

Supplementary materials of “User-Driven Strategy for In Silico Screening of Reversed-Phase Liquid Chromatography Conditions for Known Pharmaceutical-Related Small Molecules”

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Table S1. Solubilization and dilution solutions of standard compounds.

Compound	Solubilization solution	Dilution solution	Initial concentration [mg.ml ⁻¹]	Final concentration [mg.ml ⁻¹]
2,2'-Bipyridine	MeOH	H ₂ O	1	0.02
4-Nitrophenol	MeOH	H ₂ O	1	0.02
Ibuprofen	MeOH	H ₂ O	1	0.04
Metoclopramide	MeOH	H ₂ O	1	0.02
Papaverine	MeOH	H ₂ O	1	0.02
Pindolol	H ₂ O/MeOH 50:50	H ₂ O	0.5	0.02
Verapamil	H ₂ O	H ₂ O	1	0.02

Table S2. Predicted and observed retention times of the second test set of compounds in the condition with pH 2.7 and 54 minutes gradient time.

Number	Compound	Predicted t _R [min]	Observed t _R [min]
1	2,2'-bipyridine	12.35	12.17
6	pindolol	14.94	15.95
4	metoclopramide	18.02	19.19
2	4-nitrophenol	20.42	21.35
5	papaverine	23.91	25.28
7	verapamil	30.91	33.21
3	ibuprofen	43.42	45.79

Table S3. Predicted and observed retention times of the second test set of compounds in the condition with pH 7.0 and 50 minutes gradient time.

Number	Compound	Predicted t_R [min]	Observed t_R [min]
2	4-nitrophenol	11.97	12.13
6	pindolol	17.89	19.86
1	2,2'-bipyridine	24.96	25.24
4	metoclopramide	22.86	25.78
3	ibuprofen	32.27	34.48
5	papaverine	34.14	34.91
7	verapamil	37.50	41.60

Table S4. Retention times of the compounds of the test set 1 in the new conditions and the condition parameters.

Compound	Observed t_R [min]	Real pH	Target pH	Gradient time [min]
4-Nitrophenol	18.10	3	3	40
4-Nitrophenol	14.56	6.01	6	40
Ibuprofen	32.59	3	3	40
Ibuprofen	28.93	6.01	6	40
Papaverine	20.20	3	3	40
Papaverine	28.91	6.01	6	40
Pindolol	13.23	3	3	40
Pindolol	15.45	6.01	6	40