

Supplementary Materials

Towards Intelligent Drug Design System: Application of Artificial Dipeptide Receptor Library in QSAR-Oriented Studies

Andrzej Bak ^{1,*}, Violetta Kozik ¹, Malgorzata Walczak ², Justyna Fraczyk ², Zbigniew Kaminski ², Beata Kolesinska ², Adam Smolinski ³, Josef Jampilek ^{4,*}

¹ Department of Synthesis Chemistry, Faculty of Mathematics, Physics and Chemistry, University of Silesia, Szkolna 9, 40007 Katowice, Poland; violetta.kozik@us.edu.pl

² Institute of Organic Chemistry, Lodz University of Technology, Zeromskiego 116, 90924 Lodz, Poland; malgorzata.walczak@p.lodz.pl (M.W.), justyna.fraczyk@p.lodz.pl (J.F.), zbigniew.kaminski@p.lodz.pl (Z.K.), beata.kolesinska@p.lodz.pl (B.K.)

³ Central Mining Institute, Gwarkow 1, 40166 Katowice, Poland; asmolinski@gig.katowice.pl (A.S.)

⁴ Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Comenius University, Odbojarov 10, 83232 Bratislava, Slovakia

* Correspondence: andrzej.bak@us.edu.pl (A.B.); josef.jampilek@gmail.com (J.J.)

Table S1. Molecular descriptors calculated with Sybyl software.

L.p.	polar surface area	volume	polar volume	acceptor count	clogP	donor count	Ro5 violations	molecular weight	rotatable bond count
1.	63.824	1058.514	297.659	7	3.9438	1	0	348.8305	6
2.	63.913	1113.909	294.349	7	4.4428	1	0	362.8571	6
3.	59.635	1121.490	307.347	7	3.4128	1	0	362.8571	7
4.	59.223	1072.394	313.306	7	3.5518	1	0	328.8409	8
5.	49.670	1030.942	300.050	8	1.2955	0	0	342.8244	5
6.	34.303	1055.849	292.437	7	2.6775	0	0	340.8516	5
7.	83.034	1083.036	339.623	9	2.0264	1	0	358.8238	8
8.	71.756	1297.145	323.532	9	3.4444	1	0	434.9198	10
9.	127.346	1124.004	374.276	10	0.7882	2	0	374.8232	9
10.	183.253	1331.860	425.484	13	-1.1538	3	0	473.9112	12
11.	56.549	867.528	275.754	7	2.0154	0	0	287.7459	5
12.	118.914	1479.006	440.206	12	3.1768	3	1	545.0337	12
13.	176.800	1470.734	409.156	12	1.4688	3	0	486.9961	14
14.	42.977	1338.142	315.506	8	4.3696	1	0	465.4225	8
15.	43.030	1390.771	302.718	8	4.7496	1	0	479.4491	8
16.	34.469	1201.483	341.483	8	2.3295	0	0	404.3379	7
17.	70.710	1452.356	343.600	9	5.1552	1	2	511.0157	12
18.	74.499	1342.959	335.740	10	3.2898	1	0	464.9458	12
19.	95.669	1306.901	408.794	11	2.0778	2	0	443.9283	10
20.	38.187	1444.600	337.463	8	3.8386	1	0	479.4491	9

Table S2. Position on cellulose sheet and structure of array of artificial peptide receptors.

Position	ADP structure
A1	n-decanoyl-AA-NH-C ₆ H ₄ -NH-DMT-cellulose
A2	n-heptanoyl-AA-NH-C ₆ H ₄ -NH-DMT-cellulose
A3	n-decanoyl-RA-NH-C ₆ H ₄ -NH-DMT-cellulose
A4	n-heptanoyl-RA-NH-C ₆ H ₄ -NH-DMT-cellulose
A5	n-decanoyl-NA-NH-C ₆ H ₄ -NH-DMT-cellulose
A6	n-heptanoyl-NA-NH-C ₆ H ₄ -NH-DMT-cellulose
A7	n-decanoyl-DA-NH-C ₆ H ₄ -NH-DMT-cellulose
A8	n-heptanoyl-DA-NH-C ₆ H ₄ -NH-DMT-cellulose
A9	n-decanoyl-CA-NH-C ₆ H ₄ -NH-DMT-cellulose
A10	n-heptanoyl-CA-NH-C ₆ H ₄ -NH-DMT-cellulose
A11	n-decanoyl-QA-NH-C ₆ H ₄ -NH-DMT-cellulose
A12	n-heptanoyl-QA-NH-C ₆ H ₄ -NH-DMT-cellulose
A13	n-decanoyl-EA-NH-C ₆ H ₄ -NH-DMT-cellulose
A14	n-heptanoyl-EA-NH-C ₆ H ₄ -NH-DMT-cellulose
A15	n-decanoyl-GA-NH-C ₆ H ₄ -NH-DMT-cellulose
A16	n-heptanoyl-GA-NH-C ₆ H ₄ -NH-DMT-cellulose
A17	n-decanoyl-HA-NH-C ₆ H ₄ -NH-DMT-cellulose
A18	n-heptanoyl-HA-NH-C ₆ H ₄ -NH-DMT-cellulose
A19	n-decanoyl-IA-NH-C ₆ H ₄ -NH-DMT-cellulose
A20	n-heptanoyl-IA-NH-C ₆ H ₄ -NH-DMT-cellulose
B1	n-decanoyl-LA-NH-C ₆ H ₄ -NH-DMT-cellulose
B2	n-heptanoyl-LA-NH-C ₆ H ₄ -NH-DMT-cellulose
B3	n-decanoyl-KA-NH-C ₆ H ₄ -NH-DMT-cellulose
B4	n-heptanoyl-KA-NH-C ₆ H ₄ -NH-DMT-cellulose
B5	n-decanoyl-MA-NH-C ₆ H ₄ -NH-DMT-cellulose
B6	n-heptanoyl-MA-NH-C ₆ H ₄ -NH-DMT-cellulose
B7	n-decanoyl-FA-NH-C ₆ H ₄ -NH-DMT-cellulose
B8	n-heptanoyl-FA-NH-C ₆ H ₄ -NH-DMT-cellulose
B9	n-decanoyl-PA-NH-C ₆ H ₄ -NH-DMT-cellulose
B10	n-heptanoyl-PA-NH-C ₆ H ₄ -NH-DMT-cellulose
B11	n-decanoyl-SA-NH-C ₆ H ₄ -NH-DMT-cellulose
B12	n-heptanoyl-SA-NH-C ₆ H ₄ -NH-DMT-cellulose
B13	n-decanoyl-TA-NH-C ₆ H ₄ -NH-DMT-cellulose
B14	n-heptanoyl-TA-NH-C ₆ H ₄ -NH-DMT-cellulose
B15	n-decanoyl-WA-NH-C ₆ H ₄ -NH-DMT-cellulose
B16	n-heptanoyl-WA-NH-C ₆ H ₄ -NH-DMT-cellulose
B17	n-decanoyl-YA-NH-C ₆ H ₄ -NH-DMT-cellulose
B18	n-heptanoyl-YA-NH-C ₆ H ₄ -NH-DMT-cellulose
B19	n-decanoyl-VA-NH-C ₆ H ₄ -NH-DMT-cellulose
B20	n-heptanoyl-VA-NH-C ₆ H ₄ -NH-DMT-cellulose
C1	n-decanoyl-AF-NH-C ₆ H ₄ -NH-DMT-cellulose
C2	n-heptanoyl-AF-NH-C ₆ H ₄ -NH-DMT-cellulose
C3	n-decanoyl-RF-NH-C ₆ H ₄ -NH-DMT-cellulose
C4	n-heptanoyl-RF-NH-C ₆ H ₄ -NH-DMT-cellulose
C5	n-decanoyl-NF-NH-C ₆ H ₄ -NH-DMT-cellulose
C6	n-heptanoyl-NF-NH-C ₆ H ₄ -NH-DMT-cellulose
C7	n-decanoyl-DF-NH-C ₆ H ₄ -NH-DMT-cellulose
C8	n-heptanoyl-DF-NH-C ₆ H ₄ -NH-DMT-cellulose
C9	n-decanoyl-CF-NH-C ₆ H ₄ -NH-DMT-cellulose
C10	n-heptanoyl-CF-NH-C ₆ H ₄ -NH-DMT-cellulose
C11	n-decanoyl-QF-NH-C ₆ H ₄ -NH-DMT-cellulose

C12	n-heptanoyl-QF-NH-C ₆ H ₄ -NH-DMT-cellulose
C13	n-decanoyl-EF-NH-C ₆ H ₄ -NH-DMT-cellulose
C14	n-heptanoyl-EF-NH-C ₆ H ₄ -NH-DMT-cellulose
C15	n-decanoyl-GF-NH-C ₆ H ₄ -NH-DMT-cellulose
C16	n-heptanoyl-GF-NH-C ₆ H ₄ -NH-DMT-cellulose
C17	n-decanoyl-HF-NH-C ₆ H ₄ -NH-DMT-cellulose
C18	n-heptanoyl-HF-NH-C ₆ H ₄ -NH-DMT-cellulose
C19	n-decanoyl-IF-NH-C ₆ H ₄ -NH-DMT-cellulose
C20	n-heptanoyl-IF-NH-C ₆ H ₄ -NH-DMT-cellulose
D1	n-decanoyl-LF-NH-C ₆ H ₄ -NH-DMT-cellulose
D2	n-heptanoyl-LF-NH-C ₆ H ₄ -NH-DMT-cellulose
D3	n-decanoyl-KF-NH-C ₆ H ₄ -NH-DMT-cellulose
D4	n-heptanoyl-KF-NH-C ₆ H ₄ -NH-DMT-cellulose
D5	n-decanoyl-MF-NH-C ₆ H ₄ -NH-DMT-cellulose
D6	n-heptanoyl-MF-NH-C ₆ H ₄ -NH-DMT-cellulose
D7	n-decanoyl-FF-NH-C ₆ H ₄ -NH-DMT-cellulose
D8	n-heptanoyl-FF-NH-C ₆ H ₄ -NH-DMT-cellulose
D9	n-decanoyl-PF-NH-C ₆ H ₄ -NH-DMT-cellulose
D10	n-heptanoyl-PF-NH-C ₆ H ₄ -NH-DMT-cellulose
D11	n-decanoyl-SF-NH-C ₆ H ₄ -NH-DMT-cellulose
D12	n-heptanoyl-SF-NH-C ₆ H ₄ -NH-DMT-cellulose
D13	n-decanoyl-TF-NH-C ₆ H ₄ -NH-DMT-cellulose
D14	n-heptanoyl-TF-NH-C ₆ H ₄ -NH-DMT-cellulose
D15	n-decanoyl-WF-NH-C ₆ H ₄ -NH-DMT-cellulose
D16	n-heptanoyl-WF-NH-C ₆ H ₄ -NH-DMT-cellulose
D17	n-decanoyl-YF-NH-C ₆ H ₄ -NH-DMT-cellulose
D18	n-heptanoyl-YF-NH-C ₆ H ₄ -NH-DMT-cellulose
D19	n-decanoyl-VF-NH-C ₆ H ₄ -NH-DMT-cellulose
D20	n-heptanoyl-VF-NH-C ₆ H ₄ -NH-DMT-cellulose
E1	n-decanoyl-AP-NH-C ₆ H ₄ -NH-DMT-cellulose
E2	n-heptanoyl-AP-NH-C ₆ H ₄ -NH-DMT-cellulose
E3	n-decanoyl-RP-NH-C ₆ H ₄ -NH-DMT-cellulose
E4	n-heptanoyl-RP-NH-C ₆ H ₄ -NH-DMT-cellulose
E5	n-decanoyl-NP-NH-C ₆ H ₄ -NH-DMT-cellulose
E6	n-heptanoyl-NP-NH-C ₆ H ₄ -NH-DMT-cellulose
E7	n-decanoyl-DP-NH-C ₆ H ₄ -NH-DMT-cellulose
E8	n-heptanoyl-DP-NH-C ₆ H ₄ -NH-DMT-cellulose
E9	n-decanoyl-CP-NH-C ₆ H ₄ -NH-DMT-cellulose
E10	n-heptanoyl-CP-NH-C ₆ H ₄ -NH-DMT-cellulose
E11	n-decanoyl-QP-NH-C ₆ H ₄ -NH-DMT-cellulose
E12	n-heptanoyl-QP-NH-C ₆ H ₄ -NH-DMT-cellulose
E13	n-decanoyl-EP-NH-C ₆ H ₄ -NH-DMT-cellulose
E14	n-heptanoyl-EP-NH-C ₆ H ₄ -NH-DMT-cellulose
E15	n-decanoyl-GP-NH-C ₆ H ₄ -NH-DMT-cellulose
E16	n-heptanoyl-GP-NH-C ₆ H ₄ -NH-DMT-cellulose
E17	n-decanoyl-HP-NH-C ₆ H ₄ -NH-DMT-cellulose
E18	n-heptanoyl-HP-NH-C ₆ H ₄ -NH-DMT-cellulose
E19	n-decanoyl-IP-NH-C ₆ H ₄ -NH-DMT-cellulose
E20	n-heptanoyl-IP-NH-C ₆ H ₄ -NH-DMT-cellulose
F1	n-decanoyl-LP-NH-C ₆ H ₄ -NH-DMT-cellulose
F2	n-heptanoyl-LP-NH-C ₆ H ₄ -NH-DMT-cellulose
F3	n-decanoyl-KP-NH-C ₆ H ₄ -NH-DMT-cellulose
F4	n-heptanoyl-KP-NH-C ₆ H ₄ -NH-DMT-cellulose
F5	n-decanoyl-MP-NH-C ₆ H ₄ -NH-DMT-cellulose
F6	n-heptanoyl-MP-NH-C ₆ H ₄ -NH-DMT-cellulose

F7	n-decanoyl-FP-NH-C ₆ H ₄ -NH-DMT-cellulose
F8	n-heptanoyl-FP-NH-C ₆ H ₄ -NH-DMT-cellulose
F9	n-decanoyl-PP-NH-C ₆ H ₄ -NH-DMT-cellulose
F10	n-heptanoyl-PP-NH-C ₆ H ₄ -NH-DMT-cellulose
F11	n-decanoyl-SP-NH-C ₆ H ₄ -NH-DMT-cellulose
F12	n-heptanoyl-SP-NH-C ₆ H ₄ -NH-DMT-cellulose
F13	n-decanoyl-TP-NH-C ₆ H ₄ -NH-DMT-cellulose
F14	n-heptanoyl-TP-NH-C ₆ H ₄ -NH-DMT-cellulose
F15	n-decanoyl-WP-NH-C ₆ H ₄ -NH-DMT-cellulose
F16	n-heptanoyl-WP-NH-C ₆ H ₄ -NH-DMT-cellulose
F17	n-decanoyl-YP-NH-C ₆ H ₄ -NH-DMT-cellulose
F18	n-heptanoyl-YP-NH-C ₆ H ₄ -NH-DMT-cellulose
F19	n-decanoyl-VP-NH-C ₆ H ₄ -NH-DMT-cellulose
F20	n-heptanoyl-VP-NH-C ₆ H ₄ -NH-DMT-cellulose

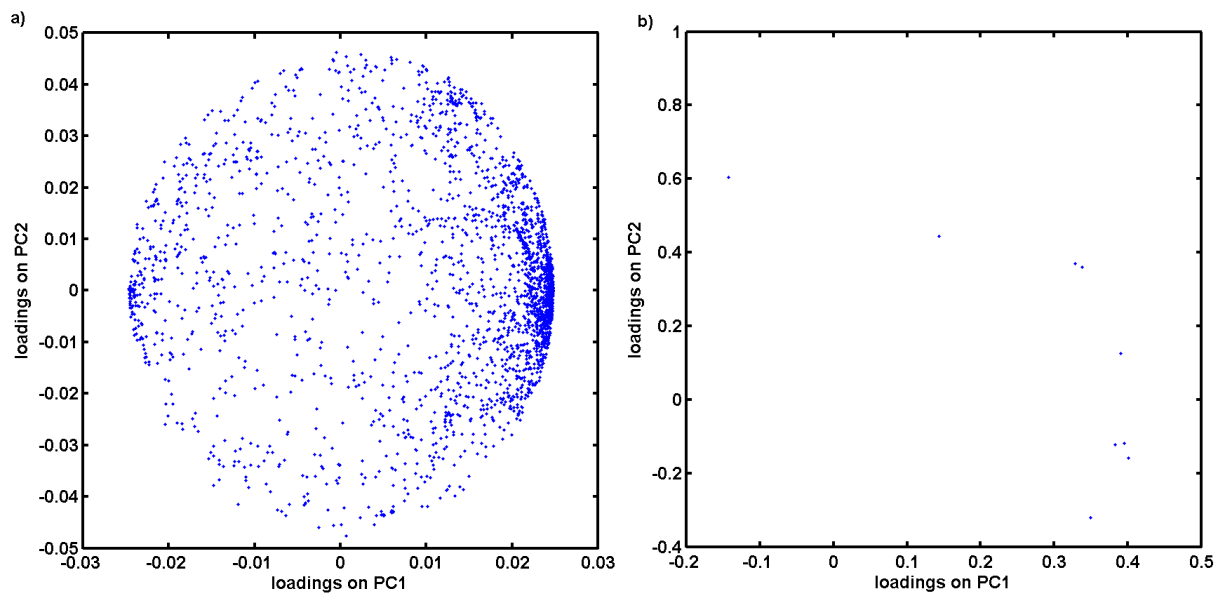


Figure S1. Projection of variables on plane defined by first and second loadings for Dragon (a) and Sybyl (b) parameters.