LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084956.D
Acq On : 19 Nov 2024 18:52
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-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\82N103024W.M
Title : SW846 8260

Signal : TIC: VN084956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	52	57	64	rVB	81240	124393	2.02%	0.425%
2	2.948	165	169	179	rVB6	24568	67512	1.09%	0.231%
3	4.430	411	421	434	rBV	29904	86913	1.41%	0.297%
4	5.553	586	612	633	rBV	1517444	6171776	100.00%	21.078%
5	7.453	920	935	946	rBV	2025962	5672795	91.92%	19.374%
6	7.553	948	952	966	rVB	41462	111840	1.81%	0.382%
7	7.835	989	1000	1022	rBV	1075237	2712954	43.96%	9.265%
8	8.159	1045	1055	1060	rBV	138924	329322	5.34%	1.125%
9	8.218	1060	1065	1078	rVB	249127	547205	8.87%	1.869%
10	8.577	1110	1126	1137	rBV4	160696	535924	8.68%	1.830%
11	8.665	1137	1141	1150	rVB3	44672	101295	1.64%	0.346%
12	9.100	1206	1215	1231	rVB	348438	733749	11.89%	2.506%
13	10.565	1456	1464	1470	rBV	555834	1013266	16.42%	3.461%
14	10.629	1470	1475	1487	rVB2	120200	331276	5.37%	1.131%
15	11.171	1557	1567	1577	rBV	180003	334797	5.42%	1.143%
16	11.776	1662	1670	1675	rVV6	32889	89211	1.45%	0.305%
17	11.865	1675	1685	1693	rVV	501810	951100	15.41%	3.248%
18	11.965	1693	1702	1711	rVB2	126682	269665	4.37%	0.921%
19	12.065	1711	1719	1729	rBV2	119178	265541	4.30%	0.907%
20	12.394	1768	1775	1782	rBV	80588	147589	2.39%	0.504%
21	12.847	1845	1852	1860	rVB	426767	744457	12.06%	2.542%
22	13.194	1901	1911	1916	rVV6	31164	85950	1.39%	0.294%
23	13.482	1948	1960	1966	rBV2	43358	97977	1.59%	0.335%
24	13.606	1973	1981	1986	rBV3	57869	110121	1.78%	0.376%
25	13.729	1996	2002	2006	rBV	91637	143048	2.32%	0.489%
26	13.788	2006	2012	2019	rVV	502769	918194	14.88%	3.136%
27	13.853	2019	2023	2034	rVB2	228169	434565	7.04%	1.484%
28	13.994	2042	2047	2060	rVB4	26410	65144	1.06%	0.222%
29	14.247	2081	2090	2094	rBV	159748	293400	4.75%	1.002%
30	14.294	2094	2098	2108	rVB	302869	524926	8.51%	1.793%
31	14.447	2114	2124	2132	rBV5	46985	119978	1.94%	0.410%
32	14.635	2150	2156	2157	rBV3	57598	93211	1.51%	0.318%
33	14.670	2157	2162	2169	rVV	714221	1267951	20.54%	4.330%
34	14.935	2202	2207	2213	rBV6	40305	75466	1.22%	0.258%
35	15.094	2228	2234	2241	rBV	144994	262551	4.25%	0.897%
36	15.264	2257	2263	2267	rBV4	122065	311876	5.05%	1.065%

LSC Area Percent Report

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241113075-01-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\82N103024W.M
Title : SW846 8260

37	15.323	2267	2273	2277	rBV	1185308	2263006	36.67%	7.729%
38	15.511	2300	2305	2315	rVB3	93983	172414	2.79%	0.589%
39	15.641	2321	2327	2334	rVB	147124	289923	4.70%	0.990%
40	15.758	2341	2347	2349	rBV3	34608	63465	1.03%	0.217%
41	16.005	2380	2389	2401	rBV2	157601	344869	5.59%	1.178%

Sum of corrected areas: 29280615

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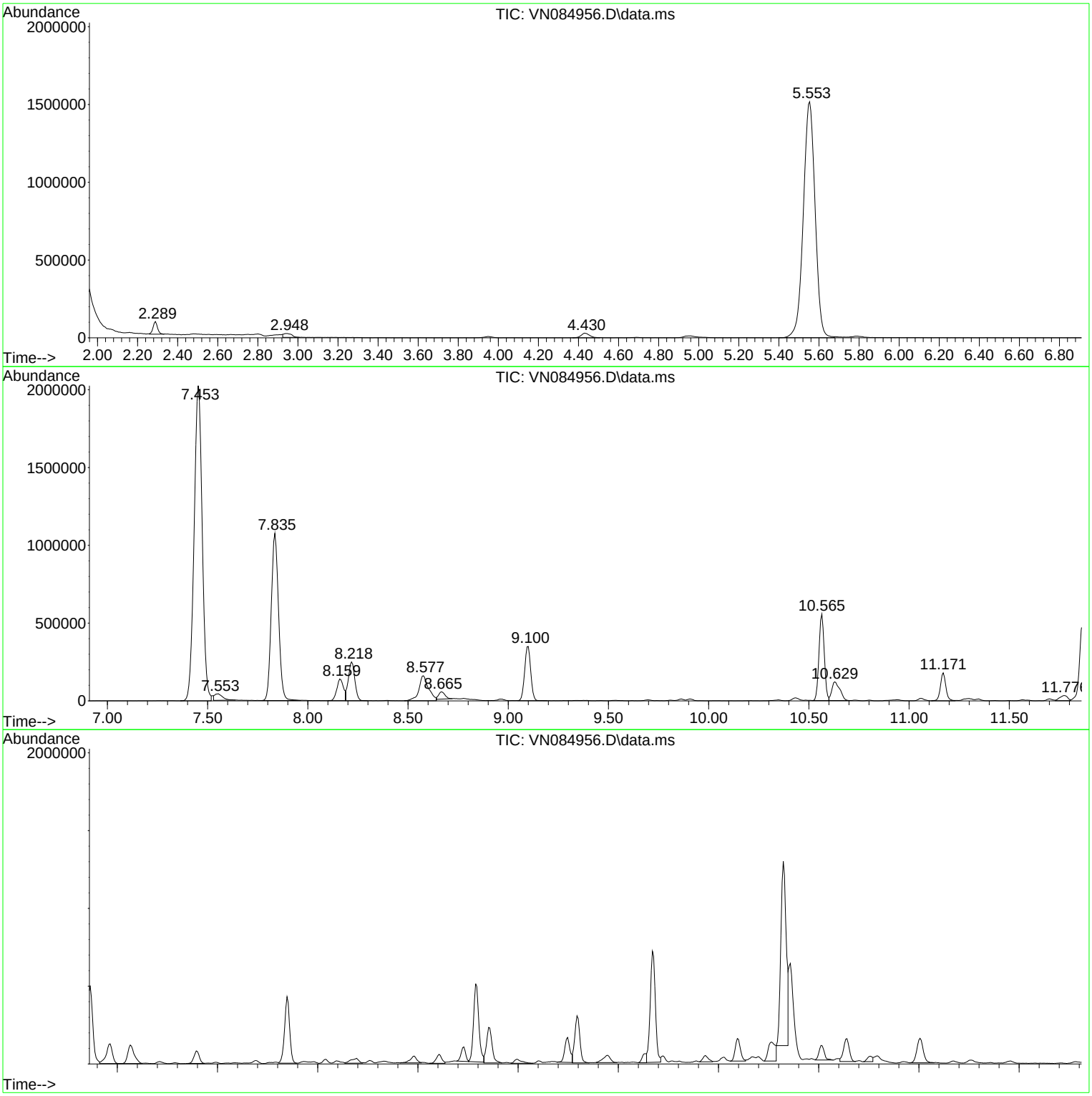
MSVOA_N
ClientSampleId :
241113075-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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Data File : VN084956.D
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Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

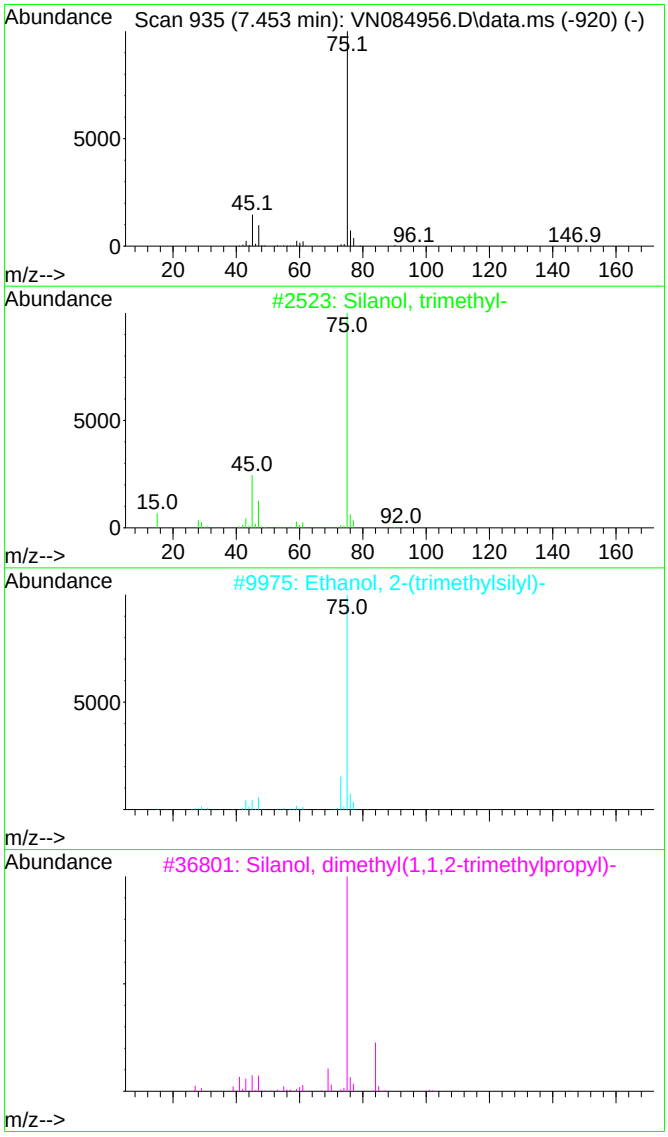
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

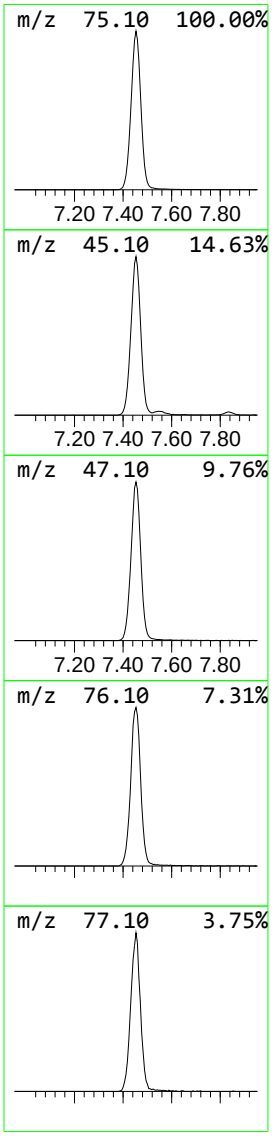
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Silanol, trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.453	518.34 ug/l	5672800	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	91
2	Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	43
3	Silanol, dimethyl(1,1,2-trimethy...	160	C8H20OSi	055644-10-5	39
4	Ethanethioamide	75	C2H5NS	000062-55-5	9
5	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9





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Data File : VN084956.D
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Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

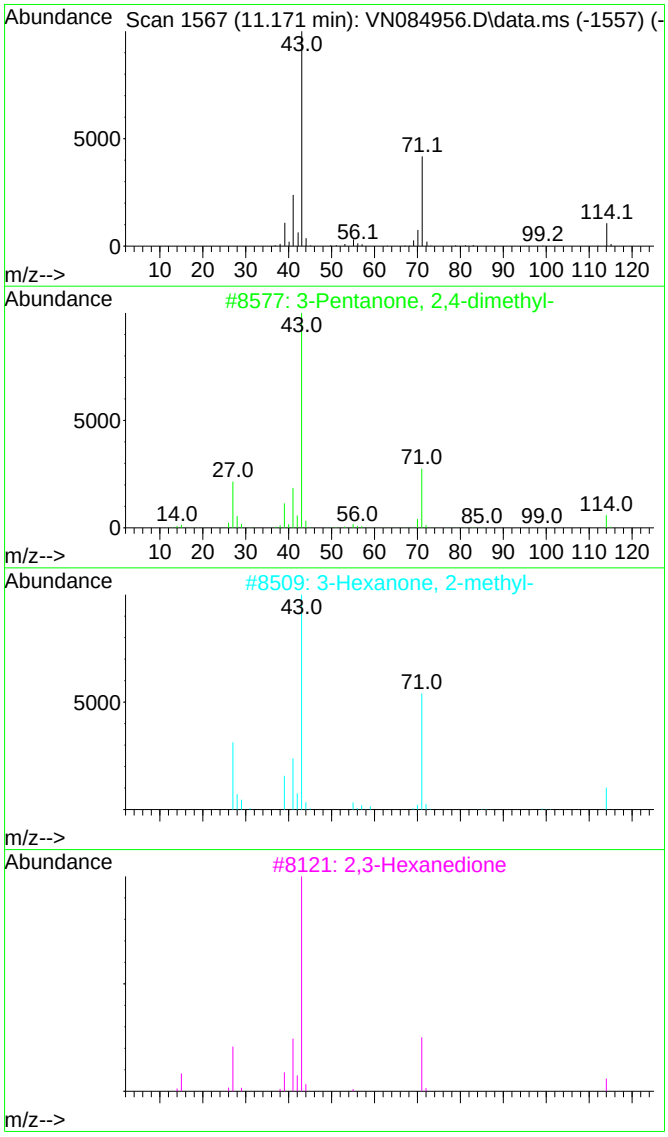
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

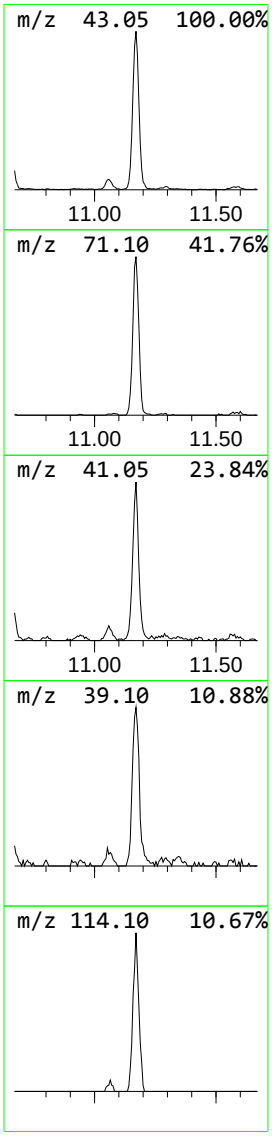
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	17.60 ug/l	334797	Chlorobenzene-d5	11.865

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	86
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	78
4	4-Heptanone	114	C7H14O	000123-19-3	59
5	Pyrrolidine	71	C4H9N	000123-75-1	59





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Data File : VN084956.D
Acq On : 19 Nov 2024 18:52
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

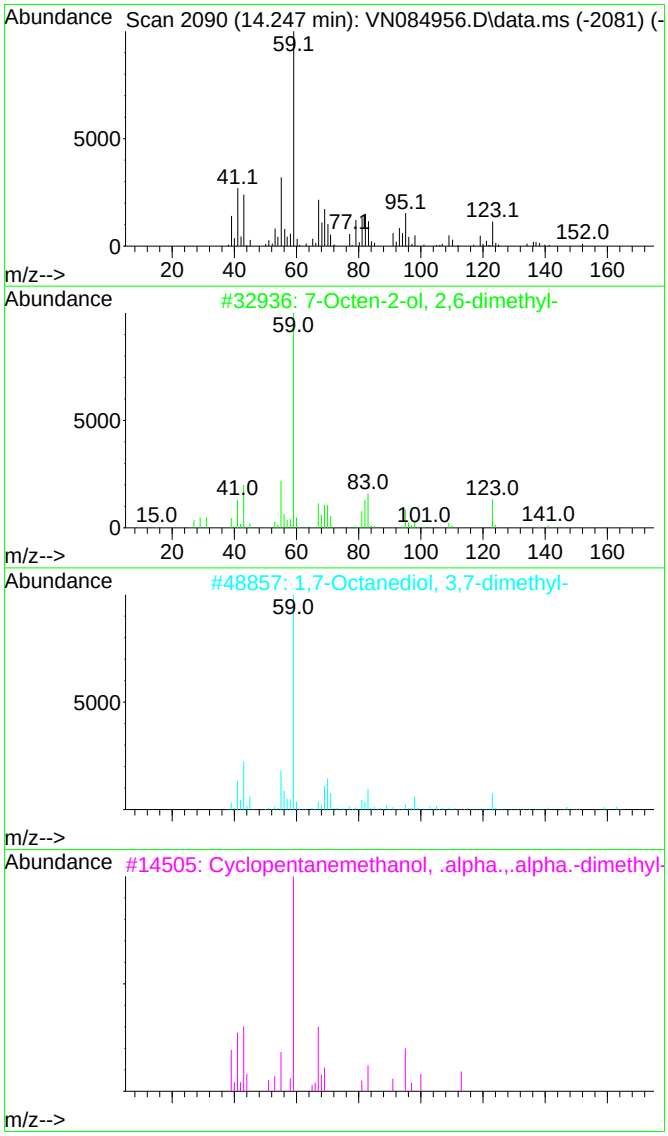
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

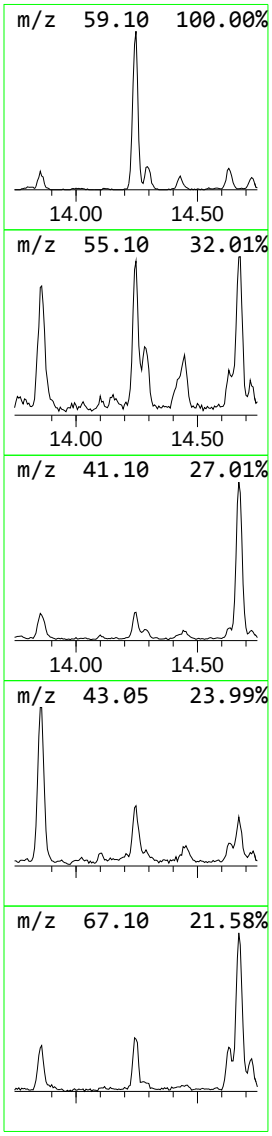
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.247	15.98 ug/l	293400	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	59
2	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	53
3	Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	45
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	45
5	2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
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Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

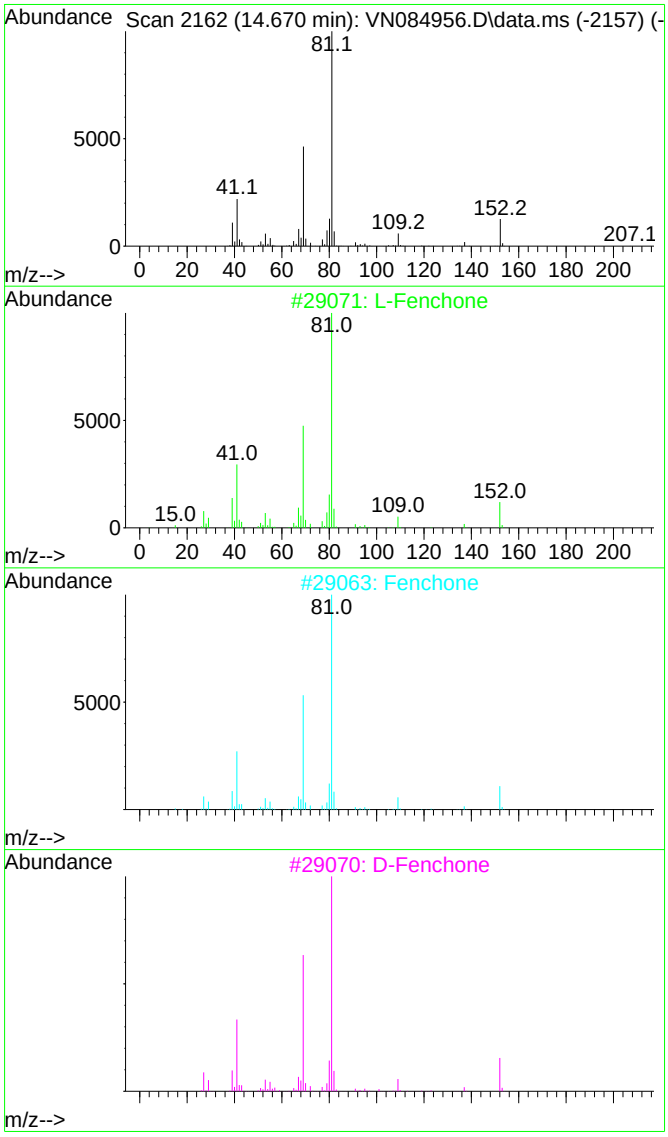
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

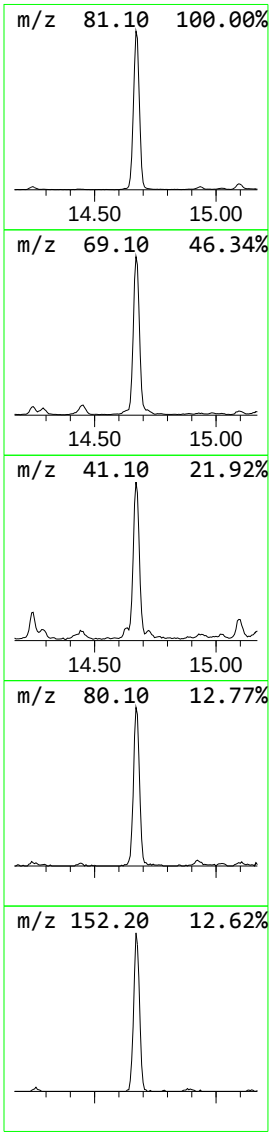
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 L-Fenchone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	69.05 ug/l	1267950	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Fenchone	152	C10H16O	007787-20-4	95
2	Fenchone	152	C10H16O	001195-79-5	95
3	D-Fenchone	152	C10H16O	004695-62-9	91
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	42





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

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

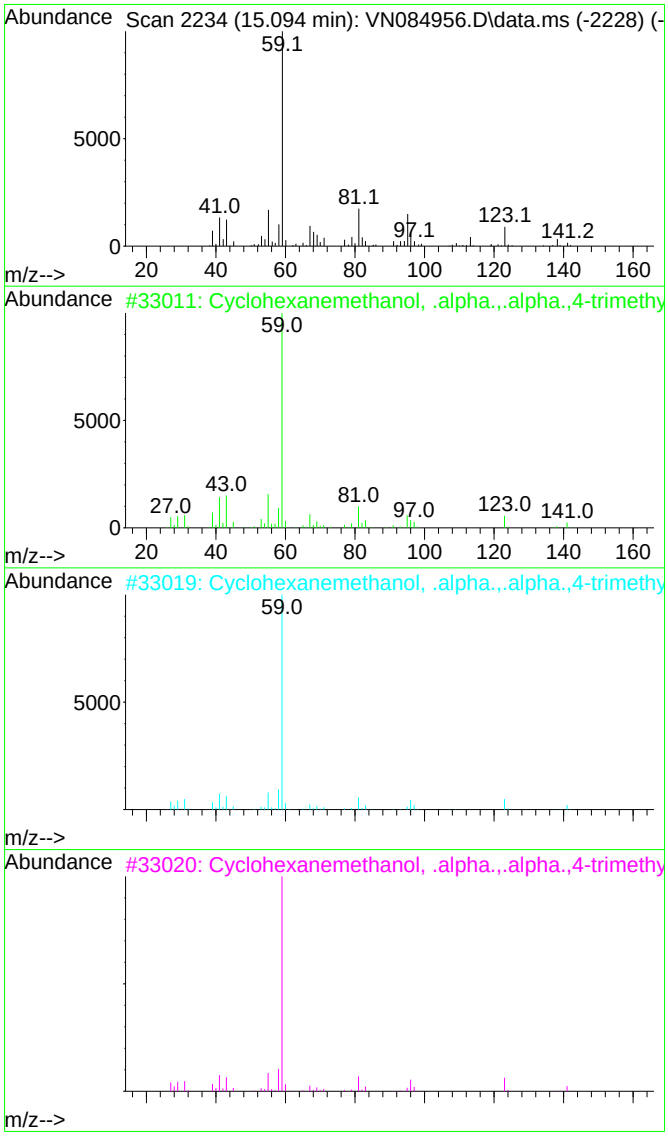
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

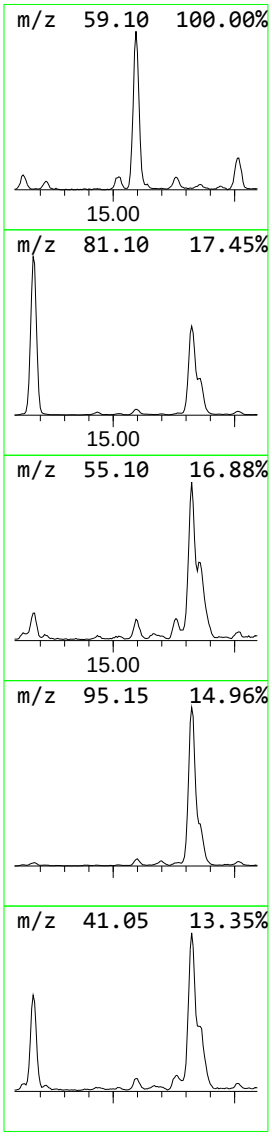
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.094	14.30 ug/l	262551	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	64
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	59
3	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	59
4	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	43
5	3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-96-4	40





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Instrument :
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ClientSampleId :
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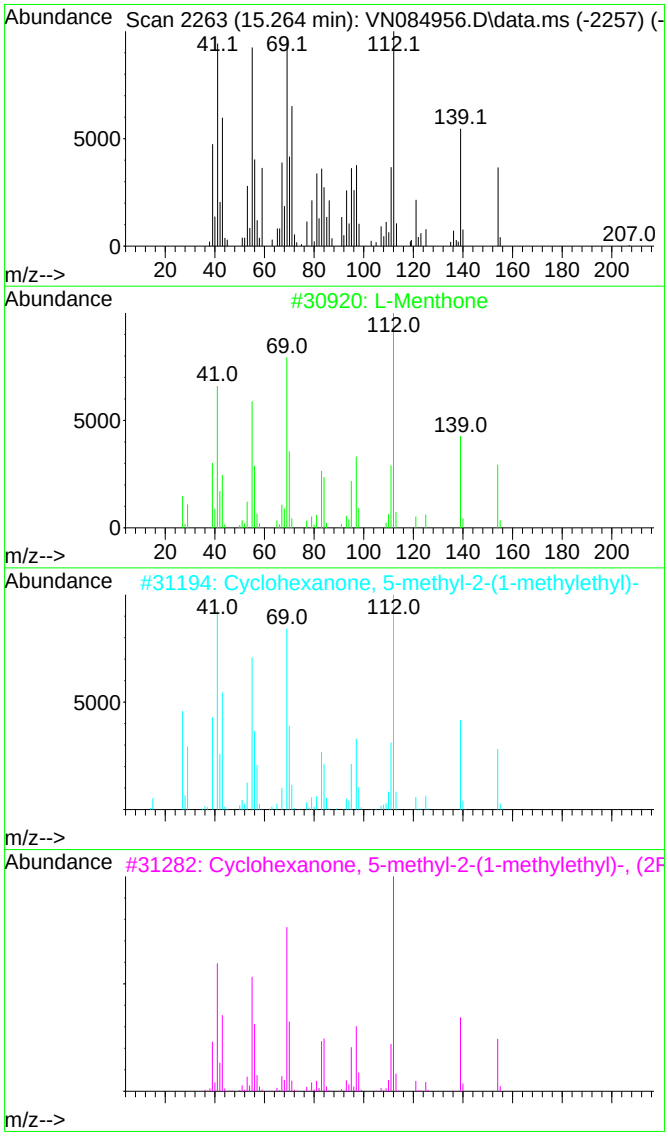
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

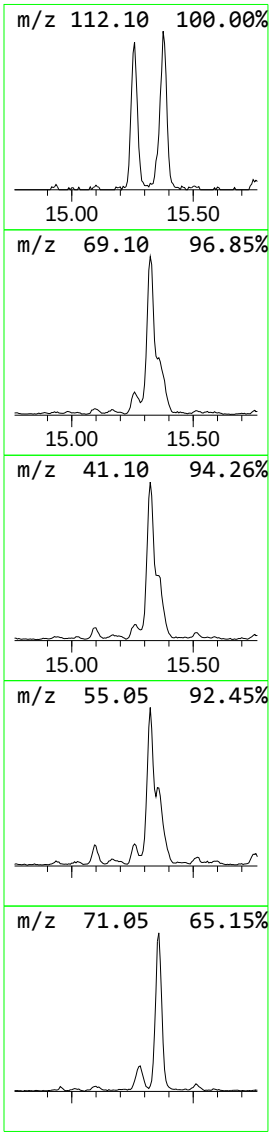
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 L-Menthone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.264	16.98 ug/l	311876	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Menthone	154	C10H18O	014073-97-3	98
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	93
3	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	93
4	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	91
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	90





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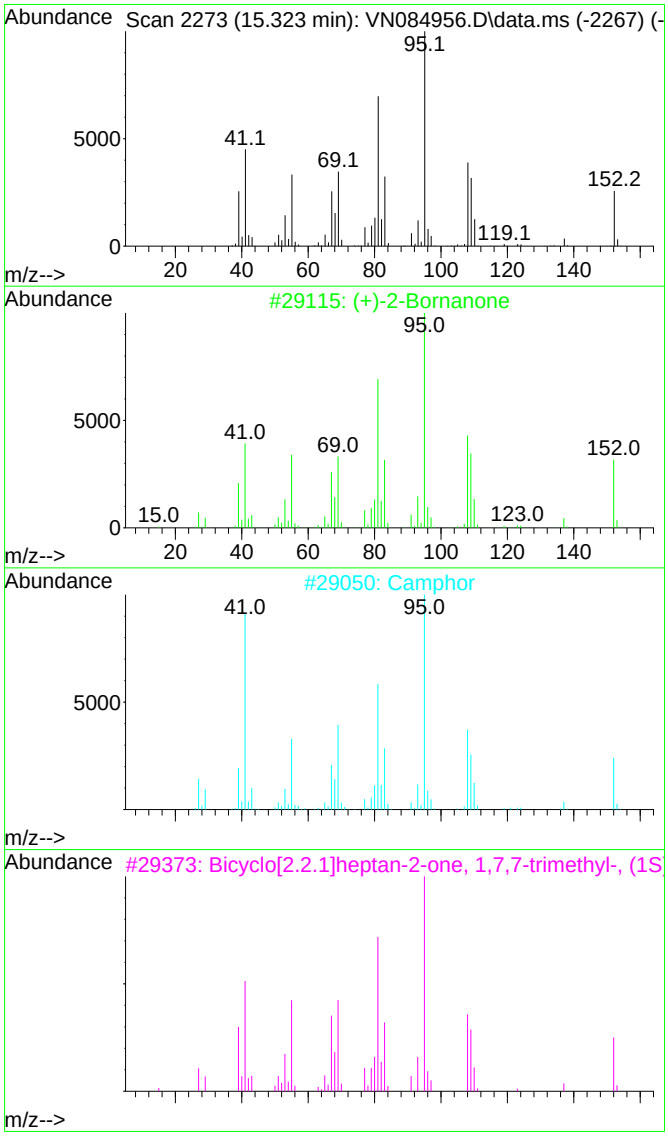
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

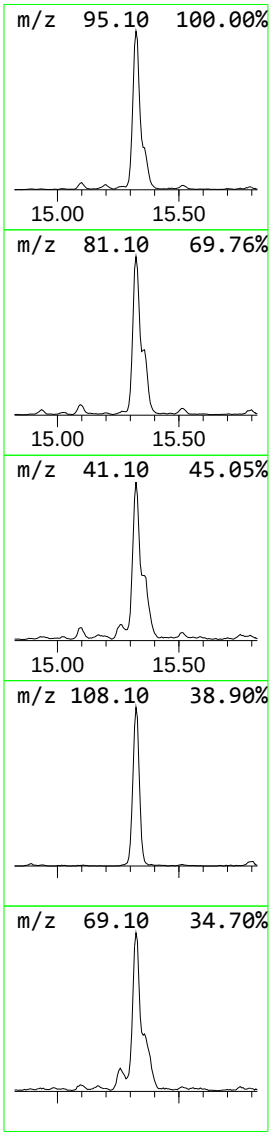
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	123.23 ug/l	2263010	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	49
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





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Data File : VN084956.D
Acq On : 19 Nov 2024 18:52
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

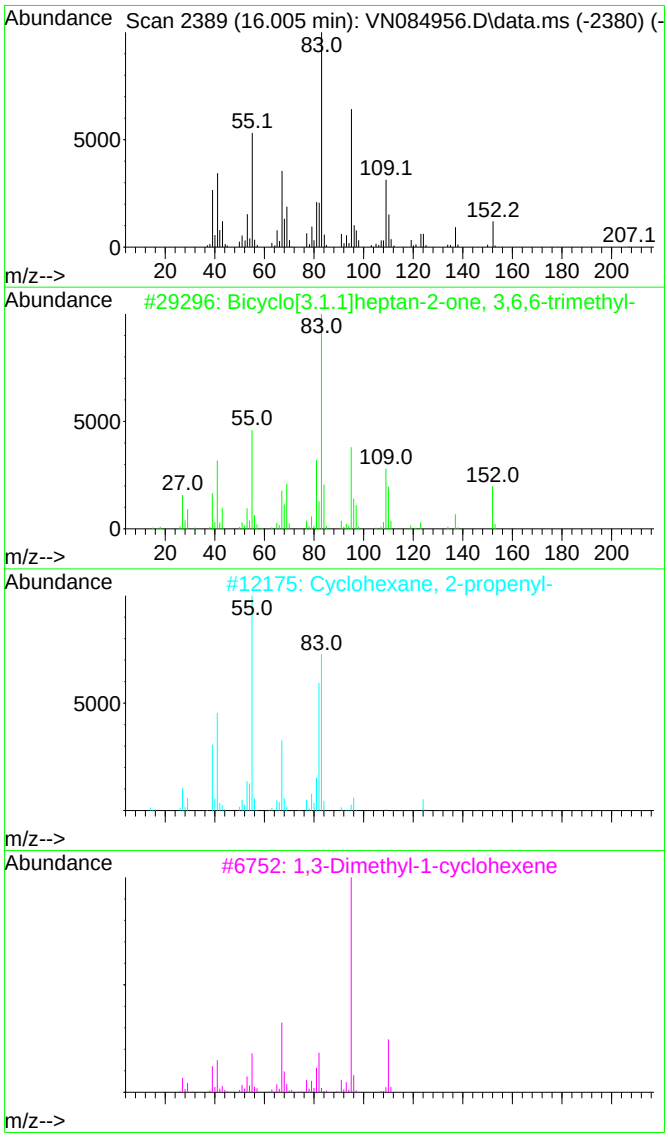
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

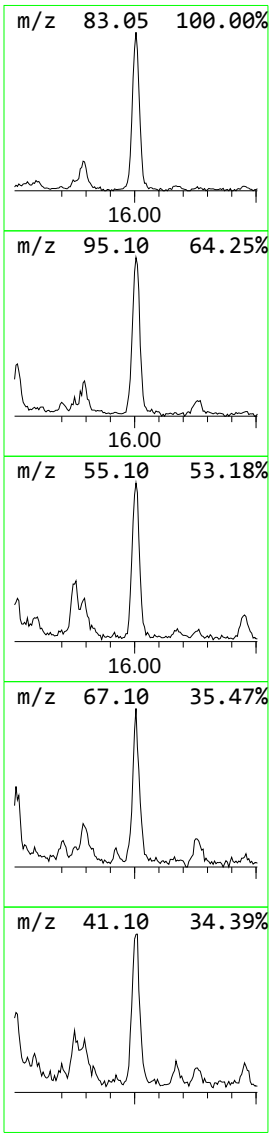
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	18.78 ug/l	344869	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	62
2	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43
3	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	41
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
5	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084956.D
Acq On : 19 Nov 2024 18:52
Operator : JC\MD
Sample : P4844-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
241113075-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.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
Silanol, trimet...	7.453	518.3	ug/l	5672800	1	8.218	547205	50.0
3-Pentanone, 2,...	11.171	17.6	ug/l	334797	3	11.865	951100	50.0
7-Octen-2-ol, 2...	14.247	16.0	ug/l	293400	4	13.794	918194	50.0
L-Fenchone	14.670	69.0	ug/l	1267950	4	13.794	918194	50.0
Cyclohexanemeth...	15.094	14.3	ug/l	262551	4	13.794	918194	50.0
L-Menthone	15.264	17.0	ug/l	311876	4	13.794	918194	50.0
(+)-2-Bornanone	15.323	123.2	ug/l	2263010	4	13.794	918194	50.0
Bicyclo[3.1.1]h...	16.006	18.8	ug/l	344869	4	13.794	918194	50.0