

Table S4

The X- and Y-axis information of the MMDF on the three types of compounds.

Structure type	Order	Original datapoints in windows		Shifted datapoints	
		Integral m/z (Da)	Decimal m/z (mDa)	Integral m/z (Da)	Decimal m/z (mDa)
Phenolic acids [M-H] ⁻	1	65	3.3	65 (+0)	3.3 (+0)
	2	89	39.7	88 (-1)	44.7 (+5)
	3	375	254.1	374 (-1)	259.1 (+5)
	4	709	271.3	709 (+0)	276.3 (+5)
	5	949	240.8	950 (+1)	235.8 (-5)
	6	683	17.7	684 (+1)	12.7 (-5)
	7	101	3.3	101 (+0)	3.3 (+0)
Phthalides [M+H] ⁺	1	165	163.8	164 (-1)	168.8 (+5)
	2	401	268.6	400 (-1)	273.6 (+5)
	3	558	282.3	559 (+1)	287.3 (+5)
	4	621	254.2	622 (+1)	254.2 (+0)
	5	461	92.6	462 (+1)	87.6 (-5)
	6	267	49.9	268 (+1)	44.9 (-5)
	7	155	85.5	154 (-1)	80.5 (-5)
Tanshinones Phase I [M+H] ⁺	1	245	59.7	244 (+1)	54.7 (-5)
	2	257	190	256 (-1)	195 (+5)
	3	305	211.1	306 (+1)	216.1 (+5)
	4	373	128.2	374 (+1)	133.2 (+5)
	5	369	96.9	370 (+1)	91.9 (-5)
	6	307	60.1	308 (+1)	55.1 (-5)
	7	245	59.7	244 (-1)	54.7 (-5)
Tanshinones Phase II [M+H] ⁺	1	453	118	452 (+1)	113 (-5)
	2	461	217	460 (+1)	222 (+5)
	3	479	227.6	480 (+1)	232.6 (+5)
	4	547	144.6	548 (+1)	149.6 (+5)
	5	483	92.2	482 (-1)	87.2 (-5)
	6	453	118	452 (-1)	113 (-5)