LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041523\
Data File : VX035093.D
Acq On : 14 Apr 2023 19:04
Operator : JC/MD
Sample : 02353-04 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1262

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_X\Method\82X032923W.M
Title : SW846 8260

Signal : TIC: VX035093.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	67	rBV	16420	21575	1.54%	0.214%
2	2.398	208	215	226	rVB	9872	22367	1.60%	0.222%
3	5.385	694	705	721	rBV	146134	432437	30.94%	4.295%
4	5.556	721	733	746	rVB	277799	773434	55.33%	7.682%
5	5.958	788	799	812	rBV	176118	469563	33.59%	4.664%
6	6.763	921	931	945	rBV	426179	1020964	73.04%	10.140%
7	6.885	945	951	959	rVB4	14108	35253	2.52%	0.350%
8	8.647	1233	1240	1249	rBV	865812	1397772	100.00%	13.883%
9	8.720	1249	1252	1258	rVB2	9700	16288	1.17%	0.162%
10	9.598	1387	1396	1411	rBV	35473	158388	11.33%	1.573%
11	10.055	1465	1471	1481	rBV	903023	1223691	87.55%	12.154%
12	11.079	1634	1639	1652	rVB	746822	962998	68.90%	9.565%
13	11.683	1734	1738	1742	rBV	12248	17481	1.25%	0.174%
14	11.756	1746	1750	1759	rVB3	9757	17045	1.22%	0.169%
15	11.890	1765	1772	1780	rBV	96003	198614	14.21%	1.973%
16	12.024	1789	1794	1803	rVB	941161	1190411	85.16%	11.823%
17	12.219	1821	1826	1831	rBV	94373	151874	10.87%	1.508%
18	12.286	1831	1837	1839	rVV3	195843	408779	29.25%	4.060%
19	12.311	1839	1841	1847	rVV3	213980	340776	24.38%	3.385%
20	12.360	1847	1849	1856	rVV	63222	136459	9.76%	1.355%
21	12.427	1856	1860	1864	rVB	37807	50766	3.63%	0.504%
22	12.969	1946	1949	1954	rVB4	14118	22630	1.62%	0.225%
23	13.042	1956	1961	1964	rBV4	11823	17262	1.23%	0.171%
24	13.213	1985	1989	1991	rBV4	12482	16650	1.19%	0.165%
25	13.268	1994	1998	2000	rVV	57716	74297	5.32%	0.738%
26	13.292	2000	2002	2007	rVB5	27520	34982	2.50%	0.347%
27	13.384	2013	2017	2020	rBV2	9882	15651	1.12%	0.155%
28	13.420	2020	2023	2028	rVV5	12452	19104	1.37%	0.190%
29	13.585	2046	2050	2059	rBV6	12904	30715	2.20%	0.305%
30	13.676	2060	2065	2067	rBV3	9470	15216	1.09%	0.151%
31	13.774	2078	2081	2088	rVB2	24605	40248	2.88%	0.400%
32	13.847	2088	2093	2099	rVB6	30608	57495	4.11%	0.571%
33	13.926	2099	2106	2110	rBV6	21040	41923	3.00%	0.416%
34	14.036	2121	2124	2127	rBV	44805	49534	3.54%	0.492%
35	14.073	2127	2130	2134	rVB2	16147	18860	1.35%	0.187%
36	14.231	2150	2156	2160	rVB	47614	78433	5.61%	0.779%

LSC Area Percent Report

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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_X\Method\82X032923W.M
Title : SW846 8260

37	14.371	2177	2179	2183	rVB2	14719	15310	1.10%	0.152%
38	14.420	2183	2187	2192	rVB7	7068	15671	1.12%	0.156%
39	14.481	2193	2197	2206	rBV5	33420	59924	4.29%	0.595%
40	14.615	2215	2219	2221	rBV2	40690	55886	4.00%	0.555%
41	14.640	2221	2223	2226	rVV	46695	54313	3.89%	0.539%
42	14.670	2226	2228	2233	rVB3	15934	21886	1.57%	0.217%
43	14.755	2239	2242	2244	rBV	36851	41091	2.94%	0.408%
44	14.780	2244	2246	2250	rVB	29954	35319	2.53%	0.351%
45	15.188	2309	2313	2314	rBV3	23223	30512	2.18%	0.303%
46	15.207	2314	2316	2320	rVB2	26429	34136	2.44%	0.339%
47	15.487	2357	2362	2367	rBV3	30695	50696	3.63%	0.504%
48	15.615	2379	2383	2386	rBV2	22665	29889	2.14%	0.297%
49	16.091	2457	2461	2467	rVB6	12175	21638	1.55%	0.215%
50	16.377	2504	2508	2515	rVB4	12492	22085	1.58%	0.219%

Sum of corrected areas: 10068291

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MSVOA_X
ClientSampleId :
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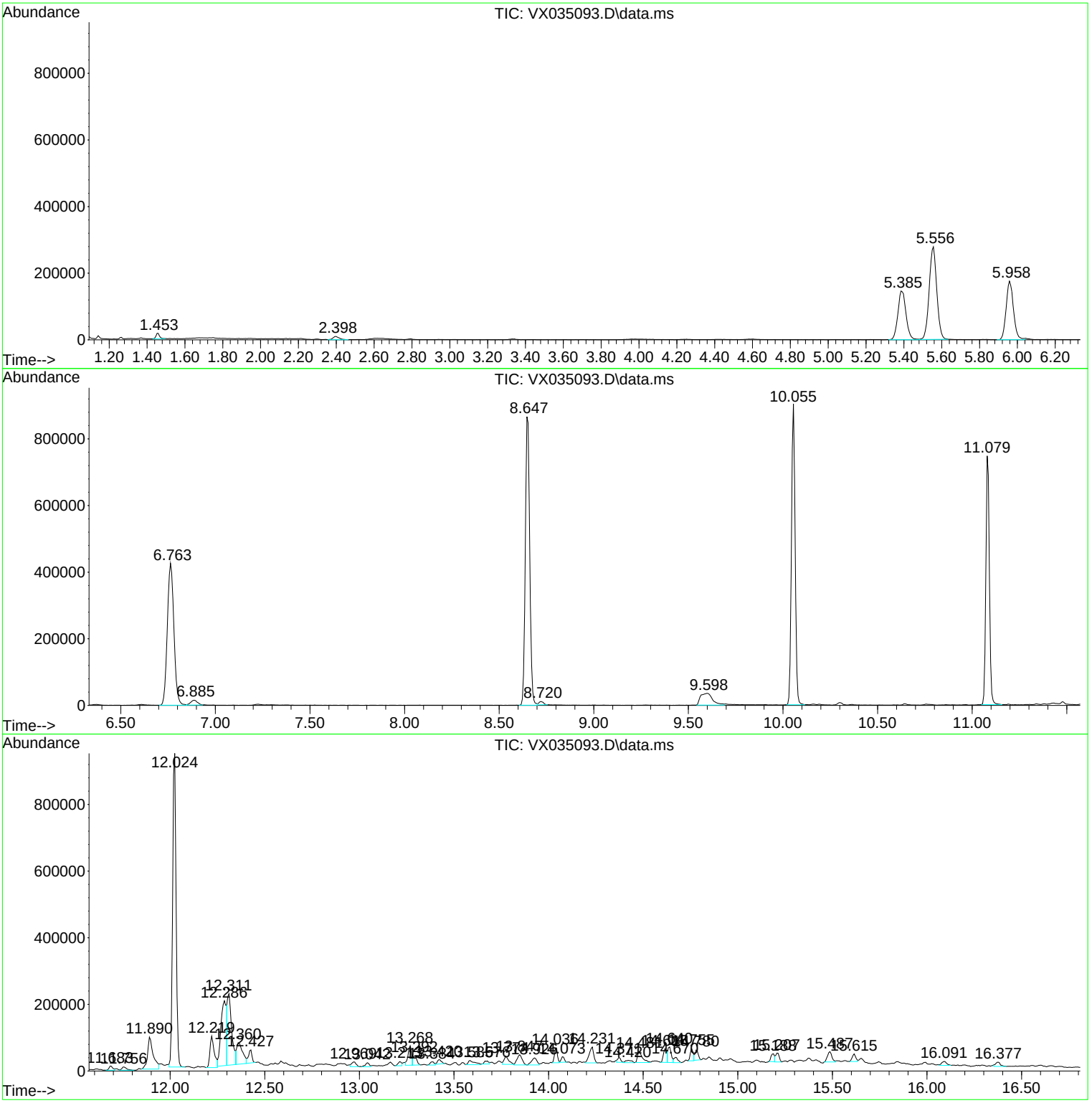
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

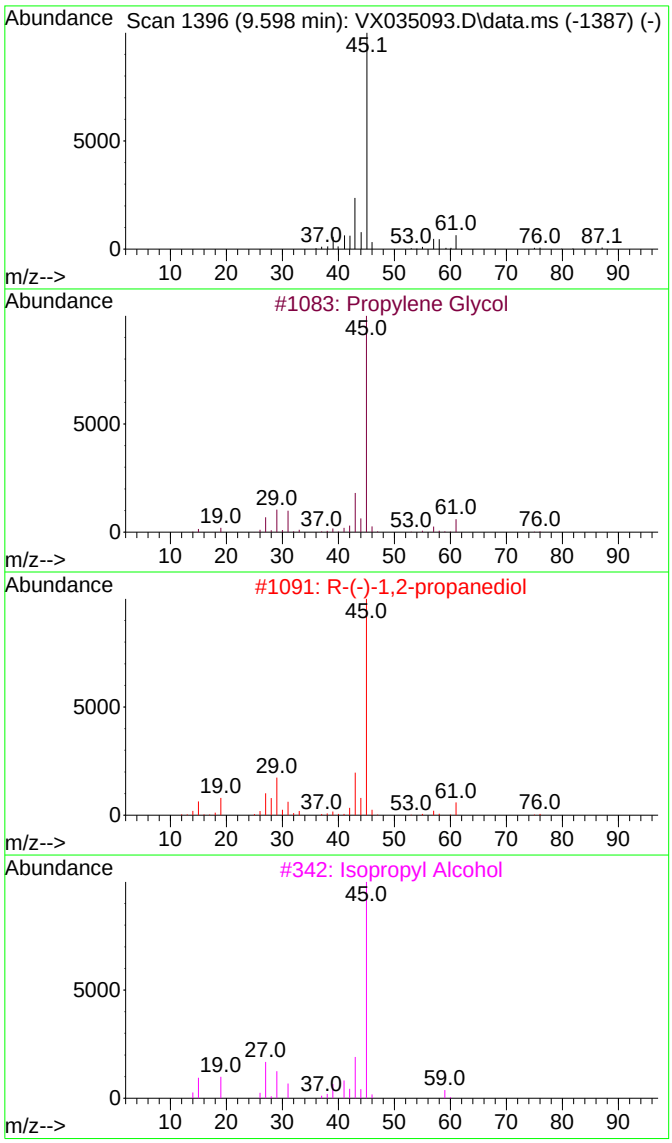
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

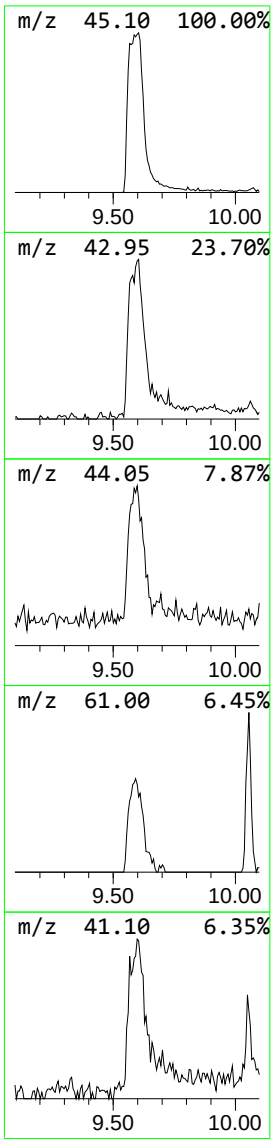
****

Peak Number 1 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.598	6.47 ug/l	158388	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	80
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5	2-Pentanol	88	C5H12O	006032-29-7	39





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Instrument :
MSVOA_X
ClientSampleId :
BUR-1262

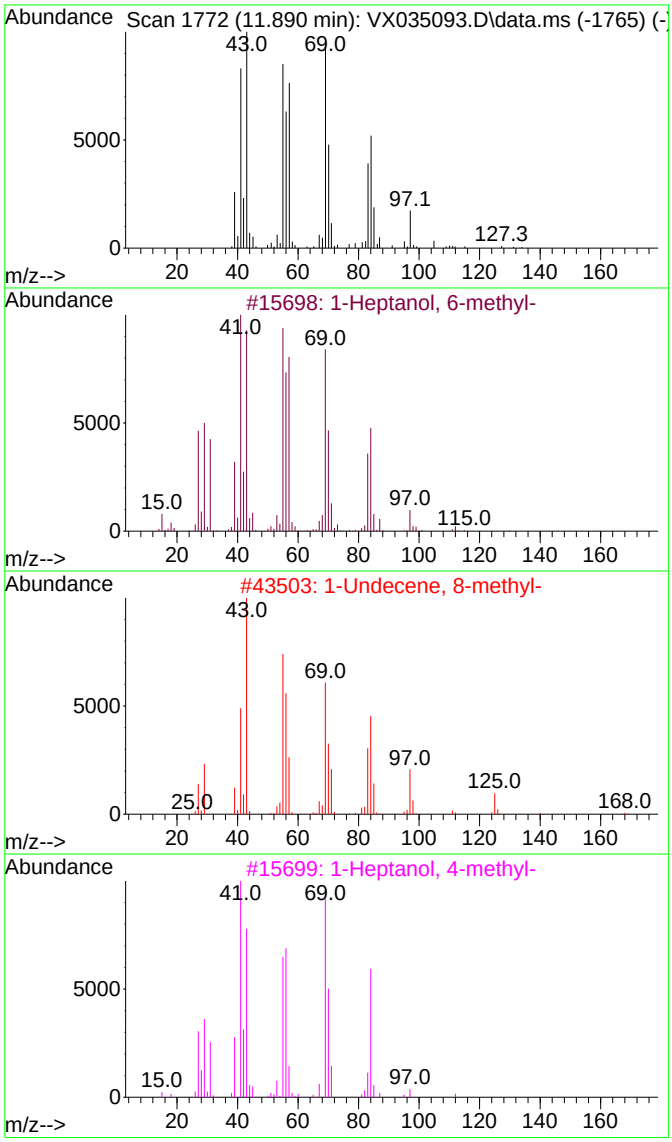
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

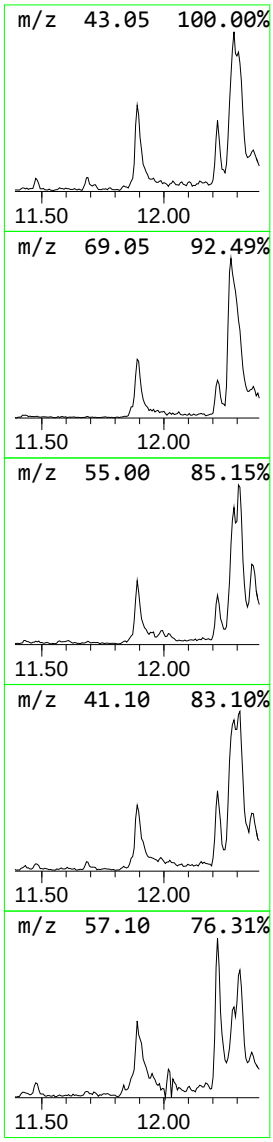
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Heptanol, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.890	8.34 ug/l	198614	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	1-Undecene, 8-methyl-	168	C12H24	074630-40-3	78
3	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
4	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	47
5	1-Hexene, 3-methyl-	98	C7H14	003404-61-3	47





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Instrument :
MSVOA_X
ClientSampleId :
BUR-1262

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

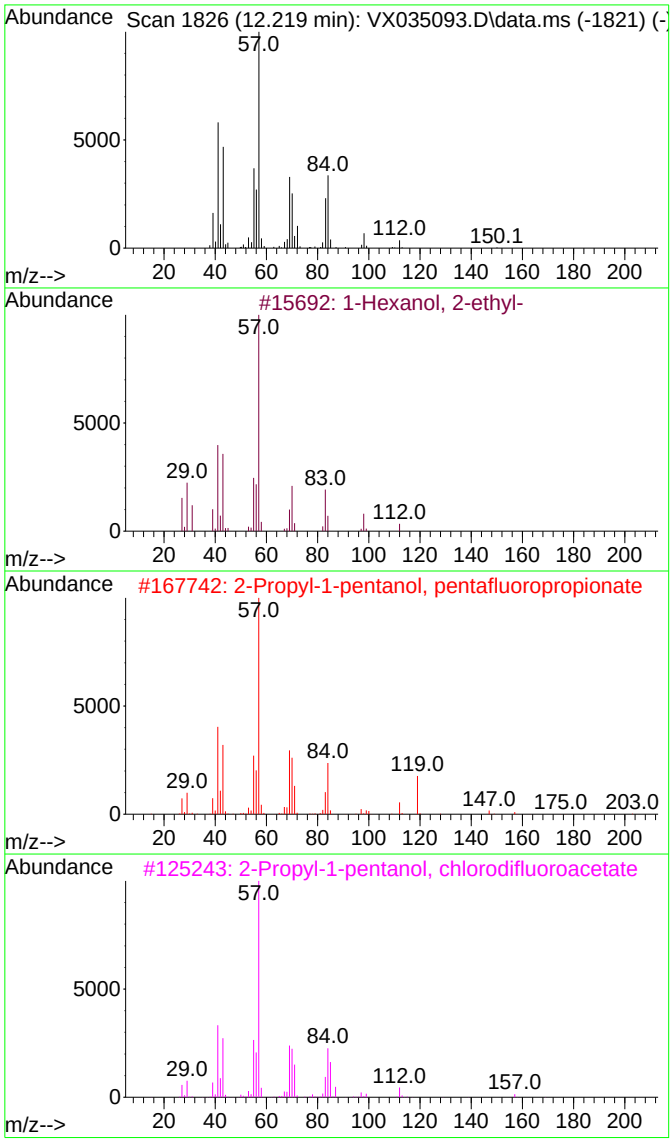
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

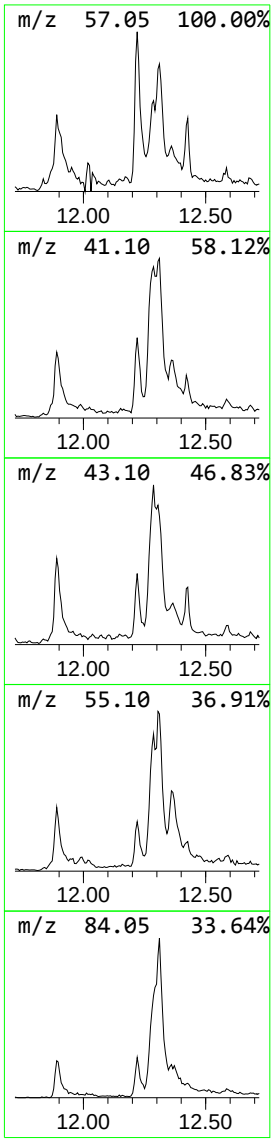
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	6.38 ug/l	151874	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
2	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	50
3	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	47
4	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	47
5	3-Octene, (E)-	112	C8H16	014919-01-8	38





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Instrument :
MSVOA_X
ClientSampleId :
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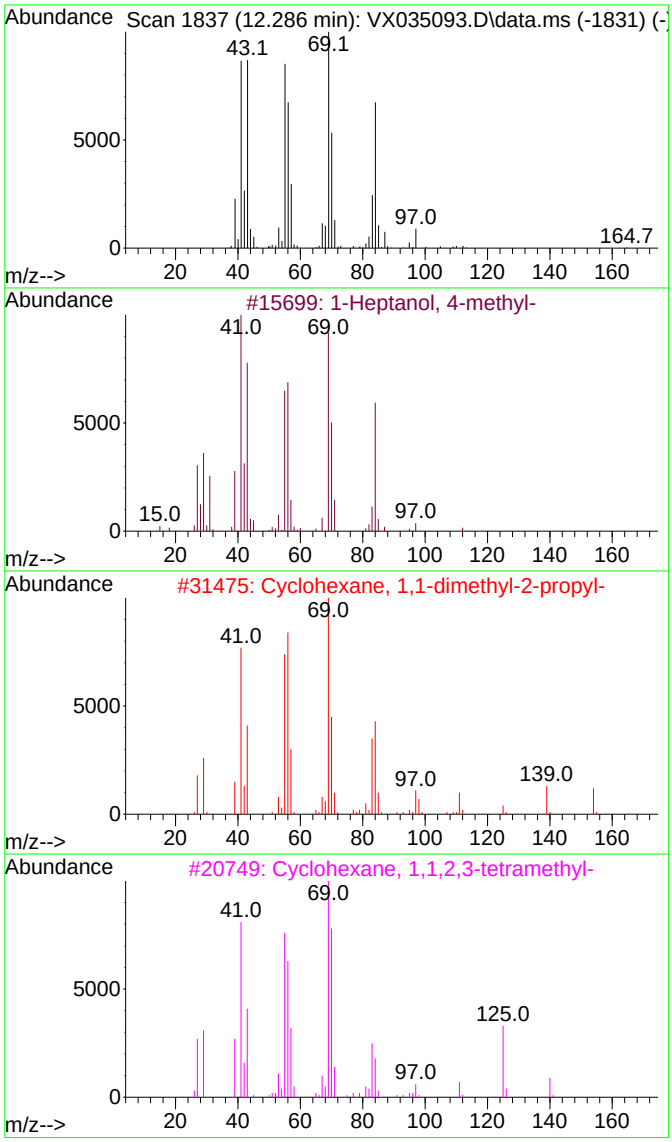
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

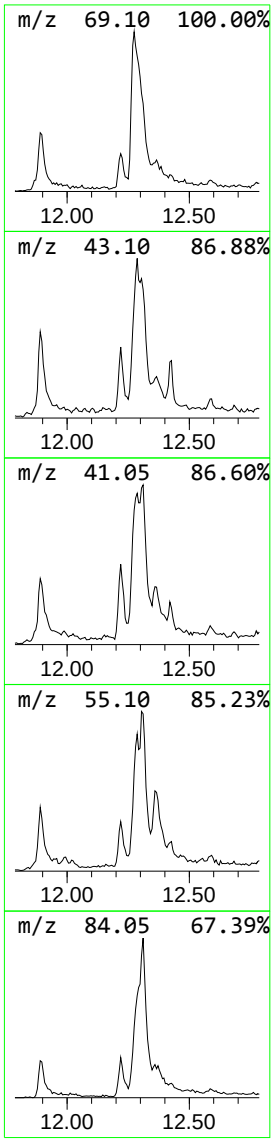
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heptanol, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.286	17.17 ug/l	408779	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	72
2	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	59
3	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	53
4	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	49
5	Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	47





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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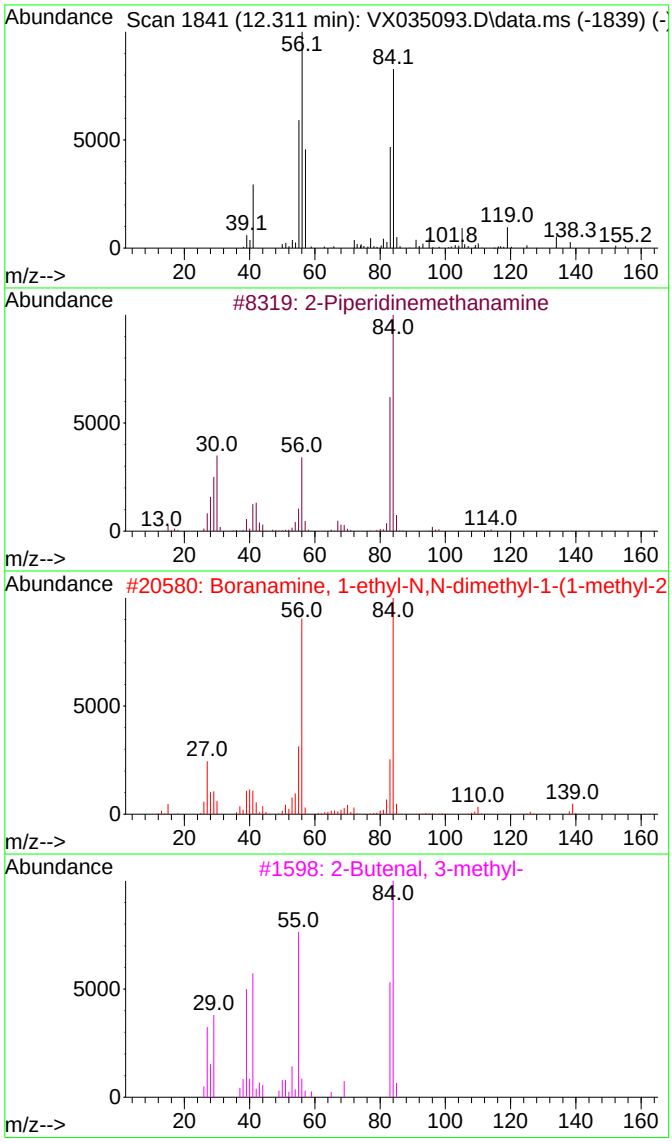
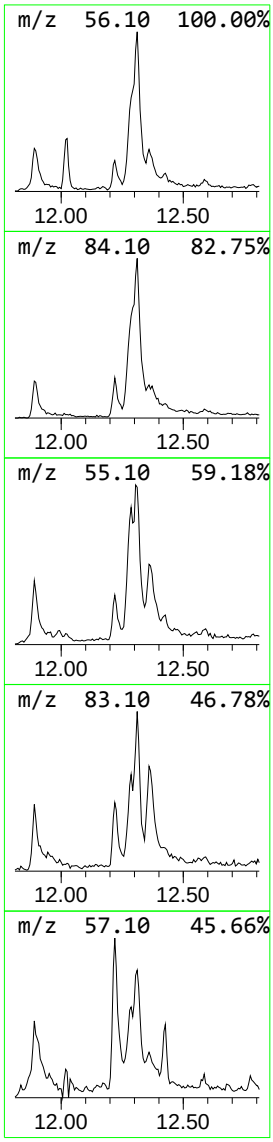
****

Peak Number 5 unknown12.311 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.311	14.31 ug/l	340776	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinemethanamine	114	C6H14N2	022990-77-8	40
2	Boranamine, 1-ethyl-N,N-dimethyl...	139	C8H18BN	042843-12-9	36
3	2-Butenal, 3-methyl-	84	C5H8O	000107-86-8	32
4	Furan, 2,3-dihydro-4-methyl-	84	C5H8O	034314-83-5	25
5	2-(1-Adamantyl)piperidine	219	C15H25N	195243-62-0	22





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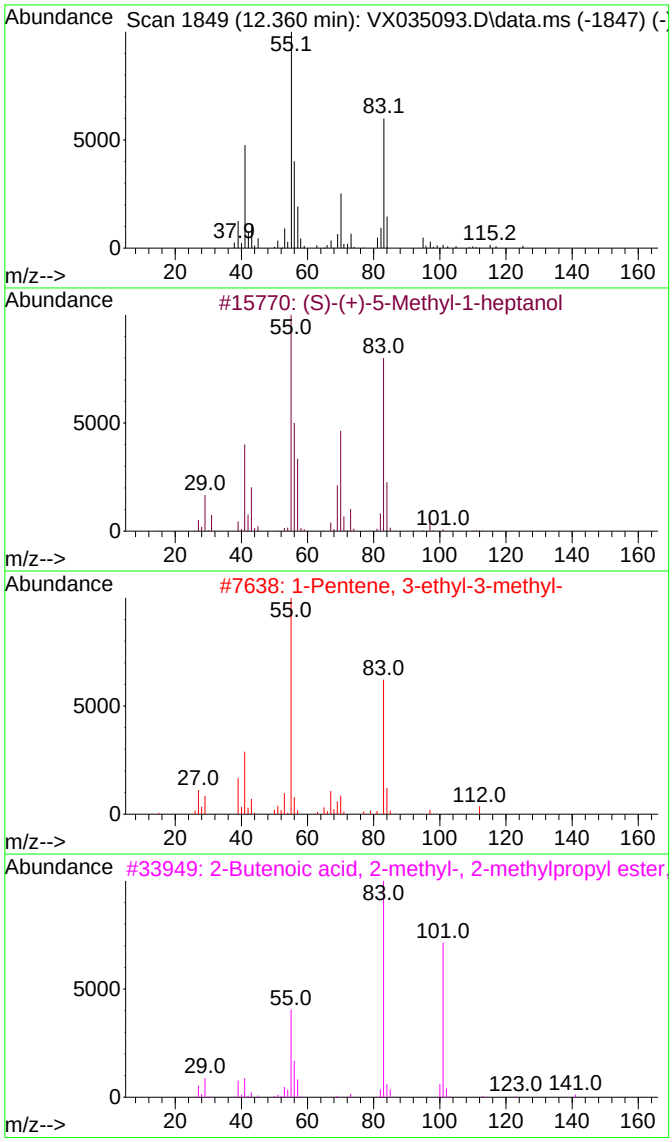
Quant Title : SW846 8260

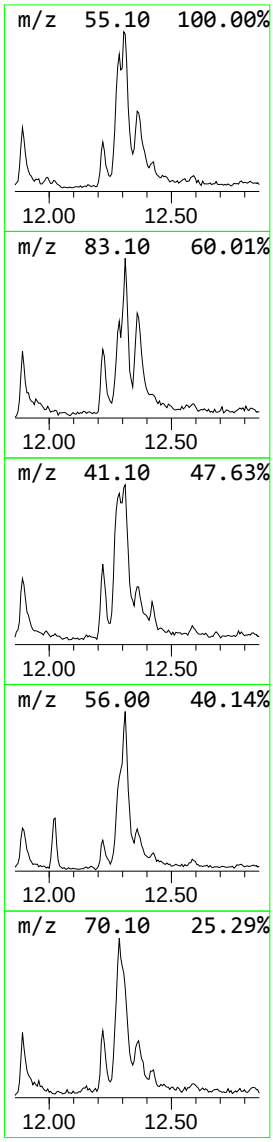
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (S)-(+)-5-Methyl-1-heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.360	5.73 ug/l	136459	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	64
2	1-Pentene, 3-ethyl-3-methyl-	112	C8H16	006196-60-7	43
3	2-Butenoic acid, 2-methyl-, 2-me...	156	C9H16O2	061692-84-0	42
4	5-Methyl-1-heptanol	130	C8H18O	007212-53-5	42
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	40





Tentatively Identified Compound (LSC) summary

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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.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
Propylene Glycol	9.598	6.5	ug/l	158388	3	10.055	1223690	50.0
1-Heptanol, 6-m...	11.890	8.3	ug/l	198614	4	12.024	1190410	50.0
1-Hexanol, 2-et...	12.219	6.4	ug/l	151874	4	12.024	1190410	50.0
1-Heptanol, 4-m...	12.286	17.2	ug/l	408779	4	12.024	1190410	50.0
unknown12.311	12.311	14.3	ug/l	340776	4	12.024	1190410	50.0
(S)-(+)-5-Methy...	12.360	5.7	ug/l	136459	4	12.024	1190410	50.0