

A Simple, Efficient and Eco-friendly Method for Preparation of 3-Substituted-2,3-dihydroquinazolin-4(1H)-one Derivatives

Zainab Almarhoon, Kholood A. Dahlous, Hazem A. Ghabbour, Ayman El-Faham*

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Table S1: Selected geometric parameters (Å, °) for compound **3a**

O1–C7	1.237 (3)	N2–C8	1.458 (3)
O2–C11	1.419 (4)	N3–C9	1.453 (3)
O2–C12	1.410 (4)	N3–C10	1.453 (4)
N1–C1	1.384 (3)	N3–C13	1.459 (4)
N2–C7	1.338 (3)		
C11–O2–C12	109.6 (2)	O1–C7–N2	120.2 (2)
C7–N2–C8	119.9 (2)	N2–C7–C6	118.6 (2)
C9–N3–C10	111.31 (19)	N2–C8–C9	113.13 (19)
C9–N3–C13	112.48 (18)	N3–C9–C8	112.14 (18)
C10–N3–C13	108.3 (2)	N3–C10–C11	111.0 (2)
N1–C1–C2	119.43 (19)	O2–C11–C10	111.5 (2)
N1–C1–C6	122.9 (2)	O2–C12–C13	111.9 (2)
O1–C7–C6	121.21 (18)	N3–C13–C12	110.1 (2)

Table S2: Hydrogen-bond geometry (Å, °) for compound **3a**

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N2–H1N2...N1 ⁱ	0.90 (3)	2.22 (3)	3.105 (3)	167 (2)
N1–H1A...N3 ⁱⁱ	0.860	2.460	3.255 (3)	153.0
N1–H1B...O1	0.860	2.090	2.698 (3)	128.0
N1–H1B...O1 ⁱⁱ	0.860	2.300	3.037 (3)	144.0
C8–H8B...O1 ⁱⁱⁱ	0.970	2.550	3.474 (3)	160.0

Symmetry codes: (i) $x, -y+1/2, z+1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y-1/2, -z+3/2$.

Figure S1: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ for compound 3a

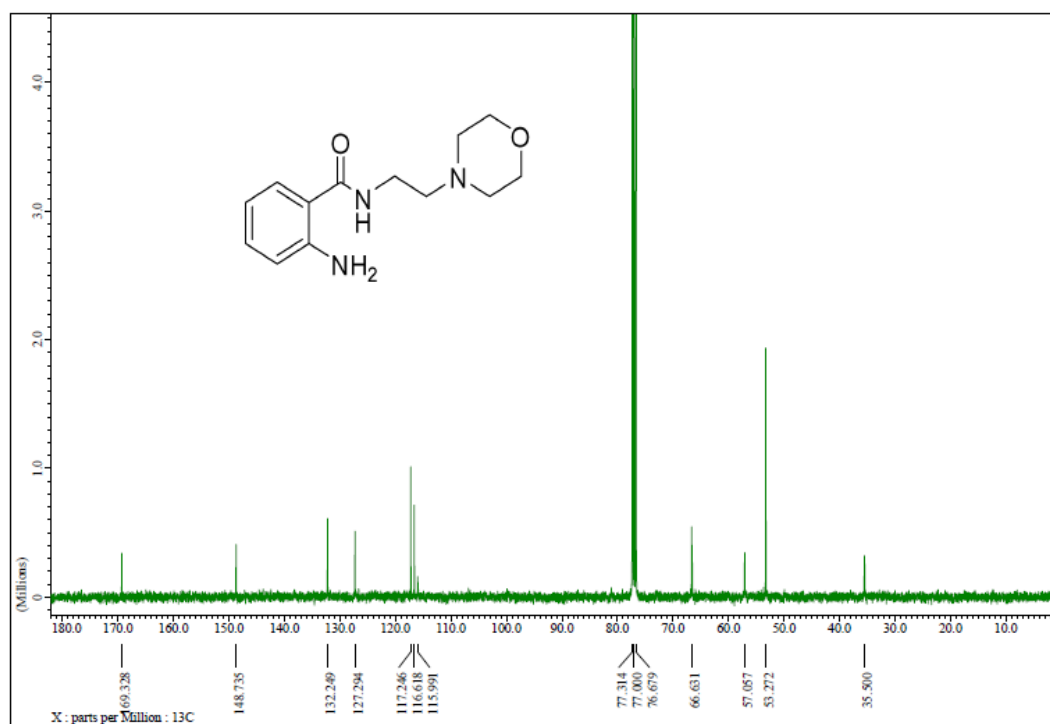
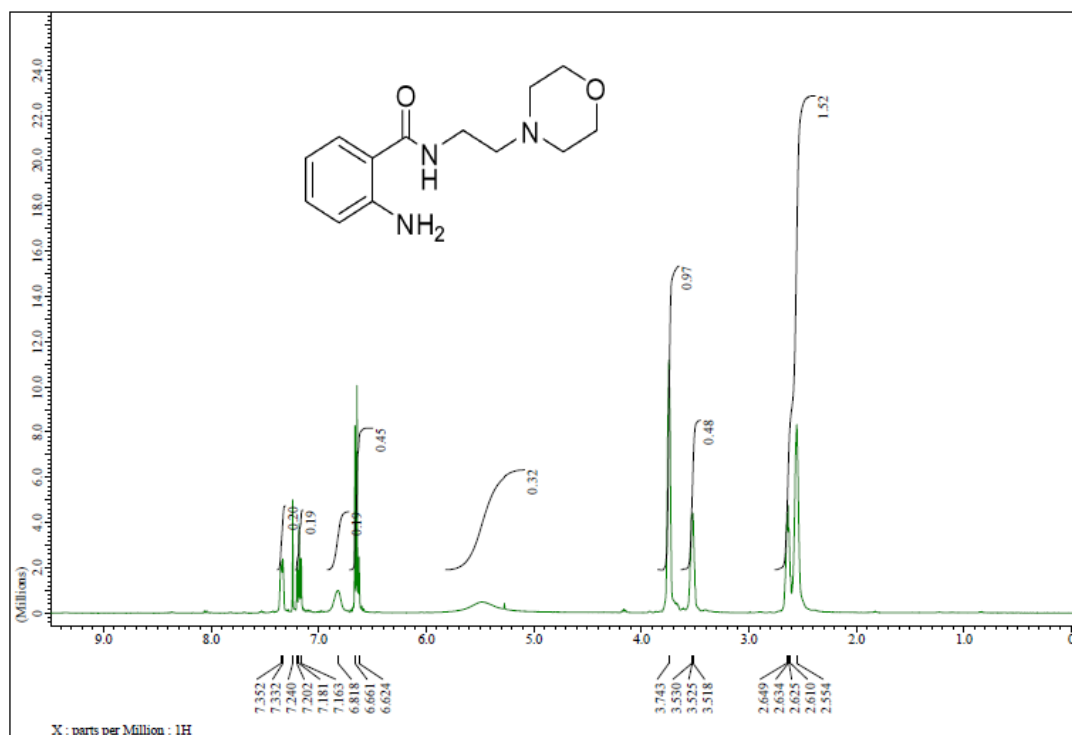


Figure S2: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ for compound 3b

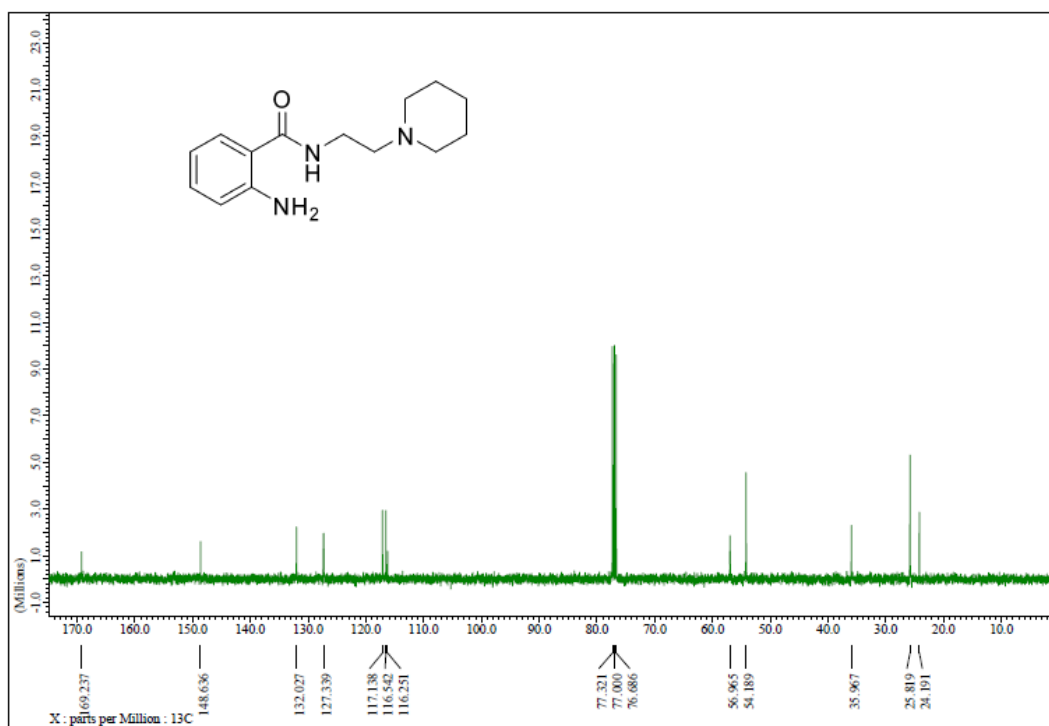
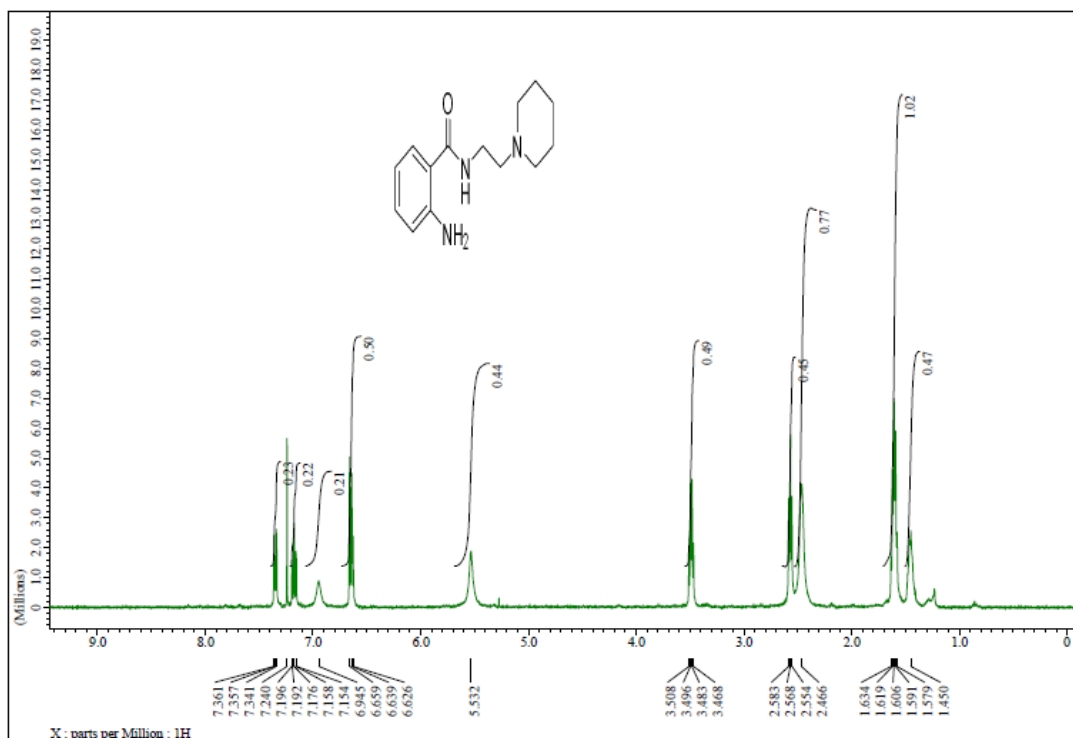


Figure S3: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ for compound 4a

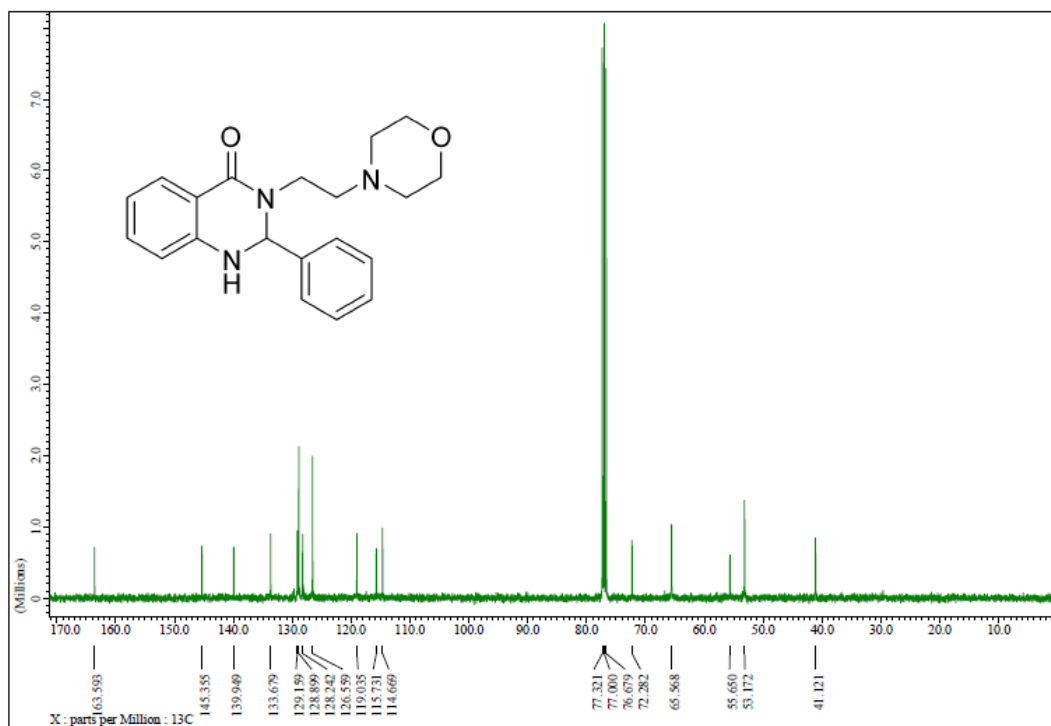
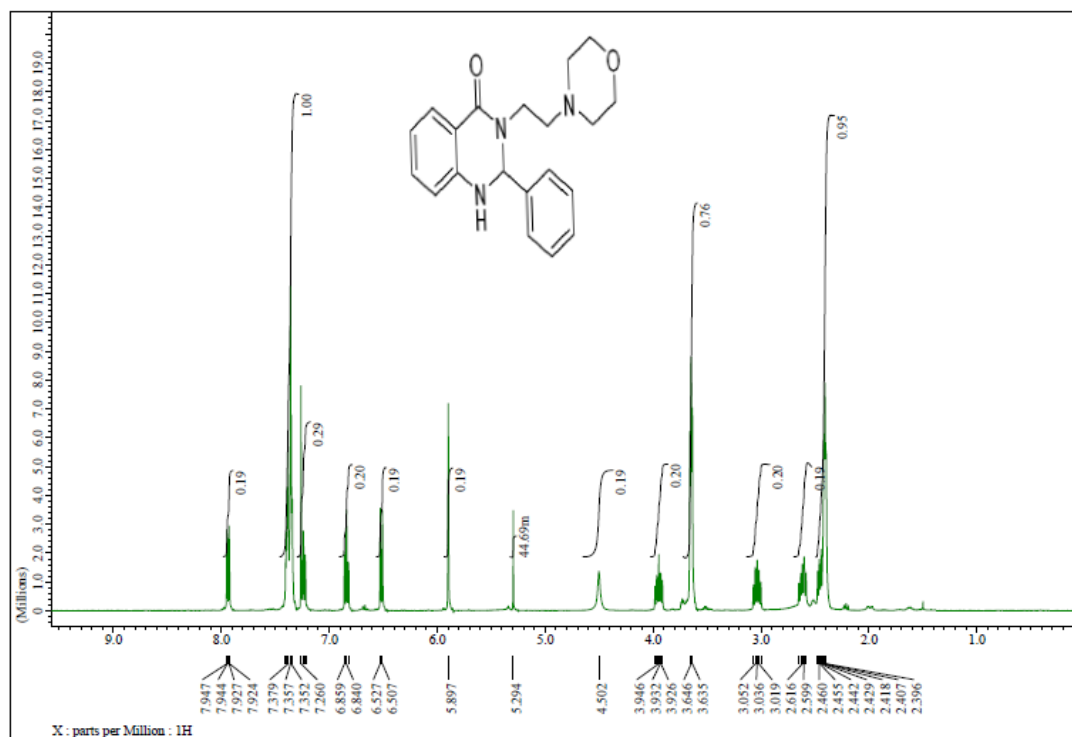


Figure S4: ^1H -NMR and ^{13}C -NMR for compound 4b

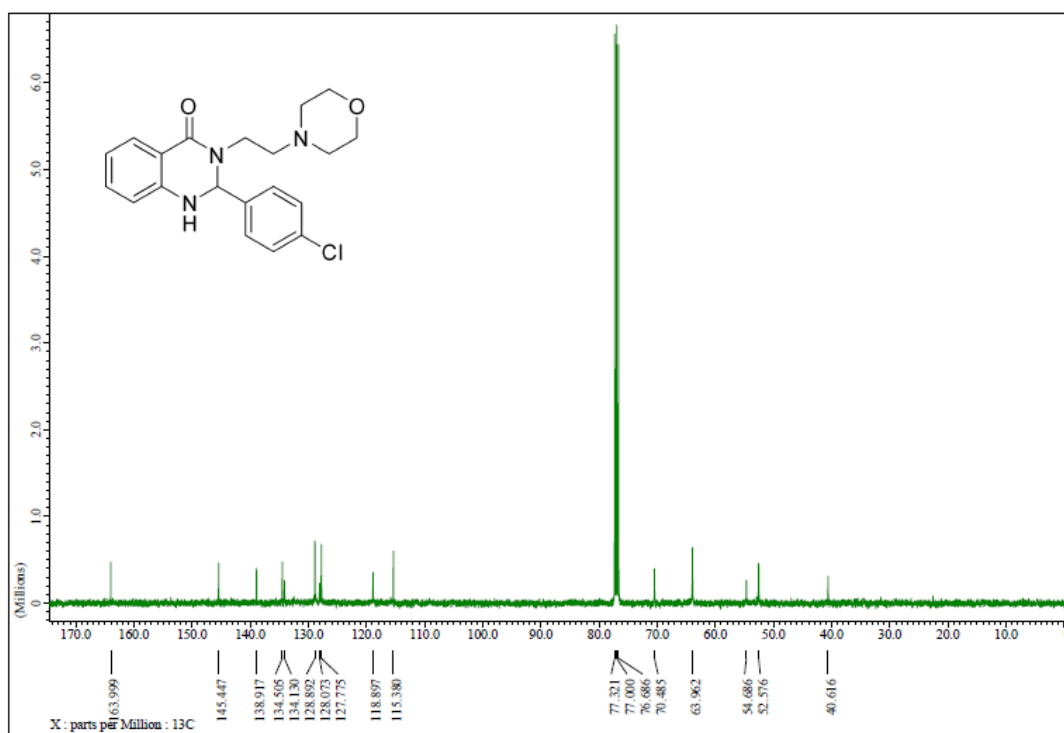
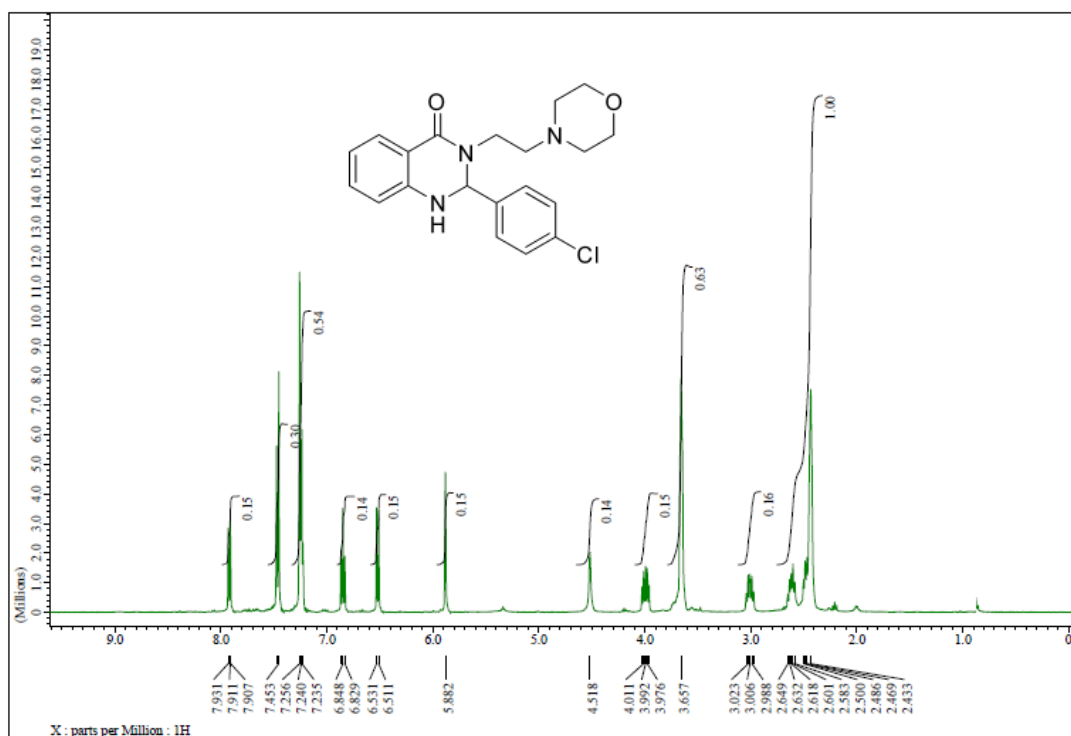


Figure S5: ¹H-NMR and ¹³C-NMR for compound 4c

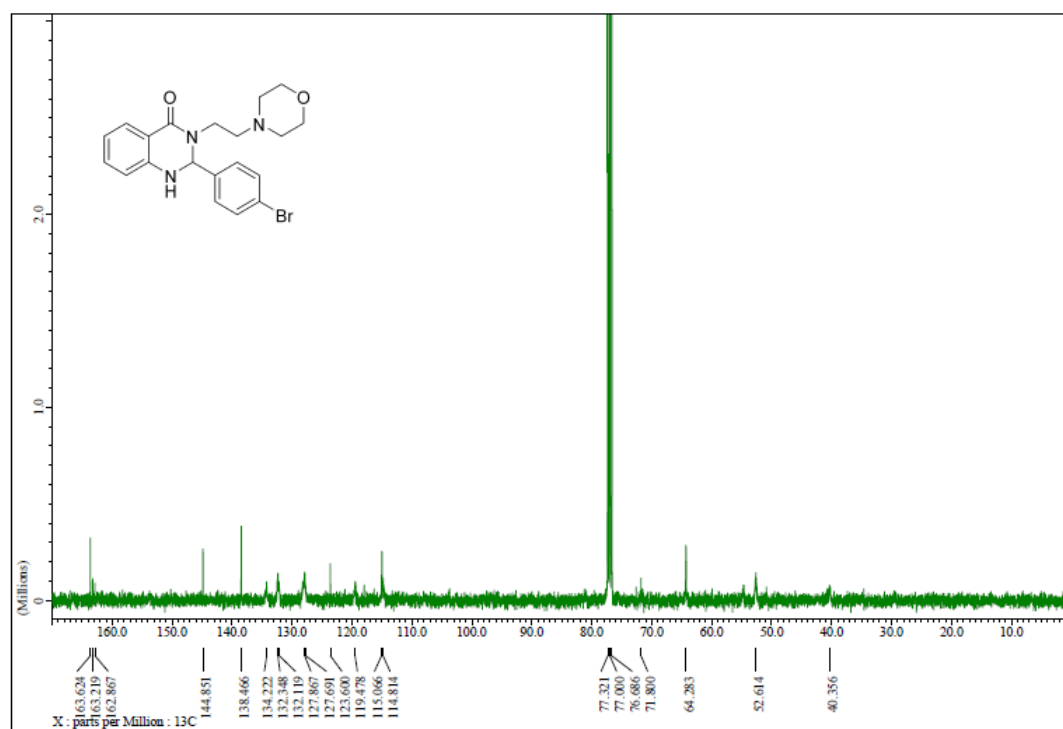
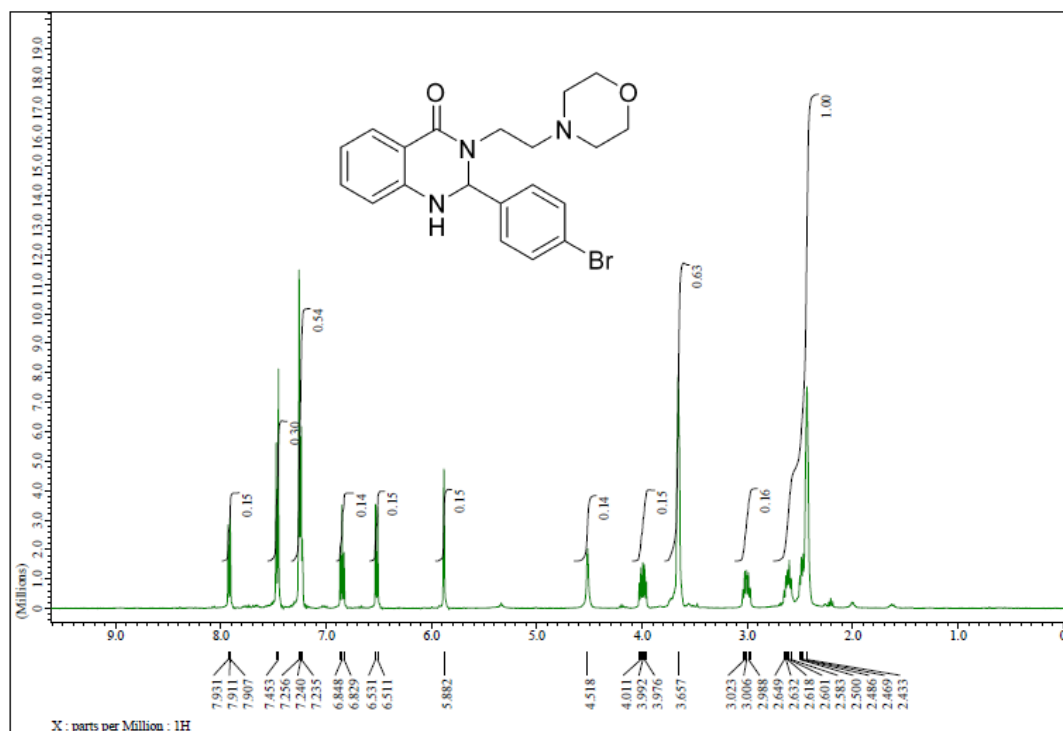


Figure S6: ¹H-NMR and ¹³C-NMR for compound 4d

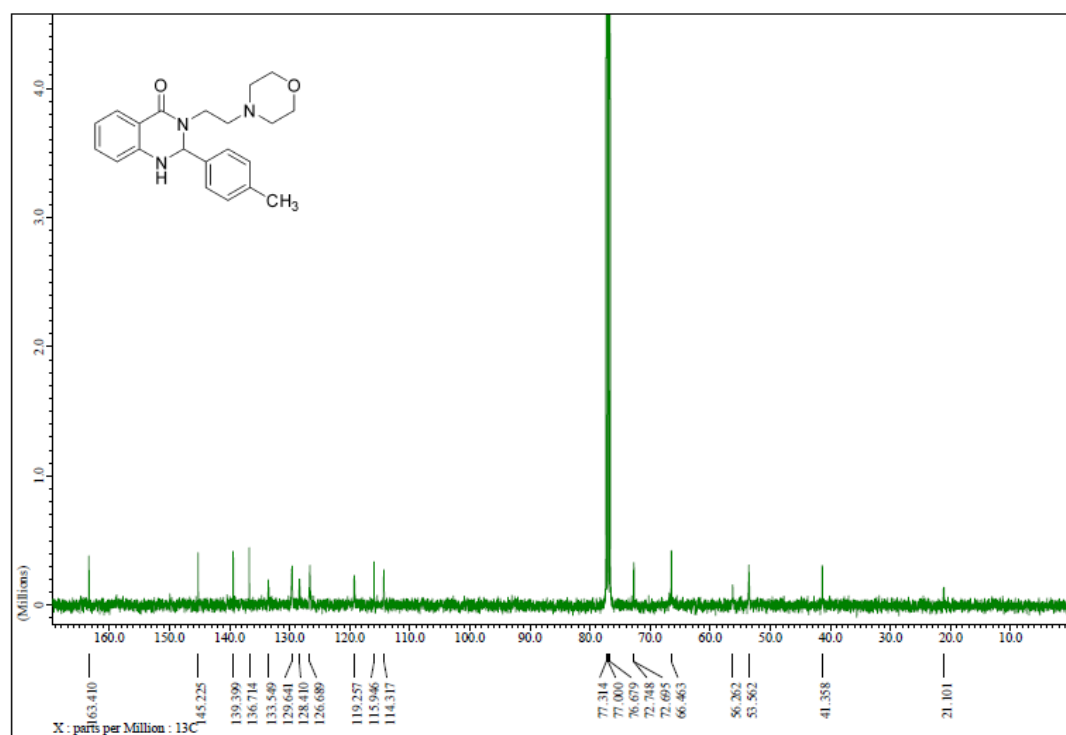
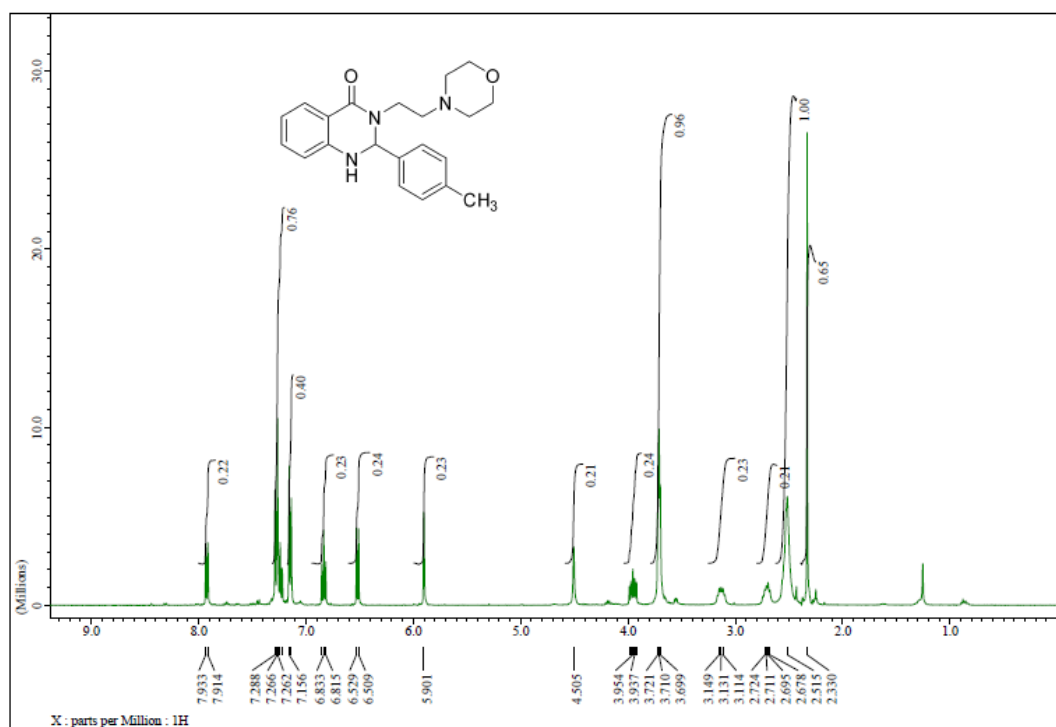


Figure S7: ^1H -NMR and ^{13}C -NMR for compound 4e

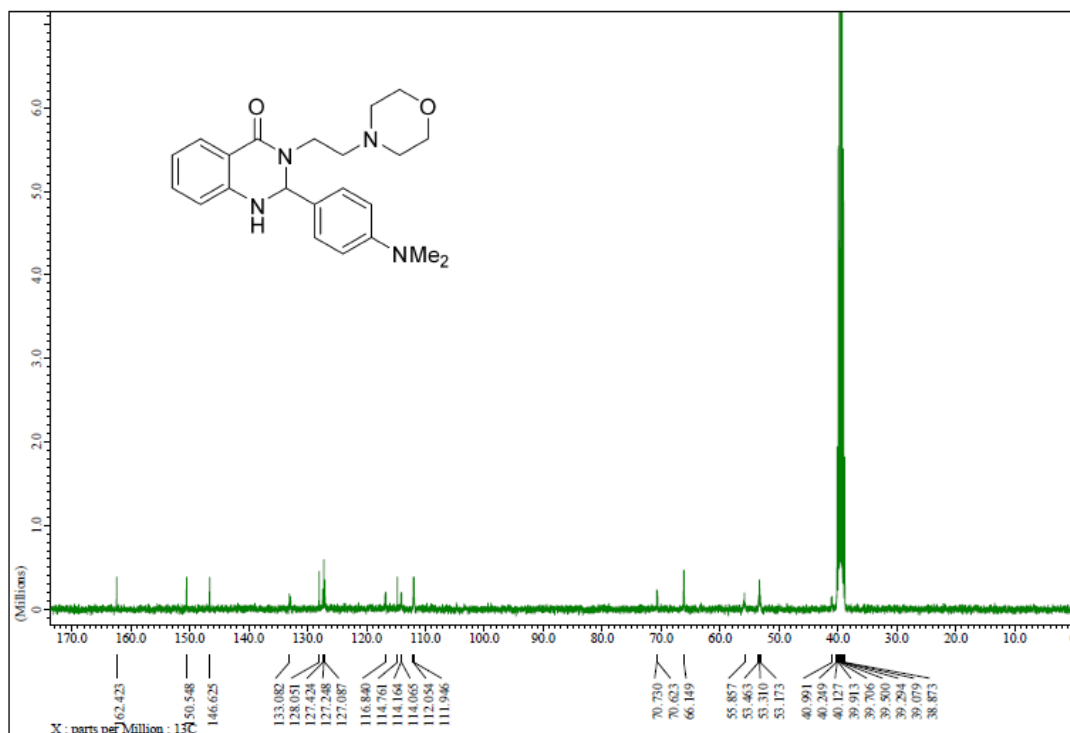
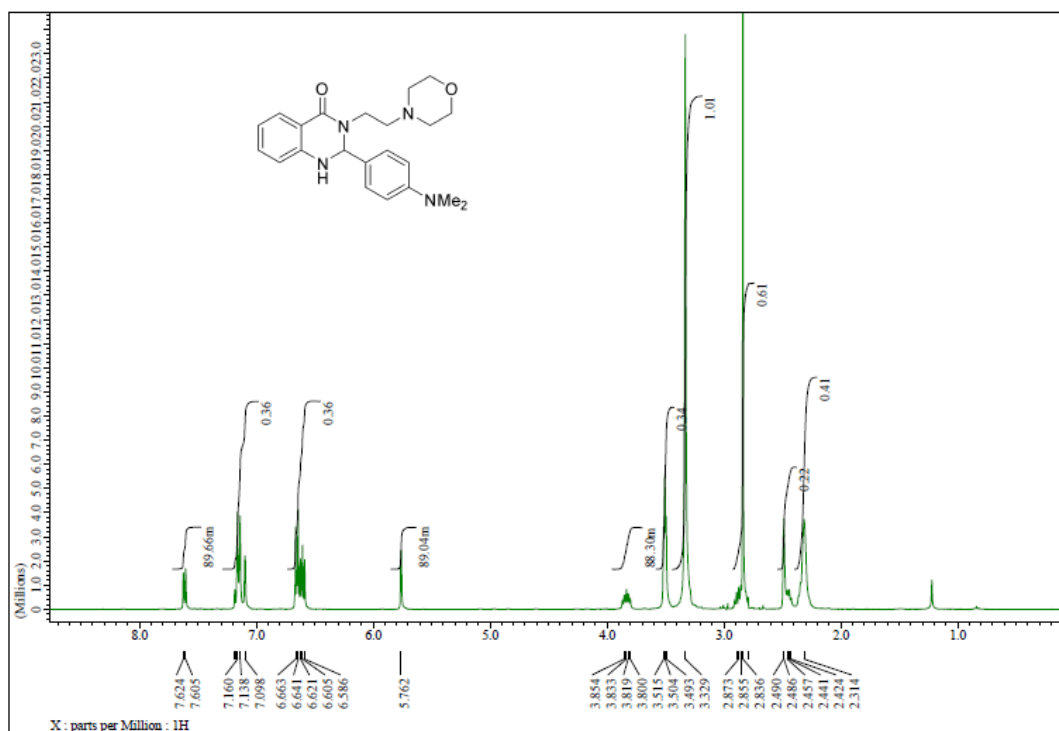


Figure S8: ¹H-NMR and ¹³C-NMR for compound 4f

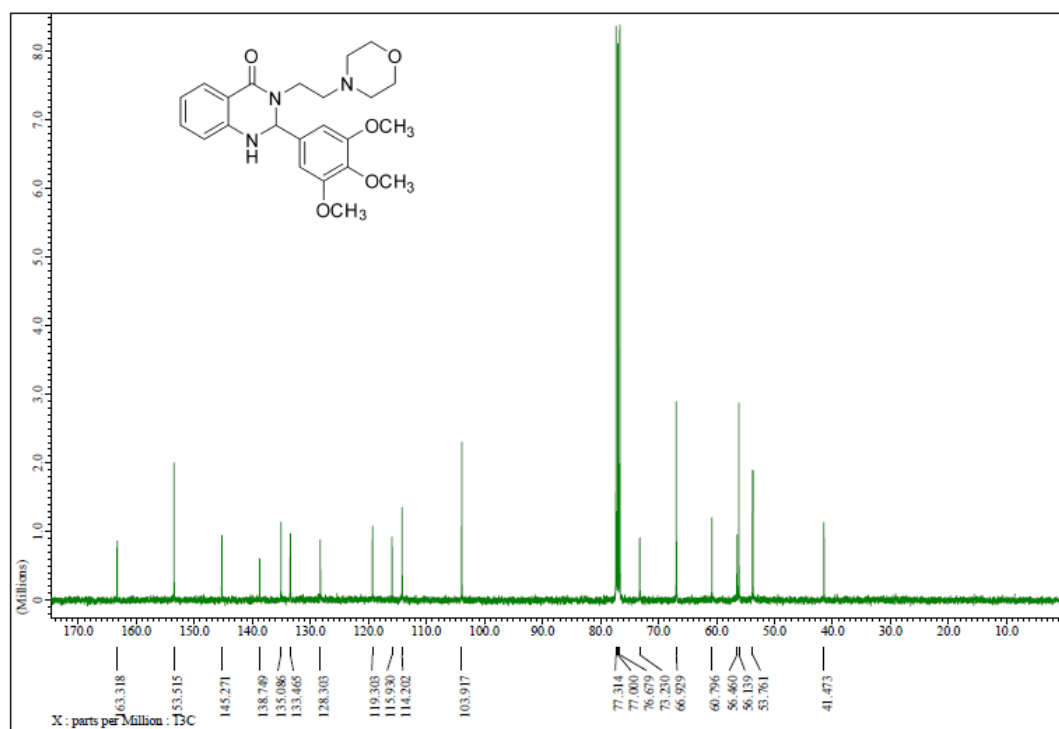
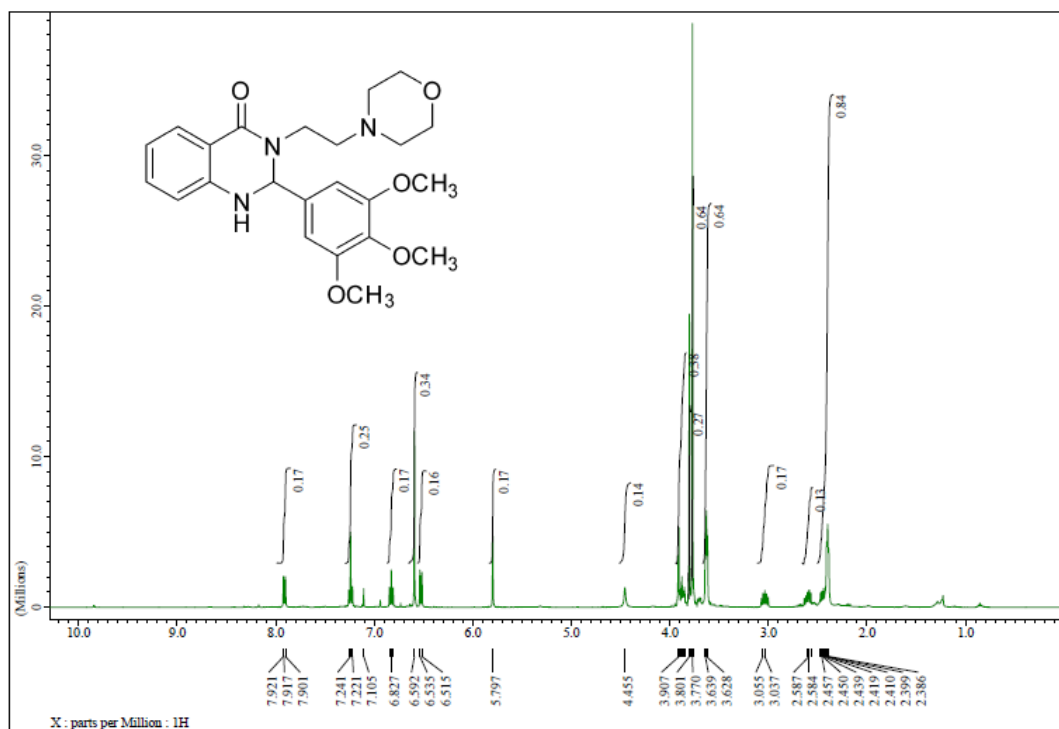


Figure S9: ¹H-NMR and ¹³C-NMR for compound 5a

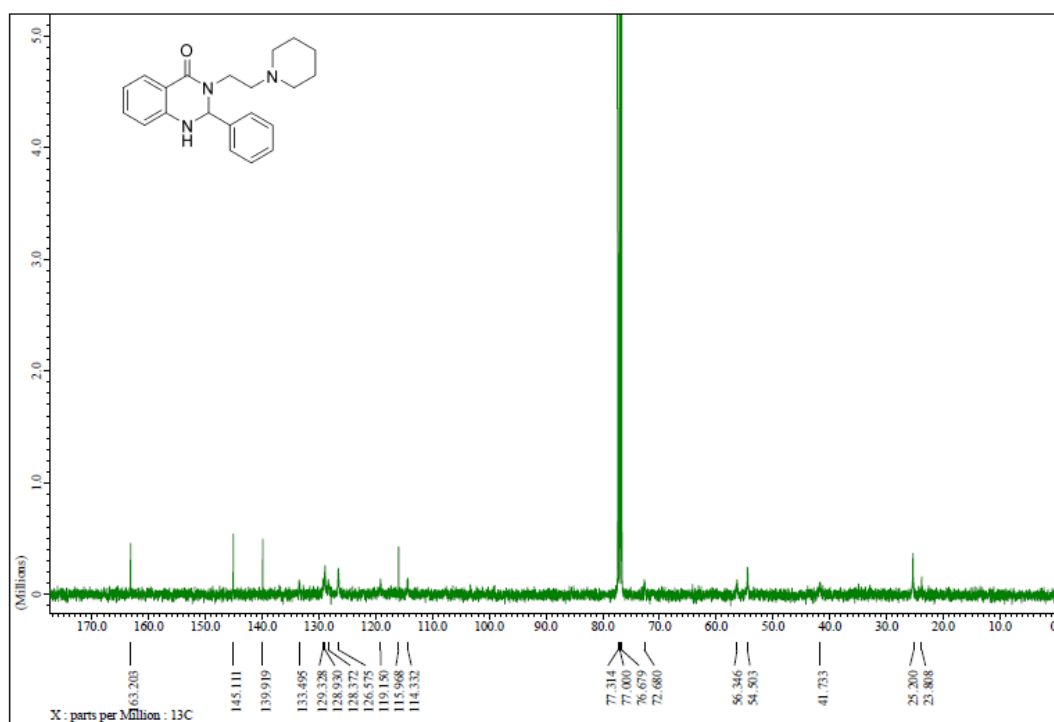
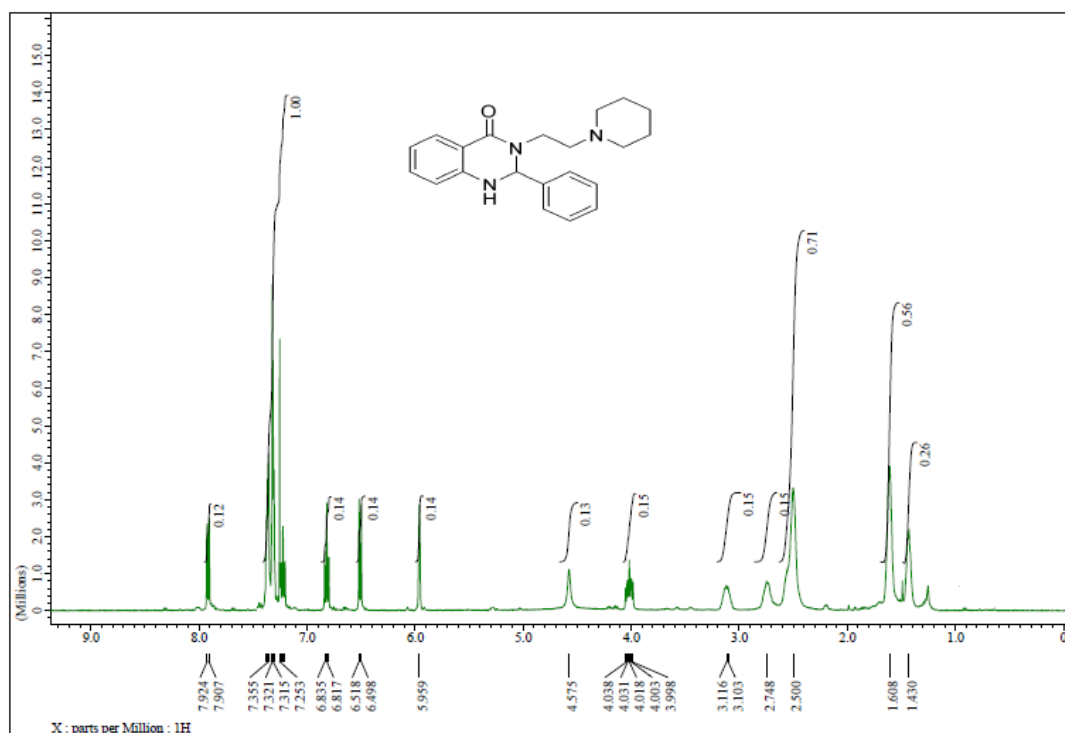


Figure S10: ^1H -NMR and ^{13}C -NMR for compound 5b

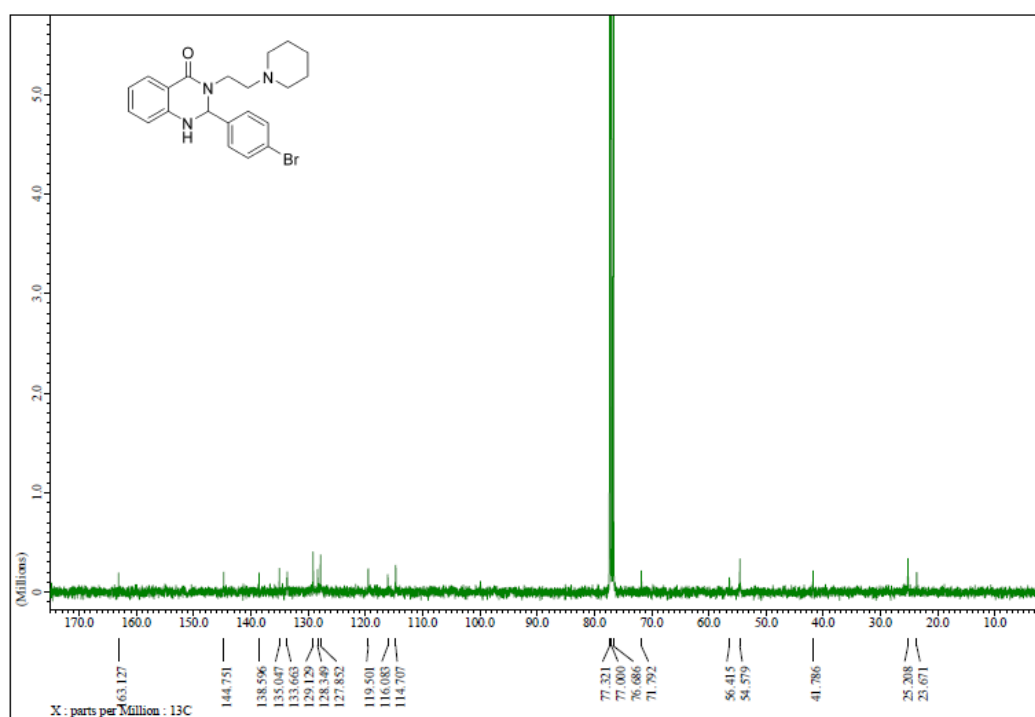
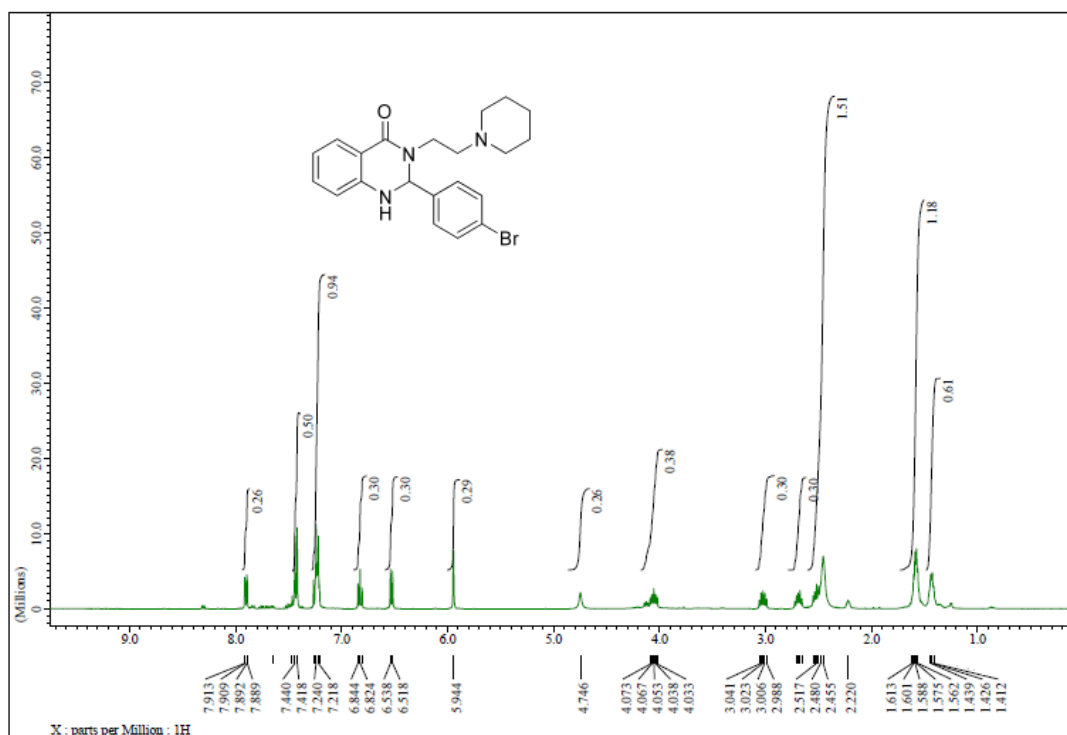


Figure S11: ^1H -NMR and ^{13}C -NMR for compound 5c

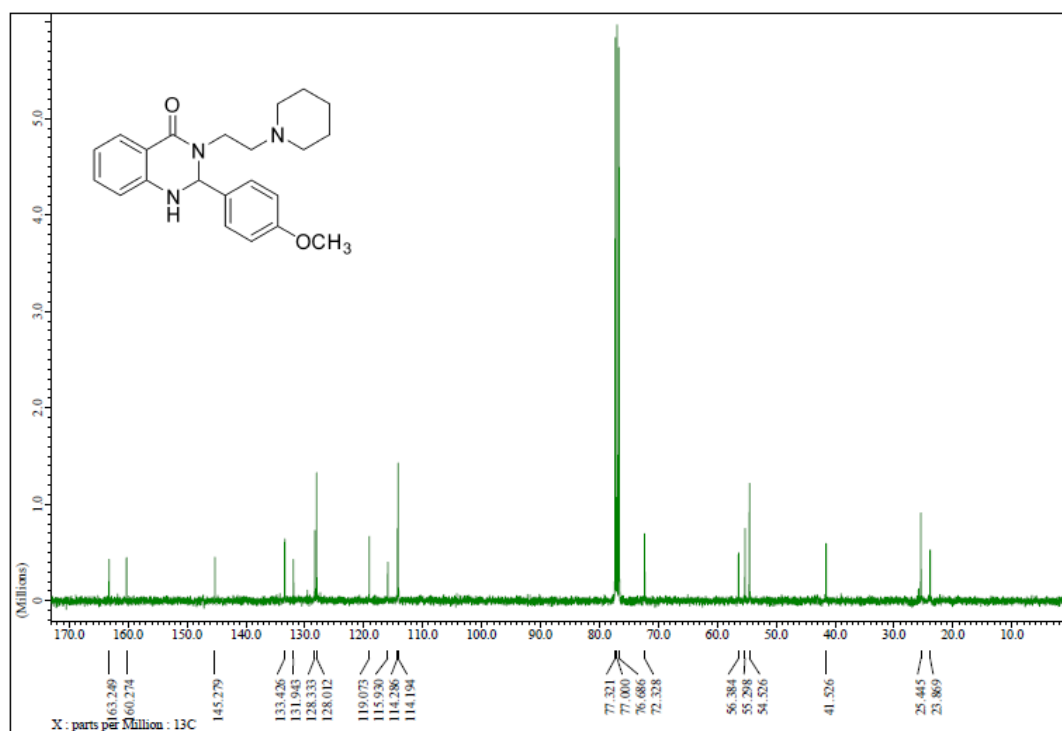
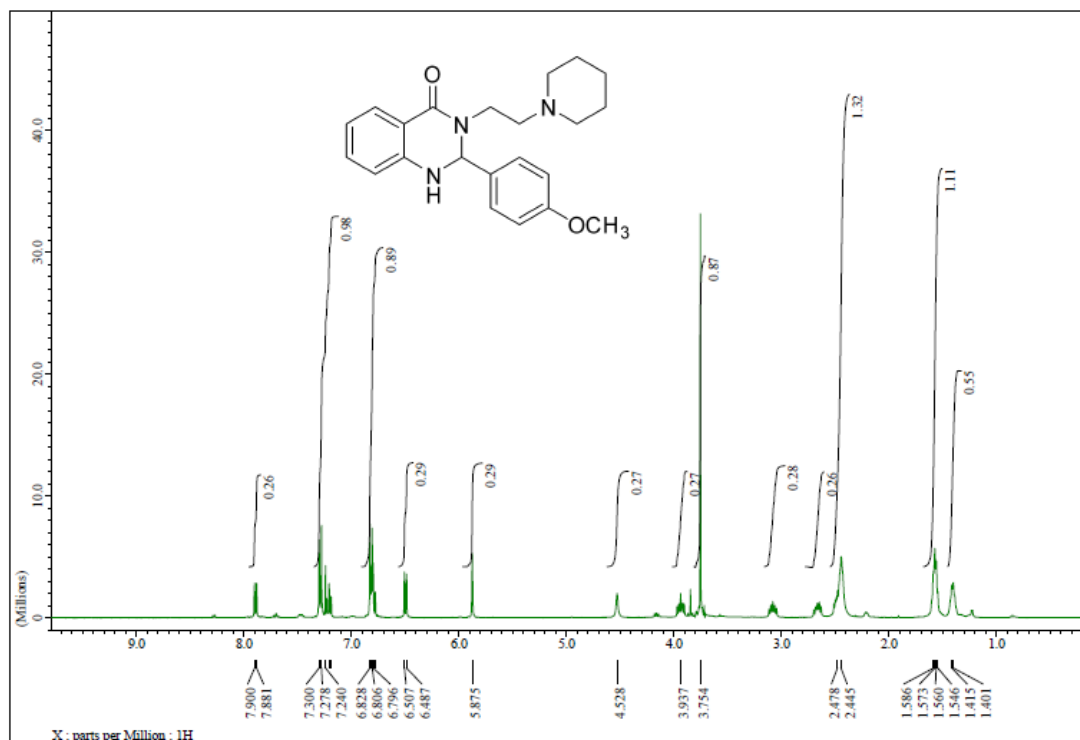


Figure S12: ^1H -NMR and ^{13}C -NMR for compound 6a

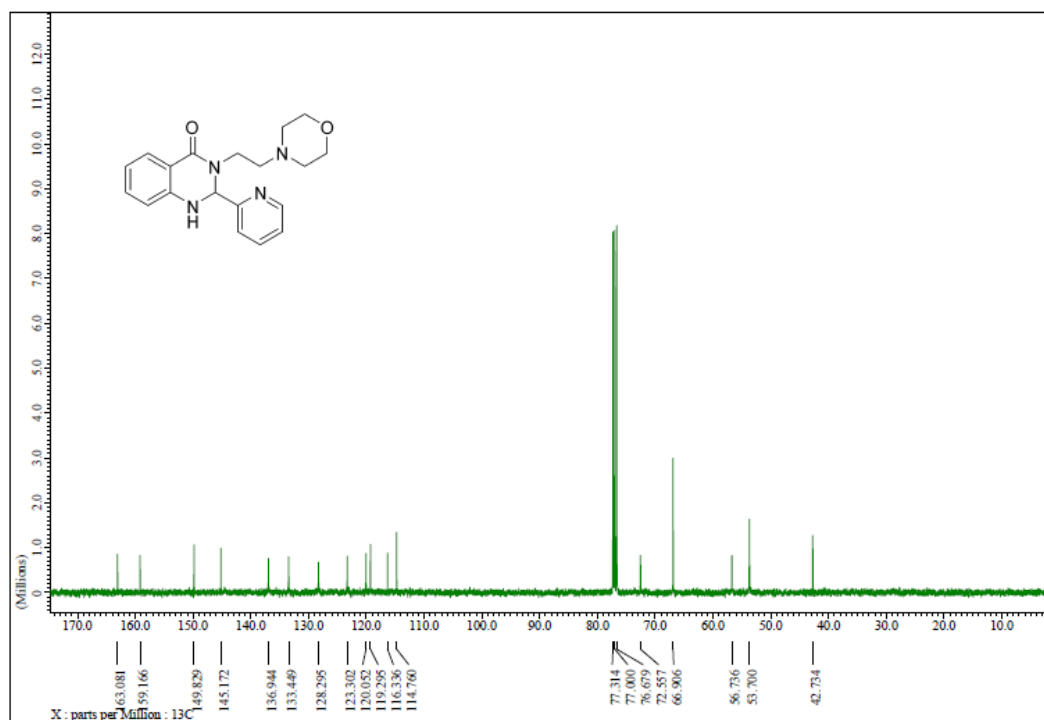
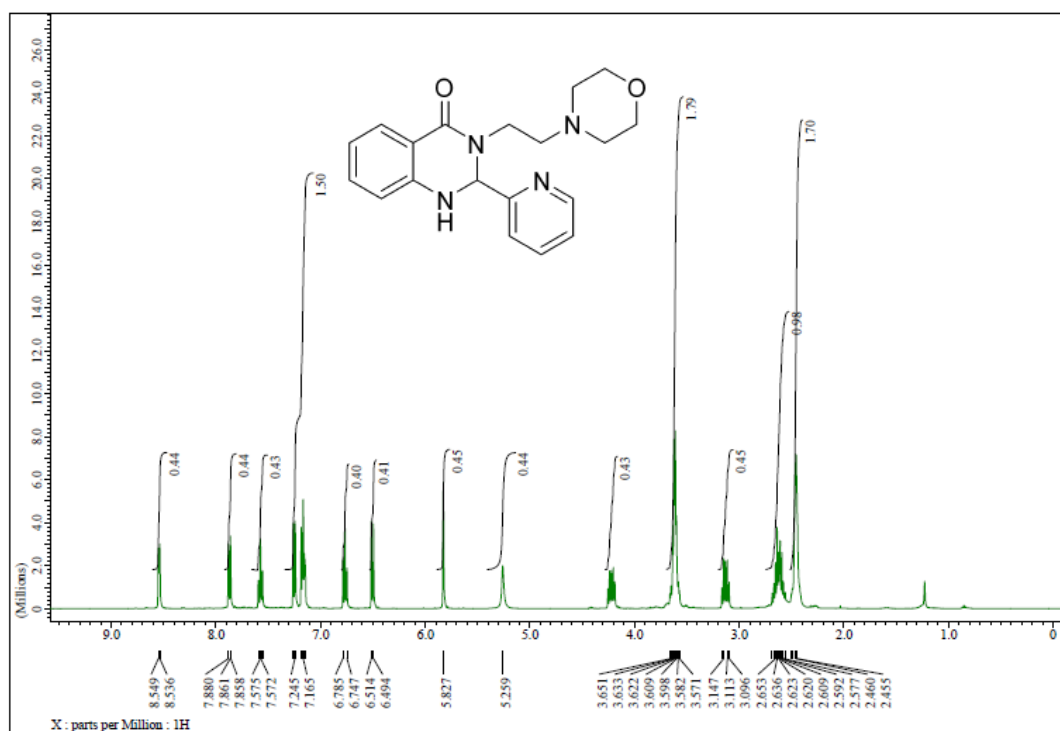


Figure S13: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ for compound **6b**

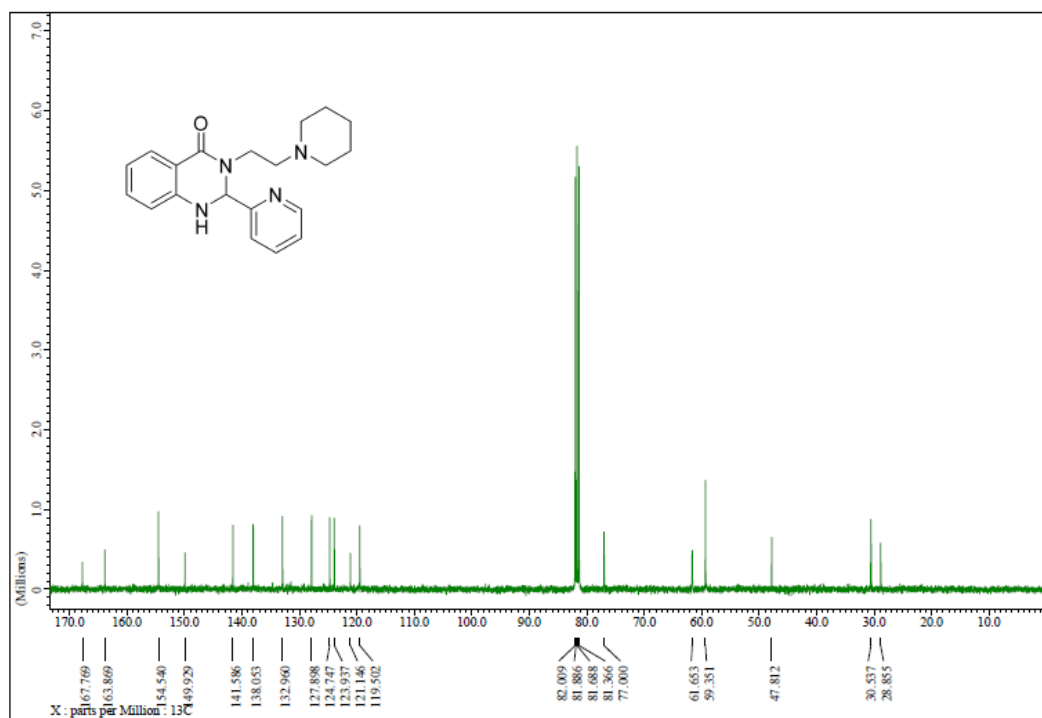
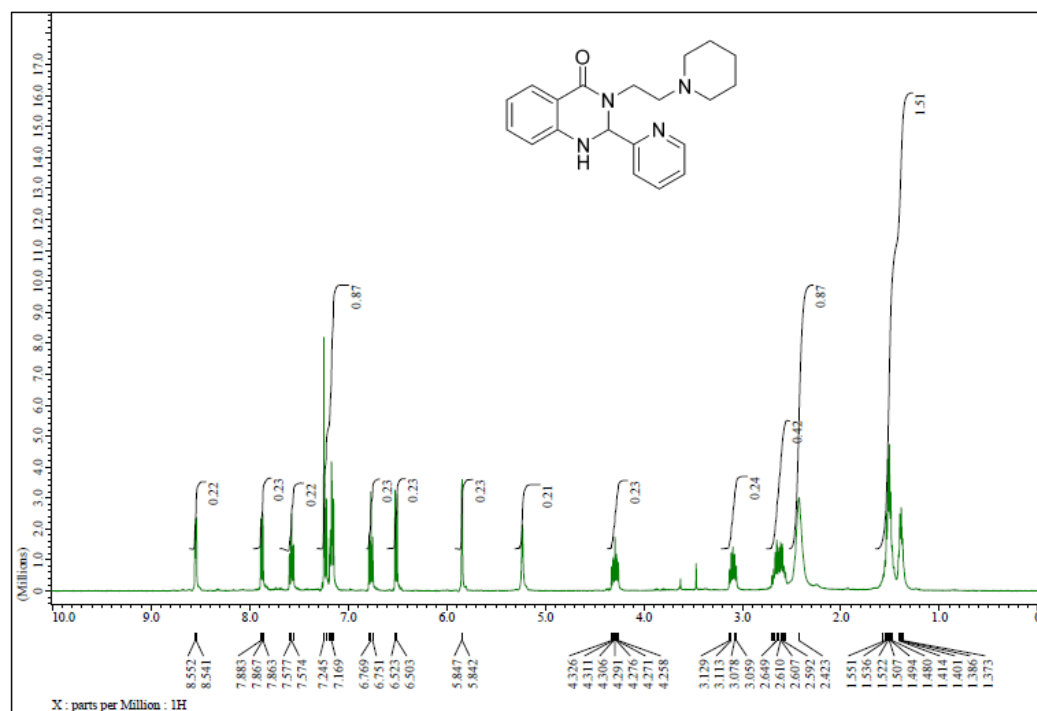


Figure S14: ^1H -NMR and ^{13}C -NMR for compound 7

