

Table 1S. Fractions Bound to Solidified and Dissolved ECM Surrogate for All Species and Modes.

No.	Compound	Mode 1		Mode 2		Mode 3		Mode 4		Mode 5		Mode 6		Sum	
		s-ECM	d-ECM	s-ECM	d-ECM										
1	acetophenone	8.1	19.6	5.1	38.0	9.6	14.3	10.1	13.0	58.0	2.9	9.21	14.9	100.0	100.0
2	aniline ^a	33.0	29.7	33.0	29.7	9.5	1.0	9.5	1.0	5.5	8.7	5.5	8.7	96.1	78.8
		0.1	16.8	0.9	0.1	1.0	0.1	0.5	1.2	0.6	1.6	0.7	1.4	3.9	21.2
3	atenolol	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
		36.4	0.0	0.0	0.0	63.6	0.0	0.0	0.0	0.0	0.0	0.0	100.0	100.0	100.0
4	BDPA	55.7	93.6	0.0	0.0	S	S	44.3	6.4	S	S	S	S	100.0	100.0
5	benzamide	21.3	70.7	8.3	9.9	0.3	6.2	63.4	5.0	0.2	7.2	6.5	1.0	100.0	100.0
6	benzenesulfonamide	0.0	0.0	0.0	0.0	26.6	0.0	0.0	0.0	35.7	0.0	35.7	0.0	98.0	0.0
		0.1	1.2	0.1	0.3	0.0	0.1	0.0	4.2	0.1	47.0	1.6	47.0	2.0	100.0
7	benzyl alcohol	92.7	0.6	1.9	20.4	2.0	19.4	1.5	20.1	0.0	19.7	1.9	19.8	100.0	100.0
8	BPCA	4.1	0.2	8.0	0.1	7.9	0.1	0.3	19.6	40.6	40.2	39.1	39.7	100.0	100.0
9	4-bromophenol	14.8	17.4	30.2	82.2	1.8	0.2	1.8	0.2	33.8	0.0	14.8	0.0	97.1	100.0

No.	Compound	Mode 1		Mode 2		Mode 3		Mode 4		Mode 5		Mode 6		Sum	
		s-ECM	d-ECM	s-ECM	d-ECM										
				0.0	0.0	1.4	0.0	1.4	0.0	0.1	0.0	S	S	S	2.9
10	4-chloro-3-methylphenol	18.5	0.2	0.0	6.2	39.2	0.0	36.6	27.6	0.0	27.3	0.0	38.7	94.3	100.0
		0.0	0.0	5.6	0.0	0.0	0.0	0.0	0.0	0.1	0	S	S	5.7	0.0
11	cinnamamide	5.9	2.1	0.0	1.6	42.5	35.5	42.5	35.5	7.5	21.0	1.6	4.2	100.0	100.0
12	3,5-dichlorophenol	25.5	83.4	2.7	0.1	38.1	5.1	11.3	8.3	1.3	0.0	16.9	1.7	95.8	98.5
		2.1	0.0	2.1	0.0	0.0	0.7	0.0	0.7	S	S	S	S	4.2	1.5
13	dimethylaniline	8.6	2.0	8.6	2.0	5.5	0.7	10.2	0.8	10.2	0.8	0.0	25.4	43.2	31.7
		0.4	5.9	1.5	22.5	0.4	5.4	0.4	7.0	26.7	14.1	27.4	13.4	56.8	68.3
14	2,2-diphenyl-ethanol	2.7	40.7	57.0	3.0	0.0	0.0	2.7	41.4	0.0	11.8	37.5	3.2	100.0	100.0
15	3-phenylpropanal	6.6	13.0	12.2	7.1	6.6	12.9	9.2	9.3	12.0	15.1	53.4	42.5	100.0	100.0
16	2-hydroxy-biphenyl	2.0	9.2	0.0	9.1	0.5	11.2	34.7	19.2	18.8	23.2	41.6	28.1	99.8	100.0
		0.0	0.0	2.3	0.0	0.1	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.2	0.0
17	4-nitroaniline	5.8	29.0	22.4	12.6	22.4	12.6	23.5	14.0	20.1	11.8	5.95	20.1	100.0	100.0
18	2-nitrotoluene	0.0	19.2	0.0	2.1	0.0	21.1	0.0	6.7	100.0	47.9	-	-	100.0	100.0
19	3-nitrotoluene	36.3	12.5	43.3	8.7	0.0	0.2	0.0	72.2	0.1	2.1	20.3	4.3	100.0	100.0
20	4-nitrotoluene	21.6	51.6	11.4	16.9	18.4	0.1	30.0	12.6	9.6	6.6	9.01	12.2	100.0	100.0

No.	Compound	Mode 1		Mode 2		Mode 3		Mode 4		Mode 5		Mode 6		Sum	
		s-ECM	d-ECM	s-ECM	d-ECM										
21	phenol	13.6	19.2	18.9	16.1	22.5	9.2	3.8	5.5	6.4	47.2	34.3	2.9	99.8	100.0
		0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0
22	phenylurea	24.0	23.7	24.7	19.4	13.7	13.6	0.7	5.2	0.7	27.6	4.3	10.4	100.0	100.0
23	sulfacetamide	19.7	0.0	0.0	1.4	0.3	2.0	0.2	1.8	3.4	82.5	S	S	23.6	87.7
		26.6	0.3	0.0	0.4	0.0	0.2	0.0	0.9	49.8	7.1	0.0	3.3	76.4	12.3
24	sulfisomidine	0.0	0.1	0.0	0.0	0.0	3.7	100.0	0.0	0.0	0.0	0.0	0.0	100.0	3.9
		0.0	54.6	0.0	0.1	0.0	40.1	0.0	0.0	0.0	0.8	0.0	0.5	0.0	96.1
25	2,4,5-trichloroaniline	55.5	0.0	39.4	0.0	0.0	20.6	0.2	22.6	0.1	56.7	4.8	0.1	100.0	100.0

^a For ionizable compounds, the neutral species is listed in the first row and the ionized species in the second row.