Developing new Pyrido[2,3-*d*]pyrimidine -Based Small-Molecule as potent ATR Inhibitors

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Fig. S14. ^{13}C NMR spectrum of **6-bromo-2-(1*H*-imidazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4e** in DMSO- d6 at r.t.

Fig. S15. HRMS spectrum of **6-bromo-2-(1*H*-imidazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4e**.

Fig. S16. Interaction study of compounds **5(a-e)** with PI3Kα mutant mimicking ATR **(PDB ID: 5UK8).**

Table S1. Selected Bond length (Å) and Bond angle (°) of compound **4(a)**.

Fig. S1. ^{1}H NMR spectrum of **6-bromo-2-(pyridin-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4a** in DMSO- d6 at r.t.

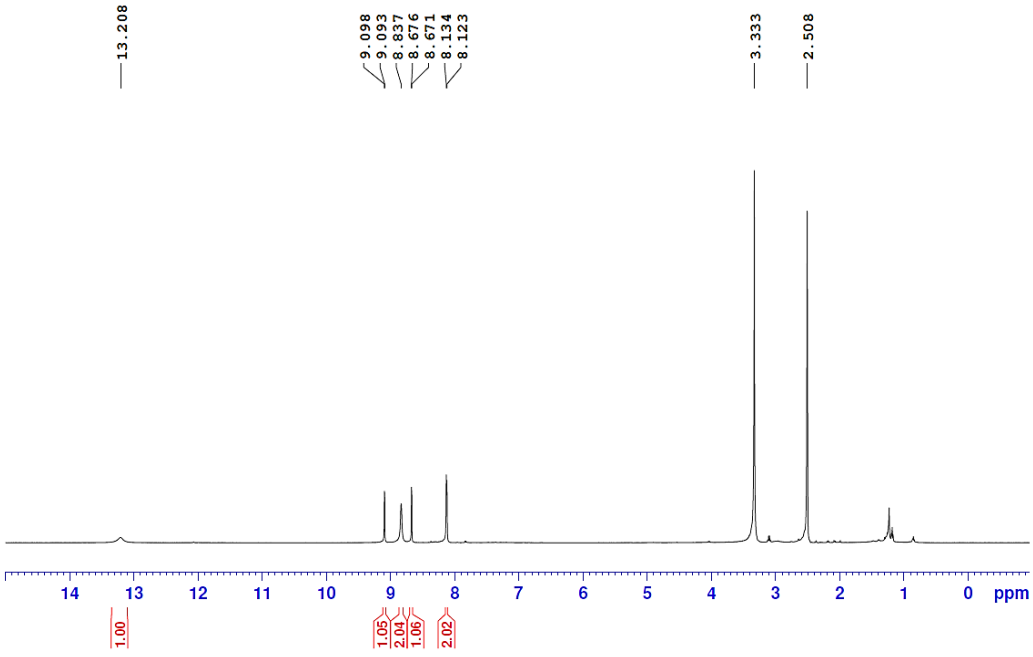


Fig. S2. ^{13}C NMR spectrum of **6-bromo-2-(pyridin-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4a** in DMSO- d6 at r.t.

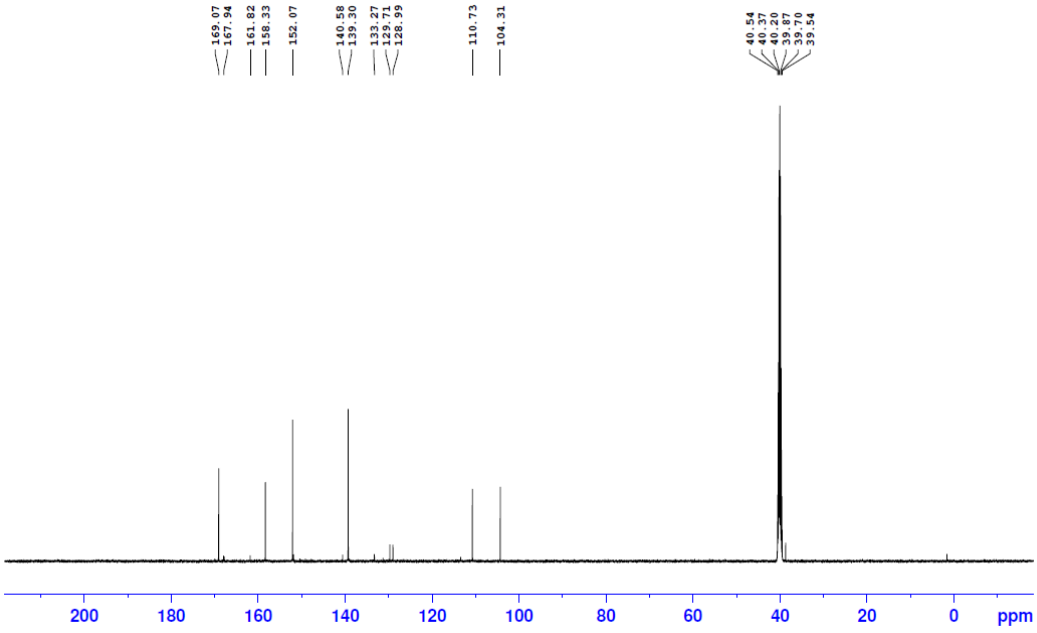


Fig. S3. HRMS spectrum of **6-bromo-2-(pyridin-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4a.**

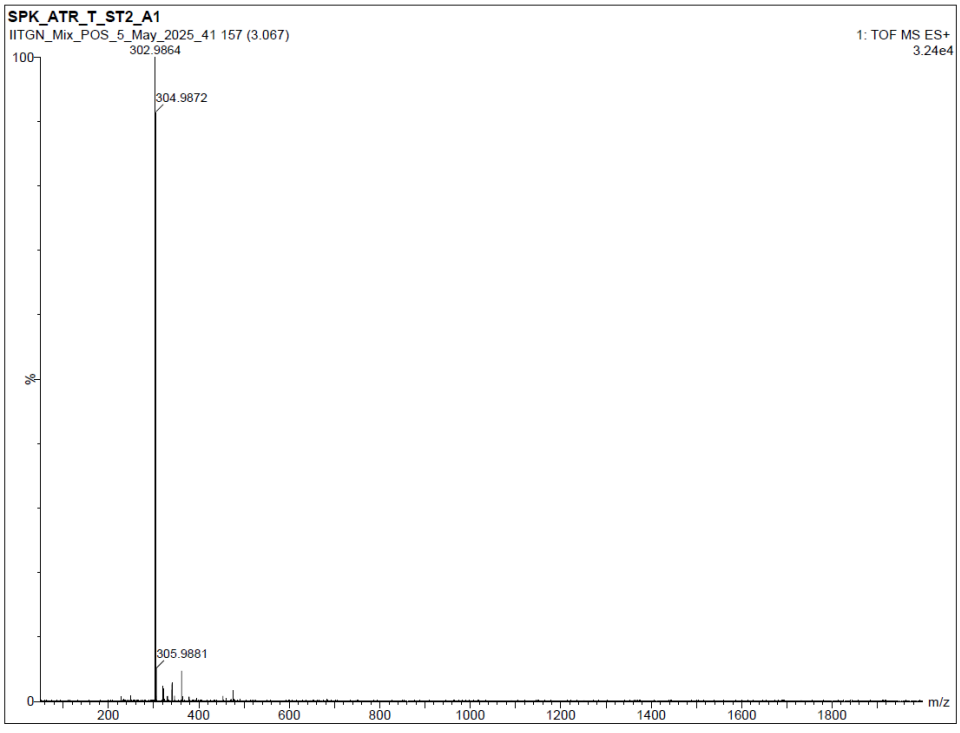


Fig. S4. [1]H NMR spectrum of **6-bromo-2-(pyridin-2-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4b** in DMSO- d6 at r.t.

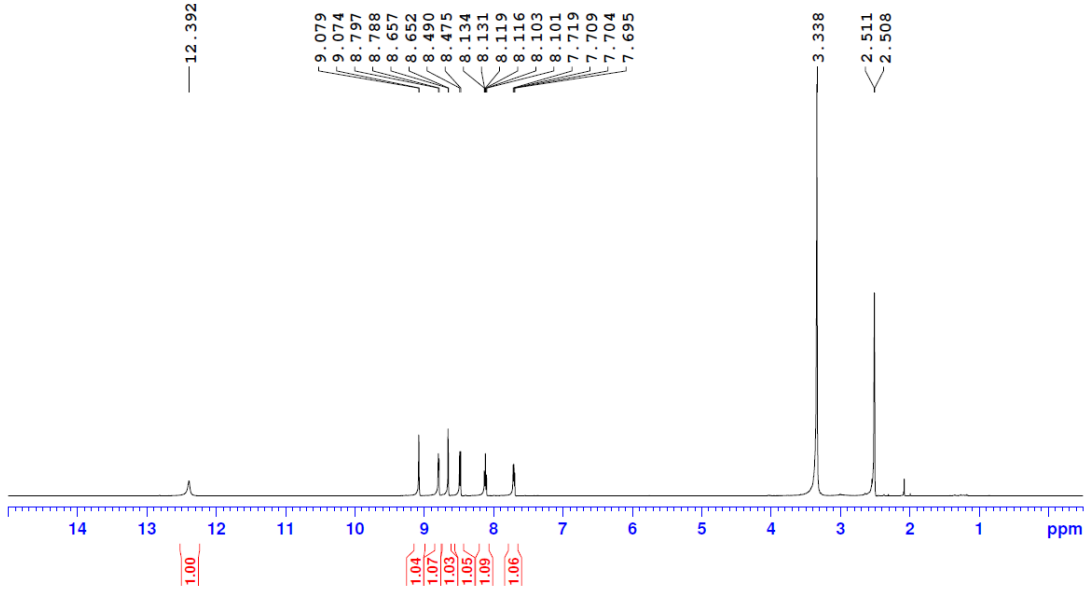


Fig. S5. [13]C NMR spectrum of **6-bromo-2-(pyridin-2-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4b** in DMSO- d6 at r.t.

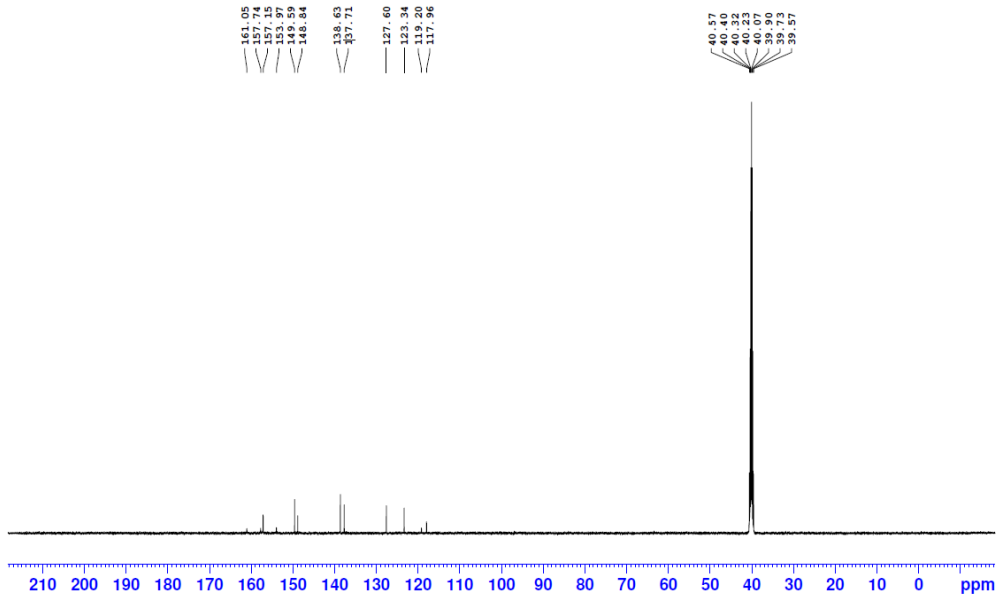


Fig. S6. HRMS spectrum of **6-bromo-2-(pyridin-2-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4b**.

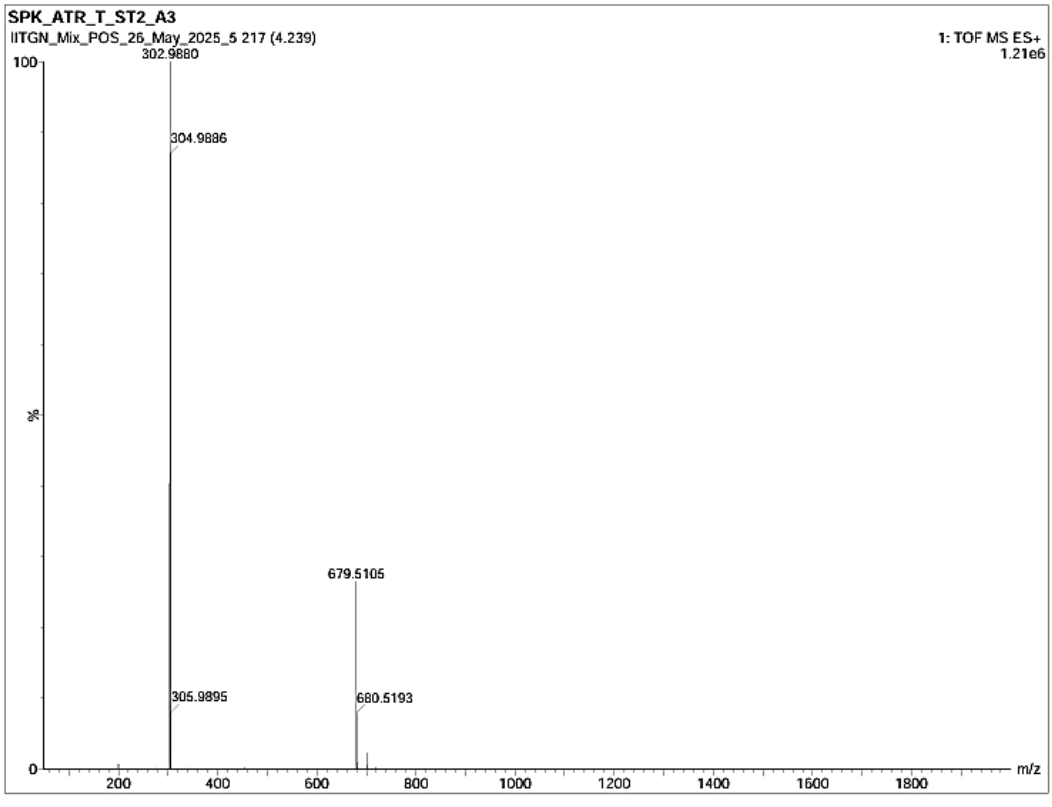


Fig. S7. ^{1}H NMR spectrum of **6-bromo-2-(1*H*-pyrazol-3-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4c** in DMSO- d6 at r.t.

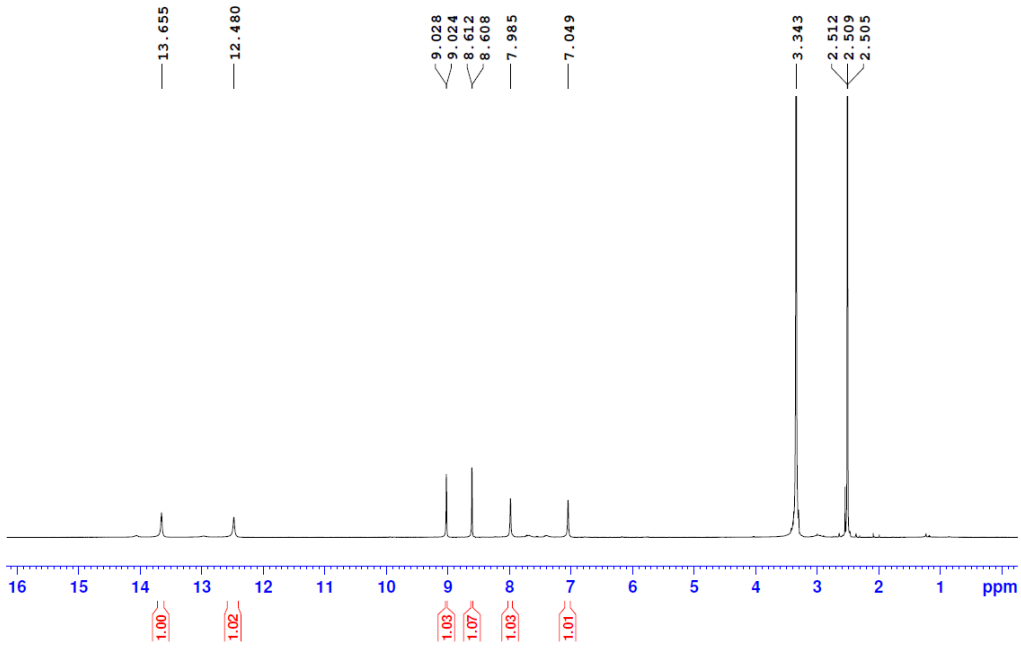


Fig. S8. ^{13}C NMR spectrum of **6-bromo-2-(1*H*-pyrazol-3-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4c** in DMSO- d6 at r.t.

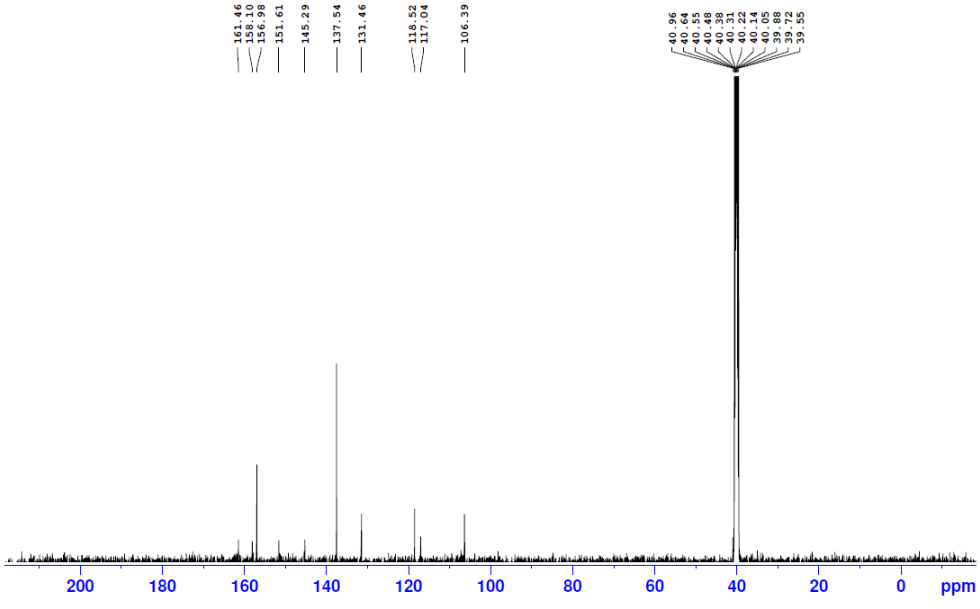


Fig. S9. HRMS spectrum of **6-bromo-2-(1*H*-pyrazol-3-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4c**.

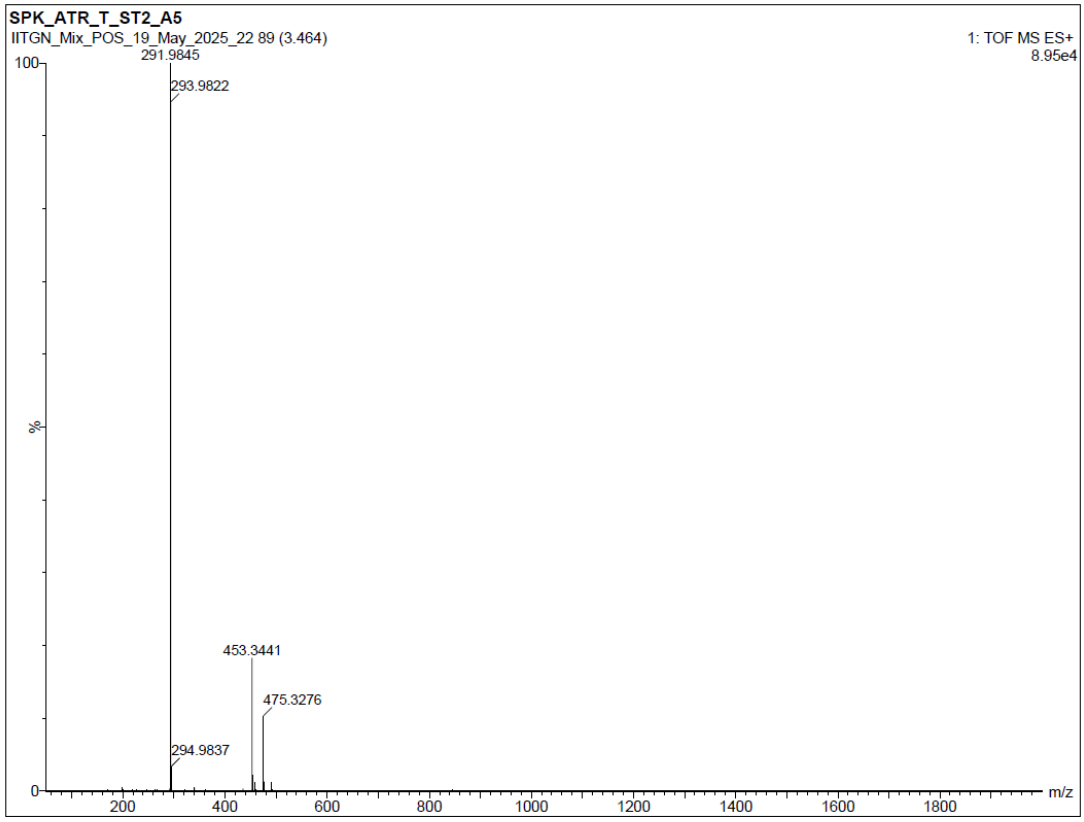


Fig. S10. ^{1}H NMR spectrum of **6-bromo-2-(1-methyl-1*H*-pyrazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4d** in DMSO- d6 at r.t.

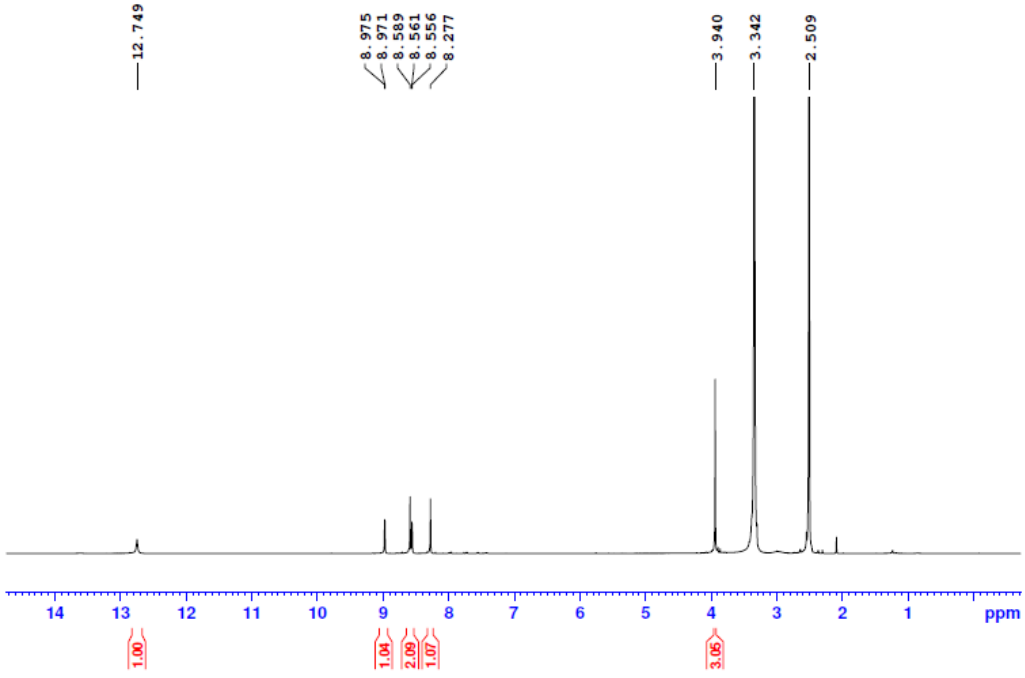


Fig. S11. ^{13}C NMR spectrum of **6-bromo-2-(1-methyl-1*H*-pyrazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4d** in DMSO- d6 at r.t.

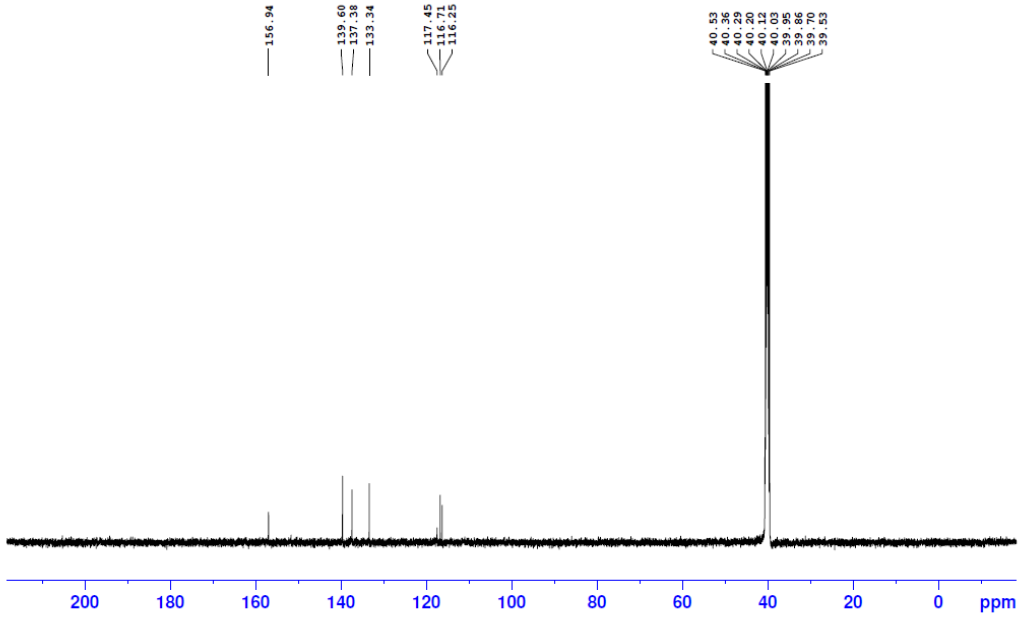


Fig. S12. HRMS spectrum of **6-bromo-2-(1-methyl-1*H*-pyrazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4d**.

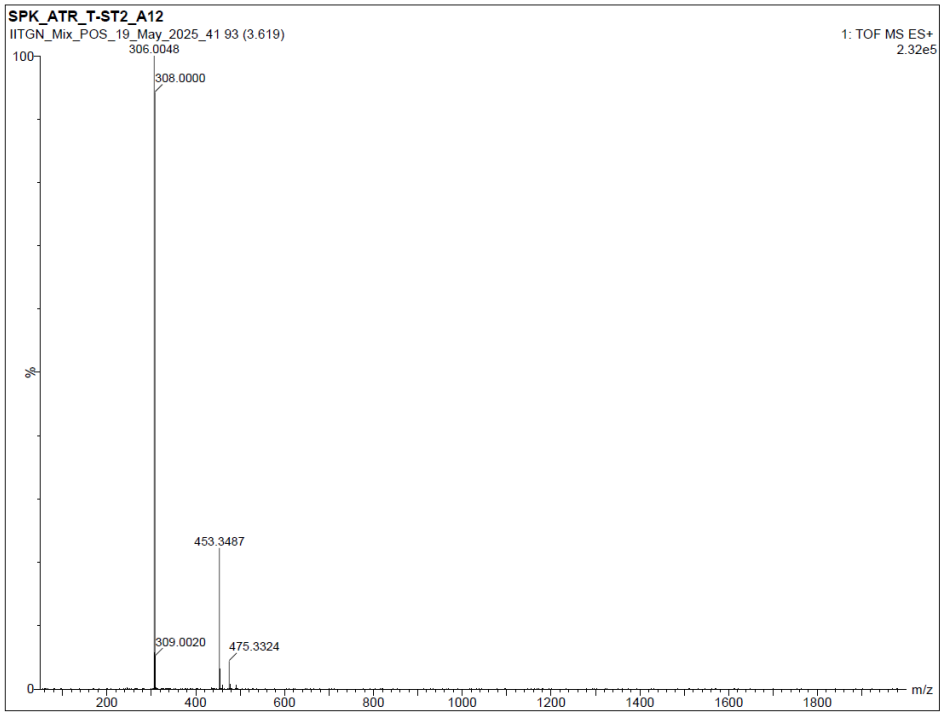


Fig. S13. [1]H NMR spectrum of **6-bromo-2-(1*H*-imidazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4e** in DMSO- d6 at r.t.

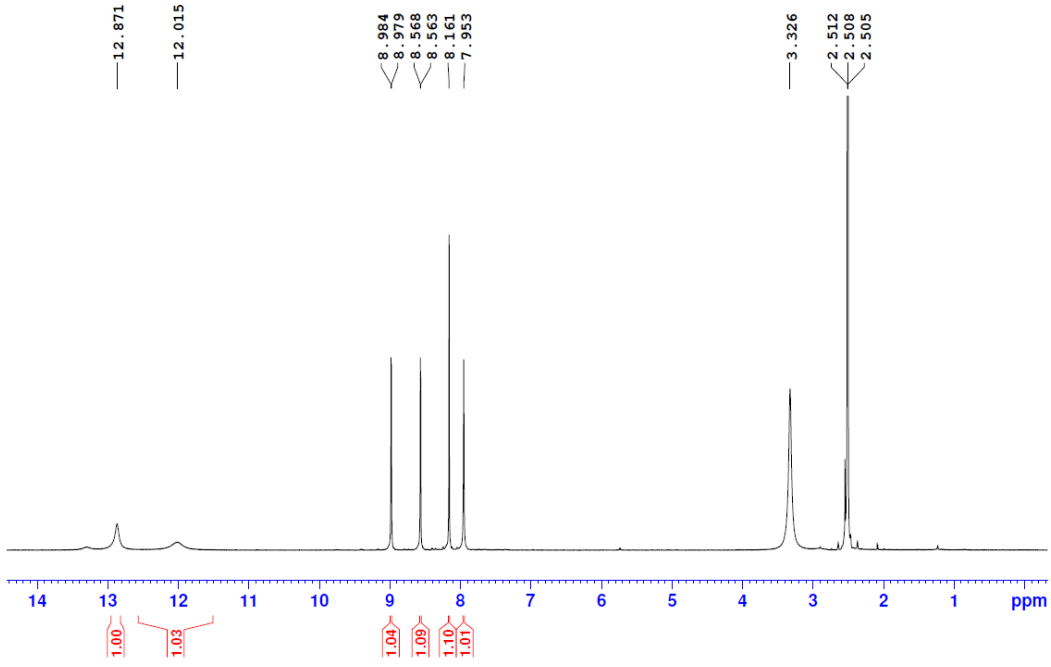


Fig. S14. [13]C NMR spectrum of **6-bromo-2-(1*H*-imidazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4e** in DMSO- d6 at r.t.

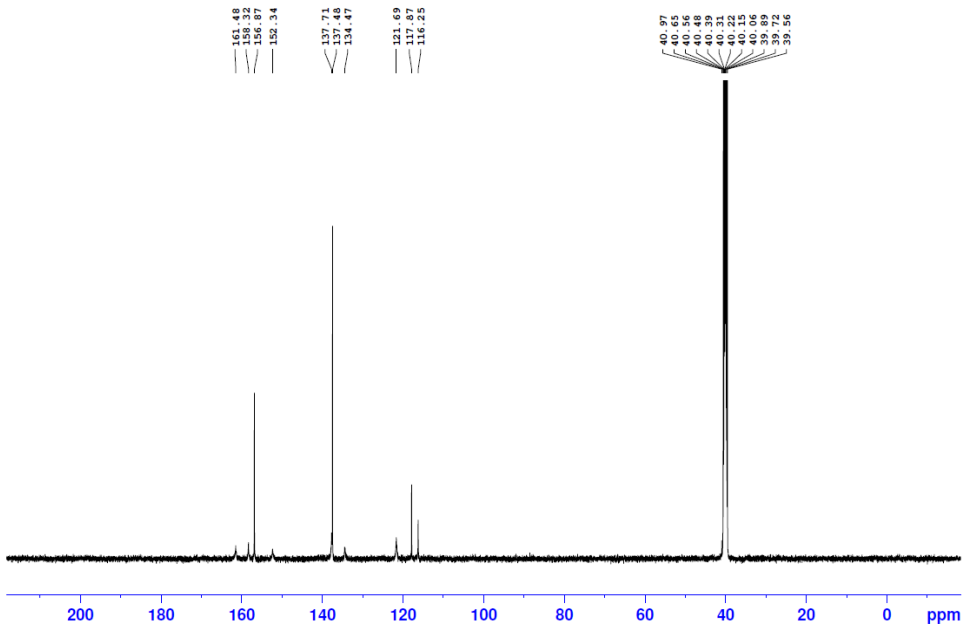


Fig. S15. HRMS spectrum of **6-bromo-2-(1*H*-imidazol-4-yl)pyrido[2,3-*d*]pyrimidin-4(3*H*)-one, 4e**.

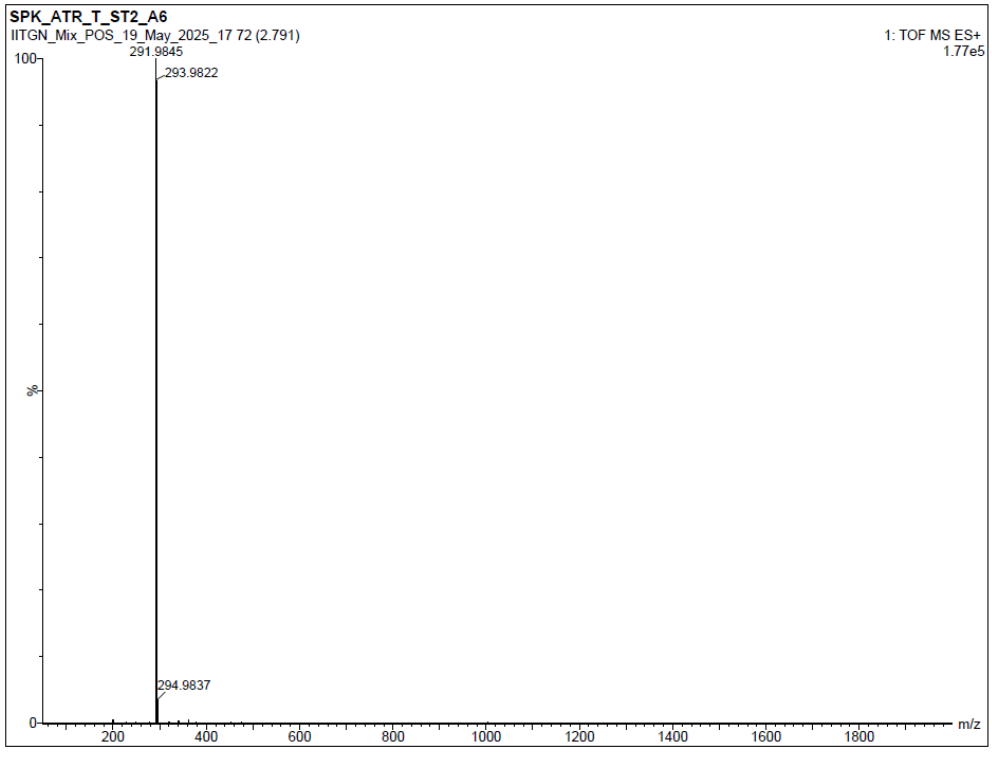
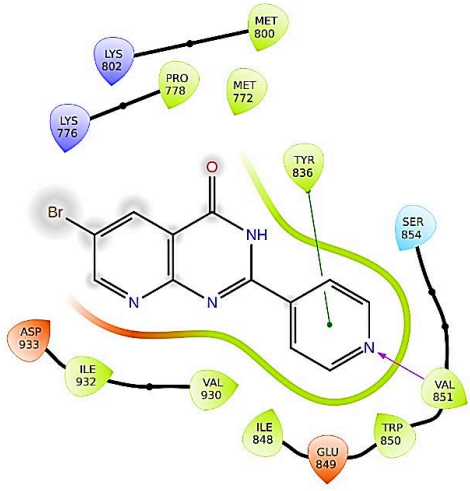
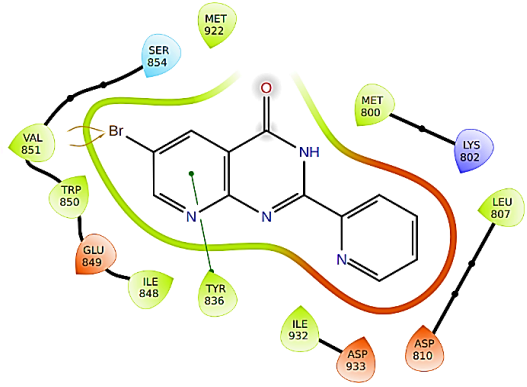


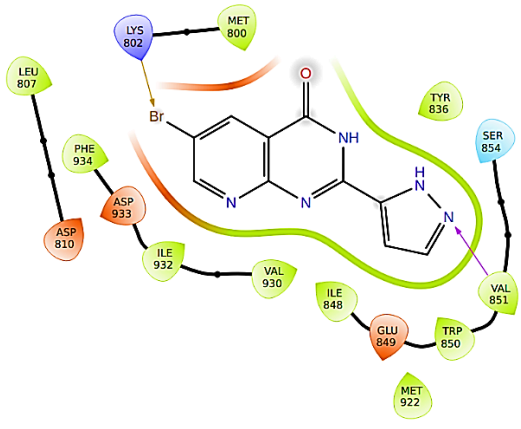
Fig. S16. Interaction study of compounds **5(a-e)** with PI3Kα mutant mimicking ATR **(PDB ID: 5UK8).**



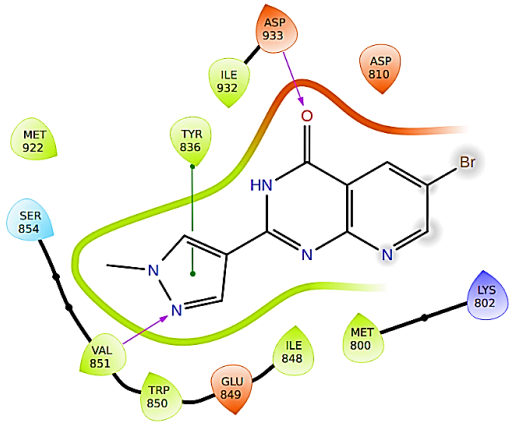
5(a)



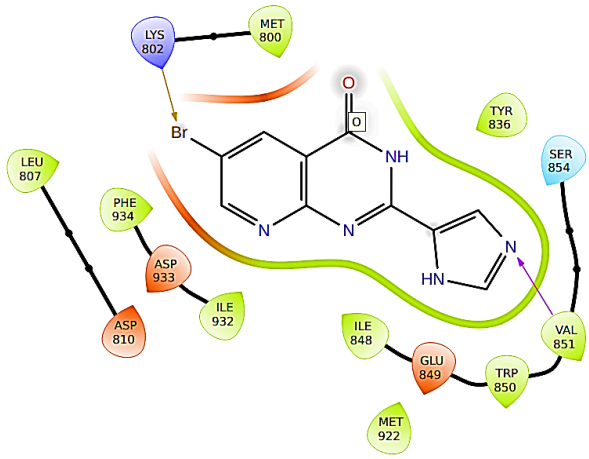
5(b)



5(c)



5(d)



5(e)

Table S1. Selected Bond length (Å) and Bond angle (°) of compound **4(a)**.

Bond length (Å)		Bond angle (°)	
C1-C2	1.3860	C2-C1-N8	120.7348
C1-N9	1.3439	C2-C1-N12	118.7939
C1-N12	1.4697	N8-C1-N12	120.4642
C2-C3	1.3937	C1-C2-C3	119.9663
C2-C10	1.5270	C1-C2-C10	118.4033
C3-C4	1.3953	C3-C2-C10	121.6302
C3-H6	1.0700	C2-C3-C4	118.4165
C4-C5	1.4031	C2-C3-C6	120.7921
C4-Br9	1.9100	C4-C3-C6	120.7910
C5-H7	1.0700	C3-C4-C5	119.2826
C5-N8	1.3454	C3-C4-Br9	120.3585
C10-N13	1.4719	C5-C4-Br9	120.3585
C10-O15	1.2584	C4-C5-H7	119.7200
C11-N12	1.3067	C4-C5-N8	129.5602
C11-N13	1.4835	H7-C5-N8	119.7197
C11-C19	1.5400	C1-N8-C5	120.9551
N13-H14	1.0000	C2-C10-N13	119.3972
C16-C20	1.4015	C2-C10-O15	120.3091
C16-H21	1.0700	N13-C10-O15	120.2912
C16-C25	1.3436	N12-C11-N13	122.9433
C17-C18	1.4015	N12-C11-C19	118.8517
C17-H22	1.0700	N13-C11-C19	118.5234
C17-C25	1.3436	C1-N12-C11	122.4905
C18-C19	1.3956	C10-N13-C11	112.1113
C18-H23	1.0700	C10-N13-H14	108.4081
C19-C22	1.3956	C11-N13-H14	108.1702
C20-H24	1.0700	C20-C16-H21	119.7660
		C21-C16-C25	119.7660

		C18-C17-H22	119.7660
		C18-C17-C25	120.4680
		H22-C17-C25	119.7660
		C17-C18-C19	119.3830
		C17-C18-C23	120.3085
		C19-C18-C23	120.3085
		C11-C19-C18	120.5834
		C11-C19-C20	120.5834

