

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074517.D
 Acq On : 16 Sep 2022 18:02
 Operator : JC\MD
 Sample : N4447-03 100X
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1659DL

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074517.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	59	rBV2	104465	199768	7.27%	0.533%
2	2.687	132	136	139	rBV3	41176	66978	2.44%	0.179%
3	7.069	868	881	890	rVB6	21954	67841	2.47%	0.181%
4	7.240	899	910	920	rBV	36874	99581	3.62%	0.266%
5	7.951	1021	1031	1036	rBV2	280502	670273	24.39%	1.789%
6	8.016	1036	1042	1051	rVV	482283	1137711	41.39%	3.037%
7	8.098	1053	1056	1064	rVB7	22426	48116	1.75%	0.128%
8	8.369	1094	1102	1111	rBV2	312321	708359	25.77%	1.891%
9	8.498	1116	1124	1131	rBV6	20159	51156	1.86%	0.137%
10	8.575	1131	1137	1141	rBV6	14115	30574	1.11%	0.082%
11	8.639	1143	1148	1155	rVB7	24257	53477	1.95%	0.143%
12	8.904	1183	1193	1204	rBV	746696	1521082	55.34%	4.060%
13	9.216	1236	1246	1252	rBV3	13207	32811	1.19%	0.088%
14	9.392	1263	1276	1282	rBV2	289729	661915	24.08%	1.767%
15	9.445	1284	1285	1293	rVB4	34543	41937	1.53%	0.112%
16	9.810	1341	1347	1355	rVB5	25953	58997	2.15%	0.157%
17	9.963	1365	1373	1377	rBV2	28851	58796	2.14%	0.157%
18	10.016	1377	1382	1385	rBV3	30412	53874	1.96%	0.144%
19	10.151	1395	1405	1418	rBV5	54278	173771	6.32%	0.464%
20	10.381	1436	1444	1458	rBV	1259306	2401633	87.38%	6.410%
21	10.557	1467	1474	1484	rVB7	72897	177968	6.47%	0.475%
22	10.722	1496	1502	1511	rVB5	79561	146947	5.35%	0.392%
23	10.816	1511	1518	1522	rBV3	54333	107603	3.91%	0.287%
24	10.857	1522	1525	1528	rVV3	31946	46397	1.69%	0.124%
25	10.904	1528	1533	1539	rVB4	49890	87776	3.19%	0.234%
26	10.992	1539	1548	1556	rBV2	109442	201595	7.33%	0.538%
27	11.098	1560	1566	1574	rBV	104209	200928	7.31%	0.536%
28	11.169	1574	1578	1581	rVV6	29221	46295	1.68%	0.124%
29	11.233	1581	1589	1594	rVV3	127694	249401	9.07%	0.666%
30	11.286	1594	1598	1604	rVV2	134510	220988	8.04%	0.590%
31	11.339	1604	1607	1611	rVB5	22346	34712	1.26%	0.093%
32	11.398	1611	1617	1621	rBV	117617	207004	7.53%	0.553%
33	11.469	1621	1629	1639	rVB5	255311	626828	22.81%	1.673%
34	11.569	1639	1646	1651	rBV	151501	237586	8.64%	0.634%
35	11.686	1657	1666	1676	rBV	1205220	2077796	75.59%	5.546%
36	11.786	1676	1683	1688	rVV3	126989	238989	8.69%	0.638%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074517.D
 Acq On : 16 Sep 2022 18:02
 Operator : JC\MD
 Sample : N4447-03 100X
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1659DL

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

37	11.898	1692	1702	1712	rVV3	1085941	2168832	78.91%	5.789%
38	11.969	1712	1714	1720	rVB3	65153	102439	3.73%	0.273%
39	12.122	1732	1740	1745	rVB4	69245	145285	5.29%	0.388%
40	12.198	1745	1753	1758	rBV4	176225	377806	13.75%	1.008%
41	12.251	1758	1762	1765	rVV3	61399	107502	3.91%	0.287%
42	12.310	1767	1772	1777	rVB	161352	262205	9.54%	0.700%
43	12.398	1777	1787	1789	rBV7	123742	302990	11.02%	0.809%
44	12.433	1789	1793	1799	rVV4	150162	360142	13.10%	0.961%
45	12.522	1803	1808	1809	rVV4	64174	105336	3.83%	0.281%
46	12.569	1812	1816	1819	rVV4	135924	294579	10.72%	0.786%
47	12.604	1819	1822	1824	rVV	202951	319139	11.61%	0.852%
48	12.627	1824	1826	1829	rVV	235071	288505	10.50%	0.770%
49	12.675	1829	1834	1839	rVV	1025148	1697679	61.76%	4.531%
50	12.710	1839	1840	1845	rVV	191426	180617	6.57%	0.482%
51	12.757	1845	1848	1853	rVB7	34890	47541	1.73%	0.127%
52	12.851	1858	1864	1870	rVB3	99549	254286	9.25%	0.679%
53	12.922	1870	1876	1882	rBV2	230370	461058	16.77%	1.231%
54	12.992	1882	1888	1895	rVV2	1485052	2474928	90.04%	6.606%
55	13.051	1895	1898	1905	rVV5	80260	125407	4.56%	0.335%
56	13.139	1908	1913	1917	rVV4	95574	158446	5.76%	0.423%
57	13.192	1917	1922	1924	rVV4	99822	187811	6.83%	0.501%
58	13.227	1924	1928	1934	rVV2	294674	507502	18.46%	1.355%
59	13.310	1934	1942	1947	rVV	450107	843041	30.67%	2.250%
60	13.357	1947	1950	1954	rVV2	101292	157949	5.75%	0.422%
61	13.410	1955	1959	1968	rVV6	74738	242580	8.83%	0.647%
62	13.510	1968	1976	1979	rVV4	213048	417529	15.19%	1.114%
63	13.551	1979	1983	1986	rVV3	206731	343408	12.49%	0.917%
64	13.616	1986	1994	2003	rVV2	1417565	2748640	100.00%	7.337%
65	13.686	2003	2006	2013	rVV	176917	273142	9.94%	0.729%
66	13.751	2015	2017	2020	rVV4	20343	30960	1.13%	0.083%
67	13.810	2024	2027	2031	rVV2	92684	152853	5.56%	0.408%
68	13.857	2031	2035	2043	rVV3	108351	213559	7.77%	0.570%
69	13.939	2043	2049	2054	rVV	1305098	1888934	68.72%	5.042%
70	13.986	2054	2057	2061	rVV4	72942	139784	5.09%	0.373%
71	14.045	2064	2067	2069	rVV3	71108	108282	3.94%	0.289%
72	14.104	2071	2077	2082	rVV8	145579	383039	13.94%	1.022%
73	14.157	2082	2086	2091	rVV4	131370	244165	8.88%	0.652%
74	14.198	2091	2093	2099	rVB2	73797	102468	3.73%	0.274%
75	14.263	2099	2104	2109	rBV3	141128	234291	8.52%	0.625%
76	14.321	2109	2114	2122	rVB7	125202	235121	8.55%	0.628%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074517.D
 Acq On : 16 Sep 2022 18:02
 Operator : JC\MD
 Sample : N4447-03 100X
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 AUD-1659DL

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
 Title : SW846 8260

77	14.416	2122	2130	2132	rBV4	99408	209090	7.61%	0.558%
78	14.480	2133	2141	2147	rVV4	335717	1049498	38.18%	2.801%
79	14.580	2151	2158	2165	rVV3	234864	649617	23.63%	1.734%
80	14.651	2167	2170	2176	rVV4	82267	141668	5.15%	0.378%
81	14.704	2177	2179	2185	rVB6	25276	37930	1.38%	0.101%
82	14.792	2187	2194	2199	rBV	588012	840441	30.58%	2.243%
83	14.857	2200	2205	2210	rBV4	120262	230412	8.38%	0.615%
84	14.910	2210	2214	2220	rVB2	122188	218839	7.96%	0.584%
85	15.074	2239	2242	2247	rVB6	35545	52229	1.90%	0.139%
86	15.133	2249	2252	2259	rVB6	53150	93969	3.42%	0.251%
87	15.198	2259	2263	2265	rBV5	44799	64246	2.34%	0.171%
88	15.339	2282	2287	2292	rVB5	74372	148538	5.40%	0.396%
89	15.404	2292	2298	2300	rBV4	77717	134061	4.88%	0.358%
90	15.439	2301	2304	2309	rVB2	65315	107755	3.92%	0.288%
91	15.633	2332	2337	2345	rVB2	171988	285560	10.39%	0.762%
92	16.257	2437	2443	2448	rVB9	23625	60165	2.19%	0.161%
93	16.380	2462	2464	2471	rVB8	20571	37494	1.36%	0.100%
94	16.533	2481	2490	2495	rBV2	65491	160041	5.82%	0.427%
95	16.598	2497	2501	2507	rVB4	48835	89059	3.24%	0.238%
96	16.745	2518	2526	2531	rBV2	51927	117144	4.26%	0.313%

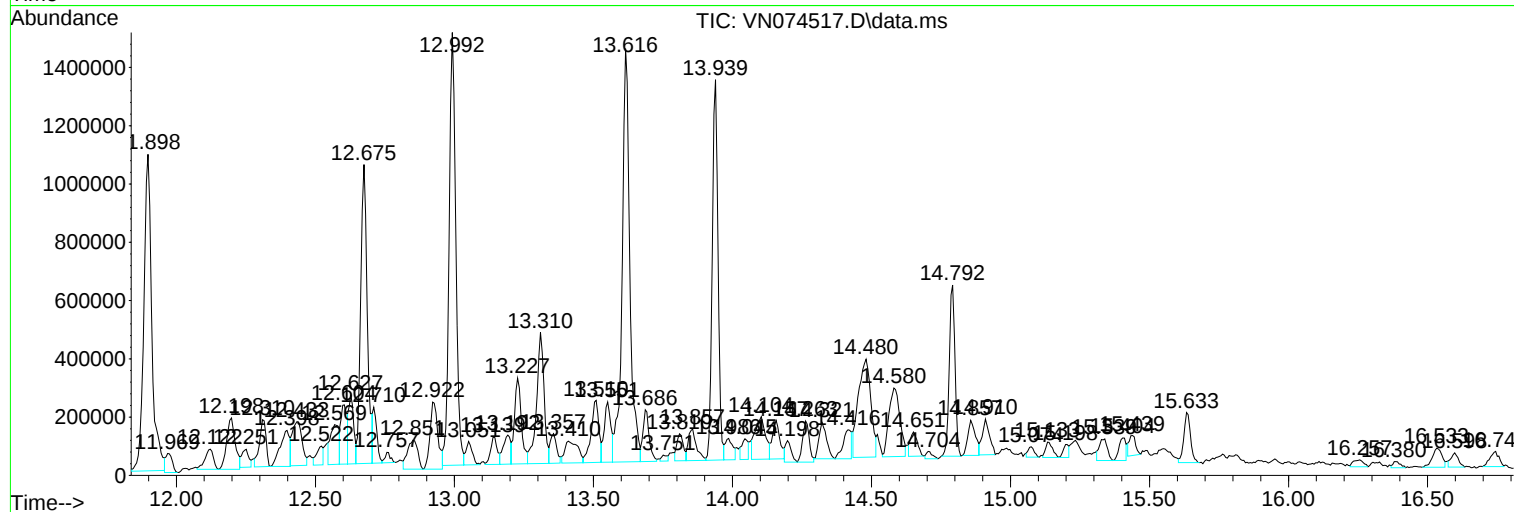
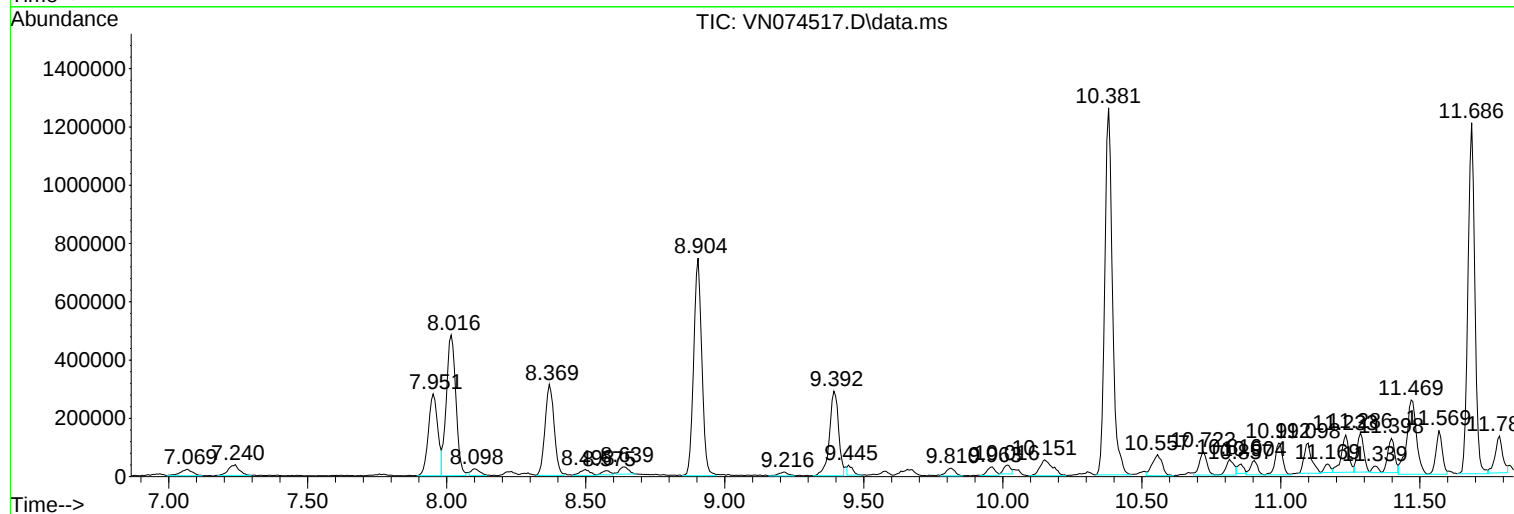
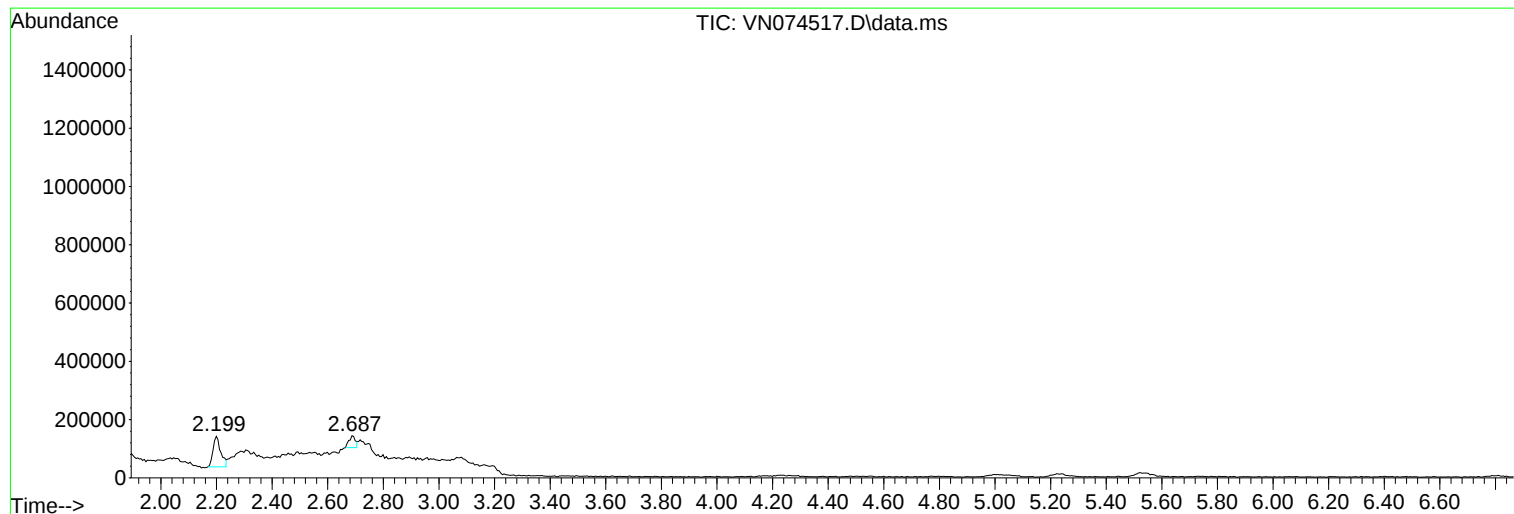
Sum of corrected areas: 37464999

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

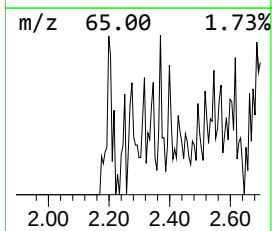
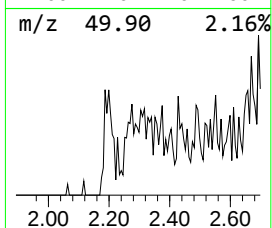
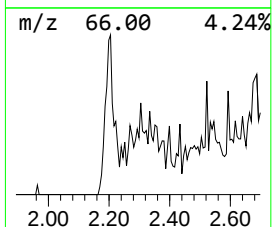
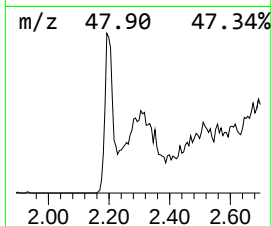
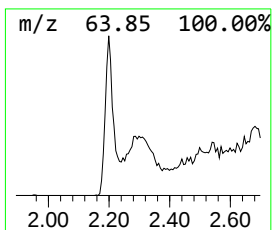
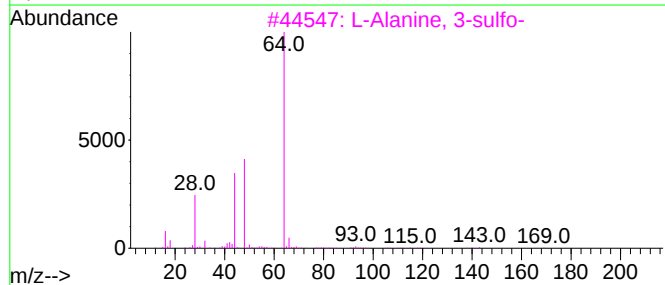
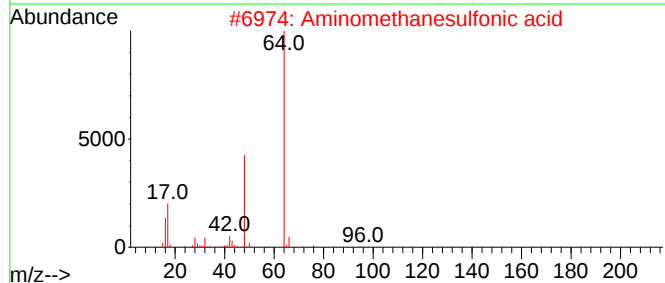
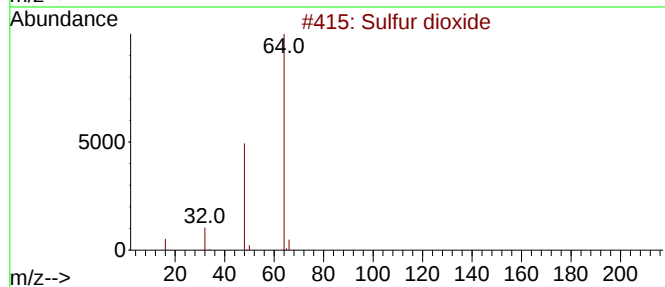
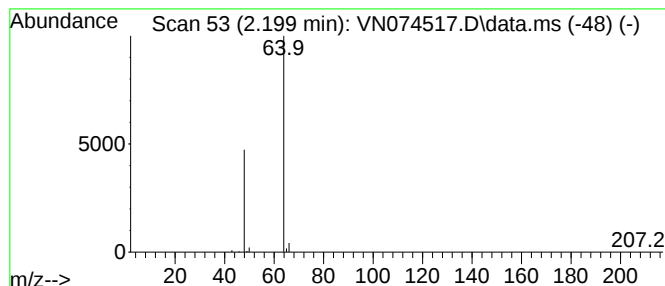
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	8.78 ug/l	199768	Pentafluorobenzene	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

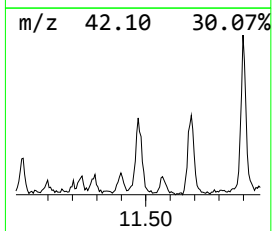
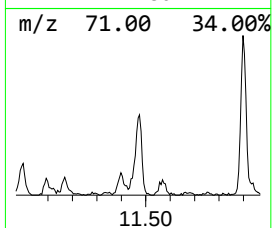
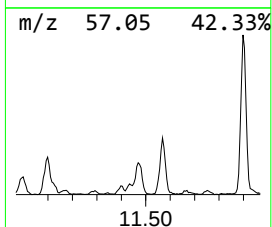
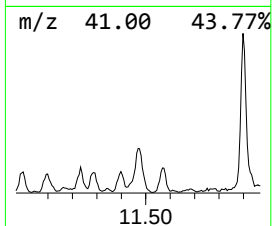
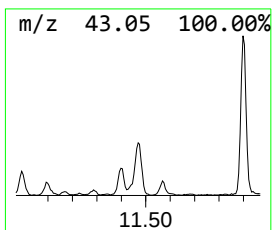
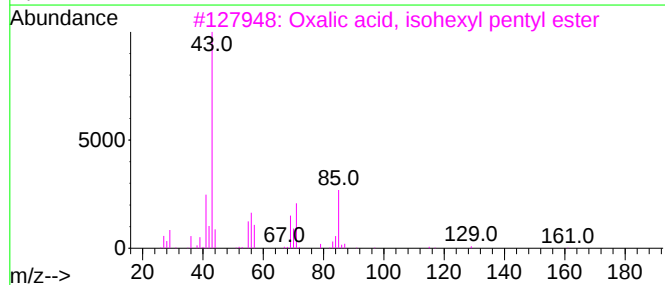
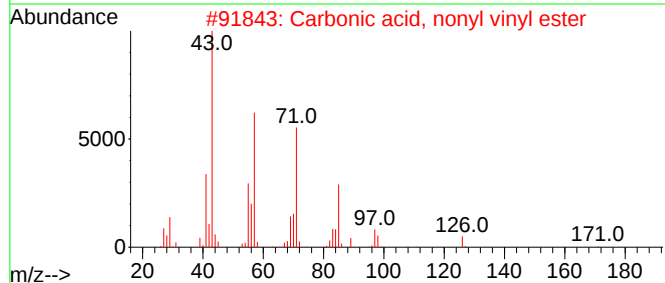
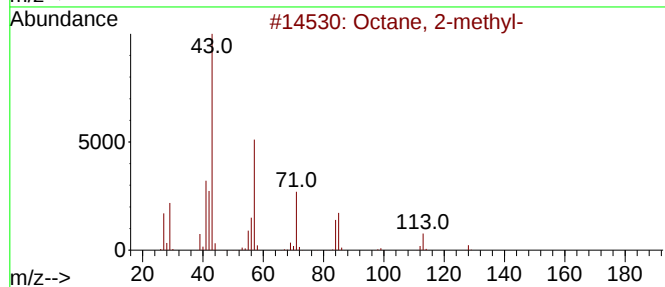
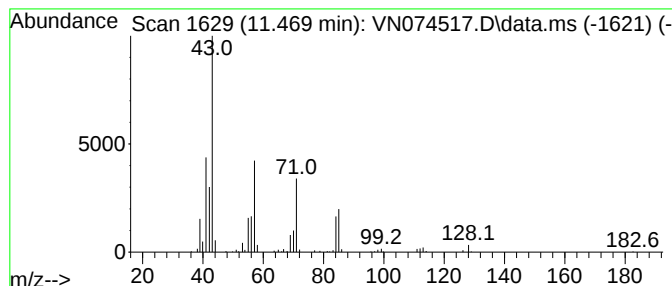
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.469	15.08 ug/l	626828	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2-methyl-	128	C9H20	003221-61-2	87
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64
3			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	64
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	64
5			Dodecane, 5-methyl-	184	C13H28	017453-93-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

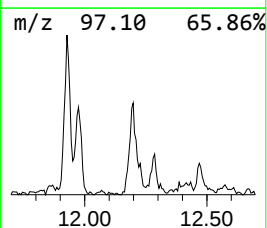
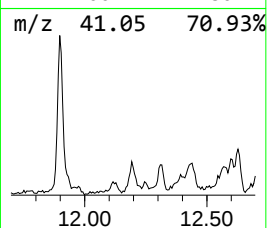
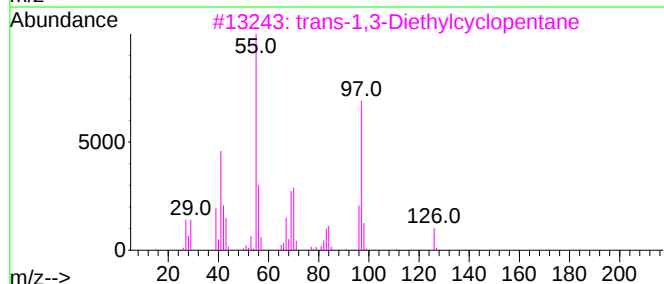
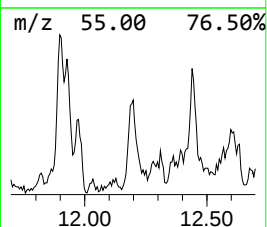
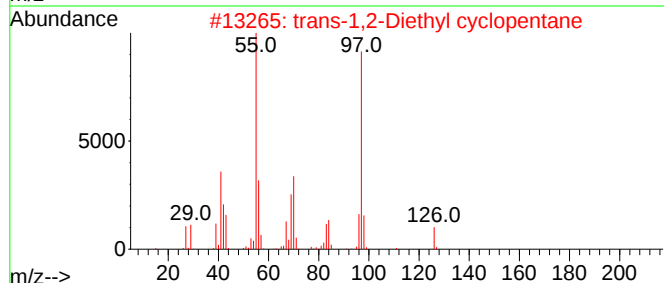
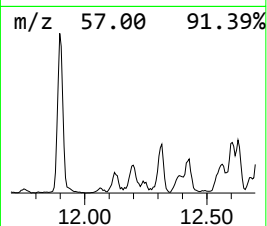
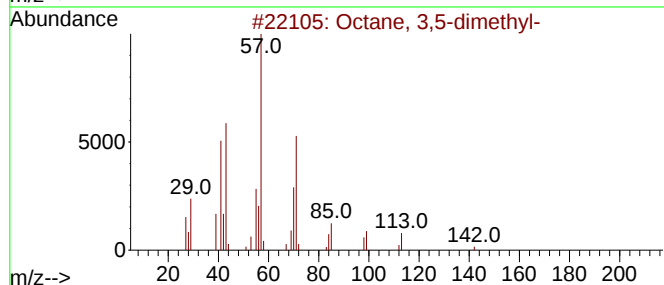
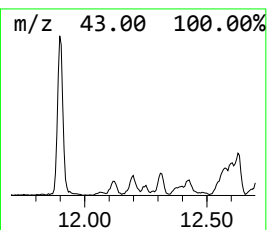
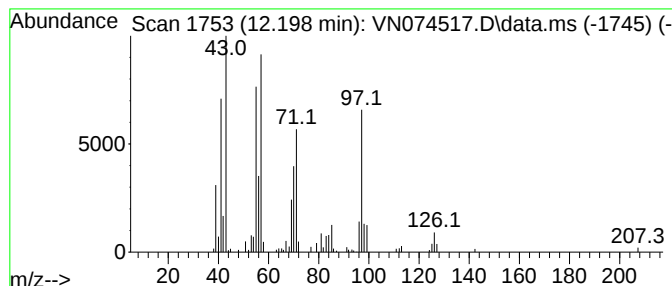
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.198 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.198	9.09 ug/l	377806	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-		142	C10H22		015869-93-9	46
2	trans-1,2-Diethyl cyclopentane		126	C9H18		000932-40-1	46
3	trans-1,3-Diethylcyclopentane		126	C9H18		1000113-87-1	45
4	Octane, 2,6-dimethyl-		142	C10H22		002051-30-1	38
5	Cyclohexane, 1,3-dimethyl-, trans-		112	C8H16		002207-03-6	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

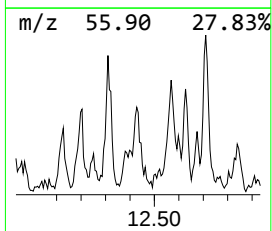
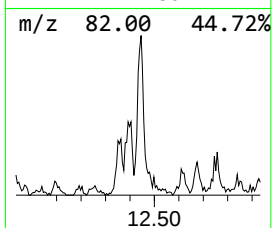
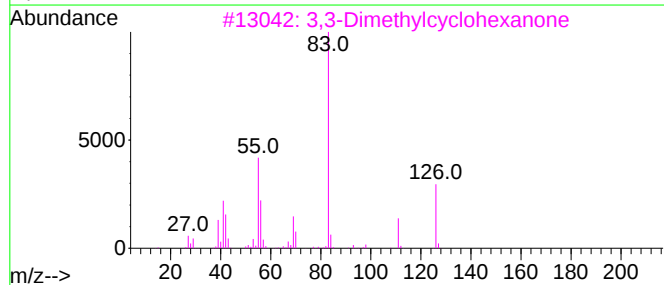
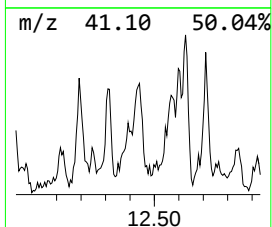
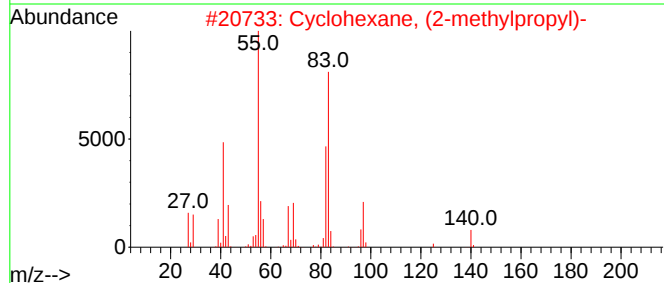
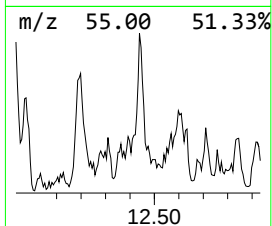
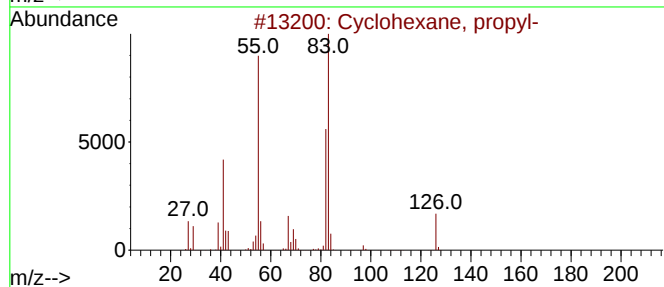
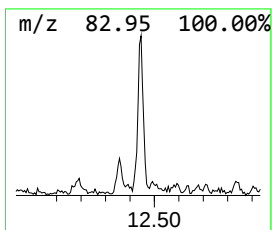
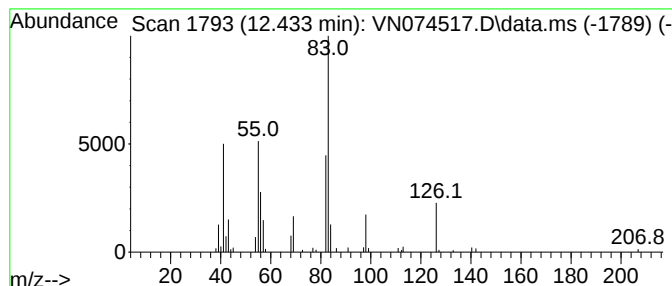
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexane, propyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.433	8.67 ug/l	360142	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, propyl-	126	C9H18	001678-92-8	64
2			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	59
3			3,3-Dimethylcyclohexanone	126	C8H14O	002979-19-3	59
4			Cyclohexane, ethyl-	112	C8H16	001678-91-7	53
5			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

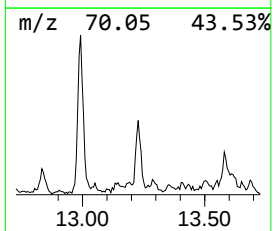
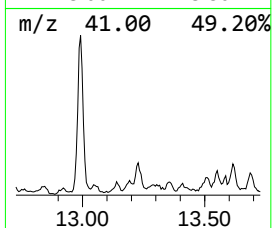
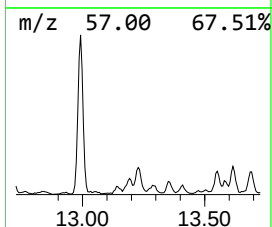
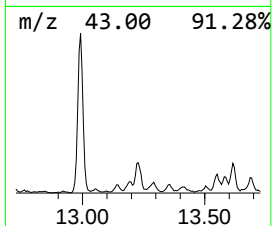
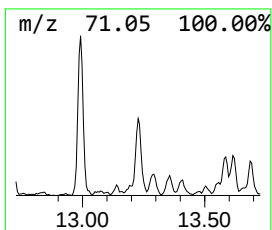
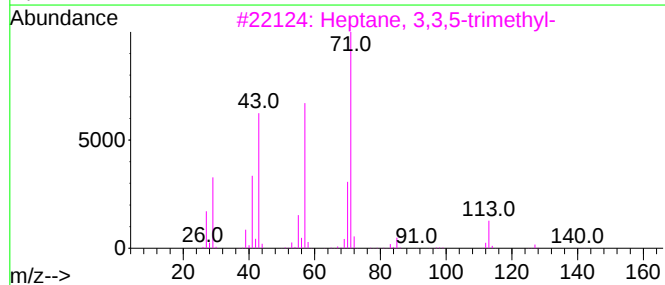
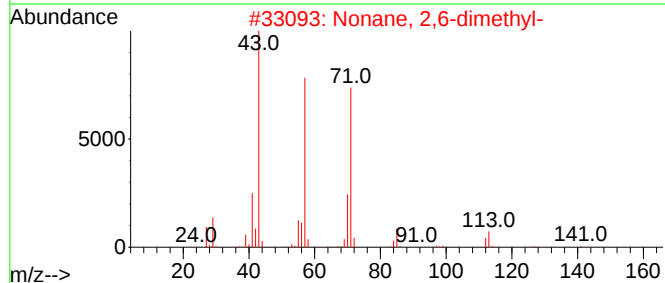
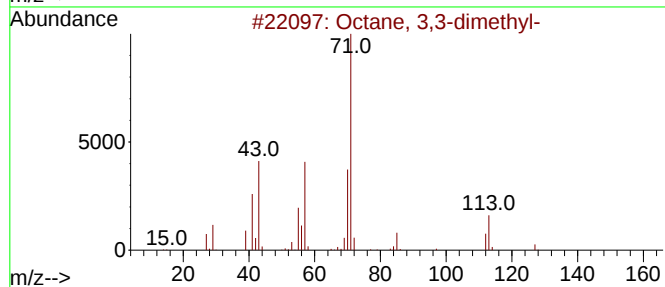
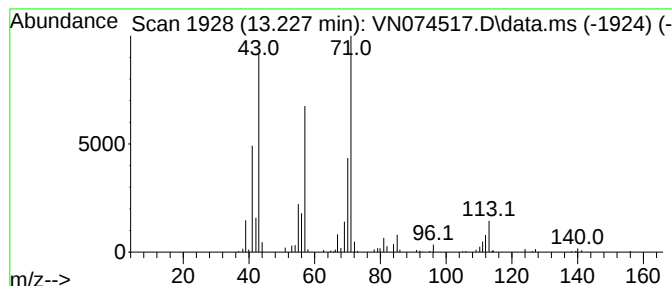
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octane, 3,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	9.23 ug/l	507502	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	78
2			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64
3			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
4			n-Amyl ether	158	C10H22O	000693-65-2	59
5			Carbonic acid, dipentyl ester	202	C11H22O3	002050-94-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

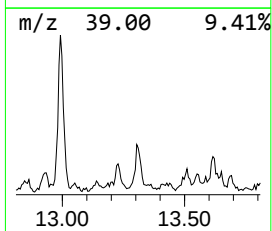
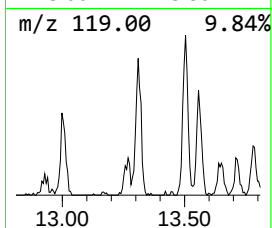
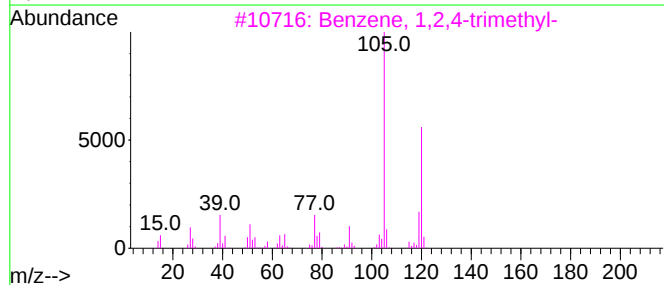
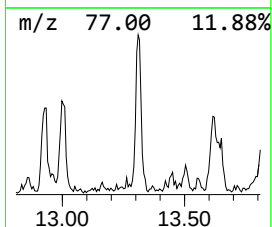
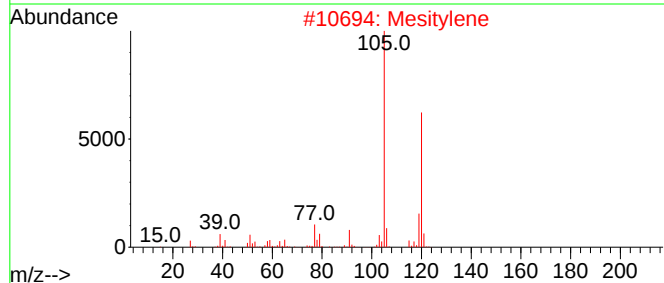
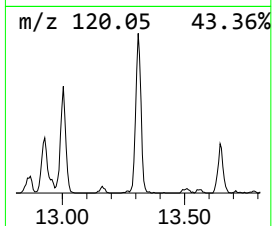
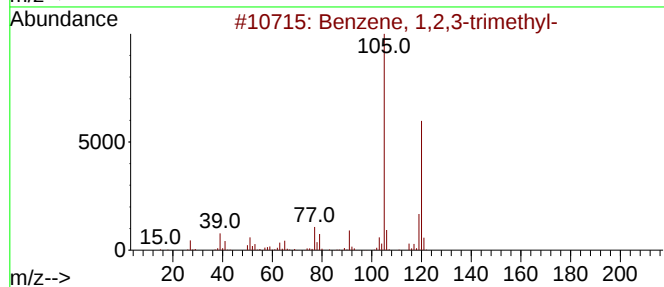
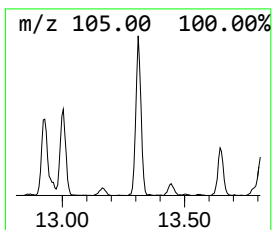
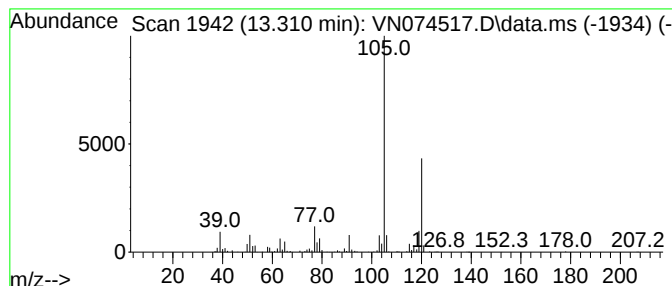
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.310	15.34 ug/l	843041	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

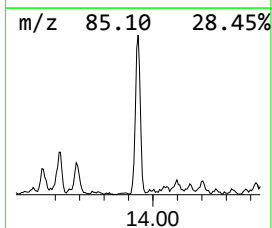
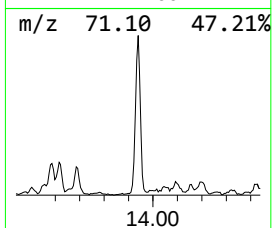
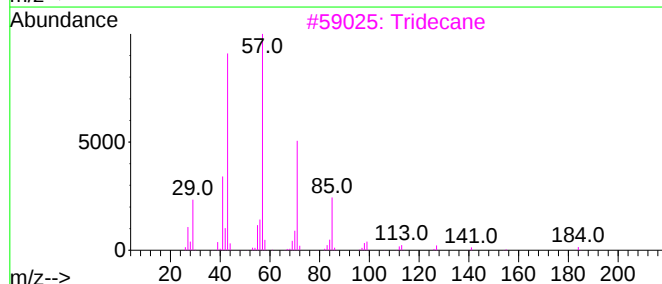
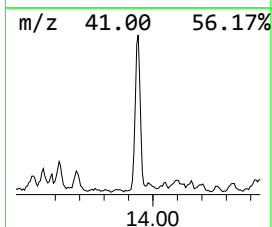
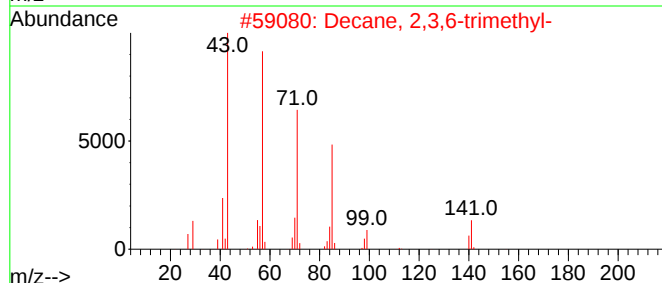
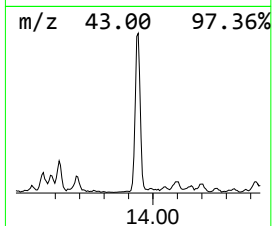
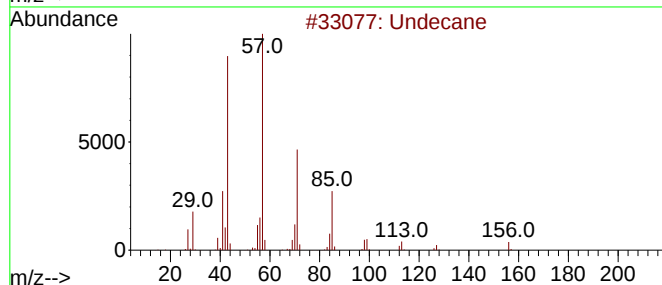
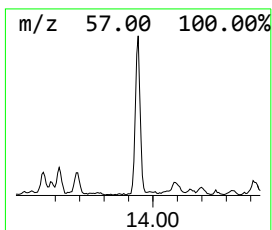
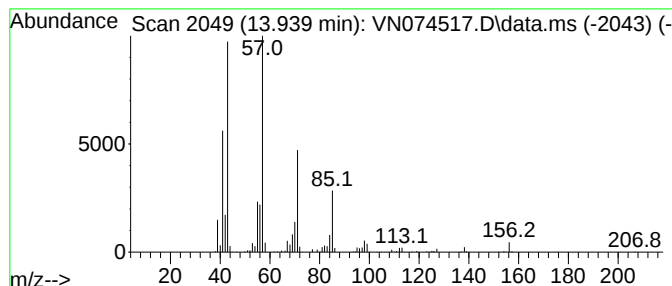
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	34.36 ug/l	1888930	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	90
2	Decane, 2,3,6-trimethyl-			184	C13H28	062238-12-4	72
3	Tridecane			184	C13H28	000629-50-5	64
4	1-Decene, 3,4-dimethyl-			168	C12H24	050871-03-9	59
5	Undecane, 2,4-dimethyl-			184	C13H28	017312-80-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

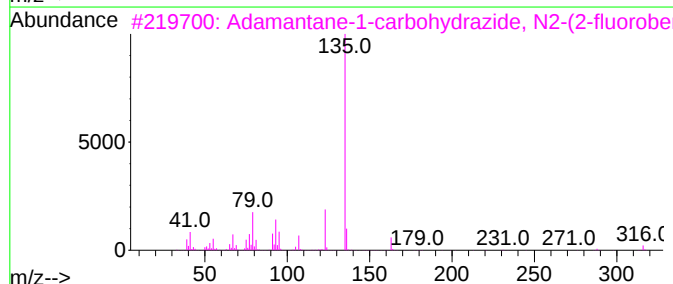
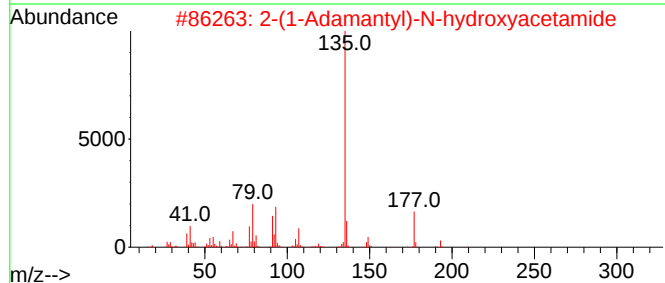
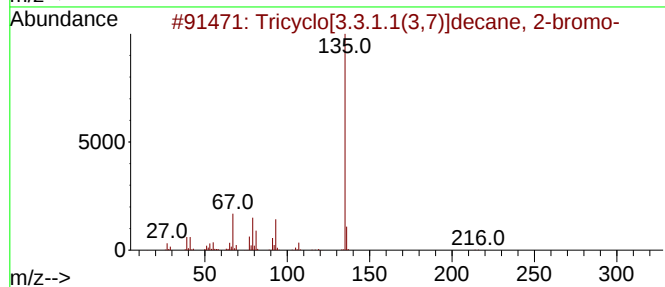
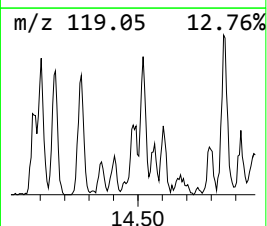
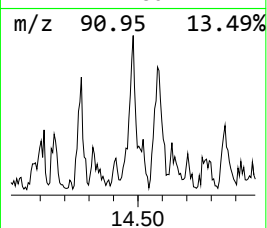
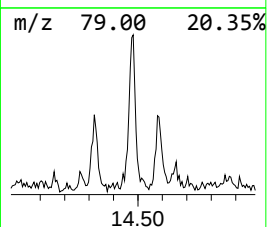
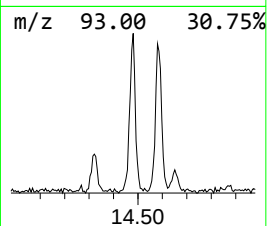
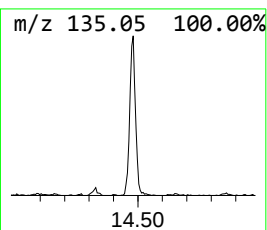
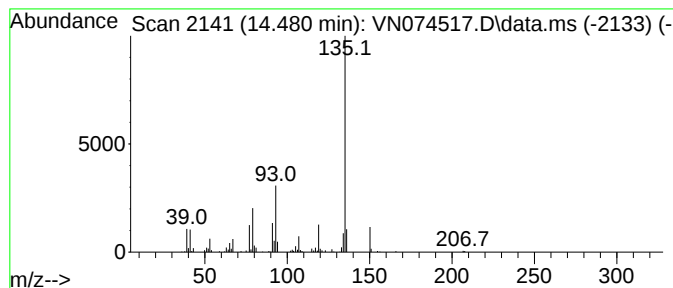
Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tricyclo[3.3.1.1(3,7)]decan... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.480	19.09 ug/l	1049500	1,4-Dichlorobenzene-d4		13.616	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tricyclo[3.3.1.1(3,7)]decane, 2-...		214	C10H15Br	007314-85-4	72
2	2-(1-Adamantyl)-N-hydroxyacetamide		209	C12H19NO2	136561-40-5	64
3	Adamantane-1-carbohydrazide, N2-...		316	C18H21FN2O2	332037-11-3	64
4	1-Adamantanecarboxylic acid chlo...		198	C11H15ClO	002094-72-6	59
5	Adamantane-1-carboxamide, N-(4-m...		261	C14H19N3O2	332042-32-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

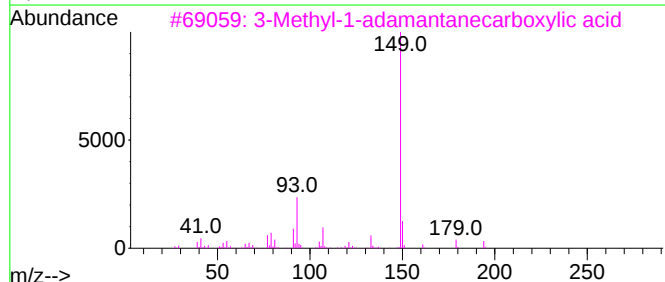
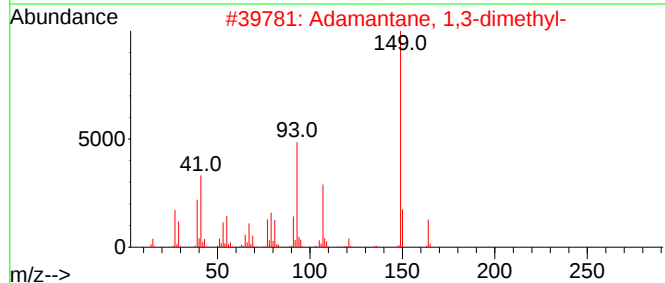
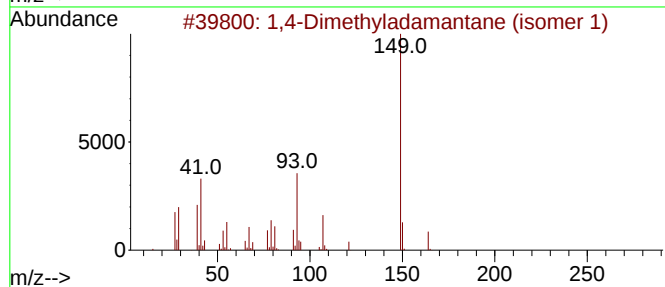
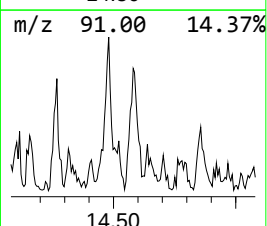
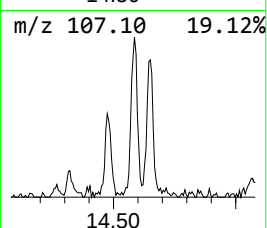
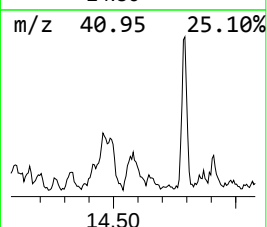
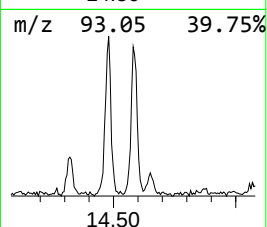
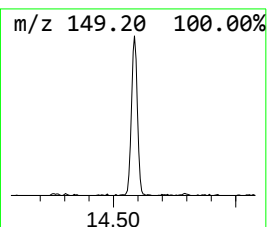
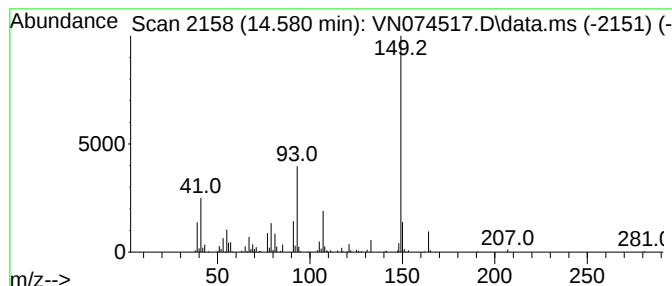
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1,4-Dimethyladamantane (iso... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	11.82 ug/l	649617	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	90
2			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	60
3			3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	50
4			1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	47
5			2'-Hydroxy-4',5'-dimethylacetoph...	164	C10H12O2	036436-65-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

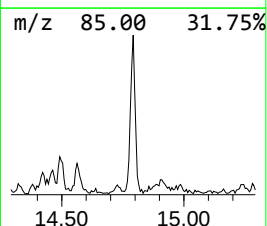
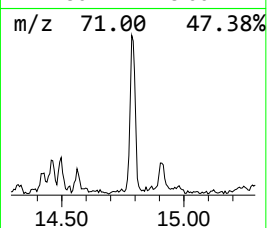
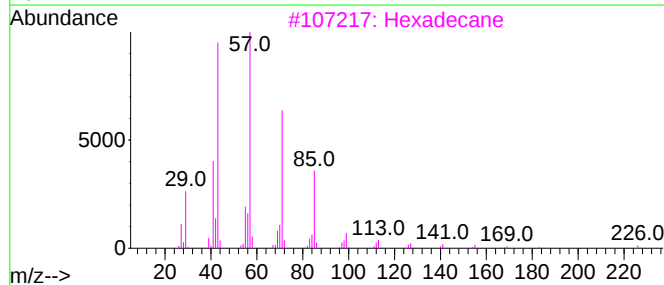
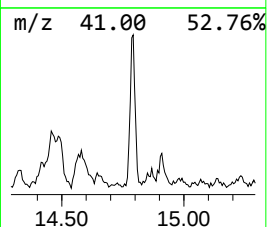
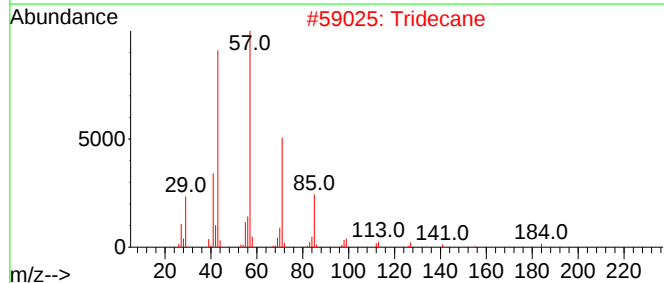
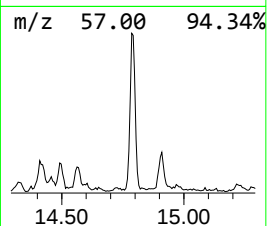
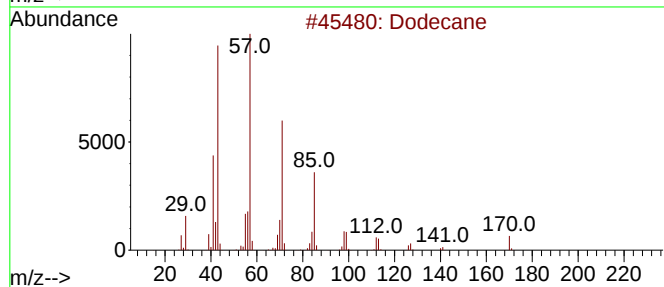
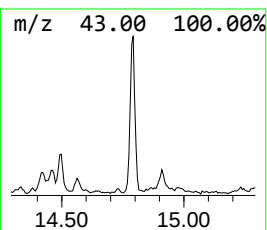
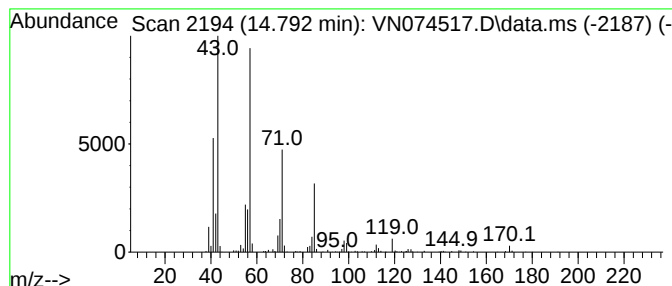
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.792	15.29 ug/l	840441	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	90
2			Tridecane	184	C13H28	000629-50-5	83
3			Hexadecane	226	C16H34	000544-76-3	72
4			Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
5			Undecane	156	C11H24	001120-21-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074517.D
Acq On : 16 Sep 2022 18:02
Operator : JC\MD
Sample : N4447-03 100X
Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1659DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	8.8	ug/l	199768	1	8.010	1137710	50.0
Octane, 2-methyl-	11.469	15.1	ug/l	626828	3	11.686	2077800	50.0
unknown12.198	12.198	9.1	ug/l	377806	3	11.686	2077800	50.0
Cyclohexane, pr...	12.433	8.7	ug/l	360142	3	11.686	2077800	50.0
Octane, 3,3-dim...	13.227	9.2	ug/l	507502	4	13.616	2748640	50.0
Benzene, 1,2,3-...	13.310	15.3	ug/l	843041	4	13.616	2748640	50.0
Undecane	13.939	34.4	ug/l	1888930	4	13.616	2748640	50.0
Tricyclo[3.3.1....	14.480	19.1	ug/l	1049500	4	13.616	2748640	50.0
1,4-Dimethylada...	14.580	11.8	ug/l	649617	4	13.616	2748640	50.0
Dodecane	14.792	15.3	ug/l	840441	4	13.616	2748640	50.0