LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061622\
Data File : VN072894.D
Acq On : 16 Jun 2022 21:39
Operator : JC\MD
Sample : N3202-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

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\82N061622W.M
Title : SW846 8260

Signal : TIC: VN072894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.493	96	103	108	rBV	23295	43622	1.24%	0.161%
2	3.793	313	324	331	rBV5	12180	35285	1.01%	0.130%
3	4.187	380	391	398	rBV3	14329	43936	1.25%	0.162%
4	4.993	514	528	542	rBV3	22445	87450	2.49%	0.322%
5	5.293	567	579	595	rBV	69509	251863	7.19%	0.927%
6	5.534	609	620	635	rBV2	82102	293308	8.37%	1.080%
7	6.416	755	770	779	rBV6	12267	45529	1.30%	0.168%
8	7.769	989	1000	1011	rVB3	51394	138458	3.95%	0.510%
9	7.951	1020	1031	1036	rBV	552555	1303061	37.17%	4.797%
10	8.016	1036	1042	1053	rVV	762427	1782394	50.85%	6.561%
11	8.104	1053	1057	1067	rVB6	18289	45718	1.30%	0.168%
12	8.369	1093	1102	1110	rBV	569167	1298575	37.05%	4.780%
13	8.463	1110	1118	1130	rVV	1025229	2314840	66.04%	8.521%
14	8.898	1183	1192	1214	rBV	1111904	2411248	68.79%	8.876%
15	9.904	1355	1363	1368	rBV	158738	308730	8.81%	1.136%
16	10.139	1395	1403	1404	rBV	292829	492417	14.05%	1.813%
17	10.169	1404	1408	1418	rVB	576414	1085131	30.96%	3.994%
18	10.375	1435	1443	1455	rBV	1907433	3505330	100.00%	12.903%
19	10.486	1455	1462	1471	rVV	595917	1124983	32.09%	4.141%
20	10.569	1473	1476	1482	rVB3	26782	49093	1.40%	0.181%
21	10.792	1507	1514	1524	rVB2	53454	107091	3.06%	0.394%
22	11.022	1546	1553	1565	rBV	67587	134941	3.85%	0.497%
23	11.145	1565	1574	1588	rVV2	106220	253352	7.23%	0.933%
24	11.551	1635	1643	1654	rBV	117306	281746	8.04%	1.037%
25	11.680	1657	1665	1678	rBV	1794007	3220888	91.89%	11.856%
26	11.798	1678	1685	1692	rVB2	98517	206190	5.88%	0.759%
27	11.898	1697	1702	1711	rVB5	28685	55088	1.57%	0.203%
28	11.980	1711	1716	1721	rBV4	21652	38042	1.09%	0.140%
29	12.298	1762	1770	1774	rBV2	30359	61488	1.75%	0.226%
30	12.475	1793	1800	1805	rBV4	35060	76128	2.17%	0.280%
31	12.669	1825	1833	1845	rBV	1435888	2493408	71.13%	9.178%
32	12.780	1846	1852	1858	rVV3	47655	100173	2.86%	0.369%
33	12.827	1858	1860	1869	rVB6	20619	46239	1.32%	0.170%
34	12.945	1872	1880	1884	rBV5	24145	51951	1.48%	0.191%
35	12.998	1884	1889	1897	rVB8	29019	61866	1.76%	0.228%
36	13.304	1937	1941	1947	rVB2	34103	59425	1.70%	0.219%

LSC Area Percent Report

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ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-30

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Title : SW846 8260

37	13.610	1986	1993	2006	rBV	1306212	2250450	64.20%	8.284%
38	13.810	2023	2027	2030	rBV2	31871	43414	1.24%	0.160%
39	13.851	2030	2034	2044	rVB	46484	78738	2.25%	0.290%
40	13.992	2053	2058	2064	rBV3	22866	40258	1.15%	0.148%
41	14.210	2090	2095	2099	rBV	41289	68009	1.94%	0.250%
42	14.263	2099	2104	2111	rVB	177001	292392	8.34%	1.076%
43	14.474	2134	2140	2144	rVV	28753	46566	1.33%	0.171%
44	14.745	2182	2186	2192	rVB3	20113	39626	1.13%	0.146%
45	14.857	2197	2205	2213	rVV4	21191	52126	1.49%	0.192%
46	15.010	2226	2231	2238	rVB6	33162	60977	1.74%	0.224%
47	15.221	2260	2267	2276	rVB4	18804	53465	1.53%	0.197%
48	15.433	2297	2303	2310	rVB	24118	51703	1.47%	0.190%
49	16.521	2482	2488	2496	rVB3	41626	100254	2.86%	0.369%
50	16.727	2517	2523	2532	rVB4	33450	79639	2.27%	0.293%

Sum of corrected areas: 27166604

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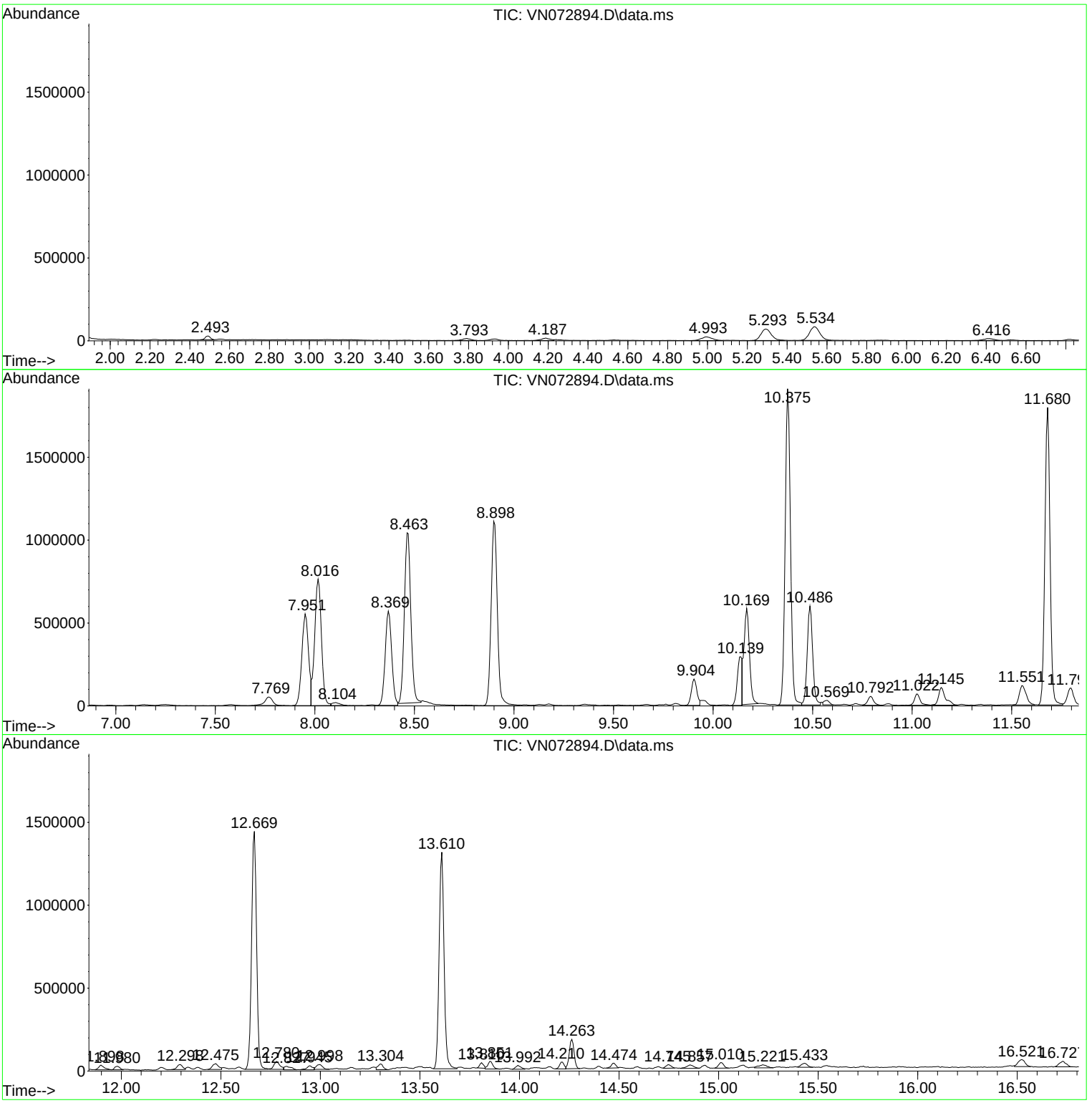
Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061622\
Data File : VN072894.D
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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

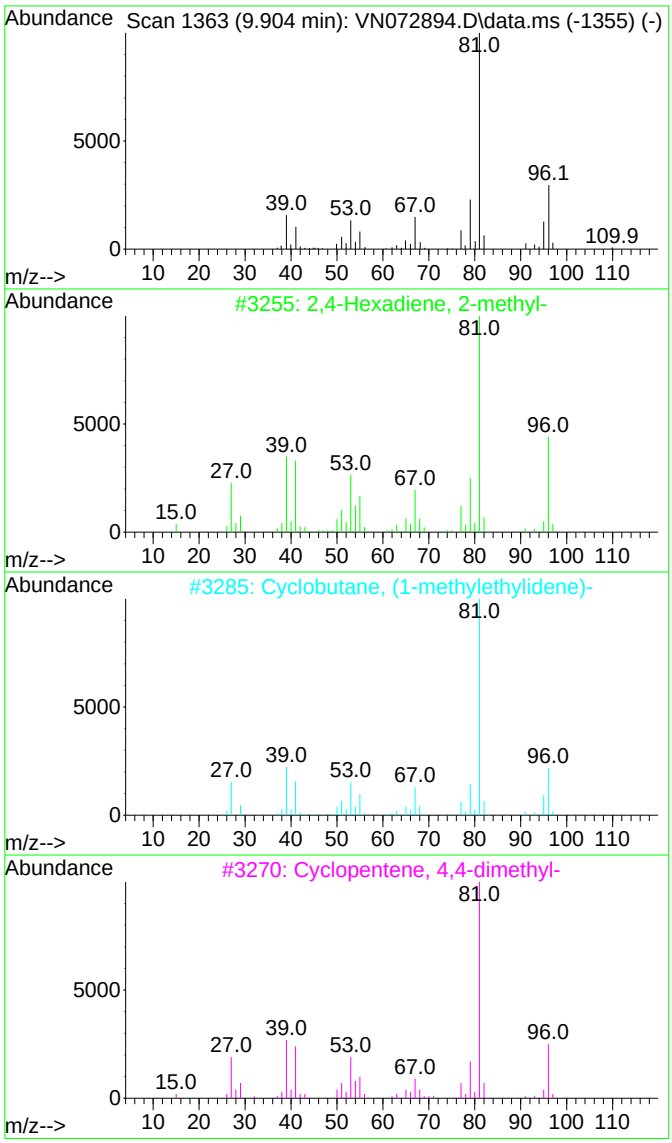
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Quant Title : SW846 8260

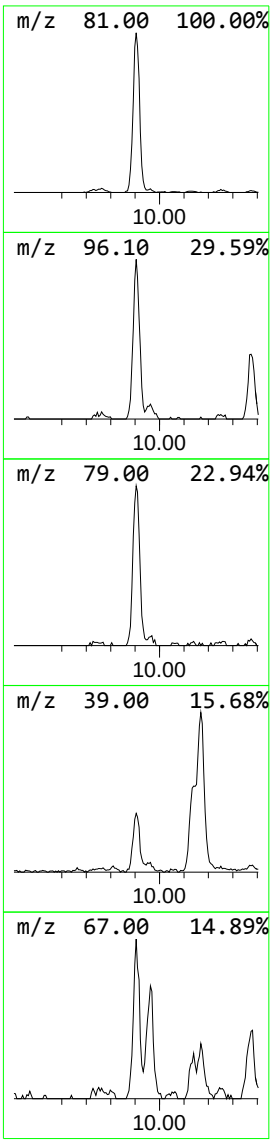
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4-Hexadiene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.904	6.40 ug/l	308730	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadiene, 2-methyl-	96	C7H12	028823-41-8	90
2	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	87
3	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	86
4	Cyclopropane, trimethylmethylene-	96	C7H12	034462-28-7	78
5	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	78





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Instrument :
MSVOA_N
ClientSampleId :
MW-30

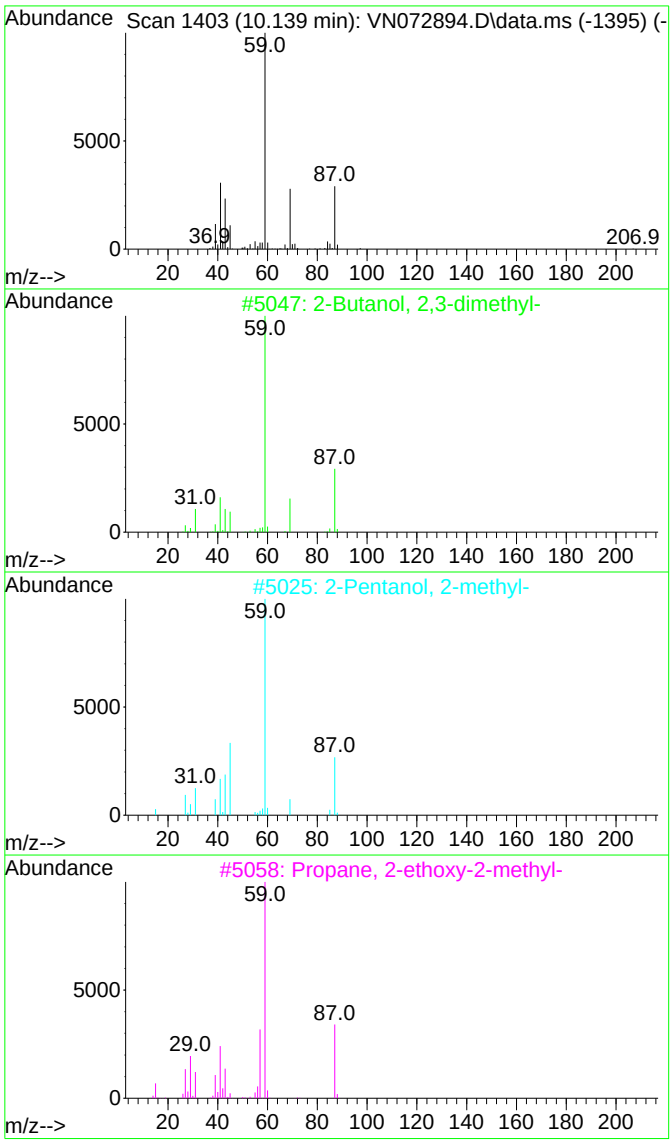
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Quant Title : SW846 8260

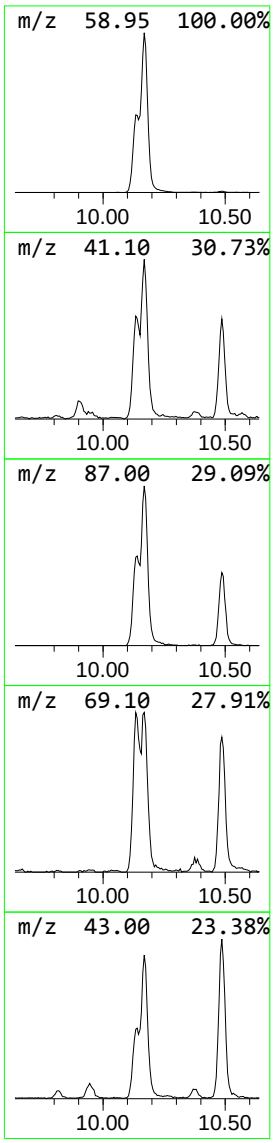
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.139	10.21 ug/l	492417	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	56
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	40
5	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40





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Instrument :
MSVOA_N
ClientSampleId :
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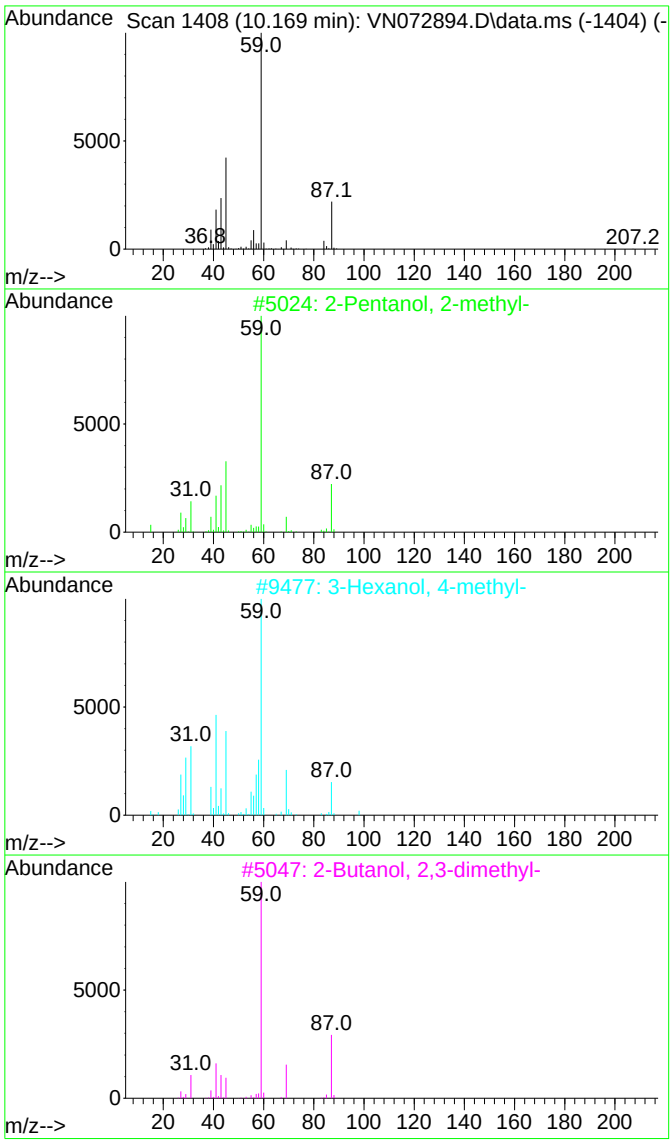
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Quant Title : SW846 8260

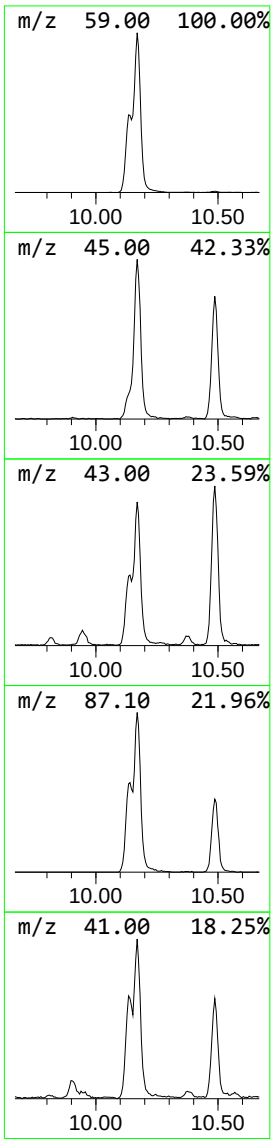
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.169	22.50 ug/l	1085130	1,4-Difluorobenzene	8.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	39
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	33
4	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	28
5	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9





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Instrument :
MSVOA_N
ClientSampleId :
MW-30

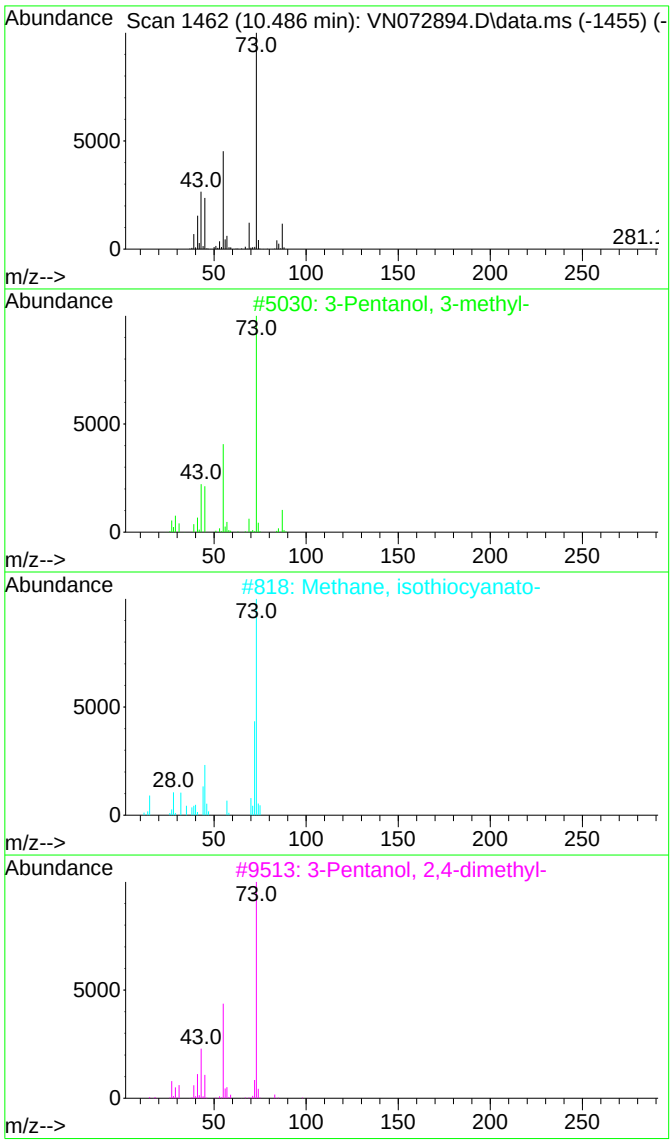
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061622W.M
Quant Title : SW846 8260

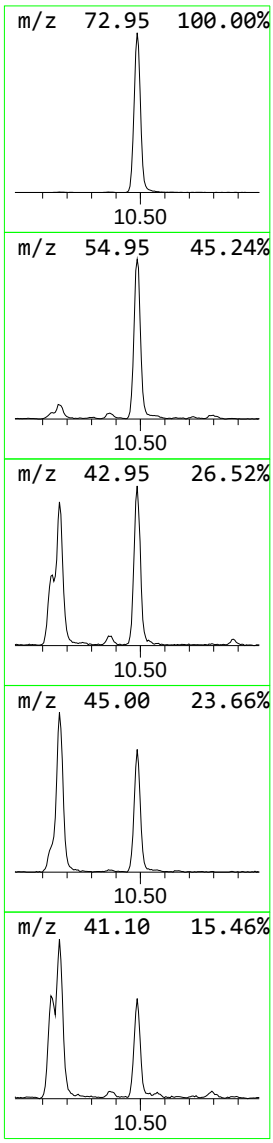
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanol, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.486	17.46 ug/l	1124980	Chlorobenzene-d5	11.681

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	78
2	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	37
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5	1,3-Dioxolane, 2-hexyl-	158	C9H18O2	001708-34-5	23





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MSVOA_N
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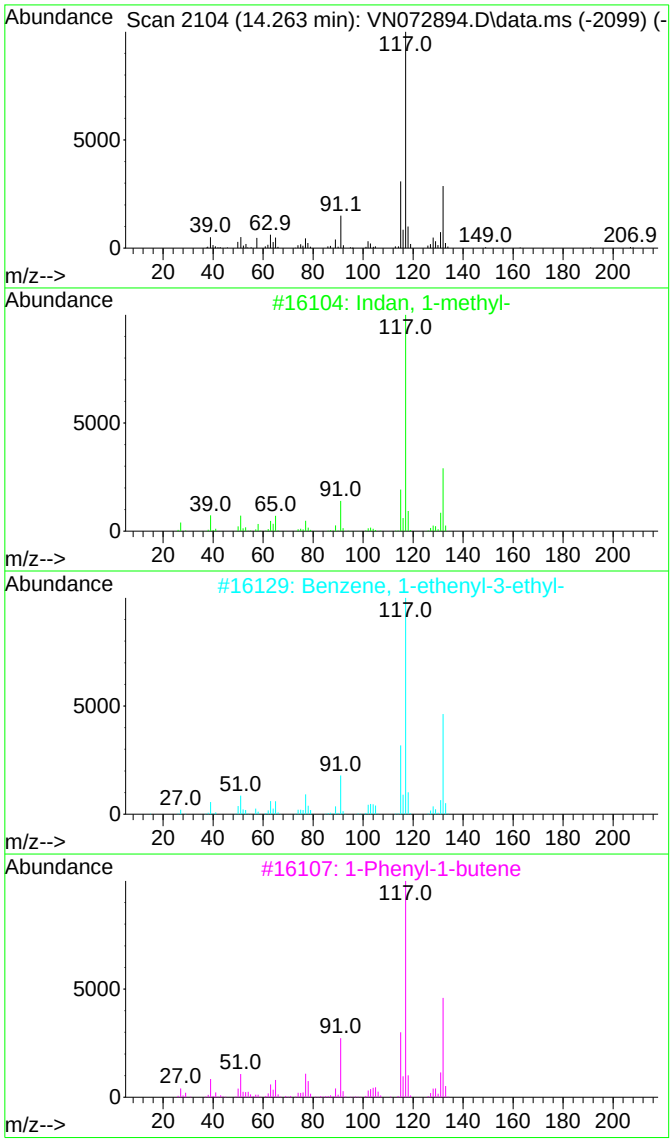
Quant Title : SW846 8260

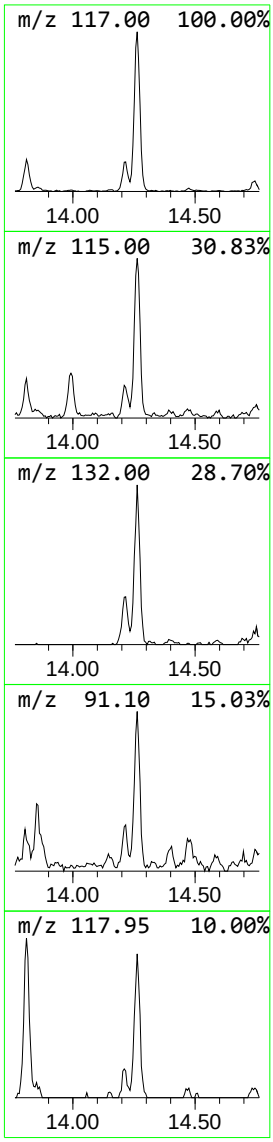
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Indan, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	6.50 ug/l	292392	1,4-Dichlorobenzene-d4	13.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86





Tentatively Identified Compound (LSC) summary

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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
2,4-Hexadiene, ...	9.904	6.4	ug/l	308730	2	8.898	2411250	50.0
2-Butanol, 2,3-...	10.139	10.2	ug/l	492417	2	8.898	2411250	50.0
2-Pentanol, 2-m...	10.169	22.5	ug/l	1085130	2	8.898	2411250	50.0
3-Pentanol, 3-m...	10.486	17.5	ug/l	1124980	3	11.681	3220890	50.0
Indan, 1-methyl-	14.263	6.5	ug/l	292392	4	13.610	2250450	50.0