

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081822\
 Data File : VN073997.D
 Acq On : 18 Aug 2022 12:07
 Operator : JC\MD
 Sample : N4241-07
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TRE-1630

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\82N081522W.M
 Title : SW846 8260

Signal : TIC: VN073997.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.487	99	102	141	rBV2	38980985	180614511	100.00%	45.822%
2	3.710	284	310	353	rBV2	24494470	124420736	68.89%	31.566%
3	4.216	385	396	427	rBV	6452792	18062978	10.00%	4.583%
4	6.981	852	866	878	rBV	1086744	3102649	1.72%	0.787%
5	8.016	1036	1042	1059	rVB	880217	1972337	1.09%	0.500%
6	8.181	1059	1070	1091	rBV	12197802	27463798	15.21%	6.968%
7	8.904	1185	1193	1214	rVB	1174097	2616284	1.45%	0.664%
8	9.092	1214	1225	1232	rBV	1088345	2221781	1.23%	0.564%
9	10.381	1432	1444	1450	rVV	1695955	3260686	1.81%	0.827%
10	11.680	1658	1665	1676	rVB	1705326	3160588	1.75%	0.802%
11	12.210	1748	1755	1763	rVV	4332756	6860025	3.80%	1.740%
12	12.669	1827	1833	1844	rVB	1498293	2543324	1.41%	0.645%
13	13.616	1987	1994	2002	rBV2	1868649	3781072	2.09%	0.959%
14	13.710	2002	2010	2018	rVB	4781347	7596285	4.21%	1.927%
15	14.863	2199	2206	2211	rBV3	937500	2209521	1.22%	0.561%
16	15.633	2332	2337	2346	rVB	1302323	2269348	1.26%	0.576%
17	16.739	2516	2525	2533	rBV2	709427	2006946	1.11%	0.509%

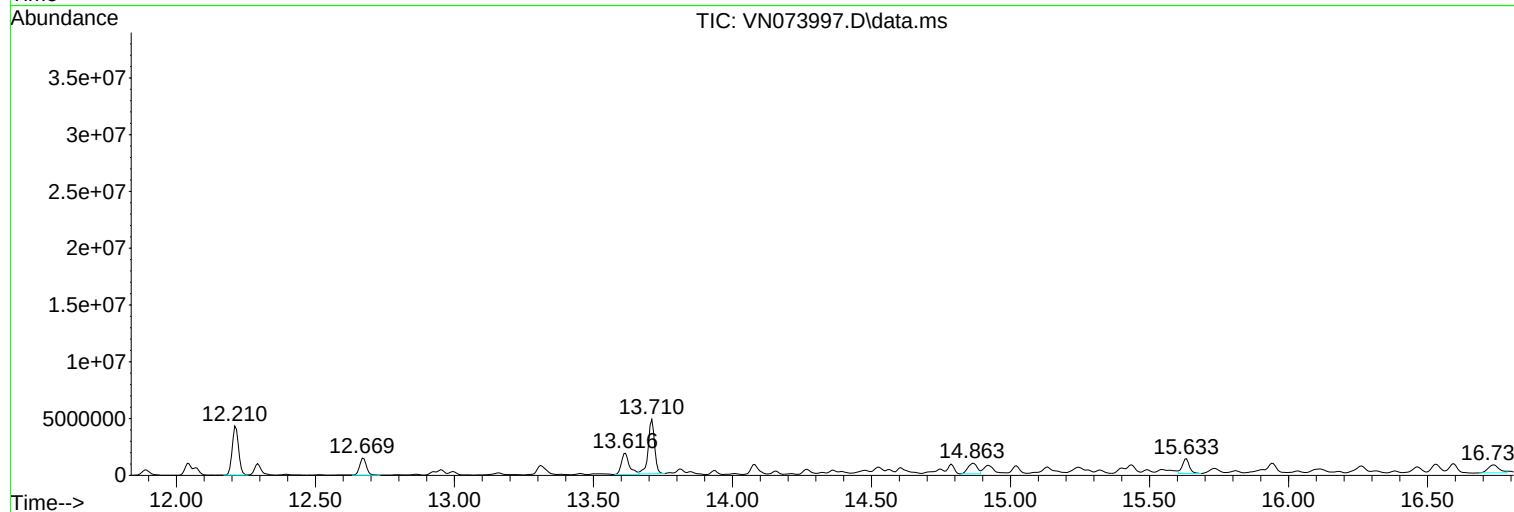
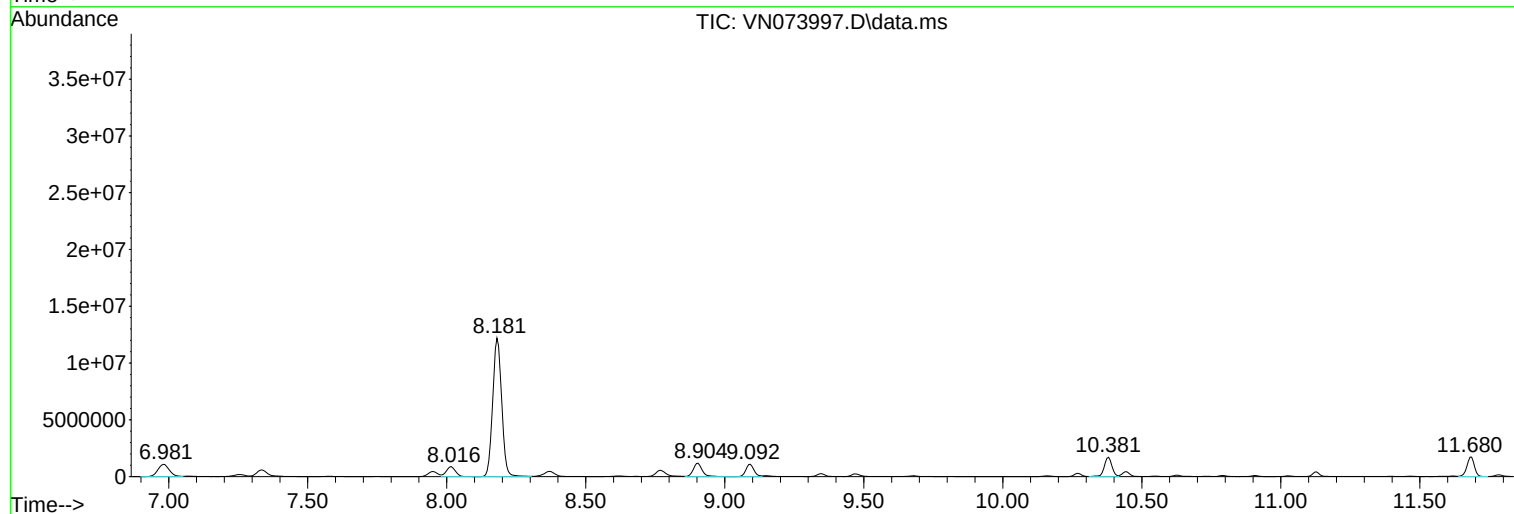
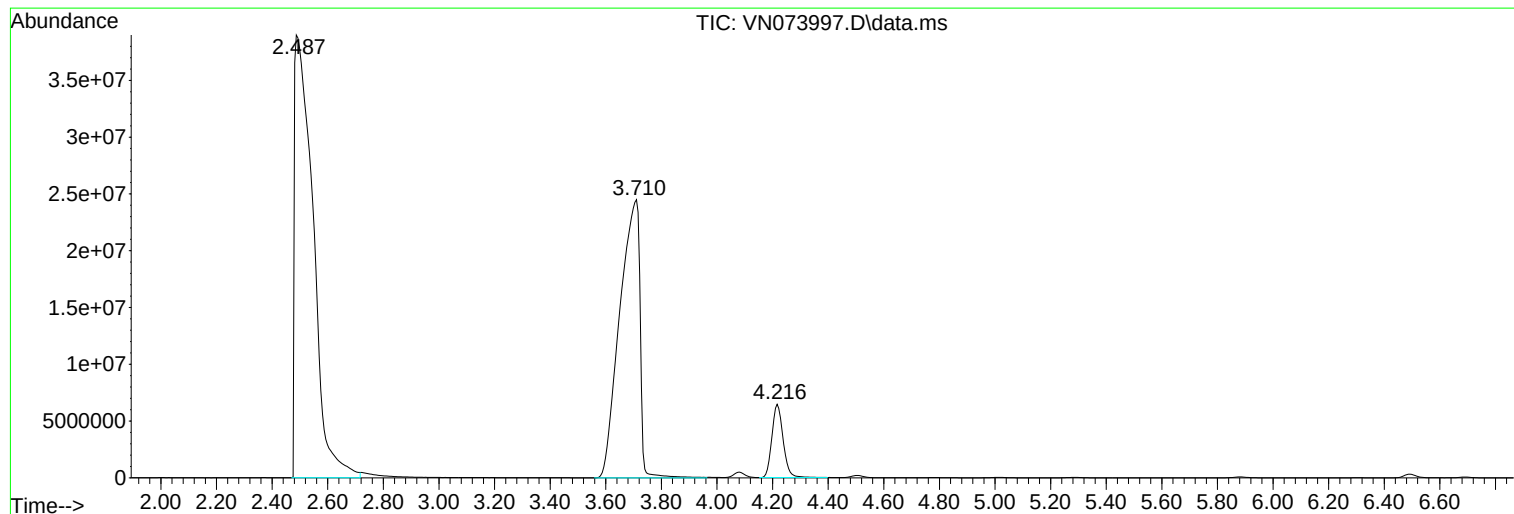
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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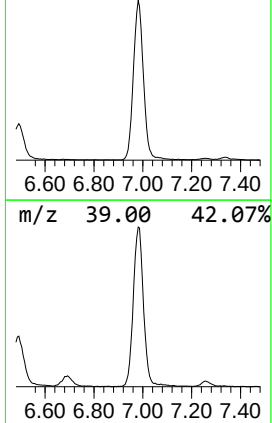
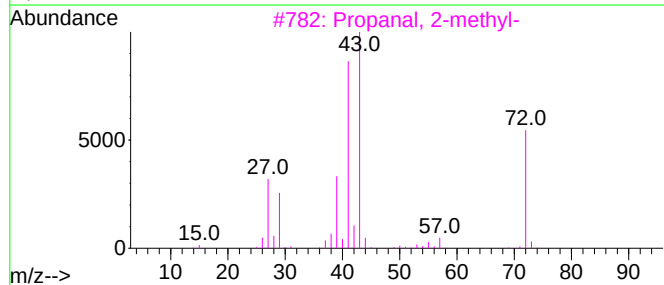
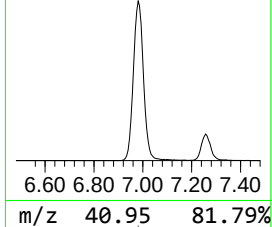
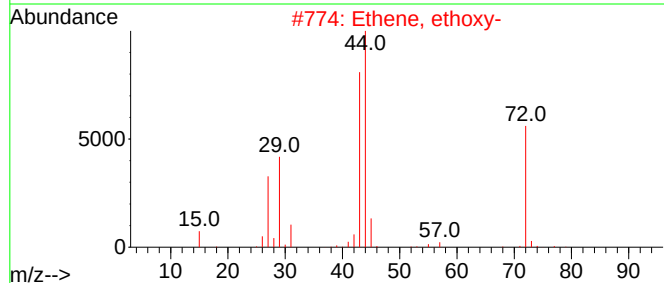
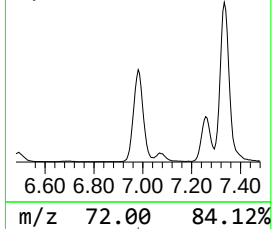
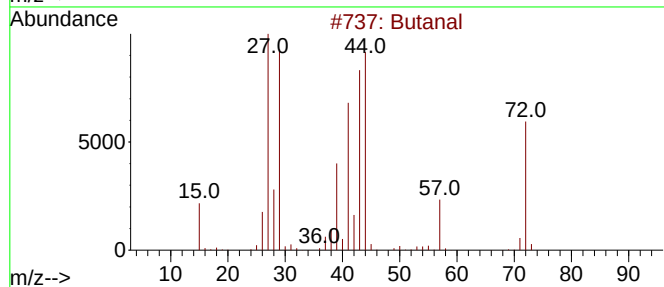
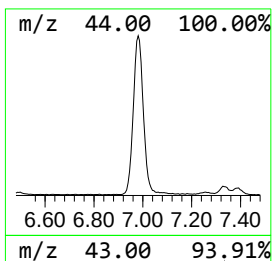
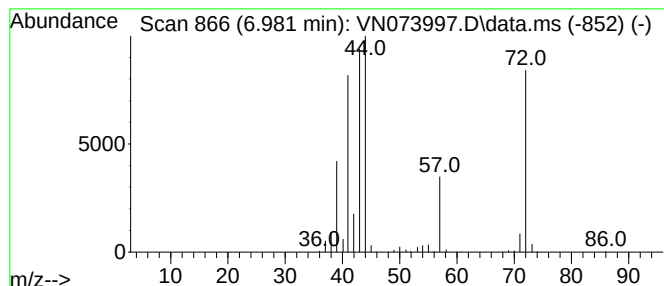
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	78.65 ug/l	3102650	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38



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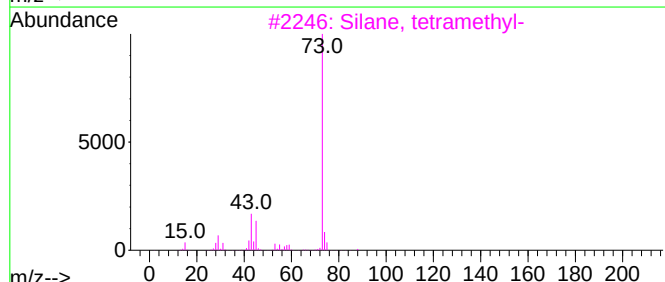
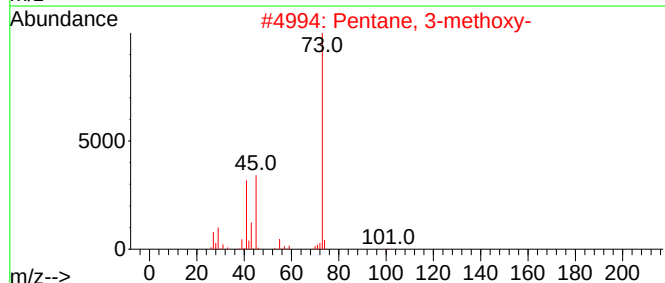
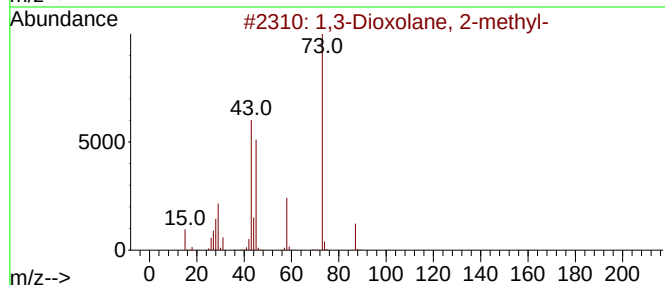
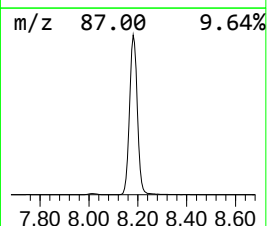
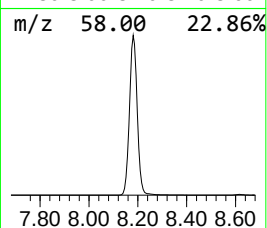
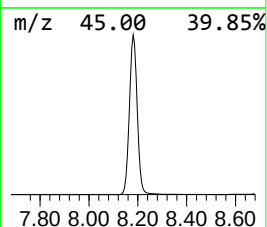
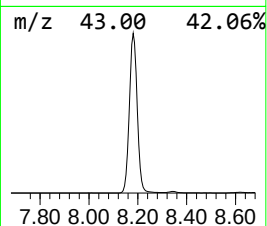
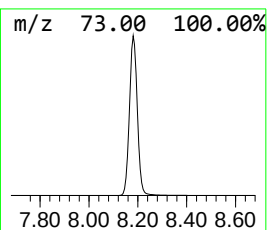
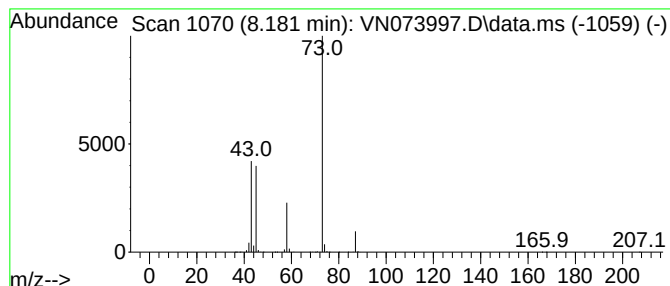
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TIC Integration Parameters: LSCINT.P

Peak Number 4 1,3-Dioxolane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.181	696.23 ug/l	27463800	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	38
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9



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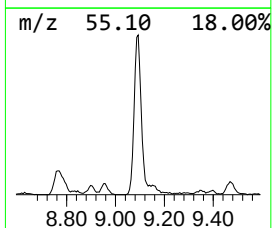
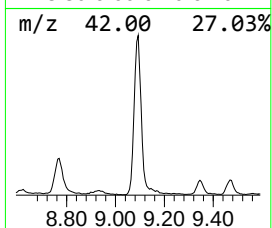
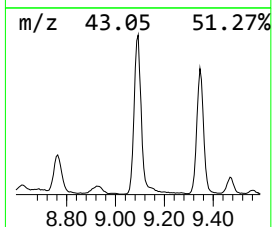
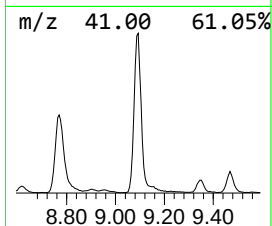
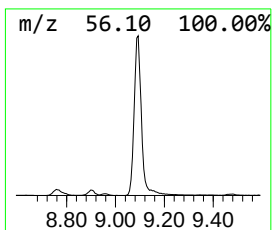
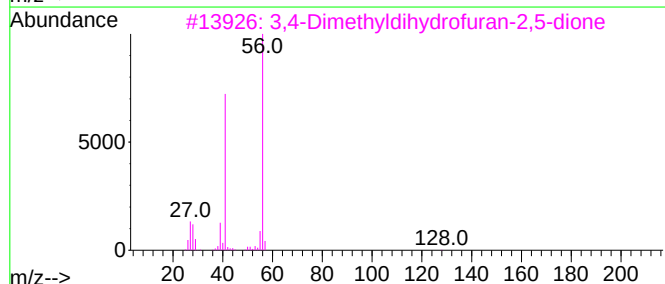
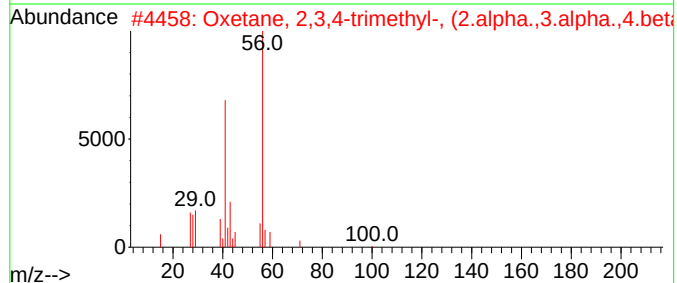
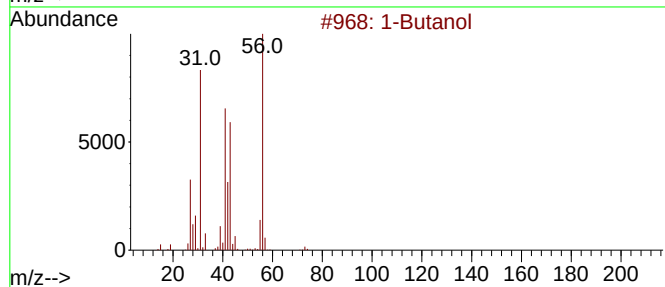
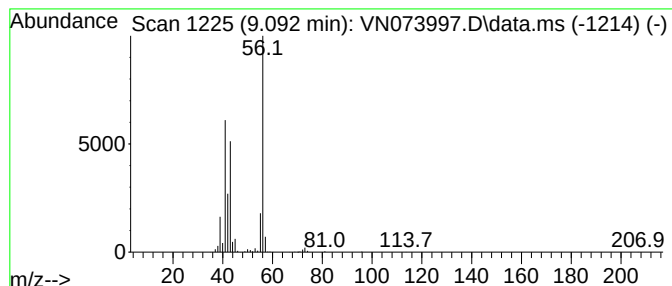
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.092	42.46 ug/l	2221780	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	33
4			.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	9
5			Formic acid, butyl ester	102	C5H10O2	000592-84-7	9



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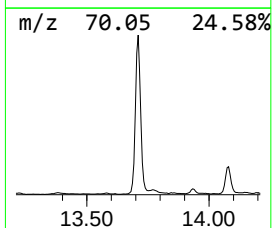
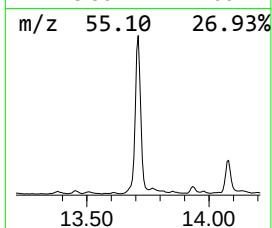
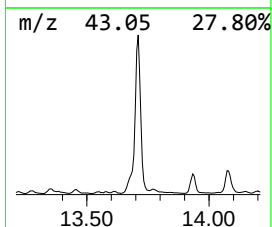
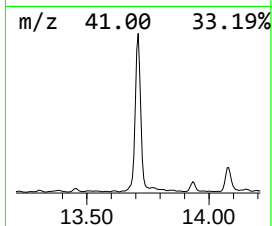
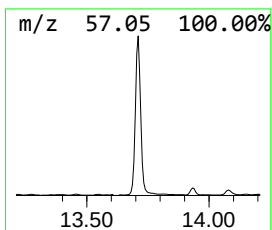
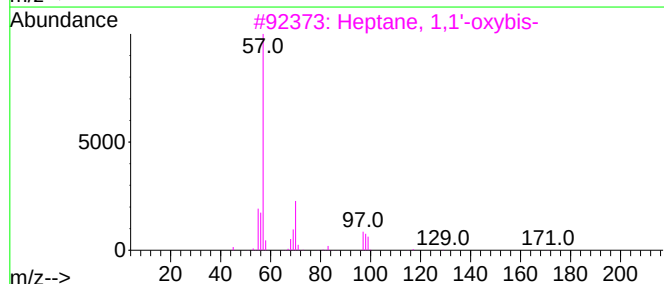
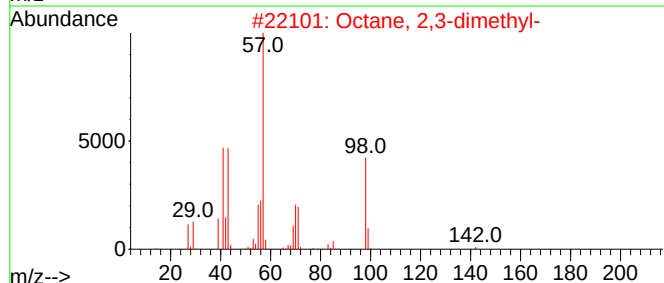
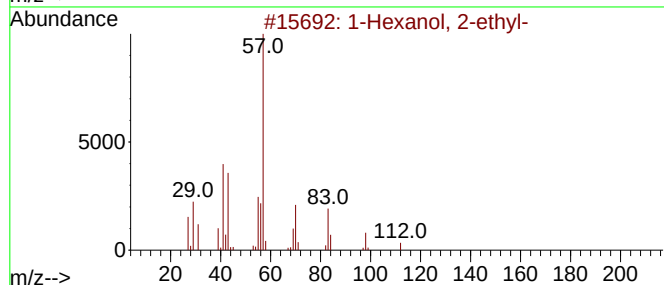
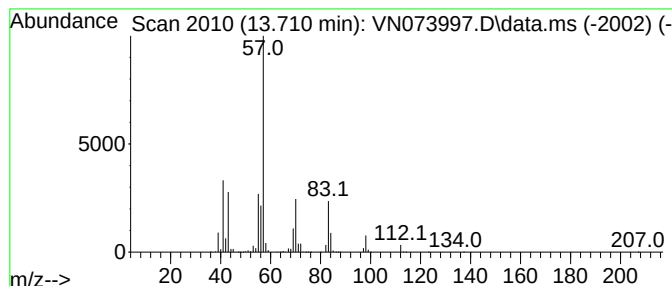
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	100.45 ug/l	7596290	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



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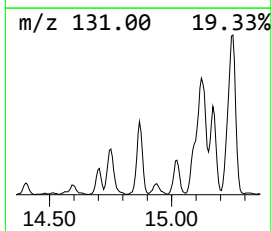
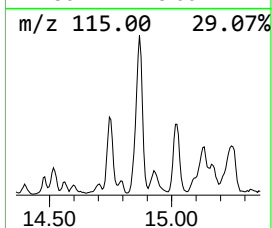
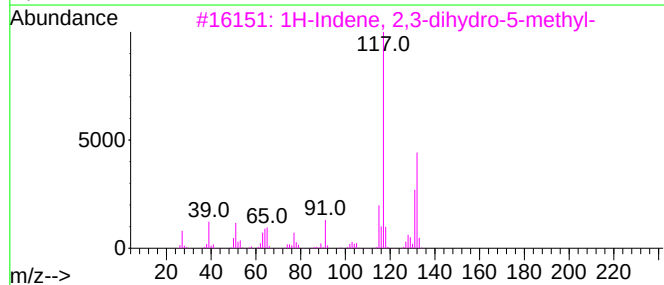
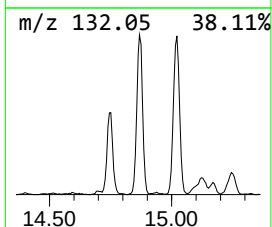
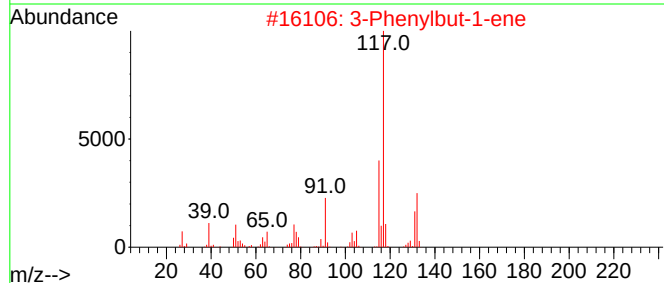
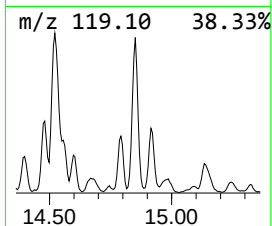
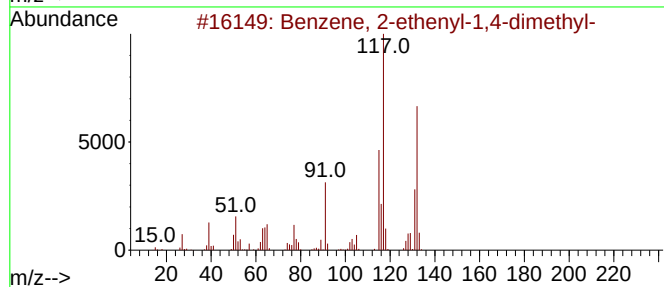
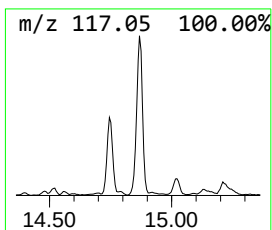
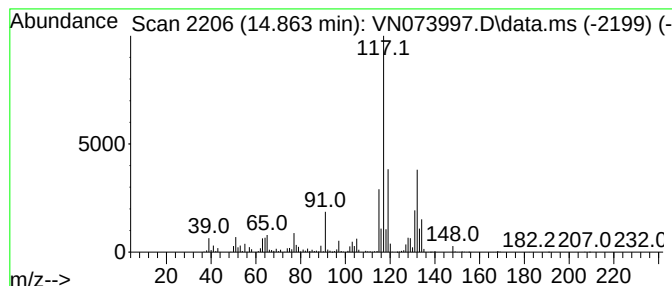
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Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.863	29.22 ug/l	2209520	1,4-Dichlorobenzene-d4			13.616
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-		132	C10H12	002039-89-6	92
2	3-Phenylbut-1-ene		132	C10H12	000934-10-1	76
3	1H-Indene, 2,3-dihydro-5-methyl-		132	C10H12	000874-35-1	70
4	1H-Indene, 2,3-dihydro-4-methyl-		132	C10H12	000824-22-6	70
5	Benzene, 1-ethenyl-4-ethyl-		132	C10H12	003454-07-7	70



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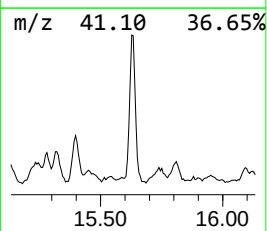
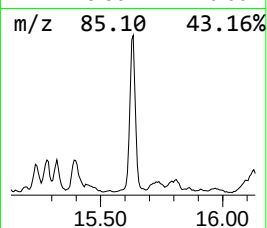
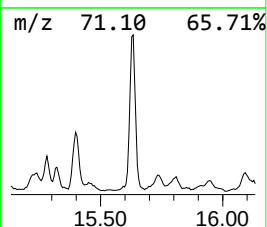
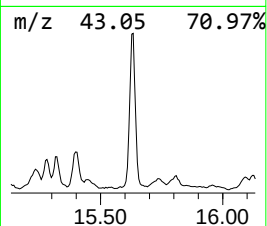
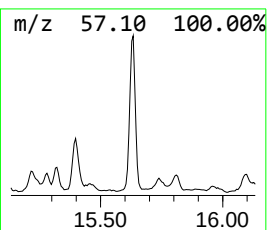
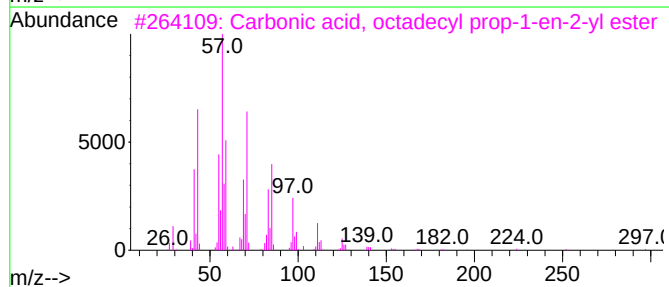
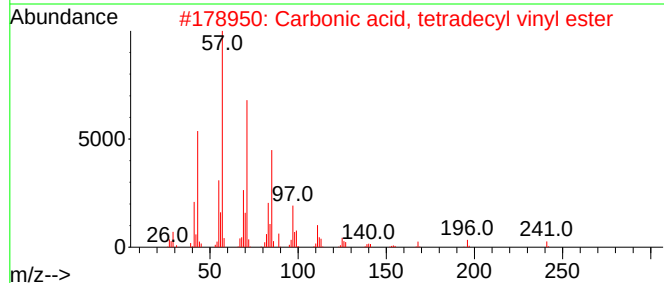
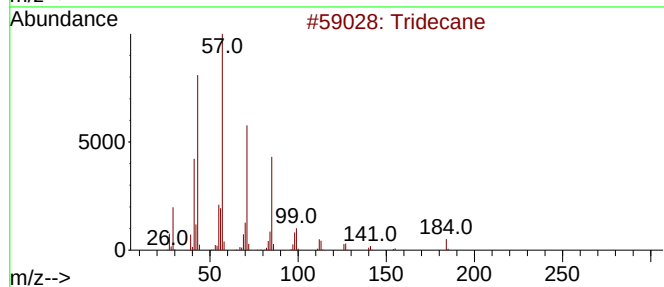
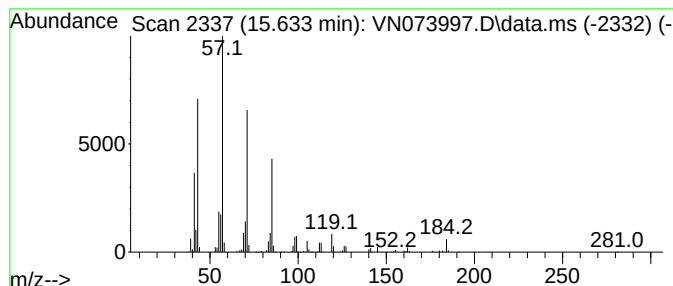
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.633	30.01 ug/l	2269350	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
4			Dodecane	170	C12H26	000112-40-3	86
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081822\
Data File : VN073997.D
Acq On : 18 Aug 2022 12:07
Operator : JC\MD
Sample : N4241-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1630

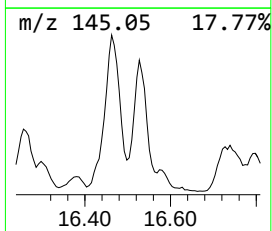
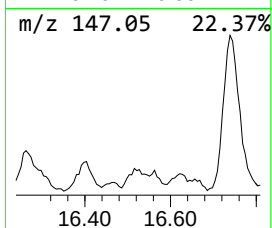
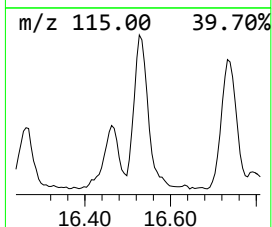
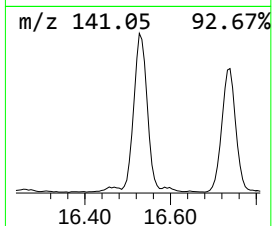
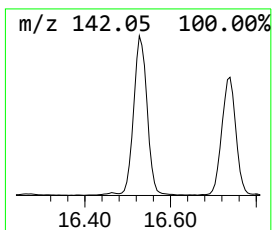
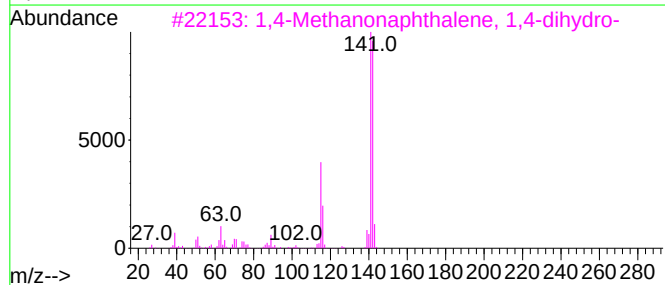
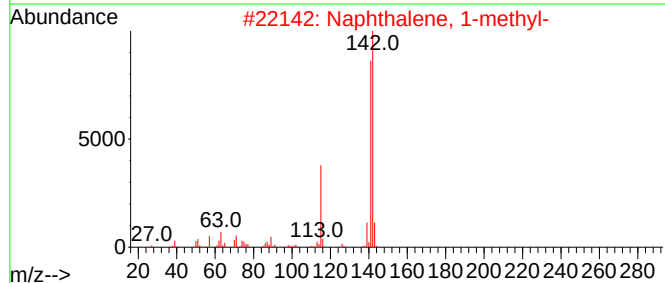
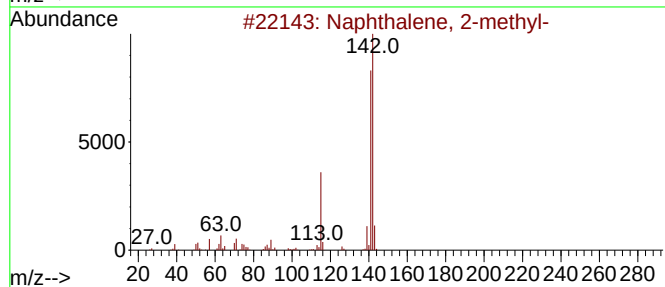
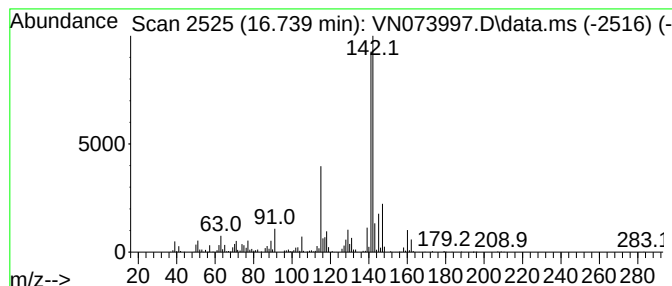
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.739	26.54 ug/l	2006950	1,4-Dichlorobenzene-d4	13.616

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	89
4			Benzocycloheptatriene	142	C11H10	000264-09-5	81
5			Benzeneacetonitrile, 4-cyano-	142	C9H6N2	000876-31-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081822\
Data File : VN073997.D
Acq On : 18 Aug 2022 12:07
Operator : JC\MD
Sample : N4241-07
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TRE-1630

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	6.981	78.7	ug/l	3102650	1	8.016	1972340	50.0
1,3-Dioxolane, ...	8.181	696.2	ug/l	27463800	1	8.016	1972340	50.0
1-Butanol	9.092	42.5	ug/l	2221780	2	8.904	2616280	50.0
1-Hexanol, 2-et...	13.710	100.5	ug/l	7596290	4	13.616	3781070	50.0
Benzene, 2-ethe...	14.863	29.2	ug/l	2209520	4	13.616	3781070	50.0
Tridecane	15.633	30.0	ug/l	2269350	4	13.616	3781070	50.0
Naphthalene, 1-...	16.739	26.5	ug/l	2006950	4	13.616	3781070	50.0