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SUPPLEMENTARY MATERIAL TO

Predicting retention indices of PAHs in reversed-phase liquid chromatography: Quantitative structure retention relationship approach

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TABLE S-I. Experimental (Exp.), predicted (Pred.) and residual (Res.) values of log *I* for PAHs

Name	log *I*					
	Polymeric			Monomeric		
	Exp.	Pred.	Res.	Exp.	Pred.	Res.
Naphthalene	2	2.0532	0.0532	2	2.0802	0.0802
Fluorene	2.7	2.7374	0.0374	2.75	2.7566	0.0066
Anthracene	3.16	3.132	-0.028	3.11	3.1157	0.0057
Fluoranthene	3.39	3.5593	0.1693	3.43	3.3816	-0.0484
Aceanthrylene	3.39	3.5146	0.1246	3.39	3.4995	0.1095
pyrene	3.55	3.6231	0.0731	3.63	3.4899	-0.1401
11H-Benzo[a]fluorene	3.81	3.749	-0.061	3.75	3.7988	0.0488
11H-Benzo[b]fluorene	3.82	3.7031	-0.1169	3.78	3.828	0.048
Cyclopenta[cd]pyrene	3.94	3.8861	-0.0539	3.95	4.0903	0.1403
Benzo[ghi]fluoranthene	3.95	3.8594	-0.0906	4.07	4.0969	0.0269
Triphenylene	3.75	3.6021	-0.1479	3.82	3.6972	-0.1228
Benzo[c]phenanthrene	3.69	3.7788	0.0888	3.91	3.7039	-0.2061
Benz[a]anthracene	4	3.995	-0.005	4	3.9853	-0.0147
Chrysene	4.06	4.1373	0.0773	3.97	3.9523	-0.0177
Benz[e]aceanthrylene	4.25	4.2389	-0.0111	4.34	4.5578	0.2178
Benz[l]aceanthrylene	4.26	4.2413	-0.0187	4.38	4.4269	0.0469
Benz[k]acephenanthrylene	4.39	4.3584	-0.0316	4.43	4.5273	0.0973
Benz[a]aceanthrylene	4.24	4.0922	-0.1478	4.45	4.4899	0.0399
Benzo[j]fluoranthene	4.26	4.3209	0.0609	4.37	4.4568	0.0868
Benzo[k]fluoranthene	4.38	4.4403	0.0603	4.5	4.5022	0.0022

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Benzo[e]pyrene	4.29	4.2252	-0.0648	4.51	4.4802	-0.0298
Perylene	4.33	4.3808	0.0508	4.52	4.497	-0.023
Benzo[a]pyrene	4.51	4.5548	0.0448	4.68	4.6848	0.0048
13H-Dibenzo[a,g]fluorene	4.53	4.5413	0.0113	4.62	4.6876	0.0676
11H-Indeno[2,1-a]phenanthrene	4.91	4.8396	-0.0704	4.74	4.8004	0.0604
13H-Dibenzo[a,h]fluorene	4.96	4.8445	-0.1155	4.77	4.8101	0.0401
Indeno[1,2,3-cd]pyrene	4.84	4.7669	-0.0731	5.23	5.2265	-0.0035
Indeno[1,2,3-cd]fluoranthene	4.93	4.9587	0.0287	5.05	5.1578	0.1078
Benzo[ghi]perylene	4.76	4.7061	-0.0539	5.36	5.3214	-0.0386
Dibenzo[def,mno]chrysene	5.08	4.9348	-0.1452	5.61	5.6305	0.0205
Dibenzo[c,g]phenanthrene	4.07	4.0412	-0.0288	4.51	4.2953	-0.2147
Benzo[b]triphenylene	4.4	4.4598	0.0598	4.73	4.7379	0.0079
Benzo[g]chrysene	4.27	4.3909	0.1209	4.71	4.7247	0.0147
Benzo[c]chrysene	4.45	4.7367	0.2867	4.85	4.7213	-0.1287
Dibenz[a,j]anthracene	4.56	4.5969	0.0369	4.84	4.653	-0.187
Pentaphene	4.67	4.8886	0.2186	4.96	4.9748	0.0148
Benzo[a]naphthacene	4.99	5.0465	0.0565	4.5	4.964	0.464
Benzo[b]chrysene	5	5.1483	0.1483	5	4.9949	-0.0051
Picene	5.18	5.1848	0.0048	5.02	4.9239	-0.0961
Dibenz[a,e]acephenanthrylene	4.8	4.5894	-0.2106	5.48	5.2584	-0.2216
Dibenzo[j,l]fluoranthene	4.79	4.7415	-0.0485	5.35	5.4208	0.0708
Naphth[2,3-a]aceanthrylene	4.91	4.7772	-0.1328	5.51	5.4563	-0.0537
Naphth[2,3-e]acephenanthrylene	5.27	5.257	-0.013	5.64	5.5046	-0.1354
Naphtho[2,3-j]fluoranthene	4.98	5.1963	0.2163	5.4	5.4736	0.0736
Dibenz[e,k]acephenanthrylene	5.28	5.2857	0.0057	5.59	5.5167	-0.0733
7H-Benzo[c]fluorene	3.49	3.4851	-0.0049	3.64	3.6692	0.0292
Benz[j]aceanthrylene	4.26	4.3223	0.0623	4.29	4.4481	0.1581
Benz[e]acephenanthrylene	4.29	4.2918	0.0018	4.44	4.4668	0.0268
Dibenzo[b,g]phenanthrene	4.33	4.4514	0.1214	4.8	4.6493	-0.1507
Dibenz[a,h]anthracene	4.73	4.9839	0.2539	4.86	4.8862	0.0262
Dibenz[a,e]aceanthrylene	4.9	4.5897	-0.3103	5.5	5.3982	-0.1018
Indeno[1,2,3-fg]naphthacene	5.07	4.7944	-0.2756	5.71	5.628	-0.082
Benzo[rst]pentaphene	5.74	5.4542	-0.2858	5.93	5.8178	-0.1122
Anthracene, 1-methyl	3.43	3.2975	-0.1325	3.57	3.5323	-0.0377
Phenanthrene, 2-methyl	3.68	3.476	-0.204	3.71	3.6171	-0.0929
Phenanthrene, 3-methyl	3.34	3.2989	-0.0411	3.47	3.362	-0.108
Phenanthrene, 4-methyl	3.26	3.3252	0.0652	3.4	3.3892	-0.0108
Phenanthrene, 9-methyl	3.38	3.3532	-0.0268	3.51	3.4003	-0.1097
Fluoranthene, 3-methyl	3.86	3.8745	0.0145	3.91	3.9518	0.0418
Pyrene, 1-methyl	3.98	3.9024	-0.0776	4.15	3.9512	-0.1988
Benz[a]anthracene, 1-methyl	4.18	4.1046	-0.0754	4.39	4.4171	0.0271
Benz[a]anthracene, 2-methyl	4.14	4.0963	-0.0437	4.43	4.3685	-0.0615
Benz[a]anthracene, 4-methyl	4.33	4.3361	0.0061	4.44	4.4917	0.0517
Benz[a]anthracene, 6-methyl	4.15	4.0944	-0.0556	4.41	4.4644	0.0544
Benz[a]anthracene, 8-methyl	4.21	4.2051	-0.0049	4.4	4.4258	0.0258
Benz[a]anthracene, 10-methyl	4.18	4.2514	0.0714	4.42	4.4419	0.0219
Benz[a]anthracene, 12-methyl	4.14	4.2485	0.1085	4.37	4.5758	0.2058

Benzo[c]phenanthrene, 3-methyl	4.09	4.0318	-0.0582	4.41	4.357	-0.053
Benzo[c]phenanthrene, 5-methyl	4.04	4.0741	0.0341	4.37	4.3441	-0.0259
Benzo[c]phenanthrene, 6-methyl	4.17	3.8761	-0.2939	4.37	4.2106	-0.1594
Chyrsene, 3-methyl	4.28	4.3594	0.0794	4.41	4.4067	-0.0033
Chyrsene, 4-methyl	4.2	4.2145	0.0145	4.36	4.3813	0.0213
Chyrsene, 6-methyl	4.17	4.2617	0.0917	4.35	4.3736	0.0236
Benzo[a]pyrene, 1-methyl	4.83	4.7796	-0.0504	5.24	5.0683	-0.1717
Benzo[a]pyrene, 4-methyl	4.84	4.7412	-0.0988	5.26	5.1368	-0.1232
Benzo[a]pyrene, 5-methyl	4.64	4.6567	0.0167	5.15	5.1626	0.0126
Benzo[a]pyrene, 11-methyl	4.66	4.6984	0.0384	5.14	5.2735	0.1335
Benzo[a]pyrene, 1,2-dimethyl	5.21	5.2264	0.0164	5.73	5.7094	-0.0206
Benzo[a]pyrene, 1,3-dimethyl	5.26	5.0922	-0.1678	5.75	5.512	-0.238
Benzo[a]pyrene, 1,4-dimethyl	5.08	4.8818	-0.1982	5.77	5.4979	-0.2721
Benzo[a]pyrene, 1,6-dimethyl	5.1	4.9867	-0.1133	5.65	5.4879	-0.1621
Benzo[a]pyrene, 3,12-dimethyl	4.94	4.9331	-0.0069	5.62	5.5425	-0.0775
Perylene, 3-methyl	4.69	4.7255	0.0355	4.57	5.0275	0.4575
Naphtho[1,2-k]fluoranthene	5	5.2213	0.2213	5.34	5.3113	-0.0287
Naphtho[2,3-k]fluoranthene	5.92	5.5952	-0.3248	5.79	5.5242	-0.2658
Dibenzo[def,p]chrysene	4.65	4.7862	0.1362	5.57	5.5884	0.0184
Benzo[a]perylene	4.93	5.2096	0.2796	5.54	5.6166	0.0766
Naphtho[1,2,3,4-def]chrysene	4.97	4.9702	0.0002	5.56	5.5666	0.0066
Dibenzo[de,qr]naphthacene	4.91	5.143	0.233	5.53	5.625	0.095
Dibenzo[fg,op]naphthacene	5.04	5.0321	-0.0079	5.52	5.699	0.179
Benzo[b]perylene	5.04	4.8086	-0.2314	5.56	5.5531	-0.0069
Naphtho[2,1,8-qra]naphthacene	5.86	5.5916	-0.2684	5.92	5.7437	-0.1763
Dibenzo[b,def]chrysene	6	5.7094	-0.2906	6	5.8644	-0.1356
Phenanthro[3,4-c]phenanthrene	4.21	4.1858	-0.0242	4.77	4.8017	0.0317
Dibenzo[g,p]chrysene	4.45	4.5961	0.1461	5.53	5.6454	0.1154
Anthracene, 2-methyl	3.69	3.4408	-0.2492	3.69	3.723	0.033
Anthracene, 9-methyl	3.41	3.4833	0.0733	3.52	3.5974	0.0774
Phenanthrene, 1-methyl	3.4	3.4359	0.0359	3.5	3.4035	-0.0965
Fluoranthene, 1-methyl	3.73	3.6879	-0.0421	3.87	3.9504	0.0804
Fluoranthene, 7-methyl	3.8	3.7781	-0.0219	3.91	3.9149	0.0049
Fluoranthene, 8-methyl	3.85	3.8324	-0.0176	3.95	3.9809	0.0309
Pyrene, 2-methyl	4.04	3.9772	-0.0628	4.21	4.3139	0.1039
Pyrene, 4-methyl	3.98	3.8308	-0.1492	4.13	4.0205	-0.1095
Benz[a]anthracene, 3-methyl	4.39	4.365	-0.025	4.51	4.6163	0.1063
Benz[a]anthracene, 5-methyl	4.28	4.2072	-0.0728	4.48	4.4358	-0.0442
Benz[a]anthracene, 7-methyl	4.17	4.2448	0.0748	4.36	4.4645	0.1045
Benz[a]anthracene, 9-methyl	4.37	4.3714	0.0014	4.52	4.5525	0.0325
Benz[a]anthracene, 11-methyl	4.17	4.0218	-0.1482	4.36	4.2997	-0.0603
Benzo[c]phenanthrene, 1-methyl	3.73	3.787	0.057	4.1	4.1087	0.0087
Benzo[c]phenanthrene, 2-methyl	3.94	3.8032	-0.1368	4.29	4.0115	-0.2785
Benzo[c]phenanthrene, 4-methyl	4.04	4.0541	0.0141	4.37	4.2163	-0.1537
Chyrsene, 1-methyl	4.39	4.3954	0.0054	4.46	4.3979	-0.0621
Chyrsene, 2-methyl	4.49	4.5481	0.0581	4.54	4.5851	0.0451

Chyrsene, 5-methyl	4.17	4.2363	0.0663	4.36	4.5387	0.1787
Triphenylene, 1-methyl	3.88	3.8721	-0.0079	4.19	4.2392	0.0492
Benzo[a]pyrene, 2-methyl	4.94	4.9836	0.0436	5.33	5.4154	0.0854
Benzo[a]pyrene, 3-methyl	4.9	4.8976	-0.0024	5.25	5.1346	-0.1154
Benzo[a]pyrene, 6-methyl	4.73	4.8103	0.0803	5.11	5.1064	-0.0036
Benzo[a]pyrene, 7-methyl	4.74	4.7999	0.0599	5.13	5.1202	-0.0098
Benzo[a]pyrene, 8-methyl	4.96	4.9365	-0.0235	5.33	5.2481	-0.0819
Benzo[a]pyrene, 9-methyl	4.78	4.8255	0.0455	5.18	5.1402	-0.0398
Benzo[a]pyrene, 10-methyl	4.73	4.6615	-0.0685	5.16	5.1126	-0.0474
Benzo[a]pyrene, 12-methyl	4.61	4.6717	0.0617	5.14	5.1044	-0.0356
Benzo[a]pyrene, 2,3-dimethyl	5.37	5.3198	-0.0502	5.74	5.7253	-0.0147
Benzo[a]pyrene, 3,6-dimethyl	5.09	5.0559	-0.0341	5.63	5.5467	-0.0833
Benzo[a]pyrene, 3,11-dimethyl	5.01	4.9604	-0.0496	5.68	5.7123	0.0323
Benzo[a]pyrene, 4,5-dimethyl	4.9	4.9148	0.0148	5.54	5.5869	0.0469
Benzo[a]pyrene, 7,10-dimethyl	4.82	4.8266	0.0066	5.51	5.53	0.02
Perylene, 1-methyl	4.28	4.4591	0.1791	4.85	4.9304	0.0804
Perylene, 2-methyl	4.5	4.5484	0.0484	5.03	5.093	0.063
Phenanthrene	3	3.1353	0.1353	3	2.8838	-0.1162
Acephenanthrene	3.37	3.4751	0.1051	3.38	3.4265	0.0465

TABLE S-II. Training and prediction sets for both columns by using Kennard and Stone algorithm

ID	Name	Status	ID	Name	Status
1	Naphthalene	Training	44	Naphtho[2,3-j]fluoranthene	Training
2	Fluorene	Training	45	Dibenz[e,k]acephenanthrylene	Training
3	Anthracene	Training	46	Naphtho[1,2-k]fluoranthene	Training
4	Fluoranthene	Training	47	Naphtho[2,3-k]fluoranthene	Training
5	Aceanthrylene	Training	48	Dibenzo[def,p]chrysene	Training
6	pyrene	Training	49	Benzo[a]perylene	Training
7	11H-Benzo[a]fluorene	Training	50	Naphtho[1,2,3,4-def]chrysene	Training
8	11H-Benzo[b]fluorene	Training	51	Dibenzo[de,qr]naphthacene	Training
9	Cyclopenta[cd]pyrene	Training	52	Dibenzo[fg,op]naphthacene	Training
10	Benzo[ghi]fluoranthene	Training	53	Benzo[b]perylene	Training
11	Triphenylene	Training	54	Naphtho[2,1,8-qra]naphthacene	Training
12	Benzo[c]phenanthrene	Training	55	Dibenzo[b,def]chrysene	Training
13	Benz[a]anthracene	Training	56	Phenanthro[3,4-c]phenanthrene	Training
14	Chrysene	Training	57	Dibenzo[g,p]chrysene	Training
15	Benz[e]aceanthrylene	Training	58	Anthracene, 2-methyl	Training
16	Benz[l]aceanthrylene	Training	59	Anthracene, 9-methyl	Training
17	Benz[k]acephenanthrylene	Training	60	Phenanthrene, 1-methyl	Training
18	Benz[a]aceanthrylene	Training	61	Fluoranthene, 1-methyl	Training
19	Benzo[j]fluoranthene	Training	62	Fluoranthene, 7-methyl	Training
20	Benzo[k]fluoranthene	Training	63	Fluoranthene, 8-methyl	Training

21	Benzo[e]pyrene	Training	64	Pyrene, 2-methyl	Training
22	Perylene	Training	65	Pyrene, 4-methyl	Training
23	Benzo[a]pyrene	Training	66	Benz[a]anthracene, 3-methyl	Training
24	13H-Dibenzo[a,g]fluorene	Training	67	Benz[a]anthracene, 5-methyl	Training
25	11H-Indeno[2,1-a]phenanthrene	Training	68	Benz[a]anthracene, 7-methyl	Training
26	13H-Dibenzo[a,h]fluorene	Training	69	Benz[a]anthracene, 9-methyl	Training
27	Indeno[1,2,3-cd]pyrene	Training	70	Benz[a]anthracene, 11-methyl	Training
28	Indeno[1,2,3-cd]fluoranthene	Training	71	Benzo[c]phenanthrene, 1-methyl	Training
29	Benzo[ghi]perylene	Training	72	Benzo[c]phenanthrene, 2-methyl	Training
30	Dibenzo[def,mno]chrysene	Training	73	Benzo[c]phenanthrene, 4-methyl	Training
31	Dibenzo[c,g]phenanthrene	Training	74	Chyrsene, 1-methyl	Training
32	Benzo[b]triphenylene	Training	75	Chyrsene, 2-methyl	Training
33	Benzo[g]chrysene	Training	76	Chyrsene, 5-methyl	Training
34	Benzo[c]chrysene	Training	77	Triphenylene, 1-methyl	Training
35	Dibenz[a,j]anthracene	Training	78	Benzo[a]pyrene, 2-methyl	Training
36	Pentaphene	Training	79	Benzo[a]pyrene, 3-methyl	Training
37	Benzo[a]naphthacene	Training	80	Benzo[a]pyrene, 6-methyl	Training
38	Benzo[b]chrysene	Training	81	Benzo[a]pyrene, 7-methyl	Training
39	Picene	Training	82	Benzo[a]pyrene, 8-methyl	Training
40	Dibenz[a,e]acephenanthrylene	Training	83	Benzo[a]pyrene, 9-methyl	Training
41	Dibenzo[j,l]fluoranthene	Training	84	Benzo[a]pyrene, 10-methyl	Training
42	Naphth[2,3-a]aceanthrylene	Training	85	Benzo[a]pyrene, 12-methyl	Training
43	Naphth[2,3-e]acephenanthrylene	Training	86	Benzo[a]pyrene, 2,3-dimethyl	Training
87	Benzo[a]pyrene, 3,6-dimethyl	Training	110	Benz[a]anthracene, 1-methyl	Prediction
88	Benzo[a]pyrene, 3,11-dimethyl	Training	111	Benz[a]anthracene, 2-methyl	Prediction
89	Benzo[a]pyrene, 4,5-dimethyl	Training	112	Benz[a]anthracene, 4-methyl	Prediction
90	Benzo[a]pyrene, 7,10-dimethyl	Training	113	Benz[a]anthracene, 6-methyl	Prediction
91	Perylene, 1-methyl	Training	114	Benz[a]anthracene, 8-methyl	Prediction
92	Perylene, 2-methyl	Training	115	Benz[a]anthracene, 10-methyl	Prediction
93	Phenanthrene	Prediction	116	Benz[a]anthracene, 12-methyl	Prediction
94	Acephenanthrene	Prediction	117	Benzo[c]phenanthrene, 3-methyl	Prediction
95	7H-Benzo[c]fluorene	Prediction	118	Benzo[c]phenanthrene, 5-methyl	Prediction

96	Benz[j]aceanthrylene	Prediction	119	Benzo[c]phenanthrene, 6-methyl	Prediction
97	Benz[e]acephenanthrylene	Prediction	120	Chyrsene, 3-methyl	Prediction
98	Dibenzo[b,g]phenanthrene	Prediction	121	Chyrsene, 4-methyl	Prediction
99	Dibenz[a,h]anthracene	Prediction	122	Chyrsene, 6-methyl	Prediction
100	Dibenz[a,e]aceanthrylene	Prediction	123	Benzo[a]pyrene, 1-methyl	Prediction
101	Indeno[1,2,3-fg]naph-thacene	Prediction	124	Benzo[a]pyrene, 4-methyl	Prediction
102	Benzo[rst]pentaphene	Prediction	125	Benzo[a]pyrene, 5-methyl	Prediction
103	Anthracene, 1-methyl	Prediction	126	Benzo[a]pyrene, 11-methyl	Prediction
104	Phenanthrene, 2-methyl	Prediction	127	Benzo[a]pyrene, 1,2-dimethyl	Prediction
105	Phenanthrene, 3-methyl	Prediction	128	Benzo[a]pyrene, 1,3-dimethyl	Prediction
106	Phenanthrene, 4-methyl	Prediction	129	Benzo[a]pyrene, 1,4-dimethyl	Prediction
107	Phenanthrene, 9-methyl	Prediction	130	Benzo[a]pyrene, 1,6-dimethyl	Prediction
108	Fluoranthene, 3-methyl	Prediction	131	Benzo[a]pyrene, 3,12-dimethyl	Prediction
109	Pyrene, 1-methyl	Prediction	132	Perylene, 3-methyl	Prediction

TABLE S-III. Evaluation metrics formulas and their accepted thresholds

Metric	Threshold
$R^2_{ext} = 1 - \frac{\sum_{i=1}^{n_{ext}} \left(y_i - \hat{y}_i\right)^2}{\sum_{n=1}^{n_{ext}} \left(y_i - \bar{y}\right)^2}$	$R^2ext > 0.7$
$Q^2_{F1} = 1 - \frac{\sum_{i=1}^{n_{ext}} \left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{n_{ext}} \left(y_i - \bar{y}_{tr}\right)^2}$	$Q^2F1 > 0.6$
$Q^2_{F2} = 1 - \frac{\sum_{i=1}^{n_{ext}} \left(y_i - \hat{y}_i\right)^2}{\sum_{i=1}^{n_{ext}} \left(y_i - \bar{y}_{ext}\right)^2}$	$Q^2F2 > 0.6$
$Q^2_{F3} = 1 - \frac{\sum_{i=1}^{n_{ext}} \left(y_i - \hat{y}_i\right)^2 / n_{ext}}{\sum_{i=1}^{n_{tr}} \left(y_i - \hat{y}_{tr}\right)^2 / n_{tr}}$	$Q^2F3 > 0.6$
$CCC = \frac{2\sum_{i=1}^{n_{ext}} \left(y_i - \bar{y}\right)\left(\hat{y}_i - \bar{\hat{y}}\right)}{\sum_{i=1}^{n_{ext}} \left(y_i - \bar{y}_{ext}\right)^2 + \sum_{i=1}^{n_{ext}} \left(\hat{y}_i - \bar{\hat{y}}\right)^2 + n_{ext}\left(\bar{y}_{ext} - \bar{\hat{y}}\right)^2}$	$CCC > 0.85$

In Table S-III, y_i is the predicted value calculated using the regression of the predicted and experimental data of the prediction set, y_n the mean experimental value in the training set and n_{ext} the number of molecules in the validation set, y_{ext} the mean experimental value in the prediction set, y is the mean predicted values.