LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031623\
Data File : VX034553.D
Acq On : 16 Mar 2023 18:09
Operator : JC/MD
Sample : 01945-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034553.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	24	27	41	rVB2	258392	429606	4.89%	1.201%
2	2.386	206	213	222	rBV2	77248	144500	1.65%	0.404%
3	2.959	297	307	325	rBV	4060310	8783055	100.00%	24.562%
4	4.574	550	572	584	rBV	2538126	8035755	91.49%	22.472%
5	5.001	631	642	663	rVB	1350054	4089967	46.57%	11.438%
6	5.385	695	705	719	rBV	141664	416187	4.74%	1.164%
7	5.550	721	732	750	rVB	247253	711749	8.10%	1.990%
8	5.952	788	798	806	rBV	170102	453097	5.16%	1.267%
9	6.172	826	834	839	rBV2	44994	149439	1.70%	0.418%
10	6.226	839	843	854	rVB	72244	191267	2.18%	0.535%
11	6.757	921	930	944	rBV	385404	941813	10.72%	2.634%
12	8.647	1233	1240	1246	rBV	830379	1280874	14.58%	3.582%
13	8.714	1246	1251	1260	rVB2	101886	182214	2.07%	0.510%
14	8.805	1260	1266	1271	rBV	100063	169166	1.93%	0.473%
15	9.378	1351	1360	1366	rBV	250266	387982	4.42%	1.085%
16	10.055	1460	1471	1483	rBV	827616	1305751	14.87%	3.652%
17	10.299	1506	1511	1518	rVV	244294	353453	4.02%	0.988%
18	10.384	1518	1525	1533	rVB3	43528	90538	1.03%	0.253%
19	10.640	1562	1567	1572	rBV	160457	212794	2.42%	0.595%
20	11.079	1633	1639	1645	rBV	706777	933467	10.63%	2.610%
21	11.750	1745	1749	1753	rVB	92704	115480	1.31%	0.323%
22	11.884	1764	1771	1778	rVB	117607	171112	1.95%	0.479%
23	12.024	1787	1794	1800	rVB	791174	1161296	13.22%	3.248%
24	12.103	1800	1807	1811	rBV2	313546	473783	5.39%	1.325%
25	12.244	1824	1830	1834	rBV	73486	105670	1.20%	0.296%
26	12.524	1872	1876	1881	rBV3	72888	134091	1.53%	0.375%
27	12.579	1881	1885	1895	rVB	177042	253485	2.89%	0.709%
28	12.768	1910	1916	1920	rVB2	201685	291423	3.32%	0.815%
29	12.902	1927	1938	1944	rBV	1327679	1815040	20.67%	5.076%
30	12.963	1944	1948	1960	rVB2	135146	253613	2.89%	0.709%
31	13.335	2005	2009	2013	rBV2	100686	136273	1.55%	0.381%
32	13.475	2027	2032	2037	rBV4	251012	423824	4.83%	1.185%
33	13.591	2045	2051	2061	rBV2	588131	1044125	11.89%	2.920%
34	13.920	2100	2105	2114	rVB5	55688	116543	1.33%	0.326%

Sum of corrected areas: 35758432

Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

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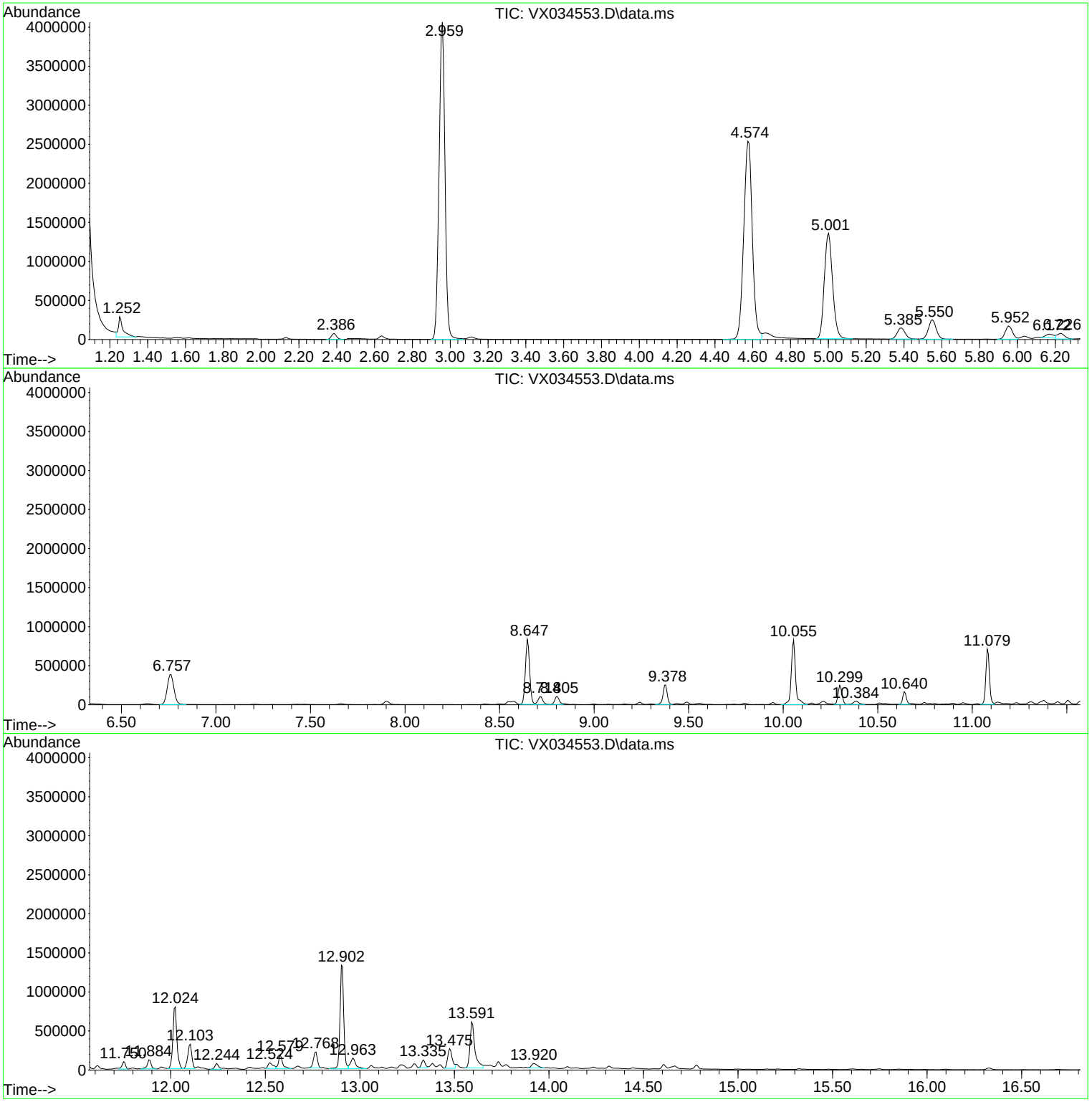
Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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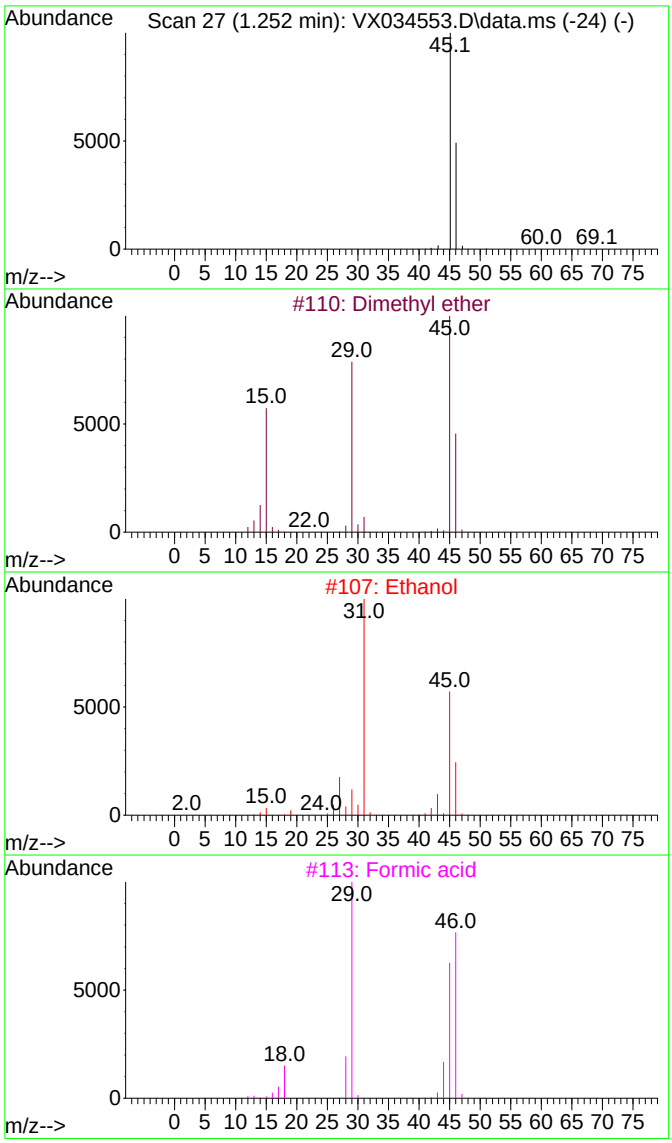
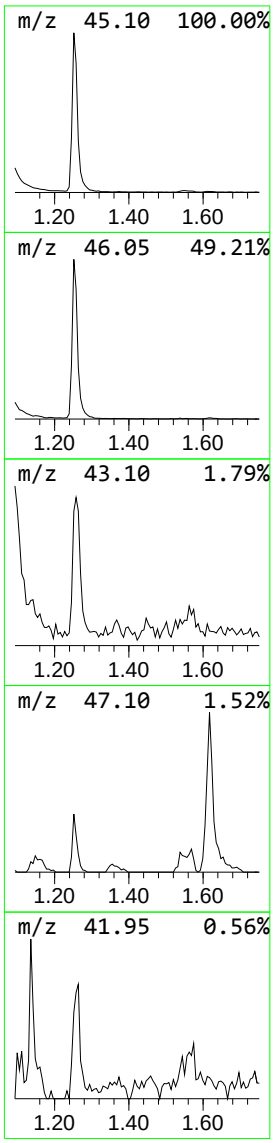
****

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	30.18 ug/l	429606	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	64
2	Ethanol	46	C2H6O	000064-17-5	7
3	Formic acid	46	CH2O2	000064-18-6	7
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





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Data File : VX034553.D
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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

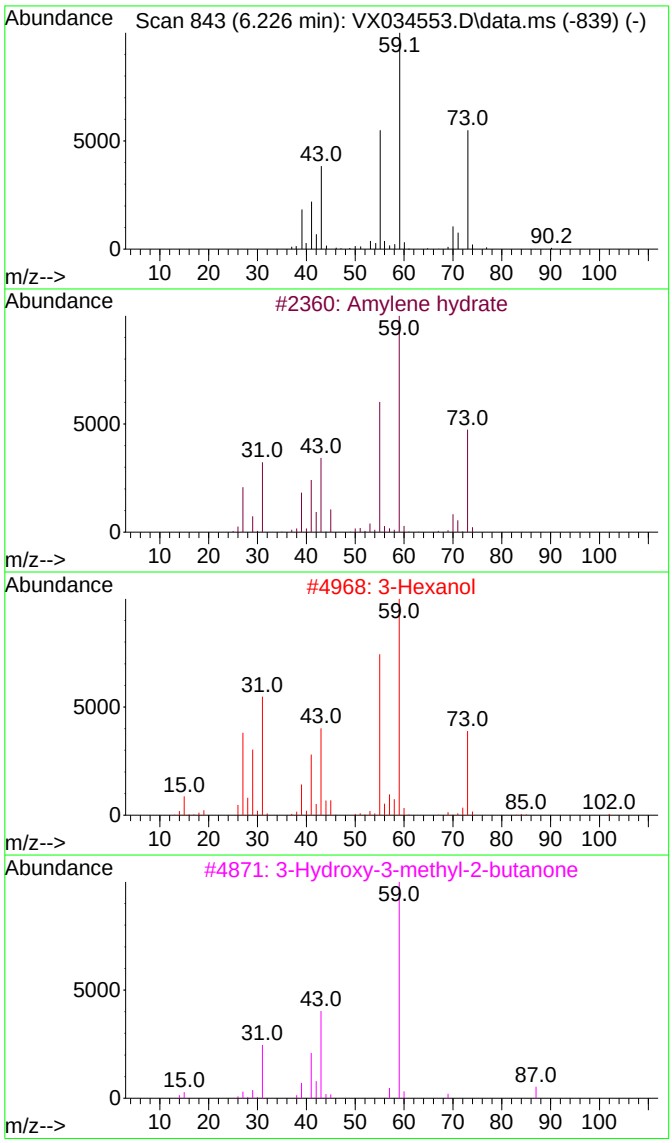
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

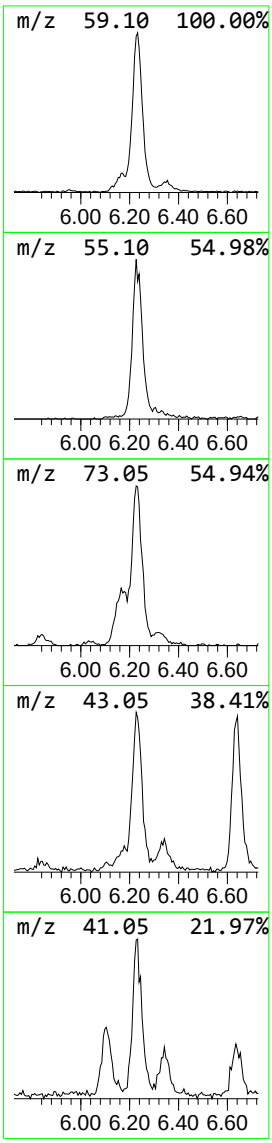
****

Peak Number 2 Amylene hydrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.226	10.15 ug/l	191267	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	78
2	3-Hexanol	102	C6H14O	000623-37-0	40
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	38
5	Carbonic acid, 3-pentyl propyl e...	174	C9H18O3	1000325-64-0	36





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ALS Vial : 23 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
230315025-02-VOA

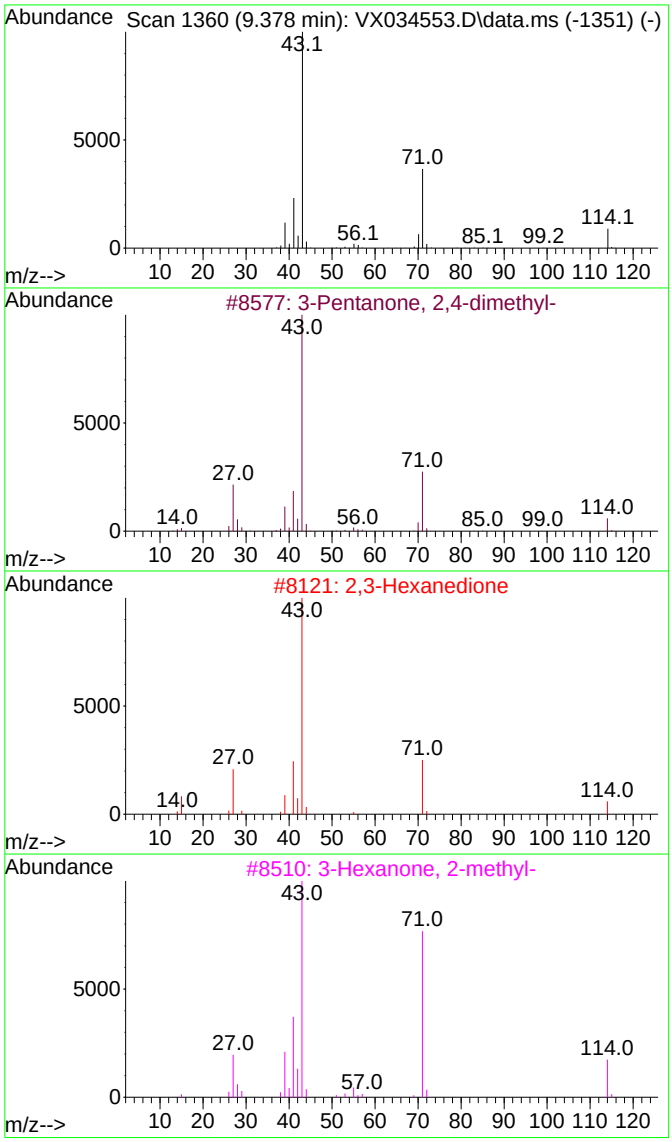
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

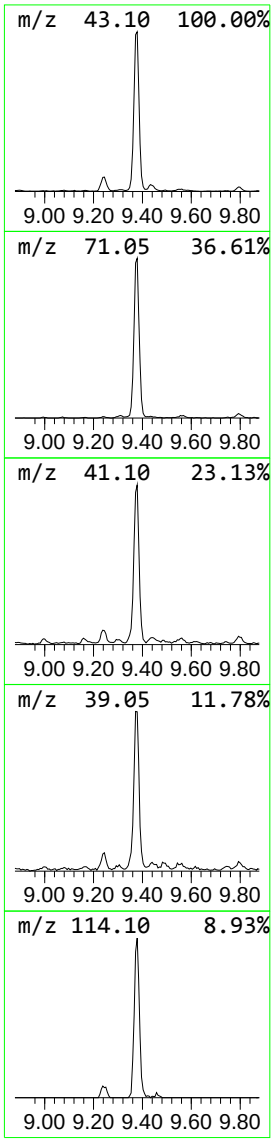
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	14.86 ug/l	387982	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	86
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	52
4	4-Heptanone	114	C7H14O	000123-19-3	50
5	2,5-Hexanedione	114	C6H10O2	000110-13-4	42





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MSVOA_X
ClientSampleId :
230315025-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

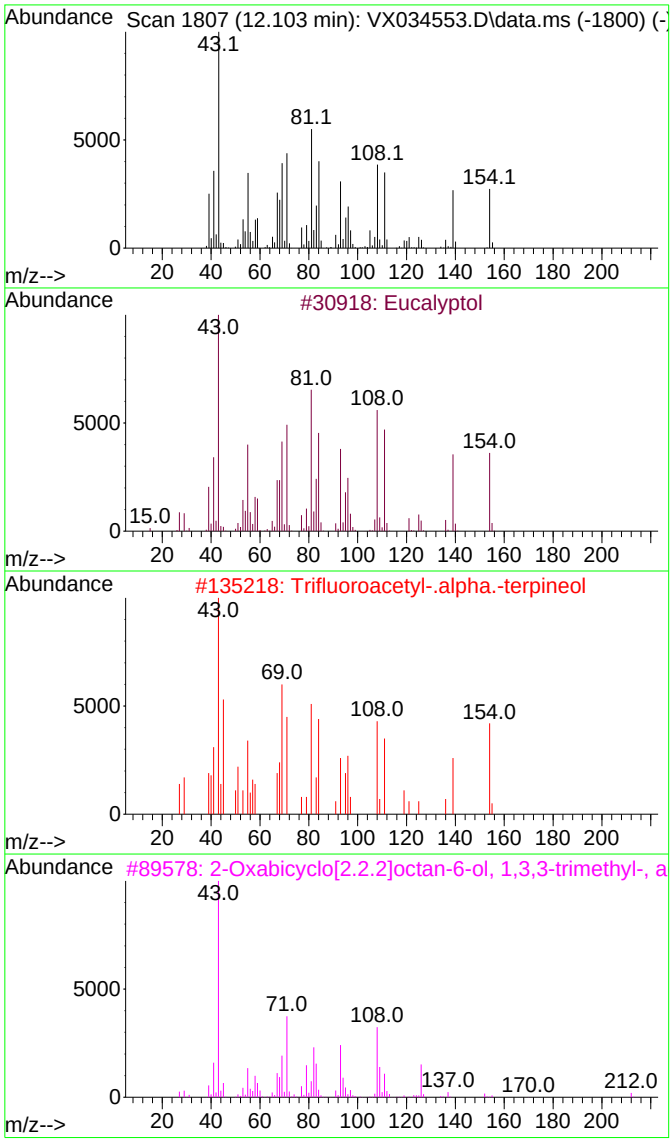
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

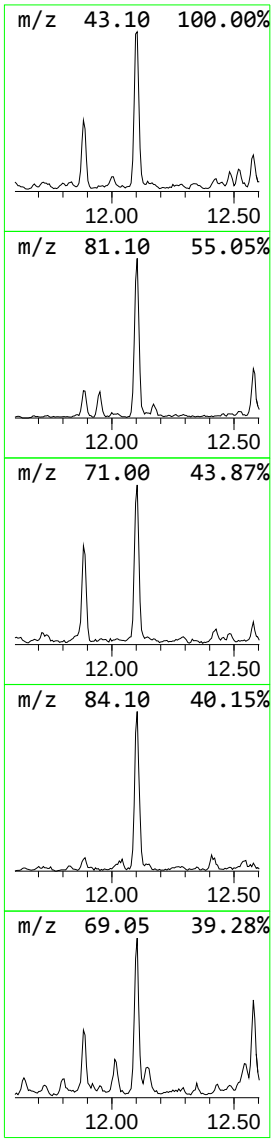
****

Peak Number 4 Eucalyptol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	20.40 ug/l	473783	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	43
3	2-Oxabicyclo[2.2.2]octan-6-ol, 1...	212	C12H20O3	057709-95-2	37
4	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	16
5	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	14





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

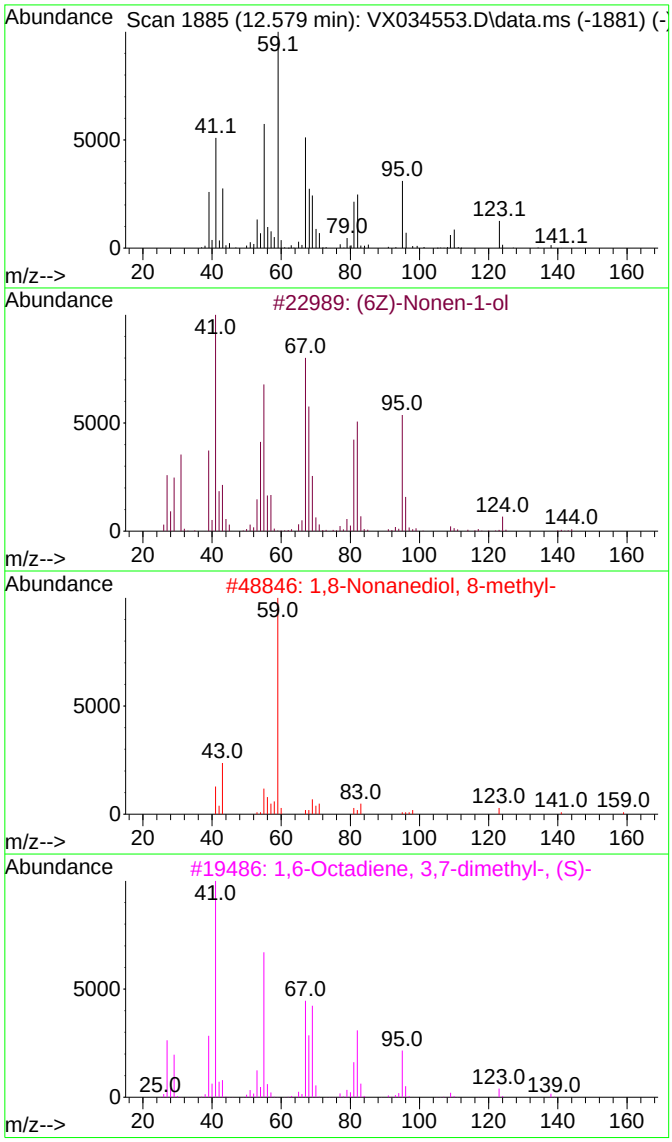
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

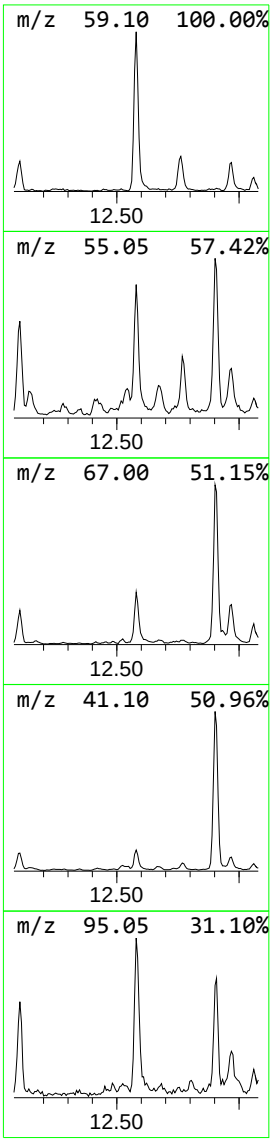
****

Peak Number 5 unknown12.579 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.579	10.91 ug/l	253485	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6Z)-Nonen-1-ol	142	C9H18O	035854-86-5	38
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38
3	1,6-Octadiene, 3,7-dimethyl-, (S)-	138	C10H18	010281-55-7	35
4	Bicyclo[2.2.1]heptane, 2-methyl-...	110	C8H14	000872-78-6	35
5	Cyclooctane, ethenyl-	138	C10H18	061142-41-4	35





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Instrument :
MSVOA_X
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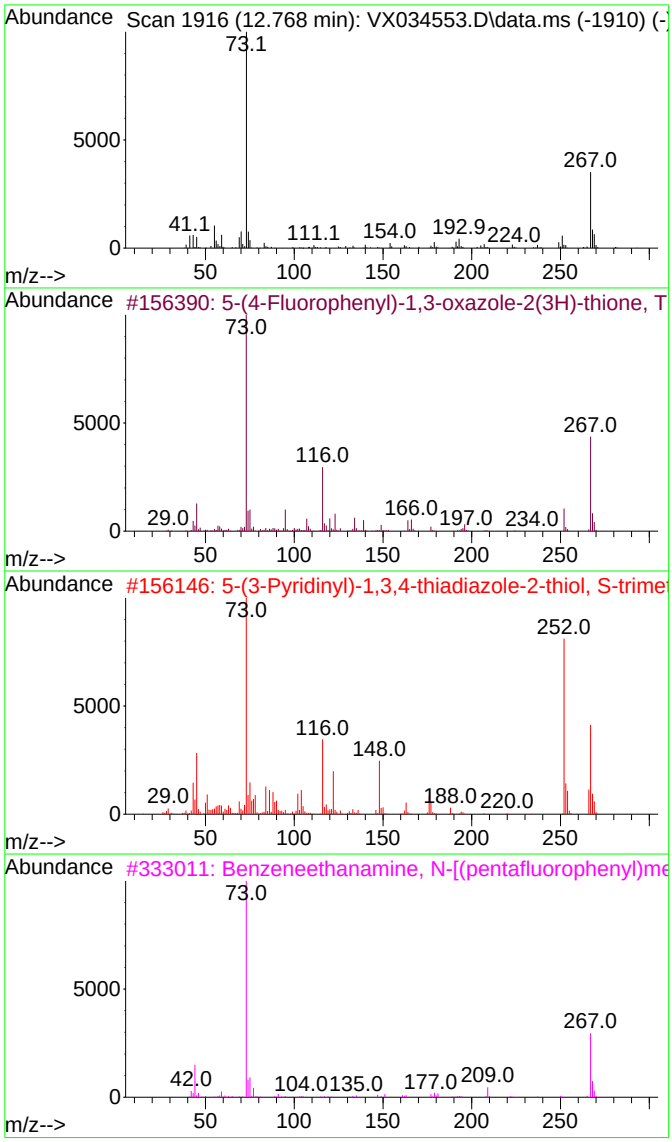
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

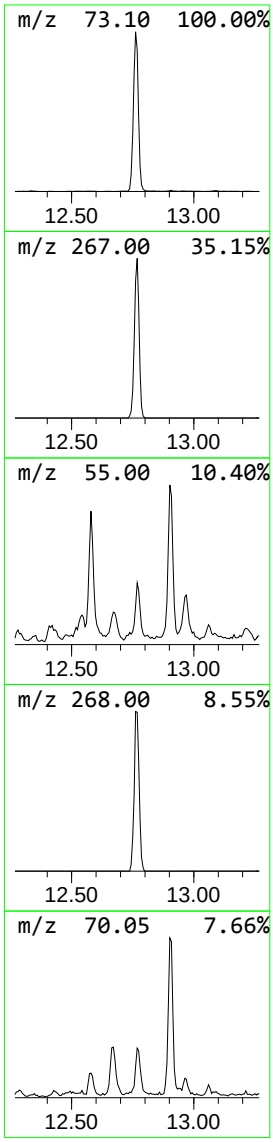
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 5-(4-Fluorophenyl)-1,3-oxaz... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	12.55 ug/l	291423	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	50
2	5-(3-Pyridinyl)-1,3,4-thiadiazol...	267	C10H13N3S2Si	1000471-43-6	40
3	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	40
4	Benzeneethanamine, N-methyl-.bet...	311	C15H29NO2Si2	029522-18-7	39
5	Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	36





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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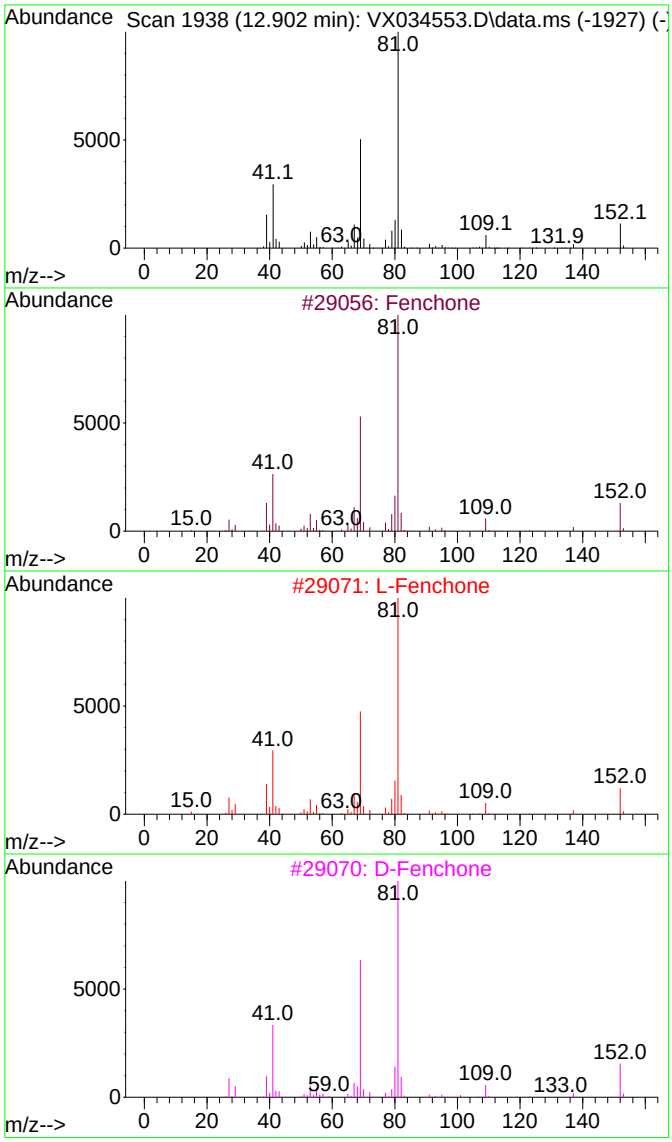
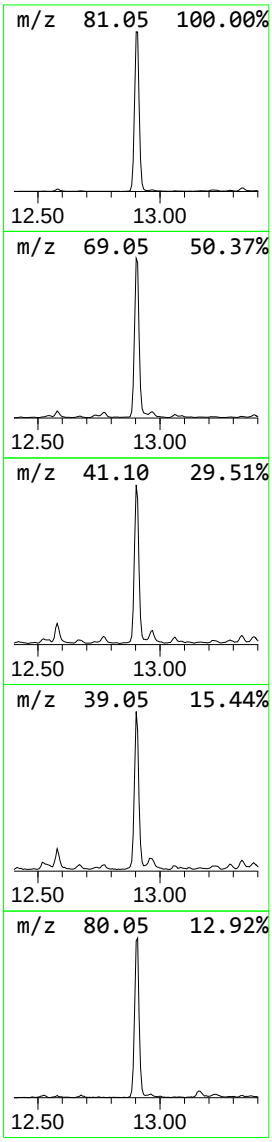
****
Peak Number 7 Fenchone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.902	78.15 ug/l	1815040	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchone	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	95
3	D-Fenchone	152	C10H16O	004695-62-9	91
4	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	59
5	Cyclohexane, 1,3-dichloro-, cis-	152	C6H10Cl2	024955-63-3	45





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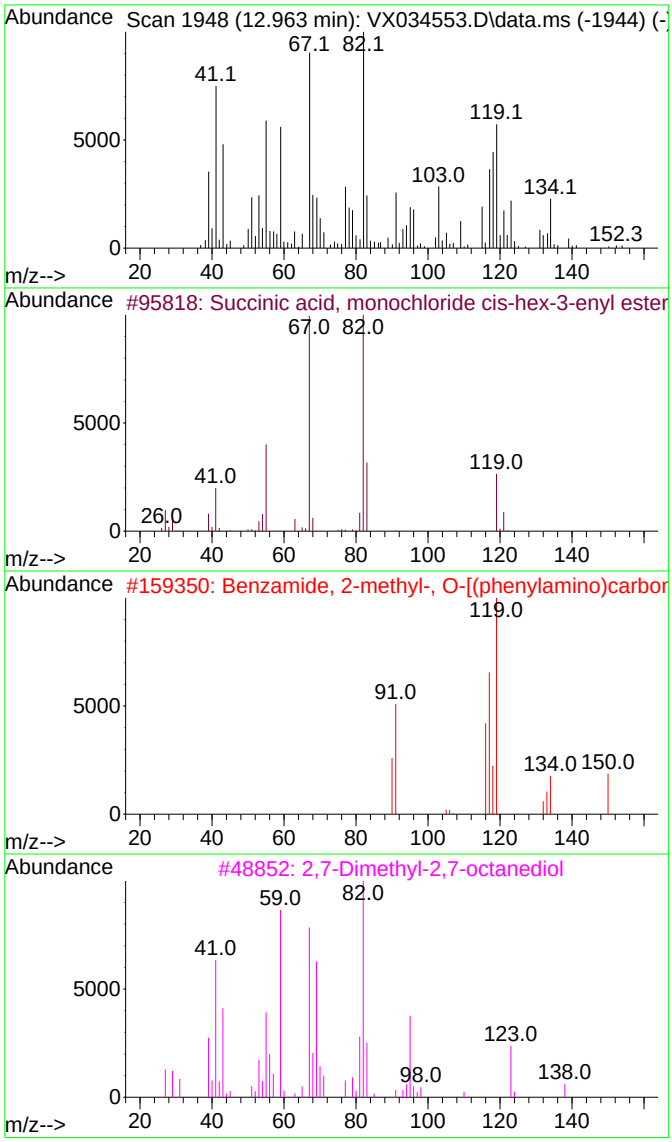
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

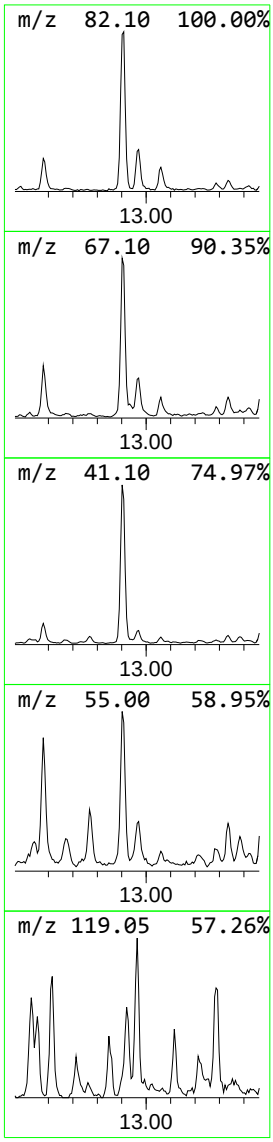
****

Peak Number 8 unknown12.963 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.963	10.92 ug/l	253613	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, monochloride cis-...	218	C10H15ClO3	1010353-42-3	43
2	Benzamide, 2-methyl-, O-[(phenyl...	269	C15H15N3O2	1010112-26-4	35
3	2,7-Dimethyl-2,7-octanediol	174	C10H22O2	019781-07-8	35
4	Hexenyl angelate, 4z-	182	C11H18O2	1000383-63-7	27
5	1,5-Cyclooctadiene, 1,2-dimethyl-	136	C10H16	006588-51-8	27





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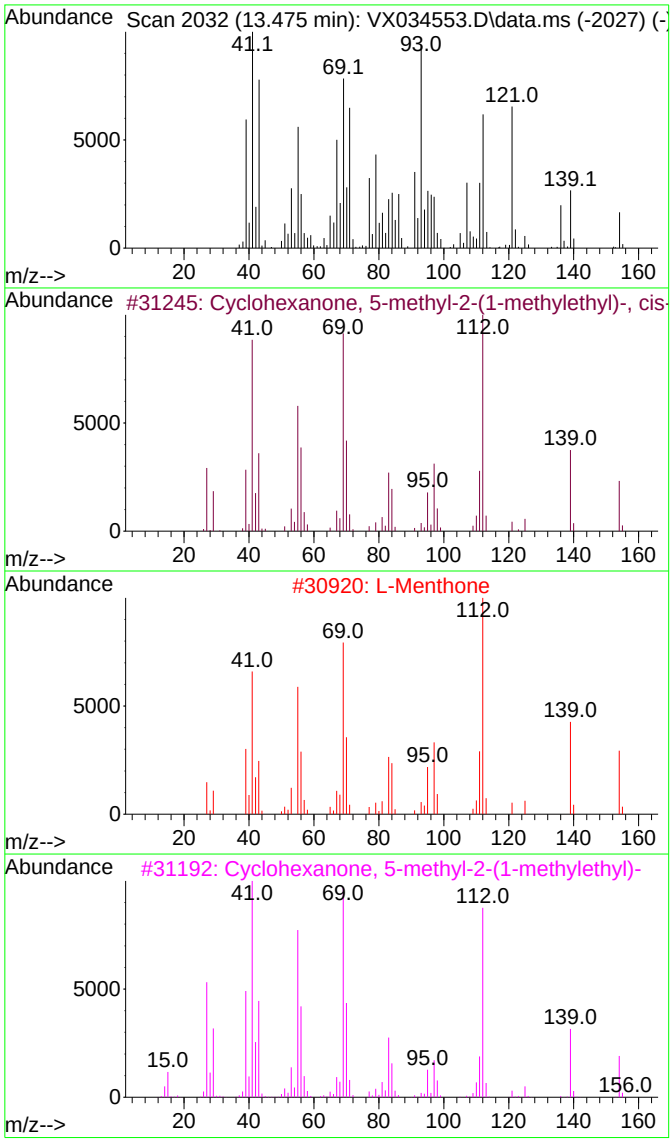
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

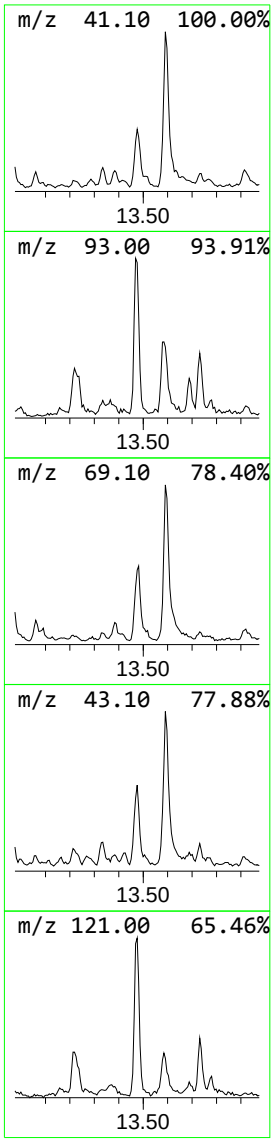
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexanone, 5-methyl-2-(... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	18.25 ug/l	423824	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	90
2	L-Menthone	154	C10H18O	014073-97-3	87
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	83
4	Camphene	136	C10H16	000079-92-5	78
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031623\
Data File : VX034553.D
Acq On : 16 Mar 2023 18:09
Operator : JC/MD
Sample : 01945-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

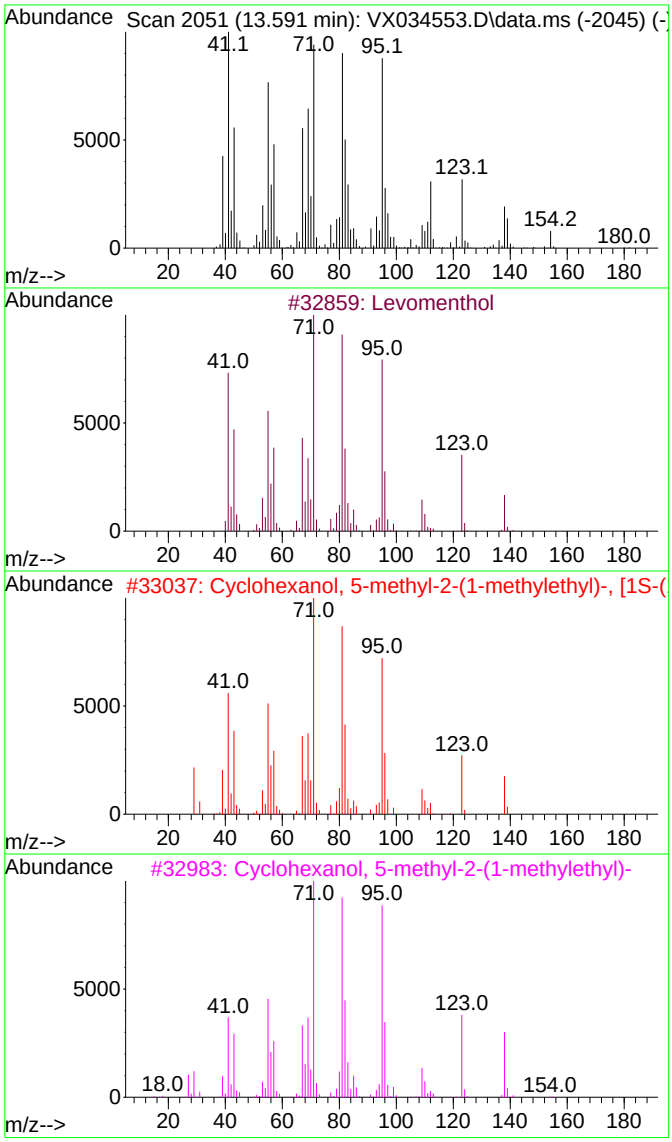
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

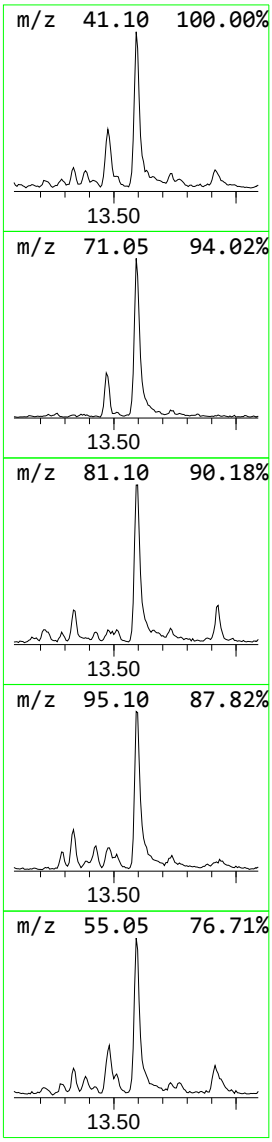
****

Peak Number 10 Levomenthol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	44.96 ug/l	1044130	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levomenthol	156	C10H20O	002216-51-5	90
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	86
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	83
4	dl-Menthol	156	C10H20O	000089-78-1	80
5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031623\
Data File : VX034553.D
Acq On : 16 Mar 2023 18:09
Operator : JC/MD
Sample : 01945-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
230315025-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
Dimethyl ether	1.252	30.2	ug/l	429606	1	5.550	711749	50.0
Amylene hydrate	6.226	10.2	ug/l	191267	2	6.763	941813	50.0
3-Pentanone, 2,...	9.378	14.9	ug/l	387982	3	10.055	1305750	50.0
Eucalyptol	12.103	20.4	ug/l	473783	4	12.024	1161300	50.0
unknown12.579	12.579	10.9	ug/l	253485	4	12.024	1161300	50.0
5-(4-Fluorophen...	12.768	12.6	ug/l	291423	4	12.024	1161300	50.0
Fenchone	12.902	78.2	ug/l	1815040	4	12.024	1161300	50.0
unknown12.963	12.963	10.9	ug/l	253613	4	12.024	1161300	50.0
Cyclohexanone, ...	13.475	18.3	ug/l	423824	4	12.024	1161300	50.0
Levomenthol	13.591	45.0	ug/l	1044130	4	12.024	1161300	50.0