LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-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_N\methods\82N070824W.M
Title : SW846 8260

Signal : TIC: VN082878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	52	58	68	rVB	109483	181076	3.60%	0.704%
2	2.824	140	148	161	rVB4	26352	78775	1.57%	0.306%
3	4.424	405	420	436	rBV	176844	544422	10.84%	2.116%
4	4.718	459	470	478	rBV2	16315	53021	1.06%	0.206%
5	5.524	590	607	641	rBV	1446340	5023855	100.00%	19.522%
6	7.435	915	932	949	rBV	1762568	4950886	98.55%	19.238%
7	7.553	949	952	963	rVB2	30472	73807	1.47%	0.287%
8	7.835	985	1000	1022	rBV	960952	2472634	49.22%	9.608%
9	8.171	1047	1057	1061	rBV2	103770	251989	5.02%	0.979%
10	8.224	1061	1066	1077	rVB	185771	409439	8.15%	1.591%
11	8.582	1116	1127	1136	rBV2	119894	376818	7.50%	1.464%
12	8.653	1136	1139	1161	rVB6	37047	137640	2.74%	0.535%
13	9.100	1206	1215	1230	rVB	283148	571800	11.38%	2.222%
14	10.441	1434	1443	1449	rBV3	22481	57981	1.15%	0.225%
15	10.565	1457	1464	1470	rBV	419294	776769	15.46%	3.018%
16	10.635	1470	1476	1488	rVB2	117234	297720	5.93%	1.157%
17	11.170	1557	1567	1578	rVV	135188	246290	4.90%	0.957%
18	11.776	1662	1670	1675	rVV4	25884	71946	1.43%	0.280%
19	11.865	1675	1685	1695	rVV	417190	821985	16.36%	3.194%
20	11.965	1695	1702	1710	rVV	141950	272872	5.43%	1.060%
21	12.070	1710	1720	1730	rVB	126491	268410	5.34%	1.043%
22	12.400	1763	1776	1782	rBV	84424	163135	3.25%	0.634%
23	12.853	1845	1853	1861	rVB	320048	583283	11.61%	2.267%
24	13.194	1902	1911	1917	rVV6	27687	76211	1.52%	0.296%
25	13.482	1948	1960	1967	rBV2	48809	103287	2.06%	0.401%
26	13.611	1974	1982	1988	rBV2	46714	90978	1.81%	0.354%
27	13.729	1996	2002	2007	rBV	110486	171464	3.41%	0.666%
28	13.794	2007	2013	2019	rVV	425421	777658	15.48%	3.022%
29	13.859	2019	2024	2036	rVB3	164256	320453	6.38%	1.245%
30	13.994	2042	2047	2060	rVB3	27385	70053	1.39%	0.272%
31	14.247	2084	2090	2094	rBV	132049	222174	4.42%	0.863%
32	14.300	2094	2099	2108	rVB2	131484	243060	4.84%	0.944%
33	14.447	2112	2124	2132	rBV5	47198	119471	2.38%	0.464%
34	14.635	2150	2156	2157	rBV3	50924	69762	1.39%	0.271%
35	14.676	2157	2163	2169	rVV	599888	1042421	20.75%	4.051%
36	14.935	2202	2207	2215	rBV4	32180	61152	1.22%	0.238%

LSC Area Percent Report

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ALS Vial : 17 Sample Multiplier: 1

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ClientSampleId :
240710076-02-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_N\methods\82N070824W.M
Title : SW846 8260

37	15.023	2215	2222	2229	rBV10	26072	64393	1.28%	0.250%
38	15.100	2229	2235	2242	rBV	214380	364777	7.26%	1.417%
39	15.264	2257	2263	2267	rBV3	99078	241808	4.81%	0.940%
40	15.329	2267	2274	2278	rBV	1069602	2167069	43.14%	8.421%
41	15.517	2301	2306	2311	rVB	101570	165257	3.29%	0.642%
42	15.641	2321	2327	2335	rVB	156912	306841	6.11%	1.192%
43	15.758	2341	2347	2350	rBV4	27271	56948	1.13%	0.221%
44	16.011	2381	2390	2399	rVV	148495	313033	6.23%	1.216%

Sum of corrected areas: 25734823

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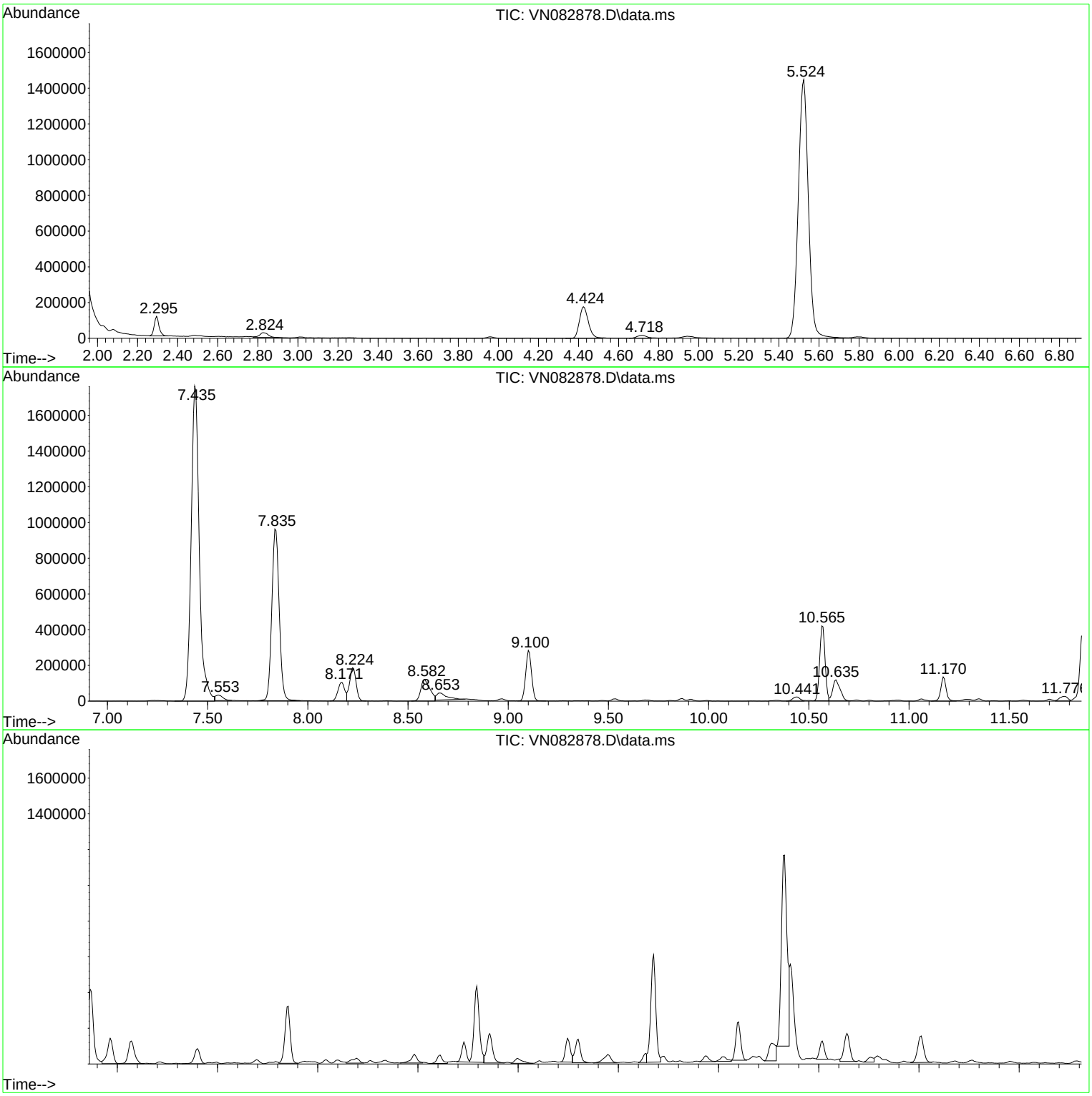
ClientSampleId :
240710076-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

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



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Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
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MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

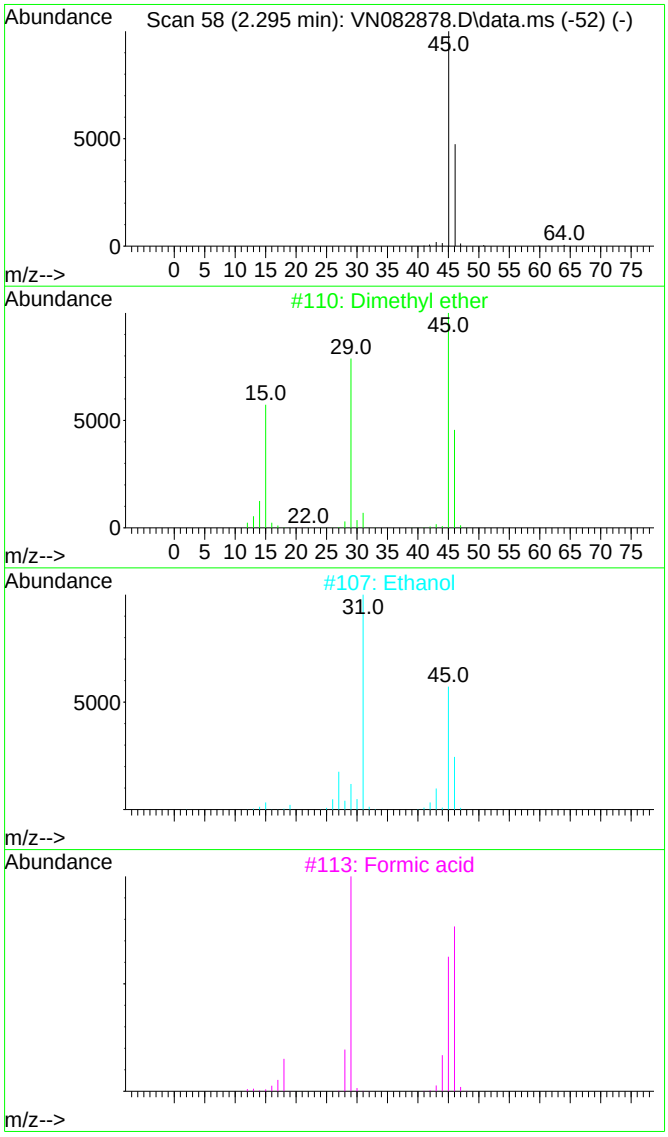
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

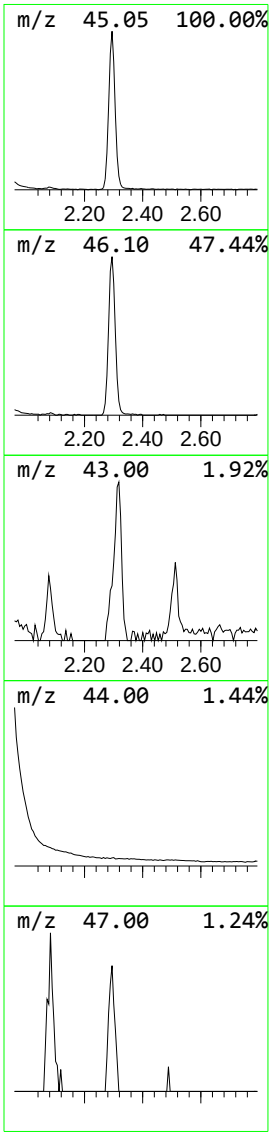
****

Peak Number 1 Dimethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	22.11 ug/l	181076	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	83
2	Ethanol	46	C2H6O	000064-17-5	9
3	Formic acid	46	CH2O2	000064-18-6	5
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





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Data File : VN082878.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

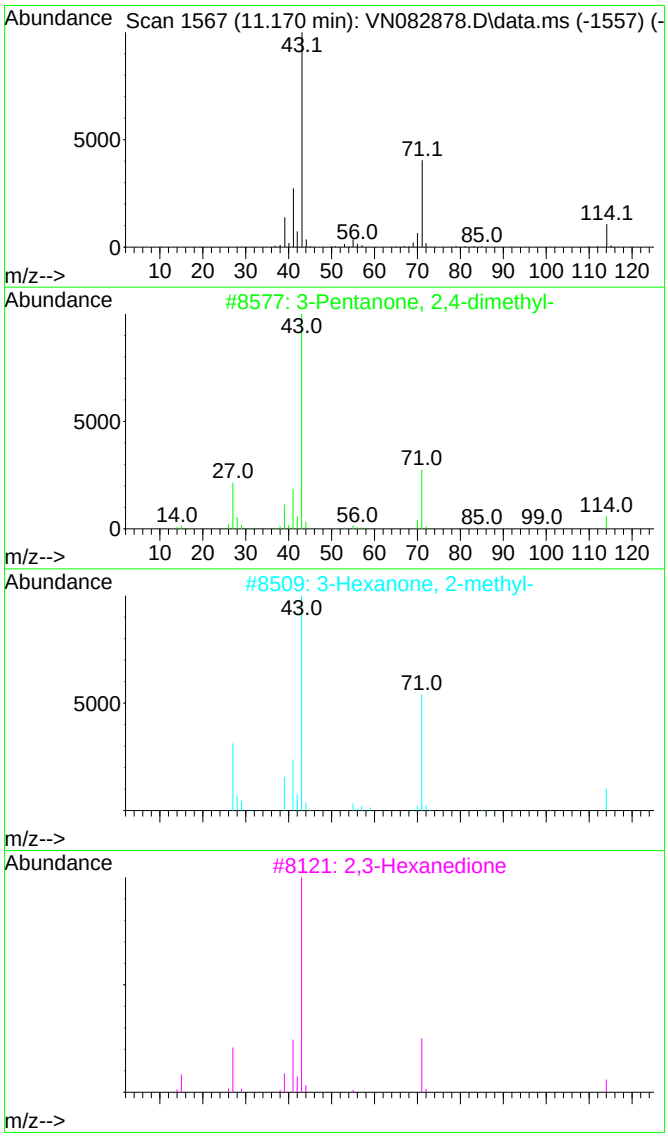
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

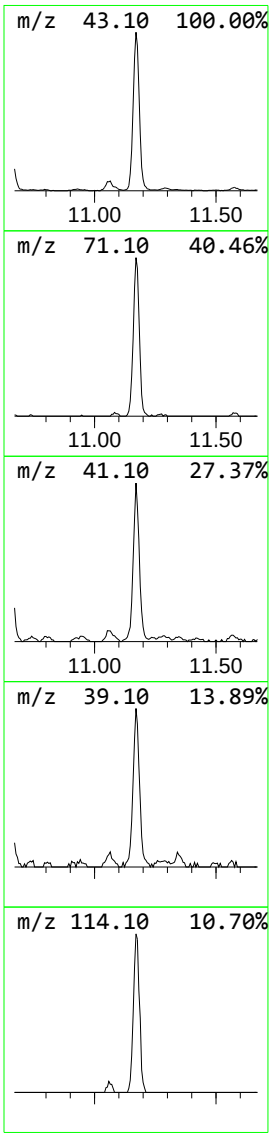
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	14.98 ug/l	246290	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	90
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
4	4-Heptanone	114	C7H14O	000123-19-3	64
5	Pyrrolidine	71	C4H9N	000123-75-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

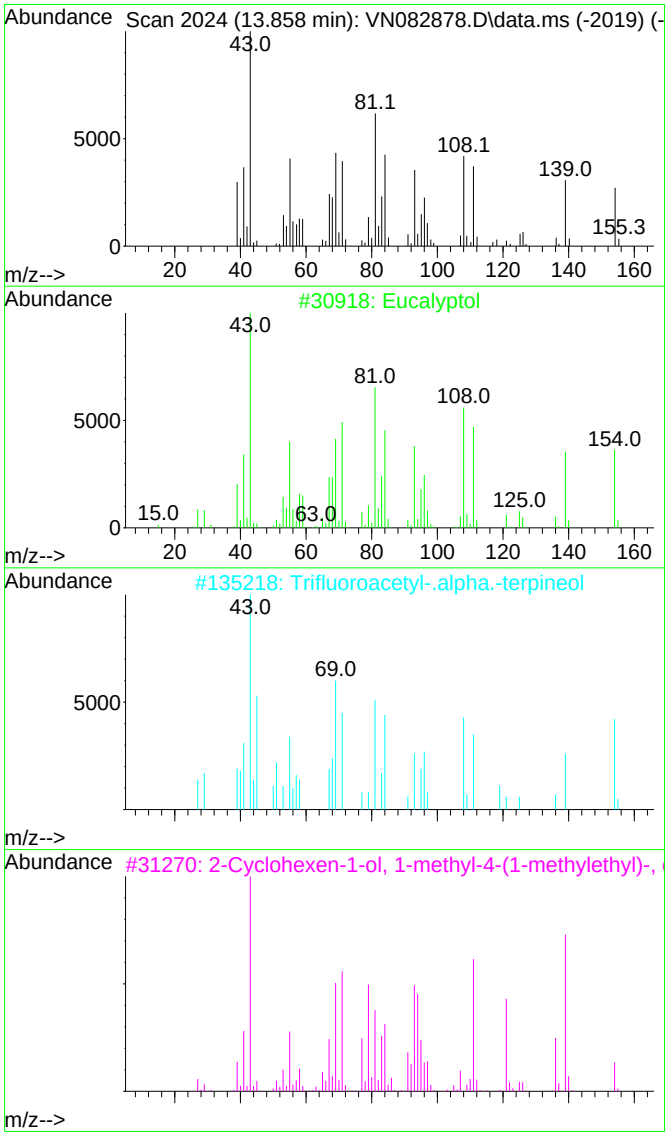
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

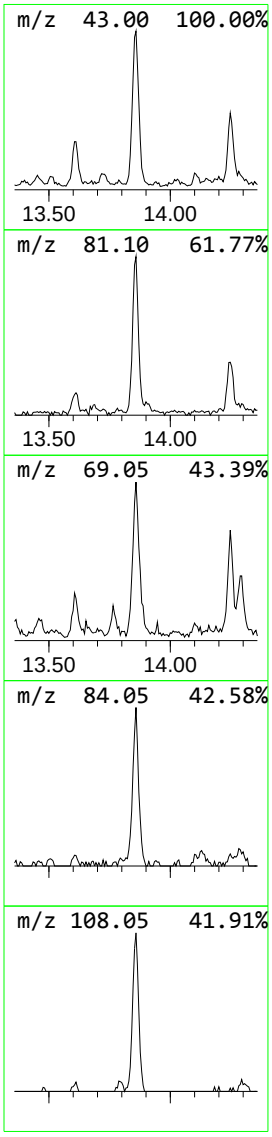
****

Peak Number 3 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.858	20.60 ug/l	320453	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	64
3	2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-82-5	37
4	Cyclopentanol, 1,2-dimethyl-3-(1...	154	C10H18O	004099-07-4	27
5	2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-81-4	25





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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

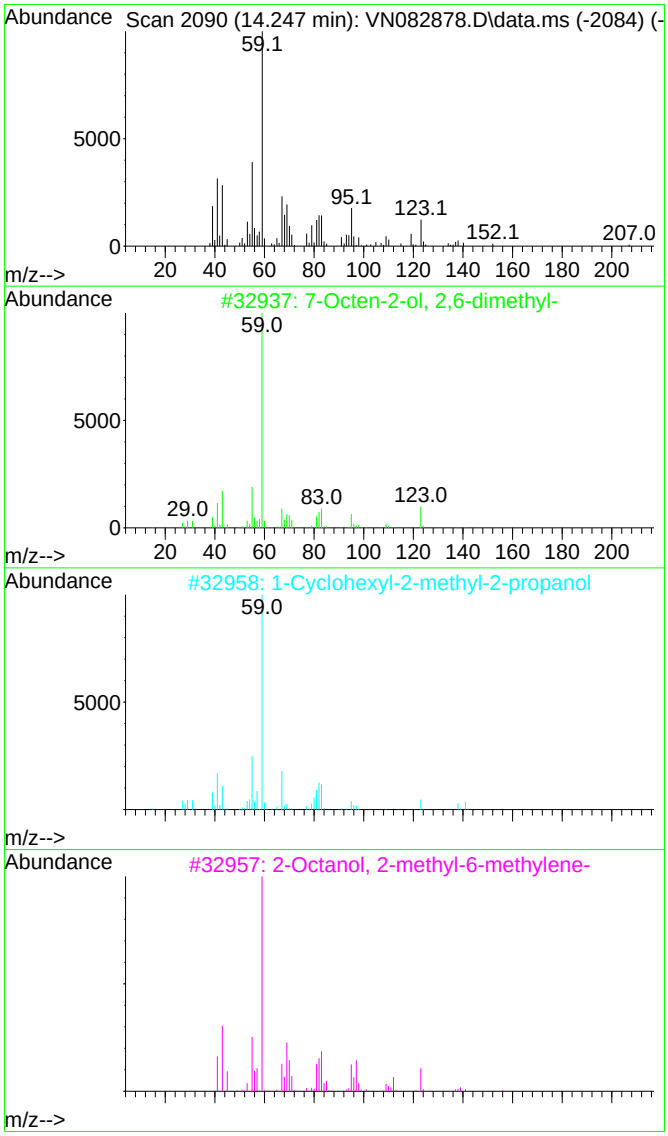
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

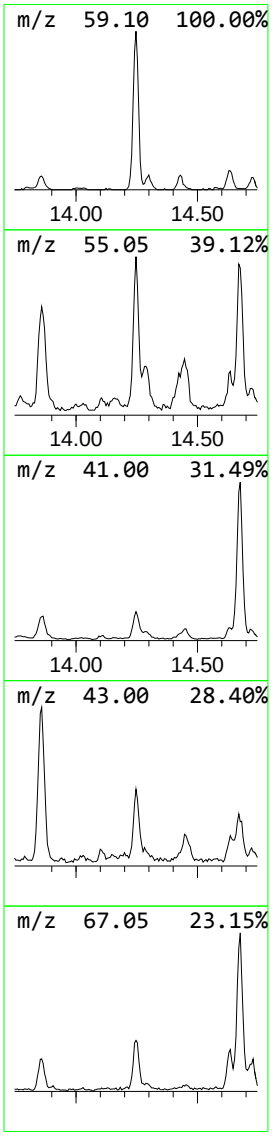
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	14.28 ug/l	222174	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	80
2	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	64
3	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	59
4	Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	50
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
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Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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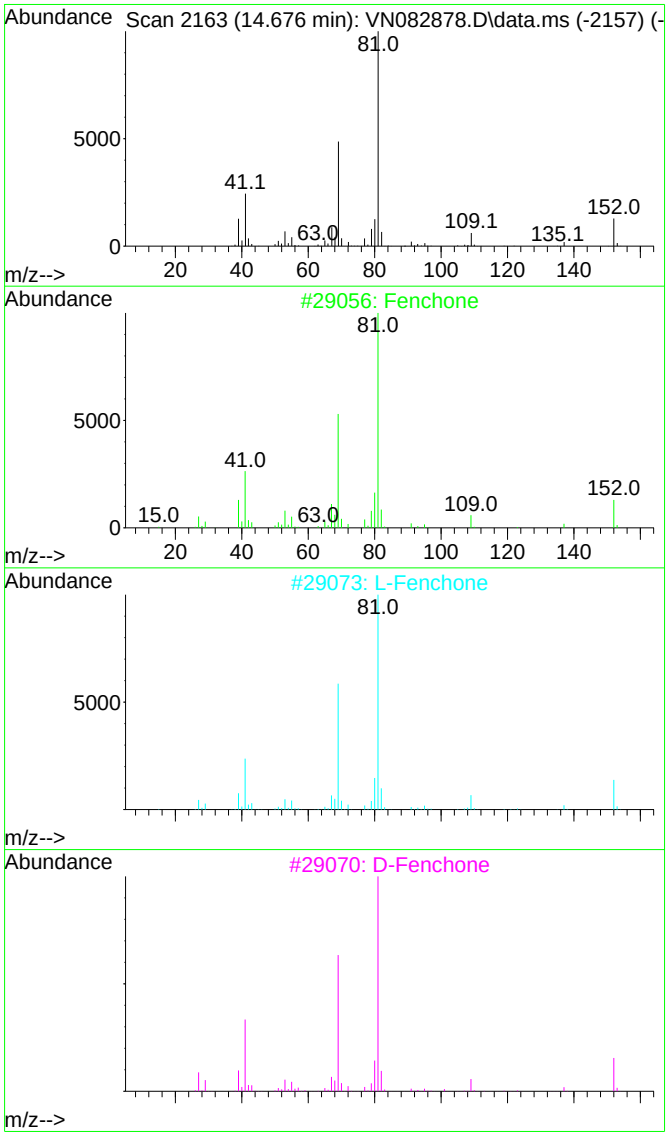
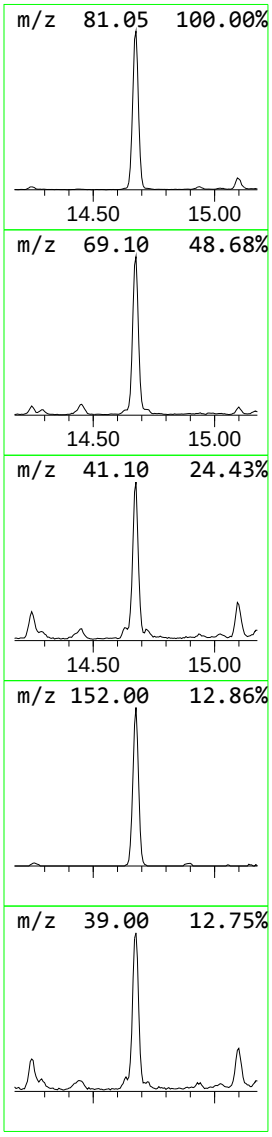
****
Peak Number 6 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	67.02 ug/l	1042420	1,4-Dichlorobenzene-d4	13.794

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	94
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42





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Instrument :
MSVOA_N
ClientSampleId :
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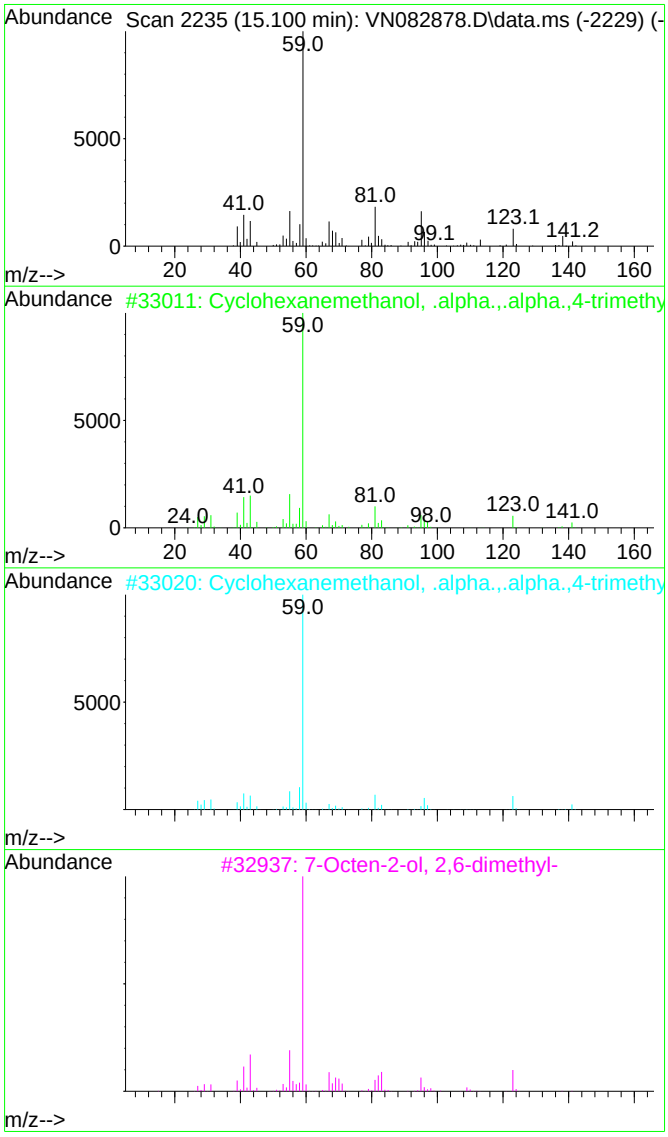
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

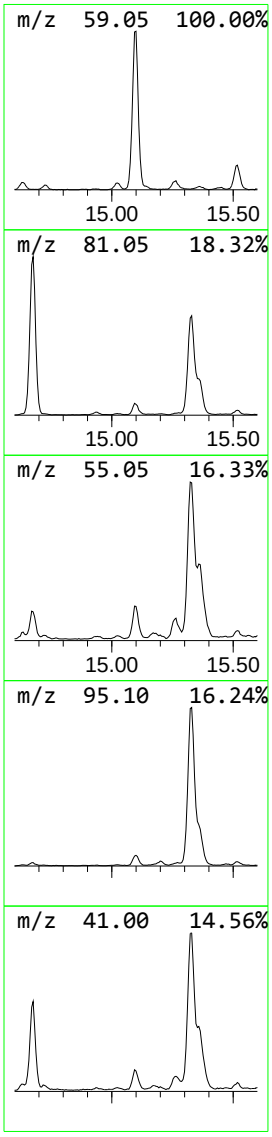
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	23.45 ug/l	364777	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	78
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	64
3	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
4	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	50
5	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	47





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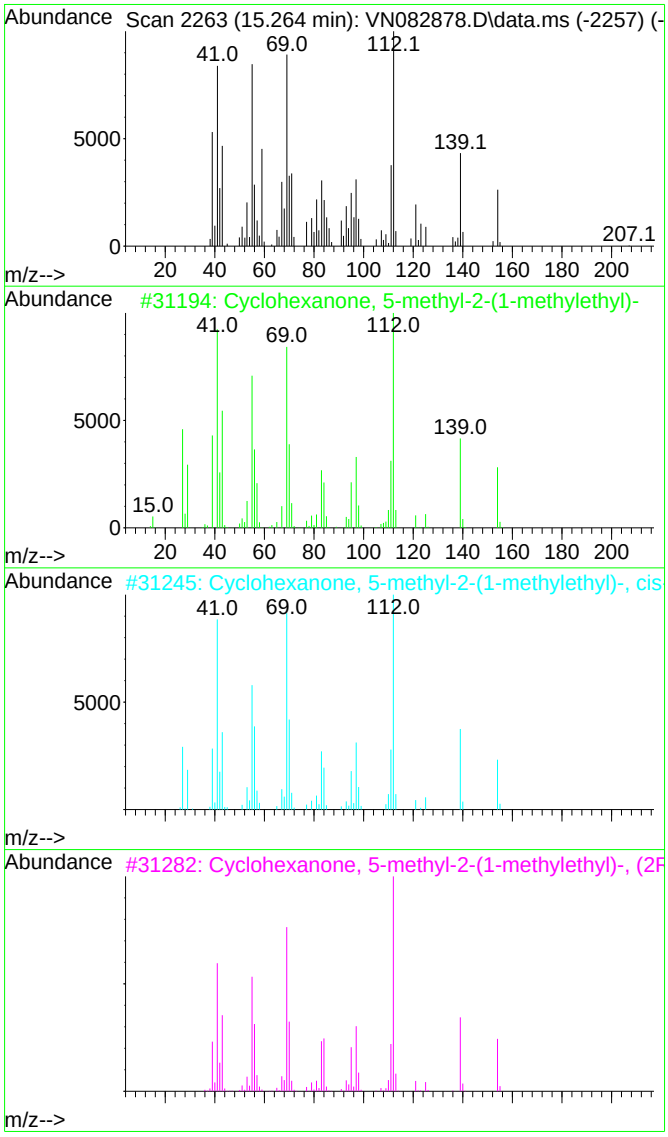
Quant Title : SW846 8260

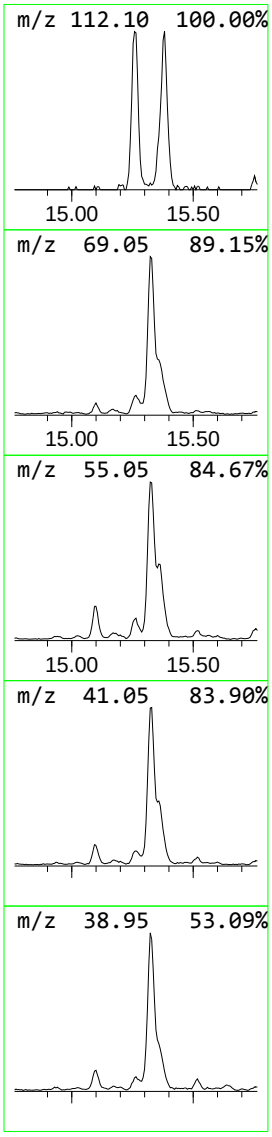
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclohexanone, 5-methyl-2-(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.264	15.55 ug/l	241808	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	97
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	95
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	95
4	L-Menthone	154	C10H18O	014073-97-3	94
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

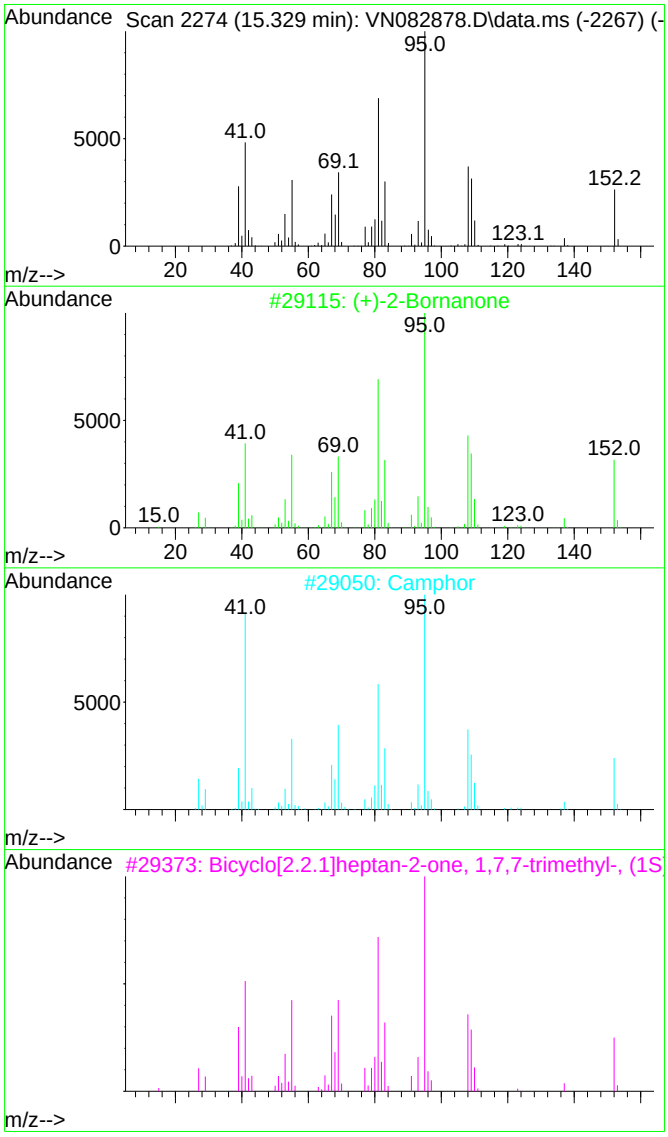
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

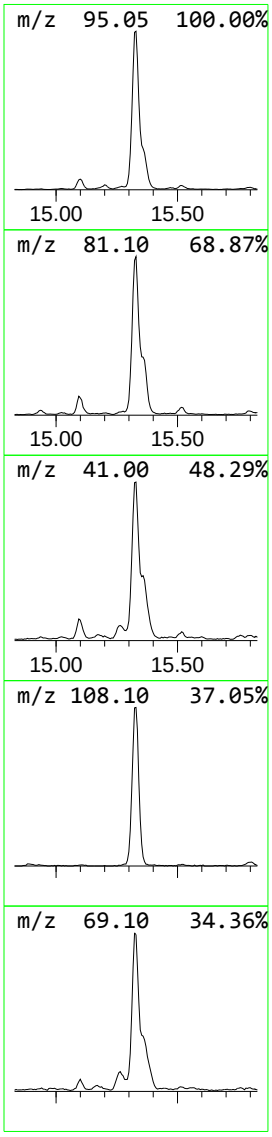
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (+)-2-Bornanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	139.33 ug/l	2167070	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	52
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.M
Quant Title : SW846 8260

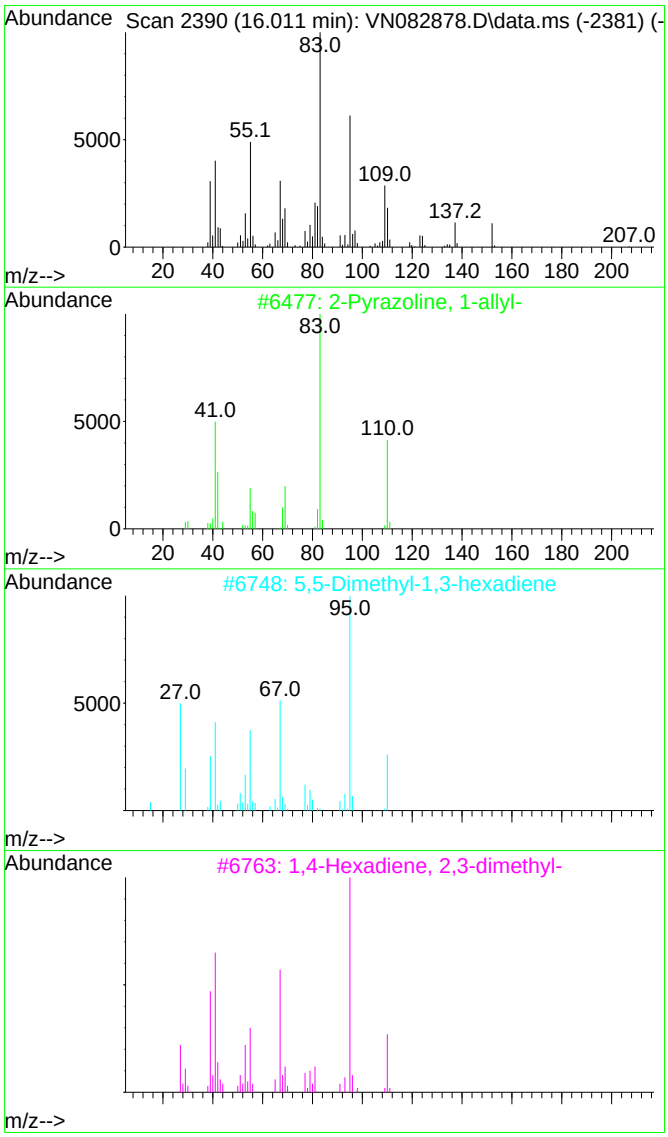
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

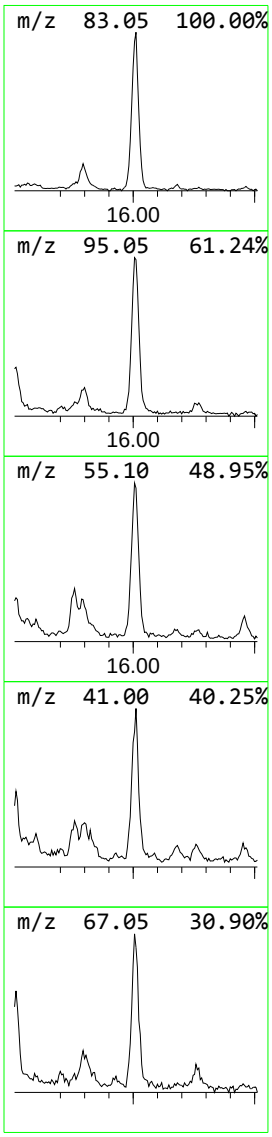
****

Peak Number 10 unknown16.011 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	20.13 ug/l	313033	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrazoline, 1-allyl-	110	C6H10N2	019804-38-7	38
2	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	35
3	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	35
4	2-Cyclohexen-1-one, 4-ethyl-3,4-...	152	C10H16O	017622-46-7	30
5	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN071124\
Data File : VN082878.D
Acq On : 11 Jul 2024 15:56
Operator : JC\MD
Sample : P3220-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240710076-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N070824W.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	2.295	22.1	ug/l	181076	1	8.224	409439	50.0
3-Pentanone, 2,...	11.171	15.0	ug/l	246290	3	11.870	821985	50.0
Eucalyptol	13.858	20.6	ug/l	320453	4	13.794	777658	50.0
7-Octen-2-ol, 2...	14.247	14.3	ug/l	222174	4	13.794	777658	50.0
Fenchone	14.676	67.0	ug/l	1042420	4	13.794	777658	50.0
Cyclohexanemeth...	15.100	23.4	ug/l	364777	4	13.794	777658	50.0
Cyclohexanone, ...	15.264	15.6	ug/l	241808	4	13.794	777658	50.0
(+)-2-Bornanone	15.329	139.3	ug/l	2167070	4	13.794	777658	50.0
unknown16.011	16.011	20.1	ug/l	313033	4	13.794	777658	50.0