

Supporting Information

ESTYBON® (ON 01910.Na)-A Clinical Stage Multi Kinase Inhibitor: Synthesis, Structure

Activity Relationship and Biological Activity.

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Table S1: Combustion analysis data for intermediates **2a-g**, **4a-g**, **5a-g**, **6a-g**, **9**, **11-15**, **19**.

Compound (# from text)	Theoretical			Found		
	C	H	N	C	H	N
2a	39.05	3.28	5.69	38.96	3.26	5.65
2b	39.05	3.28	5.69	39.16	3.30	5.72
2c	28.51	1.71	4.75	28.57	1.73	4.79
2d	33.57	2.01	5.59	33.65	2.05	5.66
2e	33.57	2.01	5.59	33.52	2.03	5.55
2f	35.93	2.15	5.99	35.99	2.11	6.06
2g	39.05	3.28	5.69	39.14	3.31	5.73
4a	52.46	4.95	7.65	52.53	4.99	7.72
4b	52.46	4.95	7.65	52.41	4.99	7.69
4c	36.23	2.61	6.04	36.29	2.64	6.09
4d	44.82	3.22	7.47	44.89	3.25	7.53
4e	44.82	3.22	7.47	44.91	3.26	7.52
4f	49.13	3.53	8.19	49.21	3.57	8.25
4g	52.46	4.95	7.65	52.52	4.99	7.71
5a	46.69	4.31	5.44	46.62	4.28	5.49
5b	46.69	4.31	5.44	46.75	4.34	5.39
5c	35.31	2.63	4.58	35.37	2.61	4.63
5d	41.31	3.08	5.35	41.36	3.11	5.42
5e	41.31	3.08	5.35	41.35	3.12	5.41
5f	44.08	3.29	5.71	44.14	3.32	5.76
5g	46.69	4.31	5.44	46.75	4.34	5.48
6a	41.52	3.83	4.84	41.59	3.87	4.89
6b	41.52	3.83	4.84	41.58	3.88	4.90
6c	31.97	2.38	4.14	32.03	2.42	4.20
6d	36.81	2.75	4.77	36.88	2.79	4.83
6e	36.81	2.75	4.77	36.85	2.76	4.72
6f	38.99	2.91	5.05	39.10	2.94	5.09
6g	41.52	3.83	4.84	41.60	3.82	4.81
9	48.23	4.55	7.03	48.31	4.52	7.08
11	58.78	4.93	4.03	58.84	4.96	4.08
12	33.34	4.35	12.96	33.42	4.38	12.88
13	53.82	4.52	3.69	53.91	4.54	3.74
14	53.53	5.02	3.67	53.48	5.05	3.72
15	68.74	6.29	-	68.82	6.33	-
19	37.53	3.44	-	37.61	3.42	-

Table S2: Combustion analysis data for final **8a-z**, **8aa- ac** molecules

Compound (# from text)	Theoretical			Found		
	C	H	N	C	H	N
8a	56.19	4.72	3.85	56.14	4.75	3.89
8b	61.24	5.74	4.20	61.30	5.78	4.21
8c	56.19	4.72	3.85	56.25	4.74	3.90
8d	61.24	5.74	4.20	61.31	5.77	4.16
8e	54.95	4.87	3.56	55.03	4.90	3.61
8f	54.95	4.87	3.56	54.89	4.88	3.58
8g	59.49	5.82	3.85	59.56	5.84	3.89
8h	59.49	5.82	3.85	59.47	5.85	3.88
8i	59.49	5.82	3.85	59.55	5.84	3.90
8j	59.49	5.82	3.85	59.56	5.84	3.89
8k	59.49	5.82	3.85	59.52	5.81	3.86
8l	53.89	5.00	3.31	53.94	5.01	3.33
8m	53.89	5.00	3.31	53.88	4.99	3.34
8n	58.00	5.89	3.56	58.06	5.91	3.59
8o	58.00	5.89	3.56	58.08	5.90	3.53
8p	58.00	5.89	3.56	58.04	5.89	3.57
8q	58.00	5.89	3.56	58.01	5.90	3.59
8r	58.00	5.89	3.56	58.06	5.91	3.59
8s	52.81	4.68	3.42	52.86	4.69	3.45
8t	56.98	5.58	3.69	57.06	5.60	3.73
8u	56.76	5.85	3.01	56.84	5.83	3.04
8v	45.77	3.84	2.97	45.85	3.86	3.00
8w	48.88	4.56	3.17	48.96	4.57	3.19
8x	54.34	5.07	3.52	54.40	5.06	3.53
8y	54.34	5.07	3.52	54.27	5.07	3.50
8z	52.55	4.41	3.40	52.62	4.44	3.42
8aa	56.68	5.29	3.67	56.62	5.31	3.68
8ab	53.78	3.95	3.92	53.86	3.96	3.95
8ac	53.78	3.95	3.92	53.76	3.95	3.94

Table S3: Combustion analysis data for sulfides and sulfoxides **17, 20, 21, 24**.

Compound (# from text)	Theoretical			Found		
	C	H	N	C	H	N
17	58.30	5.41	3.58	58.36	5.43	3.60
20	56.01	5.20	3.44	56.09	5.22	3.46
21	60.46	6.14	3.71	60.55	6.12	3.73
24	63.13	6.41	3.88	63.20	6.40	3.90

Table S4: Combustion analysis data for amino esters (**26a-l**) and amino acids (**27a-l**) and **28**.

Compound (# from text)	Theoretical			Found		
	C	H	N	C	H	N
26a	56.76	5.85	3.01	56.81	5.87	3.03
26b	56.76	5.85	3.01	56.78	5.86	3.03
26c	57.61	6.10	2.92	57.70	6.11	2.93
26d	57.61	6.10	2.92	57.67	6.10	2.91
26e	52.69	5.02	2.79	52.75	5.01	2.80
26f	51.78	4.91	2.63	51.72	4.92	2.64
26g	58.40	6.33	2.84	58.47	6.31	2.85
26h	62.09	5.77	2.59	62.15	5.76	2.60
26i	60.10	5.40	2.50	60.18	5.41	2.52
26j	58.38	5.25	2.43	58.31	5.26	2.44
26k	54.20	4.87	2.26	54.29	4.88	2.27
26l	60.93	5.82	2.45	61.00	5.81	2.47
27a	55.86	5.58	3.10	55.94	5.56	3.12
27b	55.86	5.58	3.10	55.88	5.58	3.11
27c	56.76	5.85	3.01	56.84	5.83	3.02
27d	56.76	5.85	3.01	56.78	5.86	3.01
27e	51.74	4.76	2.87	51.82	4.78	2.88
27f	50.86	4.66	2.70	50.94	4.66	2.71
27g	57.61	6.10	2.92	57.70	6.09	2.91
27h	61.47	5.54	2.65	61.55	5.55	2.65
27i	59.44	5.17	2.57	59.51	5.17	2.58
27j	57.70	5.02	2.49	57.80	5.01	2.51
27k	53.47	4.65	2.31	53.41	4.67	2.32
27l	60.31	5.60	2.51	60.40	5.61	2.50
28	49.50	5.54	2.75	49.56	5.53	2.76