LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

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\82N021624W.M
Title : SW846 8260

Signal : TIC: VN081134.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	17	22	30	rVB2	86614	122200	2.77%	0.355%
2	2.666	114	121	129	rVB	246283	443141	10.04%	1.289%
3	2.818	139	147	152	rVB3	29166	62102	1.41%	0.181%
4	4.289	387	397	408	rBV	22536	63139	1.43%	0.184%
5	4.424	410	420	431	rBV2	91639	272050	6.16%	0.791%
6	4.712	455	469	480	rBV3	40215	130144	2.95%	0.379%
7	5.024	511	522	538	rBV	111219	348114	7.89%	1.013%
8	5.518	593	606	621	rBV3	59562	213026	4.83%	0.620%
9	6.148	700	713	724	rBV4	21715	73481	1.66%	0.214%
10	7.224	883	896	910	rBV	1052558	2902902	65.77%	8.445%
11	7.483	934	940	949	rVB3	18004	45090	1.02%	0.131%
12	8.165	1047	1056	1061	rBV	276633	667061	15.11%	1.941%
13	8.224	1061	1066	1077	rVB	548721	1217405	27.58%	3.542%
14	9.100	1206	1215	1226	rBV	836675	1741925	39.46%	5.067%
15	9.271	1235	1244	1256	rBV	236723	509595	11.55%	1.482%
16	9.653	1302	1309	1317	rVB	192276	363582	8.24%	1.058%
17	10.571	1456	1465	1471	rBV	974573	1852855	41.98%	5.390%
18	10.636	1471	1476	1485	rVV	400250	761090	17.24%	2.214%
19	10.718	1485	1490	1495	rVV2	57632	109000	2.47%	0.317%
20	10.765	1495	1498	1507	rVB2	39255	71303	1.62%	0.207%
21	10.959	1524	1531	1536	rBV2	83984	152827	3.46%	0.445%
22	11.300	1582	1589	1595	rBV4	63107	137290	3.11%	0.399%
23	11.824	1673	1678	1679	rBV3	64094	78419	1.78%	0.228%
24	11.865	1679	1685	1695	rVB	1130559	2085641	47.25%	6.067%
25	11.971	1697	1703	1709	rVB4	36476	76515	1.73%	0.223%
26	12.071	1712	1720	1727	rBV2	85627	181576	4.11%	0.528%
27	12.135	1727	1731	1737	rBV6	23677	47971	1.09%	0.140%
28	12.418	1764	1779	1784	rBV5	181730	467020	10.58%	1.359%
29	12.494	1785	1792	1794	rBV4	54238	111277	2.52%	0.324%
30	12.853	1839	1853	1863	rVB	749131	1430390	32.41%	4.161%
31	12.941	1863	1868	1872	rBV2	28716	52751	1.20%	0.153%
32	13.118	1887	1898	1902	rBV	153071	329565	7.47%	0.959%
33	13.159	1902	1905	1913	rVB4	104920	173222	3.92%	0.504%
34	13.247	1913	1920	1921	rBV2	92460	138126	3.13%	0.402%
35	13.341	1930	1936	1943	rVB	1070822	1644910	37.27%	4.785%
36	13.500	1956	1963	1971	rBV	356004	718411	16.28%	2.090%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

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\82N021624W.M
Title : SW846 8260

37	13.594	1974	1979	1981	rBV5	26880	53749	1.22%	0.156%
38	13.688	1988	1995	2003	rBV	1108450	1924488	43.60%	5.599%
39	13.794	2007	2013	2020	rVV	1182053	1982047	44.90%	5.766%
40	13.877	2020	2027	2037	rVV	2741425	4413963	100.00%	12.841%
41	13.953	2037	2040	2044	rVV6	59640	104127	2.36%	0.303%
42	14.018	2045	2051	2060	rVV5	146839	437540	9.91%	1.273%
43	14.106	2061	2066	2081	rVB2	656109	1272605	28.83%	3.702%
44	14.259	2088	2092	2098	rVB6	54066	84163	1.91%	0.245%
45	14.365	2107	2110	2117	rVB3	69490	129114	2.93%	0.376%
46	14.435	2117	2122	2126	rBV6	31806	66131	1.50%	0.192%
47	14.494	2126	2132	2136	rBV6	85426	193742	4.39%	0.564%
48	14.553	2137	2142	2145	rBV3	135692	246793	5.59%	0.718%
49	14.629	2151	2155	2158	rVB3	152493	200330	4.54%	0.583%
50	14.665	2158	2161	2165	rVB3	108111	141766	3.21%	0.412%
51	14.729	2169	2172	2176	rVB2	85291	125872	2.85%	0.366%
52	14.794	2180	2183	2188	rVB5	56218	79290	1.80%	0.231%
53	14.847	2188	2192	2198	rVB9	35612	73540	1.67%	0.214%
54	14.959	2206	2211	2221	rVB	527084	803807	18.21%	2.338%
55	15.082	2221	2232	2244	rBV7	169576	623704	14.13%	1.814%
56	15.347	2272	2277	2281	rVB5	116117	181130	4.10%	0.527%
57	15.400	2281	2286	2292	rBV2	111225	205483	4.66%	0.598%
58	15.471	2293	2298	2301	rBV	141893	213659	4.84%	0.622%
59	15.594	2314	2319	2323	rBV3	80582	157068	3.56%	0.457%
60	15.659	2325	2330	2342	rVB6	80700	242112	5.49%	0.704%
61	15.776	2345	2350	2351	rBV2	41398	51320	1.16%	0.149%
62	15.835	2354	2360	2369	rVB2	186849	402053	9.11%	1.170%
63	15.941	2374	2378	2385	rVB10	44975	82560	1.87%	0.240%
64	16.118	2403	2408	2414	rBV9	42865	87344	1.98%	0.254%

Sum of corrected areas: 34374616

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Misc : 5.0mL/MSVOA_N/WATER
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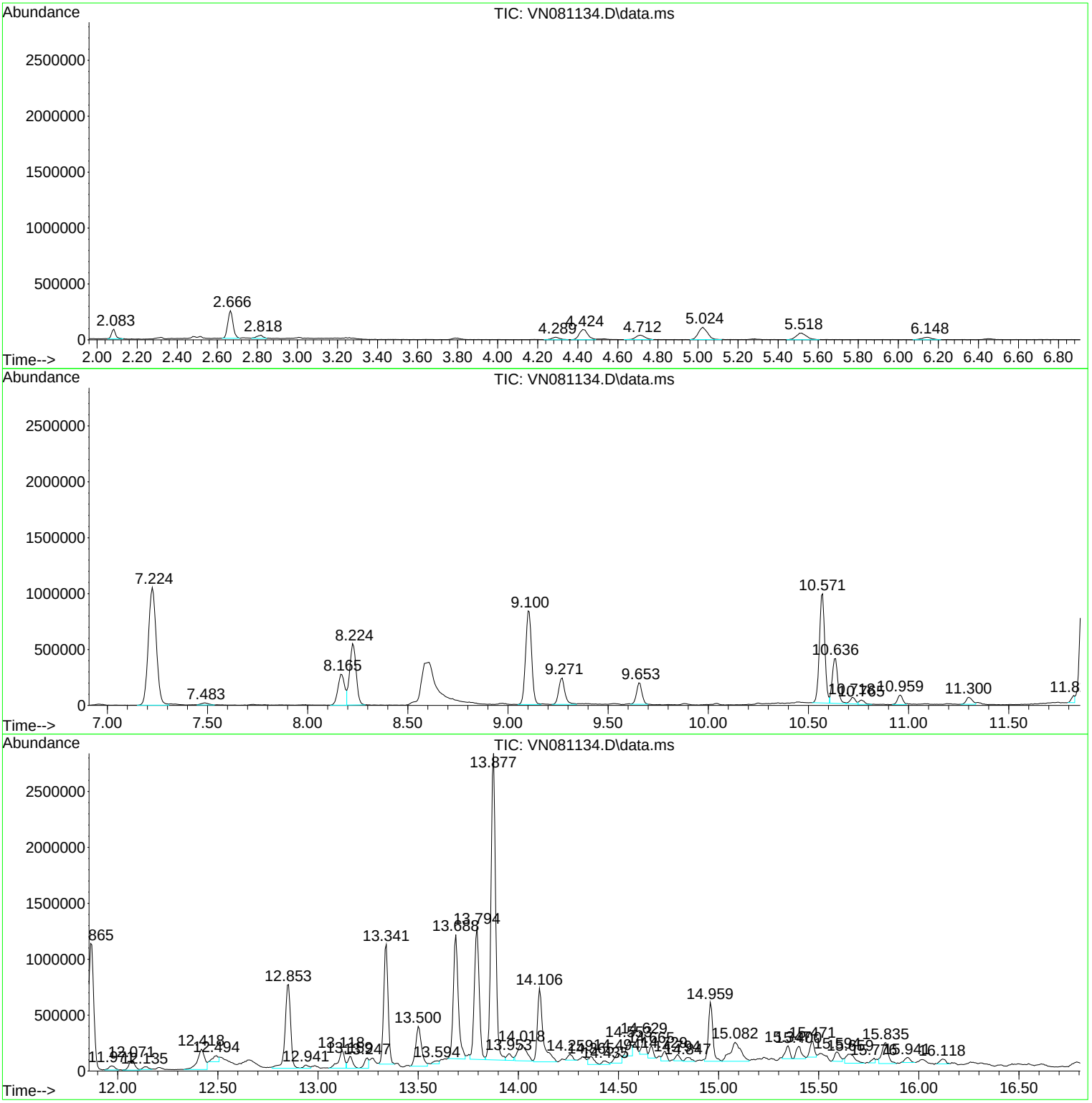
Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
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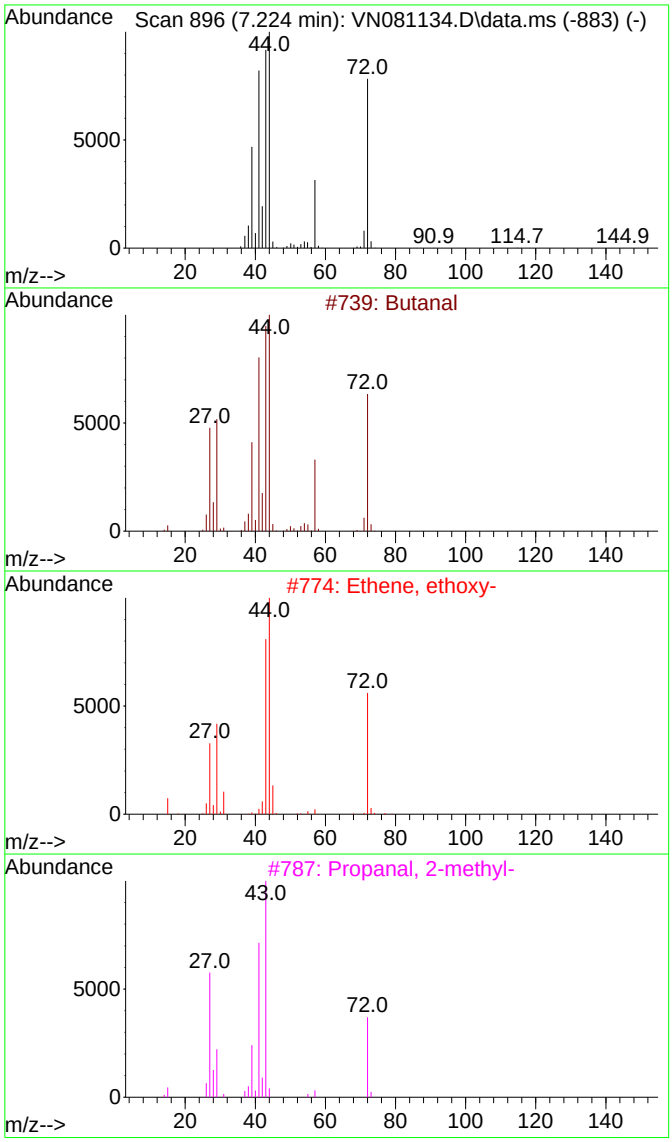
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

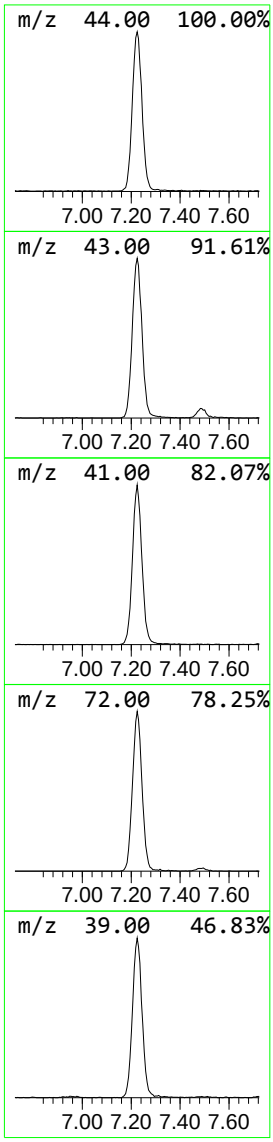
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	119.22 ug/l	2902900	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

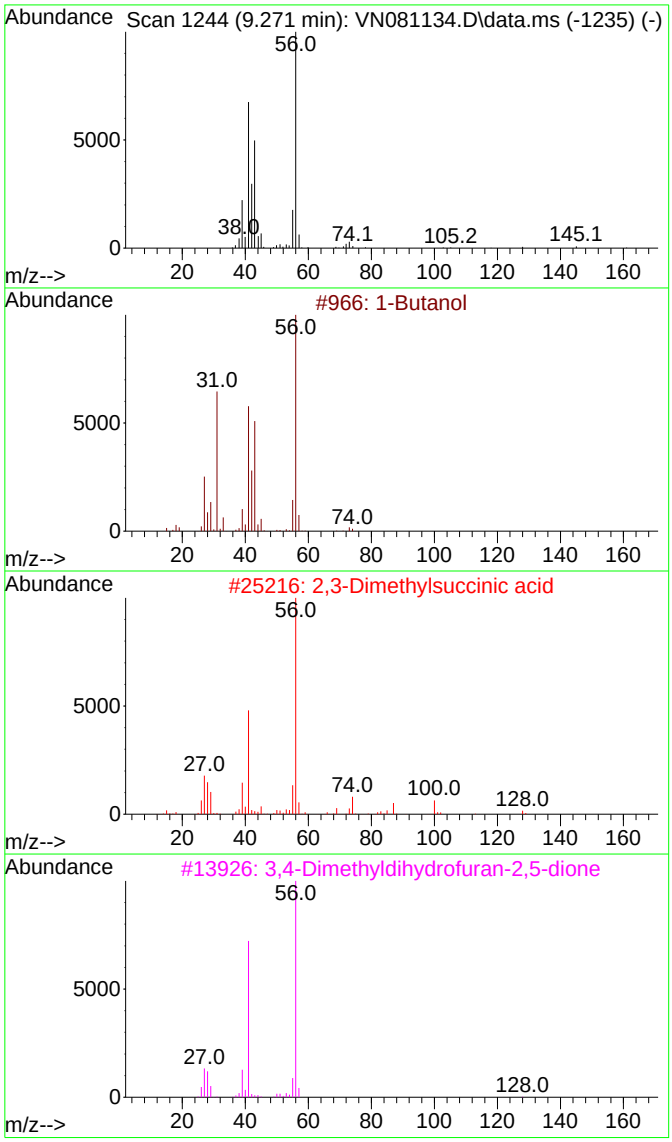
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

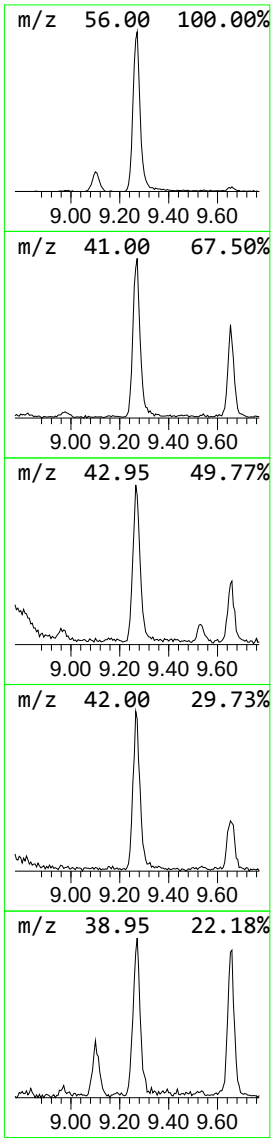
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.271	14.63 ug/l	509595	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	2,3-Dimethylsuccinic acid	146	C6H10O4	013545-04-5	42
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40
4	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	38
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

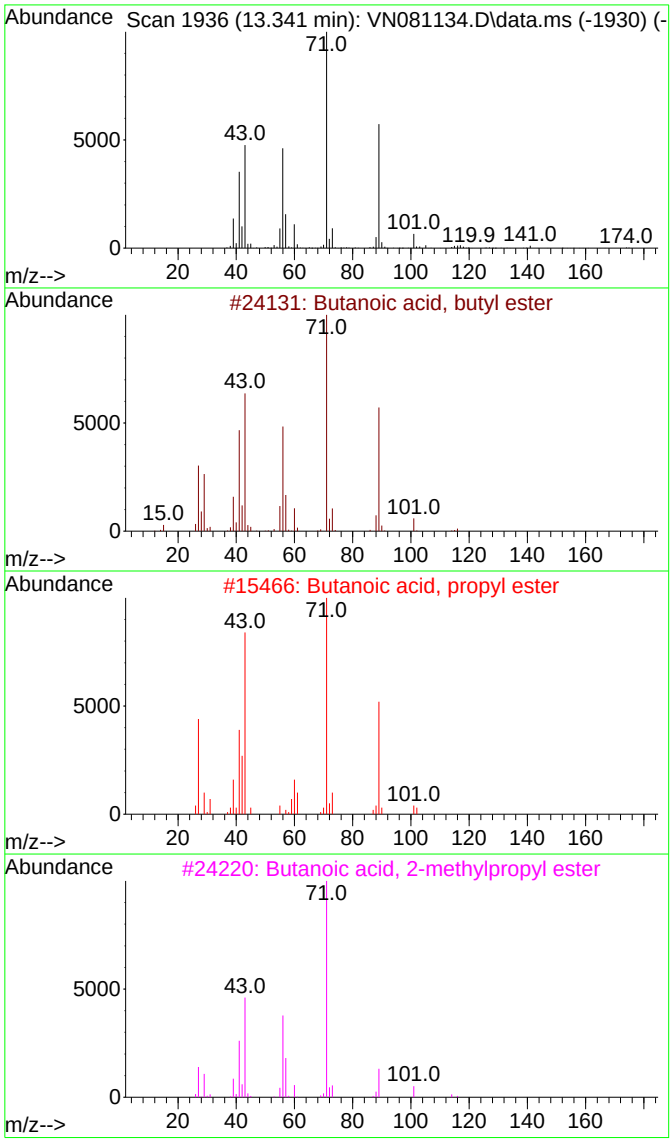
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

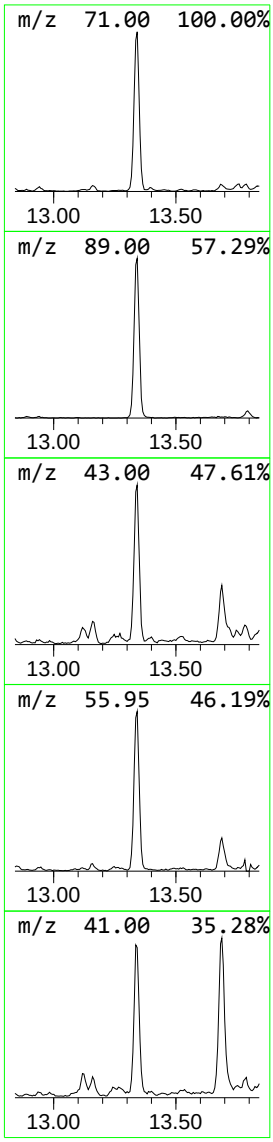
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	41.50 ug/l	1644910	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
5	Malic Acid	134	C4H6O5	006915-15-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

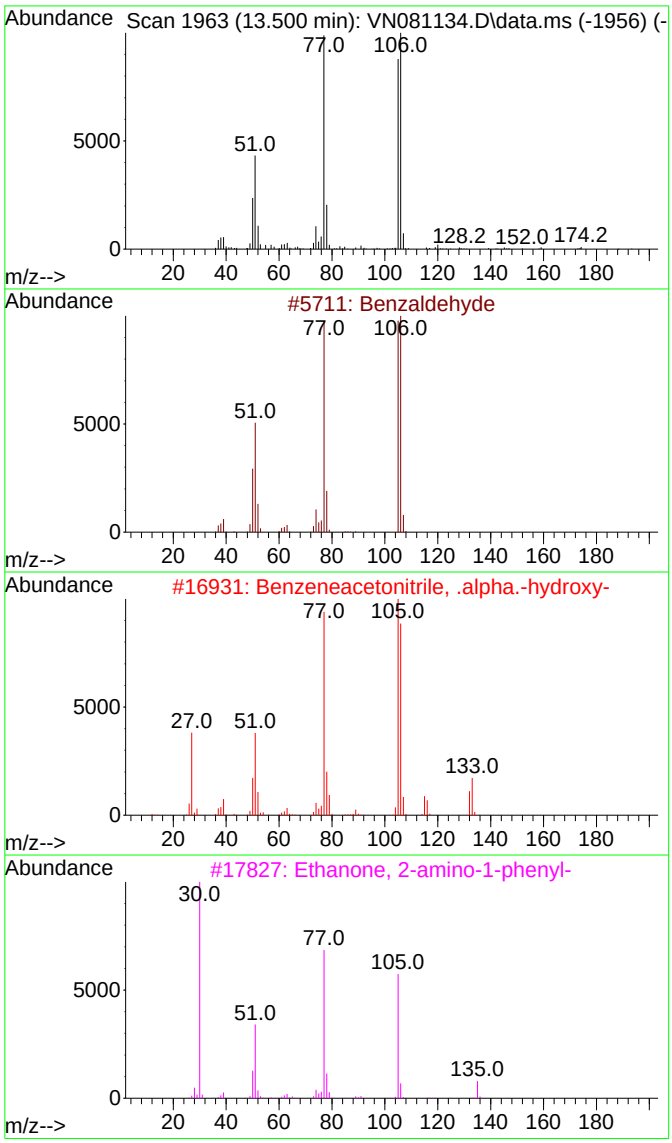
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

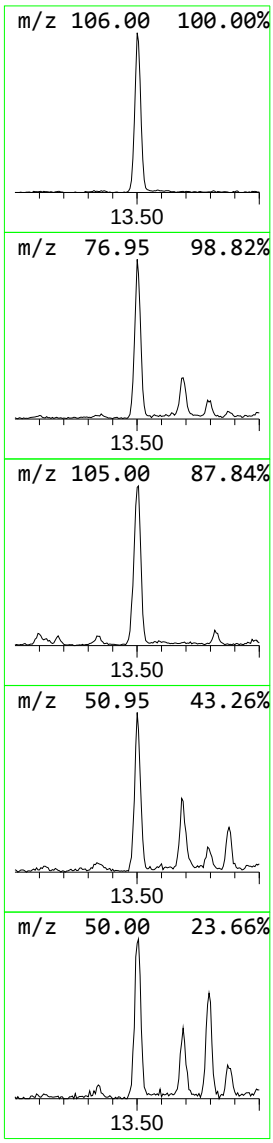
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzaldehyde Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.500	18.12 ug/l	718411	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde	106	C7H6O	000100-52-7	97
2	Benzeneacetonitrile, .alpha.-hyd...	133	C8H7NO	000532-28-5	78
3	Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	53
4	Benzoylformic acid	150	C8H6O3	000611-73-4	50
5	Hydrazine, phenylsulfinyl-	154	C6H6N2OS	017420-03-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

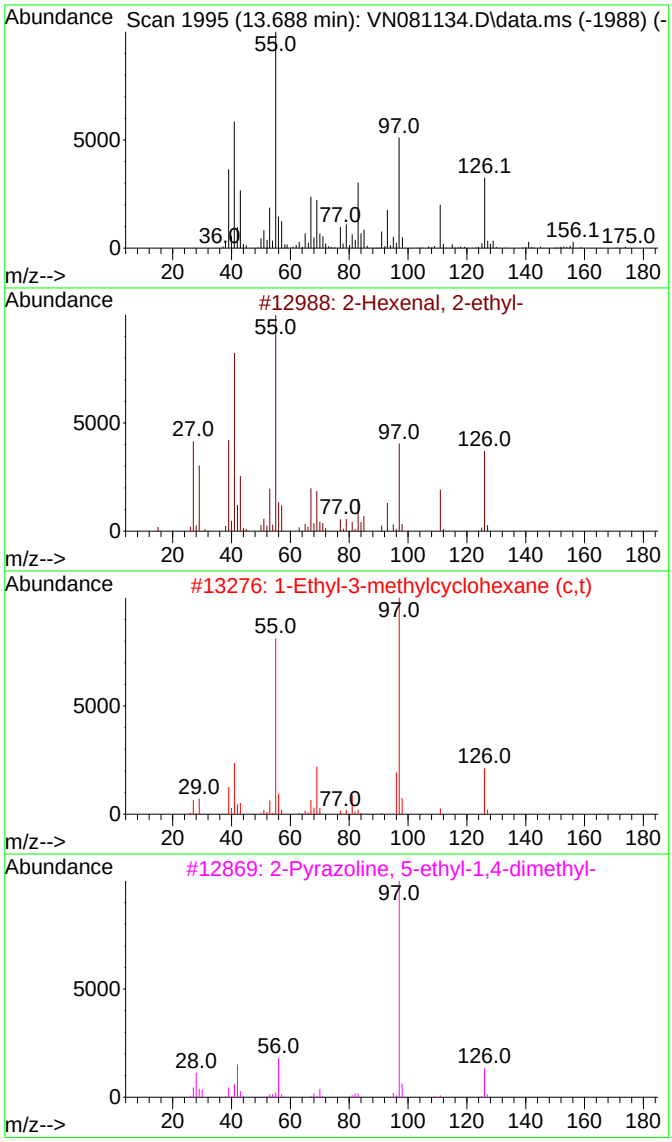
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

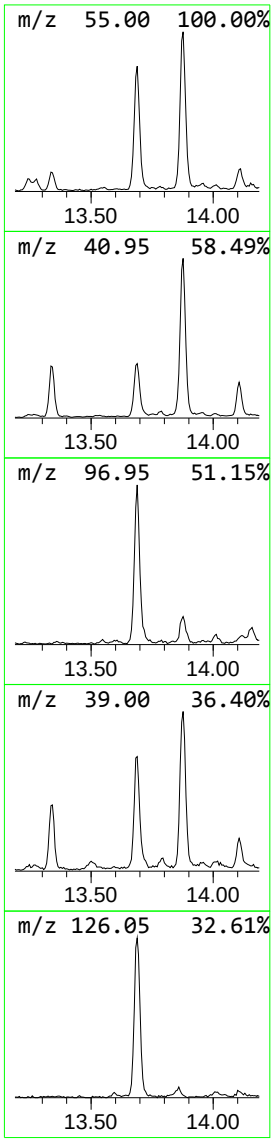
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Hexenal, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	48.55 ug/l	1924490	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	95
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	47
3	2-Pyrazoline, 5-ethyl-1,4-dimethyl-	126	C7H14N2	014339-23-2	38
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	35
5	4-Hexen-3-one, 4,5-dimethyl-	126	C8H14O	017325-90-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

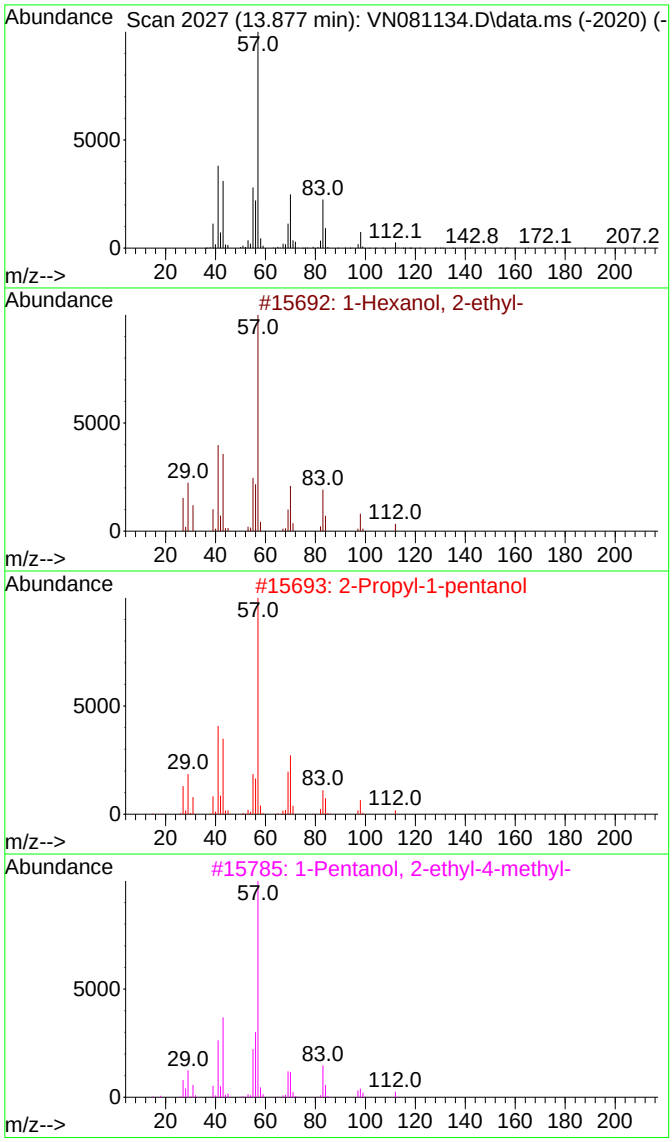
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

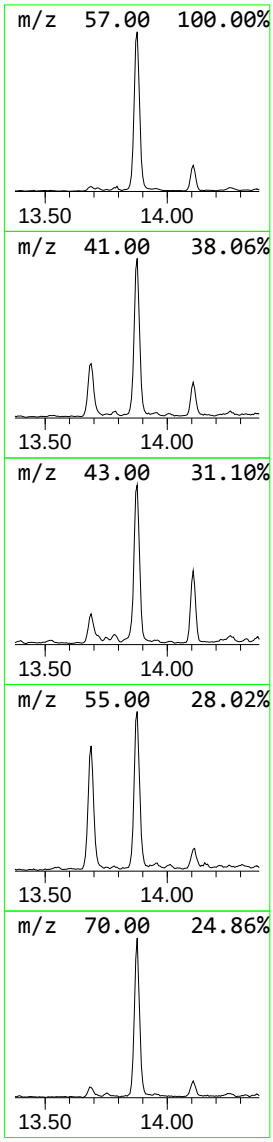
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.877	111.35 ug/l	4413960	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

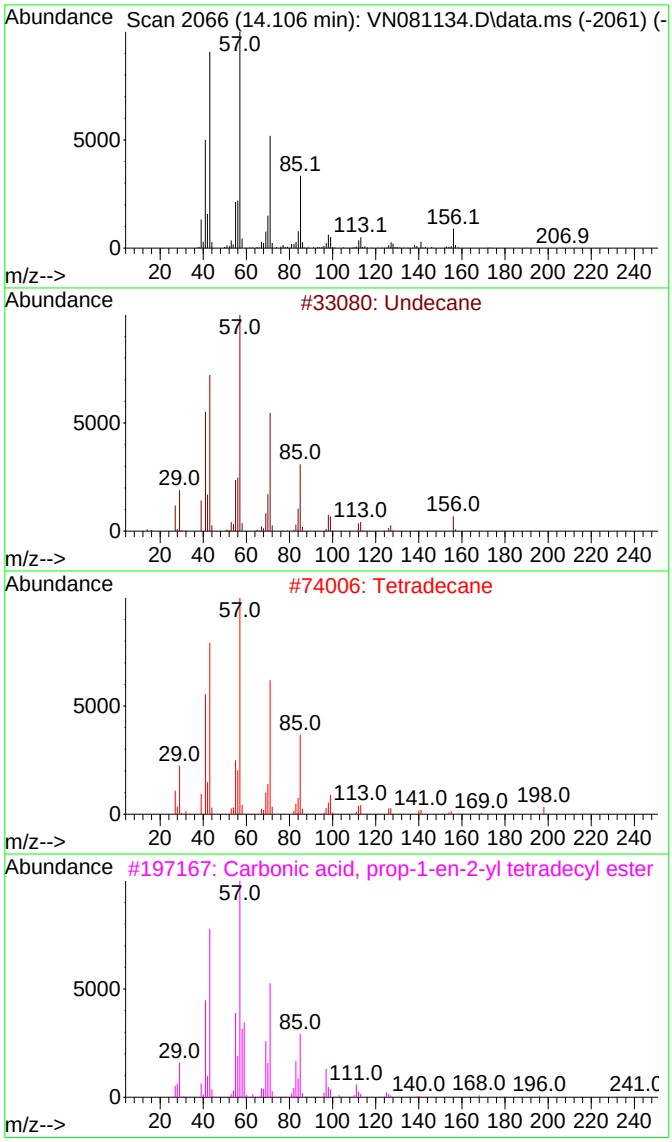
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

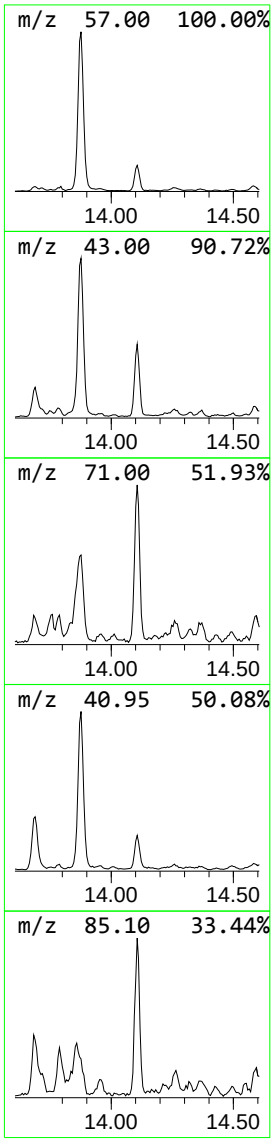
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.106	32.10 ug/l	1272610	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	96
2	Tetradecane	198	C14H30	000629-59-4	86
3	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	86
4	Tridecane	184	C13H28	000629-50-5	80
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64





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Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

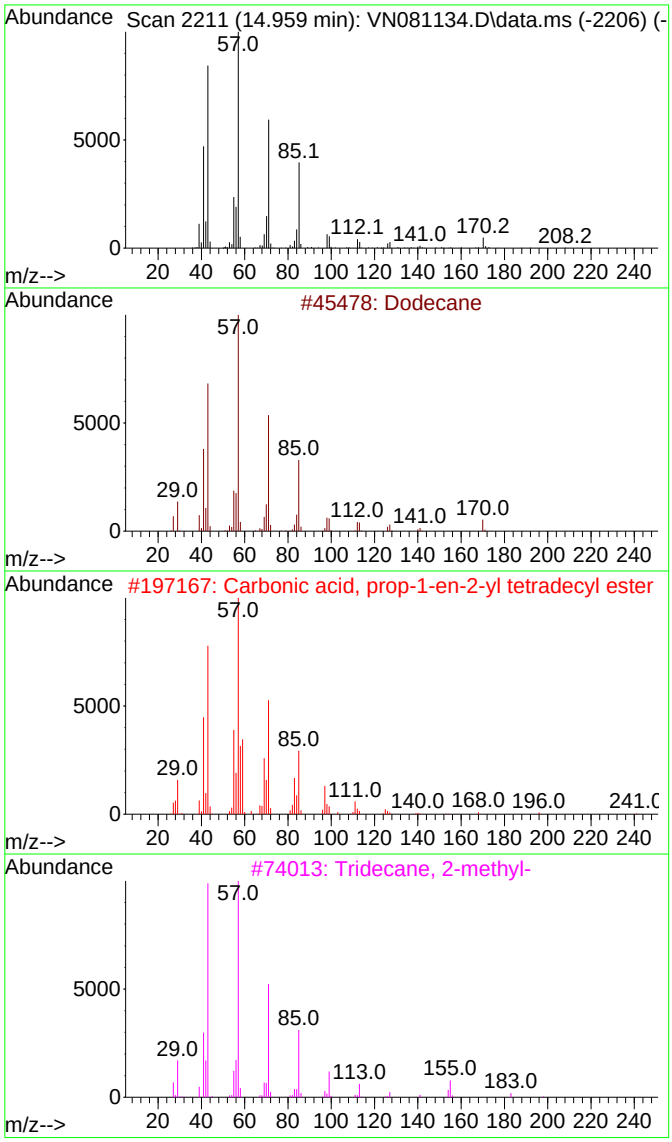
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

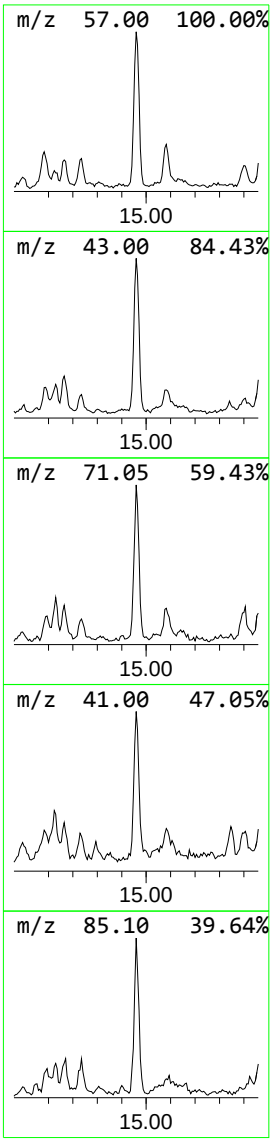
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	20.28 ug/l	803807	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	94
2	Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	64
5	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

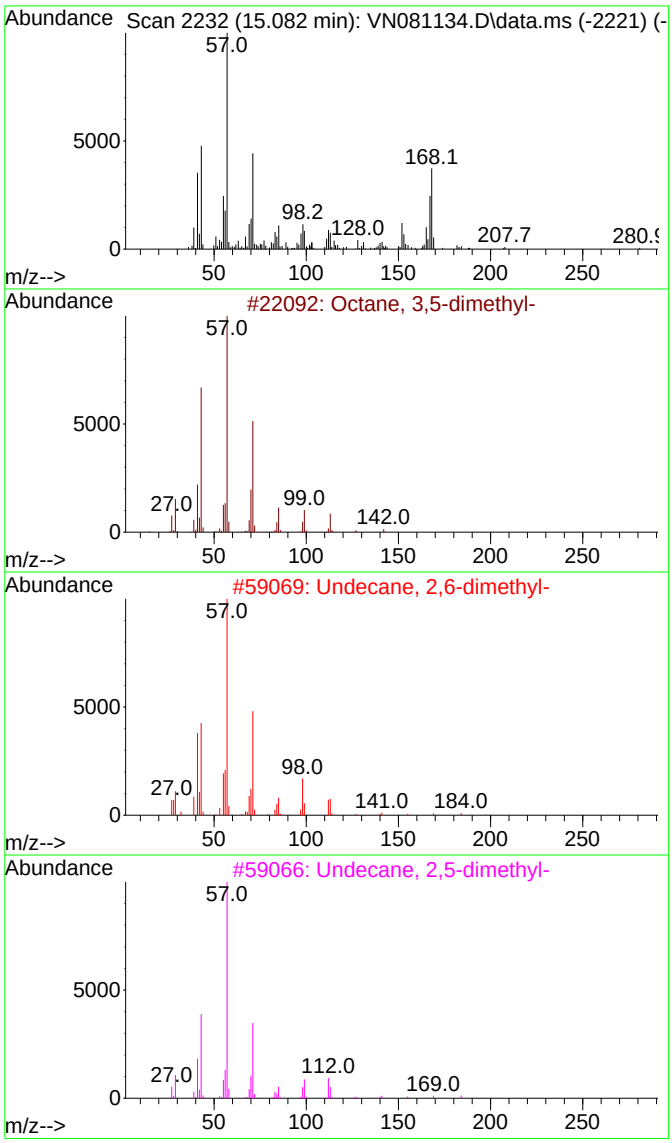
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.M
Quant Title : SW846 8260

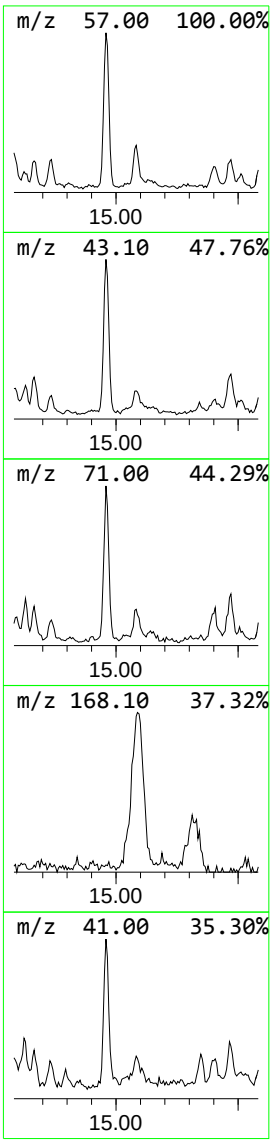
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Octane, 3,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.082	15.73 ug/l	623704	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	50
3	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	50
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	38
5	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022224\
Data File : VN081134.D
Acq On : 22 Feb 2024 14:48
Operator : JC\MD
Sample : P1540-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
AUD-1327

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021624W.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
Butanal	7.224	119.2	ug/l	2902900	1	8.224	1217410	50.0
1-Butanol	9.271	14.6	ug/l	509595	2	9.106	1741930	50.0
Butanoic acid, ...	13.341	41.5	ug/l	1644910	4	13.794	1982050	50.0
Benzaldehyde	13.500	18.1	ug/l	718411	4	13.794	1982050	50.0
2-Hexenal, 2-et...	13.688	48.5	ug/l	1924490	4	13.794	1982050	50.0
1-Hexanol, 2-et...	13.877	111.3	ug/l	4413960	4	13.794	1982050	50.0
Undecane	14.106	32.1	ug/l	1272610	4	13.794	1982050	50.0
Dodecane	14.959	20.3	ug/l	803807	4	13.794	1982050	50.0
Octane, 3,5-dim...	15.082	15.7	ug/l	623704	4	13.794	1982050	50.0