

Electronic Supplementary Information

Magnetically Retrievable Copper Ionic Liquid Nanocatalyst for Cyclooxidative Synthesis of 2-Phenylquinazolin-4(3*H*)-ones

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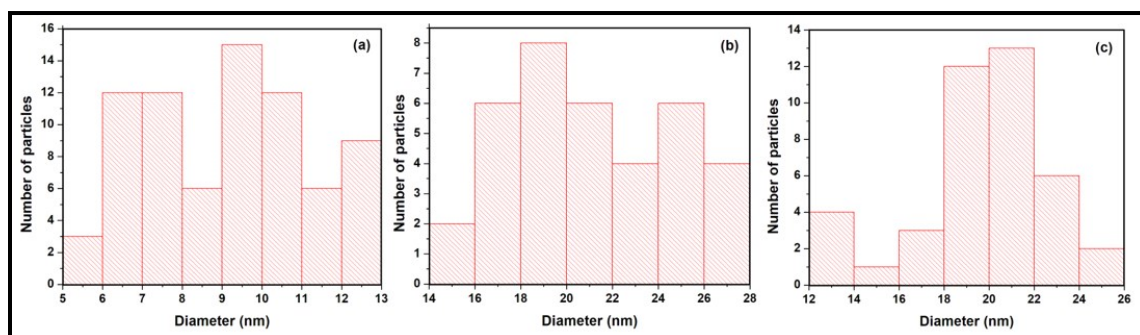


Fig. S1. Size distribution histograms of (a) MNPs, (b) SMNPs and (c) CuIL@SMNPs.

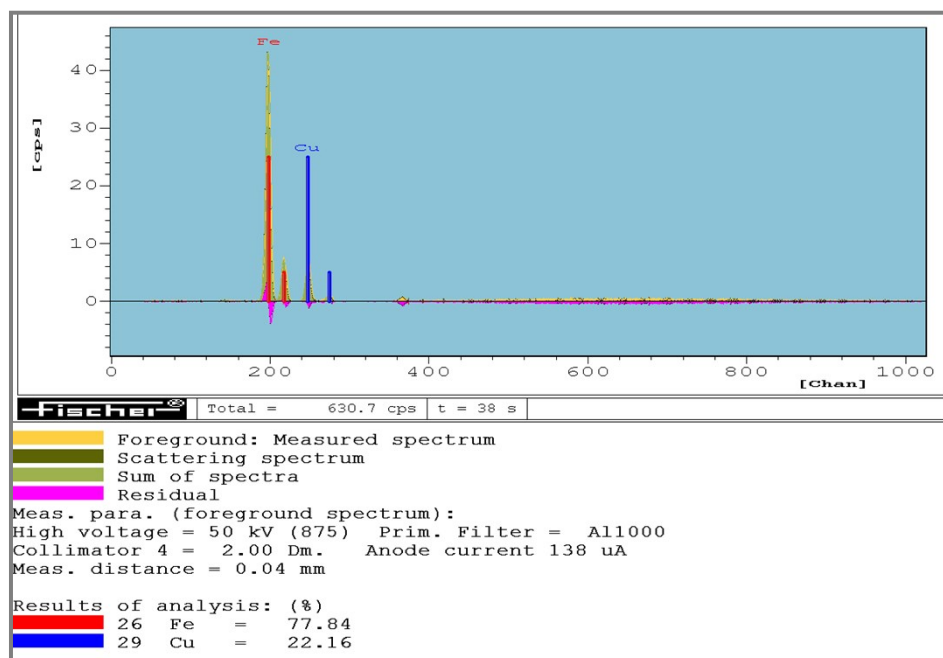


Fig. S2. Detection and quantification of copper in CuIL@SMNPs using EDXRF.

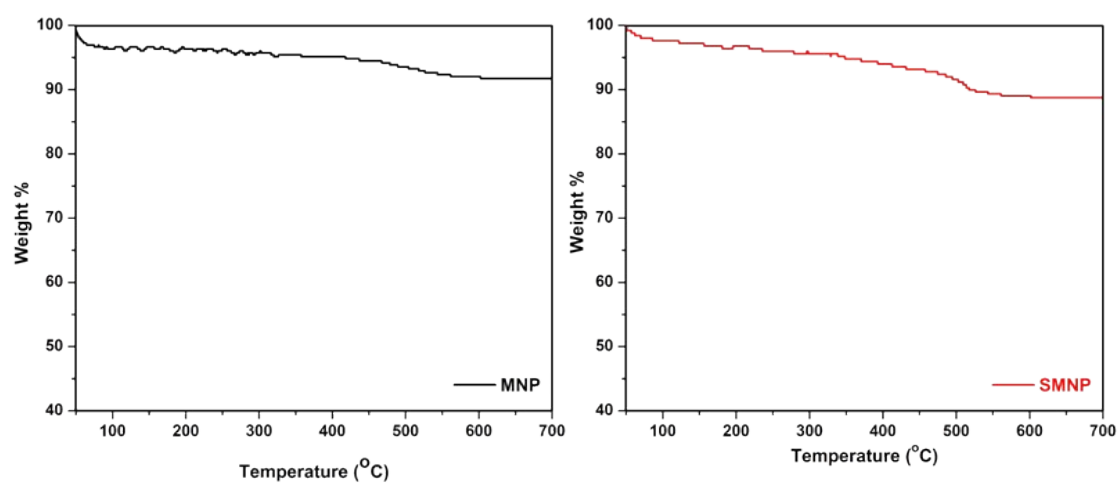


Fig. S3 TGA curves of MNP and SMNP.

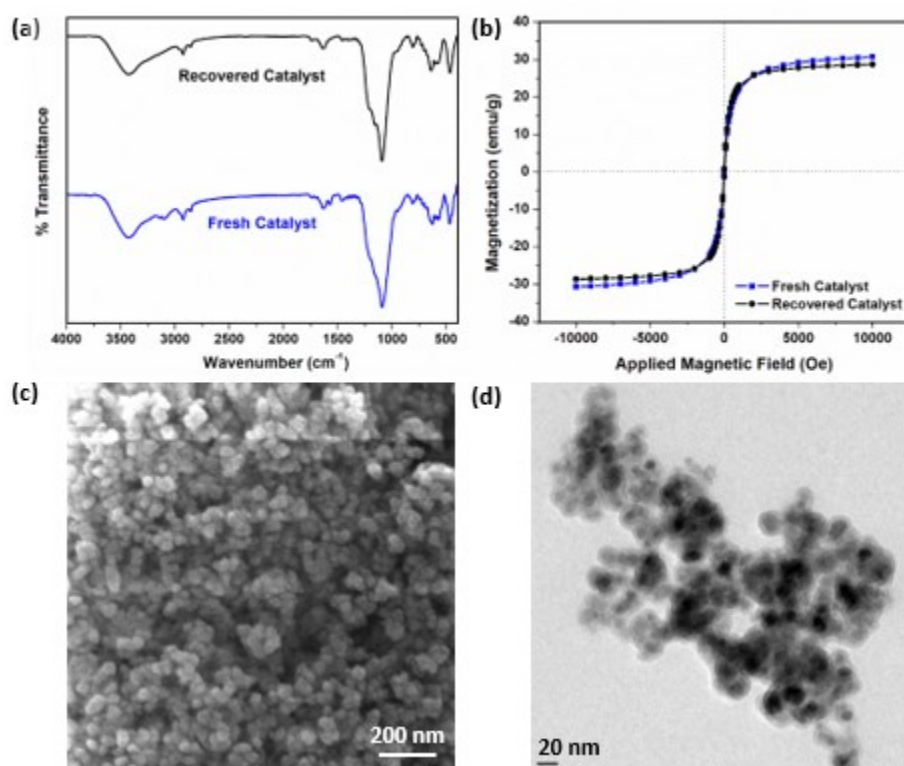


Fig. S4 (a) FT-IR, (b) VSM, (c) FE-SEM and (d) TEM analysis of the recovered catalyst after sixth run.

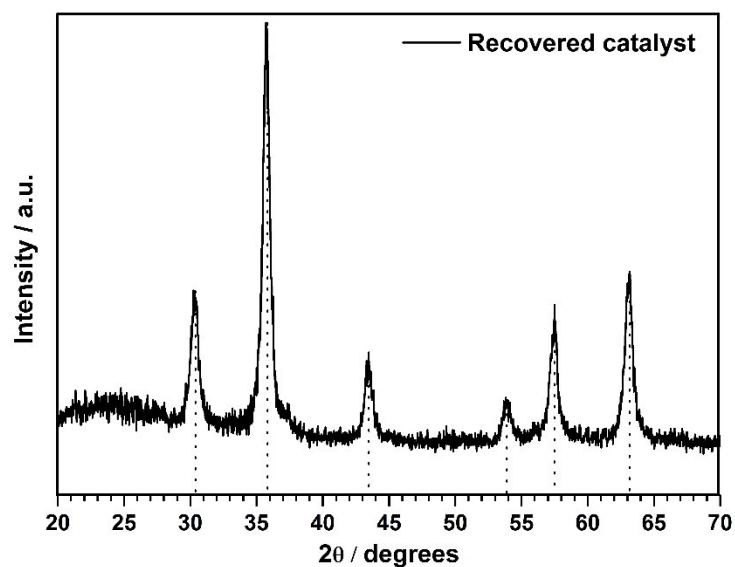
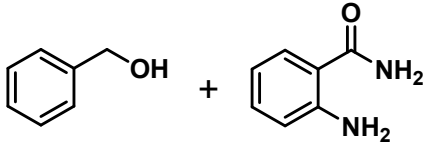
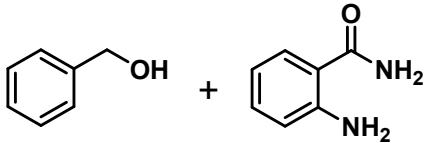
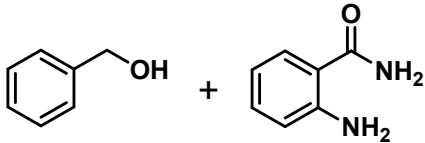
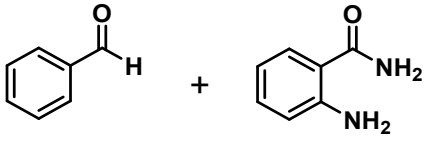
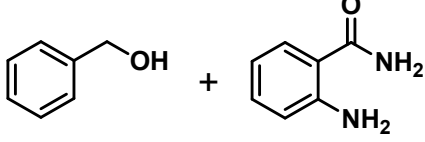
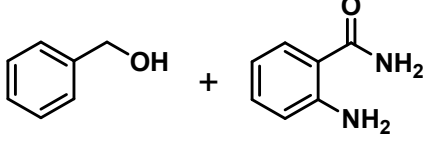
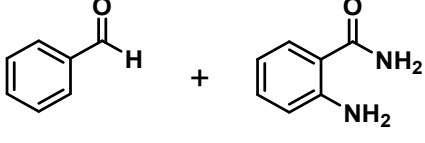
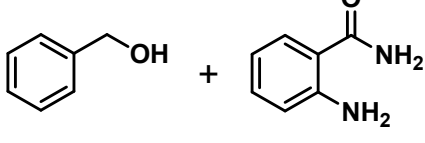
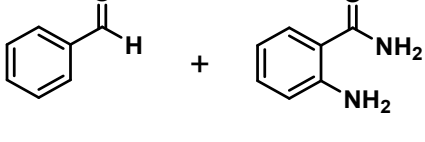
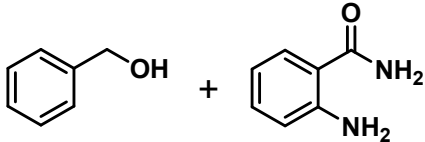
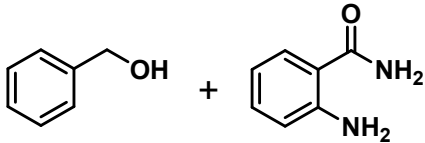
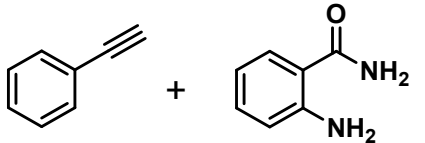
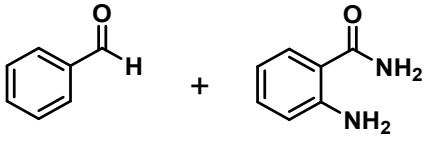
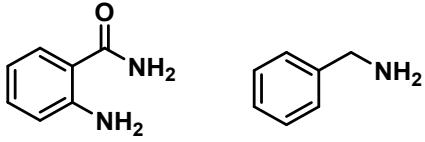
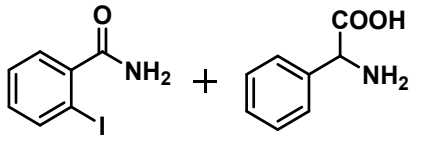
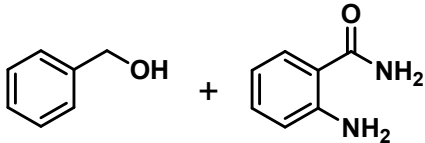
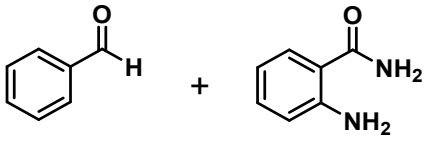


Fig. S5 XRD spectrum of recovered catalyst after 6th run.

Table S1 Comparison of the catalytic efficiency of CuIL@SMNP nanocatalyst with other previously reported catalysts for the synthesis of 2-phenylquinazolin-4(3*H*)-one.

S. No.	Reactants	Catalyst	Reaction Conditions	Yield & Reusable Cycles	Ref.
1.		Dicopper(I) complex	Cs ₂ CO ₃ , DMF, 70 °C, 6 h, N ₂	99; -	¹
2.		CuCl ₂	L-Proline, Cs ₂ CO ₃ , H ₂ O, 100 °C, 12 h	75; -	²
3.		[Cp*IrCl ₂] ₂	Xylene, 139 °C, 36 h, N ₂	93; -	³
4.		Ru(PPh ₃) ₃ (CO)(H) ₂ / Xantphos	Cronetonitrile, NH ₄ Cl, toluene, reflux, 24 h, N ₂	72; -	⁴

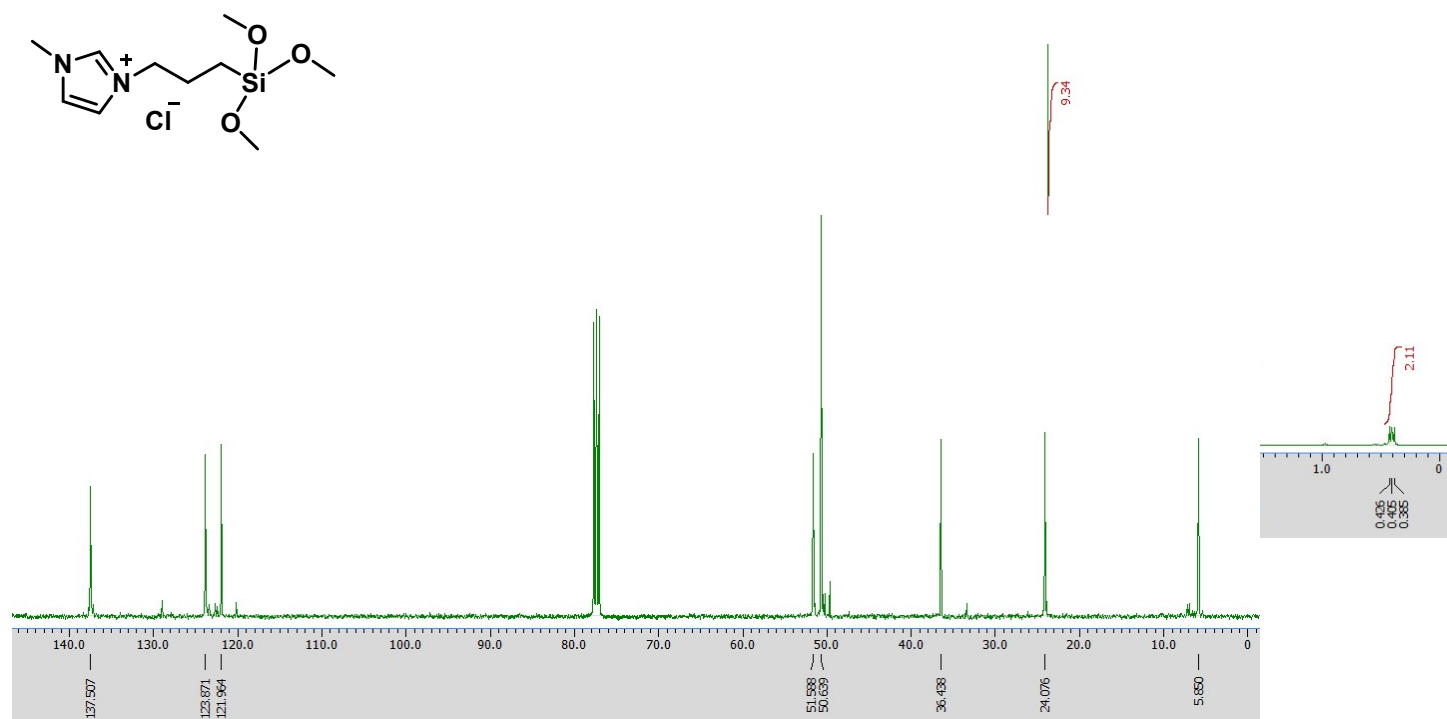
5.		$\text{Pd}(\text{OAc})_2/\text{TPPM S}$	H_2O , 100 °C, 16 h, sealed tube, air	93; -	⁵
6.		$[\text{Ni}(\text{MeTAA})]$	Na^tOBu , xylene, 100 °C, 36 h	86; -	⁶
7.		$\text{Cu}(\text{II})$ complex	NaOH , Toluene, 90 °C, 36 h	95; -	⁷
8.		CuCl_2	EtOH , 70 °C, 6 h	88; -	⁸
9.		FeCl_3	TBHP, DMSO, 60 °C, 7 h	93; -	⁹
10.		ZnI_2	TBHP, DMSO, 110 °C, 16 h	90; -	¹⁰
11.		$\text{VO}(\text{acac})_2$	DCE, 80 °C, 6 h, O_2 atmosphere	89; -	¹¹
12.		$\alpha\text{-MnO}_2$	TBHP, chlorobenzene, 80 °C, 16 h	91; 4	¹²
13.		$\text{Gd}_2\text{MoO}_6\text{-ZnO}$	Toluene, 110 °C, 8 h	90; 4	¹³

14.		Pt supported HBEA zeolite	Mesitylene, 165 °C, 24 h	95; -	14
15.		Fe-PPOP	CH ₃ CN, TBHP, 60 °C, 24 h	68; 3	15
16.		I ₂	O ₂ balloon, DMSO, H ₂ O, 110 °C, 12 h	70; -	16
17.		Bi-SO ₃ H functionalized IL	EtOH, 80 °C, 2 h	98; 4	17
18.		[BMIm]BF ₄	120 °C, 10 h	96;	18
19.		Graphene oxide/Fe ₃ O ₄ -CuI	DMSO/ethylene glycol, Cs ₂ CO ₃ , 120 °C, 12 h	61;	19
20.		Fe ₃ O ₄ -carbon dot nanocomposite	TBHP, H ₂ O, 90 °C, 16 h	94; 5	20
21.		CuIL@SMNP	EtOH, reflux, 4 h	97; 6	This work

NMR Data

Silyl-functionalized Ionic Liquid (FIL)

Colorless viscous liquid; ^1H NMR (400 MHz, CDCl_3) δ 10.20 (s, 1H), 7.59 (t, $J = 1.6$ Hz, 1H), 7.30 (t, $J = 1.7$ Hz, 1H), 4.11 (t, $J = 7.2$ Hz, 2H), 3.91 (s, 3H), 3.34 (s, 9H), 1.86-1.69 (m, 2H), 0.41 (t, $J = 8.2$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 137.5, 123.9, 122.0, 51.6, 50.6, 36.4, 24.1, 5.8



NMR data of selected organic compounds:

Note: Peaks at δ 3.4 and δ 2.5 ppm in ^1H NMR spectra are attributed to the presence of water and DMSO- d_6 , respectively. Also, the peak at δ 39.5 ppm in ^{13}C NMR is due to DMSO- d_6 . Besides, wherever CDCl_3 is used, peak at δ 7.26 ppm in ^1H and δ 77.26 ppm in ^{13}C NMR is due to CDCl_3 .

Fig. 9, 2a

White solid, m.p. 230-232 $^{\circ}\text{C}$; 20 ^1H NMR (400 MHz, DMSO- d_6) δ 12.52 (1H), 8.12 (3H), 7.74 (2H), 7.50 (4H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 162.8, 152.8, 149.2, 135.2, 133.2, 131.9, 129.1, 128.3, 128.0, 127.1, 126.4, 121.5

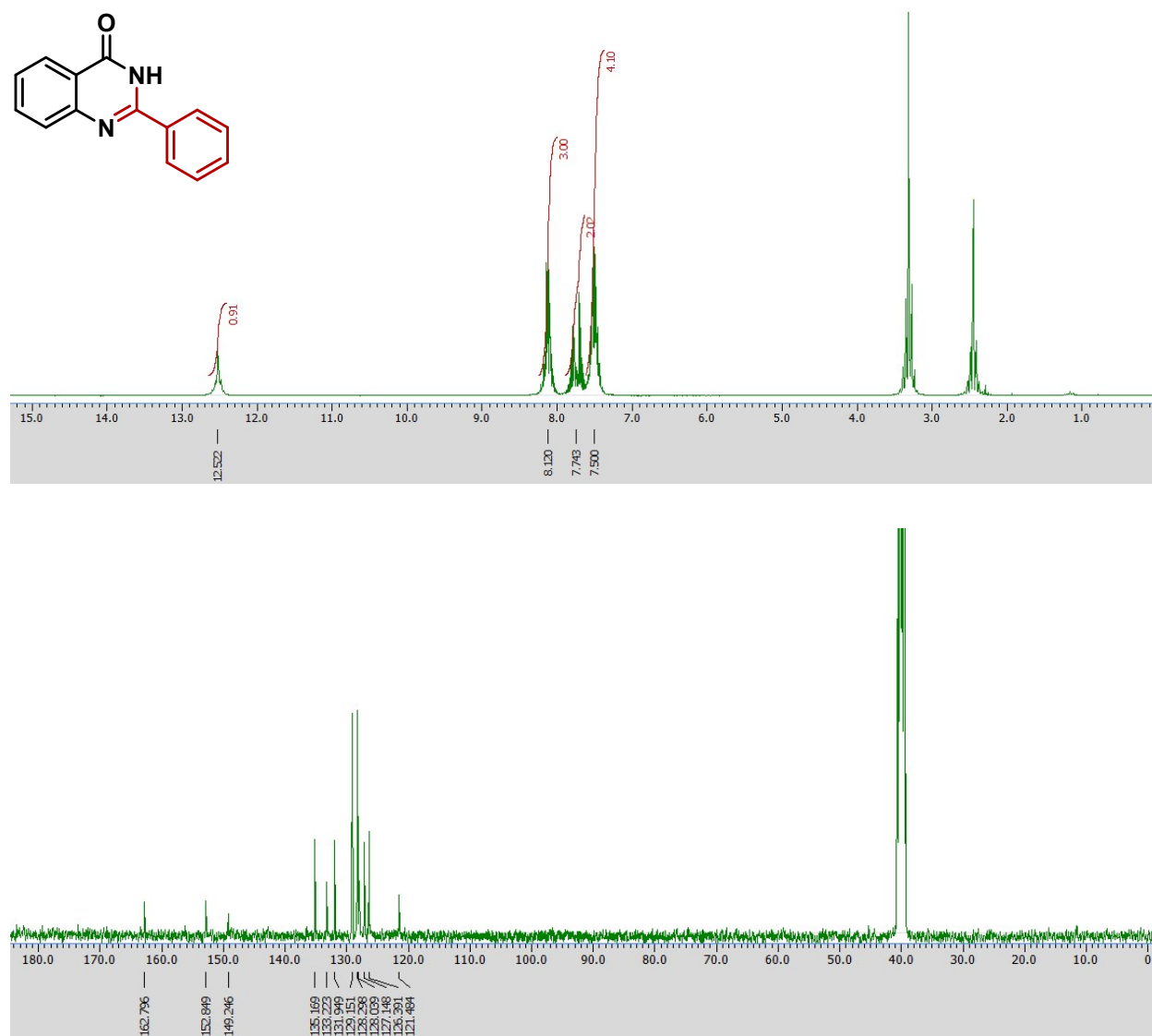


Fig. 9, 2b

White solid, m.p. 298-300 °C;²¹ ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.59 (s, 1H), 8.17-8.10 (m, 3H), 7.80 (t, *J* = 7.4 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 162.7, 151.9, 149.1, 136.8, 135.2, 132.0, 130.2, 129.2, 128.1, 127.4, 126.4, 121.5

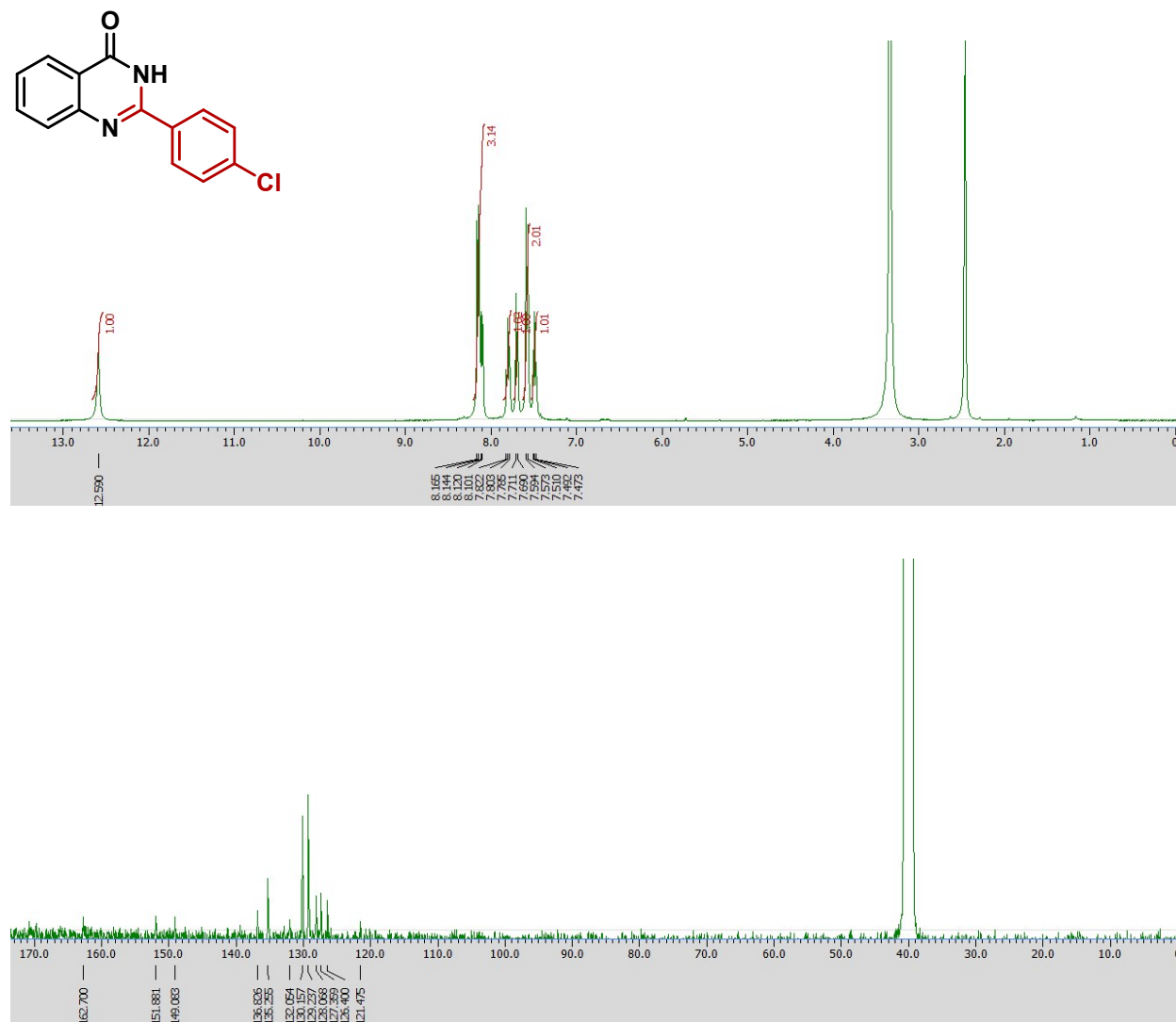


Fig. 9, 2c

White solid, m.p. 292-294 °C;²¹ ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.59 (s, 1H), 8.12-8.07 (m, 3H), 7.80 (t, *J* = 7.4 Hz, 1H), 7.71 (t, *J* = 8.2 Hz, 3H), 7.50 (t, *J* = 7.4 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 162.7, 152.0, 149.1, 135.2, 132.2, 130.3, 128.0, 127.3, 126.4, 125.8, 121.5

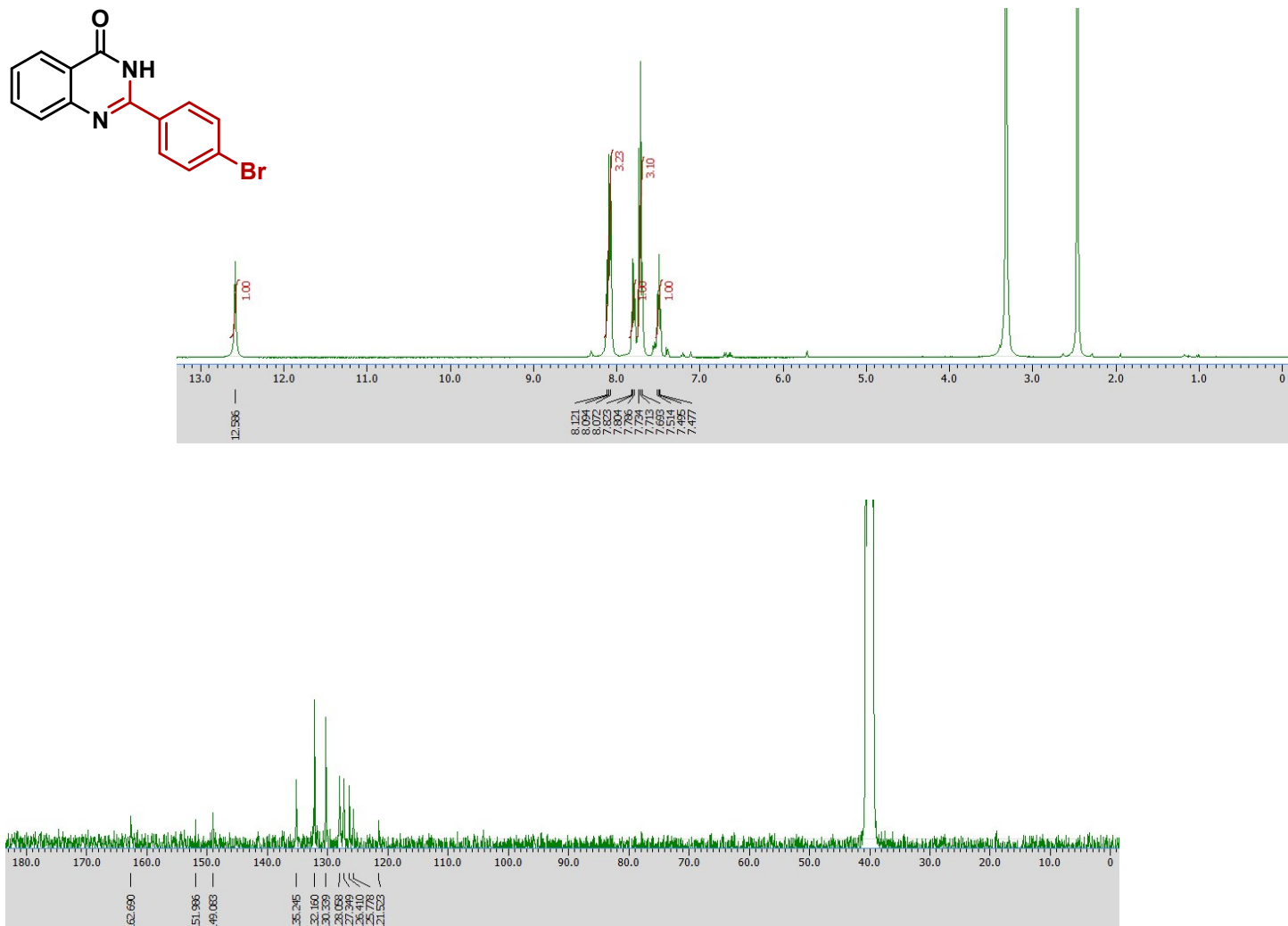


Fig. 9, 2e

White solid, m.p. 232-234 °C; ²⁰ ¹H NMR (400 MHz, CDCl₃) δ 11.62 (s, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 2H), 7.79 (dd, *J* = 15.4, 8.1 Hz, 2H), 7.50-7.47 (m, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 164.0, 151.9, 149.7, 142.3, 134.9, 130.0, 129.8, 128.0, 127.4, 126.6, 126.4, 21.7

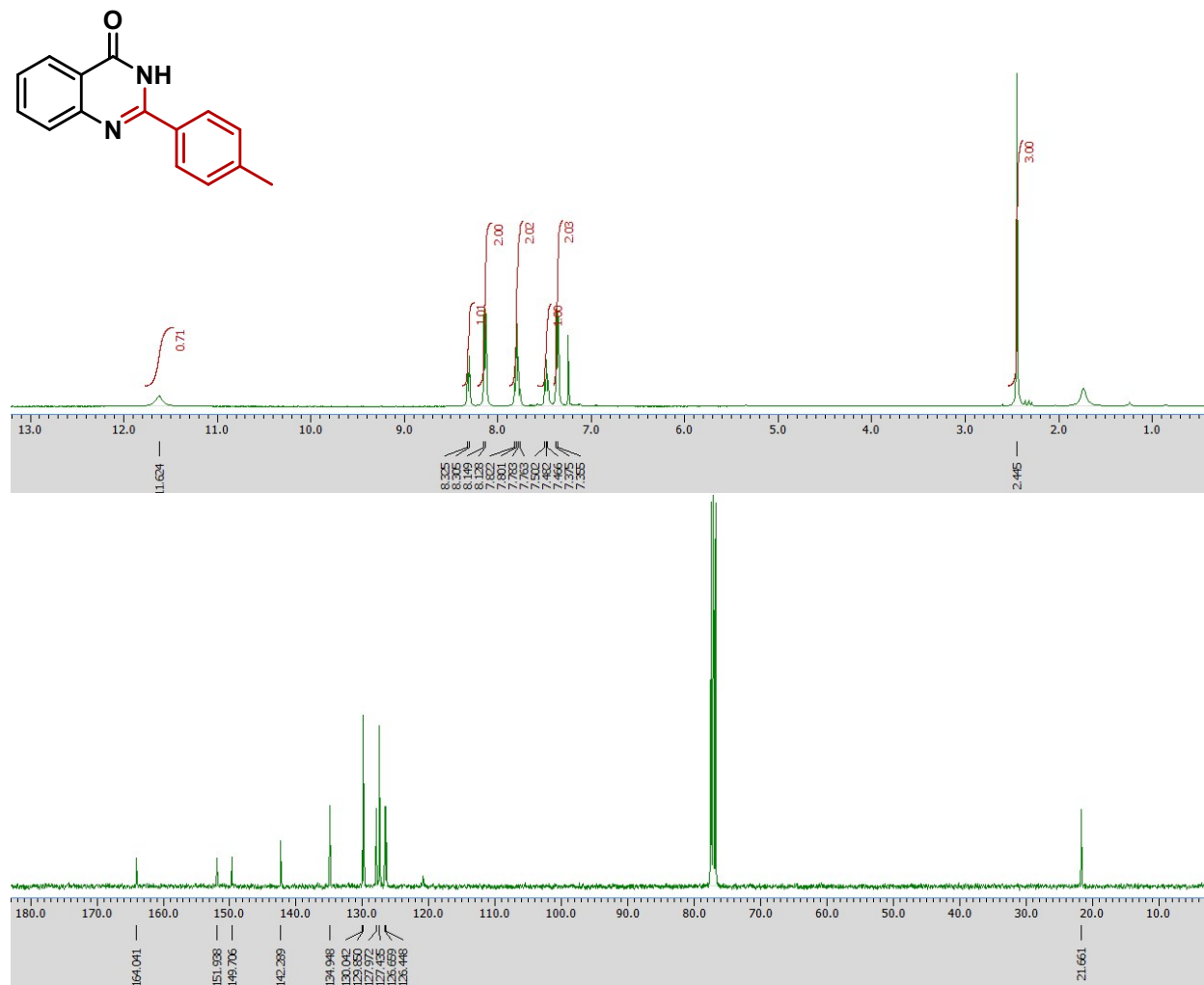


Fig. 9, 2g

Yellow solid, m.p. 222-224 °C; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 12.41 (bs, 1H), 8.08 (d, $J = 7.4$ Hz, 1H), 7.81-7.65 (m, 4H), 7.44 (t, $J = 6.9$ Hz, 1H), 7.07 (d, $J = 8.2$ Hz, 1H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 162.8, 152.3, 152.0, 149.4, 149.0, 135.1, 127.8, 126.7, 126.4, 121.6, 121.2, 111.9, 111.0, 56.2

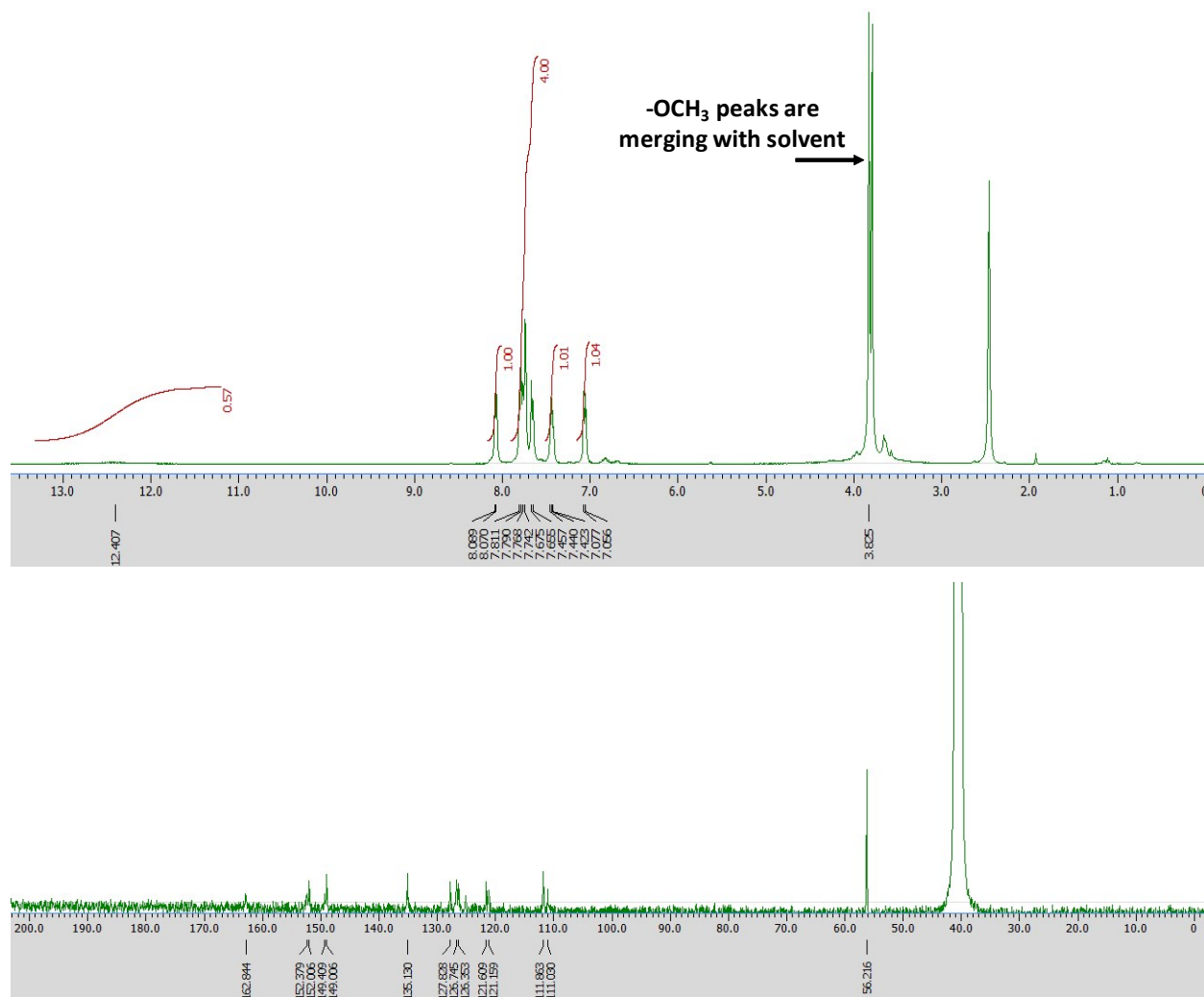
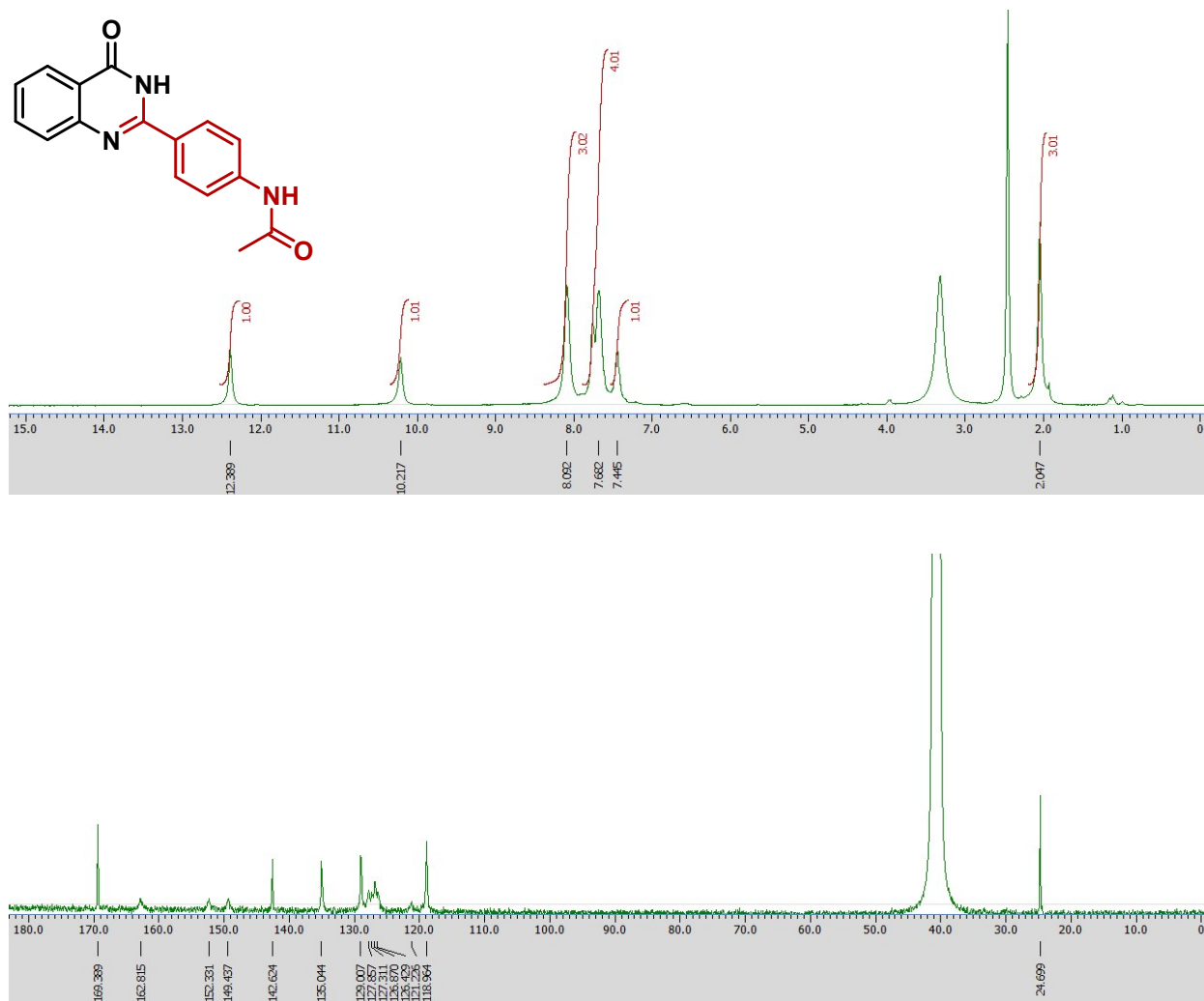


Fig. 9, 2j

Yellow solid, m.p. 324-327 °C; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 12.40 (1H), 10.22 (1H), 8.09 (3H), 7.68 (4H), 7.44 (1H), 2.05 (3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 169.4, 162.8, 152.3, 149.4, 142.6, 135.0, 129.0, 127.8, 127.3, 126.9, 126.4, 121.2, 119.0, 24.7



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