

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
 Data File : VN065307.D
 Acq On : 29 Dec 2020 15:36
 Operator : JC/MD
 Sample : L5223-07
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM-COMP

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: VN065307.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.804	10	20	35	rBV	129533	173090	2.24%	0.653%
2	2.293	159	172	218	rBV	4478299	7742421	100.00%	29.221%
3	3.255	453	471	509	rBV	773403	1854123	23.95%	6.998%
4	3.785	622	636	651	rBV	50727	131351	1.70%	0.496%
5	4.052	703	719	733	rBV	33452	90018	1.16%	0.340%
6	4.775	921	944	968	rBV2	41921	144967	1.87%	0.547%
7	6.502	1459	1481	1505	rBV2	312792	940652	12.15%	3.550%
8	6.804	1557	1575	1596	rBV2	28439	80044	1.03%	0.302%
9	7.553	1788	1808	1818	rBV	191065	469660	6.07%	1.773%
10	7.627	1819	1831	1856	rVB	373926	898214	11.60%	3.390%
11	7.997	1927	1946	1970	rBV3	434040	1116639	14.42%	4.214%
12	8.418	2064	2077	2093	rBV4	32009	77669	1.00%	0.293%
13	8.550	2103	2118	2141	rVB	512266	1064486	13.75%	4.018%
14	8.762	2172	2184	2213	rBV	79202	176763	2.28%	0.667%
15	9.135	2280	2300	2328	rVB4	54588	145018	1.87%	0.547%
16	10.058	2572	2587	2598	rBV	803386	1492474	19.28%	5.633%
17	10.126	2598	2608	2629	rVV	531529	969179	12.52%	3.658%
18	10.502	2705	2725	2747	rBV2	39897	91139	1.18%	0.344%
19	11.380	2984	2998	3020	rBV	803795	1430895	18.48%	5.400%
20	11.482	3020	3030	3038	rBV	107815	187530	2.42%	0.708%
21	11.592	3051	3064	3086	rVB	245292	466675	6.03%	1.761%
22	11.933	3154	3170	3180	rBV3	250582	559580	7.23%	2.112%
23	12.376	3294	3308	3328	rBV	593801	1032767	13.34%	3.898%
24	12.630	3376	3387	3391	rBV	62826	95995	1.24%	0.362%
25	12.659	3392	3396	3404	rVV	64387	97833	1.26%	0.369%
26	12.708	3404	3411	3422	rVB	54545	87775	1.13%	0.331%
27	13.016	3486	3507	3517	rBV3	139058	319758	4.13%	1.207%
28	13.318	3588	3601	3618	rBV	697957	1280105	16.53%	4.831%
29	13.425	3618	3634	3649	rBV	397555	659430	8.52%	2.489%
30	13.695	3707	3718	3733	rVB	338516	575272	7.43%	2.171%
31	14.556	3976	3986	3999	rBV3	44573	93922	1.21%	0.354%
32	15.096	4135	4154	4175	rBV	849990	1513702	19.55%	5.713%
33	15.965	4414	4424	4433	rBV	148417	248447	3.21%	0.938%
34	16.109	4458	4469	4485	rVB	105171	188324	2.43%	0.711%

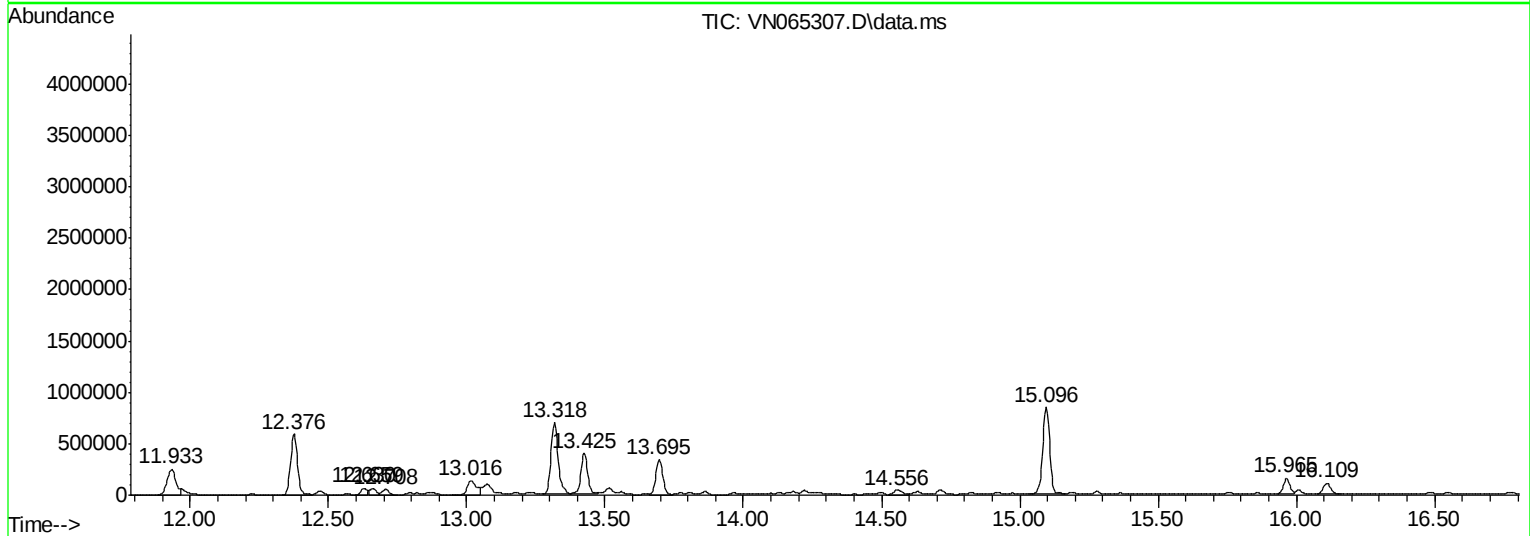
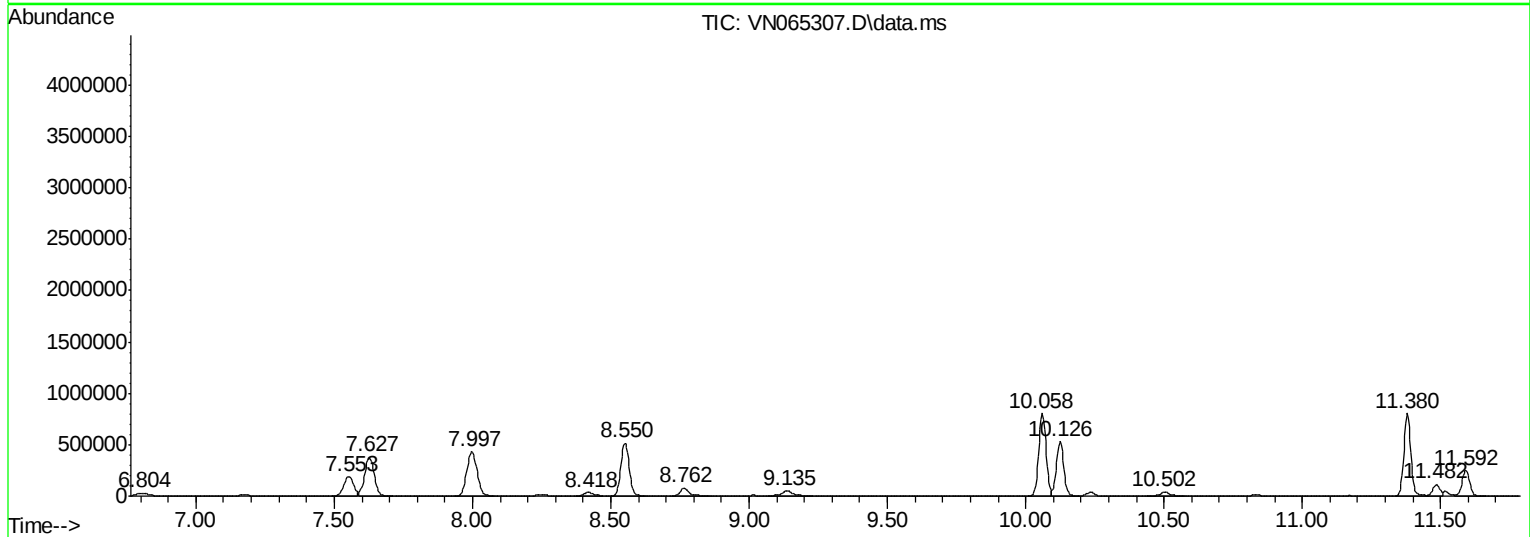
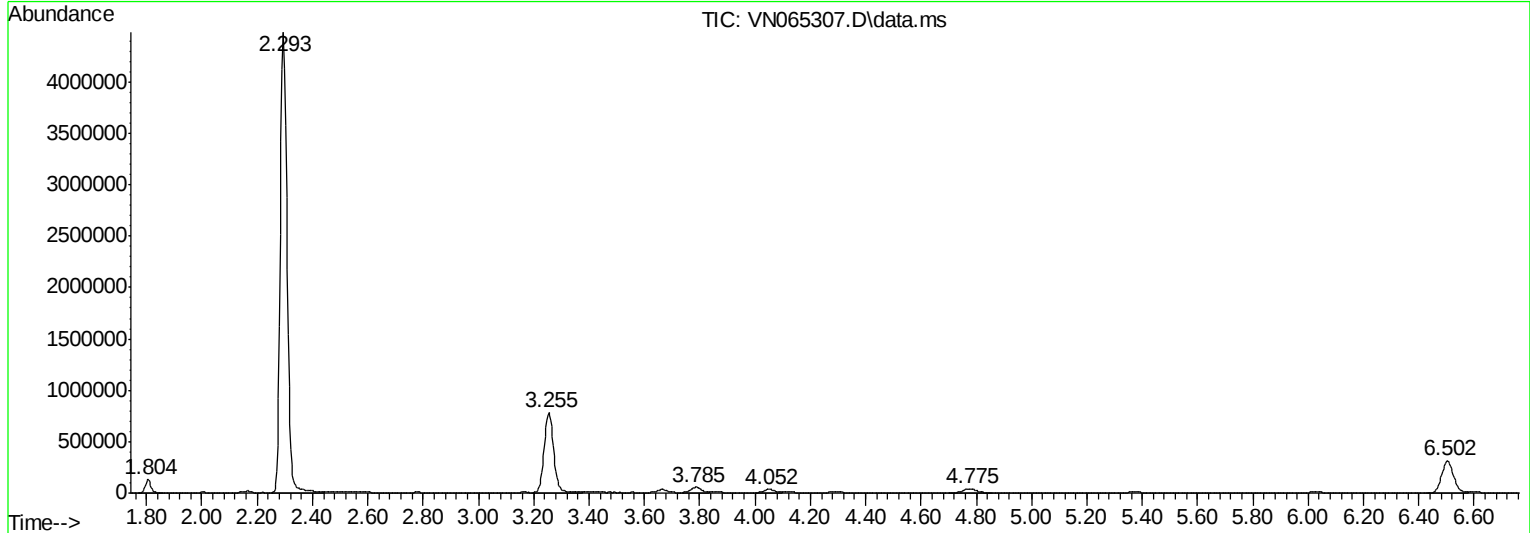
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

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



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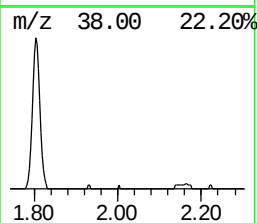
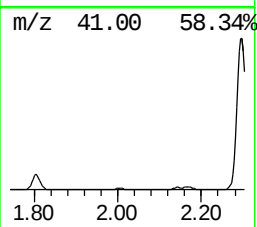
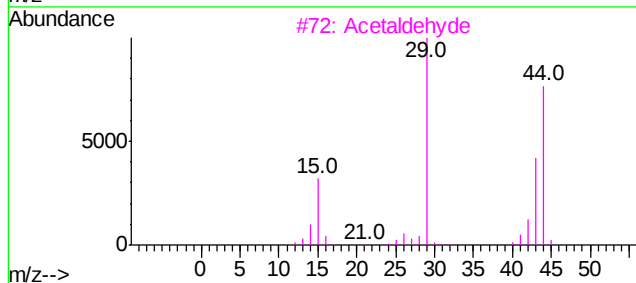
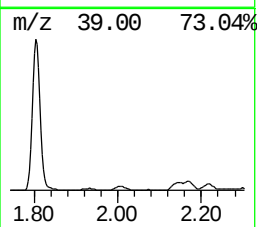
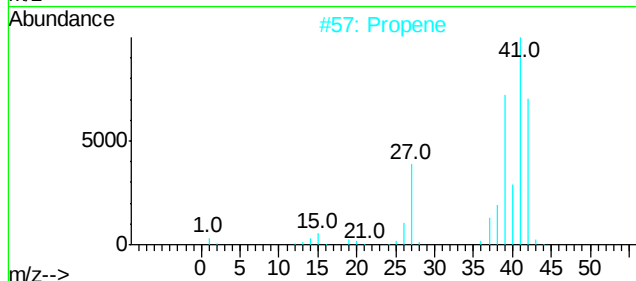
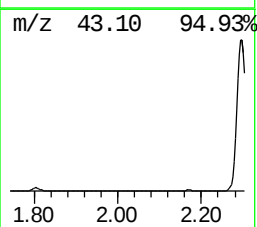
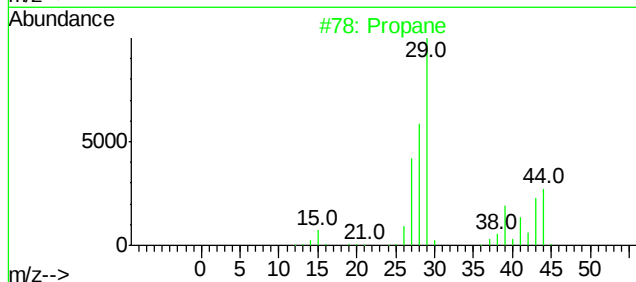
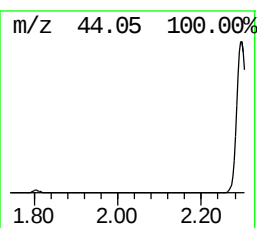
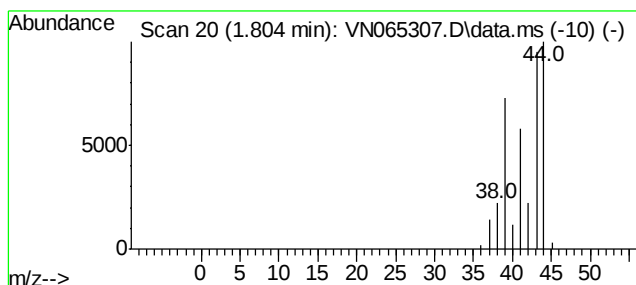
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.804	9.64 ug/l	173090	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Acetaldehyde	44	C2H4O	000075-07-0	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3



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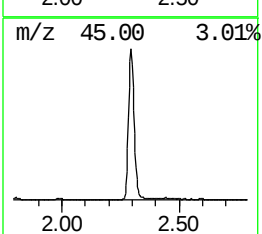
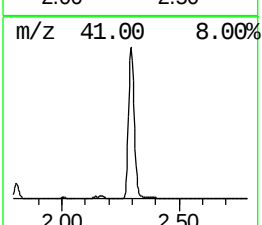
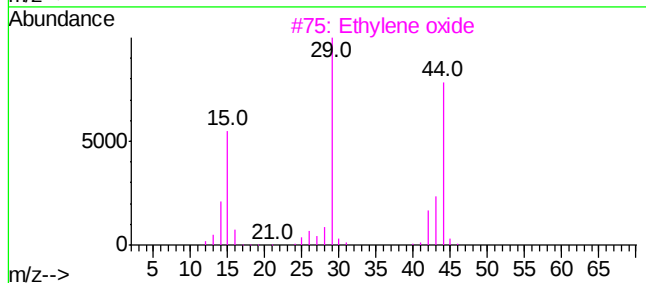
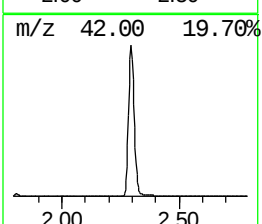
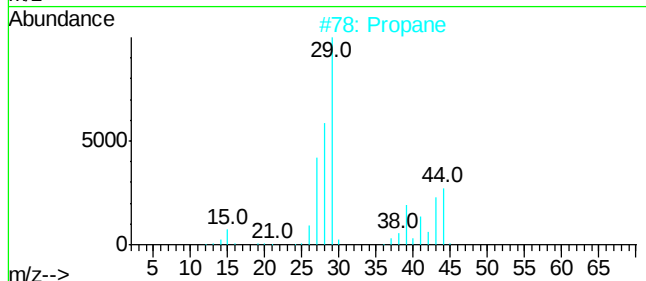
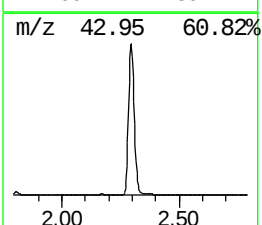
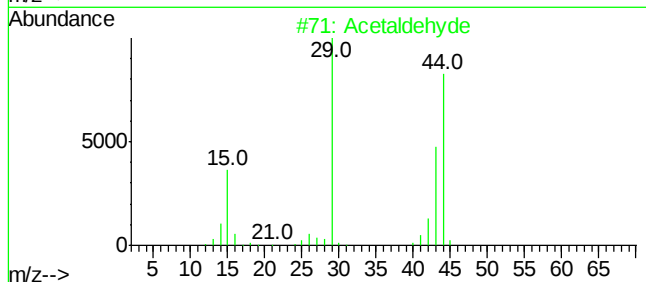
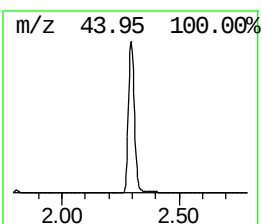
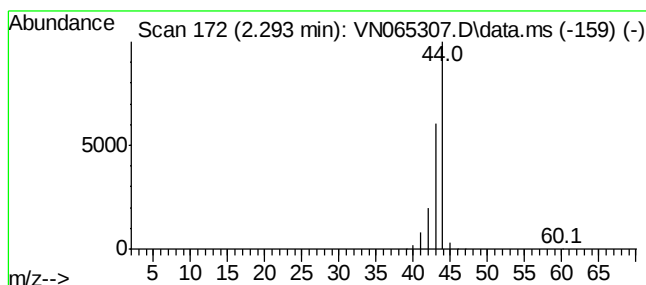
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

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

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.293	430.99 ug/l	7742420	Pentafluorobenzene	7.627

Hit# of	5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Acetaldehyde		44	C2H4O	000075-07-0	74
2	Propane		44	C3H8	000074-98-6	5
3	Ethylene oxide		44	C2H4O	000075-21-8	5
4	Alanine		89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-		44	C2HF	002713-09-9	3



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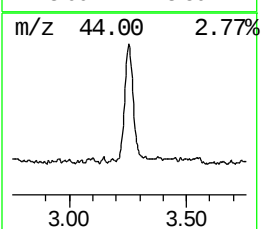
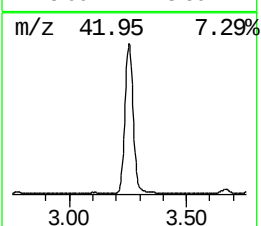
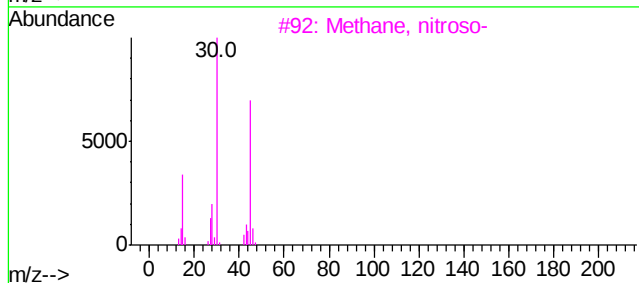
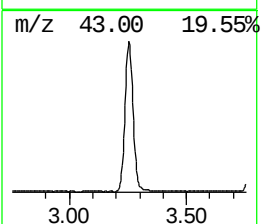
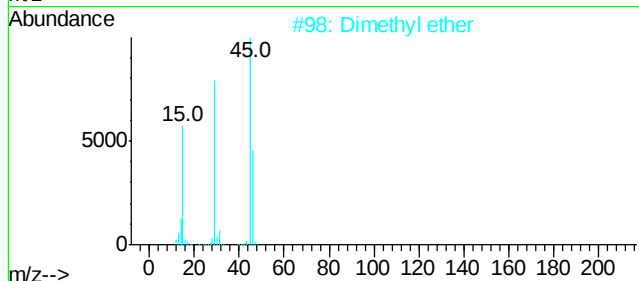
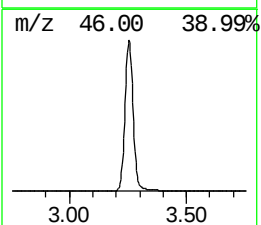
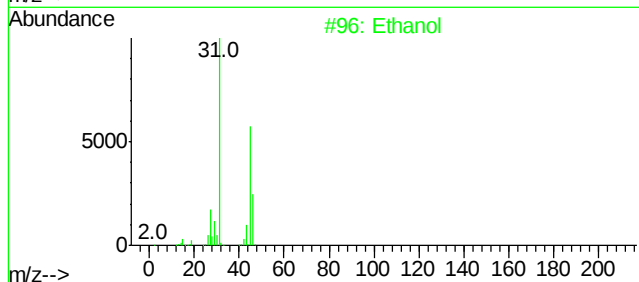
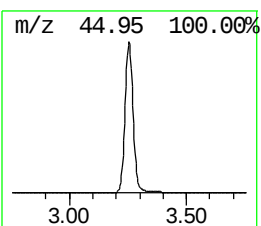
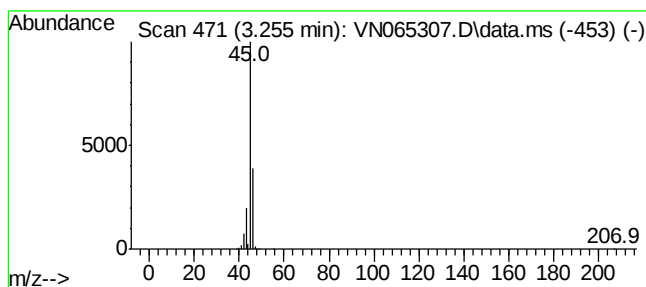
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Quant Title : SW846 8260

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

Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.255	103.21 ug/l	1854120	Pentafluorobenzene	7.627

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



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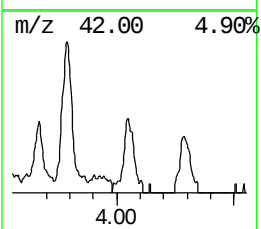
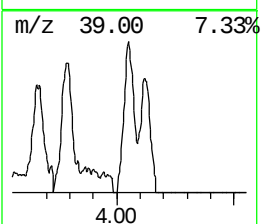
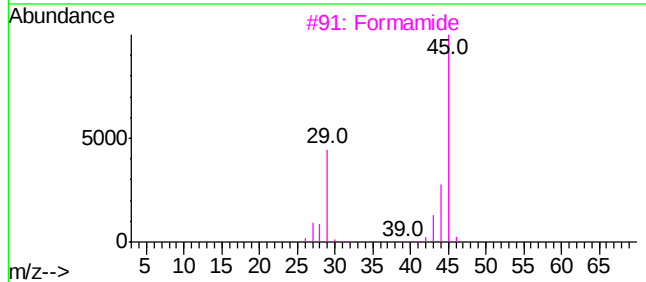
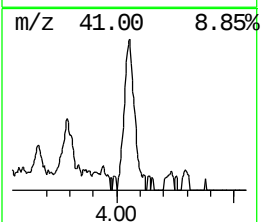
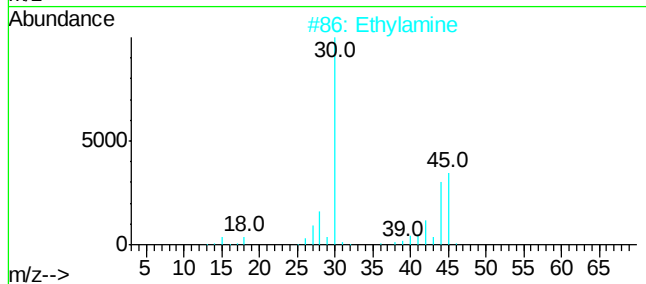
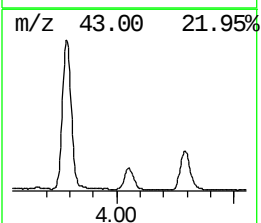
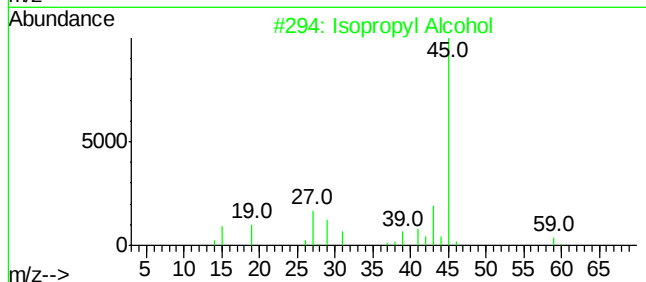
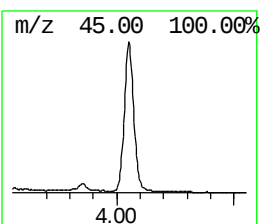
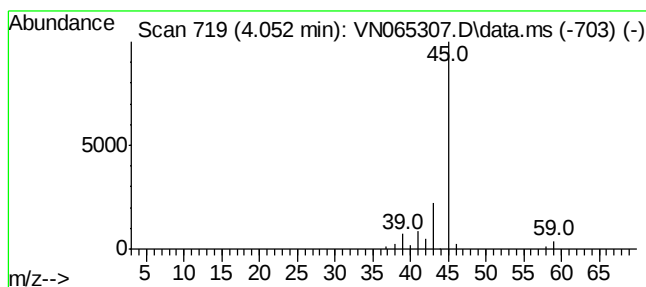
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Quant Title : SW846 8260

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

Peak Number 4 Isopropyl Alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.052	5.01 ug/l	90018	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2	Ethylamine	45	C2H7N	000075-04-7	5
3	Formamide	45	CH3NO	000075-12-7	5
4	4-Penten-2-ol	86	C5H10O	000625-31-0	4
5	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



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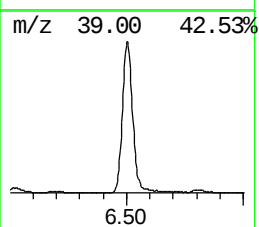
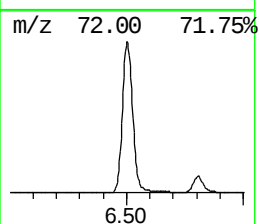
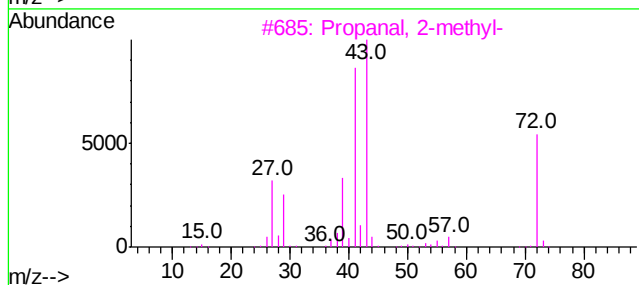
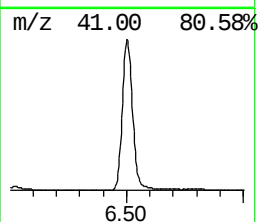
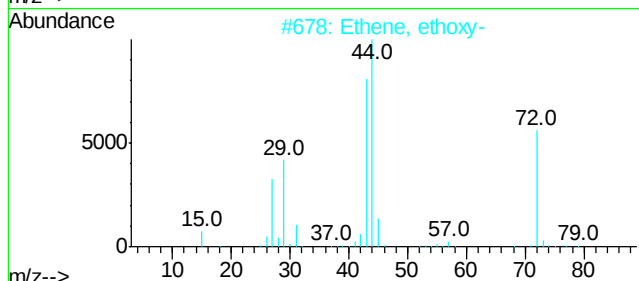
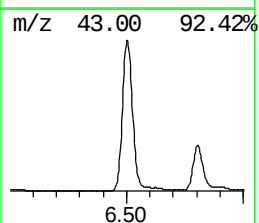
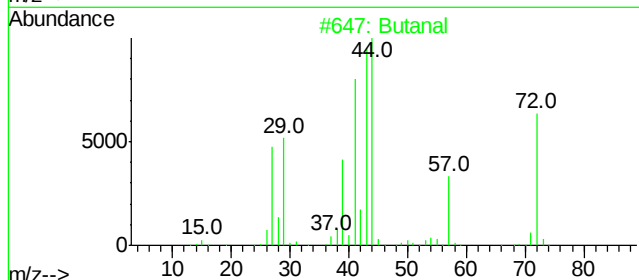
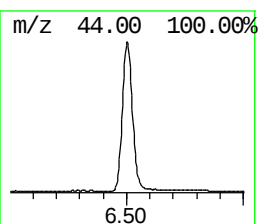
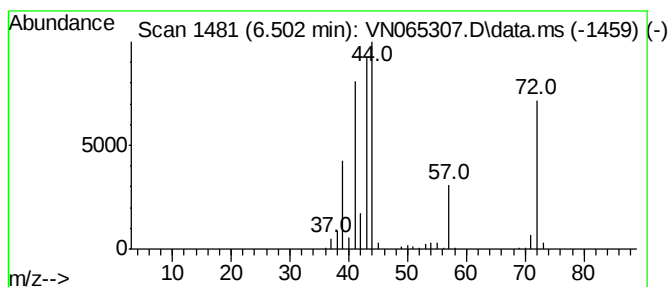
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220w.M
Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.502	52.36 ug/l	940652	Pentafluorobenzene	7.627

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	17



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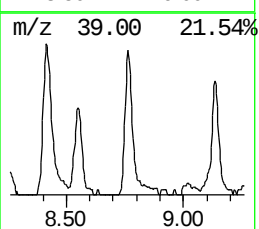
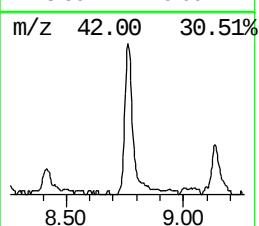
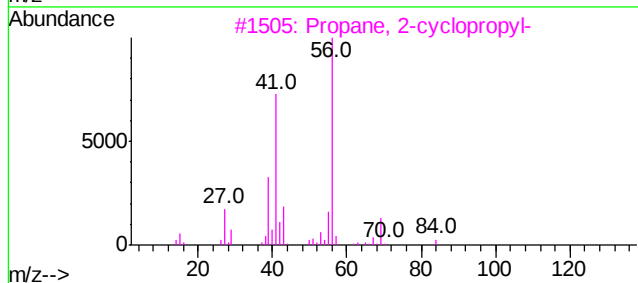
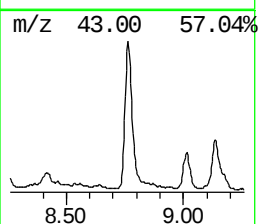
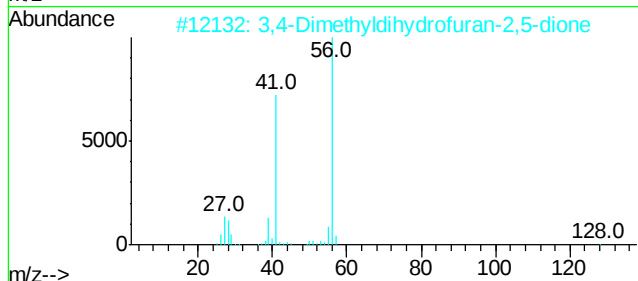
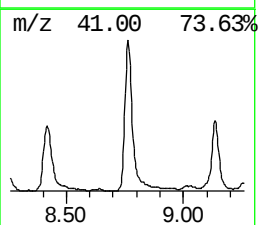
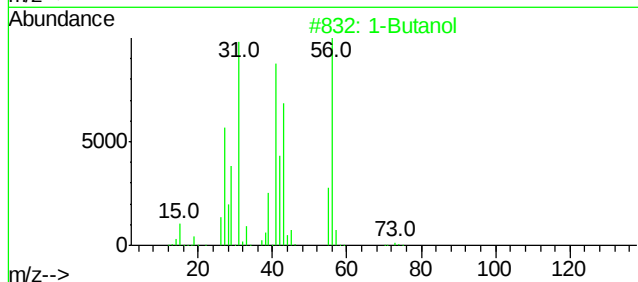
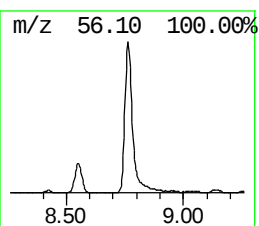
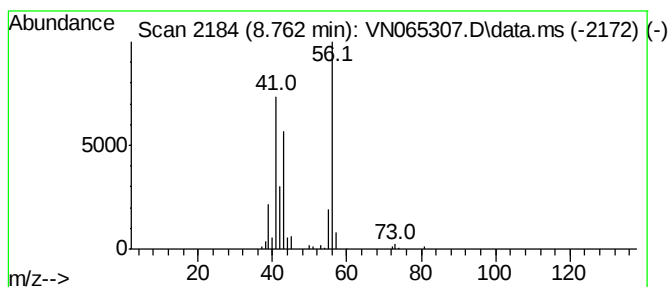
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Quant Title : SW846 8260

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

Peak Number 6 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.762	8.30 ug/l	176763	1,4-Difluorobenzene	8.550

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065307.D
Acq On : 29 Dec 2020 15:36
Operator : JC/MD
Sample : L5223-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

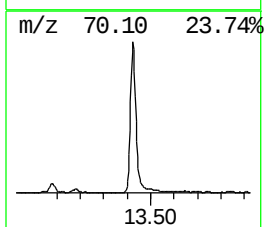
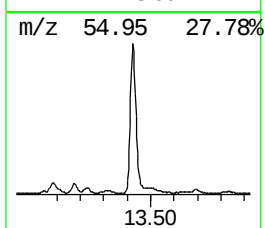
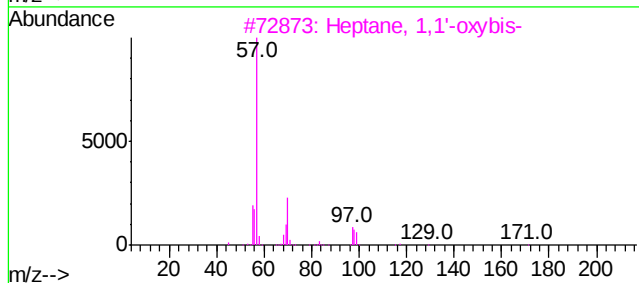
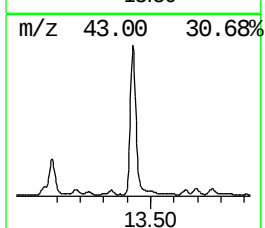
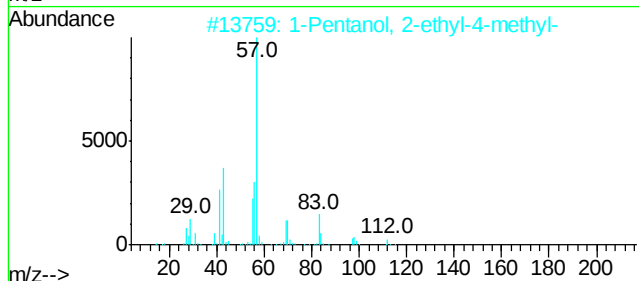
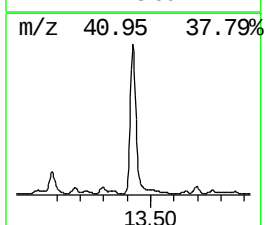
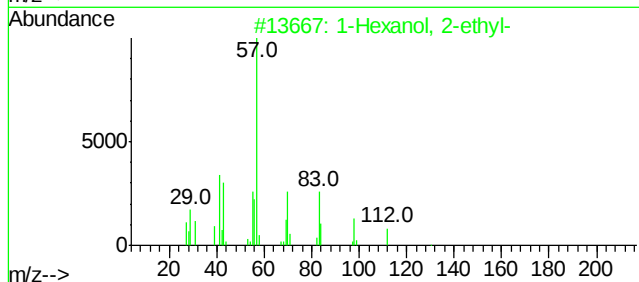
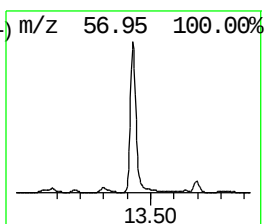
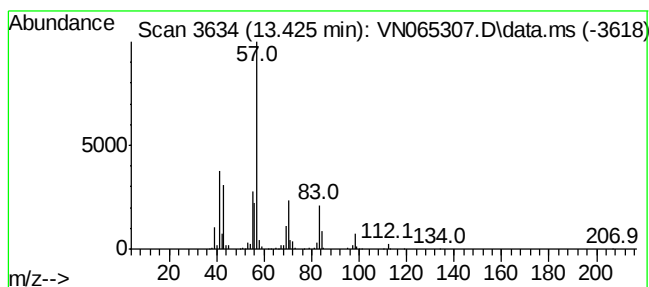
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.425	25.76 ug/l	659430	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065307.D
Acq On : 29 Dec 2020 15:36
Operator : JC/MD
Sample : L5223-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

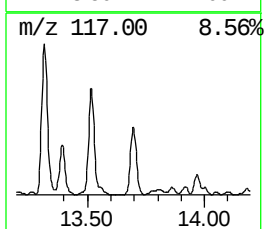
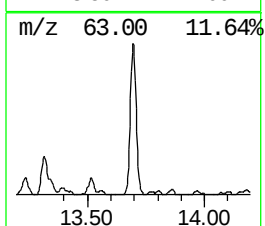
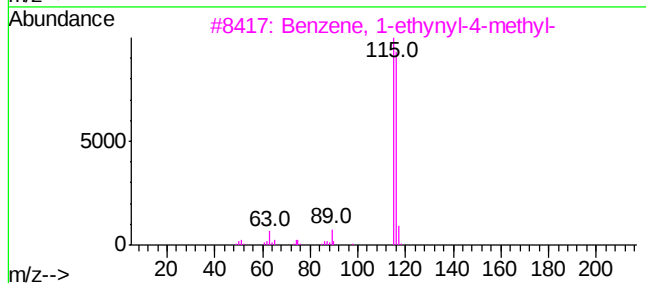
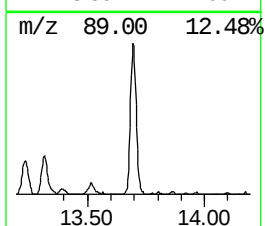
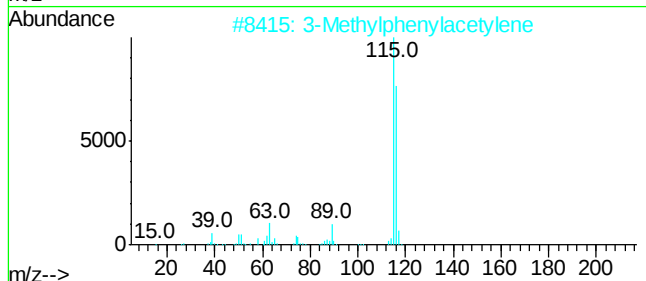
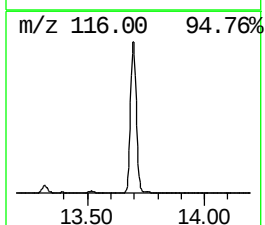
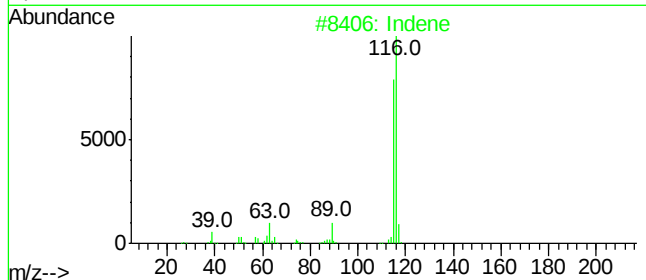
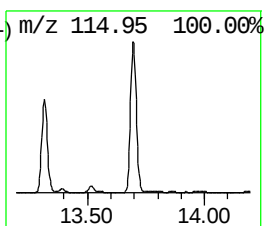
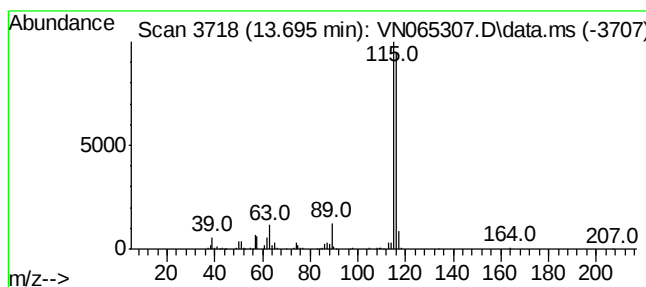
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Quant Title : SW846 8260

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

Peak Number 8 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.695	22.47 ug/l	575272	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	Mw	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065307.D
Acq On : 29 Dec 2020 15:36
Operator : JC/MD
Sample : L5223-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

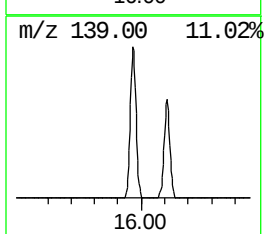
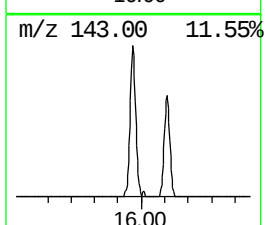
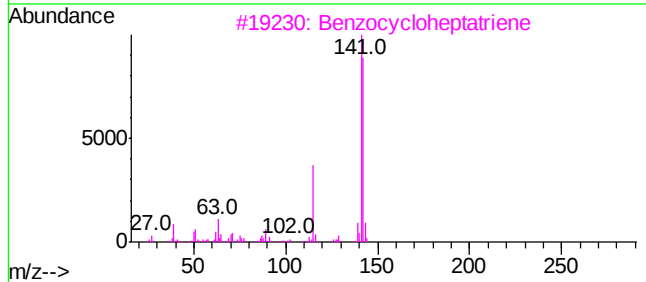
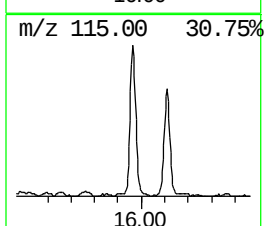
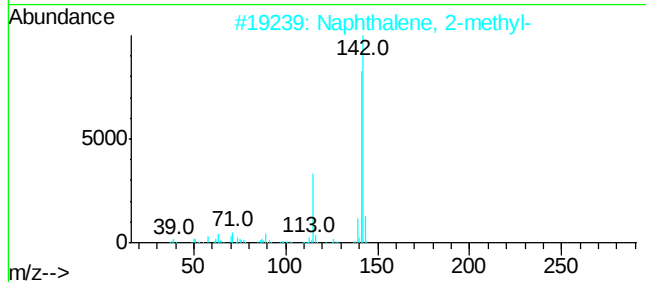
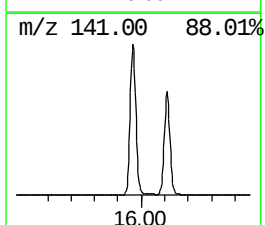
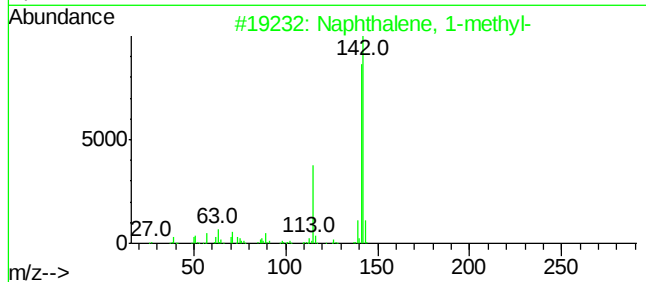
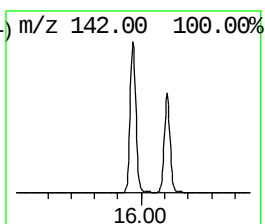
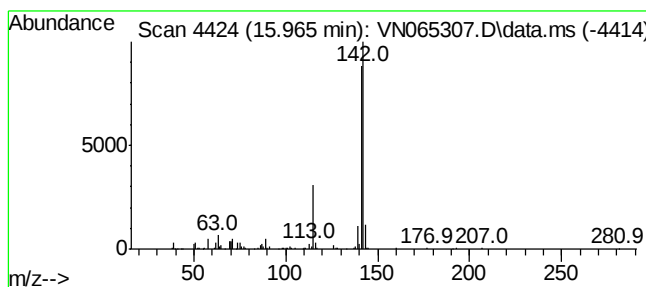
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.965	9.70 ug/l	248447	1,4-Dichlorobenzene-d4	13.318

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	Spiro(tricyclo[6.2.1.0(2,7)]unde...	186	C13H14O	1000210-02-3	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065307.D
Acq On : 29 Dec 2020 15:36
Operator : JC/MD
Sample : L5223-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

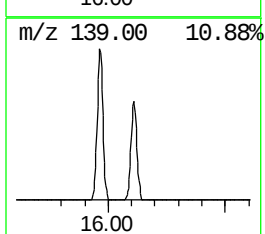
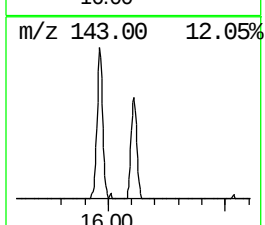
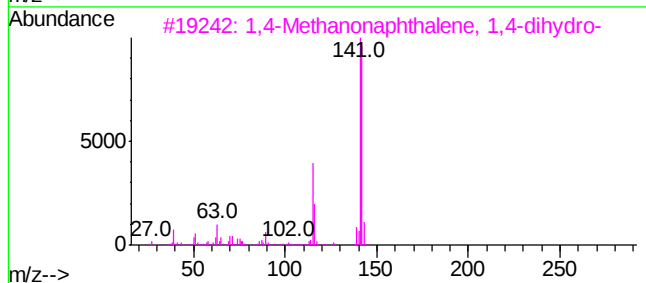
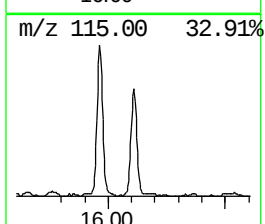
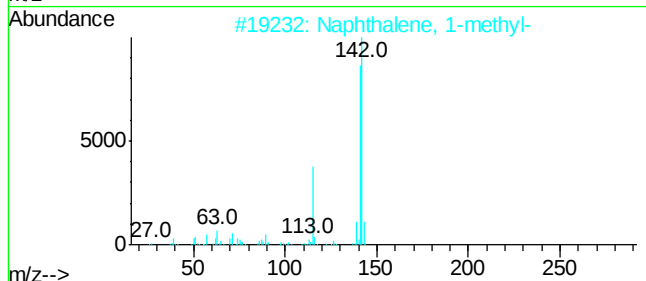
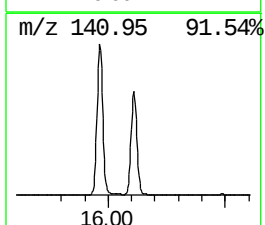
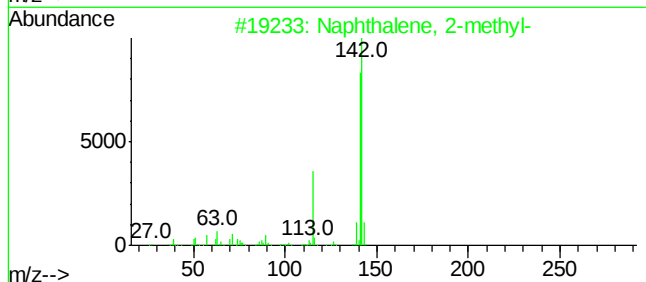
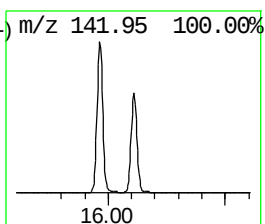
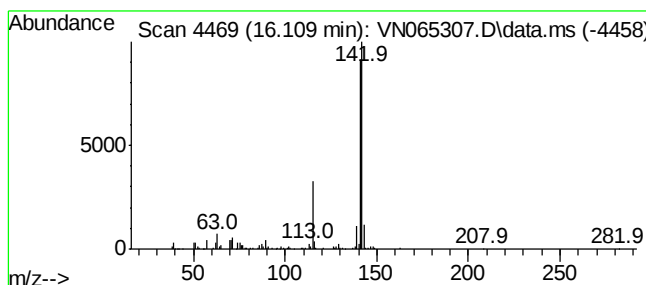
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.109	7.36 ug/l	188324	1,4-Dichlorobenzene-d4	13.318

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	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	3-Indolecarbonitrile	142	C9H6N2	005457-28-3	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122920\
Data File : VN065307.D
Acq On : 29 Dec 2020 15:36
Operator : JC/MD
Sample : L5223-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DRUM-COMP

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane	1.804	9.6	ug/l	173090	1	7.627	898214	50.0
Acetaldehyde	2.293	431.0	ug/l	7742420	1	7.627	898214	50.0
Ethanol	3.255	103.2	ug/l	1854120	1	7.627	898214	50.0
Isopropyl Alcohol	4.052	5.0	ug/l	90018	1	7.627	898214	50.0
Butanal	6.502	52.4	ug/l	940652	1	7.627	898214	50.0
1-Butanol	8.762	8.3	ug/l	176763	2	8.550	1064490	50.0
1-Hexanol, 2-et...	13.425	25.8	ug/l	659430	4	13.318	1280110	50.0
Indene	13.695	22.5	ug/l	575272	4	13.318	1280110	50.0
Naphthalene, 1-...	15.965	9.7	ug/l	248447	4	13.318	1280110	50.0
Naphthalene, 2-...	16.109	7.4	ug/l	188324	4	13.318	1280110	50.0