Electronic Supplementary Material (ESI) for New Journal of Chemistry.

New main group ferrocenyldithiocarbamates and conversion to ferrocene oxazolidine-2-thione and -2-one

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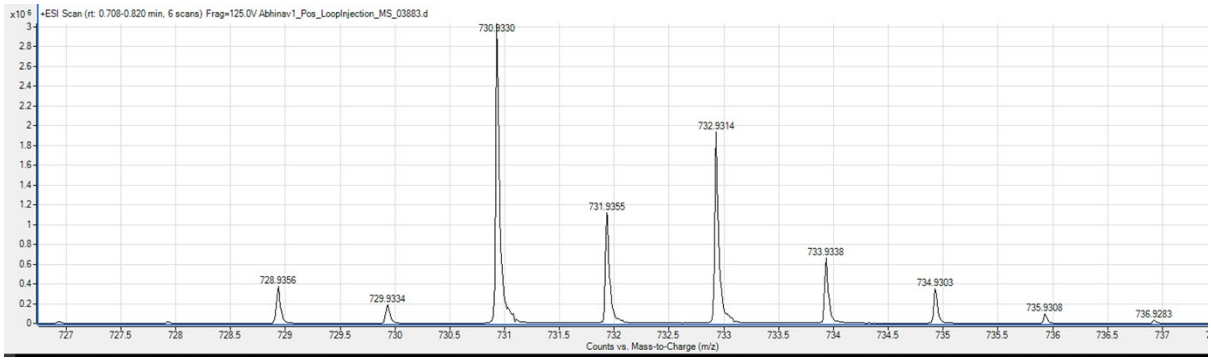
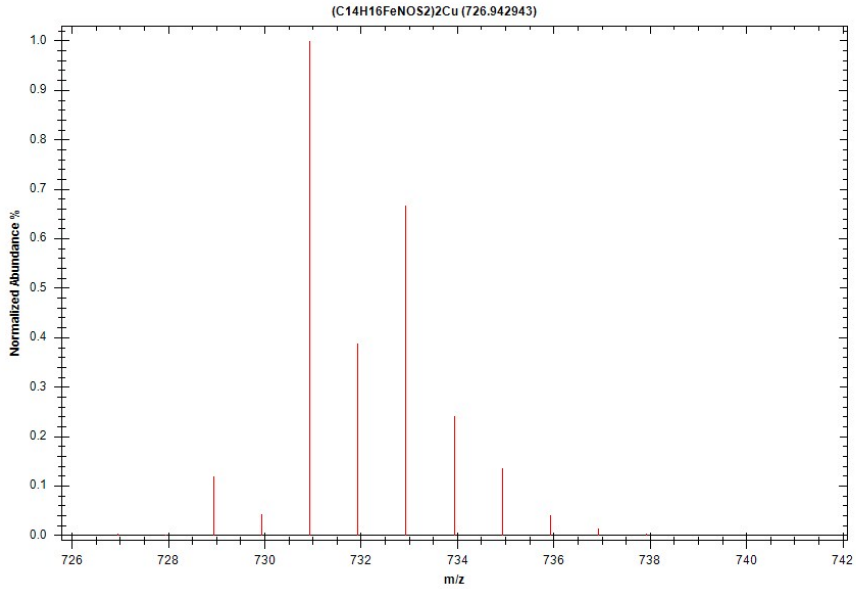
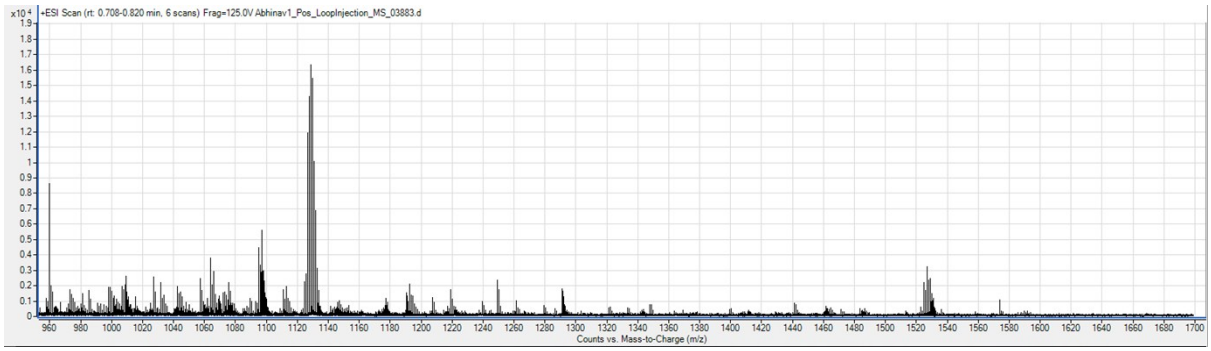
ESI-MS results related to the Comproportionation reactions of Copper Complex

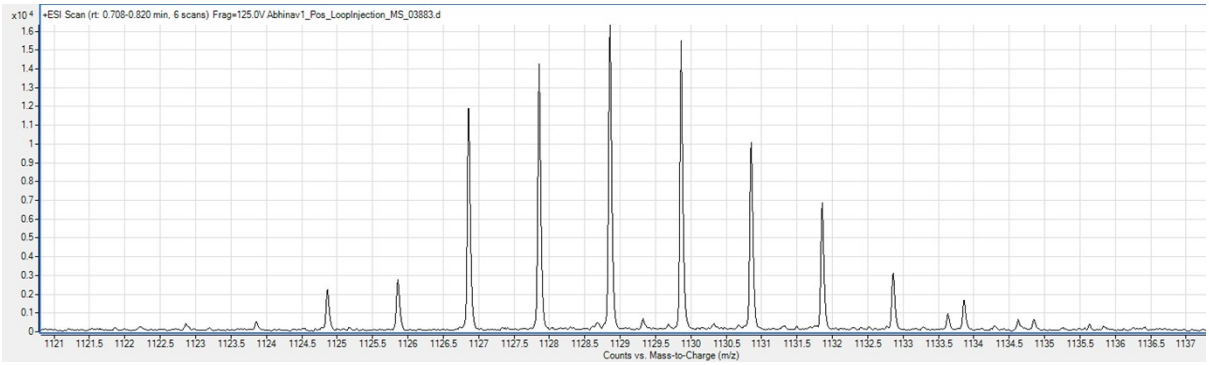
Copper complex in MeCN:

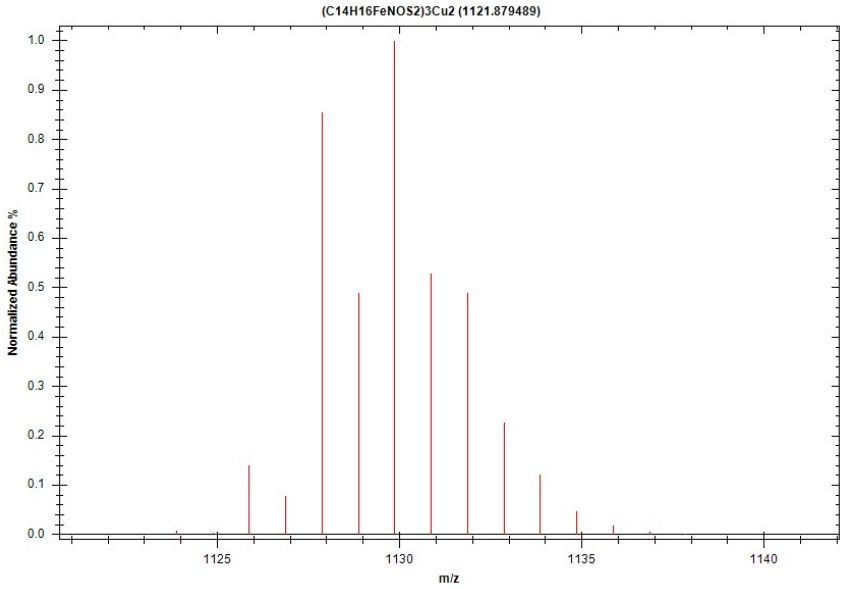




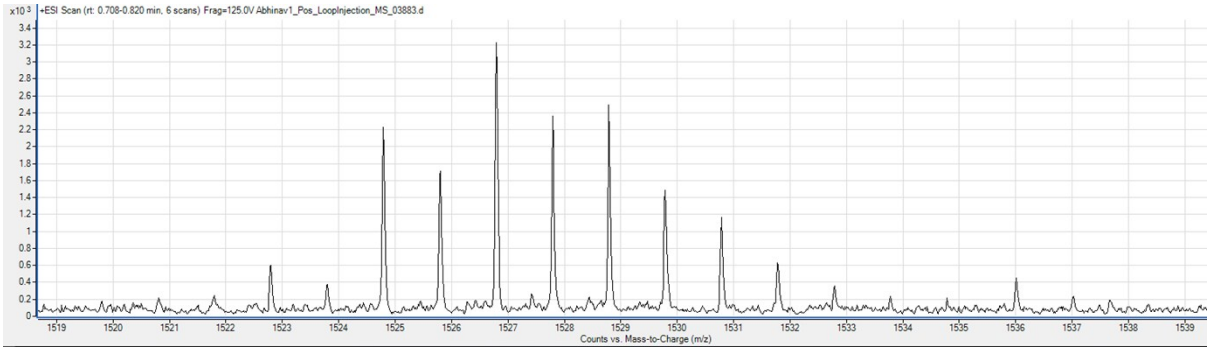
m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
726.9429	0.37	0.14	100
727.9458	0.13	0.05	34.62
728.9383	11.95	4.49	3208.31
729.9411	4.4	1.66	1181.61
730.9338	100	37.61	26848.16
731.9364	38.83	14.6	10424.64
732.932	66.79	25.12	17933.14
733.9341	24.05	9.04	6455.66
734.9305	13.59	5.11	3648.55
735.9315	4.04	1.52	1083.67
736.929	1.34	0.5	358.49
737.9291	0.32	0.12	86.11
738.9276	0.07	0.03	19.89
739.9273	0.01	0.01	3.82
740.9266	0	0	0.67

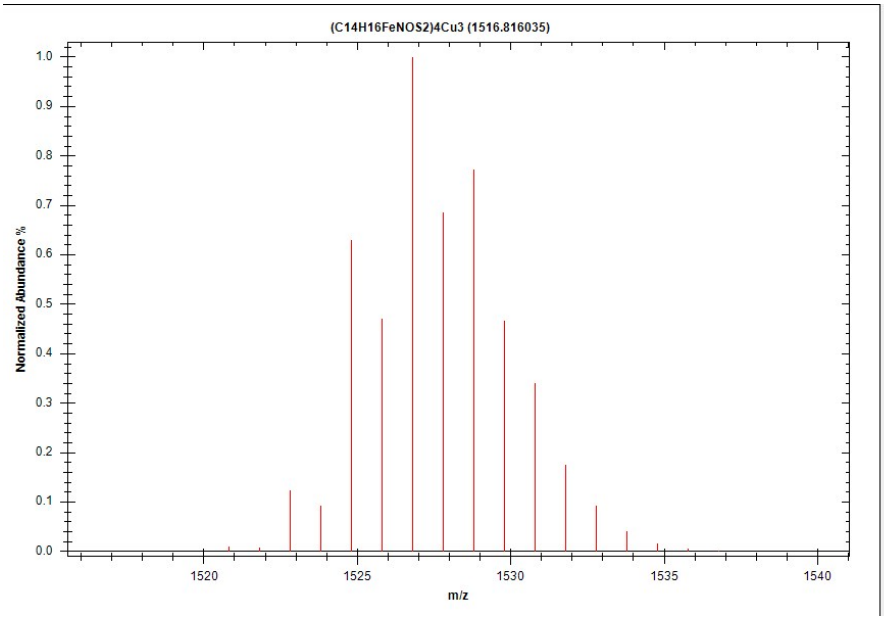




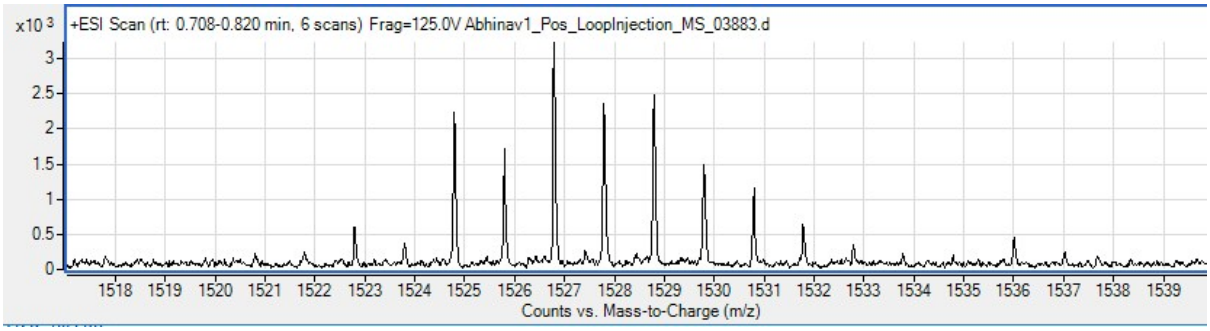


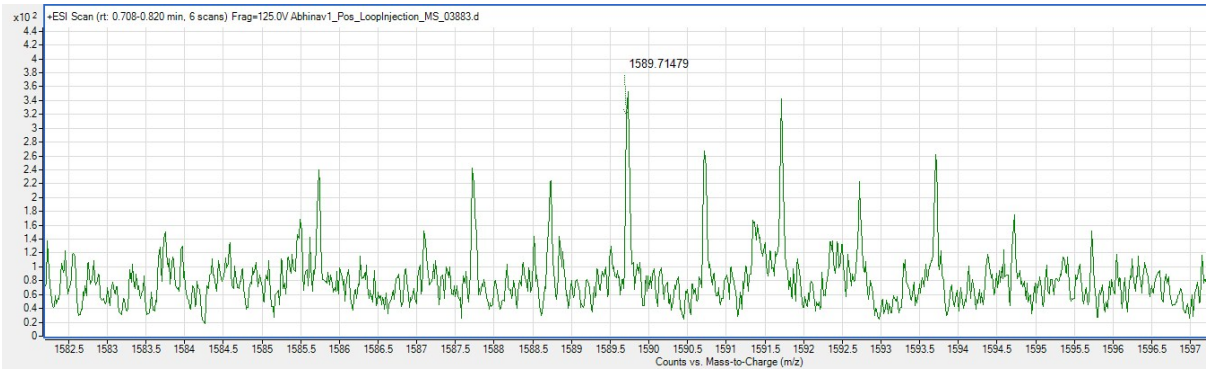
	m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
▶	1121.8795	0.02	0	100
	1122.8824	0.01	0	51.93
	1123.8749	0.85	0.21	4839.26
	1124.8777	0.46	0.11	2616.7
	1125.8704	14.04	3.5	80178.61
	1126.873	7.87	1.96	44924.42
	1127.8662	85.52	21.28	488210.19
	1128.8686	49.05	12.21	279986.22
	1129.8644	100	24.89	570875.88
	1130.8663	52.9	13.17	301982.25
	1131.863	48.93	12.18	279331.56
	1132.8641	22.62	5.63	129146.11
	1133.8617	12.26	3.05	70015.62
	1134.8619	4.68	1.17	26725.78
	1135.8601	1.79	0.45	10231.21
	1136.8598	0.56	0.14	3210.28
	1137.8585	0.17	0.04	951.79
	1138.8579	0.04	0.01	247.61
	1139.8569	0.01	0	59.62
	1140.8563	0	0	12.99
*				

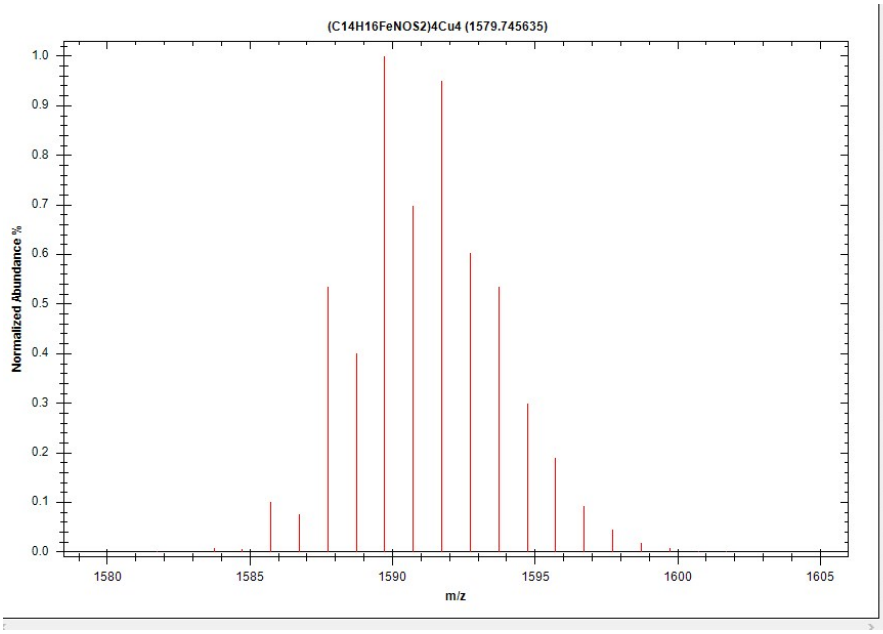




	m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
▶	1516.816	0	0	100
	1517.8189	0	0	69.23
	1518.8115	0.04	0.01	6473.21
	1519.8143	0.03	0.01	4615.35
	1520.807	1.07	0.22	160314.77
	1521.8096	0.78	0.16	117301.93
	1522.8026	12.38	2.51	1850030.75
	1523.8051	9.23	1.87	1380136
	1524.7987	62.96	12.77	9411082
	1525.8009	47.05	9.54	7033158.5
	1526.7968	100	20.28	14948656
	1527.7985	68.47	13.89	10234820
	1528.7954	77.09	15.64	11523770
	1529.7965	46.53	9.44	6956241
	1530.7941	33.97	6.89	5078094.5
	1531.7944	17.52	3.55	2619646.25
	1532.7927	9.29	1.88	1388273
	1533.7925	4.02	0.81	600322.44
	1534.7911	1.67	0.34	249319.91
	1535.7905	0.61	0.12	90669.25
	1536.7894	0.21	0.04	30933.37
	1537.7886	0.06	0.01	9567.39
	1538.7877	0.02	0	2759.85
	1539.7869	0	0	734.51
*				

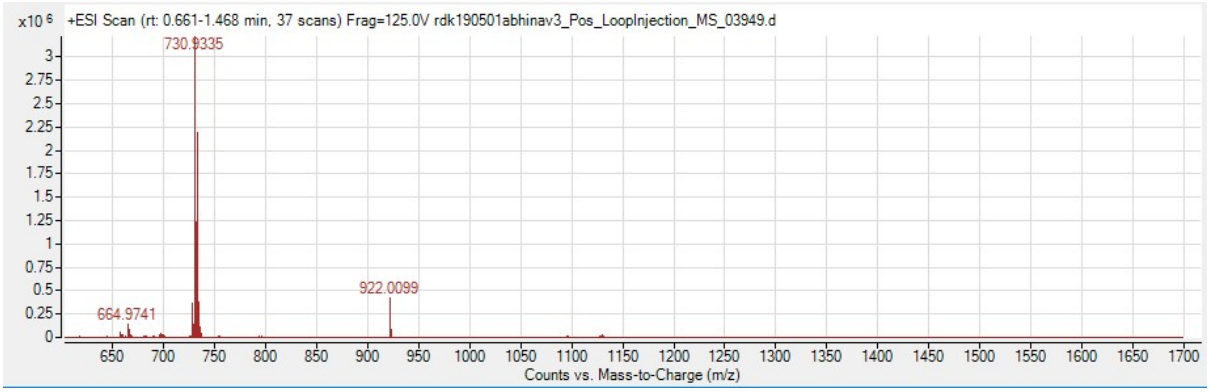


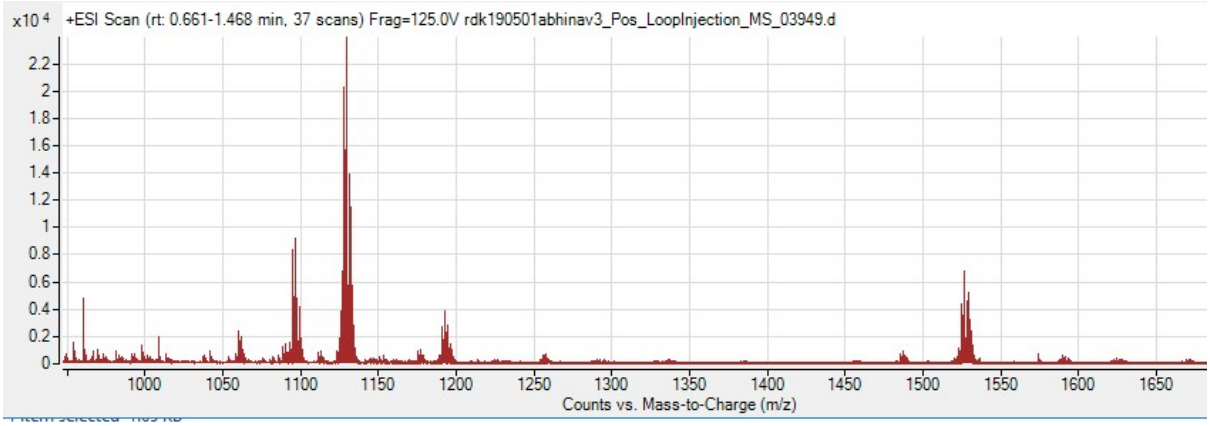


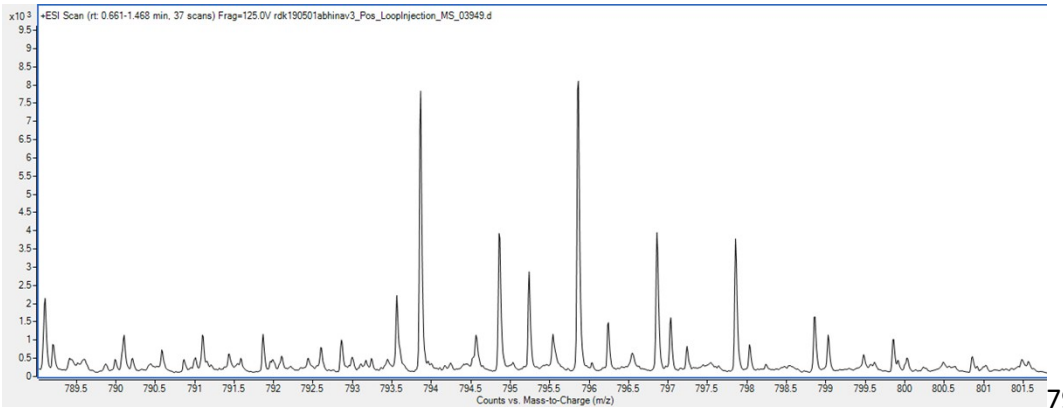


m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
1579.7456	0	0	100
1580.7485	0	0	69.23
1581.7411	0.03	0.01	6517.82
1582.7439	0.02	0	4646.24
1583.7366	0.85	0.15	163202.66
1584.7393	0.62	0.11	119360.98
1585.7323	10.04	1.8	1921552.12
1586.7348	7.48	1.34	1432468.12
1587.7284	53.46	9.6	10236440
1588.7307	39.95	7.18	7648880.5
1589.7264	100	17.97	19147238
1590.7283	69.84	12.55	13372535
1591.7249	95.02	17.07	18192840
1592.7262	60.18	10.81	11522318
1593.7235	53.37	9.59	10219213
1594.7242	29.89	5.37	5723045.5
1595.722	19.08	3.43	3653772
1596.7222	9.24	1.66	1769029.38
1597.7205	4.54	0.82	868672.38
1598.7202	1.87	0.34	358492.03
1599.7189	0.74	0.13	142162.84
1600.7183	0.26	0.05	50017.81
1601.7172	0.09	0.02	16560.2
1602.7164	0.03	0	5002.82
1603.7155	0.01	0	1413.69
1604.7147	0	0	369.88

After 1d with Cu powder in DCM, drop of filtered solution into MeCN







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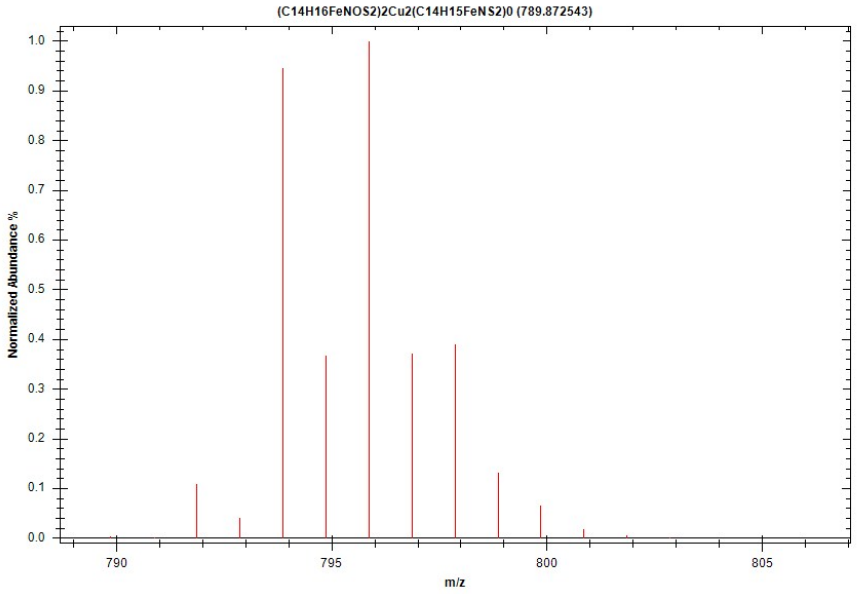
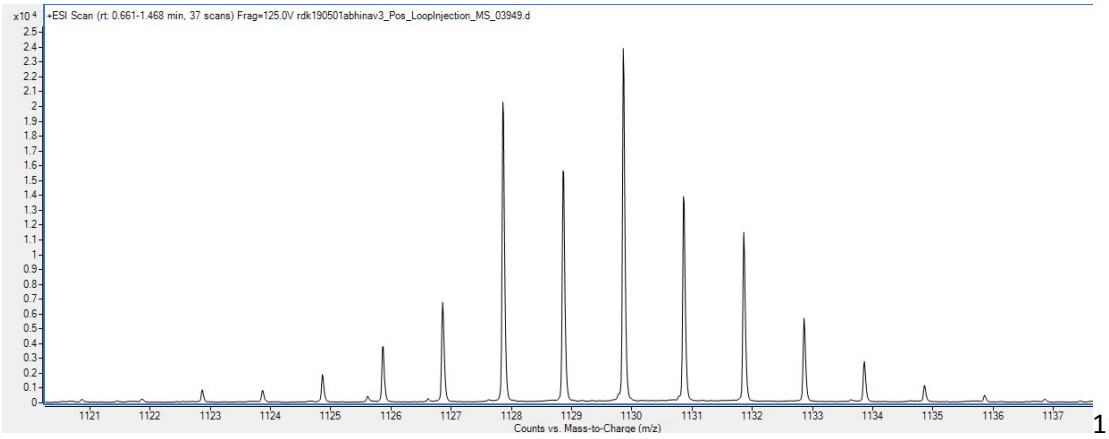
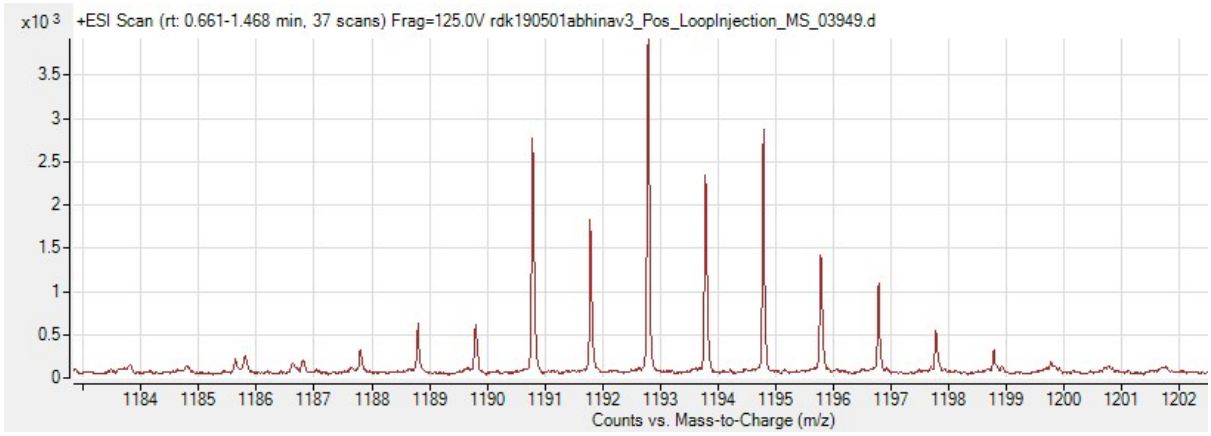
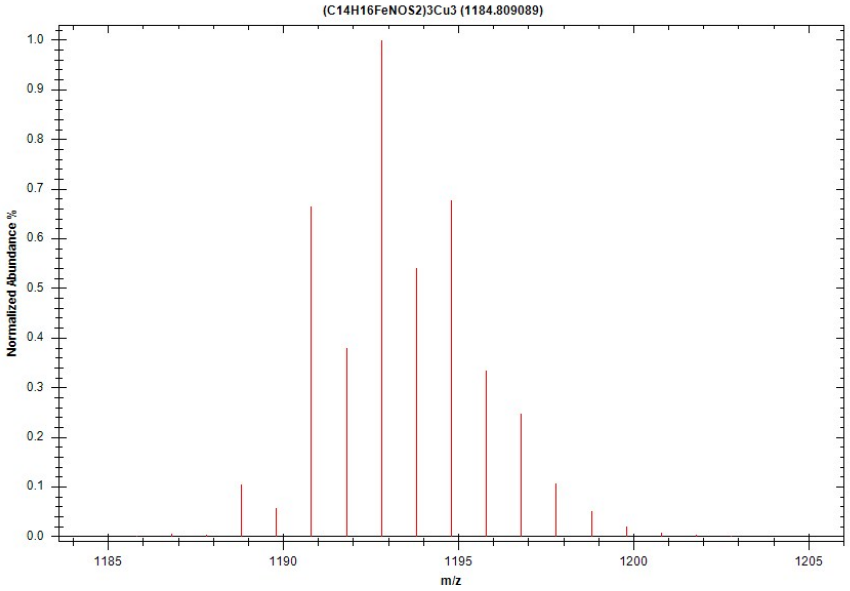


	m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
▶	789.8725	0.33	0.1	100
	790.8754	0.12	0.03	34.62
	791.868	10.88	3.15	3252.92
	792.8707	4	1.16	1197.05
	793.8636	94.55	27.39	28279.49
	794.8661	36.61	10.61	10951.79
	795.8616	100	28.97	29910.96
	796.8639	37.13	10.76	11106.42
	797.8599	38.95	11.28	11649.09
	798.8617	13.25	3.84	3963.75
	799.8584	6.64	1.92	1986.23
	800.8592	1.9	0.55	569.57
	801.8568	0.6	0.17	179.83
	802.8569	0.14	0.04	42.24
	803.8555	0.03	0.01	9.54
	804.8552	0.01	0	1.81
	805.8544	0	0	0.31
*				

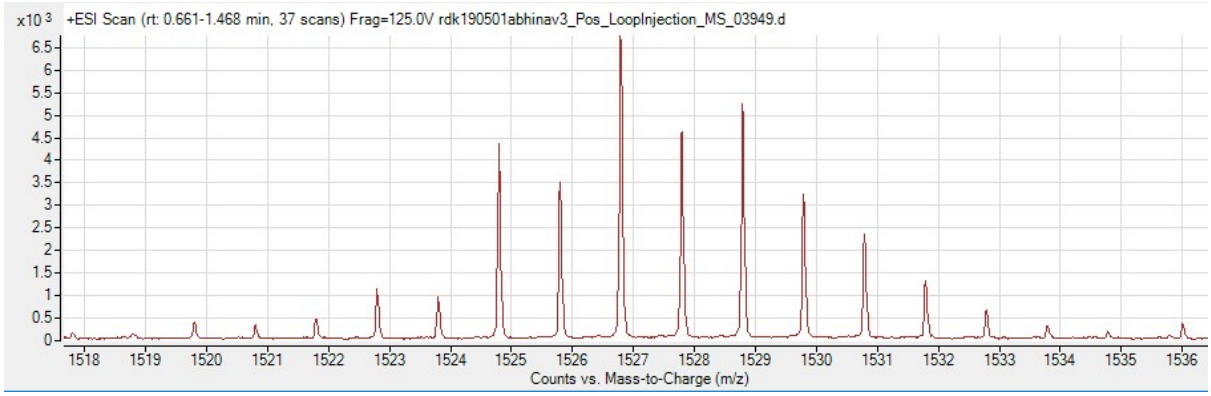


1129.86





	m/z	Abund (% largest)	Abund (% sum)	Abund (% first)
▶	1184.8091	0.01	0	100
	1185.812	0.01	0	51.93
	1186.8045	0.62	0.15	4883.87
	1187.8073	0.33	0.08	2639.87
	1188.8001	10.44	2.48	82337.55
	1189.8027	5.84	1.39	46091.82
	1190.7959	66.44	15.8	523980.47
	1191.7984	38.04	9.05	300028.44
	1192.794	100	23.78	788681.88
	1193.7961	54.13	12.87	426892.91
	1194.7924	67.71	16.1	534017.31
	1195.7939	33.46	7.96	263869.94
	1196.791	24.68	5.87	194634.27
	1197.7918	10.69	2.54	84341.94
	1198.7895	5.26	1.25	41467.39
	1199.7896	1.92	0.46	15133.49
	1200.7879	0.7	0.17	5516.25
	1201.7876	0.21	0.05	1679.82
	1202.7863	0.06	0.01	484.24
	1203.7857	0.02	0	123.45
	1204.7847	0	0	29.2
*				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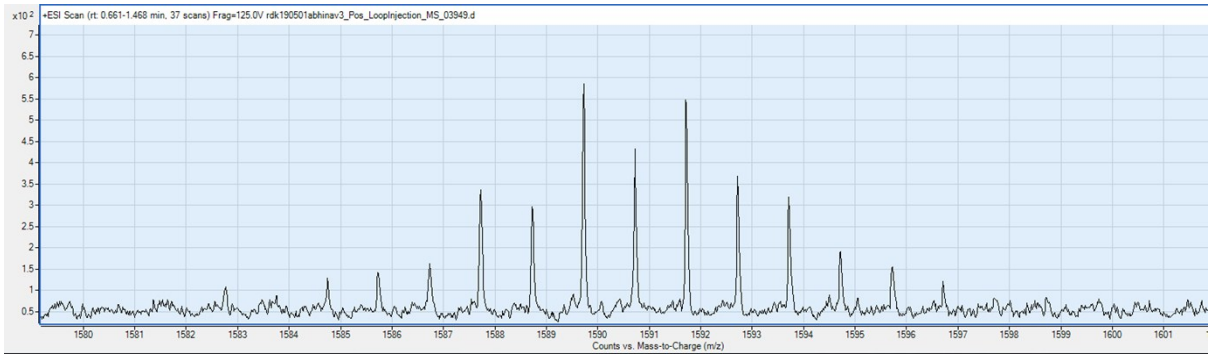
+ESI Scan (rt: 0.661-1.468 min, 37 scans) Frag=125.0V rdk190501abhinav3_Pos_LoopInjection_MS_03949.d
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536
Counts vs. Mass-to-Charge (m/z)


x10 2
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7
6.5
6
5.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601
Counts vs. Mass-to-Charge (m/z)