LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

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\82N083022W.M
Title : SW846 8260

Signal : TIC: VN074211.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.552	108	113	119	rBV	101771	169928	2.17%	0.274%
2	5.287	563	578	599	rBV2	505840	1916705	24.47%	3.089%
3	6.404	756	768	789	rBV5	61559	225102	2.87%	0.363%
4	6.969	850	864	876	rBV3	166524	520629	6.65%	0.839%
5	7.234	898	909	923	rBV2	85934	298964	3.82%	0.482%
6	7.951	1021	1031	1036	rBV3	179712	427535	5.46%	0.689%
7	8.016	1036	1042	1054	rVB2	286393	656093	8.37%	1.057%
8	8.369	1093	1102	1111	rBV3	209520	513043	6.55%	0.827%
9	8.463	1111	1118	1128	rVB3	124929	302612	3.86%	0.488%
10	8.904	1184	1193	1209	rBV	438847	914005	11.67%	1.473%
11	9.410	1271	1279	1286	rVB5	143466	300474	3.84%	0.484%
12	9.728	1327	1333	1340	rBV2	44657	88737	1.13%	0.143%
13	9.863	1350	1356	1369	rBV2	219452	444326	5.67%	0.716%
14	10.169	1397	1408	1417	rVB4	95297	231585	2.96%	0.373%
15	10.275	1418	1426	1434	rBV	116827	218405	2.79%	0.352%
16	10.380	1436	1444	1458	rBV	726785	1385920	17.69%	2.233%
17	10.557	1468	1474	1477	rBV4	70746	139868	1.79%	0.225%
18	10.592	1477	1480	1490	rVB3	62381	110118	1.41%	0.177%
19	10.804	1509	1516	1523	rBV8	26867	80081	1.02%	0.129%
20	10.998	1540	1549	1558	rBV	387895	684093	8.73%	1.102%
21	11.092	1558	1565	1566	rVV2	57436	101045	1.29%	0.163%
22	11.127	1567	1571	1580	rVV7	91664	236915	3.02%	0.382%
23	11.227	1580	1588	1593	rVV2	80070	171683	2.19%	0.277%
24	11.286	1593	1598	1604	rVB4	54945	95163	1.21%	0.153%
25	11.398	1611	1617	1622	rBV	77565	136872	1.75%	0.221%
26	11.469	1624	1629	1639	rVB4	94222	199219	2.54%	0.321%
27	11.569	1639	1646	1657	rVB	108296	229125	2.92%	0.369%
28	11.680	1657	1665	1675	rBV	704633	1293992	16.52%	2.085%
29	11.786	1675	1683	1690	rBV	900780	1850540	23.62%	2.982%
30	11.845	1690	1693	1694	rVV	133066	144974	1.85%	0.234%
31	11.886	1694	1700	1710	rVB	4503499	7834022	100.00%	12.625%
32	11.963	1710	1713	1718	rVB3	95002	150531	1.92%	0.243%
33	12.021	1718	1723	1731	rVB	236895	400912	5.12%	0.646%
34	12.121	1732	1740	1745	rVB4	41849	93237	1.19%	0.150%
35	12.198	1745	1753	1754	rBV4	127304	218487	2.79%	0.352%
36	12.304	1768	1771	1777	rVB3	88822	136902	1.75%	0.221%

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AUD-1656-WATER

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

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Title : SW846 8260

37	12.386	1777	1785	1789	rBV7	116587	283226	3.62%	0.456%
38	12.469	1795	1799	1803	rVB	168271	227654	2.91%	0.367%
39	12.516	1803	1807	1812	rVB	282142	419063	5.35%	0.675%
40	12.669	1828	1833	1838	rBV	606314	997448	12.73%	1.607%
41	12.769	1845	1850	1856	rVB7	48165	98872	1.26%	0.159%
42	12.857	1857	1865	1870	rVB	355107	612277	7.82%	0.987%
43	12.921	1870	1876	1884	rBV	1592953	3241979	41.38%	5.224%
44	12.998	1884	1889	1895	rVV2	2132430	3648338	46.57%	5.879%
45	13.157	1909	1916	1924	rBV2	277733	710314	9.07%	1.145%
46	13.221	1924	1927	1931	rVV2	194518	299814	3.83%	0.483%
47	13.263	1931	1934	1935	rVV2	172869	199405	2.55%	0.321%
48	13.304	1935	1941	1948	rVB	3182831	5290502	67.53%	8.526%
49	13.427	1954	1962	1968	rBV4	129830	350261	4.47%	0.564%
50	13.504	1968	1975	1979	rBV2	316027	615093	7.85%	0.991%
51	13.551	1979	1983	1987	rVV3	172358	270107	3.45%	0.435%
52	13.616	1987	1994	1995	rVV	893924	1340276	17.11%	2.160%
53	13.645	1995	1999	2004	rVB	2034283	3234835	41.29%	5.213%
54	13.774	2017	2021	2023	rBV2	103972	151448	1.93%	0.244%
55	13.810	2023	2027	2030	rVV2	411082	665416	8.49%	1.072%
56	13.845	2030	2033	2042	rVB3	421193	746453	9.53%	1.203%
57	13.933	2042	2048	2053	rBV2	801972	1162920	14.84%	1.874%
58	14.004	2053	2060	2064	rBV2	155997	323849	4.13%	0.522%
59	14.068	2067	2071	2073	rVV2	207731	349409	4.46%	0.563%
60	14.098	2073	2076	2081	rVV	317233	539771	6.89%	0.870%
61	14.151	2081	2085	2090	rVB	301849	473633	6.05%	0.763%
62	14.263	2098	2104	2109	rBV2	333233	547169	6.98%	0.882%
63	14.315	2109	2113	2120	rVB4	206035	368239	4.70%	0.593%
64	14.398	2122	2127	2132	rVV4	194450	414833	5.30%	0.669%
65	14.474	2132	2140	2145	rVV3	601920	1547072	19.75%	2.493%
66	14.515	2145	2147	2151	rVV	301844	386409	4.93%	0.623%
67	14.580	2151	2158	2164	rVV3	310422	794161	10.14%	1.280%
68	14.639	2165	2168	2175	rVB3	116919	214313	2.74%	0.345%
69	14.786	2188	2193	2198	rVB	649775	926947	11.83%	1.494%
70	14.851	2198	2204	2209	rBV2	422280	830142	10.60%	1.338%
71	14.904	2210	2213	2222	rVB3	206168	363850	4.64%	0.586%
72	15.015	2229	2232	2236	rVB3	55954	80608	1.03%	0.130%
73	15.133	2247	2252	2257	rBV4	160968	299261	3.82%	0.482%
74	15.215	2264	2266	2273	rVB7	85637	173526	2.22%	0.280%
75	15.310	2275	2282	2291	rVB9	156327	517520	6.61%	0.834%
76	15.433	2291	2303	2314	rBV2	760812	1907170	24.34%	3.073%

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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Title : SW846 8260

77	15.627	2331	2336	2342	rVB	459017	742622	9.48%	1.197%
78	15.751	2353	2357	2364	rBV6	44533	111455	1.42%	0.180%
79	16.098	2410	2416	2424	rBV6	36605	107817	1.38%	0.174%
80	16.233	2435	2439	2447	rVB7	35908	83600	1.07%	0.135%
81	16.309	2447	2452	2458	rVB8	41719	88653	1.13%	0.143%
82	16.386	2459	2465	2471	rVB2	69887	131767	1.68%	0.212%
83	16.527	2480	2489	2495	rBV	410050	915026	11.68%	1.475%
84	16.592	2495	2500	2507	rVB3	232517	436505	5.57%	0.703%
85	16.739	2515	2525	2533	rBV	416941	890759	11.37%	1.435%

Sum of corrected areas: 62053629

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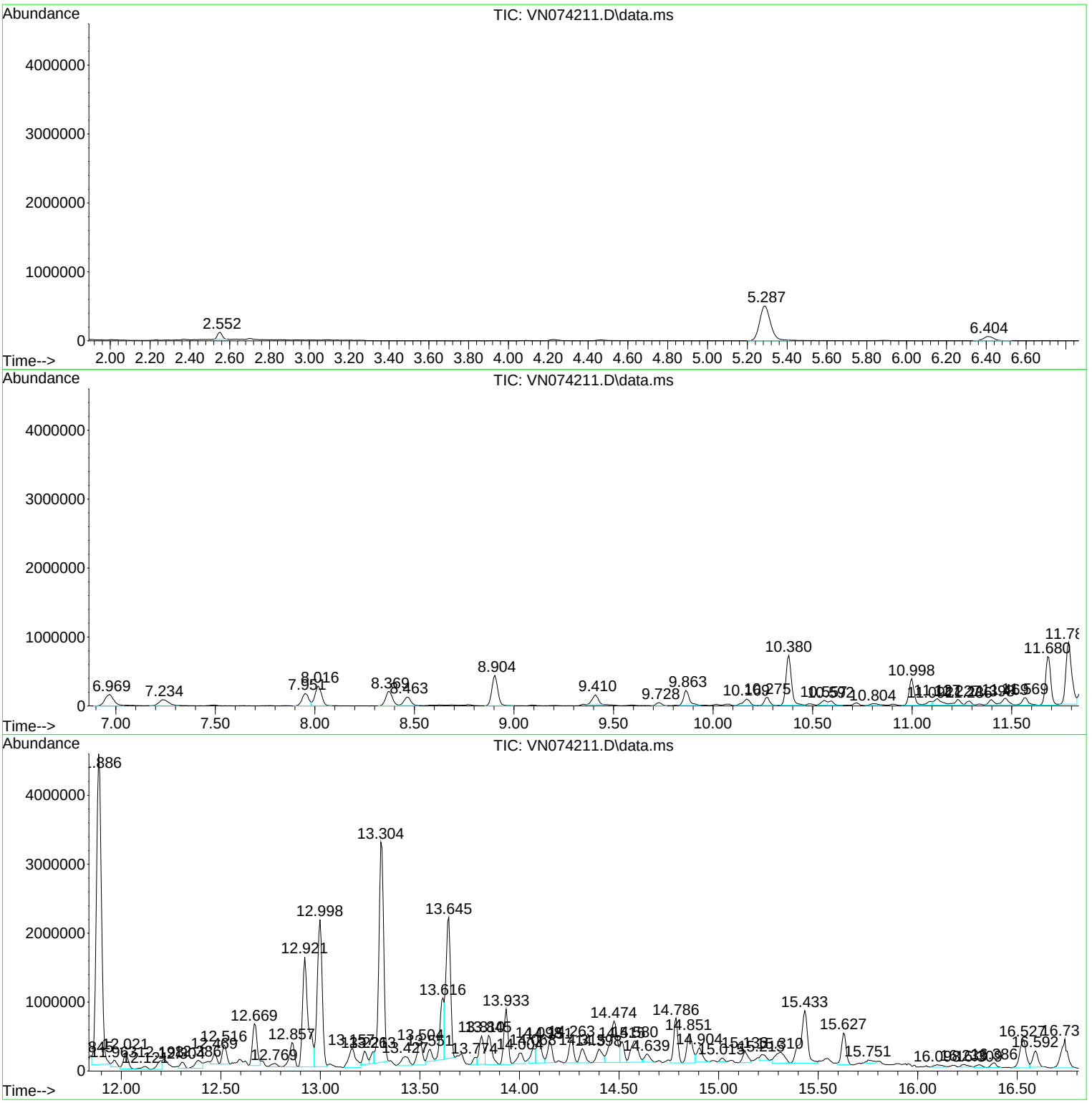
ClientSampleId :
AUD-1656-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
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Operator : JC\MD
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
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TIC Library : C:\Database\NIST20.L
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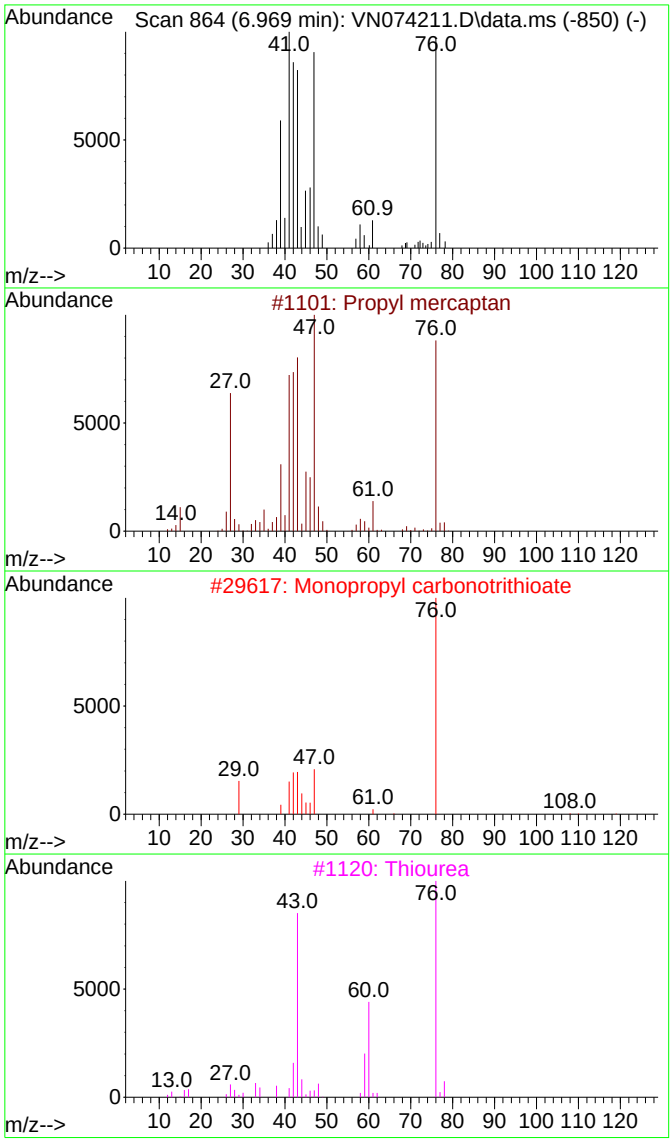
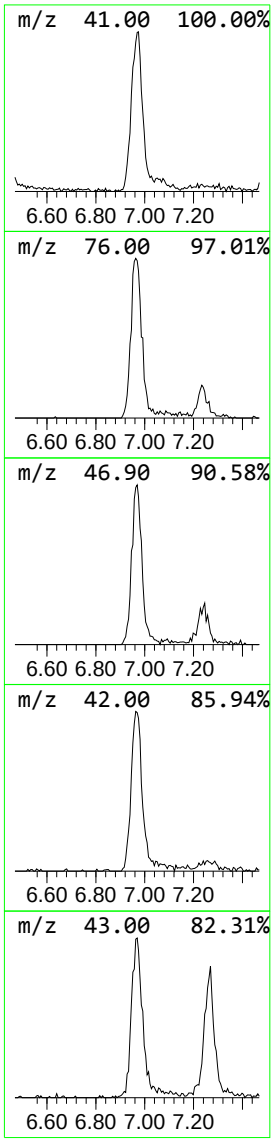
****
Peak Number 1 Propyl mercaptan Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	39.68 ug/l	520629	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	96
2	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	78
3	Thiourea	76	CH4N2S	000062-56-6	37
4	Isopropyl phosphine	76	C3H9P	004538-29-8	28
5	Cyclopropane	42	C3H6	000075-19-4	9





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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

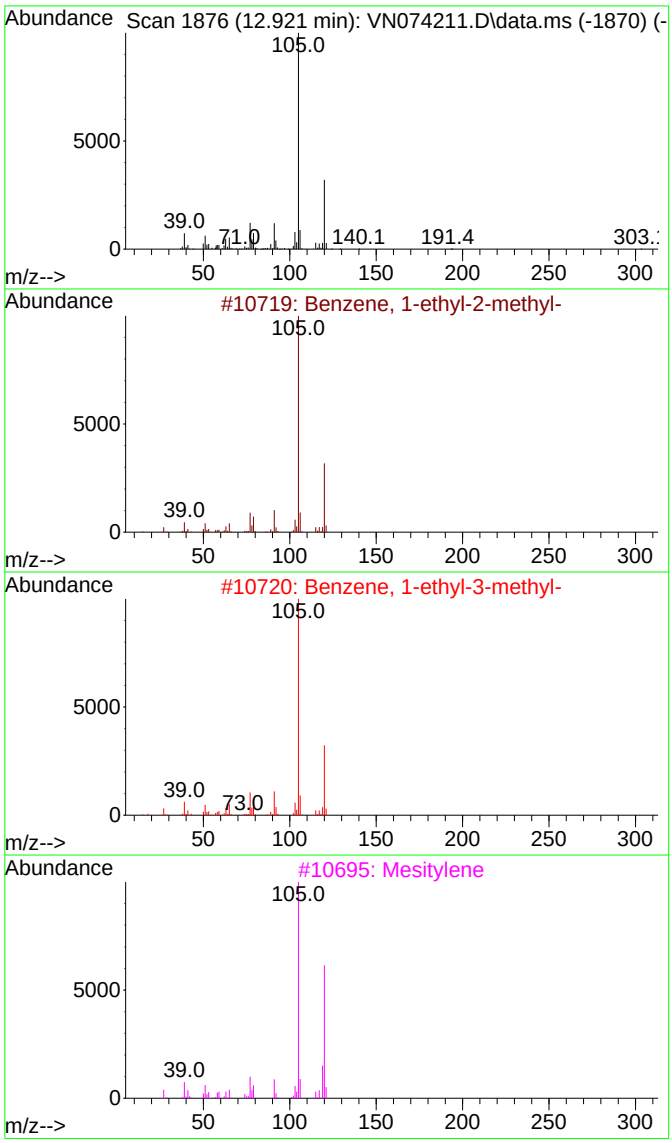
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

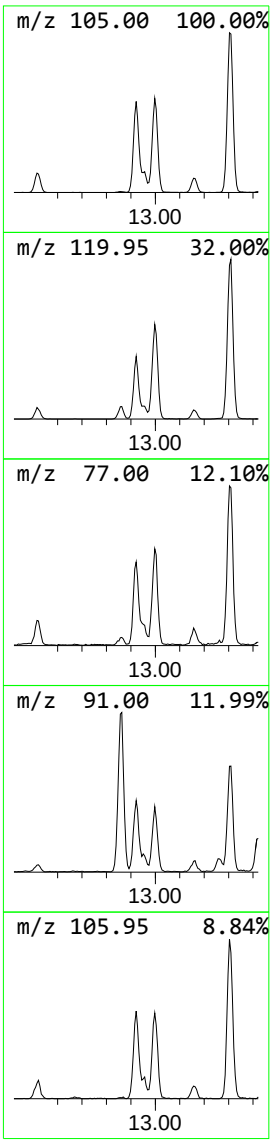
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.921	120.94 ug/l	3241980	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





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ClientSampleId :
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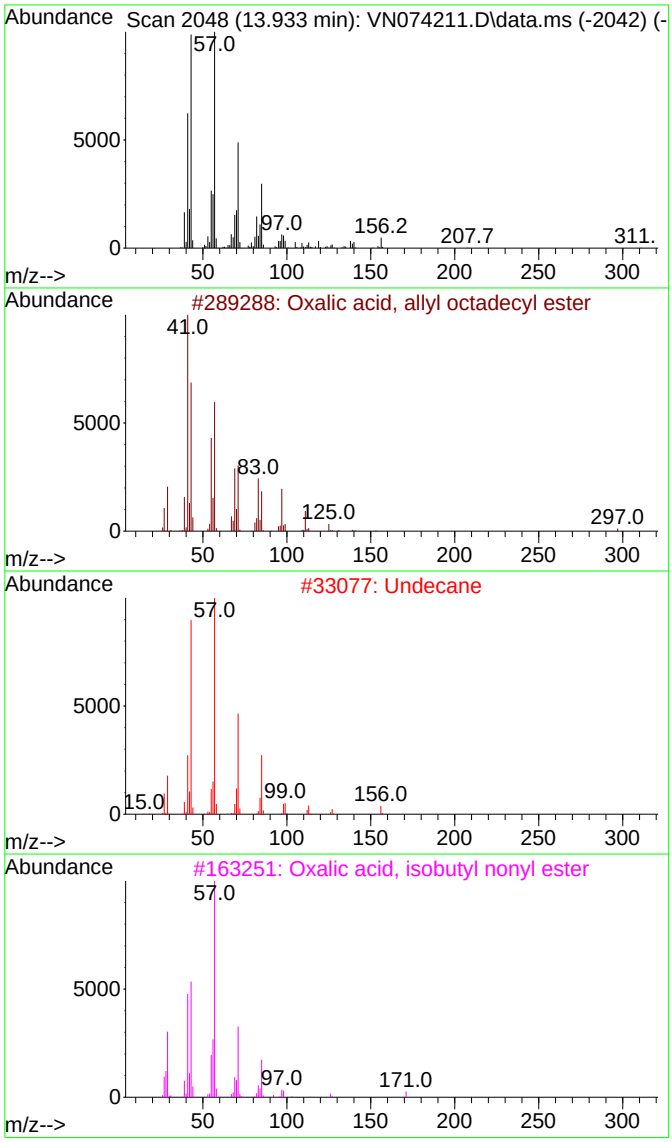
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

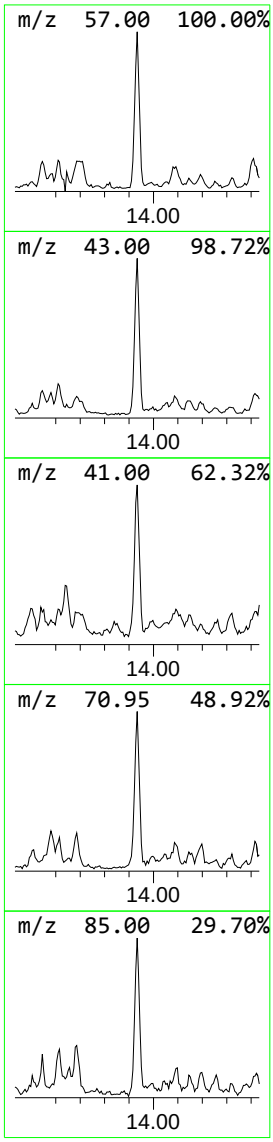
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Oxalic acid, allyl octadecy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	43.38 ug/l	1162920	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	86
2	Undecane	156	C11H24	001120-21-4	74
3	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	47
4	Ether, heptyl hexyl	200	C13H28O	007289-40-9	43
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	38





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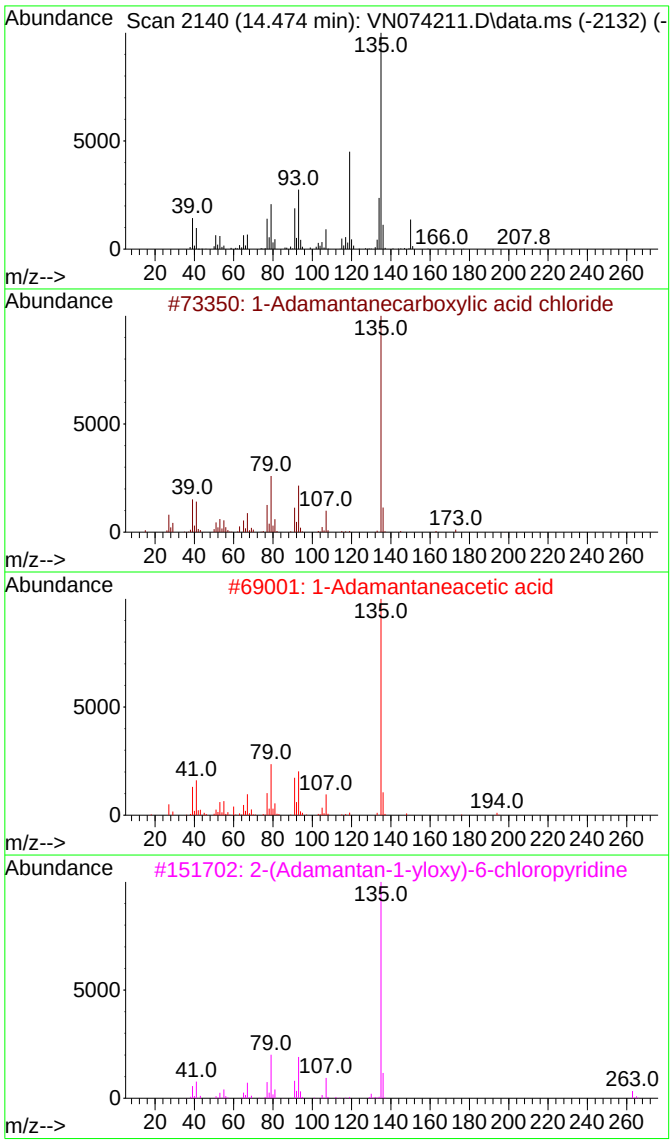
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

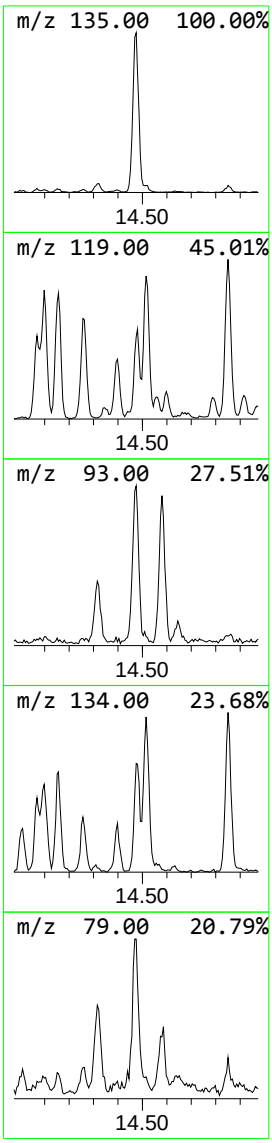
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 unknown14.474 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	57.71 ug/l	1547070	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	49
2	1-Adamantaneacetic acid	194	C12H18O2	004942-47-6	47
3	2-(Adamantan-1-yloxy)-6-chloropy...	263	C15H18ClNO	1000411-33-6	47
4	Adamantane, 1-chloro-	170	C10H15Cl	000935-56-8	47
5	3-(Adamantan-1-yl)propanoic acid	208	C13H20O2	016269-16-2	47





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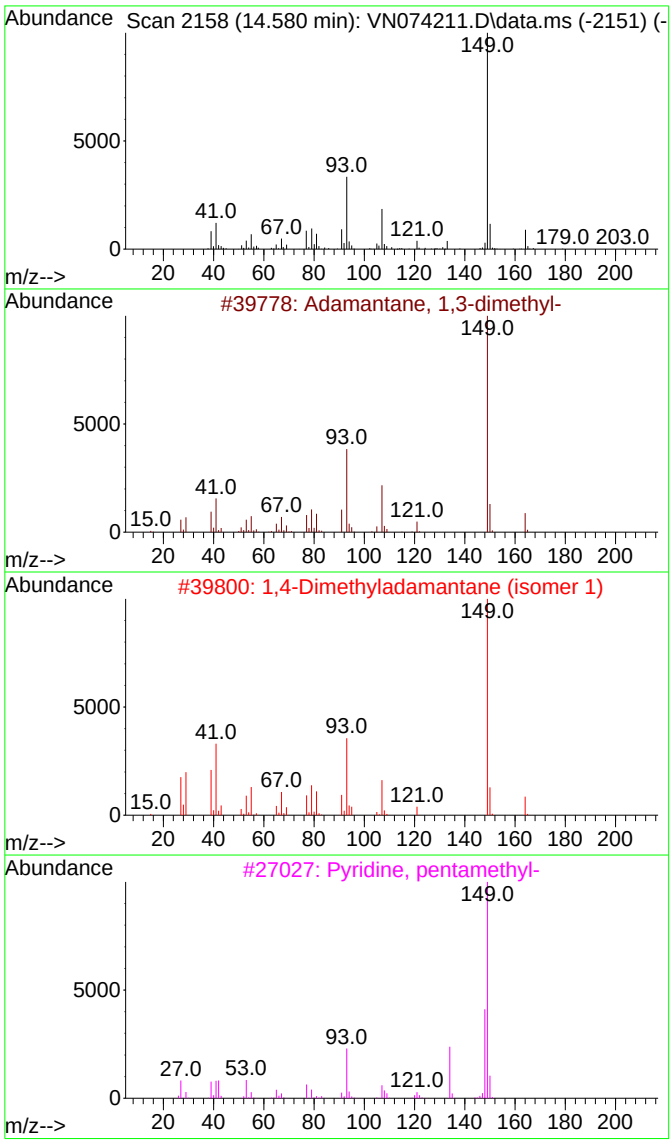
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

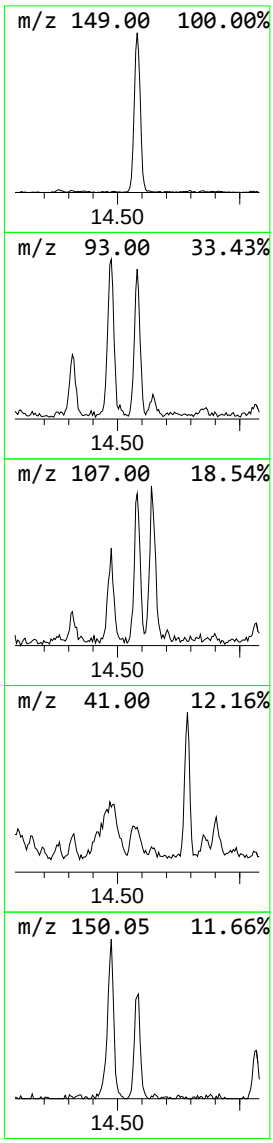
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Adamantane, 1,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.580	29.63 ug/l	794161	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	96
2	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	83
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	59
4	1H-S-Triazolo[1,5-a]pyridin-4-iu...	149	C7H7N3O	013980-64-8	50
5	Tricyclo[4.3.1.1(3,8)]undecane, ...	184	C11H17Cl	027011-46-7	47





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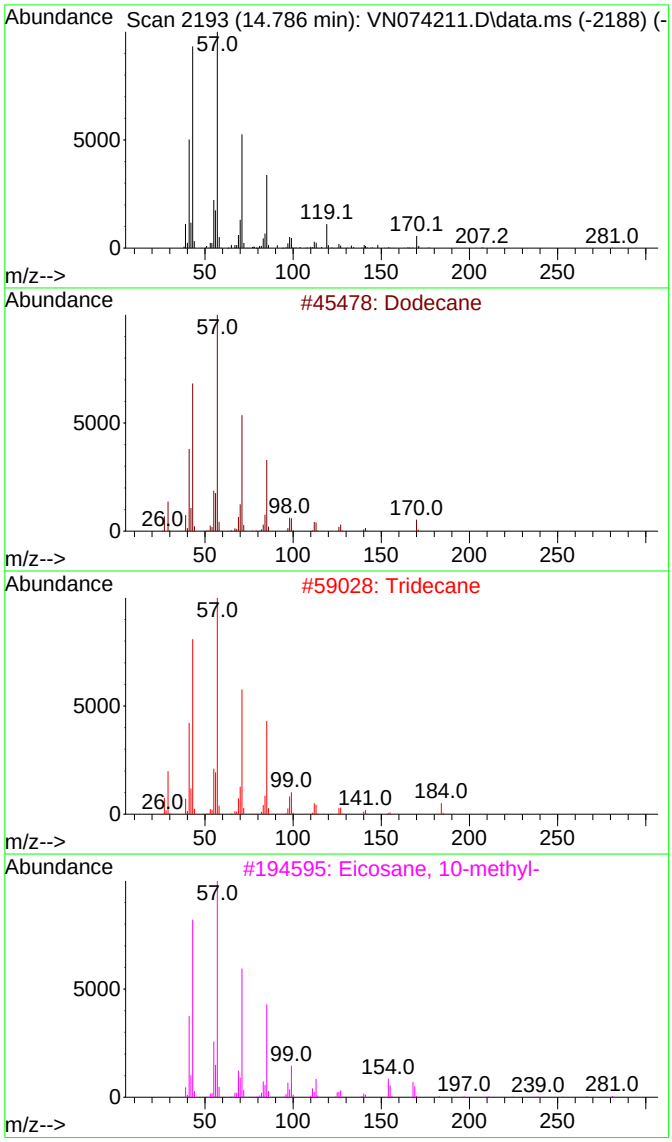
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

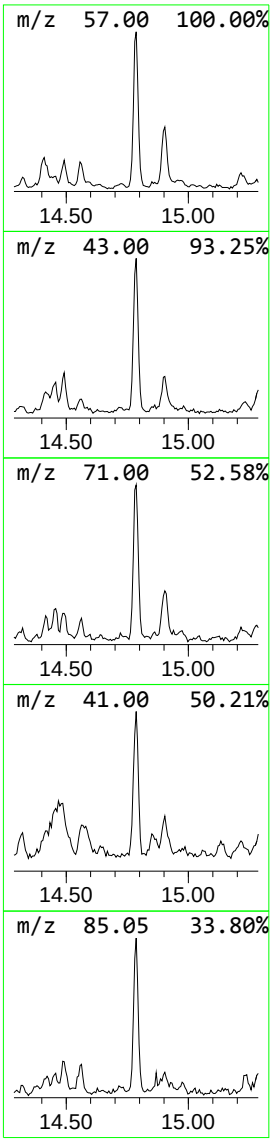
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	34.58 ug/l	926947	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	87
2	Tridecane	184	C13H28	000629-50-5	72
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
4	Undecane	156	C11H24	001120-21-4	50
5	Decane	142	C10H22	000124-18-5	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

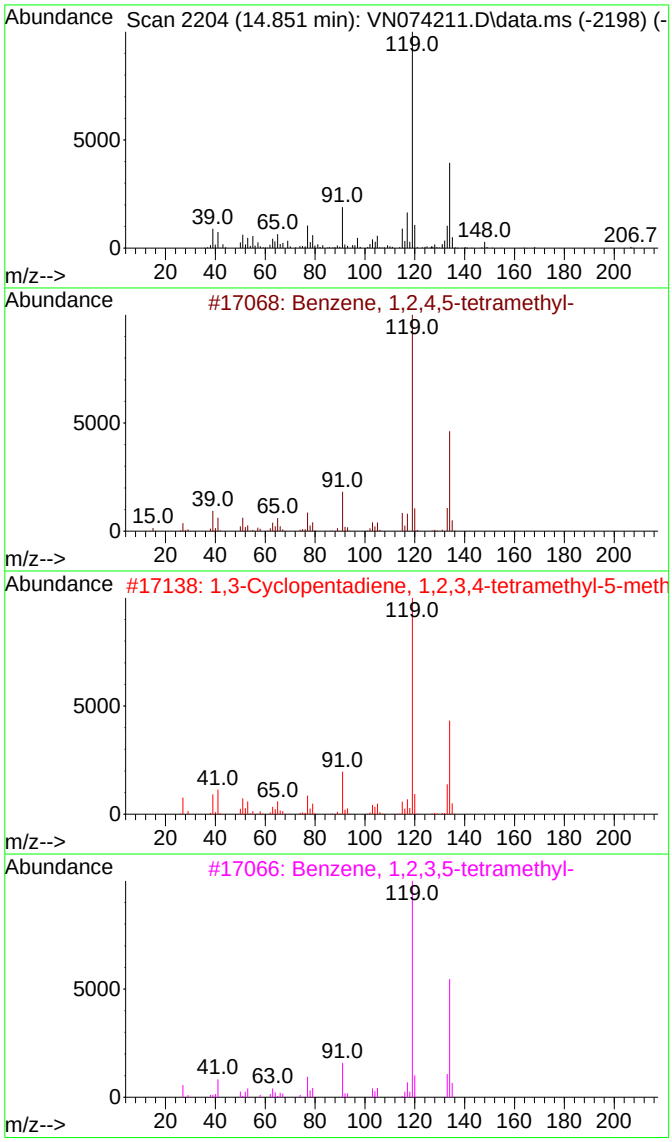
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

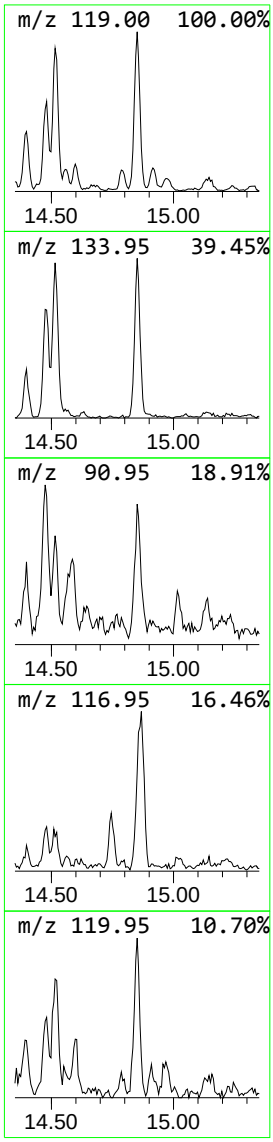
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	30.97 ug/l	830142	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	93
4	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	93
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

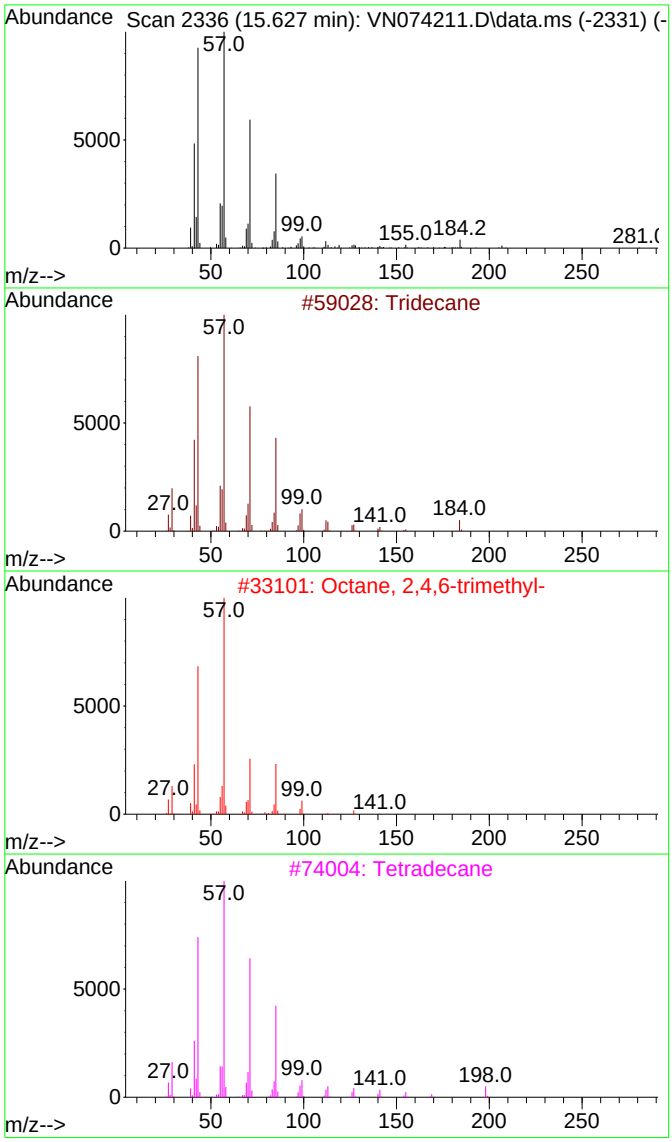
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

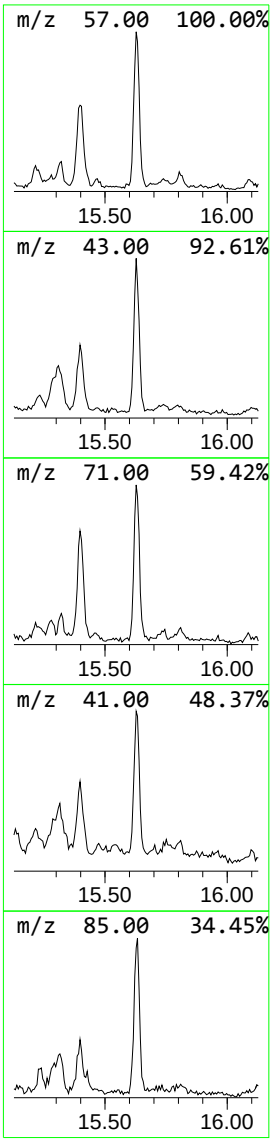
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.627	27.70 ug/l	742622	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	80
3	Tetradecane	198	C14H30	000629-59-4	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Undecane	156	C11H24	001120-21-4	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

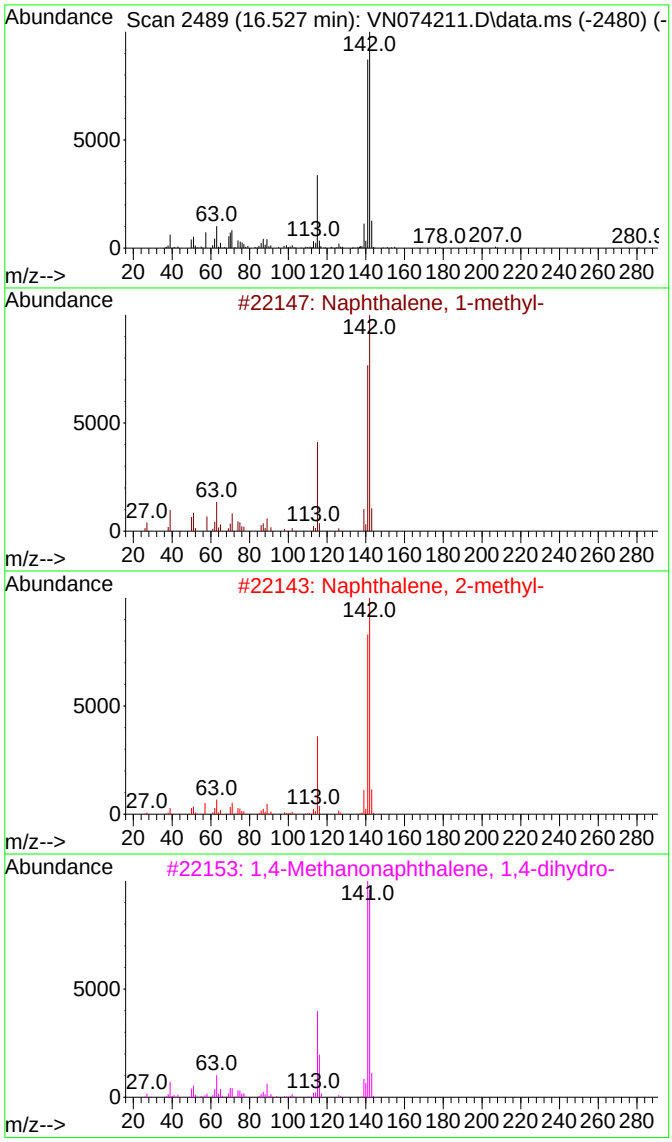
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

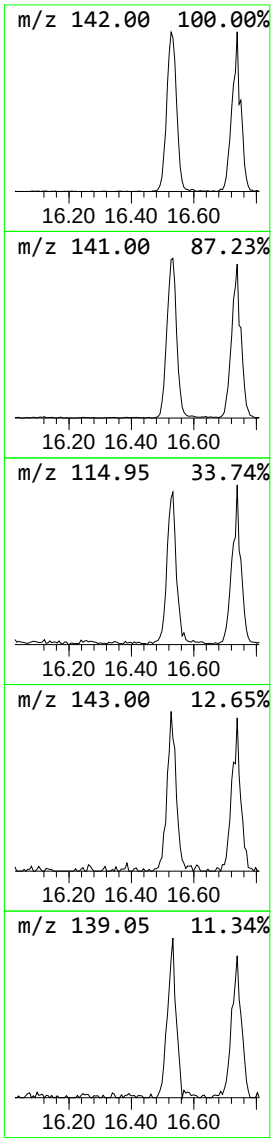
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	34.14 ug/l	915026	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

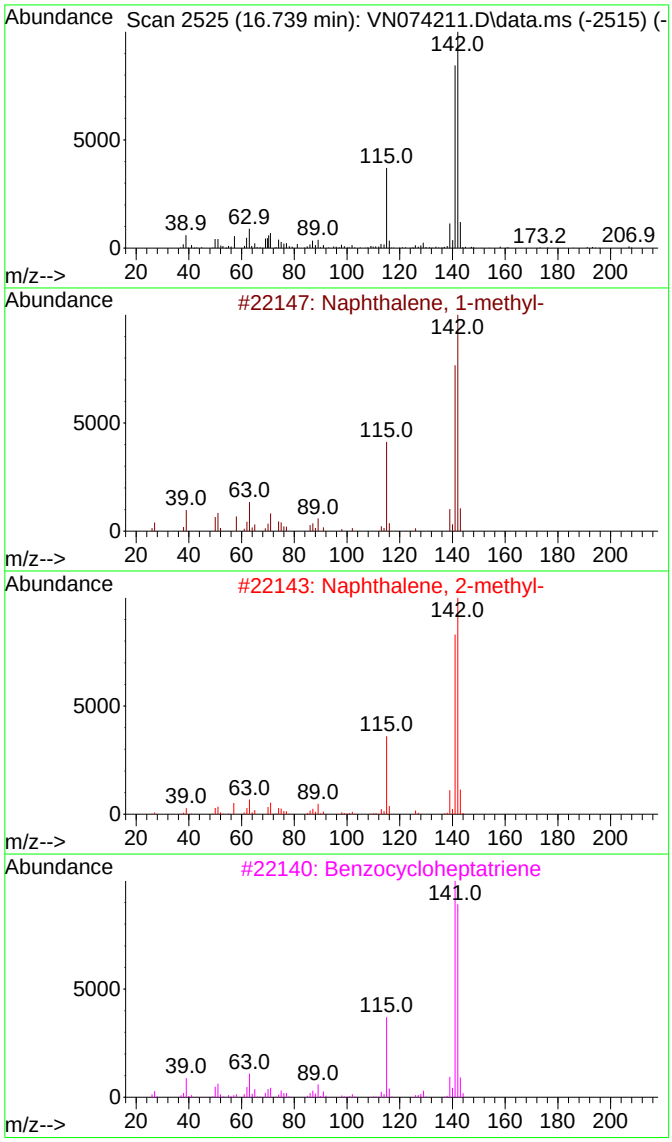
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

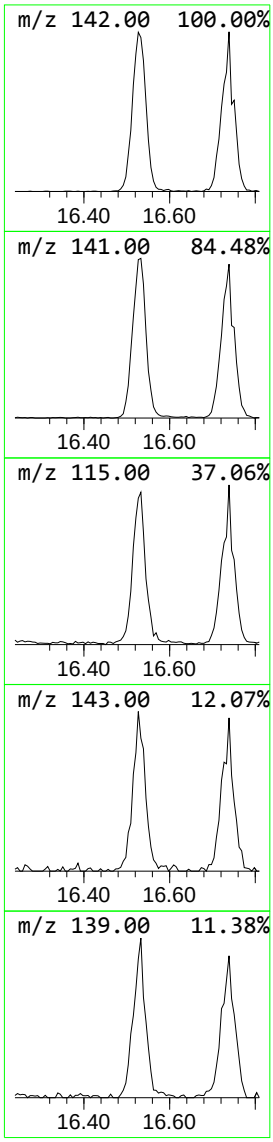
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	33.23 ug/l	890759	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	87
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083122\
Data File : VN074211.D
Acq On : 31 Aug 2022 13:56
Operator : JC\MD
Sample : N4447-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1656-WATER

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propyl mercaptan	6.969	39.7	ug/l	520629	1	8.016	656093	50.0
Benzene, 1-ethy...	12.921	120.9	ug/l	3241980	4	13.610	1340280	50.0
Oxalic acid, al...	13.933	43.4	ug/l	1162920	4	13.610	1340280	50.0
unknown14.474	14.474	57.7	ug/l	1547070	4	13.610	1340280	50.0
Adamantane, 1,3...	14.580	29.6	ug/l	794161	4	13.610	1340280	50.0
Dodecane	14.786	34.6	ug/l	926947	4	13.610	1340280	50.0
Benzene, 1,2,4,...	14.851	31.0	ug/l	830142	4	13.610	1340280	50.0
Tridecane	15.627	27.7	ug/l	742622	4	13.610	1340280	50.0
Naphthalene, 1-...	16.527	34.1	ug/l	915026	4	13.610	1340280	50.0
Naphthalene, 2-...	16.739	33.2	ug/l	890759	4	13.610	1340280	50.0