LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039602.D
Acq On : 03 Jan 2024 15:13
Operator : JC/MD
Sample : P1002-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1214

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\82X121323W.M
Title : SW846 8260

Signal : TIC: VX039602.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.374	204	211	225	rBV	331169	530611	8.86%	3.441%
2	2.526	229	236	249	rVB	33342	63414	1.06%	0.411%
3	4.227	504	515	535	rBV	104980	290617	4.85%	1.885%
4	5.385	693	705	722	rVV3	67914	198237	3.31%	1.286%
5	5.550	722	732	750	rVB2	99845	282202	4.71%	1.830%
6	5.952	789	798	812	rBV	79134	209394	3.50%	1.358%
7	6.099	814	822	836	rBV	73120	200470	3.35%	1.300%
8	6.757	921	930	945	rBV	186703	450128	7.51%	2.919%
9	7.202	996	1003	1014	rBV	109154	230451	3.85%	1.494%
10	8.647	1234	1240	1248	rBV	399838	629295	10.51%	4.081%
11	10.049	1465	1470	1483	rBV	433393	623690	10.41%	4.045%
12	10.750	1581	1585	1594	rBV3	42026	74178	1.24%	0.481%
13	11.079	1633	1639	1645	rBV	379975	478827	7.99%	3.105%
14	11.567	1714	1719	1733	rBV	4947130	5989945	100.00%	38.844%
15	11.683	1733	1738	1746	rVB	253655	294909	4.92%	1.912%
16	11.823	1756	1761	1766	rBV	1202691	1419851	23.70%	9.208%
17	11.884	1766	1771	1779	rVV	303136	402991	6.73%	2.613%
18	11.988	1779	1788	1790	rVV2	129463	200157	3.34%	1.298%
19	12.018	1790	1793	1801	rVB	464658	603556	10.08%	3.914%
20	12.098	1801	1806	1812	rBV	250682	335162	5.60%	2.173%
21	12.213	1820	1825	1836	rBV	414076	579094	9.67%	3.755%
22	12.524	1869	1876	1885	rBV2	43790	77602	1.30%	0.503%
23	13.146	1970	1978	1980	rBV	100816	150681	2.52%	0.977%
24	13.213	1985	1989	1998	rVB	172488	232453	3.88%	1.507%
25	13.579	2041	2049	2052	rBV3	53048	97300	1.62%	0.631%
26	13.676	2058	2065	2069	rBV2	76253	103998	1.74%	0.674%
27	13.731	2069	2074	2078	rBV	375519	489814	8.18%	3.176%
28	13.774	2078	2081	2086	rVB	81576	102287	1.71%	0.663%
29	15.969	2435	2441	2452	rBV2	44148	79192	1.32%	0.514%

Sum of corrected areas: 15420506

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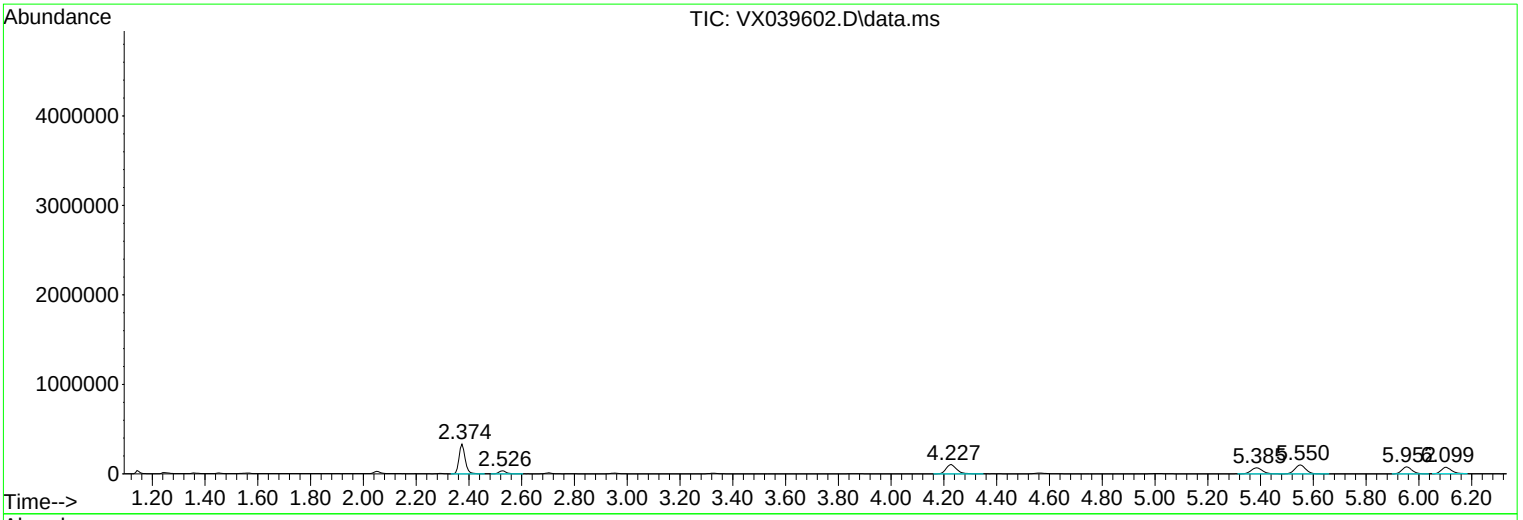
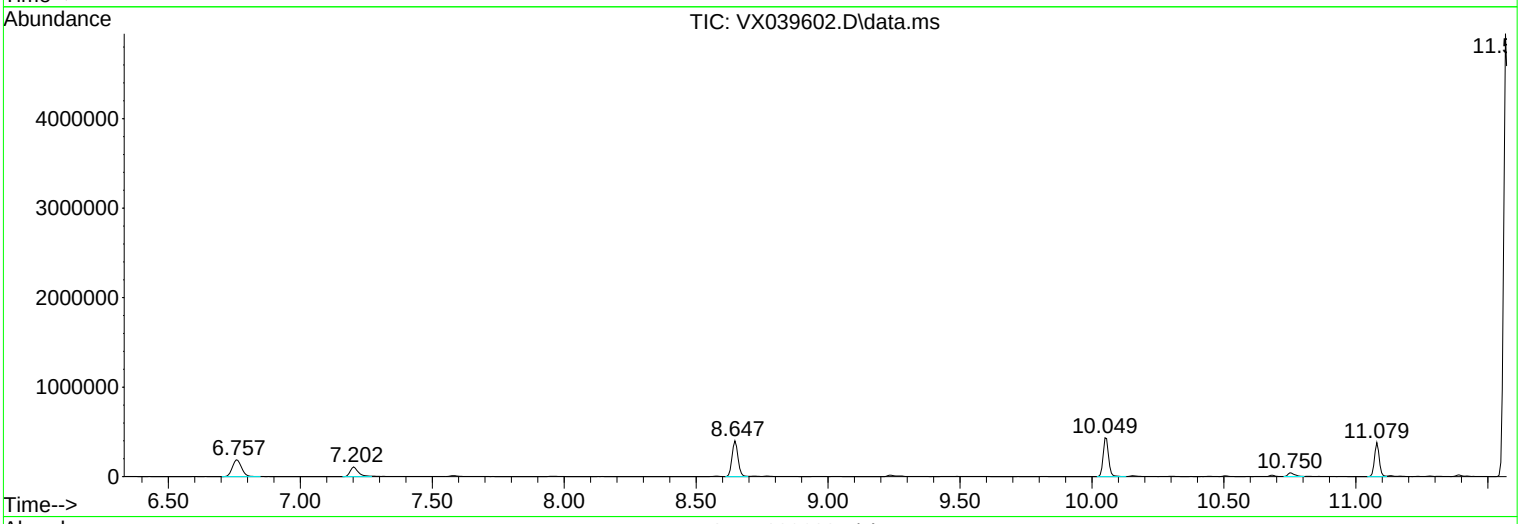
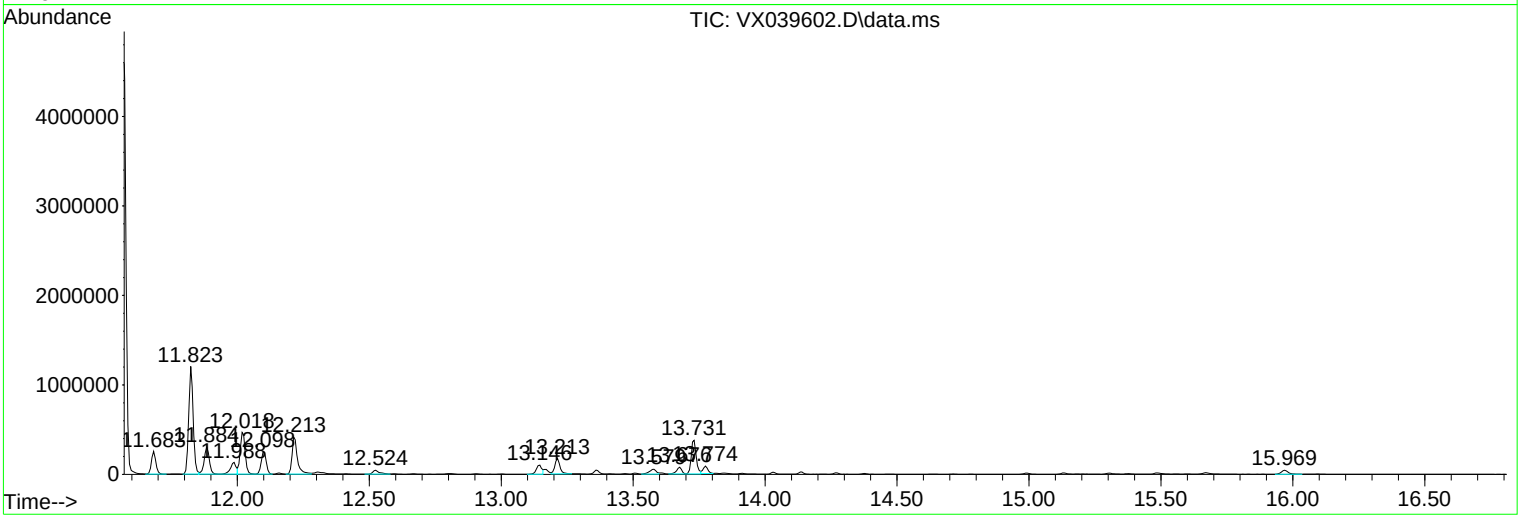
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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







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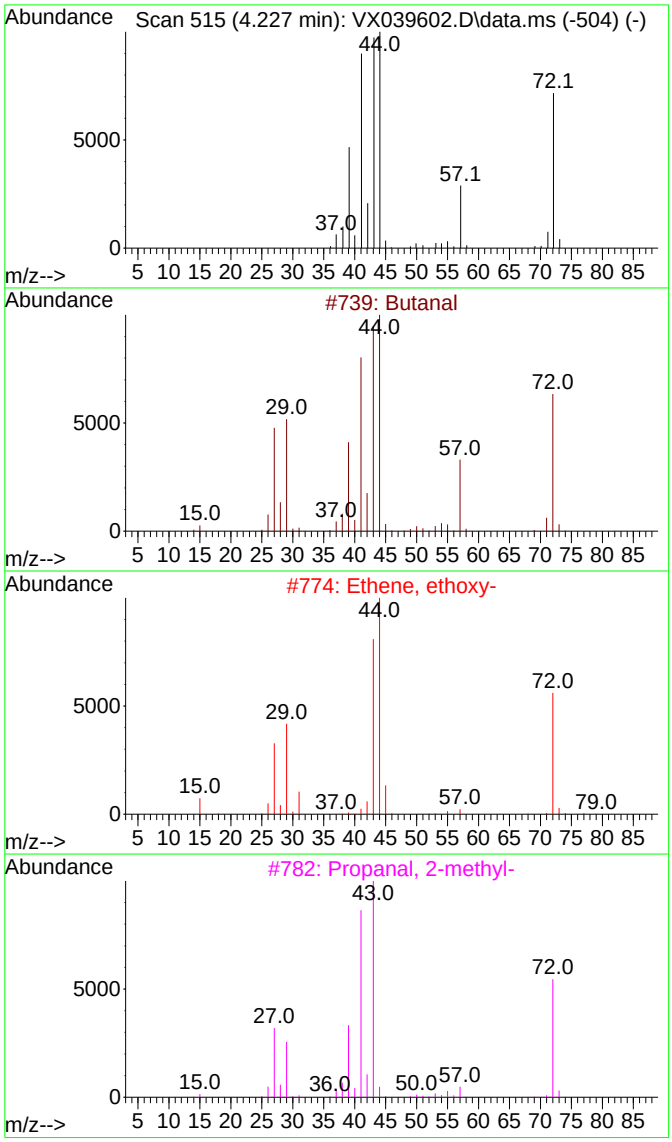
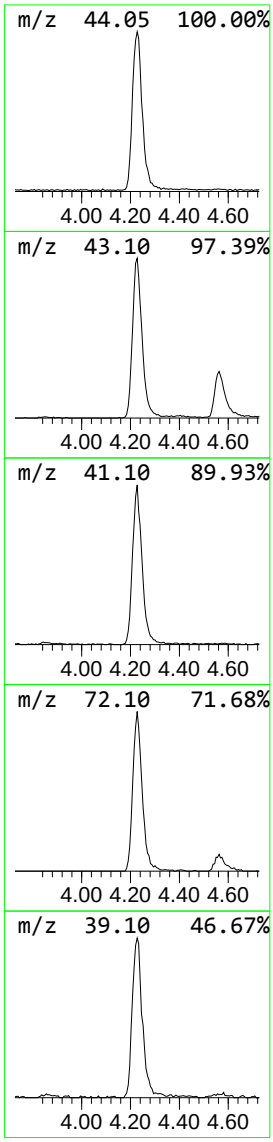
****

Peak Number 1 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	51.49 ug/l	290617	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	17





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ClientSampleId :
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Quant Title : SW846 8260

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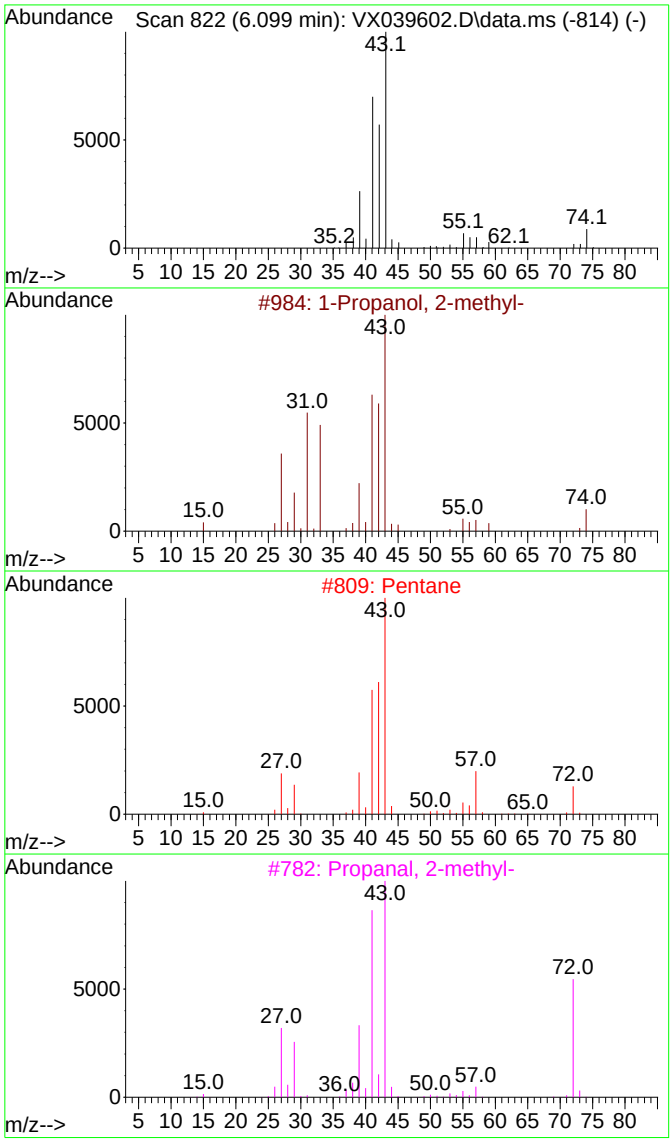
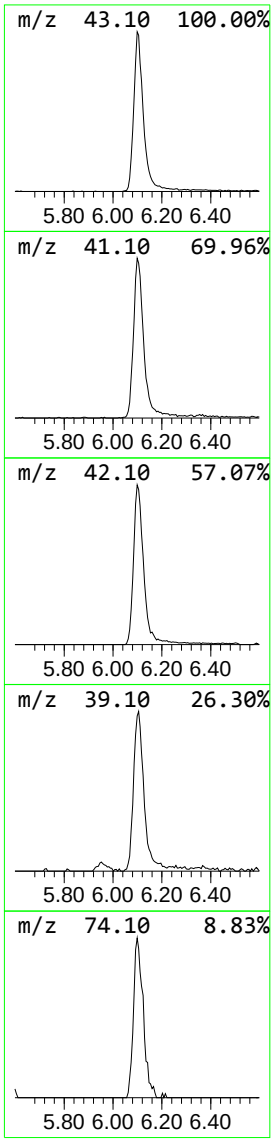
****
Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.099	35.52 ug/l	200470	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	90
2	Pentane	72	C5H12	000109-66-0	45
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27
4	Isobutylene epoxide	72	C4H8O	000558-30-5	25
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	17





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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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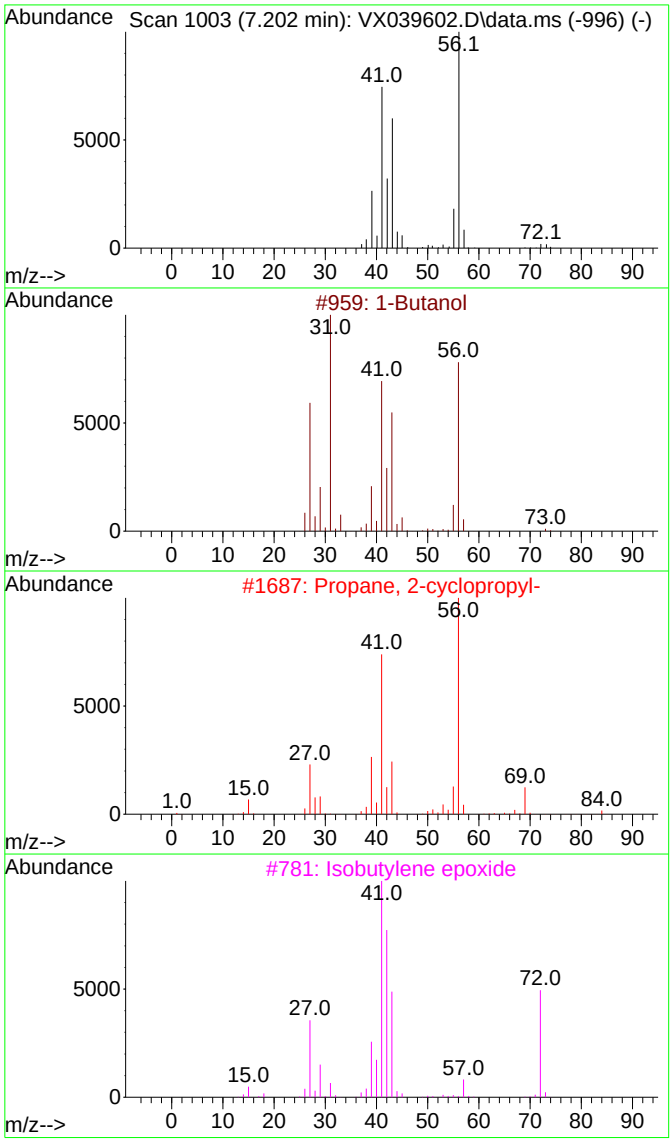
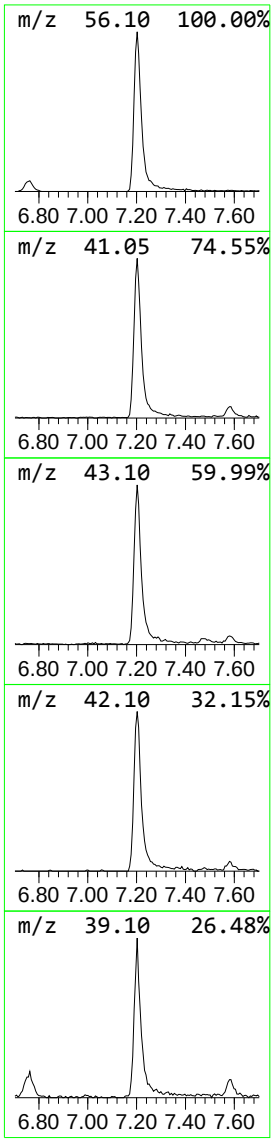
****

Peak Number 3 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.202	25.60 ug/l	230451	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3	Isobutylene epoxide	72	C4H8O	000558-30-5	9
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9





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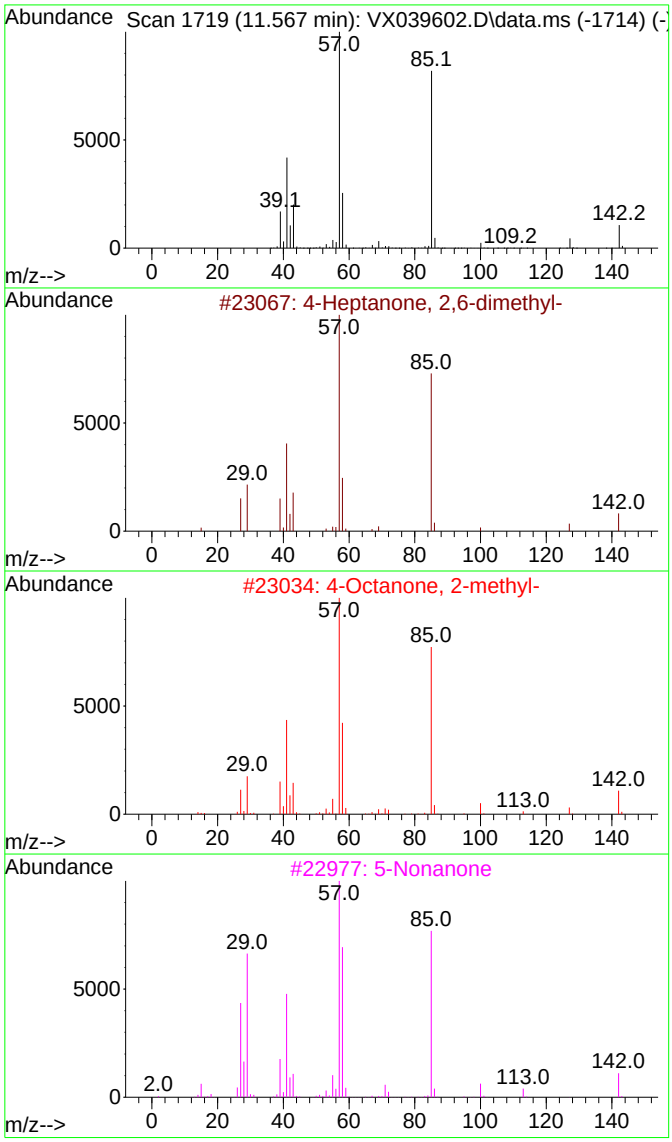
Quant Title : SW846 8260

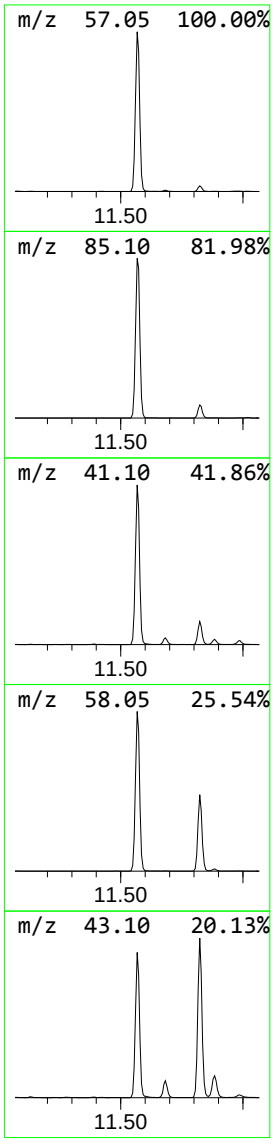
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.567	496.22 ug/l	5989950	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	94
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	72
3	5-Nonanone	142	C9H18O	000502-56-7	64
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5	3-Buten-2-ol, 2,3-dimethyl-	100	C6H12O	010473-13-9	50





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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
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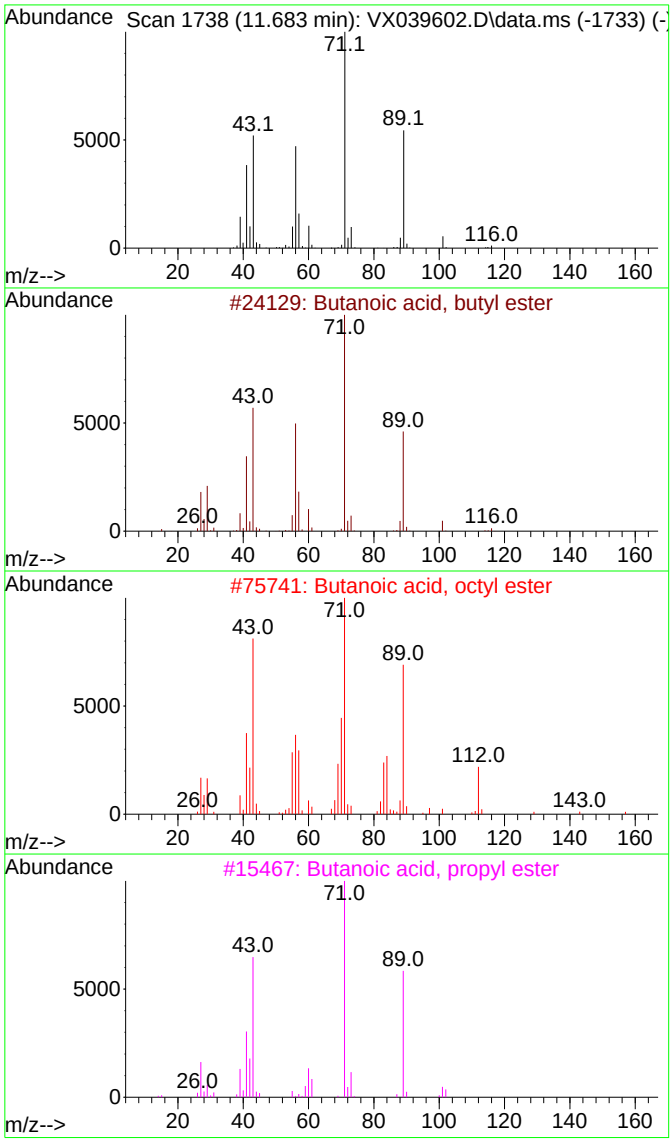
Quant Title : SW846 8260

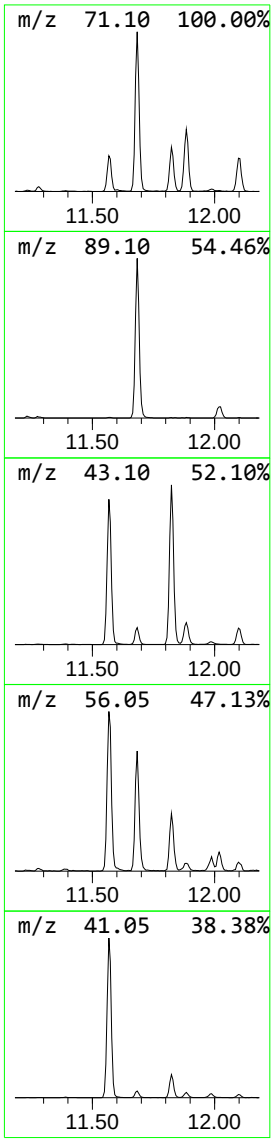
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	24.43 ug/l	294909	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56





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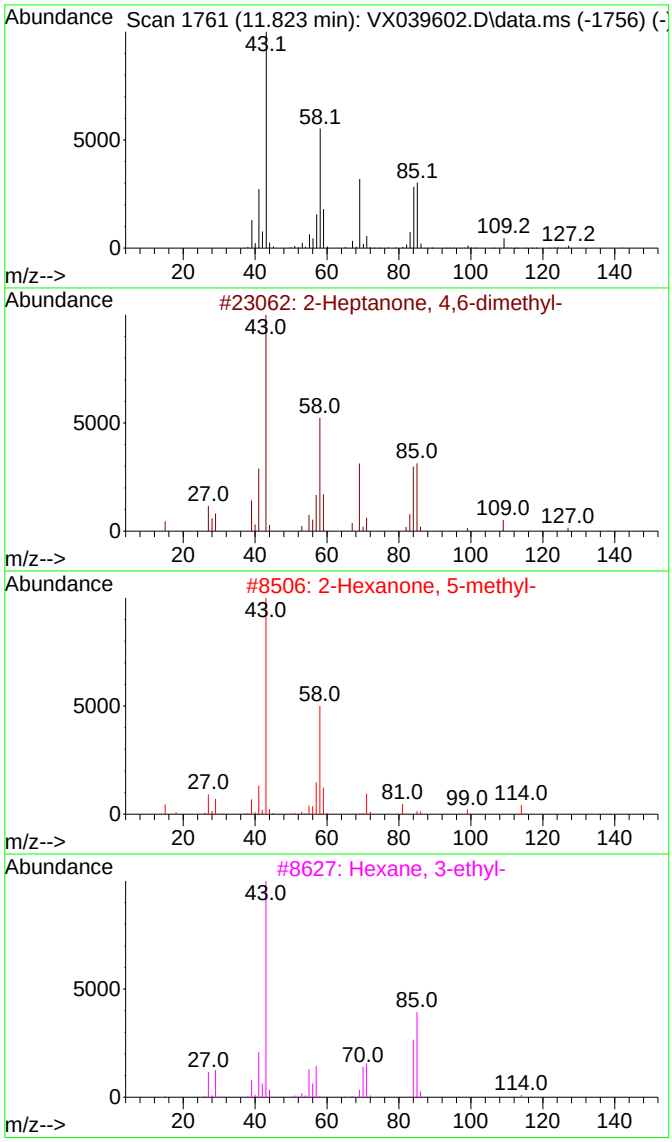
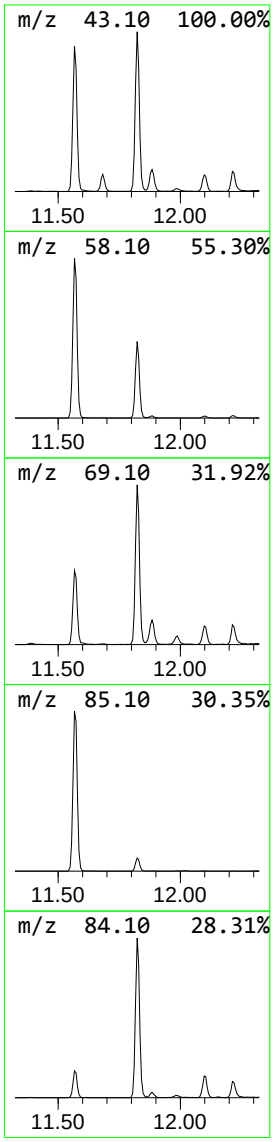
****
Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.823	117.62 ug/l	1419850	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 4,6-dimethyl-	142	C9H18O	019549-80-5	72
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
3	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
4	Carbonic acid, hexyl prop-1-en-2...	186	C10H18O3	1000382-54-2	40
5	1-Octene, 4-methyl-	126	C9H18	013151-12-7	37





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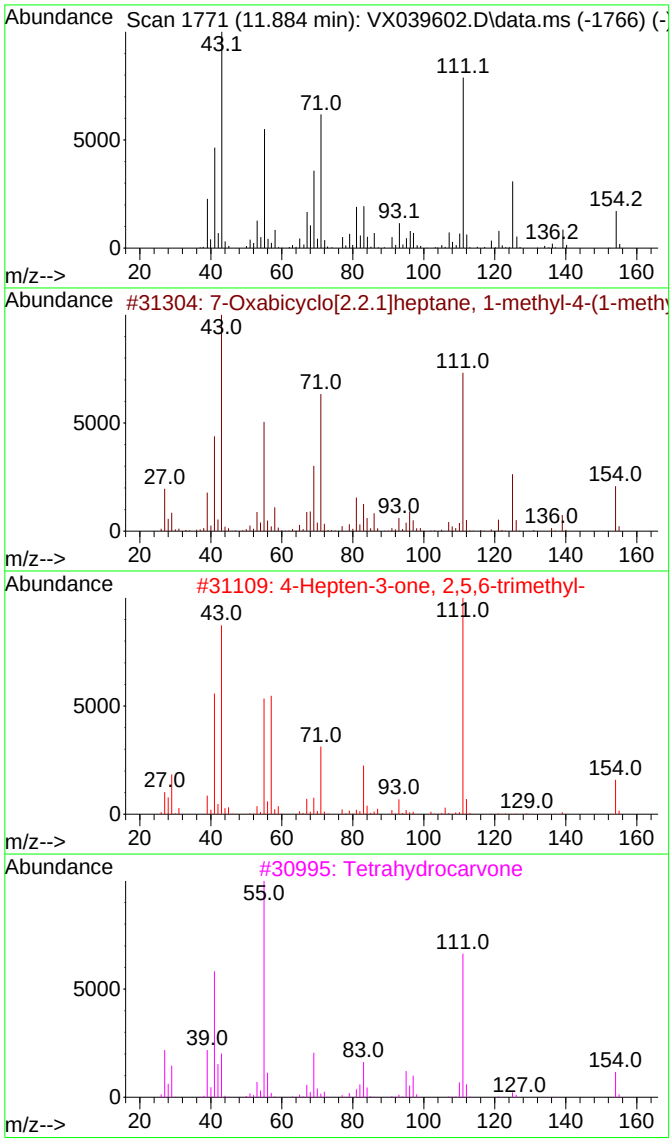
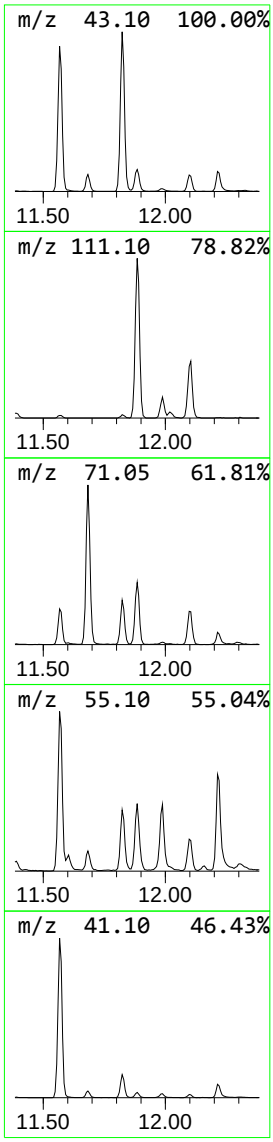
****
Peak Number 7 7-Oxabicyclo[2.2.1]heptane,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.884	33.38 ug/l	402991	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	95
2	4-Hepten-3-one, 2,5,6-trimethyl-	154	C10H18O	016466-21-0	58
3	Tetrahydrocarvone	154	C10H18O	000499-70-7	49
4	Benzenamine, 3-fluoro-	111	C6H6FN	000372-19-0	43
5	2(5H)-Furanone, 3,5,5-trimethyl-	126	C7H10O2	050598-50-0	38





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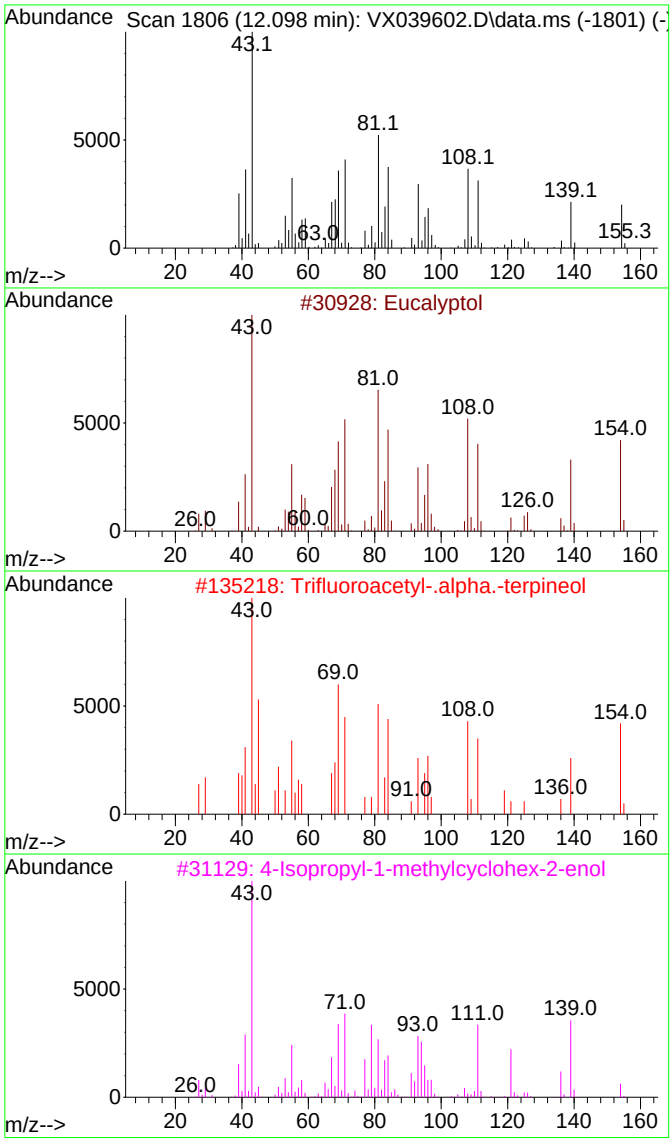
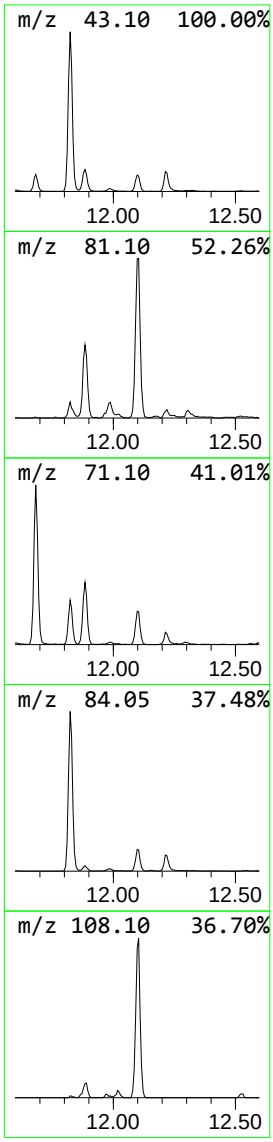
****
Peak Number 8 Eucalyptol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.098	27.77 ug/l	335162	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	50
3	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	38
4	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	25
5	3-Ethylidene- heptan-2,6-dione	154	C9H14O2	1000223-47-9	14





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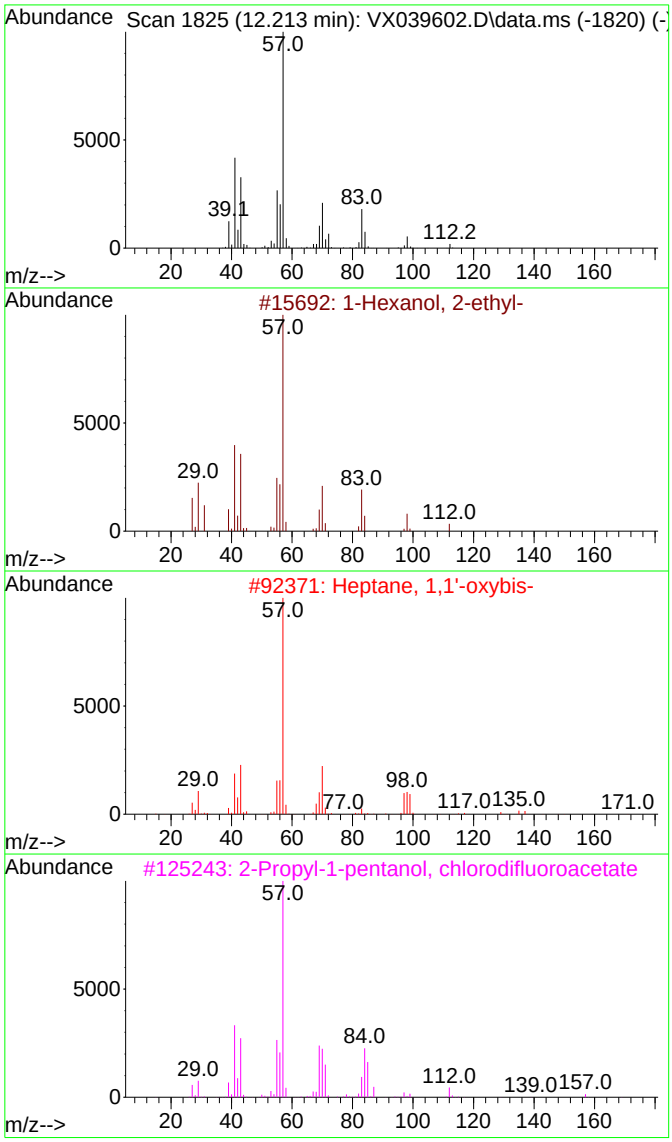
Quant Title : SW846 8260

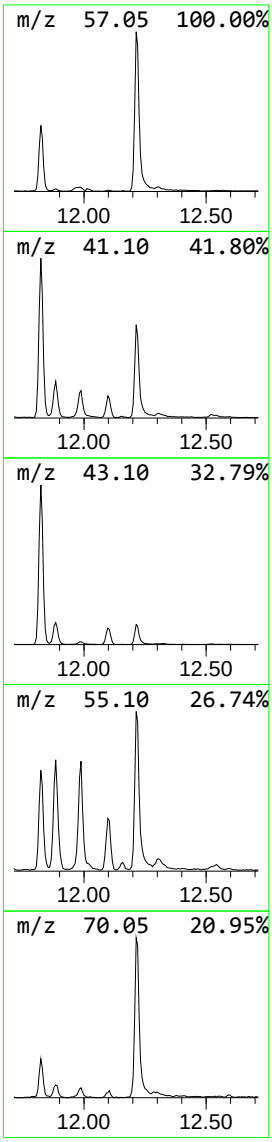
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.213	47.97 ug/l	579094	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	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039602.D
Acq On : 03 Jan 2024 15:13
Operator : JC/MD
Sample : P1002-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1214

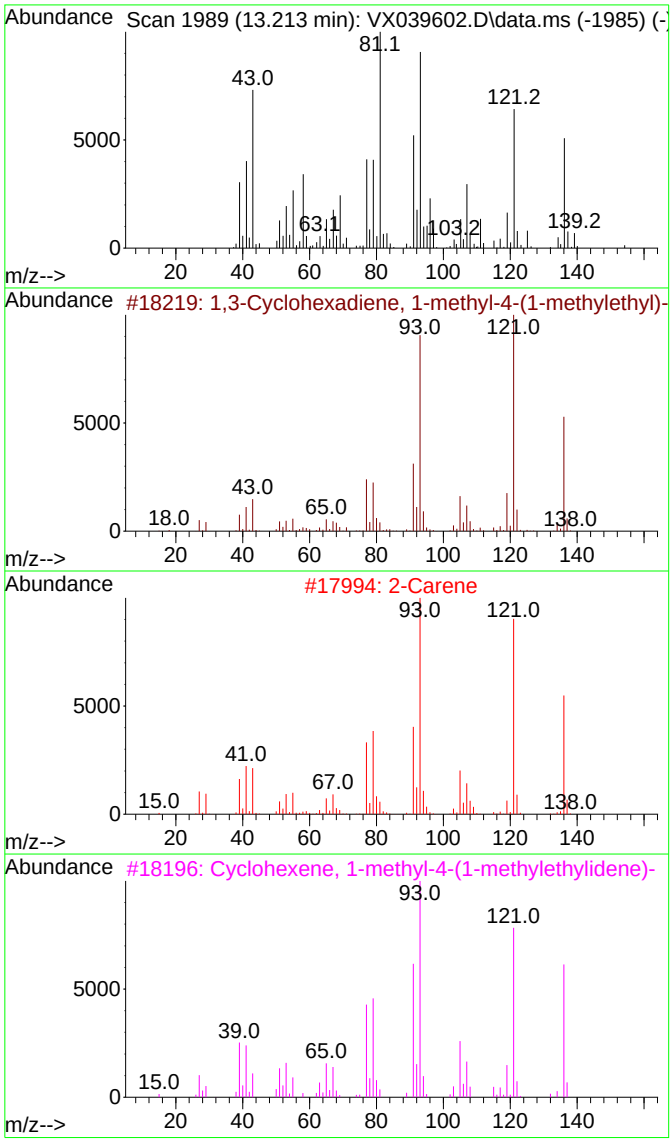
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

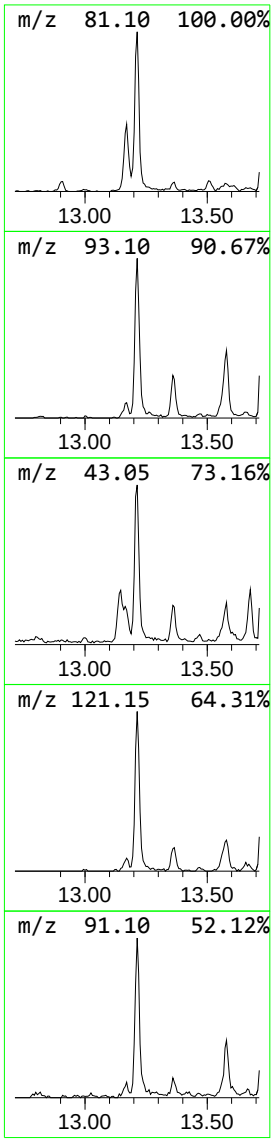
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,3-Cyclohexadiene, 1-methy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	19.26 ug/l	232453	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	93
2	2-Carene	136	C10H16	000554-61-0	91
3	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	91
4	(+)-4-Carene	136	C10H16	029050-33-7	86
5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039602.D
Acq On : 03 Jan 2024 15:13
Operator : JC/MD
Sample : P1002-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1214

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.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	4.227	51.5	ug/l	290617	1	5.550	282202	50.0
1-Propanol, 2-m...	6.099	35.5	ug/l	200470	1	5.550	282202	50.0
1-Butanol	7.202	25.6	ug/l	230451	2	6.757	450128	50.0
4-Heptanone, 2,...	11.567	496.2	ug/l	5989950	4	12.024	603556	50.0
Butanoic acid, ...	11.683	24.4	ug/l	294909	4	12.024	603556	50.0
2-Heptanone, 4,...	11.823	117.6	ug/l	1419850	4	12.024	603556	50.0
7-Oxabicyclo[2....	11.884	33.4	ug/l	402991	4	12.024	603556	50.0
Eucalyptol	12.098	27.8	ug/l	335162	4	12.024	603556	50.0
1-Hexanol, 2-et...	12.213	48.0	ug/l	579094	4	12.024	603556	50.0
1,3-Cyclohexadi...	13.213	19.3	ug/l	232453	4	12.024	603556	50.0