

Plant halides as potential norovirus 3CLpro inhibitors: An *in silico* approach

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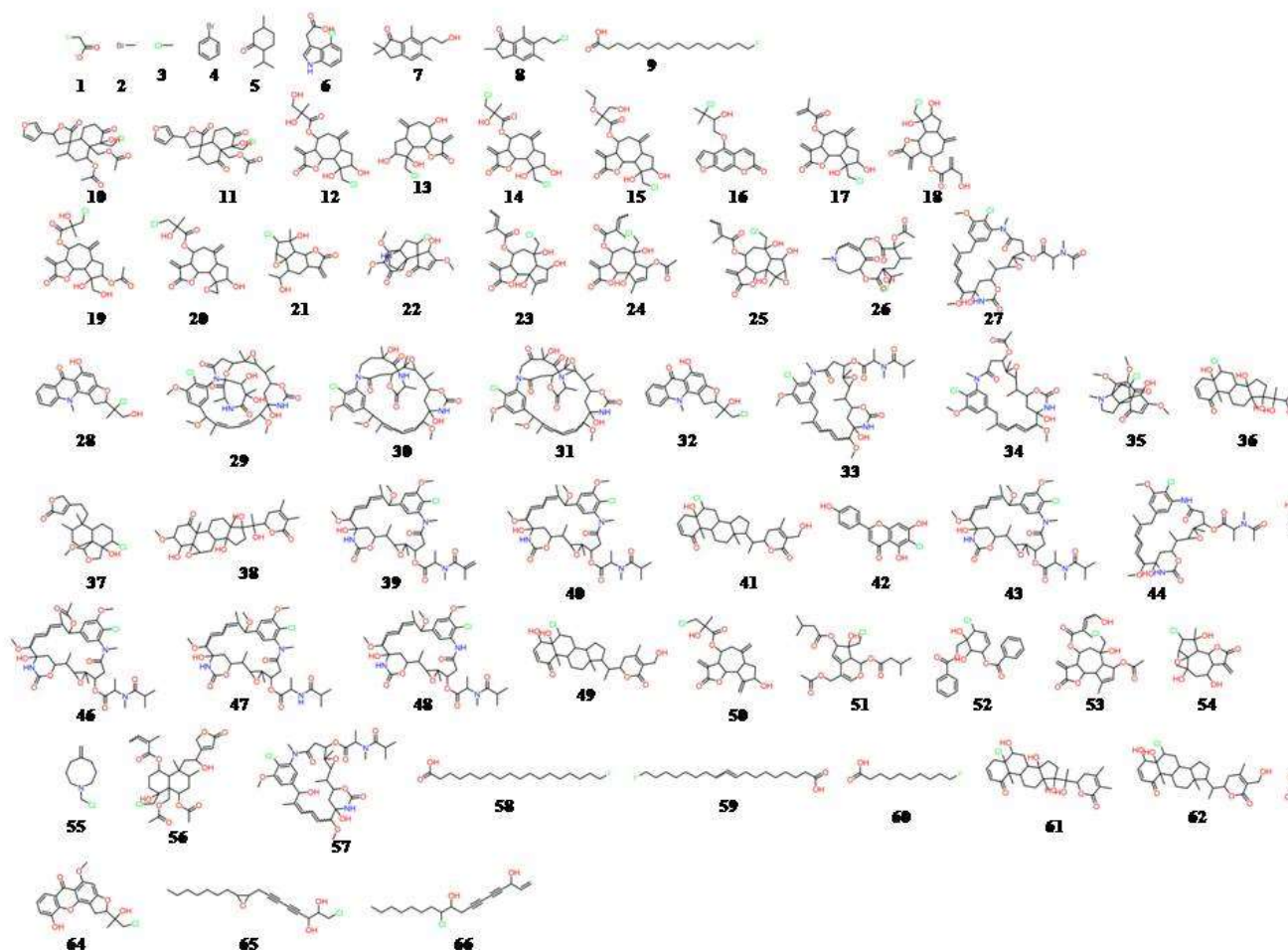


Fig. S1 — Molecular structure of halide metabolites investigated

Table S1 — ADME analysis of halide metabolites from higher plants

Molecule	Pubchem ID	Formula	MW	Heavy atoms	Aromatic heavy atoms	Fraction Csp3	Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA	iLOGP	XLOGP3	WLOGP	MLOGP
1	5236	C2H2FO2-	77.03	5	0	0.5	1	3	0	11.61	40.13	0.45	0.17	-0.87	-0.22
2	6323	CH3Br	94.94	2	0	1	0	0	0	14.79	0	1.4	0.99	1.01	1.11
3	6327	CH3Cl	50.49	2	0	1	0	0	0	11.72	0	1.21	0.82	0.85	0.84
4	7961	C6H5Br	157.01	7	6	0	0	0	0	34.14	0	1.99	2.99	2.45	3.05
5	26447	C10H18O	154.25	11	0	0.9	1	1	0	48.27	17.07	2.4	3.05	2.65	2.3
6	100413	C10H8ClNO2	209.63	14	9	0.1	2	2	2	54.85	53.09	1.29	2.14	2.45	1.67
7	134977	C15H20O2	232.32	17	6	0.53	2	2	1	69.71	37.3	2.5	2.9	2.6	2.45
8	134978	C14H17ClO	236.74	16	6	0.5	2	1	0	68.8	17.07	2.83	3.82	3.46	3.37
9	151081	C16H31FO2	274.41	19	0	0.94	15	3	1	80.85	37.3	3.73	6.63	5.92	4.32
10	158054	C24H29ClO9	496.93	34	5	0.67	7	9	1	118.2	129.34	2.56	1.45	2.4	1.2
11	158055	C22H25ClO8	452.88	31	5	0.64	5	8	1	107.5	120.11	2.07	0.56	2.04	0.75
12	162745	C19H25ClO8	416.85	28	0	0.68	5	8	4	98.25	133.52	1.91	-0.43	-0.33	0.3
13	170025	C15H19ClO5	314.76	21	0	0.67	1	5	3	76.53	86.99	1.59	0.11	0.37	1.04
14	171332	C21H29ClO8	444.9	30	0	0.71	7	8	3	107.78	122.52	2.76	0.47	0.71	0.74
15	171332	C21H29ClO8	444.9	30	0	0.71	7	8	3	107.78	122.52	2.76	0.47	0.71	0.74
16	182277	C16H15ClO5	322.74	22	13	0.31	4	5	1	83.97	72.81	2.8	2.52	3.3	1.63
17	182337	C19H23ClO6	382.84	26	0	0.58	4	6	2	95.41	93.06	2.9	1.65	1.5	1.8
18	182408	C19H23ClO7	398.83	27	0	0.58	5	7	3	96.57	113.29	2.29	0.4	0.47	1
19	327916	C21H27ClO9	458.89	31	0	0.67	7	9	3	107.98	139.59	2.64	0.14	0.24	0.69
20	442140	C19H23ClO7	398.83	27	0	0.68	4	7	2	94.89	105.59	2.18	0.56	0.71	1.09
21	442178	C15H19ClO5	314.76	21	0	0.8	1	5	2	74.85	79.29	2.2	0.58	0.61	1.13
22	442840	C18H22ClNO6	383.82	26	0	0.67	3	7	2	95.08	94.09	2.32	-0.84	0.27	-0.76
23	5281446	C20H25ClO7	412.86	28	0	0.6	4	7	3	101.42	113.29	2.45	0.85	1	1.22
24	5281447	C22H27ClO8	454.9	31	0	0.59	6	8	2	111.15	119.36	2.79	1.42	1.57	1.6
25	5281448	C20H25ClO8	428.86	29	0	0.7	4	8	3	100.9	125.82	1.95	0.24	0.22	0.52
26	5281726	C21H30ClNO8	459.92	31	0	0.71	3	9	1	115.26	119.44	3.18	1.49	0.61	0.69
27	5281828	C34H46ClN3O10	692.2	48	6	0.59	7	10	2	184.51	156.47	4.14	1.99	2.77	1.1
28	5315835	C19H18ClNO4	359.8	25	14	0.32	2	4	2	98.76	71.69	2.68	3.54	2.69	1.75
29	5477487	C36H48ClN3O13	766.23	53	6	0.61	3	13	5	199.28	214.95	2.68	3.54	0.35	1.75
30	5477698	C36H48ClN3O12	750.23	52	6	0.61	3	12	4	198.12	194.72	5.12	1.84	1.38	-0.02
31	5477781	C37H48ClN3O13	778.24	54	6	0.59	3	13	3	203.22	203	3.71	1.71	0.9	-0.66
32	5486900	C19H18ClNO4	359.8	25	14	0.32	2	4	2	98.76	71.69	2.69	3.54	2.69	1.75
33	6438456	C36H50ClN3O10	720.25	50	6	0.61	8	10	2	194.12	156.47	4.31	3.03	3.41	1.46
34	6443032	C30H39ClN2O9	607.09	42	6	0.57	4	9	2	162.19	136.16	3.29	2.06	2.93	1.54
35	10200848	C19H24ClNO6	397.85	27	0	0.68	3	7	1	99.98	85.3	2.89	-0.38	0.61	-0.54
36	13743195	C28H39ClO7	523.06	36	0	0.79	2	7	4	135.75	124.29	3.27	2.03	2.96	2.15
37	15560290	C21H31ClO5	398.92	27	0	0.86	4	5	1	103.06	64.99	3.32	3.05	3.42	2.92
38	21607601	C29H42O9	534.64	38	0	0.86	3	9	4	136.29	146.05	3.47	0.19	1.57	0.67
39	21638448	C37H50ClN3O11	748.26	52	6	0.57	9	11	2	199.54	165.7	3.9	2.38	3.15	0.81
40	21638449	C37H52ClN3O11	750.28	52	6	0.62	9	11	2	200.02	165.7	4.65	2.46	3.23	0.89
41	23266165	C28H39ClO5	491.06	34	0	0.79	3	5	2	133.31	83.83	3.52	5.22	4.58	3.76

42	23266570	C15H9ClO5	304.68	21	16	0	1	5	3	79	90.9	2.2	3.65	3.23	1.04
43	44559316	C37H52ClN3O11	750.28	52	6	0.62	9	11	2	200.02	165.7	4.65	2.46	3.23	0.89
44	44593346	C33H44ClN3O10	678.17	47	6	0.58	7	10	3	179.61	165.26	4.17	1.81	2.56	0.92
45	53463094	C28H37ClO7	521.04	36	0	0.71	2	7	4	135.24	124.29	3.14	1.41	2.73	2.06
46	54600377	C38H52ClN3O12	778.29	54	6	0.61	10	12	2	205.02	182.77	3.48	2.49	3.15	1.06
47	54611079	C36H50ClN3O11	736.25	51	6	0.61	9	11	3	195.11	174.49	3.95	2.27	2.89	0.71
48	54612244	C36H50ClN3O11	736.25	51	6	0.61	9	11	3	195.11	174.49	4.42	2.27	3.01	0.71
49	70686220	C28H39ClO6	507.06	35	0	0.79	3	6	3	134.48	104.06	3.34	4.11	3.55	2.95
50	71439502	C19H23ClO6	382.84	26	0	0.58	4	6	2	95.41	93.06	2.67	1.08	1.5	1.8
51	71522011	C22H31ClO8	458.93	31	0	0.68	12	8	1	113.63	108.36	4.01	2.04	2.86	2.09
52	100854335	C21H19ClO6	402.82	28	12	0.24	7	6	2	101.93	93.06	2.77	2.79	2.34	2.46
53	101277293	C22H27ClO8	454.9	31	0	0.59	7	8	2	111.12	119.36	2.68	1.01	1.43	1.6
54	101600034	C15H19ClO6	330.76	22	0	0.8	0	6	3	76.05	99.52	1.79	-0.48	-0.27	0.32
55	101625140	C9H16ClN	173.68	11	0	0.78	1	1	0	54.4	3.24	2.6	2.43	2.23	2.3
56	102004685	C29H41ClO10	585.08	40	0	0.72	12	10	2	146	145.66	2.67	2.5	3.01	2.27
57	102239700	C36H50ClN3O11	736.25	51	6	0.61	8	11	3	195.29	176.7	4.06	1.92	2.58	0.71
58	9858	C18H35FO2	302.47	21	0	0.94	17	3	1	90.46	37.3	4.07	7.69	6.7	4.79
59	5312955	C18H33FO2	300.45	21	0	0.83	16	3	1	89.99	37.3	4.03	7.1	6.48	4.68
60	9542	C10H19FO2	190.26	13	0	0.9	9	3	1	52.01	37.3	2.36	3.57	3.58	2.73
61	101559583	C28H39ClO7	523.06	36	0	0.79	2	7	4	135.75	124.29	4.01	2.03	2.96	2.15
62	70686220	C28H39ClO6	507.06	35	0	0.79	3	6	3	134.48	104.06	3.34	4.11	3.55	2.95
63	155551	C28H31ClO10	562.99	39	0	0.79	0	10	2	131.25	145.66	2.47	0.43	0.97	0.95
64	126454	C19H17ClO6	376.79	26	14	0.32	3	6	2	98.27	89.13	2.72	2.81	2.95	1.2
65	130756	C17H25ClO3	312.83	21	0	0.76	9	3	2	86.25	52.99	3.66	3.64	2.63	2.48
66	130664	C17H25ClO2	296.83	20	0	0.65	9	2	2	86.8	40.46	3.96	4.76	3.42	3.66

Molecule	Silicos-IT Log P	Consensus Log P	ESOL Log S (mg/ml)	ESOL Solubility (mol/l)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silico-s-IT LogS	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class	GI absorption
1	0.09	-0.08	-0.36	33.70	0.44	Very soluble	-0.57	20.70	0.27	Very soluble	0.19	118.00	1.53	Soluble	High
2	0.67	1.04	-1.05	8.42	0.09	Very soluble	-0.58	25.10	0.26	Very soluble	-1.03	8.84	0.09	Soluble	Low
3	0.63	0.87	-0.67	10.80	0.21	Very soluble	-0.4	20.00	0.40	Very soluble	-0.68	10.70	0.21	Soluble	Low
4	2.65	2.63	-3.33	0.07	0.00	Soluble	-2.65	0.35	0.00	Soluble	-3.23	0.09	0.00	Soluble	Low
5	2.64	2.61	-2.65	0.34	0.00	Soluble	-3.07	0.13	0.00	Soluble	-2.17	1.05	0.01	Soluble	High
6	2.84	2.08	-2.83	0.31	0.00	Soluble	-2.89	0.27	0.00	Soluble	-3.68	0.04	0.00	Soluble	High
7	4.48	2.99	-3.24	0.14	0.00	Soluble	-3.34	0.11	0.00	Soluble	-4.9	0.00	0.00	Moderately soluble	High
8	5.11	3.72	-3.86	0.03	0.00	Soluble	-3.87	0.03	0.00	Soluble	-5.48	0.00	0.00	Moderately soluble	High
9	5.59	5.24	-4.73	0.01	0.00	Moderately soluble	-7.21	0.00	0.00	Poorly soluble	-5.6	0.00	0.00	Moderately soluble	High
10	3.36	2.19	-3.48	0.16	0.00	Soluble	-3.77	0.08	0.00	Soluble	-5	0.01	0.00	Moderately soluble	High
11	3.44	1.77	-2.79	0.73	0.00	Soluble	-2.65	1.00	0.00	Soluble	-5.08	0.00	0.00	Moderately soluble	High

12	1.07	0.5	-1.82	6.26	0.02	Very soluble	-1.91	5.14	0.01	Very soluble	-1.37	17.70	0.04	Soluble	High
13	1.33	0.89	-1.79	5.05	0.02	Very soluble	-1.49	10.10	0.03	Very soluble	-1.49	10.10	0.03	Soluble	High
14	2.03	1.34	-2.43	1.64	0.00	Soluble	-2.61	1.09	0.00	Soluble	-2.45	1.56	0.00	Soluble	High
15	2.03	1.34	-2.43	1.64	0.00	Soluble	-2.61	1.09	0.00	Soluble	-2.45	1.56	0.00	Soluble	High
16	3.73	2.79	-3.6	0.08	0.00	Soluble	-3.7	0.07	0.00	Soluble	-5.54	0.00	0.00	Moderately soluble	High
17	2.42	2.05	-2.99	0.39	0.00	Soluble	-3.22	0.23	0.00	Soluble	-2.54	1.09	0.00	Soluble	High
18	1.83	1.2	-2.23	2.32	0.01	Soluble	-2.35	1.80	0.00	Soluble	-1.97	4.23	0.01	Soluble	High
19	1.6	1.06	-2.31	2.24	0.00	Soluble	-2.63	1.08	0.00	Soluble	-1.98	4.77	0.01	Soluble	High
20	2.14	1.34	-2.4	1.58	0.00	Soluble	-2.35	1.78	0.00	Soluble	-2.15	2.85	0.01	Soluble	High
21	1.77	1.26	-2.09	2.55	0.01	Soluble	-1.82	4.78	0.02	Very soluble	-1.54	9.02	0.03	Soluble	High
22	1.77	0.55	-1.49	12.30	0.03	Very soluble	-0.66	84.90	0.22	Very soluble	-3.45	0.14	0.00	Soluble	High
23	1.89	1.48	-2.67	0.88	0.00	Soluble	-2.81	0.64	0.00	Soluble	-1.95	4.68	0.01	Soluble	High
24	2.41	1.96	-3.16	0.32	0.00	Soluble	-3.53	0.13	0.00	Soluble	-2.56	1.26	0.00	Soluble	High
25	1.75	0.94	-2.39	1.76	0.00	Soluble	-2.44	1.55	0.00	Soluble	-1.67	9.13	0.02	Soluble	High
26	1.91	1.58	-3.43	0.17	0.00	Soluble	-3.61	0.11	0.00	Soluble	-3.1	0.36	0.00	Soluble	High
27	2.22	2.44	-5.02	0.01	0.00	Moderately soluble	-4.9	0.01	0.00	Moderately soluble	-5.19	0.00	0.00	Moderately soluble	Low
28	3.45	2.82	-4.58	0.01	0.00	Moderately soluble	-4.73	0.01	0.00	Moderately soluble	-5.17	0.00	0.00	Moderately soluble	High
29	3.45	2.82	-4.58	0.01	0.00	Moderately soluble	-4.73	0.01	0.00	Moderately soluble	-5.17	0.00	0.00	Moderately soluble	High
30	1.33	1.93	-5.54	0.00	0.00	Moderately soluble	-5.55	0.00	0.00	Moderately soluble	-5.62	0.00	0.00	Moderately soluble	Low
31	1.01	1.33	-5.63	0.00	0.00	Moderately soluble	-5.59	0.00	0.00	Moderately soluble	-5.14	0.01	0.00	Moderately soluble	Low
32	3.45	2.82	-4.58	0.01	0.00	Moderately soluble	-4.73	0.01	0.00	Moderately soluble	-5.17	0.00	0.00	Moderately soluble	High
33	2.89	3.02	-5.78	0.00	0.00	Moderately soluble	-5.98	0.00	0.00	Moderately soluble	-5.59	0.00	0.00	Moderately soluble	Low
34	2.4	2.44	-4.74	0.01	0.00	Moderately soluble	-4.55	0.02	0.00	Moderately soluble	-5.21	0.00	0.00	Moderately soluble	Low
35	1.72	0.86	-1.87	5.38	0.01	Very soluble	-0.95	44.80	0.11	Very soluble	-3.11	0.31	0.00	Soluble	High
36	3.58	2.8	-4.23	0.03	0.00	Moderately soluble	-4.27	0.03	0.00	Moderately soluble	-4.12	0.04	0.00	Moderately soluble	High
37	3.8	3.3	-3.97	0.04	0.00	Soluble	-4.08	0.03	0.00	Moderately soluble	-4.16	0.03	0.00	Moderately soluble	High
38	2.86	1.75	-3.08	0.45	0.00	Soluble	-2.82	0.82	0.00	Soluble	-3.36	0.23	0.00	Soluble	Low
39	2.59	2.57	-5.47	0.00	0.00	Moderately soluble	-5.5	0.00	0.00	Moderately soluble	-5.45	0.00	0.00	Moderately soluble	Low

						soluble				ly soluble				soluble	
40	2.58	2.76	-5.53	0.00	0.00	Moderately soluble	-5.58	0.00	0.00	Moderate ly soluble	-5.44	0.00	0.00	Moderately soluble	Low
41	4.72	4.36	-5.98	0.00	0.00	Moderately soluble	-6.73	0.00	0.00	Poorly soluble	-4.89	0.01	0.00	Moderately soluble	High
42	3.15	2.65	-4.53	0.01	0.00	Moderately soluble	-5.25	0.00	0.00	Moderate ly soluble	-5.01	0.00	0.00	Moderately soluble	High
43	2.58	2.76	-5.53	0.00	0.00	Moderately soluble	-5.58	0.00	0.00	Moderate ly soluble	-5.44	0.00	0.00	Moderately soluble	Low
44	2.25	2.34	-4.82	0.01	0.00	Moderately soluble	-4.9	0.01	0.00	Moderate ly soluble	-5.54	0.00	0.00	Moderately soluble	Low
45	3.17	2.5	-3.83	0.08	0.00	Soluble	-3.62	0.12	0.00	Soluble	-3.65	0.12	0.00	Soluble	High
46	2.56	2.55	-5.66	0.00	0.00	Moderately soluble	-5.97	0.00	0.00	Moderate ly soluble	-5.34	0.00	0.00	Moderately soluble	Low
47	2.6	2.48	-5.33	0.00	0.00	Moderately soluble	-5.57	0.00	0.00	Moderate ly soluble	-5.79	0.00	0.00	Moderately soluble	Low
48	2.6	2.61	-5.33	0.00	0.00	Moderately soluble	-5.57	0.00	0.00	Moderate ly soluble	-5.79	0.00	0.00	Moderately soluble	Low
49	3.83	3.56	-5.38	0.00	0.00	Moderately soluble	-6	0.00	0.00	Poorly soluble	-4.06	0.04	0.00	Moderately soluble	High
50	2.42	1.89	-2.63	0.90	0.00	Soluble	-2.63	0.91	0.00	Soluble	-2.54	1.09	0.00	Soluble	High
51	3.33	2.87	-3.18	0.30	0.00	Soluble	-3.94	0.05	0.00	Soluble	-3.27	0.25	0.00	Soluble	High
52	2.46	2.56	-3.95	0.05	0.00	Soluble	-4.4	0.02	0.00	Moderate ly soluble	-4.58	0.01	0.00	Moderately soluble	High
53	2.3	1.8	-2.83	0.67	0.00	Soluble	-3.11	0.36	0.00	Soluble	-2.36	2.00	0.00	Soluble	High
54	1.03	0.48	-1.59	8.53	0.03	Very soluble	-1.14	23.80	0.07	Very soluble	-1.18	22.00	0.07	Soluble	High
55	2.7	2.45	-2.38	0.72	0.00	Soluble	-2.14	1.26	0.01	Soluble	-2.56	0.47	0.00	Soluble	High
56	4.31	2.95	-4.25	0.03	0.00	Moderately soluble	-5.2	0.00	0.00	Moderate ly soluble	-4.12	0.04	0.00	Moderately soluble	Low
57	2.01	2.26	-5.17	0.00	0.00	Moderately soluble	-5.25	0.00	0.00	Moderate ly soluble	-4.76	0.01	0.00	Moderately soluble	Low
58	6.47	5.94	-5.44	0.00	0.00	Moderately soluble	-8.31	0.00	0.00	Poorly soluble	-6.4	0.00	0.00	Poorly soluble	High
59	6.29	5.72	-5.12	0.00	0.00	Moderately soluble	-7.7	0.00	0.00	Poorly soluble	-5.68	0.00	0.00	Moderately soluble	High
60	2.99	3.05	-2.67	0.40	0.00	Soluble	-4.04	0.02	0.00	Moderate ly soluble	-3.18	0.13	0.00	Soluble	High
61	3.58	2.95	-4.23	0.03	0.00	Moderately soluble	-4.27	0.03	0.00	Moderate ly soluble	-4.12	0.04	0.00	Moderately soluble	High
62	3.83	3.56	-5.38	0.00	0.00	Moderately soluble	-6	0.00	0.00	Poorly soluble	-4.06	0.04	0.00	Moderately soluble	High

63	2.29	1.42	-3.6	0.14	0.00	Soluble	-3.06	0.50	0.00	Soluble	-3.76	0.10	0.00	Soluble	Low
64	3.9	2.72	-4.15	0.03	0.00	Moderately soluble	-4.34	0.02	0.00	Moderately soluble	-5.72	0.00	0.00	Moderately soluble	High
65	4.6	3.4	-3.48	0.10	0.00	Soluble	-4.44	0.01	0.00	Moderately soluble	-3.05	0.28	0.00	Soluble	High
66	4.92	4.14	-4.09	0.02	0.00	Moderately soluble	-5.34	0.00	0.00	Moderately soluble	-3.31	0.14	0.00	Soluble	High

Molecule	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log Kp (cm/s)	Lipinski #violations	Ghose #violations	Veber ns	Egan ns	Muegge #violations	Bioavailability Score	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
1	No	No	No	No	No	No	No	-6.65	0	4	0	0	2	0.85	0	0	1	1
2	No	No	No	No	No	No	No	-6.18	0	3	0	0	3	0.55	0	1	1	3.02
3	No	No	No	No	No	No	No	-6.03	0	3	0	0	3	0.55	0	1	1	1.93
4	Yes	No	Yes	No	No	No	No	-5.13	0	3	0	0	2	0.55	0	0	1	1
5	Yes	No	No	No	No	No	No	-5.08	0	1	0	0	2	0.55	0	0	1	2.42
6	Yes	No	Yes	No	No	No	No	-6.06	0	0	0	0	0	0.85	0	0	1	1.57
7	Yes	No	No	No	No	Yes	No	-5.66	0	0	0	0	0	0.55	0	0	1	2.22
8	Yes	No	No	No	No	Yes	No	-5.03	0	0	0	0	1	0.55	0	1	2	2.61
9	Yes	No	Yes	No	No	No	No	-3.27	1	1	1	1	1	0.85	0	0	2	2.58
10	No	Yes	No	No	No	No	Yes	-8.3	0	1	0	0	0	0.55	0	2	1	6.05
11	No	Yes	No	No	No	No	No	-8.66	0	0	0	0	0	0.55	0	2	1	5.76
12	No	Yes	No	No	No	No	Yes	-9.15	0	0	0	1	0	0.55	0	4	1	5.28
13	No	Yes	No	No	No	No	No	-8.14	0	0	0	0	0	0.55	0	3	0	4.7
14	No	Yes	No	No	No	No	Yes	-8.68	0	0	0	0	0	0.55	0	4	1	5.53
15	No	Yes	No	No	No	No	Yes	-8.68	0	0	0	0	0	0.55	0	4	1	5.53
16	Yes	No	Yes	Yes	Yes	Yes	No	-6.48	0	0	0	0	0	0.55	0	2	0	3.79
17	No	Yes	No	No	No	No	Yes	-7.46	0	0	0	0	0	0.55	0	4	1	5.03
18	No	Yes	No	No	No	No	Yes	-8.45	0	0	0	0	0	0.55	0	4	1	5.09
19	No	Yes	No	No	No	No	Yes	-9	0	0	0	1	0	0.55	0	4	1	5.36
20	No	Yes	No	No	No	No	Yes	-8.34	0	0	0	0	0	0.55	0	5	1	5.49
21	No	Yes	No	No	No	No	No	-7.81	0	0	0	0	0	0.55	0	3	0	5.25
22	No	Yes	No	No	No	No	No	-9.24	0	0	0	0	0	0.56	0	1	1	5.88
23	No	Yes	No	No	No	No	Yes	-8.21	0	0	0	0	0	0.55	0	4	1	5.46
24	No	Yes	No	No	No	No	Yes	-8.07	0	0	0	0	0	0.55	0	4	1	5.7
25	No	Yes	No	No	No	No	Yes	-8.75	0	0	0	0	0	0.55	0	4	1	5.44
26	No	Yes	No	No	No	No	No	-8.05	0	0	0	0	0	0.55	0	2	1	6.43
27	No	Yes	No	No	No	No	Yes	-9.11	2	3	1	1	2	0.17	0	2	1	8.45
28	Yes	No	Yes	Yes	Yes	Yes	No	-5.98	0	0	0	0	0	0.55	0	2	2	3.73
29	Yes	No	Yes	Yes	Yes	Yes	No	-5.98	0	0	0	0	0	0.55	0	2	2	3.73
30	No	Yes	No	No	No	No	No	-9.57	2	3	1	1	3	0.17	0	2	1	8.96
31	No	Yes	No	No	No	No	No	-9.83	2	3	1	1	3	0.17	0	3	1	9.06

32	Yes	No	Yes	Yes	Yes	Yes	No	-5.98	0	0	0	0	0	0.55	0	2	2	3.69
33	No	Yes	No	No	No	No	Yes	-8.54	2	3	1	1	2	0.17	0	2	2	8.7
34	No	Yes	No	No	No	No	Yes	-8.54	2	3	0	1	1	0.17	0	2	1	7.82
35	No	Yes	No	No	No	No	No	-9	0	0	0	0	0	0.56	0	1	1	6
36	No	Yes	No	No	No	No	Yes	-8.05	1	3	0	0	0	0.55	0	1	1	6.57
37	Yes	No	No	No	No	No	No	-6.57	0	0	0	0	0	0.55	0	1	1	6.04
38	No	Yes	No	No	No	No	No	-9.43	1	3	1	1	0	0.55	0	1	1	7.16
39	No	No	No	No	No	No	Yes	-9.17	2	3	1	1	3	0.17	0	3	2	8.87
40	No	Yes	No	No	No	No	Yes	-9.13	2	3	1	1	3	0.17	0	2	2	8.95
41	No	Yes	No	No	Yes	No	No	-5.59	0	3	0	0	1	0.55	0	1	2	6.38
42	No	No	Yes	No	No	Yes	Yes	-5.57	0	0	0	0	0	0.55	0	0	1	2.88
43	No	Yes	No	No	No	No	Yes	-9.13	2	3	1	1	3	0.17	0	2	2	8.95
44	No	Yes	No	No	No	No	Yes	-9.15	2	3	1	1	2	0.17	0	2	1	8.32
45	No	Yes	No	No	No	No	No	-8.48	1	3	0	0	0	0.55	0	2	1	6.51
46	No	Yes	No	No	No	No	Yes	-9.28	2	3	1	1	3	0.17	0	2	2	9.05
47	No	Yes	No	No	No	No	Yes	-9.18	2	3	1	1	3	0.17	0	2	2	8.82
48	No	Yes	No	No	No	No	Yes	-9.18	2	3	1	1	3	0.17	0	2	2	8.82
49	No	Yes	No	No	No	No	No	-6.47	1	3	0	0	0	0.55	0	1	2	6.5
50	No	Yes	No	No	No	No	Yes	-7.87	0	0	0	0	0	0.55	0	4	1	4.96
51	No	Yes	No	No	No	Yes	Yes	-7.65	0	0	1	0	0	0.55	0	2	2	5.86
52	No	No	Yes	No	No	No	Yes	-6.78	0	0	0	0	0	0.55	0	3	1	4.7
53	No	Yes	No	No	No	No	Yes	-8.36	0	0	0	0	0	0.55	0	4	1	5.68
54	No	Yes	No	No	No	No	No	-8.66	0	0	0	0	0	0.55	0	3	0	5.35
55	Yes	No	No	No	No	No	No	-5.63	0	0	0	0	2	0.55	0	3	1	1.89
56	No	Yes	No	No	No	No	Yes	-8.09	1	3	2	1	0	0.55	0	3	2	6.52
57	No	No	No	No	No	No	Yes	-9.43	2	3	1	1	3	0.17	0	2	2	8.81
58	No	No	Yes	No	No	No	No	-2.69	1	1	1	1	2	0.85	0	0	2	2.81
59	No	No	Yes	No	Yes	No	No	-3.09	1	1	1	1	2	0.85	0	1	2	3.14
60	Yes	No	No	No	No	No	No	-4.93	0	0	0	0	1	0.85	0	0	3	1.94
61	No	Yes	No	No	No	No	Yes	-8.05	1	3	0	0	0	0.55	0	1	1	6.56
62	No	Yes	No	No	No	No	No	-6.47	1	3	0	0	0	0.55	0	1	2	6.5
63	No	Yes	No	No	No	No	No	-9.43	1	2	1	1	1	0.55	0	2	1	7.21
64	No	Yes	No	Yes	Yes	Yes	Yes	-6.6	0	0	0	0	0	0.55	0	2	1	4.28
65	Yes	No	No	No	Yes	Yes	No	-5.62	0	0	0	0	0	0.55	0	3	2	5.15
66	Yes	Yes	No	No	Yes	Yes	No	-4.73	0	0	0	0	0	0.55	0	3	2	4.98

Table S2 — Binding energies of halide metabolites

S. N	Halide compound CID	Binding Energy
1	5315835	-6.9
2	5486900	-6.1
3	327916	-6
4	100854335	-6
5	162745	-5.9
6	5281447	-5.8
7	23266570	-5.8
8	182277	-5.7
9	101600034	-5.7
10	23266165	-5.3
11	71522011	-5.3
12	442840	-5.2
13	100413	-5.1
14	171332	-5.1
15	442178	-5.1
16	15560290	-5
17	71439502	-5
18	134978	-4.9
19	170025	-4.9
20	182337	-4.9
21	182408	-4.9
22	134977	-4.8
23	5281446	-4.8
24	101277293	-4.8
25	130756	-4.7
26	442140	-4.7
27	5281448	-4.7
28	130664	-4.4
29	9542	-4.3
30	7961	-3.9
31	26447	-3.9
32	1016252140	-3.7
33	5281726	-3.6
34	5236	-2.9
35	6323	-1.5
36	6327	-1.5
