LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

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\82N122220W.M
Title : SW846 8260

Signal : TIC: VN065432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	453	474	511	rBV	2098750	5231632	8.73%	1.973%
2	3.859	643	659	701	rVB	2136660	5641700	9.41%	2.128%
3	4.129	731	743	765	rVB	363227	1008538	1.68%	0.380%
4	6.611	1496	1515	1548	rVB	457646	1378454	2.30%	0.520%
5	7.630	1820	1832	1858	rVB	352508	858735	1.43%	0.324%
6	8.007	1926	1949	1979	rBV	10394012	26441295	44.10%	9.972%
7	8.241	2006	2022	2049	rVB4	305401	903437	1.51%	0.341%
8	8.553	2103	2119	2153	rVB	534857	1132765	1.89%	0.427%
9	8.765	2168	2185	2199	rBV	1619497	3318438	5.54%	1.252%
10	10.061	2575	2588	2596	rBV	866645	1594745	2.66%	0.601%
11	10.126	2596	2608	2631	rVV	11511484	23088672	38.51%	8.708%
12	11.380	2984	2998	3018	rBV	889583	1688735	2.82%	0.637%
13	11.482	3018	3030	3045	rVV	2721666	4722434	7.88%	1.781%
14	11.592	3045	3064	3084	rVB	8263957	16362587	27.29%	6.171%
15	11.695	3085	3096	3115	rBV3	557211	1395507	2.33%	0.526%
16	11.788	3115	3125	3143	rVB	2905226	4686424	7.82%	1.768%
17	11.933	3155	3170	3186	rBV4	13239763	28523040	47.58%	10.758%
18	12.019	3187	3197	3208	rVB2	256536	625810	1.04%	0.236%
19	12.171	3235	3244	3252	rBV	681032	1114525	1.86%	0.420%
20	12.222	3252	3260	3280	rVB5	709162	1515963	2.53%	0.572%
21	12.376	3296	3308	3317	rBV	853592	1421772	2.37%	0.536%
22	12.431	3317	3325	3335	rVV	361323	678094	1.13%	0.256%
23	12.630	3378	3387	3394	rBV	626644	1061056	1.77%	0.400%
24	12.704	3402	3410	3417	rBV	712329	1059258	1.77%	0.400%
25	12.743	3418	3422	3448	rVB7	501254	1098358	1.83%	0.414%
26	12.878	3449	3464	3482	rBV4	584035	1503100	2.51%	0.567%
27	13.013	3497	3506	3514	rBV	2078843	3228257	5.38%	1.218%
28	13.064	3514	3522	3531	rVB	1912456	2910926	4.86%	1.098%
29	13.116	3531	3538	3543	rBV	597031	920744	1.54%	0.347%
30	13.235	3564	3575	3587	rVB	1963763	3412824	5.69%	1.287%
31	13.318	3589	3601	3605	rVV	1055927	1815716	3.03%	0.685%
32	13.347	3606	3610	3617	rVV	1329195	1865427	3.11%	0.704%
33	13.392	3617	3624	3645	rVB4	863595	1682109	2.81%	0.634%
34	13.518	3653	3663	3673	rBV	1008325	1658092	2.77%	0.625%
35	13.698	3704	3719	3735	rVB	18287937	35132684	58.60%	13.250%
36	13.804	3737	3752	3763	rBV7	251778	681498	1.14%	0.257%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

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\82N122220W.M
Title : SW846 8260

37	14.064	3823	3833	3851	rVB	702523	1347136	2.25%	0.508%
38	14.151	3851	3860	3868	rBV2	371340	629374	1.05%	0.237%
39	14.248	3876	3890	3905	rVB2	464161	1336767	2.23%	0.504%
40	14.569	3977	3990	3997	rBV5	394479	823284	1.37%	0.311%
41	14.630	3998	4009	4022	rVB2	639574	1256537	2.10%	0.474%
42	14.711	4023	4034	4047	rBV	890719	1498786	2.50%	0.565%
43	15.106	4136	4157	4172	rBV2	29067722	59952209	100.00%	22.611%
44	15.196	4173	4185	4201	rVB	1904048	3417706	5.70%	1.289%
45	16.119	4460	4472	4488	rVB	995798	1966965	3.28%	0.742%
46	16.309	4517	4531	4552	rVB	727944	1550704	2.59%	0.585%

Sum of corrected areas: 265142819

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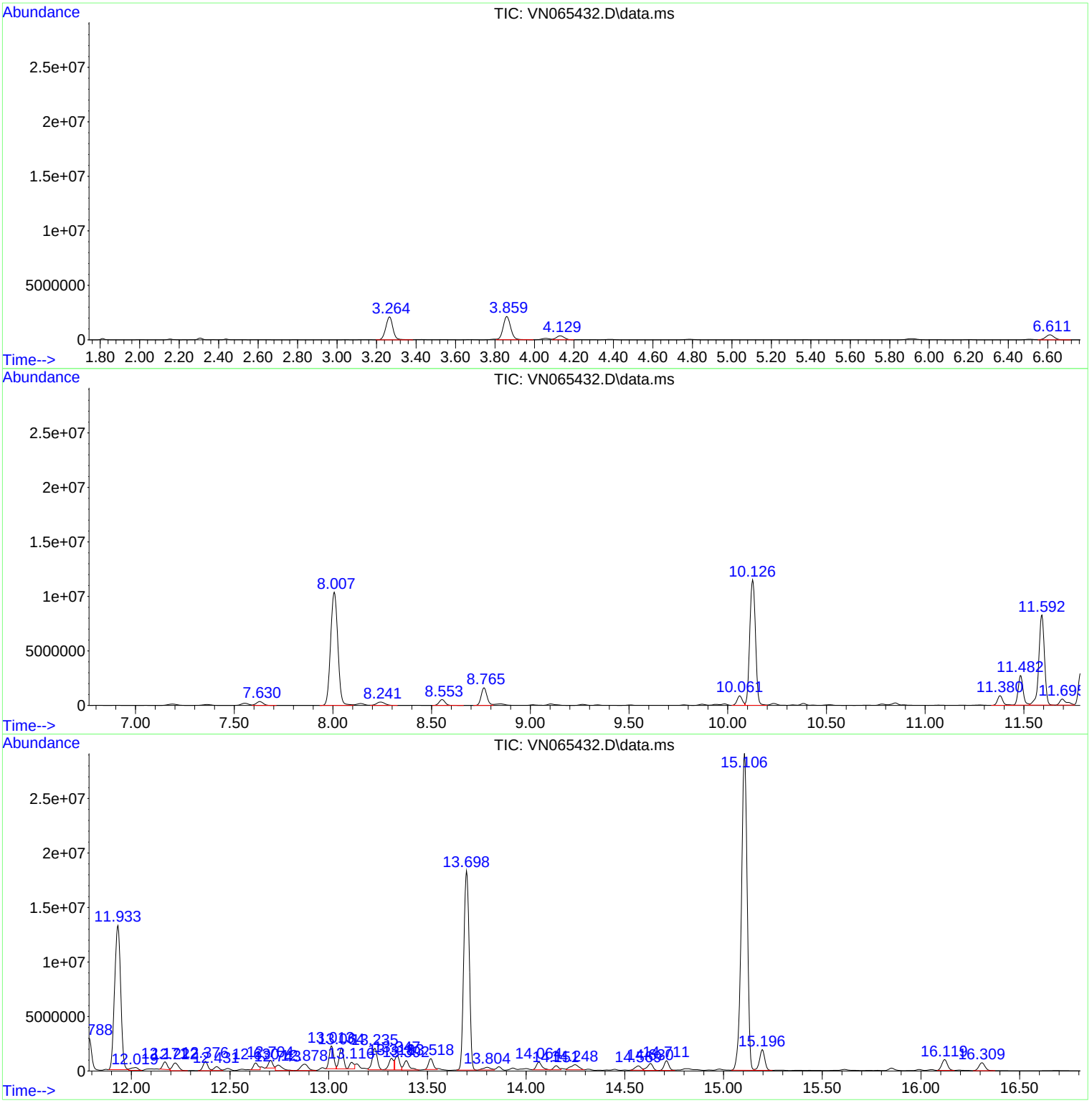
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30733

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30733

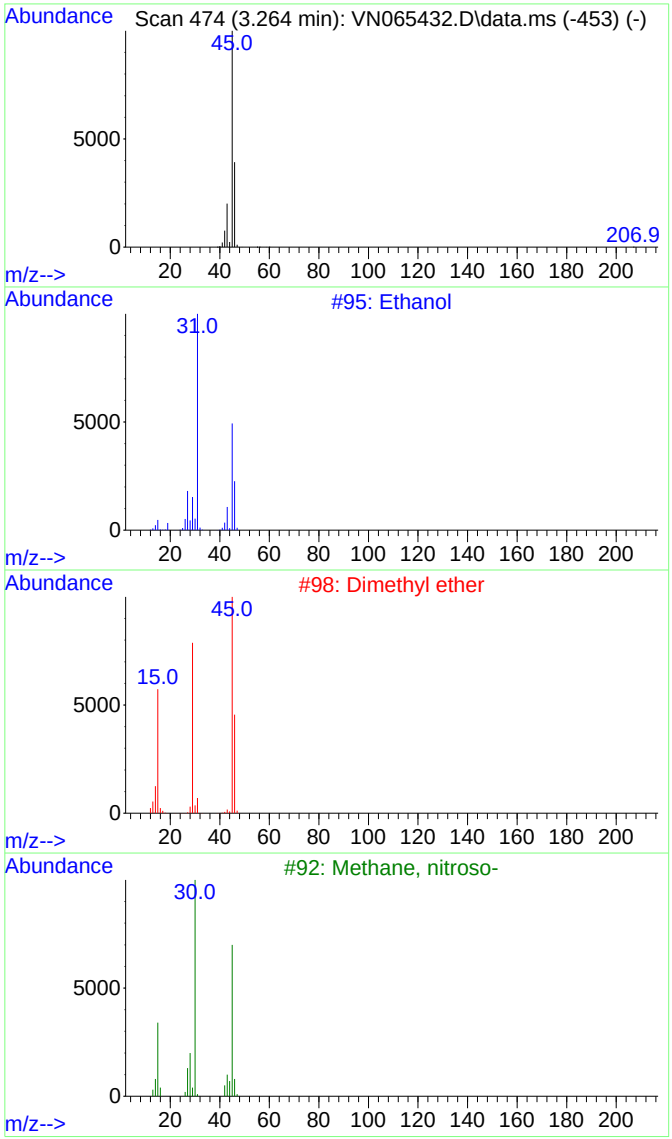
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

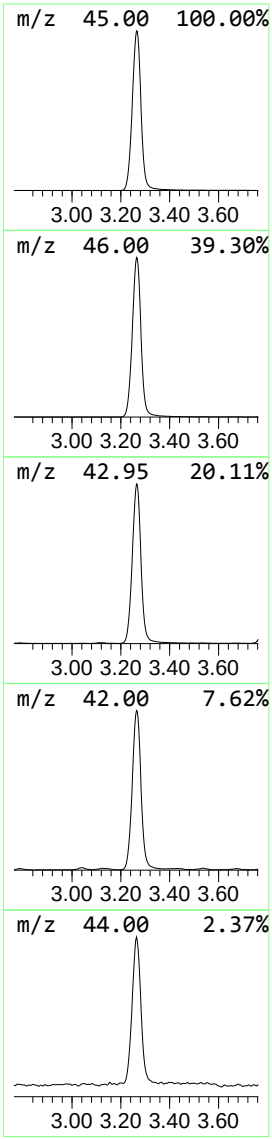
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.264	304.61 ug/l	5231630	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

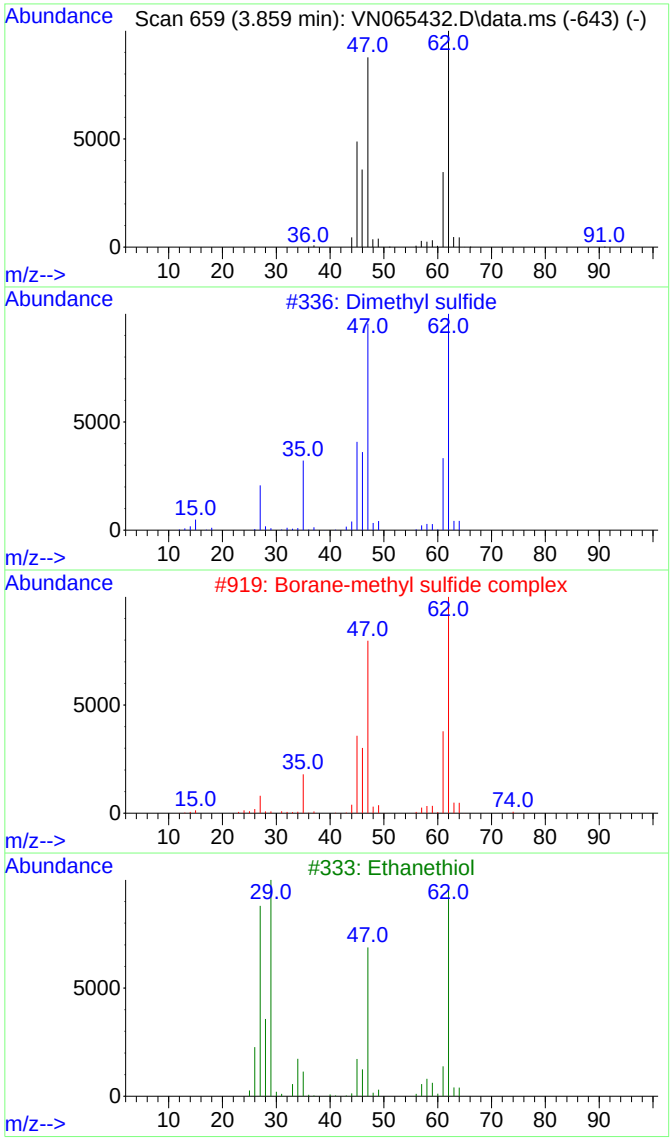
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

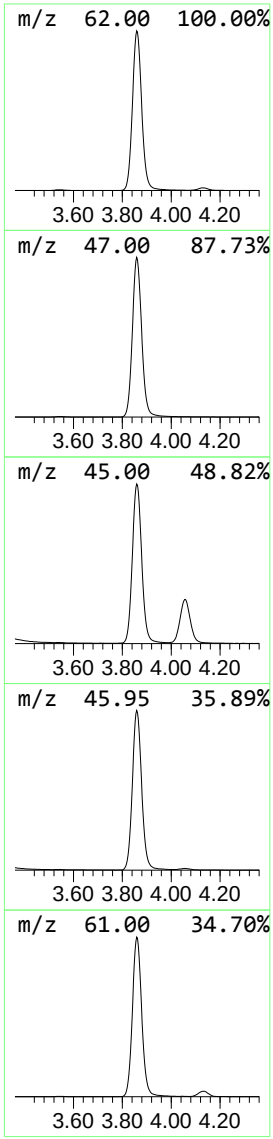
****

Peak Number 2 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.859	328.49 ug/l	5641700	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3	Ethanethiol	62	C2H6S	000075-08-1	78
4	Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5	Propane, 2-fluoro-	62	C3H7F	000420-26-8	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

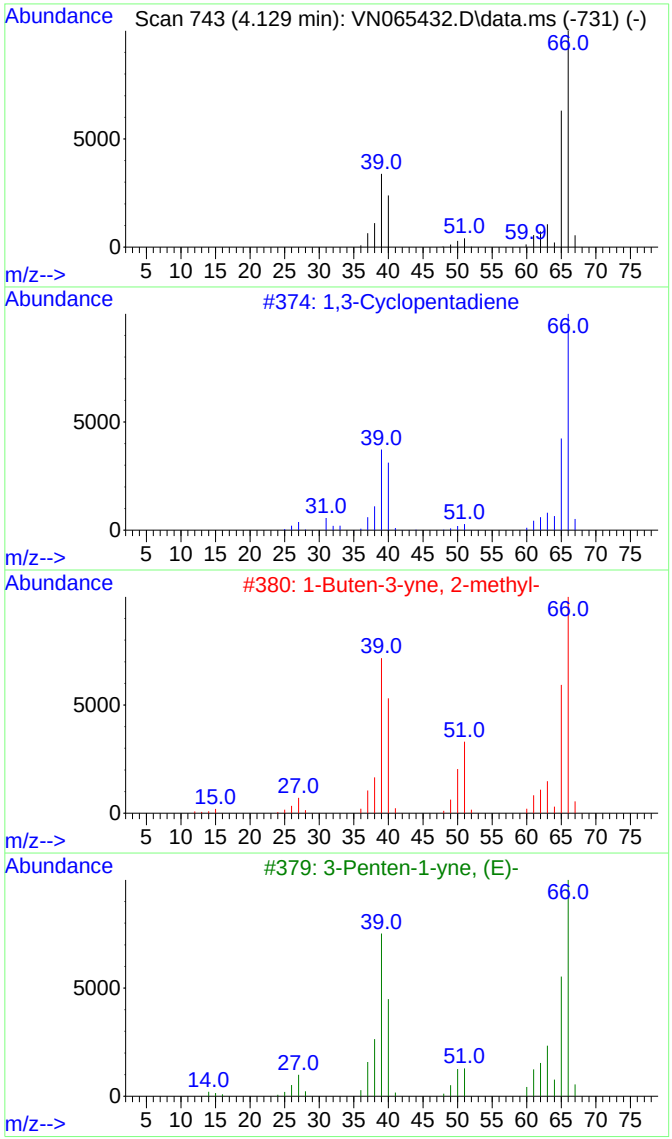
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

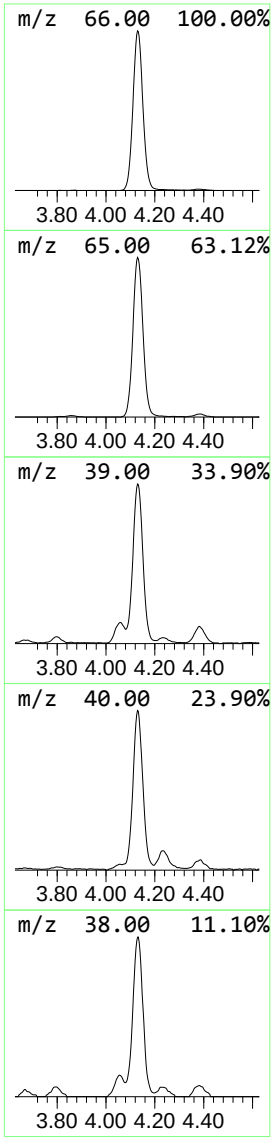
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3-Cyclopentadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.129	58.72 ug/l	1008540	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentadiene	66	C5H6	000542-92-7	91
2	1-Buten-3-yne, 2-methyl-	66	C5H6	000078-80-8	91
3	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	83
4	3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	83
5	1-Penten-3-yne	66	C5H6	000646-05-9	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

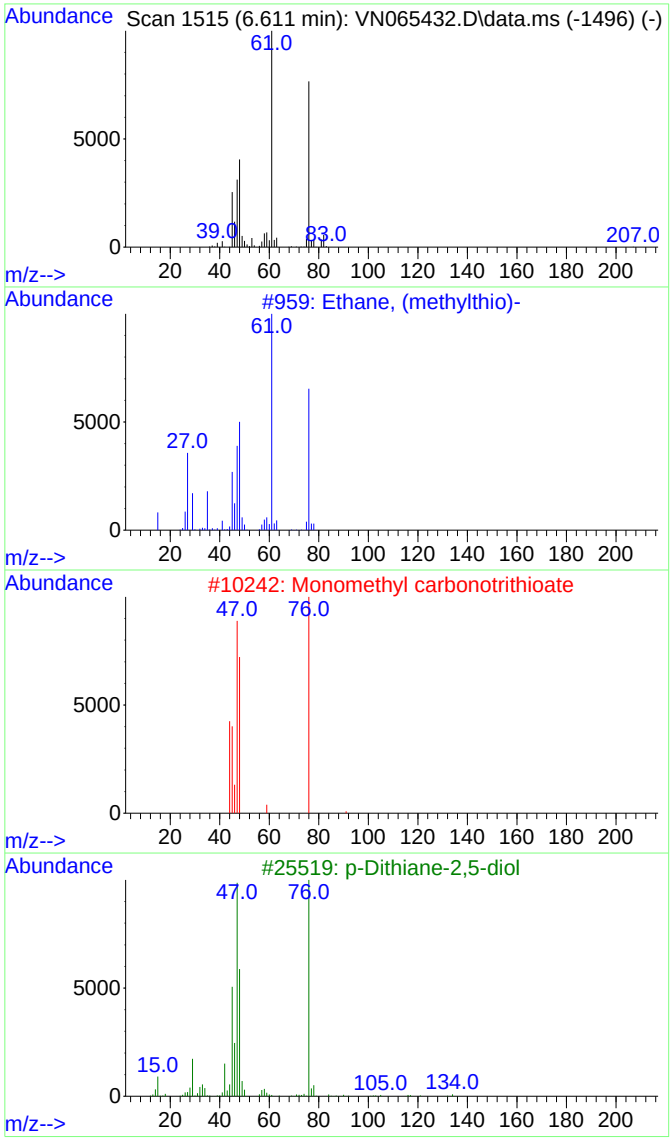
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

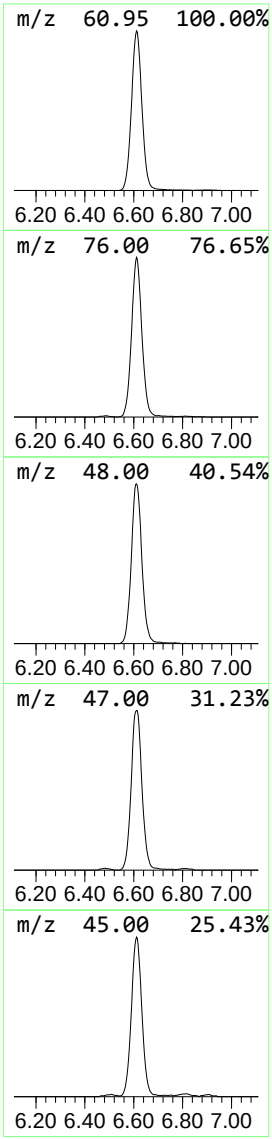
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethane, (methylthio)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.611	80.26 ug/l	1378450	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, (methylthio)-	76	C3H8S	000624-89-5	95
2	Monomethyl carbonotrithioate	124	C2H4S3	001113-26-4	45
3	p-Dithiane-2,5-diol	152	C4H8O2S2	040018-26-6	45
4	Propyl mercaptan	76	C3H8S	000107-03-9	42
5	Trimethylphosphine	76	C3H9P	000594-09-2	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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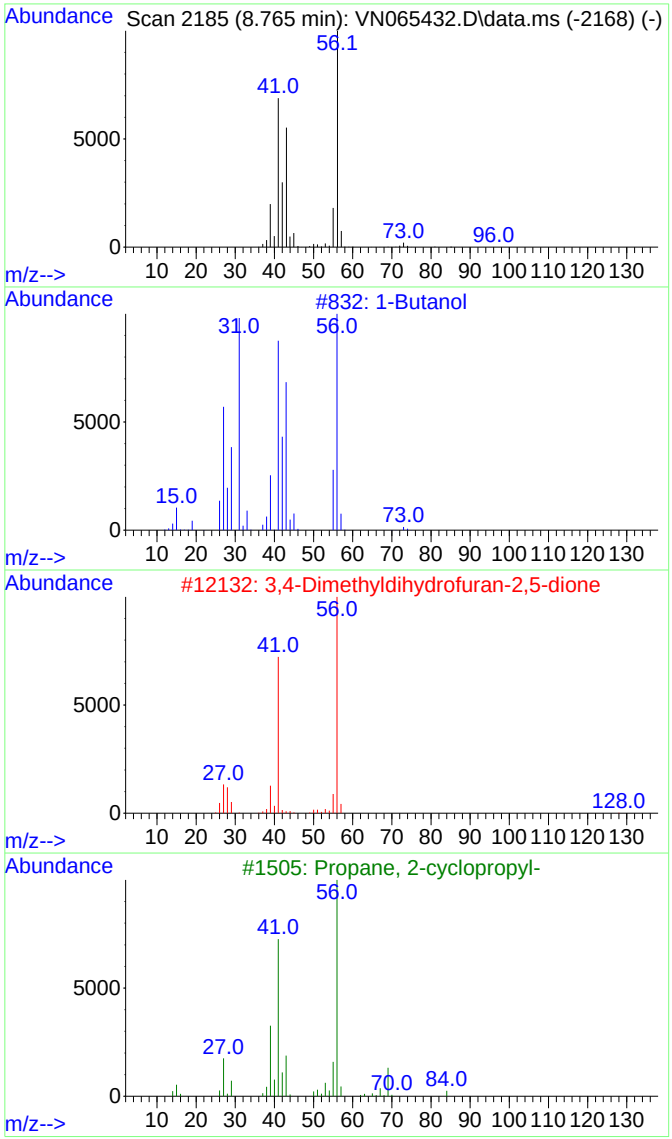
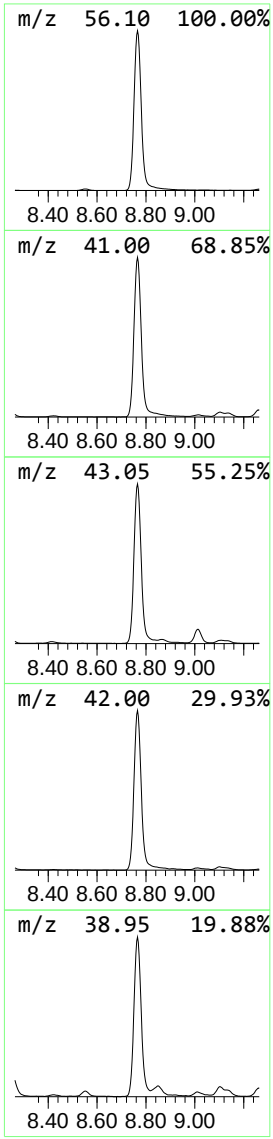
****
Peak Number 5 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	146.47 ug/l	3318440	1,4-Difluorobenzene	8.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
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Misc : 5.00mL/MSVOA_N/WATER
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Instrument : MSVOA_N
ClientSampleId : 30733

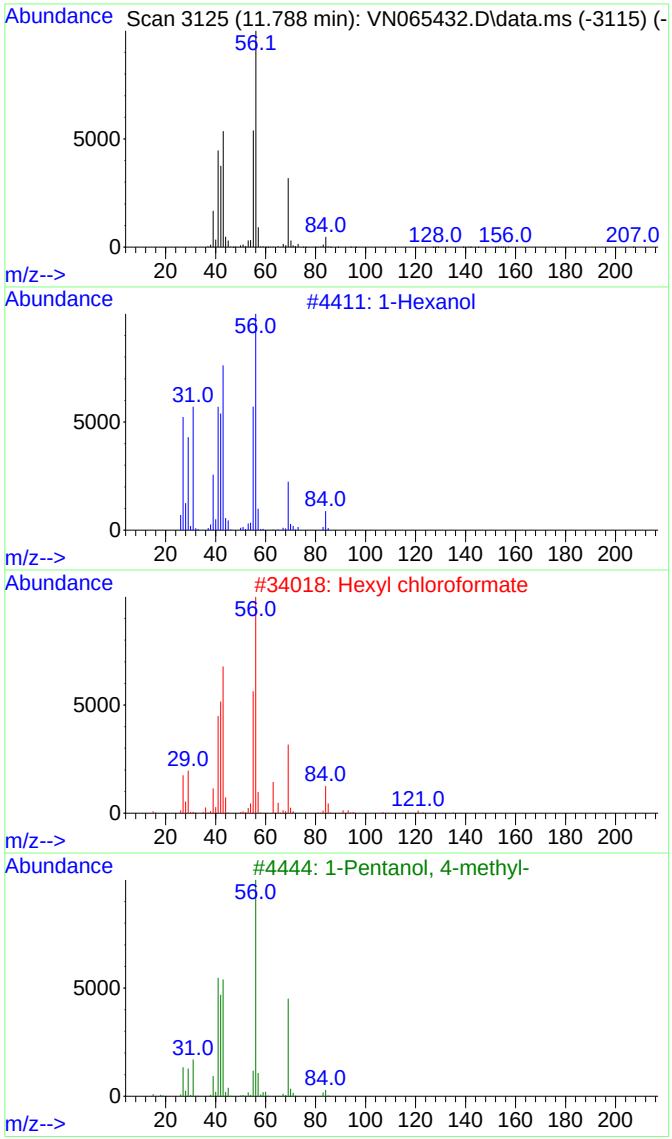
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

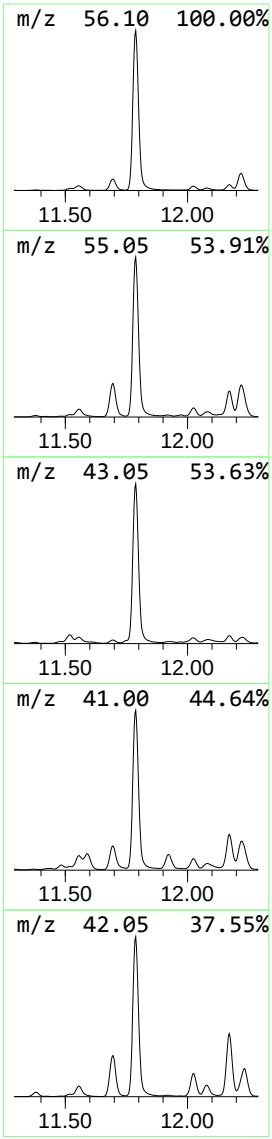
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.788	138.76 ug/l	4686420	Chlorobenzene-d5	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5	Cyclopropane, propyl-	84	C6H12	002415-72-7	72





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ClientSampleId : 30733

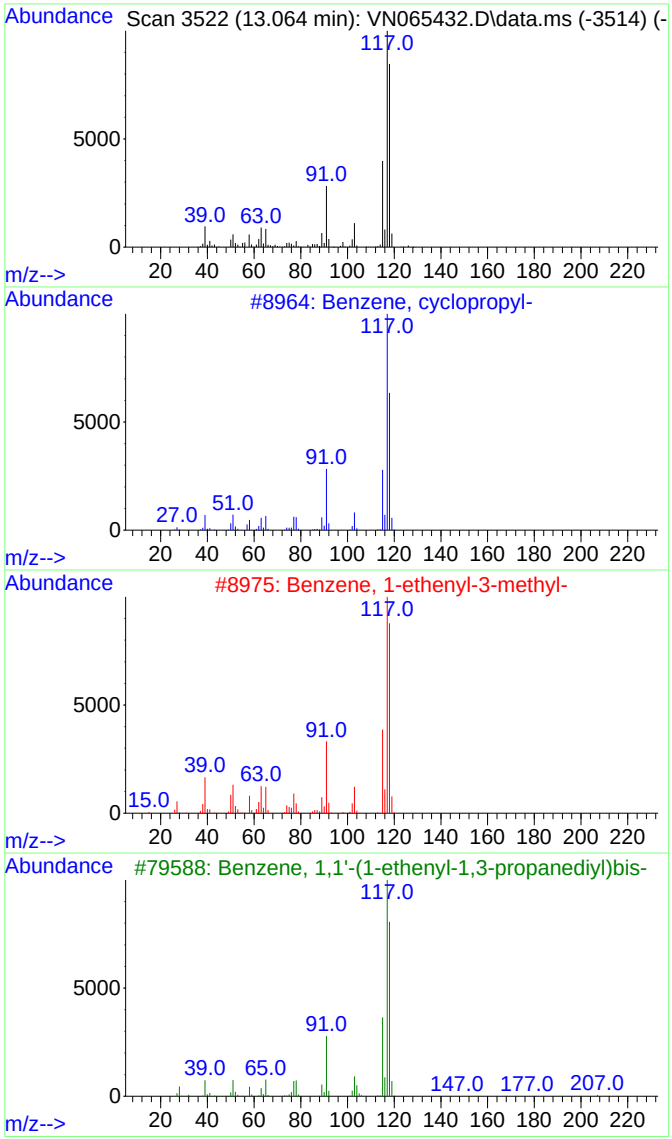
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

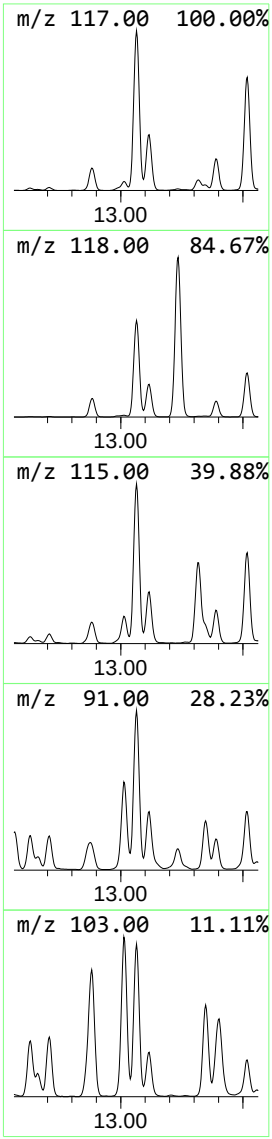
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, cyclopropyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.064	80.16 ug/l	2910930	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
2	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	90
3	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	90
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

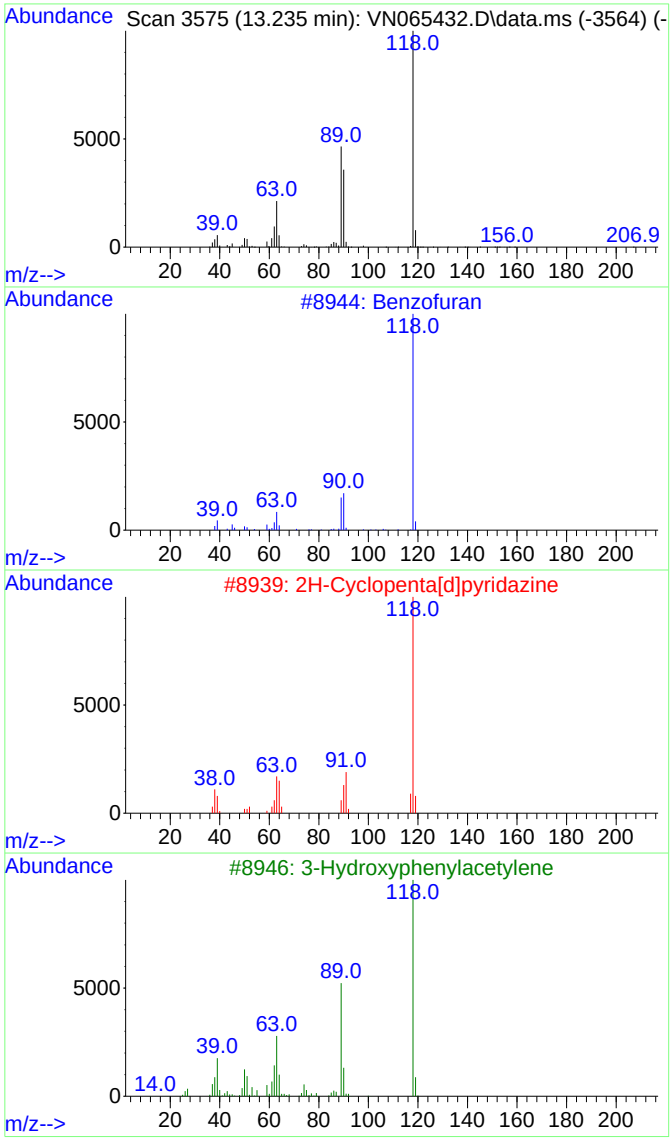
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

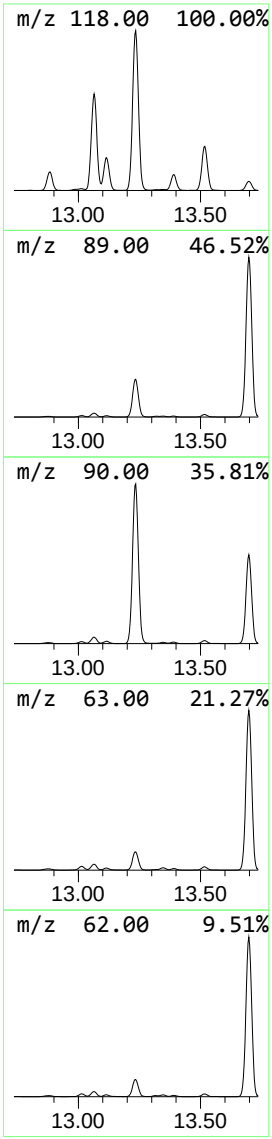
****

Peak Number 8 Benzofuran Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.235	93.98 ug/l	3412820	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzofuran	118	C8H6O	000271-89-6	91
2	2H-Cyclopenta[d]pyridazine	118	C7H6N2	000270-64-4	64
3	3-Hydroxyphenylacetylene	118	C8H6O	010401-11-3	47
4	1H-Pyrrolo[2,3-b]pyridine	118	C7H6N2	000271-63-6	45
5	3-Pyridineacetonitrile	118	C7H6N2	006443-85-2	42





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Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

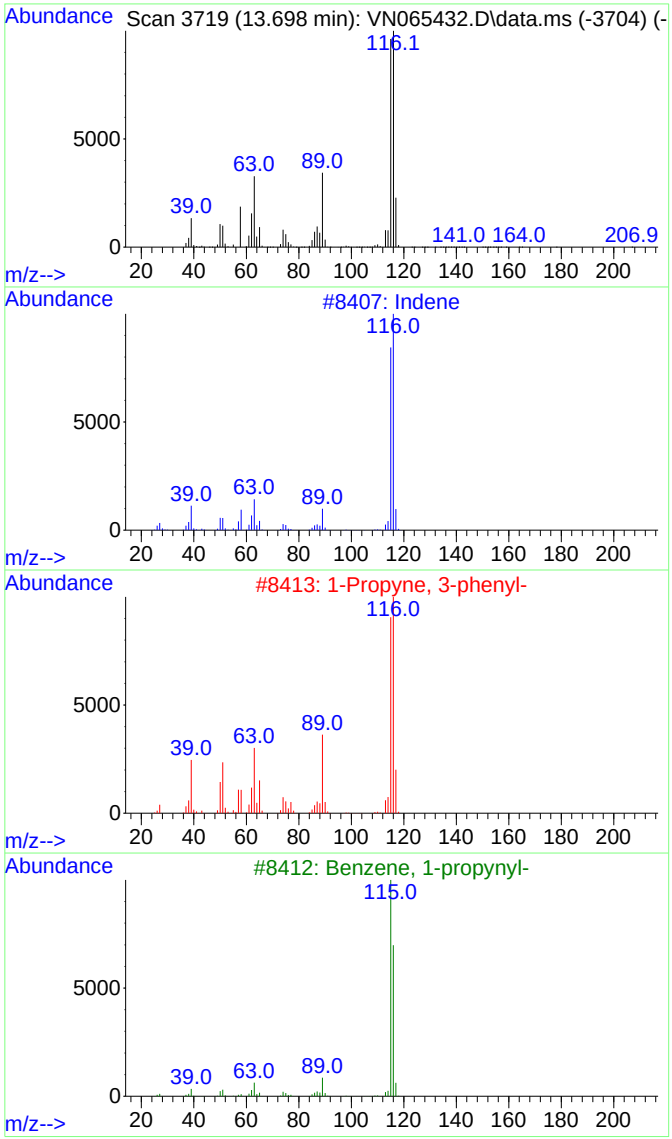
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

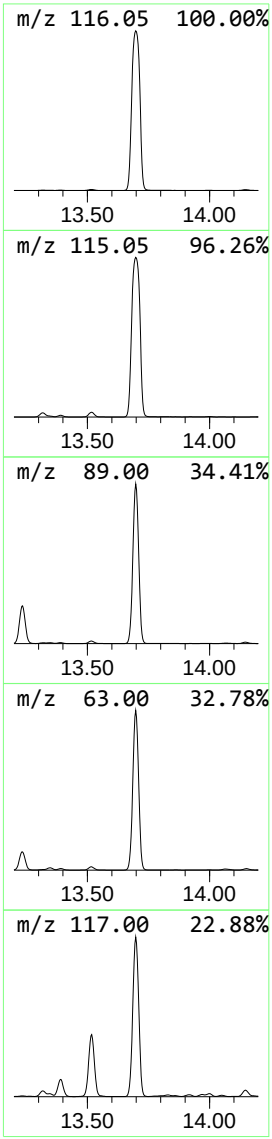
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	967.46 ug/l	35132700	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	94
3	Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80
5	3-Methylphenylacetylene	116	C9H8	000766-82-5	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

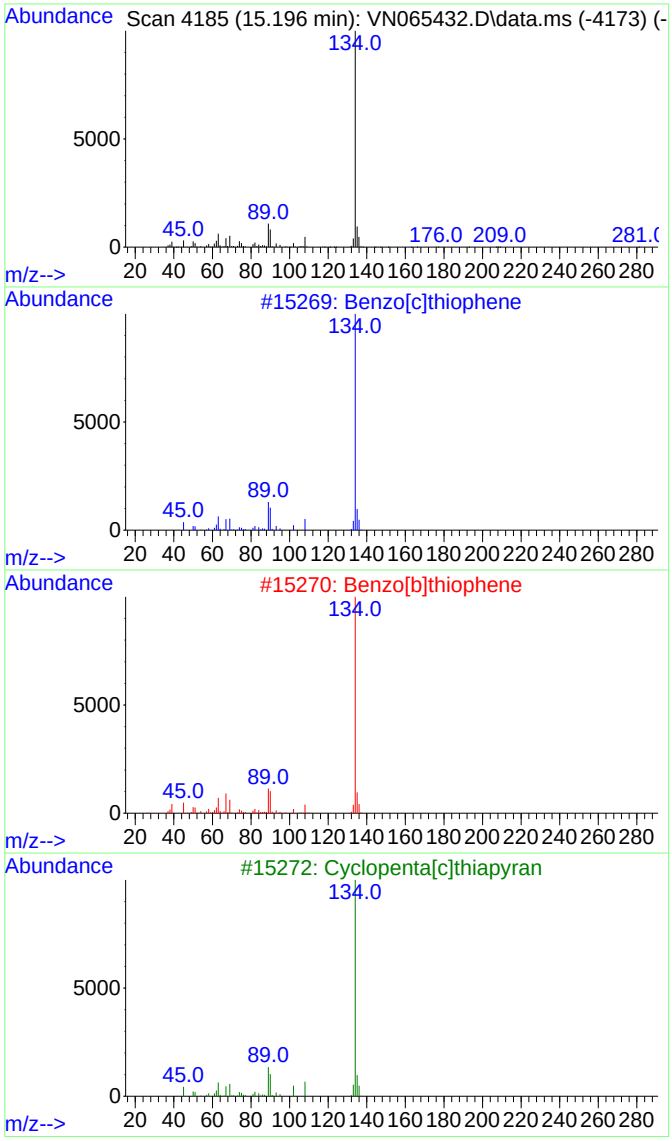
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

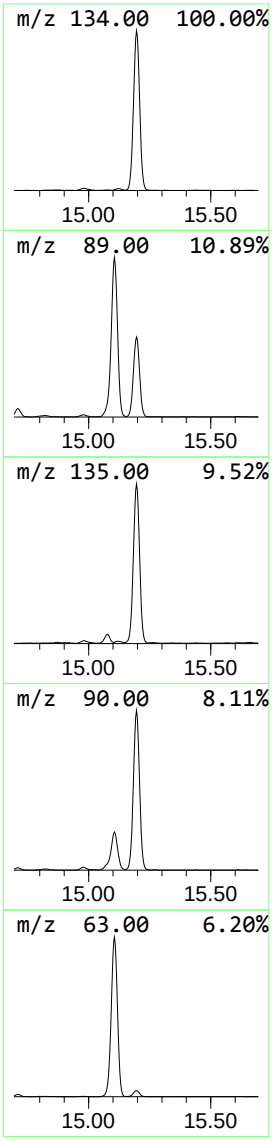
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzo[c]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	94.11 ug/l	3417710	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	94
4	[1]Benzothieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5	5H-Pyrrolo(3,2-d)pyrimidin-4-amine	134	C6H6N4	002227-98-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065432.D
Acq On : 7 Jan 2021 17:19
Operator : JC/MD
Sample : M1022-13
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30733

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.264	304.6	ug/l	5231630	1	7.630	858735	50.0
Dimethyl sulfide	3.859	328.5	ug/l	5641700	1	7.630	858735	50.0
1,3-Cyclopentad...	4.129	58.7	ug/l	1008540	1	7.630	858735	50.0
Ethane, (methyl...	6.611	80.3	ug/l	1378450	1	7.630	858735	50.0
1-Butanol	8.765	146.5	ug/l	3318440	2	8.553	1132770	50.0
1-Hexanol	11.788	138.8	ug/l	4686420	3	11.380	1688740	50.0
Benzene, cyclop...	13.064	80.2	ug/l	2910930	4	13.318	1815720	50.0
Benzofuran	13.235	94.0	ug/l	3412820	4	13.318	1815720	50.0
Indene	13.698	967.5	ug/l	35132700	4	13.318	1815720	50.0
Benzo[c]thiophene	15.196	94.1	ug/l	3417710	4	13.318	1815720	50.0