Table S1, see excel file

Table S2: Performance of assorted machine learning methods on the elution data set in 5-fold cross validation. The MPNN performs better than Linear Regression and Random Forest (applied to hand-selected features) on both measures: RMSE and the % of overall predictions with an error of less than 2 minutes.

Method	Features	Mean (STD) RMSE on test dataset	Mean (STD) % of training + test predictions with error $\leq$ 2 minutes
Linear Regression	Number of basic centers, number of acidic centers, radius of gyration, total polar surface area, total atom information content[1], total heavy atom bonds	4.68 (3.15)	78.8
Random Forest		4.88 (2.72)	85.4
MPNN	**Weave Features**	**4.62 (0.7)**	**91.2**

Table S3: The effect $\sum \epsilon_i$ of various subgraphs (with fewer than 6 atoms) to the elution time. Only subgraphs that occur more than 30 times in the entire dataset are included. Aromatic ring fragments are excluded.

Subgraph	Mean Total Effect (min)	Mean Absolute Efect (min)	Mean Relative Effect	Mean Absolute Relative Effect	Frequency	Annotation
C=CCCC	-7.42	9.52	-2.83	2.98	33	
CC=CCC	-5.96	8.10	-2.37	2.52	48	
CC(C)CO	-9.96	11.31	-2.28	2.34	37	
cccC=O	-7.01	12.72	-1.95	2.31	52	
CCNCC	-9.39	10.83	-1.88	1.95	61	
cccCO	-4.08	14.45	-1.75	2.34	46	
C=CCC	-4.89	6.00	-1.73	1.81	45	
C1CCOC1	-11.15	12.07	-1.68	1.71	54	

[1] As defined by a_IC at https://www.chemcomp.com/journal/descr.htm

C(Cn)CO	-9.88	11.12	-1.62	1.65	50	
CCCNC	-7.72	9.81	-1.60	1.68	46	
CC(=O)NC	**-6.81**	**9.99**	**-1.57**	**1.71**	**32**	**Amide**
CCC(n)O	-10.12	11.35	-1.56	1.59	49	
CC(n)OC	-9.97	11.18	-1.55	1.58	49	
CC(=O)N	-6.69	9.02	-1.54	1.64	34	
CC(Cn)O	-9.41	10.64	-1.54	1.57	38	
CCOCn	-9.89	11.05	-1.53	1.56	98	
CC(nc)O	-9.56	11.12	-1.52	1.56	98	
COCnc	-9.35	10.91	-1.50	1.54	98	
CC(C)NC	-8.43	8.89	-1.49	1.52	33	
cnCCO	-8.82	10.35	-1.48	1.52	76	
cn(c)CO	-8.93	10.81	-1.47	1.52	49	
ccCO	-3.46	11.71	-1.42	1.91	52	
C(ncn)O	-7.23	9.86	-1.42	1.48	74	
CNCC=O	-6.39	8.94	-1.41	1.54	44	
CCNC	-7.28	8.47	-1.37	1.43	124	
ccnCO	-8.27	10.33	-1.36	1.41	52	
ccC=O	-4.63	9.31	-1.32	1.63	59	
C(C(n)O)O	-7.39	8.87	-1.29	1.32	37	
CC(n)O	-7.81	8.94	-1.25	1.27	49	
CCC(C)O	-6.88	8.15	-1.24	1.29	691	
CCNC=O	-5.92	7.94	-1.22	1.32	68	
COCn	-7.61	8.73	-1.22	1.25	49	
CCCC=O	-3.27	8.72	-1.22	1.45	211	
CC(C=O)O	-1.65	10.77	-1.20	1.51	47	
cnCO	-7.19	8.68	-1.20	1.23	98	
C(CO)n	-6.87	7.97	-1.18	1.21	38	
CC(C)OC	-7.68	8.70	-1.18	1.21	101	
CCOCC	-7.56	8.72	-1.18	1.21	211	
ccCCN	-2.08	14.20	-1.17	1.72	32	
CNC	**-6.12**	**7.06**	**-1.09**	**1.14**	**58**	**Secondary Amine**
C(=O)CO	-0.86	10.57	-1.08	1.40	66	
CCCOC	-6.51	7.72	-1.05	1.09	170	
CCCCN	-4.23	10.43	-1.03	1.33	57	
COCCO	-5.83	7.19	-0.99	1.04	294	
CNC=O	-4.49	6.82	-0.98	1.09	43	
CCCCO	-5.15	7.45	-0.97	1.07	803	
CCOC	-6.08	7.03	-0.96	0.99	322	
C(n)O	-5.45	6.53	-0.92	0.95	49	
CC(CO)O	-5.04	6.86	-0.92	0.98	850	

C(CO)CO	-4.81	6.74	-0.90	0.97	462	
CC(C)O	-5.14	6.30	-0.89	0.94	461	
CCCN	-4.29	8.03	-0.88	1.06	101	
ccC(=O)O	0.69	10.53	-0.84	1.61	34	
CCC=O	-2.92	7.48	-0.83	1.03	250	
C(=O)N	-3.43	5.18	-0.81	0.89	51	
COC	-4.60	5.35	-0.81	0.83	113	
CCCO	-4.45	6.25	-0.80	0.88	1134	
C=CC	**-2.50**	**5.58**	**-0.80**	**0.96**	**52**	**Alkene**
cC=O	-1.87	6.41	-0.80	1.08	33	
CCC(C)N	-4.66	7.96	-0.77	0.95	62	
C(C(O)O)O	-3.08	5.20	-0.72	0.81	46	
CC(C=O)N	-3.45	8.10	-0.72	0.95	83	
C(CO)O	-3.37	5.44	-0.69	0.77	566	
CC(C)N	-4.10	7.48	-0.68	0.85	91	
CC=O	-1.65	6.22	-0.67	0.87	316	
CCC(O)O	-3.11	5.14	-0.66	0.74	45	
CC(O)OC	-3.38	5.01	-0.66	0.72	66	
CNCCO	-3.99	7.01	-0.64	0.78	42	
CCN	-3.18	6.33	-0.63	0.78	248	
C(C=O)CO	-1.81	9.45	-0.61	0.86	56	
CC(CO)N	-3.88	7.79	-0.61	0.82	88	
CCOCO	-3.29	4.99	-0.59	0.65	105	
CC(O)O	-2.55	4.31	-0.57	0.64	49	
CCO	-2.85	4.73	-0.57	0.65	1406	
C(C=O)N	-1.87	6.37	-0.52	0.75	95	
COCO	-2.59	4.07	-0.51	0.57	61	
CN	**-2.46**	**4.49**	**-0.50**	**0.60**	**197**	**Primary Amine**
C(O)O	**-1.64**	**3.38**	**-0.40**	**0.47**	**46**	
CCC(=O)O	1.00	9.18	-0.37	0.82	192	
C(CO)N	-1.23	6.46	-0.35	0.62	103	
CO	**-1.11**	**3.34**	**-0.34**	**0.45**	**984**	**Alcohol**
C(C(=O)O)N	-0.19	7.36	-0.32	0.69	84	
C=O	**0.52**	**4.46**	**-0.26**	**0.51**	**324**	**Ketone**
CC(=O)O	2.58	8.51	-0.21	0.72	218	
CCCOP	-0.48	5.86	-0.14	0.30	67	
C(C(=O)O)O	9.19	15.78	-0.09	0.93	34	
CCOP	1.56	5.46	-0.05	0.24	76	
C(=O)O	**3.76**	**7.51**	**-0.04**	**0.60**	**238**	**Carboxylic Acid**
C(COP)O	2.52	6.24	-0.02	0.26	70	
CCOPO	4.55	7.74	0.06	0.31	150	

COP	3.23	4.48	0.07	0.16	66	
CCOP=O	5.36	8.01	0.09	0.31	76	
P	3.05	3.09	0.10	0.11	67	
COPO	6.26	7.28	0.17	0.26	132	
OP	5.96	6.05	0.20	0.21	199	
OPOP	7.38	7.38	0.20	0.20	56	
COP=O	7.16	7.86	0.21	0.27	66	
O=P	7.19	7.23	0.24	0.25	67	
OPOPO	8.96	8.96	0.24	0.24	56	
COP(O)O	9.28	10.26	0.27	0.36	66	
O=P(O)OP	10.29	10.29	0.28	0.28	56	
O=POPO	10.29	10.29	0.28	0.28	56	
OPO	8.77	8.91	0.29	0.30	197	
COP(=O)O	10.18	10.91	0.31	0.37	132	
O=PO	10.08	10.17	0.33	0.34	199	
OP(O)O	11.49	11.69	0.37	0.39	65	
O=P(O)O	12.88	13.03	0.42	0.44	197	
O=P(O)(O)O	**15.58**	**15.78**	**0.51**	**0.53**	**65**	**Phosphate**

Table S4, see excel file