

Electronic Supplementary Information for Analyst

How useful is molecular modelling in combination with ion mobility mass spectrometry for ‘small molecule’ ion mobility collision cross sections?

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Experimental data for nitrogen-parameterised calibration set

Name	eCCS1	eCCS2	eCCS3	Mean	Std Dev	% RSD
N-ethylaniline	126.81	126.84	126.64	126.76	0.11	0.09%
Acetaminophen	129.89	128.76	128.94	129.20	0.61	0.47%
Pregabalin	137.85	137.88	137.85	137.86	0.02	0.01%
Ephedrine	135.59	135.60	135.67	135.62	0.04	0.03%
Phenacetin	139.34	139.31	139.30	139.32	0.02	0.01%
Naproxen	150.32	150.37	150.42	150.37	0.05	0.03%
Alprenolol	159.58	158.68	158.77	159.01	0.50	0.31%
5-(p-methylphenyl)-5-phenylhydantoin	163.54	163.52	163.54	163.53	0.01	0.01%
Trimethoprim	169.87	169.78	169.93	169.86	0.08	0.04%
Ondansetron	170.06	169.26	169.29	169.54	0.45	0.27%
Cinchonine	166.54	166.46	166.19	166.40	0.18	0.11%
Sulpiride	182.91	182.84	183.07	182.94	0.12	0.06%
Clozapine N-oxide	180.31	179.95	179.91	180.06	0.22	0.12%
Cortisone	184.04	184.19	183.90	184.04	0.15	0.08%
Trichlormethiazide	176.05	176.28	175.96	176.10	0.17	0.09%
Amlodipine	189.48	189.33	189.06	189.29	0.21	0.11%
Doxazosin	205.68	205.69	205.31	205.56	0.22	0.11%
Verapamil	212.14	211.59	211.75	211.83	0.28	0.13%
Sildenafil	213.57	213.43	213.01	213.34	0.29	0.14%
Reserpine	255.93	255.98	256.18	256.03	0.13	0.05%

Experimental data for helium-parameterised calibration set

Name	eCCS1	eCCS2	eCCS3	Mean	Std Dev	% RSD
N-ethylaniline	71.93	71.95	71.81	71.90	0.08	0.11%
Acetaminophen	74.54	73.72	73.85	74.04	0.44	0.60%
Ephedrine	78.46	78.47	78.51	78.48	0.03	0.03%
Phenacetin	80.22	80.21	80.19	80.21	0.02	0.02%
Pregabalin	80.26	80.28	80.26	80.27	0.01	0.01%
Naproxen	90.23	90.26	90.30	90.26	0.04	0.04%
Alprenolol	97.69	96.99	97.06	97.25	0.39	0.40%
5-(p-methylphenyl)-5-phenylhydantoin	100.55	100.53	100.55	100.54	0.01	0.01%
Cinchonine	102.04	101.97	101.76	101.92	0.15	0.14%
Trimethoprim	105.98	104.89	106.03	105.63	0.64	0.61%
Ondansetron	106.15	105.51	105.53	105.73	0.36	0.34%
Trichlormethiazide	110.01	110.21	109.95	110.06	0.14	0.12%
Clozapine N-oxide	114.45	114.26	114.22	114.31	0.12	0.11%
Sulpiride	115.97	116.35	116.53	116.28	0.29	0.25%
Cortisone	117.38	117.51	117.28	117.39	0.12	0.10%
Amlodipine	122.06	121.94	121.72	121.91	0.17	0.14%
Doxazosin	134.96	134.96	134.64	134.85	0.19	0.14%
Verapamil	141.22	140.75	140.89	140.95	0.24	0.17%
Sildenafil	141.80	141.68	141.32	141.60	0.25	0.18%
Reserpine	179.86	179.90	180.09	179.95	0.12	0.07%