

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
 Data File : VX045766.D
 Acq On : 14 Apr 2025 14:25
 Operator : JC/MD
 Sample : Q1799-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FRAC-TANK-216-PPR

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_X\Method\82X040225W.M
 Title : SW846 8260

Signal : TIC: VX045766.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	205	212	226	rBV	283805	461000	10.08%	2.907%
2	5.379	694	704	721	rBV	54286	159424	3.48%	1.005%
3	5.550	721	732	744	rBV	77839	221909	4.85%	1.399%
4	5.952	789	798	819	rBV2	63580	170116	3.72%	1.073%
5	6.757	921	930	954	rBV	134181	329332	7.20%	2.077%
6	8.647	1234	1240	1247	rVV	284289	451922	9.88%	2.850%
7	8.714	1247	1251	1262	rVB	31043	55261	1.21%	0.348%
8	10.049	1465	1470	1484	rBV	287036	405423	8.86%	2.556%
9	11.079	1634	1639	1652	rBV	225724	295415	6.46%	1.863%
10	12.018	1788	1793	1801	rBV	273449	344109	7.52%	2.170%
11	12.213	1818	1825	1828	rBV	46458	72601	1.59%	0.458%
12	12.548	1874	1880	1888	rBV	89796	129943	2.84%	0.819%
13	12.768	1910	1916	1917	rBV	120265	166076	3.63%	1.047%
14	12.786	1917	1919	1926	rVV	187432	271480	5.93%	1.712%
15	12.859	1926	1931	1945	rVV	1766897	2419574	52.88%	15.257%
16	12.969	1945	1949	1952	rVV	289032	438762	9.59%	2.767%
17	13.024	1956	1958	1960	rVV	153647	193646	4.23%	1.221%
18	13.067	1960	1965	1967	rVV2	403634	709822	15.51%	4.476%
19	13.103	1967	1971	1973	rVV	1692137	2416516	52.82%	15.237%
20	13.127	1973	1975	1985	rVV	2897932	4575202	100.00%	28.849%
21	13.213	1985	1989	1999	rVB	835686	1098797	24.02%	6.929%
22	13.774	2077	2081	2088	rVB	38088	52750	1.15%	0.333%
23	14.633	2219	2222	2227	rVB	43224	52824	1.15%	0.333%
24	14.780	2241	2246	2255	rVB	84262	111375	2.43%	0.702%
25	15.475	2354	2360	2371	rBV	28283	54059	1.18%	0.341%
26	15.609	2377	2382	2386	rBV	44214	74078	1.62%	0.467%
27	16.322	2491	2499	2510	rBV	64284	127644	2.79%	0.805%

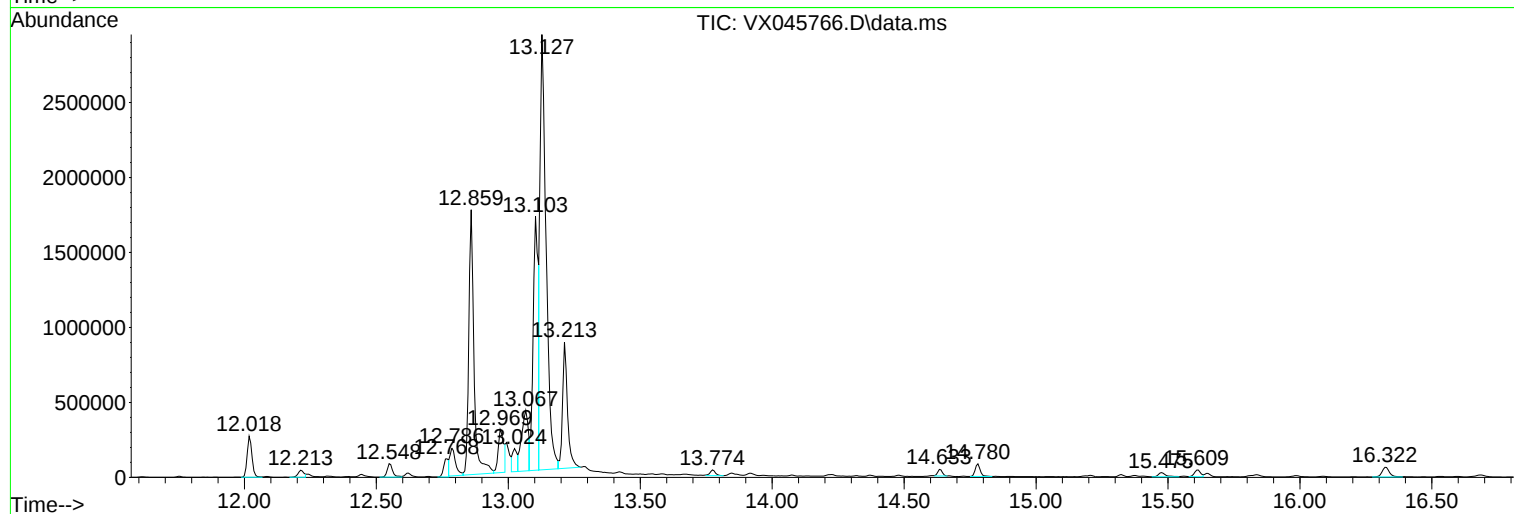
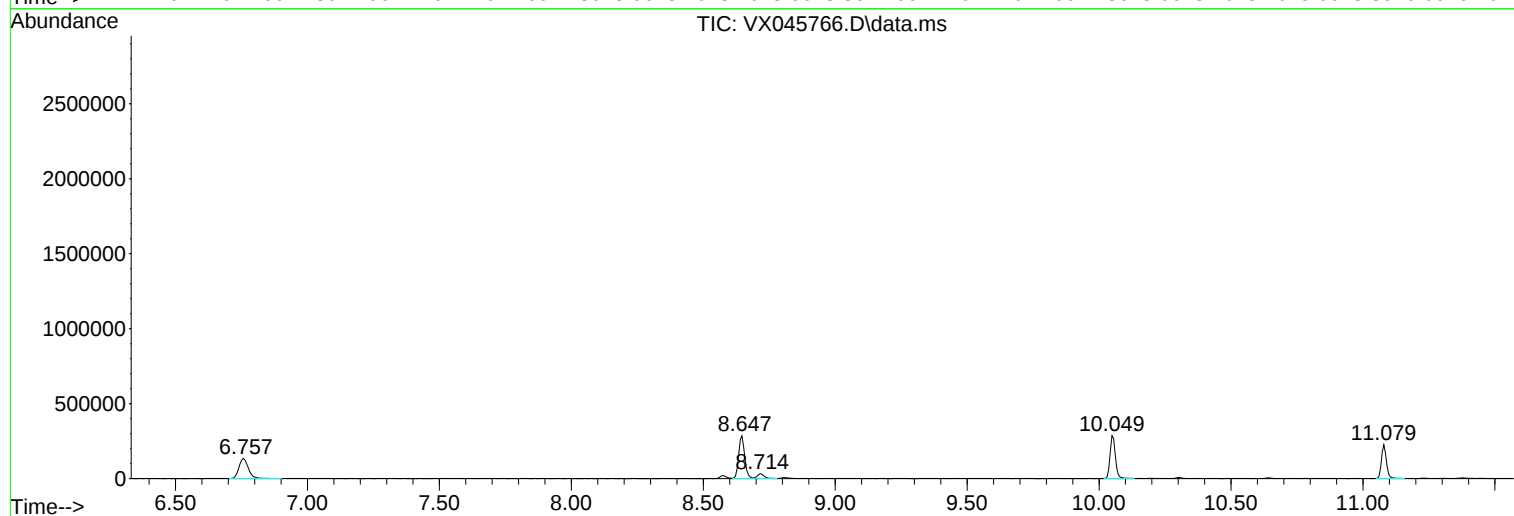
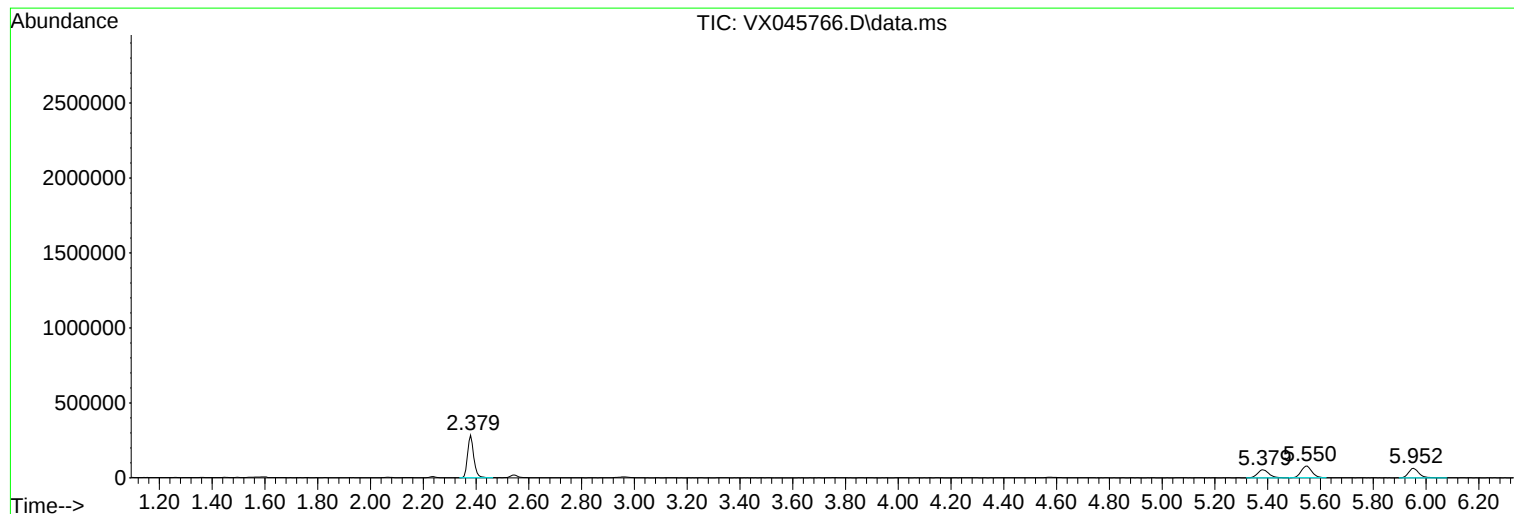
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



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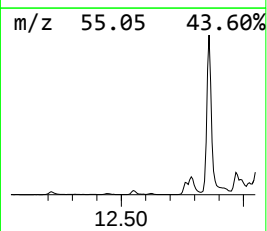
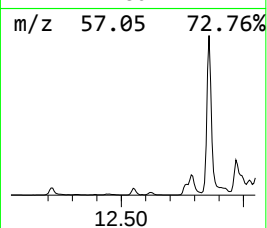
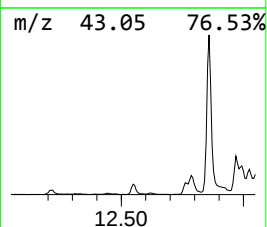
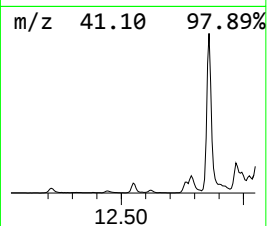
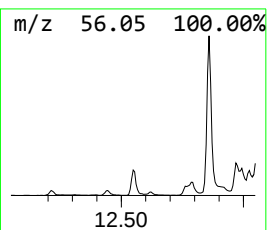
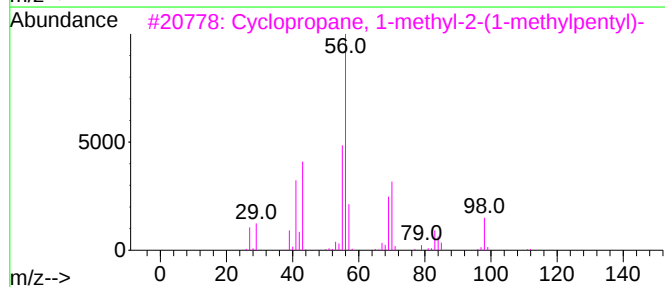
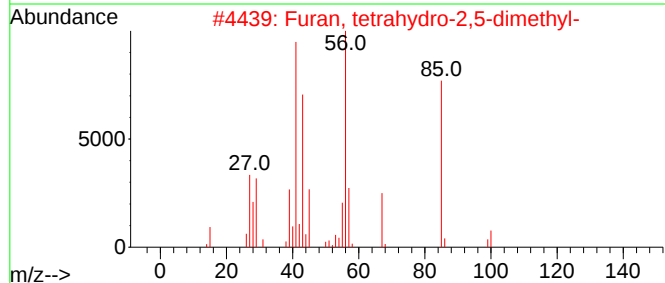
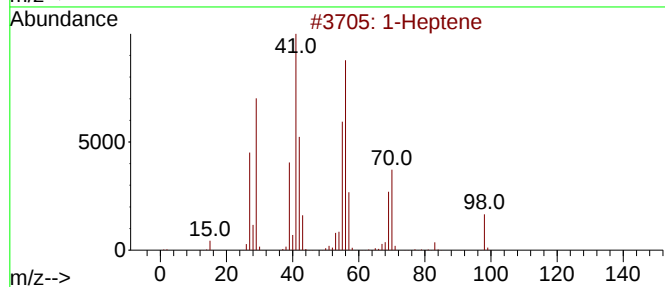
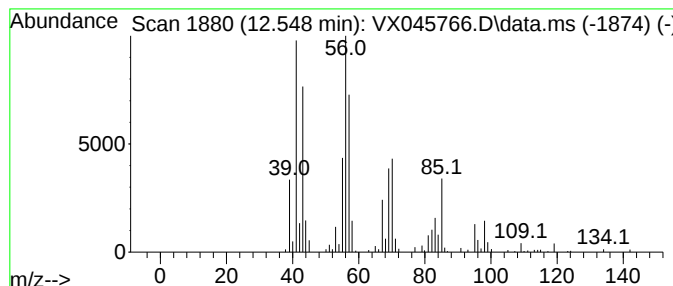
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Quant Title : SW846 8260

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

Peak Number 1 1-Heptene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.548	18.88 ug/l	129943	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptene	98	C7H14	000592-76-7	50
2			Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	47
3			Cyclopropane, 1-methyl-2-(1-meth...	140	C10H20	062238-06-6	43
4			(2,2-Dimethylcyclobutyl)methylamine	113	C7H15N	1000195-04-0	38
5			2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	38



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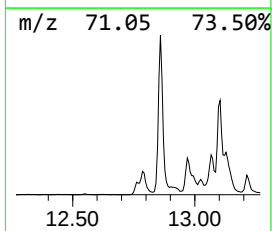
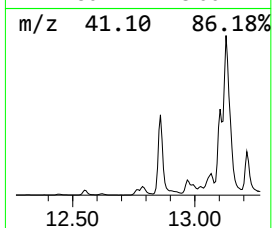
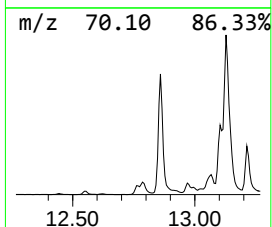
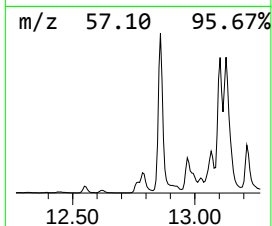
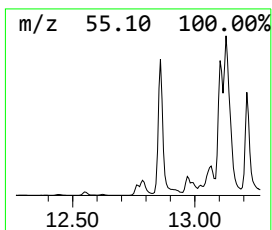
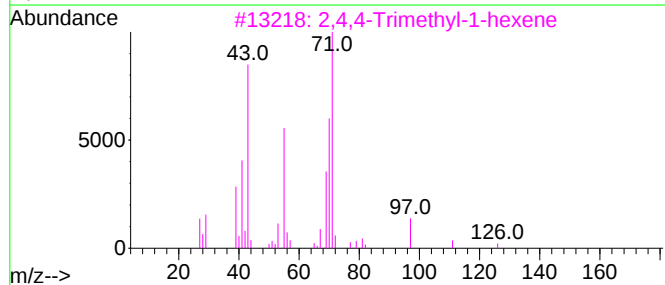
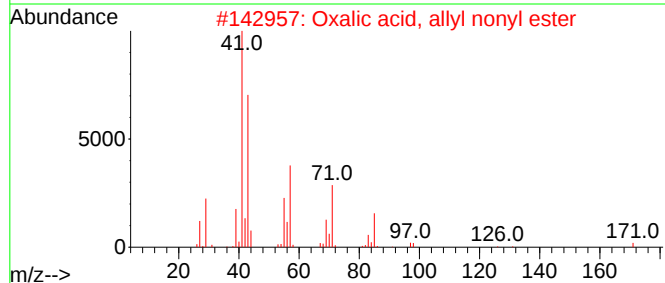
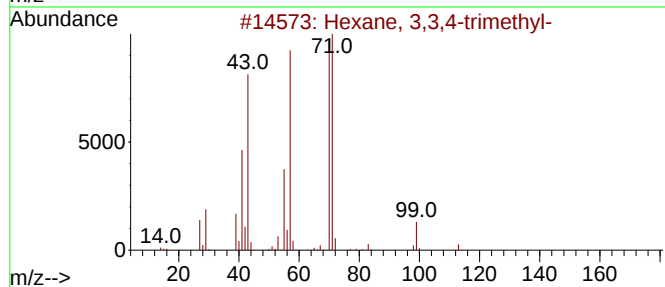
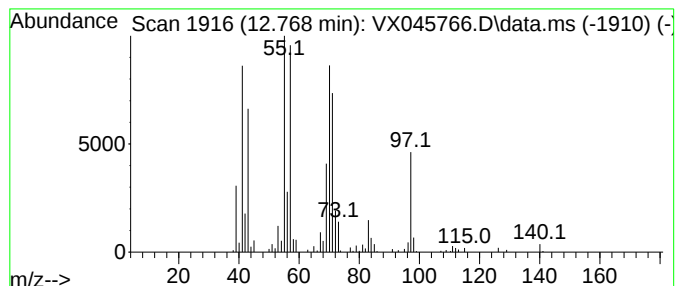
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 2 Hexane, 3,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	24.13 ug/l	166076	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	50
2		Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	43
3		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	43
4		1-Octene, 6-methyl-	126	C9H18	013151-10-5	38
5		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	35



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Instrument :
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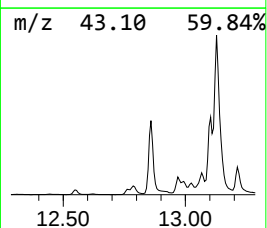
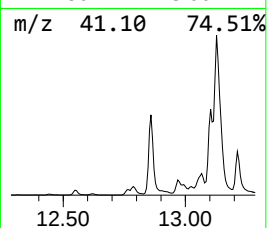
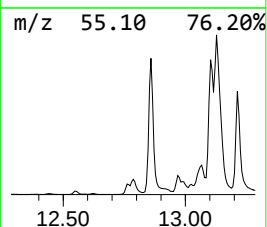
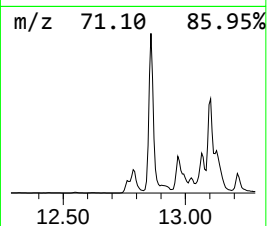
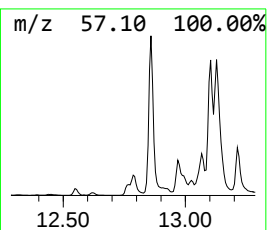
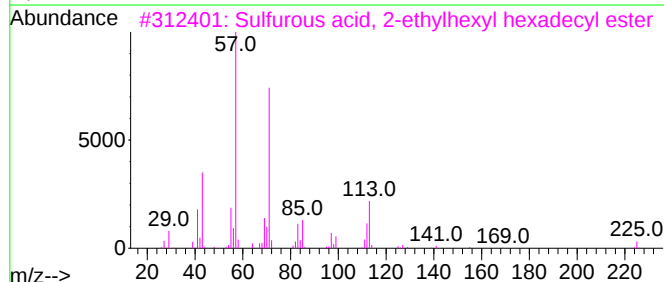
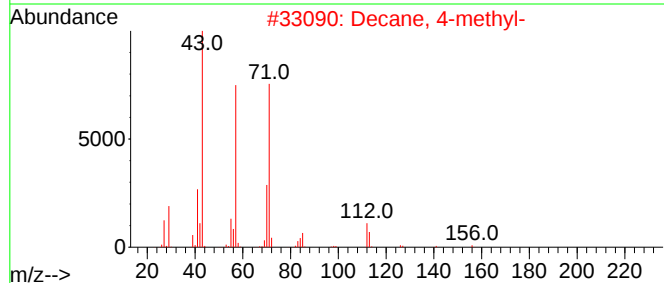
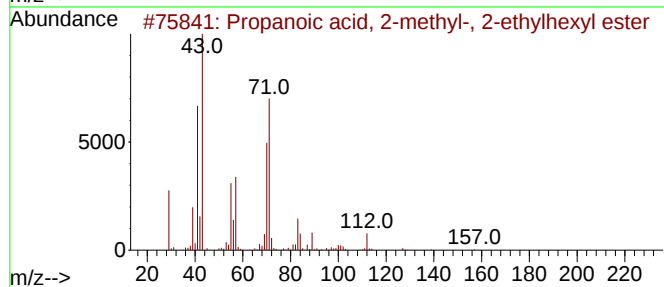
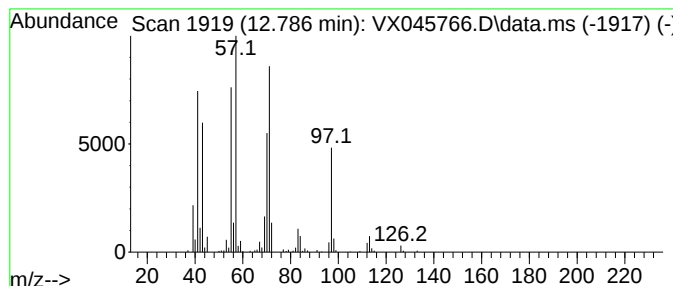
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Quant Title : SW846 8260

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

Peak Number 3 unknown12.786 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.786	39.45 ug/l	271480	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	47
2			Decane, 4-methyl-	156	C11H24	002847-72-5	43
3			Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	43
4			Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	43
5			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	38



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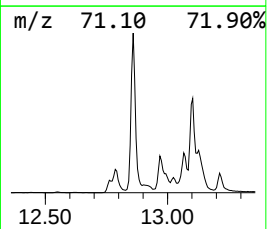
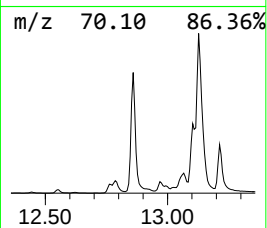
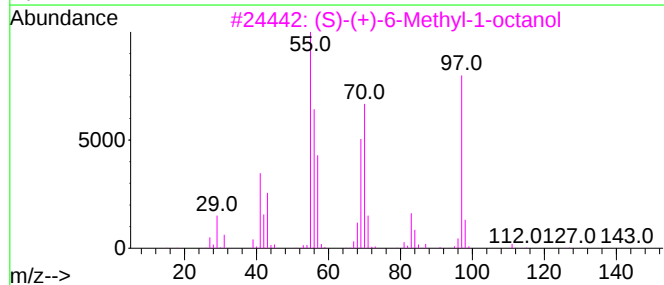
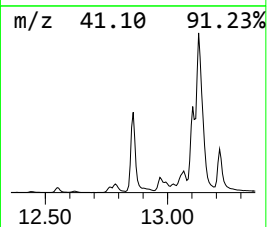
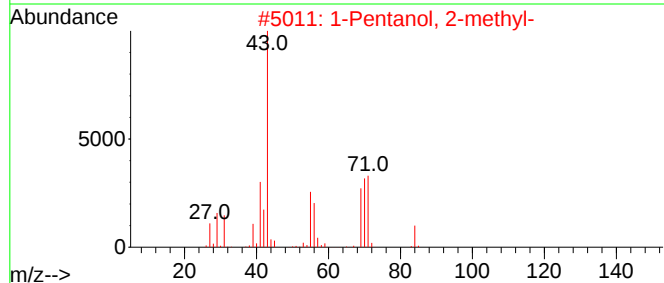
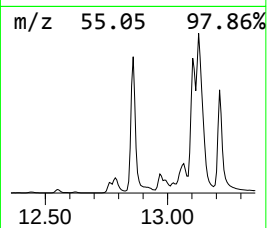
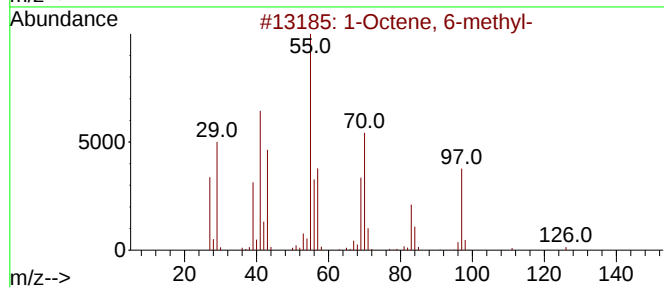
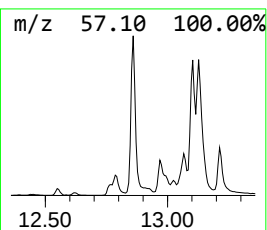
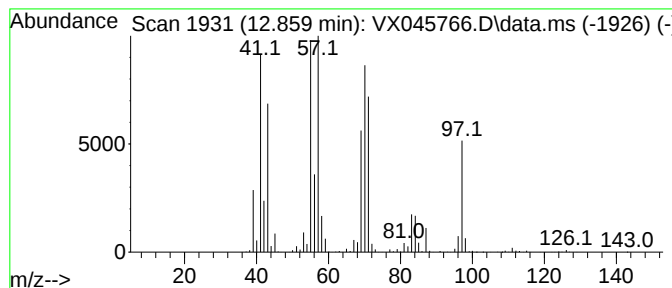
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octene, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	351.57 ug/l	2419570	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octene, 6-methyl-	126	C9H18	013151-10-5	70
2		1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	50
3		(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	50
4		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	47
5		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47



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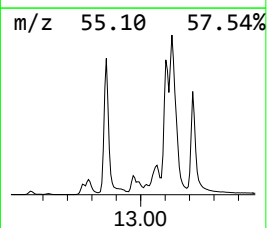
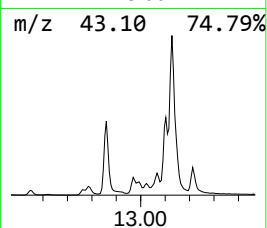
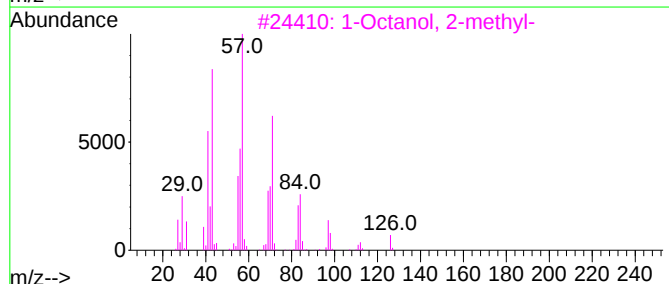
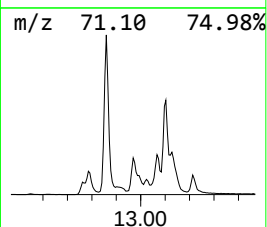
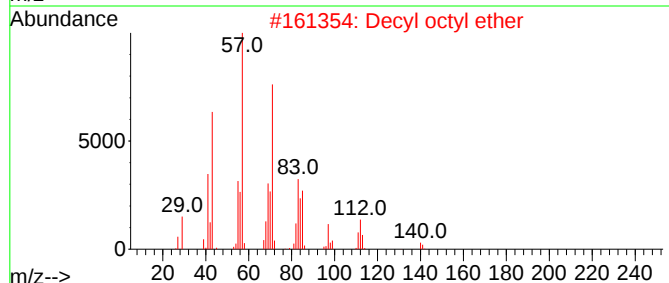
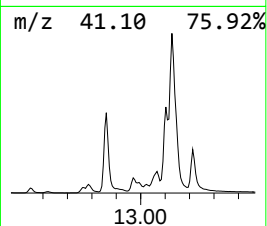
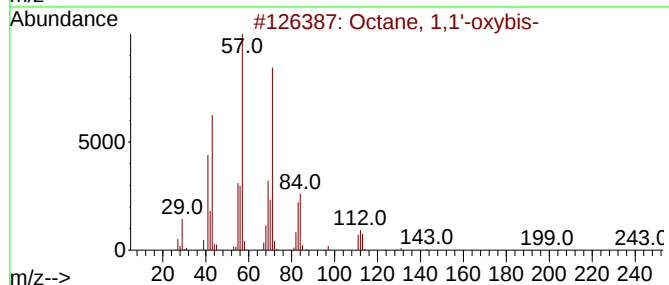
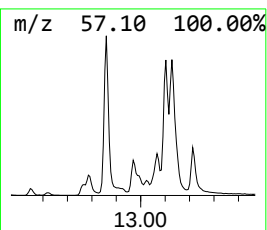
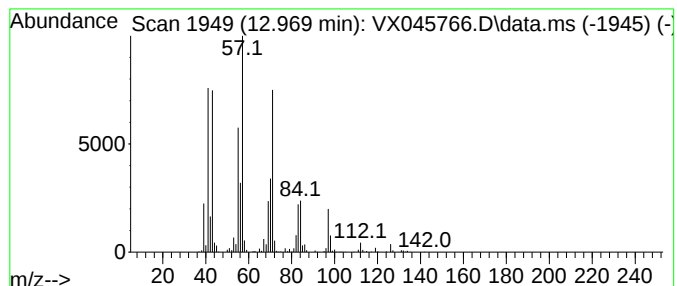
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Quant Title : SW846 8260

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

Peak Number 5 Octane, 1,1'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	63.75 ug/l	438762	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	80
2			Decyl octyl ether	270	C18H38O	1000406-38-3	72
3			1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	59
4			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	50
5			5-Methyl-2-hexanol, 2-methylprop...	186	C11H22O2	1000447-34-4	47



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FRAC-TANK-216-PPR

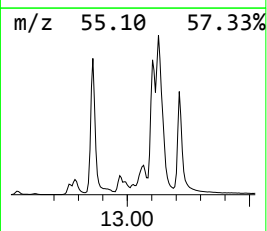
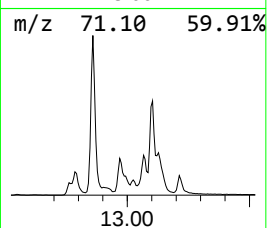
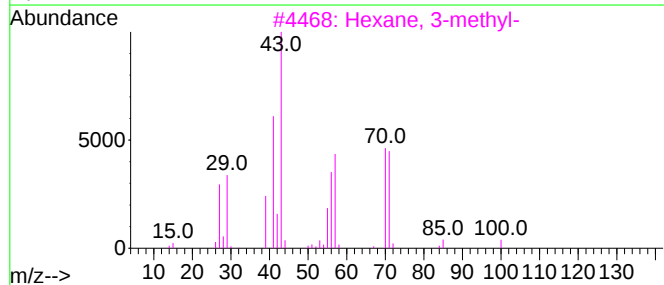
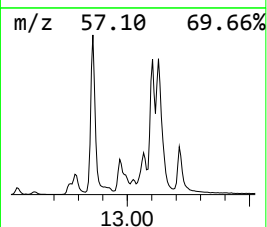
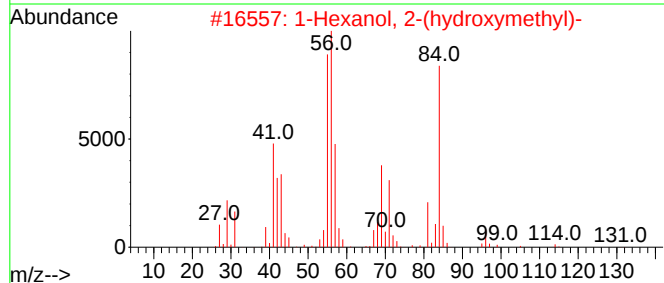
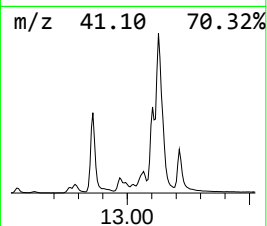
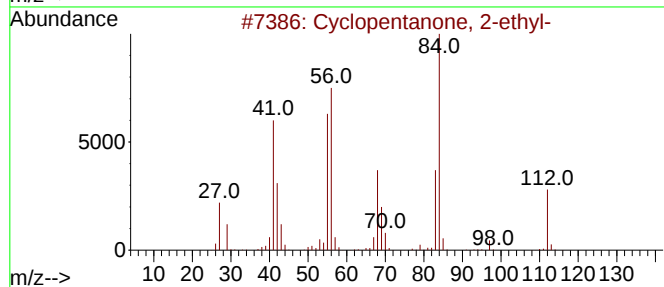
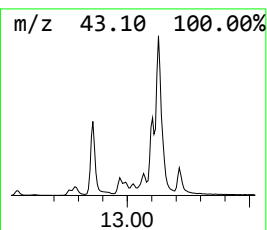
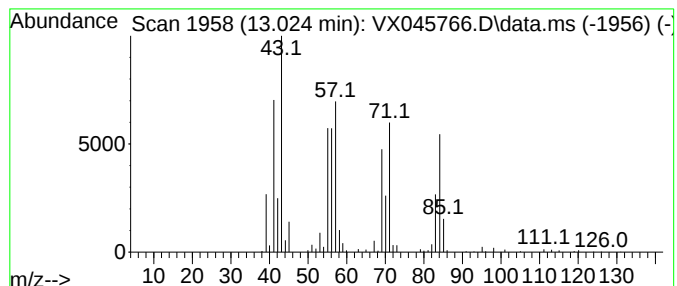
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Quant Title : SW846 8260

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

Peak Number 6 unknown13.024 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.024	28.14 ug/l	193646	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone, 2-ethyl-	112	C7H12O	004971-18-0	47
2			1-Hexanol, 2-(hydroxymethyl)-	132	C7H16O2	1000326-00-5	43
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	38
4			Cyclopentanone	84	C5H8O	000120-92-3	35
5			Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
Data File : VX045766.D
Acq On : 14 Apr 2025 14:25
Operator : JC/MD
Sample : Q1799-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

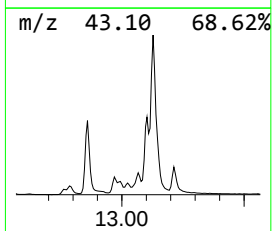
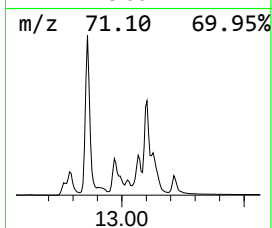
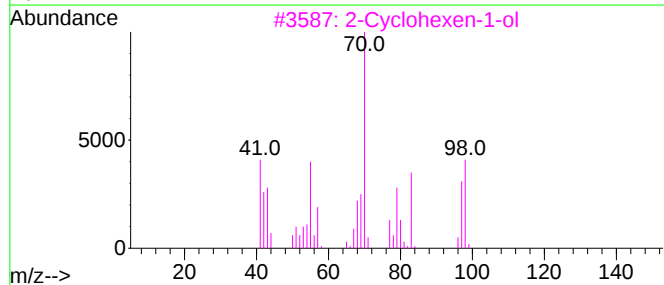
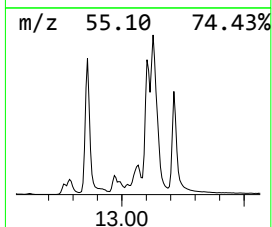
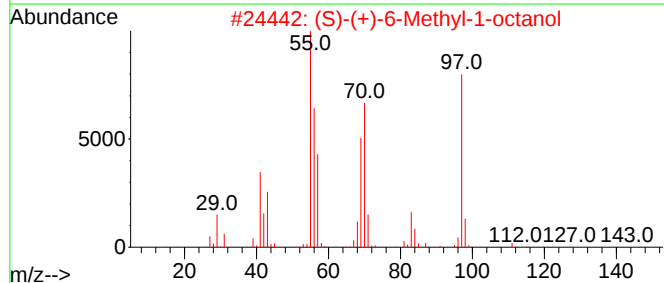
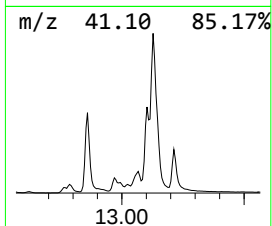
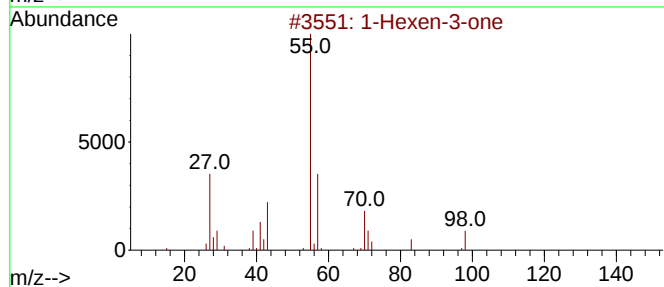
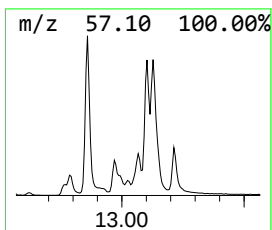
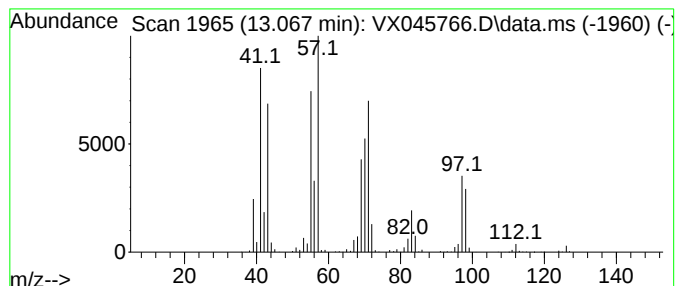
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Quant Title : SW846 8260

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

Peak Number 7 unknown13.067 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.067	103.14 ug/l	709822	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexen-3-one	98	C6H10O	001629-60-3	47
2		(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	43
3		2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	38
4		Cycloheptane, methyl-	112	C8H16	004126-78-7	38
5		Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
Data File : VX045766.D
Acq On : 14 Apr 2025 14:25
Operator : JC/MD
Sample : Q1799-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

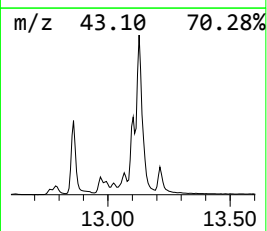
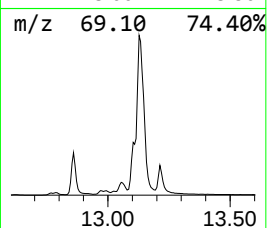
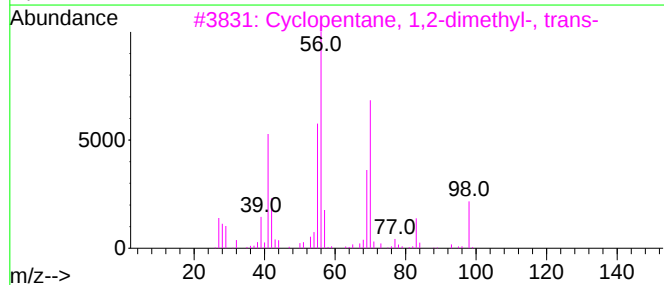
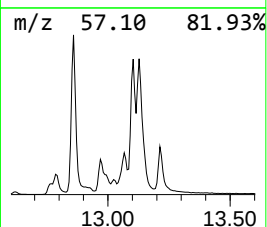
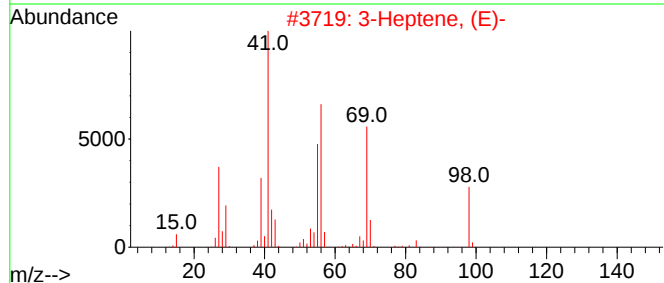
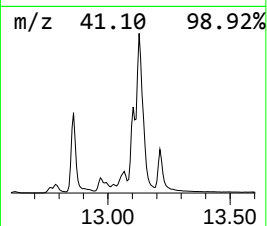
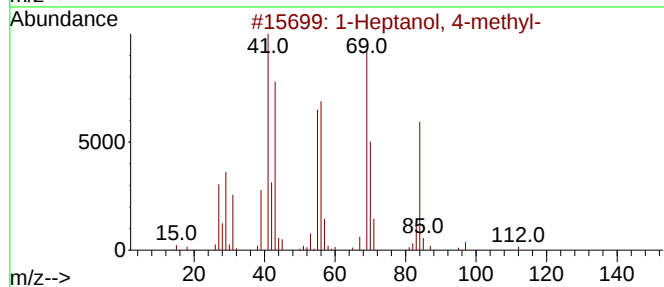
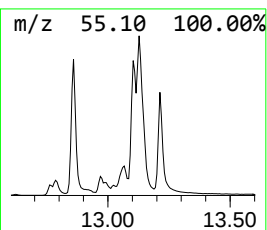
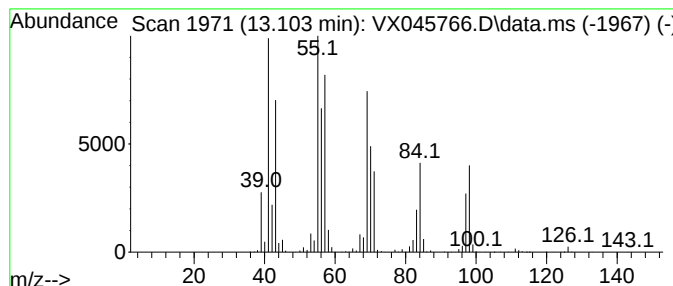
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Quant Title : SW846 8260

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

Peak Number 8 unknown13.103 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	351.13 ug/l	2416520	1,4-Dichlorobenzene-d4	12.018

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	47
2		3-Heptene, (E)-	98	C7H14	014686-14-7	46
3		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	38
4		1-Heptene	98	C7H14	000592-76-7	38
5		2-Methyl-2-pentyl methylphosphon...	182	C7H16FO2P	1000216-67-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
Data File : VX045766.D
Acq On : 14 Apr 2025 14:25
Operator : JC/MD
Sample : Q1799-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

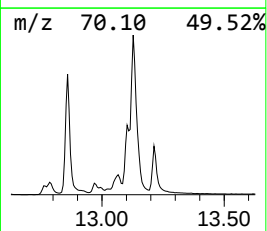
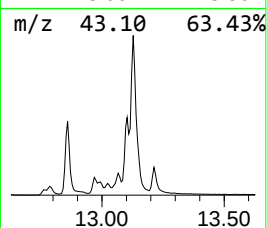
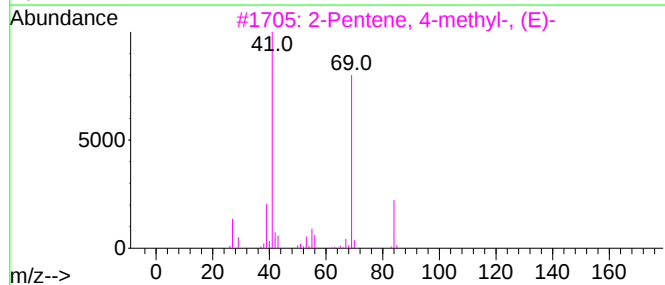
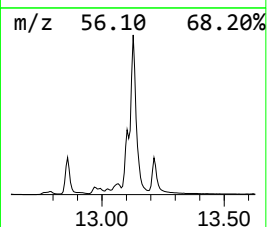
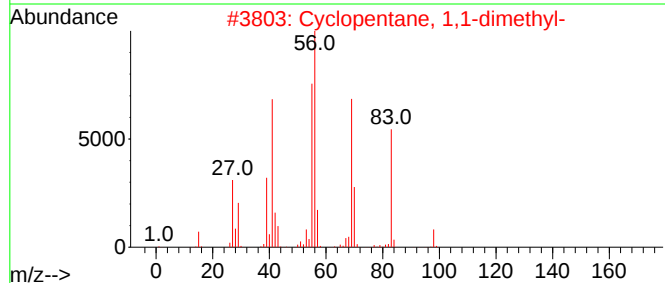
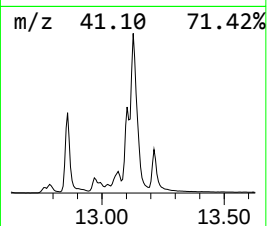
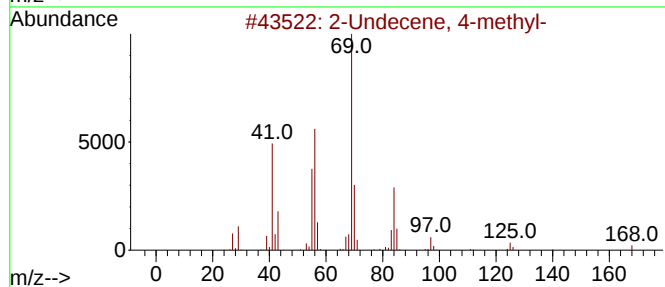
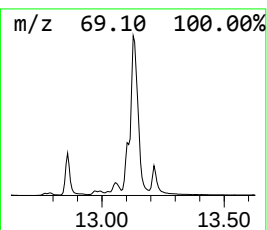
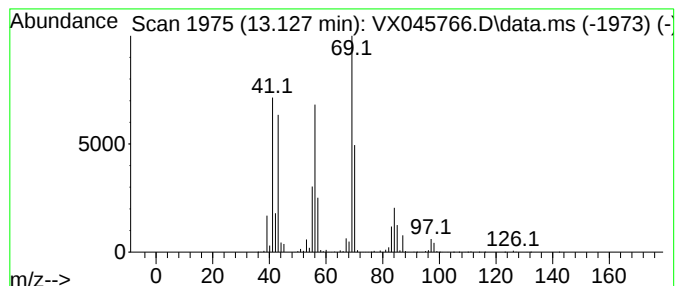
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Quant Title : SW846 8260

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

Peak Number 9 2-Undecene, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	664.79 ug/l	4575200	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Undecene, 4-methyl-	168	C12H24	091695-32-8	59
2			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	47
3			2-Pentene, 4-methyl-, (E)-	84	C6H12	000674-76-0	43
4			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	43
5			Cyanamide, dimethyl-	70	C3H6N2	001467-79-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
Data File : VX045766.D
Acq On : 14 Apr 2025 14:25
Operator : JC/MD
Sample : Q1799-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

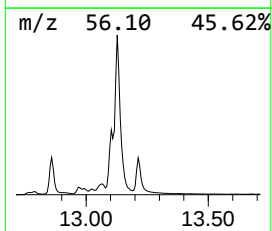
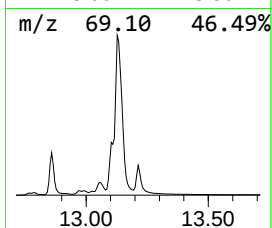
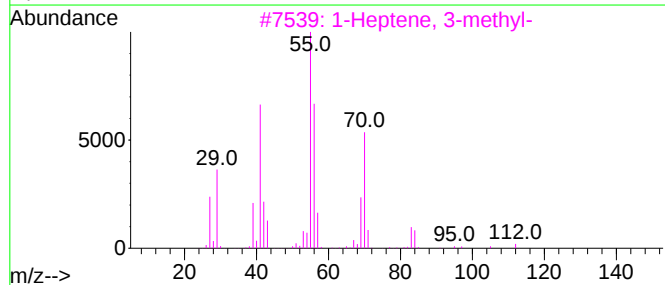
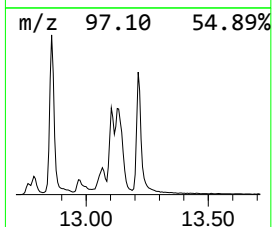
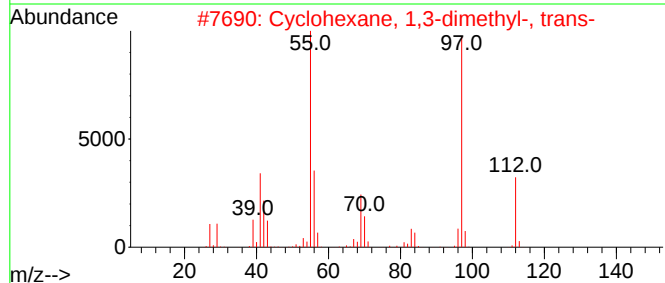
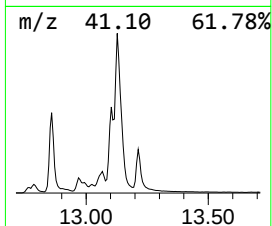
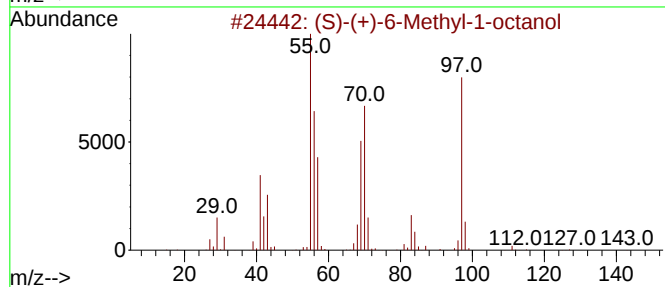
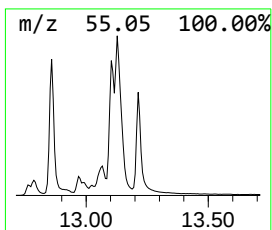
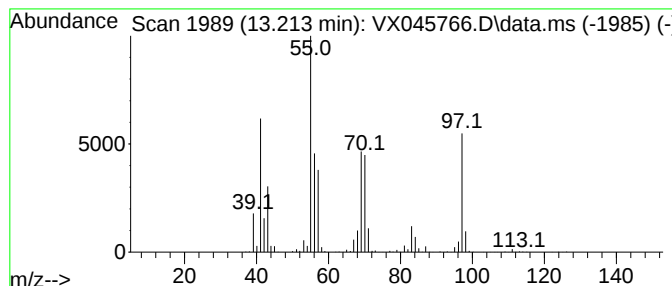
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Quant Title : SW846 8260

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

Peak Number 10 (S)-(+)-6-Methyl-1-octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	159.66 ug/l	1098800	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91		
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	53		
3	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	53		
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	50		
5	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041425\
Data File : VX045766.D
Acq On : 14 Apr 2025 14:25
Operator : JC/MD
Sample : Q1799-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FRAC-TANK-216-PPR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.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
1-Heptene	12.548	18.9	ug/l	129943	4	12.018	344109	50.0
Hexane, 3,3,4-t...	12.768	24.1	ug/l	166076	4	12.018	344109	50.0
unknown12.786	12.786	39.5	ug/l	271480	4	12.018	344109	50.0
1-Octene, 6-met...	12.859	351.6	ug/l	2419570	4	12.018	344109	50.0
Octane, 1,1'-ox...	12.969	63.8	ug/l	438762	4	12.018	344109	50.0
unknown13.024	13.024	28.1	ug/l	193646	4	12.018	344109	50.0
unknown13.067	13.067	103.1	ug/l	709822	4	12.018	344109	50.0
unknown13.103	13.103	351.1	ug/l	2416520	4	12.018	344109	50.0
2-Undecene, 4-m...	13.128	664.8	ug/l	4575200	4	12.018	344109	50.0
(S)-(+)-6-Methy...	13.213	159.7	ug/l	1098800	4	12.018	344109	50.0