

S8 Table. LipidFrag's improvement of ranks for training MS/MS spectra in positive ion mode.

	FCP- Threshold	LMGL0301	LMGP0101	LMGP0201	LMGP0301	LMGP0601	LMSP0201 LMSP0202	All
<i>Top 1</i>	0	6	25	34	6	82	156	309
	0.1	6	25	34	6	82	156	309
	0.2	6	25	34	6	82	156	309
	0.3	6	25	34	6	82	156	309
	0.4	6	25	34	6	82	156	309
	0.5	6	25	34	6	82	155	308
	0.6	6	4	34	6	82	155	287
	0.7	6	0	34	6	82	154	282
	0.8	6	0	34	6	82	148	276
	0.9	6	0	34	6	82	124	252
<i>Median Rank</i>	0	3	2	2	2	1	1	1
	0.1	3	2	2	2	1	1	1
	0.2	3	2	2	2	1	1	1
	0.3	3	2	2	2	1	1	1
	0.4	3	2	2	2	1	1	1
	0.5	3	2	2	2	1	1	1
	0.6	3	2	2	2	1	1	1
	0.7	3	2	2	2	1	1	1
	0.8	3	2	2	2	1	1	1
	0.9	3	0	2	2	1	1	1
<i>Mean Rank</i>	0	3.08	5.83	1.73	1.88	1.00	1.17	2.09
	0.1	3.08	5.83	1.73	1.88	1.00	1.00	2.07
	0.2	3.08	5.83	1.73	1.88	1.00	1.00	2.07
	0.3	3.08	5.83	1.73	1.88	1.00	1.00	2.07
	0.4	3.08	5.83	1.73	1.88	1.00	1.00	2.07
	0.5	3.08	3.00	1.73	1.88	1.00	1.00	1.60
	0.6	3.08	1.69	1.73	1.88	1.00	1.00	1.41
	0.7	3.08	2.00	1.73	1.88	1.00	1.00	1.41
	0.8	3.08	2.00	1.73	1.88	1.00	1.00	1.42
	0.9	3.08	0.00	1.73	1.88	1.00	1.00	1.43
<i>Number Spectra</i>	0	25	71	88	51	82	172	489
	0.1	25	71	88	50	82	159	475
	0.2	25	71	88	50	82	159	475
	0.3	25	71	88	50	82	159	475
	0.4	25	71	88	50	82	159	475
	0.5	25	56	88	50	82	158	459

	0.6	25	13	88	50	82	156	414
	0.7	25	9	88	49	82	155	408
	0.8	25	7	88	49	82	149	400
	0.9	25	0	88	49	82	125	369