

Development and application of a data processing method for food metabolomics analysis

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The first data comes from a previous article on the study of goat milk fat. We tested the workflow system with raw mass spectrometry data of goat milk fat from a previous study. (<https://dx.doi.org/10.1021/acs.jafc.0c02234>). The second data (mzML) were downloaded from the MetaboLights (MTBLS549). For a number of reasons, we chose a total of 23 data in positive and negative ion mode to test the metabolomic workflows system. Additional details can be found at (<http://www.ebi.ac.uk/metabolights>).

Table S1. Triacylglycerols compound identified from workflow A and workflow C.**Workflow A**

Identifier	Formula	Description	m/z	rt (min)	Adduction
[LMGL03013748]	C51H92O6	TG (13:0_15:0_20:3)	818.7305	13.69	M+NH4;1+
[LMGL03013843]	C51H92O6	TG (13:0_17:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03013842]	C51H92O6	TG (13:0_17:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03013774]	C51H92O6	TG (13:0_15:1_20:2)	818.7305	13.69	M+NH4;1+
[LMGL03013864]	C51H92O6	TG (13:0_17:1_18:2)	818.7305	13.69	M+NH4;1+
[LMGL03013885]	C51H92O6	TG (13:0_17:2_18:1)	818.7305	13.69	M+NH4;1+
[LMGL03014229]	C51H92O6	TG (14:0_16:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03014228]	C51H92O6	TG (14:0_16:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03014154]	C51H92O6	TG (14:0_14:1_20:2)	818.7305	13.69	M+NH4;1+
[LMGL03014252]	C51H92O6	TG (14:0_16:1_18:2)	818.7305	13.69	M+NH4;1+
[LMGL03014296]	C51H92O6	TG (14:0_17:1_17:2)	818.7305	13.69	M+NH4;1+
[LMGL03014985]	C51H92O6	TG (15:0_15:1_18:2)	818.7305	13.69	M+NH4;1+
[LMGL03015033]	C51H92O6	TG (15:0_16:1_17:2)	818.7305	13.69	M+NH4;1+
[LMGL03013234]	C51H92O6	TG (12:0_14:0_22:3)	818.7305	13.69	M+NH4;1+
[LMGL03013444]	C51H92O6	TG (12:0_18:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03013443]	C51H92O6	TG (12:0_18:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03013336]	C51H92O6	TG (12:0_16:0_20:3)	818.7305	13.69	M+NH4;1+
[LMGL03013262]	C51H92O6	TG (12:0_14:1_22:2)	818.7305	13.69	M+NH4;1+
[LMGL03013462]	C51H92O6	TG (12:0_18:1_18:2)	818.7305	13.69	M+NH4;1+
[LMGL03013360]	C51H92O6	TG (12:0_16:1_20:2)	818.7305	13.69	M+NH4;1+

[LMGL03013426]	C51H92O6	TG (12:0_17:2_19:1)	818.7305	13.69	M+NH4;1+
[LMGL03012718]	C51H92O6	TG (13:0_13:0_22:3)	818.7305	13.69	M+NH4;1+
[LMGL03012772]	C51H92O6	TG (14:0_14:0_20:3)	818.7305	13.69	M+NH4;1+
[LMGL03012881]	C51H92O6	TG (15:0_15:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03012880]	C51H92O6	TG (15:0_15:0_18:3)	818.7305	13.69	M+NH4;1+
[LMGL03012829]	C51H92O6	TG (14:1_14:1_20:1)	818.7305	13.69	M+NH4;1+
[LMGL03012933]	C51H92O6	TG (15:1_15:1_18:1)	818.7305	13.69	M+NH4;1+
[LMGL03010020]	C51H92O6	TG (16:1/16:1/16:1)	818.7305	13.69	M+NH4;1+
[LMGL03014633]	C51H92O6	TG (14:1_16:0_18:2)	818.7305	13.69	M+NH4;1+
[LMGL03014679]	C51H92O6	TG (14:1_17:0_17:2)	818.7305	13.69	M+NH4;1+
[LMGL03012847]	C51H92O6	TG (14:1_17:1_17:1)	818.7305	13.69	M+NH4;1+
[LMGL03014612]	C51H92O6	TG (14:1_15:1_19:1)	818.7305	13.69	M+NH4;1+
[LMGL03014657]	C51H92O6	TG (14:1_16:1_18:1)	818.7305	13.69	M+NH4;1+
[LMGL03015359]	C51H92O6	TG (15:1_16:0_17:2)	818.7305	13.69	M+NH4;1+
[LMGL03015383]	C51H92O6	TG (15:1_16:1_17:1)	818.7305	13.69	M+NH4;1+
Workflow C					
[UT000511]	C51H92O6	Triacylglycerol 14:0-16:1-18:2	818.7304	13.81	[M+NH4]+

Table S 2 The information of 442 compounds identified by Workflow B

Row ID	Formula	m/z	rt (min)	Adduction
Row 42#0	C36H67N3O19	846.4419	3.00	[M + H] ⁺
Row 705#8	C25H22N2O10S9	798.8850	15.92	[M + H] ⁺
Row 672#6	C36H38O19	775.2117	15.46	[M + H] ⁺
Row 712#0	C18H37NO22P4	744.0825	14.56	[M + H] ⁺
Row 591#7	C20H32N3O21P3	744.0820	14.47	[M + H] ⁺
Row 31#3	C37H71NO12	722.5045	2.97	[M + H] ⁺
Row 685#1	C21H22N14O13S	711.1264	14.90	[M + H] ⁺
Row 94#2	C34H59N7O8	694.4493	3.50	[M + H] ⁺
Row 35#8	C36H63N5O7	678.4783	2.94	[M + H] ⁺
Row 4#2	C33H41N11O5	672.3414	2.62	[M + H] ⁺
Row 724#9	C20H24N8O18	665.1268	17.68	[M + H] ⁺
Row 472#3	C22H23N11O10P2	664.1153	11.93	[M + H] ⁺
Row 627#10	C31H28O16	657.1476	14.94	[M + H] ⁺
Row 10#0	C36H46O11	655.3159	2.68	[M + H] ⁺
Row 26#0	C27H39N15O5	654.3315	2.86	[M + H] ⁺
Row 597#4	C25H35NO19	654.1844	14.30	[M + H] ⁺
Row 51#7	C29H57N5O11	652.4105	3.40	[M + H] ⁺
Row 637#9	C39H20N2O8	645.1299	14.60	[M + H] ⁺
Row 624#3	C33H22N4O10	635.1396	14.87	[M + H] ⁺
Row 21#10	C33H63NO10	634.4509	2.88	[M + H] ⁺
Row 638#10	C20H32N6O12S2	613.1586	14.94	[M + H] ⁺
Row 51#1	C27H53N5O10	608.3845	3.38	[M + H] ⁺
Row 502#7	C23H25N7O5S4	608.0877	12.62	[M + H] ⁺
Row 666#10	C9H22O22P4	606.9613	15.75	[M + H] ⁺
Row 658#3	C26H21O17	606.0839	15.53	[M + H] ⁺
Row 660#4	C26H21O17	606.0833	15.45	[M + H] ⁺
Row 406#3	C23H29N2O7PS4	605.0628	11.13	[M + H] ⁺
Row 37#0	C31H54N2O9	599.3896	2.96	[M + H] ⁺
Row 765#0	C19H19NO17P2	596.0187	15.79	[M + H] ⁺
Row 90#5	C29H42N10O4	595.3477	3.70	[M + H] ⁺
Row 134#5	C29H38N10O4	591.3165	4.20	[M + H] ⁺
Row 76#5	C30H48N6O6	589.3700	3.53	[M + H] ⁺
Row 92#2	C30H48N6O6	589.3700	3.47	[M + H] ⁺
Row 722#0	C21H29N6O10PS	589.1471	14.71	[M + H] ⁺
Row 9#2	C29H32N10O4	585.2693	2.71	[M + H] ⁺
Row 557#7	C23H21NO17	584.0878	13.71	[M + H] ⁺
Row 406#10	C26H21O15	574.0936	10.87	[M + H] ⁺
Row 648#6	C19H21N9O12	568.1375	15.02	[M + H] ⁺
Row 631#1	C9H19N3O17P2S2	567.9691	13.80	[M + H] ⁺
Row 11#0	C26H50N2O7P2	565.3151	2.73	[M + H] ⁺
Row 620#7	C27H24N4O8S	565.1375	15.00	[M + H] ⁺

Row 51#10	C25H49N5O9	564.3577	3.33	[M + H] ⁺
Row 44#3	C26H49N5O8	560.3633	3.11	[M + H] ⁺
Row 688#2	C30H19N3O8	550.1265	14.97	[M + H] ⁺
Row 656#7	C9H18N3O14P3S2	549.9515	15.89	[M + H] ⁺
Row 67#2	C32H48O7	545.3439	3.40	[M + H] ⁺
Row 570#1	C29H26O10	535.1630	12.50	[M + H] ⁺
Row 524#9	C29H26O10	535.1628	12.55	[M + H] ⁺
Row 214#1	C26H23N7O6	530.1794	5.54	[M + H] ⁺
Row 230#5	C26H23N7O6	530.1791	5.44	[M + H] ⁺
Row 565#7	C16H14N5O8P3S	529.9834	13.91	[M + H] ⁺
Row 576#10	C24H12O14	525.0278	13.80	[M + H] ⁺
Row 785#0	C12H11N7O13P2	523.9976	16.51	[M + H] ⁺
Row 724#6	C9H20NO18P3	523.9973	16.37	[M + H] ⁺
Row 56#10	C23H45N5O8	520.3318	3.37	[M + H] ⁺
Row 642#0	C24H38N8O5	519.3022	13.21	[M + H] ⁺
Row 442#5	C25H43N7O4	506.3466	10.01	[M + H] ⁺
Row 269#10	C30H47O6	504.3417	6.85	[M + H] ⁺
Row 50#5	C30H44O6	501.3179	3.43	[M + H] ⁺
Row 711#9	C15H14N8O12	499.0789	16.51	[M + H] ⁺
Row 694#10	C26H14N2O9	499.0787	16.45	[M + H] ⁺
Row 215#3	C33H36N2O2	493.2803	6.22	[M + H] ⁺
Row 117#7	C21H39N5O8	490.2850	4.23	[M + H] ⁺
Row 516#7	C27H20O9	489.1137	12.87	[M + H] ⁺
Row 48#3	C27H44N6O2	485.3579	3.16	[M + H] ⁺
Row 720#6	C22H37N5O7	484.2760	16.12	[M + H] ⁺
Row 560#3	C31H17NO5	484.1163	13.74	[M + H] ⁺
Row 286#3	C32H28O4	477.2040	8.47	[M + H] ⁺
Row 64#8	C21H41N5O7	476.3063	3.48	[M + H] ⁺
Row 56#7	C21H41N5O7	476.3061	3.51	[M + H] ⁺
Row 39#7	C23H43N5O5	470.3319	2.98	[M + H] ⁺
Row 831#0	C19H39N3O10	470.2704	22.65	[M + H] ⁺
Row 610#0	C24H23NO9	470.1437	12.70	[M + H] ⁺
Row 18#0	C23H25N5O6	468.1910	2.81	[M + H] ⁺
Row 573#6	C15H17N9O9	468.1215	13.77	[M + H] ⁺
Row 15#2	C21H28N3O7P	466.1749	2.76	[M + H] ⁺
Row 725#5	C8H19N9O14	466.1118	16.00	[M + H] ⁺
Row 135#0	C24H25N5O5	464.1914	4.00	[M + H] ⁺
Row 592#7	C16H27N7O9	462.1937	14.47	[M + H] ⁺
Row 546#1	C28H26O6	459.1834	12.21	[M + H] ⁺
Row 566#2	C19H26N3O10	457.1679	12.29	[M + H] ⁺
Row 624#2	C18H20N10O5	457.1679	13.65	[M + H] ⁺
Row 568#10	C18H20N10O5	457.1678	13.47	[M + H] ⁺
Row 213#8	C22H31NO9	454.2069	5.29	[M + H] ⁺
Row 15#6	C22H23N6O3P	451.1645	2.80	[M + H] ⁺

Row 527#3	C11H20N3O8PS3	450.0180	12.89	[M + H] ⁺
Row 606#6	C11H16N10O6S2	449.0767	14.37	[M + H] ⁺
Row 116#3	C19H35N5O7	446.2594	4.35	[M + H] ⁺
Row 646#10	C9H19NO15P2	444.0310	15.39	[M + H] ⁺
Row 598#6	C22H20N2O6S	441.1107	14.12	[M + H] ⁺
Row 122#8	C22H37N3O6	440.2772	4.36	[M + H] ⁺
Row 61#7	C19H37N5O6	432.2800	3.54	[M + H] ⁺
Row 25#3	C25H29N5O2	432.2379	3.01	[M + H] ⁺
Row 511#7	C15H10N8O8	431.0719	12.77	[M + H] ⁺
Row 397#8	C14H17N7O9	428.1153	10.28	[M + H] ⁺
Row 527#6	C9H19NO14P2	428.0363	12.81	[M + H] ⁺
Row 615#8	C13H22N4O8S2	427.0952	14.46	[M + H] ⁺
Row 170#0	C24H43NO5	426.3214	4.51	[M + H] ⁺
Row 128#6	C24H43NO5	426.3213	4.42	[M + H] ⁺
Row 33#1	C21H39N5O4	426.3061	2.97	[M + H] ⁺
Row 713#8	C7H13N13O9	424.1021	16.12	[M + H] ⁺
Row 510#8	C12H19N7O10	422.1260	11.99	[M + H] ⁺
Row 14#1	C21H29N5O4	416.2275	2.83	[M + H] ⁺
Row 71#7	C19H34N4O6	415.2535	3.58	[M + H] ⁺
Row 24#7	C25H26N4O2	415.2113	2.98	[M + H] ⁺
Row 340#8	C22H24N4O4	409.1870	9.05	[M + H] ⁺
Row 611#5	C9H24N6O12	409.1531	12.85	[M + H] ⁺
Row 660#0	C19H35O9	408.2341	13.75	[M + H] ⁺
Row 262#4	C17H26N8O4	407.2127	6.70	[M + H] ⁺
Row 724#2	C9H14N2O16	407.0424	15.43	[M + H] ⁺
Row 42#8	C22H29NO6	404.2072	3.08	[M + H] ⁺
Row 100#0	C17H33N5O5	388.2541	3.67	[M + H] ⁺
Row 43#6	C26H26O3	387.1925	3.00	[M + H] ⁺
Row 148#5	C19H37N4O4	386.2895	4.34	[M + H] ⁺
Row 456#10	C18H19N5O5	386.1457	11.52	[M + H] ⁺
Row 423#7	C9H20N8O7S	385.1283	11.24	[M + H] ⁺
Row 26#1	C19H35N5O3	382.2798	2.97	[M + H] ⁺
Row 715#3	C9H30N10O4S	375.2234	16.90	[M + H] ⁺
Row 511#9	C16H30N4O6	375.2231	12.17	[M + H] ⁺
Row 103#0	C17H30N4O5	371.2277	3.64	[M + H] ⁺
Row 104#5	C21H39NO4	370.2946	3.77	[M + H] ⁺
Row 312#10	C22H27NO4	370.1998	8.21	[M + H] ⁺
Row 700#7	C18H32N4O4	369.2489	21.25	[M + H] ⁺
Row 105#4	C21H37NO4	368.2789	3.86	[M + H] ⁺
Row 348#5	C17H22N2O7	367.1492	8.16	[M + H] ⁺
Row 706#10	C13H22N2O10	367.1341	17.66	[M + H] ⁺
Row 10#1	C20H31N2O2P	363.2198	2.79	[M + H] ⁺
Row 495#3	C21H20N4O2	361.1649	12.22	[M + H] ⁺
Row 305#8	C20H23NO5	358.1667	7.51	[M + H] ⁺

Row 592#0	C24H21O3	358.1543	12.45	[M + H] ⁺
Row 821#0	C17H32N4O4	357.2496	21.61	[M + H] ⁺
Row 740#4	C17H32N4O4	357.2491	21.41	[M + H] ⁺
Row 334#6	C7H19N11O6	354.1565	9.25	[M + H] ⁺
Row 639#5	C16H26N6O3	351.2121	13.53	[M + H] ⁺
Row 545#3	C8H22N12O4	351.1983	13.38	[M + H] ⁺
Row 226#3	C14H21O10	350.1206	6.59	[M + H] ⁺
Row 266#5	C14H21O10	350.1205	6.36	[M + H] ⁺
Row 448#3	C12H20N4O4S2	349.0996	11.69	[M + H] ⁺
Row 439#3	C9H18NO11P	348.0701	11.60	[M + H] ⁺
Row 425#7	C9H18NO11P	348.0699	11.38	[M + H] ⁺
Row 533#7	C8H18N12O4	347.1669	13.02	[M + H] ⁺
Row 102#1	C20H33N5	344.2791	4.05	[M + H] ⁺
Row 427#1	C9H22N5O7P	344.1339	10.57	[M + H] ⁺
Row 445#5	C16H17N5O4	344.1336	10.21	[M + H] ⁺
Row 722#3	C9H9N7O8	344.0586	17.71	[M + H] ⁺
Row 108#1	C19H35NO4	342.2636	4.14	[M + H] ⁺
Row 659#10	C8H9N2O11P	341.0029	15.60	[M + H] ⁺
Row 675#2	C8H15N6O7S	340.0805	14.53	[M + H] ⁺
Row 613#10	C10H19N3O6P2	340.0803	14.49	[M + H] ⁺
Row 354#7	C9H22N8O6	339.1756	9.68	[M + H] ⁺
Row 651#0	C15H24N6O3	337.1972	13.49	[M + H] ⁺
Row 644#10	C14H26NO8	337.1713	15.14	[M + H] ⁺
Row 398#4	C9H12N4O10	337.0637	10.71	[M + H] ⁺
Row 556#10	C8H17N9O6	336.1395	13.22	[M + H] ⁺
Row 459#8	C9H21N2O7PS	333.0863	11.45	[M + H] ⁺
Row 199#0	C20H31N2O2	332.2431	4.67	[M + H] ⁺
Row 148#10	C17H33NO5	332.2426	4.41	[M + H] ⁺
Row 284#4	C19H25NO2S	332.1696	7.31	[M + H] ⁺
Row 481#0	C15H23O8	332.1455	10.84	[M + H] ⁺
Row 364#7	C15H23O8	332.1447	9.93	[M + H] ⁺
Row 261#8	C16H17N5O3	328.1390	6.57	[M + H] ⁺
Row 244#7	C16H17N5O3	328.1386	6.46	[M + H] ⁺
Row 111#2	C15H26N4O4	327.2011	3.62	[M + H] ⁺
Row 604#10	C9H22N8O5	323.1813	14.24	[M + H] ⁺
Row 756#5	C9H13N4O9	322.0766	17.72	[M + H] ⁺
Row 298#6	C15H24N6O2	321.2018	8.60	[M + H] ⁺
Row 310#7	C15H24N6O2	321.2016	8.49	[M + H] ⁺
Row 285#2	C17H22N2O4	319.1649	6.07	[M + H] ⁺
Row 434#3	C14H21O8	318.1295	11.51	[M + H] ⁺
Row 415#7	C14H21O8	318.1292	11.29	[M + H] ⁺
Row 116#1	C18H29N5	316.2479	4.38	[M + H] ⁺
Row 39#1	C17H25N5O	316.2118	3.14	[M + H] ⁺
Row 165#0	C17H31NO4	314.2327	4.51	[M + H] ⁺

Row 123#1	C17H31NO4	314.2326	4.38	[M + H] ⁺
Row 540#7	C9H17N4O8	310.1131	13.52	[M + H] ⁺
Row 628#5	C9H17N4O8	310.1130	13.48	[M + H] ⁺
Row 605#4	C8H20N8O5	309.1655	14.36	[M + H] ⁺
Row 689#7	C13H20N6O3	309.1654	18.62	[M + H] ⁺
Row 655#4	C8H20N8O5	309.1653	15.31	[M + H] ⁺
Row 444#4	C9H18N5O7	309.1288	11.47	[M + H] ⁺
Row 143#6	C17H25NO4	308.1856	4.51	[M + H] ⁺
Row 577#0	C8H15N6O5S	308.0910	12.05	[M + H] ⁺
Row 771#0	C8H23N2O4P2S	306.0932	15.90	[M + H] ⁺
Row 575#1	C18H11NO4	306.0752	12.54	[M + H] ⁺
Row 181#3	C16H25N5O	304.2117	5.24	[M + H] ⁺
Row 474#10	C9H19O7PS	303.0675	11.70	[M + H] ⁺
Row 104#1	C16H23N5O	302.1961	4.14	[M + H] ⁺
Row 112#7	C9H23N4O5P	299.1489	4.13	[M + H] ⁺
Row 8#4	C9H22N4O5S	299.1389	2.75	[M + H] ⁺
Row 720#10	C13H23N5O3	298.1869	20.19	[M + H] ⁺
Row 155#7	C9H20N3O4PS	298.0965	4.62	[M + H] ⁺
Row 556#3	C8H15N4O8	296.0976	13.69	[M + H] ⁺
Row 563#10	C8H15N4O8	296.0974	13.47	[M + H] ⁺
Row 625#7	C9H20N5O6	295.1500	15.13	[M + H] ⁺
Row 601#3	C9H20N5O6	295.1500	14.48	[M + H] ⁺
Row 238#3	C13H19N5O3	294.1545	6.85	[M + H] ⁺
Row 534#4	C6H16N10O4	293.1451	12.39	[M + H] ⁺
Row 632#7	C12H22N2O6	291.1551	15.33	[M + H] ⁺
Row 482#8	C9H16N5O6	291.1190	11.76	[M + H] ⁺
Row 438#7	C9H16N5O6	291.1186	11.43	[M + H] ⁺
Row 423#10	C9H17N6O5	290.1344	11.21	[M + H] ⁺
Row 117#6	C19H31N2	288.2533	4.15	[M + H] ⁺
Row 47#5	C19H31N2	288.2532	3.12	[M + H] ⁺
Row 143#1	C15H27NO4	286.2012	4.60	[M + H] ⁺
Row 158#10	C15H27NO4	286.2008	4.50	[M + H] ⁺
Row 65#0	C9H23N3O5S	286.1439	3.23	[M + H] ⁺
Row 219#7	C5H16N7O5P	286.1031	5.65	[M + H] ⁺
Row 749#2	C5H6N3O9P	283.9927	15.78	[M + H] ⁺
Row 100#5	C8H22N6O5	283.1749	3.77	[M + H] ⁺
Row 75#3	C15H15N5O	282.1371	3.54	[M + H] ⁺
Row 196#7	C7H11N11O2	282.1194	5.12	[M + H] ⁺
Row 400#7	C8H17N4O7	282.1185	11.15	[M + H] ⁺
Row 192#3	C8H21N7O2S	280.1543	5.63	[M + H] ⁺
Row 203#1	C9H22N5O3P	280.1542	5.46	[M + H] ⁺
Row 316#6	C9H19N4O6	280.1390	9.06	[M + H] ⁺
Row 188#8	C9H23N7OS	278.1749	4.99	[M + H] ⁺
Row 426#5	C9H17N4O6	278.1231	9.53	[M + H] ⁺

Row 597#10	C7H12N5O5P	278.0631	14.13	[M + H] ⁺
Row 242#3	C9H21N7O3	276.1804	6.79	[M + H] ⁺
Row 307#2	C9H21N7O3	276.1802	6.49	[M + H] ⁺
Row 405#7	C9H13N4O6	274.0915	11.15	[M + H] ⁺
Row 161#7	C15H21N5	272.1853	4.57	[M + H] ⁺
Row 282#1	C7H10N8O4	271.0922	6.69	[M + H] ⁺
Row 551#0	C9H17NO8	268.1026	11.87	[M + H] ⁺
Row 174#3	C15H21O4	266.1513	5.14	[M + H] ⁺
Row 456#0	C8H17N4O6	266.1233	10.56	[M + H] ⁺
Row 386#10	C8H17N4O6	266.1230	10.44	[M + H] ⁺
Row 145#8	C9H19N3O4P	265.1183	4.47	[M + H] ⁺
Row 184#0	C9H19N3O4P	265.1182	4.59	[M + H] ⁺
Row 524#10	C7H11N4O5P	263.0522	12.58	[M + H] ⁺
Row 311#9	C8H19N7O3	262.1644	8.22	[M + H] ⁺
Row 408#4	C9H17N4O5	262.1282	11.01	[M + H] ⁺
Row 350#9	C9H17N4O5	262.1281	9.15	[M + H] ⁺
Row 590#3	C8H8N2O8	261.0369	14.28	[M + H] ⁺
Row 191#9	C9H21N7O2	260.1852	4.90	[M + H] ⁺
Row 535#5	C8H20N6P	258.1097	11.49	[M + H] ⁺
Row 482#7	C9H16N5O2P	258.1097	12.18	[M + H] ⁺
Row 284#0	C9H14N5O4	257.1131	6.68	[M + H] ⁺
Row 240#6	C9H14N5O4	257.1130	6.44	[M + H] ⁺
Row 238#5	C9H14N6O3	255.1222	5.44	[M + H] ⁺
Row 196#5	C9H14N7O2	253.1279	4.74	[M + H] ⁺
Row 386#5	C8H18N3O4S	253.1085	8.84	[M + H] ⁺
Row 410#4	C9H17NO7	252.1074	11.15	[M + H] ⁺
Row 491#4	C8H6N6O2S	251.0361	11.93	[M + H] ⁺
Row 667#7	C8H11NO6S	250.0377	16.28	[M + H] ⁺
Row 311#3	C9H19N4O4	248.1489	9.12	[M + H] ⁺
Row 237#1	C14H18N2O2	247.1438	6.03	[M + H] ⁺
Row 577#7	C9H14N2O6	247.0935	14.01	[M + H] ⁺
Row 756#3	C9H21N6O2	246.1810	23.14	[M + H] ⁺
Row 215#6	C12H21NO4	244.1541	5.87	[M + H] ⁺
Row 284#6	C6H20N4O2PS	244.1111	8.05	[M + H] ⁺
Row 345#4	C6H20N4O2PS	244.1109	9.66	[M + H] ⁺
Row 341#0	C8H23N3O3P	241.1545	7.73	[M + H] ⁺
Row 387#7	C8H23N3O3P	241.1544	10.37	[M + H] ⁺
Row 380#3	C8H23N3O3P	241.1544	10.55	[M + H] ⁺
Row 279#9	C8H23N3O3P	241.1542	7.43	[M + H] ⁺
Row 104#10	C8H20N3O5	239.1486	3.88	[M + H] ⁺
Row 759#6	C9H18O7	239.1136	20.20	[M + H] ⁺
Row 287#6	C9H14N6S	239.1058	8.37	[M + H] ⁺
Row 445#7	C9H11N5O3	238.0918	11.57	[M + H] ⁺
Row 297#3	C8H20N5O3	235.1649	8.77	[M + H] ⁺

Row 485#5	C9H15NO6	234.0968	10.85	[M + H] ⁺
Row 332#3	C9H15NO4S	234.0793	9.57	[M + H] ⁺
Row 353#10	C9H15NO4S	234.0791	9.36	[M + H] ⁺
Row 278#0	C9H19N4O3	232.1544	6.53	[M + H] ⁺
Row 234#6	C9H19N4O3	232.1542	6.29	[M + H] ⁺
Row 372#7	C8H16N5O3	231.1335	10.12	[M + H] ⁺
Row 443#3	C9H15N3O4	230.1135	11.60	[M + H] ⁺
Row 429#7	C9H15N3O4	230.1133	11.38	[M + H] ⁺
Row 268#6	C9H18N5O2	229.1545	7.58	[M + H] ⁺
Row 381#4	C9H18N5O2	229.1544	10.67	[M + H] ⁺
Row 288#4	C9H18N5O2	229.1543	7.50	[M + H] ⁺
Row 266#9	C8H14N6O2	227.1246	6.91	[M + H] ⁺
Row 156#1	C6H15N4O3P	223.0964	4.55	[M + H] ⁺
Row 156#10	C6H15N4O3P	223.0961	4.46	[M + H] ⁺
Row 346#3	C9H11N5O2	222.0970	9.88	[M + H] ⁺
Row 207#3	C9H17NO5	220.1178	5.88	[M + H] ⁺
Row 187#6	C8H13NO4S	220.0636	5.03	[M + H] ⁺
Row 242#6	C7H11N3O3S	218.0593	6.60	[M + H] ⁺
Row 300#2	C7H11N3O3S	218.0591	6.49	[M + H] ⁺
Row 367#4	C8H15N4O3	216.1227	10.28	[M + H] ⁺
Row 641#7	C8H9NO2PS	215.0161	15.53	[M + H] ⁺
Row 714#2	C6H4N3O6	215.0159	15.43	[M + H] ⁺
Row 284#10	C8H19NO3S	210.1140	7.24	[M + H] ⁺
Row 687#6	C7H7N5O3	210.0609	15.56	[M + H] ⁺
Row 715#1	C7H7N5O3	210.0608	15.48	[M + H] ⁺
Row 184#3	C9H12N4O2	209.1017	5.24	[M + H] ⁺
Row 211#10	C9H19O5	208.1324	5.35	[M + H] ⁺
Row 183#7	C9H9N4O2	206.0809	4.97	[M + H] ⁺
Row 509#5	C7H11NO4S	206.0478	11.19	[M + H] ⁺
Row 306#3	C9H10N5O	205.0968	8.97	[M + H] ⁺
Row 503#5	C9H15O5	204.0976	11.09	[M + H] ⁺
Row 347#6	C9H9N5O	204.0866	9.51	[M + H] ⁺
Row 366#9	C9H9N5O	204.0864	9.45	[M + H] ⁺
Row 726#4	C8H18N4O2	203.1499	19.82	[M + H] ⁺
Row 372#3	C9H18N2O3	203.1388	10.55	[M + H] ⁺
Row 361#4	C9H18N2O3	203.1387	10.33	[M + H] ⁺
Row 276#9	C9H21N4O	202.1798	7.10	[M + H] ⁺
Row 209#10	C9H21N4O	202.1797	5.30	[M + H] ⁺
Row 304#9	C9H17N3S	200.1214	7.99	[M + H] ⁺
Row 531#5	C6H15NO6	198.0968	11.49	[M + H] ⁺
Row 516#0	C8H11N3O3	198.0874	11.55	[M + H] ⁺
Row 110#3	C7H7N3O4	198.0523	4.21	[M + H] ⁺
Row 132#9	C9H14N4O	195.1223	4.23	[M + H] ⁺
Row 478#9	C7H6N4OS	195.0319	11.78	[M + H] ⁺

Row 420#6	C8H22N2OP	194.1538	11.07	[M + H] ⁺
Row 336#0	C8H16O3S	193.0877	7.59	[M + H] ⁺
Row 267#3	C8H16O3S	193.0875	7.46	[M + H] ⁺
Row 118#4	C9H21NO3	192.1590	4.03	[M + H] ⁺
Row 360#4	C9H13N5	192.1225	10.13	[M + H] ⁺
Row 484#7	C6H9NO4S	192.0321	12.18	[M + H] ⁺
Row 749#4	C8H10N6	191.1022	23.03	[M + H] ⁺
Row 726#10	C9H20N2O2	189.1594	20.52	[M + H] ⁺
Row 758#10	C9H18NO3	189.1342	25.16	[M + H] ⁺
Row 201#6	C8H16N2O3	189.1233	5.62	[M + H] ⁺
Row 337#7	C9H17NO3	188.1277	9.23	[M + H] ⁺
Row 223#7	C9H7N4O	188.0703	5.99	[M + H] ⁺
Row 353#5	C9H15NO3	186.1122	8.34	[M + H] ⁺
Row 322#4	C9H15NO3	186.1121	9.21	[M + H] ⁺
Row 502#3	C9H16NOP	186.1057	12.30	[M + H] ⁺
Row 283#7	C9H13O4	186.0869	7.45	[M + H] ⁺
Row 348#6	C8H11NO4	186.0760	9.51	[M + H] ⁺
Row 470#2	C4H11NO7	186.0619	10.66	[M + H] ⁺
Row 621#0	C9H11O4	184.0733	12.95	[M + H] ⁺
Row 134#6	C7H8N4O2	181.0718	4.51	[M + H] ⁺
Row 136#1	C9H10NO3	181.0718	4.45	[M + H] ⁺
Row 131#8	C9H9NO3	180.0655	4.44	[M + H] ⁺
Row 209#9	C6H13NOP2	178.0530	5.31	[M + H] ⁺
Row 359#3	C8H17NO3	176.1278	10.17	[M + H] ⁺
Row 562#9	C8H15O4	176.1026	13.27	[M + H] ⁺
Row 224#10	C8H7N4O	176.0703	5.59	[M + H] ⁺
Row 277#6	C8H18N2O2	175.1439	7.79	[M + H] ⁺
Row 692#7	C8H18N2O2	175.1438	19.11	[M + H] ⁺
Row 780#5	C8H16NO3	175.1186	24.23	[M + H] ⁺
Row 355#8	C7H14N2O3	175.1077	9.44	[M + H] ⁺
Row 427#6	C7H14N2O3	175.1075	11.21	[M + H] ⁺
Row 111#6	C9H19NO2	174.1487	4.06	[M + H] ⁺
Row 241#10	C8H12O4	173.0805	6.10	[M + H] ⁺
Row 126#6	C9H17NO2	172.1331	4.29	[M + H] ⁺
Row 386#3	C9H17NO2	172.1330	10.55	[M + H] ⁺
Row 382#7	C9H17NO2	172.1329	10.37	[M + H] ⁺
Row 835#2	C9H18N2O	171.1489	23.99	[M + H] ⁺
Row 27#7	C8H16N3O	171.1377	2.98	[M + H] ⁺
Row 254#1	C7H10N2O3	171.0762	6.19	[M + H] ⁺
Row 201#0	C9H15NO2	170.1175	4.72	[M + H] ⁺
Row 487#0	C9H13O3	170.0923	10.89	[M + H] ⁺
Row 349#3	C9H13O3	170.0921	10.07	[M + H] ⁺
Row 260#5	C7H10N2OP	170.0598	6.03	[M + H] ⁺
Row 711#7	C6H10N5O	169.0945	22.98	[M + H] ⁺

Row 230#0	C7H8N2O3	169.0606	5.17	[M + H] ⁺
Row 455#5	C5H4N4O3	169.0354	10.31	[M + H] ⁺
Row 410#9	C7H6NO4	169.0352	10.78	[M + H] ⁺
Row 231#3	C9H11NO2	166.0860	6.59	[M + H] ⁺
Row 251#4	C9H11NO2	166.0859	6.47	[M + H] ⁺
Row 126#9	C7H8N4O	165.0755	4.13	[M + H] ⁺
Row 375#4	C9H8O3	165.0544	10.39	[M + H] ⁺
Row 359#8	C7H15NO3	162.1124	9.54	[M + H] ⁺
Row 327#4	C7H15NO3	162.1121	9.31	[M + H] ⁺
Row 223#8	C7H7N5	162.0760	5.57	[M + H] ⁺
Row 131#10	C6H13NP2	162.0580	4.25	[M + H] ⁺
Row 739#10	C7H16N2O2	161.1280	21.77	[M + H] ⁺
Row 208#6	C6H9O3P	161.0377	5.77	[M + H] ⁺
Row 275#0	C8H17NO2	160.1331	6.16	[M + H] ⁺
Row 337#3	C7H13NO3	160.0966	9.78	[M + H] ⁺
Row 198#2	C6H9NO2S	160.0423	4.62	[M + H] ⁺
Row 319#4	C6H13N3P	159.0913	8.88	[M + H] ⁺
Row 551#10	C6H10N2O3	159.0760	13.16	[M + H] ⁺
Row 256#3	C7H10O4	159.0650	7.37	[M + H] ⁺
Row 235#6	C8H15NO2	158.1174	6.24	[M + H] ⁺
Row 520#7	C8H11O3	156.0764	12.92	[M + H] ⁺
Row 466#7	C8H11O3	156.0764	11.83	[M + H] ⁺
Row 297#1	C8H11O3	156.0764	6.83	[M + H] ⁺
Row 208#7	C8H9O3	154.0610	5.65	[M + H] ⁺
Row 170#3	CH8N5O2P	154.0495	5.04	[M + H] ⁺
Row 218#5	CH9N6OP	153.0655	5.08	[M + H] ⁺
Row 204#8	C7H10N4	151.0963	5.04	[M + H] ⁺
Row 311#6	C9H10P	150.0581	8.84	[M + H] ⁺
Row 347#7	C6H13NO3	148.0964	9.49	[M + H] ⁺
Row 335#4	C6H13NO3	148.0964	9.50	[M + H] ⁺
Row 473#7	C6H5N5	148.0600	11.91	[M + H] ⁺
Row 155#8	C9H8P	148.0425	4.56	[M + H] ⁺
Row 741#10	C6H14N2O2	147.1123	22.87	[M + H] ⁺
Row 513#10	C5H10N2O3	147.0759	12.29	[M + H] ⁺
Row 437#8	C7H15NO2	146.1175	11.20	[M + H] ⁺
Row 352#3	C6H11NO3	146.0808	10.07	[M + H] ⁺
Row 232#4	C9H7NO	146.0597	5.99	[M + H] ⁺
Row 181#6	C5H9NP2	146.0267	4.93	[M + H] ⁺
Row 290#6	C6H8O4	145.0492	8.52	[M + H] ⁺
Row 313#10	C6H8O4	145.0491	8.34	[M + H] ⁺
Row 225#6	C6H8O2S	145.0315	6.05	[M + H] ⁺
Row 282#8	H6N3O6	145.0315	6.82	[M + H] ⁺
Row 695#7	C8H17NO	144.1380	20.57	[M + H] ⁺
Row 291#4	C7H13NO2	144.1015	7.94	[M + H] ⁺

Row 219#3	C6H12N2P	144.0805	6.22	[M + H] ⁺
Row 354#0	C7H11NO2	142.0861	7.88	[M + H] ⁺
Row 233#1	C7H11NO2	142.0860	5.69	[M + H] ⁺
Row 810#2	C7H11NO2	142.0859	21.80	[M + H] ⁺
Row 276#1	C6H8N2O2	141.0655	6.69	[M + H] ⁺
Row 317#3	H7N7S	138.0547	9.22	[M + H] ⁺
Row 314#5	C7H6NO2	137.0454	7.21	[M + H] ⁺
Row 382#3	C8H9NO	136.0754	10.51	[M + H] ⁺
Row 371#4	C8H9NO	136.0754	10.39	[M + H] ⁺
Row 770#1	C7H7N2O	136.0615	17.12	[M + H] ⁺
Row 261#7	CH8N6P	136.0614	6.66	[M + H] ⁺
Row 585#10	CH8N6P	136.0614	13.94	[M + H] ⁺
Row 545#4	CH8N6P	136.0614	12.88	[M + H] ⁺
Row 756#10	CH8N6P	136.0614	24.72	[M + H] ⁺
Row 163#6	C8H7NO	134.0598	4.79	[M + H] ⁺
Row 191#3	C8H6P	134.0268	5.54	[M + H] ⁺
Row 698#7	C5H12N2O2	133.0969	20.62	[M + H] ⁺
Row 763#6	C5H12N2O2	133.0969	20.47	[M + H] ⁺
Row 553#8	C4H8N2O3	133.0605	12.64	[M + H] ⁺
Row 305#6	C6H13NO2	132.1016	8.69	[M + H] ⁺
Row 494#4	C6H11O3	132.0763	12.05	[M + H] ⁺
Row 746#10	C7H13O2	130.0971	23.98	[M + H] ⁺
Row 796#1	C6H11NO2	130.0860	21.86	[M + H] ⁺
Row 329#1	C6H11NO2	130.0860	8.50	[M + H] ⁺
Row 359#6	C6H11NO2	130.0860	9.80	[M + H] ⁺
Row 705#7	C6H11NO2	130.0860	22.98	[M + H] ⁺
Row 740#9	C6H11NO2	130.0859	20.47	[M + H] ⁺
Row 724#10	C6H11NO2	130.0859	20.52	[M + H] ⁺
Row 548#8	C5H7NO3	130.0497	12.59	[M + H] ⁺
Row 494#7	C5H7NO3	130.0495	12.33	[M + H] ⁺
Row 360#2	C5H7NO3	130.0495	7.42	[M + H] ⁺
Row 491#7	C5H8N2O2	129.0656	12.25	[M + H] ⁺
Row 714#7	C7H12NO	127.0975	24.16	[M + H] ⁺
Row 512#10	CH9N3PS	127.0322	12.14	[M + H] ⁺
Row 500#9	H5N4O2S	126.0216	11.97	[M + H] ⁺
Row 353#4	C8H11O	124.0864	9.94	[M + H] ⁺
Row 160#3	H7N6P	123.0549	4.89	[M + H] ⁺
Row 332#0	C8H9N	120.0806	7.64	[M + H] ⁺
Row 461#7	C4H9NO3	120.0652	11.74	[M + H] ⁺
Row 328#6	C4H8P2	119.0159	9.15	[M + H] ⁺
Row 340#3	C5H11NO2	118.0859	9.91	[M + H] ⁺
Row 782#1	C5H9NO2	116.0703	20.44	[M + H] ⁺
Row 197#6	C5H9NO2	116.0703	5.23	[M + H] ⁺
Row 759#4	C5H9NO2	116.0702	24.09	[M + H] ⁺

Row 729#10	C5H9NO2	116.0702	20.67	[M + H] ⁺
Row 437#5	C5H9NO2	116.0702	10.01	[M + H] ⁺
Row 742#9	C5H10N2O	115.0862	20.52	[M + H] ⁺
Row 534#7	C5H8N2O	113.0706	13.21	[M + H] ⁺
Row 498#6	CH10N4P	110.0710	11.97	[M + H] ⁺
