LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040512.D
Acq On : 28 Feb 2024 15:40
Operator : JC/MD
Sample : P1613-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

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\82X022624W.M
Title : SW846 8260

Signal : TIC: VX040512.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	204	212	227	rBV	156392	257467	3.87%	1.970%
2	4.806	596	610	622	rBV3	26014	77798	1.17%	0.595%
3	5.385	693	705	718	rBV	51449	147761	2.22%	1.131%
4	5.556	721	733	745	rBV	82779	233943	3.52%	1.790%
5	5.958	790	799	812	rBV	59411	156766	2.36%	1.199%
6	6.763	920	931	948	rBV2	128803	312325	4.70%	2.390%
7	8.647	1234	1240	1246	rBV	267405	417870	6.28%	3.197%
8	8.720	1246	1252	1264	rVB	221914	338671	5.09%	2.591%
9	10.055	1465	1471	1475	rBV	295721	401814	6.04%	3.074%
10	10.299	1503	1511	1519	rBV	234833	321917	4.84%	2.463%
11	10.640	1562	1567	1572	rBV	97725	120519	1.81%	0.922%
12	11.079	1633	1639	1644	rBV	263494	330250	4.96%	2.527%
13	11.573	1714	1720	1734	rBV	5633668	6652205	100.00%	50.899%
14	11.683	1734	1738	1744	rVB	175229	204100	3.07%	1.562%
15	11.823	1757	1761	1766	rBV	883337	1082743	16.28%	8.285%
16	11.884	1766	1771	1779	rVV5	82581	146302	2.20%	1.119%
17	11.975	1779	1786	1789	rVV	56935	82953	1.25%	0.635%
18	12.018	1789	1793	1801	rVV	339870	471561	7.09%	3.608%
19	12.103	1801	1807	1813	rVB	53092	75063	1.13%	0.574%
20	12.237	1824	1829	1836	rBV3	29159	67999	1.02%	0.520%
21	12.524	1871	1876	1881	rBV	89224	108073	1.62%	0.827%
22	12.817	1919	1924	1935	rBV	92411	124247	1.87%	0.951%
23	13.213	1986	1989	1997	rVB2	68134	94876	1.43%	0.726%
24	13.670	2059	2064	2069	rBV2	90222	121386	1.82%	0.929%
25	13.731	2069	2074	2079	rVV	484219	620394	9.33%	4.747%
26	13.774	2079	2081	2088	rVB2	71759	100293	1.51%	0.767%

Sum of corrected areas: 13069296

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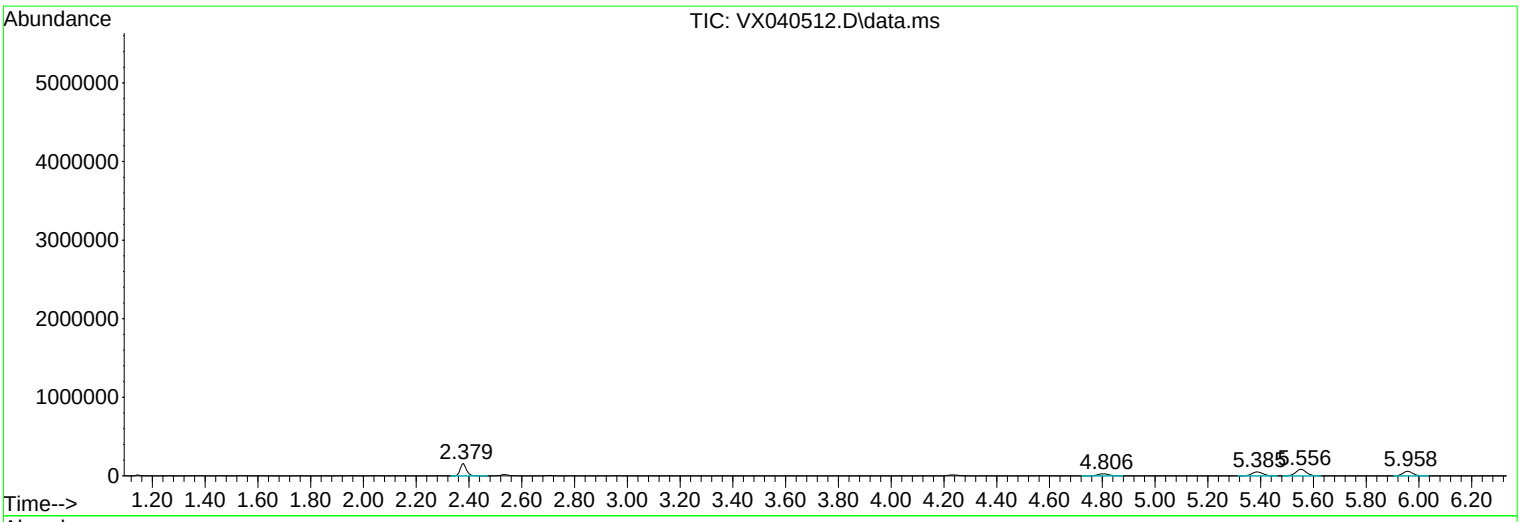
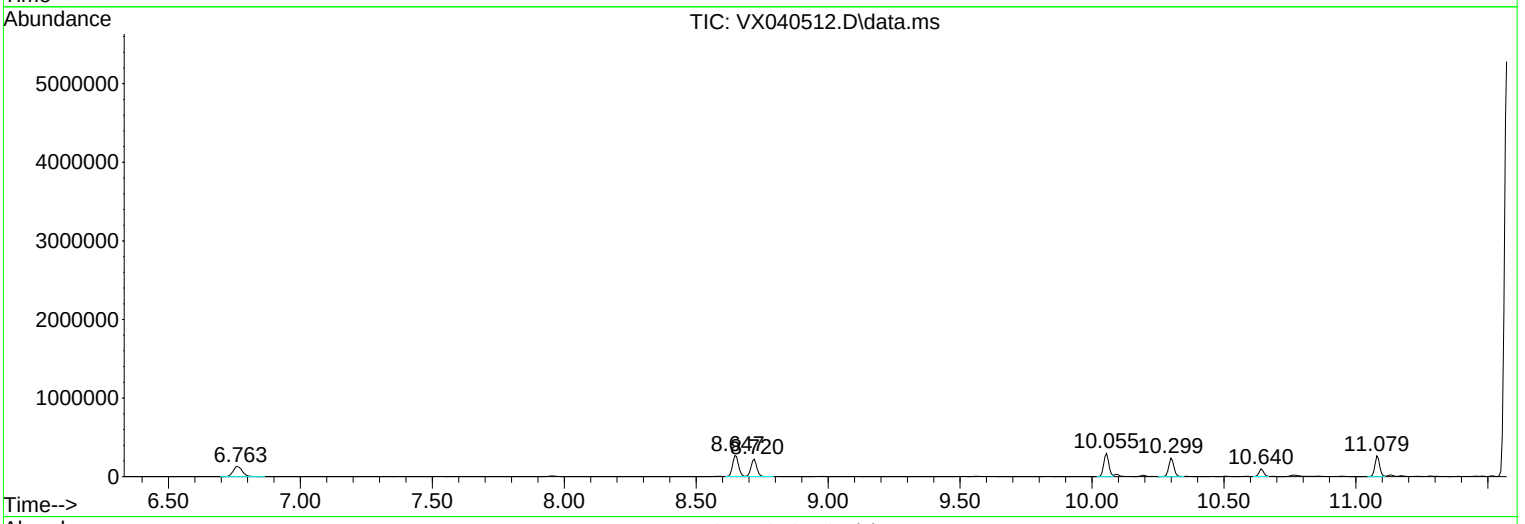
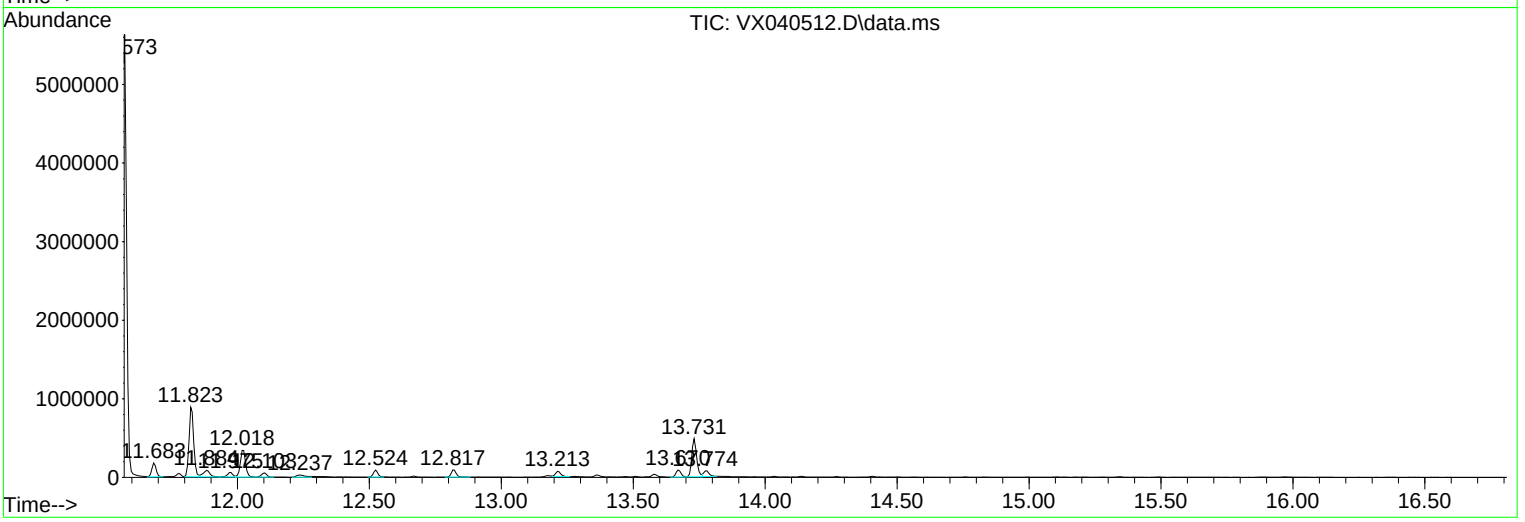
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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







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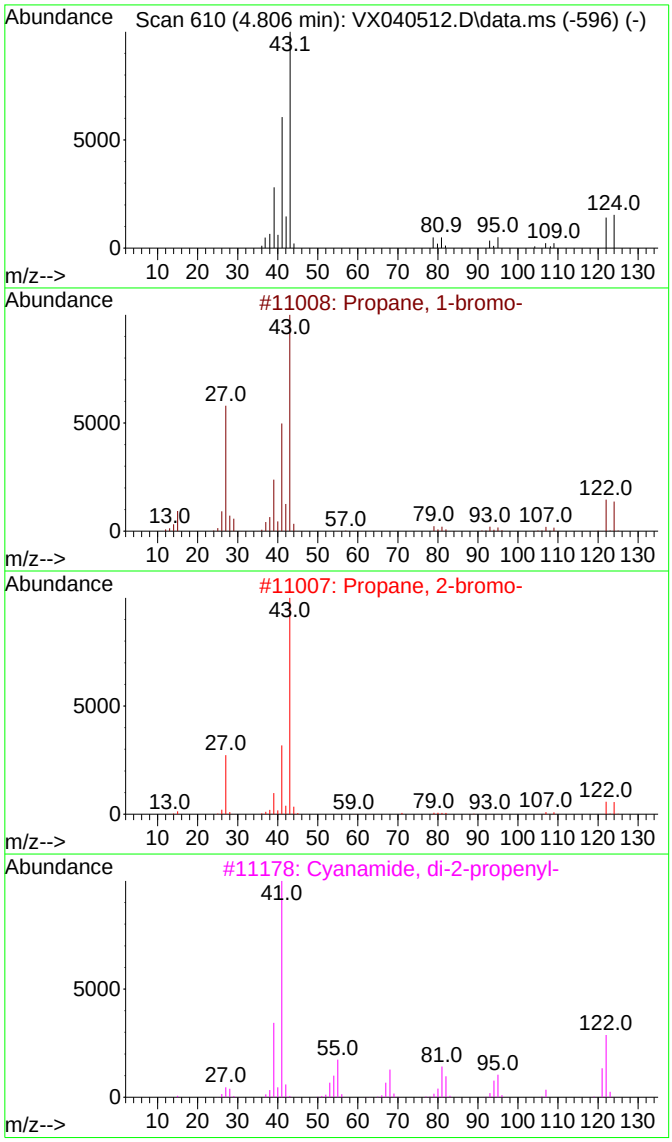
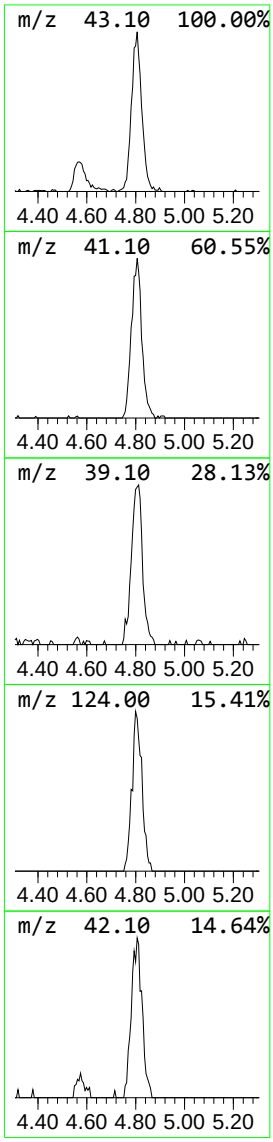
****
Peak Number 1 Propane, 1-bromo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.806	16.63 ug/l	77798	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-bromo-	122	C3H7Br	000106-94-5	87
2	Propane, 2-bromo-	122	C3H7Br	000075-26-3	52
3	Cyanamide, di-2-propenyl-	122	C7H10N2	000538-08-9	9
4	Propene	42	C3H6	000115-07-1	9
5	Acetylpyrazine	122	C6H6N2O	022047-25-2	9





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Instrument :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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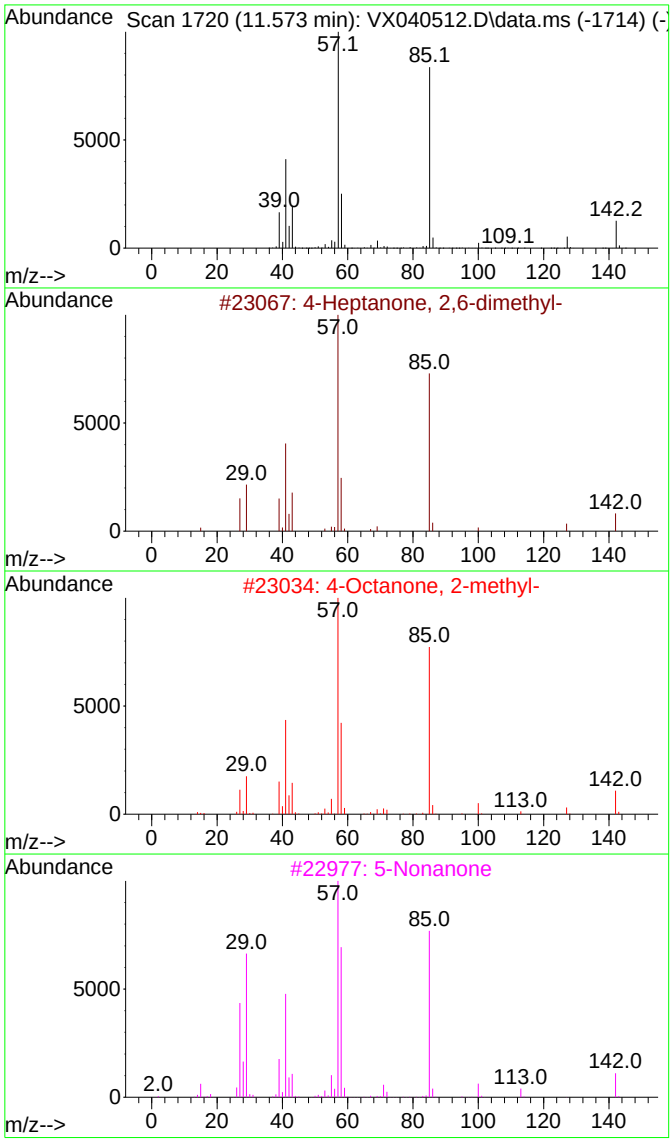
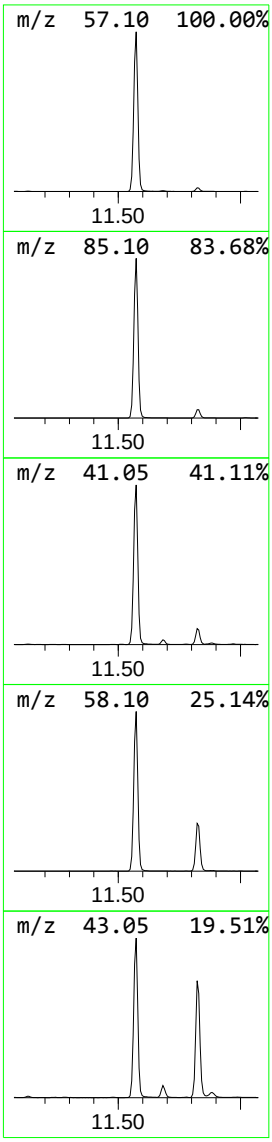
****
Peak Number 2 4-Heptanone, 2,6-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	705.34 ug/l	6652210	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	80
3	5-Nonanone	142	C9H18O	000502-56-7	64
4	t-Butyl isobutyl ketone	142	C9H18O	014705-50-1	59
5	Allyl isovalerate	142	C8H14O2	002835-39-4	59





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

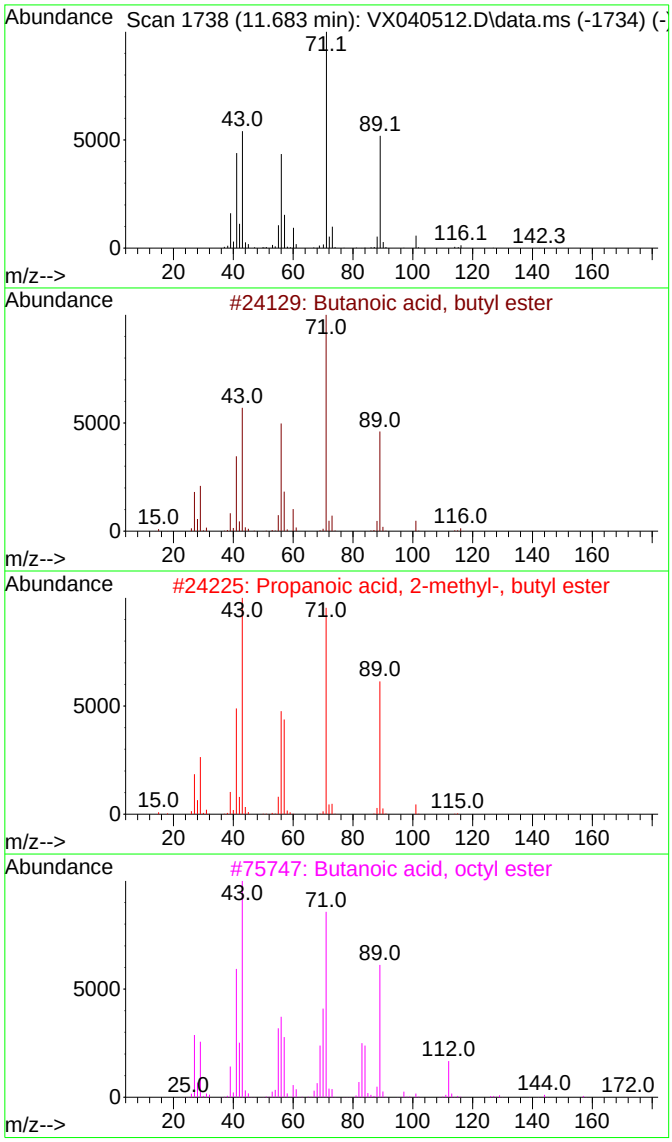
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

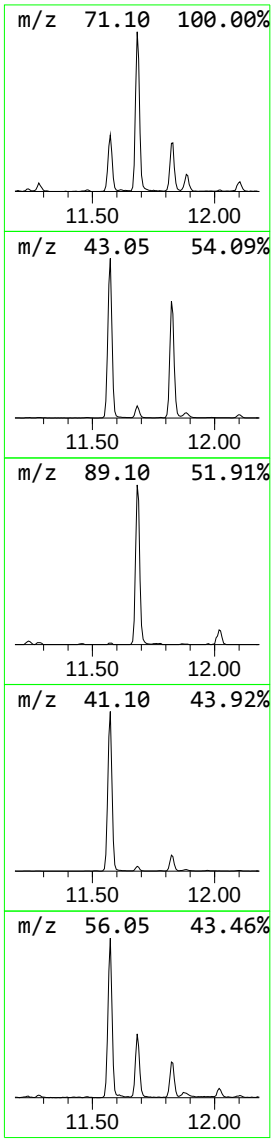
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	21.64 ug/l	204100	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	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
3	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

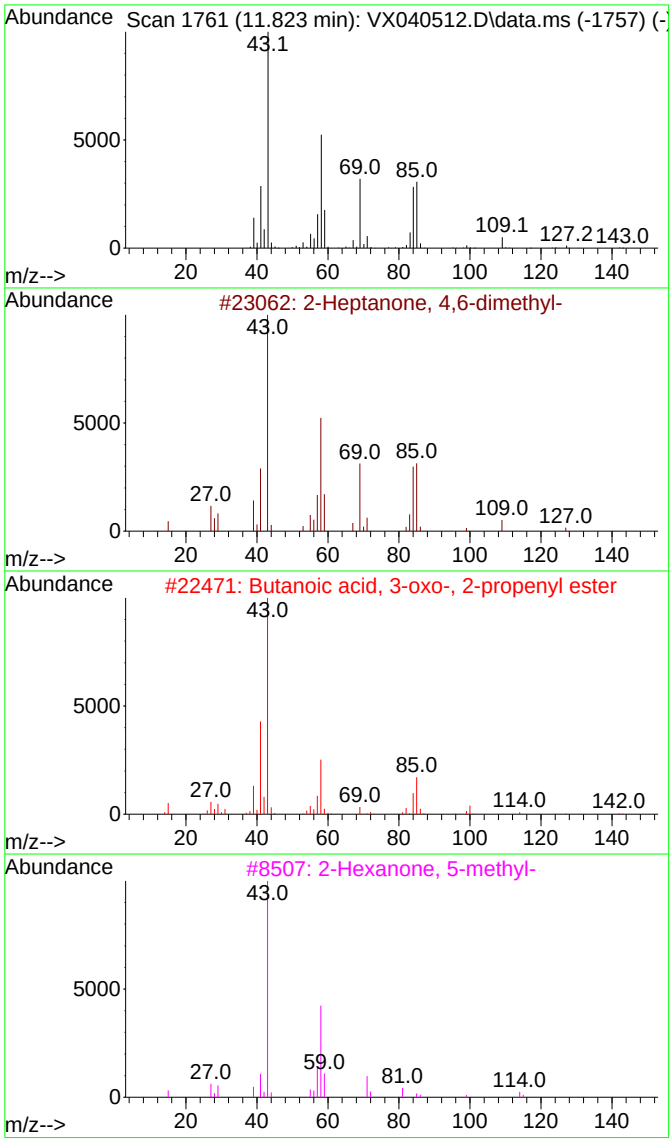
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

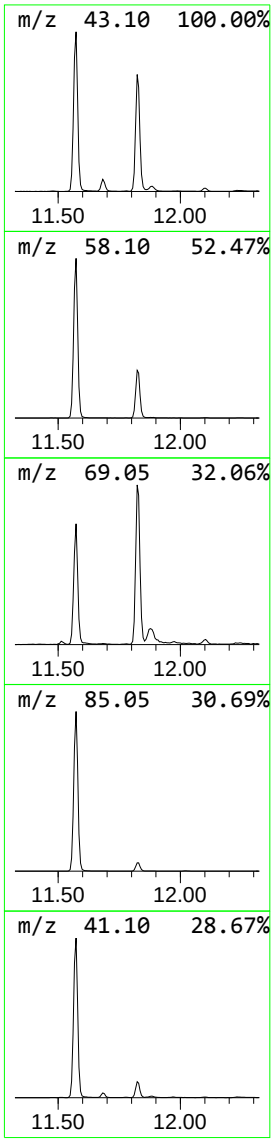
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.823	114.80 ug/l	1082740	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	90
2	Butanoic acid, 3-oxo-, 2-propeny...	142	C7H10O3	001118-84-9	64
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	50
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	43
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	43





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

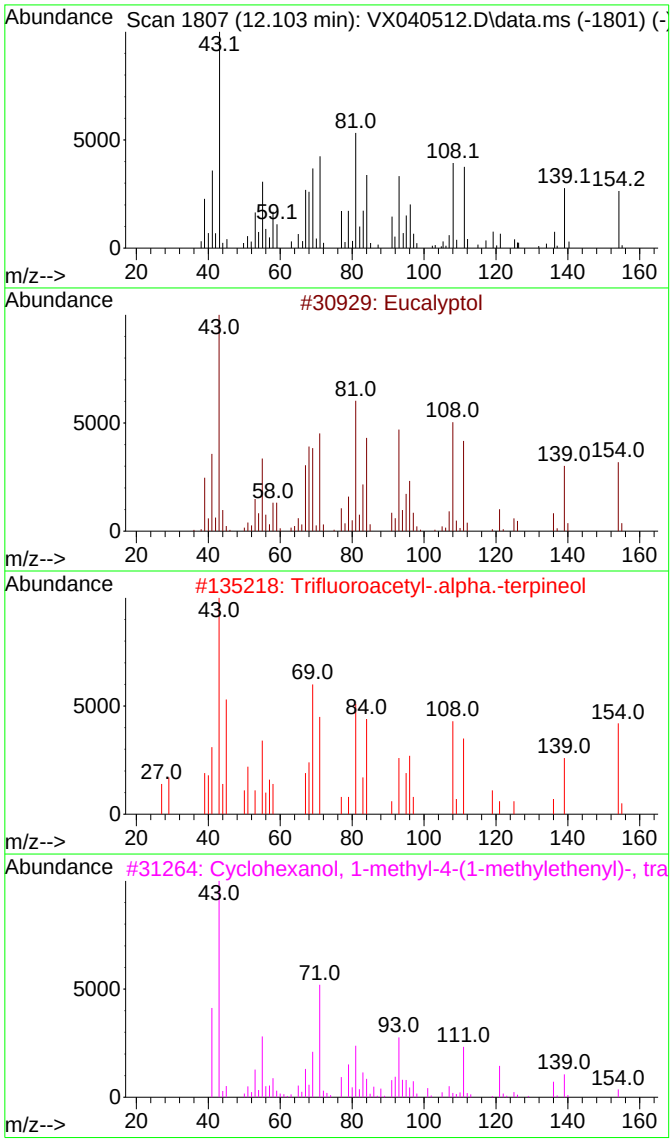
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

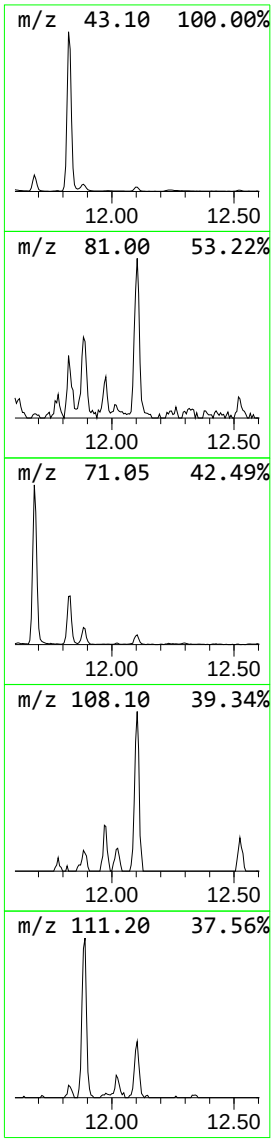
****

Peak Number 5 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	7.96 ug/l	75063	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	98
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	42
3	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	32
4	1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	27
5	7-Oxabicyclo[2.2.1]heptane, 1-me...	154	C10H18O	000470-67-7	27





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
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TIC Library : C:\Database\NIST20.L
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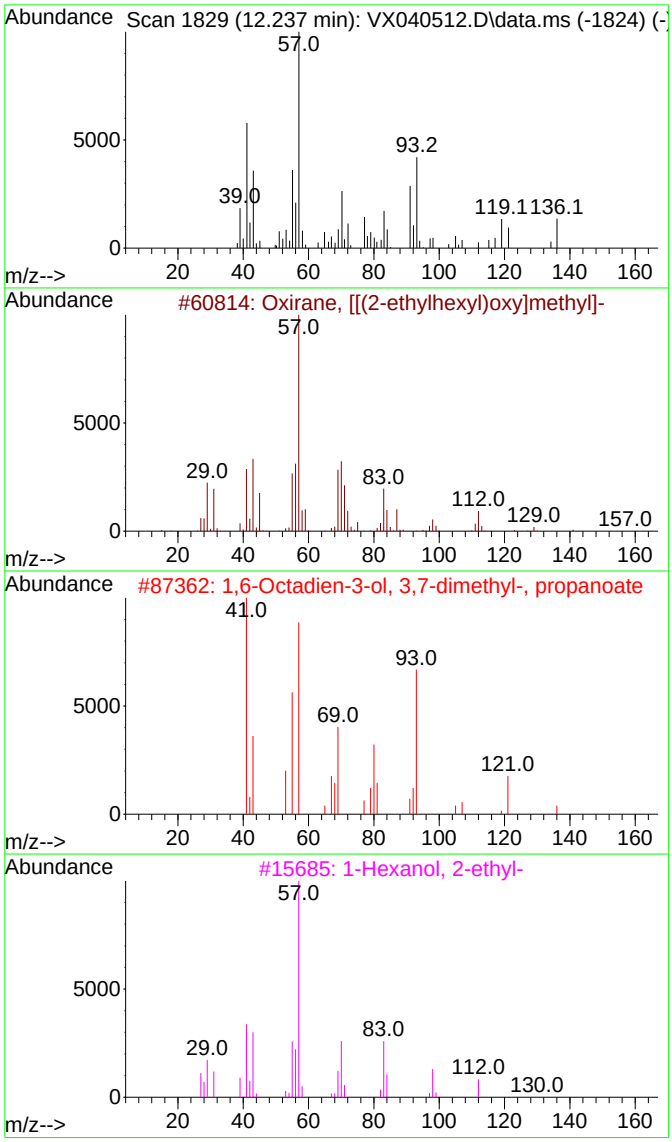
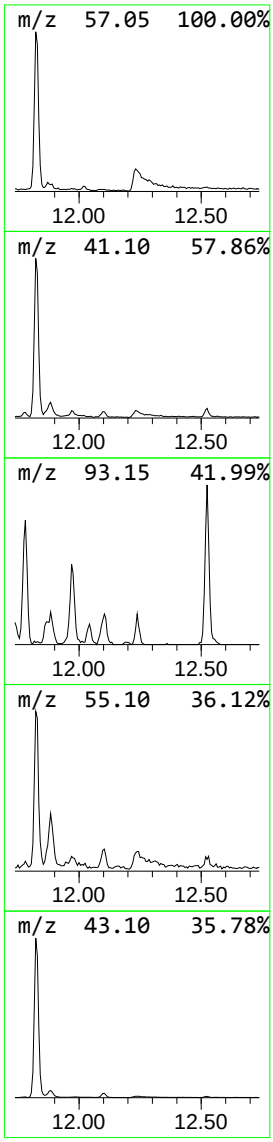
****
Peak Number 6 unknown12.238 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.238	7.21 ug/l	67999	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	35
2	1,6-Octadien-3-ol, 3,7-dimethyl-...	210	C13H22O2	000144-39-8	25
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	22
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	22
5	2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	22





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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

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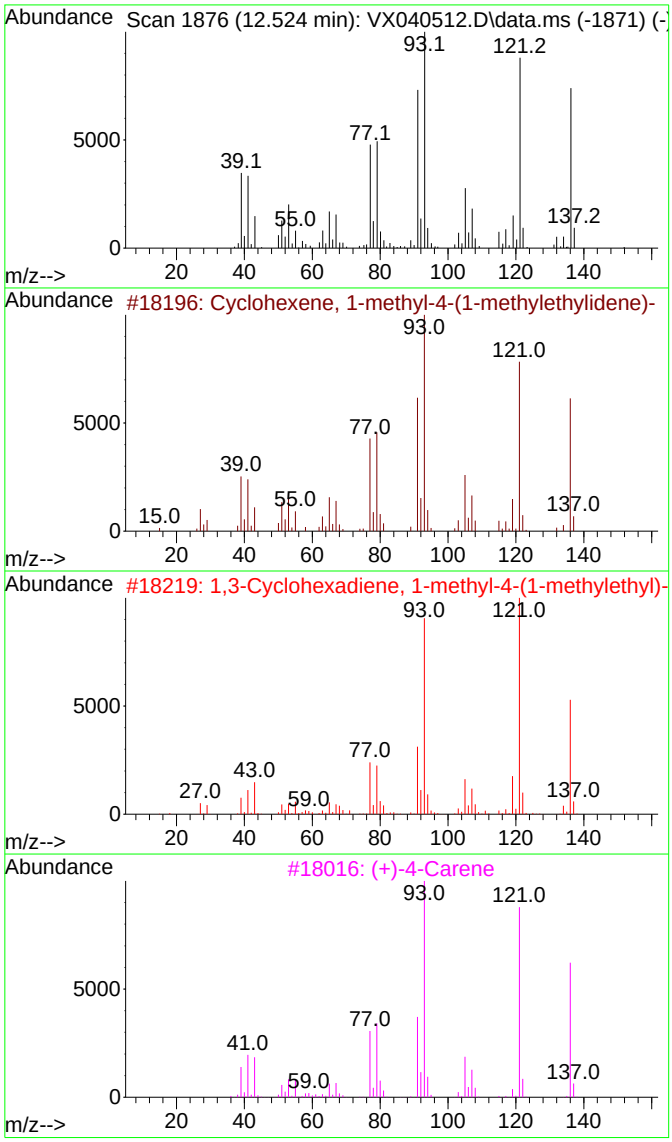
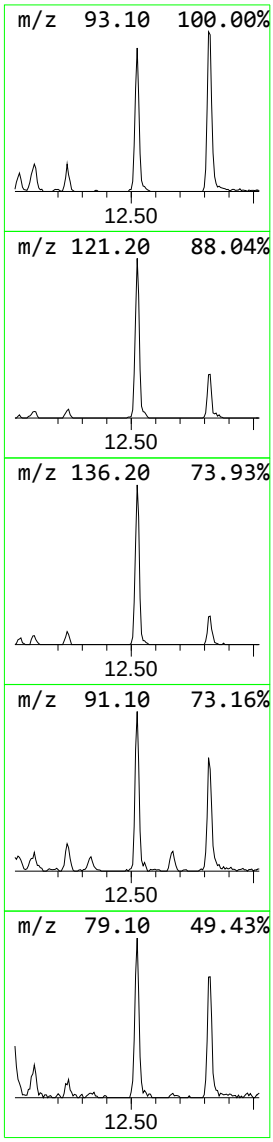
****
Peak Number 7 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.524	11.46 ug/l	108073	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	98
2	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	97
3	(+)-4-Carene	136	C10H16	029050-33-7	95
4	Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	94
5	3-Carene	136	C10H16	013466-78-9	91





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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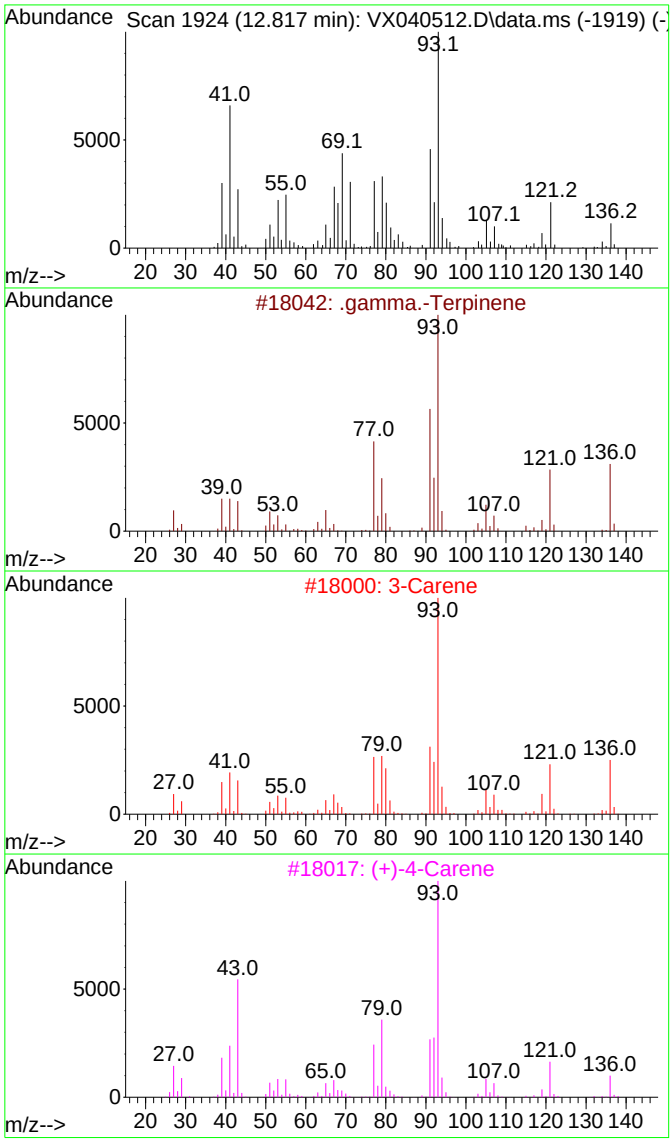
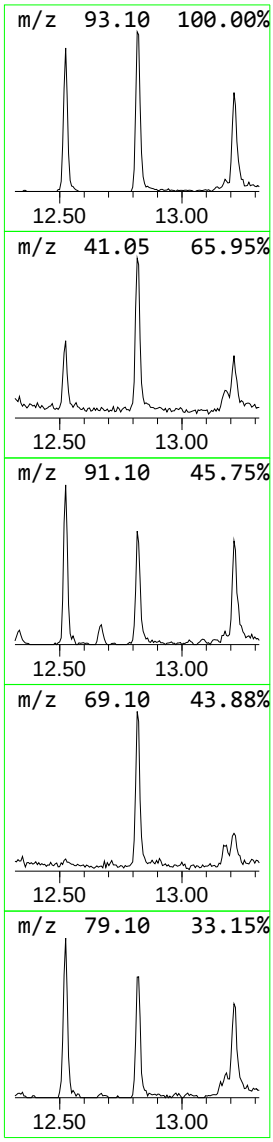
****
Peak Number 8 .gamma.-Terpinene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	13.17 ug/l	124247	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Terpinene	136	C10H16	000099-85-4	93
2	3-Carene	136	C10H16	013466-78-9	93
3	(+)-4-Carene	136	C10H16	029050-33-7	83
4	Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	76
5	Cyclopentene, 3-isopropenyl-5,5-...	136	C10H16	1000162-25-4	76





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

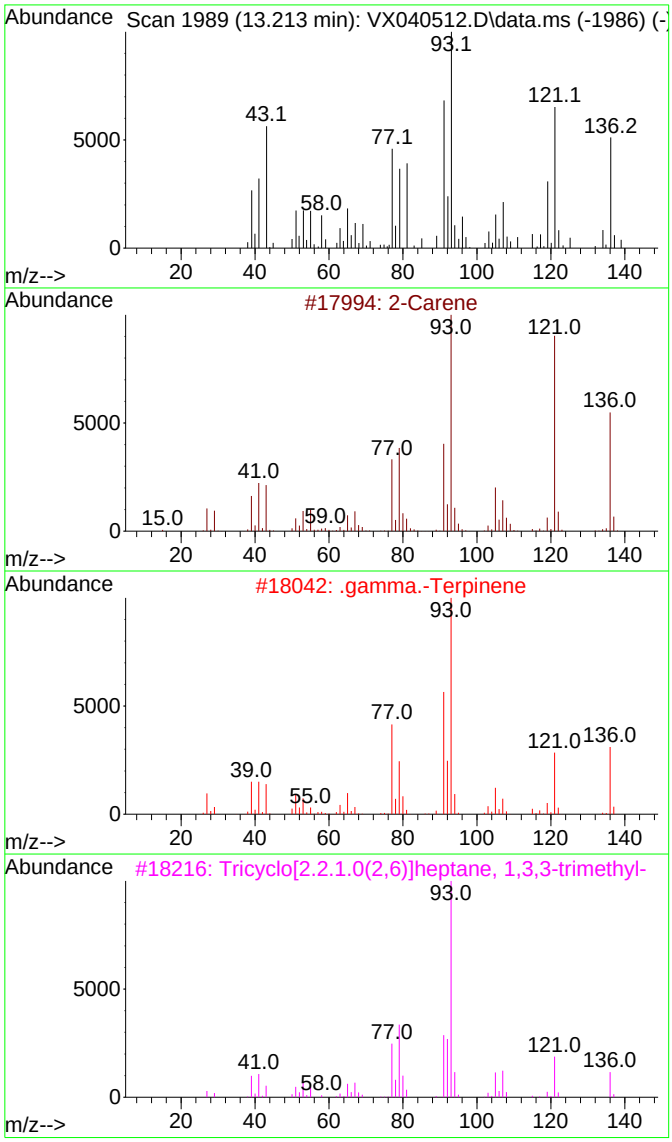
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

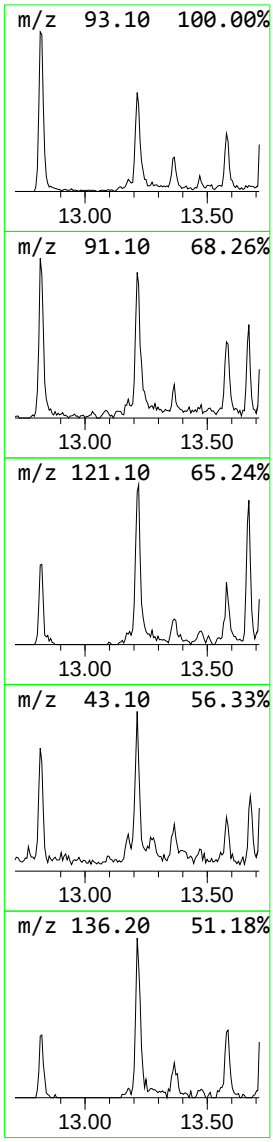
****

Peak Number 9 2-Carene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	10.06 ug/l	94876	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Carene	136	C10H16	000554-61-0	93
2	.gamma.-Terpinene	136	C10H16	000099-85-4	93
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	90
4	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	90
5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040512.D
Acq On : 28 Feb 2024 15:40
Operator : JC/MD
Sample : P1613-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

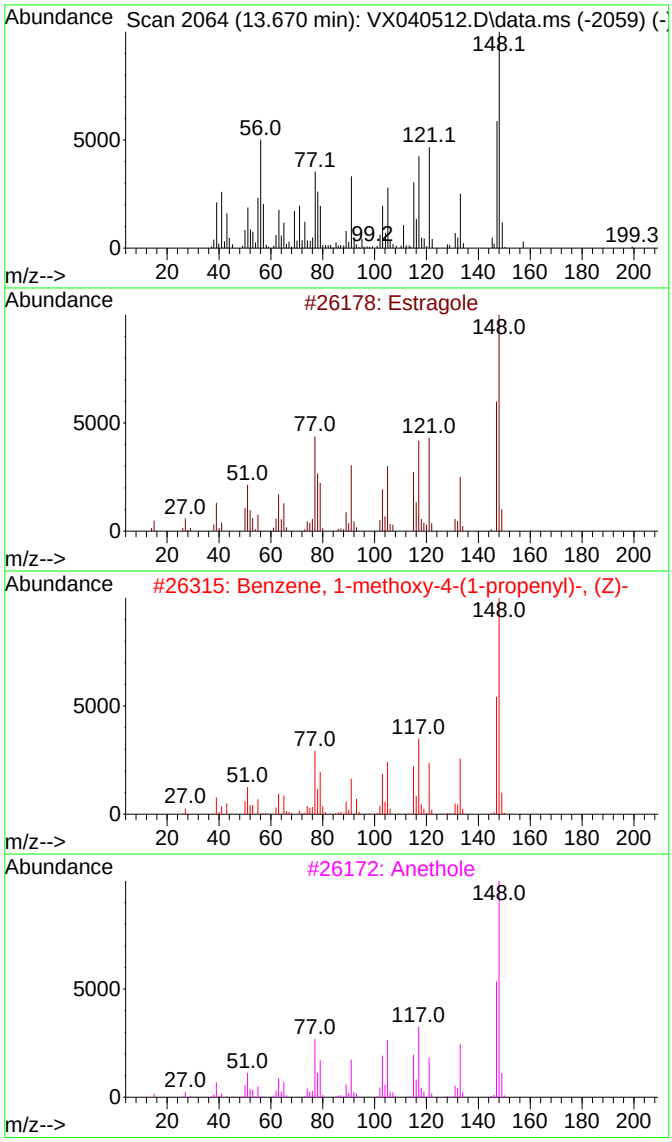
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.M
Quant Title : SW846 8260

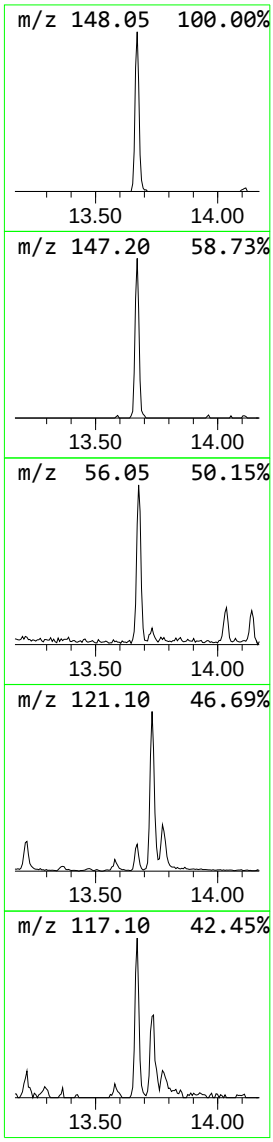
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Estragole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.670	12.87 ug/l	121386	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Estragole	148	C10H12O	000140-67-0	99
2	Benzene, 1-methoxy-4-(1-propenyl...	148	C10H12O	025679-28-1	98
3	Anethole	148	C10H12O	000104-46-1	96
4	Anethole	148	C10H12O	004180-23-8	96
5	5-Methoxyindane	148	C10H12O	1000342-73-8	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022824\
Data File : VX040512.D
Acq On : 28 Feb 2024 15:40
Operator : JC/MD
Sample : P1613-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1849

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022624W.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
Propane, 1-bromo-	4.806	16.6	ug/l	77798	1	5.556	233943	50.0
4-Heptanone, 2,...	11.573	705.3	ug/l	6652210	4	12.024	471561	50.0
Butanoic acid, ...	11.683	21.6	ug/l	204100	4	12.024	471561	50.0
2-Heptanone, 4,...	11.823	114.8	ug/l	1082740	4	12.024	471561	50.0
Eucalyptol	12.103	8.0	ug/l	75063	4	12.024	471561	50.0
unknown12.238	12.238	7.2	ug/l	67999	4	12.024	471561	50.0
Cyclohexene, 1-...	12.524	11.5	ug/l	108073	4	12.024	471561	50.0
.gamma.-Terpinene	12.817	13.2	ug/l	124247	4	12.024	471561	50.0
2-Carene	13.213	10.1	ug/l	94876	4	12.024	471561	50.0
Estragole	13.670	12.9	ug/l	121386	4	12.024	471561	50.0