Supporting Information

Data-driven prediction of protein adsorption on self-assembled monolayers toward material screening and design

Rudolf Jason Kwaria[1], Evan Angelo Quimada Mondarte[1], Hiroyuki Tahara[1], Ryongsok Chang[1] and Tomohiro Hayashi[1,2,*]

[1]*Tokyo Institute of Technology, Department of Materials Science and Engineering, School of Materials and Chemical Technology (4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa 226-8502, JAPAN)*

[2]*JST-PRESTO (4-1-8 Hon-cho, Kawaguchi, Saitama 332-0012, JAPAN)*

*corresponding author: tomo@mac.titech.ac.jp

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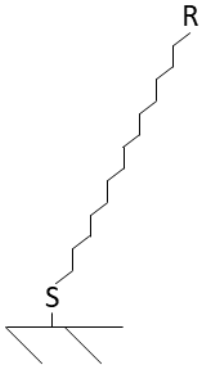
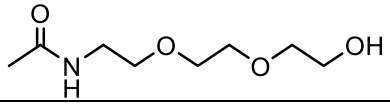
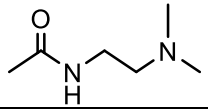
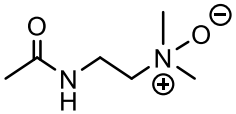
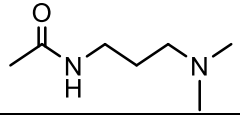
WATER CONTACT ANGLE DATASET:

TABLE S1. Results by Dobrzanska et al. [1]



No.	R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
1.		30.14	61.64	5.48	1.37	73.00	1.00	18.00	2.00	5.00	1.00	43.00
2.		30.30	63.64	1.52	3.03	66.00	0.00	16.00	5.00	0.00	1.00	34.00
3.		29.85	62.69	2.99	2.99	67.00	0.00	16.00	5.00	0.00	1.00	25.00
4.		30.43	63.77	1.45	2.90	69.00	0.00	17.00	5.00	0.00	1.00	37.00

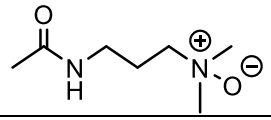
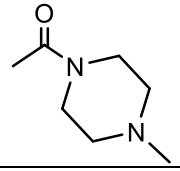
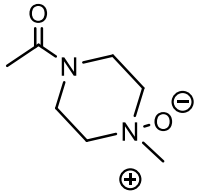
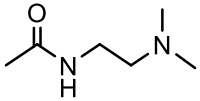
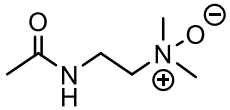
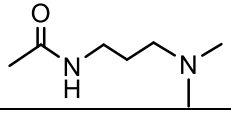
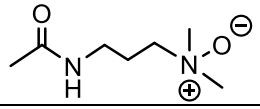
No.	R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
5.		30.00	62.86	2.86	2.86	70.00	0.00	17.00	5.00	0.00	1.00	28.00
6.		31.34	62.69	1.49	2.99	67.00	0.00	17.00	6.00	0.00	1.00	37.00
7.		30.88	61.76	2.94	2.94	68.00	0.00	17.00	6.00	0.00	1.00	29.00
8.		30.43	63.77	1.45	2.90	69.00	0.00	16.00	6.00	0.00	1.00	38.00
9.		30.00	62.86	2.86	2.86	70.00	0.00	16.00	6.00	0.00	1.00	30.00
10.		30.56	63.89	1.39	2.78	72.00	0.00	17.00	6.00	0.00	1.00	36.00
11.		30.14	63.01	2.74	2.74	73.00	0.00	17.00	6.00	0.00	1.00	28.00

TABLE S2. Results by Abe et al. [2]

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
12.	$HS-(CH_2)_{17}-CH_3$	31.58	66.67	0.00	0.00	57.00	0.00	17.00	0.00	0.00	0.00	107.00

TABLE S3. Results by Sekine et al. [3]

SAM1	**$HS(CH_2)_5CH_3$**											
SAM2	**$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
13.	0	28.57	66.67	0.00	0.00	21.00	0.00	5.00	0.00	0.00	0.00	105.00
14.	12.60	28.78	65.36	1.96	0.00	25.66	0.13	6.01	0.00	0.88	0.00	91.20
15.	16.75	28.84	65.02	2.46	0.00	27.20	0.17	6.34	0.00	1.17	0.00	74.20
16.	17.08	28.84	65.00	2.50	0.00	27.32	0.17	6.37	0.00	1.20	0.00	73.30
17.	20.40	28.88	64.76	2.86	0.00	28.55	0.20	6.63	0.00	1.43	0.00	71.80
18.	28.64	28.96	64.25	3.63	0.00	31.60	0.29	7.29	0.00	2.00	0.00	64.20
19.	38.00	29.04	63.78	4.34	0.00	35.06	0.38	8.04	0.00	2.66	0.00	47.10
20.	55.38	29.14	63.11	5.34	0.00	41.49	0.55	9.43	0.00	3.88	0.00	39.40
21.	71.60	29.22	62.65	6.03	0.00	47.49	0.72	10.73	0.00	5.01	0.00	37.10
22.	72.87	29.22	62.62	6.08	0.00	47.96	0.73	10.83	0.00	5.10	0.00	36.10
23.	78.73	29.24	62.48	6.28	0.00	50.13	0.79	11.30	0.00	5.51	0.00	35.70
24.	83.57	29.26	62.37	6.44	0.00	51.92	0.84	11.69	0.00	5.85	0.00	35.70
25.	90.61	29.28	62.24	6.65	0.00	54.53	0.91	12.25	0.00	6.34	0.00	34.70
26.	91.78	29.29	62.21	6.68	0.00	54.96	0.92	12.34	0.00	6.42	0.00	33.80
27.	100	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	30.00

TABLE S4. Results by Arima et al.[4]

SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$HS(CH_2)_{11}OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
28.	0	30.56	66.67	0.00	0.00	36.00	0.00	10.00	0.00	0.00	0.00	109.00
29.	10	30.47	66.48	0.28	0.00	36.10	0.10	10.00	0.00	0.10	0.00	102.00
30.	20	30.39	66.30	0.55	0.00	36.20	0.20	10.00	0.00	0.20	0.00	93.00
31.	50	30.14	65.75	1.37	0.00	36.50	0.50	10.00	0.00	0.50	0.00	60.00
32.	63	30.03	65.52	1.72	0.00	36.63	0.63	10.00	0.00	0.63	0.00	46.00
33.	87	29.83	65.09	2.36	0.00	36.87	0.87	10.00	0.00	0.87	0.00	36.00
34.	93	29.79	64.99	2.52	0.00	36.93	0.93	10.00	0.00	0.93	0.00	30.00
35.	100	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	22.00
SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$HS(CH_2)_{11}NH_2$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
36.	5	30.47	66.62	0.00	0.14	36.10	0.00	10.00	0.05	0.00	0.00	103.00
37.	9	30.40	66.58	0.00	0.25	36.18	0.00	10.00	0.09	0.00	0.00	99.00
38.	15	30.30	66.53	0.00	0.41	36.30	0.00	10.00	0.15	0.00	0.00	93.00
39.	28	30.09	66.41	0.00	0.77	36.56	0.00	10.00	0.28	0.00	0.00	90.00
40.	59	29.59	66.14	0.00	1.59	37.18	0.00	10.00	0.59	0.00	0.00	73.00
41.	90	29.10	65.87	0.00	2.38	37.80	0.00	10.00	0.90	0.00	0.00	55.00
42.	100	28.95	65.79	0.00	2.63	38.00	0.00	10.00	1.00	0.00	0.00	51.00

SAM1	$HS(CH_2)_{10}CH_3$											
SAM2	$HS(CH_2)_{10}COOH$											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
43.	12	30.56	66.00	0.67	0.00	36.00	0.12	10.00	0.00	0.12	0.12	103.00
44.	26	30.56	65.22	1.44	0.00	36.00	0.26	10.00	0.00	0.26	0.26	88.00
45.	50	30.56	63.89	2.78	0.00	36.00	0.50	10.00	0.00	0.50	0.50	74.04
46.	60	30.56	63.33	3.33	0.00	36.00	0.60	10.00	0.00	0.60	0.60	54.00
47.	83	30.56	62.06	4.61	0.00	36.00	0.83	10.00	0.00	0.83	0.83	36.00
48.	90	30.56	61.67	5.00	0.00	36.00	0.90	10.00	0.00	0.90	0.90	30.00
49.	100	30.56	61.11	5.56	0.00	36.00	1.00	10.00	0.00	1.00	1.00	21.00

TABLE S5. Results by Zhu et al. [5]

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
50.	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-OCH_3$	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	56.50
51.	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_6-OH$	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	29.00

TABLE S6. Results by Bain et al. [6]

SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$HS(CH_2)_{10}CH_2OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
52.	0	30.56	66.67	0.00	0.00	36.00	0.00	10.00	0.00	0.00	0.00	113.00
53.	5	30.51	66.57	0.14	0.00	36.05	0.05	10.00	0.00	0.05	0.00	101.00
54.	20	30.39	66.30	0.55	0.00	36.20	0.20	10.00	0.00	0.20	0.00	81.00
55.	32	30.29	66.08	0.88	0.00	36.32	0.32	10.00	0.00	0.32	0.00	78.00
56.	47	30.16	65.81	1.29	0.00	36.47	0.47	10.00	0.00	0.47	0.00	52.00
57.	79	29.90	65.24	2.15	0.00	36.79	0.79	10.00	0.00	0.79	0.00	29.00
58.	14	30.56	65.98	0.68	0.00	41.04	0.28	11.40	0.00	0.28	0.00	92.00
SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$[S(CH_2)_{10}CH_2OH)]_2$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
59.	19	30.56	65.78	0.89	0.00	42.84	0.38	11.90	0.00	0.38	0.00	81.00
60.	36	30.56	65.20	1.47	0.00	48.96	0.72	13.60	0.00	0.72	0.00	68.00
61.	49	30.56	64.84	1.83	0.00	53.64	0.98	14.90	0.00	0.98	0.00	55.00
62.	58	30.56	64.63	2.04	0.00	56.88	1.16	15.80	0.00	1.16	0.00	47.00
63.	100	30.56	63.89	2.78	0.00	72.00	2.00	20.00	0.00	2.00	0.00	15.00

SAM1	**$[S(CH_2)_{10}CH_3)]_2$**											
SAM2	**$HS(CH_2)_{10}CH_2OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
64.	0	31.43	65.71	0.00	0.00	70.00	0.00	20.00	0.00	0.00	0.00	110.00
65.	31	31.10	65.55	0.52	0.00	59.77	0.31	16.90	0.00	0.31	0.00	74.00
66.	35	31.05	65.53	0.60	0.00	58.45	0.35	16.50	0.00	0.35	0.00	69.00
67.	45	30.92	65.46	0.82	0.00	55.15	0.45	15.50	0.00	0.45	0.00	57.00
68.	60	30.68	65.34	1.20	0.00	50.20	0.60	14.00	0.00	0.60	0.00	41.00
69.	77	30.34	65.17	1.73	0.00	44.59	0.77	12.30	0.00	0.77	0.00	33.00
SAM1	**$[S(CH_2)_{10}CH_2OH)]_2$**											
SAM2	**$[S(CH_2)_{10}CH_3)]_2$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
70.	4	31.39	65.64	0.11	0.00	70.08	0.08	20.00	0.00	0.08	0.00	101.00
71.	14	31.30	65.45	0.40	0.00	70.28	0.28	20.00	0.00	0.28	0.00	89.00
72.	28	31.18	65.19	0.79	0.00	70.56	0.56	20.00	0.00	0.56	0.00	71.00
73.	35	31.12	65.06	0.99	0.00	70.70	0.70	20.00	0.00	0.70	0.00	61.00
74.	70	30.81	64.43	1.96	0.00	71.40	1.40	20.00	0.00	1.40	0.00	41.00
75.	78	30.74	64.28	2.18	0.00	71.56	1.56	20.00	0.00	1.56	0.00	31.00
76.	82	30.71	64.21	2.29	0.00	71.64	1.64	20.00	0.00	1.64	0.00	29.00
77.	94	30.61	64.00	2.62	0.00	71.88	1.88	20.00	0.00	1.88	0.00	16.00

TABLE S7.Results by Hayashi et al. [7]

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
78.	$HS-(CH_2)_7-CH_3$	29.63	66.67	0.00	0.00	27.00	0.00	7.00	0.00	0.00	0.00	112.00
79.	$HS-(CH_2)_{11}-OH$	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	17.00
80.	$HS-(CH_2)_{11}-NH_2$	28.95	65.79	0.00	2.63	38.00	0.00	10.00	1.00	0.00	0.00	35.00
81.	$HS-(CH_2)_{11}-COOH$	30.77	61.54	5.13	0.00	39.00	1.00	11.00	0.00	1.00	1.00	18.00
82.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)-OH$	29.55	63.64	4.55	0.00	44.00	1.00	11.00	0.00	3.00	0.00	33.00
83.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_2-OH$	29.41	62.75	5.88	0.00	51.00	1.00	12.00	0.00	5.00	0.00	32.00
84.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_3-OH$	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	32.00
85.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_3-O-CH_3$	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	69.00
86.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_3-NH_2$	28.81	62.71	5.08	1.69	59.00	0.00	13.00	1.00	6.00	0.00	25.00
87.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_3-COOH$	30.00	60.00	8.33	0.00	60.00	1.00	14.00	0.00	7.00	1.00	22.00
88.	$HS-(CH_2)_{11}-(O- CH_2- CH_2)_6-OH$	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	30.00

TABLE S8. Results by Folkers et al. [8]

SAM1	**$HS(CH_2)_{10}CH_2OH$**											
SAM2	**$HS(CH_2)_{21}CH_3$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O(%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
89.	0.00	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	5.00
90.	8.00	30.03	65.12	2.33	0.00	39.56	0.92	10.88	0.00	0.92	0.00	27.50
91.	12.00	30.17	65.23	2.15	0.00	40.84	0.88	11.32	0.00	0.88	0.00	38.50
92.	25.00	30.56	65.56	1.67	0.00	45.00	0.75	12.75	0.00	0.75	0.00	51.00
93.	40.00	30.92	65.86	1.20	0.00	49.80	0.60	14.40	0.00	0.60	0.00	66.50
94.	65.00	31.40	66.26	0.61	0.00	57.80	0.35	17.15	0.00	0.35	0.00	86.00
95.	80.00	31.63	66.45	0.32	0.00	62.60	0.20	18.80	0.00	0.20	0.00	94.00
96.	90.00	31.76	66.57	0.15	0.00	65.80	0.10	19.90	0.00	0.10	0.00	100.00
97.	95.00	31.82	66.62	0.07	0.00	67.40	0.05	20.45	0.00	0.05	0.00	107.50
98.	99.00	31.87	66.66	0.01	0.00	68.68	0.01	20.89	0.00	0.01	0.00	105.50
99.	100.00	31.88	66.67	0.00	0.00	69.00	0.00	21.00	0.00	0.00	0.00	109.00

SAM1	**$HS(CH_2)_{10}CH_2OH$**											
SAM2	**$HS(CH_2)_{21}CH_2OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O(%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
100.	0.00	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	7.50
101.	7.50	29.96	64.98	2.53	0.00	39.48	1.00	10.83	0.00	1.00	0.00	26.50
102.	10.00	30.02	65.01	2.48	0.00	40.30	1.00	11.10	0.00	1.00	0.00	38.85
103.	31.00	30.51	65.26	2.12	0.00	47.23	1.00	13.41	0.00	1.00	0.00	43.50
104.	47.50	30.80	65.40	1.90	0.00	52.68	1.00	15.23	0.00	1.00	0.00	44.25
105.	67.50	31.08	65.54	1.69	0.00	59.28	1.00	17.43	0.00	1.00	0.00	40.00
106.	77.50	31.20	65.60	1.60	0.00	62.58	1.00	18.53	0.00	1.00	0.00	34.00
107.	100.00	31.43	65.71	1.43	0.00	70.00	1.00	21.00	0.00	1.00	0.00	20.00

SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$HS(CH_2)_{21}CH_3$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O(%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
108.	0	30.56	66.67	0.00	0.00	36.00	0.00	10.00	0.00	0.00	0.00	104.75
109.	0.05	30.68	66.67	0.00	0.00	37.65	0.00	10.55	0.00	0.00	0.00	105.50
110.	0.1	30.79	66.67	0.00	0.00	39.30	0.00	11.10	0.00	0.00	0.00	104.25
111.	0.18	30.95	66.67	0.00	0.00	41.94	0.00	11.98	0.00	0.00	0.00	104.50
112.	0.23	31.04	66.67	0.00	0.00	43.59	0.00	12.53	0.00	0.00	0.00	103.75
113.	0.4	31.30	66.67	0.00	0.00	49.20	0.00	14.40	0.00	0.00	0.00	102.95
114.	0.48	31.40	66.67	0.00	0.00	51.84	0.00	15.28	0.00	0.00	0.00	103.75
115.	0.63	31.57	66.67	0.00	0.00	56.79	0.00	16.93	0.00	0.00	0.00	102.65
116.	0.75	31.69	66.67	0.00	0.00	60.75	0.00	18.25	0.00	0.00	0.00	104.40
117.	0.83	31.76	66.67	0.00	0.00	63.39	0.00	19.13	0.00	0.00	0.00	103.30
118.	0.95	31.85	66.67	0.00	0.00	67.35	0.00	20.45	0.00	0.00	0.00	104.30
119.	1	31.88	66.67	0.00	0.00	69.00	0.00	21.00	0.00	0.00	0.00	107.50

SAM1	**$HS(CH_2)_{10}CH_3$**											
SAM2	**$HS(CH_2)_{21}CH_2OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O(%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
120.	**0.00**	**30.56**	**66.67**	**0.00**	**0.00**	**36.00**	**0.00**	**10.00**	**0.00**	**0.00**	**0.00**	**107.50**
121.	2.00	30.59	66.63	0.05	0.00	36.68	0.02	10.22	0.00	0.02	0.00	104.00
122.	10.00	30.71	66.50	0.25	0.00	39.40	0.10	11.10	0.00	0.10	0.00	100.25
123.	19.00	30.83	66.37	0.45	0.00	42.46	0.19	12.09	0.00	0.19	0.00	96.00
124.	29.00	30.94	66.25	0.63	0.00	45.86	0.29	13.19	0.00	0.29	0.00	85.00
125.	44.00	31.08	66.09	0.86	0.00	50.96	0.44	14.84	0.00	0.44	0.00	79.00
126.	77.00	31.31	65.84	1.24	0.00	62.18	0.77	18.47	0.00	0.77	0.00	54.00
127.	95.00	31.41	65.74	1.39	0.00	68.30	0.95	20.45	0.00	0.95	0.00	32.50
128.	99.00	31.42	65.72	1.42	0.00	69.66	0.99	20.89	0.00	0.99	0.00	25.75

TABLE S9. Results by Herrwerth et al.[9]

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	WCA
129.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)-OMe	29.79	63.83	4.26	0.00	47.00	0.00	11.00	0.00	4.00	0.00	71.00
130.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_2$-OH	29.41	62.75	5.88	0.00	51.00	1.00	12.00	0.00	5.00	0.00	33.00
131.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_2$-OMe	29.63	62.96	5.56	0.00	54.00	0.00	12.00	0.00	6.00	0.00	69.00
132.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OH	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	34.00
133.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OMe	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	65.00
134.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OEt	29.69	62.50	6.25	0.00	64.00	0.00	14.00	0.00	8.00	0.00	84.00
135.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OPr	29.85	62.69	5.97	0.00	67.00	0.00	15.00	0.00	8.00	0.00	94.00
136.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OBu	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	107.00
137.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OH	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	32.00
138.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OMe	29.27	60.98	8.54	0.00	82.00	0.00	16.00	0.00	14.00	0.00	67.00
139.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OEt	29.41	61.18	8.24	0.00	85.00	0.00	17.00	0.00	14.00	0.00	87.00
140.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OPr	29.55	61.36	7.95	0.00	88.00	0.00	18.00	0.00	14.00	0.00	97.00
141.	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_2$-OMe	30.00	63.33	5.00	0.00	60.00	0.00	14.00	0.00	6.00	0.00	73.00
142.	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_3$-OMe	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	72.00
143.	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_4$-OMe	30.00	62.50	6.25	0.00	80.00	0.00	18.00	0.00	10.00	0.00	71.00
144.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2-CH_2)$_3$-OH	29.85	62.69	5.97	0.00	67.00	1.00	16.00	0.00	7.00	0.00	34.00
145.	HS-$(CH_2)_{11}$-(O-CH_2-CH_2-CH_2)$_3$-OMe	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	67.00

MULTI-LAB DATASET

TABLE S10. Results by Hayashi et al. [7]

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
1	$HS-(CH_2)_7-CH_3$	29.63	66.67	0.00	0.00	27.00	0.00	7.00	0.00	0.00	0.00	2.00
2	$HS-(CH_2)_{11}-OH$	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	0.58
3	$HS-(CH_2)_{11}-NH_2$	28.95	65.79	0.00	2.63	38.00	0.00	10.00	1.00	0.00	0.00	1.80
4	$HS-(CH_2)_{11}-COOH$	30.77	61.54	5.13	0.00	39.00	1.00	11.00	0.00	1.00	1.00	1.70
5	$HS-(CH_2)_{11}-(O-CH_2-CH_2)-OH$	29.55	63.64	4.55	0.00	44.00	1.00	11.00	0.00	3.00	0.00	0.10
6	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_2-OH$	29.41	62.75	5.88	0.00	51.00	1.00	12.00	0.00	5.00	0.00	0.08
7	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-OH$	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	0.00
8	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-O-CH_3$	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	0.01
9	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-NH_2$	28.81	62.71	5.08	1.69	59.00	0.00	13.00	1.00	6.00	0.00	1.40
10	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-COOH$	30.00	60.00	8.33	0.00	60.00	1.00	14.00	0.00	7.00	1.00	1.30
11	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_6-OH$	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	0.00

TABLE S11. Results by Sekine et al.[3]:

SAM1	**$HS(CH_2)_5CH_3$**											
SAM2	**$HS\text{-}(CH_2)_{11}\text{-}(O\text{-}CH_2\text{-}CH_2)_3\text{-}OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
12	4.43	28.66	66.14	0.78	0.00	22.64	0.04	5.35	0.00	0.31	0.00	2.58
13	5.29	28.67	66.05	0.92	0.00	22.96	0.05	5.42	0.00	0.37	0.00	2.60
14	5.46	28.67	66.03	0.95	0.00	23.02	0.05	5.44	0.00	0.38	0.00	2.51
15	5.85	28.68	65.99	1.01	0.00	23.16	0.06	5.47	0.00	0.41	0.00	2.73
16	6.30	28.69	65.95	1.08	0.00	23.33	0.06	5.50	0.00	0.44	0.00	2.66
17	6.35	28.69	65.94	1.09	0.00	23.35	0.06	5.51	0.00	0.44	0.00	2.63
18	6.93	28.70	65.88	1.18	0.00	23.56	0.07	5.55	0.00	0.48	0.00	2.31
19	7.55	28.71	65.82	1.27	0.00	23.80	0.08	5.60	0.00	0.53	0.00	2.62
20	8.19	28.72	65.76	1.36	0.00	24.03	0.08	5.66	0.00	0.57	0.00	1.87
21	9.55	28.74	65.63	1.56	0.00	24.53	0.10	5.76	0.00	0.67	0.00	2.02
22	10.17	28.75	65.57	1.64	0.00	24.76	0.10	5.81	0.00	0.71	0.00	2.62
23	10.37	28.75	65.55	1.67	0.00	24.84	0.10	5.83	0.00	0.73	0.00	2.24
24	10.95	28.76	65.50	1.75	0.00	25.05	0.11	5.88	0.00	0.77	0.00	2.38
25	12.64	28.78	65.35	1.97	0.00	25.68	0.13	6.01	0.00	0.88	0.00	2.81
26	13.20	28.79	65.31	2.04	0.00	25.88	0.13	6.06	0.00	0.92	0.00	1.94
27	13.42	28.79	65.29	2.07	0.00	25.97	0.13	6.07	0.00	0.94	0.00	1.97
28	15.45	28.82	65.12	2.31	0.00	26.72	0.15	6.24	0.00	1.08	0.00	2.09
29	16.54	28.83	65.04	2.44	0.00	27.12	0.17	6.32	0.00	1.16	0.00	2.03
30	16.80	28.84	65.02	2.47	0.00	27.22	0.17	6.34	0.00	1.18	0.00	2.07
31	18.29	28.85	64.91	2.63	0.00	27.77	0.18	6.46	0.00	1.28	0.00	1.62
32	20.64	28.88	64.74	2.88	0.00	28.64	0.21	6.65	0.00	1.44	0.00	1.75

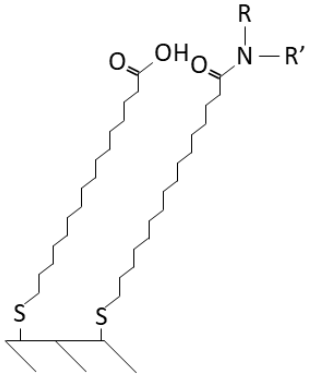
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
33	23.23	28.91	64.57	3.14	0.00	29.59	0.23	6.86	0.00	1.63	0.00	1.93
34	24.99	28.93	64.46	3.31	0.00	30.25	0.25	7.00	0.00	1.75	0.00	1.68
35	25.21	28.93	64.45	3.33	0.00	30.33	0.25	7.02	0.00	1.77	0.00	1.78
36	28.08	28.95	64.28	3.58	0.00	31.39	0.28	7.25	0.00	1.97	0.00	1.70
37	28.28	28.96	64.27	3.60	0.00	31.46	0.28	7.26	0.00	1.98	0.00	1.26
38	35.43	29.02	63.90	4.15	0.00	34.11	0.35	7.83	0.00	2.48	0.00	1.08
39	41.05	29.06	63.64	4.54	0.00	36.19	0.41	8.28	0.00	2.87	0.00	0.77
40	41.38	29.06	63.63	4.56	0.00	36.31	0.41	8.31	0.00	2.90	0.00	0.44
41	41.52	29.06	63.62	4.57	0.00	36.36	0.42	8.32	0.00	2.91	0.00	0.29
42	46.55	29.09	63.42	4.87	0.00	38.22	0.47	8.72	0.00	3.26	0.00	0.57
43	47.77	29.10	63.37	4.94	0.00	38.68	0.48	8.82	0.00	3.34	0.00	0.15
44	50.84	29.12	63.26	5.11	0.00	39.81	0.51	9.07	0.00	3.56	0.00	0.32
45	51.69	29.12	63.23	5.15	0.00	40.13	0.52	9.14	0.00	3.62	0.00	0.54
46	56.67	29.15	63.07	5.40	0.00	41.97	0.57	9.53	0.00	3.97	0.00	0.25
47	70.03	29.21	62.69	5.97	0.00	46.91	0.70	10.60	0.00	4.90	0.00	0.18
48	74.06	29.23	62.59	6.12	0.00	48.40	0.74	10.92	0.00	5.18	0.00	0.17
49	76.31	29.24	62.53	6.20	0.00	49.23	0.76	11.10	0.00	5.34	0.00	0.10
50	78.07	29.24	62.49	6.26	0.00	49.89	0.78	11.25	0.00	5.47	0.00	0.10
51	78.75	29.24	62.48	6.28	0.00	50.14	0.79	11.30	0.00	5.51	0.00	0.08
52	79.45	29.25	62.46	6.31	0.00	50.40	0.79	11.36	0.00	5.56	0.00	0.09
53	81.05	29.25	62.43	6.36	0.00	50.99	0.81	11.48	0.00	5.67	0.00	0.06
54	81.30	29.25	62.42	6.37	0.00	51.08	0.81	11.50	0.00	5.69	0.00	0.09
55	82.47	29.26	62.40	6.40	0.00	51.52	0.82	11.60	0.00	5.77	0.00	0.05
56	85.11	29.27	62.34	6.49	0.00	52.49	0.85	11.81	0.00	5.96	0.00	0.08
57	85.48	29.27	62.34	6.50	0.00	52.63	0.85	11.84	0.00	5.98	0.00	0.04

No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
58	85.92	29.27	62.33	6.51	0.00	52.79	0.86	11.87	0.00	6.01	0.00	0.03
59	86.93	29.27	62.31	6.54	0.00	53.16	0.87	11.95	0.00	6.08	0.00	0.09
60	87.59	29.27	62.29	6.56	0.00	53.41	0.88	12.01	0.00	6.13	0.00	0.03
61	88.98	29.28	62.27	6.60	0.00	53.92	0.89	12.12	0.00	6.23	0.00	0.10
62	89.43	29.28	62.26	6.61	0.00	54.09	0.89	12.15	0.00	6.26	0.00	0.07
63	90.08	29.28	62.25	6.63	0.00	54.33	0.90	12.21	0.00	6.31	0.00	0.07
64	91.48	29.29	62.22	6.67	0.00	54.85	0.91	12.32	0.00	6.40	0.00	0.07
65	92.49	29.29	62.20	6.70	0.00	55.22	0.92	12.40	0.00	6.47	0.00	0.15
66	92.56	29.29	62.20	6.70	0.00	55.25	0.93	12.41	0.00	6.48	0.00	0.10
67	93.32	29.29	62.19	6.72	0.00	55.53	0.93	12.47	0.00	6.53	0.00	0.16
68	93.81	29.29	62.18	6.74	0.00	55.71	0.94	12.51	0.00	6.57	0.00	0.16
69	96.55	29.30	62.13	6.81	0.00	56.72	0.97	12.72	0.00	6.76	0.00	0.07
70	97.17	29.30	62.12	6.82	0.00	56.95	0.97	12.77	0.00	6.80	0.00	0.03
71	97.60	29.30	62.11	6.84	0.00	57.11	0.98	12.81	0.00	6.83	0.00	0.11
72	97.88	29.30	62.10	6.84	0.00	57.22	0.98	12.83	0.00	6.85	0.00	0.06

TABLE S12. Results by Herrwerth et al.[9]:

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
73	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)-OMe	29.79	63.83	4.26	0.00	47.00	0.00	11.00	0.00	4.00	0.00	0.44
74	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_2$-OH	29.41	62.75	5.88	0.00	51.00	1.00	12.00	0.00	5.00	0.00	0.00
75	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_2$-OMe	29.63	62.96	5.56	0.00	54.00	0.00	12.00	0.00	6.00	0.00	0.00
76	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OH	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	0.00
77	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OMe	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	0.00
78	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OEt	29.69	62.50	6.25	0.00	64.00	0.00	14.00	0.00	8.00	0.00	1.20
79	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OPr	29.85	62.69	5.97	0.00	67.00	0.00	15.00	0.00	8.00	0.00	1.58
80	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_3$-OBu	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	1.54
81	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OH	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	0.00
82	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OMe	29.27	60.98	8.54	0.00	82.00	0.00	16.00	0.00	14.00	0.00	0.00
83	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OEt	29.41	61.18	8.24	0.00	85.00	0.00	17.00	0.00	14.00	0.00	1.02
84	HS-$(CH_2)_{11}$-(O-CH_2-CH_2)$_6$-OPr	29.55	61.36	7.95	0.00	88.00	0.00	18.00	0.00	14.00	0.00	1.38
85	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_2$-OMe	30.00	63.33	5.00	0.00	60.00	0.00	14.00	0.00	6.00	0.00	1.04
86	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_3$-OMe	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	0.98
87	HS-$(CH_2)_{11}$-(O-CH(CH_3)-CH_2)$_4$-OMe	30.00	62.50	6.25	0.00	80.00	0.00	18.00	0.00	10.00	0.00	0.84
88	HS-$(CH_2)_{11}$-(O-CH_2-CH_2-CH_2)$_3$-OH	29.85	62.69	5.97	0.00	67.00	1.00	16.00	0.00	7.00	0.00	0.00
89	HS-$(CH_2)_{11}$-(O-CH_2-CH_2-CH_2)$_3$-OMe	30.00	62.86	5.71	0.00	70.00	0.00	16.00	0.00	8.00	0.00	0.00

TABLE S13. Results by Ostuni et al. [10]

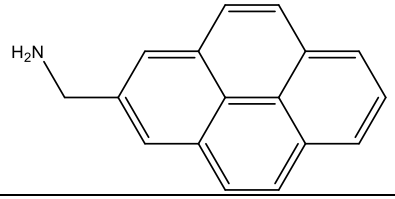


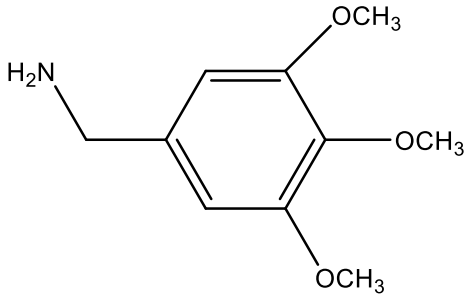
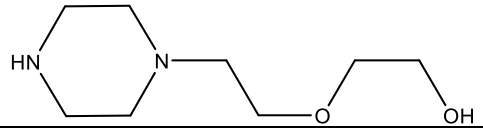
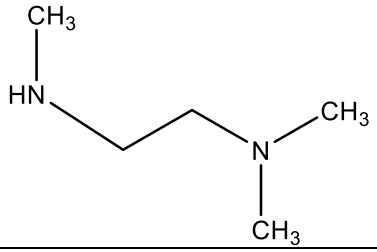
Schematic of Mixed SAMs in paper published by Ostuni, et. al.

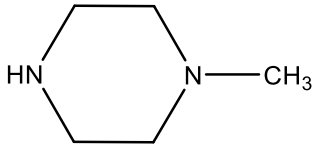
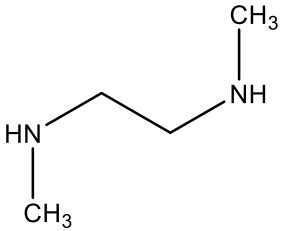
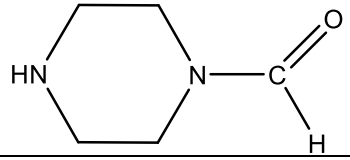
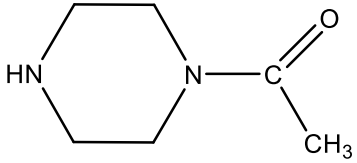
The SAM is a 1:1 mixture of -CONR'R and -CO_2H/CO_2^- groups

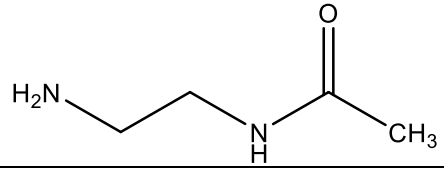
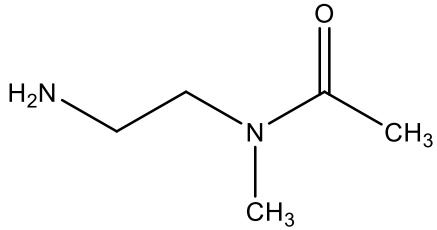
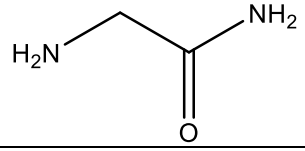
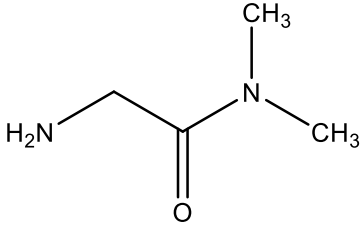
The -CONR'R part of the SAMs were synthesized by reacting the SAMs

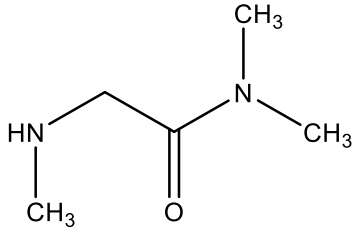
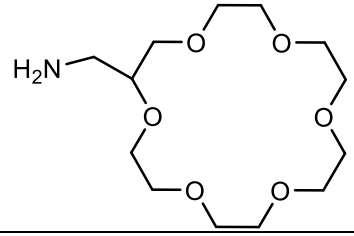
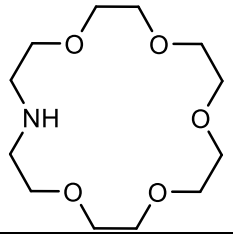
with amines of the form HNR'R

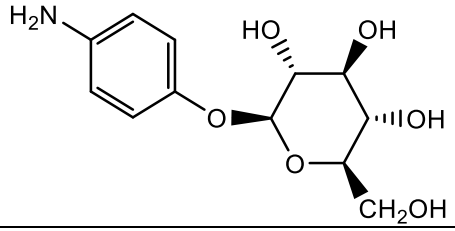
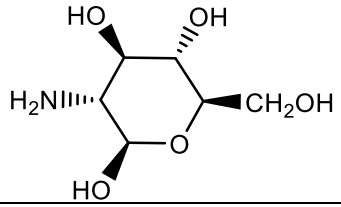
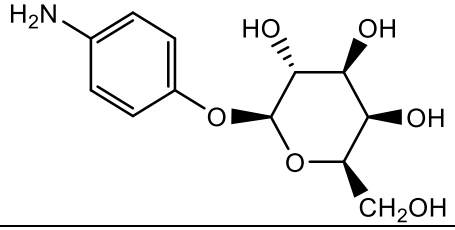
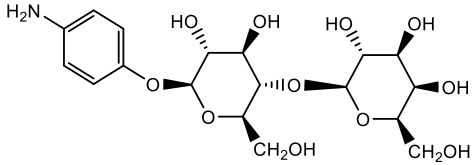
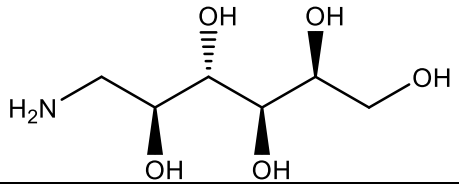
No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
90	$H_2N(CH_2)_{10}CH_3$	31.62	63.97	2.21	0.74	68.00	0.50	20.00	1.00	0.50	1.00	2.00
91		37.69	57.69	2.31	0.77	65.00	0.50	25.00	1.00	0.50	1.00	2.12

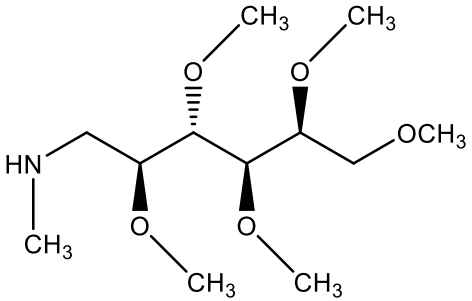
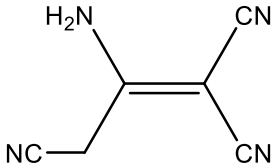
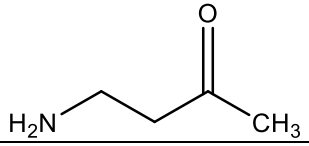
No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
92		32.81	60.16	4.69	0.78	64.00	0.50	18.50	1.00	3.50	1.00	1.50
93	$H_2NCH_2CH_2OCH_3$	30.97	62.83	3.54	0.88	56.50	0.50	15.50	1.00	1.50	1.00	1.06
94	$H_2NCH_2CH_2OH$	30.91	62.73	3.64	0.91	55.00	1.00	15.50	1.00	1.00	1.00	0.94
95	$H(NCH_2CH_2OCH_3)_2$	30.89	62.60	4.07	0.81	61.50	0.50	16.00	1.50	2.50	1.00	1.00
96	$H_2N(CH_2CH_2O)_3CH_3$	30.71	62.20	4.72	0.79	63.50	0.50	16.50	1.00	3.50	1.00	0.03
97	$H_2N(CH_2CH_2O)_3H$	30.65	62.10	4.84	0.81	62.00	1.00	16.50	1.00	3.00	1.00	0.03
98	$H_2N(CH_2CH_2O)_6CH_3$	30.41	61.49	6.08	0.68	74.00	0.50	18.00	1.00	6.50	1.00	0.01
99	$H_2N(CH_2CH_2O)_6H$	30.34	61.38	6.21	0.69	72.50	1.00	18.00	1.00	6.00	1.00	0.01
100		31.01	62.02	3.88	1.55	64.50	1.00	17.00	3.00	2.00	1.00	0.07
101		30.83	63.33	2.50	1.67	60.00	0.50	15.50	3.00	0.50	1.00	0.80

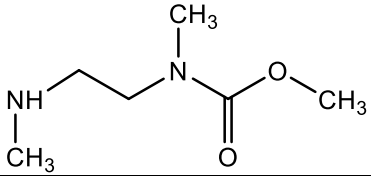
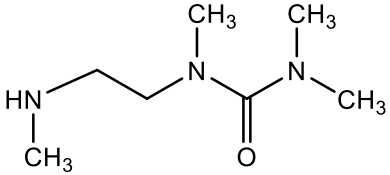
No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
102	$H_2N(CH_2CH_2O)_2CH_2CH_2NH_2$	30.40	62.40	4.00	1.60	62.50	0.50	16.50	1.50	2.50	1.00	0.74
103		31.36	62.71	2.54	1.69	59.00	0.50	16.00	3.00	0.50	1.00	0.32
104		30.77	63.25	2.56	1.71	58.50	0.50	15.50	2.50	0.50	1.00	0.17
105	$HN(CH_3)_2$	31.19	63.30	2.75	0.92	54.50	0.50	15.00	1.50	0.50	1.00	1.08
106		31.62	61.54	3.42	1.71	58.50	0.50	16.00	3.00	0.50	1.50	0.78
107		31.67	61.67	3.33	1.67	60.00	0.50	16.50	3.00	0.50	1.50	0.76

No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
108		31.03	62.07	3.45	1.72	58.00	0.50	16.00	2.00	0.50	1.50	0.80
109		31.15	62.30	3.28	1.64	61.00	0.50	16.00	3.00	0.50	1.50	0.24
110		30.91	61.82	3.64	1.82	55.00	0.50	15.50	1.50	0.50	1.50	1.16
111	 $H_2N(Gly)_1N(CH_3)_2$	31.03	62.07	3.45	1.72	58.00	0.50	15.50	2.50	0.50	1.50	0.66
112	$H_2N(Gly)_3N(CH_3)_2$	31.75	60.32	4.76	1.59	63.00	0.50	17.50	2.50	0.50	2.50	0.44

No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
113	 $H(CH_3)N(Sar)_1N(CH_3)_2$	31.09	62.18	3.36	1.68	59.50	0.50	15.50	3.00	0.50	1.50	0.18
114	$H(CH_3)N(Sar)_3N(CH_3)_2$	31.78	60.47	4.65	1.55	64.50	0.50	17.50	3.00	0.50	2.50	0.04
115	$H(CH_3)N(Sar)_4N(CH_3)_2$	32.09	59.70	5.22	1.49	67.00	0.50	18.50	3.00	0.50	3.00	0.03
116	$H(CH_3)N(Sar)_5N(CH_3)_2$	32.37	58.99	5.76	1.44	69.50	0.50	19.50	3.00	0.50	3.50	0.03
117		30.82	60.96	6.16	0.68	73.00	0.50	18.50	1.00	6.50	1.00	1.18
118		30.99	61.27	5.63	0.70	71.00	0.50	18.00	1.50	5.50	1.00	0.22

No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
119		32.59	58.52	6.67	0.74	67.50	2.50	20.50	1.00	4.50	1.00	1.34
120		30.65	60.48	6.45	0.81	62.00	2.50	17.50	1.00	3.50	1.00	1.10
121		32.59	58.52	6.67	0.74	67.50	2.50	20.50	1.00	4.50	1.00	0.98
122		31.85	56.69	9.55	0.64	78.50	4.00	23.00	1.00	8.00	1.00	0.64
123		30.16	61.11	6.35	0.79	63.00	3.00	17.50	1.00	3.00	1.00	1.36

No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
124		30.56	61.81	5.56	0.69	72.00	0.50	17.50	1.50	5.50	1.00	0.06
125		33.63	58.41	2.65	3.54	56.50	0.50	17.00	3.00	0.00	1.50	1.16
126	$HN(CH_2CH_2CN)_2$	32.48	60.68	2.56	2.56	58.50	0.50	17.00	2.50	0.50	1.00	1.16
127	$HN(CH_2CN)_2$	32.43	60.36	2.70	2.70	55.50	0.50	16.00	2.50	0.50	1.00	1.46
128	$H_2NCH_2CH_2CN$	31.82	61.82	2.73	1.82	55.00	0.50	16.00	1.50	0.50	1.00	1.44
129		31.58	62.28	3.51	0.88	57.00	0.50	16.50	1.00	0.50	1.50	1.48
130	$H_2NC(CH_2CH_2CH_2OH)_3$	30.88	62.50	4.41	0.74	68.00	2.00	19.50	1.00	2.00	1.00	1.14

No.	HNR'R	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
131		30.89	61.79	4.07	1.63	61.50	0.50	15.50	3.00	1.50	1.50	1.16
132	$H(CH_3)NCH_2CH(OCH_3)_2$	31.03	62.93	3.45	0.86	58.00	0.50	15.50	1.50	1.50	1.00	0.72
133		30.71	62.20	3.15	2.36	63.50	0.50	15.50	4.50	0.50	1.50	0.50

SINGLE-LAB DATASET

TABLE S14. Results by Hayashi et al.[7]:

No.	Structure	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
1	$HS-(CH_2)_7-CH_3$	29.63	66.67	0.00	0.00	27.00	0.00	7.00	0.00	0.00	0.00	2.00
2	$HS-(CH_2)_{11}-OH$	29.73	64.86	2.70	0.00	37.00	1.00	10.00	0.00	1.00	0.00	0.58
3	$HS-(CH_2)_{11}-NH_2$	28.95	65.79	0.00	2.63	38.00	0.00	10.00	1.00	0.00	0.00	1.80
4	$HS-(CH_2)_{11}-COOH$	30.77	61.54	5.13	0.00	39.00	1.00	11.00	0.00	1.00	1.00	1.70
5	$HS-(CH_2)_{11}-(O-CH_2-CH_2)-OH$	29.55	63.64	4.55	0.00	44.00	1.00	11.00	0.00	3.00	0.00	0.10
6	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_2-OH$	29.41	62.75	5.88	0.00	51.00	1.00	12.00	0.00	5.00	0.00	0.08
7	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-OH$	29.31	62.07	6.90	0.00	58.00	1.00	13.00	0.00	7.00	0.00	0.00
8	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-O-CH_3$	29.51	62.30	6.56	0.00	61.00	0.00	13.00	0.00	8.00	0.00	0.01
9	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-NH_2$	28.81	62.71	5.08	1.69	59.00	0.00	13.00	1.00	6.00	0.00	1.40
10	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_3-COOH$	30.00	60.00	8.33	0.00	60.00	1.00	14.00	0.00	7.00	1.00	1.30
11	$HS-(CH_2)_{11}-(O-CH_2-CH_2)_6-OH$	29.11	60.76	8.86	0.00	79.00	1.00	16.00	0.00	13.00	0.00	0.00

TABLE S15. Results by Sekine et al.[3]:

SAM1	**$HS(CH_2)_5CH_3$**											
SAM2	**$HS\text{-}(CH_2)_{11}\text{-}(O\text{-}CH_2\text{-}CH_2)_3\text{-}OH$**											
No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
12	4.43	28.66	66.14	0.78	0.00	22.64	0.04	5.35	0.00	0.31	0.00	2.58
13	5.29	28.67	66.05	0.92	0.00	22.96	0.05	5.42	0.00	0.37	0.00	2.60
14	5.46	28.67	66.03	0.95	0.00	23.02	0.05	5.44	0.00	0.38	0.00	2.51
15	5.85	28.68	65.99	1.01	0.00	23.16	0.06	5.47	0.00	0.41	0.00	2.73
16	6.30	28.69	65.95	1.08	0.00	23.33	0.06	5.50	0.00	0.44	0.00	2.66
17	6.35	28.69	65.94	1.09	0.00	23.35	0.06	5.51	0.00	0.44	0.00	2.63
18	6.93	28.70	65.88	1.18	0.00	23.56	0.07	5.55	0.00	0.48	0.00	2.31
19	7.55	28.71	65.82	1.27	0.00	23.80	0.08	5.60	0.00	0.53	0.00	2.62
20	8.19	28.72	65.76	1.36	0.00	24.03	0.08	5.66	0.00	0.57	0.00	1.87
21	9.55	28.74	65.63	1.56	0.00	24.53	0.10	5.76	0.00	0.67	0.00	2.02
22	10.17	28.75	65.57	1.64	0.00	24.76	0.10	5.81	0.00	0.71	0.00	2.62
23	10.37	28.75	65.55	1.67	0.00	24.84	0.10	5.83	0.00	0.73	0.00	2.24
24	10.95	28.76	65.50	1.75	0.00	25.05	0.11	5.88	0.00	0.77	0.00	2.38
25	12.64	28.78	65.35	1.97	0.00	25.68	0.13	6.01	0.00	0.88	0.00	2.81
26	13.20	28.79	65.31	2.04	0.00	25.88	0.13	6.06	0.00	0.92	0.00	1.94
27	13.42	28.79	65.29	2.07	0.00	25.97	0.13	6.07	0.00	0.94	0.00	1.97
28	15.45	28.82	65.12	2.31	0.00	26.72	0.15	6.24	0.00	1.08	0.00	2.09
29	16.54	28.83	65.04	2.44	0.00	27.12	0.17	6.32	0.00	1.16	0.00	2.03
30	16.80	28.84	65.02	2.47	0.00	27.22	0.17	6.34	0.00	1.18	0.00	2.07
31	18.29	28.85	64.91	2.63	0.00	27.77	0.18	6.46	0.00	1.28	0.00	1.62
32	20.64	28.88	64.74	2.88	0.00	28.64	0.21	6.65	0.00	1.44	0.00	1.75

No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
33	23.23	28.91	64.57	3.14	0.00	29.59	0.23	6.86	0.00	1.63	0.00	1.93
34	24.99	28.93	64.46	3.31	0.00	30.25	0.25	7.00	0.00	1.75	0.00	1.68
35	25.21	28.93	64.45	3.33	0.00	30.33	0.25	7.02	0.00	1.77	0.00	1.78
36	28.08	28.95	64.28	3.58	0.00	31.39	0.28	7.25	0.00	1.97	0.00	1.70
37	28.28	28.96	64.27	3.60	0.00	31.46	0.28	7.26	0.00	1.98	0.00	1.26
38	35.43	29.02	63.90	4.15	0.00	34.11	0.35	7.83	0.00	2.48	0.00	1.08
39	41.05	29.06	63.64	4.54	0.00	36.19	0.41	8.28	0.00	2.87	0.00	0.77
40	41.38	29.06	63.63	4.56	0.00	36.31	0.41	8.31	0.00	2.90	0.00	0.44
41	41.52	29.06	63.62	4.57	0.00	36.36	0.42	8.32	0.00	2.91	0.00	0.29
42	46.55	29.09	63.42	4.87	0.00	38.22	0.47	8.72	0.00	3.26	0.00	0.57
43	47.77	29.10	63.37	4.94	0.00	38.68	0.48	8.82	0.00	3.34	0.00	0.15
44	50.84	29.12	63.26	5.11	0.00	39.81	0.51	9.07	0.00	3.56	0.00	0.32
45	51.69	29.12	63.23	5.15	0.00	40.13	0.52	9.14	0.00	3.62	0.00	0.54
46	56.67	29.15	63.07	5.40	0.00	41.97	0.57	9.53	0.00	3.97	0.00	0.25
47	70.03	29.21	62.69	5.97	0.00	46.91	0.70	10.60	0.00	4.90	0.00	0.18
48	74.06	29.23	62.59	6.12	0.00	48.40	0.74	10.92	0.00	5.18	0.00	0.17
49	76.31	29.24	62.53	6.20	0.00	49.23	0.76	11.10	0.00	5.34	0.00	0.10
50	78.07	29.24	62.49	6.26	0.00	49.89	0.78	11.25	0.00	5.47	0.00	0.10
51	78.75	29.24	62.48	6.28	0.00	50.14	0.79	11.30	0.00	5.51	0.00	0.08
52	79.45	29.25	62.46	6.31	0.00	50.40	0.79	11.36	0.00	5.56	0.00	0.09
53	81.05	29.25	62.43	6.36	0.00	50.99	0.81	11.48	0.00	5.67	0.00	0.06
54	81.30	29.25	62.42	6.37	0.00	51.08	0.81	11.50	0.00	5.69	0.00	0.09
55	82.47	29.26	62.40	6.40	0.00	51.52	0.82	11.60	0.00	5.77	0.00	0.05
56	85.11	29.27	62.34	6.49	0.00	52.49	0.85	11.81	0.00	5.96	0.00	0.08
57	85.48	29.27	62.34	6.50	0.00	52.63	0.85	11.84	0.00	5.98	0.00	0.04

No.	Percentage of SAM2 (%)	%C (%)	%H (%)	%O (%)	%N (%)	nAT	O-H Bond	C-C Bond	C-N Bond	C-O Bond	C=O Bond	Fibrinogen Adsorption
58	85.92	29.27	62.33	6.51	0.00	52.79	0.86	11.87	0.00	6.01	0.00	0.03
59	86.93	29.27	62.31	6.54	0.00	53.16	0.87	11.95	0.00	6.08	0.00	0.09
60	87.59	29.27	62.29	6.56	0.00	53.41	0.88	12.01	0.00	6.13	0.00	0.03
61	88.98	29.28	62.27	6.60	0.00	53.92	0.89	12.12	0.00	6.23	0.00	0.10
62	89.43	29.28	62.26	6.61	0.00	54.09	0.89	12.15	0.00	6.26	0.00	0.07
63	90.08	29.28	62.25	6.63	0.00	54.33	0.90	12.21	0.00	6.31	0.00	0.07
64	91.48	29.29	62.22	6.67	0.00	54.85	0.91	12.32	0.00	6.40	0.00	0.07
65	92.49	29.29	62.20	6.70	0.00	55.22	0.92	12.40	0.00	6.47	0.00	0.15
66	92.56	29.29	62.20	6.70	0.00	55.25	0.93	12.41	0.00	6.48	0.00	0.10
67	93.32	29.29	62.19	6.72	0.00	55.53	0.93	12.47	0.00	6.53	0.00	0.16
68	93.81	29.29	62.18	6.74	0.00	55.71	0.94	12.51	0.00	6.57	0.00	0.16
69	96.55	29.30	62.13	6.81	0.00	56.72	0.97	12.72	0.00	6.76	0.00	0.07
70	97.17	29.30	62.12	6.82	0.00	56.95	0.97	12.77	0.00	6.80	0.00	0.03
71	97.60	29.30	62.11	6.84	0.00	57.11	0.98	12.81	0.00	6.83	0.00	0.11
72	97.88	29.30	62.10	6.84	0.00	57.22	0.98	12.83	0.00	6.85	0.00	0.06

Appropriateness test of machine learning

To verify the appropriateness of the modeling and the possibility of the over-fitting, we performed training and prediction, in which the data were split to test (randomly selected five data) and training (the rest of data)

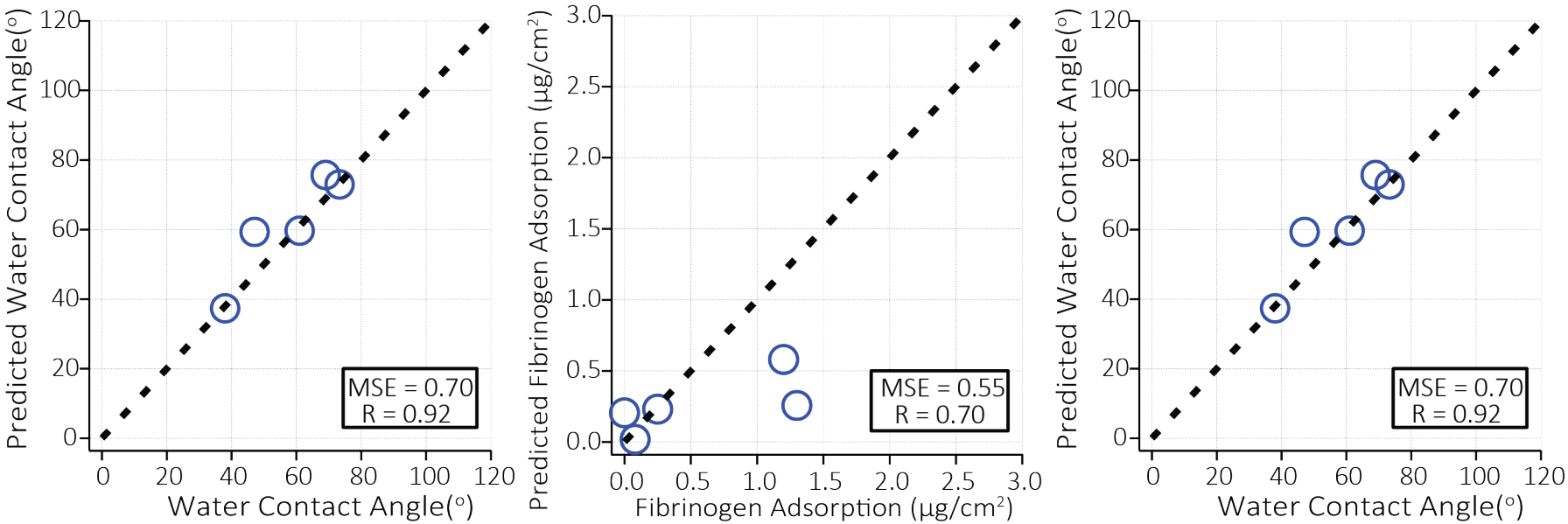


Figure S1. Prediction of WCA (left) the amount of adsorbed fibrinogen on SAMs [multi- (middle) and single- (right) lab datasets]

Importance analysis using the multi-lab dataset

The importance of the descriptors was calculated by using the multi-lab dataset. Compared with the results with the single-lab dataset, the importance obtained with the multi-lab dataset shows significant coefficients of variation (standard deviation divided by value).

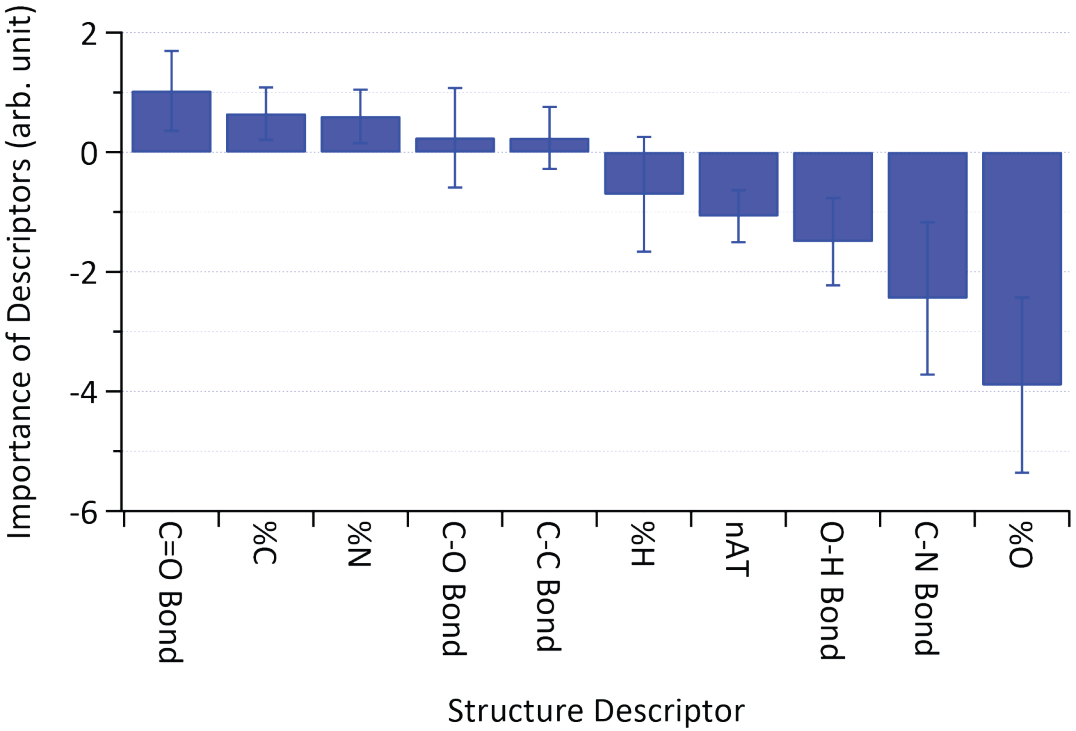


Figure S2. Results of importance analysis after the training with the multi-lab dataset. Error bars stand for standard deviation (N = 2000).

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