Supplementary Information

Additive SMILES-Based Carcinogenicity Models: Probabilistic Principles in search for Robust Prediction

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Supplementary Materials

Table 1. Three splits into subtraining, calibration, and test sets, which were studied.

	CAS No Split1	CAS No Split2	CAS No Split3
	Subtraining set		
1.	75-07-0	75-07-0	75-07-0
2.	60-35-5	60-35-5	60-35-5
3.	34627-78-6	53-96-3	53-96-3
4.	4075-79-0	7008-42-6	7008-42-6
5.	53-96-3	79-06-1	79-06-1
6.	79-06-1	3688-53-7	107-13-1
7.	107-13-1	81-49-2	3688-53-7
8.	3688-53-7	3775-55-1	81-49-2
9.	81-49-2	99-57-0	3775-55-1
10.	3775-55-1	117-79-3	99-57-0
11.	712-68-5	97-56-3	121-88-0
12.	99-57-0	10589-74-9	117-79-3
13.	121-88-0	140-57-8	2432-99-7
14.	117-79-3	1912-24-9	10589-74-9
15.	60142-96-3	115-02-6	115-02-6
16.	2432-99-7	17967-53-9	17967-53-9
17.	10589-74-9	50-32-8	71-43-2
18.	17967-53-9	3296-90-0	92-87-5
19.	30516-87-1	542-88-1	50-32-8
20.	71-43-2	2475-45-8	14504-15-5
21.	92-87-5	75-27-4	2475-45-8
22.	50-32-8	51333-22-3	74-96-4
23.	14504-15-5	3068-88-0	3068-88-0
24.	3296-90-0	63-25-2	63-25-2
25.	85-68-7	56-23-5	56-23-5
26.	3068-88-0	120-80-9	60391-92-6
27.	331-39-5	305-03-3	305-03-3
28.	63-25-2	77439-76-0	37087-94-8
29.	56-23-5	37087-94-8	5131-60-2
30.	305-03-3	95-83-0	75-88-7
31.	37087-94-8	150-68-5	50892-23-4
32.	75-88-7	10473-70-8	108-90-7
33.	50892-23-4	1897-45-6	107-30-2
34.	65089-17-0	102-50-1	150-68-5
35.	108-90-7	80-08-0	126-99-8

Table 1. Cont.

36.	107-30-2	50-29-3	1897-45-6
37.	150-68-5	53-43-0	102-50-1
38.	126-99-8	853-23-6	120-71-8
39.	1897-45-6	63019-65-8	80-08-0
40.	102-50-1	16338-97-9	853-23-6
41.	120-71-8	720-69-4	16338-97-9
42.	1163-19-5	95-80-7	720-69-4
43.	853-23-6	96-12-8	96-12-8
44.	16338-97-9	10318-26-0	10318-26-0
45.	720-69-4	106-93-4	106-93-4
46.	4106-66-5	1717-00-6	106-46-7
47.	96-12-8	107-06-2	107-06-2
48.	10318-26-0	62-73-7	101-90-6
49.	106-93-4	56-53-1	3276-41-3
50.	7572-29-4	101-90-6	119-84-6
51.	106-46-7	5803-51-0	5803-51-0
52.	105-55-5	59-35-8	91-93-0
53.	3276-41-3	55738-54-0	60-11-7
54.	91-93-0	121-69-7	59-35-8
55.	4164-28-7	26049-69-4	513-37-1
56.	513-37-1	513-37-1	106-89-8
57.	106-89-8	106-89-8	150-69-6
58.	150-69-6	140-88-5	16301-26-1
59.	16301-26-1	64-17-5	57497-29-7
60.	75-21-8	16301-26-1	75-21-8
61.	117-81-7	57497-29-7	86386-73-4
62.	110559-84-7	75-21-8	69112-98-7
63.	86386-73-4	96724-44-6	110-00-9
64.	69112-98-7	86386-73-4	67730-11-4
65.	93957-54-1	363-17-7	56-40-6
66.	98-01-1	3570-75-0	87-68-3
67.	56-40-6	110-00-9	319-84-6
68.	319-84-6	98-01-1	67-72-1
69.	67-72-1	67730-11-4	26049-70-7
70.	18774-85-1	56-40-6	122-66-7
71.	26049-70-7	87-68-3	53-95-2
72.	122-66-7	67-72-1	129-43-1
73.	53-95-2	680-31-9	96724-45-7
74.	129-43-1	26049-70-7	13743-07-2
75.	96724-45-7	53-95-2	71752-70-0
76.	71752-70-0	84545-30-2	100643-96-7
77.	100643-96-7	100643-96-7	76180-96-6
78.	76180-96-6	76180-96-6	115-11-7
79.	115-11-7	15503-86-3	542-56-3
80.	542-56-3	115-11-7	54-85-3
81.	303-34-4	542-56-3	303-34-4
82.	76956-02-0	54-85-3	108-78-1
83.	148-82-3	303-34-4	148-82-3
84.	149-30-4	76956-02-0	149-30-4
85.	5834-17-3	108-78-1	934-00-9
86.	934-00-9	148-82-3	298-81-7
87.	298-81-7	60-56-0	598-55-0
88.	598-55-0	5834-17-3	55-80-1
89.	21638-36-8	298-81-7	21638-36-8
90.	63412-06-6	1634-04-4	63412-06-6
91.	598-57-2	21340-68-1	14026-03-0
92.	33868-17-6	21638-36-8	598-57-2
93.	443-48-1	63412-06-6	76014-81-8

Table 1. Cont.

94.	39801-14-4	14026-03-0	64091-91-4
95.	50-07-7	76014-81-8	90-94-8
96.	3771-19-5	64091-91-4	2385-85-5
97.	2243-62-1	90-94-8	39801-14-4
98.	139-94-6	39801-14-4	50-07-7
99.	99-59-2	50-07-7	58139-48-3
100.	2122-86-3	58139-48-3	2243-62-1
101.	2578-75-8	389-08-2	139-94-6
102.	53757-28-1	2243-62-1	99-59-2
103.	24554-26-5	91-59-8	91-23-6
104.	600-24-8	139-94-6	600-24-8
105.	1836-75-5	99-59-2	1836-75-5
106.	607-57-8	59-87-0	607-57-8
107.	75-52-5	75198-31-1	555-84-0
108.	38777-13-8	36133-88-7	38777-13-8
109.	83335-32-4	4812-22-0	83335-32-4
110.	89911-78-4	555-84-0	89911-79-5
111.	96806-35-8	51-75-2	89911-78-4
112.	56222-35-6	38777-13-8	96806-35-8
113.	760-60-1	83335-32-4	760-60-1
114.	937-25-7	89911-78-4	937-25-7
115.	75881-22-0	96806-35-8	13256-11-6
116.	38347-74-9	760-60-1	75881-22-0
117.	64005-62-5	937-25-7	38347-74-9
118.	1133-64-8	13256-11-6	91308-70-2
119.	51542-33-7	38347-74-9	1133-64-8
120.	60599-38-4	1133-64-8	60599-38-4
121.	62-75-9	55-18-5	62-75-9
122.	156-10-5	62-75-9	156-10-5
123.	10595-95-6	156-10-5	20917-49-1
124.	20917-49-1	42579-28-2	42579-28-2
125.	42579-28-2	86451-37-8	86451-37-8
126.	86451-37-8	70415-59-7	70415-59-7
127.	26921-68-6	16219-98-0	55984-51-5
128.	70415-59-7	59-89-2	16219-98-0
129.	16219-98-0	5632-47-3	614-00-6
130.	614-00-6	930-55-2	59-89-2
131.	59-89-2	81795-07-5	5632-47-3
132.	26541-51-5	3096-50-2	100-75-4
133.	611-23-4	101-80-4	930-55-2
134.	303-47-9	60102-37-6	26541-51-5
135.	3096-50-2	62-44-2	611-23-4
136.	60102-37-6	60-80-0	303-47-9
137.	62-44-2	77-09-8	3096-50-2
138.	77-09-8	7227-91-0	77-09-8
139.	7227-91-0	842-07-9	7227-91-0
140.	90-43-7	50-33-9	50-33-9
141.	51-03-6	122-60-1	90-43-7
142.	29069-24-7	51-03-6	51-03-6
143.	50-24-8	1955-45-9	1955-45-9
144.	671-16-9	29069-24-7	29069-24-7
145.	1120-71-4	816-57-9	57-57-8
146.	57-57-8	75-56-9	13010-07-6
147.	13010-07-6	599-79-1	81-54-9
148.	51-52-5	2318-18-5	2425-85-6
149.	2425-85-6	10048-13-2	480-54-6
150.	480-54-6	18883-66-4	2318-18-5
151.	94-59-7	96-09-3	10048-13-2

Table 1. Cont.

152.	2318-18-5	95-06-7	18883-66-4
153.	10048-13-2	23031-25-6	95-06-7
154.	18883-66-4	127-18-4	116-14-3
155.	96-09-3	116-14-3	109-99-9
156.	95-06-7	509-14-8	509-14-8
157.	127-18-4	139-65-1	52-24-4
158.	109-99-9	62-56-6	139-65-1
159.	62-56-6	68-76-8	88-19-7
160.	88-19-7	538-23-8	68-76-8
161.	68-76-8	88-06-2	76-25-5
162.	76-25-5	96-18-4	75-25-2
163.	75-25-2	2489-77-2	137-17-7
164.	51-79-6	51-79-6	51-79-6
165.	88-12-0	593-60-2	88-12-0
	Calibration set		
1.	18523-69-8	18523-69-8	18523-69-8
2.	7008-42-6	34627-78-6	34627-78-6
3.	2835-39-4	4075-79-0	4075-79-0
4.	760-56-5	107-13-1	760-56-5
5.	82-28-0	1162-65-8	82-28-0
6.	119-34-6	760-56-5	712-68-5
7.	121-66-4	82-28-0	119-34-6
8.	97-56-3	712-68-5	121-66-4
9.	61-82-5	119-34-6	97-56-3
10.	115-02-6	60142-96-3	60142-96-3
11.	103-33-3	61-82-5	61-82-5
12.	88133-11-3	25843-45-2	1912-24-9
13.	271-89-6	30516-87-1	103-33-3
14.	542-88-1	88133-11-3	25843-45-2
15.	2475-45-8	71-43-2	30516-87-1
16.	75-27-4	92-87-5	88133-11-3
17.	74-96-4	271-89-6	271-89-6
18.	51333-22-3	14504-15-5	3296-90-0
19.	106-99-0	2784-94-3	542-88-1
20.	75-65-0	106-99-0	2784-94-3
21.	60391-92-6	75-65-0	51333-22-3
22.	115-28-6	115-28-6	106-99-0
23.	101-79-1	101-79-1	75-65-0
24.	77439-76-0	5131-60-2	85-68-7
25.	5131-60-2	75-88-7	115-28-6
26.	593-70-4	65089-17-0	101-79-1
27.	54749-90-5	107-30-2	77439-76-0
28.	52214-84-3	126-99-8	65089-17-0
29.	637-07-0	52214-84-3	593-70-4
30.	123-73-9	637-07-0	10473-70-8
31.	50-18-0	120-71-8	52214-84-3
32.	80-08-0	123-73-9	637-07-0
33.	50-29-3	50-18-0	123-73-9
34.	63019-65-8	1163-19-5	50-18-0
35.	95-80-7	4106-66-5	50-29-3
36.	56654-52-5	56654-52-5	1163-19-5
37.	1717-00-6	7572-29-4	63019-65-8
38.	91-94-1	106-46-7	95-80-7
39.	107-06-2	91-94-1	56654-52-5
40.	62-73-7	111-46-6	1717-00-6
41.	685-91-6	3276-41-3	7572-29-4
42.	111-46-6	119-84-6	91-94-1

Table 1. Cont.

43.	56-53-1	94-58-6	62-73-7
44.	119-84-6	91-93-0	685-91-6
45.	94-58-6	65176-75-2	111-46-6
46.	5803-51-0	60-11-7	56-53-1
47.	65176-75-2	551-92-8	94-58-6
48.	60-11-7	123-91-1	65176-75-2
49.	59-35-8	57-63-6	551-92-8
50.	551-92-8	150-69-6	26049-69-4
51.	26049-69-4	100-41-4	123-91-1
52.	123-91-1	96-45-7	13256-06-9
53.	13256-06-9	117-81-7	57-63-6
54.	57-63-6	110559-84-7	140-88-5
55.	140-88-5	38434-77-4	64-17-5
56.	64-17-5	69112-98-7	100-41-4
57.	57497-29-7	93957-54-1	96-45-7
58.	100-41-4	556-52-5	117-81-7
59.	96-45-7	517-28-2	96724-44-6
60.	96724-44-6	118-74-1	110559-84-7
61.	38434-77-4	319-84-6	38434-77-4
62.	363-17-7	122-66-7	363-17-7
63.	110-00-9	306-83-2	93957-54-1
64.	67730-11-4	129-43-1	3570-75-0
65.	556-52-5	33389-36-5	556-52-5
66.	517-28-2	71752-70-0	517-28-2
67.	118-74-1	5208-87-7	118-74-1
68.	87-68-3	21416-87-5	680-31-9
69.	680-31-9	53-86-1	26049-68-3
70.	26049-68-3	86315-52-8	306-83-2
71.	306-83-2	78-59-1	33389-36-5
72.	13743-07-2	3778-73-2	5208-87-7
73.	33389-36-5	143-50-0	21416-87-5
74.	5208-87-7	5989-27-5	84545-30-2
75.	84545-30-2	77500-04-0	53-86-1
76.	53-86-1	149-30-4	15503-86-3
77.	15503-86-3	57-39-6	86315-52-8
78.	86315-52-8	934-00-9	78-59-1
79.	54-85-3	150-76-5	3778-73-2
80.	78-59-1	598-55-0	143-50-0
81.	3778-73-2	55-80-1	5989-27-5
82.	143-50-0	70-25-7	76956-02-0
83.	5989-27-5	129-15-7	57-39-6
84.	108-78-1	63642-17-1	60-56-0
85.	57-39-6	452-86-8	150-76-5
86.	60-56-0	56-49-5	1634-04-4
87.	150-76-5	101-14-4	70-25-7
88.	1634-04-4	838-88-0	129-15-7
89.	21340-68-1	598-57-2	63642-17-1
90.	70-25-7	33868-17-6	98-85-1
91.	63642-17-1	443-48-1	452-86-8
92.	98-85-1	3771-19-5	56-49-5
93.	452-86-8	139-13-9	101-14-4
94.	56-49-5	2578-75-8	838-88-0
95.	101-14-4	531-82-8	33868-17-6
96.	838-88-0	24554-26-5	443-48-1
97.	101-61-1	91-23-6	315-22-0
98.	76014-81-8	98-95-3	3771-19-5
99.	64091-91-4	600-24-8	389-08-2
100.	2385-85-5	1836-75-5	59-87-0

Table 1. Cont.

101.	315-22-0	607-57-8	75198-31-1
102.	58139-48-3	67-20-9	2122-86-3
103.	389-08-2	75-52-5	36133-88-7
104.	91-59-8	551-88-2	2578-75-8
105.	139-13-9	5522-43-0	24554-26-5
106.	59-87-0	607-35-2	4812-22-0
107.	75198-31-1	16813-36-8	602-87-9
108.	36133-88-7	89911-79-5	98-95-3
109.	4812-22-0	92177-50-9	67-20-9
110.	602-87-9	56222-35-6	51-75-2
111.	91-23-6	55090-44-3	75-52-5
112.	98-95-3	75881-20-8	551-88-2
113.	67-20-9	75881-22-0	5522-43-0
114.	555-84-0	684-93-5	607-35-2
115.	51-75-2	55556-92-8	16813-36-8
116.	551-88-2	82018-90-4	92177-50-9
117.	607-35-2	75881-18-4	75896-33-2
118.	16813-36-8	91308-70-2	56222-35-6
119.	89911-79-5	91308-69-9	55090-44-3
120.	92177-50-9	51542-33-7	75881-20-8
121.	96806-34-7	60599-38-4	684-93-5
122.	55090-44-3	924-16-3	55556-92-8
123.	13256-11-6	1116-54-7	82018-90-4
124.	684-93-5	621-64-7	75881-18-4
125.	92177-49-6	10595-95-6	91308-69-9
126.	55556-92-8	614-95-9	64005-62-5
127.	82018-90-4	20917-49-1	51542-33-7
128.	75881-18-4	26921-68-6	1116-54-7
129.	91308-70-2	55984-51-5	55-18-5
130.	91308-69-9	614-00-6	621-64-7
131.	1116-54-7	68107-26-6	10595-95-6
132.	55-18-5	78246-24-9	26921-68-6
133.	621-64-7	303-47-9	78246-24-9
134.	55984-51-5	14698-29-4	14698-29-4
135.	68107-26-6	13752-51-7	101-80-4
136.	78246-24-9	1825-21-4	13752-51-7
137.	5632-47-3	50-24-8	60102-37-6
138.	14698-29-4	671-16-9	62-44-2
139.	101-80-4	1120-71-4	842-07-9
140.	13752-51-7	57-57-8	122-60-1
141.	1825-21-4	13010-07-6	50-24-8
142.	842-07-9	51-52-5	671-16-9
143.	50-33-9	81-54-9	1120-71-4
144.	122-60-1	2425-85-6	816-57-9
145.	1955-45-9	127-47-9	51-52-5
146.	816-57-9	480-54-6	127-47-9
147.	81-54-9	18559-94-9	18559-94-9
148.	127-47-9	533-31-3	533-31-3
149.	18559-94-9	77-46-3	96-09-3
150.	599-79-1	811-97-2	77-46-3
151.	533-31-3	40548-68-3	127-18-4
152.	77-46-3	109-99-9	811-97-2
153.	23031-25-6	52-24-4	40548-68-3
154.	116-14-3	62-55-5	62-55-5
155.	40548-68-3	789-61-7	789-61-7
156.	509-14-8	141-90-2	141-90-2
157.	52-24-4	88-19-7	62-56-6
158.	62-55-5	76-25-5	88-06-2

Table 1. Cont.

159.	789-61-7	75-25-2	42011-48-3
160.	141-90-2	137-17-7	95-63-6
161.	137-17-7	95-63-6	2489-77-2
162.	95-63-6	55-63-0	55-63-0
163.	55-63-0	126-72-7	126-72-7
164.	126-72-7	66-22-8	66-22-8
165.	108-05-4	108-05-4	108-05-4
166.	75-02-5	75-02-5	75-02-5
167.	2832-40-8	2832-40-8	2832-40-8
	Test set		
1.	29611-03-8	29611-03-8	29611-03-8
2.	1162-65-8	57-06-7	1162-65-8
3.	57-06-7	2835-39-4	57-06-7
4.	38514-71-5	38514-71-5	2835-39-4
5.	140-57-8	121-88-0	38514-71-5
6.	1912-24-9	121-66-4	140-57-8
7.	25843-45-2	2432-99-7	33372-39-3
8.	33372-39-3	103-33-3	75-27-4
9.	2784-94-3	33372-39-3	869-01-2
10.	869-01-2	74-96-4	331-39-5
11.	120-80-9	85-68-7	120-80-9
12.	95-83-0	869-01-2	95-83-0
13.	10473-70-8	331-39-5	54749-90-5
14.	117-10-2	60391-92-6	117-10-2
15.	1192-28-5	50892-23-4	1192-28-5
16.	53-43-0	108-90-7	53-43-0
17.	79-43-6	593-70-4	4106-66-5
18.	101-90-6	54749-90-5	79-43-6
19.	55738-54-0	117-10-2	105-55-5
20.	121-69-7	1192-28-5	55738-54-0
21.	106-88-7	79-43-6	121-69-7
22.	13073-35-3	685-91-6	4164-28-7
23.	398-32-3	105-55-5	106-88-7
24.	32852-21-4	4164-28-7	13073-35-3
25.	3570-75-0	13256-06-9	398-32-3
26.	67730-10-3	106-88-7	32852-21-4
27.	26049-71-8	13073-35-3	98-01-1
28.	21416-87-5	398-32-3	67730-10-3
29.	77500-04-0	32852-21-4	18774-85-1
30.	55-80-1	67730-10-3	26049-71-8
31.	129-15-7	18774-85-1	77500-04-0
32.	14026-03-0	26049-71-8	5834-17-3
33.	90-94-8	26049-68-3	21340-68-1
34.	531-82-8	96724-45-7	101-61-1
35.	51325-35-0	13743-07-2	91-59-8
36.	62-23-7	98-85-1	139-13-9
37.	5522-43-0	101-61-1	53757-28-1
38.	75896-33-2	2385-85-5	531-82-8
39.	75881-20-8	315-22-0	51325-35-0
40.	88208-16-6	2122-86-3	62-23-7
41.	91308-71-3	53757-28-1	96806-34-7
42.	53609-64-6	51325-35-0	92177-49-6
43.	924-16-3	602-87-9	88208-16-6
44.	40580-89-0	62-23-7	91308-71-3
45.	614-95-9	96806-34-7	53609-64-6
46.	100-75-4	75896-33-2	924-16-3
47.	930-55-2	92177-49-6	40580-89-0
48.	81795-07-5	88208-16-6	614-95-9

Table 1. Cont.

49.	60-80-0	91308-71-3	68107-26-6
50.	75-56-9	64005-62-5	81795-07-5
51.	22571-95-5	53609-64-6	1825-21-4
52.	811-97-2	40580-89-0	60-80-0
53.	139-65-1	100-75-4	75-56-9
54.	538-23-8	26541-51-5	94-59-7
55.	88-06-2	611-23-4	599-79-1
56.	96-18-4	90-43-7	22571-95-5
57.	42011-48-3	94-59-7	23031-25-6
58.	2489-77-2	22571-95-5	538-23-8
59.	66-22-8	42011-48-3	96-18-4
60.	593-60-2	75-01-4	593-60-2
61.	75-01-4	88-12-0	75-01-4

Table 2. Experimental and calculated with Eq. 3 log(TD_{50}): split1, limS=4, first probe of the Monte Carlo method optimization.

CAS No	SMILES	DCW(4)	Expr	Calc
	Subtraining set			
75-07-0	CC=O	-1.6442255	-0.541	-0.782
60-35-5	CC(N)=O	2.4339941	-0.484	-0.326
34627-78-6	CC(=O)OC(C=C)c1ccc2OCOc2c1	8.9723429	0.945	0.405
4075-79-0	O=C(C)Nc1ccc(cc1)c2ccccc2	16.8254890	2.253	1.283
53-96-3	CC(=O)NC1C=CC2=C3C=CC=CC3=CC2=C1	23.7041967	2.263	2.052
79-06-1	C=CC(N)=O	6.1553307	1.278	0.090
107-13-1	C=CC#N	0.4363647	0.497	-0.549
3688-53-7	O=[N+]([O-])c2ccc(/C=C(\c1ccco1)C(N)=O)o2	19.7219116	0.926	1.607
81-49-2	O=C2c1ccccc1C(=O)c3c2c(N)c(Br)cc3Br	10.6082785	0.918	0.588
3775-55-1	Nc1nnc(o1)c2oc(cc2)[N+]([O-])=O	19.5286009	1.728	1.585
712-68-5	Nc1nnc(s1)c2oc(cc2)[N+]([O-])=O	21.4765044	2.506	1.803
99-57-0	Nc1cc(ccc1O)[N+]([O-])=O	8.7582849	-0.736	0.381
121-88-0	Nc1ccc(cc1O)[N+]([O-])=O	8.7582849	0.143	0.381
117-79-3	Nc2ccc3C(=O)c1ccccc1C(=O)c3c2	10.4267880	0.344	0.568
60142-96-3	NCC1(CC(=O)O)CCCCC1	-3.0738151	-1.533	-0.942
2432-99-7	O=C(O)CCCCCCCCCCN	-2.3822437	-0.737	-0.864
10589-74-9	CCCCCN(N=O)C(N)=O	28.9999825	2.462	2.644
17967-53-9	CC(C)[N+](\[O-])=N/C(C)C	41.1617896	4.686	4.004
30516-87-1	CC1=CN(C(=O)NC1=O)C2CC(/N=[N+]=[N-])C(CO)O2	-2.1058355	-1.637	-0.834
71-43-2	c1ccccc1	3.2902364	-0.335	-0.230
92-87-5	Nc1ccc(cc1)c2ccc(N)cc2	15.6117993	2.027	1.147
50-32-8	c1cc2c3ccc4cccc5ccc(cc2cc1)c3c45	28.9921674	2.421	2.643
14504-15-5	NC(=O)Cc2c([O-])on[n+]2Cc1ccccc1	4.7178230	-0.260	-0.071
3296-90-0	OCC(CBr)(CBr)CO	10.1582969	0.373	0.538
85-68-7	O=C(OCc1ccccc1)c2ccccc2C(=O)OCCCC	9.6647886	-0.522	0.482
3068-88-0	O=C1CC(C)O1	7.0229065	0.795	0.187
331-39-5	Oc1ccc(/C=C/C(=O)O)cc1O	2.7387186	-0.217	-0.292
63-25-2	CNC(=O)Oc2cccc1ccccc12	12.8497971	1.154	0.839
56-23-5	ClC(Cl)(Cl)Cl	12.2869593	1.827	0.776
305-03-3	O=C(O)CCCc1ccc(cc1)N(CCCl)CCCl	26.8564822	2.531	2.404
37087-94-8	CC1CC(C)CN(C1)S(=O)(=O)c2cc(C(=O)O)c(Cl)cc2	22.7615129	1.835	1.947
75-88-7	ClCC(F)(F)F	11.1755831	0.133	0.651
50892-23-4	Cc2cccc(Nc1cc(Cl)nc(SCC(=O)O)n1)c2C	19.0894905	1.871	1.536
65089-17-0	Cc2cccc(Nc1cc(Cl)nc(SCC(=O)NCCO)n1)c2C	17.8867308	1.752	1.402
108-90-7	Clc1ccccc1	0.8393418	-0.341	-0.504
107-30-2	COCCl	21.7058832	1.166	1.829
150-68-5	Clc1ccc(NC(=O)N(C)C)cc1	7.6668178	0.181	0.259

Table 2. Cont.

126-99-8	C=C(Cl)C=C	0.3865032	-0.150	-0.555
1897-45-6	Clc1c(C#N)c(Cl)c(C#N)c(Cl)c1Cl	-1.4730550	-0.931	-0.763
102-50-1	Nc1ccc(OC)cc1C	3.4796799	-0.535	-0.209
120-71-8	Nc1cc(C)ccc1OC	6.7795818	0.146	0.160
1163-19-5	Brc2c(Oc1c(Br)c(Br)c(Br)c(Br)c1Br)c(Br)c(Br)c(Br)c2Br	0.8059877	-0.542	-0.508
853-23-6	CC(=O)OC2CCC3(C)C4CCC1(C)C(CCC1=O)C4CC=C3C2	23.1543517	1.022	1.991
16338-97-9	C=CCN(CC=C)N=O	26.5787909	0.571	2.373
720-69-4	O=[N+]([O-])c1ccc(o1)c2nc(N)nc(N)n2	15.5122743	2.114	1.136
4106-66-5	Nc1ccc2c3ccccc3oc2c1	18.8006239	1.869	1.504
96-12-8	BrC(CBr)CCl	24.2664740	2.960	2.115
10318-26-0	OC(C(O)CBr)C(O)C(O)CBr	21.0738102	1.566	1.758
106-93-4	BrCCBr	13.4511485	2.092	0.906
7572-29-4	ClC#CCl	24.1260754	1.423	2.099
106-46-7	Clc1ccc(Cl)cc1	4.3705653	-0.642	-0.109
105-55-5	CCNC(=S)NCC	12.9520877	0.741	0.850
3276-41-3	O=NN1CC=CCO1	17.2055032	0.100	1.325
91-93-0	COc1cc(ccc1/N=C=O)c2ccc(\N=C=O)c(OC)c2	1.4504491	-0.740	-0.436
4164-28-7	CN(C)[N+]([O-])=O	20.1348499	2.217	1.653
513-37-1	C/C(C)=C\Cl	19.4680508	0.455	1.578
106-89-8	ClCC1CO1	15.6927349	1.495	1.156
150-69-6	CCOc1ccc(cc1)NC(N)=O	4.9437759	-0.474	-0.045
16301-26-1	[O-]\[N+](CC)=N\CC	29.8573580	3.667	2.740
75-21-8	C1CO1	4.1677964	0.316	-0.132
117-81-7	CCC(CCCC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	-2.5987356	-0.263	-0.889
110559-84-7	O=C(NCC(C)=O)N(CC)N=O	25.1884351	2.981	2.218
86386-73-4	OC(Cn1cncn1)(Cn2cncn2)c3ccc(F)cc3F	6.0321942	0.579	0.076
69112-98-7	NC(=O)N(CCF)N=O	24.3033326	3.034	2.119
93957-54-1	O=C(O)CC(O)CC(O)/C=C/c2c(c1ccccc1n2C(C)C)c3ccc(F)cc3	14.6992645	0.517	1.045
98-01-1	O=Cc1ccco1	6.3091859	-0.852	0.107
56-40-6	NCC(=O)O	-1.3873663	-2.534	-0.753
319-84-6	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	18.2269649	1.414	1.440
67-72-1	ClC(Cl)(Cl)C(Cl)(Cl)Cl	14.7243688	0.631	1.048
18774-85-1	CCCCCCN(N=O)C(N)=O	28.1722194	2.529	2.552
26049-70-7	NNc1nc(cs1)c2ccc(cc2)[N+]([O-])=O	20.6520759	1.867	1.711
122-66-7	N(Nc1ccccc1)c2ccccc2	18.1209496	1.518	1.428
53-95-2	CC(=O)N(O)C1C=CC2=C3C=CC=CC3=CC2=C1	23.9896850	2.384	2.084
129-43-1	O=C3c1ccccc1C(=O)c2c3cccc2O	2.8757163	0.380	-0.277
96724-45-7	O=C(NCC)N(N=O)CCO	21.7630490	2.458	1.835
71752-70-0	O=C(N)N(N=O)CCCO	17.2624478	2.177	1.332
100643-96-7	O=C2Nc1ccc(cc1C2(C)C)C=3CCC(=O)NN=3	22.0312469	2.107	1.865
76180-96-6	Nc3nc2c(ccc1ncccc12)n3C	21.3468133	2.388	1.788
115-11-7	C=C(C)C	0.3184457	-1.801	-0.562
542-56-3	CC(C)CON=O	8.3162583	0.280	0.332
303-34-4	CC(C)(O)C(O)(C(C)OC)C(=O)OCC1=CCN2CCC(OC(=O)C(\C)=C\C)C12	31.4970206	3.024	2.923
76956-02-0	OCc3nc(NCCCOc2cc(CN1CCCCC1)ccc2)n(C)n3	12.5193481	-0.125	0.802
148-82-3	O=C(O)C(N)Cc1ccc(cc1)N(CCCl)CCCl	41.9895654	3.512	4.096
149-30-4	S=C1Nc2ccccc2S1	4.9343382	-0.313	-0.046
5834-17-3	COc1cc2c3ccccc3oc2cc1N	15.3424654	0.866	1.117
934-00-9	COc1cccc(O)c1O	-1.6426353	0.459	-0.782
298-81-7	COc1c3occc3cc2C=CC(=O)Oc12	12.9007718	0.824	0.844
598-55-0	NC(=O)OC	2.7475976	0.123	-0.291
21638-36-8	O=[N+]([O-])c2ccc(/C=N/N1CC(C)NC1=O)o2	15.3657507	1.649	1.120
63412-06-6	O=C(N(C)N=O)c1ccccc1	25.3611674	1.706	2.237
598-57-2	[O-][N+](=O)CN	9.4966339	0.641	0.464

Table 2. Cont.

33868-17-6	N#CN(C)N=O	24.8721377	2.249	2.183
443-48-1	Cc1ncc([N+]([O-])=O)n1CCO	2.0019404	-0.501	-0.374
39801-14-4	ClC13C5(Cl)C2(Cl)C4C(Cl)(C(Cl)(Cl)C12Cl)C3(Cl)C4(Cl)C5(Cl)Cl	23.6405290	2.544	2.045
50-07-7	NC(=O)OCC3C=1C(=O)C(N)=C(C)C(=O)C=1N4CC2NC2C34OC	46.6793245	5.509	4.621
3771-19-5	O=C(O)C(C)(C)Oc1ccc(cc1)C3CCCc2ccccc23	15.0473711	1.451	1.084
2243-62-1	Nc2cccc1c2cccc1N	6.3106925	0.357	0.107
139-94-6	O=C(Nc1ncc(s1)[N+]([O-])=O)NCC	6.7942596	0.218	0.161
99-59-2	Nc1cc(ccc1OC)[N+]([O-])=O	15.7194316	0.494	1.159
2122-86-3	O=C1NN=C(O1)c2oc(cc2)[N+]([O-])=O	17.1616511	1.360	1.321
2578-75-8	O=C(C)Nc1nnc(s1)c2ccc(o2)[N+]([O-])=O	19.6066702	1.459	1.594
53757-28-1	[O-][N+](=O)c1ccc(o1)c2cscn2	17.5109445	1.407	1.360
24554-26-5	O=CNc1nc(cs1)c2ccc(o2)[N+]([O-])=O	18.1182161	1.750	1.428
600-24-8	CC(CC)[N+]([O-])=O	10.7916363	-0.443	0.608
1836-75-5	Clc2cc(Cl)ccc2Oc1ccc(cc1)[N+]([O-])=O	5.0065304	-0.170	-0.038
607-57-8	[O-][N+](=O)C1C=CC2=C3C=CC=CC3=CC2=C1	33.1141590	2.870	3.104
75-52-5	[O-][N+](C)=O	19.9552121	0.179	1.633
38777-13-8	CC(C)Oc1ccccc1OC(=O)N(C)N=O	30.1163221	2.816	2.769
83335-32-4	FC(F)(F)CCCN(CCCC(F)(F)F)N=O	20.6003220	2.551	1.705
89911-78-4	O=NN(CCO)CC(O)CO	23.8214739	1.439	2.065
96806-35-8	O=C(NCCCl)N(N=O)CC(C)O	30.0147037	2.380	2.758
56222-35-6	CC(O)CN(CCO)N=O	22.4227138	1.181	1.909
760-60-1	CC(C)CN(N=O)C(=O)N	24.4205969	1.487	2.132
937-25-7	O=NN(C)c1ccc(F)cc1	31.5388819	2.781	2.928
75881-22-0	CN(CCCCCCCCCC)N=O	21.5702225	2.201	1.813
38347-74-9	O=C1OCCN1N=O	16.7506150	2.479	1.275
64005-62-5	O=NN(CCCCC)C(=O)OCC	29.8114261	2.270	2.735
1133-64-8	O=NN2CCCCC2c1cccnc1	25.2879439	1.206	2.229
51542-33-7	CN(N=O)C(=O)Nc1nc2ccccc2s1	28.6323803	2.320	2.603
60599-38-4	O=C(C)CN(CC(=O)C)N=O	28.7233886	2.508	2.613
62-75-9	CN(C)N=O	28.9349431	2.888	2.637
156-10-5	O=Nc2ccc(Nc1ccccc1)cc2	18.9993753	-0.006	1.526
10595-95-6	CCN(C)N=O	32.7168392	3.244	3.060
20917-49-1	O=NN1CCCCCCC1	23.6797366	3.575	2.049
42579-28-2	O=C1NC(=O)CN1N=O	19.2961524	0.469	1.559
86451-37-8	CN(N=O)CC(O)CO	21.1388672	2.317	1.765
26921-68-6	CN(N=O)CCO	25.9729565	1.907	2.306
70415-59-7	CN(N=O)CCCO	20.2587809	1.852	1.667
16219-98-0	O=NN(C)c1ccccn1	24.9818346	2.807	2.195
614-00-6	O=NN(C)c1ccccc1	26.3316239	2.982	2.346
59-89-2	O=NN1CCOCC1	21.4019649	3.028	1.795
26541-51-5	O=NN1CCSCC1	24.3742548	1.390	2.127
611-23-4	Cc1ccccc1N=O	10.7414983	0.378	0.603
303-47-9	O=C(O)C(Cc1ccccc1)NC(=O)c2cc(Cl)c3CC(C)OC(=O)c3c2O	27.3969214	3.593	2.465
3096-50-2	CC(=O)Nc2ccc3c1ccccc1C(=O)c3c2	9.8204373	1.585	0.500
60102-37-6	CN1CCC2OC(=O)C3(CC(C)C(C)(O)C(=O)OCC(=CC1)C2=O)OC3C	22.8541422	2.617	1.957
62-44-2	CCOc1ccc(cc1)NC(C)=O	6.9861875	-0.843	0.183
77-09-8	Oc1ccc(cc1)C3(OC(=O)c2ccccc23)c4ccc(O)cc4	6.3745131	-0.452	0.115
7227-91-0	CN(C)/N=N/c1ccccc1	15.5075709	1.810	1.136
90-43-7	Oc2ccccc2c1ccccc1	4.7845818	-0.134	-0.063
51-03-6	CCCc1cc2OCOc2cc1COCCOCCOCCCC	8.6169629	-0.272	0.365
29069-24-7	ClCCN(CCCl)c1ccc(cc1)CCCC(=O)OCC(=O)C5(O)CCC4C3CCC2=CC(=O)C=CC2(C)C3C(O)CC45C	26.4791878	1.527	2.362
50-24-8	OCC(=O)C4(O)CCC3C2CCC1=CC(=O)C=CC1(C)C2C(O)CC34C	24.1947047	2.372	2.107

Table 2. Cont.

671-16-9	CC(C)NC(=O)c1ccc(CNNC)cc1	15.0574555	1.742	1.085
1120-71-4	O=S1(=O)CCCO1	6.0564342	1.503	0.079
57-57-8	O=C1CCO1	10.5571479	1.693	0.582
13010-07-6	N/C(=N/[N+]([O-])=O)N(CCC)N=O	36.6885548	2.126	3.504
51-52-5	S=C1NC(CCC)=CC(=O)N1	10.2034731	1.094	0.543
2425-85-6	[O-][N+](=O)c3cc(C)ccc3N\N=C1\c2ccccc2C=CC1=O	-6.2022200	-0.581	-1.292
480-54-6	O=C1OCC3=CCN2CCC(OC(=O)C(/CC(C)C1(O)CO)=C\C)C23	4.9508078	-0.390	-0.045
94-59-7	C=CCc1ccc2OCOc2c1	5.7835004	-0.434	0.048
2318-18-5	O=C1OC2CCN(C)CC=C(COC(=O)C(C)(O)C(C)C\C1=C\C)C2=O	23.6803007	2.332	2.049
10048-13-2	Oc2cccc3Oc1c4C5C=COC5Oc4cc(OC)c1C(=O)c23	35.8981610	3.329	3.415
18883-66-4	OC1OC(CO)C(O)C(O)C1NC(=O)N(C)N=O	39.1285358	2.440	3.776
96-09-3	c1ccccc1C2CO2	7.7920177	0.336	0.273
95-06-7	C=C(Cl)CSC(=S)N(CC)CC	8.2349252	0.933	0.323
127-18-4	Cl/C(Cl)=C(\Cl)Cl	15.8707394	0.215	1.176
109-99-9	C1CCCO1	3.2078794	-0.752	-0.239
62-56-6	NC(N)=S	11.0889155	-0.112	0.642
88-19-7	Cc1ccccc1S(=O)(N)=O	-2.1709891	-1.364	-0.841
68-76-8	O=C1C=C(C(=O)C(=C1N2CC2)N3CC3)N4CC4	40.6549214	4.662	3.947
76-25-5	OCC(=O)C54OC(C)(C)OC5CC3C2CCC1=CC(=O)C=CC1(C)C2(F)C(O)CC34C	43.7916285	3.914	4.298
75-25-2	BrC(Br)Br	5.8279398	-0.409	0.053
51-79-6	NC(=O)OCC	5.1255209	0.334	-0.025
88-12-0	O=C1CCCN1C=C	16.7959985	0.967	1.280
	Calibration set			
18523-69-8	C\C(C)=N\Nc1ncc(s1)c2ccc(o2)[N+]([O-])=O	15.7962887	1.644	1.168
7008-42-6	CN3c2c(c(cc1OC(C)(C)C=Cc12)OC)C(=O)c4ccccc34	23.9804592	2.804	2.083
2835-39-4	CC(C)CC(=O)OCC=C	4.9735733	0.063	-0.042
760-56-5	NC(=O)N(CC=C)N=O	21.9012133	2.578	1.850
82-28-0	O=C3c1ccccc1C(=O)c2c3ccc(C)c2N	17.3450396	0.603	1.341
119-34-6	O=[N+]([O-])c1cc(N)ccc1O	9.7056304	-0.302	0.487
121-66-4	[O-][N+](=O)c1cnc(N)s1	10.4559636	0.513	0.571
97-56-3	Cc2cc(/N=N/c1ccccc1C)ccc2N	14.9214206	1.746	1.070
61-82-5	Nc1nncn1	8.4764466	0.927	0.350
115-02-6	N#[N+]\C=C(/[O-])OCC(N)C(=O)O	16.6905834	2.339	1.268
103-33-3	N(=N/c1ccccc1)\c2ccccc2	13.6683807	0.879	0.930
88133-11-3	Nc1nc(c(CCOCC)c2ncnn12)c3ccccc3	6.2415469	-0.286	0.100
271-89-6	c1cccc2occc12	7.3775200	-0.555	0.227
542-88-1	ClCOCCl	26.3207801	4.507	2.345
2475-45-8	Nc3ccc(N)c2C(=O)c1c(N)ccc(N)c1C(=O)c23	8.2016002	0.235	0.319
75-27-4	BrC(Cl)Cl	15.6604646	0.354	1.153
74-96-4	BrCC	7.1144910	-0.136	0.197
51333-22-3	OCC(=O)C53OC(OC5CC2C1CCC4=CC(=O)C=CC4(C)C1C(O)CC23C)CCC	24.6288783	3.170	2.155
106-99-0	C=CC=C	-2.4847352	-0.683	-0.876
75-65-0	CC(C)(C)O	-1.1616802	0.060	-0.728
60391-92-6	O=C(N)N(N=O)CC(=O)O	22.4120388	1.533	1.908
115-28-6	ClC2(Cl)C1(Cl)C(Cl)=C(Cl)C2(Cl)C(C1C(=O)O)C(=O)O	10.5026263	0.979	0.576
101-79-1	Clc2ccc(Oc1ccc(N)cc1)cc2	13.5687773	0.767	0.919
77439-76-0	ClC=1C(=O)OC(O)C=1C(Cl)Cl	24.3423352	2.572	2.123
5131-60-2	Nc1ccc(Cl)c(N)c1	5.3139941	-0.344	-0.004
593-70-4	ClCF	10.5959992	0.396	0.587
54749-90-5	OC1OC(CO)C(O)C(O)C1NC(=O)N(CCCl)N=O	31.9896113	3.923	2.978
52214-84-3	ClC2(Cl)CC2c1ccc(OC(C)(C)C(=O)O)cc1	20.0158390	2.123	1.640
637-07-0	Clc1ccc(OC(C)(C)C(=O)OCC)cc1	3.8349646	0.157	-0.169
123-73-9	C\C=C\C=O	4.9703123	1.222	-0.042

Table 2. Cont.

50-18-0	O=P1(NCCCO1)N(CCCl)CCCl	19.9930944	2.072	1.637
80-08-0	Nc1ccc(cc1)S(=O)(=O)c2ccc(N)cc2	10.1590864	1.045	0.538
50-29-3	Clc1ccc(cc1)C(c2ccc(Cl)cc2)C(Cl)(Cl)Cl	9.0943378	0.622	0.419
63019-65-8	CC(=O)N(C(C)=O)C2C=CC=C1c3ccccc3C=C12	20.4197854	1.145	1.685
95-80-7	Nc1cc(N)c(C)cc1	4.6373599	1.694	-0.080
56654-52-5	O=C(NCCCC)N(CCCC)N=O	21.9450360	1.672	1.855
1717-00-6	CC(Cl)(Cl)F	-3.0596285	-1.653	-0.940
91-94-1	Nc1ccc(cc1Cl)c2ccc(N)c(Cl)c2	13.5727307	0.955	0.919
107-06-2	ClCCCl	20.7099520	1.090	1.717
62-73-7	COP(=O)(OC)O\C=C(\Cl)Cl	22.6999204	1.725	1.940
685-91-6	CCN(CC)C(C)=O	12.0480263	1.115	0.749
111-46-6	OCCOCCO	-5.3166083	-1.194	-1.192
56-53-1	Oc1ccc(cc1)C(\CC)=C(\CC)c2ccc(O)cc2	20.1502302	3.080	1.655
119-84-6	O=C1CCc2ccccc2O1	-2.0947876	-1.302	-0.832
94-58-6	CCCc1ccc2OCOc2c1	7.0532301	0.060	0.190
5803-51-0	COc2ccc(cc2/C=C/c1ccc(N)cc1)OC	18.2640447	2.549	1.444
65176-75-2	COc5c(OC)cc(O)c2c5Oc1c3C4C=COC4Oc3cc(OC)c1C2=O	27.2013851	3.024	2.443
60-11-7	CN(C)c2ccc(/N=N/c1ccccc1)cc2	25.0188899	1.833	2.199
59-35-8	O=[N+]([O-])c1ccc(o1)c2nc(C)cc(C)n2	23.6523030	2.198	2.046
551-92-8	O=[N+]([O-])c1cnc(C)n1C	11.8799028	0.919	0.730
26049-69-4	CN(C)Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O	32.0887363	2.793	2.989
123-91-1	C1COCCO1	3.8263120	-0.481	-0.170
13256-06-9	CCCCCN(CCCCC)N=O	20.8293992	1.665	1.731
57-63-6	Oc3cc4CCC2C(CCC1(C)C2CCC1(O)C#C)c4cc3	23.6026061	3.171	2.041
140-88-5	C=CC(=O)OCC	-0.4544704	-0.075	-0.649
64-17-5	CCO	-2.0986452	-2.296	-0.833
57497-29-7	[O-]\[N+](CC)=N\C	35.5286934	3.669	3.374
100-41-4	CCc1ccccc1	-0.2763213	-1.612	-0.629
96-45-7	S=C1NCCN1	15.6987509	1.099	1.157
96724-44-6	O=NN(CC)C(=O)NCCO	24.0147978	2.490	2.087
38434-77-4	N#CN(CC)N=O	27.9326312	1.430	2.525
363-17-7	FC(F)(F)C(=O)NC1C=CC2=C3C=CC=CC3=CC2=C1	21.8934039	2.233	1.850
110-00-9	c1ccco1	11.1441338	2.235	0.648
67730-11-4	Cc1cccn2c3nc(N)ccc3nc12	17.7533734	1.626	1.387
556-52-5	OCC1CO1	8.2028179	1.238	0.319
517-28-2	Oc2cc3CC4(O)COc1c(O)c(O)ccc1C4c3cc2O	1.6535029	-0.520	-0.413
118-74-1	Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	18.0729350	1.868	1.422
87-68-3	Cl/C(Cl)=C(/Cl)\C(\Cl)=C(/Cl)Cl	5.0800268	0.598	-0.030
680-31-9	CN(C)P(=O)(N(C)C)N(C)C	24.8394682	3.717	2.179
26049-68-3	NNc1nc(cs1)c2oc(cc2)[N+]([O-])=O	20.4685616	1.851	1.690
306-83-2	ClC(Cl)C(F)(F)F	5.3073777	-1.190	-0.005
13743-07-2	NC(=O)N(N=O)CCO	22.3036387	2.737	1.895
33389-36-5	O=[N+]([O-])c1ccc(s1)c2nc(NCCO)c3ccccc3n2	20.5124644	2.228	1.695
5208-87-7	C=CC(O)c1ccc2OCOc2c1	5.6164087	0.986	0.030
84545-30-2	FC(F)(F)C\N=C(/N)Nc1ccn(CCCCC(N)=O)n1	-1.1528528	-0.582	-0.727
53-86-1	Clc1ccc(cc1)C(=O)n3c2ccc(cc2c(CC(=O)O)c3C)OC	20.8646978	2.493	1.735
15503-86-3	[O-][N+]13CC=C2COC(=O)[C@@](O)(CO)[C@H](C)C/C(=C\C)C(=O)OC(CC1)C23	23.0174870	2.710	1.975
86315-52-8	CS(=O)c3ccc(c1nc2cnccc2n1)c(OC)c3	12.4221377	0.610	0.791
54-85-3	O=C(NN)c1ccncc1	6.9743574	-0.039	0.182
78-59-1	O=C1C=C(C)CC(C)(C)C1	7.5076649	-0.942	0.241
3778-73-2	O=P1(NCCCl)OCCCN1CCCl	22.8638696	2.548	1.958
143-50-0	O=C2C1(Cl)C3(Cl)C5(Cl)C1(Cl)C4(Cl)C2(Cl)C3(Cl)C4(Cl)C5(Cl)Cl	20.4516977	2.219	1.688
5989-27-5	CC1=CCC(CC1)C(C)=C	4.0566866	-0.175	-0.145
108-78-1	Nc1nc(N)nc(N)n1	3.6878686	-0.765	-0.186

Table 2. Cont.

57-39-6	CC1CN1P(=O)(N2CC2C)N3CC3C	27.2097154	1.684	2.444
60-56-0	S=C1NC=CN1C	14.2653106	2.001	0.997
150-76-5	Oc1ccc(OC)cc1	0.9123388	-0.724	-0.496
1634-04-4	CC(C)(C)OC	5.6530612	-0.901	0.034
21340-68-1	Clc1ccc(cc1)c2ccc(OC(C)(C)C(=O)OC)cc2	17.6806284	1.805	1.379
70-25-7	O=[N+]([O-])\N=C(\N)N(C)N=O	28.6725181	2.263	2.607
63642-17-1	NC(CCCNC(=O)N(C)N=O)C(=O)O	28.8570438	2.443	2.628
98-85-1	CC(O)c1ccccc1	-0.4434130	-0.574	-0.648
452-86-8	Cc1cc(O)c(O)cc1	0.8376489	-0.301	-0.504
56-49-5	Cc2ccc3cc1c5ccccc5ccc1c4CCc2c34	28.4179889	2.738	2.579
101-14-4	Nc2ccc(Cc1ccc(N)c(Cl)c1)cc2Cl	10.3247375	1.141	0.556
838-88-0	Cc2cc(Cc1ccc(N)c(C)c1)ccc2N	14.6440072	1.487	1.039
101-61-1	CN(C)c2ccc(Cc1ccc(cc1)N(C)C)cc2	19.3590719	1.191	1.566
76014-81-8	OC(CCCN(C)N=O)c1cccnc1	30.8490216	3.308	2.851
64091-91-4	O=C(CCCN(C)N=O)c1cccnc1	29.2949689	3.317	2.677
2385-85-5	ClC53C1(Cl)C4(Cl)C2(Cl)C1(Cl)C(Cl)(Cl)C5(Cl)C2(Cl)C3(Cl)C4(Cl)Cl	27.1109046	2.489	2.433
315-22-0	O=C1OCC3=CCN2CCC(OC(=O)C(C)C(C)(O)C1(C)O)C23	26.1356689	2.539	2.324
58139-48-3	O=[N+]([O-])c1ccc(s1)c3nc(N2CCOCC2)c4ccccc4n3	22.4025459	1.833	1.907
389-08-2	O=C(O)C2=CN(CC)c1nc(C)ccc1C2=O	2.9489805	0.063	-0.268
91-59-8	Nc1ccc2ccccc2c1	4.7774007	0.366	-0.064
139-13-9	OC(=O)CN(CC(=O)O)CC(=O)O	1.4031307	-0.967	-0.441
59-87-0	O=[N+]([O-])c1ccc(/C=N/NC(N)=O)o1	15.4159812	1.453	1.125
75198-31-1	O=[N+]([O-])c1ccc(o1)c2cnc3ccccn23	16.2049151	1.227	1.214
36133-88-7	[O-][N+](=O)c1ccc(o1)c2nc(CNC(C)=O)on2	12.4300126	0.627	0.792
4812-22-0	CC\C=C(/CC)[N+]([O-])=O	13.7273230	1.174	0.937
602-87-9	[O-][N+](=O)c1ccc2CCc3cccc1c23	9.4562186	1.361	0.459
91-23-6	COc1ccccc1[N+]([O-])=O	-2.4235018	0.992	-0.869
98-95-3	[O-][N+](=O)c1ccccc1	11.5415934	0.684	0.692
67-20-9	O=[N+]([O-])c2ccc(/C=N/N1CC(=O)NC1=O)o2	9.0897766	0.165	0.418
555-84-0	O=[N+]([O-])c2ccc(/C=N/N1CCNC1=O)o2	11.4825719	1.630	0.686
51-75-2	ClCCN(C)CCCl	30.5203075	4.137	2.814
551-88-2	CCC(CC)[N+]([O-])=O	12.8577847	0.694	0.839
607-35-2	[O-][N+](=O)c1cccc2cccnc12	12.5000850	1.249	0.799
16813-36-8	O=C1NC(=O)N(N=O)CC1	21.4966956	3.163	1.805
89911-79-5	O=NN(CC(C)O)CC(O)CO	26.1835997	3.523	2.329
92177-50-9	OC(CNCC(C)=O)C(O)N=O	22.4907916	3.699	1.916
96806-34-7	O=C(NCCCl)N(N=O)CCO	28.0419947	2.740	2.537
55090-44-3	CN(CCCCCCCCCCCC)N=O	20.6335287	2.629	1.709
13256-11-6	CN(CCc1ccccc1)N=O	26.1136794	4.216	2.321
684-93-5	NC(=O)N(C)N=O	25.2656253	3.046	2.227
92177-49-6	O=C(N=O)CCNCCO	15.4212329	1.910	1.126
55556-92-8	O=NN1CC=CCC1	21.4577569	3.271	1.801
82018-90-4	FC(F)(F)CN(CC)N=O	20.7170961	1.792	1.718
75881-18-4	CC1CN(N=O)CC(C)N1C	39.3778121	3.018	3.804
91308-70-2	CC(O)CN(CC=C)N=O	26.6342790	2.216	2.380
91308-69-9	C=CCN(N=O)CCO	19.8460294	2.423	1.621
1116-54-7	OCCN(N=O)CCO	16.1731320	1.627	1.210
55-18-5	CCN(CC)N=O	25.0720908	3.586	2.205
621-64-7	CCCN(CCC)N=O	28.5592505	2.845	2.595
55984-51-5	CC(=O)CN(C)N=O	26.5154639	3.829	2.366
68107-26-6	CN(CCCCCCCCCCC)N=O	21.1018756	1.956	1.761
78246-24-9	O=NN2CCCC2c1c[n+]([O-])ccc1	21.5748823	2.344	1.814
5632-47-3	O=NN1CCNCC1	22.9448185	1.118	1.967
14698-29-4	O=C(O)C2=CN(CC)c1cc3OCOc3cc1C2=O	7.1612743	0.194	0.203
101-80-4	Nc1ccc(cc1)Oc2ccc(N)cc2	16.4624683	1.323	1.242
13752-51-7	S=C(SN1CCOCC1)N2CCOCC2	11.7032524	0.437	0.710

Table 2. Cont.

1825-21-4	Clc1c(OC)c(Cl)c(Cl)c(Cl)c1Cl	16.7076547	1.053	1.270
842-07-9	O=C3C=Cc1ccccc1/C3=N\Nc2ccccc2	8.1054887	0.927	0.308
50-33-9	O=C3C(CCCC)C(=O)N(c1ccccc1)N3c2ccccc2	3.0841934	-0.575	-0.253
122-60-1	c2ccc(OCC1CO1)cc2	5.8485539	0.533	0.056
1955-45-9	O=C1OCC1(C)C	4.2138276	-0.324	-0.127
816-57-9	NC(=O)N(CCC)N=O	22.6119432	1.541	1.930
81-54-9	O=C2c1ccccc1C(=O)c3c2c(O)cc(O)c3O	11.7313515	-0.423	0.713
127-47-9	CC=1CCCC(C)(C)C=1/C=CC(\C)=C\C=C\C(\C)=C\CO C(C)=O	12.3716885	0.420	0.785
18559-94-9	OCc1cc(ccc1O)C(O)CNC(C)(C)C	3.2247443	0.777	-0.238
599-79-1	O=S(=O)(Nc1ccccn1)c3ccc(N\N=C2/C=CC(=O)C(=C2) C(=O)O)cc3	2.6830187	-0.601	-0.298
533-31-3	Oc1ccc2OCOc2c1	5.4856314	-0.990	0.015
77-46-3	O=S(=O)(c1ccc(NC(C)=O)cc1)c2ccc(NC(C)=O)cc2	14.4156550	0.777	1.014
23031-25-6	Oc1cc(cc(O)c1)C(O)CNC(C)(C)C	6.0019117	-0.260	0.073
116-14-3	F/C(F)=C(\F)F	2.7326963	-0.029	-0.293
40548-68-3	O=NN1CCCCO1	18.8342347	0.679	1.508
509-14-8	O=[N+]([O-])C([N+]([O-])=O)([N+](=O)[O-])[N+]([O-])=O	19.9621805	2.642	1.634
52-24-4	S=P(N1CC1)(N2CC2)N3CC3	28.4599896	3.062	2.584
62-55-5	CC(N)=S	8.4251325	0.815	0.344
789-61-7	NC=3Nc2c(ncn2C1CC(O)C(CO)O1)C(=S)N=3	25.3320122	2.130	2.234
141-90-2	O=C1C=CNC(=S)N1	17.6865810	1.032	1.379
137-17-7	Cc1cc(C)c(N)cc1C	0.3523384	0.605	-0.559
95-63-6	Cc1cc(C)c(C)cc1	3.1538748	-1.559	-0.245
55-63-0	O=[N+]([O-])OC(CO[N+]([O-])=O)CO[N+](=O)[O-]	8.5730907	0.094	0.360
126-72-7	BrCC(Br)COP(=O)(OCC(Br)CBr)OCC(Br)CBr	21.6072056	2.260	1.818
108-05-4	CC(=O)OC=C	0.4943662	-0.598	-0.543
75-02-5	C=CF	-0.6009610	0.362	-0.665
2832-40-8	O=C2C=CC(C)=C\C2=N\Nc1ccc(NC(C)=O)cc1	5.1582118	-0.149	-0.021
	Test set			
29611-03-8	O=C2Oc1c4C5C=COC5Oc4cc(OC)c1C=3CCC(O)C2=3	37.2419668	5.102	3.566
1162-65-8	O=C2Oc1c4C5C=COC5Oc4cc(OC)c1C=3CCC(=O)C2 =3	37.9690087	4.991	3.647
57-06-7	C=CC\N=C=S	0.5282930	0.014	-0.539
38514-71-5	Nc1nc(cs1)c2oc(cc2)[N+]([O-])=O	16.1535617	1.558	1.208
140-57-8	CC(C)(C)c1ccc(OCC(C)OS(=O)OCCCl)cc1	6.9764303	0.539	0.182
1912-24-9	Clc1nc(NCC)nc(NC(C)C)n1	11.2226837	0.833	0.657
25843-45-2	[O-]\[N+](C)=N\C	32.4681999	3.201	3.032
33372-39-3	O=[N+]([O-])c1ccc(s1)c2nc(N(CCO)CCO)c3ccccc3n2	22.0260018	2.060	1.864
2784-94-3	CNc1ccc(cc1[N+]([O-])=O)N(CCO)CCO	-0.0656579	-0.439	-0.605
869-01-2	O=C(N)N(CCCC)N=O	25.3510763	2.448	2.236
120-80-9	Oc1ccccc1O	-0.0151194	0.114	-0.600
95-83-0	Nc1cc(Cl)ccc1N	8.8914505	-0.176	0.396
10473-70-8	Clc1ccc(NC(=O)N(C)C)cc1	7.6668178	1.512	0.259
117-10-2	Oc3cccc2C(=O)c1cccc(O)c1C(=O)c23	2.2118706	-0.009	-0.351
1192-28-5	O\N=C1\CCCC1	5.4517784	0.385	0.011
53-43-0	O=C2CCC1C3CC=C4CC(O)CCC4(C)C3CCC12C	13.1419721	0.538	0.871
79-43-6	ClC(Cl)C(=O)O	6.7872450	-0.096	0.161
101-90-6	c1ccc(cc1OCC2CO2)OCC3CO3	17.1281712	1.769	1.317
55738-54-0	CN(C)CNc2nnc(/C=C/c1ccc(o1)[N+]([O-])=O)o2	9.7862431	1.096	0.496
121-69-7	CN(C)c1ccccc1	8.7503763	-0.013	0.380
106-88-7	CCC1CO1	5.3651210	-0.484	0.002
13073-35-3	OC(=O)C(N)CCSCC	15.6037032	1.517	1.146
398-32-3	O=C(C)Nc1ccc(cc1)c2ccc(F)cc2	22.0327470	2.356	1.865
32852-21-4	O=CNNc1nc(C)cs1	6.1212428	1.038	0.086
3570-75-0	O=CNNc1nc(cs1)c2ccc(o2)[N+]([O-])=O	22.4332160	1.701	1.910
67730-10-3	Nc1ccc2nc3ccccn3c2n1	13.0355578	0.639	0.859

Table 2. Cont.

26049-71-8	NNc1nc(cs1)c2ccc(N)cc2	16.3483477	2.302	1.230
21416-87-5	O=C2CN(CC(C)N1CC(=O)NC(=O)C1)CC(=O)N2	10.5466160	1.399	0.581
77500-04-0	Cc1nc3c(nc1)ccc2c3nc(N)n2C	23.2794448	2.109	2.005
55-80-1	CN(C)c2ccc(/N=N/c1cc(C)ccc1)cc2	27.2082826	1.863	2.444
129-15-7	[O-][N+](=O)c3c(C)ccc2C(=O)c1ccccc1C(=O)c23	11.1318117	0.499	0.646
14026-03-0	CC1CCCCN1N=O	22.1230424	0.987	1.875
90-94-8	CN(C)c1ccc(cc1)C(=O)c2ccc(cc2)N(C)C	15.4754897	1.677	1.132
531-82-8	O=C(C)Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O	22.4493722	1.153	1.912
51325-35-0	O=[N+]([O-])c1ccc(o1)c2nc(NC(C)=O)nc(NC(C)=O)n2	18.7810092	1.337	1.502
62-23-7	O=[N+]([O-])c1ccc(cc1)C(=O)O	11.6562372	-0.235	0.705
5522-43-0	[O-][N+](=O)c4ccc1ccc2cccc3ccc4c1c23	14.2090349	1.871	0.990
75896-33-2	OC1CCN(N=O)C1	27.8276236	2.162	2.513
75881-20-8	CN(CCCCCCCCCCCCCC)N=O	19.6968349	2.192	1.604
88208-16-6	O=NN(CC=C)CC(O)CO	24.1429095	2.288	2.101
91308-71-3	C=CCN(CC(=O)C)N=O	29.3465230	2.628	2.683
53609-64-6	CC(O)CN(CC(C)O)N=O	24.7848396	2.283	2.173
924-16-3	CCCCN(CCCC)N=O	30.8956853	2.360	2.856
40580-89-0	O=NN1CCCCCCCCCCC1	15.8409546	1.290	1.173
614-95-9	O=NN(CC)C(=O)OCC	26.0539800	3.209	2.315
100-75-4	O=NN1CCCCC1	23.0864884	1.902	1.983
930-55-2	O=NN1CCCC1	21.0203400	2.098	1.752
81795-07-5	CC1SC(C)SC(C)N1N=O	22.5025937	2.600	1.918
60-80-0	O=C2C=C(C)N(C)N2c1ccccc1	13.3054506	-0.815	0.889
75-56-9	CC1CO1	11.0792966	-0.107	0.641
22571-95-5	CC(C)C(O)(C(C)O)C(=O)OCC1=CCN2CCC(OC(=O)C(\C)=C\C)C12	23.3746230	2.300	2.015
811-97-2	FCC(F)(F)F	-4.6111637	-2.467	-1.114
139-65-1	Nc1ccc(cc1)Sc2ccc(N)cc2	10.6556332	1.766	0.593
538-23-8	O=C(CCCCCCC)OC(COC(=O)CCCCCCC)COC(=O)CCCCCC	-6.8111993	-1.067	-1.360
88-06-2	Clc1cc(Cl)cc(Cl)c1O	4.0429184	-0.312	-0.146
96-18-4	ClCC(Cl)CCl	22.1125091	2.038	1.874
42011-48-3	O=C(Nc1nc(cs1)c2ccc(o2)[N+]([O-])=O)C(F)(F)F	13.7807006	1.656	0.943
2489-77-2	CN(C)C(=S)NC	21.0749620	0.661	1.758
66-22-8	O=C1C=CNC(=O)N1	7.6978985	-0.777	0.263
593-60-2	BrC=C	6.2037631	0.762	0.095
75-01-4	C=CCl	15.1872444	1.010	1.100