

S3 Table. Statistics on training MS/MS spectra from negative ion mode.

	<i>LMGP0101</i> <i>LMGP0201</i> <i>(PC, PE)</i>	<i>LMGP0301</i> <i>(PS)</i>	<i>LMGP0401</i> <i>(PG)</i>	<i>LMGP0601</i> <i>(PI)</i>	<i>LMSP0201</i> <i>LMSP0202</i> <i>(Cer)</i>
<i>Number of MS2 spectra used for training</i>	128	36	41	78	189
<i>Mean number of informative MS2 peaks</i>	7.01	6.81	8.98	11.73	9.40
<i>Median number of informative MS2 peaks</i>	7	7	9	13	10
<i>Standard deviation of informative MS2 peaks</i>	2.26	1.74	2.60	2.88	3.15