

Table S8. Probable identification of the metabolites selected from the dataset based on VIP scores derived from the PCA and PLS-DA analysis and annotated after METLIN searches.

Rt (min)	m/z	Molecular formula	Possible adducts	Most probable Metlin match
1.41	261.1243	C14H18N2O4 C17H19NaO2 C14H16N2O3 C17H17NaO C17H18O C13H12N2O2 C16H13Na C14H22O2 C12H13NO3	M+H-H2O M+H-H2O M+H M+H M+Na M+CH3OH+H M+CH3OH+H M+K M+ACN+H	C14H18N2O4 [M+H-H2O]
1.57	147.0556	C8H8N2O2 C8H6N2O C7H2N2	M+H-H2O M+H M+CH3OH+H	C8H8N2O2 [M+H-H2O]
1.98	201.1032	C12H14N2O2 C15H15Na C12H12N2O C12H18	M+H-H2O M+H-H2O M+H M+K	C12H12N2O [M+H]
2.27	197.1084	C8H19N2NaOS C8H17N2NaS C8H18N2S	M+H-H2O M+H M+Na	C8H18N2S [M+Na] C10H13FN2O [M+H]
2.46	201.0679	C14H11NaO C14H9Na C14H10	M+H-H2O M+H M+Na	C10H13ClO2 [M+H]
3.46	560.3941	C32H50N5NaO2 C32H49NO5 C33H45N5O C30H50NNaO5 C31H46N5NaO C31H50O6 C32H46N4O2 C30H47N4NaO2	M+H M+CH3OH+H M+CH3OH+H M+CH3OH+H M+CH3OH+H M+ACN+H M+ACN+H M+ACN+H	C33H53NO6 CAS: 511-36-4 [M+H]
5.16	479.2703	C26H41NO5S C24H42NNaO5S C21H38N5NaO6 C25H38N5NaOS	M+H-H2O, M+H M+H-H2O, M+H M+H-H2O, M+H M+H-H2O, M+H	C19H36N8O5 [M+Na]
5.16	515.2924	C22H45NO12	M+H-H2O M+H M+Na	C21H38N8O7 [M+H]
5.16	554.2464	C23H41NO15 C24H37N5O11 C21H41N5O11S	M+H-H2O M+H-H2O M+H-H2O	C24H35N5O10 [M+H]

		C19H42N5NaO11S C23H39NO14 C20H43NO14S C24H35N5O10 C21H39N5O10S C19H40N5NaO10S C19H41N5O10S C22H42N3NaO8S C22H35NO13 C19H39NO13S C23H31N5O9 C20H35N5O9S C18H36N5NaO9S C24H41N3O9 C20H45N5O6S2 C22H42N3NaO9 C22H32N4O10 C25H33N2NaO8 C17H37N4NaO10S C21H37N4NaO5S2 C22H43N3O8S C20H44N3NaO8S	M+H-H2O M+H M+H M+H M+H M+H M+Na M+Na M+CH3OH+H M+CH3OH+H M+CH3OH+H M+CH3OH+H M+CH3OH+H M+K M+K M+K M+ACN+H M+ACN+H M+ACN+H M+ACN+H M+ACN+H M+2Na-H M+2Na-H	
5.39	398.3423	C27H45NO2 C27H43NO C26H39N C21H44NNaS C25H40O	M+H-H2O M+H M+CH3OH+H M+CH3OH+H M+ACN+H	C27H43NO CAS: 80-78-4
5.99	430.2957	C26H41NO5 C27H37N5O C25H38N5NaO C22H42N5NaOS C26H39NO4 C27H35N5 C25H36N5Na C22H40N5NaS C25H37N5 C22H41N5S C25H35NO3 C22H41N5O C24H36O4 C25H32N4 C23H33N4Na	M+H-H2O M+H-H2O M+H-H2O M+H-H2O M+H M+H M+H M+H M+Na M+Na M+CH3OH+H M+K M+ACN+H M+ACN+H M+ACN+H	C26H39NO4 C27H35N5 [M+H]
5.99	465.3098	C26H43NO6 C27H39N5O2	M+H-H2O, M+H, M+Na M+H-H2O, M+H, M+Na	C29H40N2O3 CAS: 112648-68-7, [M+H]

		C25H40N5NaO2 C22H44N5NaO2S	M+H-H2O, M+H, M+Na M+H-H2O, M+H, M+Na	C27H42N2O3 [M+Na]
5.99	337.2531	C24H34O2 C24H32O C23H28	M+H-H2O M+H M+CH3OH+H	C24H32O [M+H]
6.14	352.2404	C24H32O2	M+H-H2O M+H	C21H34ClNO [M+H]
6.93	223.1177	C7H17N3O5 C10H18NNaO3	M+H-H2O M+H M+H-H2O M+H	C9H18O6 CAS: 5391-17-3 [M+H]
6.93	372.2679	C24H36O3	M+H-H2O M+H	C22H36FNO CAS: 166100-37-4 [M+Na]
6.95	426.3213	C24H45NO6 C23H42N5NaO2 C24H43NO5 C23H40N5NaO C23H41N5O C23H39NO4 C24H35N5 C22H36N5Na C23H46N3Na C23H36N4O C21H37N4NaO	M+H-H2O M+H-H2O M+H M+H M+Na M+CH3OH+H M+CH3OH+H M+CH3OH+H M+K M+ACN+H M+ACN+H	C22H45NO5 [M+Na]
7.09	456.3072	C25H44O7 C23H45NaO7 C24H41N4NaO3	M+H-H2O, M+Na M+H-H2O, M+Na M+H-H2O, M+Na	C26H43NO4 [M+Na]
7.28	470.2908	C18H42N5NaO6 C18H43N5O6	M+Na M+2Na-H	C26H42ClN3O [M+Na]
10.79	677.2932	C32H47N4NaO8 C31H41NO13 C30H38N5NaO9 C26H49N4NaO12	M+K M+ACN+H M+ACN+H M+2Na-H	C29H46N6O9S [M+Na]

Note: Metabolites generated from the VIP list (a statistically generated list) have a confidence level of >95%. Most probable Metlin match was determined using *m/z* values, retention time, precursor ion, fragmentation patterns, and mass error. These are probable identifications. Additional potential metabolites that differ from those in this list by standard adducts (e.g. Na-H) are not included.