

Selection of a Respiratory Syncytial Virus Fusion Inhibitor Clinical Candidate

Part 2: Discovery of a Morpholino-propylamino- benzimidazole derivative (TMC353121)

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Supporting Information

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Supplement to the chemistry experimental section:

Table of C,H,N Analysis for the target compounds

Compound N°	Formula		C%	H%	N%
21a	$C_{31}H_{40}N_6O_2, 0.4 H_2O$	Theory	69.48	7.67	15.68
		Found	69.8	7.56	15.32
21b	$C_{29}H_{36}N_6O_2, 0.3H_2O$	Theory	68.83	7.29	16.61
		Found	69.17	7.48	16.24
21c	$C_{28}H_{34}N_6O$	Theory	71.46	7.28	17.86
		Found	71.54	7.29	17.55
22	$C_{28}H_{33}N_5OS$	Theory	68.96	6.82	14.36
		Found	68.82	6.81	14.23

24	$C_{29}H_{33}N_5O, 0.3 H_2O$	Theory	73.64	7.16	14.81
		Found	73.28	7.3	14.82
25	$C_{29}H_{35}N_5O, 0.3 H_2O$	Theory	73.32	7.55	14.74
		Found	73.28	7.61	14.62
26b	$C_{28}H_{34}N_6O, 0.5 H_2O$	Theory	70.12	7.36	17.52
		Found	70.43	7.45	17.36
26c	$C_{27}H_{32}N_6O, 0.4 H_2O$	Theory	69.92	7.13	18.12
		Found	70.2	7.17	17.78
27	$C_{27}H_{31}N_5O_2, 1 H_2O$	Theory	68.19	6.99	14.73
		Found	67.82	7.23	14.34
37	$C_{28}H_{34}N_6O$	Theory	71.46	7.28	17.86
		Found	71.19	7.47	17.62
41a	$C_{29}H_{36}N_6O_2, 2.8 H_2O$	Theory	63.21	7.61	15.25
		Found	63.14	7.34	14.97
48a	$C_{31}H_{41}N_7O, 0.45 H_2O$	Theory	69.49	7.88	18.3
		Found	69.34	7.8	17.92
48c	$C_{27}H_{33}N_5O$	Theory	73.11	7.5	15.79
		Found	72.9	7.73	15.67
48d	$C_{31}H_{33}N_5O$	Theory	75.73	6.77	14.25
		Found	75.81	6.78	14.14
48e	$C_{30}H_{38}N_6O_2$	Theory	70.01	7.44	16.33
		Found	69.86	7.48	16.03
48f	$C_{26}H_{31}N_5O_3, 0.35 H_2O$	Theory	66.75	6.83	14.97
		Found	66.48	6.76	14.73
55a	$C_{30}H_{38}N_6O_3, 0.5 H_2O$	Theory	66.77	7.28	15.57
		Found	66.45	7.07	15.33
55b	$C_{31}H_{40}N_6O_3, 0.3 H_2O$	Theory	67.69	7.44	15.28
		Found	67.93	7.44	14.9
55c	$C_{32}H_{42}N_6O_3$	Theory	68.79	7.58	15.04
		Found	68.85	7.66	14.77
55d	$C_{34}H_{45}N_7O_3$	Theory	68.09	7.56	16.35
		Found	67.69	7.44	16.08
56a	$C_{29}H_{36}N_6O_2$	Theory	69.57	7.25	17.79
		Found	69.24	7.3	16.71
56b	$C_{30}H_{38}N_6O_3, 1.35 H_2O$	Theory	64.93	7.39	15.14
		Found	64.67	7.37	14.8
56c	$C_{31}H_{40}N_6O_3$	Theory	68.36	7.4	15.43
		Found	67.87	7.39	15.31
56d	$C_{32}H_{42}N_6O_3$	Theory	68.79	7.58	15.04
		Found	68.87	7.46	14.99

