

Qualitative Compound Report

Analysis Info

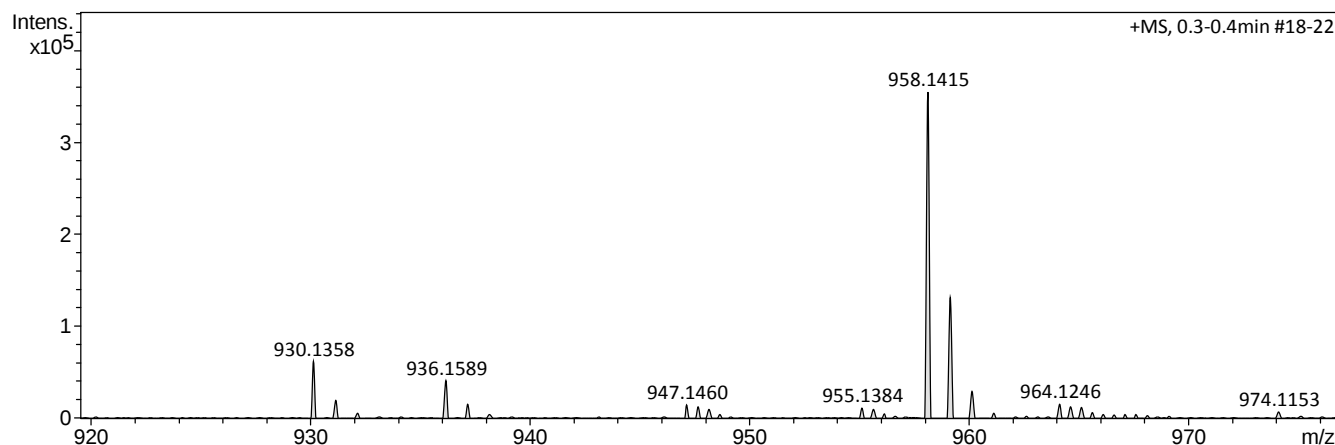
Analysis Name D:\Data\ggc\25-020310_P1-C-1_01_10057.d
Method lc_ms directos tunelow300924.m
Sample Name 25-020310
Comment NFC-FAZT1(may)
Sv: MeOH + HCOOH
Uhrig

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	C33H42IN5NaO17	930.1513	16.6	39.8	1	0.00	14.5	even	ok
	2	C33H37N3NaO27	930.1507	16.0	40.7	2	0.00	16.5	even	ok
	3	C33H37IN7O17	930.1285	-7.8	43.3	3	2.01	18.5	even	ok
	4	C33H32N5O27	930.1279	-8.5	44.3	4	0.59	20.5	even	ok
	5	C33H33IN13O12	930.1411	5.7	52.8	5	42.99	23.5	even	ok
	6	C33H28N11O22	930.1405	5.1	52.9	6	100.00	25.5	even	ok
	7	C33H25N13NaO19	930.1282	-8.2	55.2	7	0.73	27.5	even	ok
	8	C33H30IN15NaO9	930.1288	-7.5	55.5	8	2.32	25.5	even	ok
	9	C33H24N17O17	930.1531	18.6	62.0	9	0.00	30.5	even	ok
	10	C33H29IN19O7	930.1537	19.2	62.5	10	0.00	28.5	even	ok
	11	C33H21N19NaO14	930.1408	5.3	64.4	11	47.13	32.5	even	ok
	12	C33H26IN21NaO4	930.1414	6.0	65.3	12	18.87	30.5	even	ok
	13	C33H16N21O14	930.1180	-19.1	68.0	13	0.00	36.5	even	ok
	14	C33H21IN23O4	930.1186	-18.5	68.7	14	0.00	34.5	even	ok
	15	C33H17N25NaO9	930.1533	18.9	73.9	15	0.00	37.5	even	ok
936.1589	1	C33H44IN3NaO19	936.1506	-8.8	12.1	1	0.06	12.5	even	ok
	2	C33H47INO22	936.1629	4.3	13.4	2	78.69	10.5	even	ok
	3	C33H43IN7O17	936.1755	17.7	14.7	3	0.00	15.5	even	ok
	4	C33H40IN9NaO14	936.1632	4.6	15.6	4	54.26	17.5	even	ok
	5	C33H35IN11O14	936.1404	-19.7	18.5	5	0.00	21.5	even	ok
	6	C33H39NNaO29	936.1500	-9.5	19.6	6	0.01	14.5	even	ok
	7	C33H35N7NaO24	936.1626	3.9	20.4	7	100.00	19.5	even	ok
	8	C33H38N5O27	936.1749	17.1	21.0	8	0.00	17.5	even	ok
	9	C33H36IN15NaO9	936.1757	18.0	23.1	9	0.00	22.5	even	ok
	10	C33H31N13NaO19	936.1751	17.4	25.4	10	0.00	24.5	even	ok
	11	C33H31IN17O9	936.1530	-6.3	26.4	11	4.41	26.5	even	ok
	12	C33H26N15O19	936.1524	-6.9	28.7	12	1.52	28.5	even	ok
	13	C33H28IN19NaO6	936.1407	-19.4	28.8	13	0.00	28.5	even	ok
	14	C33H23N17NaO16	936.1401	-20.1	30.0	14	0.00	30.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
947.1460	15	C33H27IN23O4	936.1656	7.1	35.3	15	0.89	31.5	even	ok
	16	C33H22N21O14	936.1650	6.5	36.2	16	2.47	33.5	even	ok
	17	C33H24IN25NaO	936.1533	-6.0	37.9	17	5.07	33.5	even	ok
	18	C33H19N23NaO11	936.1527	-6.6	38.0	18	1.91	35.5	even	ok
	19	C33H18N27O9	936.1775	19.9	44.6	19	0.00	38.5	even	ok
	1	C33H21IN26NaO	947.1329	-13.8	112.7	1	0.00	35.5	even	ok
	2	C33H16N24NaO11	947.1323	-14.5	114.9	2	0.00	37.5	even	ok
	3	C33H24IN24O4	947.1452	-0.8	115.6	3	100.00	33.5	even	ok
	4	C33H19N22O14	947.1446	-1.5	118.0	4	61.90	35.5	even	ok
	5	C33H28IN18O9	947.1326	-14.1	125.4	5	0.00	28.5	even	ok
	6	C33H23N16O19	947.1320	-14.7	127.8	6	0.00	30.5	even	ok
	7	C33H33IN16NaO9	947.1553	9.9	128.8	7	0.00	24.5	even	ok
	8	C33H28N14NaO19	947.1547	9.3	131.1	8	0.00	26.5	even	ok
	9	C33H36N2NaO29	947.1296	-17.3	134.9	9	0.00	16.5	even	ok
	10	C33H39O32	947.1419	-4.3	137.6	10	2.18	14.5	even	ok
955.1384	11	C33H37IN10NaO14	947.1428	-3.4	138.6	11	4.30	19.5	even	ok
	12	C33H32N8NaO24	947.1422	-4.0	140.9	12	1.95	21.5	even	ok
	13	C33H40IN8O17	947.1551	9.6	141.5	13	0.00	17.5	even	ok
	14	C33H35N6O27	947.1545	9.0	144.0	14	0.00	19.5	even	ok
	15	C33H41IN4NaO19	947.1302	-16.6	148.3	15	0.00	14.5	even	ok
	16	C33H44IN2O22	947.1425	-3.7	151.3	16	1.44	12.5	even	ok
	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	C33H48IO24	955.1575	20.0	712.0	3	0.00	9.5	even	ok
	4	C33H45IN2NaO21	955.1452	7.1	713.1	4	0.00	11.5	even	ok
	5	C33H40IN4O21	955.1224	-16.7	713.8	5	0.00	15.5	even	ok
	6	C33H36N6NaO26	955.1571	19.6	713.9	6	0.00	18.5	even	ok
	7	C33H31N8O26	955.1344	-4.2	714.6	7	0.00	22.5	even	ok
	8	C33H28N10NaO23	955.1221	-17.1	715.8	8	0.00	24.5	even	ok
	9	C33H36IN10O16	955.1350	-3.6	717.0	9	0.00	20.5	even	ok
958.1415	10	C33H27N14O21	955.1470	9.0	717.7	10	0.00	27.5	even	ok
	11	C33H33IN12NaO13	955.1227	-16.5	718.2	11	0.00	22.5	even	ok
	12	C33H24N16NaO18	955.1347	-3.9	719.0	12	0.00	29.5	even	ok
	13	C33H32IN16O11	955.1476	9.6	720.3	13	0.00	25.5	even	ok
	14	C33H29IN18NaO8	955.1353	-3.3	721.7	14	0.00	27.5	even	ok
	15	C33H20N22NaO13	955.1472	9.2	722.5	15	0.00	34.5	even	ok
	16	C33H15N24O13	955.1245	-14.6	723.4	16	0.00	38.5	even	ok
	17	C33H25IN24NaO3	955.1478	9.9	725.3	17	0.00	32.5	even	ok
	18	C33H20IN26O3	955.1251	-13.9	726.2	18	0.00	36.5	even	ok
	1	C33H46INNaO22	958.1448	3.5	16.7	1	100.00	10.5	even	ok
	2	C33H42IN7NaO17	958.1574	16.6	19.0	2	0.00	15.5	even	ok
	3	C33H37IN9O17	958.1347	-7.1	22.3	3	0.57	19.5	even	ok
	4	C33H34IN11NaO14	958.1224	-20.0	23.0	4	0.00	21.5	even	ok
	5	C33H37N5NaO27	958.1568	16.0	27.0	5	0.00	17.5	even	ok
	6	C33H33IN15O12	958.1472	6.0	29.0	6	3.34	24.5	even	ok
	7	C33H32N7O27	958.1341	-7.8	29.6	7	0.15	21.5	even	ok
964.1246	8	C33H30IN17NaO9	958.1349	-6.9	30.7	8	0.76	26.5	even	ok
	9	C33H28N13O22	958.1466	5.3	34.0	9	7.31	26.5	even	ok
	10	C33H25N15NaO19	958.1343	-7.5	34.6	10	0.23	28.5	even	ok
	11	C33H29IN21O7	958.1598	19.1	37.3	11	0.00	29.5	even	ok
	12	C33H26IN23NaO4	958.1475	6.3	39.4	12	1.66	31.5	even	ok
	13	C33H24N19O17	958.1592	18.5	40.4	13	0.00	31.5	even	ok
	14	C33H21N21NaO14	958.1469	5.6	41.7	14	4.00	33.5	even	ok
	15	C33H21IN25O4	958.1248	-17.5	43.1	15	0.00	35.5	even	ok
	16	C33H16N23O14	958.1242	-18.1	45.4	16	0.00	37.5	even	ok
	17	C33H17N27NaO9	958.1595	18.7	49.9	17	0.00	38.5	even	ok
	1	C33H19IN29O	964.1367	12.5	223.7	1	0.00	38.5	even	ok
	2	C33H15N23NaO13	964.1112	-13.9	224.8	2	0.00	37.5	even	ok
	3	C33H18N21O16	964.1235	-1.1	225.9	3	100.00	35.5	even	ok
	4	C33H20IN25NaO3	964.1118	-13.3	229.1	4	0.00	35.5	even	ok
	5	C33H23IN23O6	964.1241	-0.5	230.0	5	93.10	33.5	even	ok
	6	C33H22N15O21	964.1109	-14.2	232.7	6	0.00	30.5	even	ok
	7	C33H34N5O29	964.1334	9.1	235.0	7	0.00	19.5	even	ok

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
	8	C33H27N13NaO21	964.1337	9.4	236.1	8	0.00	26.5	even	ok
	9	C33H27IN17O11	964.1115	-13.5	236.5	9	0.00	28.5	even	ok
	10	C33H32IN15NaO11	964.1343	10.0	239.8	10	0.00	24.5	even	ok
	11	C33H35NNaO31	964.1085	-16.7	239.9	11	0.00	16.5	even	ok
	12	C33H31N7NaO26	964.1211	-3.6	243.2	12	2.56	21.5	even	ok
	13	C33H36IN9NaO16	964.1217	-3.0	246.6	13	3.33	19.5	even	ok
	14	C33H39IN7O19	964.1340	9.8	247.8	14	0.00	17.5	even	ok
	15	C33H40IN3NaO21	964.1091	-16.0	253.5	15	0.00	14.5	even	ok
	16	C33H43INO24	964.1214	-3.3	254.8	16	1.08	12.5	even	ok