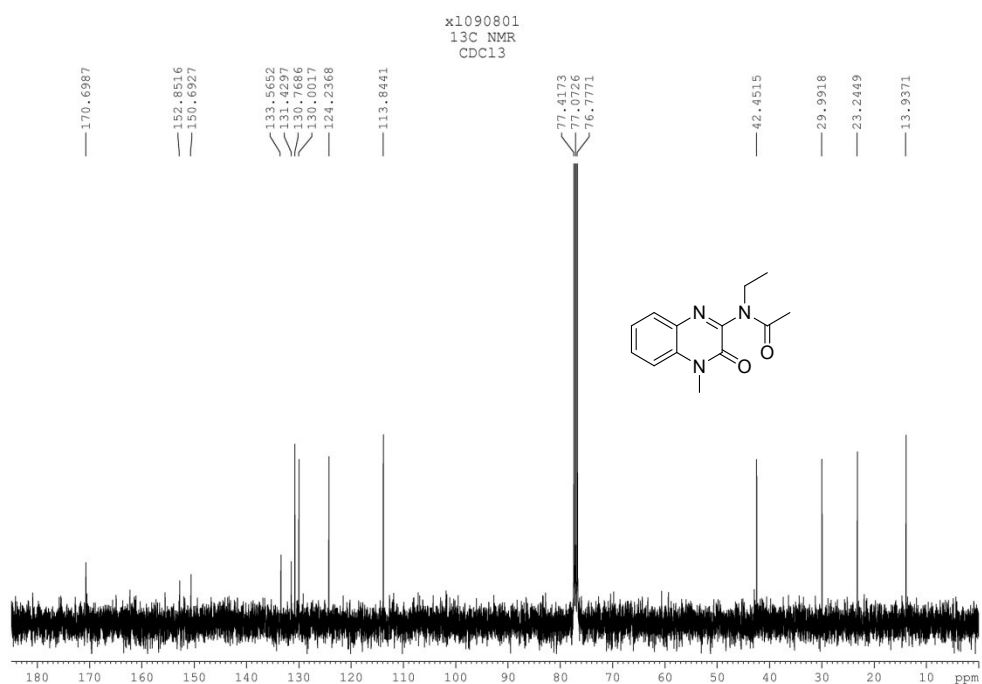


Fig. 43 ¹³C NMR spectrum of compound 3av

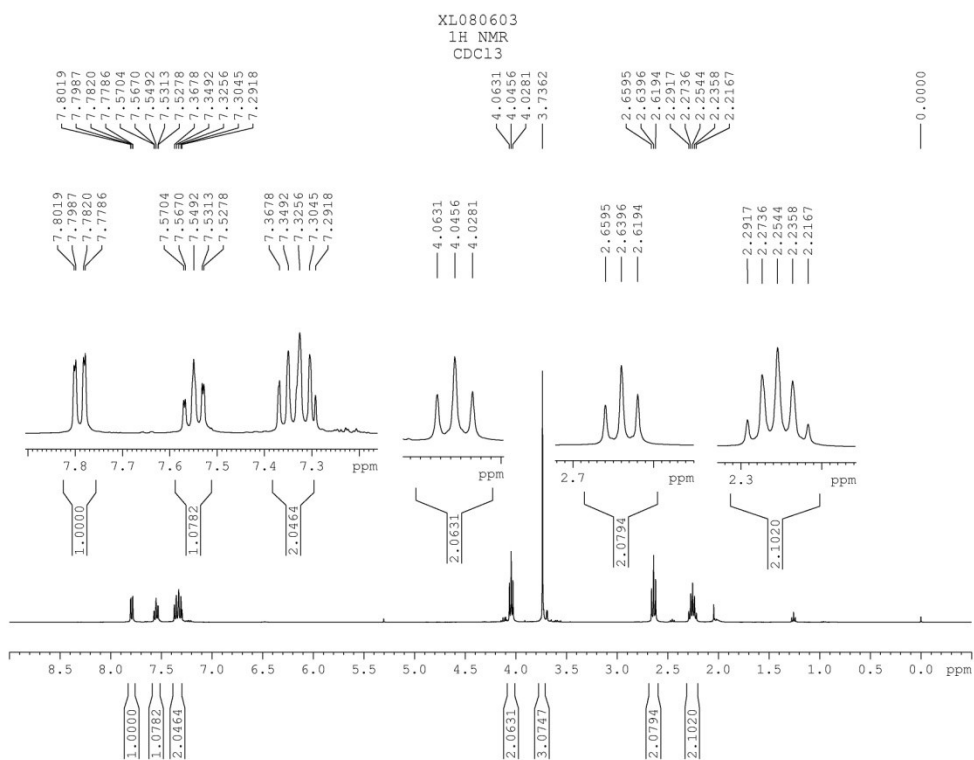


Fig. 44 ¹H NMR spectrum of compound 3av

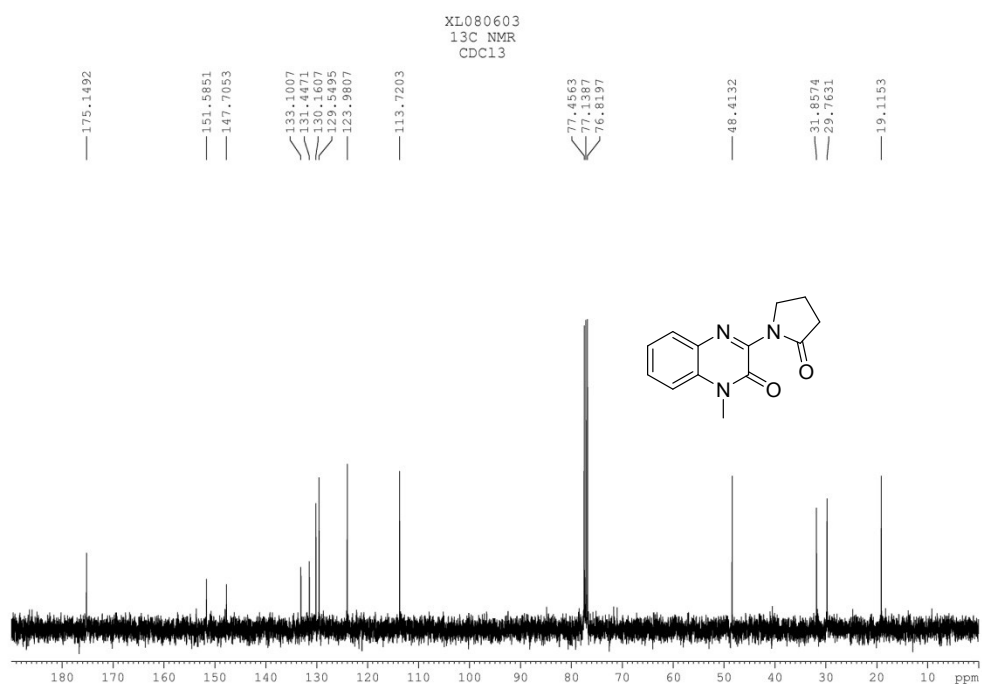


Fig. 45 ¹³C NMR spectrum of compound 3aw

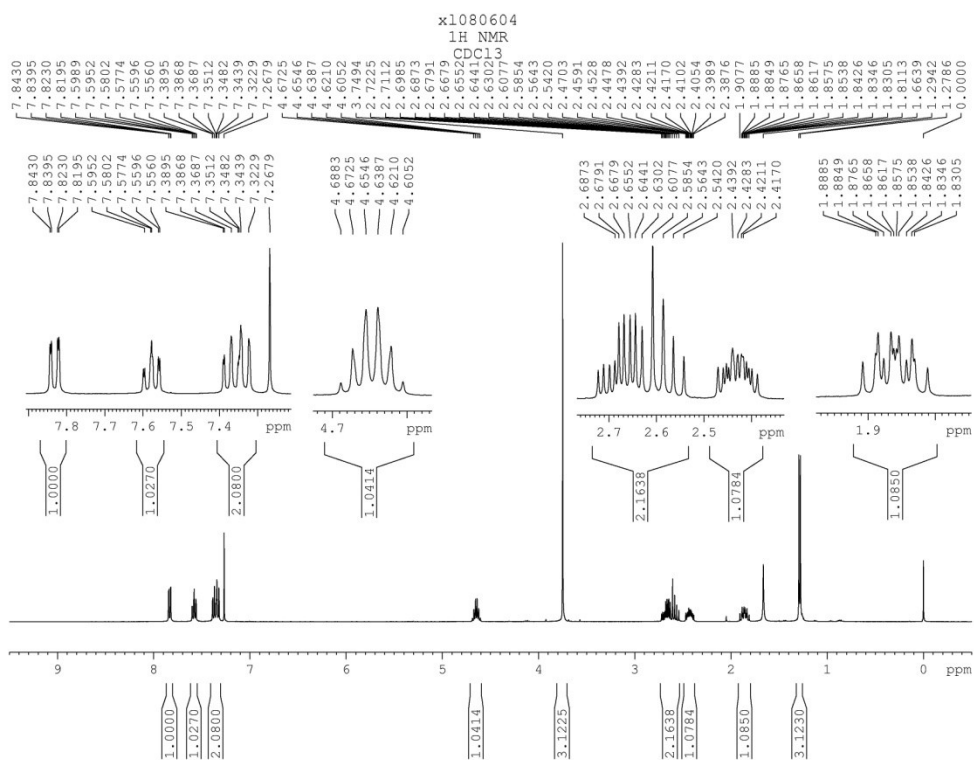


Fig. 46 ¹H NMR spectrum of compound 3ax

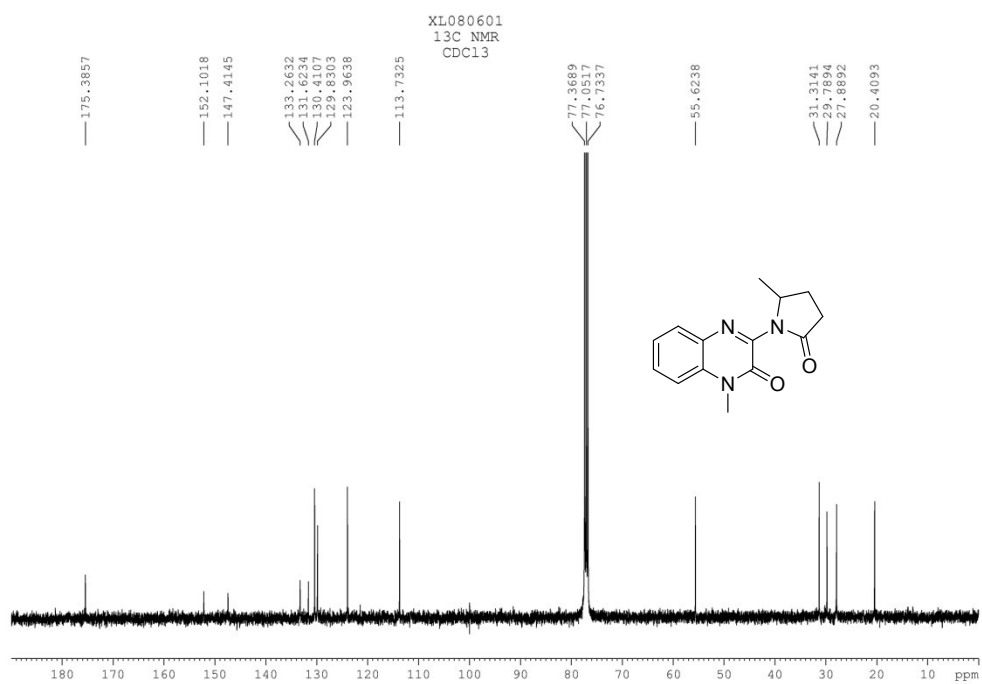


Fig. 47 ¹³C NMR spectrum of compound 3ax

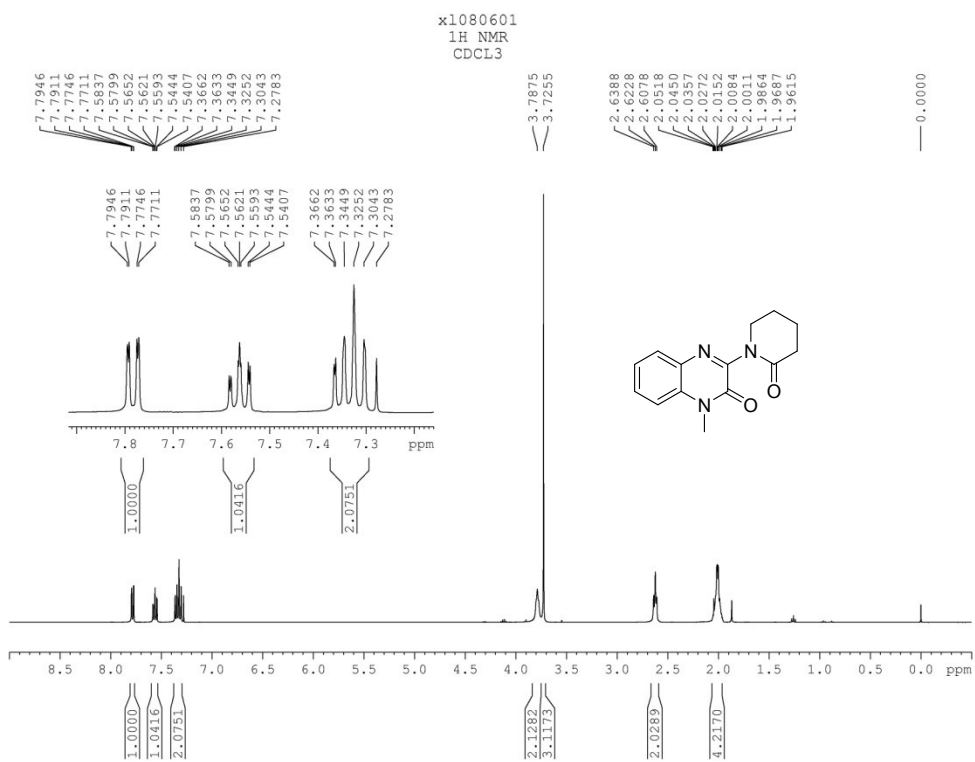


Fig. 48 ¹H NMR spectrum of compound 3ay

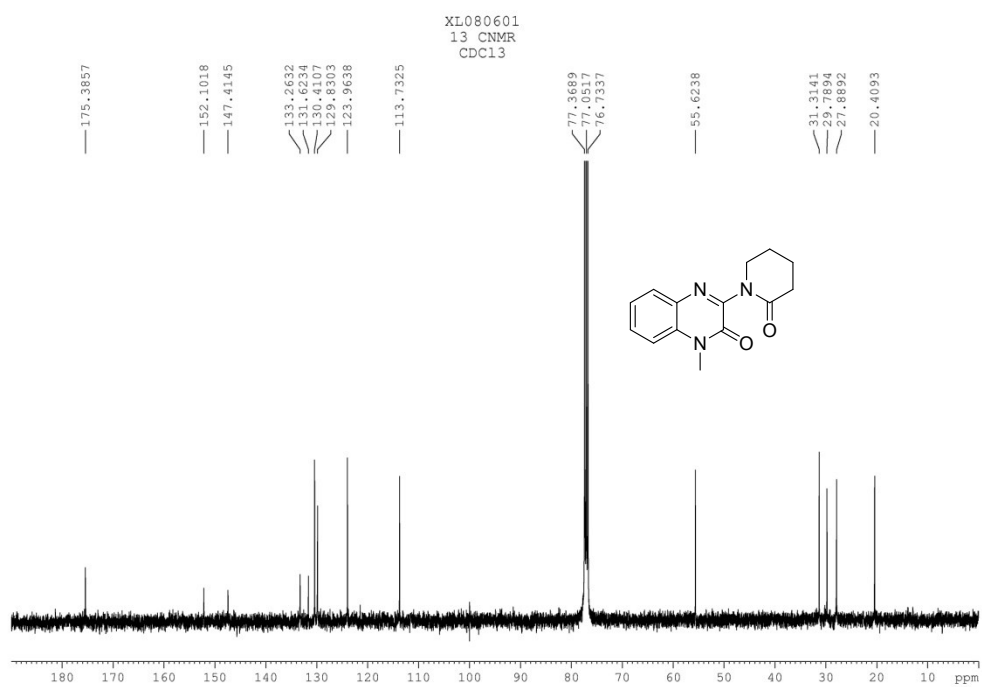


Fig. 49 ¹³C NMR spectrum of compound 3ay

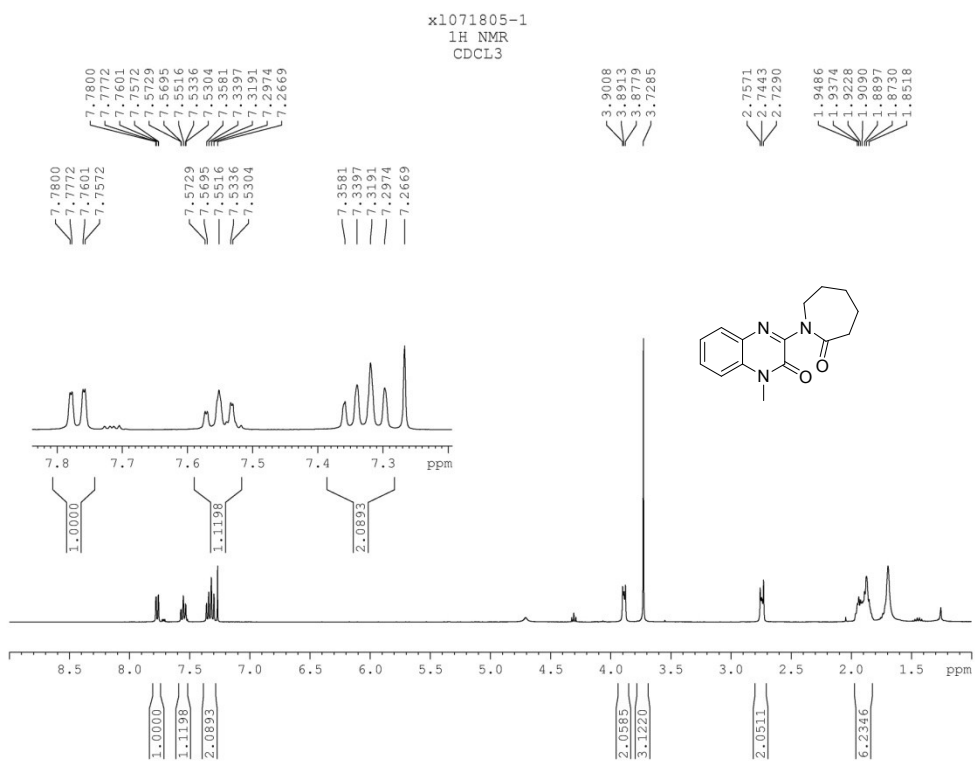


Fig. 50 ¹H NMR spectrum of compound 3az

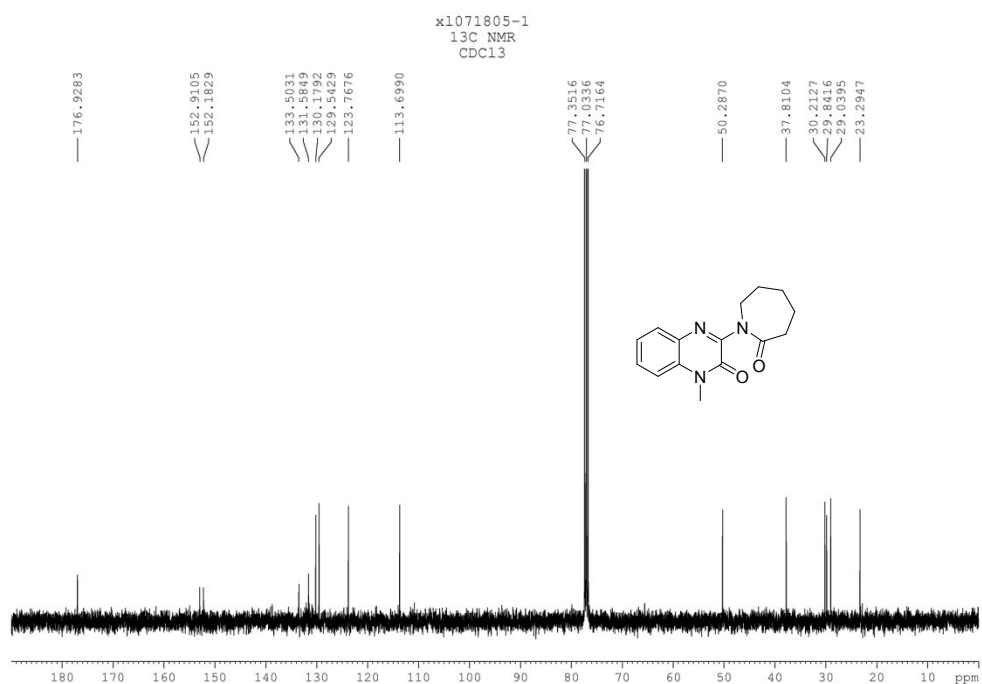


Fig. 51 ¹³C NMR spectrum of compound 3az

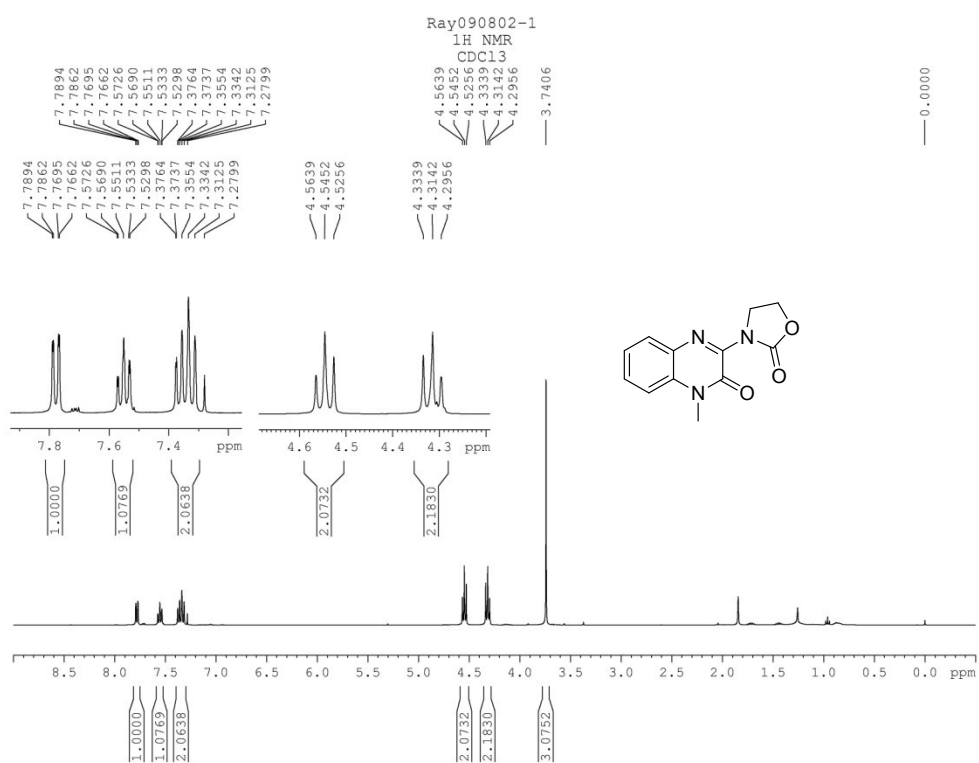


Fig. 52 ¹H NMR spectrum of compound 3az'

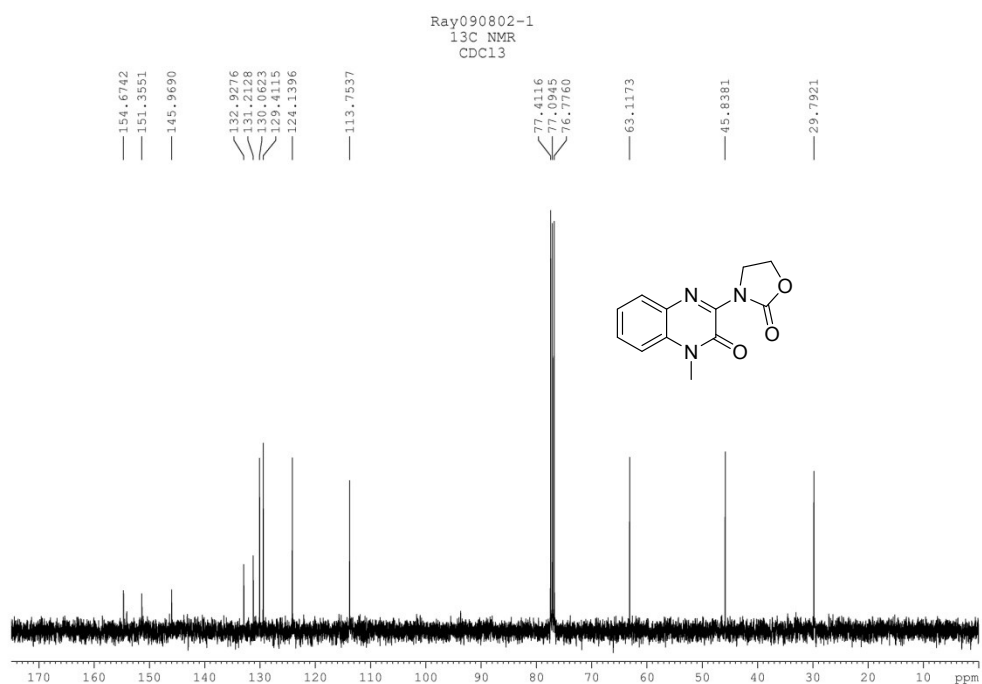


Fig. 53 ¹³C NMR spectrum of compound 3az'

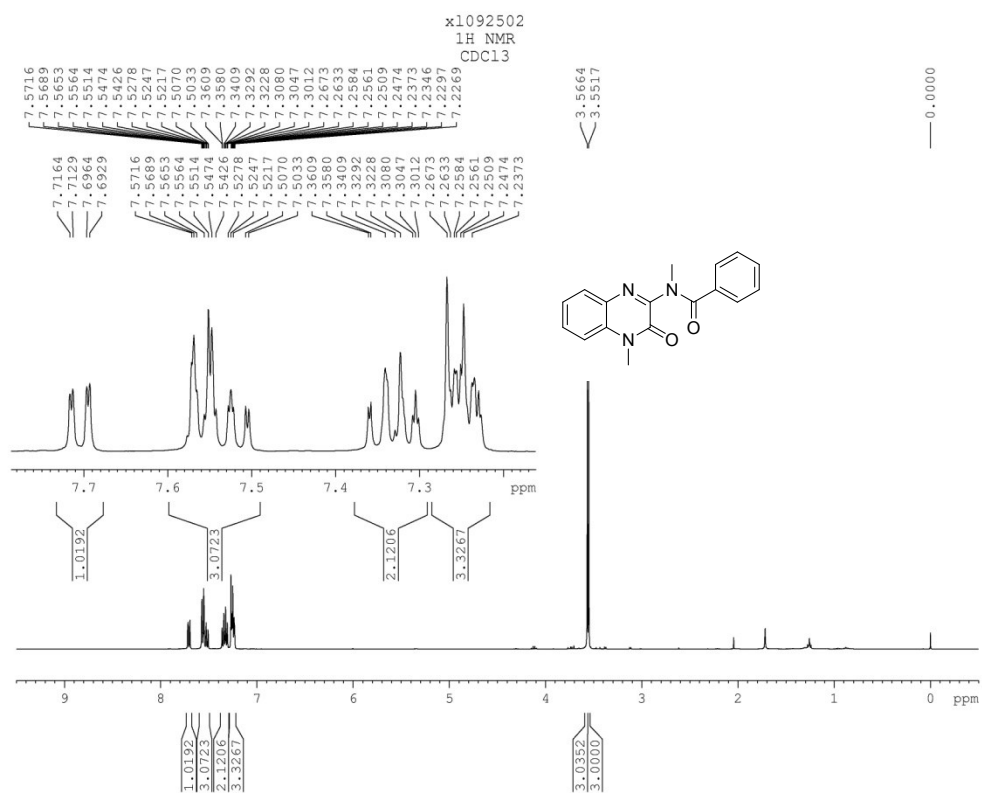


Fig. 54 ¹H NMR spectrum of compound 3az''

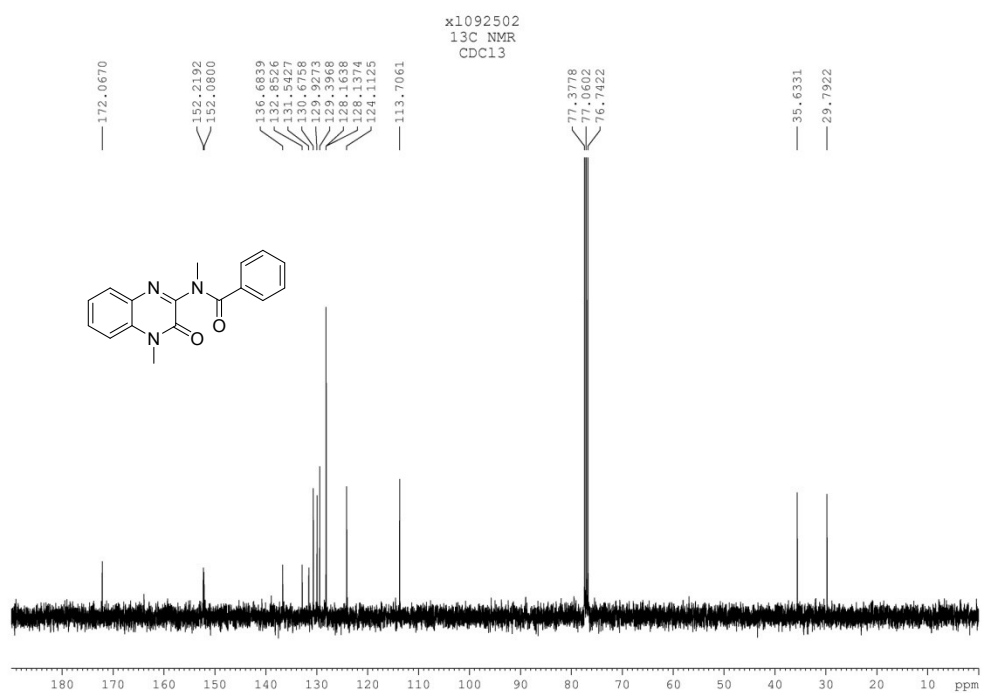


Fig. 55 ¹³C NMR spectrum of compound 3az''

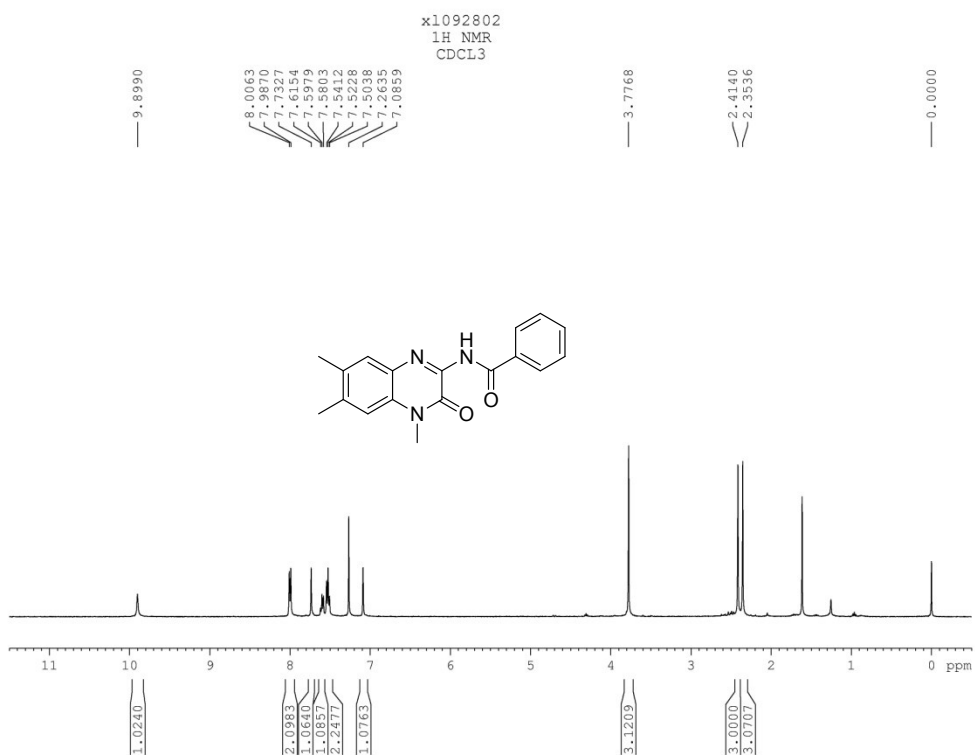


Fig. 56 ¹H NMR spectrum of compound 3ba

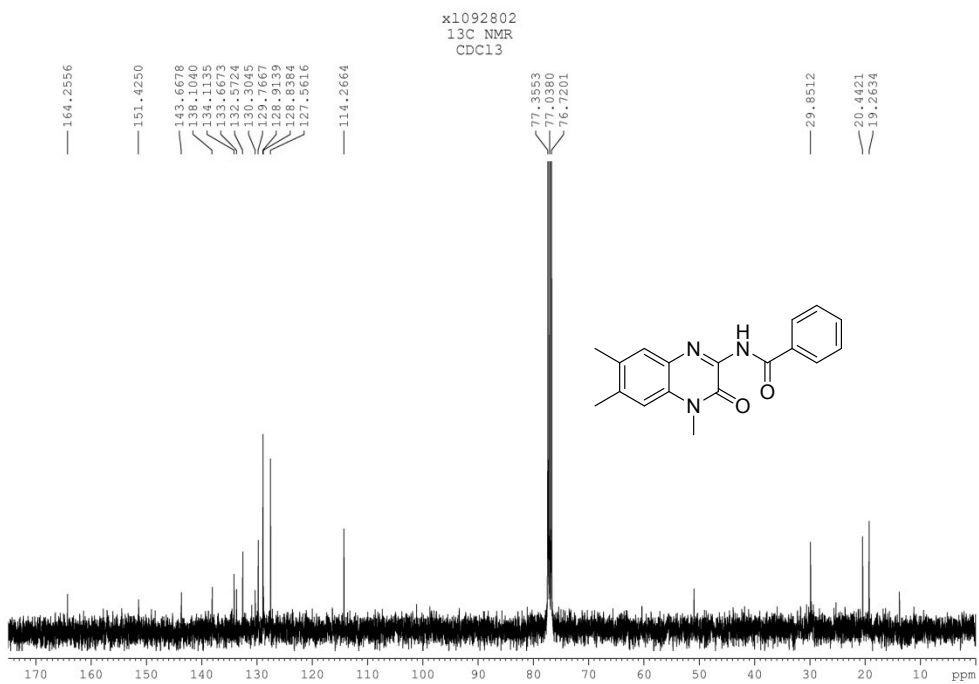


Fig. 57 ¹³C NMR spectrum of compound 3ba

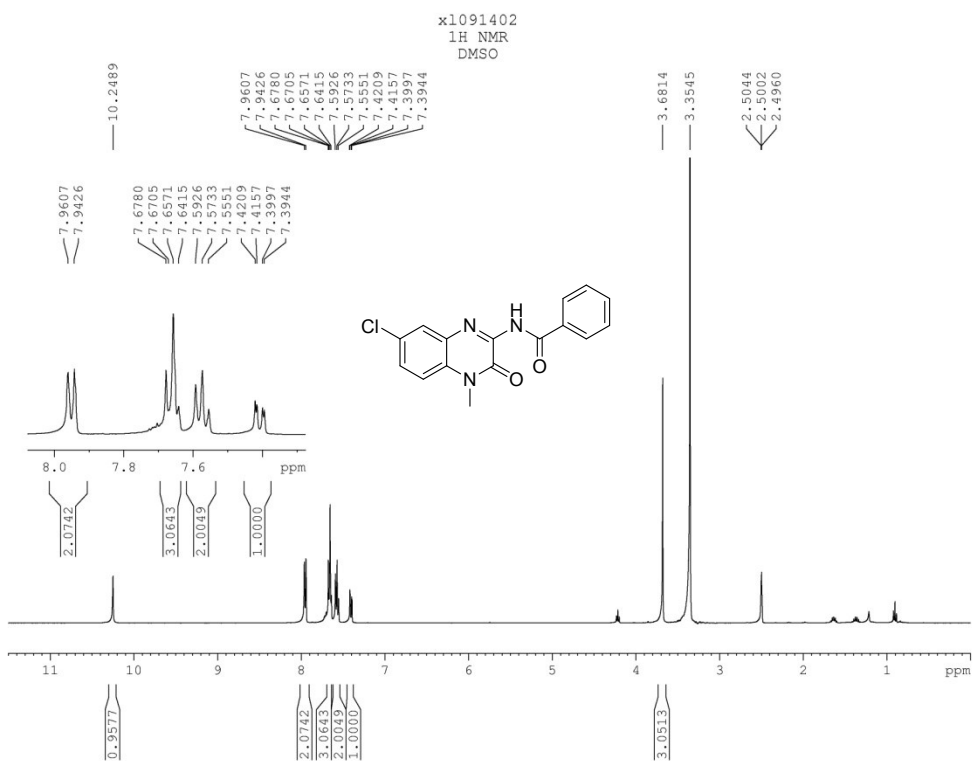


Fig. 58 ¹H NMR spectrum of compound 3ca

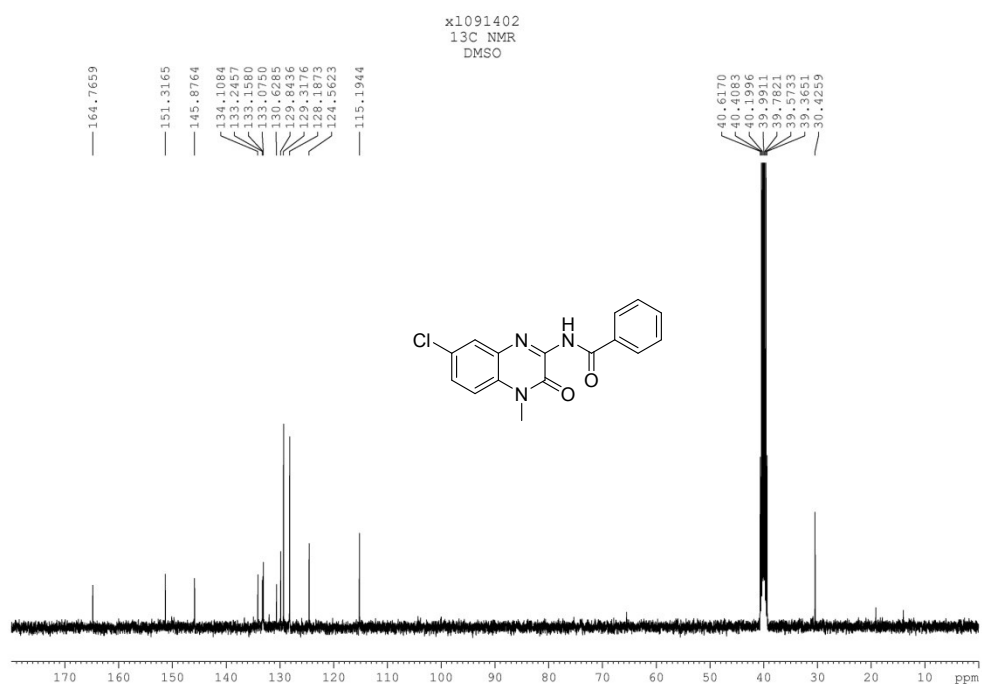


Fig. 59 ¹³C NMR spectrum of compound 3ca

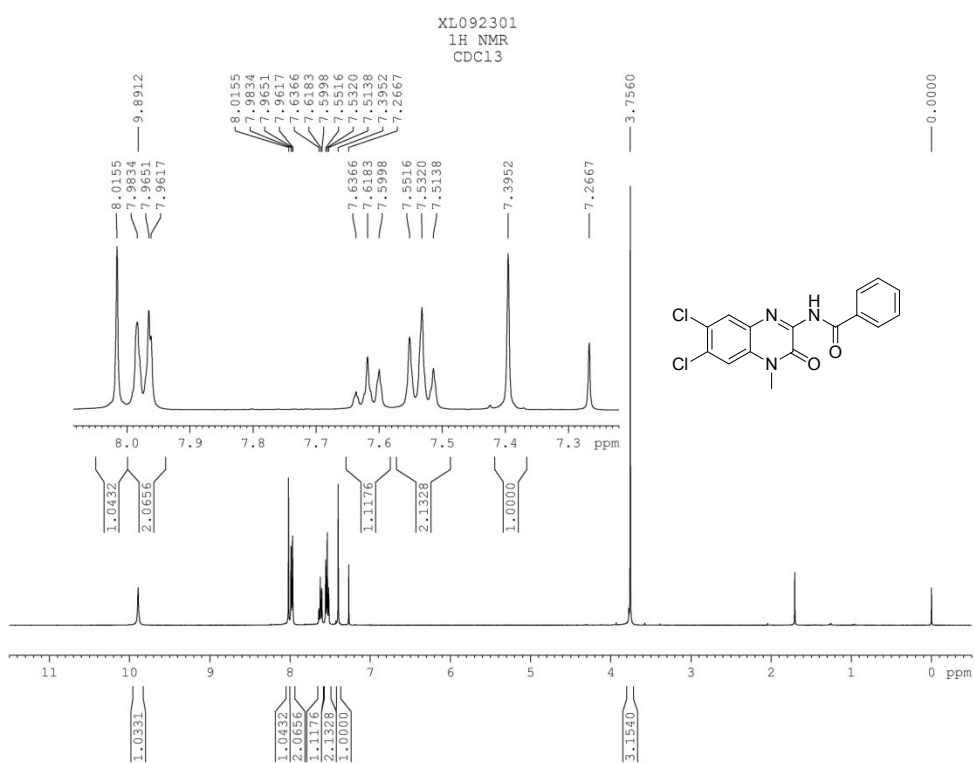


Fig. 60 ¹H NMR spectrum of compound 3da

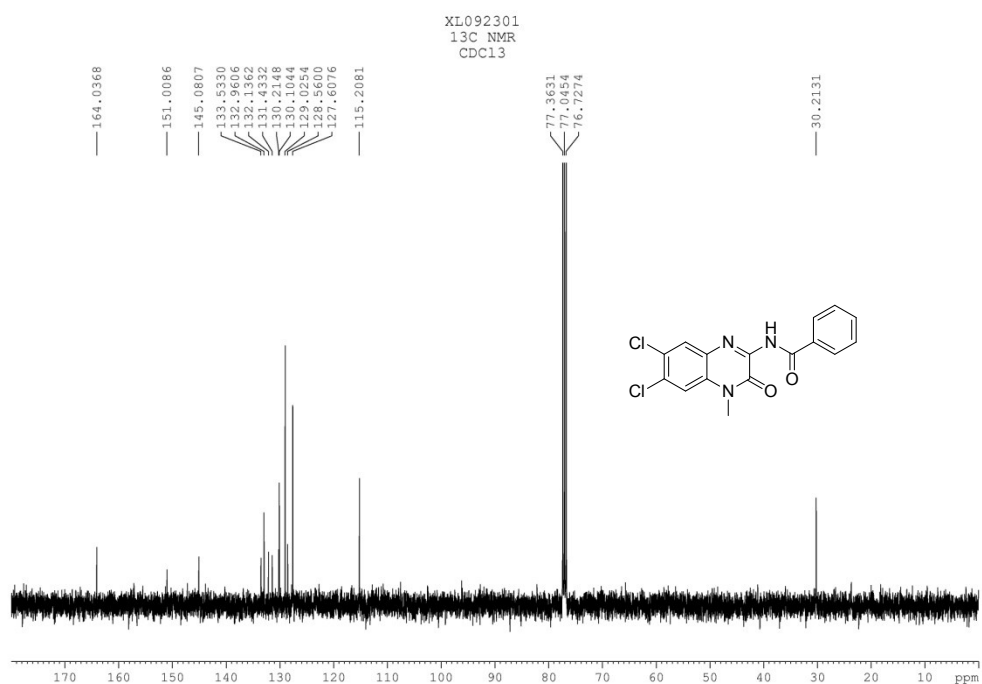


Fig. 61 ¹³C NMR spectrum of compound 3da

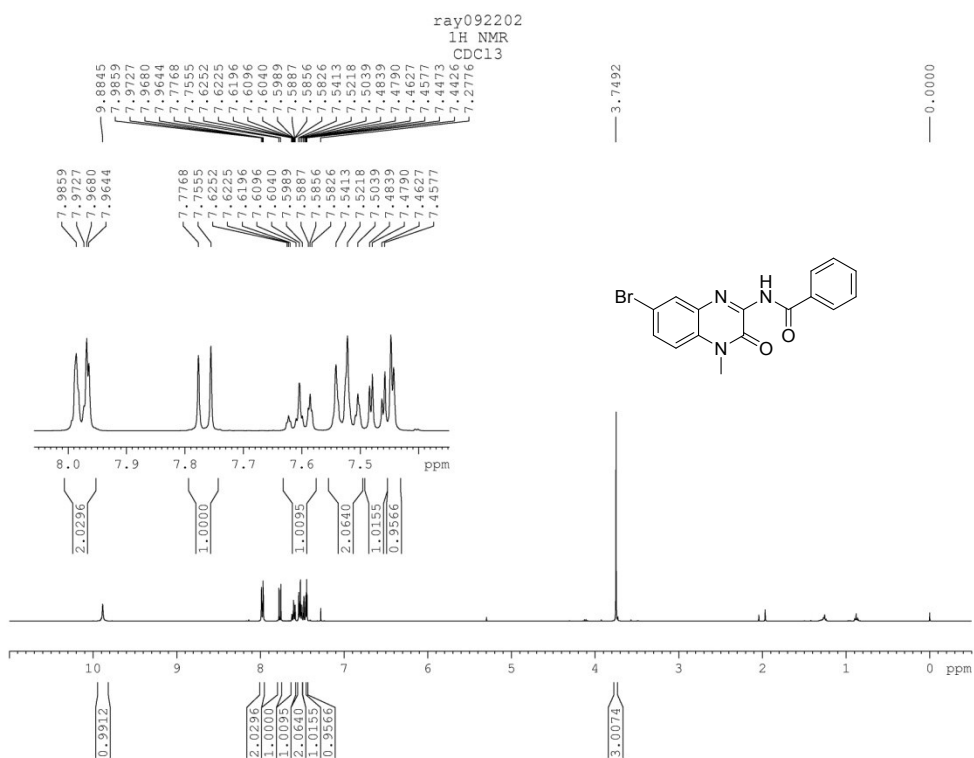


Fig. 62 ¹H NMR spectrum of compound 3ea

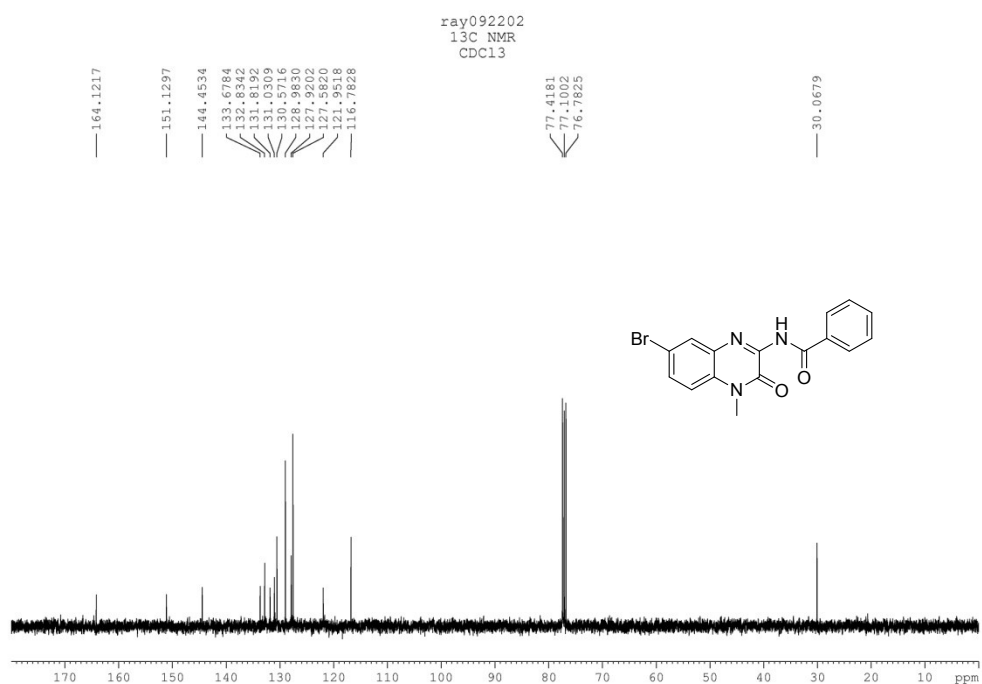


Fig. 63 ¹³C NMR spectrum of compound 3ea

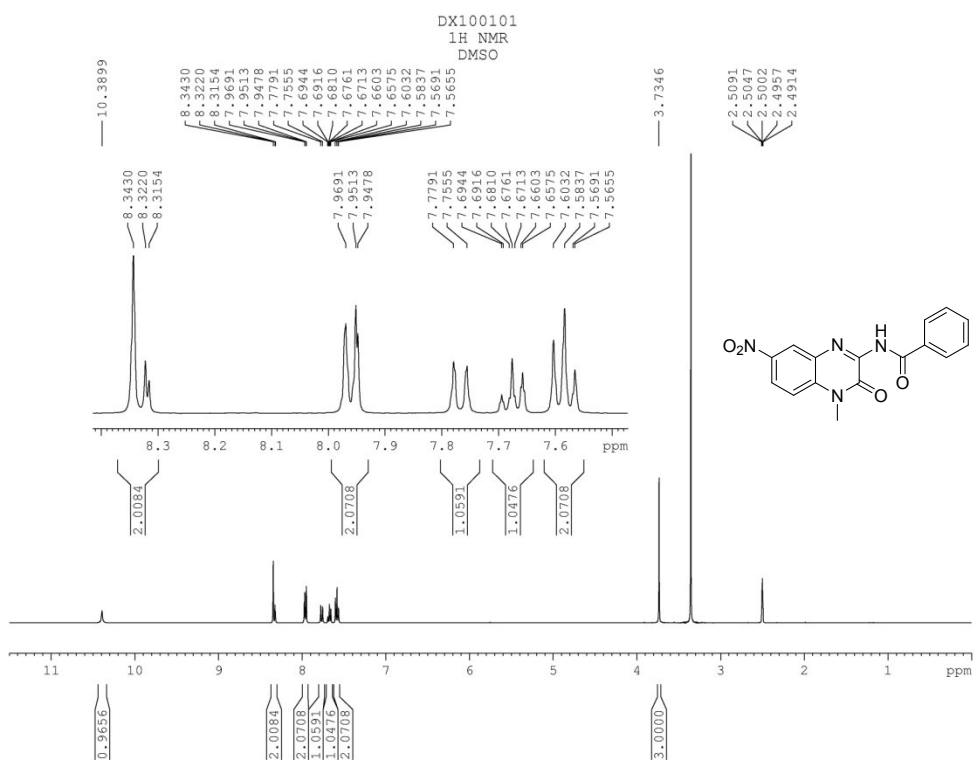


Fig. 64 ¹H NMR spectrum of compound 3fa

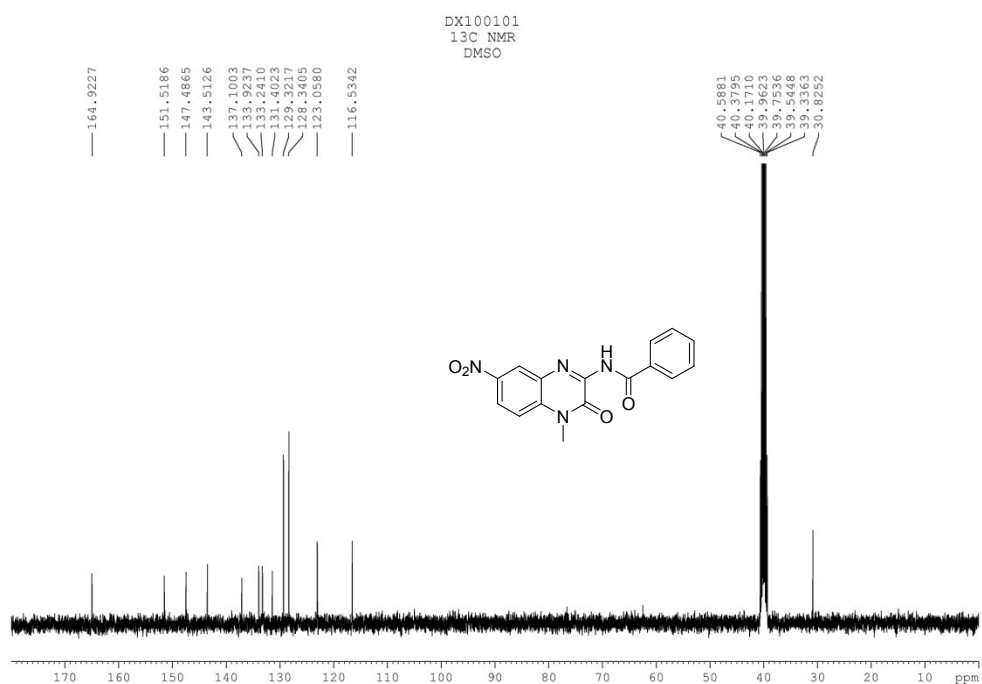


Fig. 65 ¹³C NMR spectrum of compound 3fa

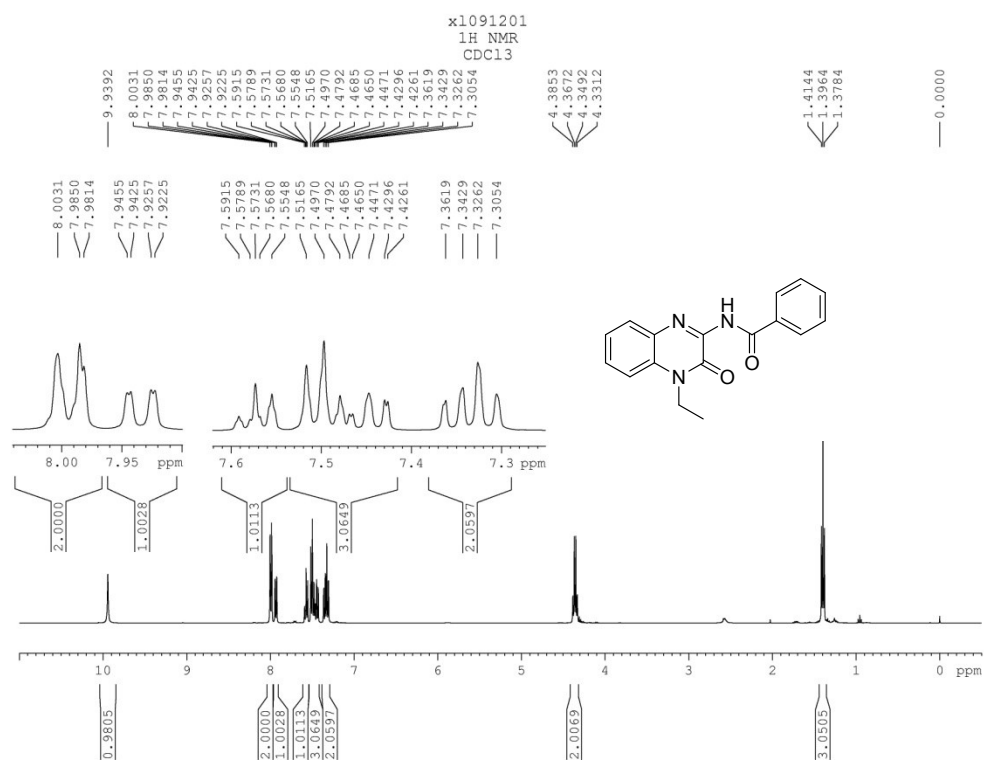


Fig. 66 ¹H NMR spectrum of compound 3ga

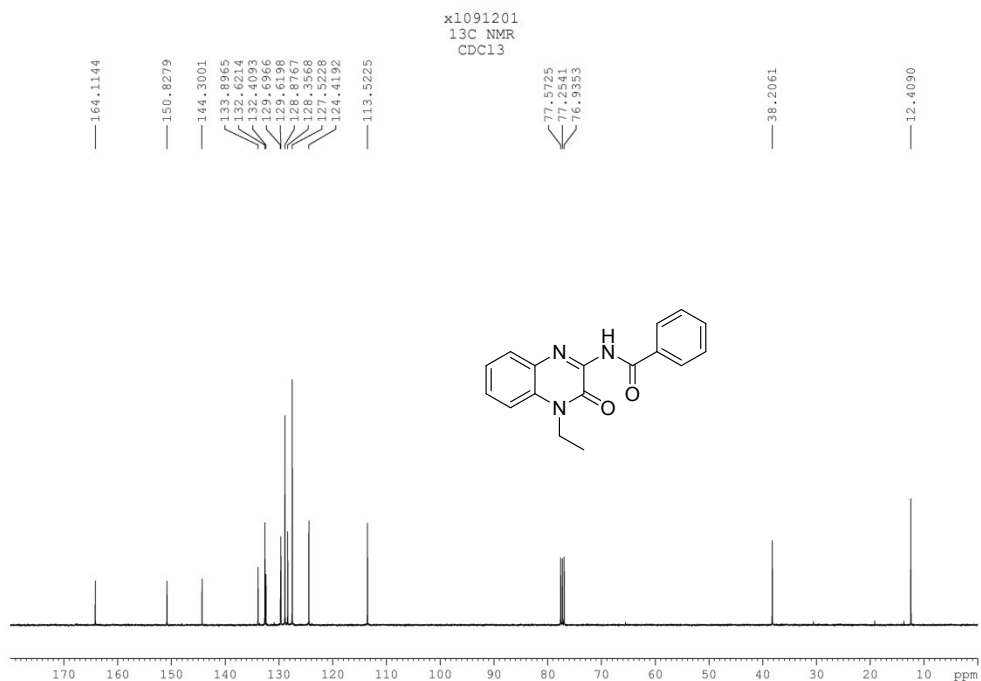


Fig. 67 ¹³C NMR spectrum of compound 3ga

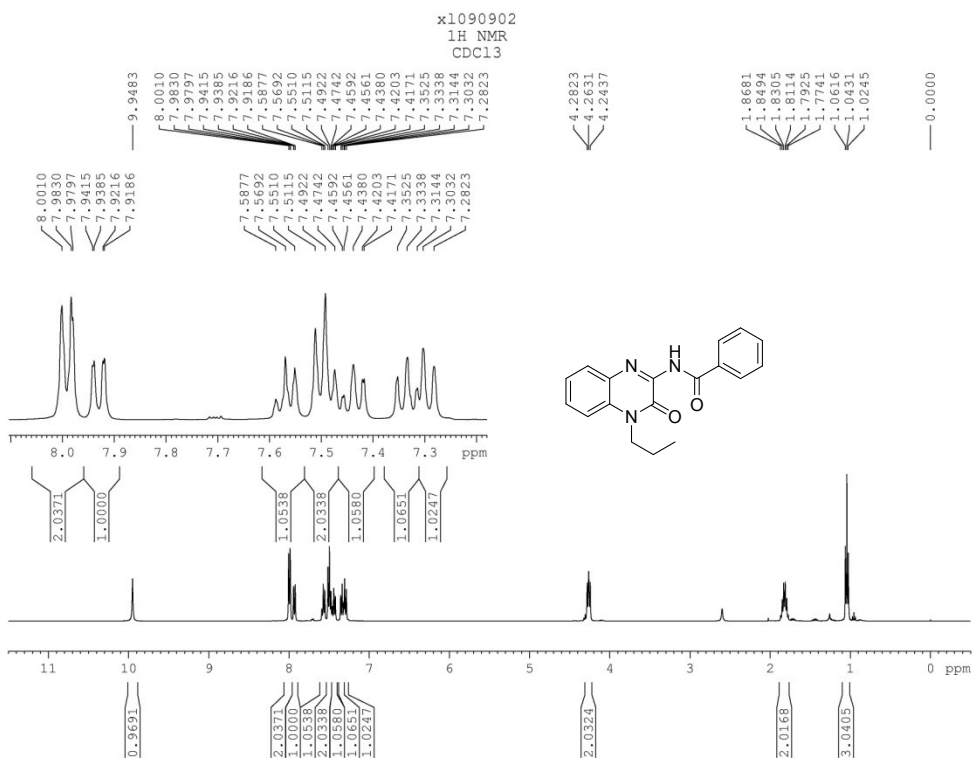


Fig. 68 ¹H NMR spectrum of compound 3ga

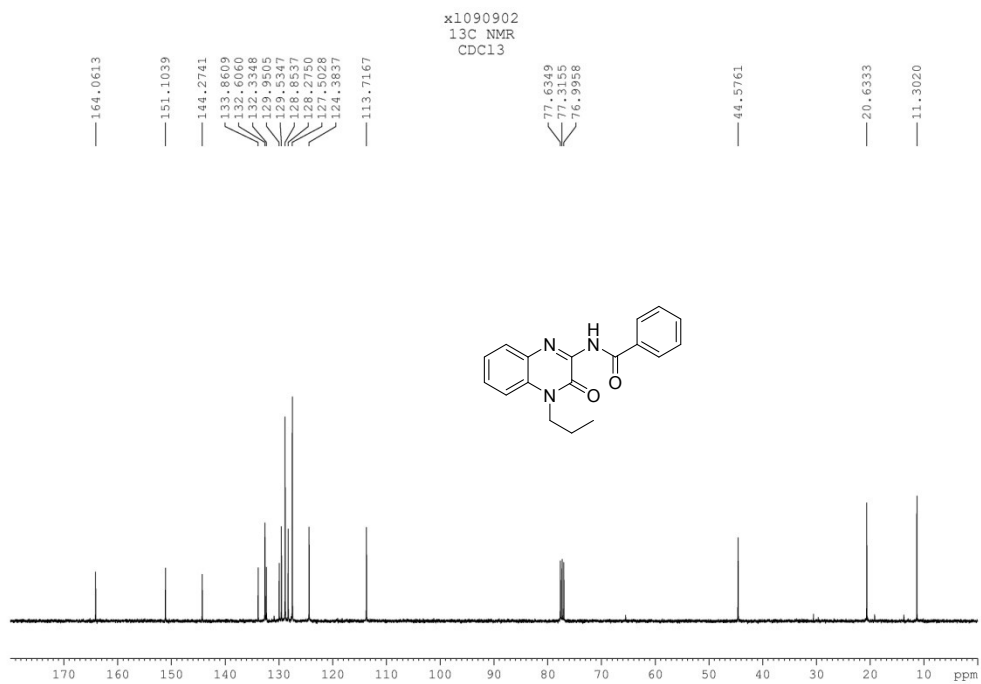


Fig. 69 ¹³C NMR spectrum of compound 3ha

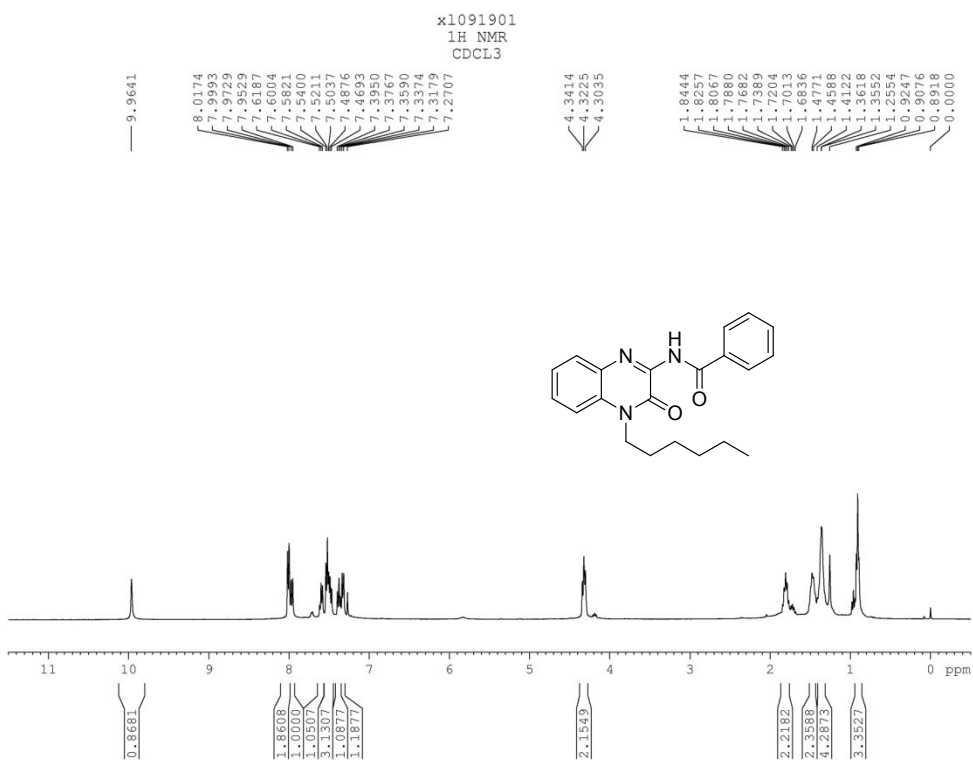


Fig. 70 ¹H NMR spectrum of compound 3ia

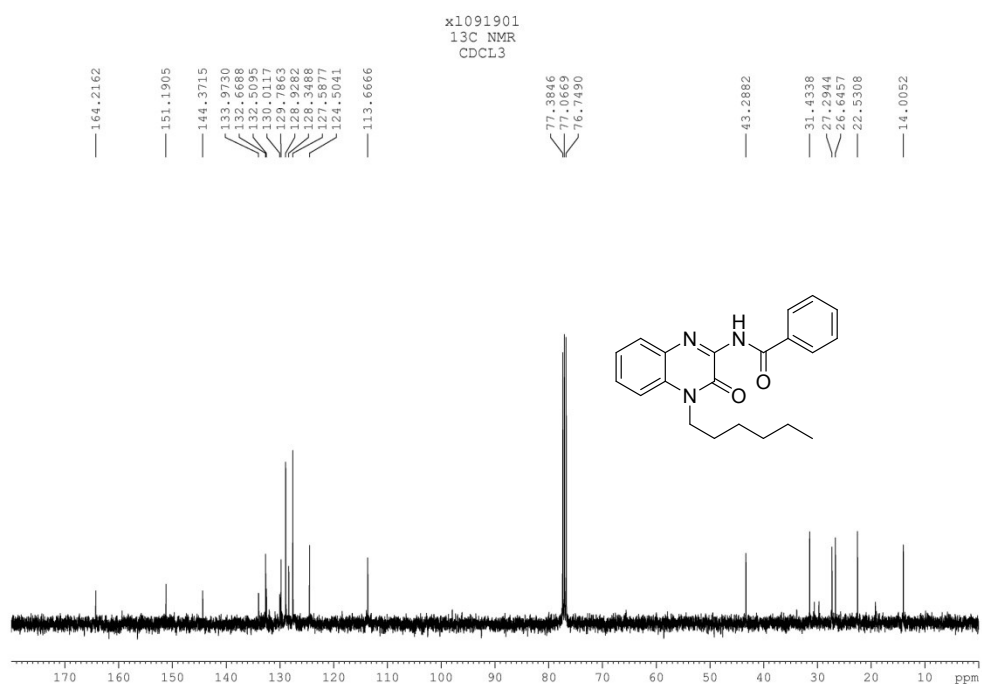


Fig. 71 ¹³C NMR spectrum of compound 3ia

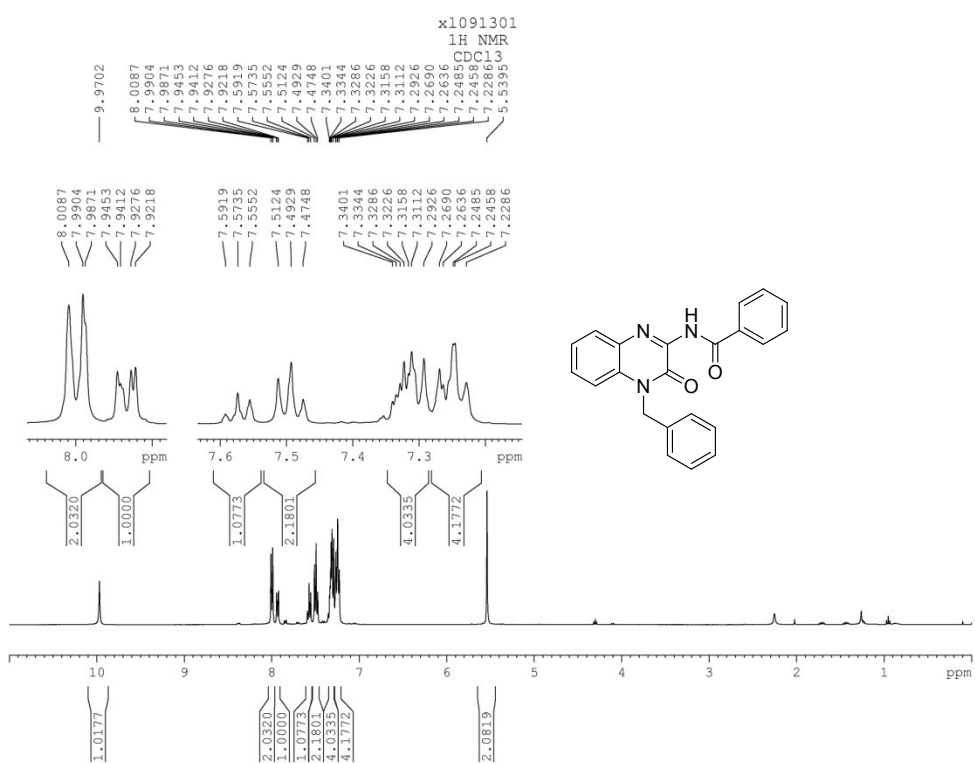


Fig. 72 ¹H NMR spectrum of compound 3ja

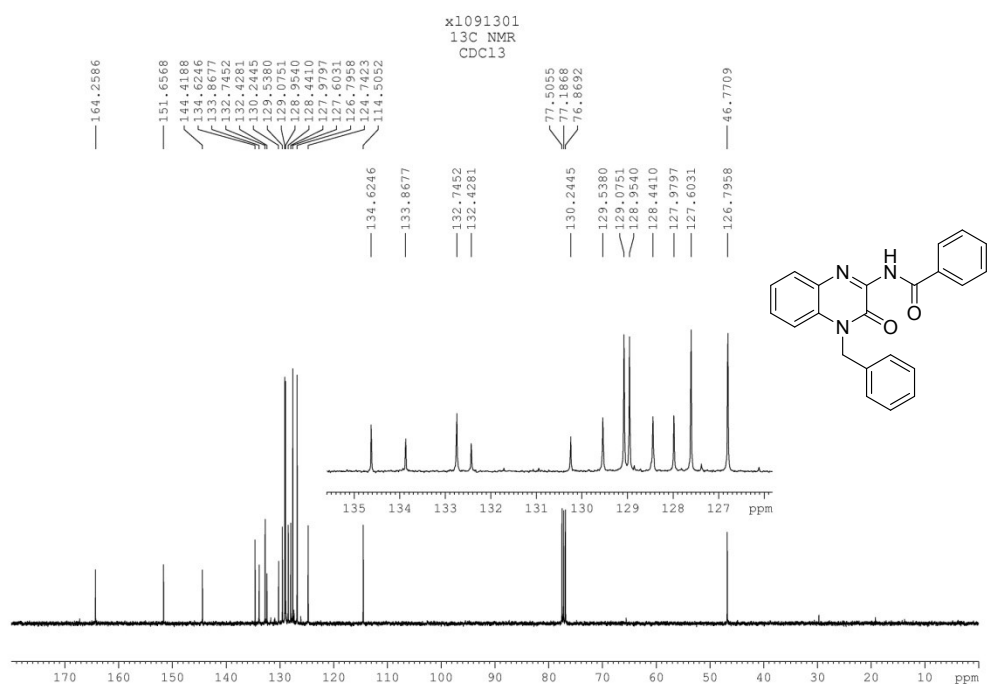


Fig. 73 ¹³C NMR spectrum of compound 3ja

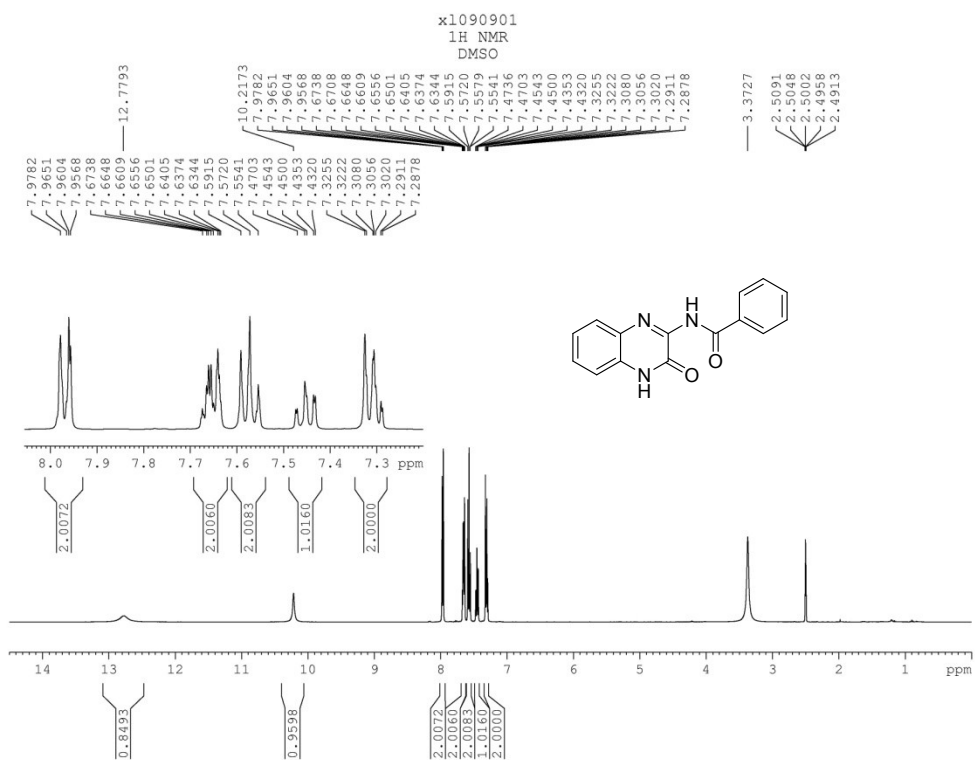


Fig. 74 ¹H NMR spectrum of compound 3ka

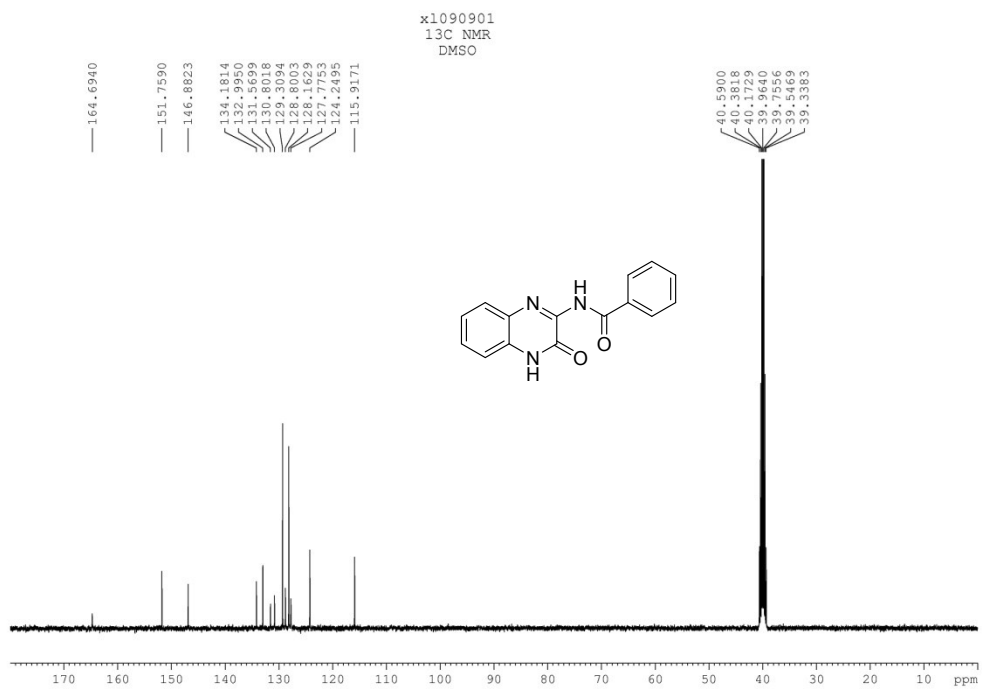


Fig. 75 ¹H NMR spectrum of compound 4

3. NMR and HR MS of the adduct 4 of BHT and benzamide radical

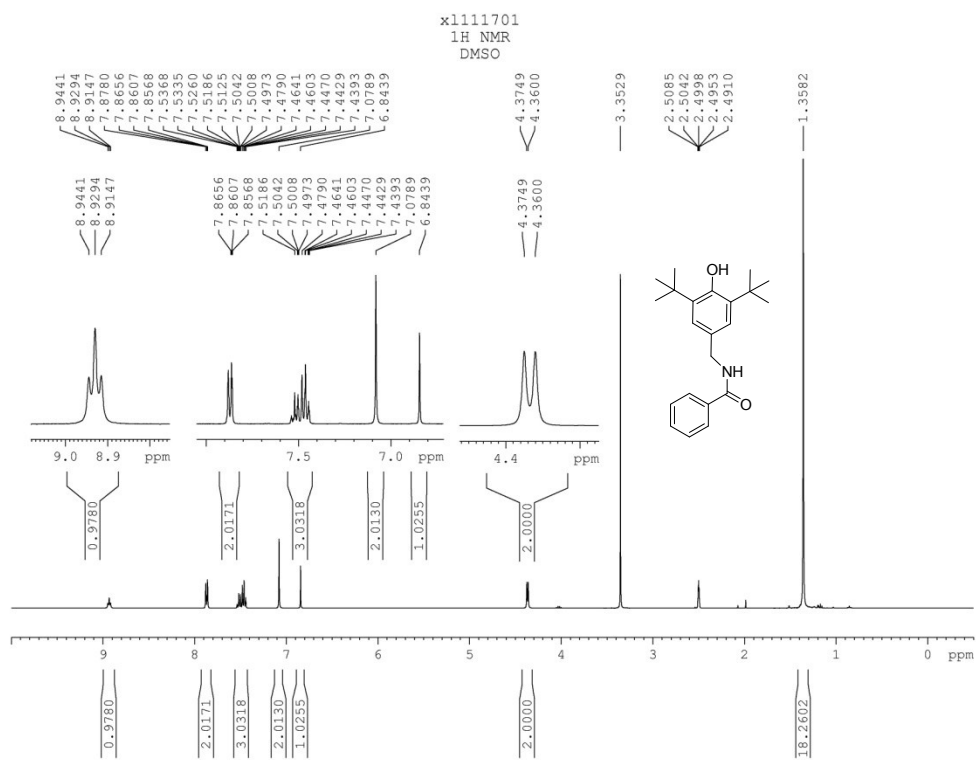


Fig. 76 ¹H NMR spectrum of compound 4

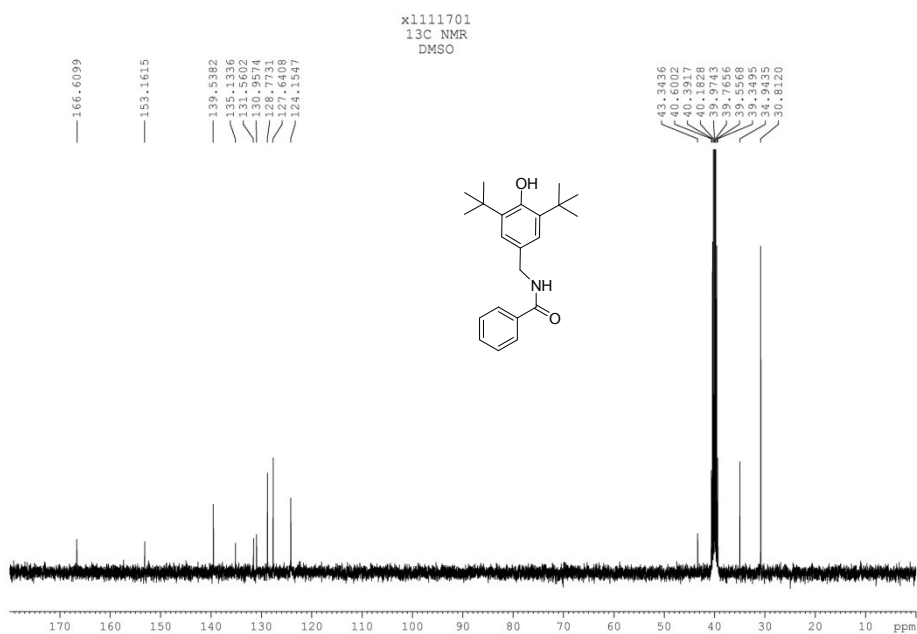


Fig. 77 ¹³C NMR spectrum of compound 4

20 #32 RT: 0.50 AV: 1 NL: 6.60E6
T: FTMS + p ESI Full ms [150.00-2000.00]

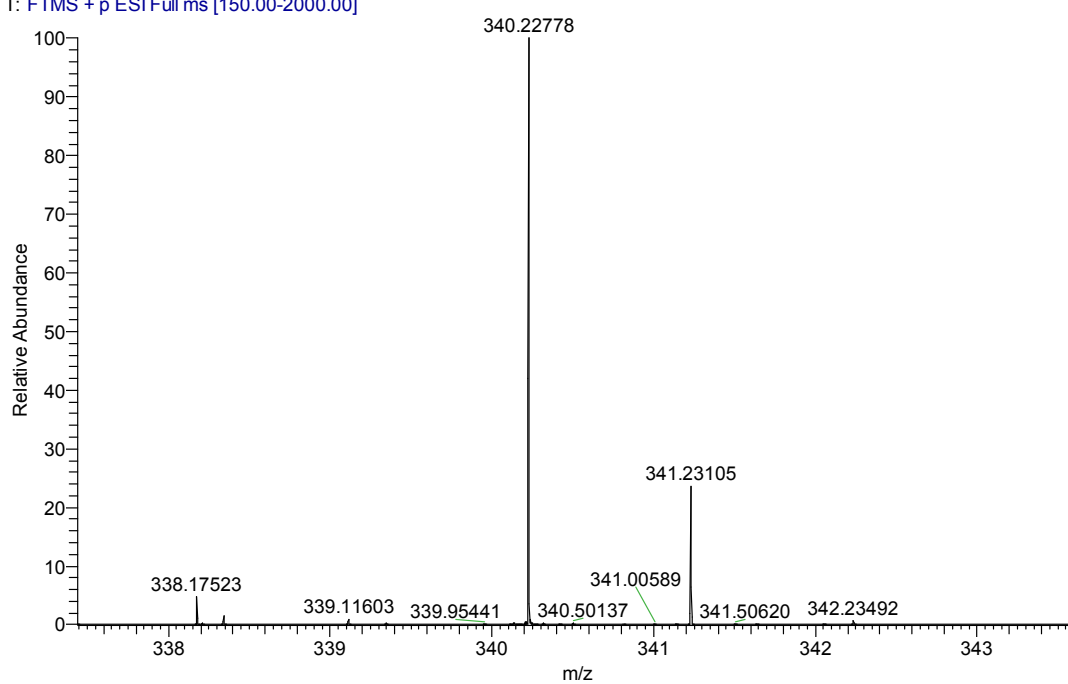


Fig. 78 HR MS of the adduct **4** of BHT and benzamide radical