

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
 Data File : VX046399.D
 Acq On : 29 May 2025 15:10
 Operator : JC/MD
 Sample : Q2137-01
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MOO-25-0151

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	318	326	336	rVB	9955	17933	1.49%	0.384%
2	3.690	417	427	437	rBV5	5143	16967	1.41%	0.363%
3	5.385	694	705	716	rBV2	44214	132556	11.01%	2.839%
4	5.544	716	731	749	rVB2	65731	208241	17.29%	4.461%
5	5.806	764	774	785	rBV2	5736	17471	1.45%	0.374%
6	5.952	788	798	814	rBV	53661	143386	11.91%	3.071%
7	6.757	920	930	947	rBV	117694	285861	23.74%	6.123%
8	8.647	1233	1240	1247	rBV	243619	392327	32.58%	8.404%
9	8.714	1247	1251	1265	rVB	50975	87907	7.30%	1.883%
10	10.055	1465	1471	1485	rBV	241364	355905	29.55%	7.623%
11	11.079	1634	1639	1651	rVB	200014	262388	21.79%	5.620%
12	12.018	1788	1793	1803	rBV	244816	325055	26.99%	6.963%
13	12.219	1821	1826	1834	rBV	19977	37363	3.10%	0.800%
14	12.421	1855	1859	1869	rVB4	21135	47943	3.98%	1.027%
15	12.695	1899	1904	1909	rVB3	12395	17610	1.46%	0.377%
16	12.988	1946	1952	1959	rBV	505981	630481	52.35%	13.505%
17	13.164	1974	1981	1986	rBV	11796	16572	1.38%	0.355%
18	13.256	1989	1996	2008	rVV2	65434	106459	8.84%	2.280%
19	13.433	2020	2025	2031	rVB	17014	26264	2.18%	0.563%
20	13.591	2047	2051	2055	rBV2	11977	14073	1.17%	0.301%
21	13.841	2088	2092	2098	rVB5	7292	14851	1.23%	0.318%
22	13.920	2098	2105	2110	rBV5	5935	12625	1.05%	0.270%
23	14.036	2120	2124	2128	rBV	20899	22537	1.87%	0.483%
24	14.091	2128	2133	2137	rBV	9671	13544	1.12%	0.290%
25	14.438	2184	2190	2198	rBV	942226	1204295	100.00%	25.796%
26	14.609	2215	2218	2222	rBV3	11780	16513	1.37%	0.354%
27	14.695	2225	2232	2236	rVB3	8946	14918	1.24%	0.320%
28	14.755	2236	2242	2245	rBV	52073	59996	4.98%	1.285%
29	14.847	2252	2257	2264	rVB9	6846	18364	1.52%	0.393%
30	14.981	2275	2279	2283	rVB	21370	28729	2.39%	0.615%
31	15.073	2290	2294	2302	rVB4	13100	26027	2.16%	0.557%
32	15.207	2314	2316	2320	rVV	13551	16437	1.36%	0.352%
33	15.487	2357	2362	2367	rBV	34139	50548	4.20%	1.083%
34	15.774	2404	2409	2416	rVB2	7180	13142	1.09%	0.282%
35	16.091	2457	2461	2467	rBV8	4941	13252	1.10%	0.284%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M

Title : SW846 8260

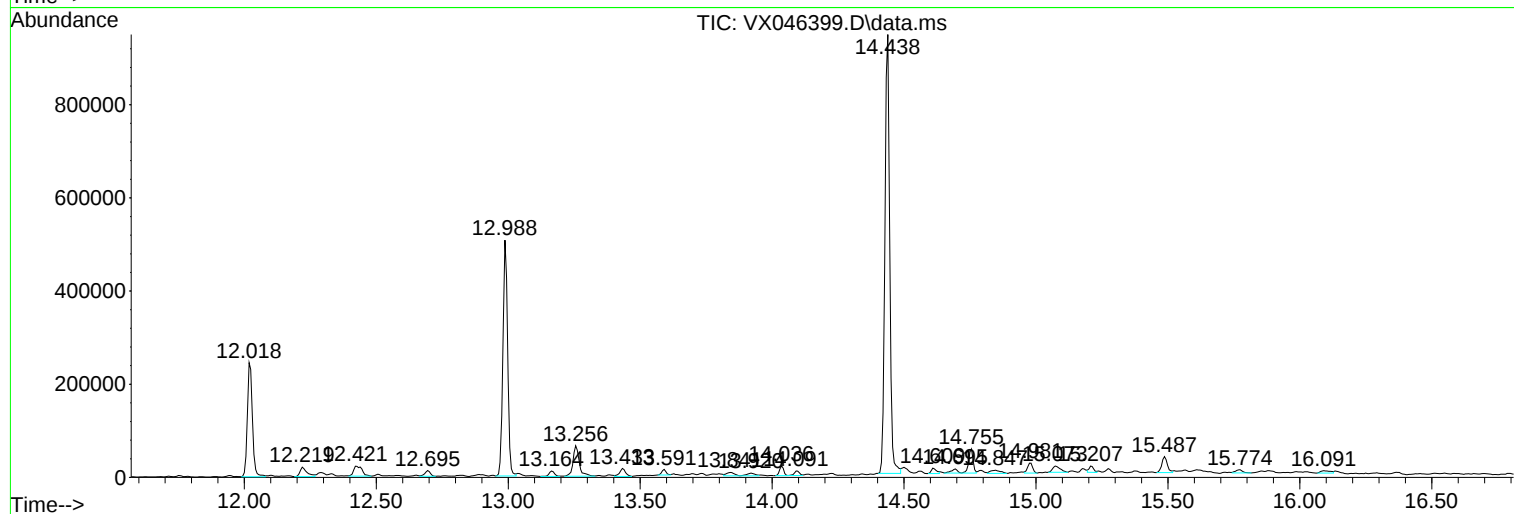
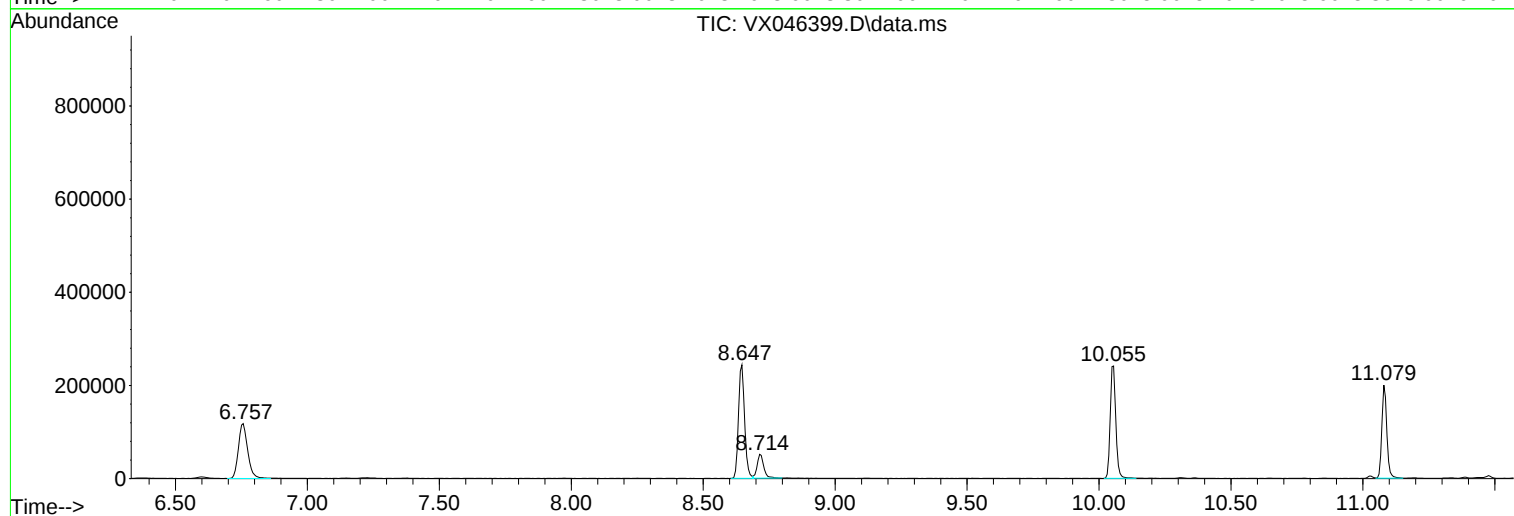
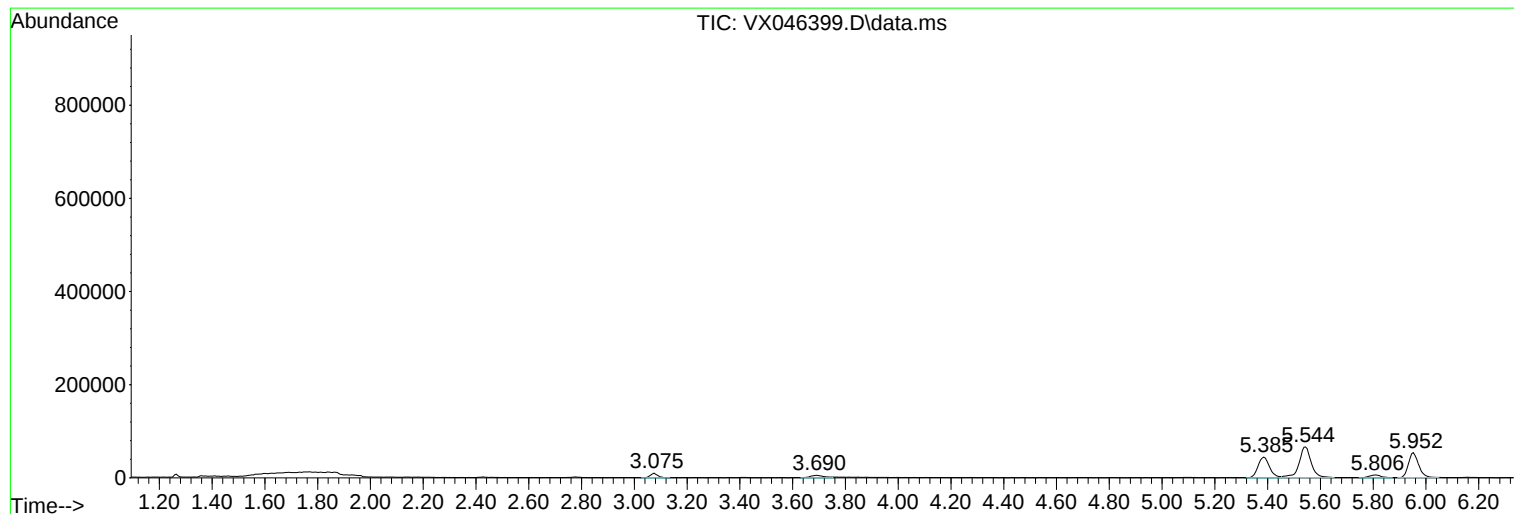
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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



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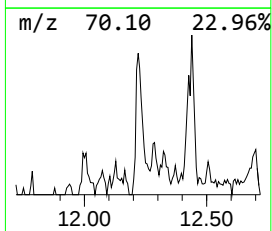
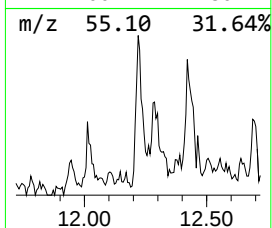
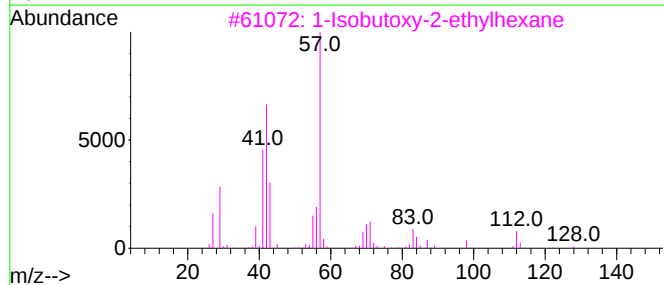
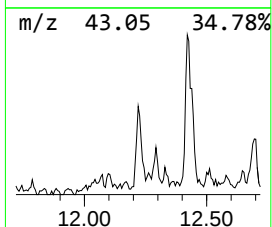
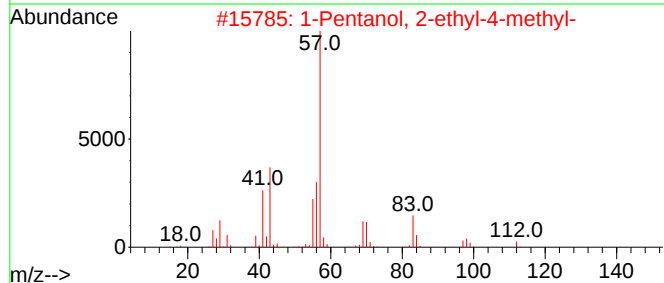
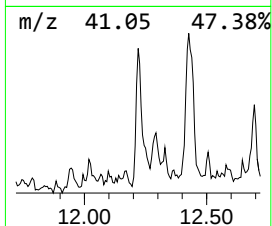
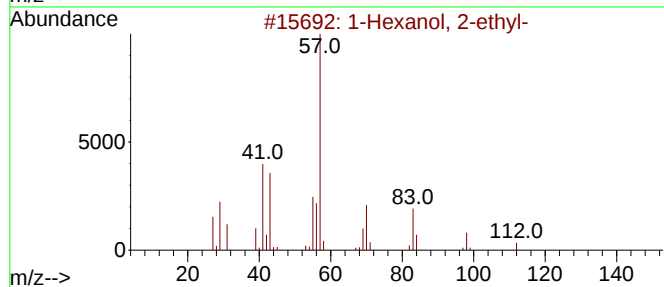
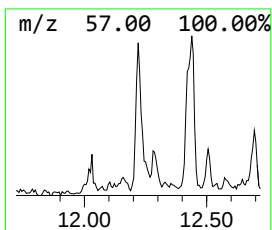
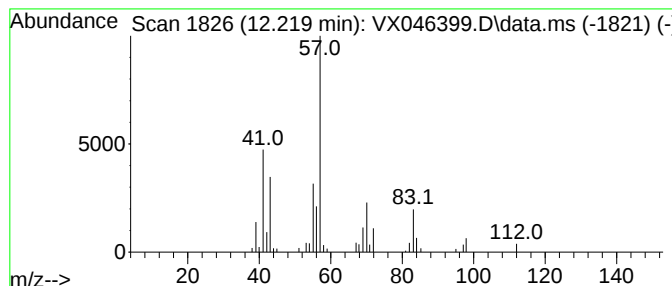
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	5.75 ug/l	37363	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
4		2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	47
5		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-25-0151

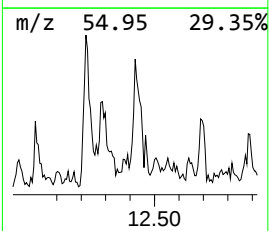
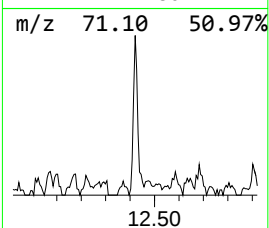
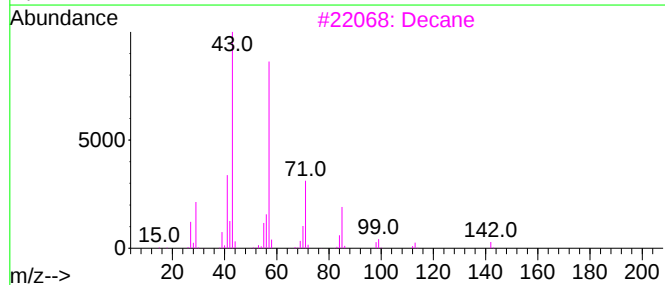
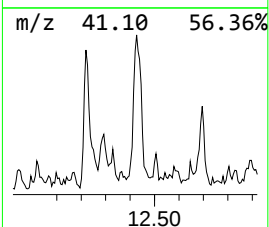
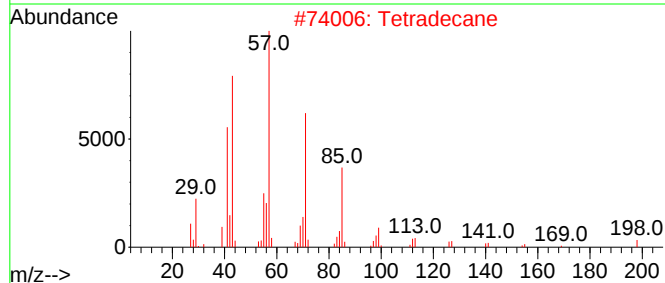
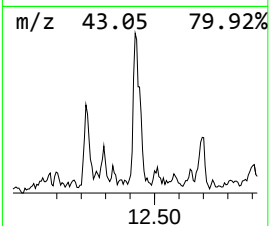
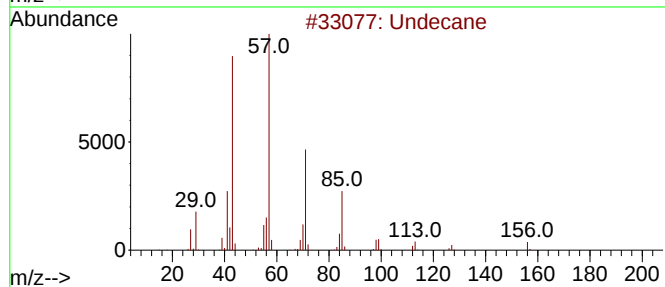
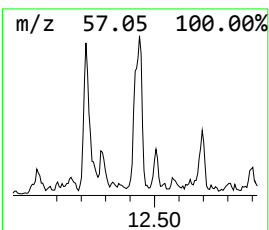
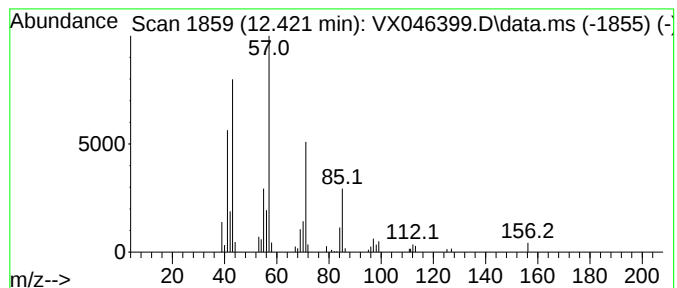
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	7.37 ug/l	47943	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	83
2	Tetradecane	198	C14H30	000629-59-4	80
3	Decane	142	C10H22	000124-18-5	72
4	Tridecane	184	C13H28	000629-50-5	64
5	Hexadecane	226	C16H34	000544-76-3	64



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-25-0151

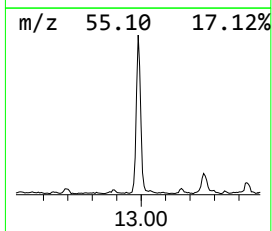
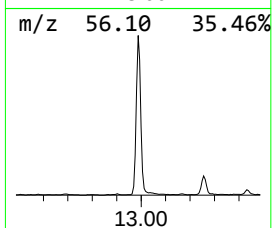
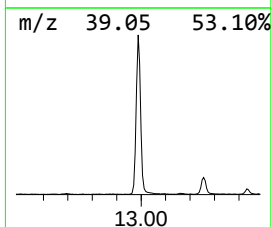
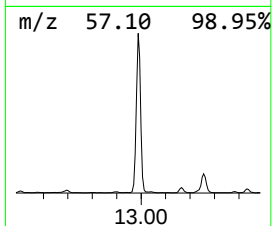
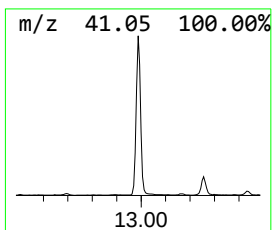
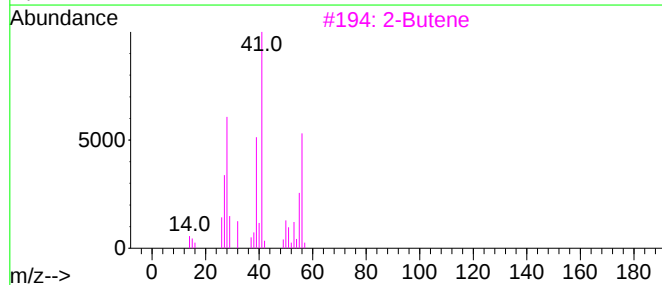
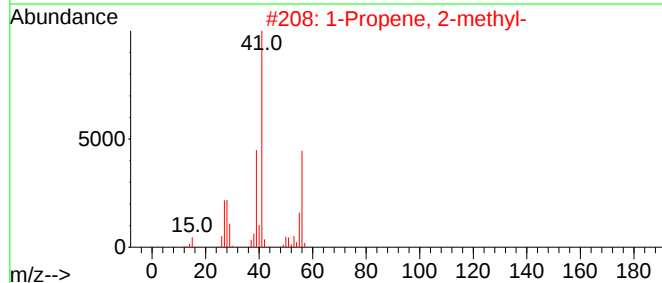
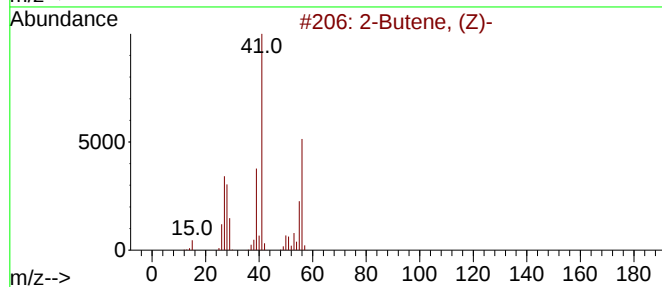
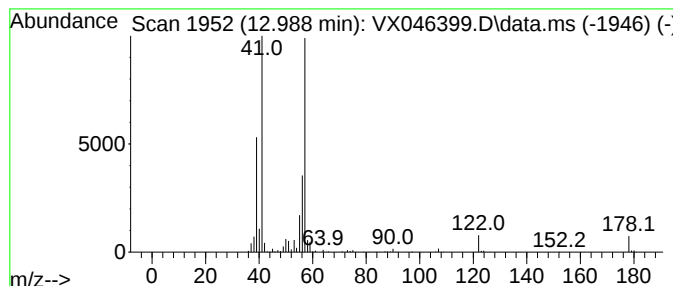
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 3 2-Butene, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.988	96.98 ug/l	630481	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butene, (Z)-	56	C4H8	000590-18-1	58
2			1-Propene, 2-methyl-	56	C4H8	000115-11-7	58
3			2-Butene	56	C4H8	000107-01-7	53
4			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	32
5			Cyclobutane	56	C4H8	000287-23-0	30



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Instrument :
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ClientSampleId :
MOO-25-0151

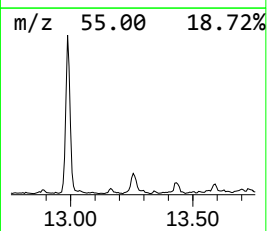
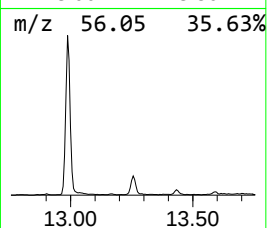
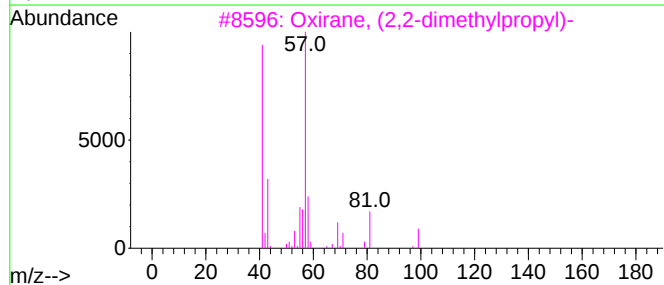
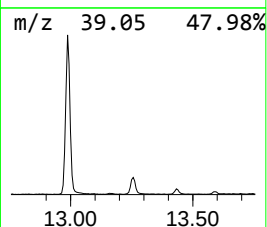
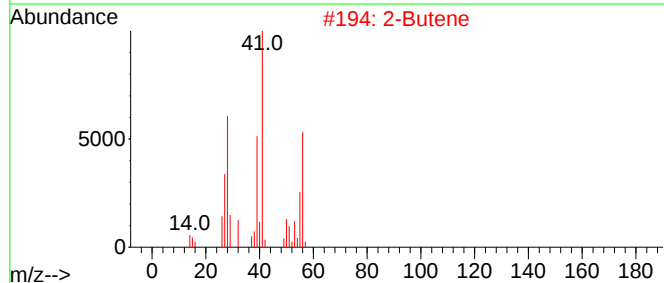
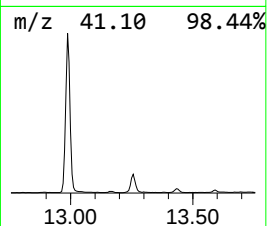
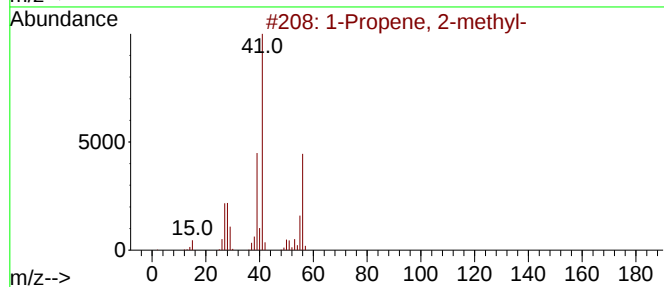
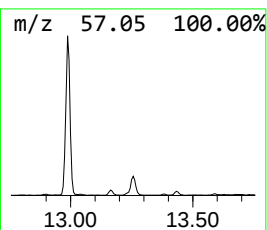
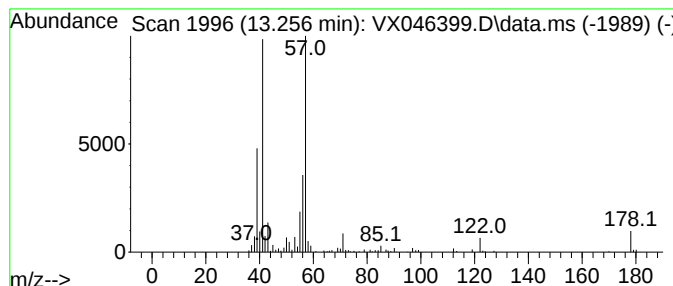
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Peak Number 4 1-Propene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.256	16.38 ug/l	106459	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-			56	C4H8	000115-11-7	52
2	2-Butene			56	C4H8	000107-01-7	50
3	Oxirane, (2,2-dimethylpropyl)-			114	C7H14O	002245-29-6	37
4	1-Butene			56	C4H8	000106-98-9	30
5	4,4-Dimethyl-3-oxopentanenitrile			125	C7H11NO	059997-51-2	28



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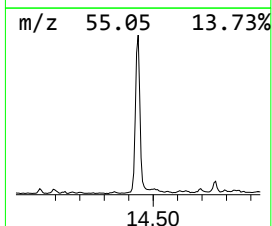
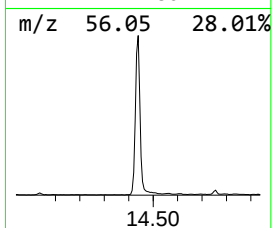
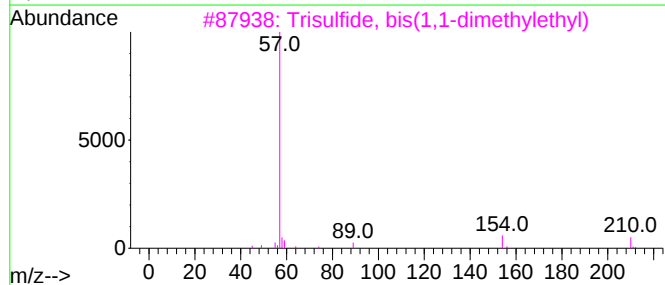
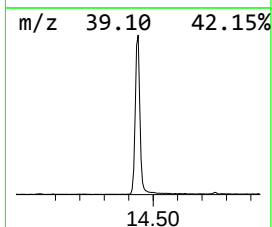
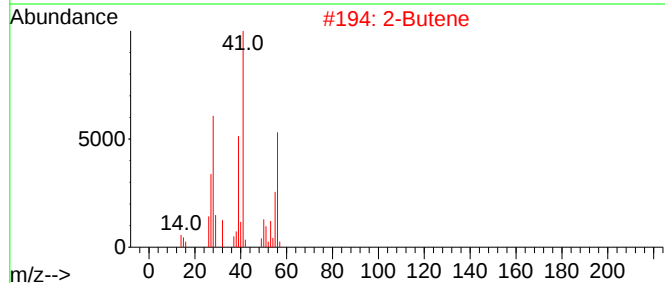
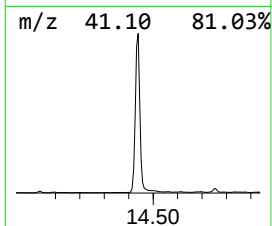
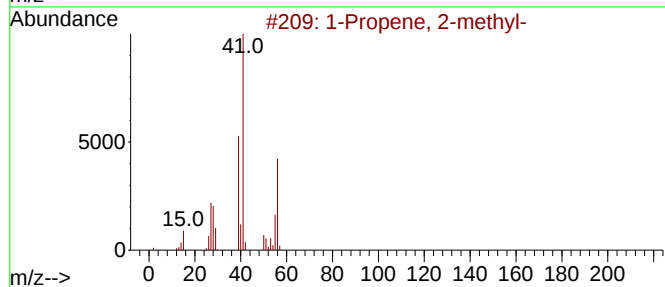
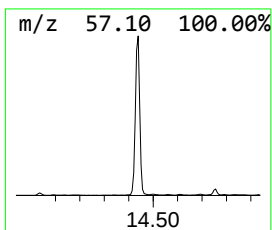
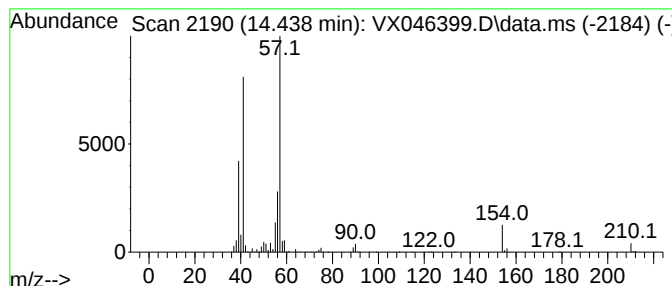
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.438 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.438	185.25 ug/l	1204300	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propene, 2-methyl-	56	C4H8	000115-11-7	46
2			2-Butene	56	C4H8	000107-01-7	43
3			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	38
4			Nitroxide, bis(1,1-dimethylethyl)	144	C8H18NO	002406-25-9	28
5			4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	23



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046399.D
Acq On : 29 May 2025 15:10
Operator : JC/MD
Sample : Q2137-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-25-0151

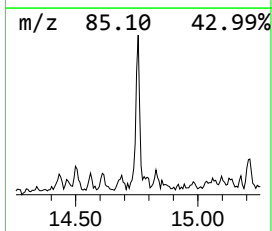
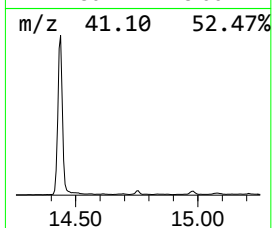
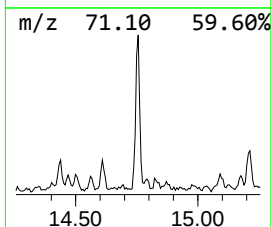
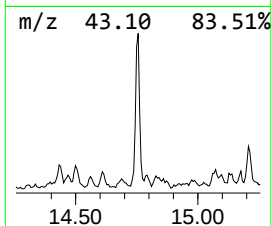
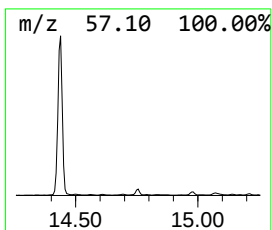
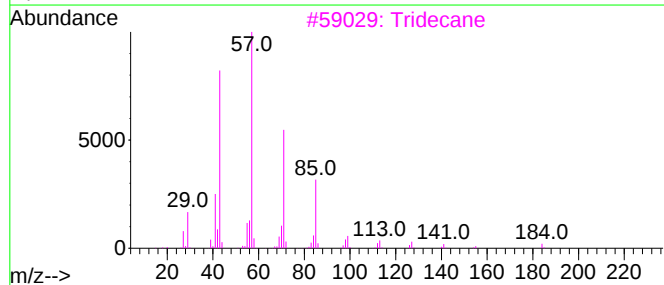
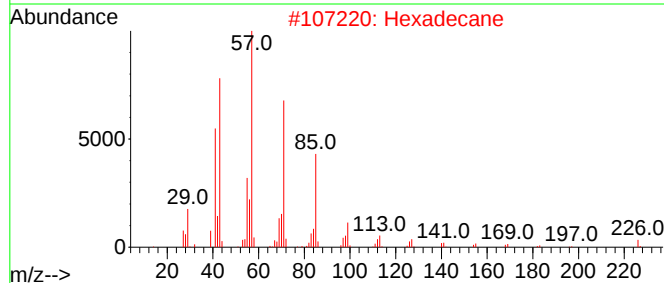
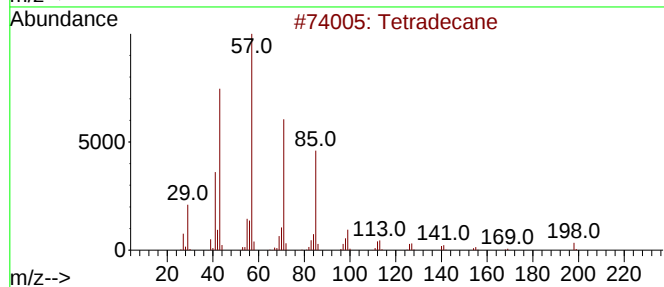
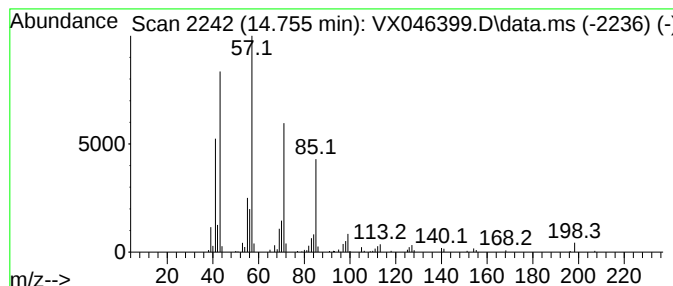
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Quant Title : SW846 8260

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

Peak Number 6 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.756	9.23 ug/l	59996	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	96
2		Hexadecane	226	C16H34	000544-76-3	91
3		Tridecane	184	C13H28	000629-50-5	80
4		Nonadecane	268	C19H40	000629-92-5	80
5		Decane, 1-iodo-	268	C10H21I	002050-77-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046399.D
Acq On : 29 May 2025 15:10
Operator : JC/MD
Sample : Q2137-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-25-0151

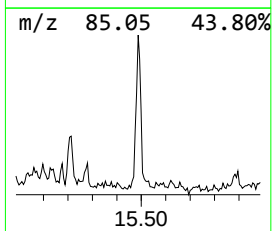
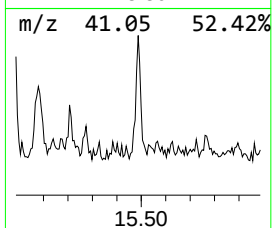
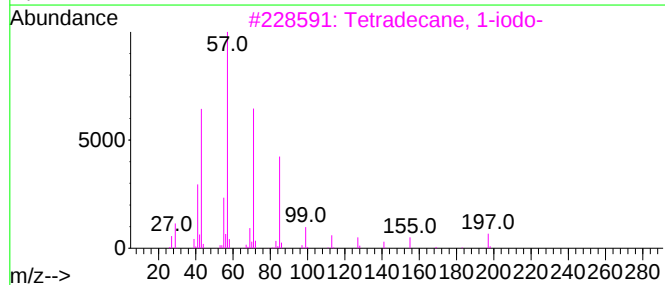
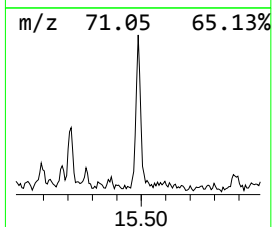
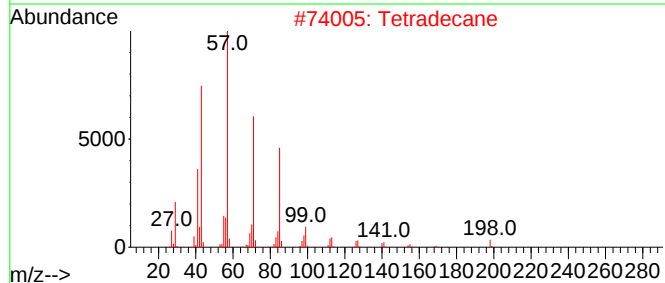
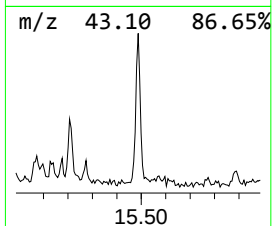
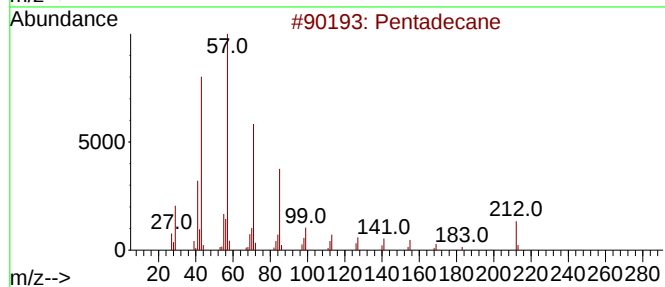
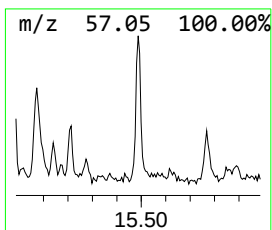
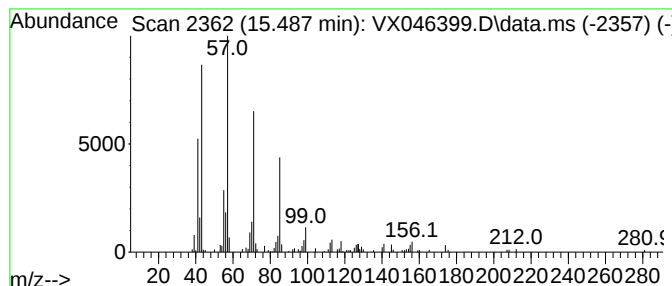
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Quant Title : SW846 8260

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

Peak Number 7 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	7.78 ug/l	50548	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane	212	C15H32	000629-62-9	93
2		Tetradecane	198	C14H30	000629-59-4	83
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
4		Heptadecane	240	C17H36	000629-78-7	80
5		Hexadecane	226	C16H34	000544-76-3	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052925\
Data File : VX046399.D
Acq On : 29 May 2025 15:10
Operator : JC/MD
Sample : Q2137-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MOO-25-0151

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.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-Hexanol, 2-et...	12.219	5.8	ug/l	37363	4	12.024	325055	50.0
Undecane	12.421	7.4	ug/l	47943	4	12.024	325055	50.0
2-Butene, (Z)-	12.988	97.0	ug/l	630481	4	12.024	325055	50.0
1-Propene, 2-me...	13.256	16.4	ug/l	106459	4	12.024	325055	50.0
unknown14.438	14.438	185.3	ug/l	1204300	4	12.024	325055	50.0
Tetradecane	14.756	9.2	ug/l	59996	4	12.024	325055	50.0
Pentadecane	15.487	7.8	ug/l	50548	4	12.024	325055	50.0