LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

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: VN065431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.303	162	175	204	rBV	976153	1641493	4.33%	1.140%
2	3.267	454	475	513	rBV	1972173	4973370	13.11%	3.454%
3	3.791	621	638	647	rBV	249160	625106	1.65%	0.434%
4	3.859	647	659	701	rVB	604436	1612220	4.25%	1.120%
5	4.055	703	720	735	rBV	143213	408943	1.08%	0.284%
6	6.505	1461	1482	1500	rBV	251710	762881	2.01%	0.530%
7	6.611	1500	1515	1542	rVB	131847	407902	1.08%	0.283%
8	7.553	1792	1808	1819	rBV	199050	492717	1.30%	0.342%
9	7.627	1819	1831	1860	rVB	342913	829514	2.19%	0.576%
10	8.004	1928	1948	1978	rBV	3620259	8776394	23.14%	6.095%
11	8.553	2103	2119	2139	rBV	534862	1114949	2.94%	0.774%
12	8.766	2166	2185	2227	rBV	1499142	3259867	8.59%	2.264%
13	10.061	2574	2588	2596	rBV	873126	1618209	4.27%	1.124%
14	10.126	2596	2608	2632	rVB	4007551	7337421	19.34%	5.096%
15	11.380	2985	2998	3018	rBV	907846	1623966	4.28%	1.128%
16	11.482	3019	3030	3045	rVV	1029177	1963104	5.17%	1.363%
17	11.589	3045	3063	3084	rVB	3689288	7443064	19.62%	5.169%
18	11.695	3085	3096	3114	rBV4	491640	1018571	2.69%	0.707%
19	11.788	3114	3125	3144	rBV	1940002	3154457	8.32%	2.191%
20	11.923	3154	3167	3185	rBV4	5035467	10799431	28.47%	7.501%
21	12.100	3209	3222	3234	rVV9	137058	507448	1.34%	0.352%
22	12.171	3236	3244	3252	rVV	594034	1006068	2.65%	0.699%
23	12.222	3252	3260	3279	rVB3	568087	1215466	3.20%	0.844%
24	12.376	3297	3308	3317	rBV	817450	1328482	3.50%	0.923%
25	12.431	3317	3325	3336	rVB	257935	431067	1.14%	0.299%
26	12.630	3378	3387	3394	rBV	601857	1006518	2.65%	0.699%
27	12.704	3402	3410	3418	rBV	929599	1418892	3.74%	0.985%
28	12.868	3449	3461	3478	rBV4	421614	1060583	2.80%	0.737%
29	13.013	3497	3506	3515	rBV	2060288	3287855	8.67%	2.284%
30	13.064	3515	3522	3531	rVB	1028729	1598063	4.21%	1.110%
31	13.116	3531	3538	3542	rBV	284810	410554	1.08%	0.285%
32	13.232	3565	3574	3588	rVB	692025	1282371	3.38%	0.891%
33	13.315	3589	3600	3605	rBV	983957	1691864	4.46%	1.175%
34	13.347	3605	3610	3618	rVB	1068872	1554482	4.10%	1.080%
35	13.518	3653	3663	3672	rBV	743566	1223701	3.23%	0.850%
36	13.698	3706	3719	3736	rVB	10267745	18271433	48.16%	12.690%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

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	3824	3833	3850	rVB4	468959	934746	2.46%	0.649%
38	14.563	3977	3988	3997	rBV3	235654	522809	1.38%	0.363%
39	14.630	3998	4009	4022	rVB2	428874	838085	2.21%	0.582%
40	14.711	4023	4034	4044	rBV	629224	1093605	2.88%	0.760%
41	15.103	4137	4156	4172	rBV	18863077	37935205	100.00%	26.347%
42	15.196	4174	4185	4199	rVB	836524	1552998	4.09%	1.079%
43	15.852	4379	4389	4406	rVB	182474	387302	1.02%	0.269%
44	16.119	4460	4472	4487	rBV	978705	1944769	5.13%	1.351%
45	16.309	4517	4531	4554	rVB	763491	1613695	4.25%	1.121%

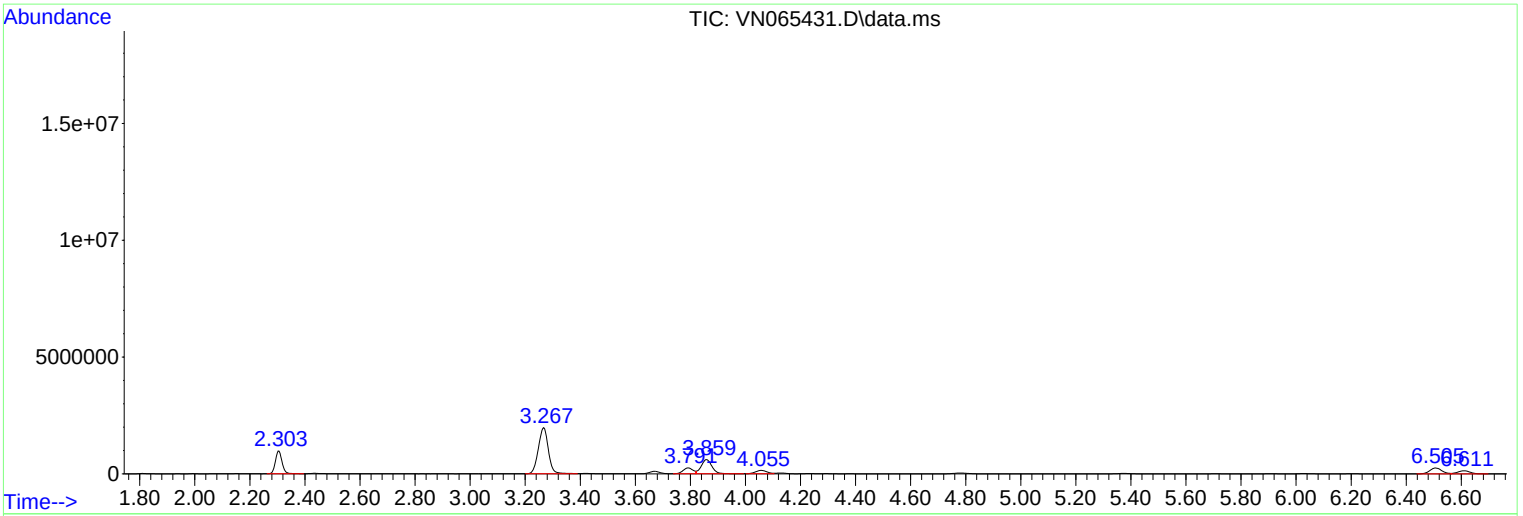
Sum of corrected areas: 143981640

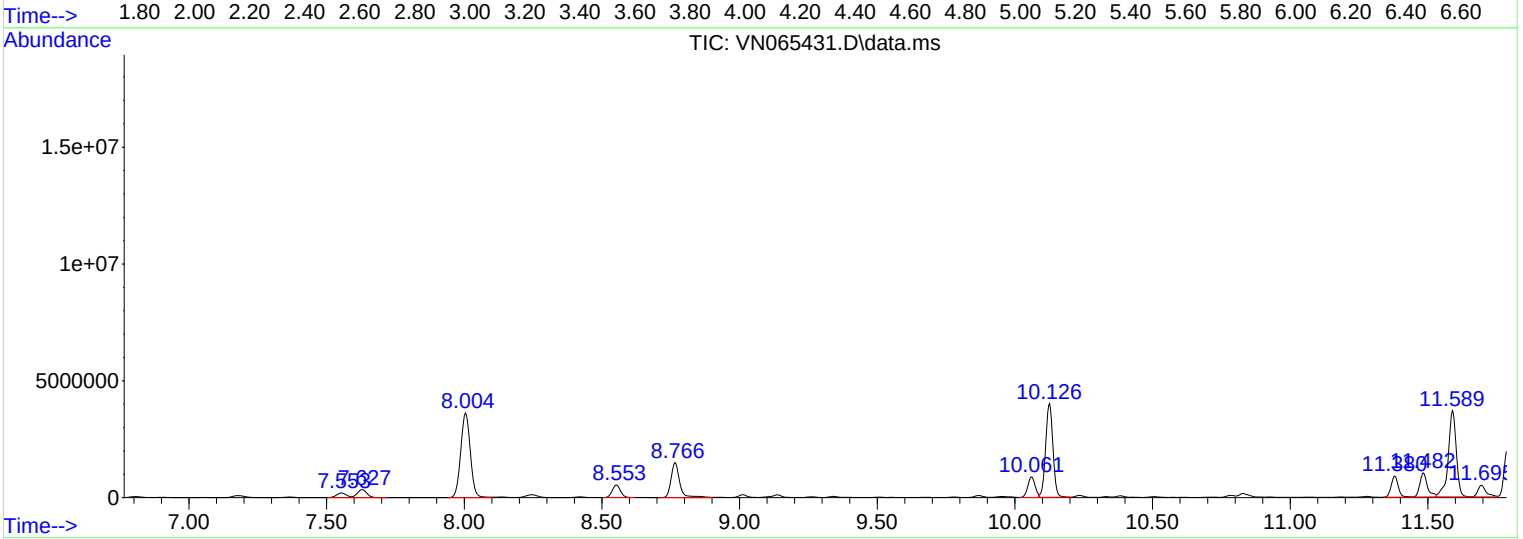
Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

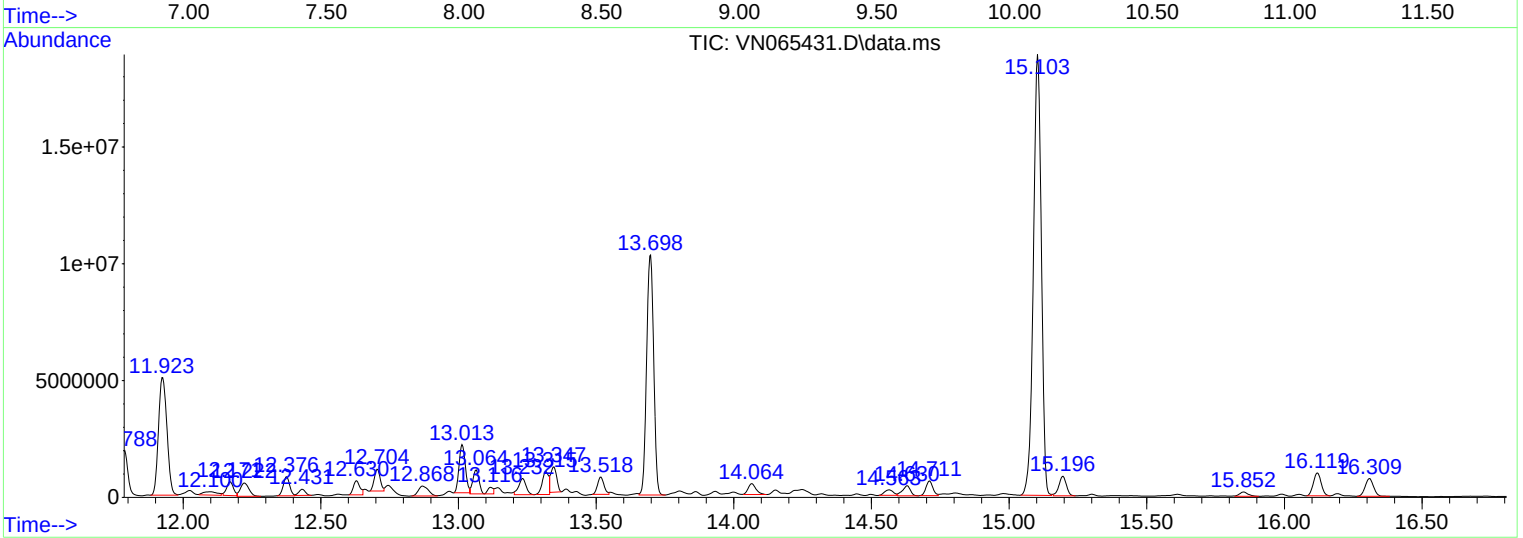
Instrument :
MSVOA_N
ClientSampleId :
30732

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 : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

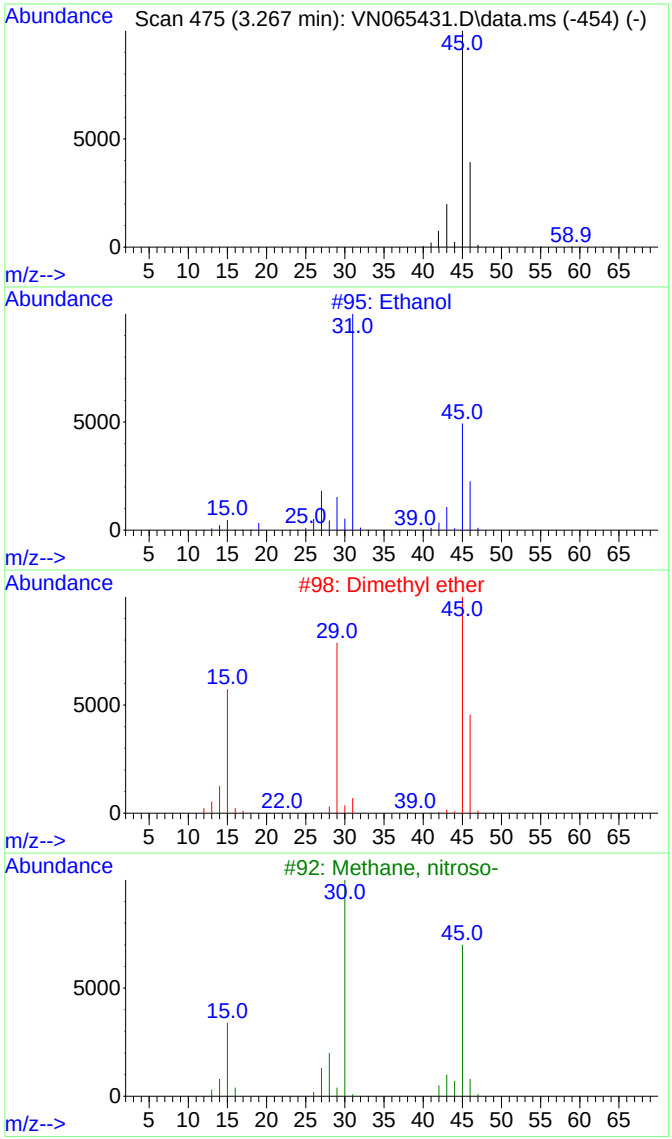
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

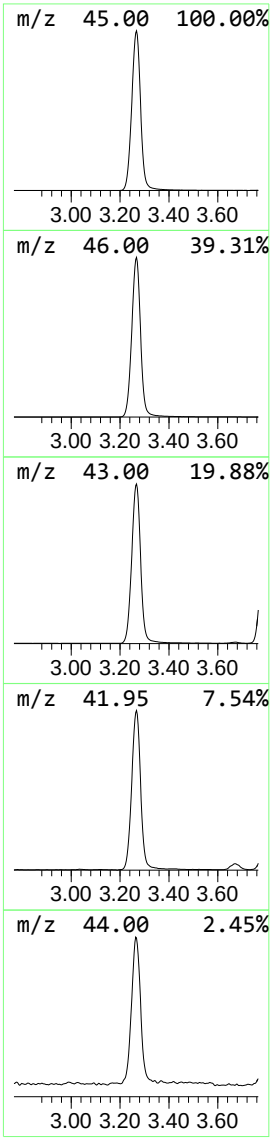
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.267	299.78 ug/l	4973370	Pentafluorobenzene	7.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	83
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 : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

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

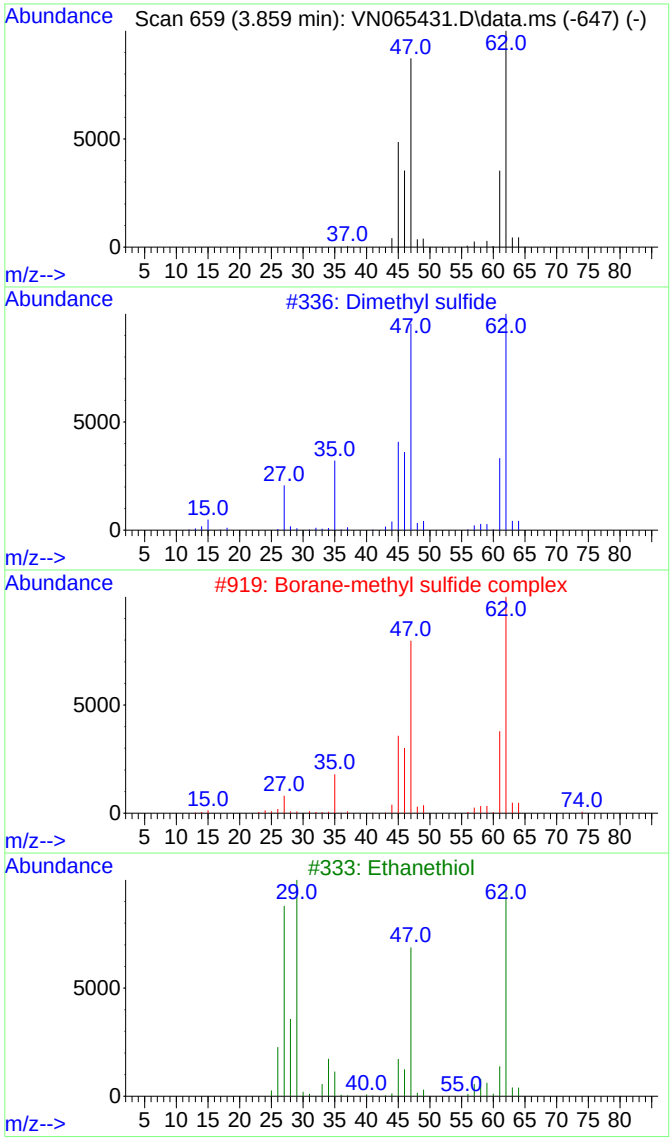
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

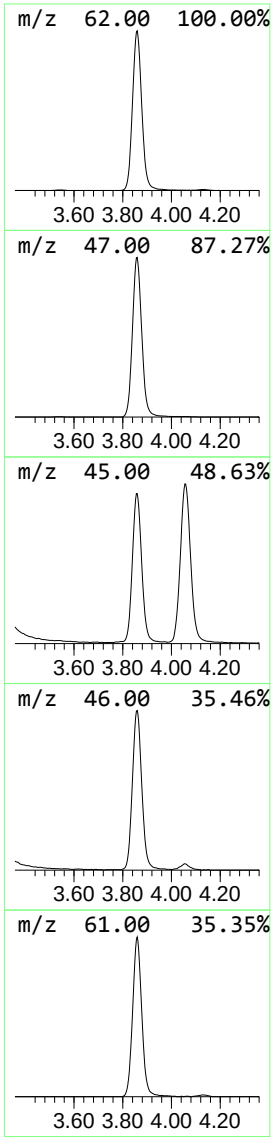
****

Peak Number 3 Dimethyl sulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.859	97.18 ug/l	1612220	Pentafluorobenzene	7.631

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 : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

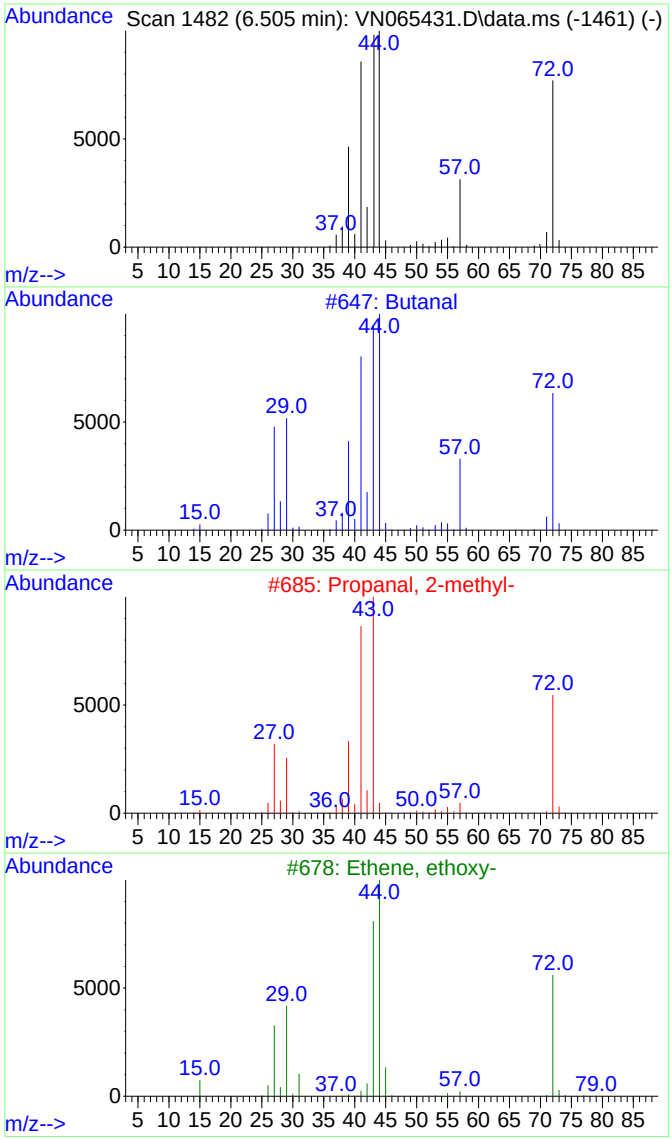
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

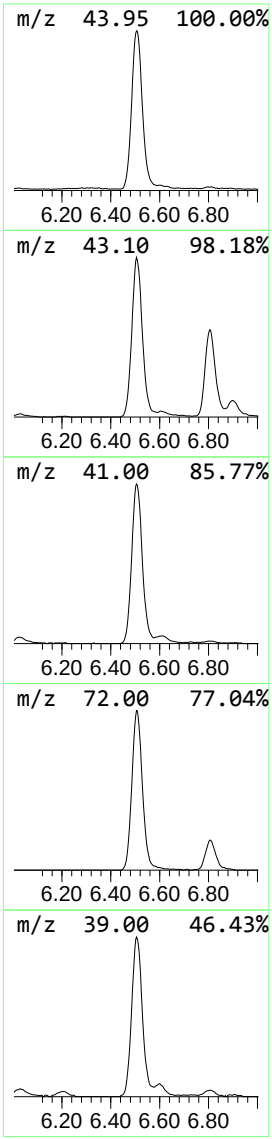
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.505	45.98 ug/l	762881	Pentafluorobenzene	7.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

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

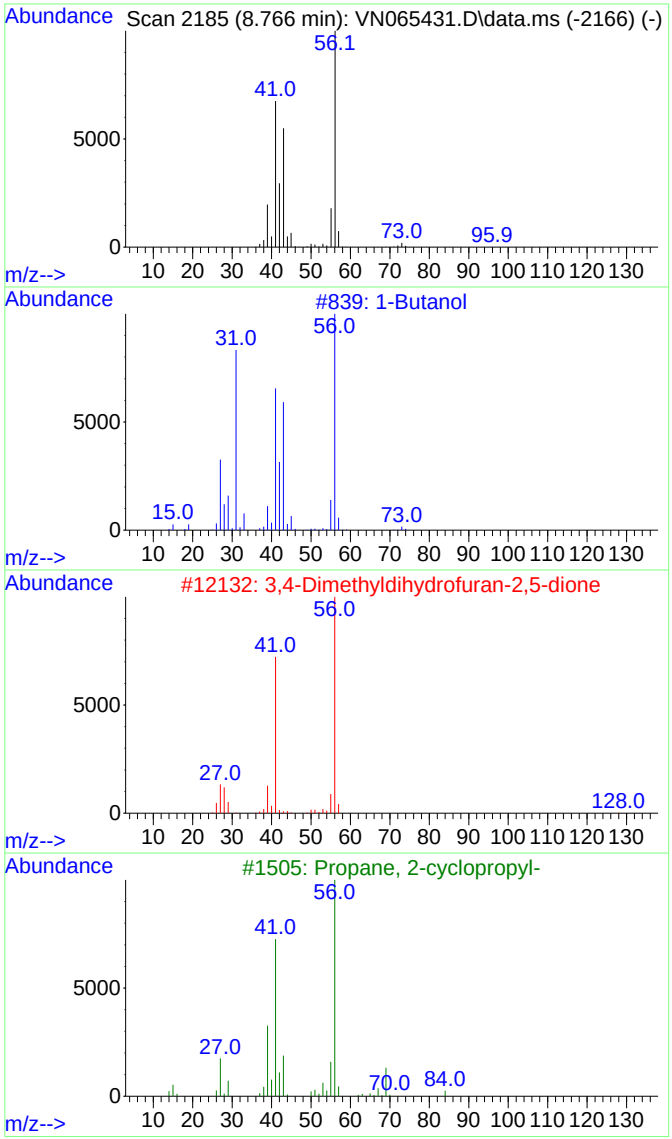
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

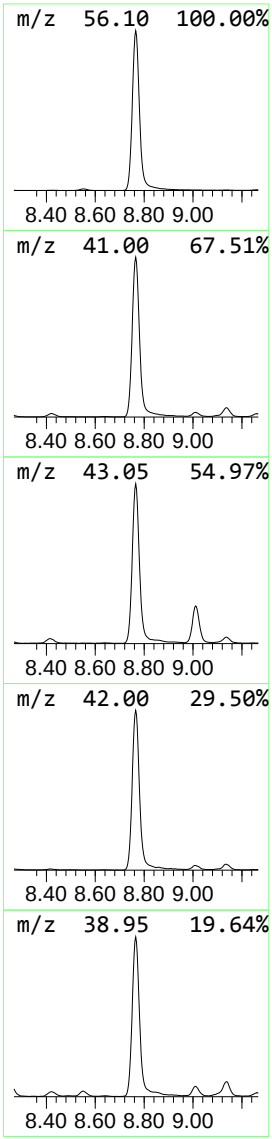
****

Peak Number 5 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.766	146.19 ug/l	3259870	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	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

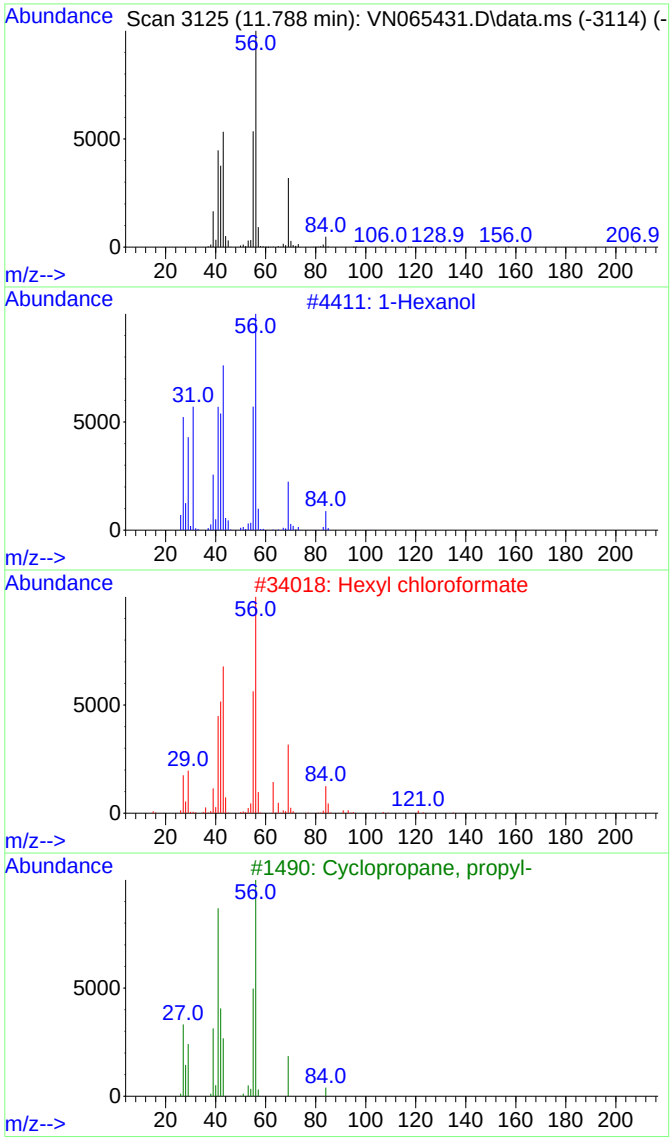
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

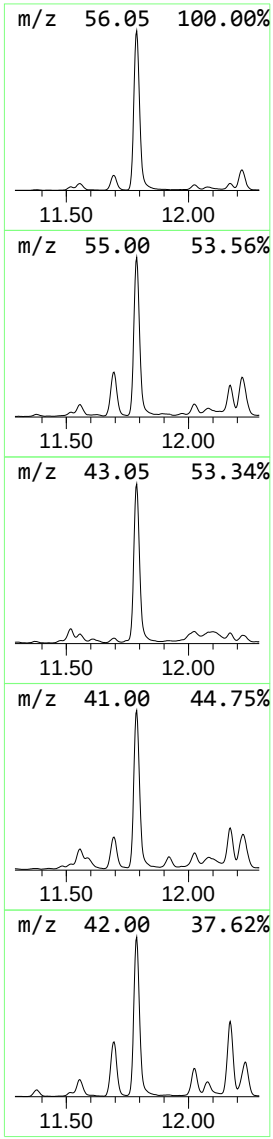
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.788	97.12 ug/l	3154460	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	Cyclopropane, propyl-	84	C6H12	002415-72-7	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30732

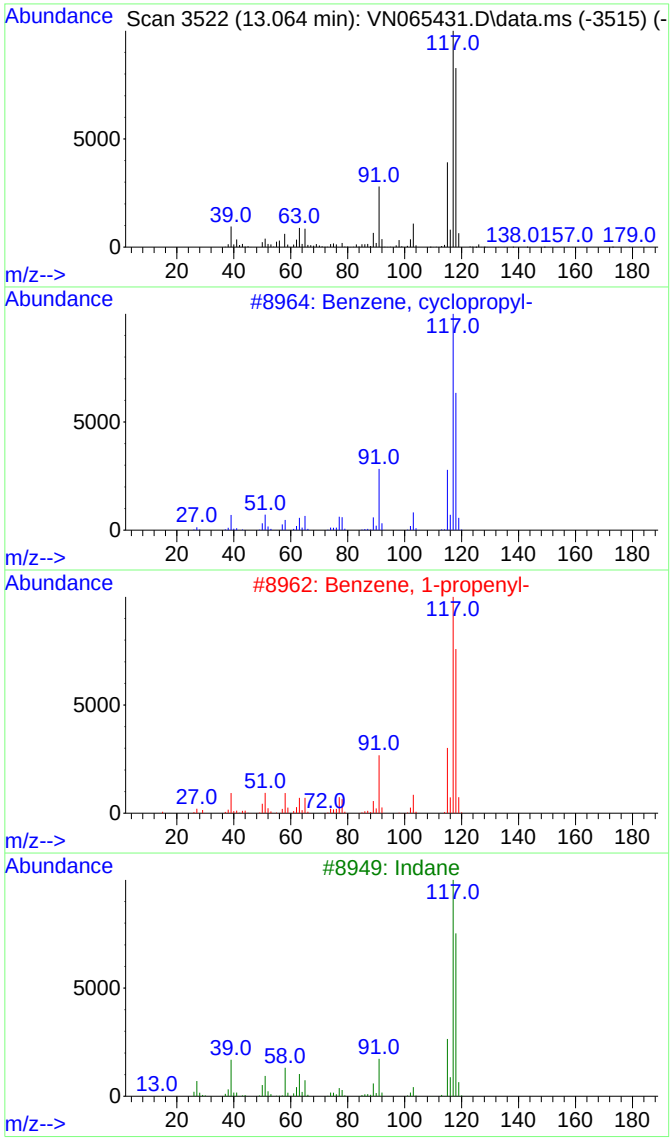
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

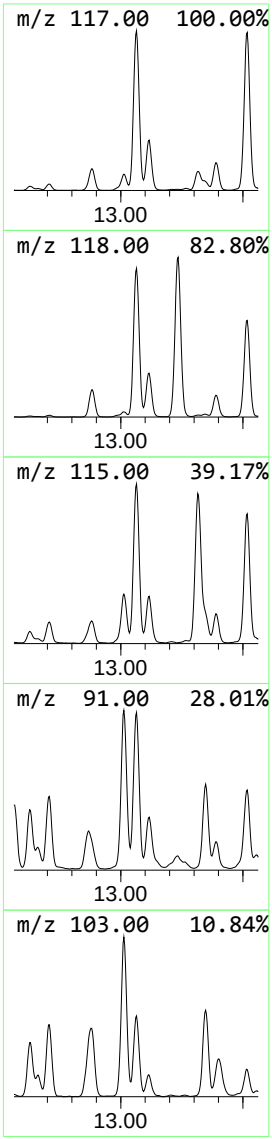
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.064	47.23 ug/l	1598060	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
2	Benzene, 1-propenyl-	118	C9H10	000637-50-3	81
3	Indane	118	C9H10	000496-11-7	81
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
5	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
30732

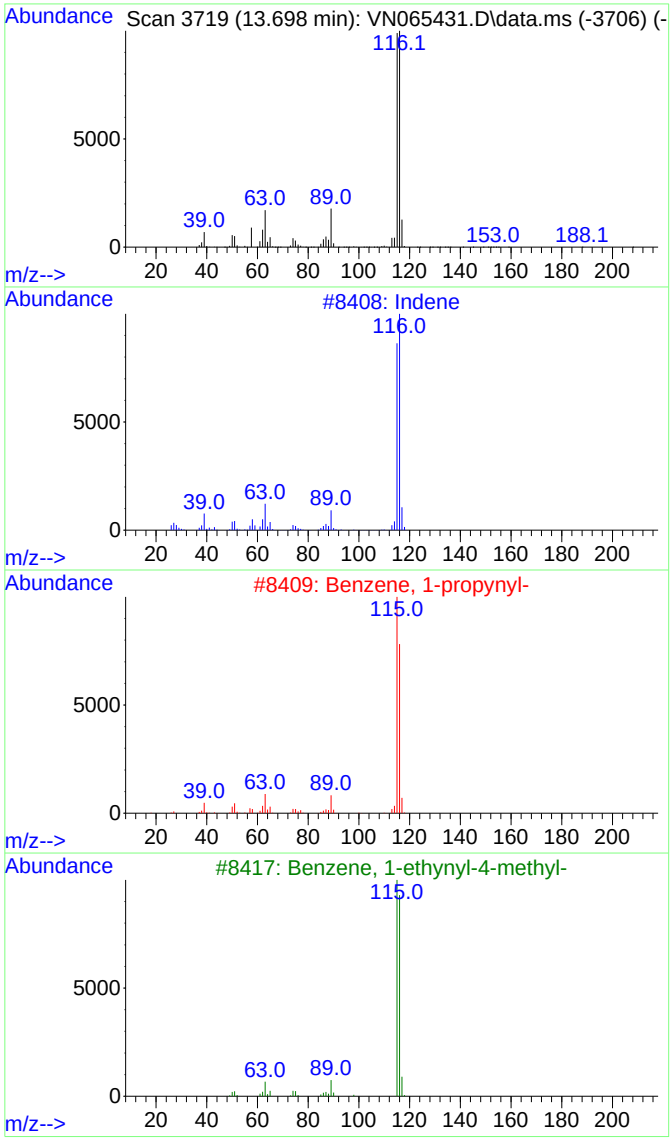
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

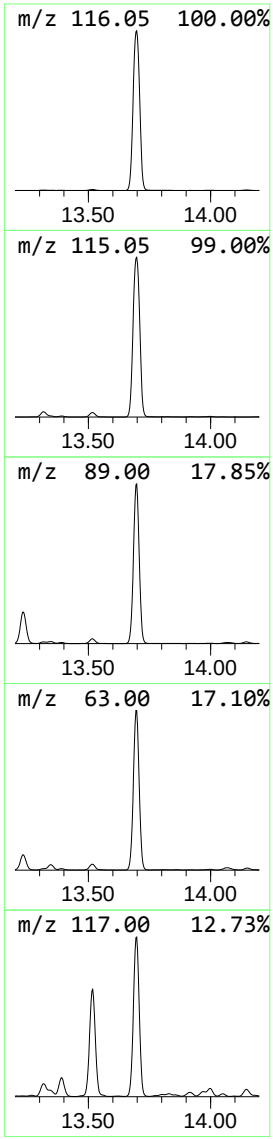
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.698	539.98 ug/l	18271400	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	96
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80
4	1-indanol trifluoroacetate ester	230	C11H9F3O2	1000376-43-6	64
5	3-Methylphenylacetylene	116	C9H8	000766-82-5	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

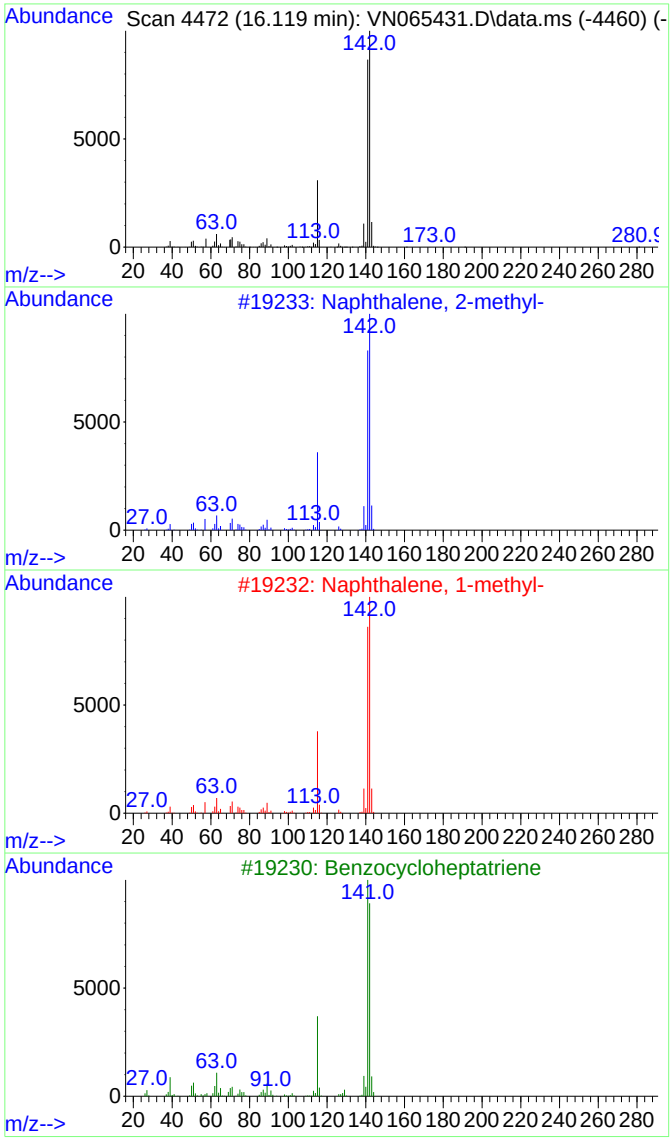
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

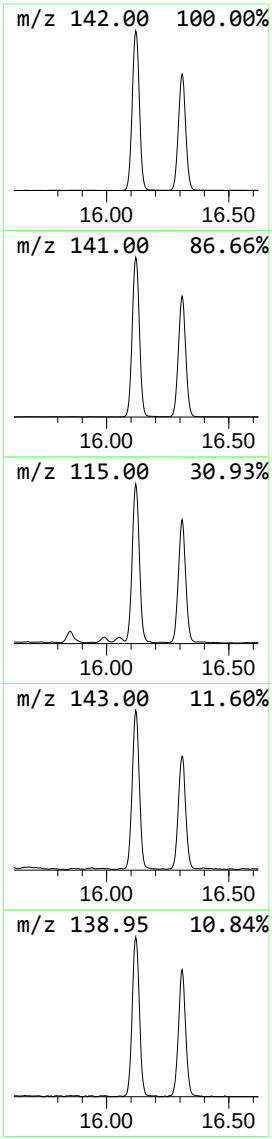
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.119	57.47 ug/l	1944770	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

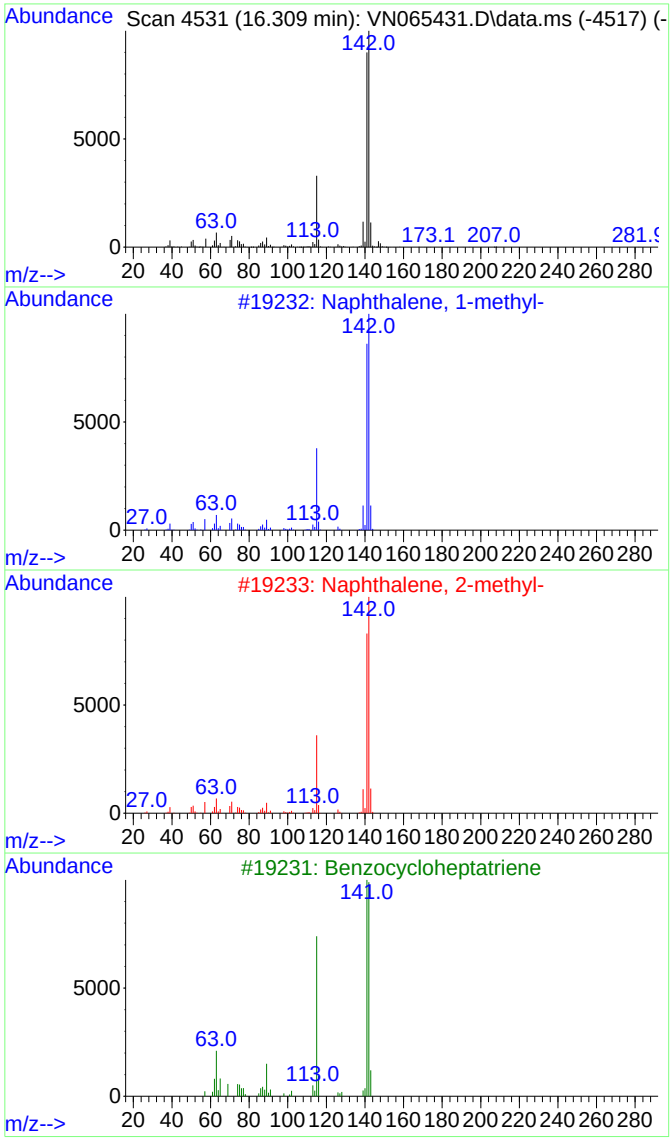
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

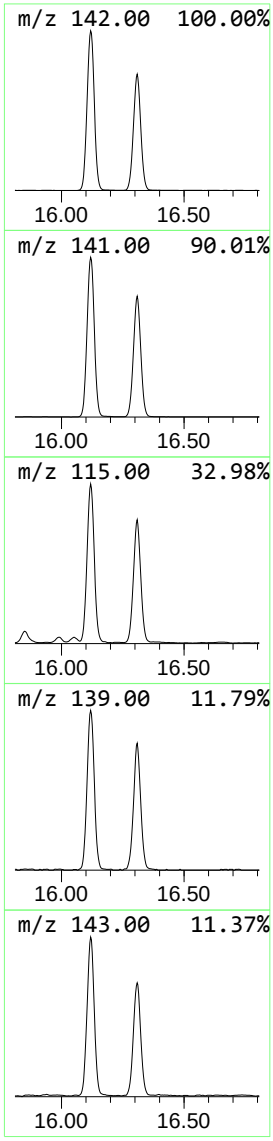
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.309	47.69 ug/l	1613700	1,4-Dichlorobenzene-d4	13.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010721\
Data File : VN065431.D
Acq On : 7 Jan 2021 16:54
Operator : JC/MD
Sample : M1022-12
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 30732

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	3.267	299.8	ug/l	4973370	1	7.631	829514	50.0
Dimethyl sulfide	3.859	97.2	ug/l	1612220	1	7.631	829514	50.0
Butanal	6.505	46.0	ug/l	762881	1	7.631	829514	50.0
1-Butanol	8.766	146.2	ug/l	3259870	2	8.553	1114950	50.0
1-Hexanol	11.788	97.1	ug/l	3154460	3	11.380	1623970	50.0
Benzene, cyclop...	13.064	47.2	ug/l	1598060	4	13.315	1691860	50.0
Indene	13.698	540.0	ug/l	18271400	4	13.315	1691860	50.0
Naphthalene, 2-...	16.119	57.5	ug/l	1944770	4	13.315	1691860	50.0
Naphthalene, 1-...	16.309	47.7	ug/l	1613700	4	13.315	1691860	50.0