LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-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\82N051524W.M
Title : SW846 8260

Signal : TIC: VN082163.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	53	58	71	rVB	192667	321266	5.92%	0.995%
2	2.824	140	148	162	rVB2	80874	182328	3.36%	0.565%
3	4.424	405	420	435	rBV	375538	1151214	21.21%	3.566%
4	4.706	458	468	483	rBV3	33894	108801	2.00%	0.337%
5	5.512	589	605	639	rBV	1286316	4577827	84.33%	14.182%
6	7.430	917	931	938	rBV	1896638	5428166	100.00%	16.816%
7	7.835	982	1000	1019	rBV	982397	2548464	46.95%	7.895%
8	8.165	1046	1056	1061	rBV	155808	370751	6.83%	1.149%
9	8.224	1061	1066	1078	rVB	275585	606521	11.17%	1.879%
10	8.582	1113	1127	1136	rBV2	198318	612497	11.28%	1.897%
11	8.659	1136	1140	1158	rVB4	62600	179680	3.31%	0.557%
12	9.100	1205	1215	1227	rBV	409120	832336	15.33%	2.579%
13	9.529	1282	1288	1299	rVB	60345	123223	2.27%	0.382%
14	10.447	1433	1444	1452	rBV2	48953	109473	2.02%	0.339%
15	10.565	1456	1464	1471	rVV	656395	1219892	22.47%	3.779%
16	10.629	1471	1475	1487	rVB3	115361	301218	5.55%	0.933%
17	11.065	1540	1549	1558	rBV3	31272	71021	1.31%	0.220%
18	11.171	1558	1567	1576	rBV	169827	318029	5.86%	0.985%
19	11.770	1662	1669	1675	rVV6	31811	89579	1.65%	0.278%
20	11.865	1675	1685	1694	rVV	601131	1160624	21.38%	3.596%
21	11.965	1694	1702	1709	rVV2	173673	351103	6.47%	1.088%
22	12.070	1710	1720	1730	rVB2	131325	295125	5.44%	0.914%
23	12.400	1763	1776	1782	rBV	103122	198166	3.65%	0.614%
24	12.694	1820	1826	1832	rVB2	35379	64215	1.18%	0.199%
25	12.847	1845	1852	1861	rVB	462646	835432	15.39%	2.588%
26	13.194	1902	1911	1918	rVB6	43428	120878	2.23%	0.374%
27	13.482	1948	1960	1973	rVB2	65595	168722	3.11%	0.523%
28	13.606	1973	1981	1987	rBV4	66989	130558	2.41%	0.404%
29	13.729	1996	2002	2006	rBV	53743	91840	1.69%	0.285%
30	13.794	2006	2013	2020	rVV	549303	1047248	19.29%	3.244%
31	13.859	2020	2024	2036	rVB2	150364	299202	5.51%	0.927%
32	13.994	2042	2047	2060	rVB2	50943	116026	2.14%	0.359%
33	14.247	2084	2090	2094	rVV3	122301	228958	4.22%	0.709%
34	14.300	2094	2099	2108	rVB	233721	418348	7.71%	1.296%
35	14.447	2114	2124	2132	rBV6	54035	137329	2.53%	0.425%
36	14.676	2156	2163	2169	rVV	994879	1676829	30.89%	5.195%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-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\82N051524W.M
Title : SW846 8260

37	14.935	2202	2207	2216	rVB6	42404	93749	1.73%	0.290%
38	15.023	2217	2222	2229	rBV5	42090	93168	1.72%	0.289%
39	15.100	2229	2235	2242	rVV	134573	242703	4.47%	0.752%
40	15.282	2257	2266	2267	rBV4	116581	260055	4.79%	0.806%
41	15.329	2267	2274	2291	rVB2	1546398	3785633	69.74%	11.728%
42	15.517	2301	2306	2312	rVB2	61993	107249	1.98%	0.332%
43	15.641	2319	2327	2337	rVB	379072	739796	13.63%	2.292%
44	15.800	2349	2354	2369	rVB7	50624	146170	2.69%	0.453%
45	16.005	2382	2389	2398	rBV	147828	318323	5.86%	0.986%

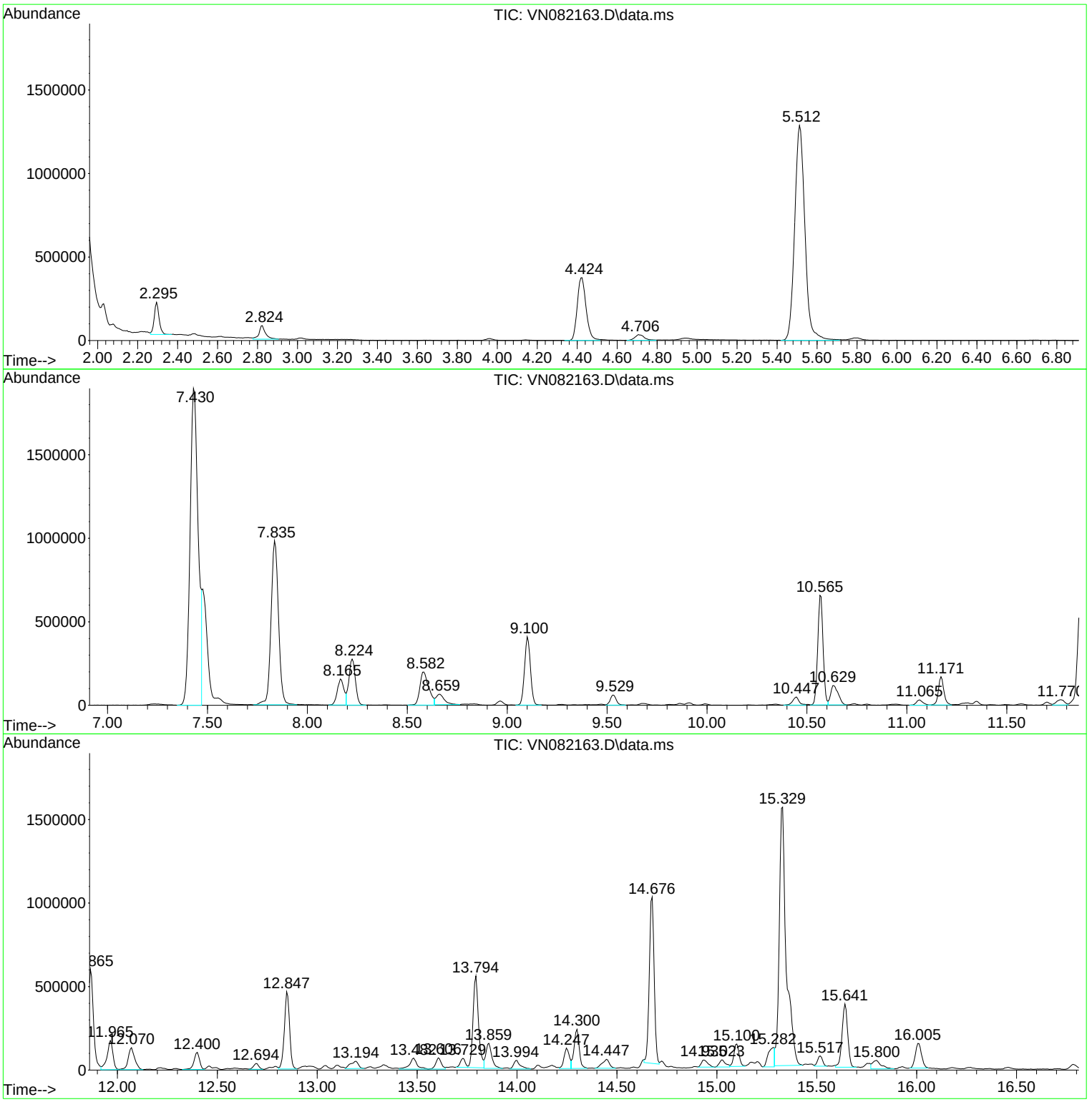
Sum of corrected areas: 32279735

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

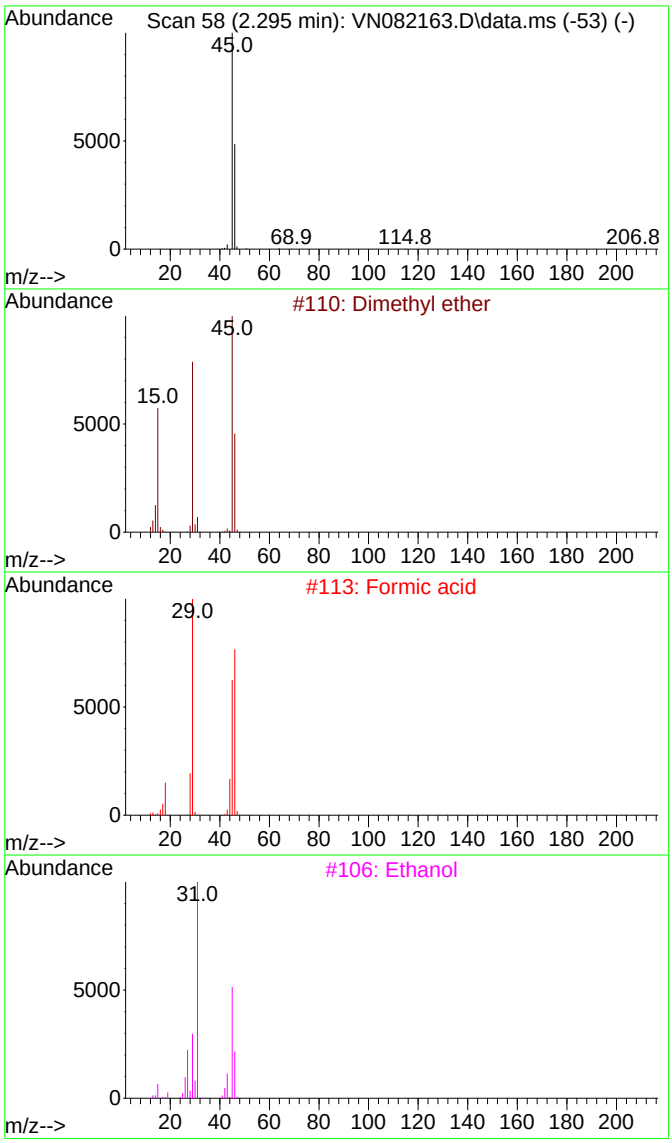
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

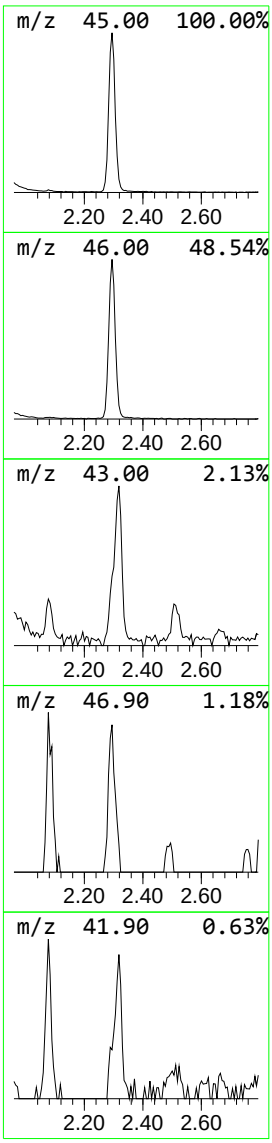
****

Peak Number 1 Dimethyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	26.48 ug/l	321266	Pentafluorobenzene	8.224

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

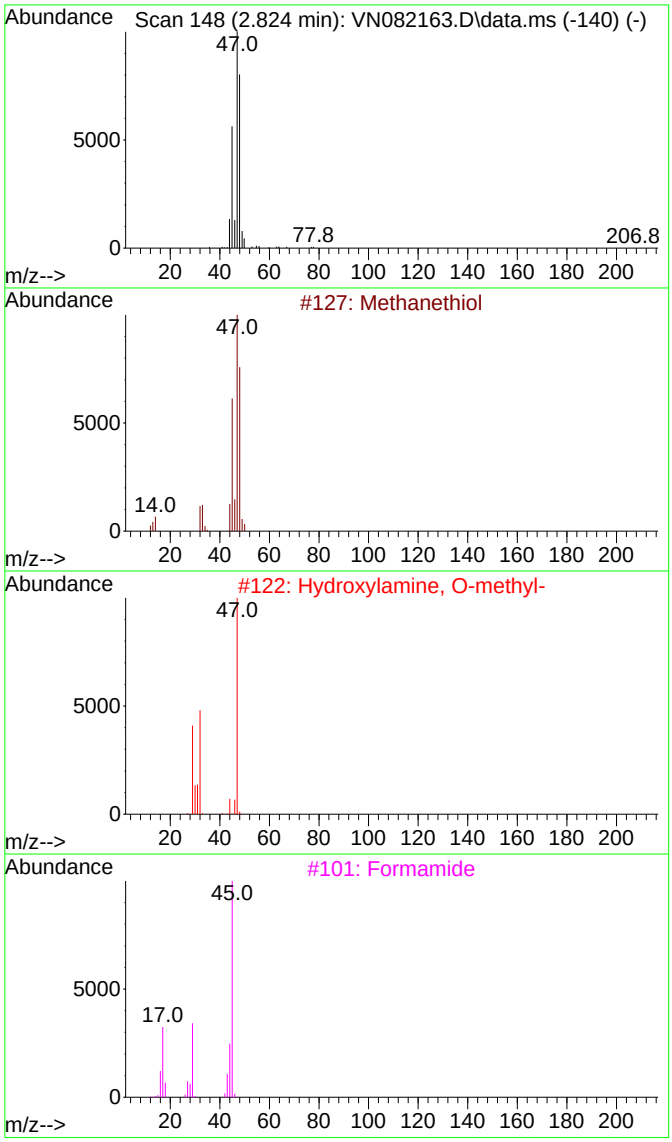
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

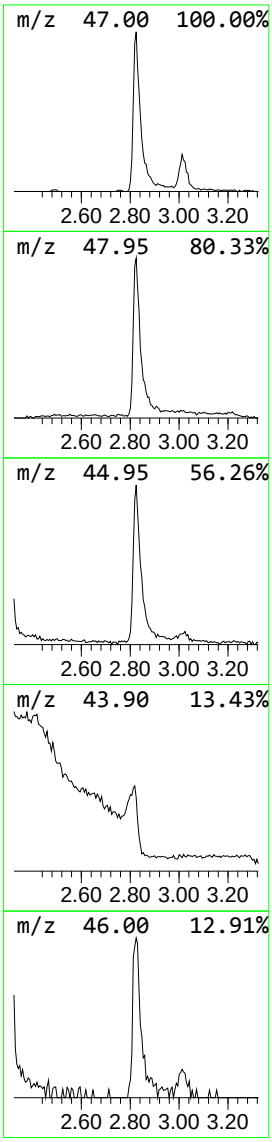
****

Peak Number 2 Methanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.824	15.03 ug/l	182328	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	9
3	Formamide	45	CH3NO	000075-12-7	4
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	4
5	Boronic acid, ethyl-	74	C2H7BO2	004433-63-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

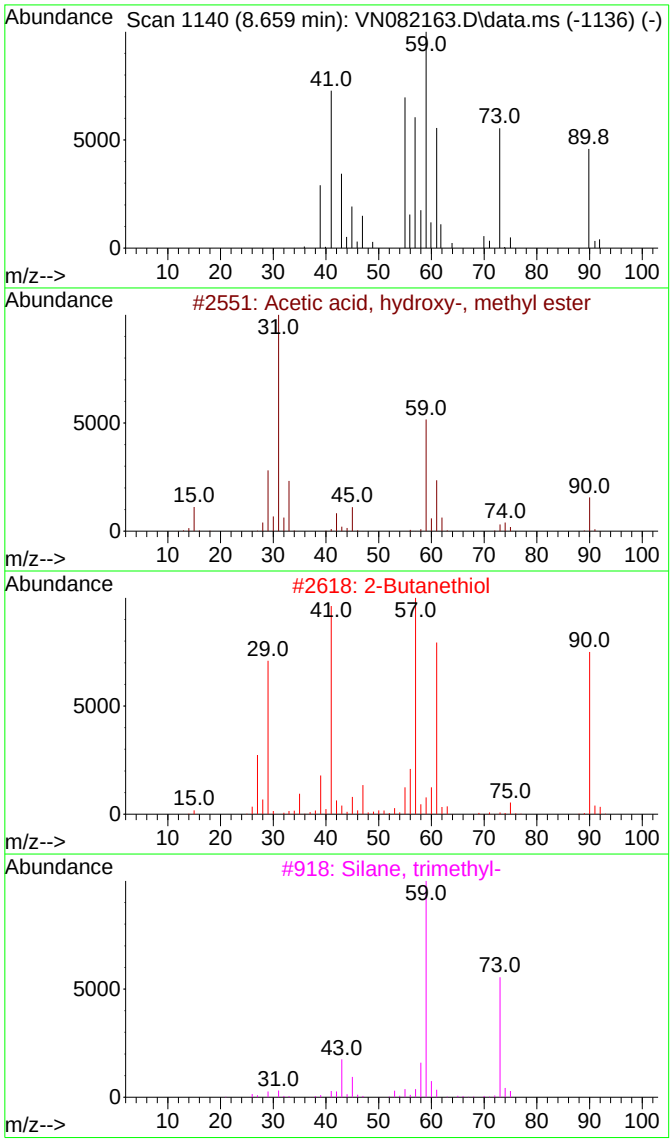
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

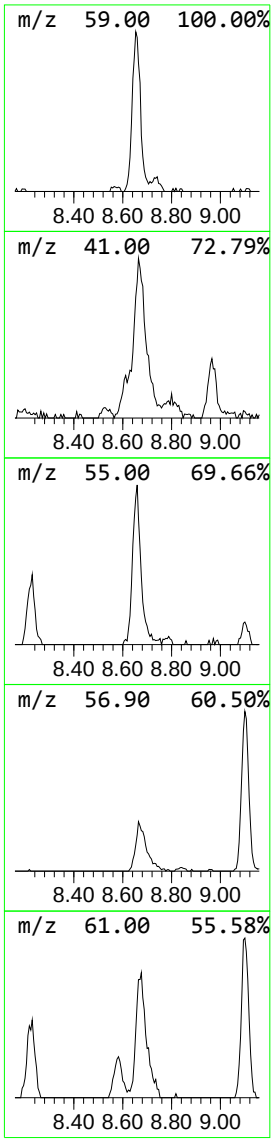
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Acetic acid, hydroxy-, meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.659	14.81 ug/l	179680	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, hydroxy-, methyl ester	90	C3H6O3	000096-35-5	72
2	2-Butanethiol	90	C4H10S	000513-53-1	38
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	32
4	Vinyldimethyl(hydroxymethyl)silane	116	C5H12OSi	120491-40-9	28
5	Methyl fluoroacetate	92	C3H5FO2	000453-18-9	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

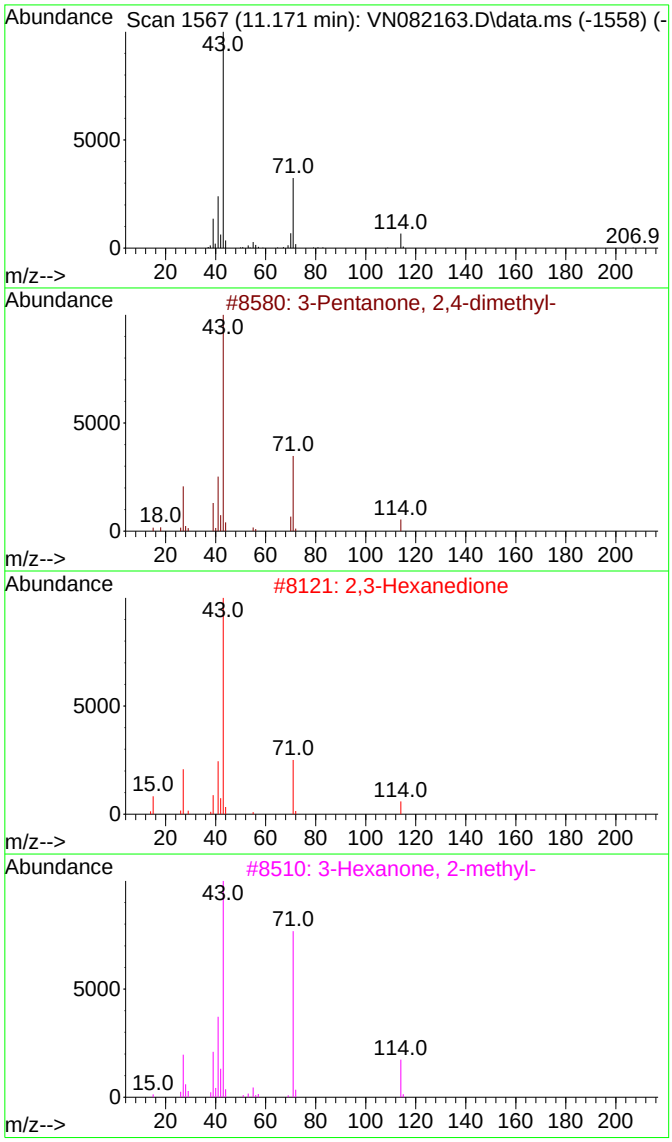
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

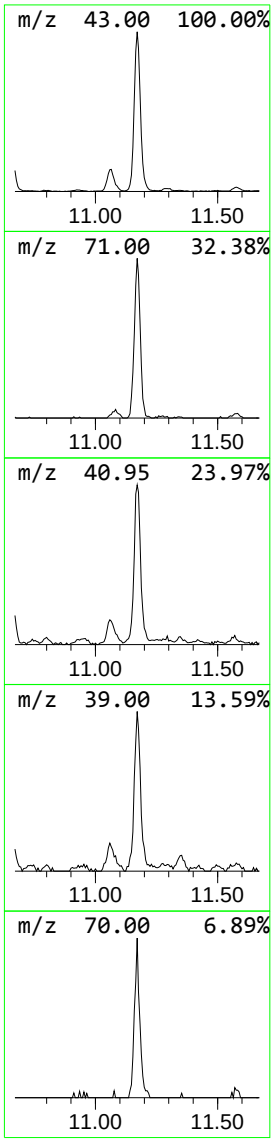
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	13.70 ug/l	318029	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	50
4	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	45
5	Pentane, 2-methyl-	86	C6H14	000107-83-5	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

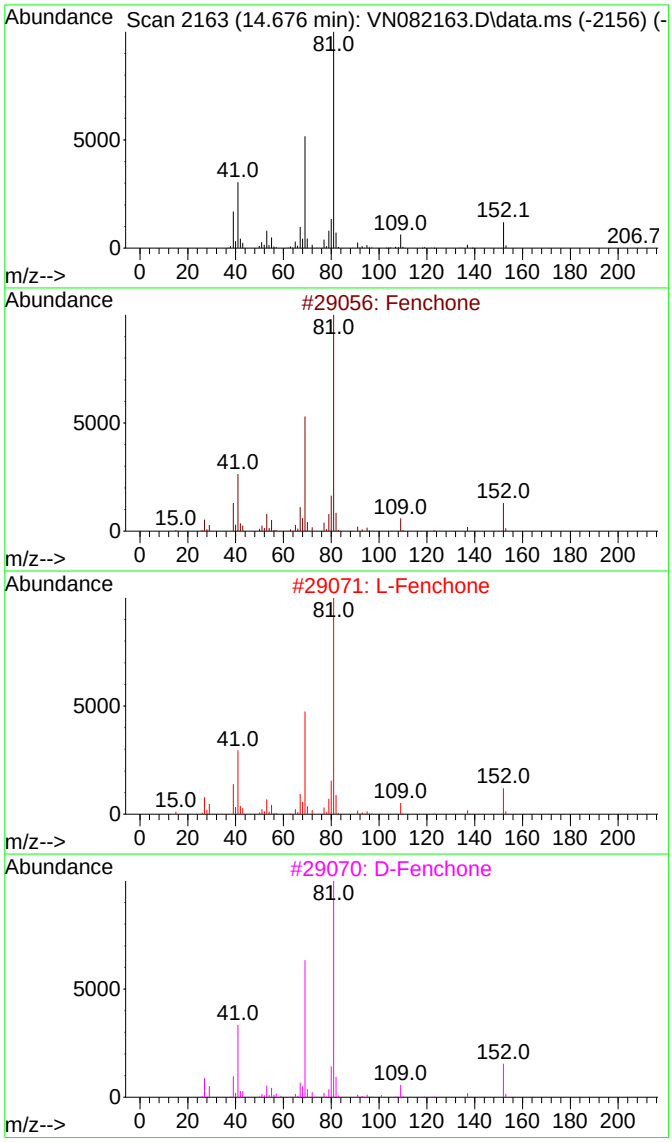
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

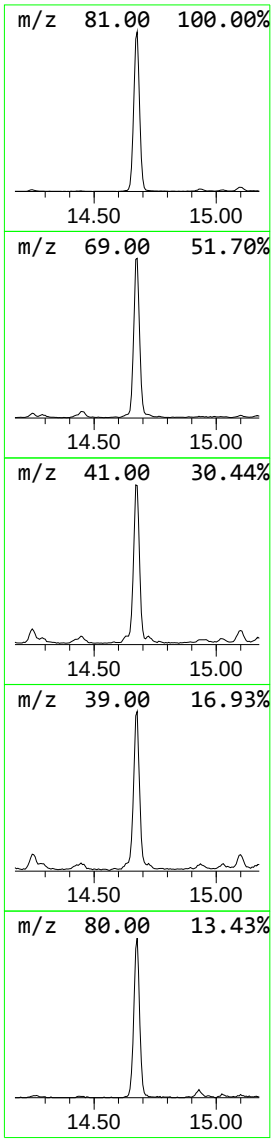
****

Peak Number 6 Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.676	80.06 ug/l	1676830	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	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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

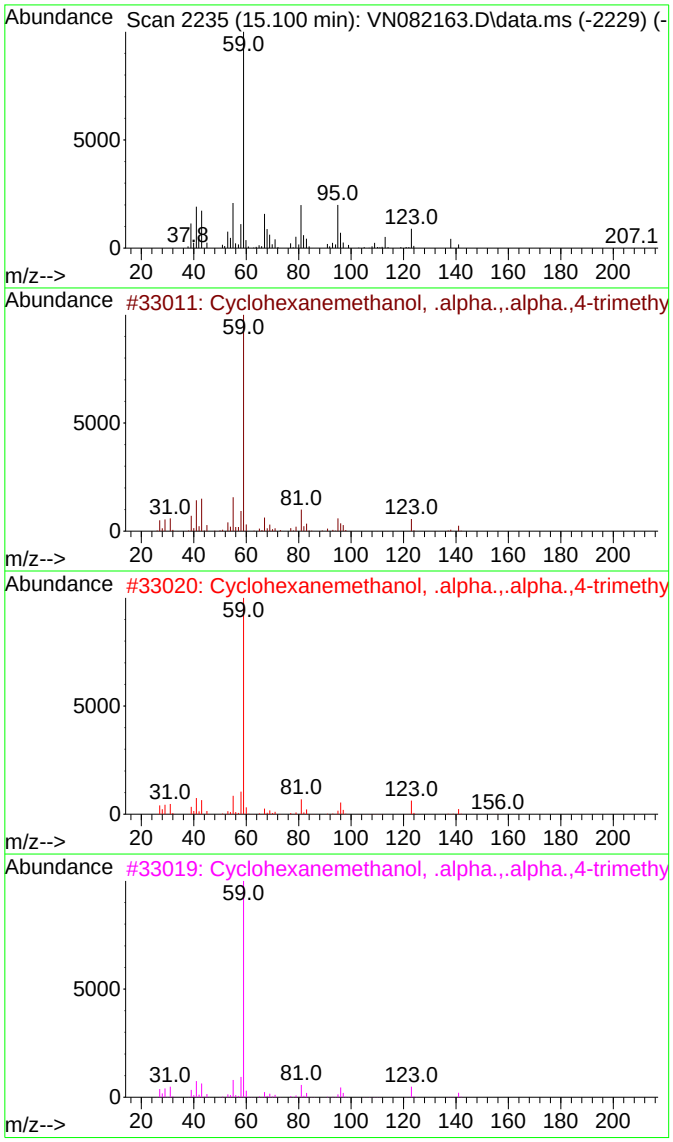
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

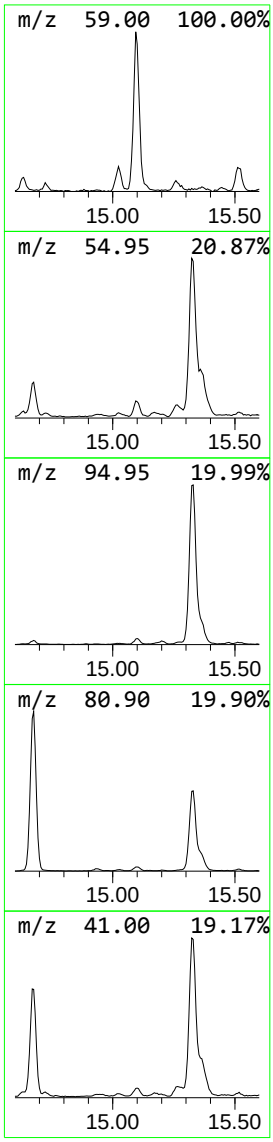
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	11.59 ug/l	242703	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	59
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	53
3	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	53
4	2-Decanol, methyl ether	172	C11H24O	1000333-83-9	47
5	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

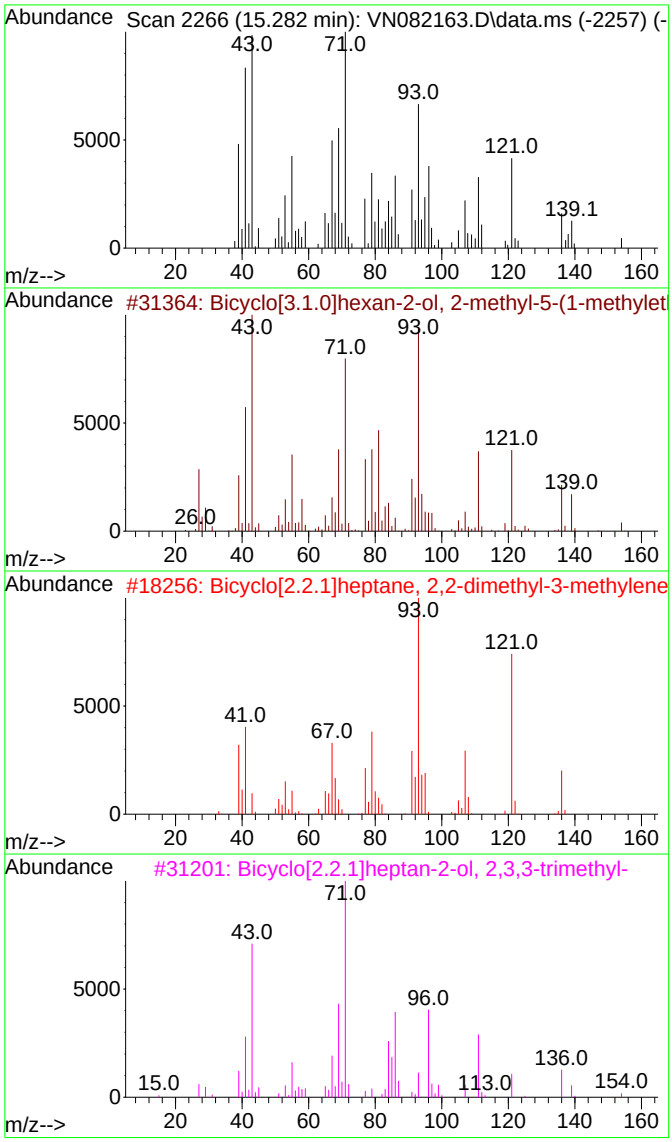
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

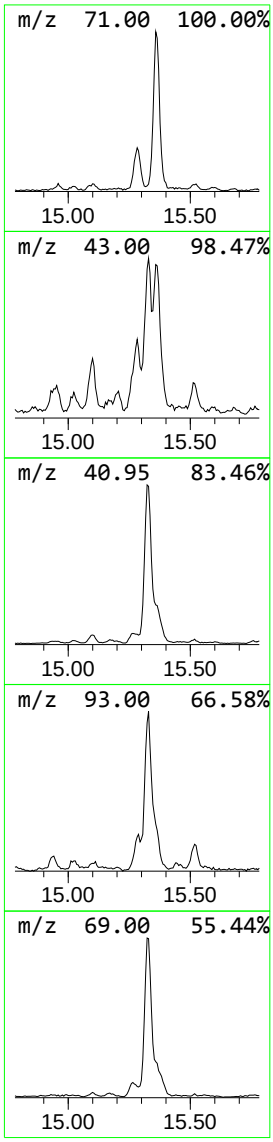
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bicyclo[3.1.0]hexan-2-ol, 2... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.282	12.42 ug/l	260055	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.0]hexan-2-ol, 2-meth...	154	C10H18O	015537-55-0	83
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	72
3	Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	64
4	Bicyclo[4.1.0]heptane, 7-(1-meth...	136	C10H16	053282-47-6	51
5	Camphene	136	C10H16	000079-92-5	48





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

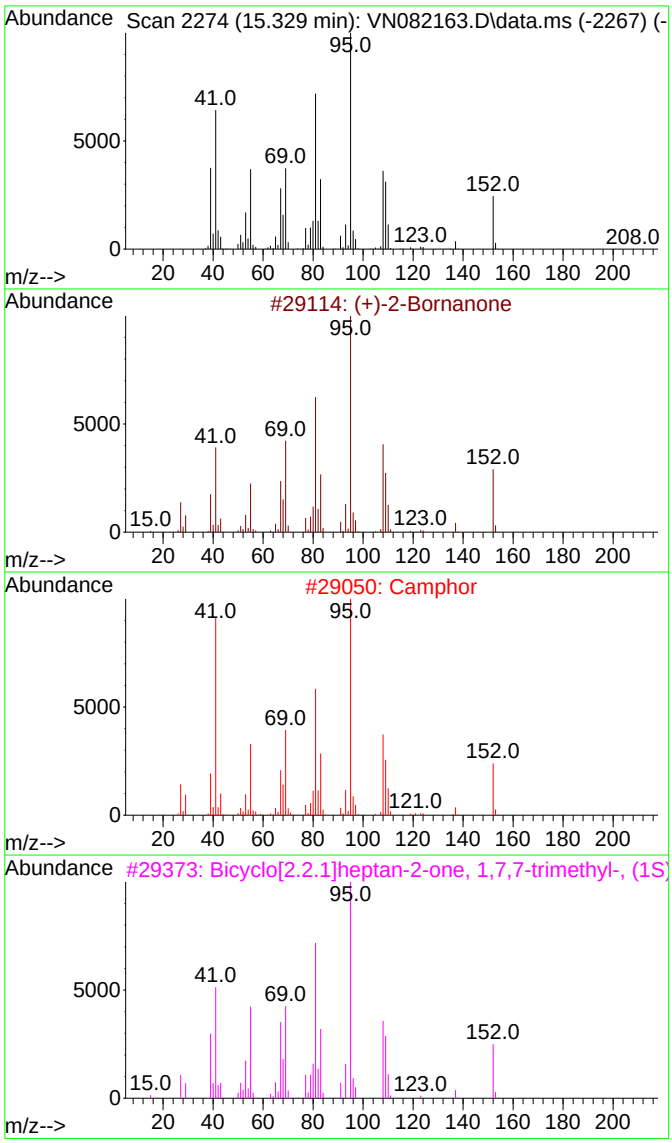
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

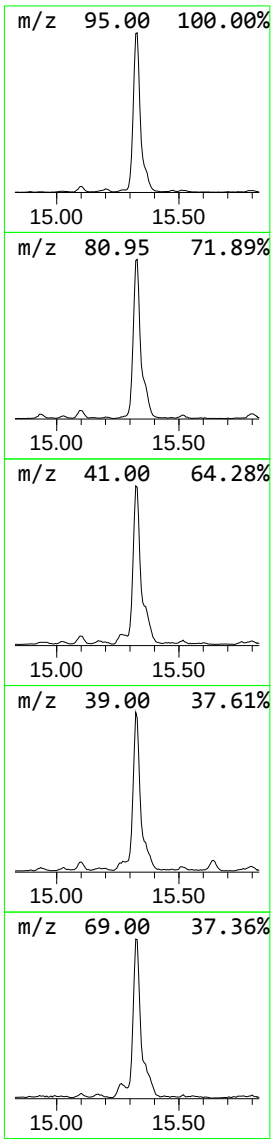
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.329	180.74 ug/l	3785630	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	58
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

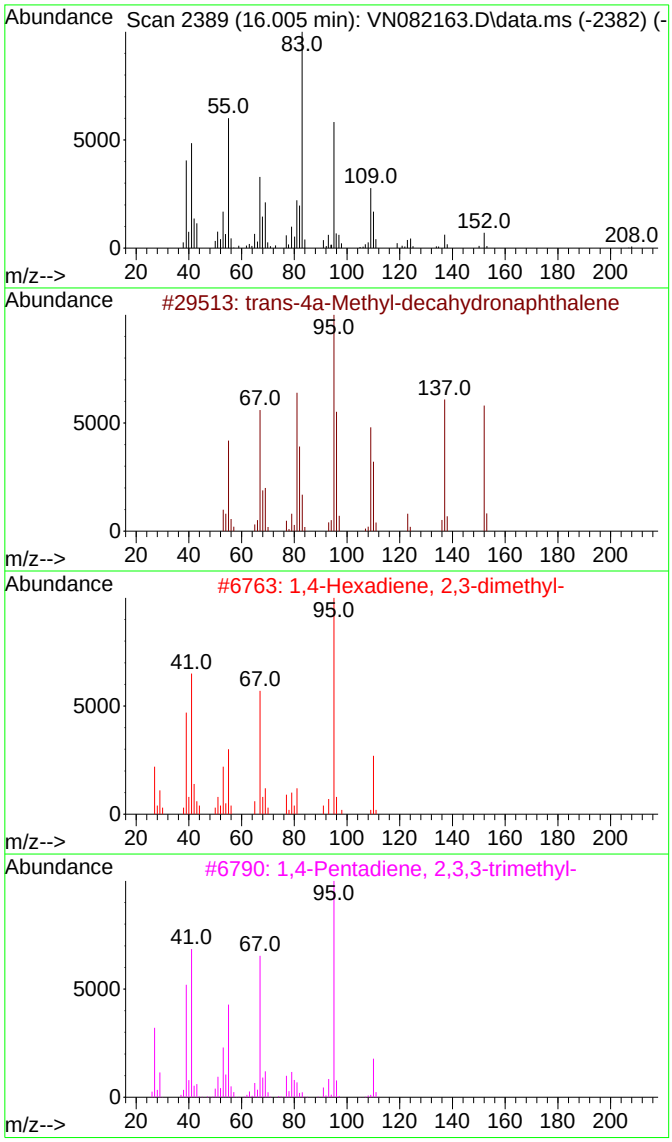
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.M
Quant Title : SW846 8260

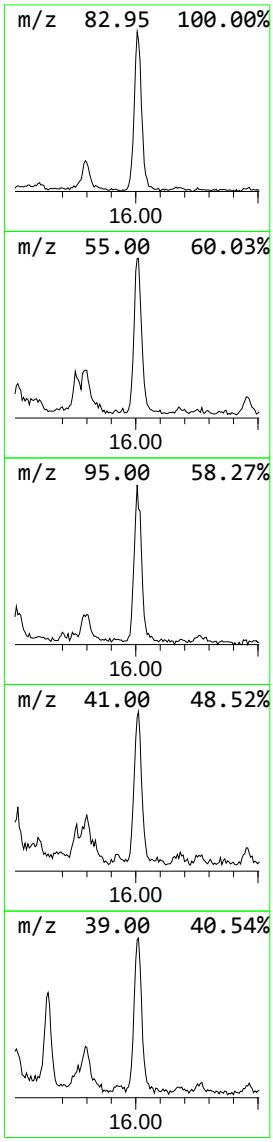
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.006 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	15.20 ug/l	318323	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
2	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	46
3	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	35
4	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	30
5	trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051624\
Data File : VN082163.D
Acq On : 16 May 2024 15:43
Operator : JC\MD
Sample : P2502-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
240515064-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051524W.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	26.5	ug/l	321266	1	8.224	606521	50.0
Methanethiol	2.824	15.0	ug/l	182328	1	8.224	606521	50.0
Acetic acid, hy...	8.659	14.8	ug/l	179680	1	8.224	606521	50.0
3-Pentanone, 2,...	11.171	13.7	ug/l	318029	3	11.865	1160620	50.0
Fenchone	14.676	80.1	ug/l	1676830	4	13.794	1047250	50.0
Cyclohexanemeth...	15.100	11.6	ug/l	242703	4	13.794	1047250	50.0
Bicyclo[3.1.0]h...	15.282	12.4	ug/l	260055	4	13.794	1047250	50.0
(+)-2-Bornanone	15.329	180.7	ug/l	3785630	4	13.794	1047250	50.0
unknown16.006	16.006	15.2	ug/l	318323	4	13.794	1047250	50.0