Table 2-1. Overview of formula annotated features detected in FF5.3 with positive ionization MS-TOF.

Feature	RT (minute)	m/z ($[M+H]^+$)	intensity (%)	formulas
FF5.3-pos-1	20.0	279.2300	5	$C_{12}H_{31}N_4OP$
				$C_{14}H_{26}N_6$
				$C_{16}H_{28}N_3O$
FF5.3-pos-2	19.7	281.2470	5	$C_{16}H_{30}N_3O$
				$C_{18}H_{32}O_2$
FF5.3-pos-3	19.8	294.2791	3	$C_{19}H_{35}NO$
FF5.3-pos-4	19.9	323.2567	49	$C_{13}H_{34}N_6OS$
				$C_{14}H_{35}N_4O_2P$
				$C_{16}H_{37}NO_3P$
FF5.3-pos-5	19.7	377.3211	6	$C_{13}H_{36}N_{12}O$
				$C_{20}H_{44}N_2O_2S$
				$C_{20}H_{46}N_2P_2$
FF5.3-pos-6	19.7	404.3141	4	$C_{18}H_{41}N_7OS$
				$C_{19}H_{42}N_5O_2P$
				$C_{21}H_{44}N_2O_3P$
FF5.3-pos-7	20	411.3253	3	$C_{13}H_{38}N_{12}O_3$
				$C_{16}H_{44}N_8P_2$
				$C_{21}H_{42}N_6S$
FF5.3-pos-8	19.5	428.3154	5	$C_{13}H_{33}N_{17}$
				$C_{14}H_{42}N_{11}PS$
				$C_{21}H_{42}N_5O_2P$
FF5.3-pos-9	19.5	450.2966	3	$C_{12}H_{33}N_{16}O_3$
				$C_{18}H_{40}N_7O_4P$
				$C_{22}H_{44}NO_6P$
FF5.3-pos-10	19.8	451.3179	3	$C_{11}H_{34}N_{18}O_2$
				$C_{18}H_{42}N_8O_3S$
				$C_{20}H_{39}N_{10}P$
FF5.3-pos-11	20.0	451.3179	6	$C_{11}H_{34}N_{18}O_2$
				$C_{18}H_{44}N_8OP_2$
				$C_{20}H_{39}N_{10}P$
FF5.3-pos-12	19.6	453.4043	3	$C_{19}H_{51}N_9OP$
				$C_{23}H_{48}N_8O$
				$C_{27}H_{52}N_2O_3$
FF5.3-pos-13	19.8	482.3231	6	$C_{11}H_{35}N_{19}O_3$
				$C_{14}H_{41}N_{15}P_2$
				$C_{20}H_{48}N_7PS_2$

Note: Only the top three candidate formulae are shown. Intensities are normalized to sum of all feature intensities. Acronyms: RT: retention time.

Table 2-2. Overview of formula annotated features detected in FF5.3 with negative ionization MS-TOF

Feature	RT (minute)	m/z ($[M-H]^-$)	intensity (%)	formulas
FF5.3-neg-1	19.2	279.2322	5	$C_{16}H_{30}N_3O$
				$C_{18}H_{32}O_2$
FF5.3-neg-2	20.2	293.2480	17	$C_{17}H_{32}N_3O$
				$C_{19}H_{34}O_2$
FF5.3-neg-3	20.1	299.2584	1	$C_{16}H_{34}N_3O_2$
				$C_{18}H_{36}O_3$
FF5.3-neg-4	20.6	307.2636	16	$C_{18}H_{34}N_3O$
				$C_{20}H_{36}O_2$
FF5.3-neg-5	19.9	321.2429	7	$C_{14}H_{35}N_4O_2P$
				$C_{16}H_{37}NO_3P$
				$C_{20}H_{34}O_3$
FF5.3-neg-6	19.8	368.3164	1	$C_{20}H_{41}N_4O_2$
				$C_{22}H_{43}NO_3$
FF5.3-neg-7	19.2	399.2744	7	$C_{11}H_{38}N_{12}P_2$
				$C_{17}H_{37}N_8OP$
				$C_{18}H_{36}N_6O_4$
FF5.3-neg-8	19.8	402.3007	2	$C_{19}H_{42}N_5O_2P$
				$C_{21}H_{44}N_2O_3P$
				$C_{23}H_{39}N_4O_2$
FF5.3-neg-9	19.5	426.3008	17	$C_{12}H_{37}N_{13}O_4$
				$C_{15}H_{43}N_9OP_2$
				$C_{17}H_{43}N_6O_4S$
FF5.3-neg-10	20.3	537.4872	1	$C_{30}H_{62}N_6O_2$
				$C_{32}H_{64}N_3O_3$
FF5.3-neg-11	20.5	539.5035	1	$C_{30}H_{64}N_6O_2$
				$C_{32}H_{66}N_3O_3$
				$C_{34}H_{68}O_4$
FF5.3-neg-12	20.5	549.4876	2	$C_{24}H_{62}N_{12}S$
				$C_{31}H_{62}N_6O_2$
				$C_{35}H_{66}O_4$
FF5.3-neg-13	20.3	561.4859	3	$C_{25}H_{62}N_{12}S$
				$C_{31}H_{66}N_2O_6$
				$C_{32}H_{62}N_6O_2$
FF5.3-neg-14	20.3	563.5032	5	$C_{25}H_{64}N_{12}S$
				$C_{32}H_{64}N_6O_2$
				$C_{34}H_{66}N_3O_3$
FF5.3-neg-15	20.9	563.5031	2	$C_{25}H_{64}N_{12}S$
				$C_{28}H_{67}N_7O_2P$
				$C_{32}H_{64}N_6O_2$
FF5.3-neg-16	19.9	601.4824	2	$C_{18}H_{59}N_{20}OP$
				$C_{19}H_{58}N_{18}O_4$

				$C_{20}H_{54}N_{22}$
FF5.3-neg-17	19.6	785.6392	3	$C_{19}H_2N_3O_7P_{13}$
				$C_20HNO_10P_{12}$
				$C_{42}H_{87}N_6O_5P$
FF5.3-neg-18	19.0	833.5164	3	$C_{10}H_{14}NOPS_{20}$
				$C_{12}H_9N_3S_{20}$
				$C_{19}HNO_3S_{17}$
FF5.3-neg-19	19.4	857.5162	2	$C_{32}H_{70}N_{14}O_{13}$
				$C_{33}H_{66}N_{18}O_9$
				$C_{40}H_{62}N_{18}O_4$

Note: Only the top three candidate formulae are shown. Intensities are normalized to sum of all feature intensities. Acronyms: RT: retention time.

Table 2-3. Overview of chemical structure annotated features detected in FC18.3 with positive ionization MS-TOF.

Feature	RT (minute)	m/z ($[M+H]^+$)	intensity (%)	formula	compound	PC identifier
FC18.3-pos-1	5.2	281.2472	37	$C_{18}H_{32}O_2$	(9Z,12Z)-octadeca-9,12-dienoic acid (*linoleic acid*)	5280450
				$C_{18}H_{32}O_2$	(9Z,12Z,15Z)-octadeca-9,12,15-triene-1,1-diol	88317388
				$C_{18}H_{32}O_2$	(8Z,12Z)-octadeca-8,12-dienoic acid	58249011
				$C_{18}H_{32}O_2$	octadeca-6,9,12-triene-1,1-diol	53672256
				$C_{18}H_{32}O_2$	octadeca-8,11-dienoic acid, 8Z,11Z-octadecadienoic acid	16614
FC18.3-pos-2	5.3	394.3314	14	$C_{24}H_{43}NO_3$	1-decoxy-3-[[1-(4-methoxyphenyl)-2-methylpropan-2-yl]amino]propan-2-ol	18667769
				$C_{24}H_{43}NO_3$	2-amino-2-[2-(4-tridecoxyphenyl)ethyl]propane-1,3-diol	11223128
				$C_{24}H_{43}NO_3$	(9Z,12Z,15Z)-N,N-bis(3-hydroxypropyl)octadeca-9,12,15-trienamide	117844693
				$C_{24}H_{43}NO_3$	2-amino-2-(2-methylpropyl)-3-oxoicos-11-ynoic acid	129727379
				$C_{24}H_{43}NO_3$	1-[4-[2-[(4R)-2,7-dimethyloctan-4-yl]oxyethyl]phenoxy]-3-(propan-2-ylamino)propan-2-ol	57647621
FC18.3-pos-3	5.3	428.3154	27	$C_{27}H_{41}NO_3$	(2S)-2-[[(9Z,12Z)-octadeca-9,12-dienoyl]amino]-3-phenylpropanoic acid	89824941
				$C_{27}H_{41}NO_3$	3-(4-hydroxyphenyl)-2-[[(9Z,12Z,15Z)-octadeca-9,12,15-trienyl]amino]propanoic acid	69817144
				$C_{27}H_{41}NO_3$	(3-anilino-2-hydroxypropyl) (9Z,12Z,15Z)-octadeca-9,12,15-trienoate	102505987
				$C_{27}H_{41}NO_3$	(2S)-3-(4-hydroxyphenyl)-2-[[(9Z,12Z,15Z)-octadeca-9,12,15-trien-3-yl]amino]propanoic acid	69817185
				$C_{27}H_{41}NO_3$	(2S)-3-(4-hydroxyphenyl)-2-(octadeca-9,12,15-trien-2-ylamino)propanoic acid	54445037
FC18.3-pos-4	5.4	323.2581	22	$C_{20}H_{34}O_3$	(15S)-15-hydroxyicosa-8,11,13-trienoic acid	3246874
				$C_{20}H_{34}O_3$	15-hydroxyicosa-2,4,6-trienoic acid	133910
				$C_{20}H_{34}O_3$	20-hydroxyicosa-2,4,6-trienoic acid	53763823
				$C_{20}H_{34}O_3$	5-hydroxyicosa-6,8,11-trienoic acid	1768
				$C_{20}H_{34}O_3$	(12R)-12-hydroxyicosa-2,4,6-trienoic acid	54236448

Only the top five candidate structures are shown. Intensities are normalized to sum of all feature intensities. Acronyms: RT: retention time; PC: PubChem.

Table 2-4. Overview of chemical structure annotated features detected in FC18.3 with negative ionization MS-TOF

Feature	RT (minute)	m/z ($[M-H]^-$)	intensity (%)	formula	compound	PC identifier
FC18.3-neg-1	5.2	279.2328	88	$C_{18}H_{32}O_2$	(9Z,12Z)-octadeca-9,12-dienoic acid (*linoleic acid*)	5280450
				$C_{18}H_{32}O_2$	hexadeca-7,11-dienyl acetate	39848
				$C_{18}H_{32}O_2$	octadec-17-ynoic acid	1449
				$C_{18}H_{32}O_2$	octadeca-9,11-dienoic acid	74607
				$C_{18}H_{32}O_2$	octadeca-2,4-dienoic acid	154212
FC18.3-neg-2	5.3	392.3165	6	$C_{24}H_{43}NO_3$	1-decoxy-3-[[1-(4-methoxyphenyl)-2-methylpropan-2-yl]amino]propan-2-ol	18667769
				$C_{24}H_{43}NO_3$	2-amino-2-[2-(4-tridecoxyphenyl)ethyl]propane-1,3-diol	11223128
				$C_{24}H_{43}NO_3$	[[(Z)-2-ethyloctadec-9-enoyl]amino] 2-methylprop-2-enoate	87083461
				$C_{24}H_{43}NO_3$	(2S)-4-methyl-2-[[(9Z,12Z)-octadeca-9,12-dienoyl]amino]pentanoic acid	89824815
				$C_{24}H_{43}NO_3$	(3-hydroxy-1-methylpiperidin-4-yl) octadeca-9,12-dienoate	77481390
FC18.3-neg-3	5.3	426.3008	6	$C_{27}H_{41}NO_3$	(2S)-2-[[(9Z,12Z)-octadeca-9,12-dienoyl]amino]-3-phenylpropanoic acid	89824941
				$C_{27}H_{41}NO_3$	3-(4-hydroxyphenyl)-2-[[(9Z,12Z,15Z)-octadeca-9,12,15-trienyl]amino]propanoic acid	69817144
				$C_{27}H_{41}NO_3$	(2S)-3-(4-hydroxyphenyl)-2-[[(9Z,12Z,15Z)-octadeca-9,12,15-trien-3-yl]amino]propanoic acid	69817185
				$C_{27}H_{41}NO_3$	3-[4-(3-methylcyclooctyl)phenyl]-2-[(1-propylcyclopentanecarbonyl)amino]propanoic acid	123374824
				$C_{27}H_{41}NO_3$	3-(4-cyclononylphenyl)-2-[(1-propylcyclopentanecarbonyl)amino]propanoic acid	123840724

Note: only the top five candidate structures are shown. Intensities are normalized to sum of all feature intensities. Acronyms: RT: retention time; PC: PubChem.