

Unravelling the potency of 4,5-diamino-4H- 1,2,4 triazole-3-thiol derivatives for kinase inhibition through a rational approach

Supplementary Information

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Mass Spectrometry

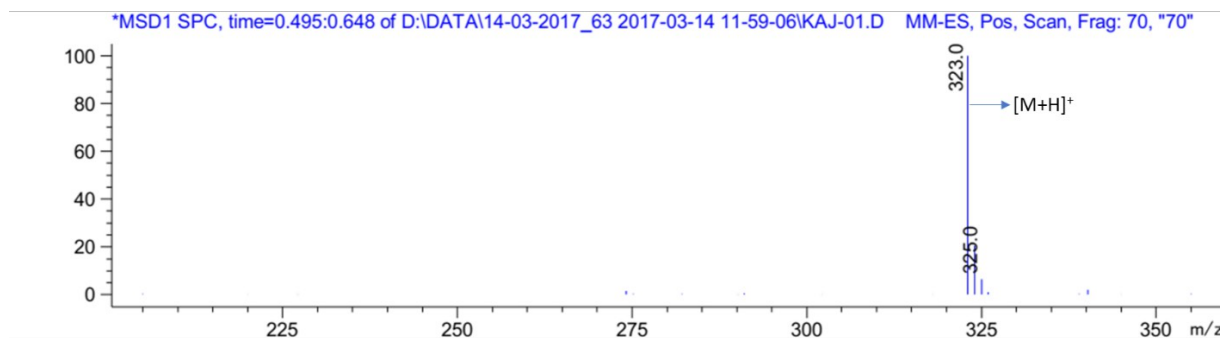


Figure-S1. Mass Spectra of Compound-1

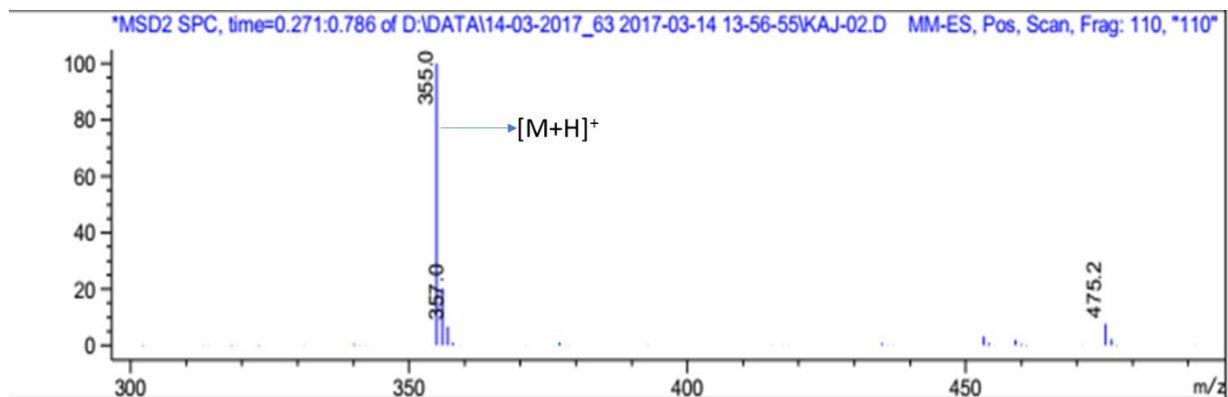


Figure-S2. Mass Spectra of Compound-2

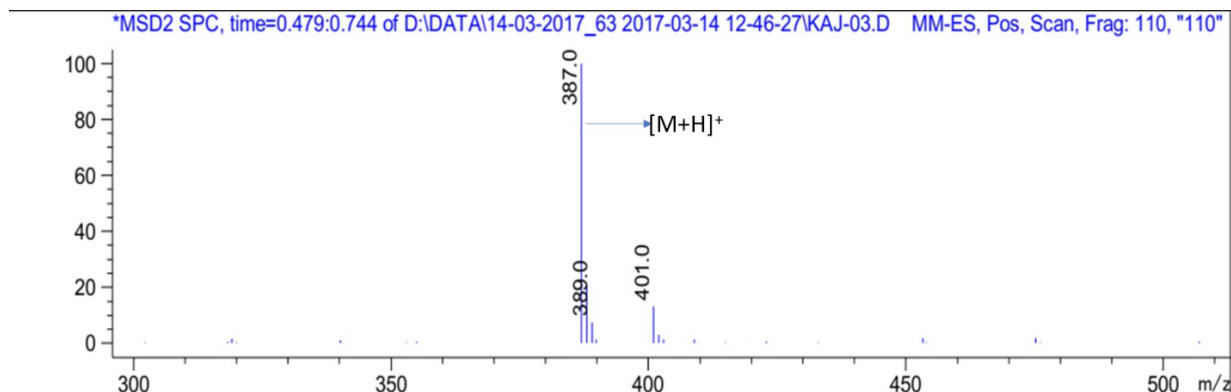


Figure-S3. Mass Spectra of Compound-3

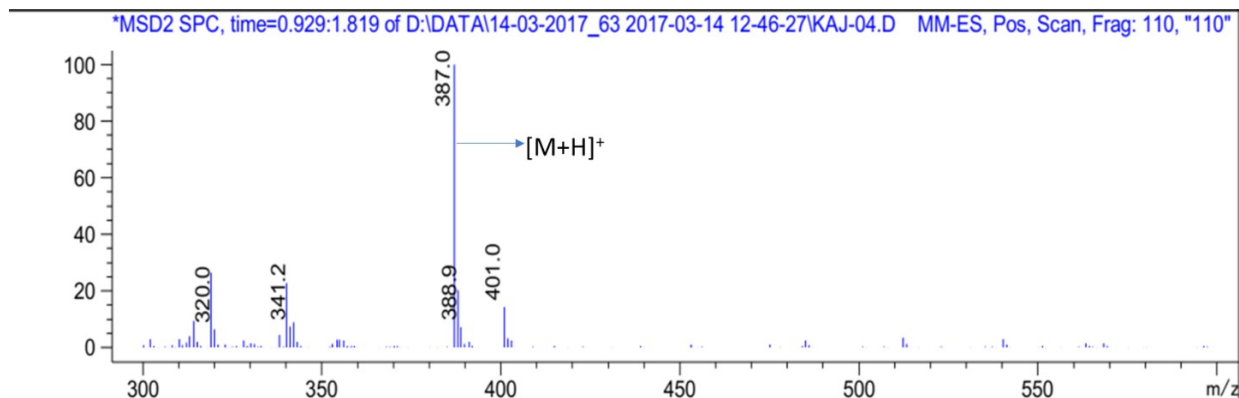


Figure-S4. Mass Spectra of Compound-4

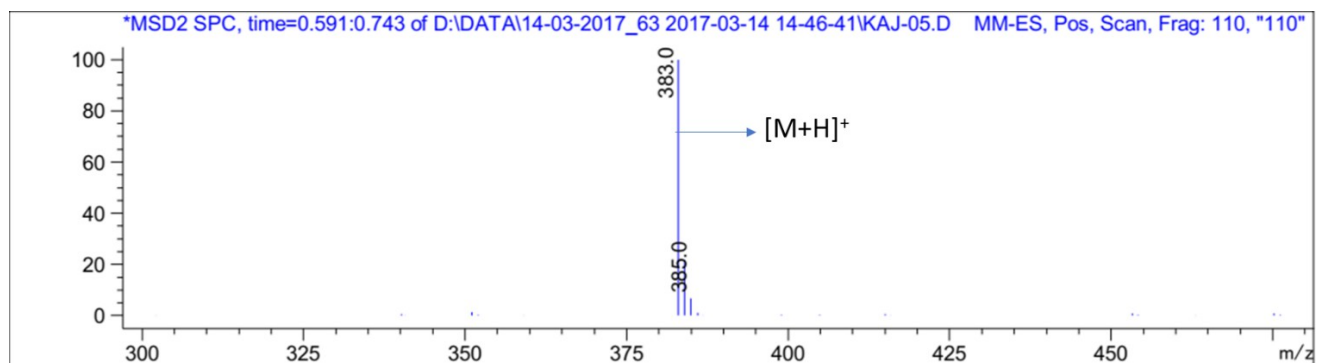


Figure-S5. Mass Spectra of Compound-5

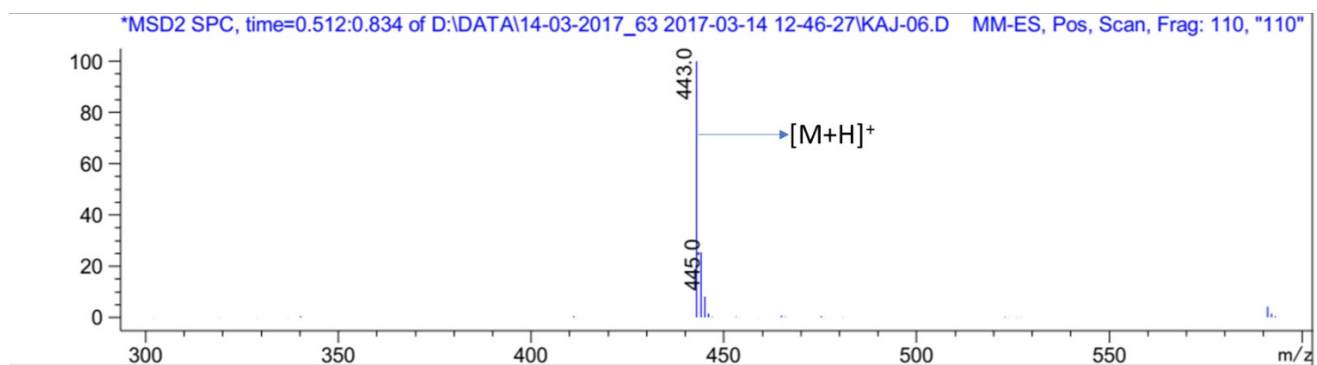


Figure-S6. Mass Spectra of Compound-6

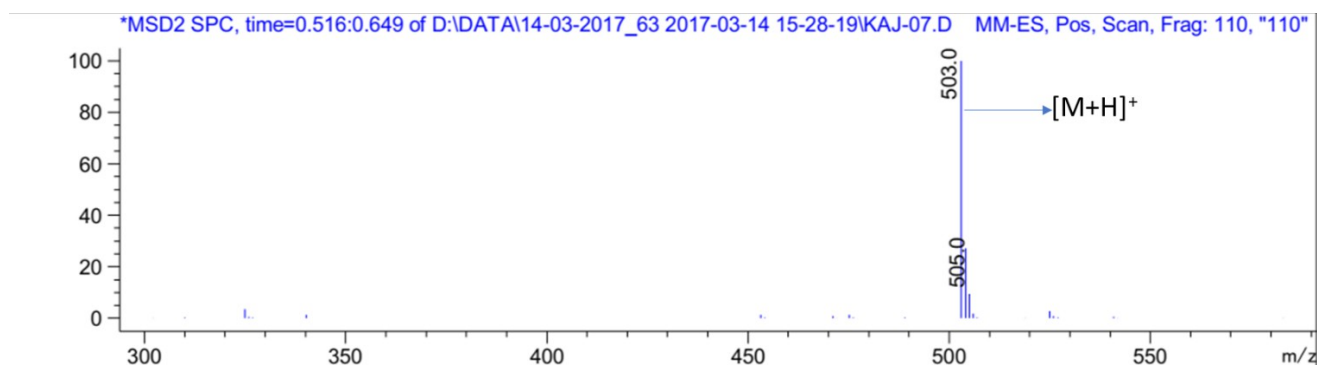


Figure-S7. Mass Spectra of Compound-7

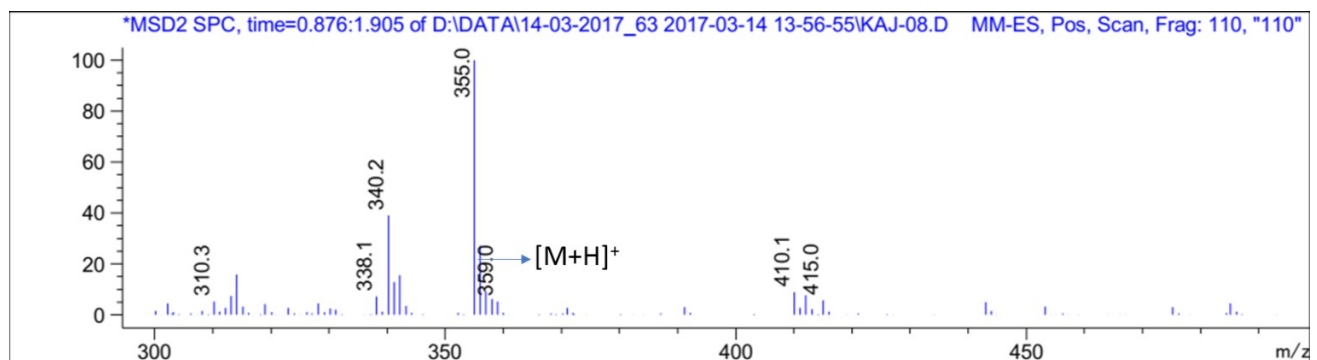


Figure-S8. Mass Spectra of Compound-8

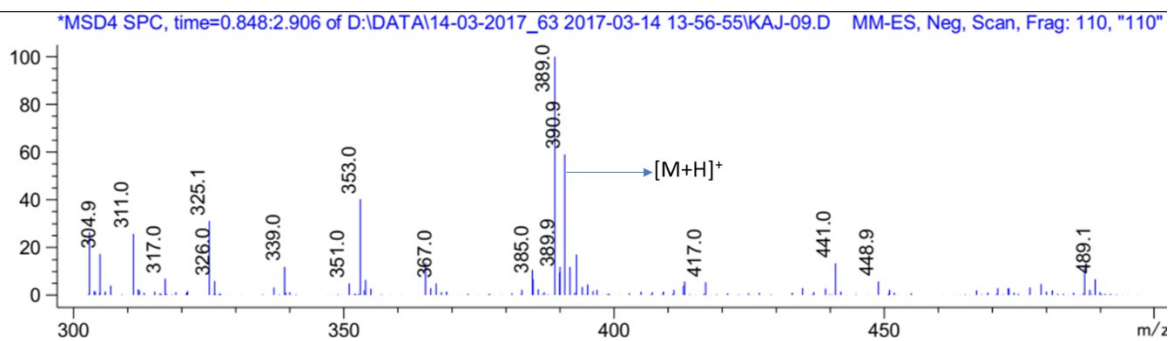


Figure-S9. Mass Spectra of Compound-9

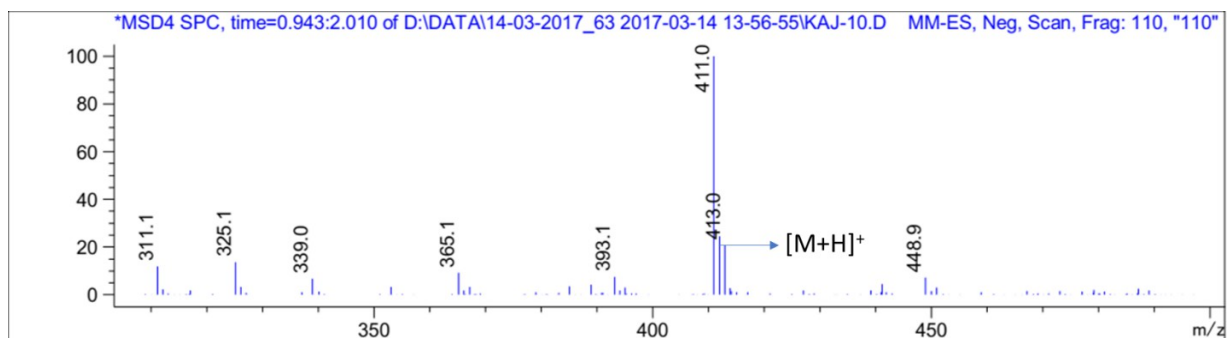


Figure-S10. Mass Spectra of Compound-10

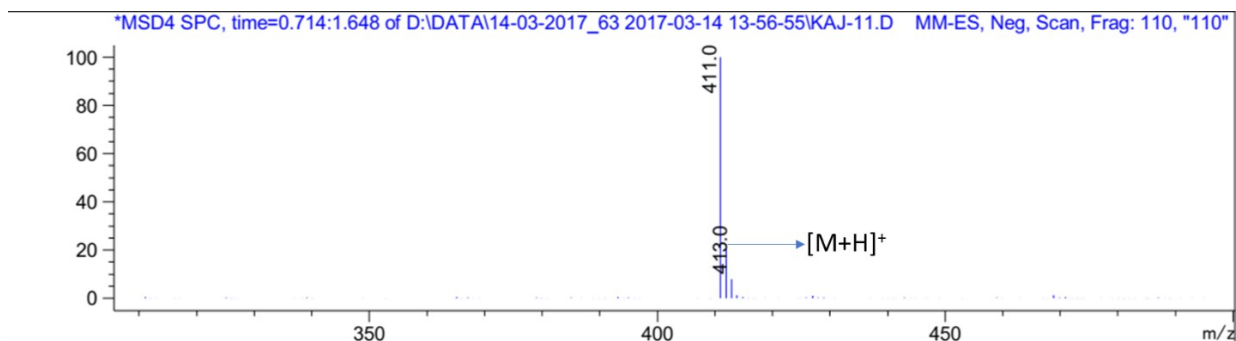


Figure-S11. Mass Spectra of Compound-11

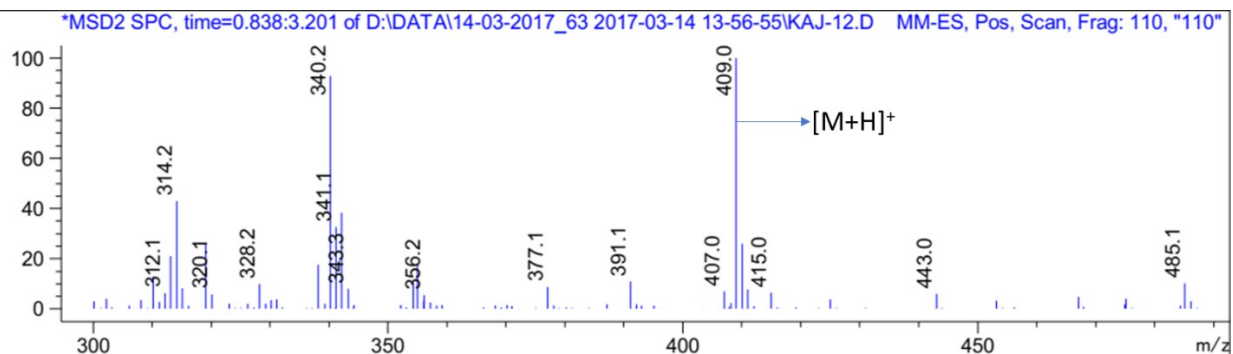


Figure-S12. Mass Spectra of Compound-12

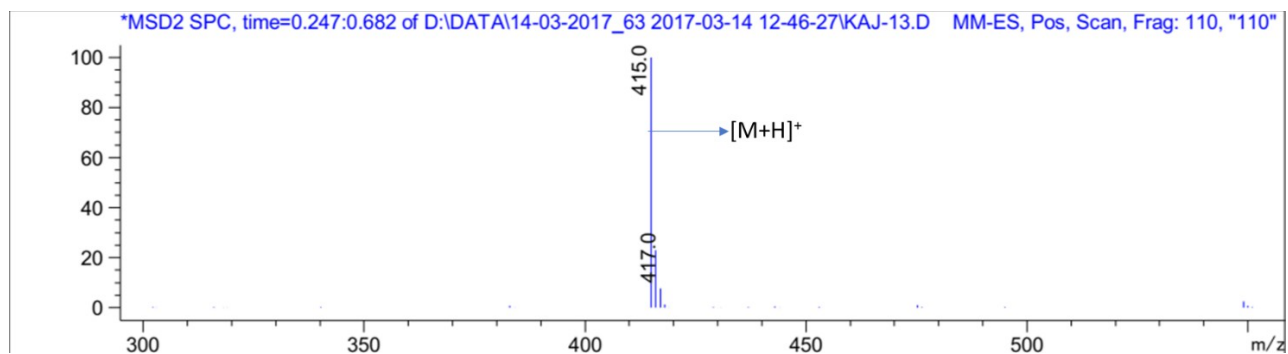


Figure-S13. Mass Spectra of Compound-13

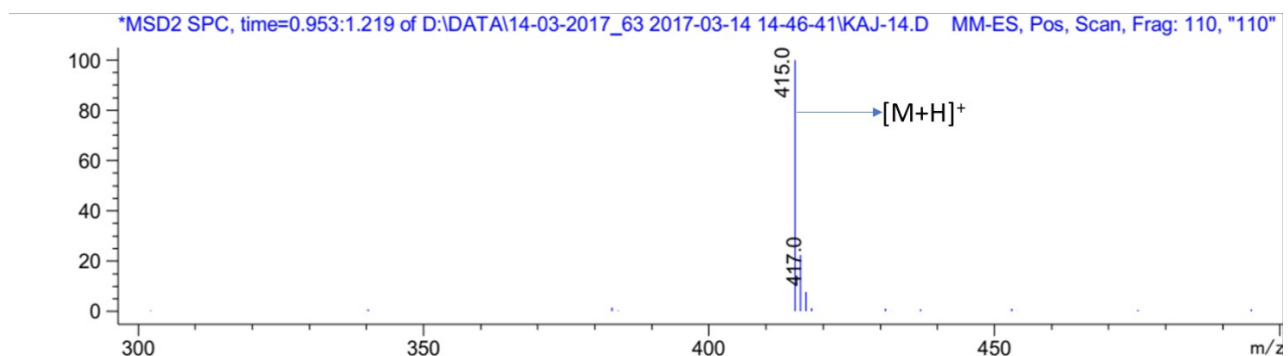


Figure-S14. Mass Spectra of Compound-14

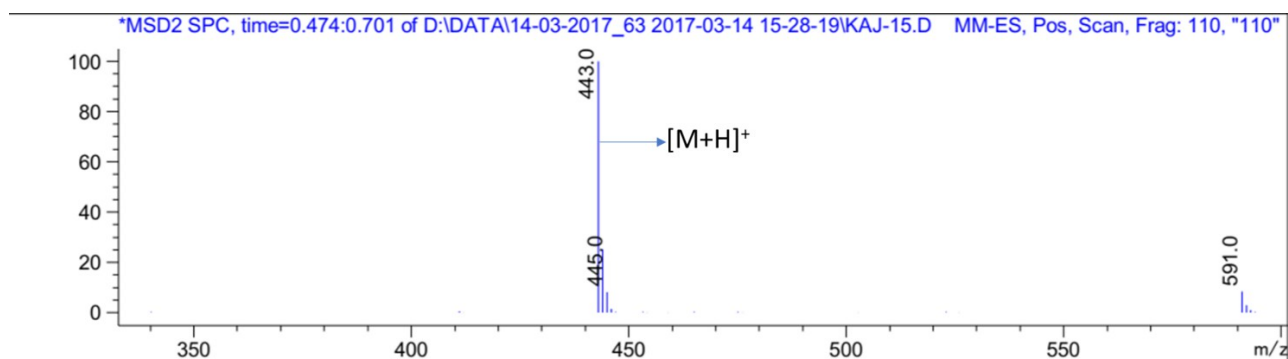


Figure-S15. Mass Spectra of Compound-15

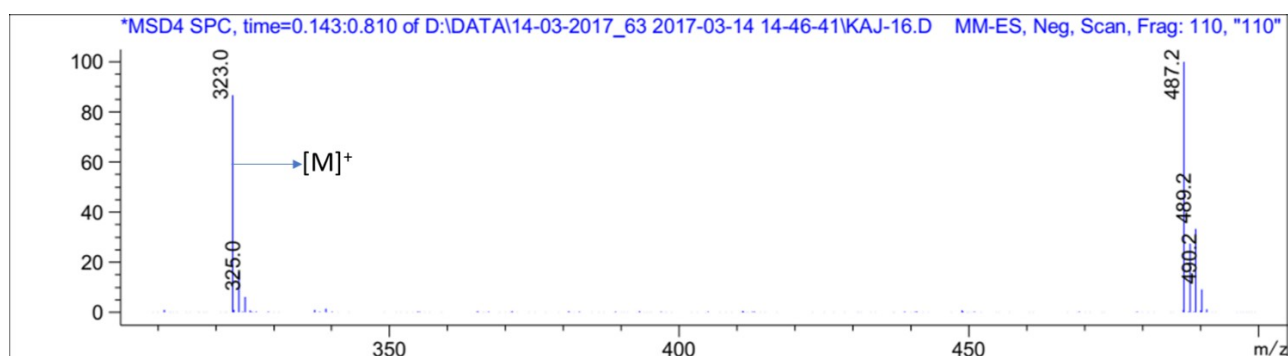


Figure-S16. Mass Spectra of Compound-16

H¹ NMR Spectra

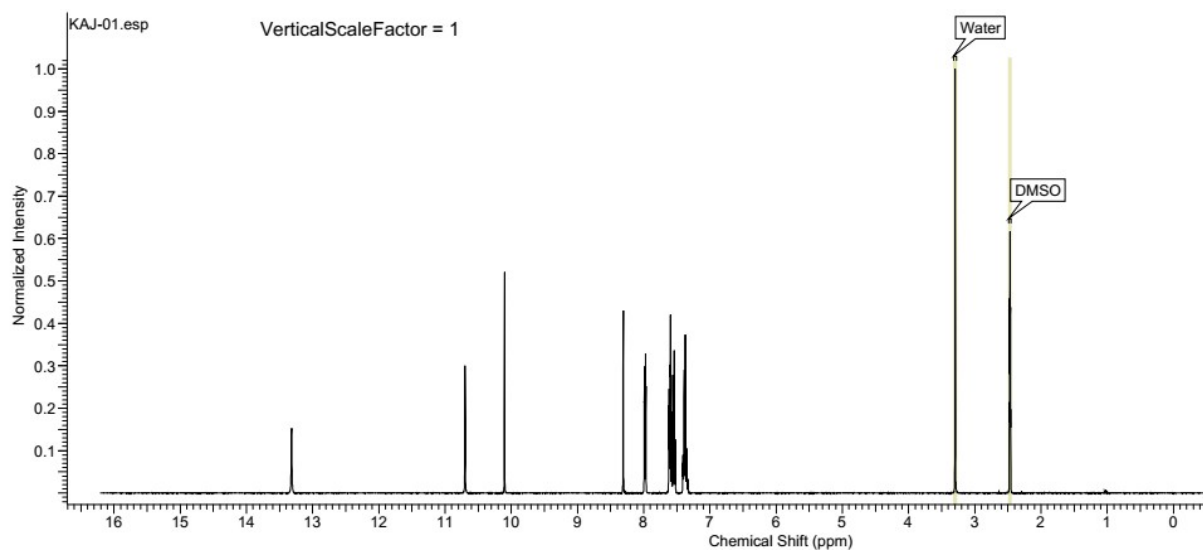


Figure-S17. H¹ NMR Spectra of Compound-1

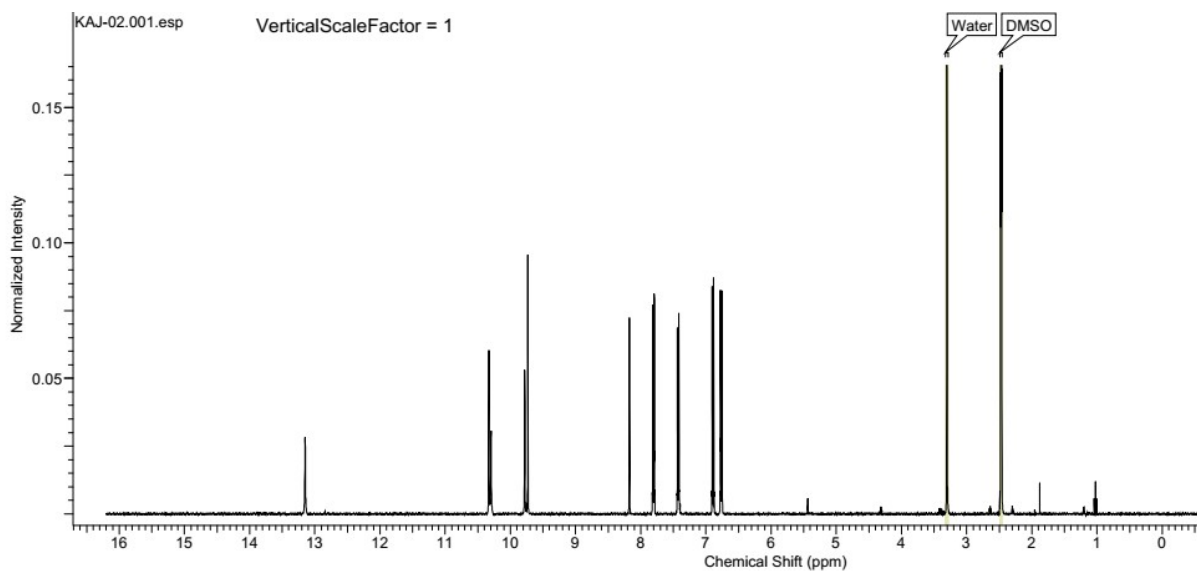


Figure-S18. H¹ NMR Spectra of Compound-2

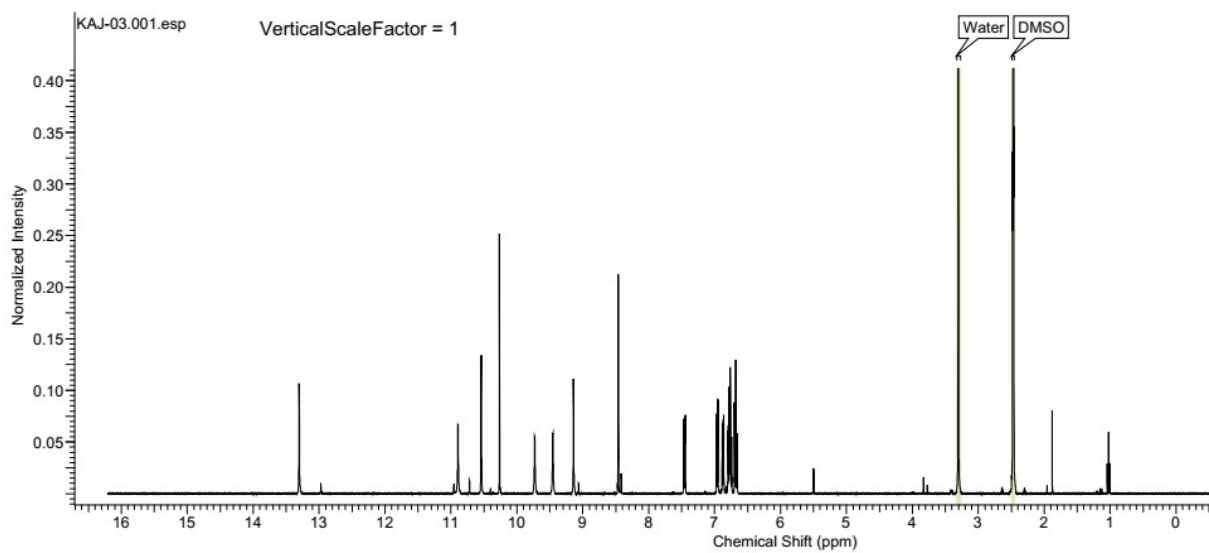


Figure-S19. ¹H NMR Spectra of Compound-3

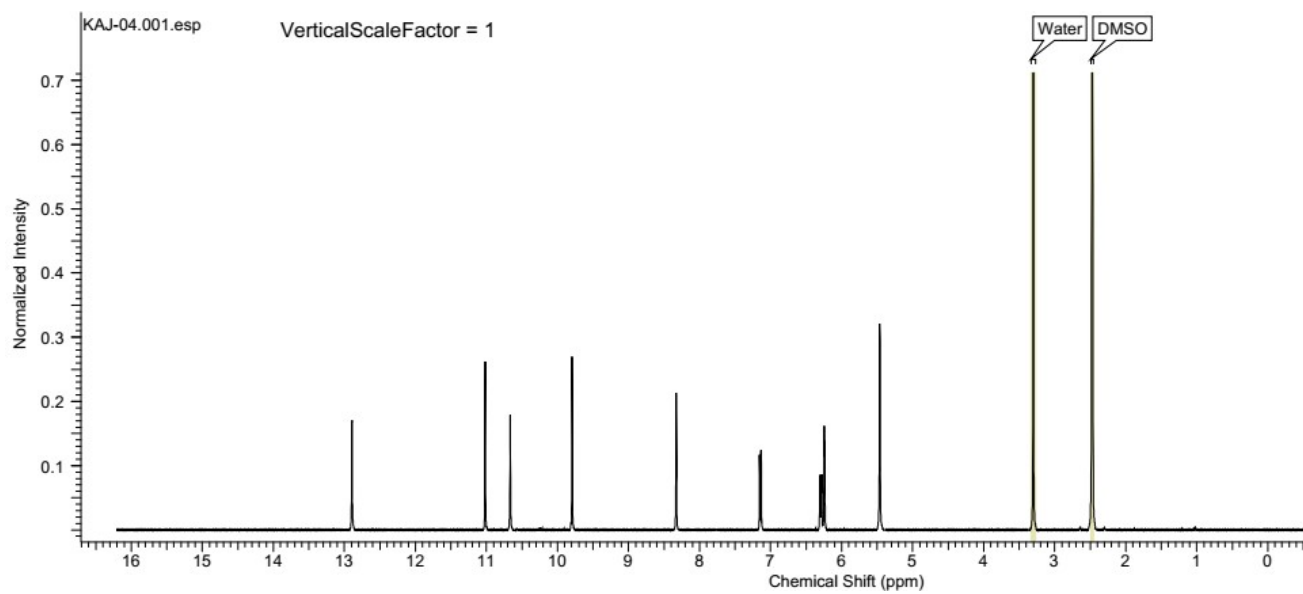


Figure-S20. ¹H NMR Spectra of Compound-4

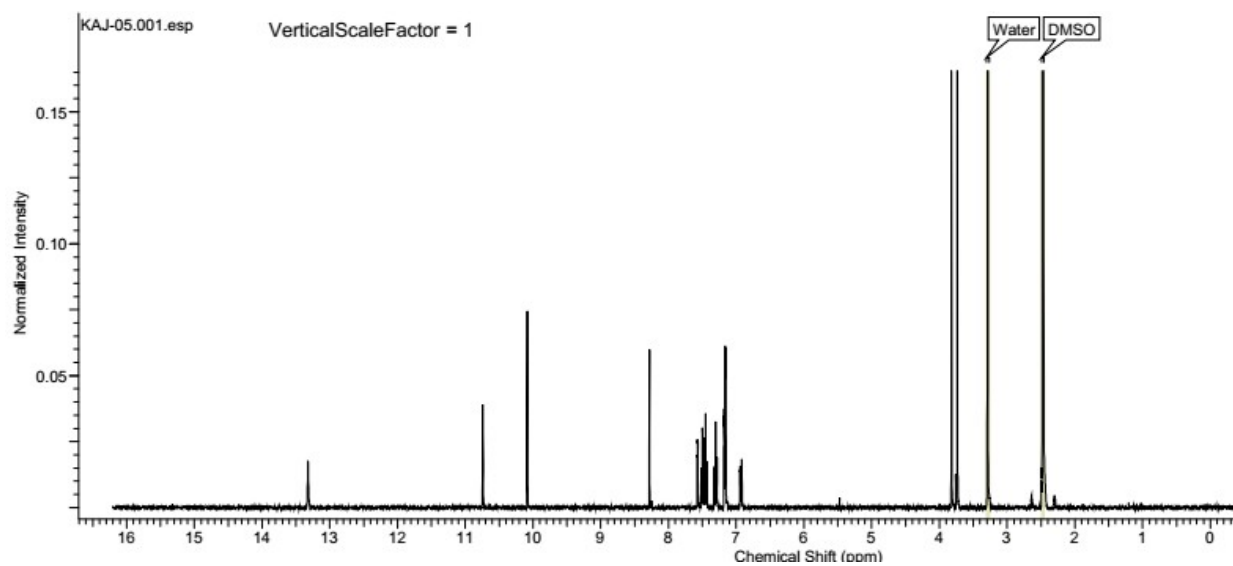


Figure-S21. ¹H NMR Spectra of Compound-5

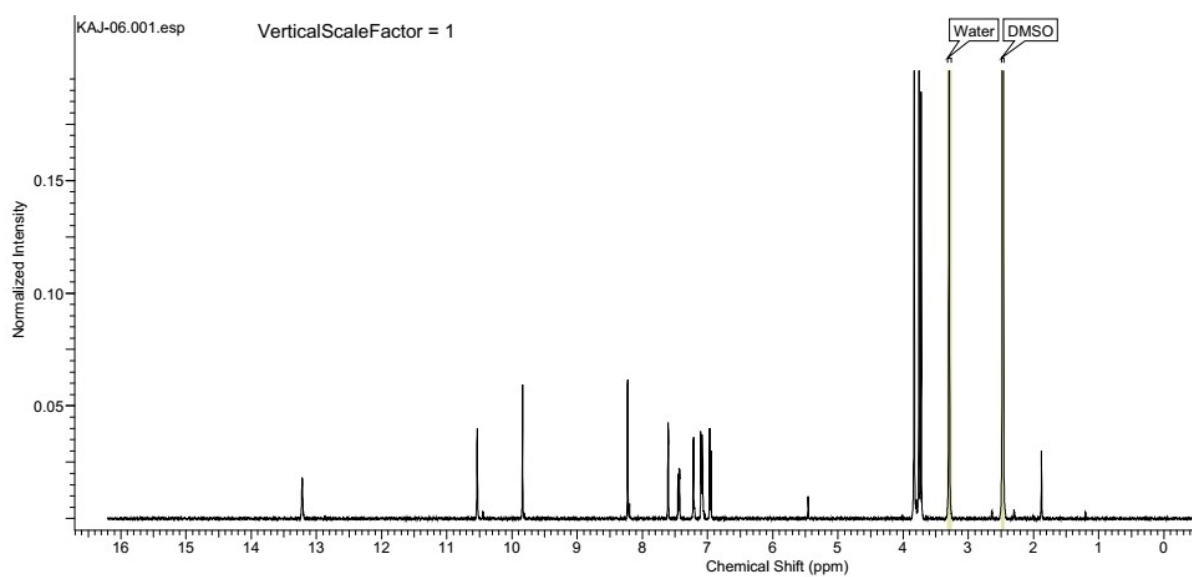


Figure-S22. ¹H NMR Spectra of Compound-6

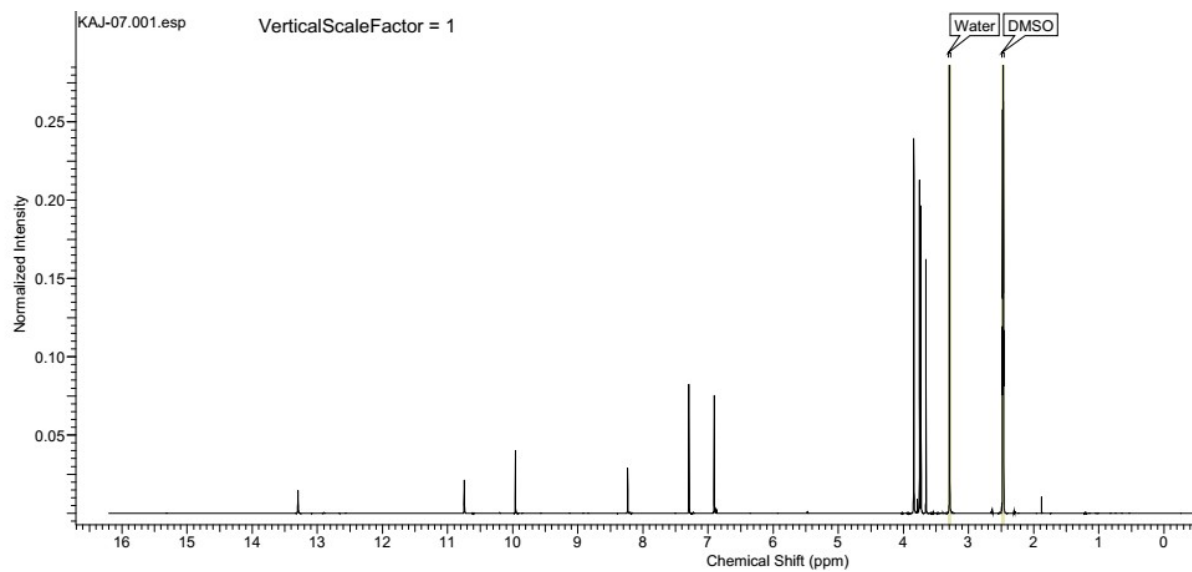


Figure-S23. H^1 NMR Spectra of Compound-7

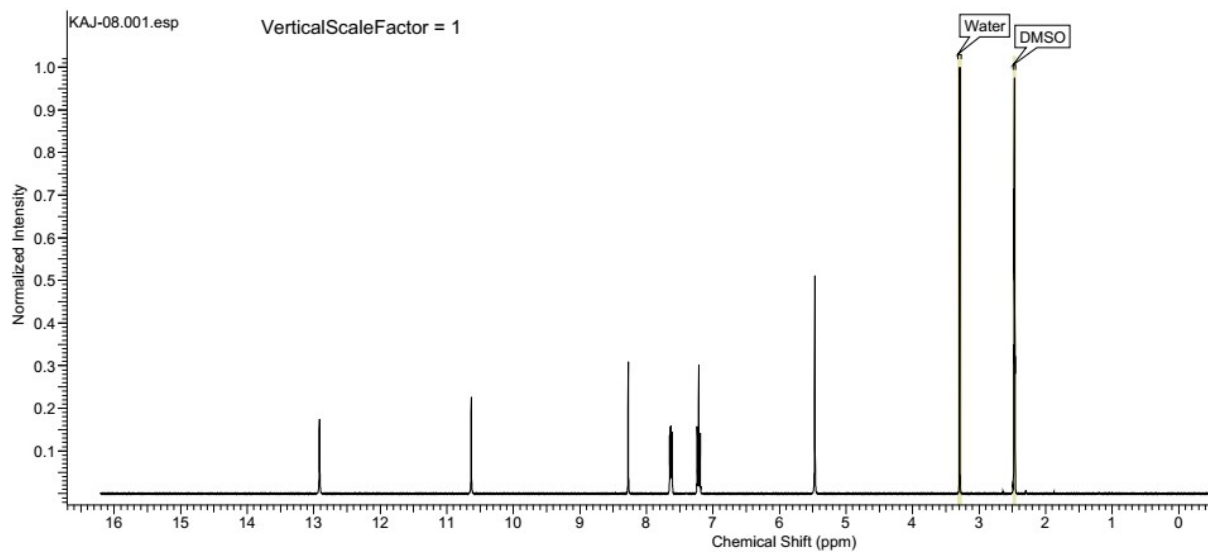


Figure-S24. H^1 NMR Spectra of Compound-8

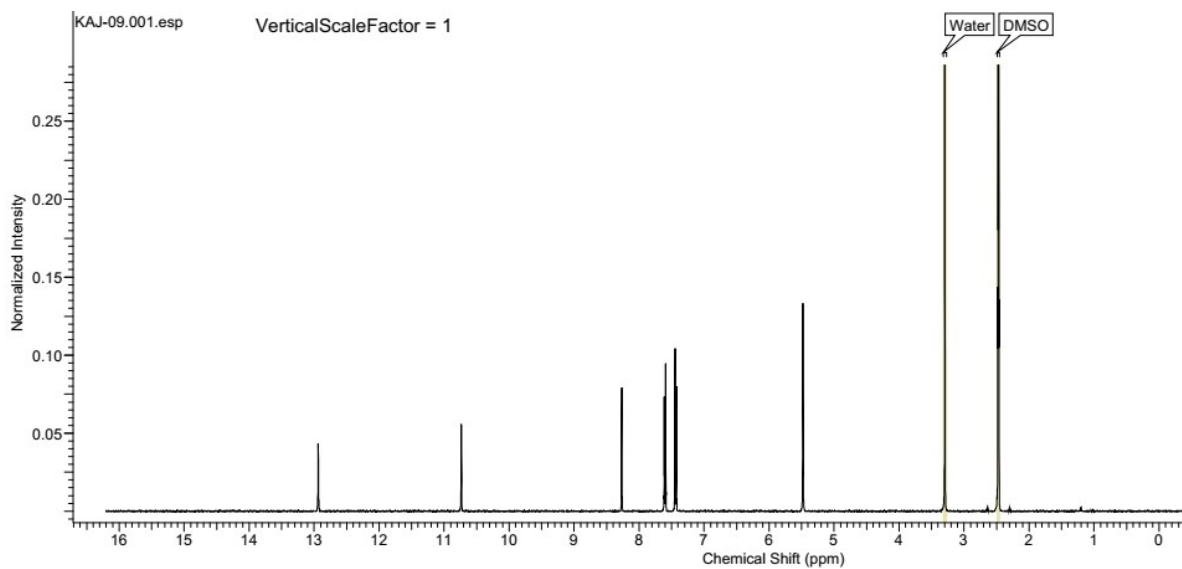


Figure-S25. ¹H NMR Spectra of Compound-9

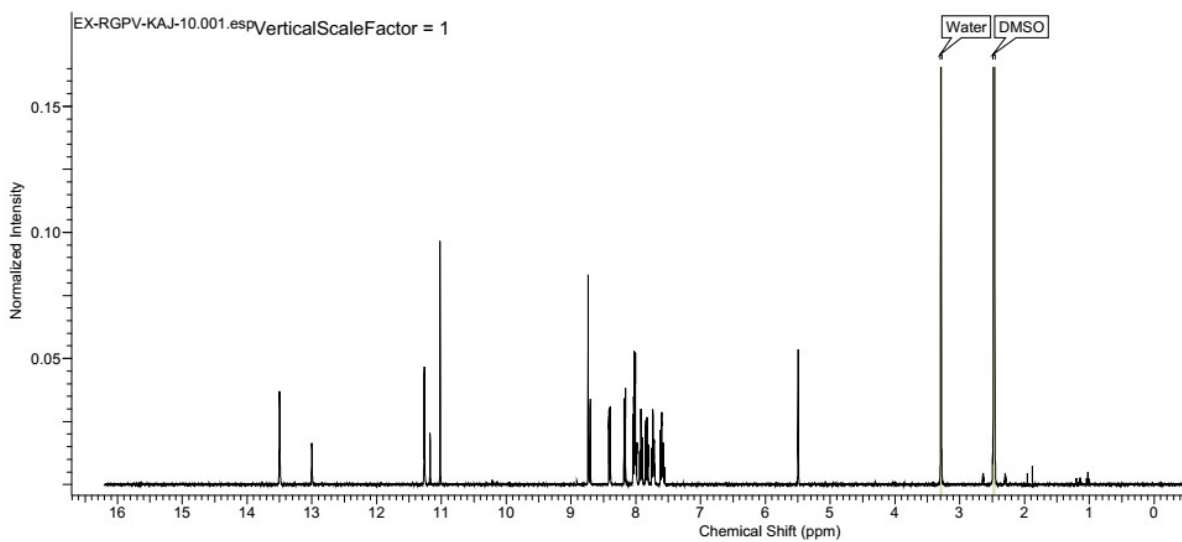


Figure-S26. ¹H NMR Spectra of Compound-10

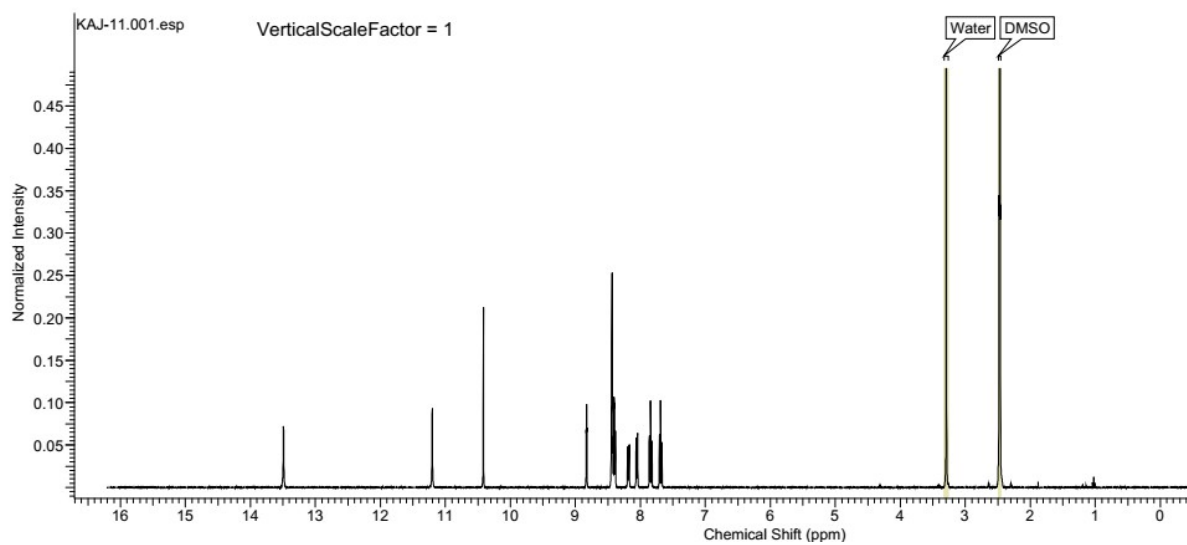


Figure-S27. H^1 NMR Spectra of Compound-11

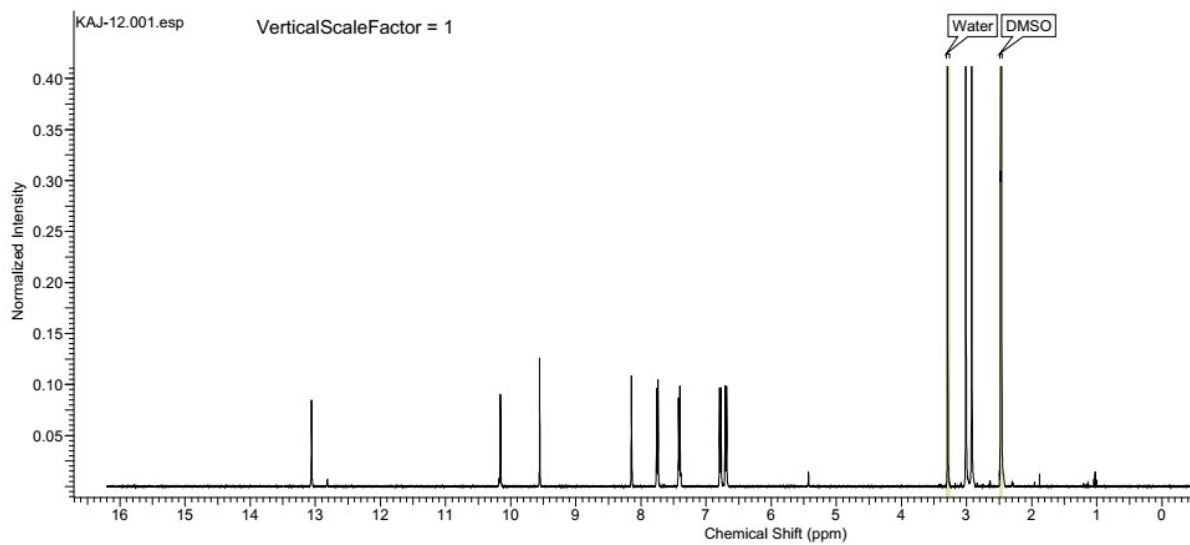


Figure-S28. H^1 NMR Spectra of Compound-12

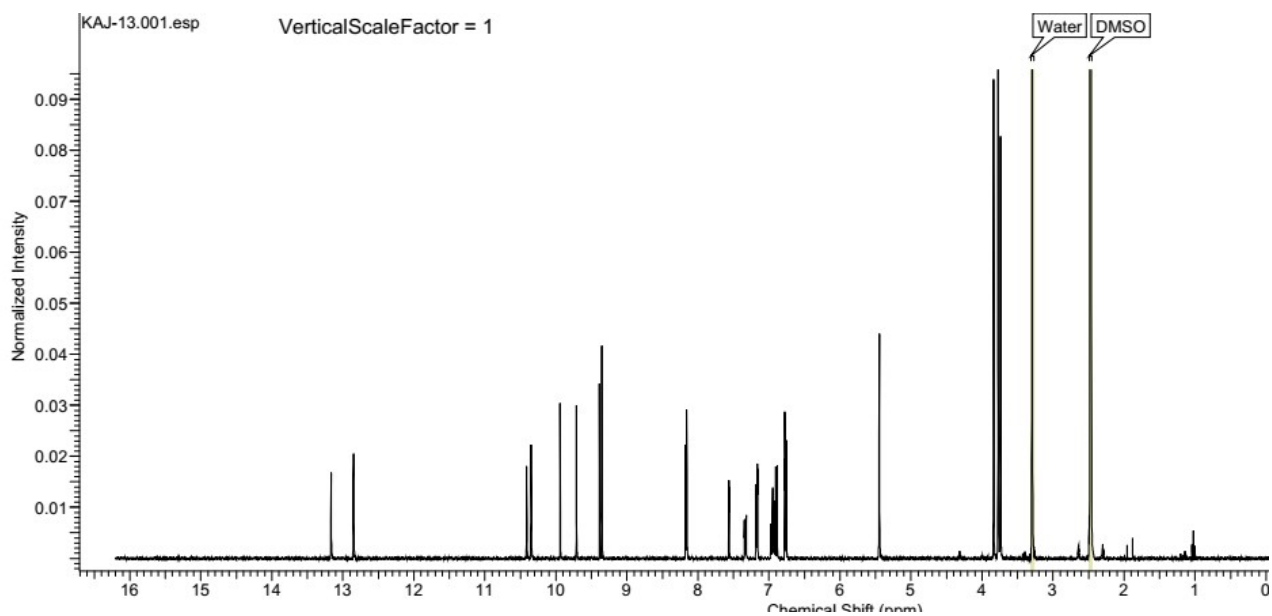


Figure-S29. ¹H NMR Spectra of Compound-13

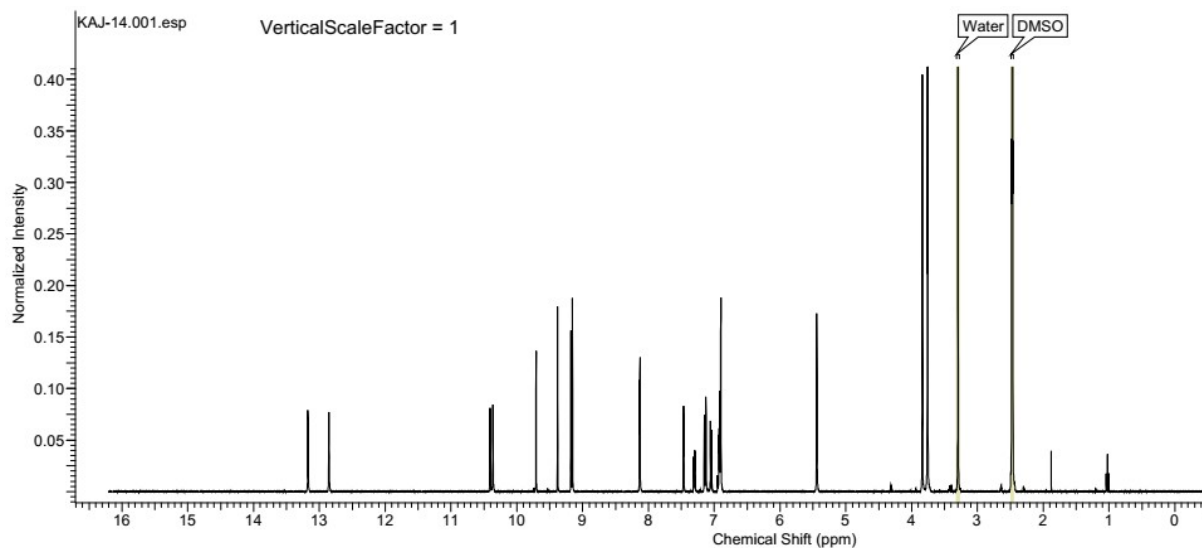


Figure-S30. ¹H NMR Spectra of Compound-14

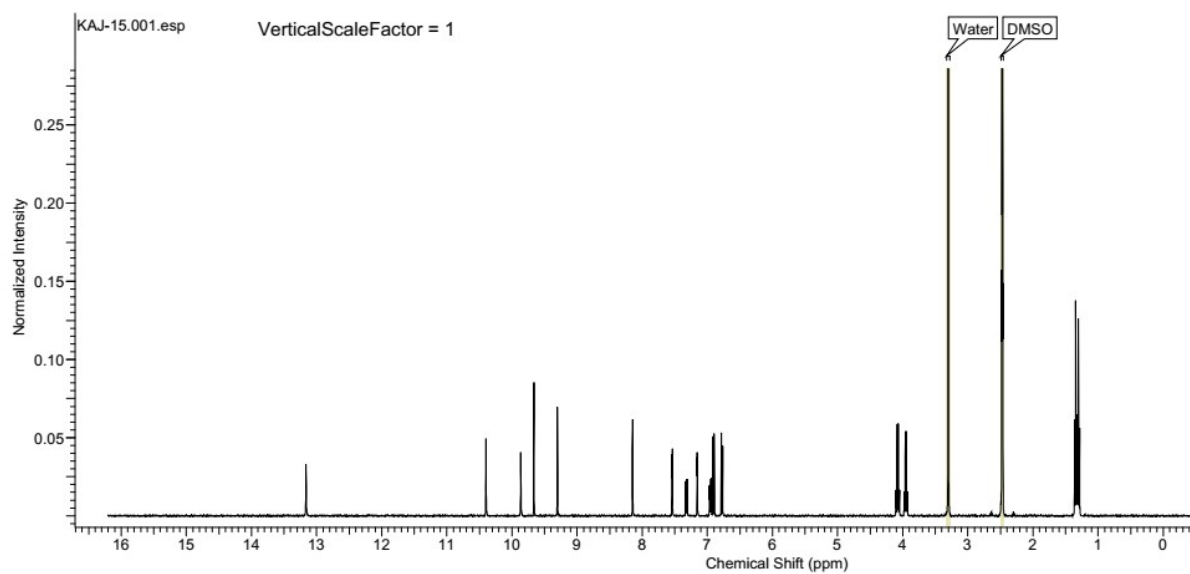


Figure-S31. H^1 NMR Spectra of Compound-15

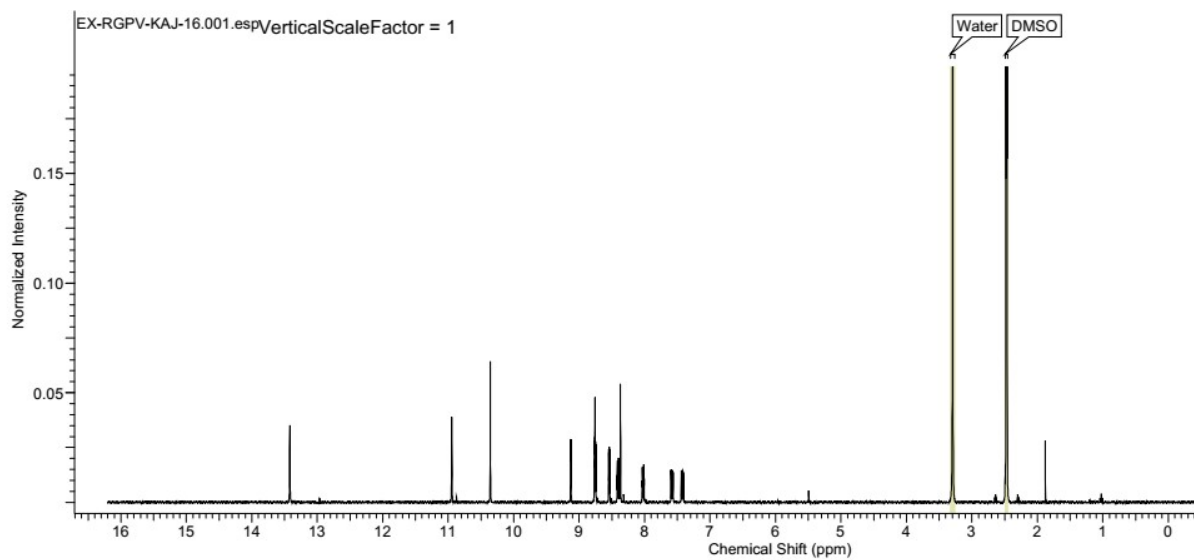


Figure-S32. H^1 NMR Spectra of Compound-16

Table-S1 : Kinase Inhibition Assay for-DYRK1A (IC₅₀-Values)

Conc. (μM)	Conc. (nM)	LOG Conc.	% Activity of Compd-3 (Mean)	<u>S</u> <u>D</u>	% Activity of Compd-4 (Mean)	<u>SD</u>	% Activity of Compd-5 (Mean)	<u>SD</u>
0.003	3	0.477121	95	6	101	5	94	4
0.01	10	1.000000	101	12	98	1	105	7
0.017	17	1.230449	95	23	97	6	101	5
0.024	24	1.380211	115	11	87	6	99	7
0.031	31	1.491362	105	15	90	6	104	5
0.038	38	1.579784	79	10	66	3	88	3
0.045	45	1.653213	44	4	50	6	99	3
0.052	52	1.716003	16	3	16	0	75	6
0.059	59	1.770852	6	1	9	1	72	4
0.066	66	1.819544	2	0	12	0	58	4
		IC ₅₀ (nM)	2868		2240		>100000	
		IC ₅₀ (uM)	2.87 μM		2.24 μM		>100	

Table-S2 Kinase Inhibition Assay for-CLK-1 (IC₅₀-Values)

Conc. (μM)	Conc. (nM)	LOG Conc.	% Activity of Compd-3 (Mean)	<u>S</u> <u>D</u>	% Activity of Compd-4 (Mean)	<u>SD</u>	% Activity of Compd-5 (Mean)	<u>SD</u>
0.003	3	0.477121	97	16	88	26	110	13
0.01	10	1.000000	119	10	106	2	117	7
0.03	30	1.477121	105	13	106	2	100	16
0.1	100	2.000000	111	3	104	9	105	6
0.3	300	2.477121	107	1	84	3	79	11
1	1000	3.000000	55	11	72	10	50	1
3	3000	3.477121	35	2	51	14	32	4
10	10000	4.000000	17	0	17	1	18	3
30	30000	4.477121	7	0	8	1	19	2
100	100000	5.000000	3	0	5	1	17	2
		IC ₅₀ (nM)	1376		2575		974.9	
		IC ₅₀ (uM)	1.38μM		2.58 μM		0.97 μM	

