

Qualitative Compound Report

Analysis Info

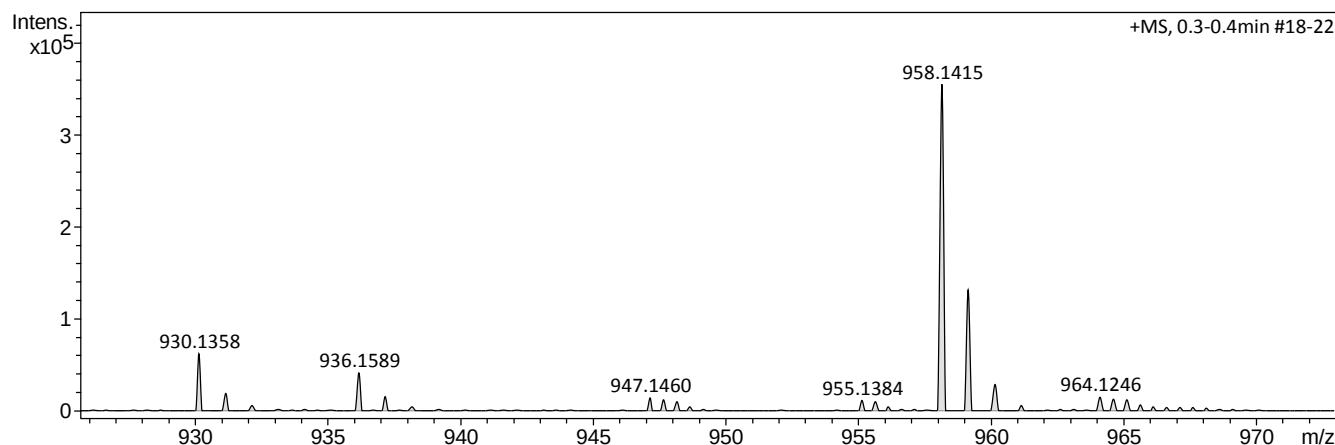
Analysis Name D:\Data\ggc\25-020310_P1-C-1_01_10057.d
Method lc_ms directos tunelow300924.m
Sample Name 25-020310
Comment NFC-FAZT1(may)
Sv: MeOH + HCOOH
Uhrig

Acquisition Date 2/24/2025 3:18:41 PM

Operator EB - MV
Instrument micrOTOF-Q

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
930.1358	1	C33H37N3NaO27	930.1507	16.0	40.7	1	0.00	16.5	even	ok
	2	C33H32N5O27	930.1279	-8.5	44.3	2	0.59	20.5	even	ok
	3	C33H28N11O22	930.1405	5.1	52.9	3	100.00	25.5	even	ok
	4	C33H25N13NaO19	930.1282	-8.2	55.2	4	0.73	27.5	even	ok
	5	C33H24N17O17	930.1531	18.6	62.0	5	0.00	30.5	even	ok
	6	C33H21N19NaO14	930.1408	5.3	64.4	6	47.13	32.5	even	ok
	7	C33H16N21O14	930.1180	-19.1	68.0	7	0.00	36.5	even	ok
	8	C33H17N25NaO9	930.1533	18.9	73.9	8	0.00	37.5	even	ok
	9	C33H18N27O9	936.1775	19.9	44.6	9	0.00	38.5	even	ok
936.1589	1	C33H39NNaO29	936.1500	-9.5	19.6	1	0.01	14.5	even	ok
	2	C33H35N7NaO24	936.1626	3.9	20.4	2	100.00	19.5	even	ok
	3	C33H38N5O27	936.1749	17.1	21.0	3	0.00	17.5	even	ok
	4	C33H31N13NaO19	936.1751	17.4	25.4	4	0.00	24.5	even	ok
	5	C33H26N15O19	936.1524	-6.9	28.7	5	1.52	28.5	even	ok
	6	C33H23N17NaO16	936.1401	-20.1	30.0	6	0.00	30.5	even	ok
	7	C33H22N21O14	936.1650	6.5	36.2	7	2.47	33.5	even	ok
	8	C33H19N23NaO11	936.1527	-6.6	38.0	8	1.91	35.5	even	ok
	9	C33H18N27O9	936.1775	19.9	44.6	9	0.00	38.5	even	ok
947.1460	1	C33H16N24NaO11	947.1323	-14.5	114.9	1	0.00	37.5	even	ok
	2	C33H19N22O14	947.1446	-1.5	118.0	2	100.00	35.5	even	ok
	3	C33H23N16O19	947.1320	-14.7	127.8	3	0.00	30.5	even	ok
	4	C33H28N14NaO19	947.1547	9.3	131.1	4	0.00	26.5	even	ok
	5	C33H36N2NaO29	947.1296	-17.3	134.9	5	0.00	16.5	even	ok
	6	C33H39O32	947.1419	-4.3	137.6	6	3.52	14.5	even	ok
	7	C33H32N8NaO24	947.1422	-4.0	140.9	7	3.15	21.5	even	ok
	8	C33H35N6O27	947.1545	9.0	144.0	8	0.00	19.5	even	ok
	9	C33H31N8O26	955.1344	-4.2	714.6	4	0.00	22.5	even	ok
955.1384	1	C33H40NaO31	955.1446	6.4	656.4	1	100.00	13.5	even	ok
	2	C33H35N2O31	955.1218	-17.4	656.9	2	0.00	17.5	even	ok
	3	C33H36N6NaO26	955.1571	19.6	713.9	3	0.00	18.5	even	ok
	4	C33H31N8O26	955.1344	-4.2	714.6	4	0.00	22.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
958.1415	5	C33H28N10NaO23	955.1221	-17.1	715.8	5	0.00	24.5	even	ok
	6	C33H27N14O21	955.1470	9.0	717.7	6	0.00	27.5	even	ok
	7	C33H24N16NaO18	955.1347	-3.9	719.0	7	0.00	29.5	even	ok
	8	C33H20N22NaO13	955.1472	9.2	722.5	8	0.00	34.5	even	ok
	9	C33H15N24O13	955.1245	-14.6	723.4	9	0.00	38.5	even	ok
	1	C33H37N5NaO27	958.1568	16.0	27.0	1	0.00	17.5	even	ok
	2	C33H32N7O27	958.1341	-7.8	29.6	2	2.08	21.5	even	ok
	3	C33H28N13O22	958.1466	5.3	34.0	3	100.00	26.5	even	ok
	4	C33H25N15NaO19	958.1343	-7.5	34.6	4	3.11	28.5	even	ok
	5	C33H24N19O17	958.1592	18.5	40.4	5	0.00	31.5	even	ok
964.1246	6	C33H21N21NaO14	958.1469	5.6	41.7	6	54.74	33.5	even	ok
	7	C33H16N23O14	958.1242	-18.1	45.4	7	0.00	37.5	even	ok
	8	C33H17N27NaO9	958.1595	18.7	49.9	8	0.00	38.5	even	ok
	1	C33H15N23NaO13	964.1112	-13.9	224.8	1	0.00	37.5	even	ok
	2	C33H18N21O16	964.1235	-1.1	225.9	2	100.00	35.5	even	ok
	3	C33H22N15O21	964.1109	-14.2	232.7	3	0.00	30.5	even	ok
	4	C33H34N5O29	964.1334	9.1	235.0	4	0.00	19.5	even	ok
	5	C33H27N13NaO21	964.1337	9.4	236.1	5	0.00	26.5	even	ok
	6	C33H35NNaO31	964.1085	-16.7	239.9	6	0.00	16.5	even	ok
	7	C33H31N7NaO26	964.1211	-3.6	243.2	7	2.56	21.5	even	ok