

Příloha číslo 1: Tabulka - výsledky metabolické analýzy z těl žíral vystavených koncentraci mikroplastů 1 mg/kg suché půdy (c1) a koncentraci 0,0265 mg/kg suché půdy (c2); C18 = nepolární metabolity; Fold change = míra velikosti změny mezi kontrolním vzorkem a vzorkem s mikroplasty; Skóre = pravděpodobnost správného určení sumárního vzorce

Název vzorku	Počet nalezených změných znaků	Retenční čas	Hmotnost	Fold change	Látka	Skóre [%] TGT	Hmotnost@retenční čas		
C18_t14_c1	1	9.626	247.1575	7163.0	C11 H24 N2 O2 P	64.12	247.1575@9.626001		
		13.018	285.3039	-3.6	C18 H39 N O	98.24	285.3039@13.018002		
		9.626	247.1575	-6.1	C11 H24 N2 O2 P	64.12	247.1575@9.626001		
C18_t14_c2	3	12.858	634.5164	-222777.7	C36 H62 N10	77.98	634.5164@12.858001		
		11.906	324.1968	-2.1	C17 H29 N2 O2 P	84.42	324.1968@11.906001		
		12.182	488.2202	2.1	C30 H32 O6	98.43	488.2202@12.182002		
C18_t28_c1	5	12.183	368.1630	2.1	C22 H24 O5	82.96	368.163@12.183		
		5.645	134.0943	-3.6	C6 H14 O3	87.69	134.0943@5.644999		
		9.060	670.4158	-3.8	C33 H48 N15 O	98.59	670.4158@9.059999		
		12.646	680.5020	-2.2	C43 H68 O6	91.79	680.502@12.645998		
		11.706	280.1704	-4.4	C13 H28 O4 S	97.11	280.1704@11.705998		
		11.906	324.1968	-3.5	C17 H29 N2 O2 P	84.42	324.1968@11.906001		
		11.881	442.2596	-2.4	C24 H44 O P2 S	88.59	442.2596@11.880998		
C18_t28_c2	33	12.182	488.2202	3.0	C30 H32 O6	98.43	488.2202@12.182002		
		12.146	422.3251	2.3	C23 H42 N4 O3	97.81	422.3251@12.145998		
		12.064	712.4155	2.7	C36 H60 N2 O12	99.26	712.4155@12.063999		
		12.139	290.2463	2.3	C16 H34 O4	97.07	290.2463@12.139002		
		12.534	335.3187	3.3	C22 H41 N O	83.75	335.3187@12.533		
		12.140	290.2461	2.6	C17 H30 N4	83.42	290.2461@12.140		
		12.183	368.1630	2.7	C22 H24 O5	82.96	368.163@12.183		
		12.020	310.1577	2.2	C20 H22 O3	82.82	310.1577@12.020002		
		12.442	257.2724	-4.4	C16 H35 N O	97.84	257.2724@12.442		
		5.645	134.0943	-5.9	C6 H14 O3	87.69	134.0943@5.644999		
		11.995	229.2388	-3.7	C14 H31 N O	85.99	229.2388@11.994999		
		11.821	458.4924	-8.3	C33 H62	41.24	458.4924@11.821		
		13.015	285.3038	-4.3	C18 H39 N O	98.66	285.3038@13.015		
		11.821	458.4925	-7.5	C33 H62	41.24	458.4925@11.821		
		12.600	736.6106	-3.3	1-Octadecanoyl-2-[9Z,12Z-octadecadienyl]-3-O-[[(N,N,N-trimethyl) homoserine]-glycerol	99.33	736.6106@12.600001		
		12.437	800.6056	-4.2	C44 H85 N2 O8 P	92.82	800.6056@12.436998		
		10.376	271.2515	-10.5	C16 H33 N O2	99.63	271.2515@10.376001		
		8.838	259.2147	-3.4	C14 H29 N O3	89.14	259.2147@8.837999		
		12.656	724.6092	-2.9	C40 H81 N6 O3 P	98.62	724.6092@12.656001		
		12.092	770.5578	-3.1	C47 H72 N5 O4	98.01	770.5578@12.091999		
		10.623	273.2670	-4.9	Sphinganine	98.4	273.267@10.6232		
		9.488	152.0839	-2.2	C9 H12 O2	86.71	152.0839@9.488001		
		12.437	764.6053	-3.6	C46 H78 N5 O4	94.14	764.6053@12.436998		
		12.498	710.5950	-3.0	C37 H77 N9 O2 P	61.43	710.595@12.498		
		12.434	486.5132	-4.6	C30 H66 N2 O2	77.6	486.5132@12.434001		
		12.437	800.6048	-4.2	C45 H81 N6 O4 P	92.09	800.6048@12.436998		
		14.486	610.3580	-3.3	C40 H51 O3 P	96.93	610.358@14.485996		
		12.657	362.3026	-2.1	C21 H38 N4 O	83.62	362.3026@12.656999		
		12.166	243.2567	-2.2	C15 H33 N O	86.57	243.2567@12.166		
		C18_t56_c1	49	16.362	512.3639	-408122.1	C30 H58 P2 S	47.62	512.3639@16.362
				7.417	335.1472	-2.4	C15 H15 N10	82.22	335.1472@7.417
				10.609	381.1253	-30902.8	C22 H22 O4 P	79.16	381.1253@10.609
				10.608	246.1292	460.4	C12 H22 O3 S	97.32	246.1292@10.608001
10.708	246.1294			520.2	C12 H22 O3 S	97.32	246.1294@10.708		
10.629	246.1283			392.7	C12 H22 O3 S	98.55	246.1283@10.628999		
10.590	937.5901			56.3	C53 H85 N4 O6 S2	94.76	937.5901@10.589999		
10.638	760.3581			98.7	C43 H53 N7 P3	66.19	760.3581@10.638		
10.590	470.1935			8.2	C24 H28 N3 O7	95.17	470.1935@10.589999		
10.685	760.3583			49.2	C43 H53 N7 P3	66.19	760.3583@10.684999		
9.219	496.3396			608386.3	26-Hydroxybrassinolide	99.24	496.3396@9.219001		
9.335	772.4421			61.3	C39 H62 N7 O7 S	99.4	772.4421@9.335		
10.789	991.6025			4.7	C59 H95 O2 P4 S	90.47	991.6025@10.7890005		
10.628	947.5737			13.4	C36 H63 N30 O2	61.36	947.5737@10.627999		
10.211	264.1389			15.7	C12 H24 O4 S	97.18	264.1389@10.2109995		
9.211	496.3394			3104815.8	C27 H42 N7 O2	98.91	496.3394@9.2109995		
10.728	917.5646			60.4	C54 H84 N3 O3 P S2	65.77	917.5646@10.727999		
10.140	232.1124			96.5	2-Oxo-10-methylthiododecanoic acid	97.87	232.1124@10.14		
10.781	705.4774			16.8	C35 H63 N9 O4 S	98.95	705.4774@10.780999		
10.626	330.1059			99915.9	C11 H26 N O4 P2 S	97.85	330.1059@10.626		
9.122	357.1713			227528.9	C18 H24 N5 O P	95.56	357.1713@9.122001		
10.513	246.1293			117.5	C12 H22 O3 S	95.51	246.1293@10.513		
12.073	212.1771			2.4	C13 H24 O2	86.24	212.1771@12.072999		
10.586	346.0565			749871.1	C20 H12 N O3 S	88.31	346.0565@10.5859995		
10.940	675.4652			9.6	C32 H53 N17	81.67	675.4652@10.940001		
11.020	246.1283			134.5	C12 H22 O3 S	98.55	246.1283@11.020001		
10.165	306.0902			5.5	C13 H22 O4 S2	96.74	306.0902@10.165		
10.637	495.2591			38.1	C16 H31 N16 O S	94.27	495.2591@10.637		
10.186	244.1160			199595.3	C12 H20 O3 S	94.79	244.116@10.186		
10.630	532.2119			42.4	C18 H37 N11 O4 P2	73.12	532.2119@10.629999		
10.586	346.0574			748454.8	C20 H12 N O3 S	88.31	346.0574@10.5859995		
10.785	736.4909			10.7	C49 H70 O P2	47.62	736.4909@10.785001		
10.040	278.1183			243945.0	3-(7'-Methylthio)heptymalic acid	96.11	278.1183@10.04		
10.720	686.3092			38.6	C38 H49 N5 O P S2	94.23	686.3092@10.72		
9.427	772.4462			26.5	C39 H62 N7 O7 S	99.4	772.4462@9.427001		
10.604	160.0192			51187.5	C8 H5 N2 P	85.79	160.0192@10.603999		
10.557	784.3222			20.7	C48 H50 O4 P2 S	89.92	784.3222@10.557		
10.674	347.0557			295981.6	C17 H18 N O P S2	47.62	347.0557@10.674		
10.578	849.4691			11.5	C48 H65 N8 O2 S2	85.73	849.4691@10.578001		
10.629	330.1067			100066.2	C12 H22 N5 P2 S	98.25	330.1067@10.628999		
7.367	162.0310			12.1	4-Hydroxycoumarin	85.88	162.031@7.3669996		
10.713	798.3356			30.4	C25 H38 N26 O4 S	68.44	798.3356@10.712999		
10.743	761.4765			4.7	C46 H69 N2 O5 S	88.85	761.4765@10.742999		
10.448	292.1702			17.0	C16 H25 N2 O P	86.37	292.1702@10.447999		
9.312	539.3442			138187.1	C33 H51 N O P2	74.87	539.3442@9.312		
10.785	392.0882			15.1	C19 H8 N10 O	83.21	392.0882@10.785001		
9.342	531.3283			10.7	C31 H43 N6 S	86.66	531.3283@9.342001		
10.774	885.5894			28095.7	C43 H72 N19 P	64.19	885.5894@10.774001		
9.064	610.3321			628303.8	C28 H51 N7 O2 P3	78.34	610.3321@9.064		
C18_t56_c1	49	16.362	512.3639	-408122.1	C30 H58 P2 S	47.62	512.3639@16.362		
		10.609	381.1253	-30902.8	C22 H22 O4 P	79.16	381.1253@10.609		
		10.608	246.1292	290.6	C12 H22 O3 S	97.32	246.1292@10.608001		
		10.708	246.1294	399.3	C12 H22 O3 S	97.32	246.1294@10.708		
		10.629	246.1283	295.0	C12 H22 O3 S	98.55	246.1283@10.628999		
		9.308	496.3397	1531658.5	26-Hydroxybrassinolide	99.24	496.3397@9.308		
		10.590	937.5901	18.5	C53 H85 N4 O6 S2	94.76	937.5901@10.589999		
		10.638	760.3581	117.6	C43 H53 N7 P3	66.19	760.3581@10.638		

	10.590	470.1935	7.5	C24 H28 N3 O7	C24 H28 N3 O7	95.17	470.1935@10.589999
	10.685	760.3583	66.3	C43 H53 N7 P3	C43 H53 N7 P3	66.19	760.3583@10.684999
	9.335	772.4421	65.9	C39 H62 N7 O7 S	C39 H62 N7 O7 S	99.4	772.4421@9.335
	10.789	991.6025	8.5	C59 H95 O2 P4 S	C59 H95 O2 P4 S	90.47	991.6025@10.7890005
	10.628	947.5737	19.2	C36 H63 N30 O2	C36 H63 N30 O2	61.36	947.5737@10.627999
	10.211	264.1389	15.9	C12 H24 O4 S	C12 H24 O4 S	97.18	264.1389@10.2109995
	9.211	496.3394	1898667.6	C27 H42 N7 O2	C27 H42 N7 O2	98.91	496.3394@9.2109995
	10.728	917.5646	64.9	C54 H84 N3 O3 P S2	C54 H84 N3 O3 P S2	65.77	917.5646@10.727999
	10.140	232.1124	138.1	2-Oxo-10-methylthiododecanoic acid	C11 H20 O3 S	97.87	232.1124@10.14
	10.781	705.4774	15.8	C35 H63 N9 O4 S	C35 H63 N9 O4 S	98.95	705.4774@10.780999
	10.626	330.1059	121769.3	C11 H26 N O4 P2 S	C11 H26 N O4 P2 S	97.85	330.1059@10.626
	9.122	357.1713	339934.0	C18 H24 N5 O P	C18 H24 N5 O P	95.56	357.1713@9.122001
	10.513	246.1293	127.9	C12 H22 O3 S	C12 H22 O3 S	95.51	246.1293@10.513
	12.073	212.1771	2.7	trans-?2-11-methyl-Dodecenoic Acid	C13 H24 O2	86.24	212.1771@12.072999
	10.586	346.0565	1102082.1	C20 H12 N O3 S	C20 H12 N O3 S	88.31	346.0565@10.5859995
	10.940	675.4652	9.1	C32 H53 N17	C32 H53 N17	81.67	675.4652@10.940001
	11.020	246.1283	124.0	C12 H22 O3 S	C12 H22 O3 S	98.55	246.1283@11.020001
	10.165	306.0902	5.5	C13 H22 O4 S2	C13 H22 O4 S2	96.74	306.0902@10.165
	10.637	495.2591	44.3	C16 H31 N16 O S	C16 H31 N16 O S	94.27	495.2591@10.637
	10.186	244.1160	257142.1	C12 H20 O3 S	C12 H20 O3 S	94.79	244.1160@10.186
	10.630	532.2119	33.4	C18 H37 N11 O4 P2	C18 H37 N11 O4 P2	73.12	532.2119@10.629999
	10.586	346.0574	1102038.4	C20 H12 N O3 S	C20 H12 N O3 S	88.31	346.0574@10.5859995
	10.785	736.4909	13.1	C49 H70 O P2	C49 H70 O P2	47.62	736.4909@10.785001
	10.040	278.1183	477506.8	3-(7'-Methylthio)heptylmalic acid	C12 H22 O5 S	96.11	278.1183@10.04
	10.720	686.3092	28.0	C38 H49 N5 O P S2	C38 H49 N5 O P S2	94.23	686.3092@10.72
	9.427	772.4462	33.9	C39 H62 N7 O7 S	C39 H62 N7 O7 S	99.4	772.4462@9.427001
	10.604	160.0192	59829.9	C8 H5 N2 P	C8 H5 N2 P	85.79	160.0192@10.603999
	10.557	784.3222	18.8	C48 H50 O4 P2 S	C48 H50 O4 P2 S	89.92	784.3222@10.557
	10.674	347.0557	341942.1	C17 H18 N O P S2	C17 H18 N O P S2	47.62	347.0557@10.674
	10.578	849.4691	5.6	C48 H65 N8 O2 S2	C48 H65 N8 O2 S2	85.73	849.4691@10.578001
	10.629	330.1067	96026.8	C12 H22 N5 P2 S	C12 H22 N5 P2 S	98.25	330.1067@10.628999
	7.367	162.0310	12.5	4-Hydroxycoumarin	C9 H6 O3	85.88	162.0310@7.3669996
	10.713	798.3356	33.0	C25 H38 N26 O4 S	C25 H38 N26 O4 S	68.44	798.3356@10.712999
	10.743	761.4765	4.2	C46 H69 N2 O5 S	C46 H69 N2 O5 S	88.85	761.4765@10.742999
	10.448	292.1702	18.6	C16 H25 N2 O P	C16 H25 N2 O P	86.37	292.1702@10.447999
	9.312	539.3442	130864.7	C33 H51 N O P2	C33 H51 N O P2	74.87	539.3442@9.312
	10.785	392.0882	14.0	C19 H8 N10 O	C19 H8 N10 O	83.21	392.0882@10.785001
	9.342	531.3283	12.2	C31 H43 N6 S	C31 H43 N6 S	86.66	531.3283@9.342001
	10.774	885.5894	21055.7	C43 H72 N19 P	C43 H72 N19 P	64.19	885.5894@10.774001
	9.064	610.3321	396580.4	C28 H51 N7 O2 P3	C28 H51 N7 O2 P3	78.34	610.3321@9.064

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Příloha číslo 2: Tabulka - výsledky metabolické analýzy z těl žížal vystavených koncentraci mikroplastů 1 mg/kg suché půdy (c1) a koncentraci 0,0265 mg/kg suché půdy (c2); HILIC = polární metabolity; Fold change = míra velikosti změny mezi kontrolním vzorkem a vzorkem s mikroplasty; Skóre = pravděpodobnost správného určení sumárního vzorce

Název vzorku	Počet nalezených změných znaků	Retenční čas	Hmotnost	Fold change	Látka	Vzorec	Skóre [%] TGT	Hmotnost@retenční čas
HILIC_t14_c1	4	7.155	230.1628	31.7	Isoleucyl-Valine	C11 H22 N2 O3	87.09	230.1628@7.1549993
		8.799	531.3271	129.8	C23 H39 N12 O3	C23 H39 N12 O3	80.4	531.3271@8.798999
		12.464	174.0890	7.5	C8 H14 O4	C8 H14 O4	84.86	174.089@12.464
		2.516	506.1653	-388713.6	C22 H26 N4 O10	C22 H26 N4 O10	99.33	506.1653@2.516
HILIC_t14_c2	4	7.155	230.1628	33.5	Isoleucyl-Valine	C11 H22 N2 O3	87.09	230.1628@7.1549993
		8.799	531.3271	165.9	C23 H39 N12 O3	C23 H39 N12 O3	80.4	531.3271@8.798999
		12.464	174.0890	16.1	C8 H14 O4	C8 H14 O4	84.86	174.089@12.464
		2.516	506.1653	-58863.4	C22 H26 N4 O10	C22 H26 N4 O10	99.33	506.1653@2.516
HILIC_t28_c1	1	8.738	413.2041	12530.7	C11 H31 N10 O3 P2	C11 H31 N10 O3 P2	55.19	413.2041@8.738
HILIC_t28_c2	2	1.373	294.1858	-5.1	C17 H26 O4	C17 H26 O4	84.92	294.1858@1.3729999
		8.738	413.2041	4860.1	C11 H31 N10 O3 P2	C11 H31 N10 O3 P2	55.19	413.2041@8.738
HILIC_t56_c1	62	13.299	134.0214	4.8	3-Dehydro-L-threonate	C4 H6 O5	87.12	134.0214@13.298997
		11.861	160.0846	3.7	N-alpha-Acetyl-L-2,4-diaminobutyrate	C6 H12 N2 O3	87.48	160.0846@11.860999
		12.828	246.1211	6.7	2,4-Bis(acetamido)-2,4,6-trideoxy-beta-L-altropyranose	C10 H18 N2 O5	86.51	246.1211@12.828002
		12.278	176.0795	3.4	D-Alanyl-D-serine	C6 H12 N2 O4	87.46	176.0795@12.278
		10.196	202.1314	2.6	Alanyl-Isoleucine	C9 H18 N2 O3	87.38	202.1314@10.196
		10.924	204.1106	2.8	Seriny-Valine	C8 H16 N2 O4	87.12	204.1106@10.923998
		11.794	190.0951	3.3	Alanyl-Threonine	C7 H14 N2 O4	87.27	190.0951@11.794001
		13.286	116.0108	6.4	Formylpyruvate	C4 H4 O4	87.65	116.0108@13.286
		12.172	192.0743	2.4	Seriny-Serine	C6 H12 N2 O5	87.05	192.0743@12.171998
		9.471	275.0999	2.8	1,6-Anhydro-N-acetyl-beta-muramate	C11 H17 N O7	83.99	275.0999@9.471
		12.474	217.1060	3.1	N-a-Acetylcitrulline	C8 H15 N3 O4	87.1	217.106@12.474
		10.803	259.1531	3.3	Glutaminy-Isoleucine	C11 H21 N3 O4	99.71	259.1531@10.8029995
		11.845	196.0580	5.6	L-Galactonate	C6 H12 O7	86.42	196.058@11.845
		11.828	176.0794	3.4	D-Alanyl-D-serine	C6 H12 N2 O4	87.22	176.0794@11.828002
		11.806	146.0690	2.7	Isoglutamine	C5 H10 N2 O3	87.64	146.069@11.806
		12.753	260.1370	6.1	C10 H14 N9	C10 H14 N9	85.06	260.137@12.753
		10.842	147.0530	3.6	C5 H9 N O4	C5 H9 N O4	87.45	147.053@10.842001
		10.919	174.1001	2.4	N2-Acetyl-L-ornithine	C7 H14 N2 O3	87.54	174.1001@10.919001
		10.458	220.0877	2.7	C10 H13 N4 P	C10 H13 N4 P	86.57	220.0877@10.458001
		10.597	236.0828	3.0	C10 H13 N4 O P	C10 H13 N4 O P	98.33	236.0828@10.597
		10.861	129.0424	2.4	4-Oxo-L-proline	C5 H7 N O3	87.61	129.0424@10.860999
		10.455	236.0826	3.7	Methionyl-Serine	C8 H16 N2 O4 S	98.7	236.0826@10.455001
		12.729	246.0847	15.2	C11 H21 P3	C11 H21 P3	86.99	246.0847@12.729002
		12.385	233.1009	5.6	C8 H15 N3 O5	C8 H15 N3 O5	85.41	233.1009@12.385
		9.404	190.0411	2.1	C6 H12 N2 O P2	C6 H12 N2 O P2	86.37	190.0411@9.404
		10.530	245.1370	2.3	Asparaginy-Isoleucine	C10 H19 N3 O4	86.17	245.137@10.53
		12.825	264.0777	4.9	C11 H13 N4 O2 P	C11 H13 N4 O2 P	86.03	264.0777@12.824998
		10.807	259.1531	2.7	Glutaminy-Isoleucine	C11 H21 N3 O4	99.71	259.1531@10.807001
		13.302	72.0210	6.8	C3 H4 O2	C3 H4 O2	87.95	72.021@13.302001
		12.944	434.1381	4.0	C19 H18 N10 O S	C19 H18 N10 O S	96.83	434.1381@12.944
		9.405	130.0190	2.0	C4 H6 N2 O S	C4 H6 N2 O S	75.82	130.019@9.405
		13.013	381.0675	3.5	C13 H15 N7 O3 S2	C13 H15 N7 O3 S2	98.31	381.0675@13.013
		12.192	162.0638	2.5	Glycyl-Serine	C5 H10 N2 O4	87.5	162.0638@12.192
		10.320	232.1054	4.2	Aspartyl-Valine	C9 H16 N2 O5	86.75	232.1054@10.320001
		9.531	372.2367	3.5	C16 H26 N11	C16 H26 N11	85.16	372.2367@9.530999
		12.852	260.1369	4.6	C11 H20 N2 O5	C11 H20 N2 O5	99.55	260.1369@12.852
		10.919	289.1633	2.6	C12 H23 N3 O5	C12 H23 N3 O5	84.78	289.1633@10.919001
		11.872	158.0689	2.5	C6 H10 N2 O3	C6 H10 N2 O3	87.02	158.0689@11.872
		10.155	293.1372	2.3	Glutaminy-Phenylalanine	C14 H19 N3 O4	82.8	293.1372@10.155
		12.250	277.1272	3.4	C10 H19 N3 O6	C10 H19 N3 O6	82.29	277.1272@12.25
		11.871	233.1010	2.9	Asparaginy-Threonine	C8 H15 N3 O5	86.8	233.101@11.871001
		10.847	232.0305	2.6	C5 H6 N5 O6	C5 H6 N5 O6	81.04	232.0305@10.847
		10.858	298.0774	6.9	C8 H10 N8 O5	C8 H10 N8 O5	83.24	298.0774@10.858001
		10.395	206.0721	2.4	Glycyl-Methionine	C7 H14 N2 O3 S	98.26	206.0721@10.395002
		12.000	261.1321	5.0	C9 H13 N10	C9 H13 N10	84.73	261.1321@12.0
		10.241	156.0894	3.9	C7 H12 N2 O2	C7 H12 N2 O2	87.54	156.0894@10.240999
		11.724	231.1218	3.4	Valyl-Asparagine	C9 H17 N3 O4	86.23	231.1218@11.724
		12.240	368.1426	7.5	C15 H31 O4 P3	C15 H31 O4 P3	83.87	368.1426@12.24
		10.833	245.1370	2.5	Asparaginy-Isoleucine	C10 H19 N3 O4	86.56	245.137@10.833001
		10.805	289.1632	3.1	C11 H17 N10	C11 H17 N10	84.98	289.1632@10.804999
		11.177	360.2006	4.1	C10 H25 N12 O P	C10 H25 N12 O P	86.92	360.2006@11.177001
		11.533	321.1529	3.1	C14 H30 N O P3	C14 H30 N O P3	85.88	321.1529@11.532999
		11.238	204.0744	3.5	C7 H12 N2 O5	C7 H12 N2 O5	85.97	204.0744@11.238001
		11.747	321.1167	3.4	C10 H13 N10 O3	C10 H13 N10 O3	85.89	321.1167@11.747
		12.279	216.1473	3.9	Valyl-Valine	C10 H20 N2 O3	86.62	216.1473@12.279001
		10.490	291.0950	2.3	C10 H11 N8 O3	C10 H11 N8 O3	85.5	291.095@10.489999
		11.993	384.1220	2.3	C12 H20 N9 O2 P2	C12 H20 N9 O2 P2	47.61	384.122@11.992998
		9.834	303.1792	4.9	C12 H19 N10	C12 H19 N10	84.78	303.1792@9.834
		10.870	309.1052	2.4	C8 H21 N7 P2 S	C8 H21 N7 P2 S	47.6	309.1052@10.870001
		11.664	338.0850	4.5	C13 H19 N5 P3	C13 H19 N5 P3	86.78	338.085@11.6640005
		12.294	247.1165	3.6	Glutaminy-Threonine	C9 H17 N3 O5	85.97	247.1165@12.294001
		-2.845	1.3230	280.1	C8 H14 N3 O6 S	C8 H14 N3 O6 S	93.28	280.061@1.323
HILIC_t56_c2	5	2.376	1.7040	222.0	C9 H7 N2 O3 P	C9 H7 N2 O3 P	86.46	222.0198@1.7040004
		2.015	2.0170	343.3	C21 H45 N O2	C21 H45 N O2	83.26	343.3454@2.017
		-3.936	1.5170	442.3	C22 H43 N4 O3 P	C22 H43 N4 O3 P	78.09	442.3087@1.5170001
		-80216.670	3.1200	499.3	C29 H45 N3 O4	C29 H45 N3 O4	97.6	499.3411@3.1199996
		-31777.752	10.5860	455.3	C25 H37 N5 O3	C25 H37 N5 O3	81.6	455.289@10.5859995