

Supplementary Data

Kinase and GPCR Polypharmacology to Identify Efficient Anticancer Medicines

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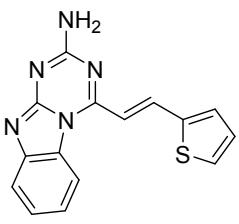
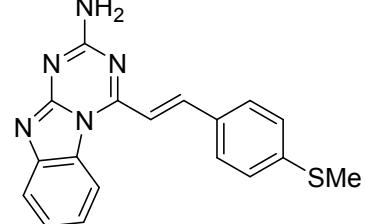
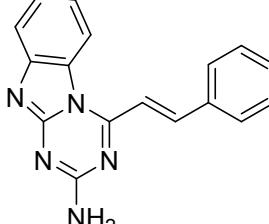
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Appendix I

I. Virtual Screening of M3R Antagonists and CK1 δ Inhibitors

Protein-ligand docking simulations for virtual screening began with the calculation of 3D grids of interaction energy for all possible atom types. These uniquely defined potential grids for M3R and CK1 δ were used for docking simulations of all 328,937 molecules in the docking library. As the center for the common grids in the orthosteric binding pocket and that in the hinge region, we used the center of mass coordinates of tiotropium and compound **16b** in the original X-ray crystal structures of M3R-tiotropium and CK1 δ -**16b** complexes, respectively. The calculated grid maps were of dimension $61 \times 61 \times 61$ points with the spacing of 0.375 Å, which yielded a receptor model including the protein atoms within 22.9 Å of the grid center. Using these two receptor models, docking simulations of individual molecules in the docking library were carried out to select 1000 top-scored ones for both target proteins. The ranks of compounds **1** and **2** were 32 and 55, respectively, in terms of the binding free energy in the orthosteric binding pocket of M3R. **1** and **2** ranked 484 and 519 in the virtual screening of CK1 δ inhibitors, which was carried out with the same scoring function as used in identifying the M3R antagonists.

II. Dose-Response Curves for Inhibitory and Antagonistic Activity

1  NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=CS4)=N1	2  NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(SC)=C)=N1	3  NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=CC=C4)=N1
4	5	6

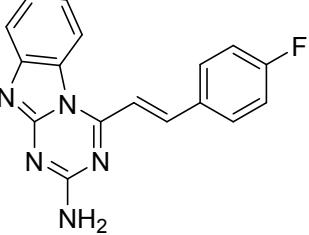
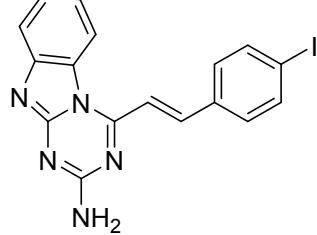
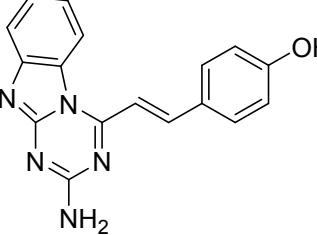
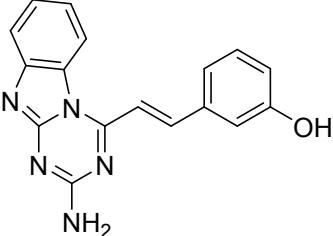
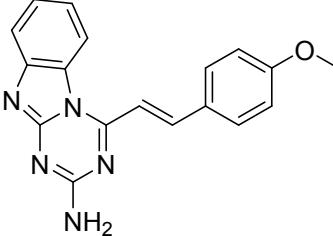
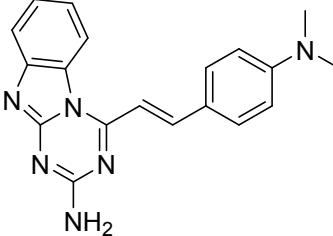
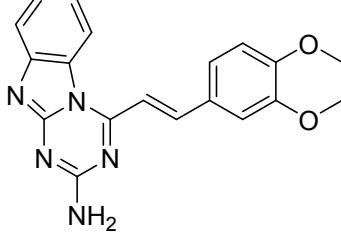
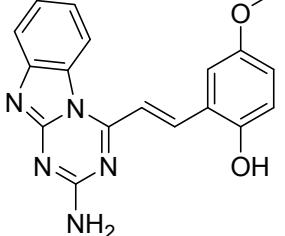
		
NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(F)C=C 4)=N1	NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(I)C=C 4)=N1	NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(O)C=C 4)=N1
7 	8 	9 
NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=CC(O)=C 4)=N1	NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(OC)=C C=C4)=N1	NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(N(C)C C=C4)=N1
10 	11 	
NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(OC)C OC)=C4)=N1	NC1=NC2=NC(C=CC=C3)=C 3N2C(/C=C/C4=CC=C(OC)=C C=C4O)=N1	

Figure S1. Structures and SMILES strings information of compounds.

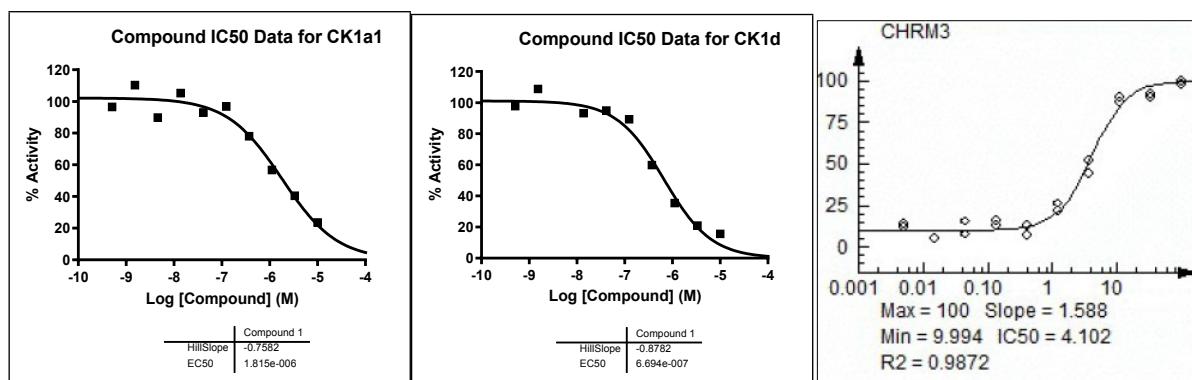


Figure S2. Dose-response curves of compound 1 for CK1 α 1, CK1 δ , and M3R.

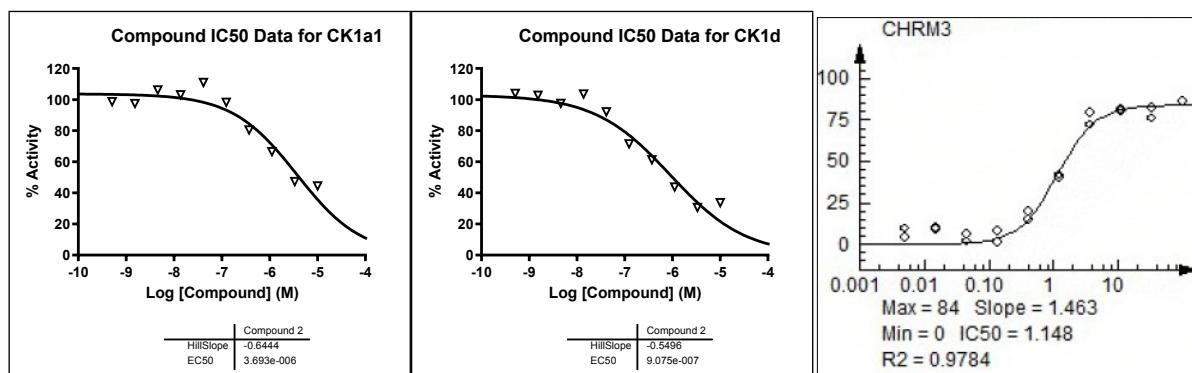


Figure S3. Dose-response curves of compound 2 for CK1 α 1, CK1 δ , and M3R.

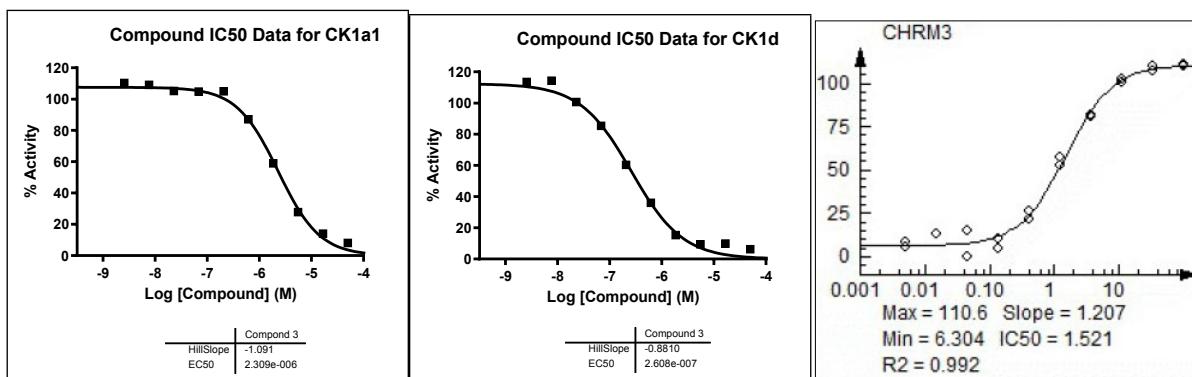


Figure S4. Dose-response curves of compound 3 for CK1 α 1, CK1 δ , and M3R.

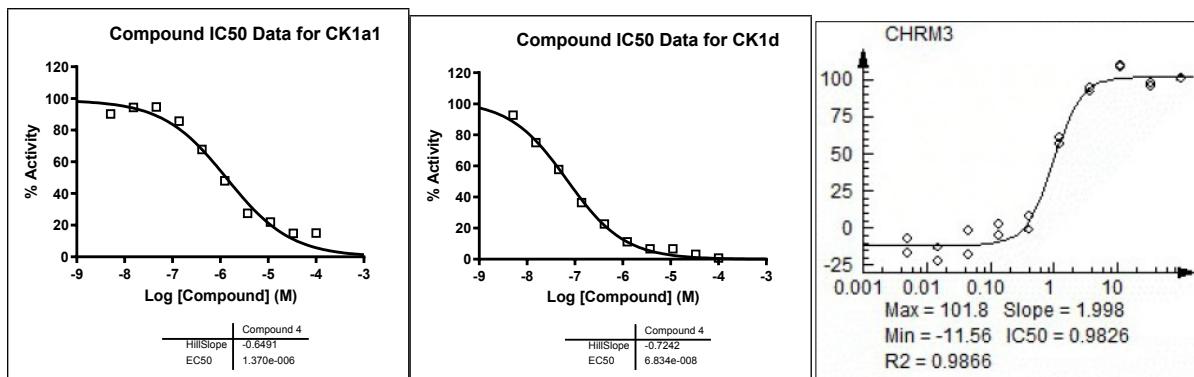


Figure S5. Dose-response curves of compound 4 for CK1 α 1, CK1 δ , and M3R.

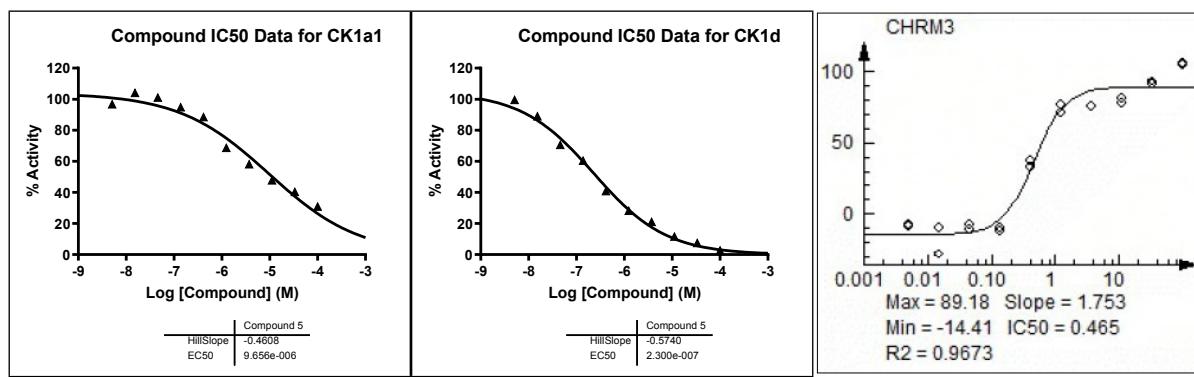


Figure S6. Dose-response curves of compound 5 for CK1 α 1, CK1 δ , and M3R.

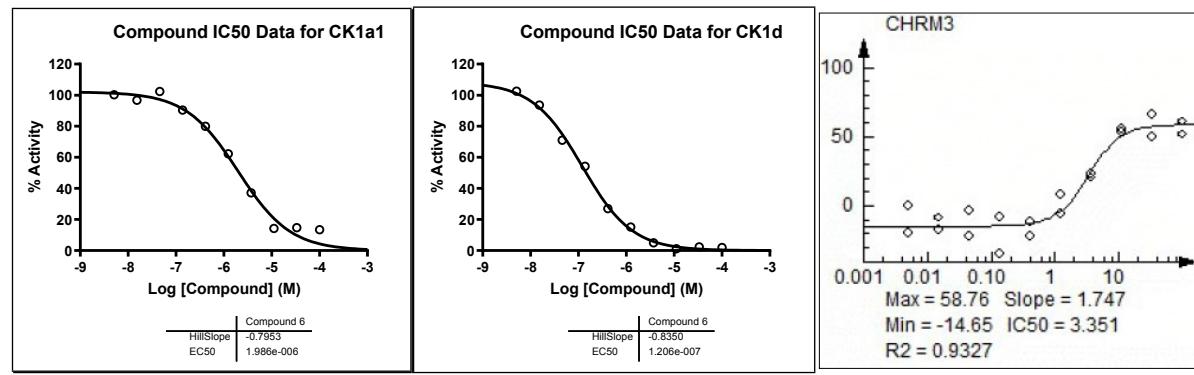


Figure S7. Dose-response curves of compound 6 for CK1 α 1, CK1 δ , and M3R.

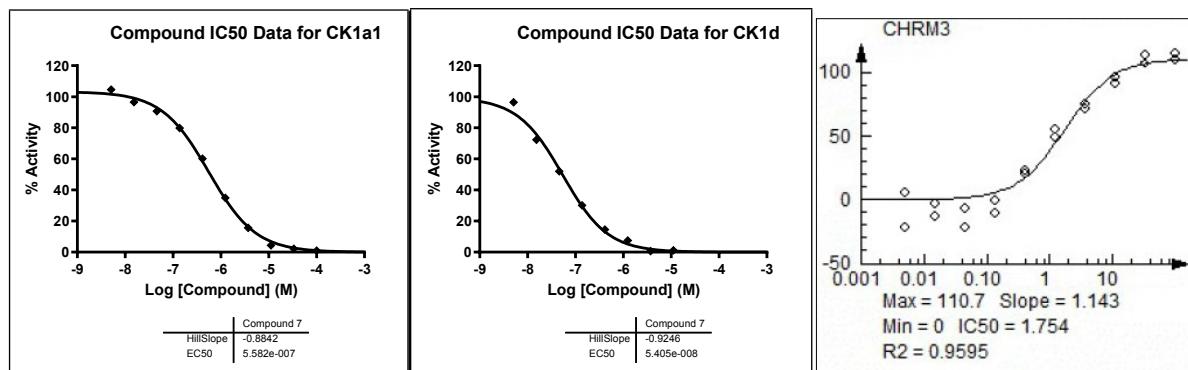


Figure S8. Dose-response curves of compound 7 for CK1 α 1, CK1 δ , and M3R.

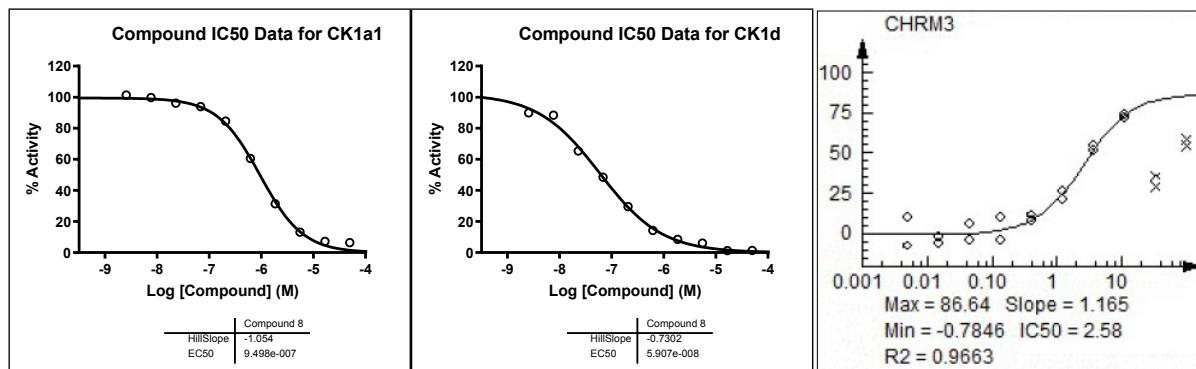


Figure S9. Dose-response curves of compound 8 for CK1 α 1, CK1 δ , and M3R.

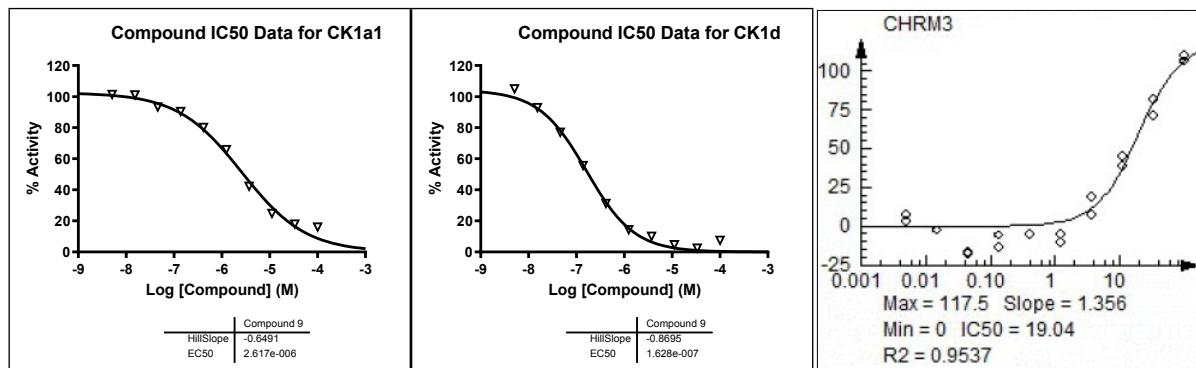


Figure S10. Dose-response curves of compound 9 for CK1 α 1, CK1 δ , and M3R.

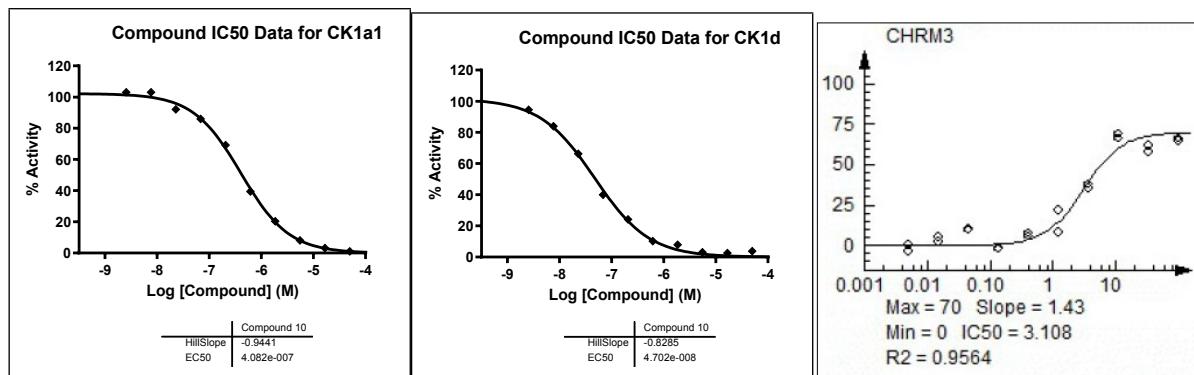


Figure S11. Dose-response curves of compound **10** for CK1 α 1, CK1 δ , and M3R.

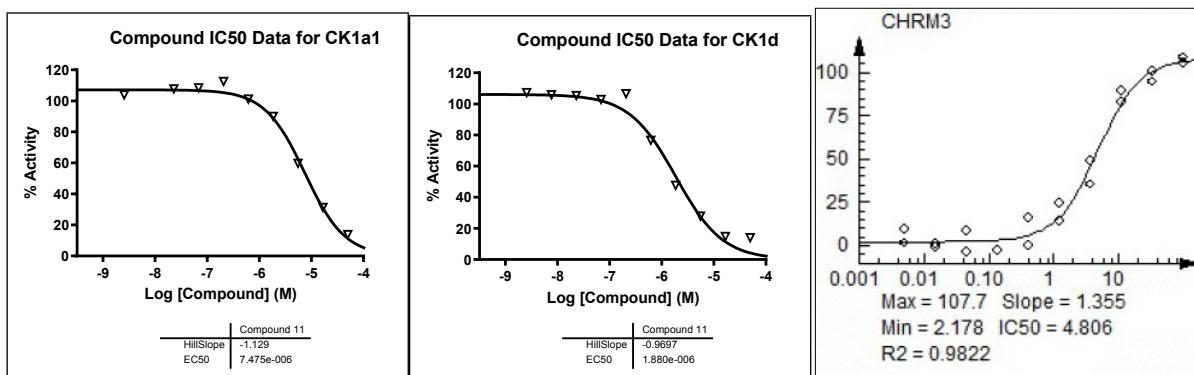


Figure S12. Dose-response curves of compound **11** for CK1 α 1, CK1 δ , and M3R.

III. Evaluation of ATP Competitiveness in the Inhibition of CK1 δ

The experiments were designed to obtain the IC₅₀ values for compound **1** at varying ATP concentrations. The kinase assays were performed at room temperature. Compound **1** was tested in 10-dose IC₅₀ mode with 3-fold serial dilution starting at 100 μ M. A positive control D4476 was also tested in 10-dose IC₅₀ mode with 3-fold serial dilution starting at 20 μ M. Reactions were carried out at 1, 10, 25, 50, and 100 μ M of ATP. The results were summarized in Figure S13 and Table S1.

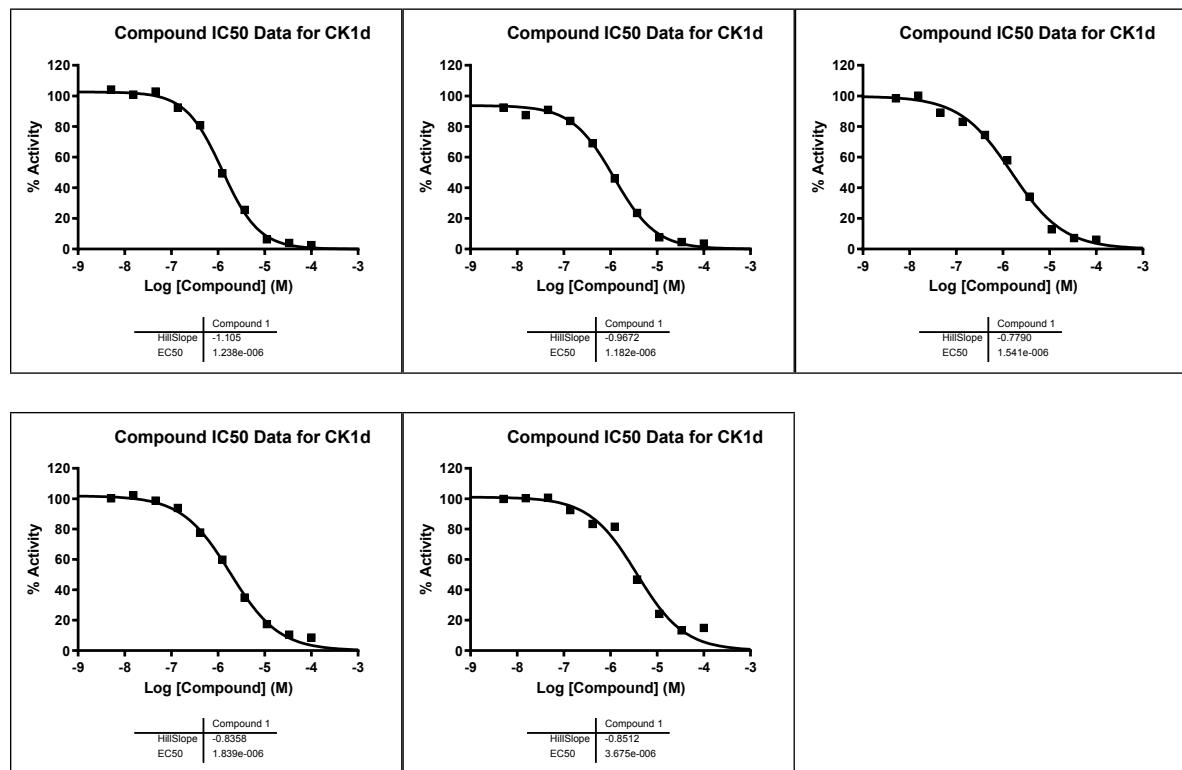


Figure S13. Curve fits of compound **1** for CK1 δ at 1, 10, 25, 50 and 100 μ M ATP.

[ATP] (μ M)	IC ₅₀ (M)	
	compound 1	D4476
1	1.24E-06	4.37E-07
10	1.18E-06	5.34E-07
25	1.54E-06	5.58E-07
50	1.84E-06	6.70E-07
100	3.68E-06	1.11E-06

Table S1. Effects of ATP concentration on the IC₅₀ values of **1** and D4476 with respect to CK1 δ .

IV. Kinase Selectivity Profiles

Kinase:	% Enzyme Activity (relative to DMSO controls)						Control Compound IC ₅₀ (M):	Control Compound ID:		
	1		2		10					
	Data 1	Data 2	Data 1	Data 2	Data 1	Data 2				
ABL1	89.89	88.77	75.26	74.91	101.52	101.33	3.03E-08	Staurosporine		
ABL2/ARG	75.97	74.69	56.15	55.67	85.29	85.24	1.44E-08	Staurosporine		
ACK1	68.80	67.02	80.47	80.46	70.94	68.65	2.00E-08	Staurosporine		
AKT1	86.95	86.35	83.01	83.00	96.88	95.92	4.26E-09	Staurosporine		
AKT2	83.29	80.84	78.28	77.93	92.08	90.35	5.21E-09	Staurosporine		
AKT3	82.71	81.10	58.73	57.74	95.75	93.88	2.94E-09	Staurosporine		
ALK	66.84	65.73	66.28	65.72	76.47	76.22	1.12E-09	Staurosporine		
ALK1/ACVRL1	97.18	94.77	90.79	90.29	94.13	93.56	8.96E-09	LDN193189		
ALK2/ACVR1	103.22	103.07	117.39	115.93	109.78	105.14	1.64E-08	LDN193189		
ALK3/BMPR1A	105.81	104.74	102.74	102.06	100.03	98.77	2.68E-09	LDN193189		
ALK4/ACVR1B	100.07	99.01	97.14	96.65	97.28	95.22	1.27E-07	LDN193189		
ALK5/TGFB1	92.28	90.96	89.36	87.64	99.31	98.73	1.36E-07	LDN193189		
ALK6/BMPR1B	97.78	95.15	104.07	103.37	94.83	94.53	6.64E-09	LDN193189		
ARAF	87.57	84.92	90.32	87.77	87.66	86.31	1.91E-08	GW5074		
ARK5/NUAK1	87.16	86.74	88.36	86.51	90.54	89.90	1.10E-09	Staurosporine		
ASK1/MAP3K5	96.78	95.71	99.56	97.48	93.92	92.54	2.78E-08	Staurosporine		
Aurora A	77.32	71.47	61.95	52.24	105.88	105.55	9.31E-10	Staurosporine		
Aurora B	84.66	84.56	91.65	89.05	99.17	95.77	4.50E-09	Staurosporine		
Aurora C	88.79	88.53	89.87	89.71	91.94	89.83	4.59E-09	Staurosporine		
AXL	75.00	73.03	79.99	79.03	77.93	77.14	9.23E-09	Staurosporine		
BLK	61.25	60.17	40.35	40.17	127.89	124.39	2.74E-09	Staurosporine		
BMPR2	76.26	74.73	91.14	86.44	83.54	82.88	2.12E-07	Staurosporine		
BMX/ETK	82.65	80.94	75.44	75.10	96.71	95.37	5.25E-09	Staurosporine		
BRAF	86.59	85.44	86.67	86.51	84.18	83.19	1.24E-08	GW5074		
BRK	79.49	78.57	84.19	81.59	78.88	78.02	1.54E-07	Staurosporine		
BRSK1	92.85	91.86	83.84	82.46	103.06	100.22	4.90E-10	Staurosporine		
BRSK2	96.92	96.76	95.88	95.61	95.51	93.91	1.59E-09	Staurosporine		
BTK	74.70	73.84	57.26	56.21	86.13	85.74	2.25E-08	Staurosporine		
c-Kit	99.37	98.86	99.51	99.05	93.50	92.02	4.46E-08	Staurosporine		
c-MER	65.05	63.92	65.20	64.71	66.42	66.26	5.60E-09	Staurosporine		
c-MET	102.94	101.40	104.29	92.95	101.71	92.07	6.72E-08	Staurosporine		
c-Src	77.20	76.14	75.77	75.12	81.56	80.27	2.30E-09	Staurosporine		
CAMK1a	80.89	80.03	93.15	92.43	122.80	116.97	7.47E-09	Staurosporine		
CAMK1b	93.51	93.14	87.29	86.38	98.82	97.06	8.67E-09	Staurosporine		

CAMK1d	69.43	69.00	46.94	46.40	100.16	98.58	3.41E-10	Staurosporine
CAMK1g	73.45	72.33	74.32	73.62	82.81	81.33	7.74E-09	Staurosporine
CAMK2a	93.20	90.71	102.47	100.41	91.29	90.19	1.58E-11	Staurosporine
CAMK2b	95.72	94.29	92.64	91.27	97.87	97.39	5.30E-11	Staurosporine
CAMK2d	104.69	101.70	90.75	90.63	107.60	105.78	2.38E-11	Staurosporine
CAMK2g	94.16	93.36	84.80	83.51	94.76	94.62	2.21E-10	Staurosporine
CAMK4	71.53	68.40	64.03	63.07	74.73	74.56	1.34E-07	Staurosporine
CAMKK1	142.81	141.32	109.11	108.48	129.61	126.35	7.77E-08	Staurosporine
CAMKK2	91.45	91.31	96.65	91.70	84.04	82.86	2.39E-08	Staurosporine
CDC7/DBF4	100.61	95.93	108.03	103.30	89.83	81.08	2.21E-08	Staurosporine
CDK1/cyclin A	92.73	91.14	91.74	91.36	96.02	90.91	2.46E-09	Staurosporine
CDK1/cyclin B	81.64	79.88	66.91	66.64	90.46	90.17	1.69E-09	Staurosporine
CDK1/cyclin E	92.28	91.78	84.12	78.62	94.81	94.80	3.18E-09	Staurosporine
CDK14/cyclin Y (PFTK1)	97.10	95.88	98.03	96.35	89.29	88.39	1.77E-07	Staurosporine
CDK16/cyclin Y (PCTAIRE)	104.22	103.73	101.97	101.97	109.33	105.23	1.37E-08	Staurosporine
CDK17/cyclin Y (PCTK2)	96.68	96.64	96.19	93.93	99.90	99.72	1.14E-08	Staurosporine
CDK18/cyclin Y (PCTK3)	97.85	97.14	98.30	95.88	98.81	95.39	2.14E-08	Staurosporine
CDK19/cyclin C	77.96	77.27	84.99	81.87	81.63	79.55	5.49E-11	Staurosporine
CDK2/cyclin A	76.07	75.85	66.67	66.41	81.96	78.54	5.73E-10	Staurosporine
CDK2/Cyclin A1	91.34	90.58	95.55	95.18	96.63	94.77	2.05E-09	Staurosporine
CDK2/cyclin E	101.17	100.09	95.52	95.44	102.38	101.76	3.92E-09	Staurosporine
CDK2/cyclin E2	84.01	83.06	73.53	73.49	82.56	81.48	2.62E-09	Staurosporine
CDK2/cyclin O	83.25	80.62	65.00	64.96	78.01	77.73	2.30E-09	Staurosporine
CDK3/cyclin E	88.65	88.49	76.63	75.74	83.57	83.08	3.25E-09	Staurosporine
CDK3/cyclin E2	88.04	84.39	69.71	68.22	89.17	88.28	3.47E-09	Staurosporine
CDK4/cyclin D1	91.35	88.47	88.14	87.66	94.92	94.46	1.49E-08	Staurosporine
CDK4/cyclin D3	105.08	103.09	122.18	119.77	108.00	105.08	3.96E-08	Staurosporine
CDK5/p25	82.06	81.91	76.74	76.04	87.00	83.44	1.73E-09	Staurosporine
CDK5/p35	96.72	95.67	95.37	94.43	97.07	96.61	1.90E-09	Staurosporine
CDK6/cyclin D1	91.39	91.19	90.37	88.19	93.78	93.01	4.24E-09	Staurosporine
CDK6/cyclin D3	84.48	83.30	87.82	87.17	93.10	91.18	6.37E-08	Staurosporine
CDK7/cyclin H	99.35	98.83	111.55	111.44	102.76	100.68	4.31E-08	Staurosporine
CDK9/cyclin K	98.54	95.02	77.58	76.77	102.22	101.80	1.61E-08	Staurosporine
CDK9/cyclin T1	93.24	93.05	79.03	78.67	107.14	104.00	6.19E-09	Staurosporine
CDK9/cyclin T2	81.07	80.28	50.06	49.38	98.35	95.09	5.44E-09	Staurosporine
CHK1	135.42	134.26	163.40	160.36	97.90	97.63	3.29E-10	Staurosporine
CHK2	88.98	88.17	86.16	85.74	87.86	83.35	8.09E-09	Staurosporine
CK1a1	19.23	18.86	24.04	23.91	5.53	4.19	2.88E-06	Staurosporine
CK1a1L	37.48	36.84	63.88	60.12	13.37	11.82	2.18E-06	Staurosporine

CK1d	4.27	4.21	6.18	5.70	2.73	2.54	1.65E-07	D4476
CK1epsilon	11.15	10.69	19.08	18.41	3.40	3.29	1.43E-07	D4476
CK1g1	55.17	54.99	58.65	56.41	18.53	18.48	5.98E-06	Staurosporine
CK1g2	46.42	44.37	62.39	62.20	31.67	30.94	1.49E-06	Staurosporine
CK1g3	39.54	38.68	62.66	61.25	18.38	16.82	1.32E-06	Staurosporine
CK2a	76.00	74.94	57.66	57.24	94.74	84.31	4.17E-08	GW5074
CK2a2	83.08	82.48	85.09	80.64	101.89	100.71	3.16E-07	Staurosporine
CLK1	51.51	51.46	94.20	90.11	93.34	90.72	1.11E-08	Staurosporine
CLK2	106.39	103.71	135.01	135.00	91.18	88.66	3.95E-09	Staurosporine
CLK3	105.76	103.70	104.67	104.20	102.18	101.64	1.47E-06	Staurosporine
CLK4	47.15	45.43	83.55	83.17	77.21	74.70	3.67E-08	Staurosporine
COT1/MAP3K8	90.22	90.16	93.92	92.88	88.55	88.12	1.16E-05	Ro-31-8220
CSK	86.08	85.64	85.95	85.90	99.79	98.10	1.59E-08	Staurosporine
CTK/MATK	91.88	90.24	77.49	74.42	96.74	94.99	2.10E-06	Staurosporine
DAPK1	68.88	68.86	60.90	59.82	63.66	62.80	3.73E-09	Staurosporine
DAPK2	110.40	107.45	103.89	98.72	110.03	104.71	3.68E-09	Staurosporine
DCAMKL1	83.32	82.96	79.40	78.08	82.54	81.92	1.60E-07	Staurosporine
DCAMKL2	96.15	94.89	98.93	98.91	98.04	97.99	9.58E-08	Staurosporine
DDR1	84.67	84.34	89.60	88.33	90.04	89.61	3.17E-09	Staurosporine
DDR2	111.09	106.28	96.50	95.19	107.16	105.79	4.49E-10	Staurosporine
DLK/MAP3K12	103.72	97.83	100.32	99.75	81.54	81.05	2.71E-07	Staurosporine
DMPK	107.14	106.39	105.40	105.07	114.39	114.12	2.44E-08	Staurosporine
DMPK2	92.96	89.64	88.38	84.50	101.15	100.45	2.20E-10	Staurosporine
DRAK1/STK17A	98.44	96.93	101.40	100.31	105.88	104.08	7.00E-08	Staurosporine
DYRK1/DYRK1A	79.98	79.94	100.22	98.05	88.69	87.59	3.19E-09	Staurosporine
DYRK1B	75.45	73.63	96.58	93.39	88.66	82.55	1.18E-09	Staurosporine
DYRK2	87.60	85.61	92.79	92.69	86.86	86.14	1.23E-07	Staurosporine
DYRK3	82.93	82.80	87.66	85.71	82.79	82.30	8.33E-09	Staurosporine
DYRK4	67.79	65.63	42.63	42.30	99.89	99.63	1.02E-06	GW5074
EGFR	41.65	41.54	85.81	85.76	79.47	79.22	7.90E-08	Staurosporine
EPHA1	94.55	93.46	102.15	97.93	99.13	98.37	1.22E-07	Staurosporine
EPHA2	81.62	81.57	87.06	86.50	87.58	87.58	4.67E-08	Staurosporine
EPHA3	101.14	100.35	99.03	94.28	97.01	94.72	3.50E-08	Staurosporine
EPHA4	90.50	89.92	94.11	94.11	97.69	97.54	1.15E-08	Staurosporine
EPHA5	85.45	84.73	75.15	75.12	97.21	96.98	1.61E-08	Staurosporine
EPHA6	101.07	99.95	98.34	97.81	109.32	105.09	8.05E-08	Staurosporine
EPHA7	90.96	90.27	89.41	88.19	90.02	90.01	3.14E-08	Staurosporine
EPHA8	99.00	97.78	91.94	87.75	107.17	105.34	1.38E-07	Staurosporine
EPHB1	99.06	97.91	101.03	99.70	101.02	100.44	3.51E-08	Staurosporine
EPHB2	88.53	85.21	96.70	95.88	95.40	94.68	5.64E-08	Staurosporine

EPHB3	93.86	93.75	90.98	90.29	106.77	105.45	1.55E-06	Staurosporine
EPHB4	81.85	80.34	86.81	85.25	100.12	98.87	1.91E-07	Staurosporine
ERBB2/HER2	88.04	87.40	80.67	79.11	93.84	93.20	2.24E-07	Staurosporine
ERBB4/HER4	90.10	88.68	85.45	80.89	82.38	82.32	1.68E-07	Staurosporine
ERK1	102.79	98.37	104.72	101.27	94.30	91.77	1.10E-08	SCH772984
ERK2/MAPK1	104.35	101.89	102.22	102.12	98.68	98.08	9.26E-09	SCH772984
ERK5/MAPK7	83.96	81.62	79.58	79.08	85.71	85.14	5.04E-06	Staurosporine
ERK7/MAPK15	98.60	96.21	81.69	80.14	98.91	97.18	2.42E-09	Staurosporine
ERN1/IRE1	99.69	99.69	95.96	95.63	98.63	96.69	5.08E-08	Staurosporine
ERN2/IRE2	75.62	75.48	83.60	83.26	86.91	85.21	2.30E-08	Staurosporine
FAK/PTK2	92.30	91.56	91.09	90.94	92.94	92.63	1.35E-08	Staurosporine
FER	81.97	80.61	69.01	68.43	98.03	97.63	8.59E-10	Staurosporine
FES/FPS	88.86	88.36	84.90	84.87	101.51	100.08	1.96E-09	Staurosporine
FGFR1	93.69	92.53	98.14	97.89	108.51	105.62	3.58E-09	Staurosporine
FGFR2	88.07	88.02	107.23	96.76	95.76	94.97	1.35E-09	Staurosporine
FGFR3	64.58	63.91	56.62	55.54	101.90	99.44	8.05E-09	Staurosporine
FGFR4	59.91	59.19	45.26	44.93	88.57	87.19	9.23E-08	Staurosporine
FGR	72.11	71.80	73.96	73.06	80.17	79.46	5.84E-10	Staurosporine
FLT1/VEGFR1	96.44	94.60	94.79	92.86	83.53	83.42	3.21E-08	Staurosporine
FLT3	70.21	69.98	68.07	67.75	84.94	84.93	1.06E-09	Staurosporine
FLT4/VEGFR3	80.38	78.89	76.79	75.41	89.67	88.92	2.25E-09	Staurosporine
FMS	91.85	91.36	98.37	98.21	91.80	91.72	2.13E-09	Staurosporine
FRK/PTK5	102.37	101.81	100.17	98.51	103.86	101.30	1.02E-08	Staurosporine
FYN	67.85	66.98	52.57	52.49	82.96	82.77	1.68E-09	Staurosporine
GCK/MAP4K2	89.70	87.70	87.82	85.34	90.51	88.77	9.74E-10	Staurosporine
GLK/MAP4K3	102.19	100.01	86.52	84.42	100.03	97.74	1.07E-10	Staurosporine
GRK1	98.39	97.08	91.46	90.86	106.20	101.34	4.93E-08	Staurosporine
GRK2	98.07	96.34	100.64	100.28	96.53	94.54	1.06E-06	Staurosporine
GRK3	108.23	104.79	106.61	105.85	97.34	96.76	6.62E-07	Staurosporine
GRK4	85.48	84.69	91.27	91.26	98.44	94.26	1.03E-07	Staurosporine
GRK5	87.08	85.79	94.22	93.73	90.36	89.49	3.17E-08	Staurosporine
GRK6	90.59	90.32	87.94	87.65	93.77	92.49	4.21E-08	Staurosporine
GRK7	94.78	94.44	88.52	88.23	97.50	95.90	5.23E-09	Staurosporine
GSK3a	75.67	72.21	80.36	79.27	92.95	92.43	3.67E-09	Staurosporine
GSK3b	77.46	76.56	89.64	86.16	67.73	63.25	5.64E-09	Staurosporine
Haspin	99.45	97.12	99.99	99.61	96.93	96.36	9.82E-08	Staurosporine
HCK	69.52	68.47	56.25	54.49	86.63	85.57	1.86E-09	Staurosporine
HGK/MAP4K4	93.12	88.24	118.24	114.86	79.71	79.43	3.13E-10	Staurosporine
HIPK1	75.53	73.97	83.25	82.65	86.12	82.16	5.23E-07	Ro-31-8220
HIPK2	107.38	105.27	95.45	93.97	105.96	101.45	2.40E-06	Staurosporine

HIPK3	86.04	84.28	107.27	106.66	110.34	109.10	3.16E-07	Staurosporine
HIPK4	100.64	96.14	107.87	106.80	110.58	109.74	8.81E-07	Staurosporine
HPK1/MAP4K1	104.19	104.09	94.96	93.93	107.70	103.74	1.19E-07	Ro-31-8220
IGF1R	79.64	79.09	86.44	85.91	87.74	87.57	2.02E-08	Staurosporine
IKKa/CHUK	91.09	91.00	91.36	91.35	97.96	97.67	9.21E-08	Staurosporine
IKKb/IKBKB	86.92	84.70	81.39	80.65	98.91	96.73	3.73E-07	Staurosporine
IKKe/IKBKE	90.64	90.26	83.94	82.61	105.92	104.68	3.27E-10	Staurosporine
IR	95.47	94.49	94.46	91.74	109.07	107.86	1.12E-08	Staurosporine
IRAK1	201.41	192.28	199.25	192.86	106.23	105.75	1.57E-08	Staurosporine
IRAK4	78.26	72.66	145.39	134.40	87.07	83.08	3.06E-09	Staurosporine
IRR/INSRR	65.79	62.41	66.86	66.65	92.96	92.79	4.90E-09	Staurosporine
ITK	100.54	97.88	96.09	95.87	99.75	95.81	1.07E-08	Staurosporine
JAK1	92.37	91.80	99.45	97.42	92.94	90.82	5.99E-10	Staurosporine
JAK2	84.95	82.69	76.36	74.75	103.35	103.25	1.74E-10	Staurosporine
JAK3	85.92	85.57	70.99	70.14	103.37	103.13	1.24E-10	Staurosporine
JNK1	95.59	95.27	95.27	94.08	94.96	91.15	3.44E-07	Staurosporine
JNK2	94.00	93.93	96.23	95.98	94.58	94.43	7.22E-07	Staurosporine
JNK3	100.26	96.51	96.77	93.79	85.68	85.14	6.65E-07	JNKi VIII
KDR/VEGFR2	93.31	92.62	91.25	90.14	96.98	96.79	6.31E-09	Staurosporine
KHS/MAP4K5	94.51	94.25	106.09	103.18	103.02	98.40	4.53E-10	Staurosporine
KSR1	84.67	84.49	79.22	78.54	89.43	89.08	8.55E-06	Staurosporine
KSR2	86.21	85.11	67.67	66.53	99.28	97.48	9.29E-06	Staurosporine
LATS1	96.37	95.31	99.58	97.38	99.81	97.96	1.39E-08	Staurosporine
LATS2	80.34	77.58	78.03	77.91	92.34	90.04	3.43E-09	Staurosporine
LCK	74.58	73.93	59.81	58.35	103.84	102.42	4.37E-09	Staurosporine
LCK2/ICK	100.07	99.23	105.74	100.99	109.01	105.94	6.64E-08	Staurosporine
LIMK1	88.63	88.60	94.01	93.73	99.22	97.51	9.41E-10	Staurosporine
LIMK2	97.05	96.11	93.20	92.78	95.14	94.70	6.36E-08	Staurosporine
LKB1	81.76	80.78	108.79	108.66	113.45	110.58	1.11E-07	Staurosporine
LOK/STK10	84.94	83.86	88.72	88.50	90.28	88.87	4.51E-08	Ro-31-8220
LRRK2	83.58	83.48	92.27	90.96	79.94	78.19	4.94E-09	Staurosporine
LYN	83.41	83.03	82.37	82.17	103.61	103.21	1.21E-09	Staurosporine
LYN B	79.61	79.16	77.60	76.11	93.02	92.62	1.98E-09	Staurosporine
MAK	79.98	79.44	90.93	90.59	91.15	89.60	2.23E-08	Staurosporine
MAPKAPK2	80.92	80.37	53.21	52.57	93.33	92.21	9.68E-08	Staurosporine
MAPKAPK3	94.70	92.55	59.22	54.37	96.97	94.53	2.40E-06	Staurosporine
MAPKAPK5/PRA K	82.91	82.77	68.37	67.48	98.58	98.39	2.04E-07	Staurosporine
MARK1	95.19	93.83	94.46	91.60	97.37	96.27	1.39E-10	Staurosporine
MARK2/PAR-1Ba	92.71	90.06	92.55	90.48	100.94	99.02	1.01E-10	Staurosporine

MARK3	97.46	96.27	97.69	95.37	99.47	96.58	1.21E-10	Staurosporine
MARK4	95.68	95.03	95.42	94.49	98.27	97.67	7.44E-12	Staurosporine
MEK1	96.19	95.42	95.42	94.74	102.05	100.91	1.57E-08	Staurosporine
MEK2	90.43	89.17	90.13	88.88	100.45	99.47	2.85E-08	Staurosporine
MEK3	100.09	98.82	96.97	96.90	108.12	107.76	5.42E-09	Staurosporine
MEK5	104.00	103.69	104.59	102.53	99.42	99.23	1.70E-08	Staurosporine
MEKK1	101.13	98.01	114.47	112.59	102.91	100.27	1.39E-06	Staurosporine
MEKK2	94.06	89.12	114.43	113.53	106.69	102.54	1.40E-07	Staurosporine
MEKK3	73.12	72.74	103.37	97.73	103.54	96.88	1.90E-08	Staurosporine
MEKK6	111.00	109.01	127.01	122.09	44.09	42.65	1.79E-07	Staurosporine
MELK	68.28	65.65	60.29	59.57	79.01	78.79	5.92E-10	Staurosporine
MINK/MINK1	111.60	105.02	100.25	94.95	83.15	80.73	3.84E-10	Staurosporine
MKK4	97.72	92.60	99.27	98.72	100.33	99.20	2.16E-06	Staurosporine
MKK6	86.69	85.18	80.72	80.58	88.04	87.71	3.90E-09	Staurosporine
MKK7	100.06	99.96	97.88	96.17	94.74	90.74	9.21E-07	Staurosporine
MLCK/MYLK	89.93	89.67	93.70	93.18	90.17	89.28	5.59E-08	Staurosporine
MLCK2/MYLK2	92.63	91.79	95.65	95.17	103.09	100.97	2.12E-08	Staurosporine
MLK1/MAP3K9	72.27	71.96	78.48	77.35	86.81	86.12	1.13E-09	Staurosporine
MLK2/MAP3K10	90.53	84.00	70.25	68.84	94.47	93.61	4.20E-09	Staurosporine
MLK3/MAP3K11	93.27	93.16	103.79	103.72	95.90	95.60	4.01E-09	Staurosporine
MLK4	94.94	90.80	103.30	102.86	95.70	95.19	1.75E-06	Staurosporine
MNK1	115.13	113.36	143.18	132.24	114.41	113.58	7.15E-08	Staurosporine
MNK2	104.63	104.33	83.81	82.77	110.80	109.33	2.15E-08	Staurosporine
MRCKa/CDC42BP A	94.52	94.47	93.49	90.34	117.86	117.47	2.00E-09	Staurosporine
MRCKb/CDC42BP B	111.41	111.26	109.83	104.41	113.84	111.44	1.63E-09	Staurosporine
MSK1/RPS6KA5	84.41	82.54	72.99	72.29	96.57	91.24	5.14E-10	Staurosporine
MSK2/RPS6KA4	92.94	92.92	92.49	89.15	103.18	102.44	3.92E-09	Staurosporine
MSSK1/STK23	93.27	92.32	89.12	87.85	99.70	95.64	1.95E-06	Staurosporine
MST1/STK4	96.08	91.56	90.19	87.49	98.65	98.07	2.08E-09	Staurosporine
MST2/STK3	95.38	94.01	97.51	96.43	93.22	88.19	5.77E-09	Staurosporine
MST3/STK24	93.42	93.03	90.49	87.08	81.10	81.02	4.02E-09	Staurosporine
MST4	80.78	80.55	84.67	83.20	86.75	86.38	1.52E-08	Staurosporine
MUSK	83.02	81.55	88.84	88.74	87.21	85.11	1.16E-07	Staurosporine
MYLK3	102.09	101.74	106.00	103.53	100.55	99.15	1.50E-07	Staurosporine
MYLK4	77.35	76.11	69.35	68.79	96.20	93.45	5.95E-08	Staurosporine
MYO3A	101.02	98.24	97.99	97.72	97.27	97.14	3.51E-08	Staurosporine
MYO3b	112.76	109.98	116.57	113.57	110.62	107.59	4.86E-09	Staurosporine
NEK1	119.39	111.15	138.27	134.93	156.57	147.33	7.67E-09	Staurosporine
NEK11	77.80	77.78	74.95	73.34	92.54	90.29	1.12E-06	Staurosporine

NEK2	81.53	81.14	52.92	52.72	69.56	68.16	1.94E-07	Staurosporine
NEK3	75.04	75.01	43.17	42.63	80.39	76.96	1.51E-05	Staurosporine
NEK4	96.35	91.53	75.42	68.04	96.90	94.89	2.01E-07	Staurosporine
NEK5	103.97	102.67	98.56	98.02	102.26	98.56	7.41E-08	Staurosporine
NEK6	89.95	89.89	85.01	84.83	96.47	93.54	6.52E-06	PKR Inhibitor
NEK7	120.15	120.07	108.60	107.07	103.80	101.69	1.43E-05	PKR Inhibitor
NEK8	93.96	89.42	99.64	96.00	97.69	92.16	1.68E-08	Staurosporine
NEK9	82.94	78.81	75.27	73.57	104.43	103.79	1.89E-07	Staurosporine
NIM1	90.90	90.34	83.27	83.17	110.38	107.67	1.47E-07	Staurosporine
NLK	107.34	101.59	105.24	104.77	106.03	105.52	1.28E-07	Staurosporine
OSR1/OXSR1	84.87	84.49	84.78	80.46	91.41	90.95	4.58E-08	Staurosporine
P38a/MAPK14	123.02	115.91	118.39	115.25	117.14	112.87	1.56E-08	SB202190
P38b/MAPK11	94.37	90.53	102.68	96.73	94.52	90.20	1.52E-08	SB202190
P38d/MAPK13	114.43	112.92	118.96	114.24	102.11	101.77	1.68E-07	Staurosporine
P38g	100.43	97.06	110.90	110.72	100.82	98.50	8.88E-08	Staurosporine
p70S6K/RPS6KB1	88.92	88.77	82.35	82.00	94.87	93.85	8.65E-10	Staurosporine
p70S6Kb/RPS6KB2	85.20	84.59	71.69	71.50	97.62	96.17	1.33E-09	Staurosporine
PAK1	92.75	92.28	180.17	172.94	89.43	88.30	4.53E-10	Staurosporine
PAK2	96.95	96.69	104.49	104.04	104.61	103.63	2.26E-09	Staurosporine
PAK3	98.82	97.65	95.39	94.55	101.41	101.22	1.72E-09	Staurosporine
PAK4	100.91	97.90	103.27	103.08	91.39	88.98	2.00E-08	Staurosporine
PAK5	85.36	85.26	63.05	62.10	96.42	94.29	3.43E-09	Staurosporine
PAK6	85.72	83.86	92.44	91.64	83.48	82.25	5.74E-08	Staurosporine
PASK	90.51	89.95	89.13	86.76	92.79	90.65	6.97E-09	Staurosporine
PBK/TOPK	83.11	80.78	70.85	69.35	98.09	96.61	5.39E-08	Staurosporine
PDGFRa	90.39	89.35	85.80	84.57	94.34	92.80	6.50E-10	Staurosporine
PDGFRb	79.08	78.58	75.41	73.77	84.24	82.89	1.93E-09	Staurosporine
PDK1/PDPK1	97.42	92.30	89.21	87.79	108.53	106.86	3.45E-10	Staurosporine
PEAK1	87.26	85.42	85.57	84.81	86.95	86.03	2.85E-09	Staurosporine
PHKg1	91.37	89.80	92.18	90.30	91.58	91.13	3.08E-09	Staurosporine
PHKg2	87.74	86.83	89.24	88.14	89.42	85.29	5.31E-10	Staurosporine
PIM1	73.47	73.21	57.77	56.91	93.08	91.91	3.98E-09	Staurosporine
PIM2	81.31	81.18	53.05	52.55	103.87	102.78	1.36E-08	Staurosporine
PIM3	70.83	70.75	78.98	78.93	84.87	84.62	1.42E-10	Staurosporine
PKA	109.72	93.05	103.32	93.85	98.56	97.87	2.83E-10	Staurosporine
PKAcb	89.24	89.11	73.55	73.42	100.68	100.18	8.23E-10	Staurosporine
PKAcg	104.39	103.54	97.10	97.08	108.17	104.92	1.57E-09	Staurosporine
PKCa	97.98	97.78	97.46	97.01	92.74	92.30	5.95E-10	Staurosporine
PKCb1	83.33	82.30	83.26	81.90	80.07	79.40	4.81E-09	Staurosporine

PKCb2	90.69	89.61	89.35	86.47	81.68	80.38	3.69E-09	Staurosporine
PKCd	81.04	80.60	68.71	68.46	92.53	92.04	1.61E-10	Staurosporine
PKCepsilon	109.48	106.94	105.38	104.42	112.71	109.82	1.56E-10	Staurosporine
PKCeta	109.29	107.37	108.09	106.09	117.30	113.41	4.78E-10	Staurosporine
PKCg	82.33	81.24	79.31	78.93	81.53	80.47	1.14E-09	Staurosporine
PKCiota	93.45	91.40	97.08	96.33	104.43	102.58	1.59E-08	Staurosporine
PKCmu/PRKD1	83.88	83.29	83.42	83.31	90.13	85.43	1.13E-09	Staurosporine
PKCnu/PRKD3	84.12	83.48	79.90	79.79	93.54	92.46	1.26E-09	Staurosporine
PKCtheta	81.66	79.47	72.33	71.60	79.74	79.68	2.44E-09	Staurosporine
PKCzeta	85.60	85.18	82.75	81.11	90.89	89.05	3.49E-08	Staurosporine
PKD2/PRKD2	73.83	73.76	76.25	75.21	81.89	81.42	1.00E-09	Staurosporine
PKG1a	98.62	98.11	122.08	121.68	89.76	89.07	1.14E-09	Staurosporine
PKG1b	115.29	112.26	126.52	125.46	99.86	98.05	3.66E-09	Staurosporine
PKG2/PRKG2	95.06	90.99	109.12	101.83	104.01	100.30	3.32E-09	Staurosporine
PKN1/PRK1	97.91	95.76	95.10	92.97	96.61	95.60	2.76E-10	Staurosporine
PKN2/PRK2	88.96	86.78	81.74	80.95	94.38	91.32	9.10E-10	Staurosporine
PKN3/PRK3	91.85	90.78	91.93	89.03	94.23	94.10	1.04E-08	Staurosporine
PLK1	78.11	78.01	75.53	75.02	86.23	84.60	1.16E-07	Staurosporine
PLK2	73.16	72.29	88.03	87.84	89.10	88.89	4.55E-07	Staurosporine
PLK3	75.97	74.70	81.62	81.10	83.47	82.66	2.88E-09	BI2536
PLK4/SAK	80.16	77.62	88.49	88.19	80.94	80.76	6.35E-09	Staurosporine
PRKX	71.40	70.18	74.76	73.54	91.21	91.17	1.70E-09	Staurosporine
PYK2	96.65	96.56	96.52	96.31	99.51	99.26	9.08E-09	Staurosporine
RAF1	98.54	98.40	99.86	98.59	94.39	92.44	7.55E-09	GW5074
RET	80.22	78.94	73.07	72.12	94.78	94.28	2.17E-09	Staurosporine
RIPK2	87.97	85.51	95.26	93.25	94.87	93.81	1.82E-07	Staurosporine
RIPK3	107.99	101.18	108.19	102.59	104.60	102.49	3.77E-07	GW5074
RIPK4	73.79	73.16	78.87	76.36	84.52	81.02	1.47E-07	Staurosporine
RIPK5	72.13	71.06	68.80	68.33	76.06	72.43	1.99E-08	Staurosporine
ROCK1	88.04	87.97	90.88	89.38	86.53	84.45	5.23E-10	Staurosporine
ROCK2	82.33	81.12	86.09	84.51	84.49	84.33	5.26E-10	Staurosporine
RON/MST1R	84.01	82.89	77.28	76.60	87.24	84.91	7.82E-08	Staurosporine
ROS/ROS1	74.74	74.67	82.37	76.86	78.09	77.02	3.52E-10	Staurosporine
RSK1	69.97	69.00	38.78	38.25	90.91	89.65	1.56E-10	Staurosporine
RSK2	81.77	80.93	68.00	67.46	91.11	87.54	2.87E-10	Staurosporine
RSK3	97.33	96.79	99.36	97.59	97.11	94.94	2.79E-10	Staurosporine
RSK4	89.34	88.06	80.26	79.97	94.48	93.82	1.77E-10	Staurosporine
SBK1	120.21	113.55	107.82	107.52	107.78	106.39	7.82E-08	Staurosporine
SGK1	90.18	90.02	91.63	90.17	102.27	100.82	8.21E-09	Staurosporine
SGK2	85.10	85.00	90.19	89.20	95.56	93.17	1.82E-08	Staurosporine

SGK3/SGKL	88.80	85.75	91.15	90.61	98.19	96.11	3.62E-08	Staurosporine
SIK1	90.37	86.56	84.50	83.31	95.84	90.29	1.04E-09	Staurosporine
SIK2	101.19	100.42	102.55	98.22	96.95	96.28	8.67E-10	Staurosporine
SIK3	100.76	89.22	116.23	103.81	91.68	91.47	1.01E-09	Staurosporine
SLK/STK2	94.75	94.33	96.67	95.04	99.32	96.42	1.34E-08	Staurosporine
SNARK/NUAK2	84.33	81.82	88.88	87.57	89.39	88.15	2.24E-09	Staurosporine
SNRK	97.16	96.20	96.50	94.01	97.46	97.40	9.26E-09	Staurosporine
SRMS	90.40	89.84	87.00	86.59	94.71	91.10	2.60E-06	Staurosporine
SRPK1	96.39	96.35	97.51	96.58	99.19	98.33	3.60E-08	Staurosporine
SRPK2	90.09	89.97	86.91	86.15	88.09	86.25	2.37E-07	Staurosporine
SSTK/TSSK6	95.83	95.62	100.59	99.71	100.69	91.16	8.07E-08	Staurosporine
STK16	91.34	90.76	92.01	88.07	95.79	95.02	4.21E-07	Staurosporine
STK21/CIT	101.81	98.63	116.95	113.69	90.65	87.60	4.25E-07	Staurosporine
STK22D/TSSK1	88.42	87.31	78.94	78.35	84.60	83.95	5.15E-11	Staurosporine
STK25/YSK1	142.12	139.62	123.86	123.58	98.14	96.27	2.73E-09	Staurosporine
STK32B/YANK2	130.81	130.20	132.11	125.91	129.33	124.13	4.07E-08	Staurosporine
STK32C/YANK3	82.69	82.48	85.11	82.21	78.08	78.04	1.85E-07	Staurosporine
STK33	91.00	87.68	87.86	86.77	74.58	73.78	3.38E-08	Staurosporine
STK38/NDR1	86.09	85.63	62.37	61.46	95.41	94.64	7.15E-10	Staurosporine
STK38L/NDR2	87.22	86.13	76.91	75.99	97.05	96.37	1.07E-09	Staurosporine
STK39/STLK3	74.94	74.38	89.31	86.98	73.49	71.49	4.29E-08	Staurosporine
SYK	86.39	86.26	96.86	95.17	94.13	92.41	2.73E-10	Staurosporine
TAK1	95.80	95.28	93.66	93.42	97.28	97.04	7.18E-08	Staurosporine
TAOK1	100.05	98.41	101.89	101.80	98.29	96.27	1.16E-09	Staurosporine
TAOK2/TAO1	97.60	97.53	97.50	95.95	96.63	95.71	5.42E-09	Staurosporine
TAOK3/JIK	96.38	95.97	112.57	110.83	103.34	97.60	2.30E-09	Staurosporine
TBK1	110.63	109.56	125.20	121.83	106.97	105.78	2.60E-09	Staurosporine
TEC	81.01	80.50	51.30	51.25	96.29	94.28	5.66E-08	Staurosporine
TESK1	80.64	76.36	70.70	69.23	92.71	92.46	2.07E-07	Staurosporine
TESK2	105.46	105.46	106.70	106.05	108.11	102.81	6.22E-06	Staurosporine
TGFBR2	84.37	83.99	98.85	97.88	88.71	87.45	6.23E-08	LDN193189
TIE2/TEK	71.13	70.82	38.55	37.32	107.57	103.17	4.33E-08	Staurosporine
TLK1	83.72	80.33	97.18	92.44	89.98	86.08	1.85E-08	Staurosporine
TLK2	94.60	94.15	92.07	91.81	92.62	92.48	1.82E-09	Staurosporine
TNIK	66.27	65.52	69.50	67.94	74.29	68.05	6.49E-10	Staurosporine
TNK1	90.88	89.83	86.94	86.03	90.45	90.06	5.23E-09	Staurosporine
TRKA	94.26	94.12	79.13	76.38	90.34	88.33	4.43E-09	Staurosporine
TRKB	74.44	69.24	84.88	84.56	85.13	84.18	8.30E-11	Staurosporine
TRKC	78.37	77.10	82.78	81.15	94.91	94.87	1.91E-10	Staurosporine
TSSK2	71.47	70.77	48.49	47.53	105.45	104.29	5.49E-09	Staurosporine

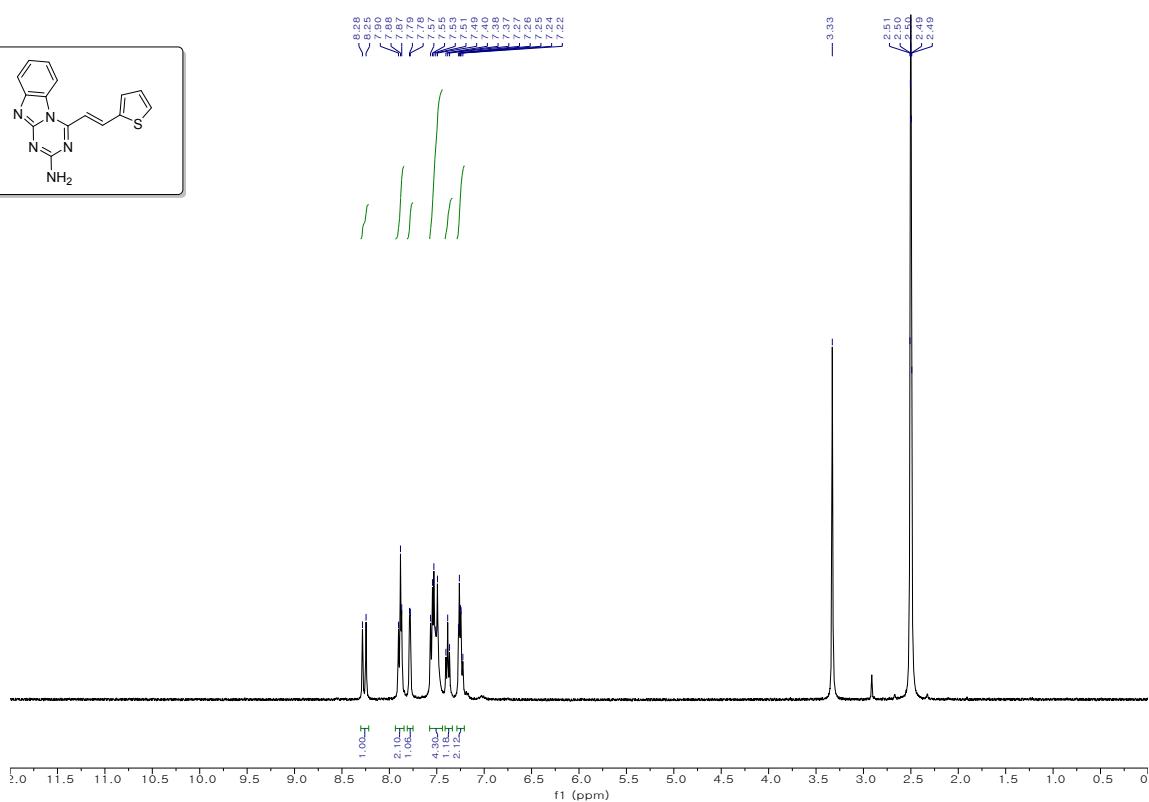
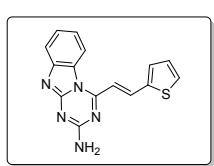
TSSK3/STK22C	79.10	76.68	79.21	78.93	91.41	88.18	7.18E-09	Staurosporine
TTBK1	98.94	96.42	89.38	89.12	91.38	90.83	7.62E-06	SB202190
TTBK2	97.60	95.52	84.95	84.48	99.43	96.23	3.61E-06	SB202190
TXK	77.99	76.85	74.15	73.12	79.41	79.39	2.22E-08	Staurosporine
TYK1/LTK	91.54	88.07	94.41	93.59	107.29	106.12	1.67E-08	Staurosporine
TYK2	86.49	83.05	90.58	88.63	97.51	95.64	1.71E-10	Staurosporine
TYRO3/SKY	96.87	95.68	99.38	98.53	95.56	94.99	4.48E-09	Staurosporine
ULK1	108.32	107.55	109.48	108.58	103.44	102.70	2.59E-08	Staurosporine
ULK2	102.34	101.36	102.39	101.90	91.42	86.49	4.01E-09	Staurosporine
ULK3	105.85	102.19	106.14	101.04	106.72	101.81	1.96E-09	Staurosporine
VRK1	97.92	95.30	98.98	97.67	95.37	95.09	6.11E-07	Ro-31-8220
VRK2	81.84	80.42	83.05	77.08	70.94	68.71	4.79E-06	Ro-31-8220
WEE1	75.88	75.13	77.70	74.55	76.27	74.17	7.49E-08	Wee-1 Inhibitor
WNK1	106.80	100.80	100.41	98.30	115.48	107.00	1.04E-05	Staurosporine
WNK2	110.52	109.69	110.61	107.96	109.42	109.37	3.24E-06	Staurosporine
WNK3	93.41	90.05	91.79	89.49	100.78	95.65	9.13E-07	Wee-1 Inhibitor
YES/YES1	77.65	77.01	77.16	74.45	96.12	92.85	2.21E-09	Staurosporine
YSK4/MAP3K19	93.15	91.11	87.20	85.08	92.99	92.52	4.00E-09	Staurosporine
ZAK/MLTK	59.02	57.07	58.65	55.55	79.03	78.80	8.72E-07	GW5074
ZAP70	88.19	85.70	71.87	71.04	102.16	101.72	5.82E-09	Staurosporine
ZIPK/DAPK3	106.39	104.56	92.00	86.83	110.18	107.75	3.57E-09	Staurosporine

Table S2. Kinase selectivity profiles of compounds **1**, **2**, **10**. Experiment was performed by Reaction Biology Corp. (Malvern, PA, USA). Compounds were tested in single dose duplicate mode at a concentration of 10 μ M against panel of 371 kinases. Control compound Staurosporine was tested in 10-dose IC₅₀ mode with 4-fold serial dilution starting at 20, 40, or 100 μ M. Alternate control compounds were tested in 10-dose IC₅₀ mode with 3 or 4-fold serial dilution starting at 10, 20, or 100 μ M. Reactions were carried out at 1 μ M ATP.

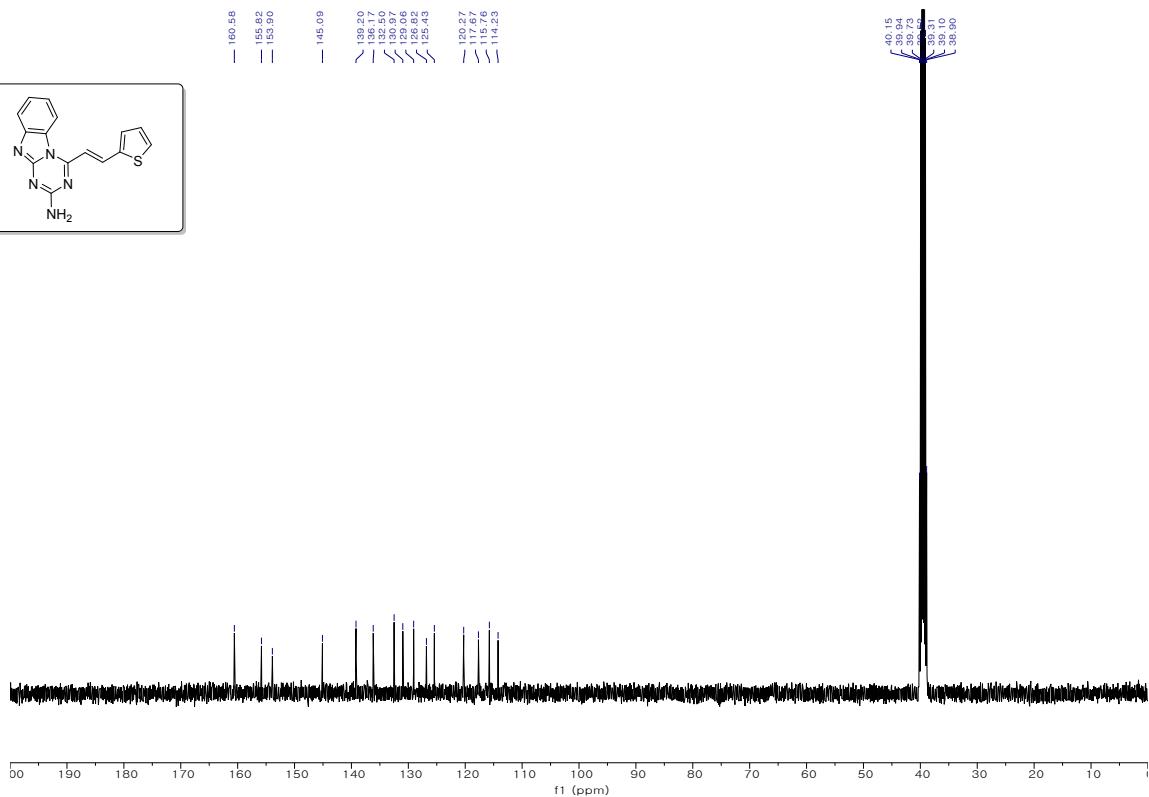
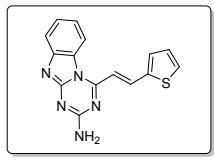
Appendix I

**Spectral Copies of ^1H - and ^{13}C - NMR Data for the
Reported Compounds**

(*E*)-4-(2-(thiophen-2-yl)vinyl)benzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-2-amine (1)

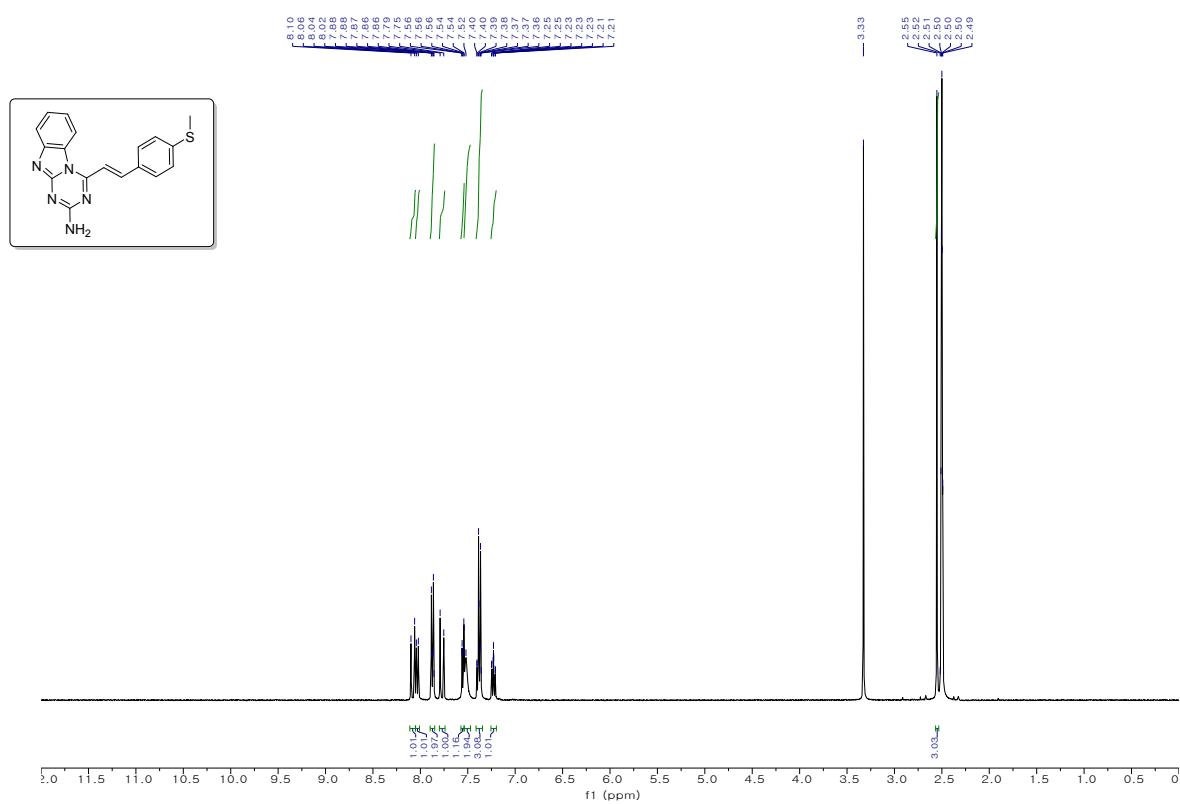


400 MHz, ^1H NMR in DMSO- d_6

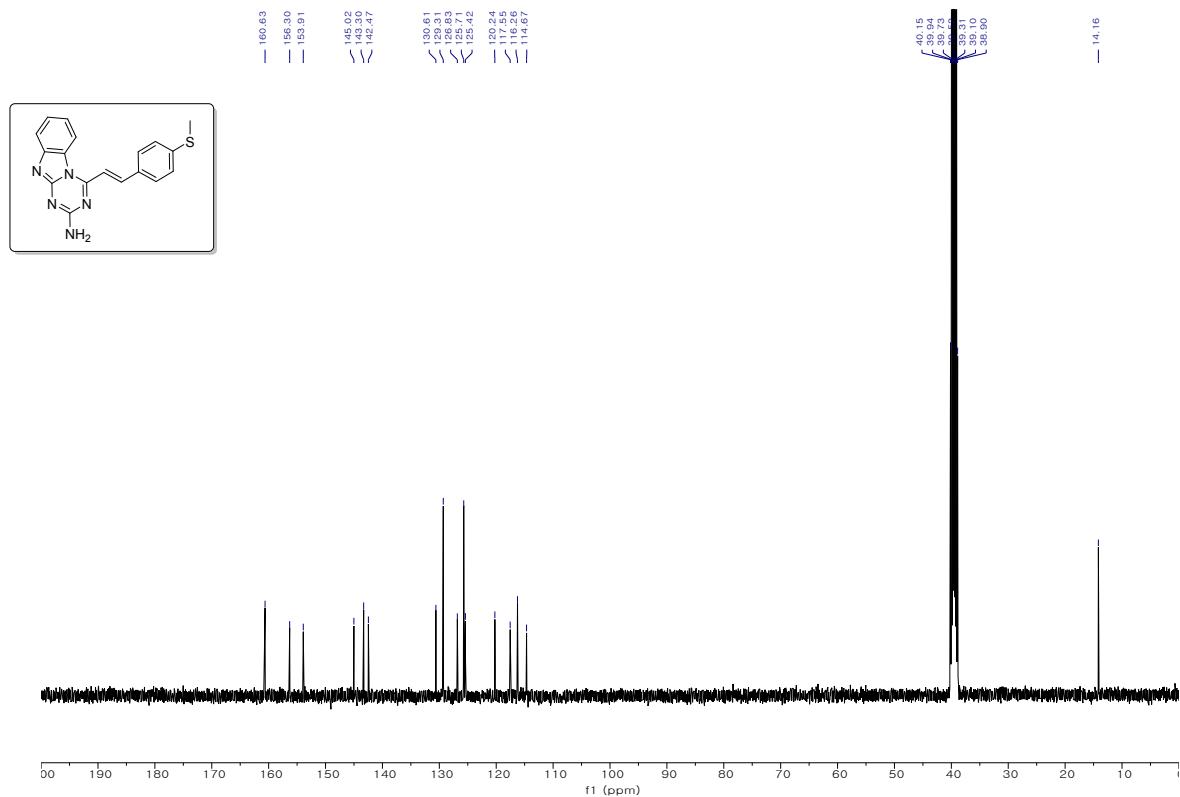


100 MHz, ^{13}C NMR in DMSO- d_6

(E)-4-(4-(methylthio)styryl)benzo[4,5]imidazo[1,2-a][1,3,5]triazin-2-amine (2)

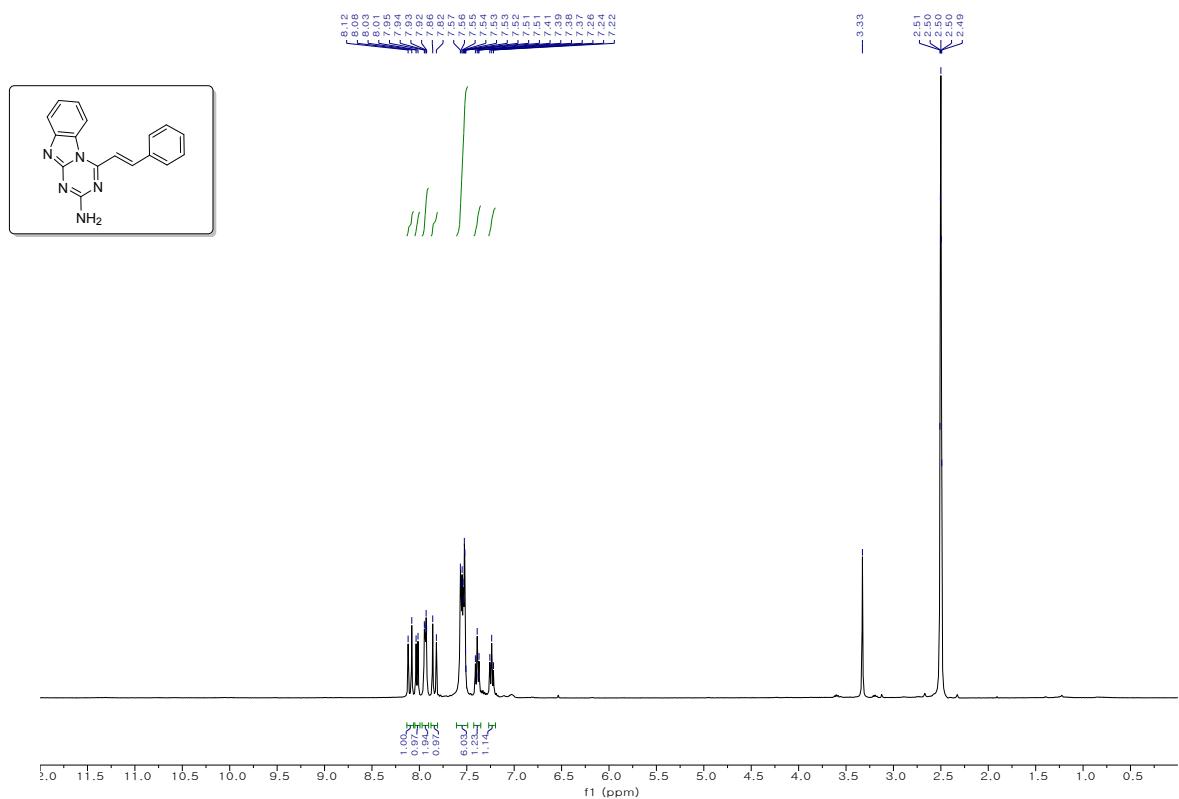


400 MHz, ^1H NMR in DMSO- d_6

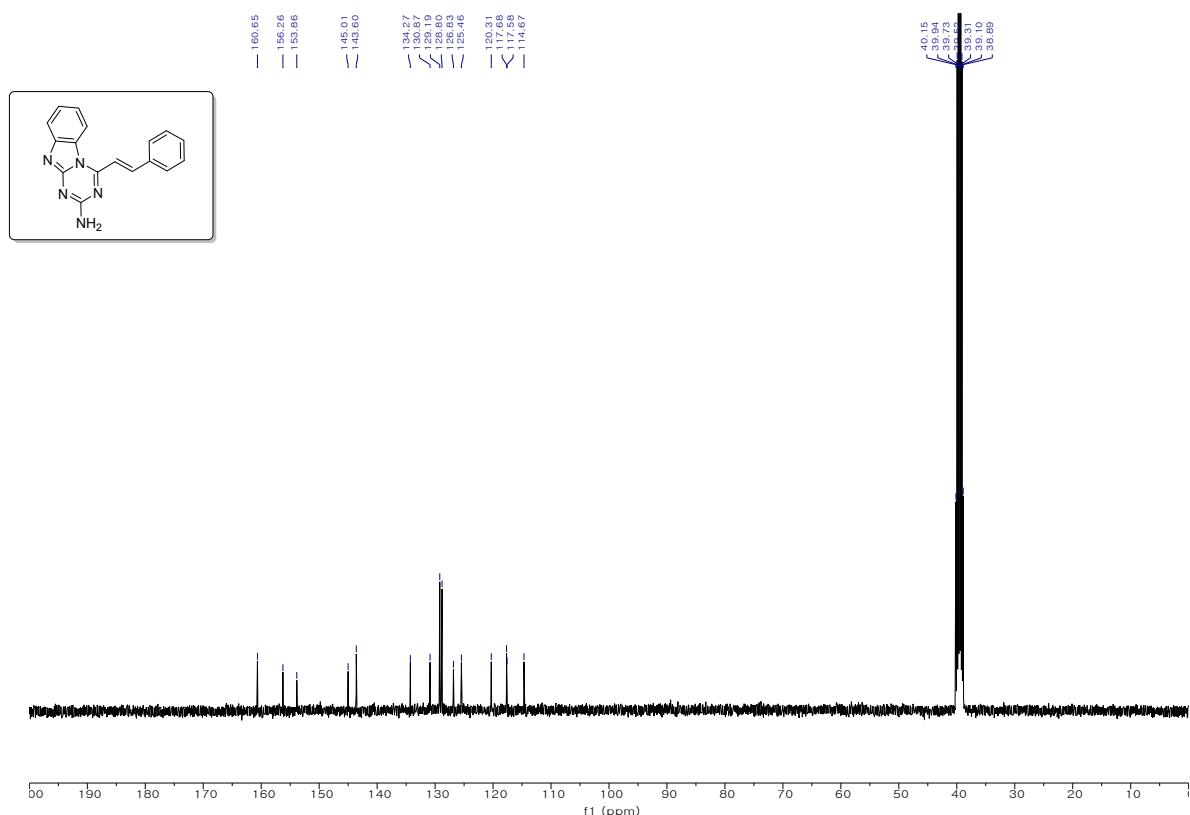


100 MHz, ^{13}C NMR in DMSO- d_6

(E)-4-styrylbenzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-2-amine (**3**)

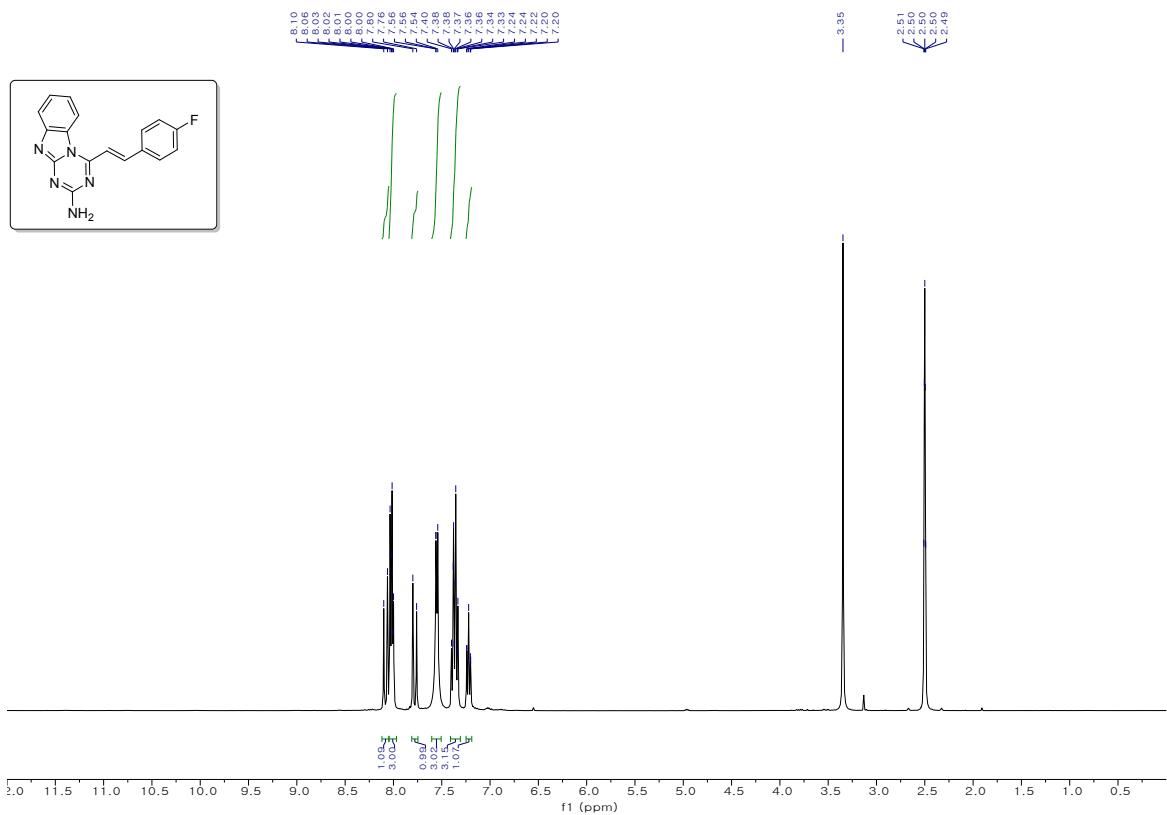


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

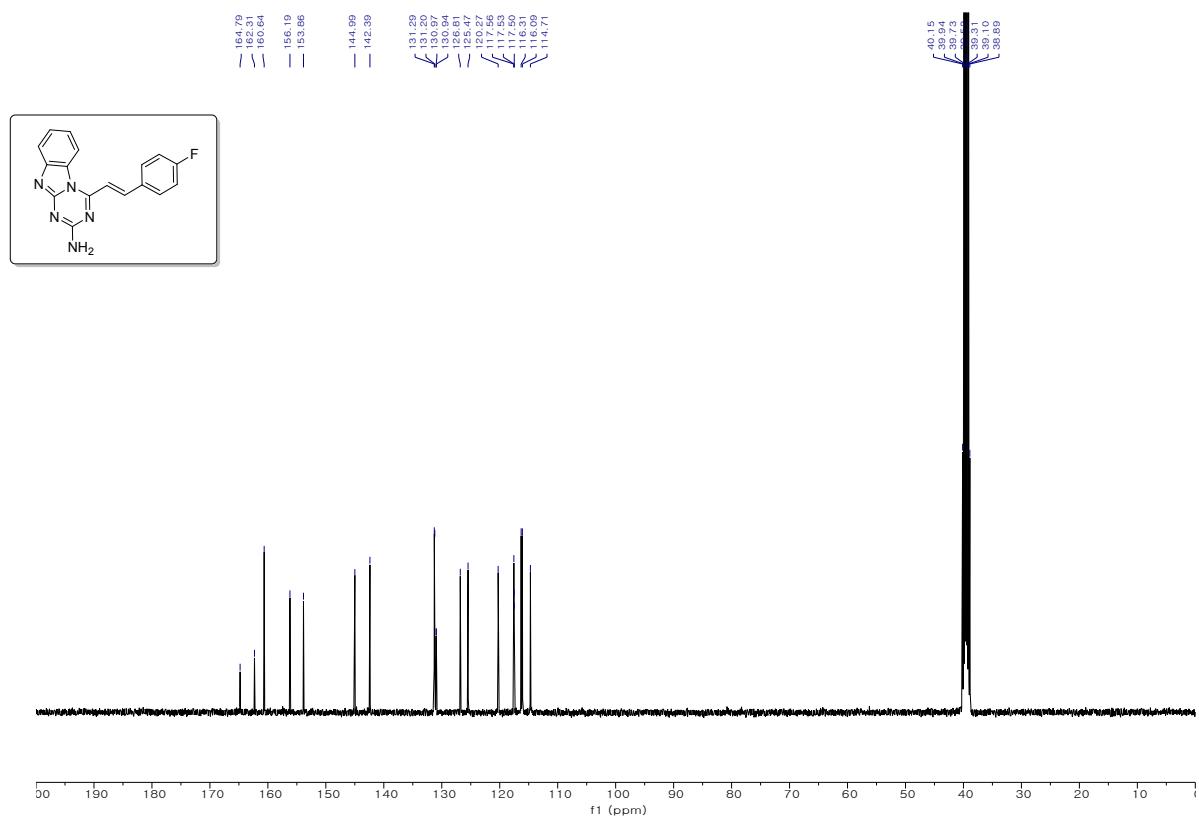


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

(E)-4-(4-fluorostyryl)benzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-2-amine (4)

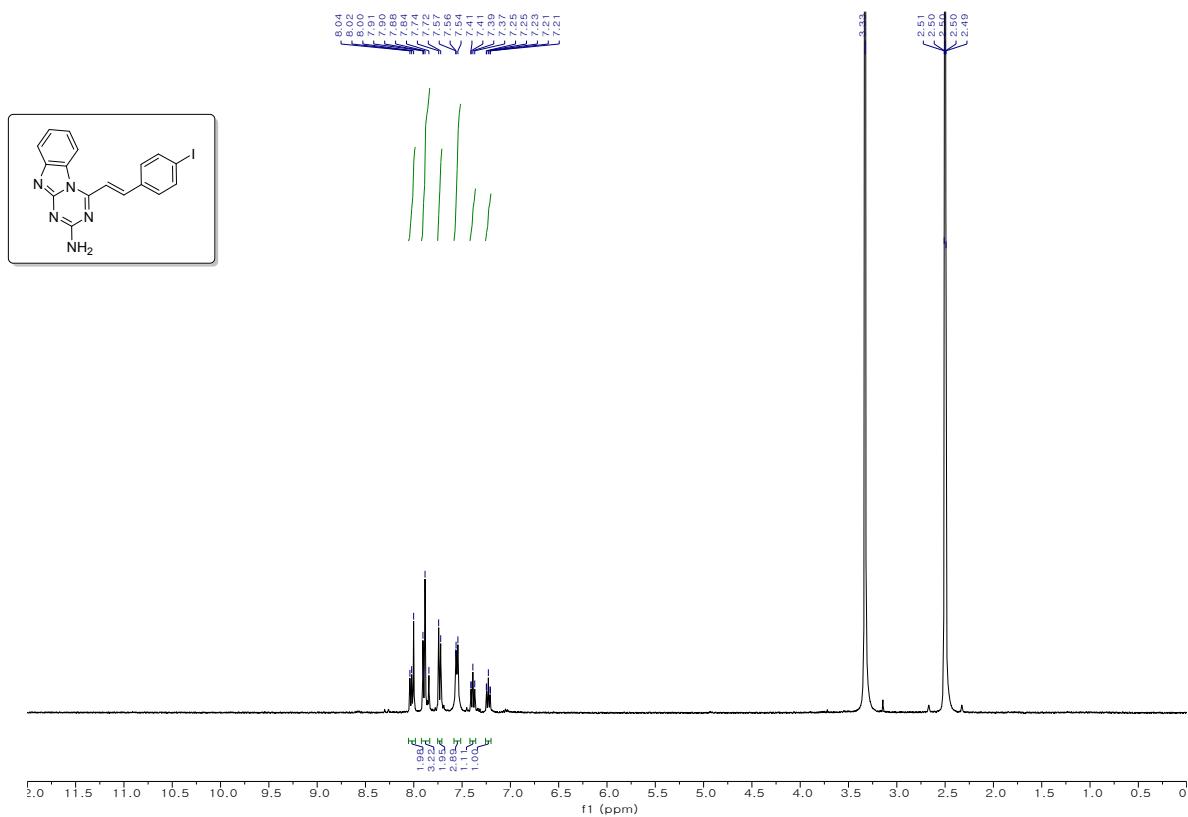


400 MHz, ^1H NMR in DMSO- d_6

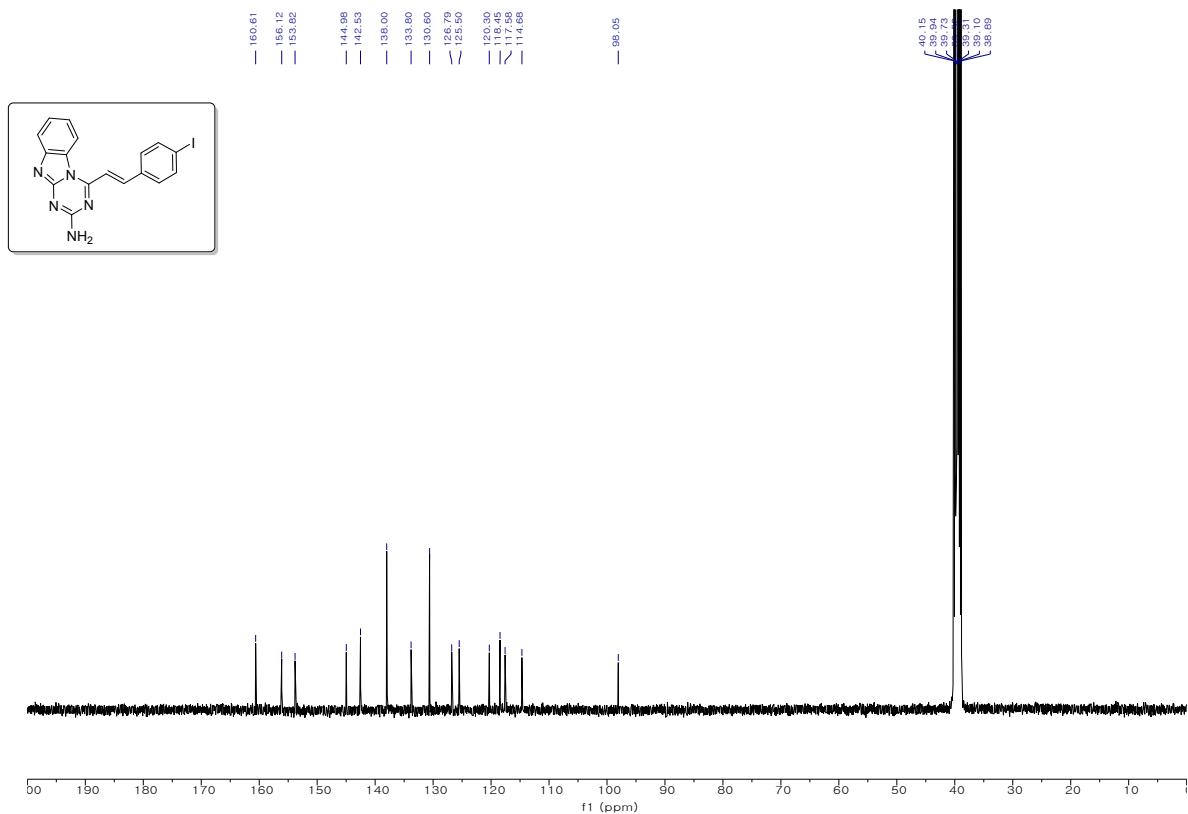


100 MHz, ^{13}C NMR in DMSO- d_6

(E)-4-(4-iodostyryl)benzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-2-amine (5)

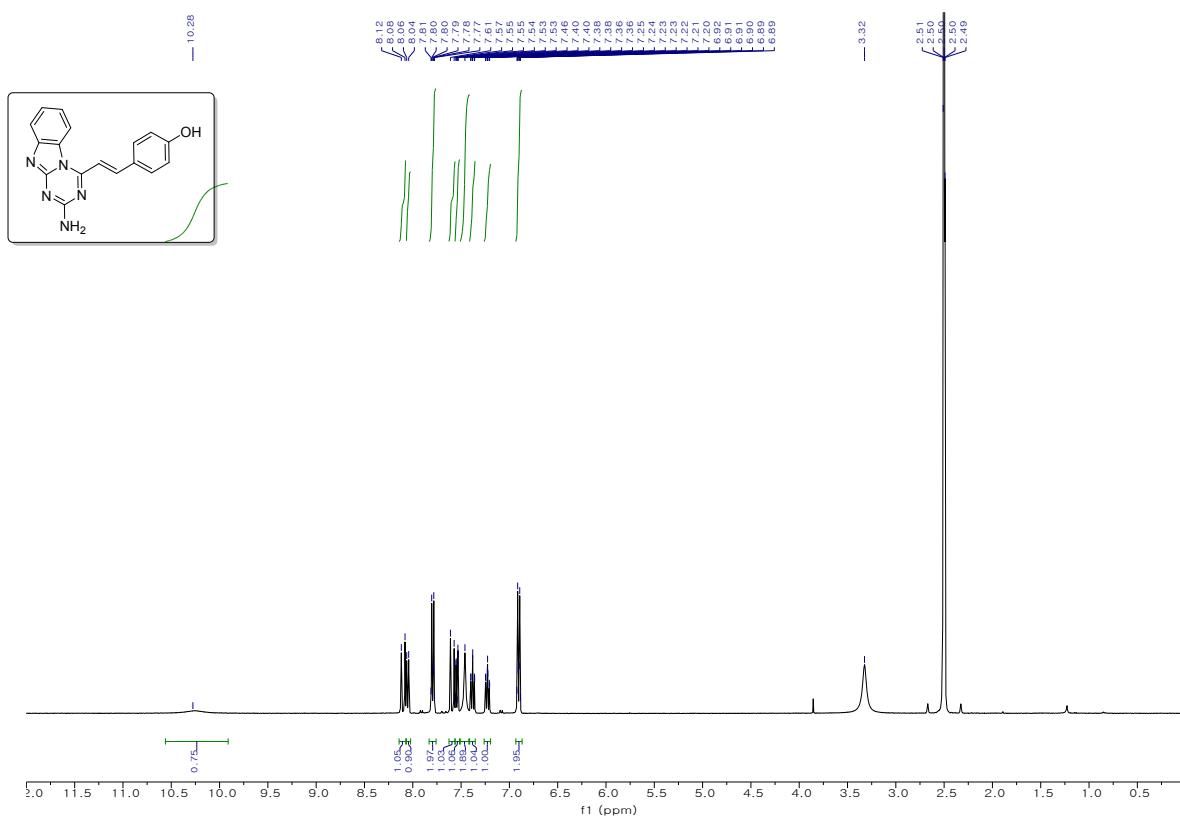


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

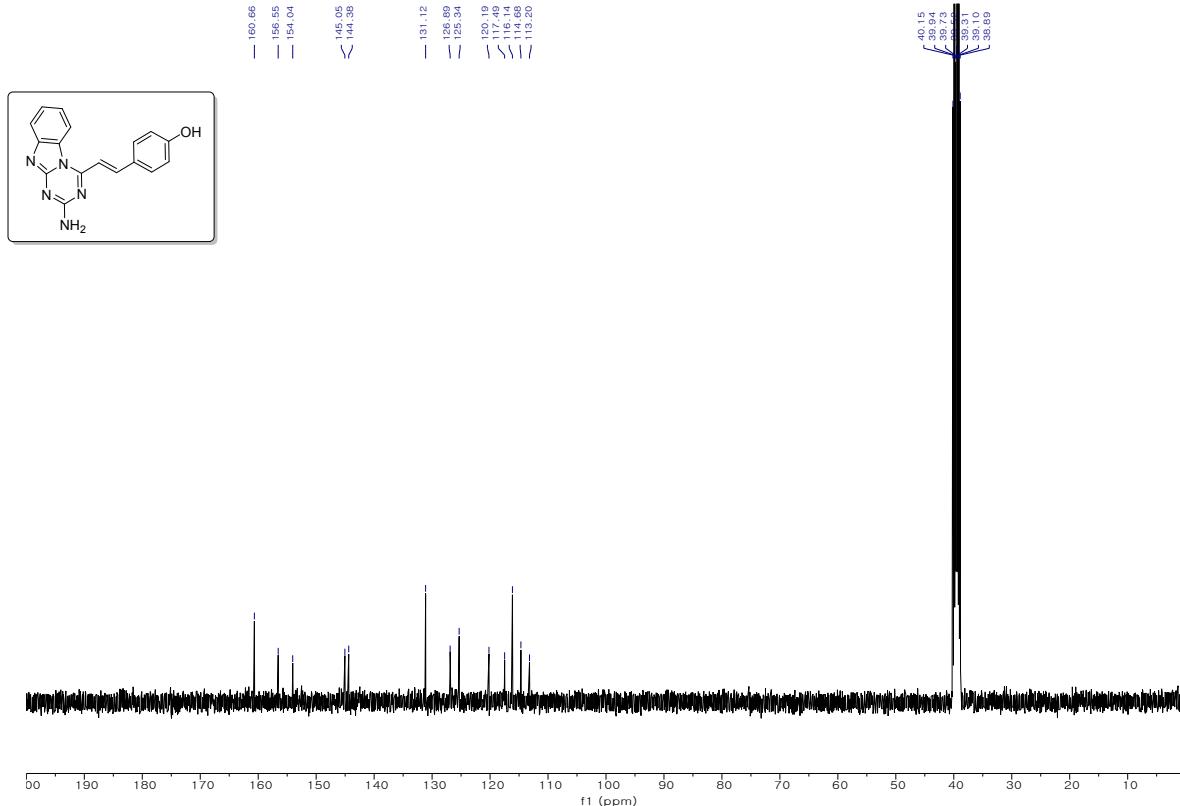


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

(E)-4-(2-(2-aminobenzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-4-yl)vinyl)phenol (6)

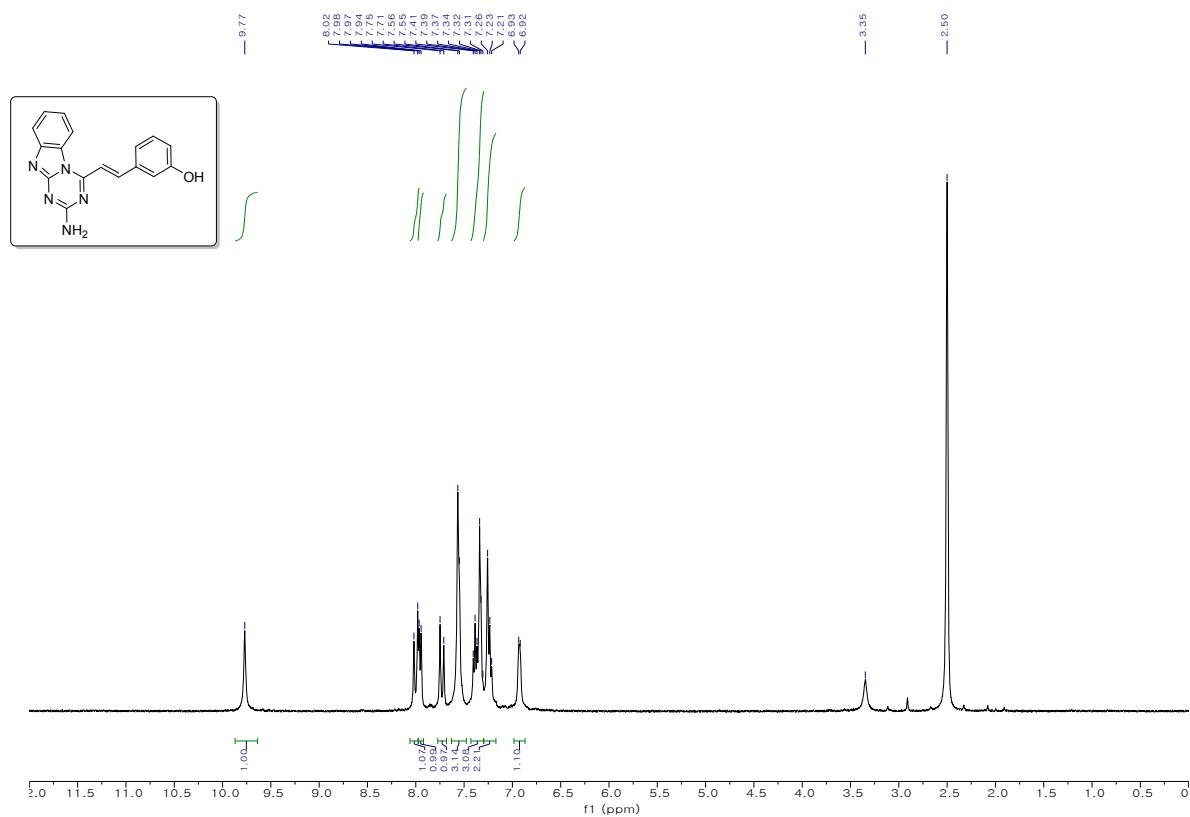


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

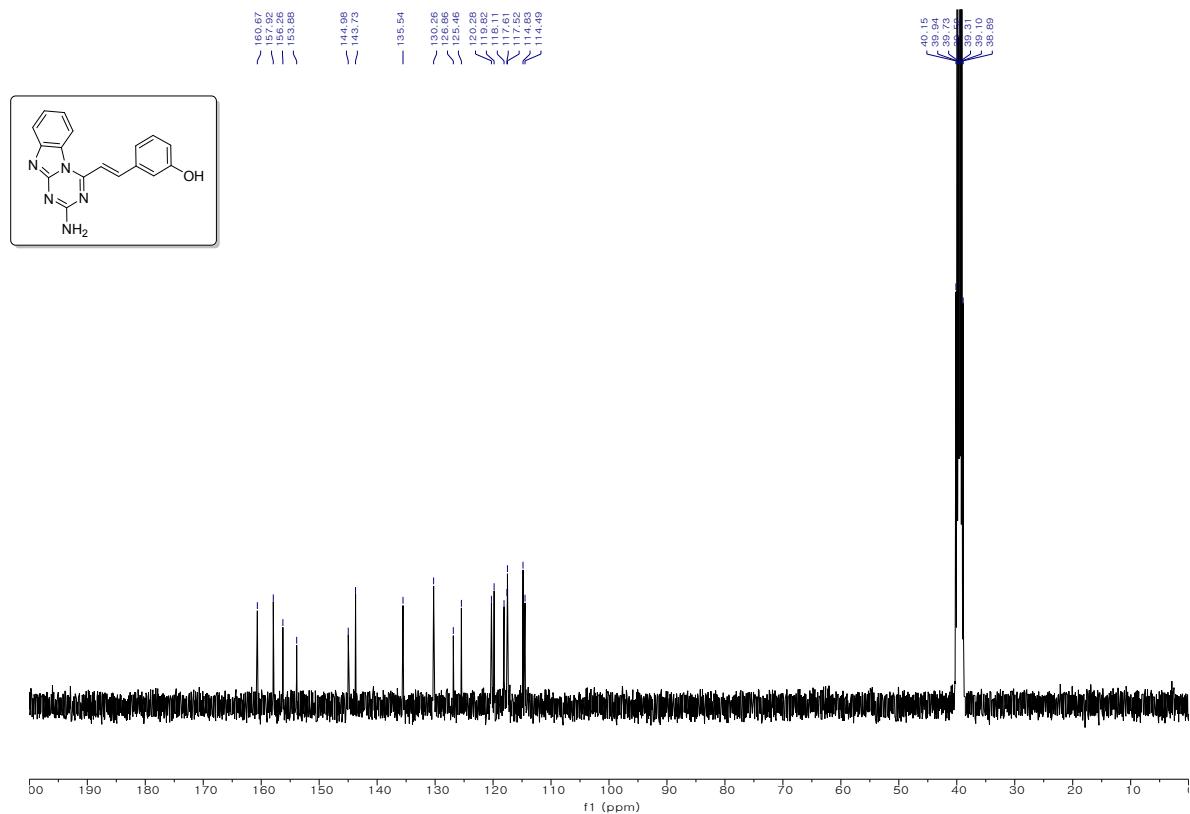


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

(E)-3-(2-(2-aminobenzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-4-yl)vinyl)phenol (7)

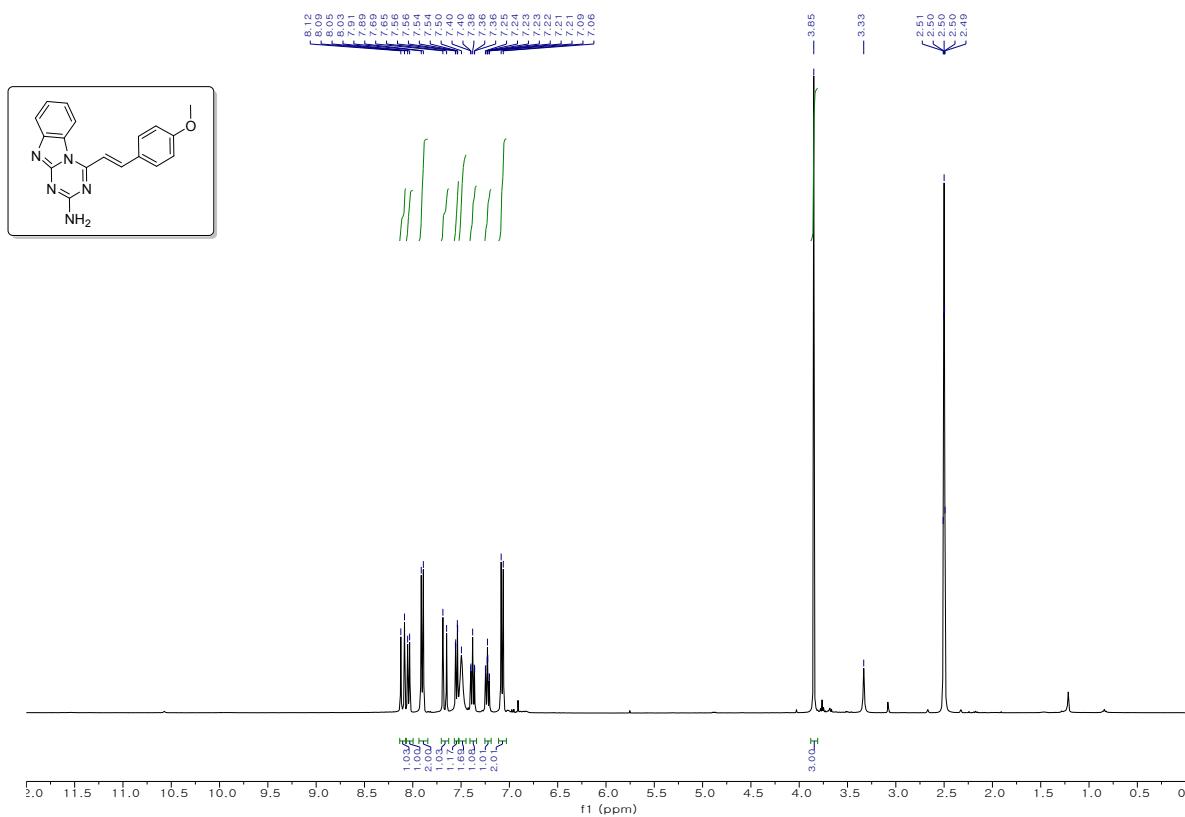


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

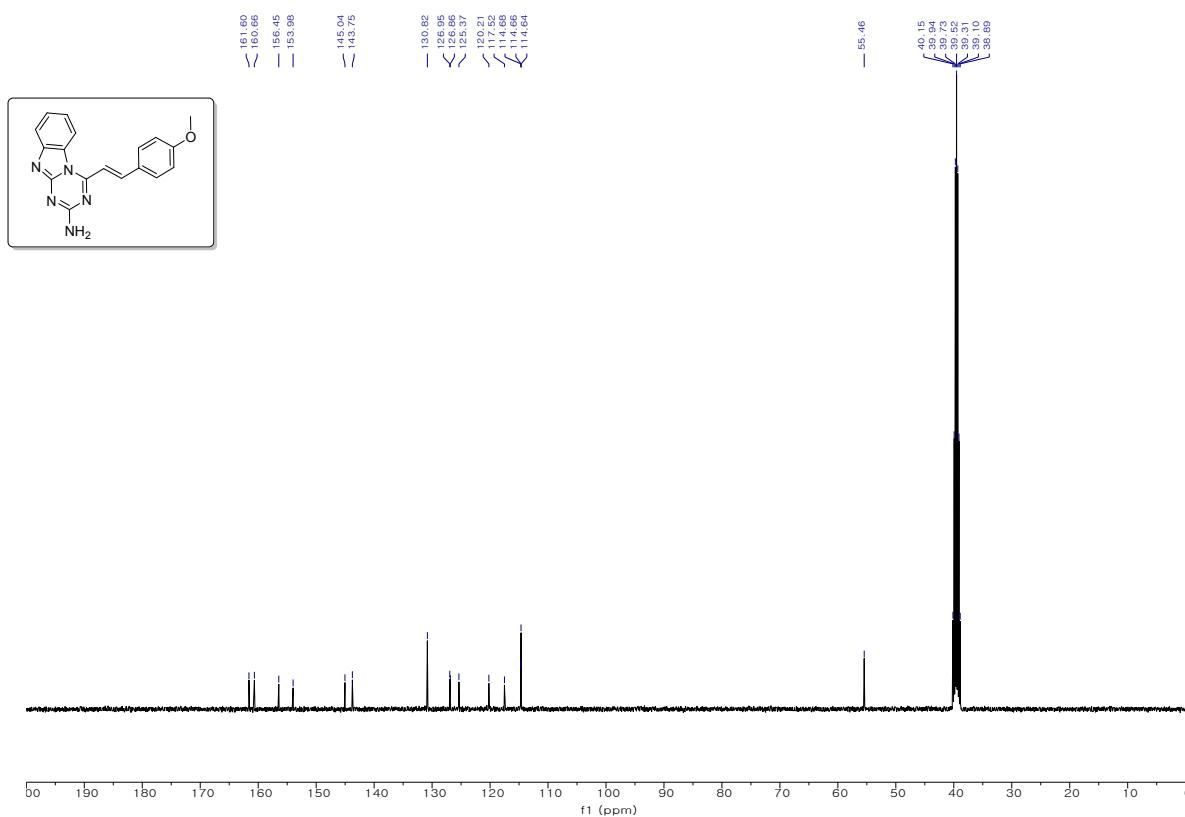


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

(E)-4-(4-methoxystyryl)benzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-2-amine (8)

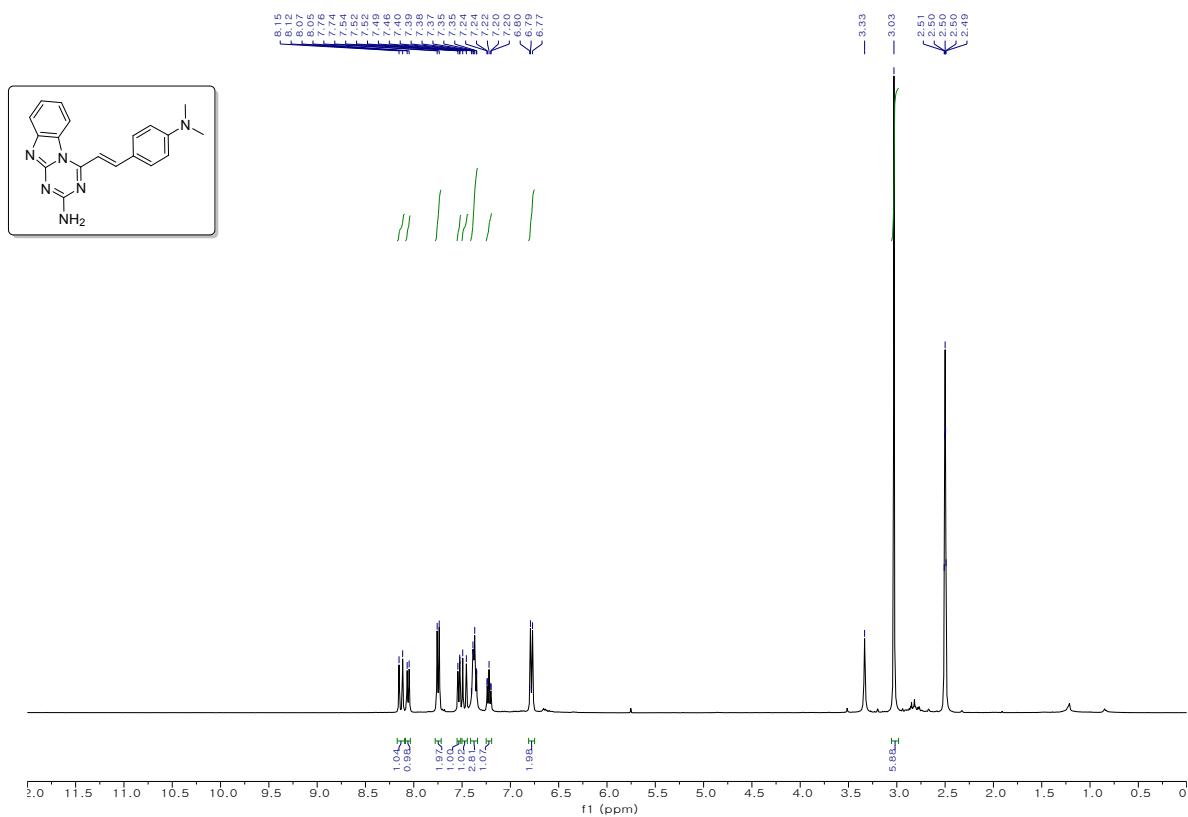


400 MHz, ^1H NMR in DMSO- d_6

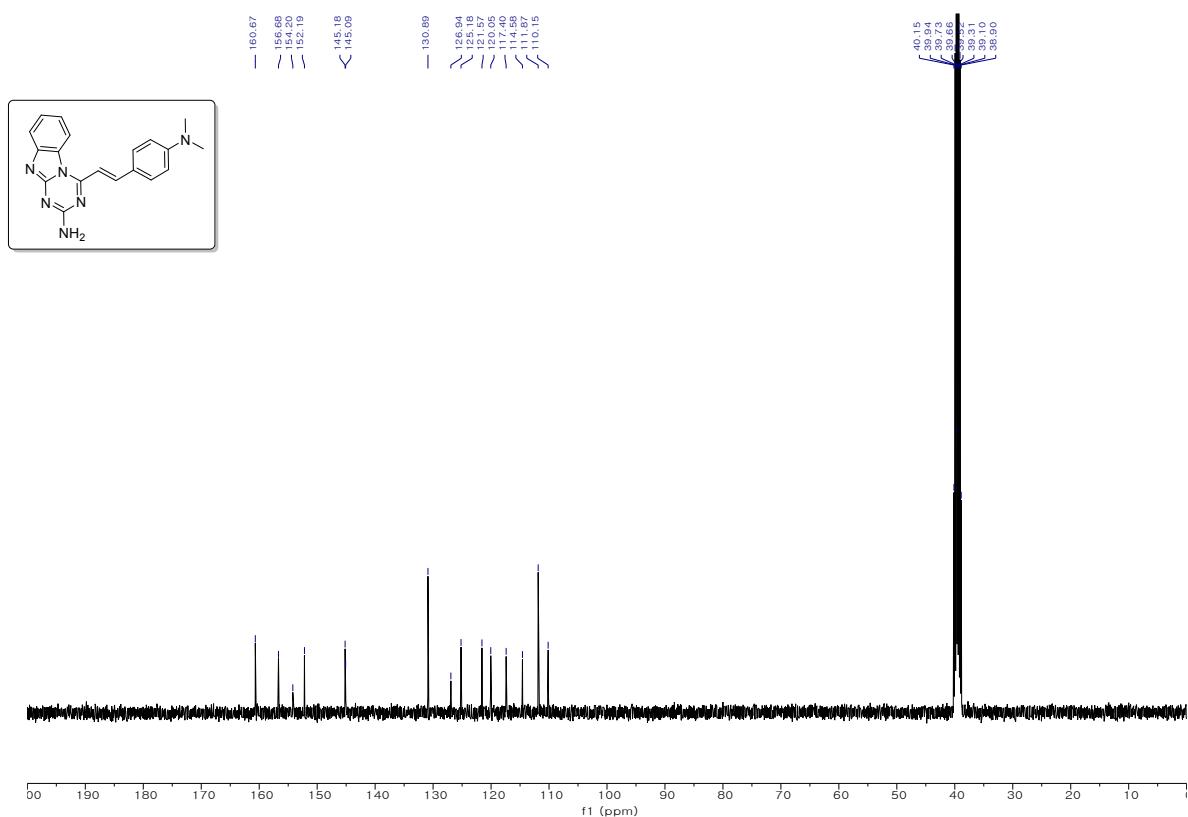


100 MHz, ^{13}C NMR in DMSO- d_6

(E)-4-(4-(dimethylamino)styryl)benzo[4,5]imidazo[1,2-a][1,3,5]triazin-2-amine (9)

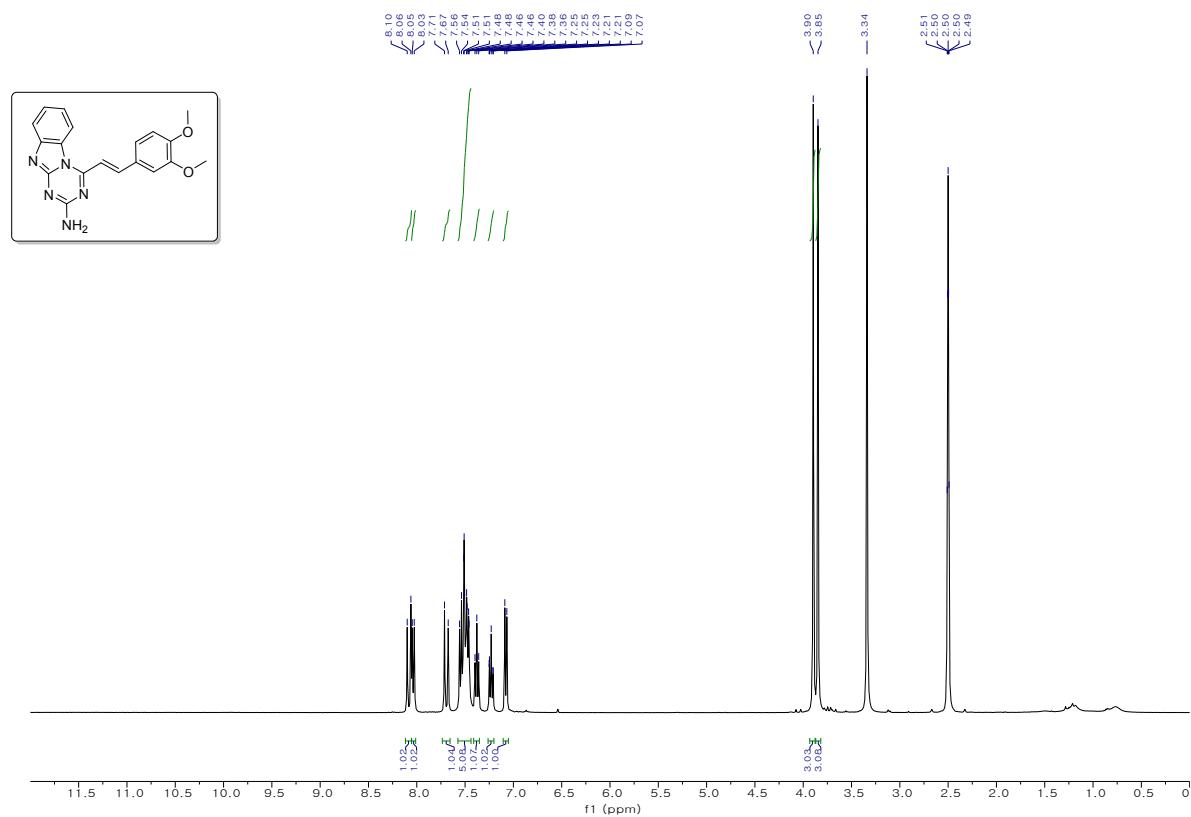


400 MHz, ^1H NMR in $\text{DMSO}-d_6$

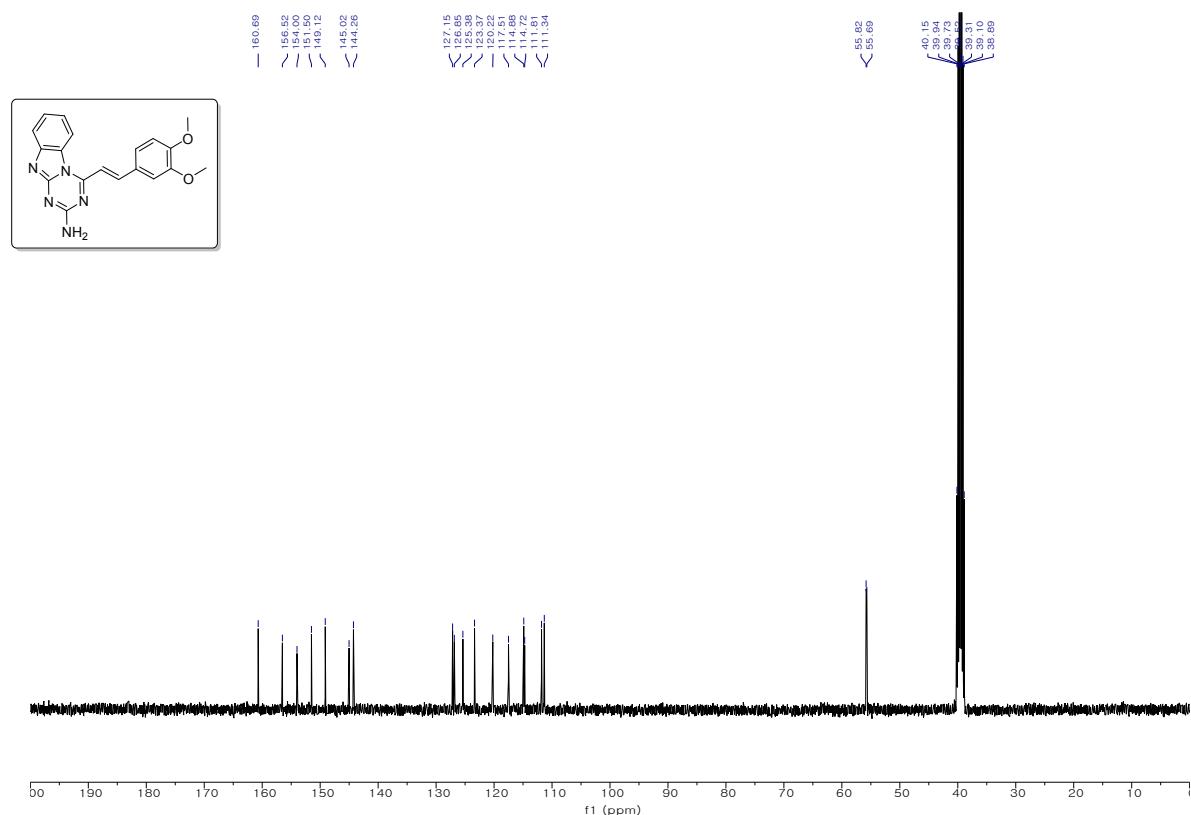


100 MHz, ^{13}C NMR in $\text{DMSO}-d_6$

(E)-4-(3,4-dimethoxystyryl)benzo[4,5]imidazo[1,2-a][1,3,5]triazin-2-amine (10)

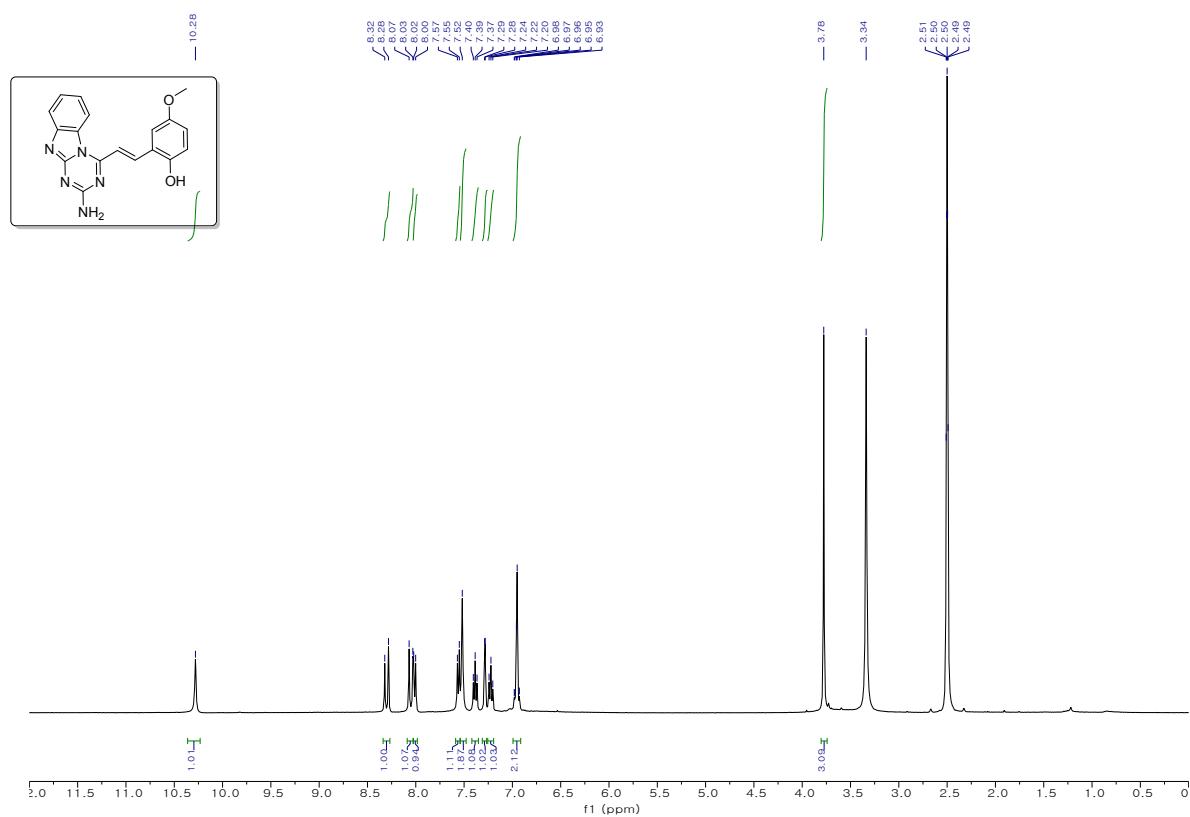


400 MHz, ¹H NMR in DMSO-*d*₆

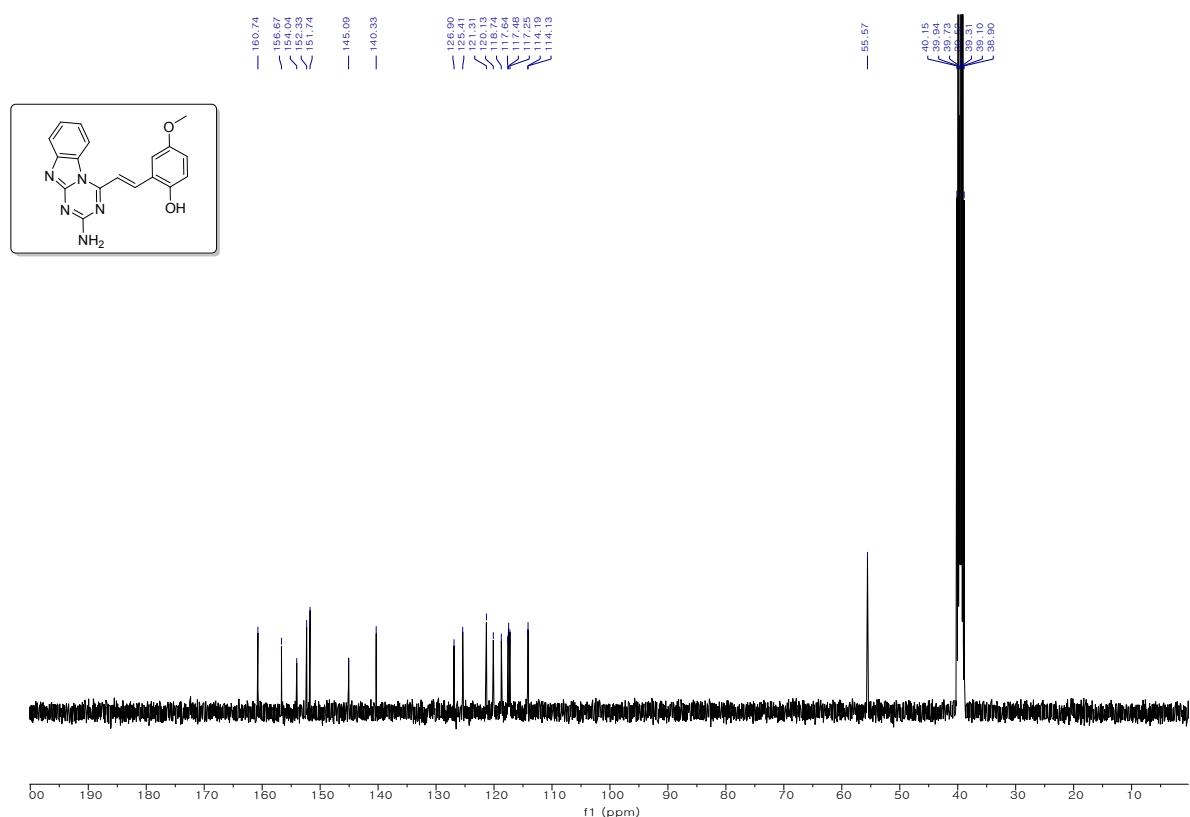


100 MHz, ¹³C NMR in DMSO-*d*₆

(E)-2-(2-(2-aminobenzo[4,5]imidazo[1,2-*a*][1,3,5]triazin-4-yl)vinyl)-4-methoxyphenol (11)



400 MHz, ¹H NMR in DMSO-*d*₆



100 MHz, ¹³C NMR in DMSO-*d*₆