

Design, Synthesis and Biological Evaluation of N^4 -Sulfonamido-Succinamic, Phthalamic, Acrylic and Benzoyl Acetic Acid Derivatives as Potential DPP IV Inhibitors

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Supplementary Material

Table 2. Docking Scoring Functions for the Synthesized Compounds 6-21 Inside the DPP IV Binding Pocket

Docking Pose	Ligscore 1	Ligscore 2	PLP1	PLP2	Jain	PMF	Dock score
6	5.84	5.95	90.46	77.3	1.73	105.01	96.165
6	5.84	5.98	89.07	83.86	3.57	105.38	92.092
6	4.92	4.77	45.69	35.71	0.19	35.32	91.711
6	4.31	4.39	34.32	31.91	0.85	30.5	90.703
6	5.01	5.23	45.49	33.74	-0.5	57.15	89.026
6	5.69	5.63	89.4	80.62	3.36	101.25	88.547
6	6.53	6.15	73.32	66.11	0.71	95.39	87.364
6	5.53	5.72	78.43	64.33	0.36	98.67	86.671
6	5.81	5.45	56.5	54.82	-0.49	82.02	84.357
6	5.27	5.46	44.9	43.59	0.01	80.03	84.234
7	4.64	5.23	46.01	36.56	-0.55	48.87	91.305
7	4.65	5.24	45.99	36.56	-0.55	48.54	90.828
7	4.84	4.61	38.89	31.6	-0.36	21.18	89.625
7	6.37	6.41	69.27	54.37	0.56	91.09	88.898
7	5.36	4.66	32.97	30.57	0.14	43.51	88.273
7	4.5	4.5	35.55	24.77	-0.11	19.71	87.963
7	5.36	4.66	32.97	30.57	0.14	43.59	87.556
7	4.64	4.44	31.45	21.22	0	34.49	85.49
7	4.41	4.63	38.12	26.8	-0.19	29.4	84.961
7	4.41	4.45	34.53	24.78	-0.13	22.87	84.842
8	5.57	5.21	54.39	52.43	-0.23	78.33	97.76
8	5.89	5.49	52.6	55.84	1.64	77.03	93.967
8	5.62	5.45	62.51	63.69	1.07	101.12	92.271
8	5.9	5.49	52.6	55.84	1.64	77.32	90.088

(Table 2) contd....

Docking Pose	Ligscore 1	Ligscore 2	PLP1	PLP2	Jain	PMF	Dock score
8	4.54	4.43	41.98	38.73	-0.48	55.33	89.176
8	5.95	5.75	63.99	56.46	2.51	91.58	87.839
8	5.53	5.15	42.4	40.3	1.03	64.46	86.881
8	5.6	5.39	49.15	47.47	1.02	54.1	86.806
8	5.53	5.15	42.4	40.29	1.03	64.46	86.217
8	5.19	4.81	35.19	40.33	0.57	57.47	86.092
9	5.8	5.59	68.2	72.09	3.77	116.16	93.835
9	5.33	5.24	72.2	70.03	2.27	99.97	88.018
9	6.48	6.46	67.14	70.45	2.88	83.5	83.584
9	5.29	5.08	74.1	71.23	3.14	105.95	82.887
9	5.7	5.64	77.45	73.69	3.36	96.76	82.315
9	4.86	4.89	67.44	67	3.78	94.46	81.918
9	5.95	5.64	71.22	66.85	2.26	95.96	81.596
9	6.38	6.26	72.15	70.96	2.78	103.29	80.633
9	5.41	5.47	75.25	73.01	2.09	99.6	80.604
9	6.17	5.6	74.21	67.02	2.44	90.58	80.503
10	6.02	5.31	68.41	65.51	1.29	77.87	87.256
10	6.02	5.49	61.76	58.58	0.75	70.04	86.903
10	5.83	5.81	46.1	38.43	1.58	77.61	86.239
10	5.19	4.65	41.39	43.5	-0.34	53.88	85.408
10	5.69	5.14	58.31	53.92	0.64	73.64	85.074
10	5.67	5.15	54.5	51.18	0.33	69.39	84.842
10	5.56	5.16	54.91	52.01	0.47	59.18	84.682
10	5.72	5.02	50.37	50.13	0.98	52.71	84.299
10	5.71	5.18	54.68	51.92	0.1	76.02	83.276
10	5.06	5.03	48.75	52.24	1.41	68.26	83.151
11	5.99	5.94	44.67	44.1	2.46	67.26	97.483
11	5.5	5	46.02	44.86	1.06	63.56	92.506
11	5.7	5.6	44.85	46.26	1.32	71.52	91.423
11	5.87	5.66	55.02	47.25	0.11	66.97	90.924
11	5.96	5.51	43.89	51.19	1.58	61.99	90.738
11	6.21	5.68	50.92	45.77	2.14	66.46	90.216
11	5.27	4.9	45.64	40.46	-0.08	33.28	89.877
11	4.7	4.46	41.17	36.11	-0.17	40.09	88.974
11	5.87	5.67	54.82	47.02	0.12	67.09	88.391
11	5.86	5.18	47.72	41.73	-0.36	68.04	88.266
12	5.08	4.95	44.8	35.5	0.05	39.39	99.523

(Table 2) contd....

Docking Pose	Ligscore 1	Ligscore 2	PLP1	PLP2	Jain	PMF	Dock score
12	6.09	5.66	45.44	44.45	1.98	61.31	98.211
12	4.94	4.88	47.79	39.02	-0.09	53.6	96.334
12	5.93	6.11	89.43	82.83	3.64	111.75	95.496
12	5.21	5.03	61.05	50.98	0.39	46.43	93.352
12	5.65	5.83	72.88	65.51	3.09	104.47	93.117
12	5.61	5.3	67.46	55.72	-0.14	102.07	92.36
12	5.63	5.32	68.77	56.15	0	100.5	91.571
12	5.66	5.55	70.61	53.68	0.16	105.01	91.274
12	5.93	6.11	89.43	82.83	3.64	111.74	90.807
13	5.28	4.95	45.34	46.9	2.05	68.29	90.52
13	5.5	6.13	59.88	60.33	2.38	75.58	89.048
13	6.02	6.01	63.85	62.39	1.25	115.11	88.912
13	4.55	4.31	35.13	32.25	-1	43.37	88.585
13	6.02	6.04	64.01	62.5	1.17	115.7	87.97
13	5.39	5.15	49.45	52.31	2.01	79.89	87.925
13	6.1	5.95	68.93	72.56	1.65	119.63	87.374
13	6.21	5.93	70.74	71.53	2.21	98.88	87.034
13	5.71	5.88	64.17	64.81	1.63	109.12	86.581
13	5.77	5.4	53.53	56.61	3.08	81.57	86.412
14	5.43	4.93	52.94	53.51	2	71.01	99.06
14	5.34	4.83	56.01	60.37	0.64	94.65	98.275
14	5.34	4.82	56.04	60.39	0.64	94.34	95.901
14	5.21	5.15	56.58	58.25	0	92.59	93.389
14	5	4.92	38.43	35.69	1.78	60.5	93.185
14	5.42	4.93	52.76	53.41	2.07	72.12	92.565
14	5.69	4.94	46.4	49.07	2.53	47.28	92.264
14	5.41	4.91	52.54	53.25	2.04	73.68	91.599
14	5.46	4.9	44.22	46.23	-0.73	82.88	91.569
14	5.71	5.55	38.11	34.73	0.02	52.2	91.097
15	6.29	5.88	70.44	66.84	4.29	97.09	89.674
15	5.96	5.86	57.68	43.82	-0.83	65.12	86.862
15	5.67	5.47	71.72	65.16	2.13	86.77	86.402
15	5.67	5.47	71.72	65.16	2.13	86.76	86.398
15	5.57	5.38	65.65	59.77	2.11	78.21	86.116
15	5.55	5.3	54.29	51.46	0.69	80.95	85.273
15	5.24	5.16	50.87	50.69	0.83	79.66	84.784
15	5.77	5.26	54.41	44.66	0.17	93.82	84.49

(Table 2) contd....

Docking Pose	Ligscore 1	Ligscore 2	PLP1	PLP2	Jain	PMF	Dock score
15	5.4	4.94	46.15	43.5	0.93	63.9	84.359
15	5.54	5.44	73.05	70.14	2.3	103.19	83.934
16	5.27	5.23	45.25	43.21	1.68	64.79	95.841
16	5.74	5.48	58.16	53.25	1.18	58.48	95.714
16	5.77	5.2	46.33	39.02	1.93	52.62	95.291
16	5.42	5.21	70.57	64.85	1.29	71.38	94.027
16	5.44	5.46	64.41	53.67	-0.12	105.45	89.172
16	5.99	5.92	57.62	47.75	3.33	72.74	88.435
16	6.01	5.82	50.74	56.89	2.01	95.69	88.105
16	5.95	5.6	55.32	51.37	1.46	85.07	87.023
16	5.99	5.92	57.62	47.75	3.33	72.74	86.466
16	5.97	5.53	58.3	53.56	1.35	86.84	85.186
17	5.5	5.27	56.05	60.31	2.35	83.94	106.087
17	5.56	5.37	53.74	47.84	-0.6	75.96	99.158
17	5.96	5.47	59.89	62.92	1.29	86.27	98.741
17	6.09	5.82	58.93	56.92	1.95	92.61	97.304
17	5.85	6.03	88.22	75.01	1.35	113.22	97.046
17	5.92	5.57	61.17	62.12	2.79	72.26	96.505
17	5.77	5.58	73.44	60.72	0.13	105.43	96.078
17	5.77	5.58	73.42	60.7	0.13	105.25	95.179
17	5.49	5.31	62.01	52.78	1.22	56.94	94.073
17	5.89	5.72	70.45	67.26	0.49	104.58	93.283
18	6.79	6.43	75.94	73.34	2.26	87.24	93.175
18	6.27	6.12	62.31	56.76	1.97	106.05	91.459
18	6.58	6.42	75.65	84.92	3.92	83.27	89.783
18	6.58	6.43	75.65	84.93	3.92	83.45	88.519
18	5.87	4.9	56.62	54.91	0.44	67.39	86.336
18	5.67	5.57	71.28	70.12	0.98	109.37	85.931
18	6.5	6.38	94.66	76.79	3.74	103.37	84.618
18	6.61	6.36	73.62	70.61	3.34	83.94	84.456
18	5.71	6.3	62.09	55.22	0.81	93.59	84.395
18	5.06	4.68	48.32	38.16	-0.07	27.2	83.593
19	6.26	6.01	63.99	63.38	2.68	91.97	101.664
19	6.02	5.49	52.35	54.95	2.18	86.84	97.882
19	5.37	5.27	53.65	52.22	0.65	84.83	94.197
19	5.38	5.27	53.37	51.88	0.75	81.43	93.958
19	5.48	5.25	63.9	58.15	2	88.53	92.626

(Table 2) contd....

Docking Pose	Ligscore 1	Ligscore 2	PLP1	PLP2	Jain	PMF	Dock score
19	5.99	5.69	54.91	57.53	3.2	95.69	90.825
19	5.37	5.18	49.92	42.63	-0.76	73.21	90.313
19	5.47	5.22	39.82	46.78	3.05	63.4	90.297
19	5.42	5.38	60.97	62.44	0.72	102.83	90.092
19	5.51	5.35	60.85	64.68	1.53	102.84	89.374
20	5.68	5.89	56.34	55.83	0.44	82.31	90.238
20	5.9	6.02	52.17	60.94	2.83	73.58	90.153
20	4.92	5	46.8	37.3	-1.09	42.06	88.693
20	4.94	5.37	60.11	53.63	0.62	102.86	86.841
20	6.04	6.01	63.19	73.86	2.77	87.82	86.278
20	5.96	5.39	59.49	52.98	1.39	81.47	86.269
20	6.06	6.34	68.65	59.73	2.47	86.29	84.716
20	5.79	5.61	59.64	63.59	1.34	73.13	84.178
20	5	5.36	47.94	46.07	-0.63	46.32	83.276
20	5.58	5.19	50.98	38.15	0.13	60.94	83.036
21	5.59	5.32	50.28	55.31	2.54	79.81	103.344
21	6.03	5.89	49.13	45.5	0.9	62.77	97.012
21	5.43	5.28	40.08	40.23	1.49	65.25	89.284
21	5.23	4.85	55.73	44.43	0.4	95.16	88.451
21	5.48	5.08	58.5	56.6	1.17	90.27	87.765
21	5.72	5.43	63.36	53	1.15	100.75	86.864
21	5.99	5.98	68.15	63.33	1.58	69.58	86.634
21	5.65	6.02	70.14	58.15	0.66	71.86	86.583
21	5.55	5.05	41.5	32.47	0.45	34.41	85.654
21	5.91	5.59	54.45	47.67	2.35	63.74	85.479