

## SUPPLEMENTARY INFORMATION

### QSAR Model for Predicting the Cannabinoid Receptor 1 Binding Affinity and Dependence Potential of Synthetic Cannabinoids

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Luna (C18) 5 $\mu$ m 150 x 4.6 mm	Mobile Phase A: 0.1% formic acid in water Mobile Phase B: 0.1% formic acid in acetonitrile 0-30 min; A/B = 10/90	210 nm	Concentration : 5 mg/ml in acetonitrile; 5 $\mu$ l injection
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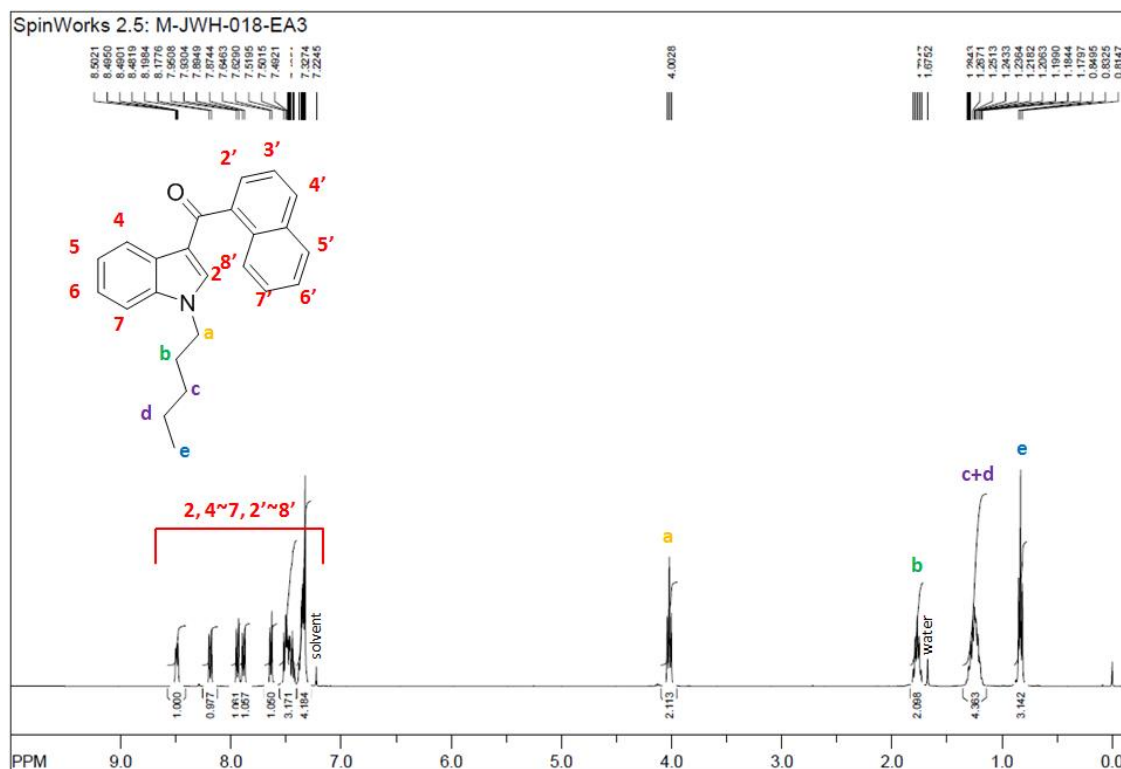
Results: 99.06% purity

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.235	BB	0.0834	63.13132	0.1802	?
2	3.679	BV	0.0902	4.26878e-1	1.218e-3	?
3	3.835	VV	0.0778	2.30263	6.571e-3	?
4	3.968	VB	0.0946	9.23103	0.0263	?
5	4.478	BV	0.1196	58.67265	0.1674	?
6	4.754	VBA	0.0972	2.81685	8.039e-3	?
7	5.474	BV	0.1117	6.31314	0.0180	?
8	5.682	VB	0.1058	1.80776	5.159e-3	?
9	6.311	BV	0.1482	52.76944	0.1506	?
10	6.771	VB	0.1943	8.98942	0.0257	?
11	7.799	BV	0.1867	47.05533	0.1343	?
12	8.485	VB	0.1939	3.47119e4	99.0618	CB13
13	11.344	BB	0.2269	12.12432	0.0346	?
14	12.658	BB	0.3155	29.82164	0.0851	?
15	15.858	BB	0.3055	5.08271	0.0145	?
16	17.099	BB	0.3294	16.73203	0.0478	?
17	25.586	BB	0.3974	11.48984	0.0328	?

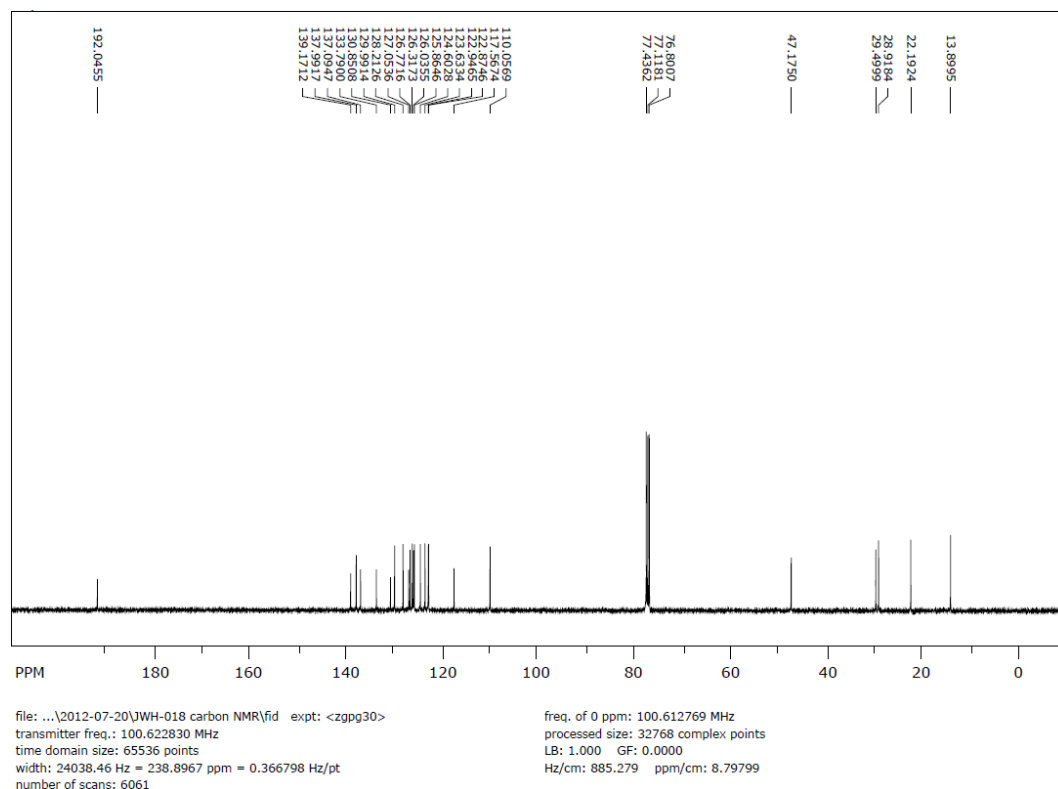
Synthesis of JWH-018

JWH-018 was synthesized by alkylation of indole with pentyl bromide followed by acylation of the resulting 1-pentylindole with 1-naphthoyl chloride as described [4].

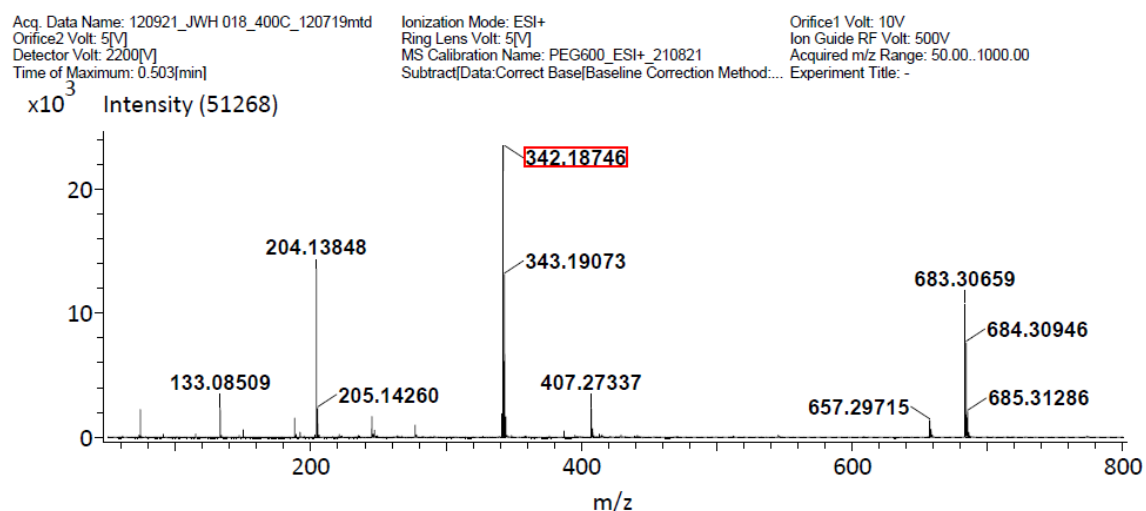
(a) <sup>1</sup>H-NMR spectrum of JWH-018.



(b)  $^{13}\text{C}$ -NMR spectrum of JWH-018.



(c) High Resolution Mass spectrum of JWH-018.



### Synthesis of CP47,497 and its homologs (CP47,497-C6, C8, and C9)

CP47,497 and its homologs (CP47,497-C6, C8, and C9) were synthesized by the following procedure. The derivatives of 1-methoxy CP47,497 were prepared

according to the reported method [5]. Treatment of 1-methoxy CP47,497 derivatives with 1-propanthiol and n-butyllithium in HMPA gave the desired compounds (CP47,497-C6, C8, and C9).

**2-((1S,3R)-3-hydroxycyclohexyl)-5-(2-methyloctan-2-yl)phenol (CP47,497)**

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.09 (d, J = 8.4 Hz, 1H), 6.87 (dd, J = 8.4 Hz, 2.1 Hz, 1H), 6.70 (d, J = 2.1 Hz, 1H), 3.69-3.86 (m, 1H), 2.79-2.99 (m, 1H), 2.13-2.27 (m, 2H), 1.98-2.13 (m, 2H), 1.80-1.98 (m, 2H), 1.49-1.75 (m, 4H), 1.26 (s, 6H), 1.01-1.30 (m, 8H), 0.79-0.94 (m, 3H) LRMS(EI) m/z 317.9

**2-((1S,3R)-3-hydroxycyclohexyl)-5-(2-methylheptan-2-yl)phenol (CP47,497-C6)**

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) : δ 7.08 (d, J = 7.8 Hz, 1H), 6.86 (dd, J = 7.8 Hz, 2.1 Hz, 1H), 6.70 (d, J = 2.1 Hz, 1H), 3.71-3.90 (m, 1H), 2.80-3.00 (m, 1H), 2.11-2.40 (m, 2H), 1.95-2.10 (m, 2H), 1.78-1.94 (m, 2H), 1.30-1.74 (m, 4H), 1.25 (s, 6H), 0.98-1.40 (m, 6H), 0.80-0.90 (m, 3H) ; HRMS(ESI) m/z calcd for C<sub>20</sub>H<sub>32</sub>O<sub>2</sub> [M+1]<sup>+</sup> : 304.2402, found 305.2479

**2-((1S,3R)-3-hydroxycyclohexyl)-5-(2-methylnonan-2-yl)phenol (CP47,497-C8)**

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) : δ 7.08 (d, J = 8.1 Hz, 1H), 6.86 (dd, J = 8.1 Hz, 1.8 Hz, 1H), 6.69 (d, J = 1.8 Hz, 1H), 3.70-3.83 (m, 1H), 2.81-2.94 (m, 1H), 2.12-2.41 (m, 2H), 1.95-2.13 (m, 2H), 1.78-1.96 (m, 2H), 1.37-1.63 (m, 4H), 1.25 (s, 6H), 0.98-1.38 (m, 10H), 0.80-0.98 (m, 3H) ; HRMS(ESI) m/z calcd for C<sub>22</sub>H<sub>36</sub>O<sub>2</sub> [M+1]<sup>+</sup> : 332.2715, found 333.2787

**2-((1S,3R)-3-hydroxycyclohexyl)-5-(2-methyldecan-2-yl)phenol (CP47,497-C9)**

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) : δ 7.08 (d, J = 8.1 Hz, 1H), 6.86 (dd, J = 8.1 Hz, 1.8 Hz, 1H), 6.69 (d, J = 1.8 Hz, 1H), 3.70-3.84 (m, 1H), 2.81-2.94 (m, 1H), 1.78-2.3 (m, 6H), 1.36-1.60 (m, 6H), 1.24 (s, 6H), 0.97-1.36 (m, 12H), 0.86 (t, J = 6.6 Hz, 3H) ; HRMS(ESI) m/z calcd for C<sub>23</sub>H<sub>38</sub>O<sub>2</sub> [M+1]<sup>+</sup> : 346.2872, found 347.2943

**Table S1.** CB1R-binding affinity raw data for 15 synthetic cannabinoids.

	THC			AM694			CP47,497			CP47,497-C6			CP47,497-C8			CP47,497-C9			JWH-018			JWH-015					
M	1			2			3			4			5			6			7			8					
10 <sup>-4</sup>				169	0	124	71	-2	83	60	217	203															
10 <sup>-5</sup>	49	0	0	337	55	56	293	250	588	650	579	736	0	0	0	0	0	0	0	0	0	0	0	24			
10 <sup>-6</sup>	356	287	285	831	367	599	716	572	771	917	1018	1100	268	95	208	316	587	294	121	158	230	408	816	737			
10 <sup>-7</sup>	514	616	724	1098	740	717	1106	755	826	791	1108	1039	920	775	662	553	2601	916	130	394	433	656	1162	1060			
10 <sup>-8</sup>	981	961	1235	868	1056	897	923	1235	1164	848	1136	1031	1058	1225	739	1129	1249	979	972	966	854	899	968	1122			
10 <sup>-9</sup>	700	891	991	1184	1254	1172	875	1118	1317	868	623	998	1176	1554	776	1070	1338	896	615	572	1095	676	499	1312			
10 <sup>-10</sup>	532	570	837	1765	1174	884	552	1031	1173	738	604	1136	1033	1215	626	1159	1303	708	784	853	1634	987	919	755			
10 <sup>-11</sup>				1169	1131	1148	1237	962	1118							791	831	748				1190	1365	1006			
Ki(M)	2.06E-07			2.83E-07			8.62E-07			1.18E-05			1.15E-07			4.81E-07			2.26E-08			0.005558					
	JWH-073			RCS-4			JWH-081			JWH-210			CRA13			CRA13-F			CRA13-OH								
M	9			10			11			12			13			14			15								
10 <sup>-4</sup>				202	23	199							649	702	762	57	299	499	1025	-347	597						
10 <sup>-5</sup>	43	-27	35	702	871	868	-143	245	170	-39	35	-3	729	761	644	454	205	1313	1067	1038	1363						
10 <sup>-6</sup>	785	728	267	877	909	770	-19	358	60	-10	107	91	1189	1643	1165	1321	686	659	1327	1777	1321						
10 <sup>-7</sup>	1429	1049	1179	801	971	1164	747	1041	810	319	571	646	1872	1516	1656	1540	1702	2137	1747	1929	1631						
10 <sup>-8</sup>	1763	1647	1301	918	1068	861	1380	1776	1311	1018	1049	790	2211	2054	1450	1494	2873	2297	1651	1886	2226						
10 <sup>-9</sup>	1414	1640	1417	1154	1323	1403	1606	1532	1748	1006	1475	1435	1880	2255	1602	2122	2491	2402	1514	1504	1972						
10 <sup>-10</sup>	1670	1706	1320	1203	1203	1288	1218	1433	1030	1164	1403	1241	1462	2009	1796	3161	3175	2689									
10 <sup>-11</sup>	1733	1797	1443	1174	1100	1187	1255	1588	1188	1162	1368	1269	1936	1656	1899	2118	2352	2418									
Ki(M)	2.28E-07			1.16E-05			6.16E-08			2.20E-08			4.80E-07			8.00E-08			5.42E-06								

**Table S2.** List of descriptors used for QSAR models.

Descriptor Name	Descriptor Type	Descriptor class	Definition
XLogP	XLogP	Constitutional Descriptor	Prediction of logP based on the atom-type method called XLogP
VP.7	ChiPath	Topological Descriptor	Evaluates chi path descriptors Valence path orders 7
SPC.5	ChiPathCluster	Topological Descriptor	Evaluates chi path cluster descriptors, Simple path cluster, order 5
TopoPSA	TPSA	Topological Descriptor	Calculation of topological polar surface area based on fragment contributions (TPSA)
WTPT.4	WeightedPath	Topological Descriptor	Evaluates the weighted path descriptors.sum of path lengths starting from oxygens
Kier1	KappaShapeIndices	Topological Descriptor	Kier and Hall kappa molecular shape indices compare the molecular graph with minimal and maximal molecular graphs, First kappa shape index
MW	Weight	Constitutional Descriptor	Molecular weight

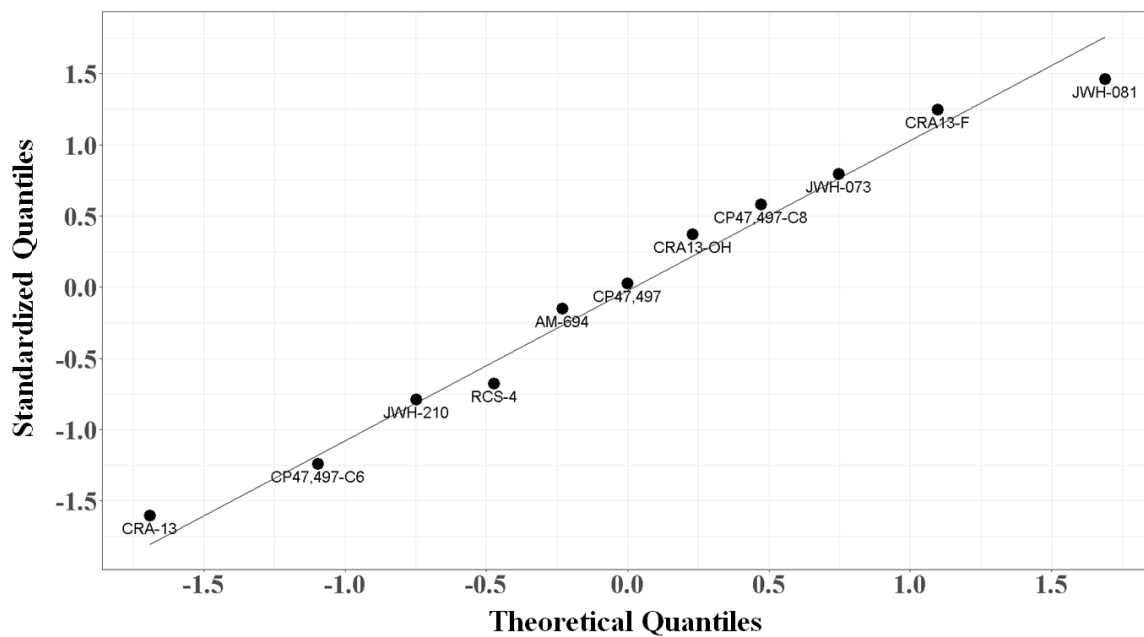
BCUTc.11	BCUT	Hybrid descriptor	Eigenvalue based descriptor noted for its utility in chemical diversity, nhigh lowest partial charge weighted BCUTS(nhigh : The number of highest eigenvalue)
MLogP	MannholdLogP	Constitutional descriptor	Prediction of logP based on the number of carbon and hetero atoms.
Wlambda3.un ity	WHIM	Hybrid descriptor	Holistic descriptors described by Todeschini et al (Todeschini, R. and Gramatica, P. Persepectives in Drug Discovery and Design. 1998. null). Wlambda3 directional WHIM descriptors.
WPSA.1	CPSA	Electronic & geometrical descriptor	Calculates Charged Partial Surface Area (CPSA) sum of surface area on positive parts of molecule * total molecular surface area / 1000
FP SA.3	CPSA	Electronic & geometrical descriptor	Calculates Charged Partial Surface Area (CPSA) Charge weighted partial positive surface area/ total molecular surface area
apol	APolDescriptor	Electronic descriptor	Sum of the atomic polarizabilities (including implicit hydrogens).
geomShape	PetitjeanShapeIndex	Topological descriptor	Evaluates the Petitjean shape indices, (geometric shape index)
nHBAcc	HBondAcceptorCount	Electronic descriptor	This descriptor calculates the number of hydrogen bond acceptors using a slightly simplified version of the PHACIR atom types.
ATSc4	AutocorrelationDescriptorCharge	Topological descriptor	Calculates the Autocorrelation of a Topological Structure autocorrelation descriptor, where the weight equal to the charges.



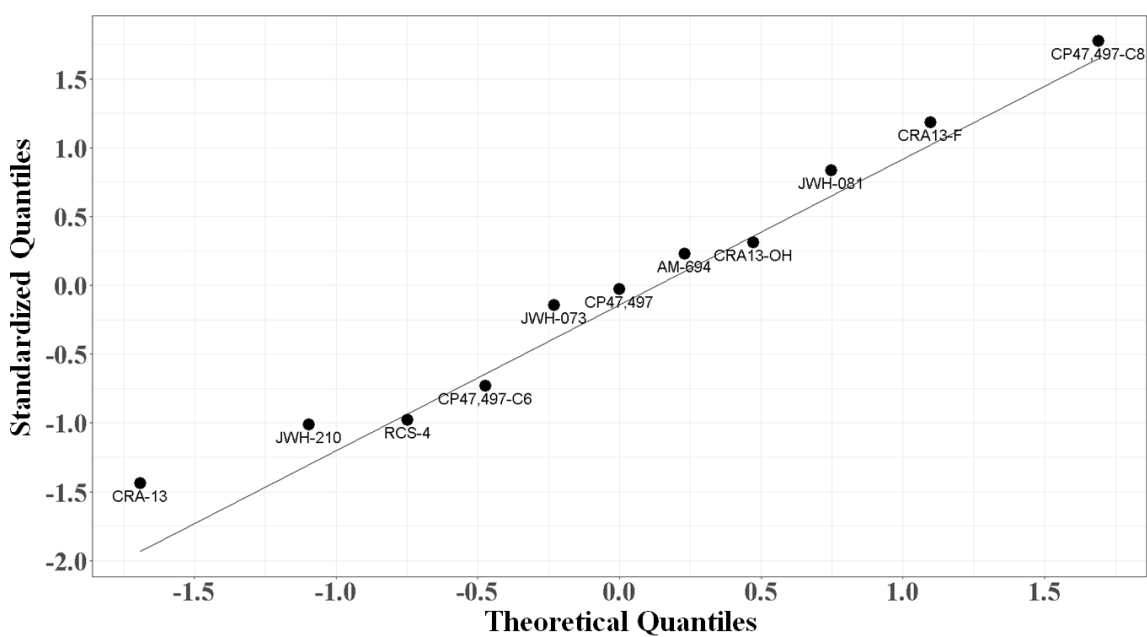
**Table S3.** Statistical Analysis of MLR models.

MLR Model number	Descriptor	R <sup>2</sup>	Adjusted R <sup>2</sup> <sub>adj</sub>	Predicted R <sup>2</sup> <sub>pred</sub>	training set RMSE	test set RMSE	Q <sup>2</sup>
1	XLogP	0.611	0.567	-0.857	0.558	1.071	0.527
2	VP.7	0.528	0.475	-0.776	0.614	1.047	0.463
3	SPC.5	0.376	0.307	0.008	0.706	0.783	0.25
4	WPSA.1	0.372	0.302	0.216	0.708	0.695	0.272
5	TopoPSA	0.319	0.244	0.539	0.737	0.533	0.224
6	apol	0.252	0.168	-0.755	0.773	1.041	0.037
7	WTPT.4	0.227	0.141	0.546	0.786	0.529	0.156
8	MLogP	0.203	0.114	0.117	0.798	0.738	-0.075
9	MW	0.17	0.078	-0.477	0.814	0.955	-0.033
10	Kier1	0.163	0.07	-0.793	0.818	1.052	-0.121
11	BCUTc.11	0.152	0.058	0.799	0.823	0.352	-0.043
12	geomShape	0.15	0.056	-0.3	0.824	0.896	-0.032
13	nHBAcc	0.14	0.044	-0.247	0.829	0.877	-0.005
14	FPSA.3	0.132	0.035	0.556	0.833	0.524	-0.092
15	Wlambda3.unity	0.107	0.008	-0.983	0.844	1.106	-0.188
16	ATSc4	0.097	-0.003	0.466	0.849	0.574	-0.078
17	VP.7, XLogP	0.696	0.621	-0.607	0.492	0.996	0.546
18	SPC.5, XLogP	0.679	0.599	0.097	0.506	0.746	0.52
19	WPSA.1, XLogP	0.655	0.569	-0.334	0.525	0.907	0.468
20	TopoPSA, XLogP	0.714	0.643	0.098	0.478	0.746	0.59
21	apol, XLogP	0.625	0.532	-0.635	0.547	1.005	0.455
22	WTPT.4, XLogP	0.738	0.672	-0.378	0.458	0.922	0.656
23	MLogP, XLogP	0.615	0.518	-0.965	0.555	1.101	0.439
24	MW, XLogP	0.647	0.559	-0.986	0.531	1.107	0.515
25	Kier1, XLogP	0.616	0.519	-0.718	0.554	1.03	0.41
26	BCUTc.11, XLogP	0.686	0.607	0.049	0.501	0.766	0.556
27	geomShape, XLogP	0.694	0.618	-0.374	0.494	0.921	0.544
28	nHBAcc, XLogP	0.636	0.544	-0.402	0.539	0.93	0.503
29	FPSA.3, XLogP	0.618	0.522	-1.123	0.553	1.145	0.217
30	Wlambda3.unity, XLogP	0.619	0.524	-1.23	0.551	1.173	0.358
<b>31</b>	<b>ATSc4, XLogP</b>	<b>0.812</b>	<b>0.765</b>	<b>0.133</b>	<b>0.387</b>	<b>0.732</b>	<b>0.698</b>
32	VP.7, ATSc4, XLogP	0.838	0.768	0.04	0.36	0.77	0.613
33	SPC.5, ATSc4, XLogP	0.834	0.762	0.465	0.364	0.575	0.664
34	WPSA.1, ATSc4, XLogP	0.834	0.762	0.42	0.365	0.598	0.655
35	TopoPSA, ATSc4, XLogP	0.813	0.733	0.083	0.387	0.752	0.531
36	apol, ATSc4, XLogP	0.829	0.756	0.039	0.369	0.77	0.559
37	WTPT.4, ATSc4, XLogP	0.82	0.743	0.13	0.379	0.733	0.609
38	MLogP, ATSc4, XLogP	0.818	0.74	0.269	0.382	0.672	0.649
39	MW, ATSc4, XLogP	0.821	0.744	0.098	0.378	0.746	0.646
40	Kier1, ATSc4, XLogP	0.844	0.777	0.09	0.353	0.75	0.658
41	BCUTc.11, ATSc4, XLogP	0.817	0.739	0.28	0.382	0.667	0.618
42	geomShape, ATSc4, XLogP	0.813	0.732	0.157	0.387	0.721	0.599
43	nHBAcc, ATSc4, XLogP	0.816	0.737	0.029	0.383	0.774	0.648
44	FPSA.3, ATSc4, XLogP	0.838	0.769	-0.158	0.359	0.846	0.54
45	Wlambda3.unity, ATSc4, XLogP	0.829	0.756	-0.153	0.369	0.843	0.628

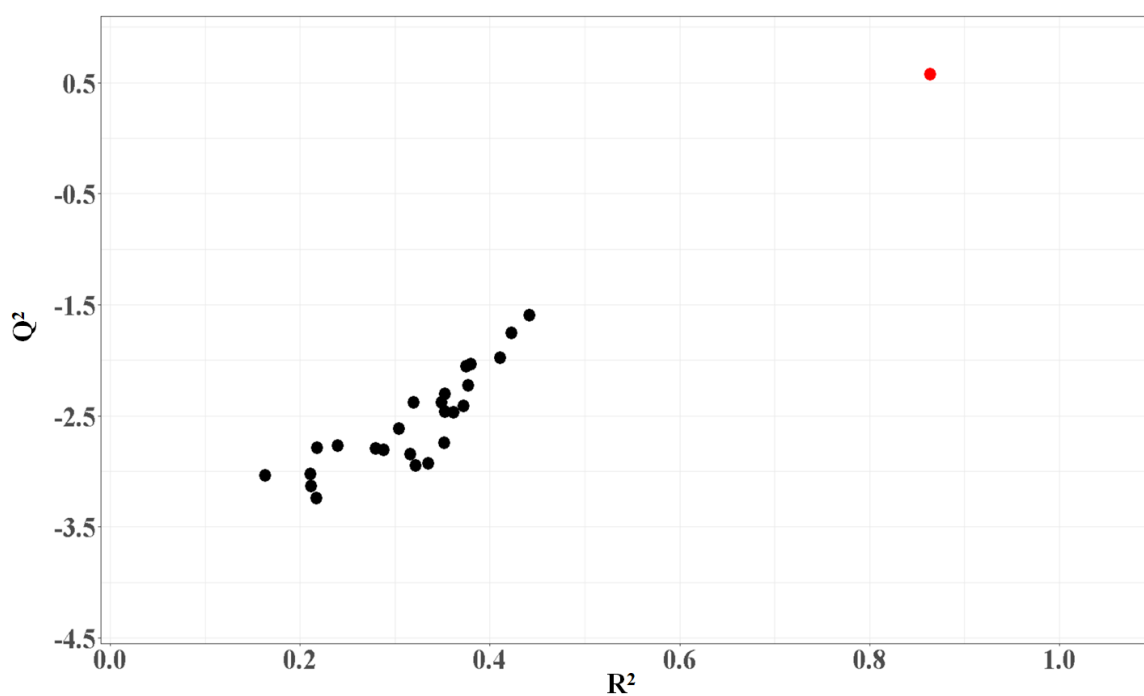
(R<sup>2</sup>: coefficient of determination data set, R<sup>2</sup><sub>adj</sub>: adjusted R<sup>2</sup>, R<sup>2</sup><sub>pred</sub>: R<sup>2</sup> for external test set, RMSE: root mean squared Error, Q<sup>2</sup>: cross-validated coefficient of determination (Leave-One-Out method))



**Figure S1.** Q-Q plot of the residuals from MLR model 31 showing a normal distribution.

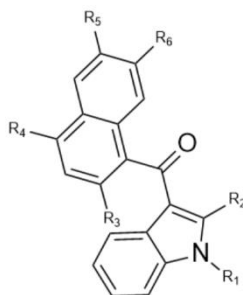


**Figure S2.** Q-Q plot of the residuals from PLSR model showing a normal distribution.



**Figure S3.** Y-Randomization analysis of the generated PLSR model. Black dots indicate Y-randomization models, and a red dot indicates the PLSR model.

**Table S4.** CB1R-binding affinity ( $pK_i$ ) of JWH-series compounds predicted by the PLSR model.



Compound Name	R <sub>1</sub>	R <sub>2</sub>	R <sub>3</sub>	R <sub>4</sub>	R <sub>5</sub>	R <sub>6</sub>	$pK_i$ value of literature	Predicted $pK_i$	<sup>1</sup> Residual	Eclidean Distance (APD=4.753)
*JWH-007	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	H	H	H	8.022	<b>7.490</b>	0.532	2.036
JWH-015	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	H	H	H	6.785	6.436	0.349	3.540
JWH-016	C <sub>4</sub> H <sub>9</sub>	CH <sub>3</sub>	H	H	H	H	7.658	7.323	0.335	3.186
*JWH-019	C <sub>6</sub> H <sub>13</sub>	H	H	H	H	H	8.009	<b>7.962</b>	0.047	4.280
JWH-043	C <sub>2</sub> H <sub>5</sub>	CH <sub>3</sub>	H	H	H	H	5.928	6.049	-0.121	4.233
JWH-046	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	H	H	CH <sub>3</sub>	6.465	6.750	-0.285	3.762
JWH-047	C <sub>4</sub> H <sub>9</sub>	CH <sub>3</sub>	H	H	H	CH <sub>3</sub>	7.231	7.349	-0.118	2.930
JWH-048	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	H	H	CH <sub>3</sub>	7.971	7.924	0.047	2.231

JWH-049	C <sub>6</sub> H <sub>13</sub>	CH <sub>3</sub>	H	H	H	CH <sub>3</sub>	7.259	8.679	-1.420	4.466
JWH-071	C <sub>2</sub> H <sub>5</sub>	H	H	H	H	H	5.873	5.594	0.279	4.171
JWH-072	C <sub>3</sub> H <sub>7</sub>	H	H	H	H	H	5.979	6.167	-0.188	2.057
JWH-076	C <sub>3</sub> H <sub>7</sub>	H	H	H	H	CH <sub>3</sub>	6.67	6.471	0.199	2.099
JWH-078	C <sub>2</sub> H <sub>5</sub>	H	H	OCH <sub>3</sub>	H	H	6.088	5.595	0.493	4.180
JWH-079	C <sub>3</sub> H <sub>7</sub>	H	H	OCH <sub>3</sub>	H	H	7.201	6.211	0.990	3.933
JWH-080	C <sub>4</sub> H <sub>9</sub>	H	H	OCH <sub>3</sub>	H	H	8.252	6.528	1.724	2.163
JWH-082	C <sub>6</sub> H <sub>13</sub>	H	H	OCH <sub>3</sub>	H	H	8.276	7.689	0.587	4.130
JWH-094	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	OCH <sub>3</sub>	H	H	6.322	6.294	0.028	3.614
JWH-096	C <sub>4</sub> H <sub>9</sub>	CH <sub>3</sub>	H	OCH <sub>3</sub>	H	H	7.472	7.344	0.128	2.852
*JWH-098	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	OCH <sub>3</sub>	H	H	8.347	<b>8.300</b>	0.047	2.864
JWH-120	C <sub>3</sub> H <sub>7</sub>	H	H	CH <sub>3</sub>	H	H	5.977	6.398	-0.421	3.388
*JWH-122	C <sub>5</sub> H <sub>11</sub>	H	H	CH <sub>3</sub>	H	H	9.161	<b>7.966</b>	1.195	4.015
JWH-148	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	CH <sub>3</sub>	H	H	6.91	6.620	0.290	4.447
JWH-149	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	CH <sub>3</sub>	H	H	8.301	7.778	0.523	2.802
JWH-153	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	H	OCH <sub>3</sub>	H	6.602	7.614	-1.012	3.537
JWH-159	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	H	H	OCH <sub>3</sub>	7.347	7.433	-0.086	2.755
JWH-160	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	H	H	OCH <sub>3</sub>	5.805	6.242	-0.437	3.744
JWH-163	C <sub>3</sub> H <sub>7</sub>	H	H	H	OCH <sub>3</sub>	H	5.627	5.977	-0.350	3.440
JWH-164	C <sub>5</sub> H <sub>11</sub>	H	H	H	H	OCH <sub>3</sub>	8.18	7.565	0.615	1.360
JWH-165	C <sub>3</sub> H <sub>7</sub>	H	H	H	H	OCH <sub>3</sub>	6.69	6.222	0.468	3.965
*JWH-166	C <sub>5</sub> H <sub>11</sub>	H	H	H	OCH <sub>3</sub>	H	7.357	<b>7.085</b>	0.272	1.677
JWH-180	C <sub>3</sub> H <sub>7</sub>	H	H	C <sub>3</sub> H <sub>7</sub>	H	H	7.585	7.519	0.066	3.776
JWH-181	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	C <sub>3</sub> H <sub>7</sub>	H	H	8.886	8.971	-0.085	3.569
JWH-182	C <sub>5</sub> H <sub>11</sub>	H	H	C <sub>3</sub> H <sub>7</sub>	H	H	9.187	9.191	-0.004	2.851
JWH-189	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	C <sub>3</sub> H <sub>7</sub>	H	H	7.284	7.753	-0.469	3.236
JWH-211	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	C <sub>2</sub> H <sub>5</sub>	H	H	7.155	7.295	-0.140	3.935
JWH-212	C <sub>3</sub> H <sub>7</sub>	H	H	C <sub>2</sub> H <sub>5</sub>	H	H	7.481	7.223	0.258	2.837
JWH-213	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	C <sub>2</sub> H <sub>5</sub>	H	H	8.824	8.408	0.416	2.396
JWH-234	C <sub>5</sub> H <sub>11</sub>	H	H	H	H	C <sub>2</sub> H <sub>5</sub>	8.076	8.077	-0.001	2.626
JWH-235	C <sub>3</sub> H <sub>7</sub>	H	H	H	H	C <sub>2</sub> H <sub>5</sub>	6.471	6.998	-0.527	2.291
JWH-236	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	H	H	C <sub>2</sub> H <sub>5</sub>	5.869	7.282	-1.413	4.504
JWH-239	C <sub>3</sub> H <sub>7</sub>	H	H	C <sub>4</sub> H <sub>9</sub>	H	H	6.466	8.009	-1.543	3.599
JWH-240	C <sub>5</sub> H <sub>11</sub>	H	H	C <sub>4</sub> H <sub>9</sub>	H	H	7.854	9.132	-1.278	4.054
JWH-241	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	C <sub>4</sub> H <sub>9</sub>	H	H	6.833	8.301	-1.468	2.507
JWH-258	C <sub>5</sub> H <sub>11</sub>	H	H	OC <sub>2</sub> H <sub>5</sub>	H	H	8.337	8.234	0.103	2.784
JWH-259	C <sub>3</sub> H <sub>7</sub>	H	H	OC <sub>2</sub> H <sub>5</sub>	H	H	6.658	6.423	0.235	2.435
JWH-260	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	OC <sub>2</sub> H <sub>5</sub>	H	H	7.538	8.028	-0.490	4.556

JWH-261	C <sub>3</sub> H <sub>7</sub>	CH <sub>3</sub>	H	OC <sub>2</sub> H <sub>5</sub>	H	H	6.115	6.796	-0.681	2.617
JWH-262	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	H	H	H	C <sub>2</sub> H <sub>5</sub>	7.553	8.485	-0.932	3.254
JWH-267	C <sub>5</sub> H <sub>11</sub>	H	OCH <sub>3</sub>	H	H	H	6.419	7.256	-0.837	3.240
JWH-268	C <sub>5</sub> H <sub>11</sub>	CH <sub>3</sub>	OCH <sub>3</sub>	H	H	H	5.86	7.838	-1.978	4.255

(\* Compound currently in US schedule I; <sup>1</sup>Residual: difference between the observed and predicted pK<sub>i</sub> values.)

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