

Supplementary Information

Highly Active 4-Aminoquinoline-Pyrimidine Based Molecular Hybrids as Potential Next Generation Antimalarial Agents

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List of Contents

1. ¹ H and ¹³ C NMR of compounds	2-31
2. HRMS data of selected compounds.....	32-34
3. HPLC data of selected compounds.....	35-36

1. ^1H and ^{13}C NMR of compounds:

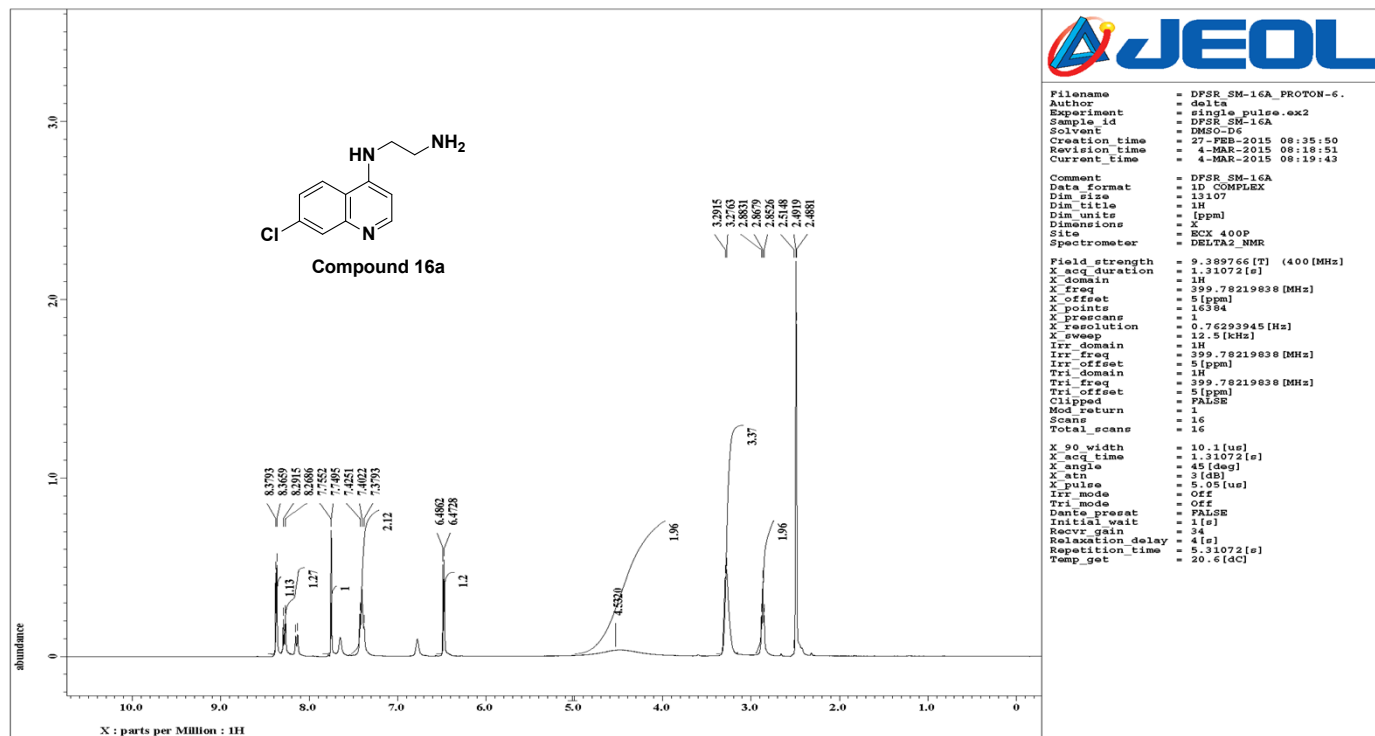


Fig 1: ^1H NMR of compound 16a

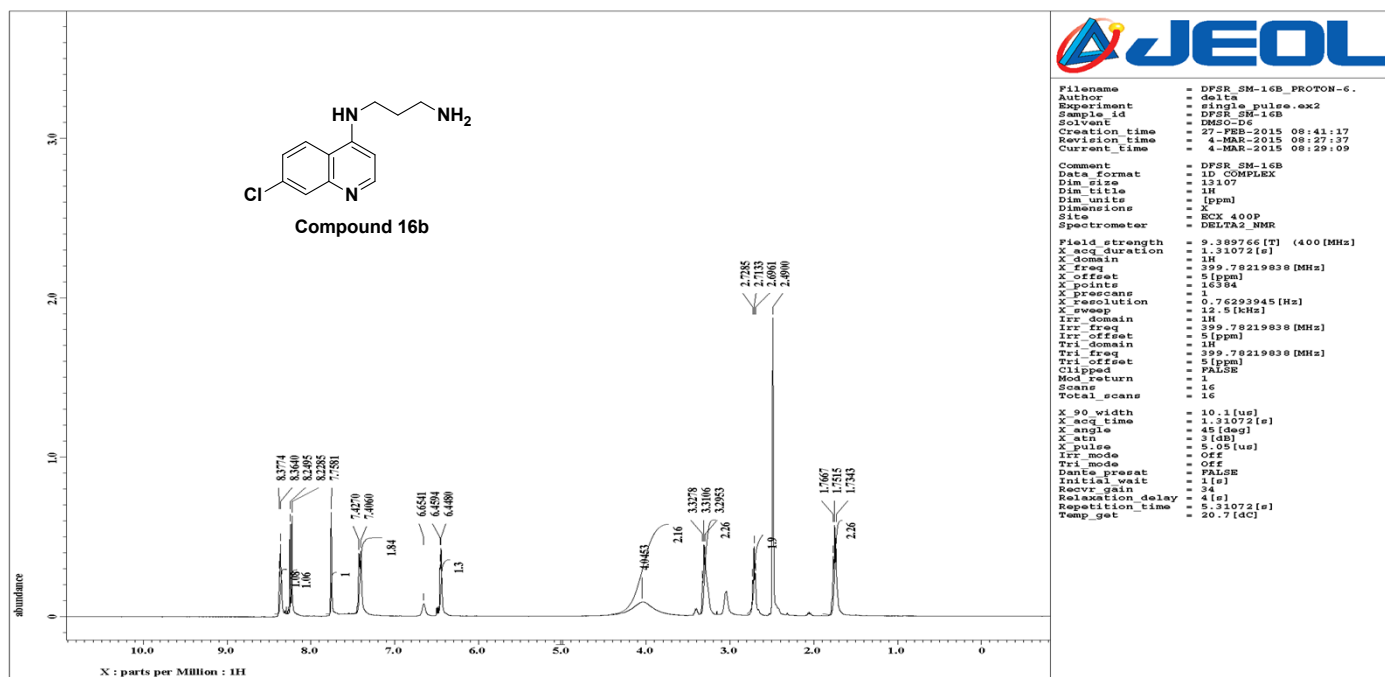


Fig 2: ^1H NMR of compound 16b

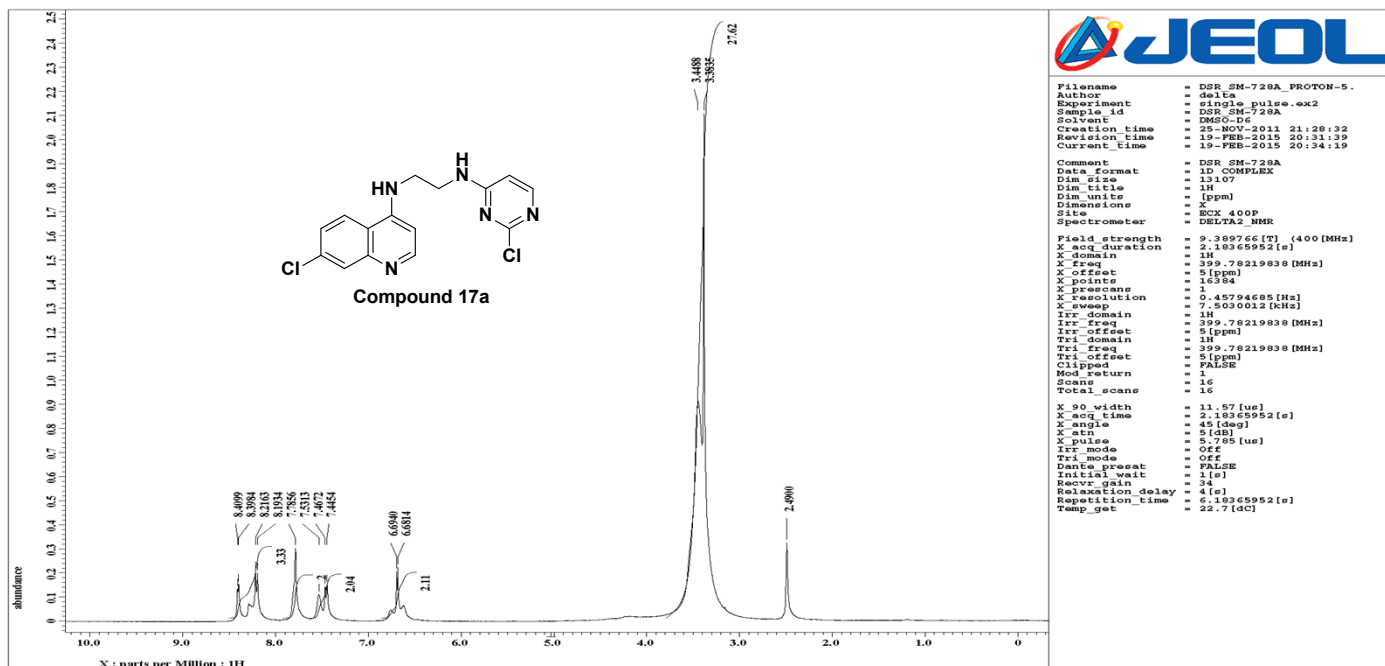


Fig 3: ¹H NMR of compound 17a

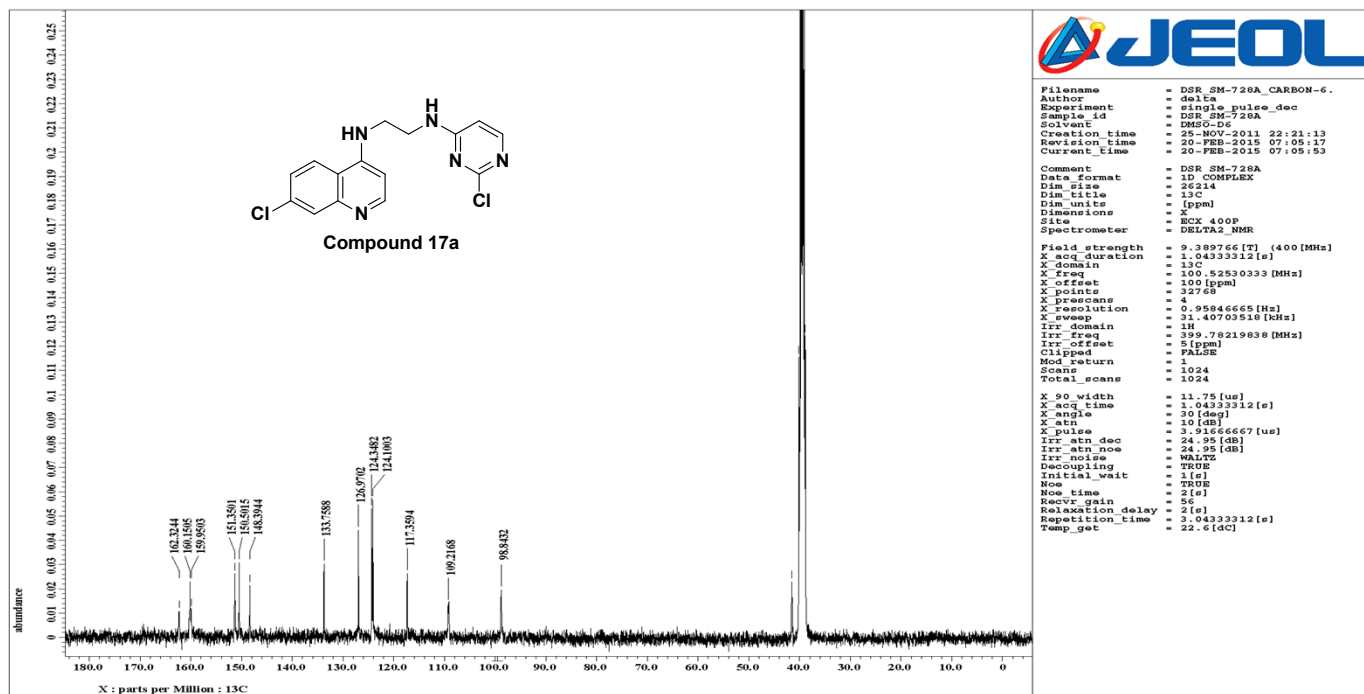


Fig 4: ¹³C NMR of compound 17a

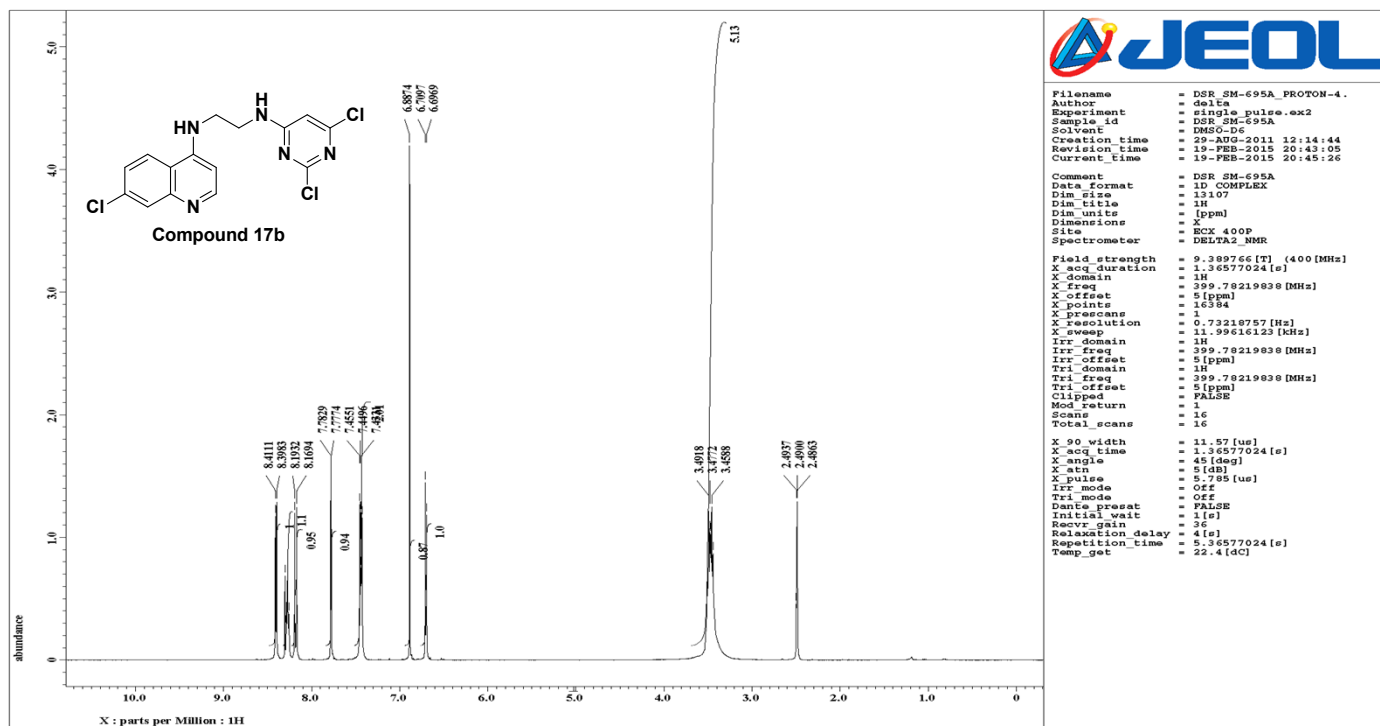


Fig 5: ¹H NMR of compound 17b

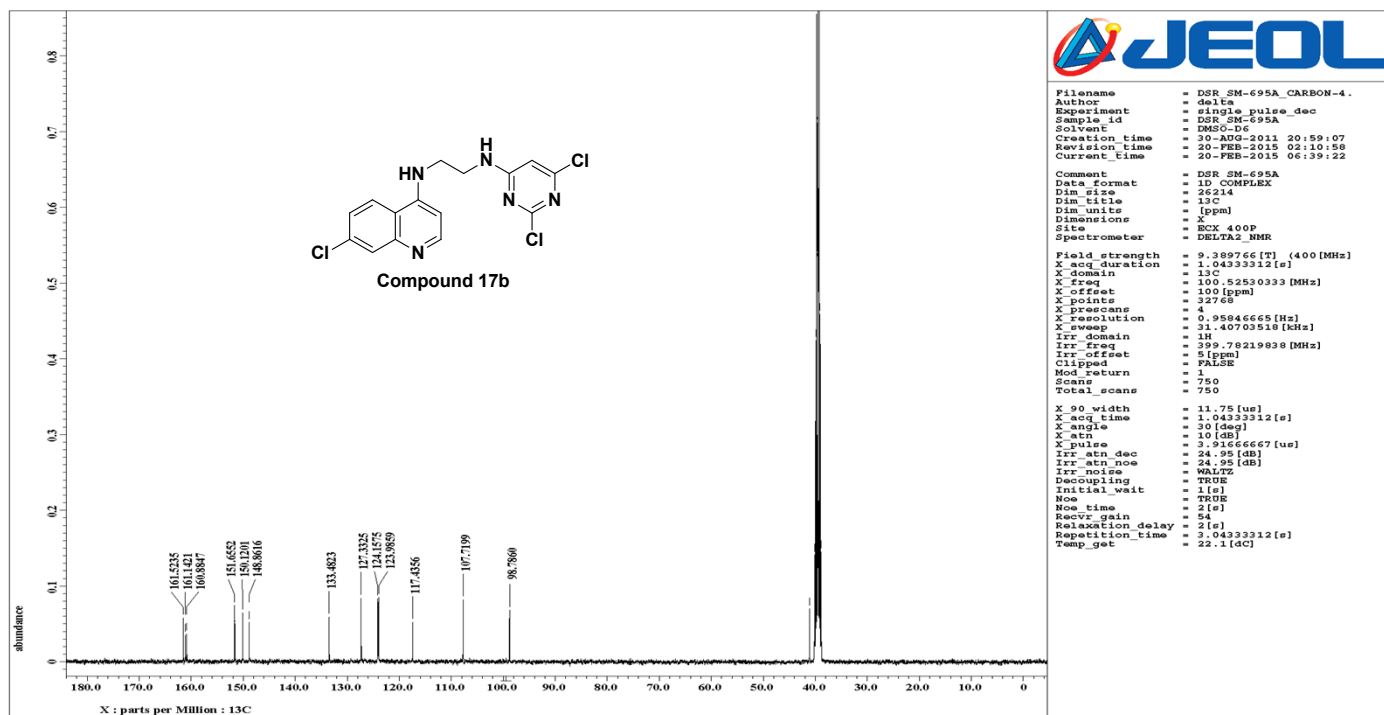


Fig 6: ¹³C NMR of compound 17b

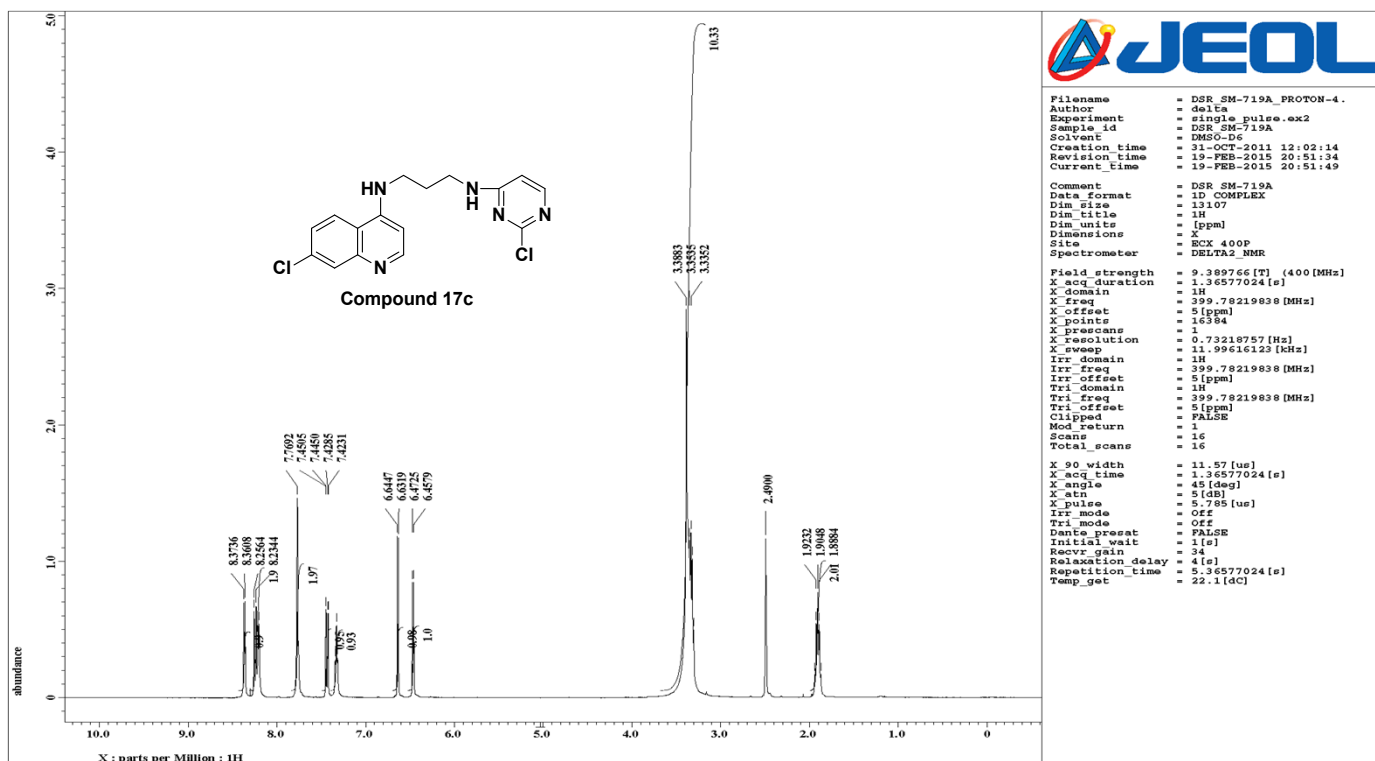


Fig 7: ¹H NMR of compound 17c

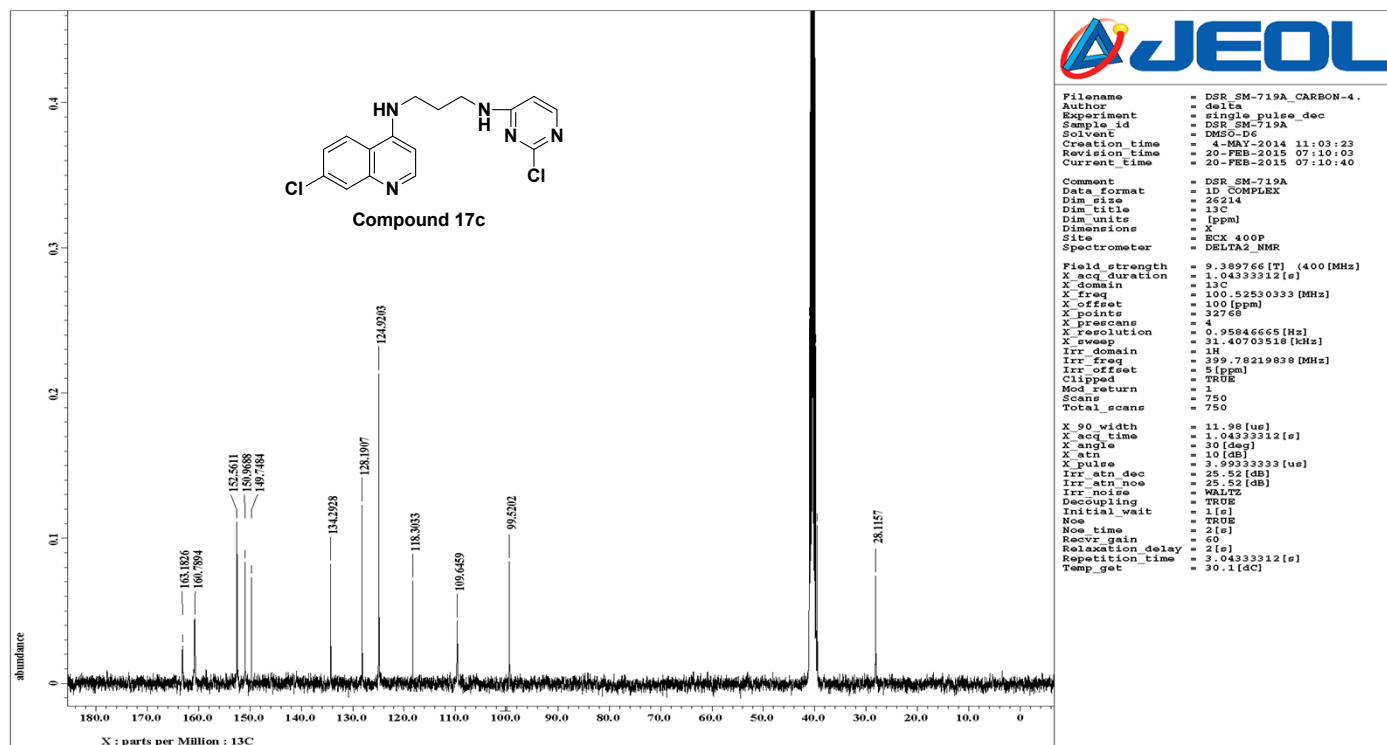


Fig 8: ¹³C NMR of compound 17c

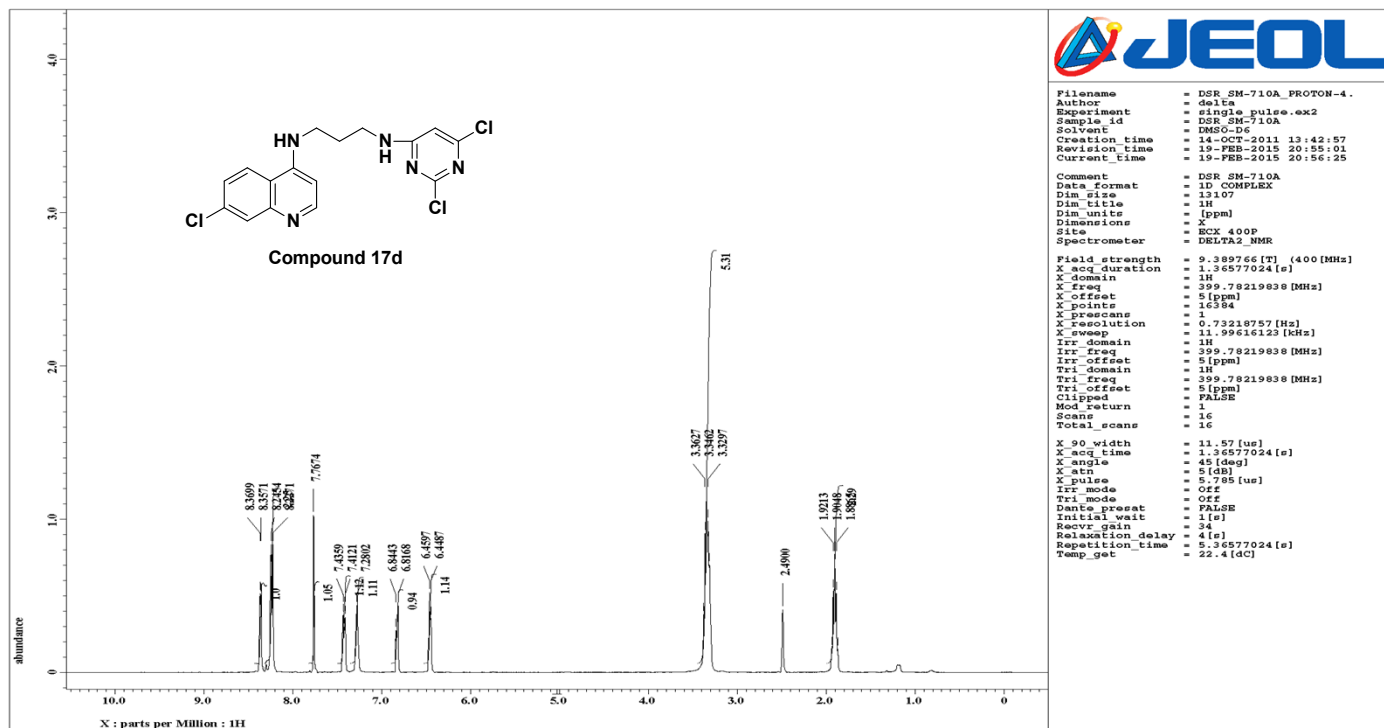


Fig 9: ¹H NMR of compound 17d

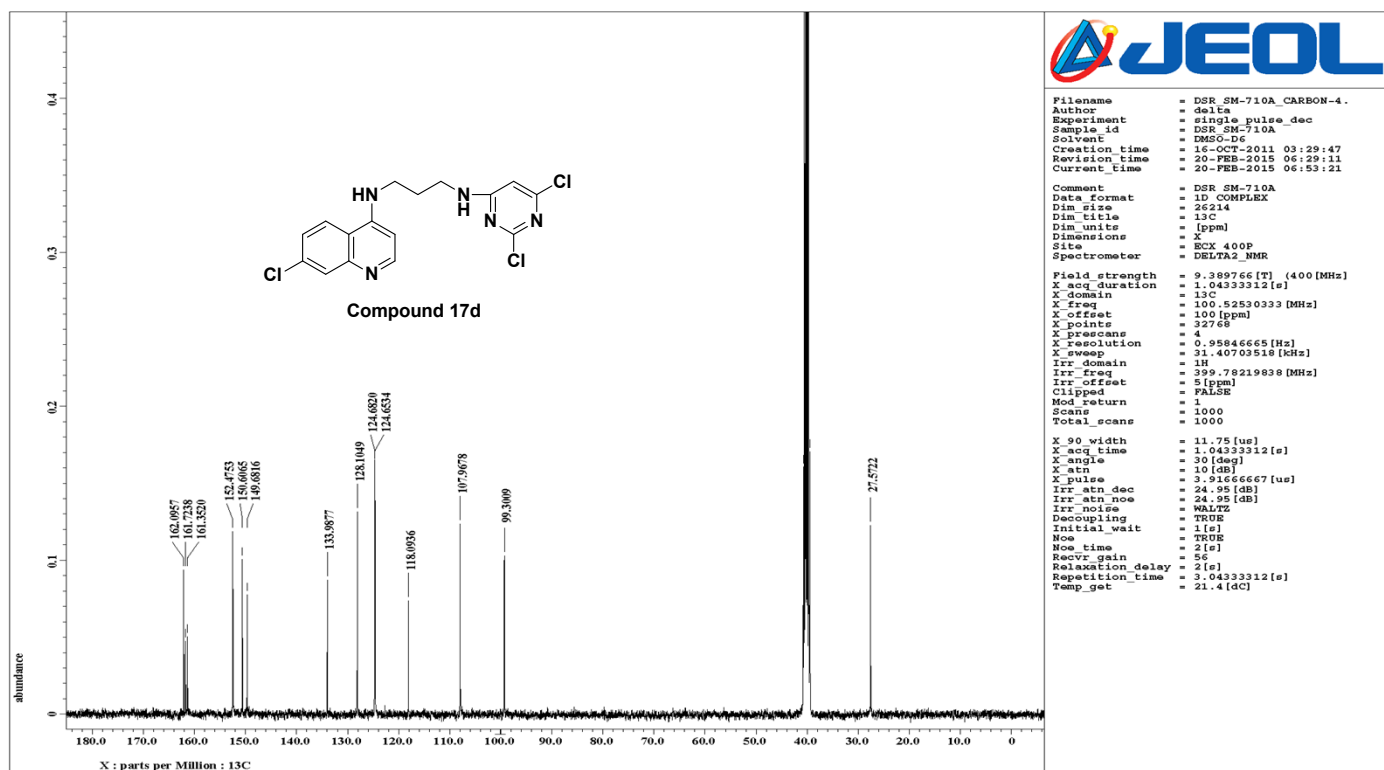


Fig 10: ¹³C NMR of compound 17d

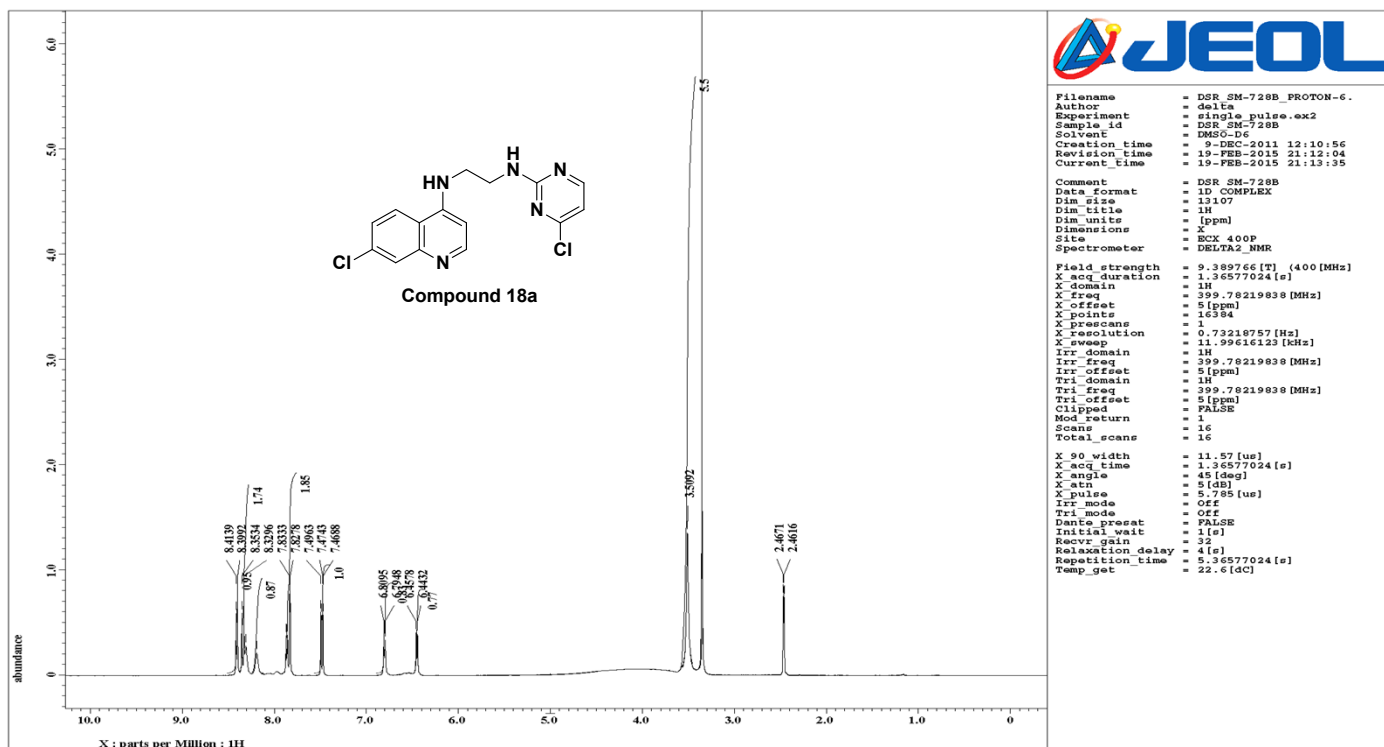


Fig 11: ¹H NMR of compound 18a

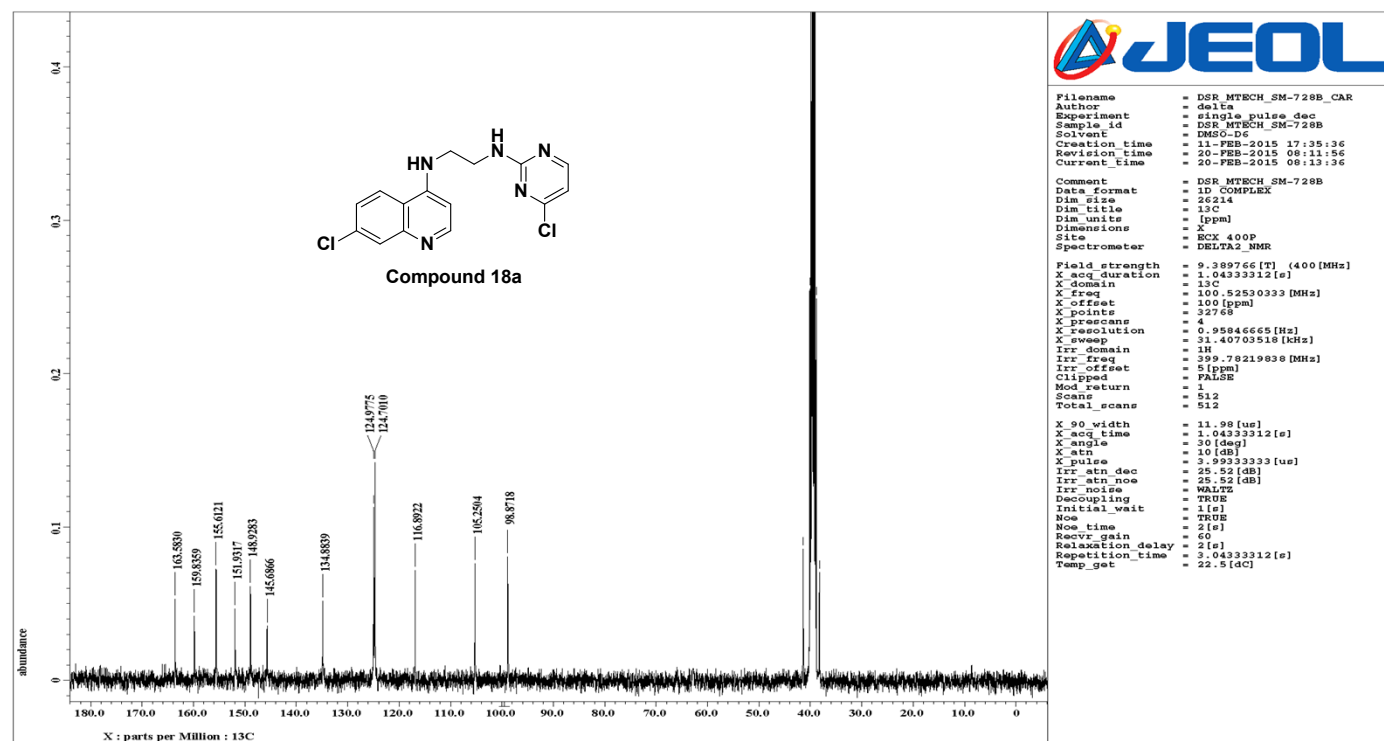


Fig 12: ¹³C NMR of compound 18a

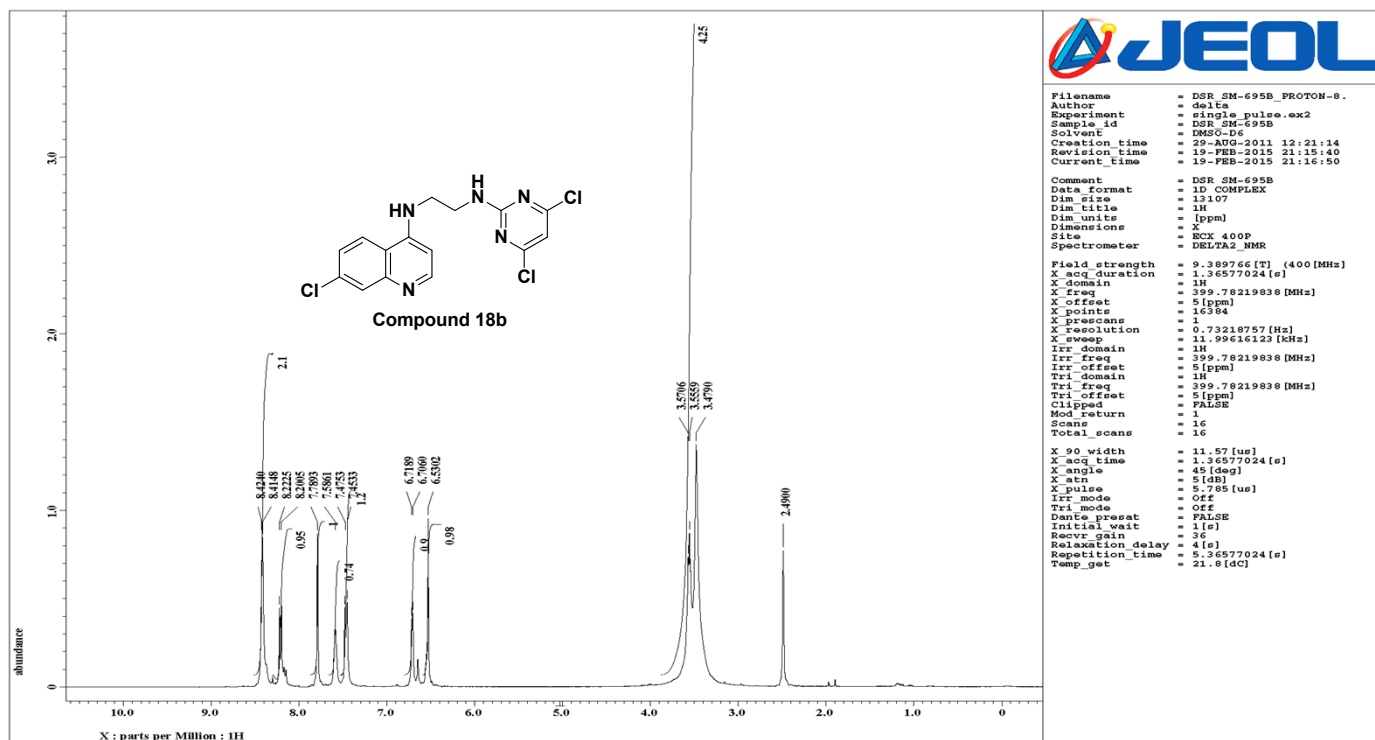


Fig 13: ¹H NMR of compound 18b

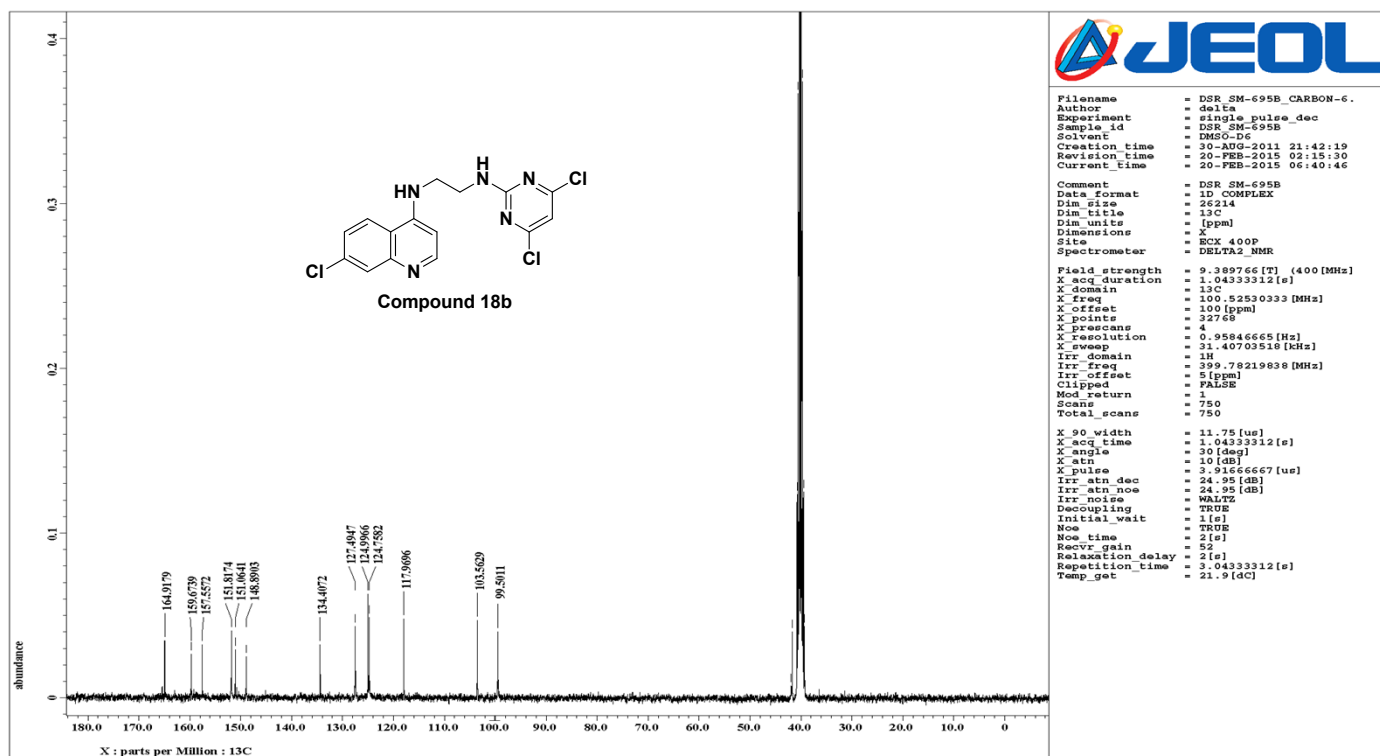


Fig 14: ¹³C NMR of compound 18b

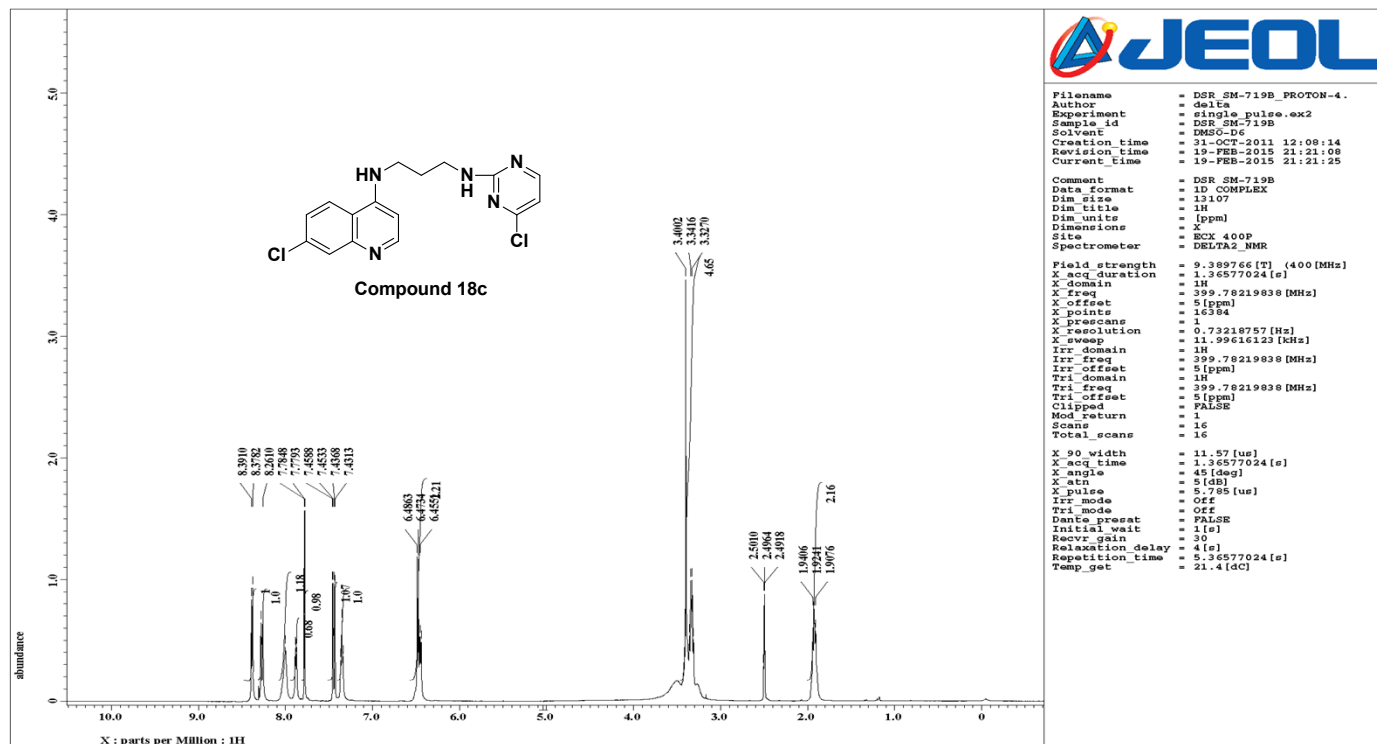


Fig 15: ¹H NMR of compound 18c

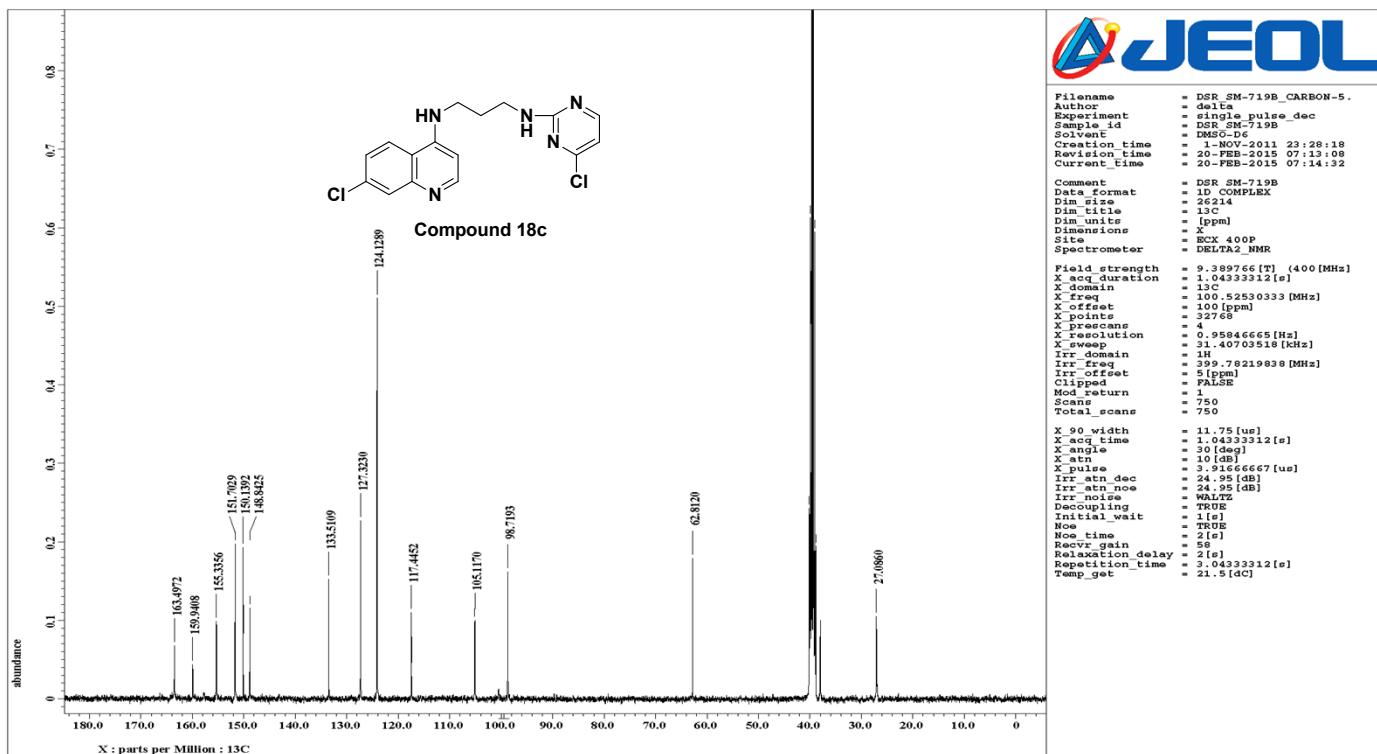


Fig 16: ¹³C NMR of compound 18c

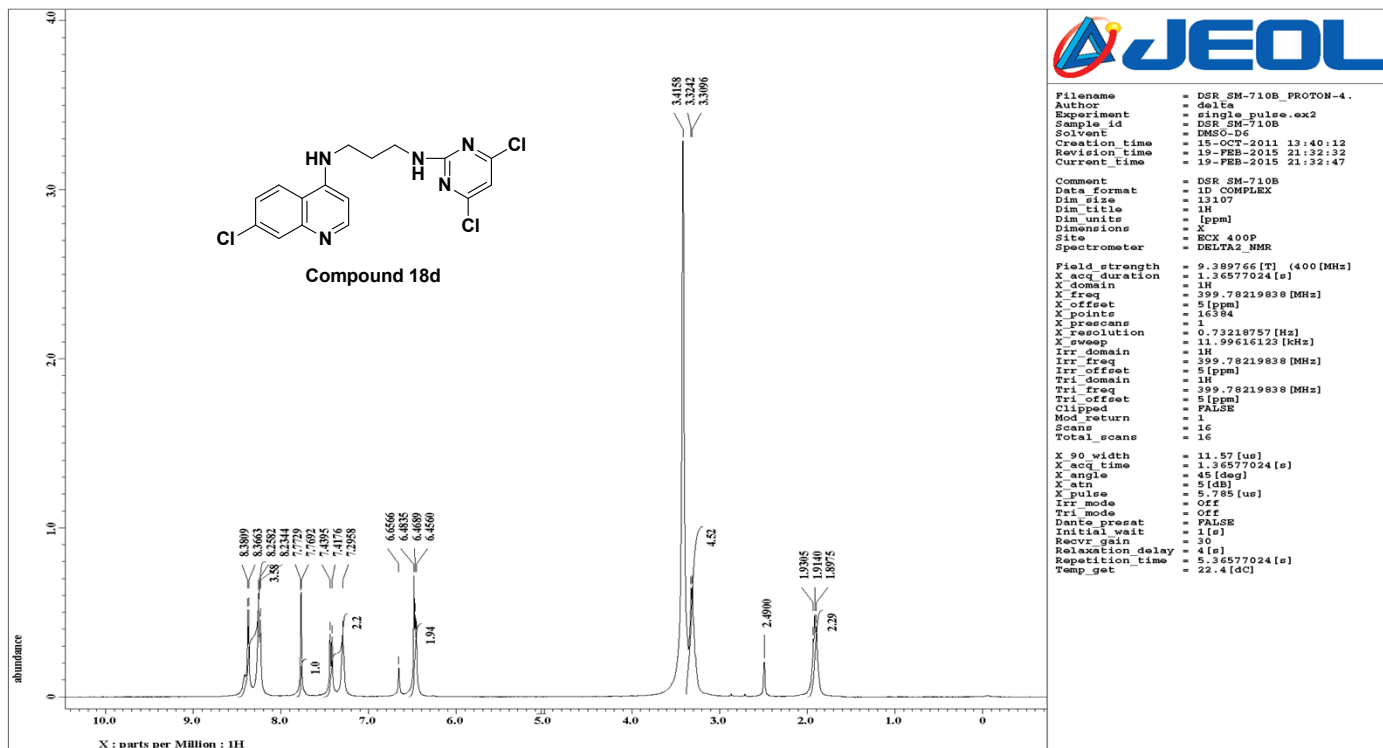


Fig 17: ¹H NMR of compound 18d

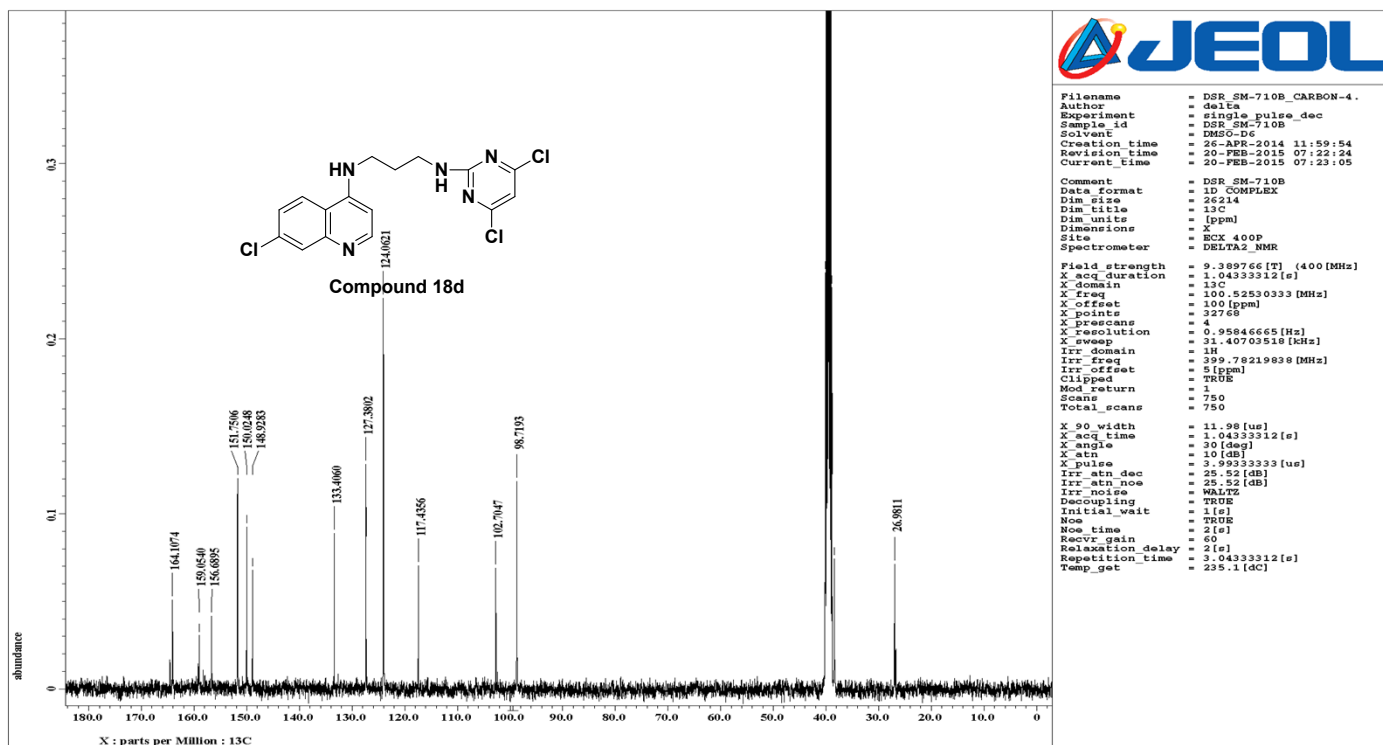


Fig 18: ¹³C NMR of compound 18d

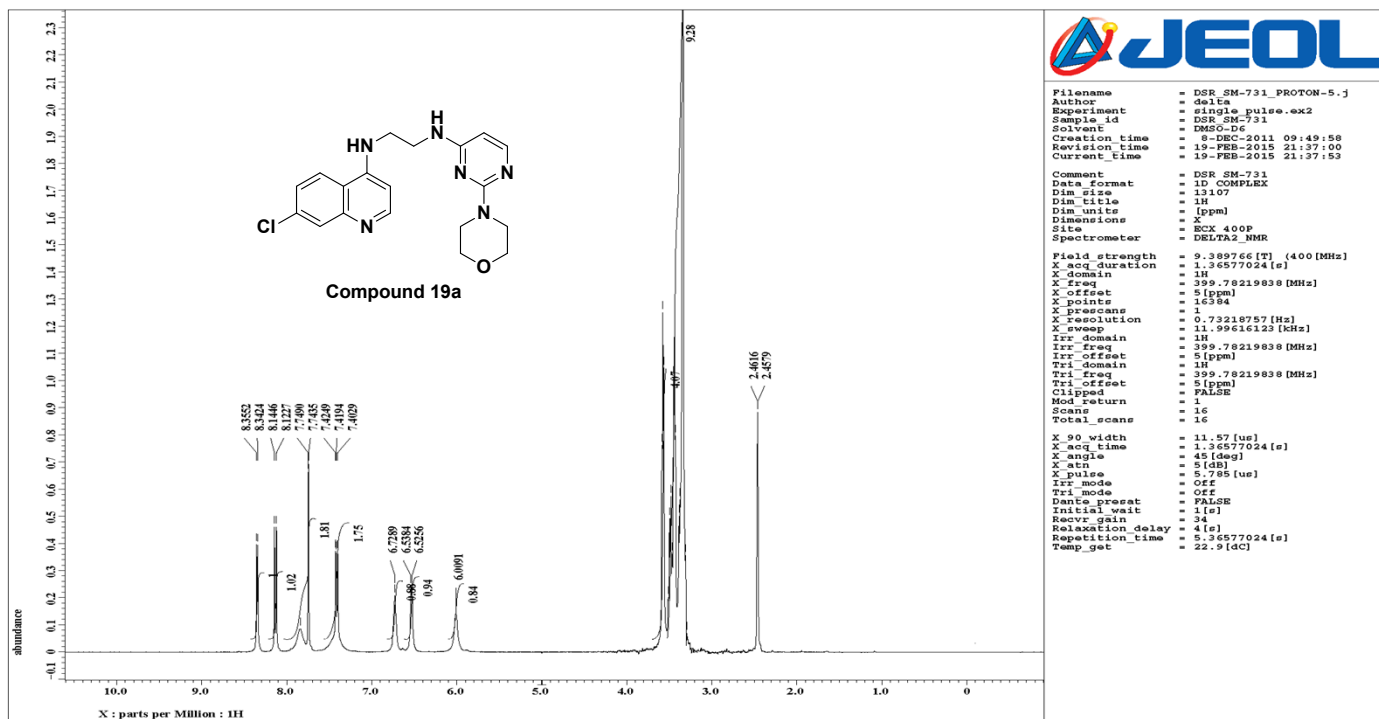


Fig 19: ¹H NMR of compound 19a

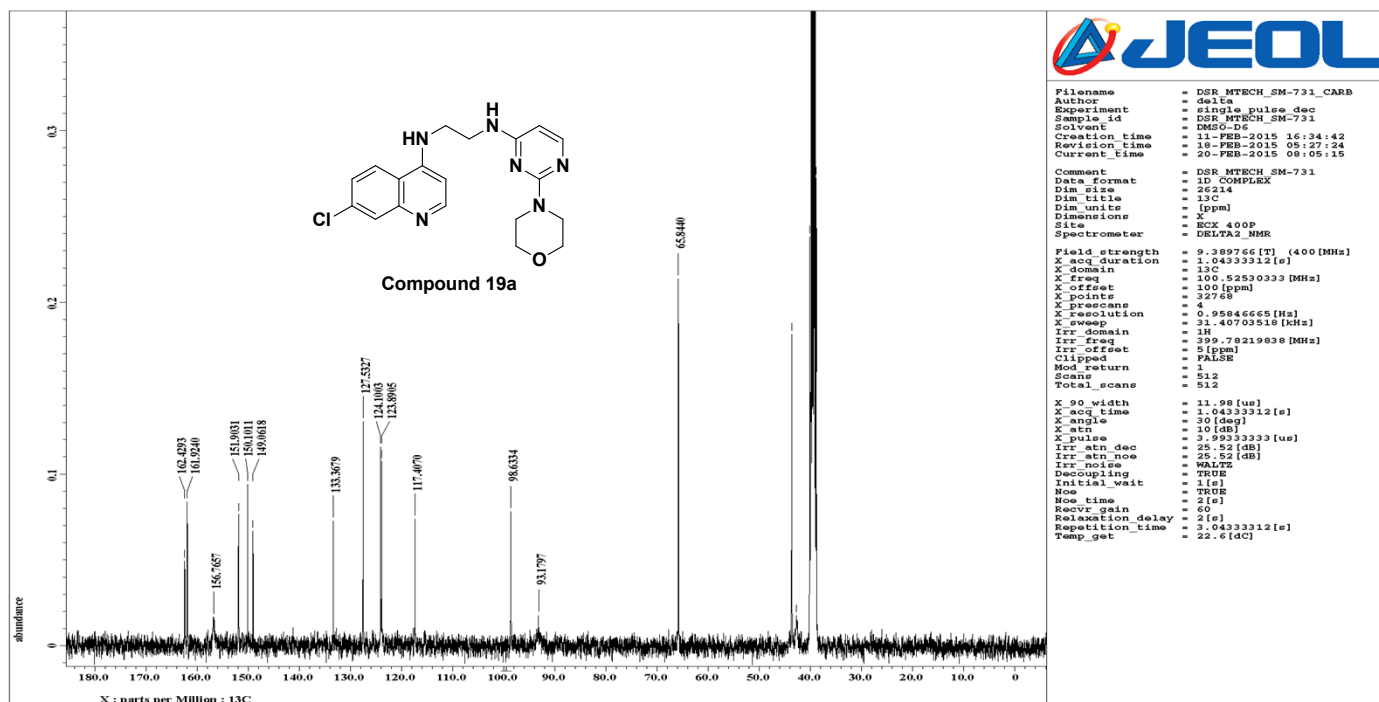


Fig 20: ¹³C NMR of compound 19a

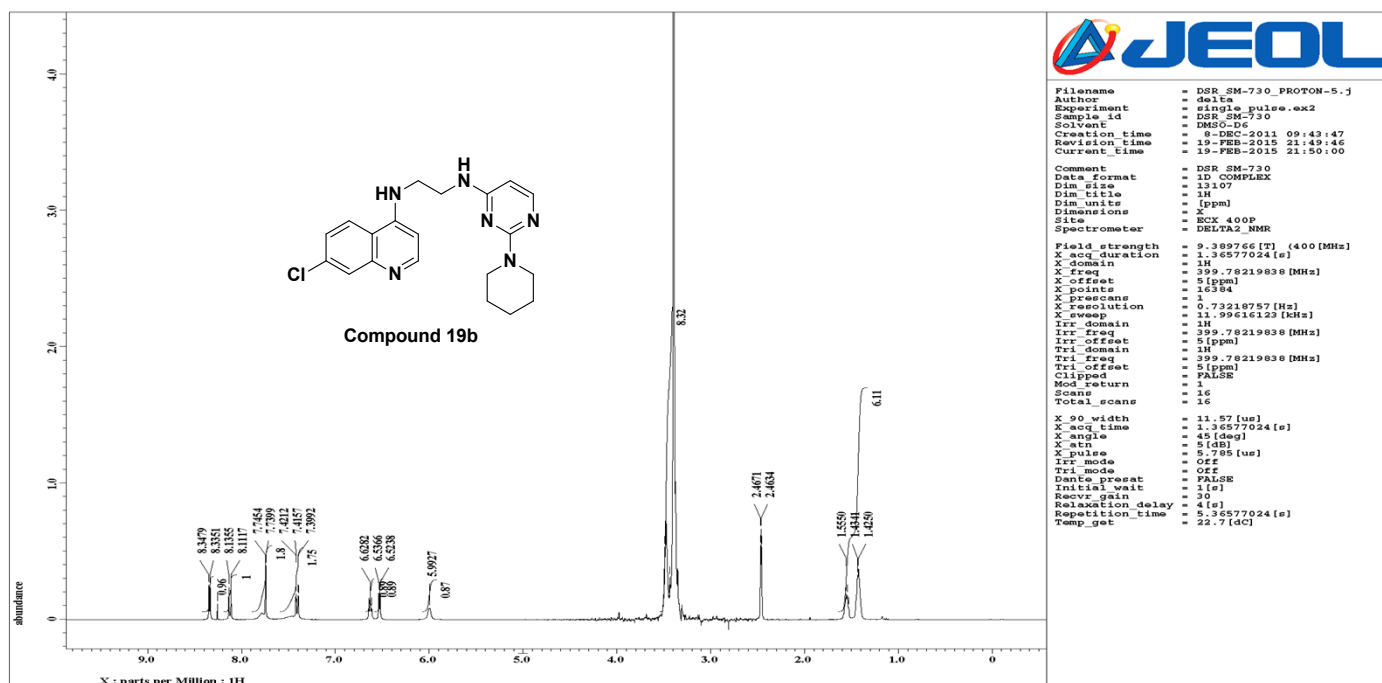


Fig 21: ¹H NMR of compound 19b

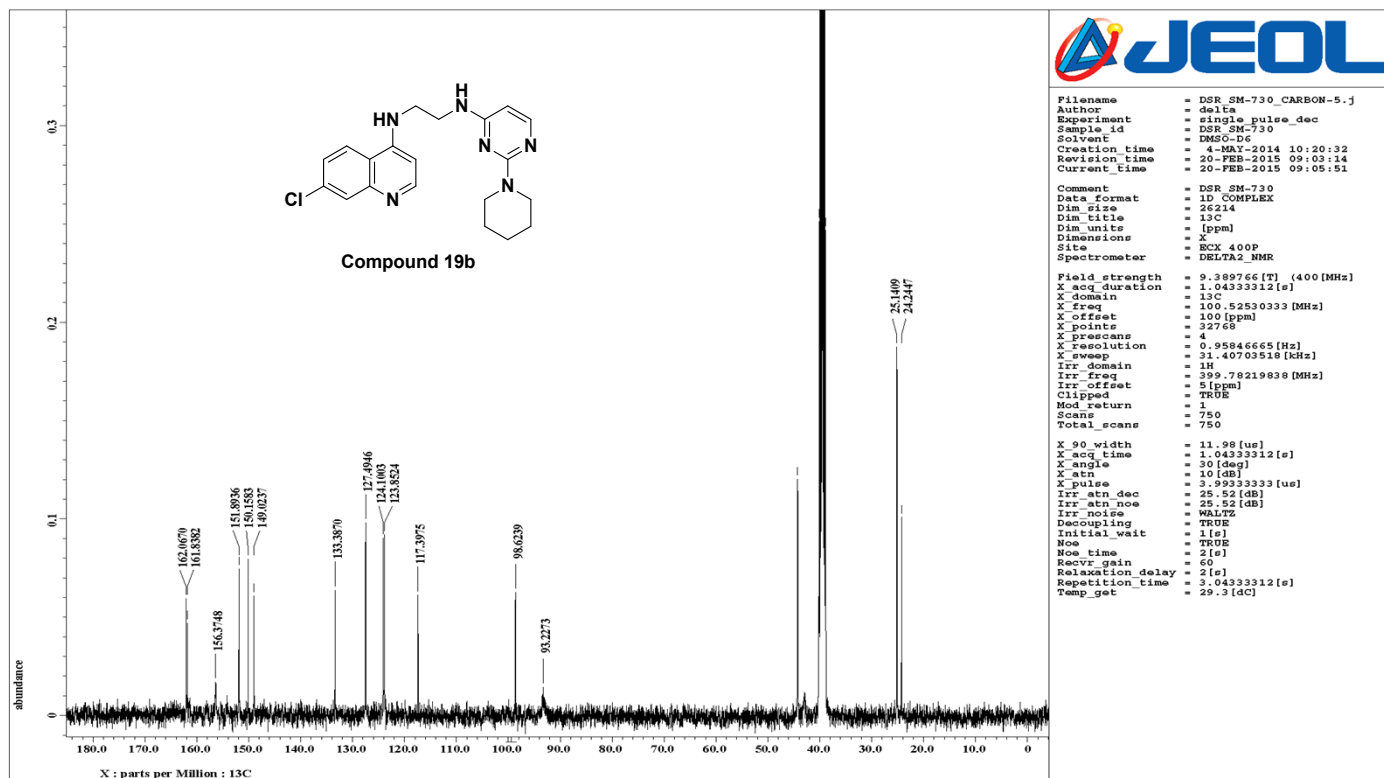
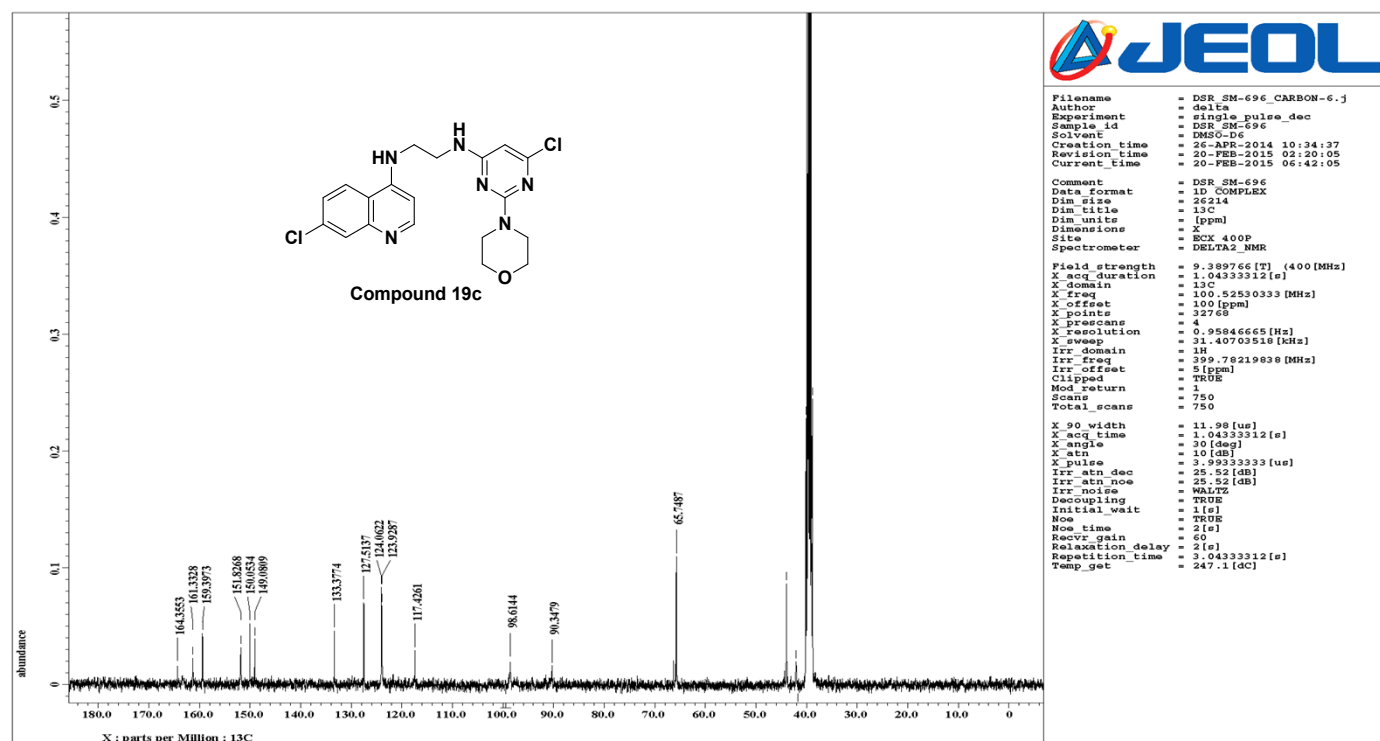
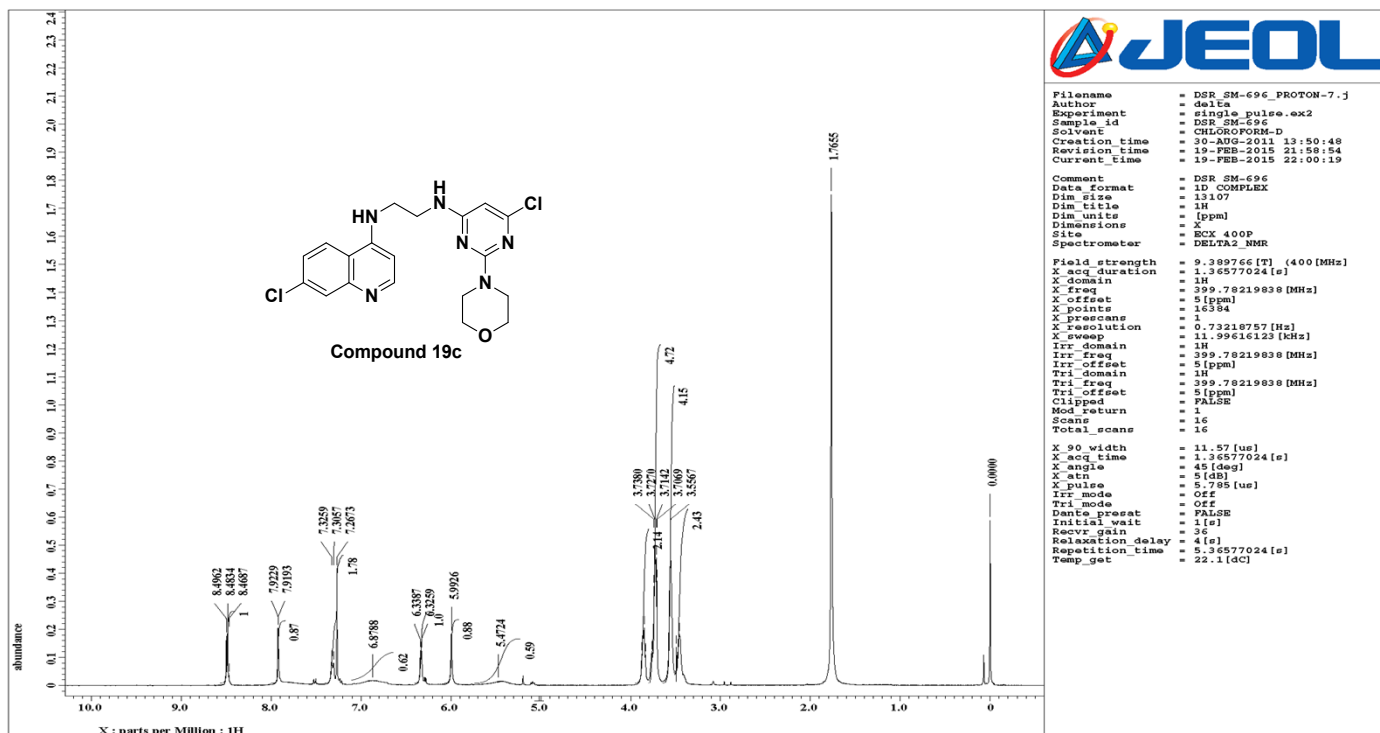


Fig 22: ¹³C NMR of compound 19b



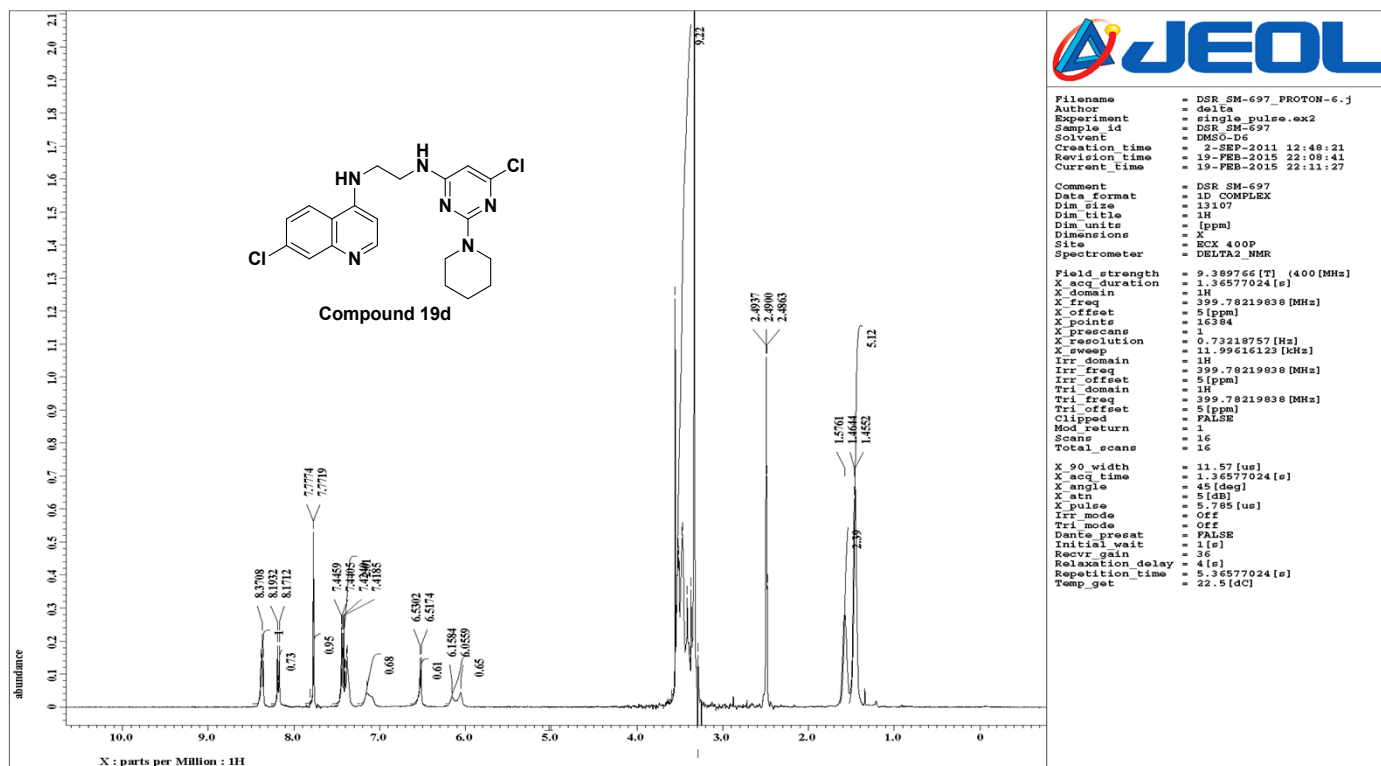


Fig 25: ¹H NMR of compound 19d

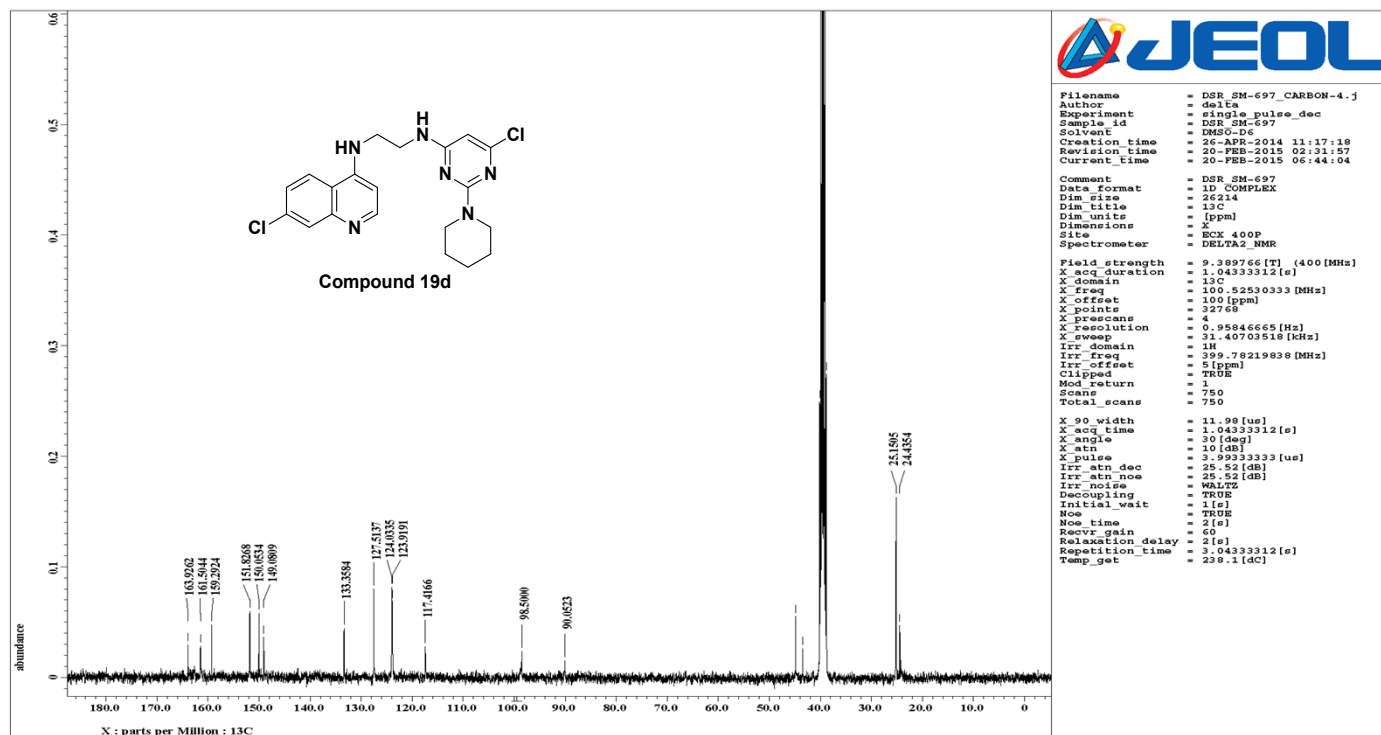


Fig 26: ¹³C NMR of compound 19d

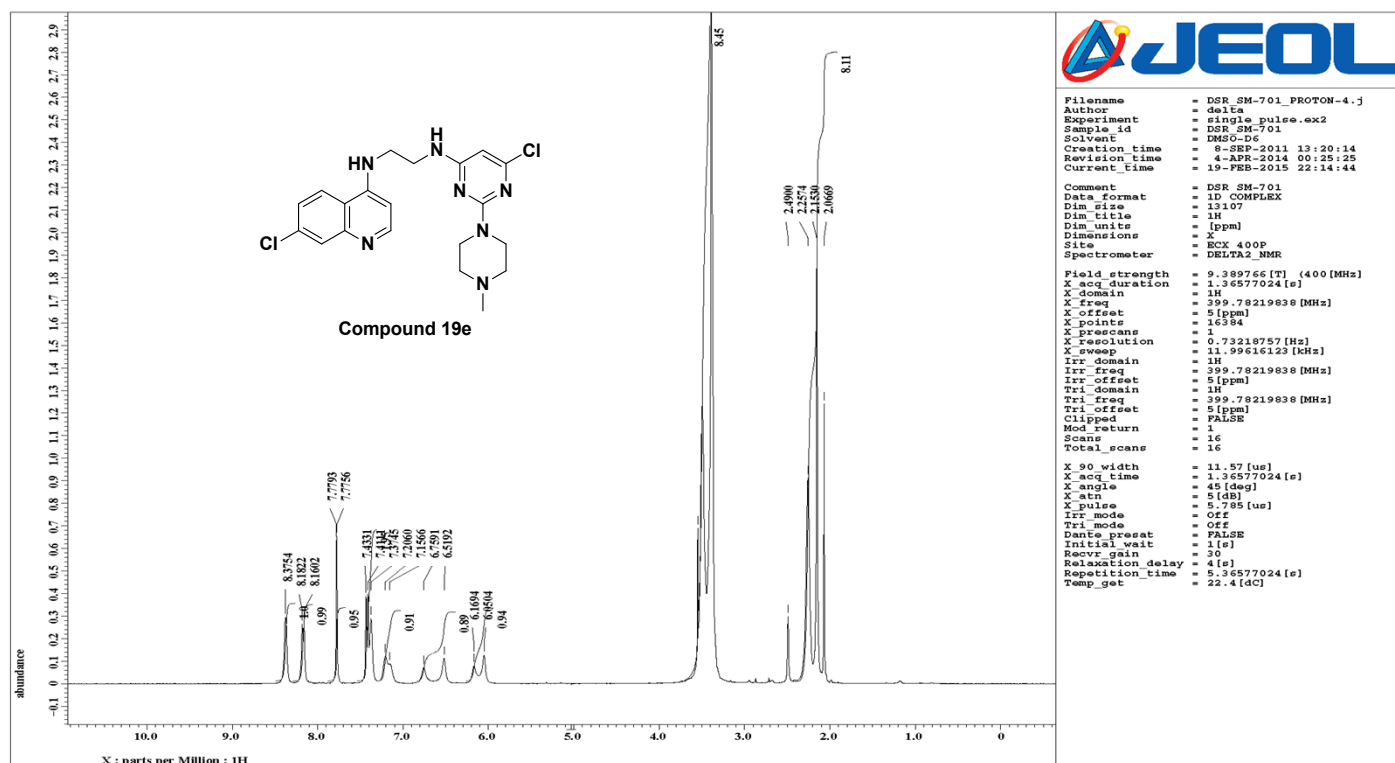


Fig 27: ¹H NMR of compound 19e

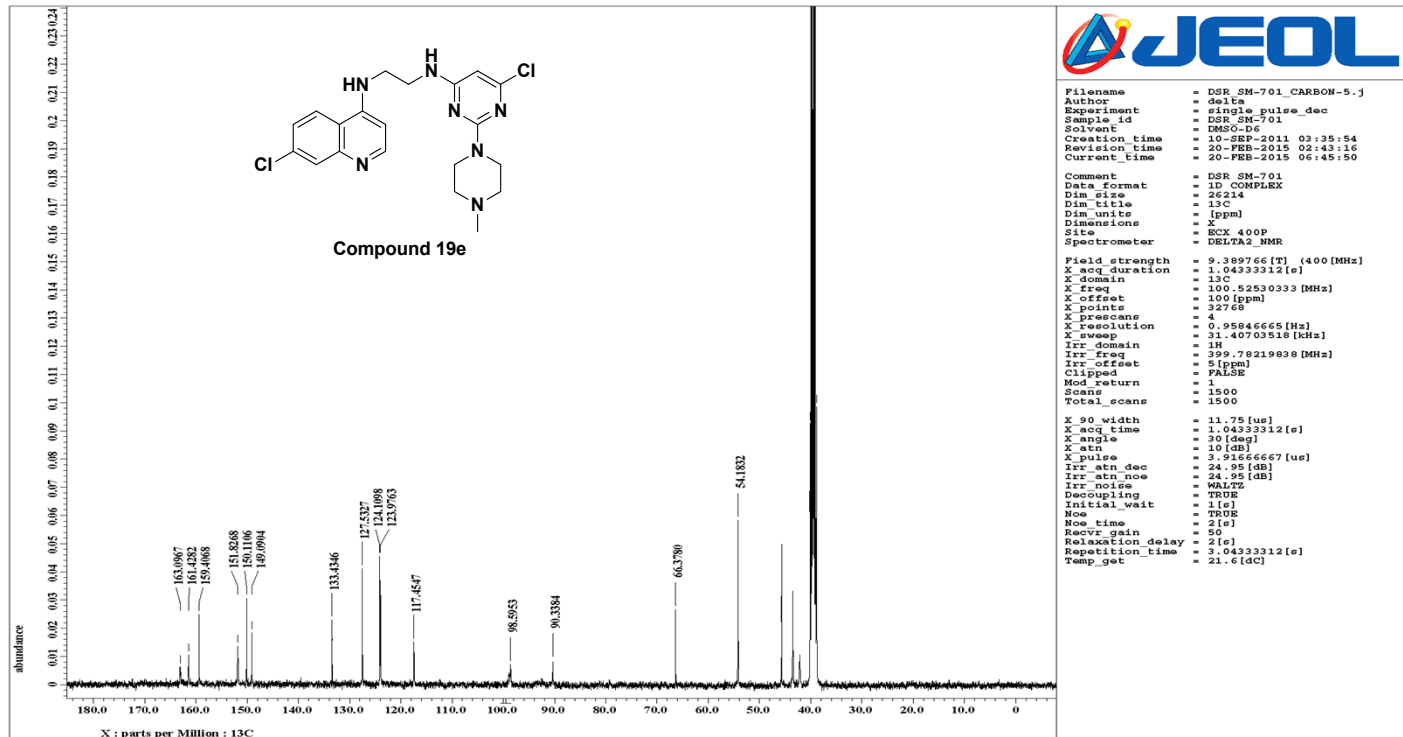


Fig 28: ¹³C NMR of compound 19e

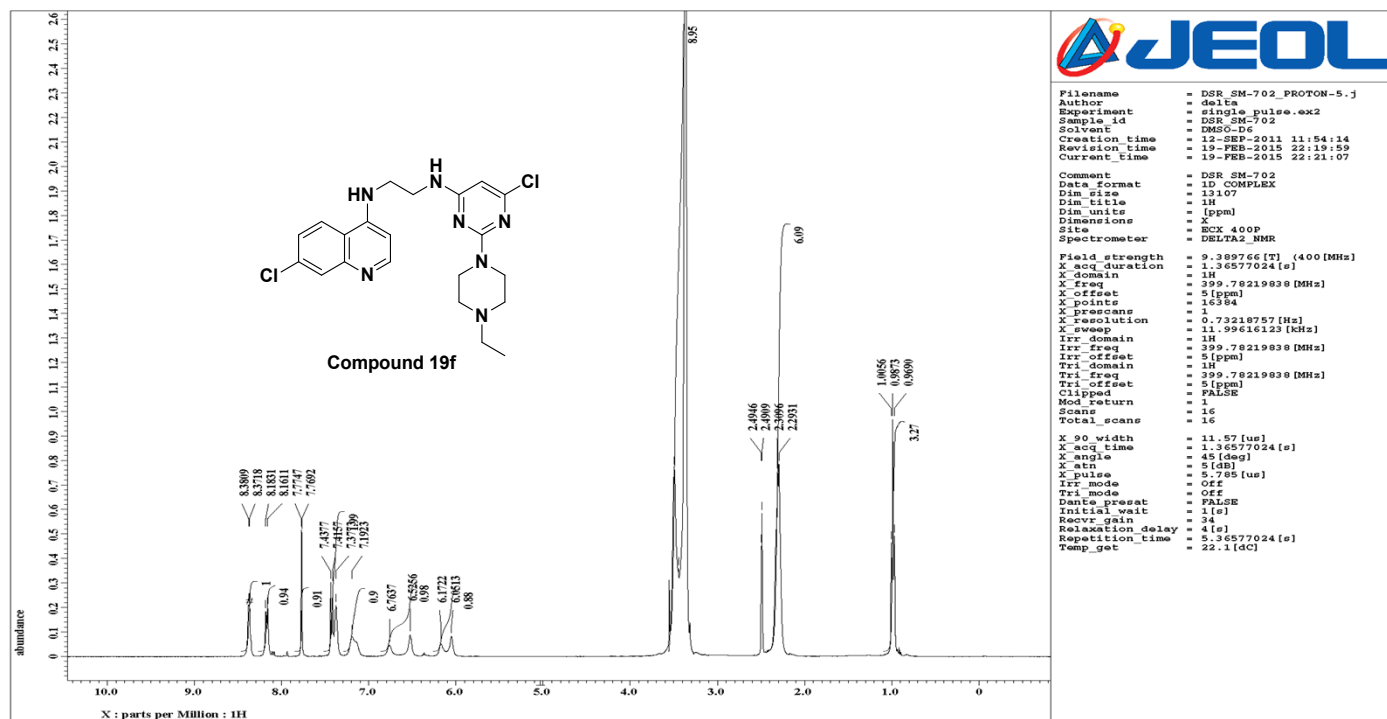


Fig 29: ¹H NMR of compound 19f

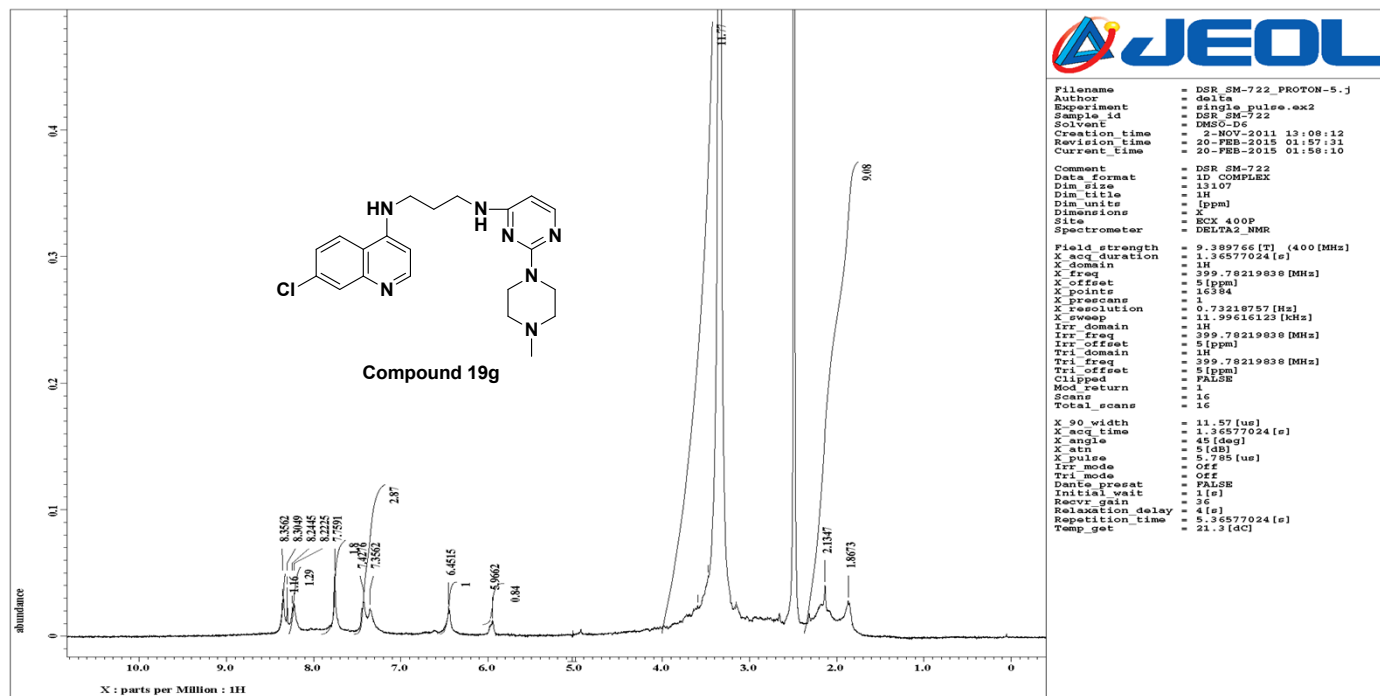


Fig 30: ¹H NMR of compound 19g

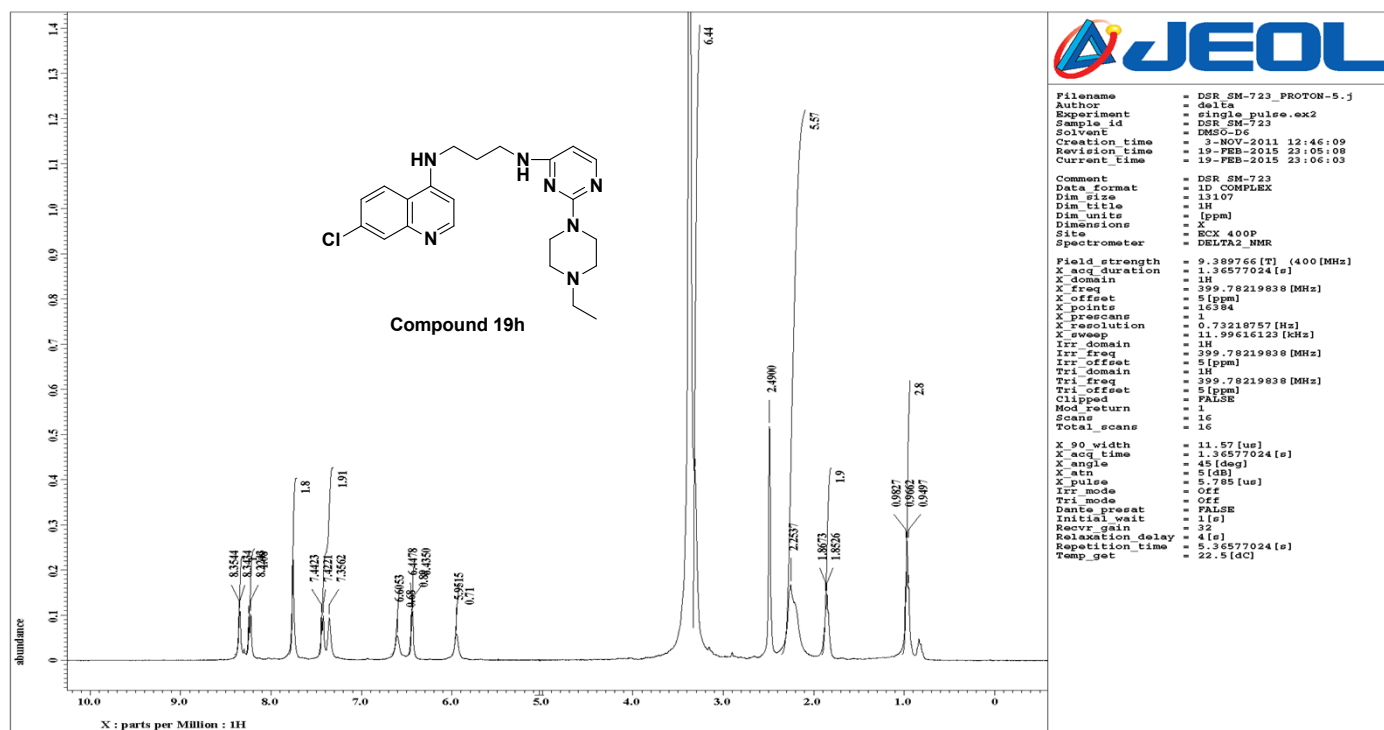


Fig 31: ¹H NMR of compound 19h

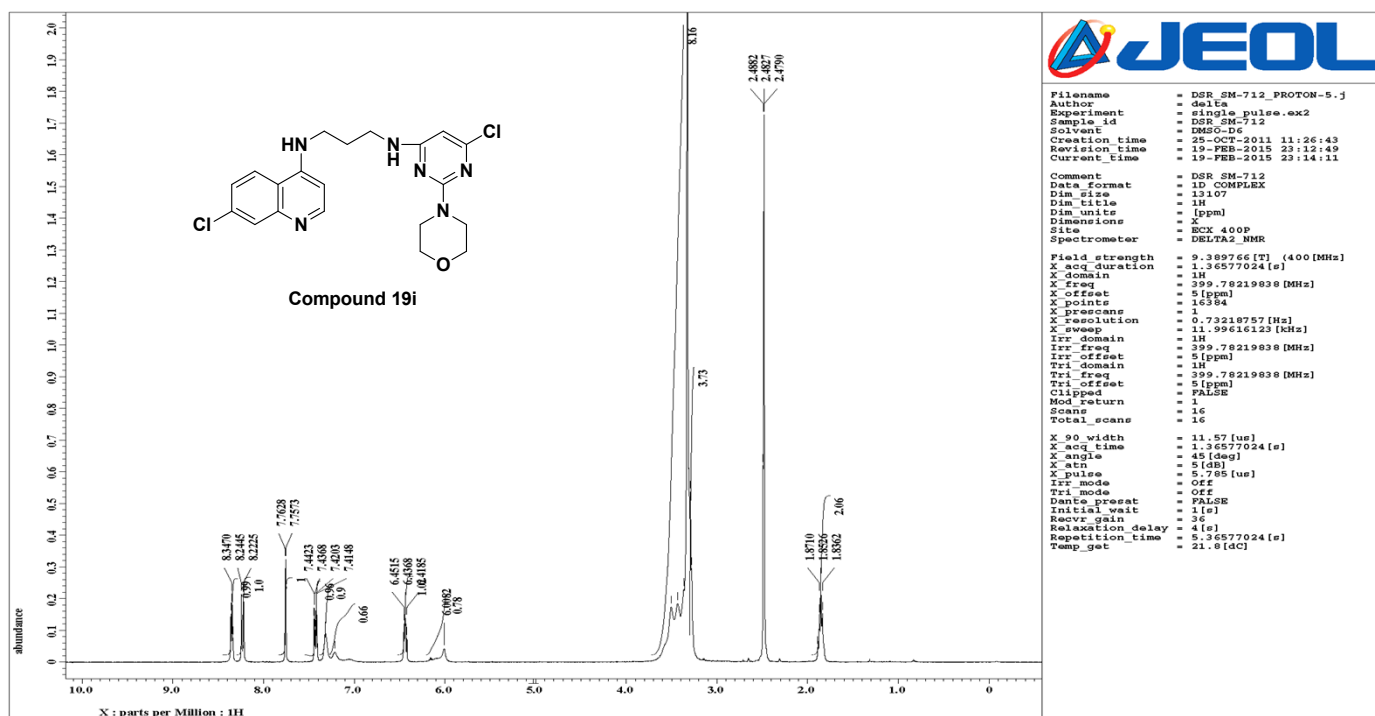


Fig 32: ¹H NMR of compound 19i

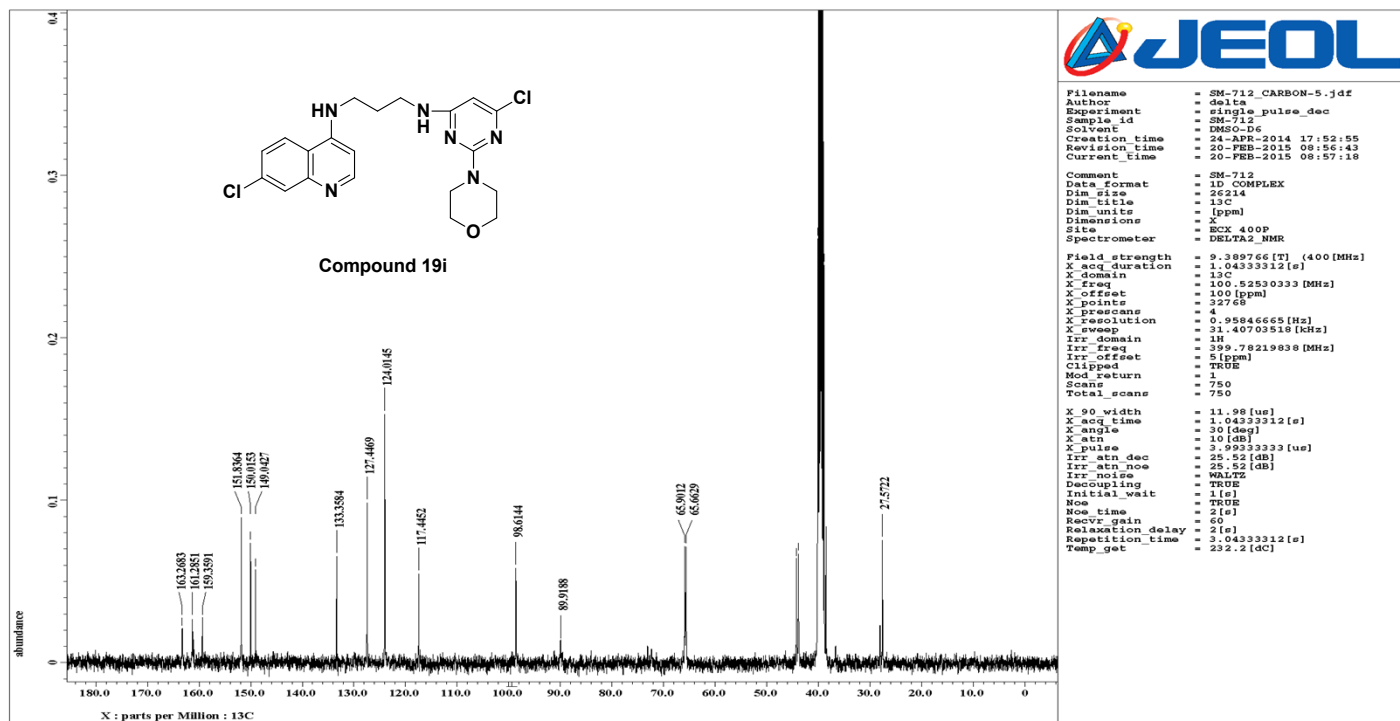


Fig 33: ¹³C NMR of compound 19i

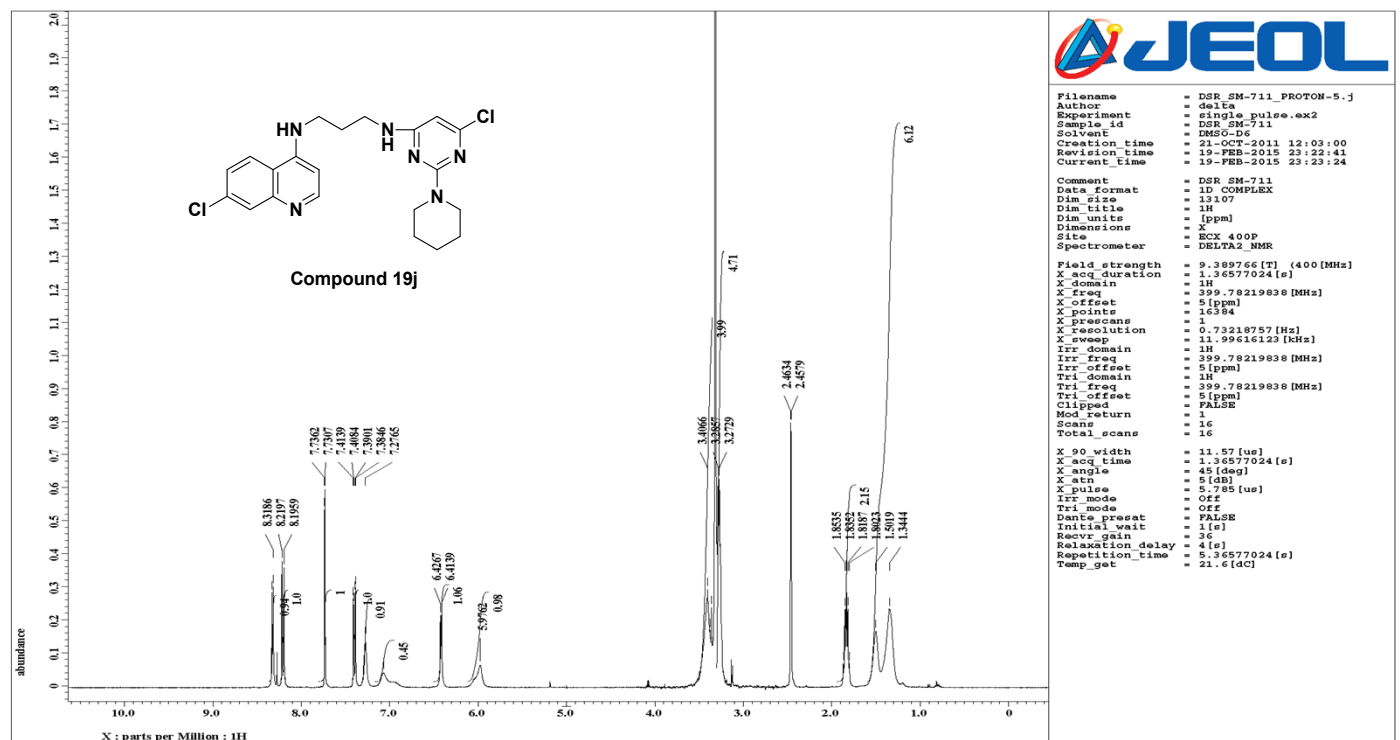


Fig 34: ¹H NMR of compound 19j

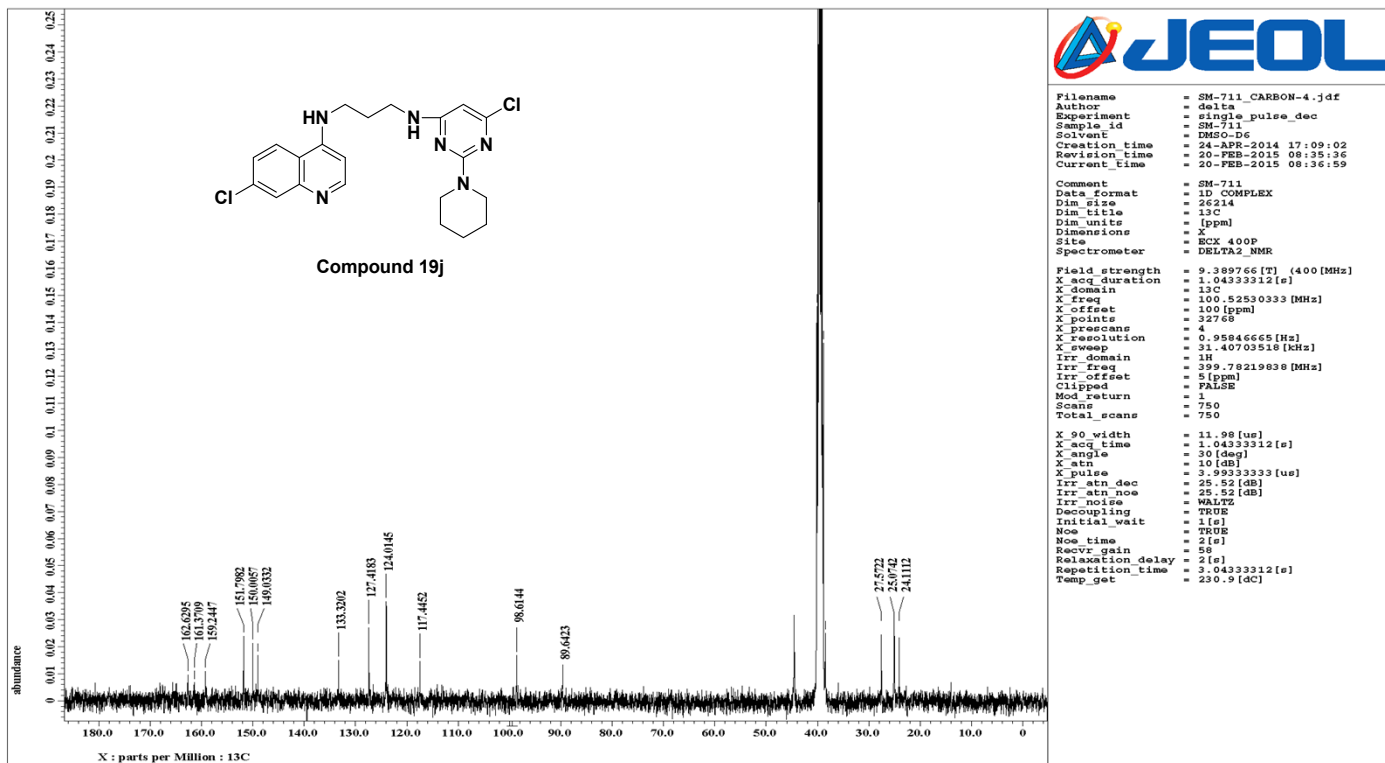


Fig 35: ¹³C NMR of compound 19j

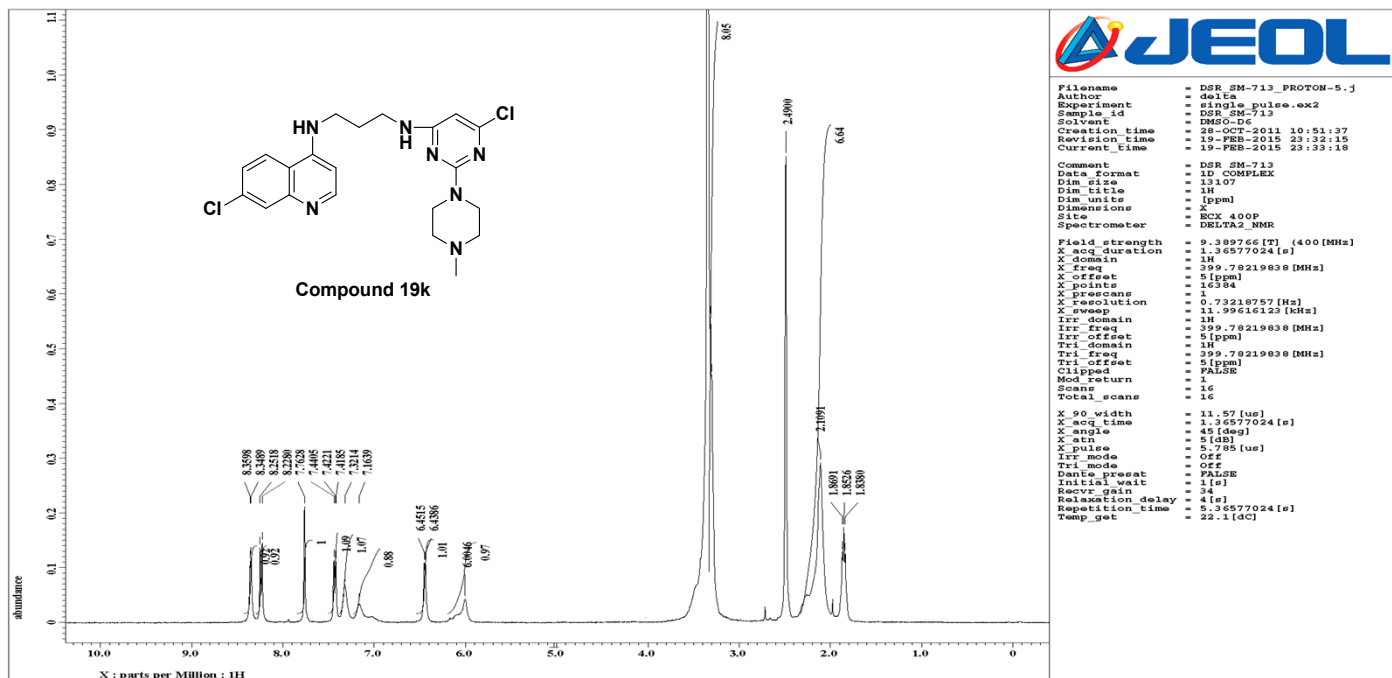


Fig 36: ¹H NMR of compound 19k

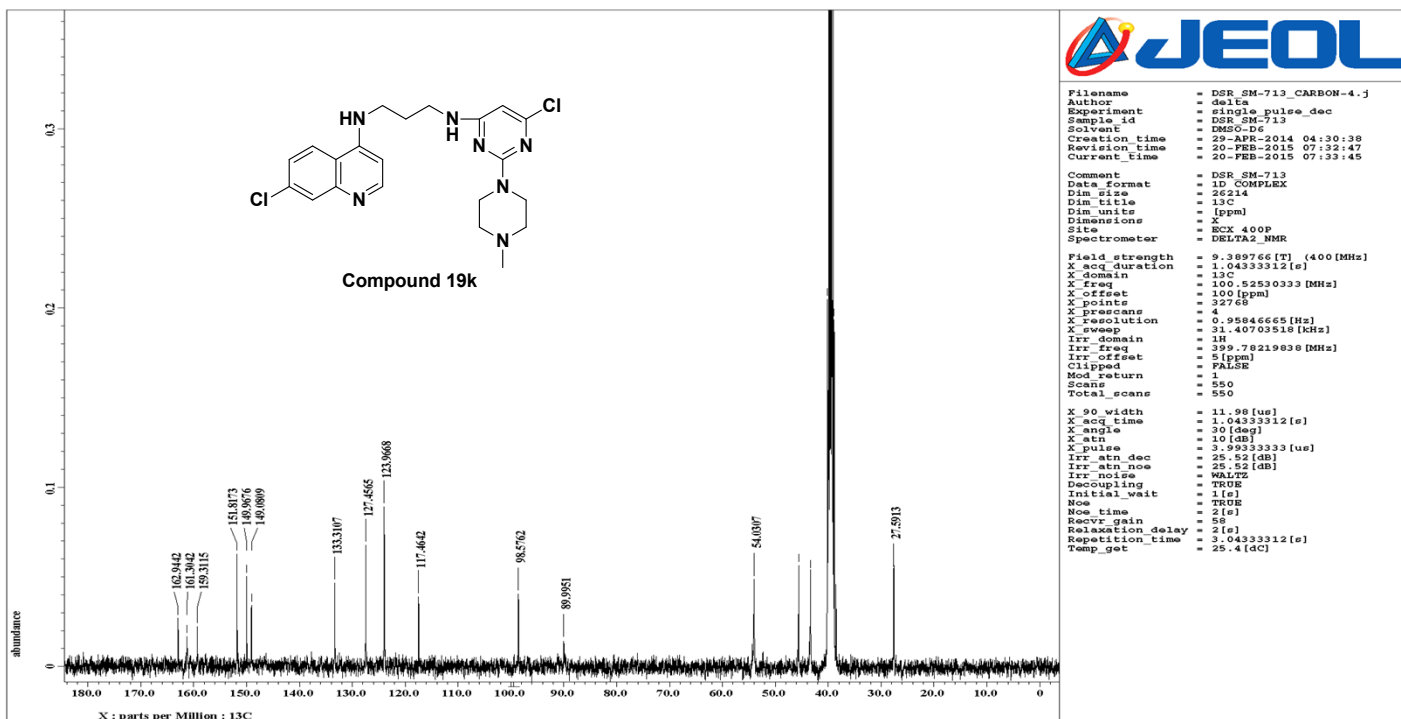


Fig 37: ¹³C NMR of compound 19k

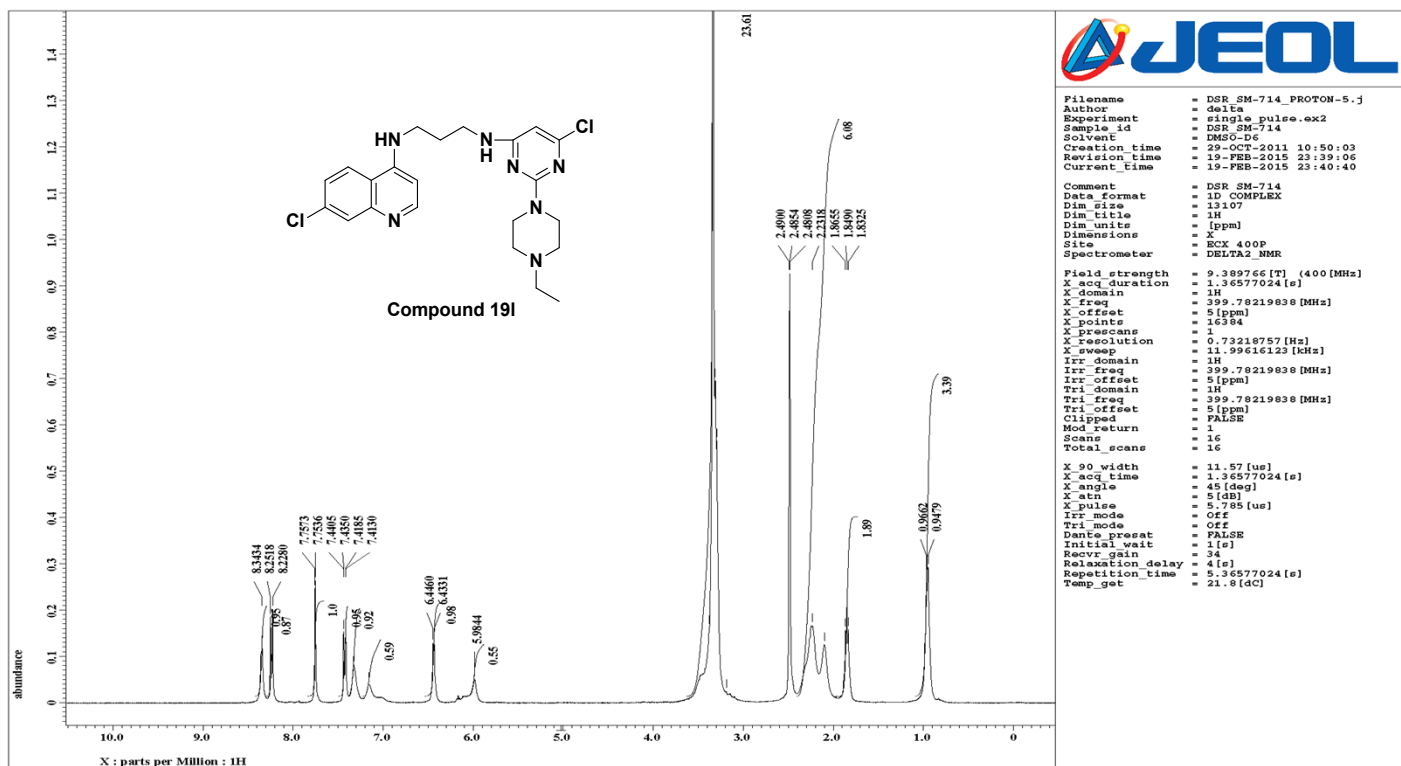


Fig 38: ¹H NMR of compound 19l

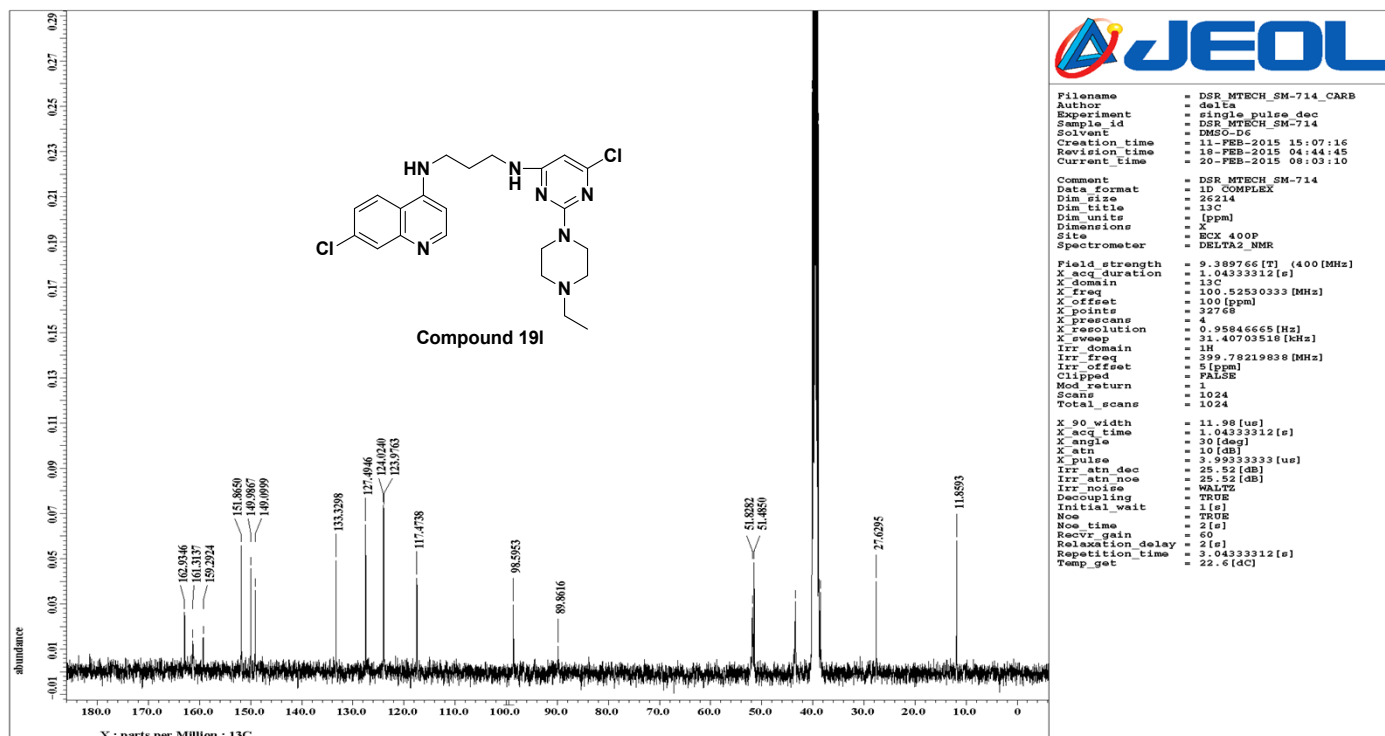


Fig 39: ¹³C NMR of compound 19l

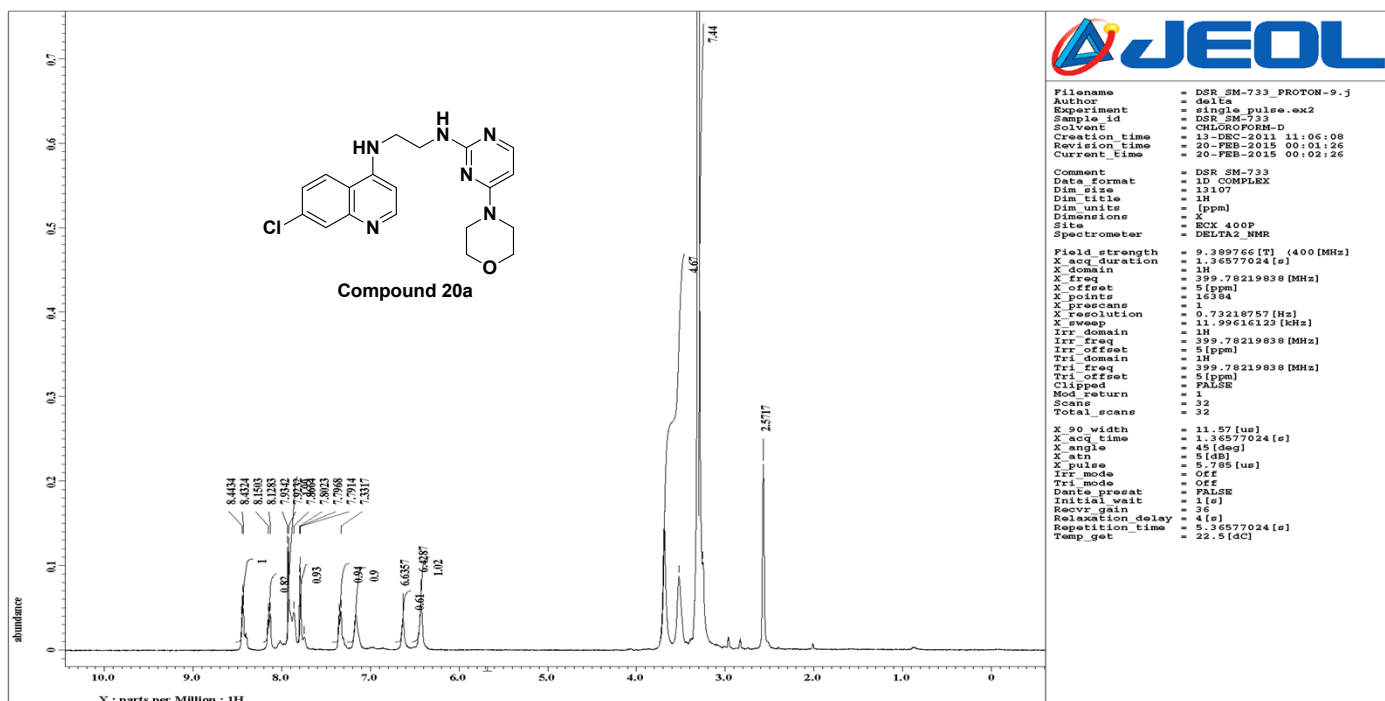


Fig 40: ¹H NMR of compound 20a

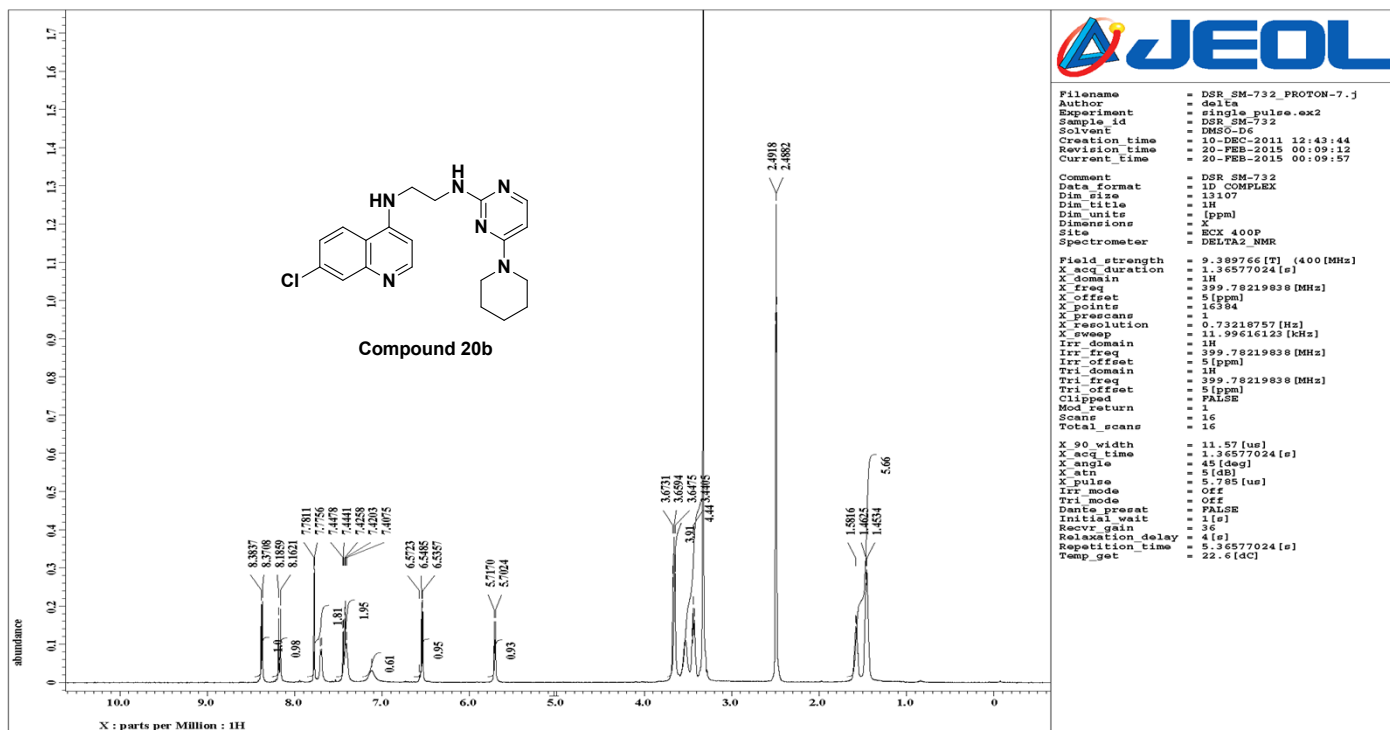


Fig 41: ¹H NMR of compound 20b

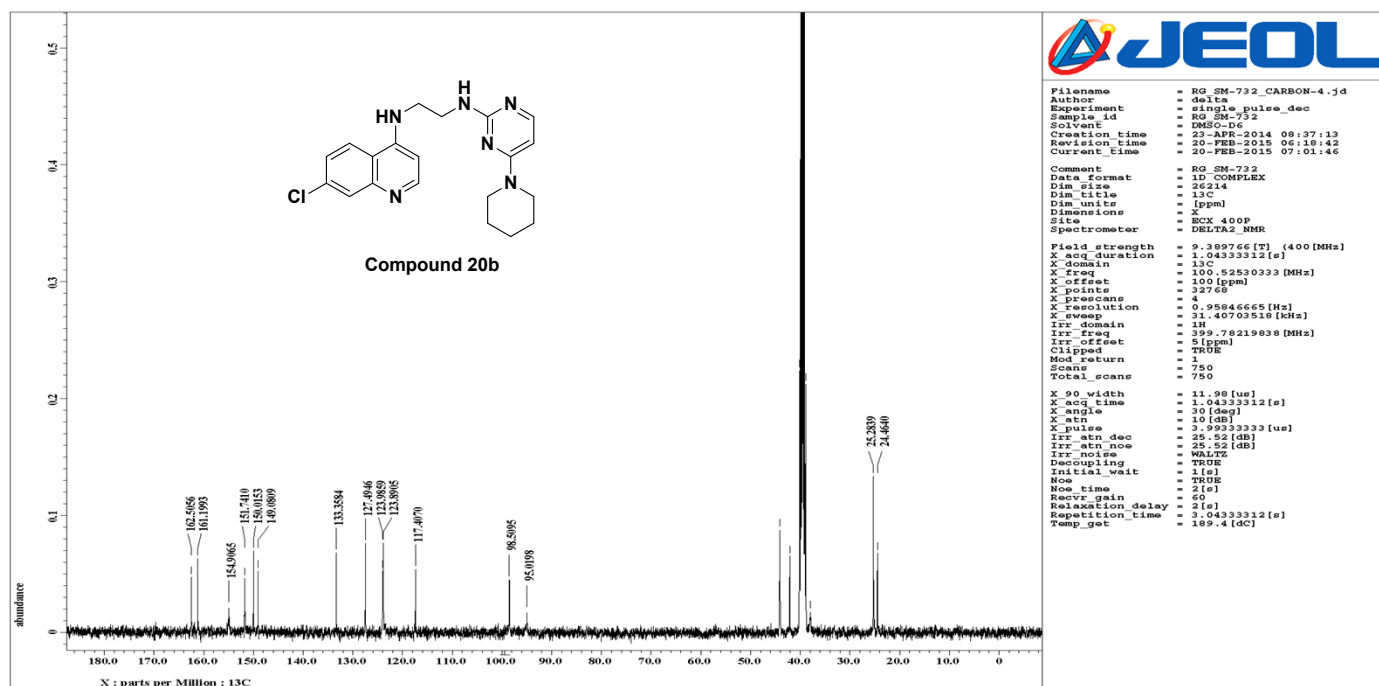


Fig 42: ¹³C NMR of compound 20b

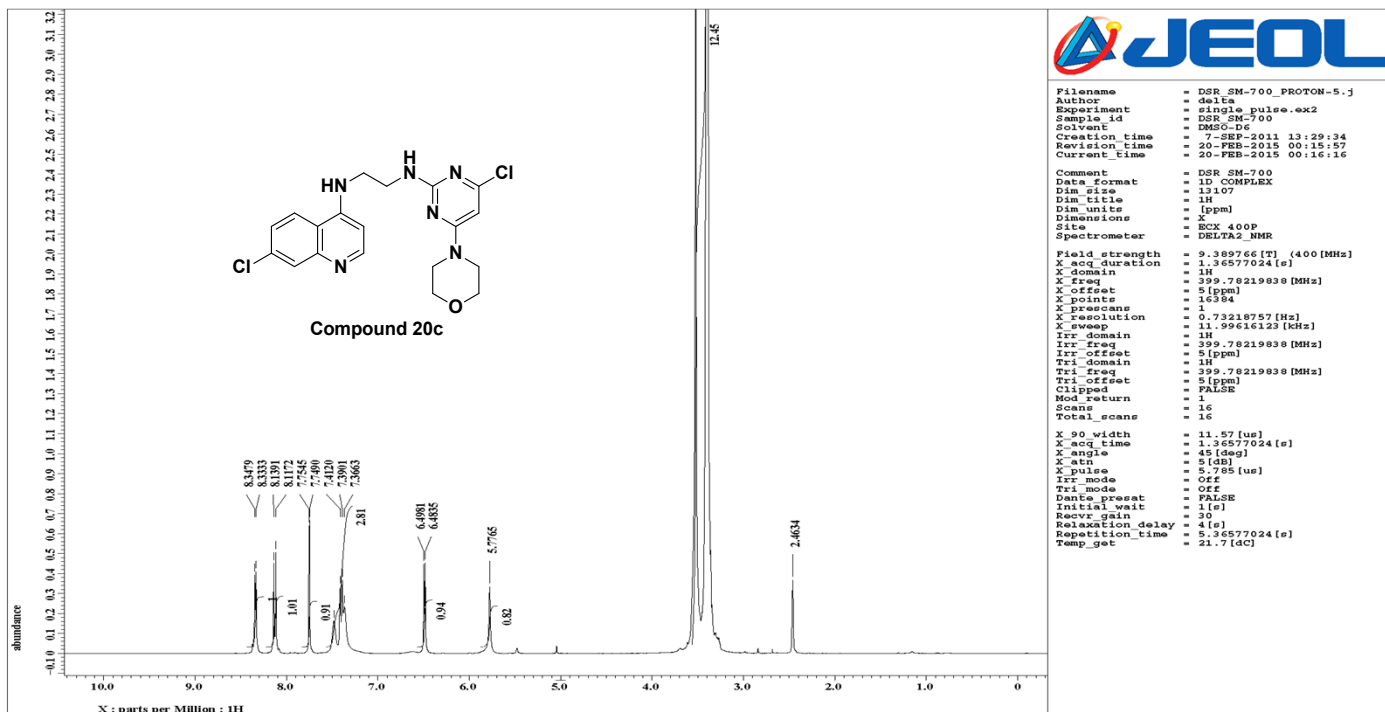


Fig 43: ¹H NMR of compound 20c

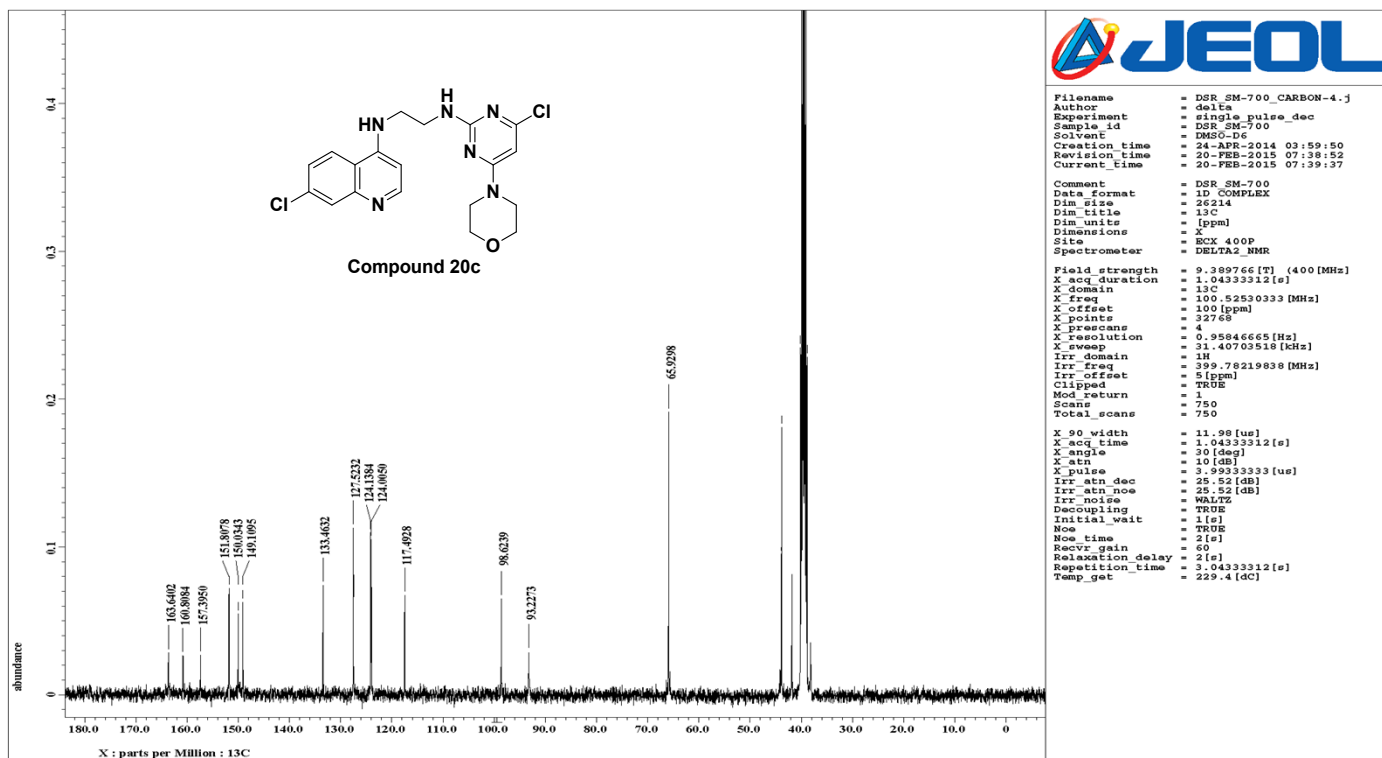


Fig 44: ¹³C NMR of compound 20c

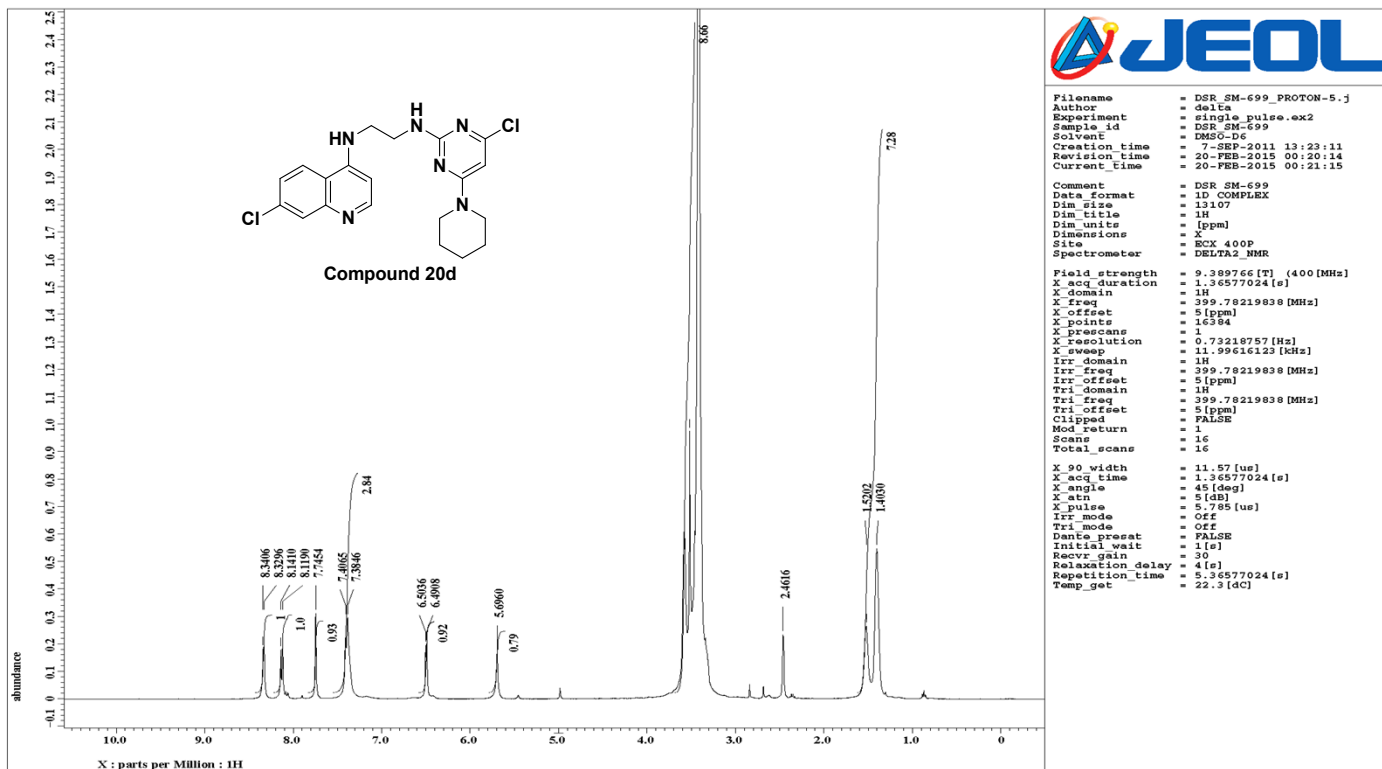


Fig 45: ¹H NMR of compound 20d

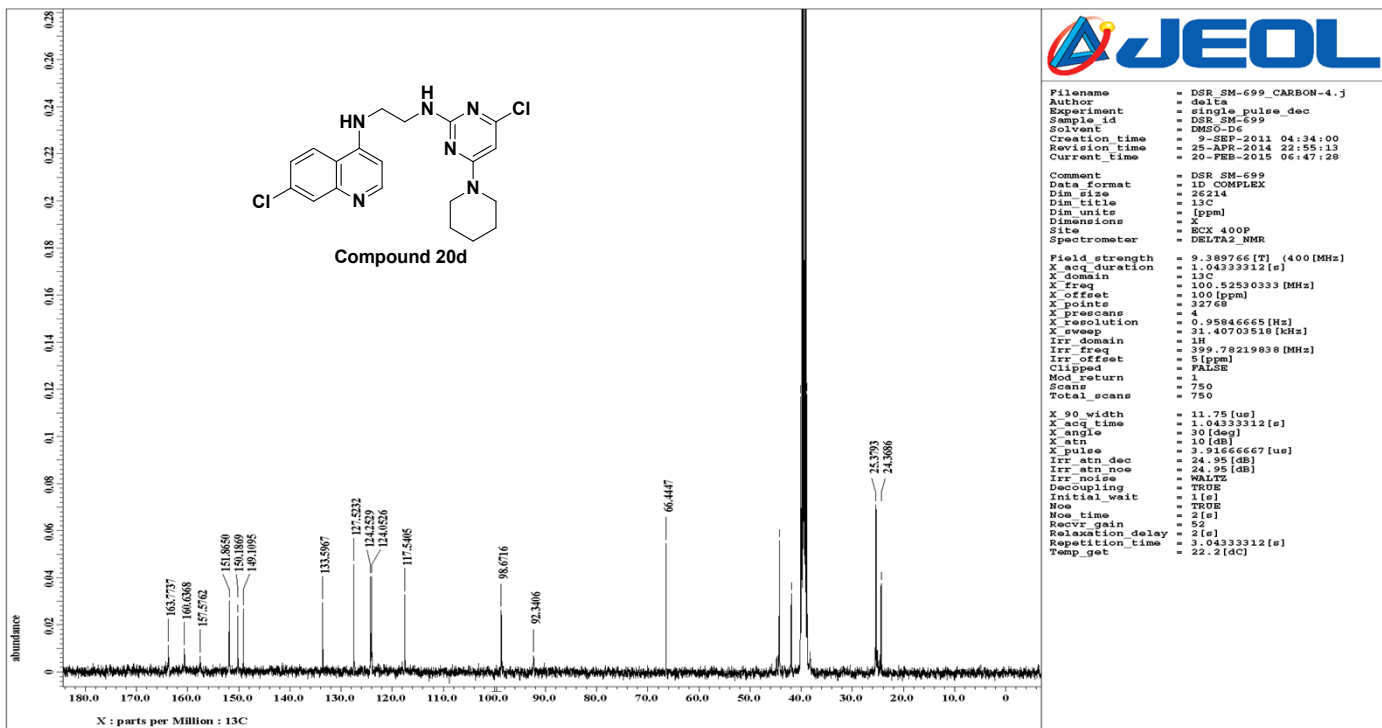


Fig 46: ¹³C NMR of compound 20d

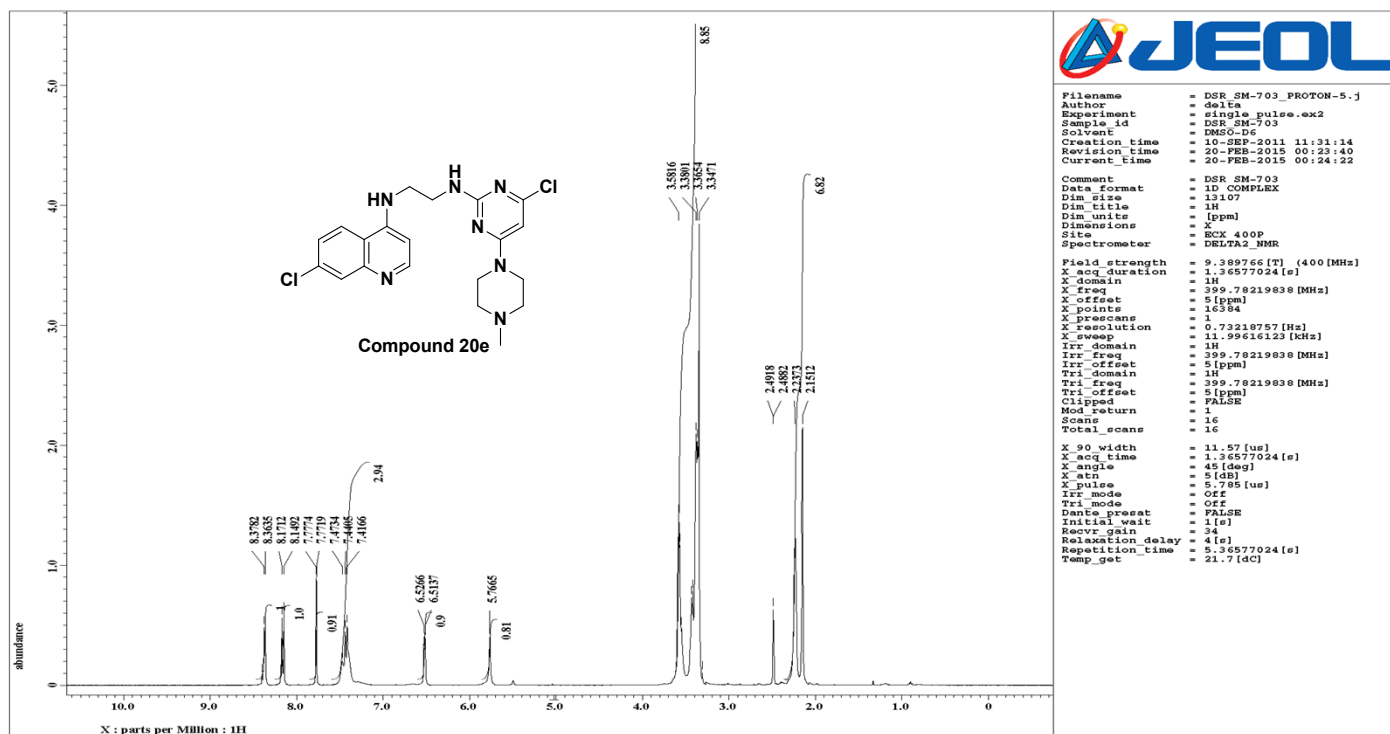


Fig 47: ¹H NMR of compound 20e

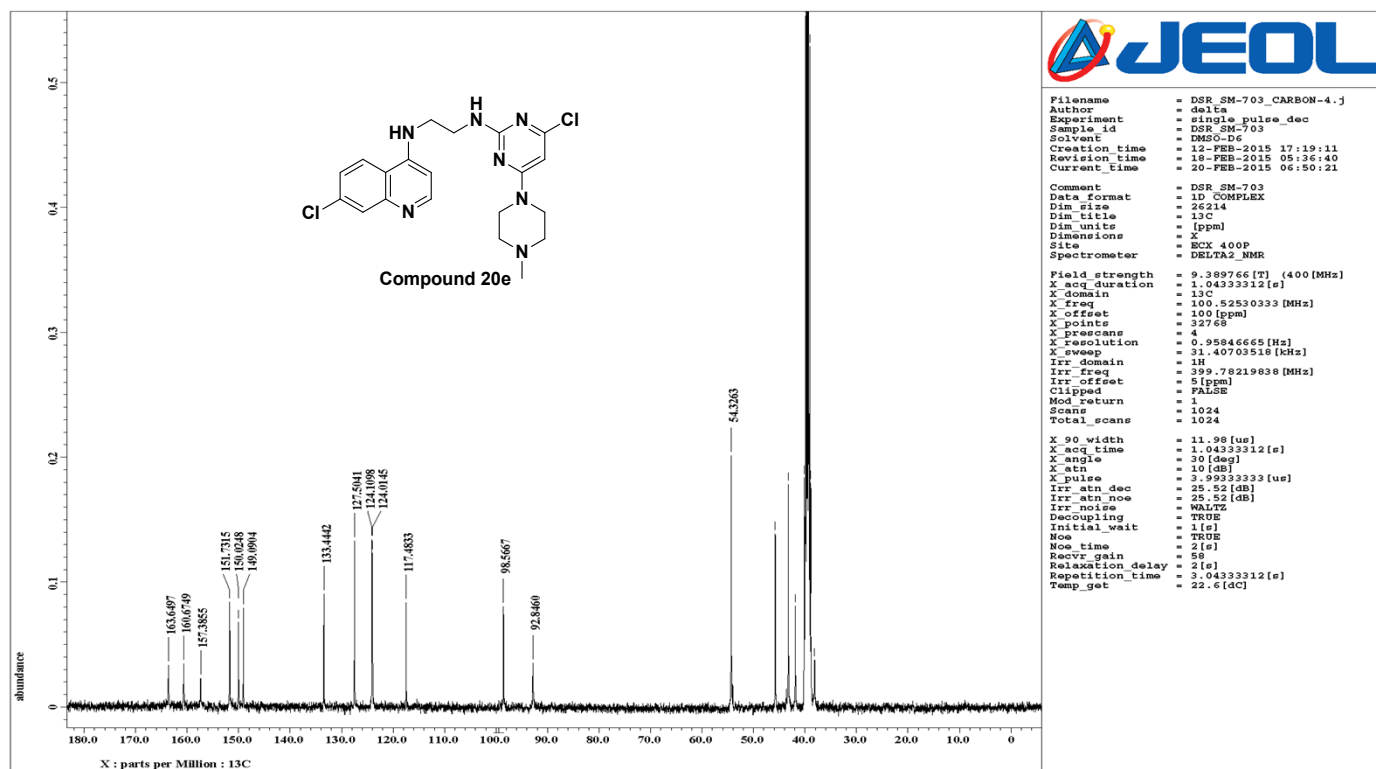


Fig 48: ¹³C NMR of compound 20e

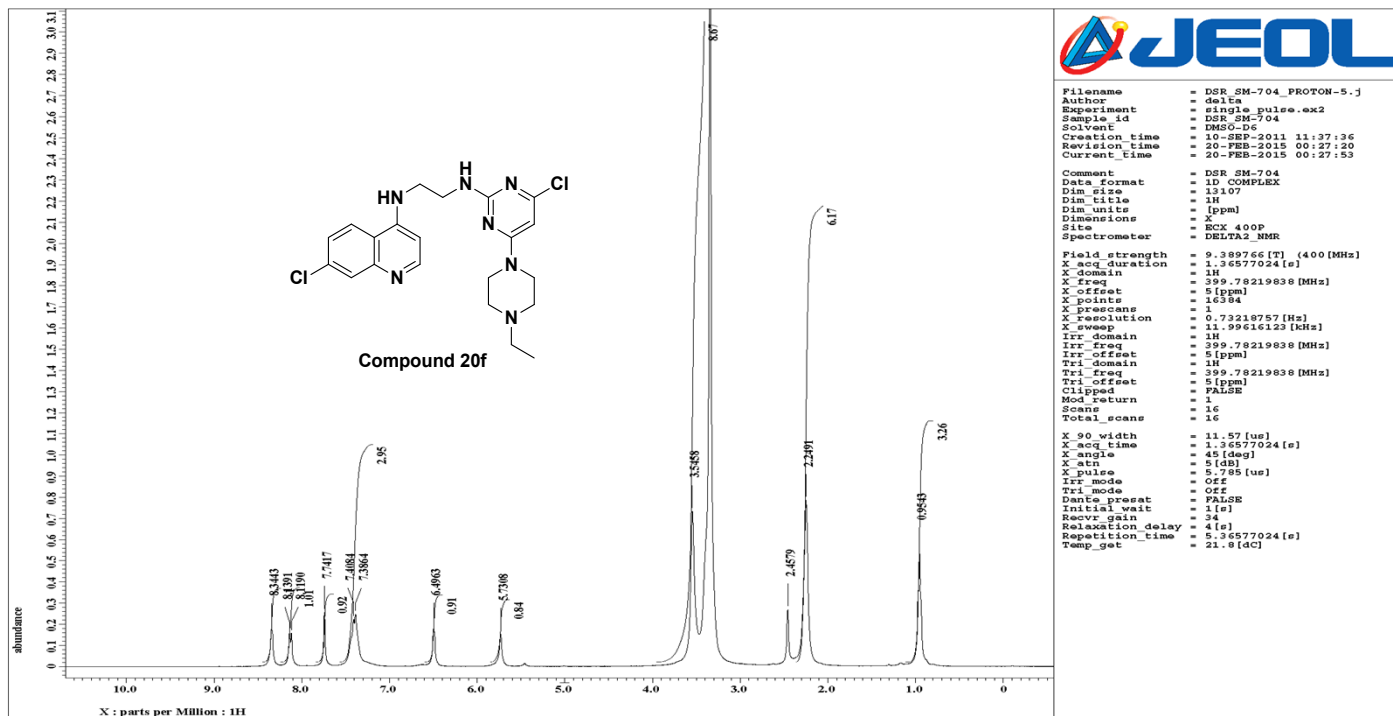


Fig 49: ¹H NMR of compound 20f

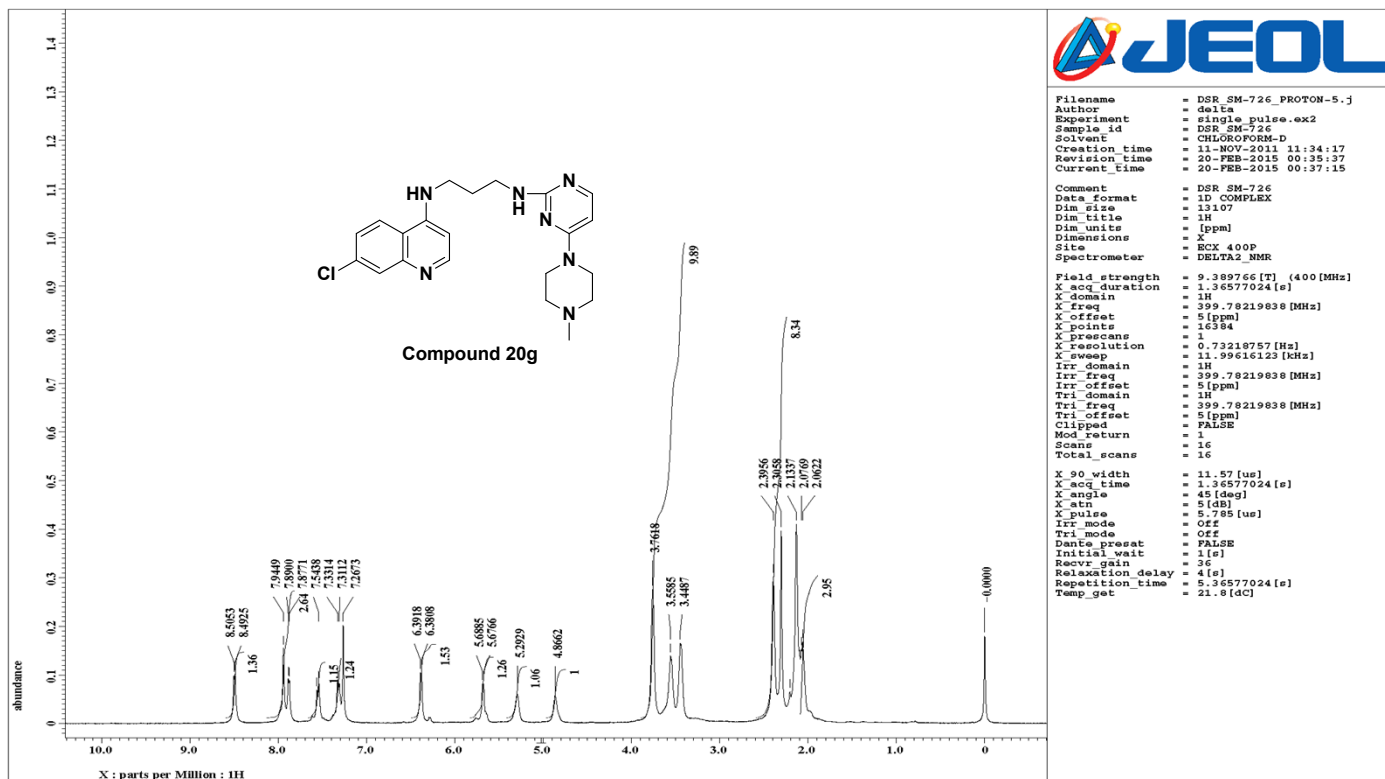


Fig 50: ¹H NMR of compound 20g

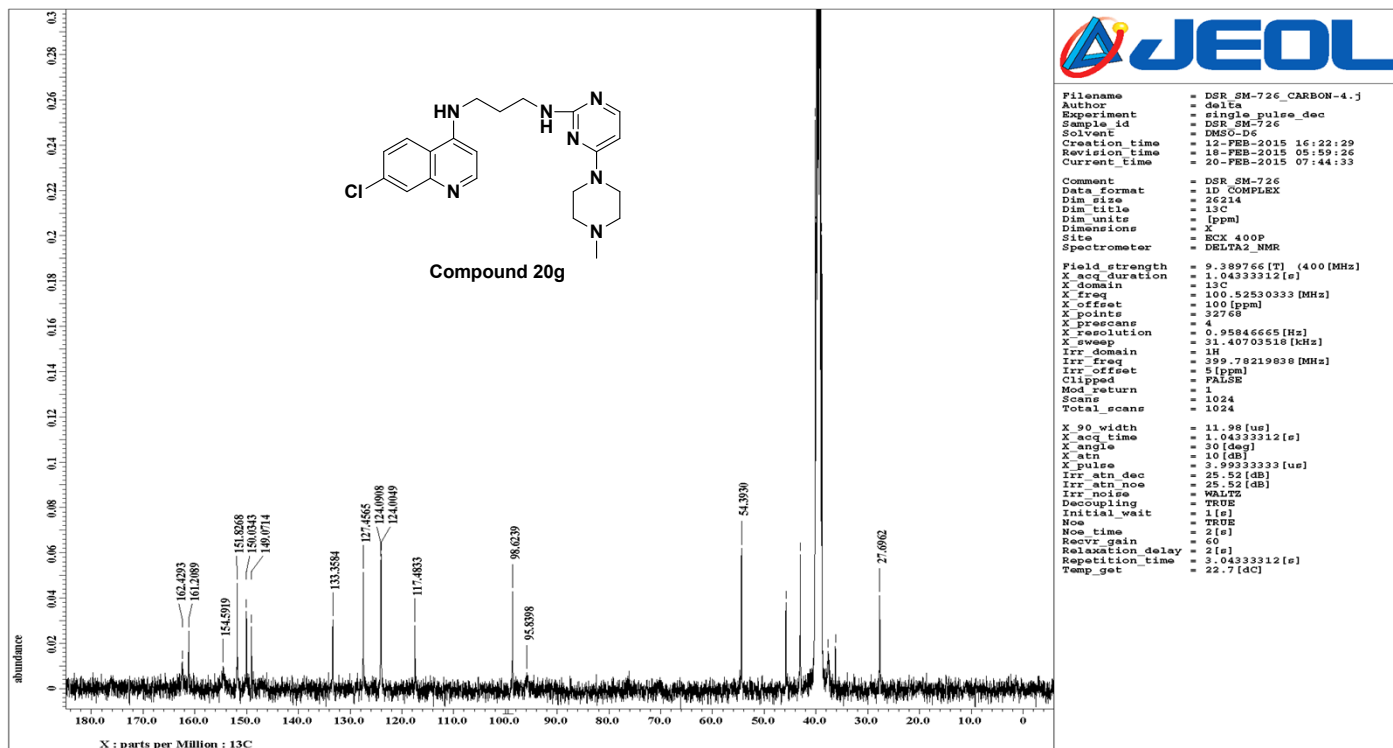


Fig 51: ¹³C NMR of compound 20g

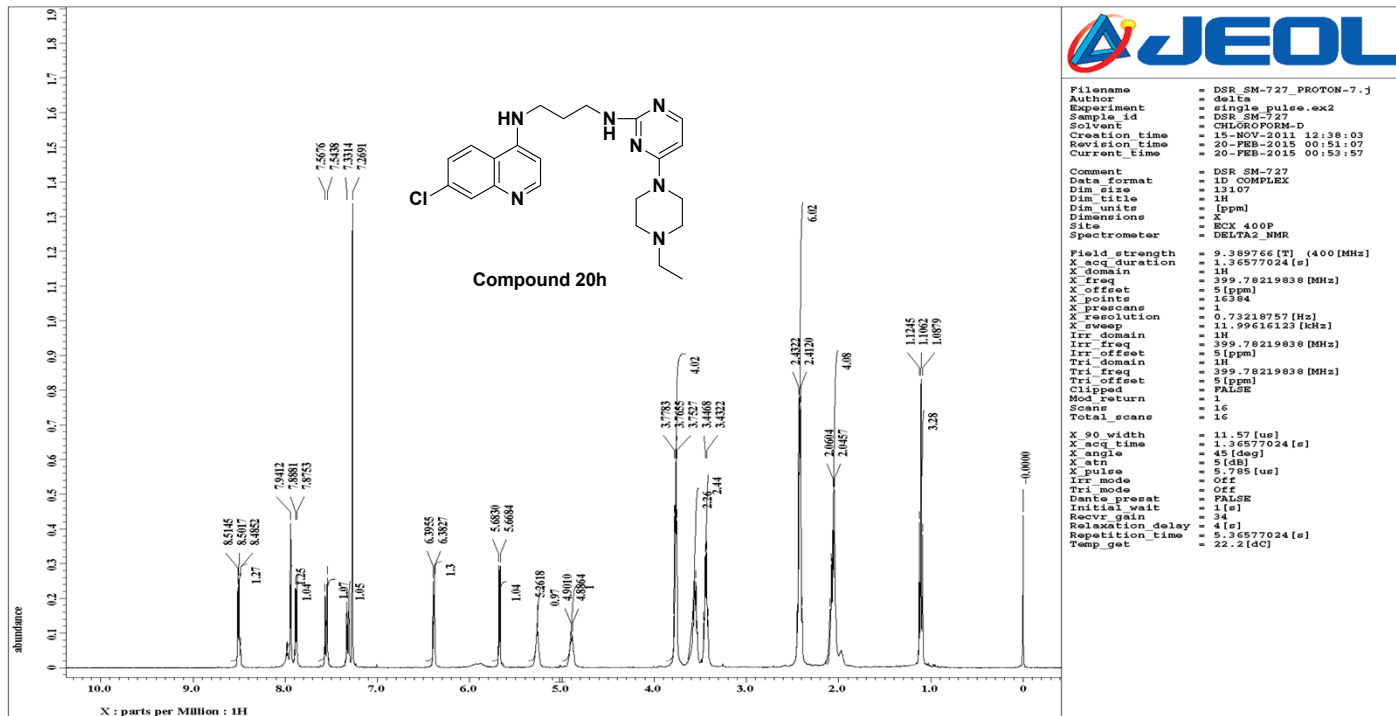


Fig 52: ¹H NMR of compound 20h

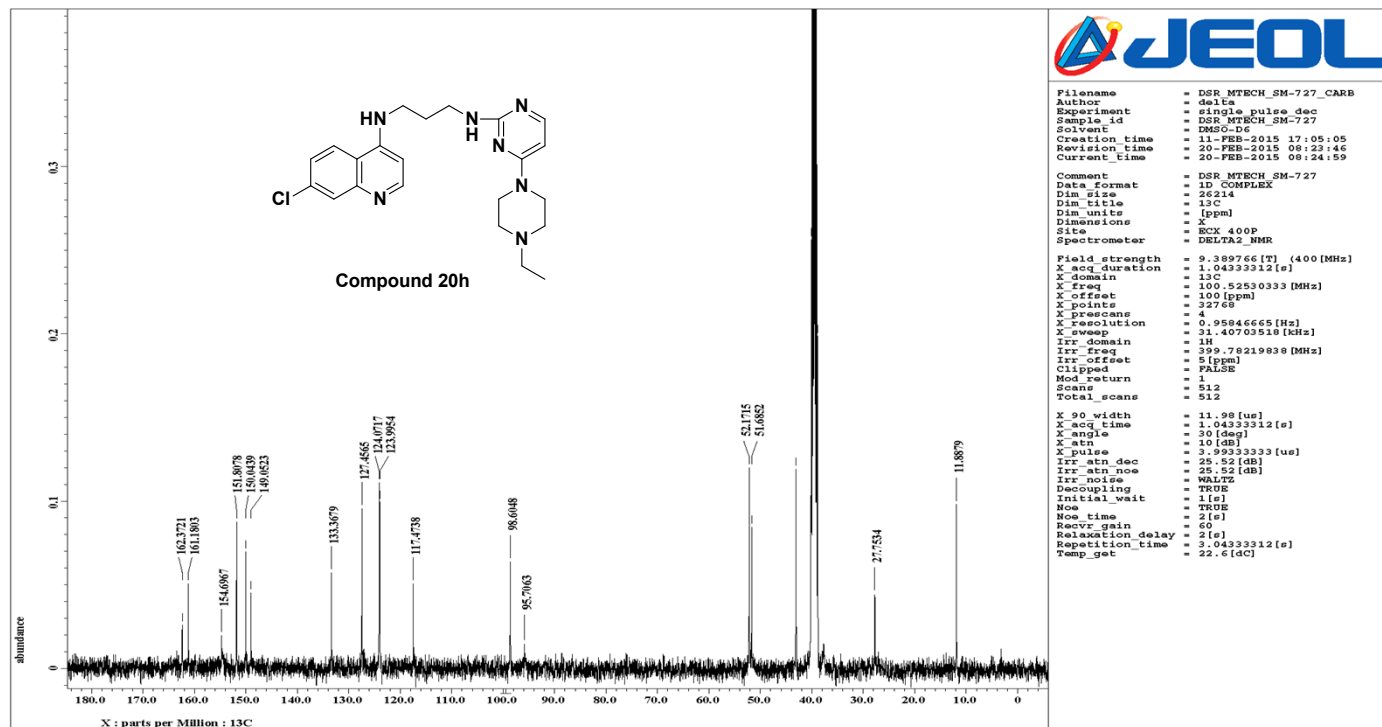


Fig 53: ¹³C NMR of compound 20h

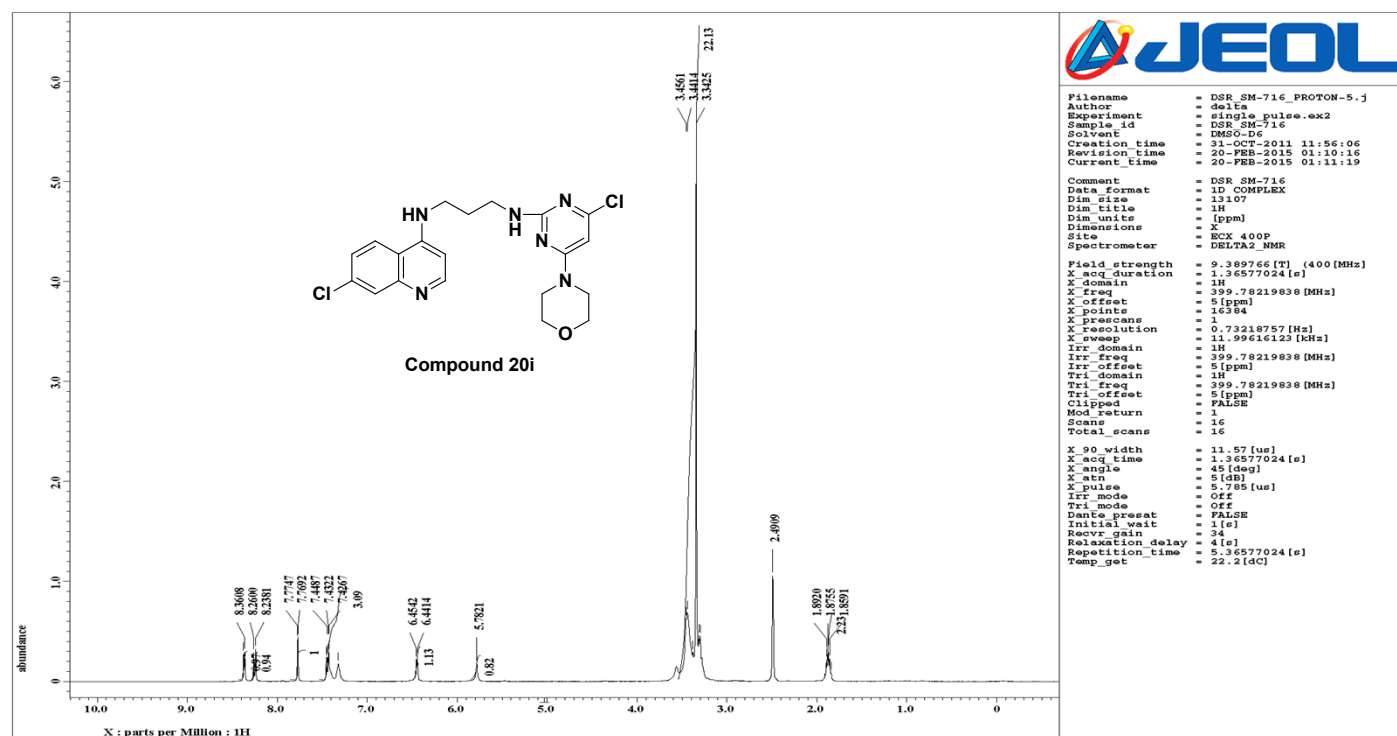


Fig 54: ¹H NMR of compound 20i

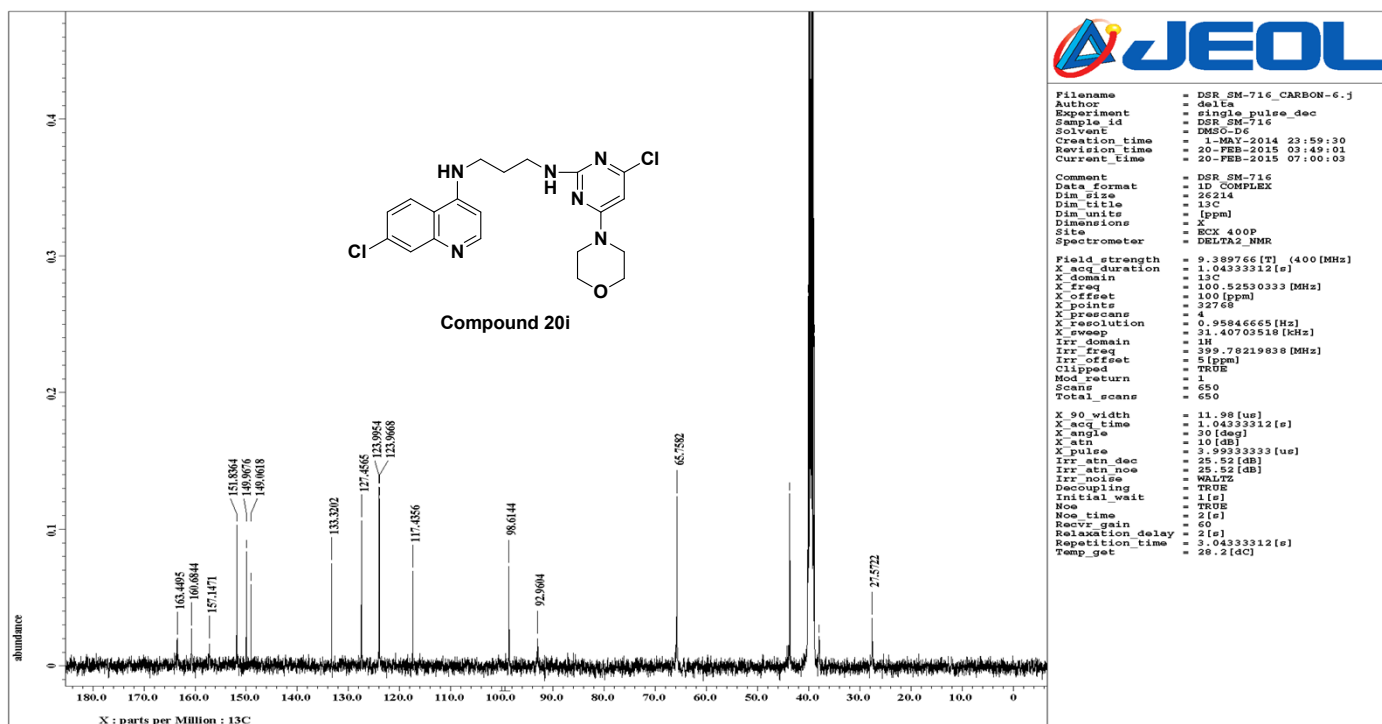


Fig 55: ^{13}C NMR of compound 20i

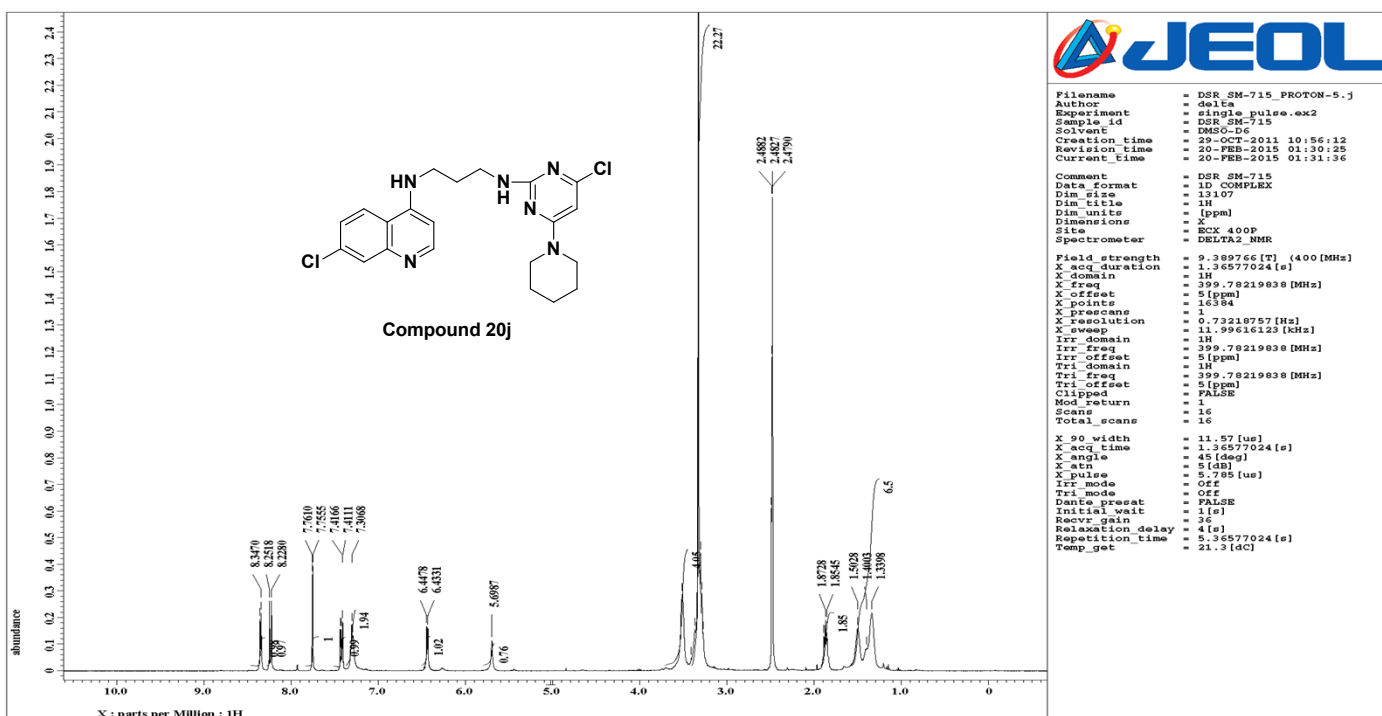


Fig 56: ^1H NMR of compound 20j

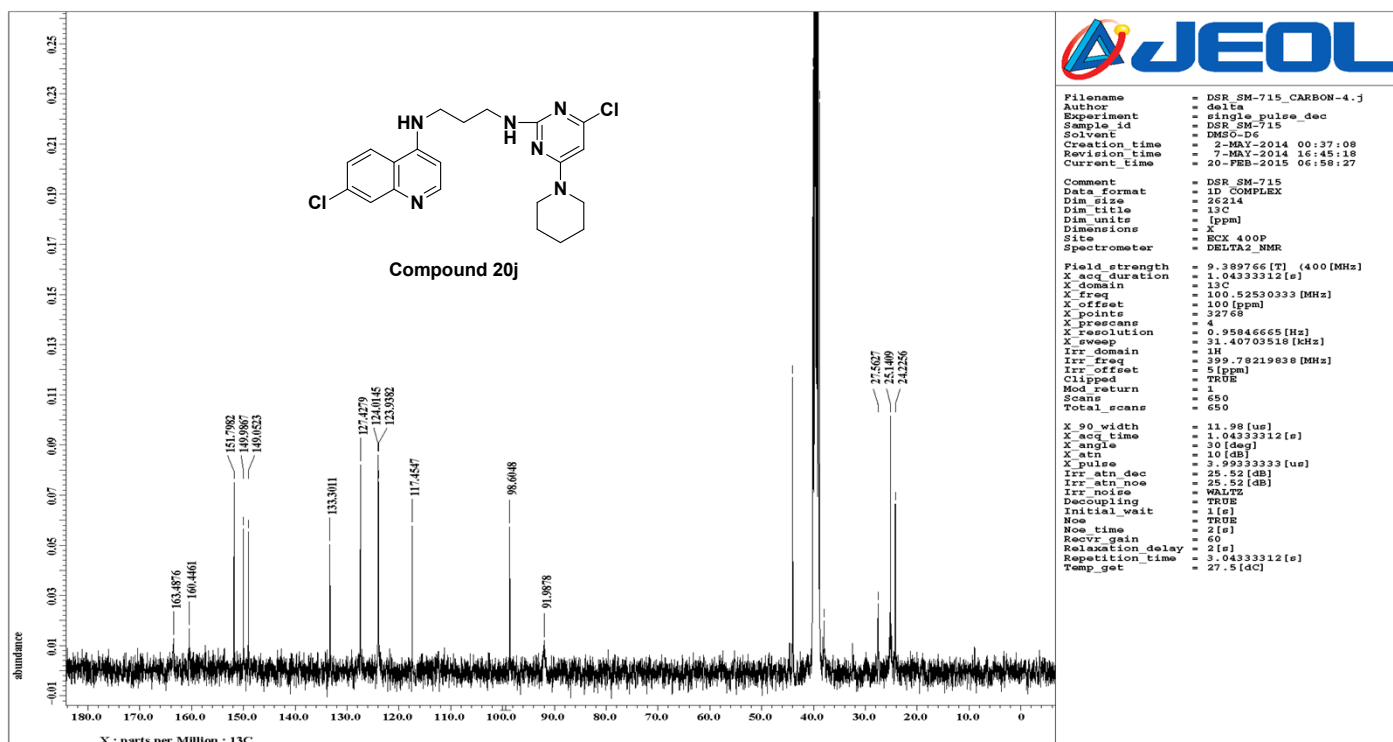


Fig 57: ¹³C NMR of compound 20j

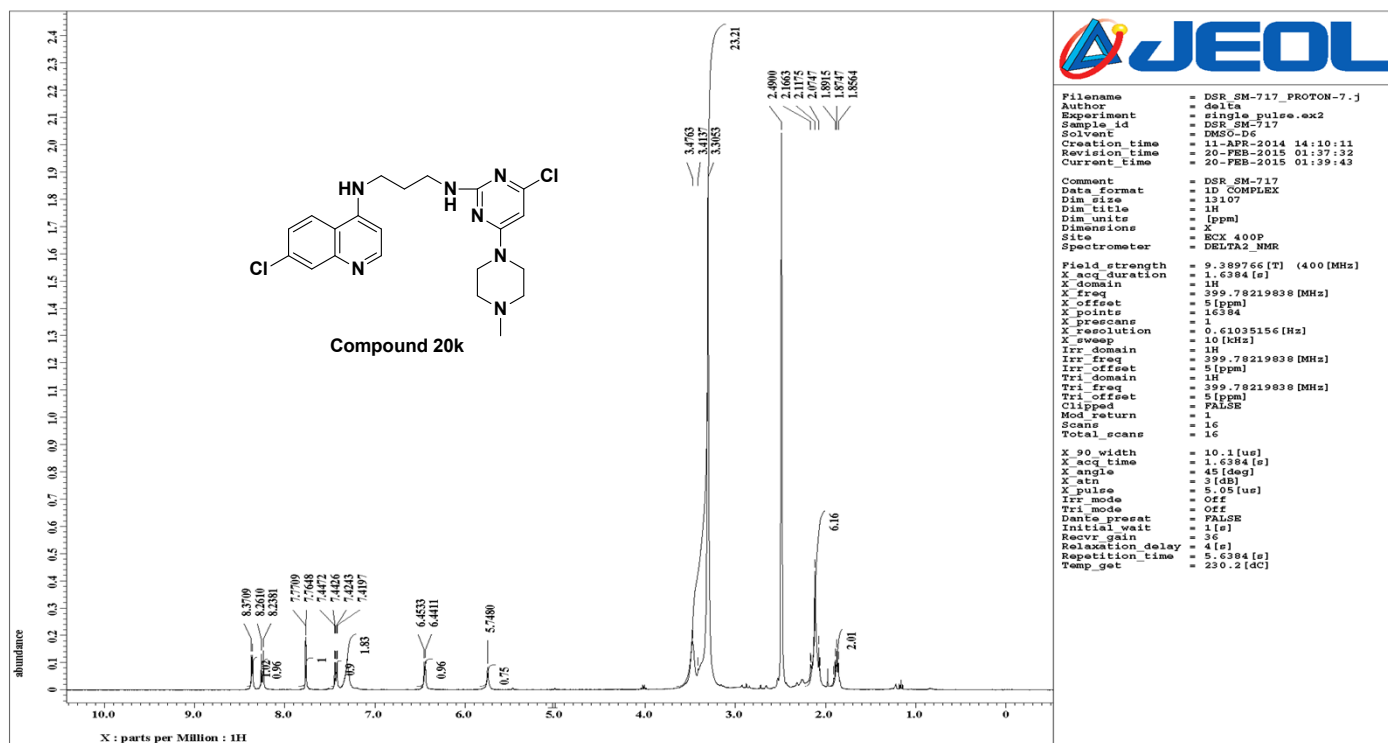


Fig 58: ¹H NMR of compound 20k

2. HRMS data of selected compounds:

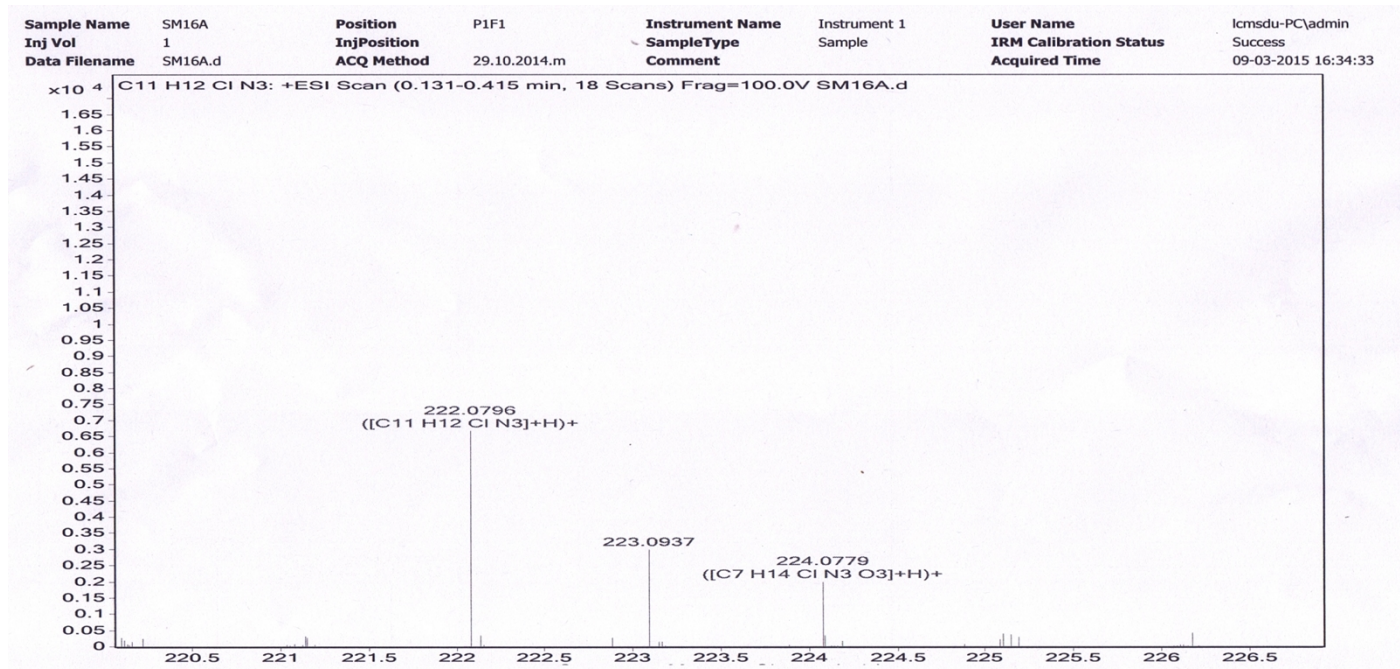


Fig 61: HRMS data of compound 16a

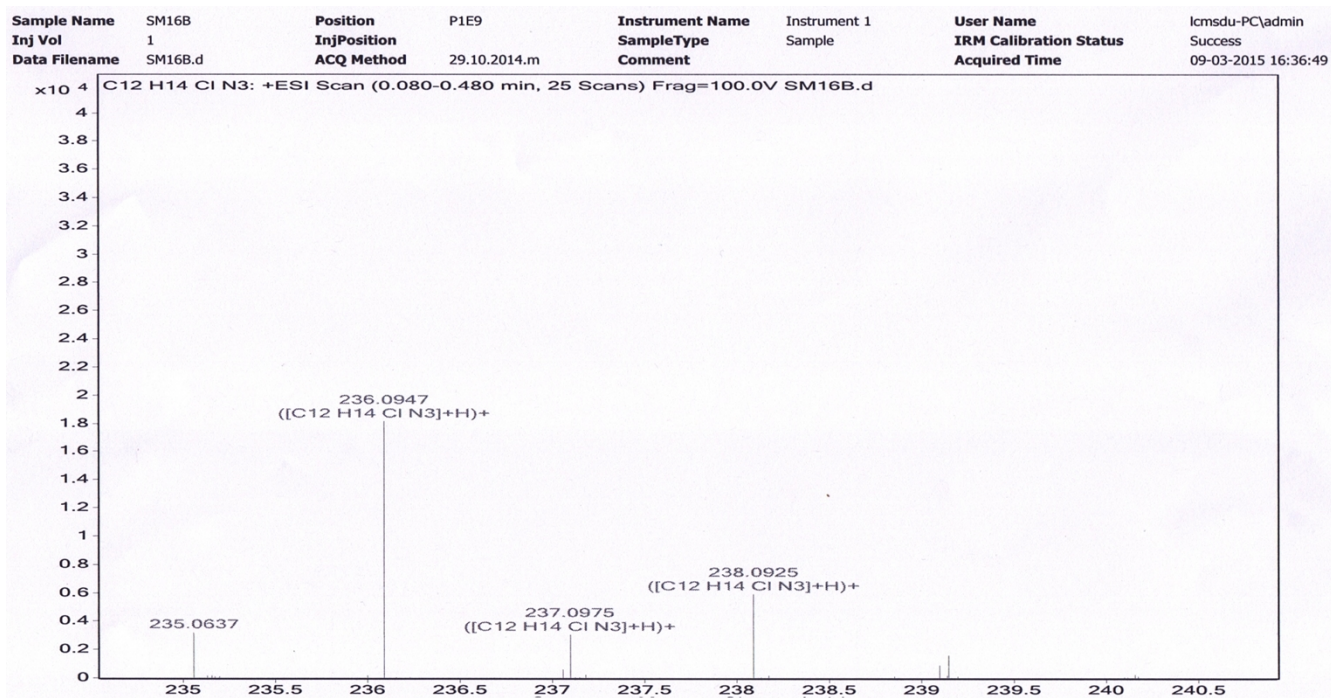


Fig 62: HRMS data of compound 16b

Qualitative Compound Report

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IRM Calibration Status	Success	DA Method	Default.m
Comment			

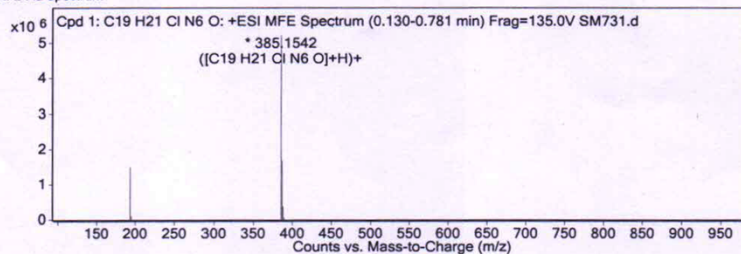
Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125)	

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C19 H21 Cl N6 O	0.225	384.1471	C19 H21 Cl N6 O	C19 H21 Cl N6 O	-1.38	C19 H21 Cl N6 O

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C19 H21 Cl N6 O	385.1542	0.225	Find by Molecular Feature	384.1471

MFE MS Spectrum



MFE MS Zoomed Spectrum

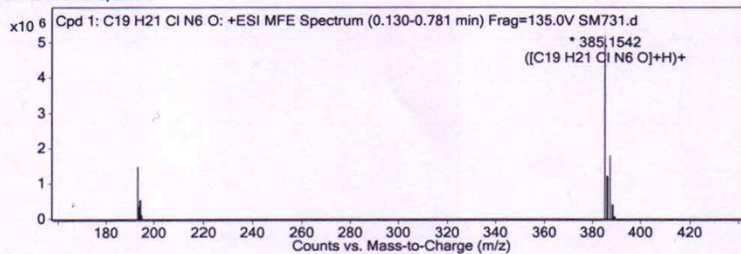


Fig 63: HRMS data of compound 19a

Qualitative Compound Report

Data File	SM-733.d	Sample Name	SM-733
Sample Type	Sample	Position	P2A7
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IRM Calibration Status	Success	DA Method	Default.m
Comment			

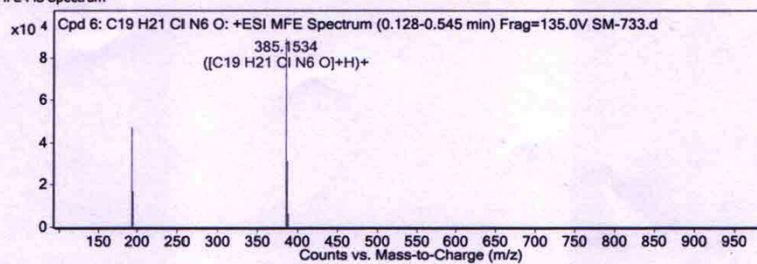
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125)		

Compound Table

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Compound Label	m/z	RT	Algorithm	Mass
Cpd 6: C19 H21 Cl N6 O	385.1534	0.228	Find by Molecular Feature	384.1462

MFE MS Spectrum



MFE MS Zoomed Spectrum

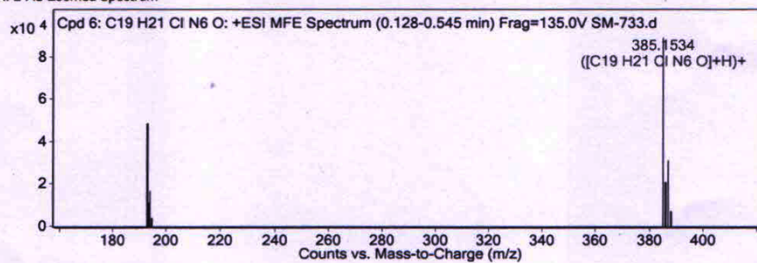


Fig 64: HRMS data of compound 20a

3. HPLC of selected compounds:

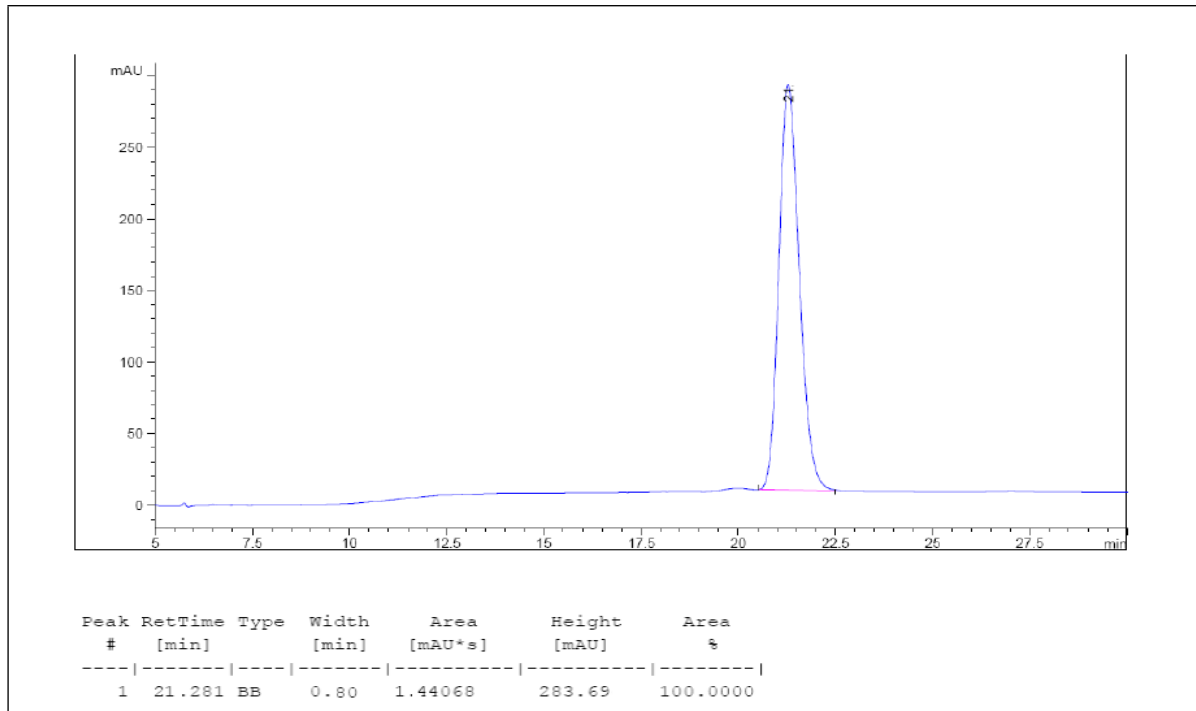


Fig 65: HPLC of compound 17d

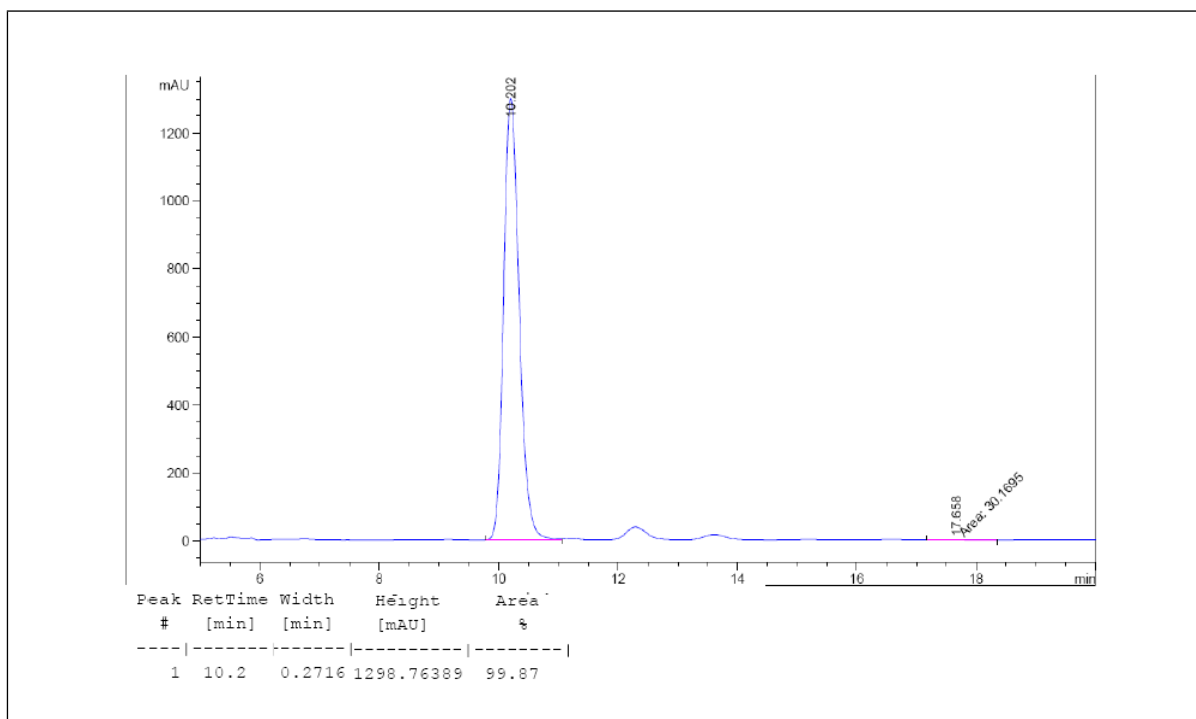


Fig 66: HPLC of compound 19i

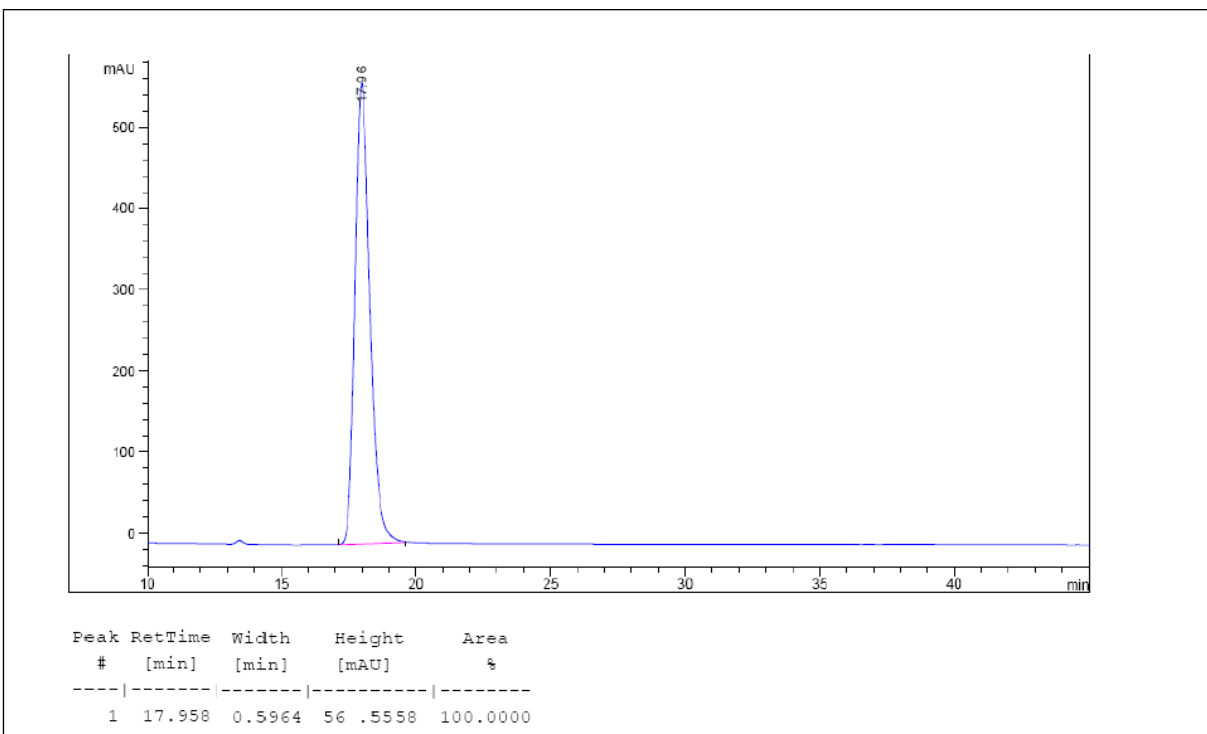


Fig 67: HPLC of compound 19j

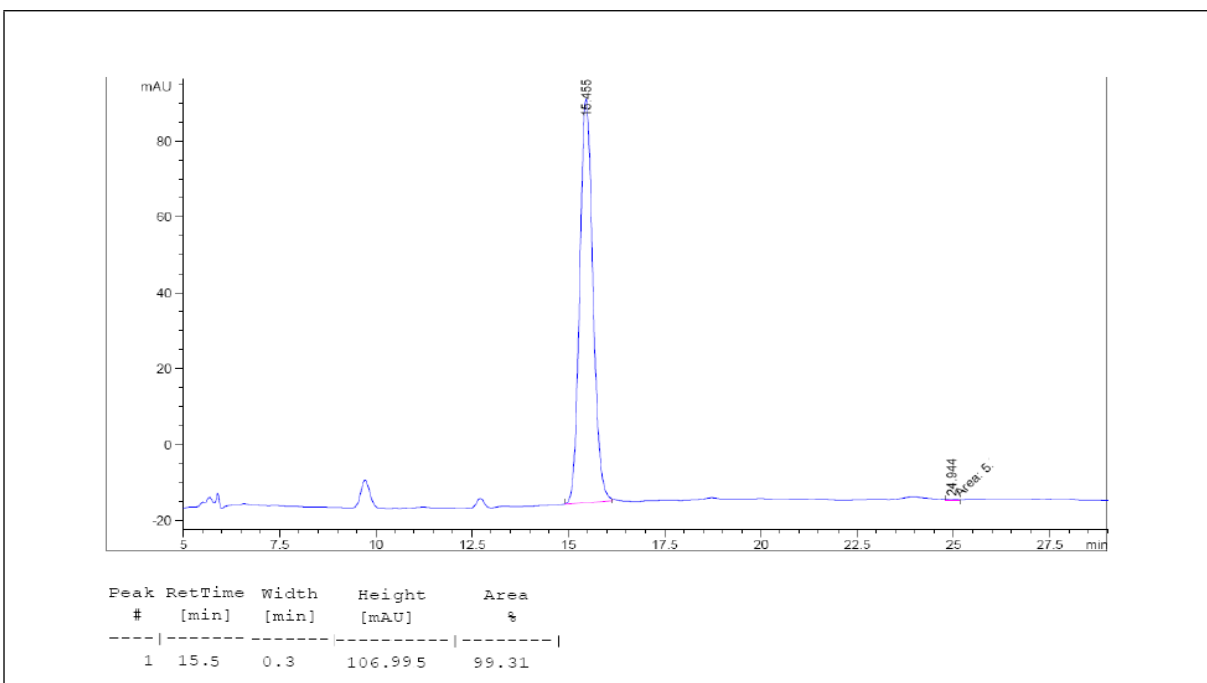


Fig 68: HPLC of compound 19k