

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
 Data File : VN076666.D
 Acq On : 14 Feb 2023 17:24
 Operator : JC\MD
 Sample : 01549-13
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1929

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\82N021323W.M
 Title : SW846 8260

Signal : TIC: VN076666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.096	21	27	33	rBV2	91128	138923	6.76%	0.944%
2	2.331	59	67	72	rBV4	12355	25139	1.22%	0.171%
3	2.525	96	100	107	rVB2	15788	27788	1.35%	0.189%
4	2.678	119	126	132	rBV	150700	276626	13.46%	1.880%
5	2.831	143	152	153	rBV6	16401	34988	1.70%	0.238%
6	2.843	153	154	162	rVB5	23330	30034	1.46%	0.204%
7	4.307	393	403	413	rBV2	31788	93170	4.53%	0.633%
8	4.449	418	427	437	rBV	32940	101743	4.95%	0.691%
9	4.737	467	476	485	rBV2	13734	41751	2.03%	0.284%
10	6.731	806	815	828	rBV4	43915	139831	6.80%	0.950%
11	7.237	891	901	914	rBV4	94683	275611	13.41%	1.873%
12	8.172	1049	1060	1065	rBV	259882	643308	31.29%	4.372%
13	8.231	1065	1070	1079	rVB	483003	1036293	50.41%	7.043%
14	8.589	1118	1131	1145	rBV2	340412	1039911	50.58%	7.067%
15	9.107	1210	1219	1231	rBV	705803	1459435	70.99%	9.919%
16	9.278	1243	1248	1256	rBV6	10619	27200	1.32%	0.185%
17	10.572	1459	1468	1474	rBV	1099855	2055892	100.00%	13.972%
18	10.631	1474	1478	1487	rVB	89512	176630	8.59%	1.200%
19	11.360	1596	1602	1606	rBV7	12615	29275	1.42%	0.199%
20	11.719	1650	1663	1665	rBV7	12686	39385	1.92%	0.268%
21	11.866	1681	1688	1699	rVB	981483	1809163	88.00%	12.295%
22	11.960	1701	1704	1713	rVB5	13899	29733	1.45%	0.202%
23	12.072	1716	1723	1730	rBV	41200	88098	4.29%	0.599%
24	12.407	1773	1780	1782	rBV4	30832	60645	2.95%	0.412%
25	12.519	1789	1799	1802	rBV5	65093	187738	9.13%	1.276%
26	12.848	1845	1855	1864	rVB	787398	1487848	72.37%	10.112%
27	13.101	1894	1898	1899	rBV4	21549	24674	1.20%	0.168%
28	13.348	1934	1940	1944	rBV3	78593	146230	7.11%	0.994%
29	13.483	1960	1963	1969	rBV2	26038	43079	2.10%	0.293%
30	13.624	1983	1987	1988	rBV4	22081	24199	1.18%	0.164%
31	13.683	1995	1997	2009	rVB4	42642	116039	5.64%	0.789%
32	13.795	2009	2016	2021	rVV	920977	1553526	75.56%	10.558%
33	13.871	2023	2029	2040	rVB3	184106	519842	25.29%	3.533%
34	14.036	2048	2057	2068	rBV5	106868	338475	16.46%	2.300%
35	15.218	2253	2258	2262	rBV8	22598	53973	2.63%	0.367%
36	15.348	2276	2280	2287	rVB9	30438	63887	3.11%	0.434%

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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\82N021323W.M
Title : SW846 8260

37	15.654	2325	2332	2343	rVB9	46999	148576	7.23%	1.010%
38	15.836	2354	2363	2371	rBV4	108934	325450	15.83%	2.212%

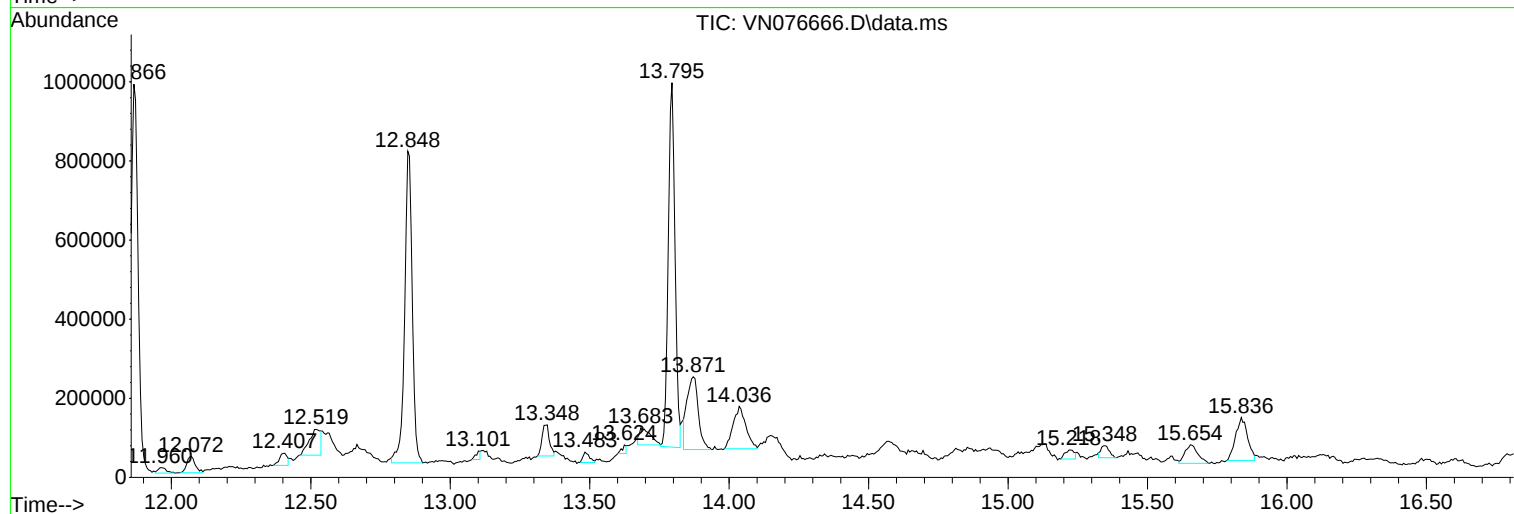
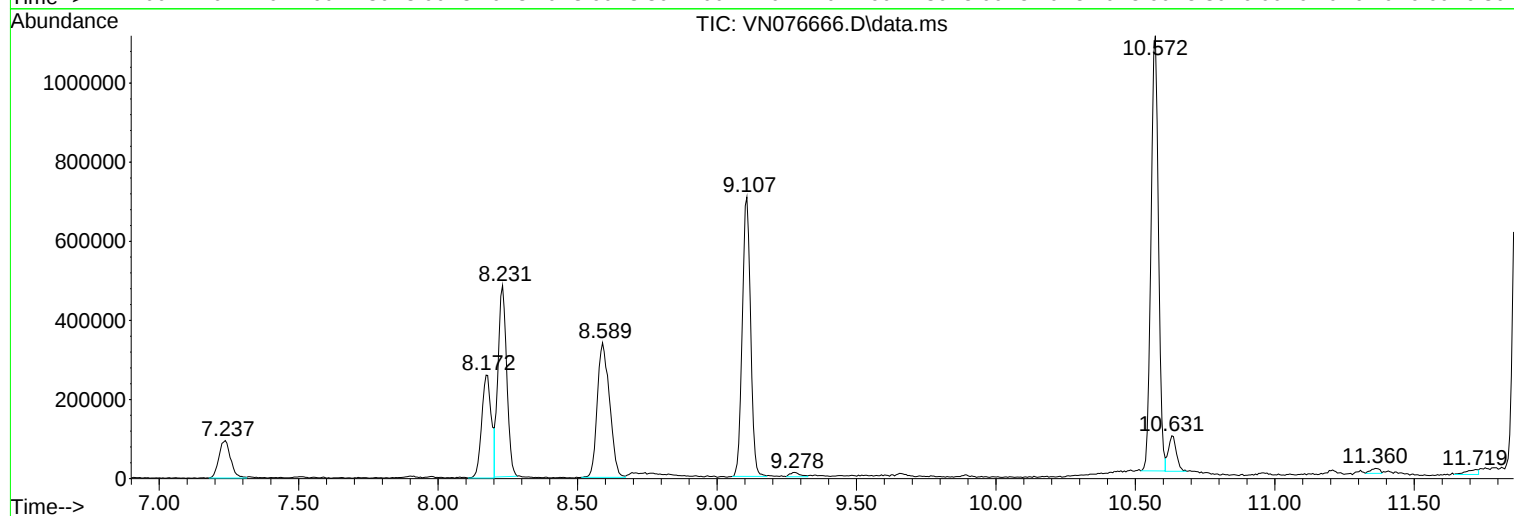
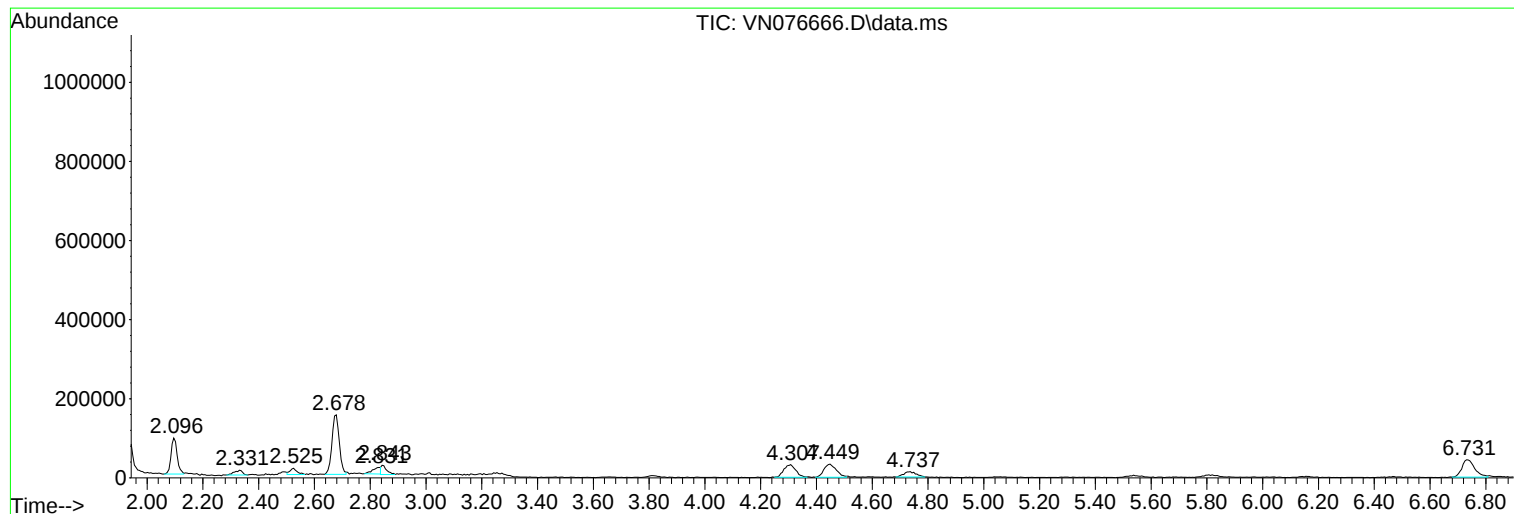
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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



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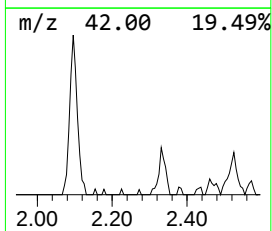
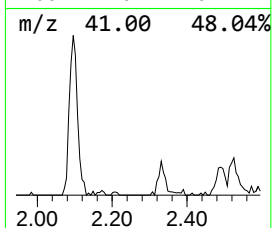
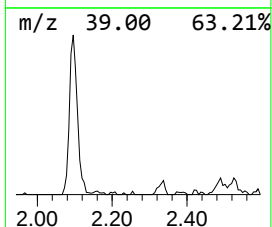
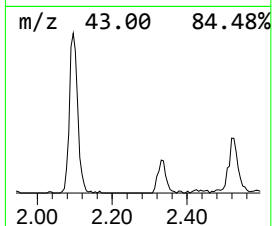
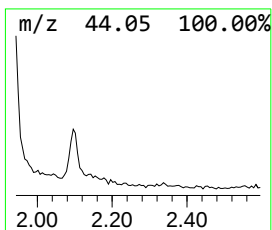
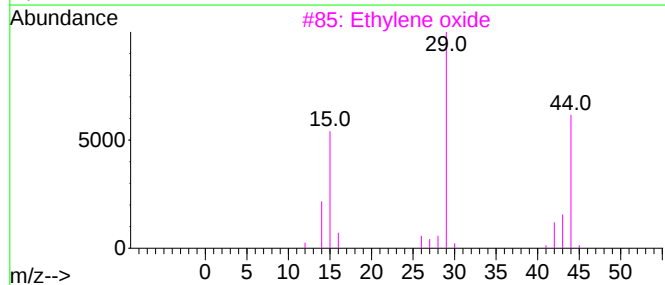
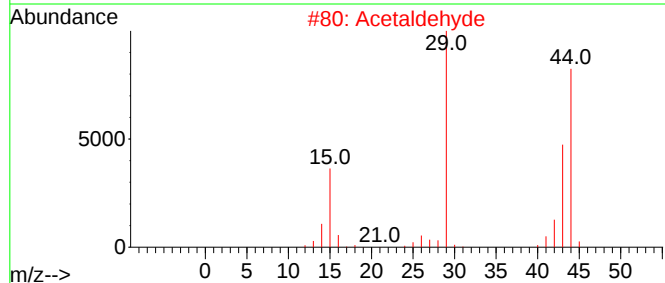
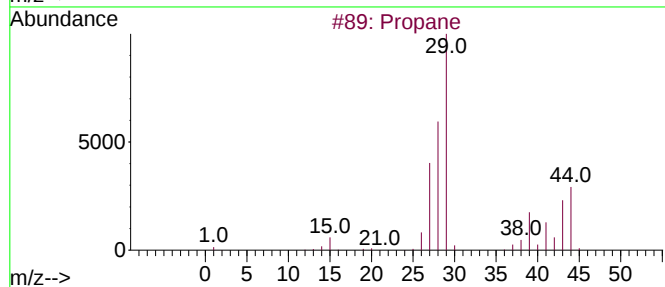
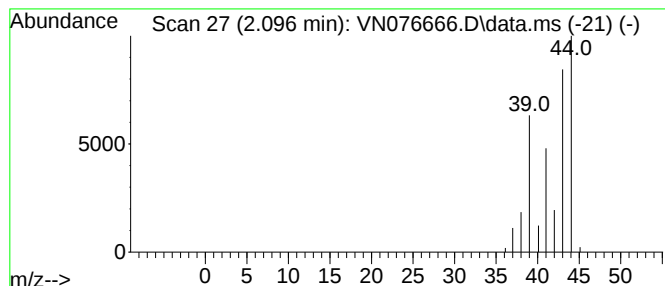
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 1 Propane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.096	6.70 ug/l	138923	Pentafluorobenzene	8.231

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane	44	C3H8	000074-98-6	83
2		Acetaldehyde	44	C2H4O	000075-07-0	7
3		Ethylene oxide	44	C2H4O	000075-21-8	5
4		Acetonitrile-d3	44	C2D3N	002206-26-0	4
5		Hydrogen isocyanate	43	CHNO	000075-13-8	3



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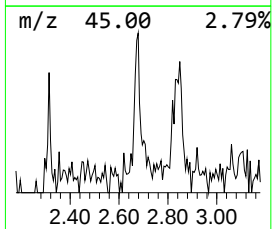
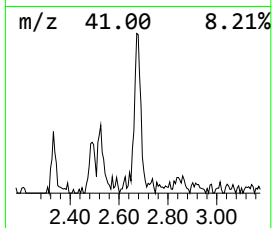
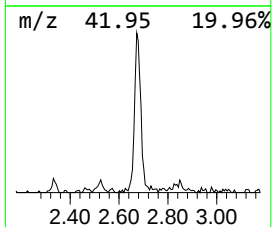
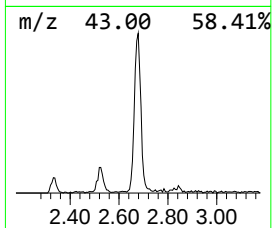
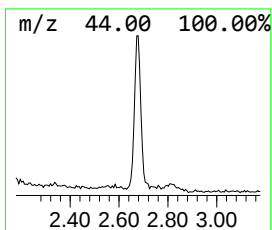
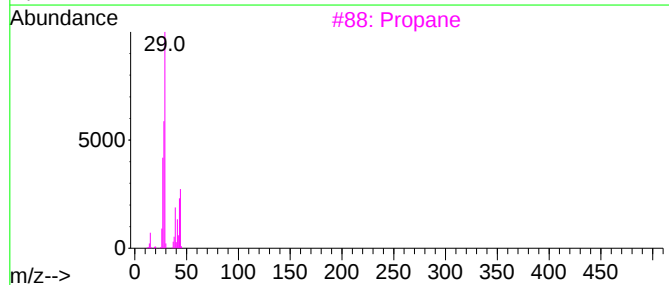
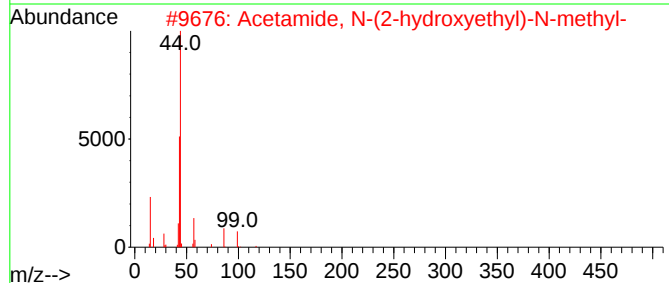
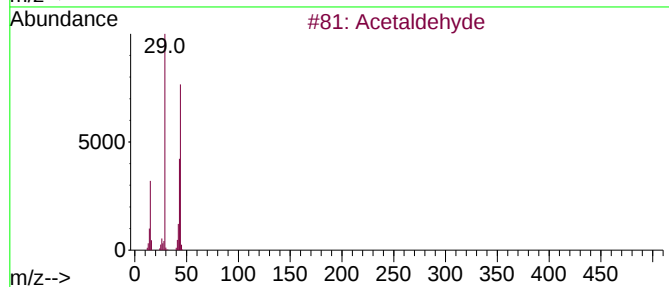
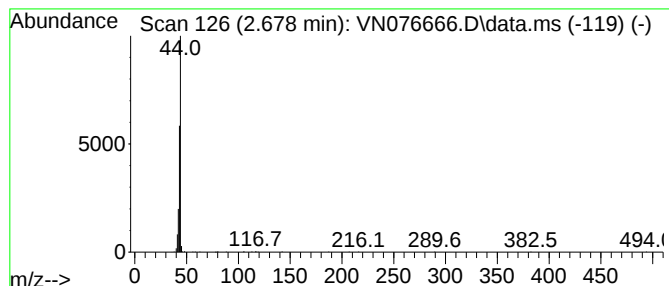
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.678	13.35 ug/l	276626	Pentafluorobenzene	8.231

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Acetamide, N-(2-hydroxyethyl)-N-...	117	C5H11NO2	015567-95-0	7
3			Propane	44	C3H8	000074-98-6	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			3,6-Dimethylpiperazine-2,5-dione	142	C6H10N2O2	005625-46-7	4



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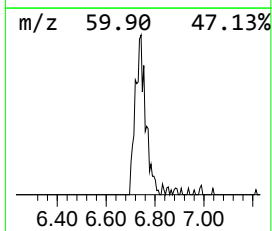
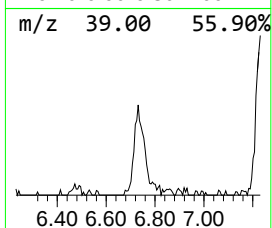
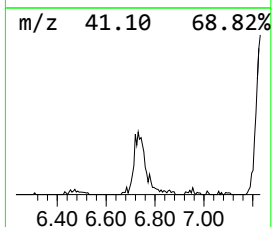
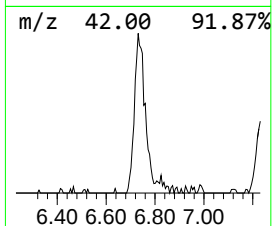
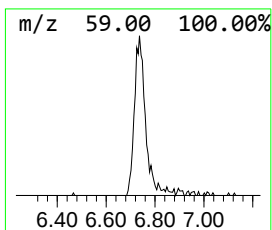
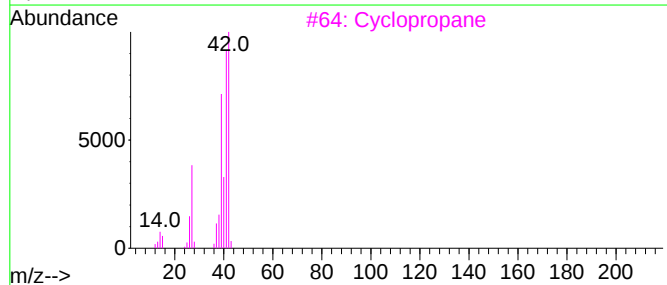
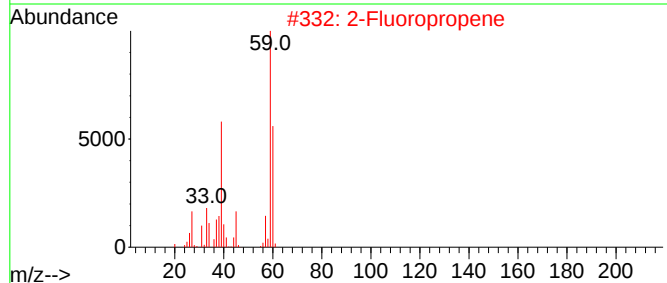
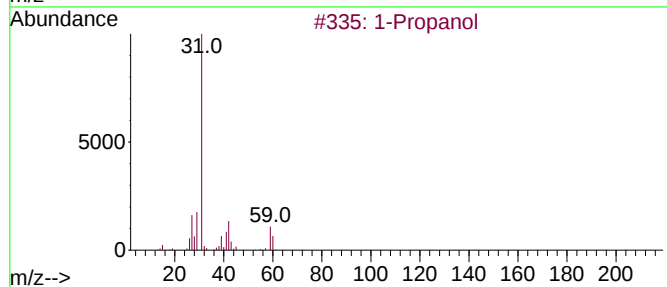
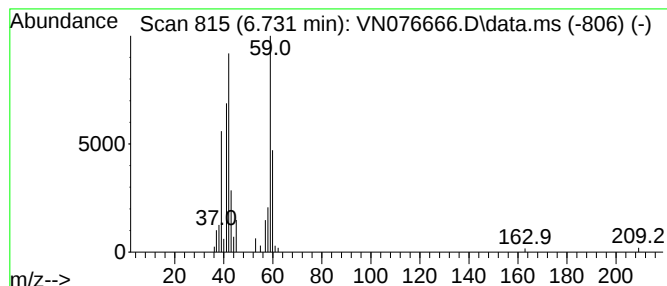
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.731	6.75 ug/l	139831	Pentafluorobenzene	8.231

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	50
2	2-Fluoropropene			60	C3H5F	001184-60-7	46
3	Cyclopropane			42	C3H6	000075-19-4	32
4	Allyl fluoride			60	C3H5F	000818-92-8	30
5	3-Buten-1-ol			72	C4H8O	000627-27-0	25



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ALS Vial : 16 Sample Multiplier: 1

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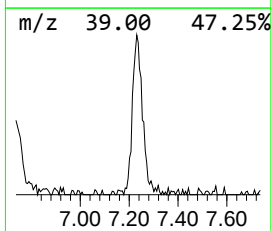
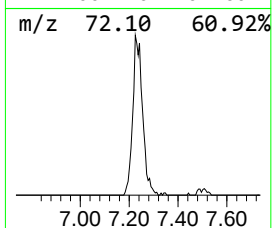
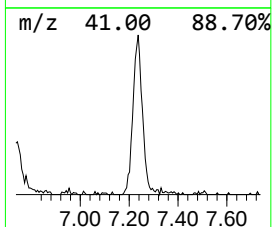
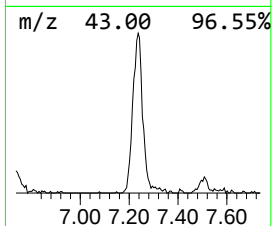
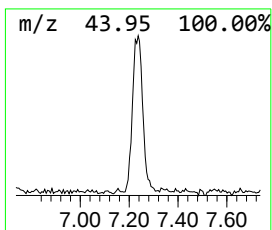
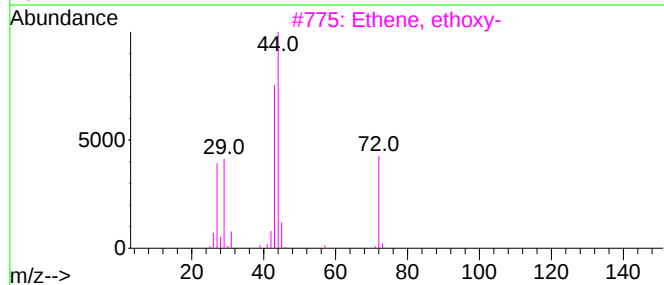
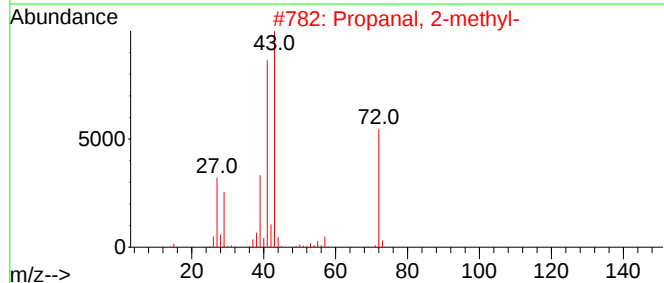
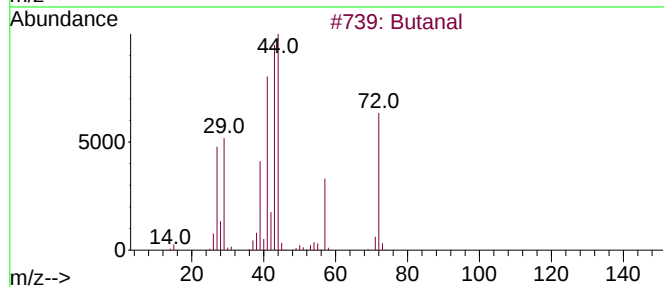
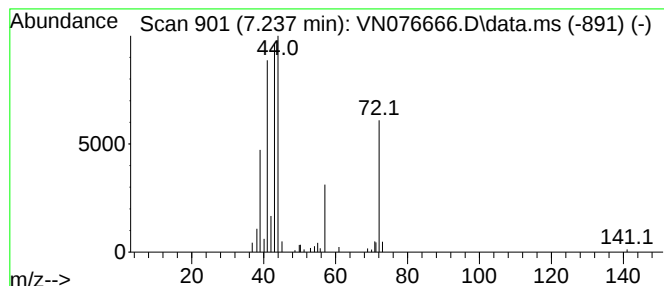
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.237	13.30 ug/l	275611	Pentafluorobenzene	8.231

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	91
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	50
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	25
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25



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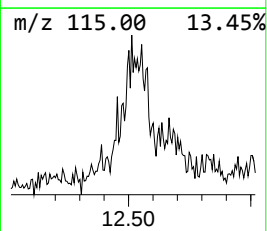
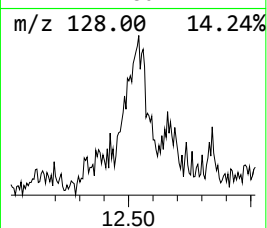
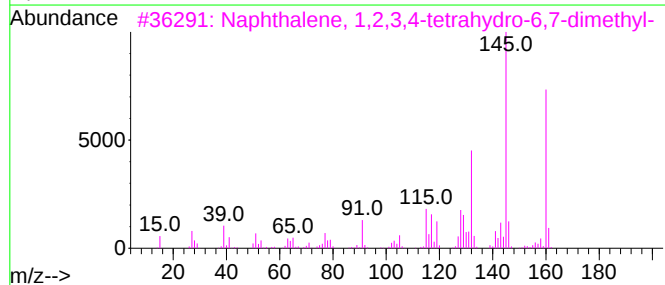
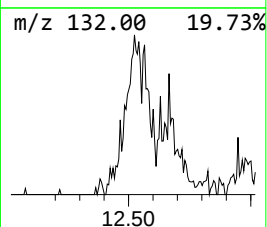
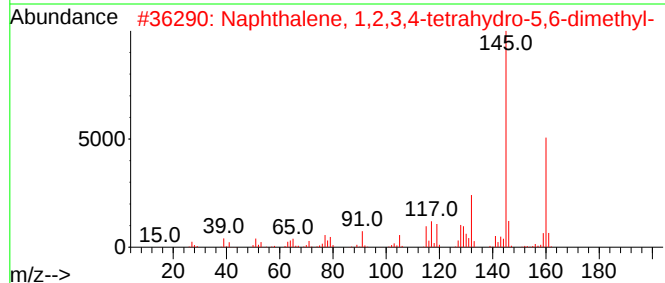
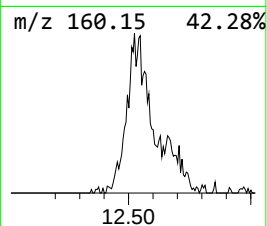
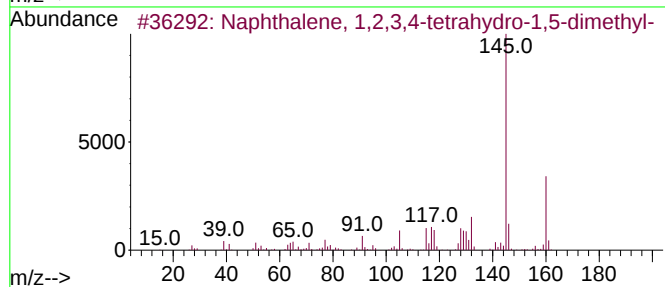
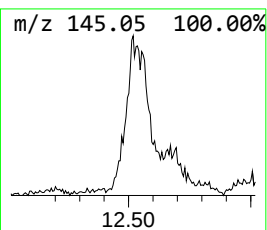
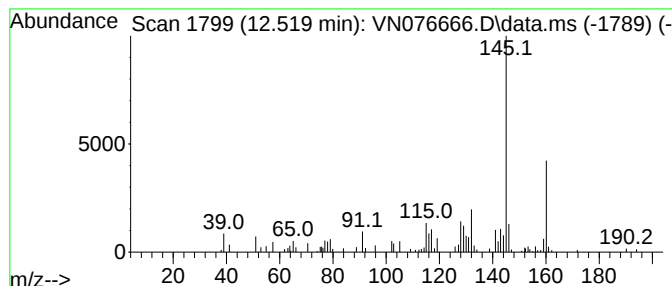
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Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.519	5.19 ug/l	187738	Chlorobenzene-d5		11.866	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	021564-91-0	93
2	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	020027-77-4	91
3	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	001076-61-5	87
4	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	004175-54-6	87
5	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	021693-54-9	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076666.D
Acq On : 14 Feb 2023 17:24
Operator : JC\MD
Sample : 01549-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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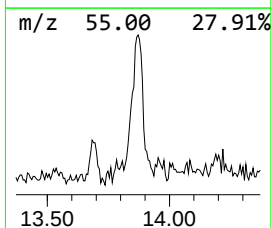
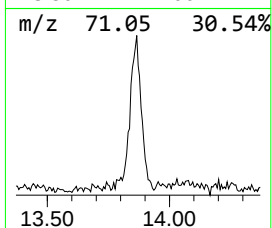
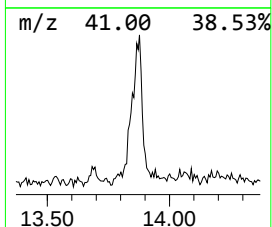
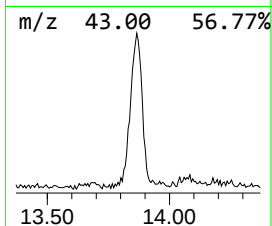
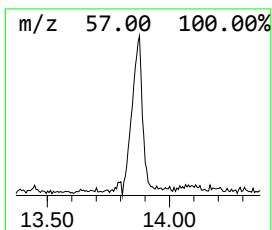
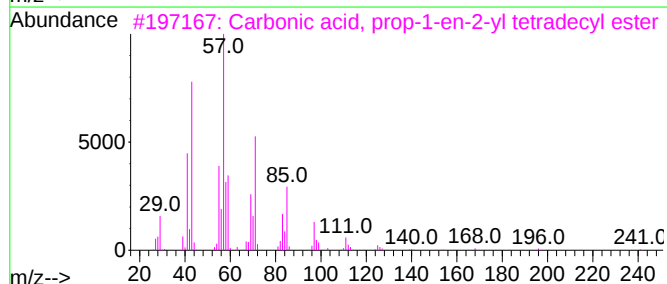
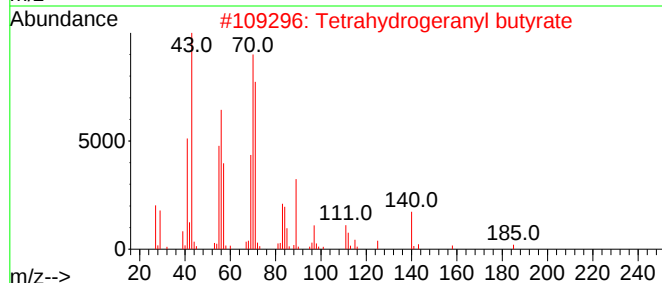
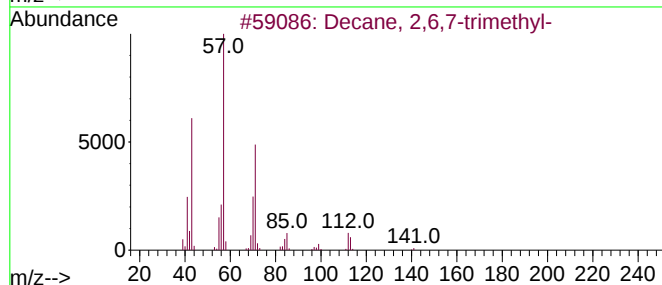
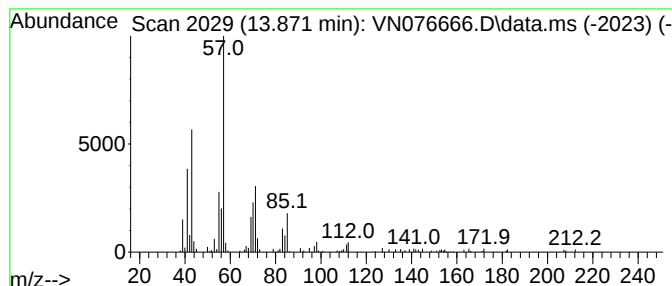
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Quant Title : SW846 8260

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

Peak Number 6 Decane, 2,6,7-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	16.73 ug/l	519842	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
2			Tetrahydrogeranyl butyrate	228	C14H28O2	1000428-75-4	53
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	50
4			Nonane, 4-methyl-	142	C10H22	017301-94-9	50
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076666.D
Acq On : 14 Feb 2023 17:24
Operator : JC\MD
Sample : 01549-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1929

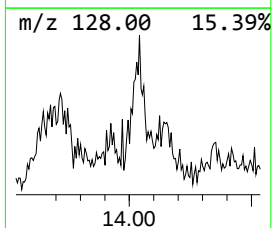
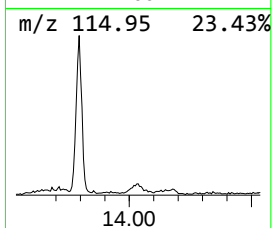
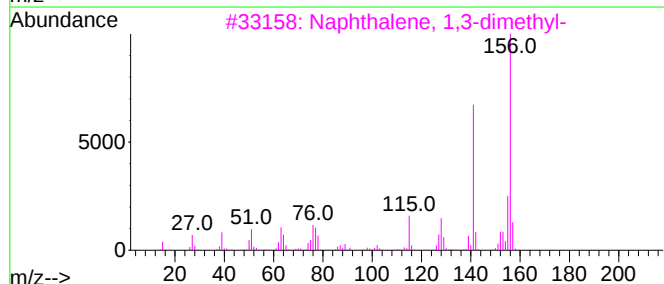
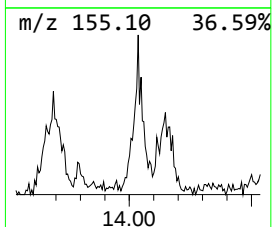
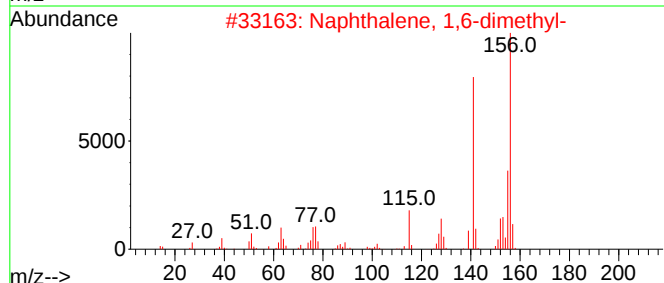
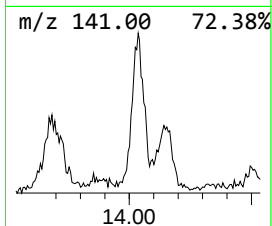
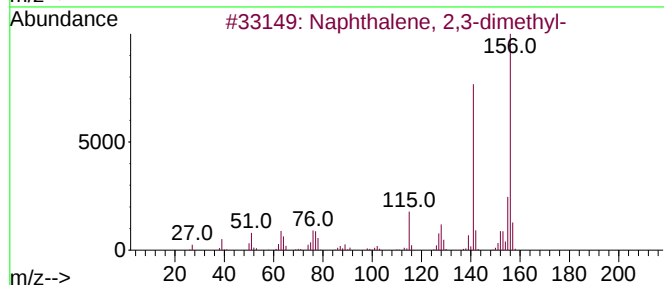
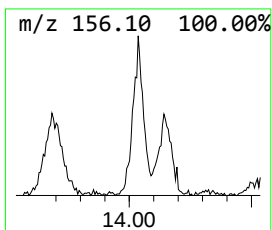
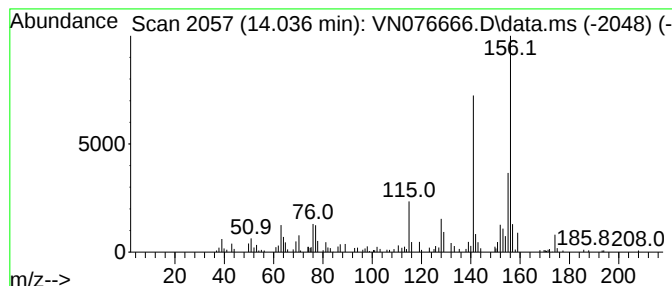
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.036	10.89 ug/l	338475	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076666.D
Acq On : 14 Feb 2023 17:24
Operator : JC\MD
Sample : 01549-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1929

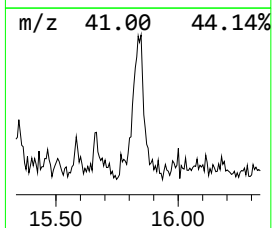
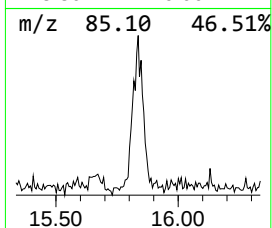
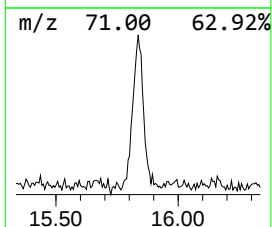
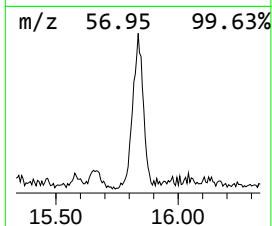
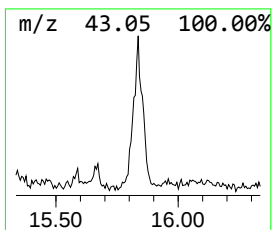
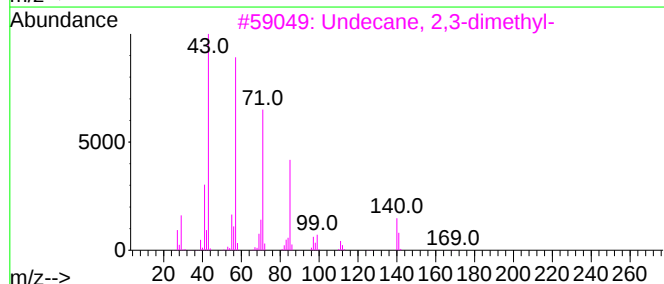
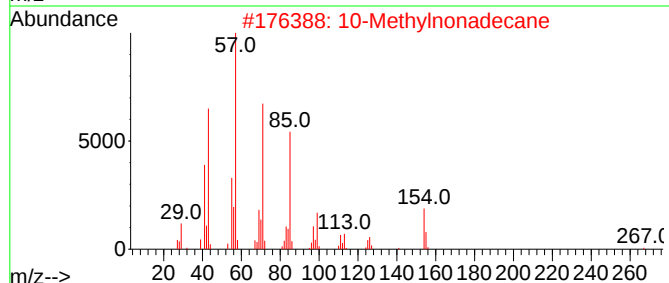
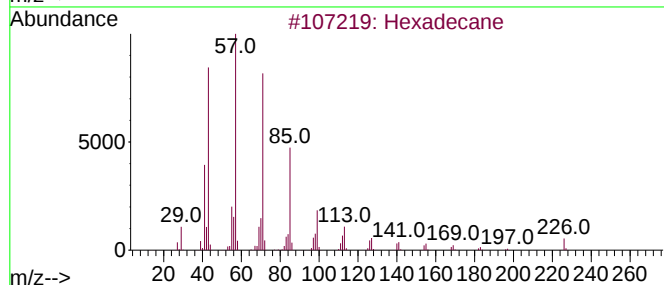
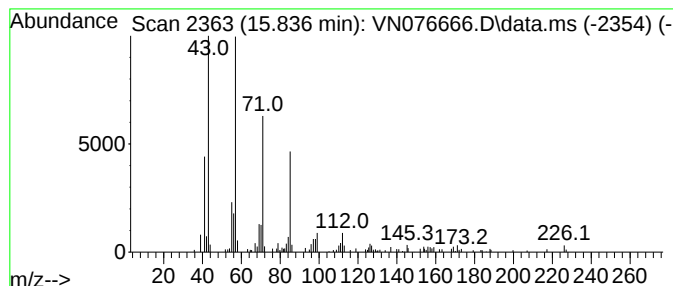
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Quant Title : SW846 8260

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

Peak Number 8 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.836	10.47 ug/l	325450	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			10-Methylnonadecane	282	C20H42	056862-62-5	87
3			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	72
4			Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	64
5			Tridecane	184	C13H28	000629-50-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021423\
Data File : VN076666.D
Acq On : 14 Feb 2023 17:24
Operator : JC\MD
Sample : 01549-13
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.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
Propane	2.096	6.7	ug/l	138923	1	8.231	1036290	50.0
Acetaldehyde	2.678	13.4	ug/l	276626	1	8.231	1036290	50.0
1-Propanol	6.731	6.8	ug/l	139831	1	8.231	1036290	50.0
Butanal	7.237	13.3	ug/l	275611	1	8.231	1036290	50.0
Naphthalene, 1,...	12.519	5.2	ug/l	187738	3	11.866	1809160	50.0
Decane, 2,6,7-t...	13.871	16.7	ug/l	519842	4	13.795	1553530	50.0
Naphthalene, 2,...	14.036	10.9	ug/l	338475	4	13.795	1553530	50.0
Hexadecane	15.836	10.5	ug/l	325450	4	13.795	1553530	50.0