molecules

MDPI

Supplementary materials

Evaluation of Physicochemical Properties of Ipsapirone Derivatives Based on Chromatographic and Chemometric Approaches

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Table S1. Summary of QSRR model of HSA based on the theoretical descriptors.

QSRR equation						
$\log K_{HSA}$ = 0.230(±0.335) F05[C-N] 0.060(±0.330) RDF155u 5.899(±0.821) LLS_01 + 1.955(±1.240)						
Eq.	**R^2**	**$RMSE_{tr}$**	**Q^2_{LLO}**	**R^2_{EXT}**	**$RMSE_{Ext}$**	**CCC_{Ext}**
1	0.786	0.274	0.670	0.7093	0.302	0.7954

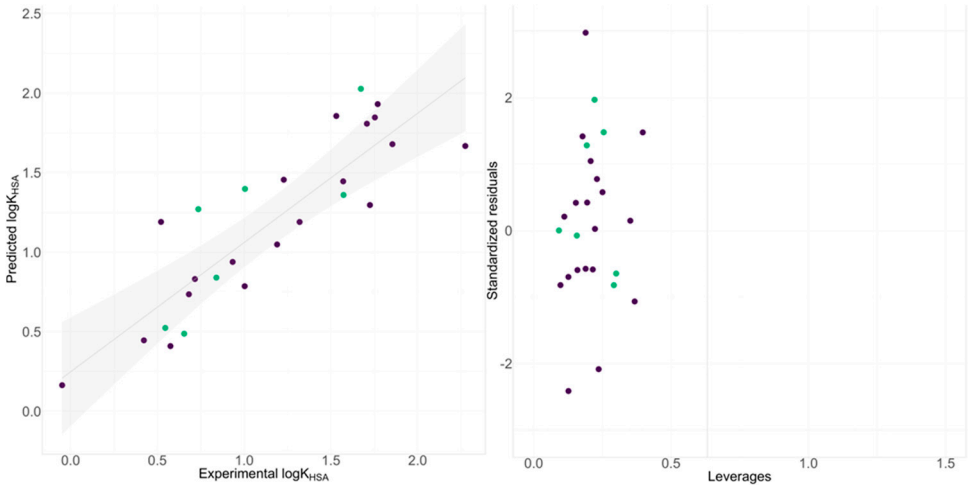

Table S2. List and SMILE notation of target structures.

No	Smiles	linker	R
1	O=C1N(CCCN2CCN(C3=CC=CC=C3)CC2)S(C4=CC=CC=C41)(=O)=O	butyl	H
2	O=C1N(CCCN2CCN(C3=CC=CC=C3OC)CC2)S(C4=CC=CC=C41)(=O)=O	butyl	2-OMe-Ph
3	O=C1N(CCCN2CCN(C3=CC=CC(Cl)=C3Cl)CC2)S(C4=CC=CC=C41)(=O)=O	butyl	2,3-diCl-Ph
4	O=C1N(CCCN2CCN(C3=CC=C(Cl)C=C3)CC2)S(C4=CC=CC=C41)(=O)=O	butyl	4-Cl-Ph
5	O=C1N(CCCCCN2CCN(C3=CC=CC=C3)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	H
6	O=C1N(CCCCCN2CCN(C3=CC=CC=C3OC)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	2-OMe-Ph
7	O=C1N(CCCCCN2CCN(C3=CC=CC(Cl)=C3Cl)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	2,3-diCl-Ph
8	O=C1N(CCCCCN2CCN(C3=CC=C(Cl)C=C3)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	4-Cl-Ph
9	O=C1N(CCCCCN2CCN(C3=NC=CC=N3)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	2-pirymidyl
10	O=C1N(CCCCCN2CCN(C3=CC=CC=N3)CC2)S(C4=CC=CC=C41)(=O)=O	pentyl	2-pirydyl
11	O=C1N(CCCCCN2CCN(C3=C(C=CC=C4)C4=CC=C3)CC2)S(C5=CC=CC=C51)(=O)=O	pentyl	1-naphthyl
12	O=C1N(CCCCCCN2CCN(C3=CC=CC=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	H
13	O=C1N(CCCCCCN2CCN(C3=CC=CC=C3OC)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	2-OMe-Ph
14	O=C1N(CCCCCCN2CCN(C3=CC(OC)=CC=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	3-OMe-Ph
15	O=C1N(CCCCCCN2CCN(C3=CC=C(OC)C=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	4-OMe-Ph
16	O=C1N(CCCCCCN2CCN(C3=CC=CC(Cl)=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	3-Cl-Ph
17	O=C1N(CCCCCCN2CCN(C3=CC=C(Cl)C=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	4-Cl-Ph
18	O=C1N(CCCCCCN2CCN(C3=CC=C(Cl)C(Cl)=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	3,4-diCl-Ph
19	O=C1N(CCCCCCN2CCN(C3=CC=CC(C(F)(F)F)=C3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	3-CF_3-Ph
20	O=C1N(CCCCCCN2CCN(C3=CC=CC=C3F)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	2-F-Ph
21	O=C1N(CCCCCCN2CCN(C3=C(C=CC=C4)C4=CC=C3)CC2)S(C5=CC=CC=C51)(=O)=O	heksyl	1-naphthyl
22	O=C1N(CCCCCCN2CCN(C3=CC=CC=N3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	1-pirydyl
23	O=C1N(CCCCCCN2CCN(C3=NC=CC=N3)CC2)S(C4=CC=CC=C41)(=O)=O	heksyl	1-pirymidynyl
24	O=C1N(CCCCCCN2CCN(C3=NSC4=C3C=CC=C4)CC2)S(C5=CC=CC=C51)(=O)=O	heksyl	3-benzisothiazole
25	O=C1N(CCCCCCN2CCN(C3=CC=CC4=C3C=CS4)CC2)S(C5=CC=CC=C51)(=O)=O	heksyl	1-benzothiophen
26	O=C1N(CC2=CC=C(CN3CCN(C4=CC=CC=C4OC)CC3)C=C2)S(C5=CC=CC=C51)(=O)=O	xylene	H

General structure of investigated molecules

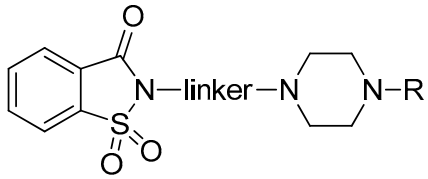

Table S3. Calibration mixtures for biomimetic chromatography.

Compound	t_{mean}	SD	CHI $_{C18}$
	C_{18}-HPLC		
Theophylline	2.19	0.024	18.4
Benzimidazole	2.60	0.009	34.3
Colichicine	3.27	0.006	42.0
Acetophenone	3.58	0.007	65.1
Indole	3.99	0.005	71.5
Propiophenone	4.13	0.005	77.5
Butyrophenone	4.54	0.006	87.5
Valerophenone	4.91	0.006	96.2
	IAM-HPLC		
Paracetamol	2.27	0.075	2.9
Acetanilidine	2.84	0.047	11.5
Acetophenone	3.16	0.038	17.2
Propiohenone	3.79	0.023	25.9
Butyrophenone	4.26	0.015	32.0
Valerophenone	4.65	0.011	37.3
Hexanophenone	4.98	0.010	41.8
Heptanophenone	5.25	0.010	45.7
Octanophenone	5.49	0.010	49.4
	HSA-HPLC		
Nizatidine	2.10	0.027	35.0%
Carbamazepine	5.31	0.069	75.0%
Nicardipine	11.09	0.216	95.0%
Indometacine	20.80	0.010	99.0%
Diclofenac	33.67	0.256	99.8%