

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090225\
 Data File : VN087708.D
 Acq On : 02 Sep 2025 12:49
 Operator : JC\MD
 Sample : Q2991-01
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 309

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\82N082125W.M

Title : SW846 8260

Signal : TIC: VN087708.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.141	1042	1052	1056	rBV2	187899	456591	1.71%	0.814%
2	8.194	1056	1061	1073	rVV2	467978	1122767	4.20%	2.002%
3	8.418	1090	1099	1109	rBV	283378	659563	2.47%	1.176%
4	8.559	1114	1123	1134	rVB2	212264	503423	1.88%	0.897%
5	8.941	1179	1188	1199	rBV2	180328	361487	1.35%	0.644%
6	9.077	1201	1211	1222	rBV	478191	1001882	3.75%	1.786%
7	10.541	1451	1460	1465	rBV	760389	1414168	5.29%	2.521%
8	10.606	1465	1471	1485	rVB	1863508	3448119	12.89%	6.147%
9	11.841	1673	1681	1690	rBV	600307	1157651	4.33%	2.064%
10	11.941	1690	1698	1707	rBV	3697494	6110224	22.85%	10.893%
11	12.047	1707	1716	1728	rVV	13929376	26746339	100.00%	47.681%
12	12.376	1761	1772	1782	rBV	3939047	6913402	25.85%	12.324%
13	12.829	1843	1849	1859	rVB	458013	885972	3.31%	1.579%
14	13.076	1885	1891	1895	rBV	183694	352850	1.32%	0.629%
15	13.135	1895	1901	1909	rVB4	298503	688741	2.58%	1.228%
16	13.459	1950	1956	1967	rVB	349699	618675	2.31%	1.103%
17	13.770	2003	2009	2017	rBV2	639597	1307575	4.89%	2.331%
18	14.082	2056	2062	2068	rBV	601575	947393	3.54%	1.689%
19	14.935	2197	2207	2214	rBV4	328457	610500	2.28%	1.088%
20	15.023	2214	2222	2229	rBV6	122379	394892	1.48%	0.704%
21	15.800	2349	2354	2365	rVB2	181470	392688	1.47%	0.700%

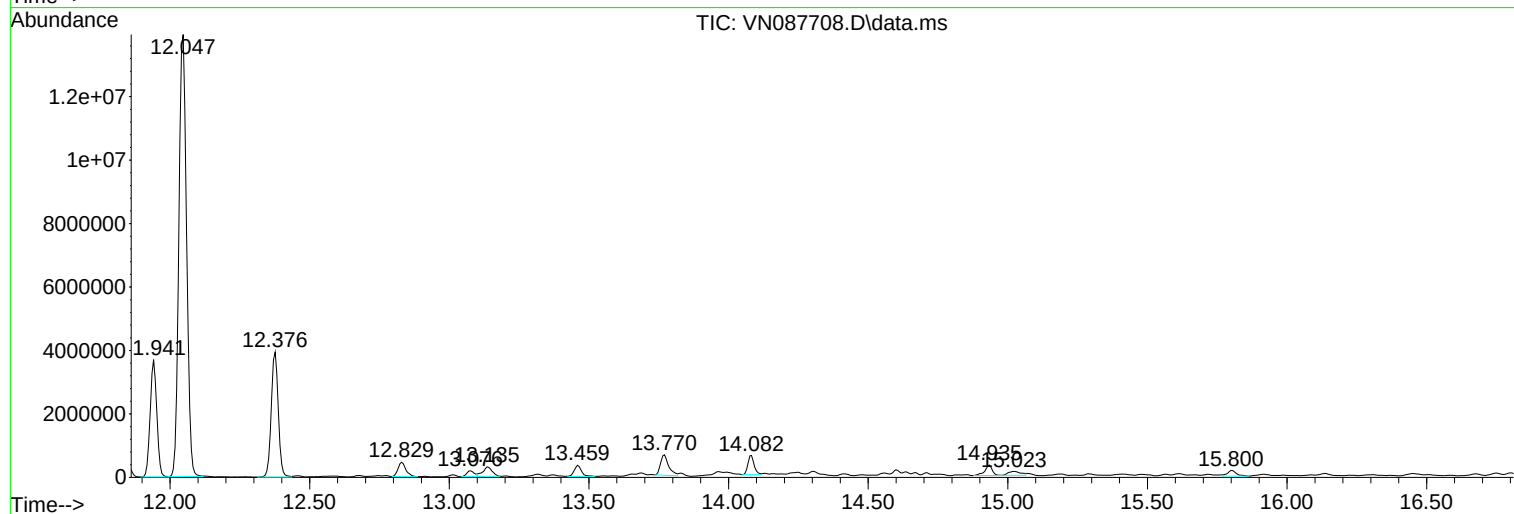
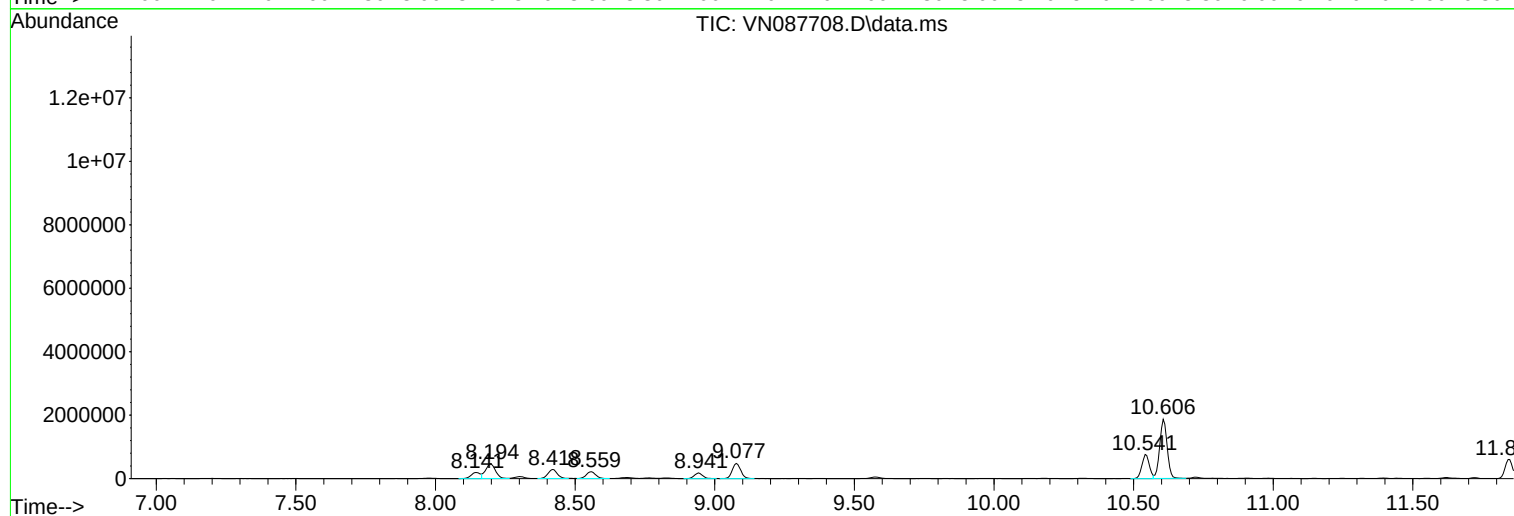
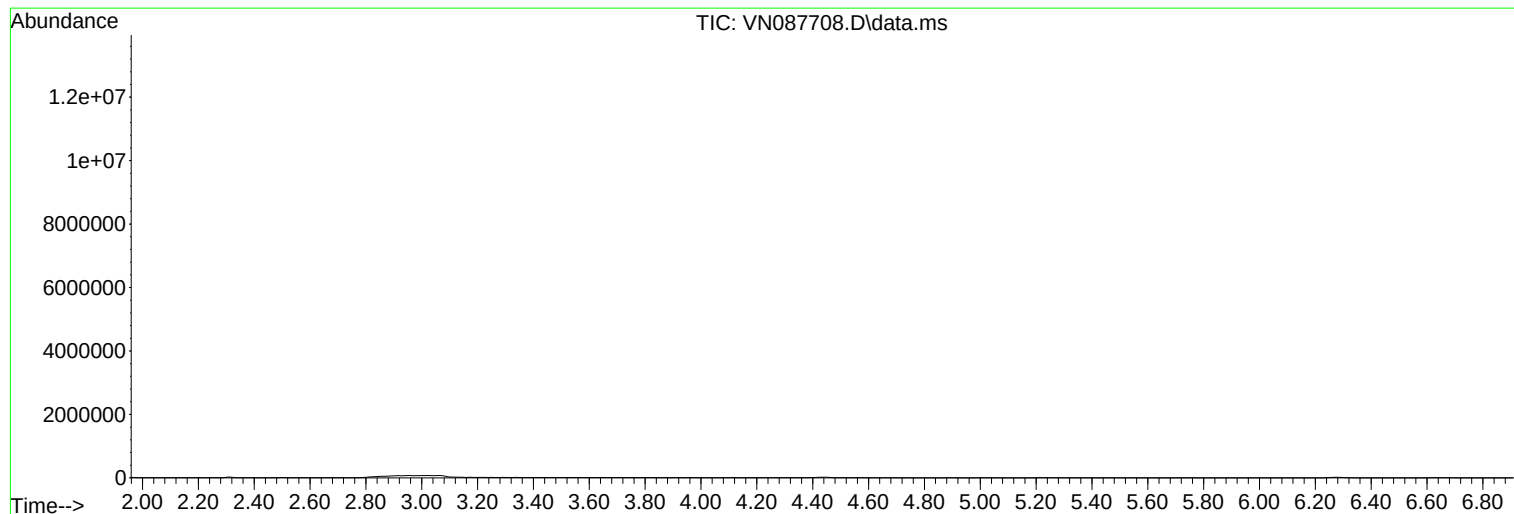
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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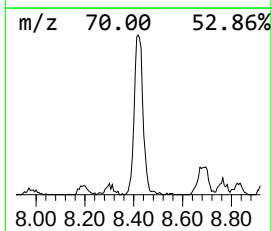
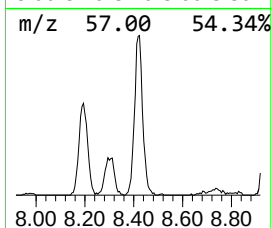
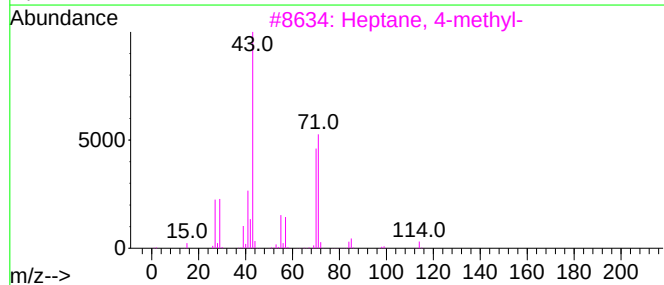
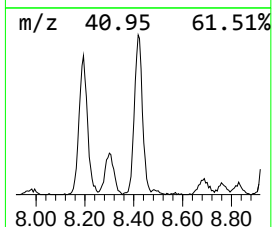
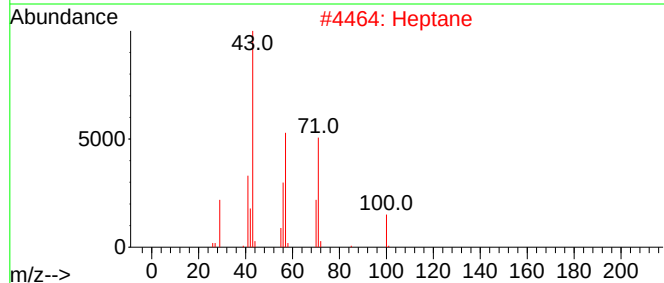
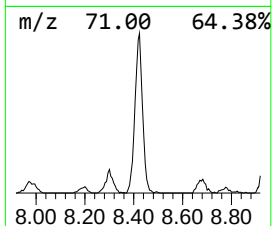
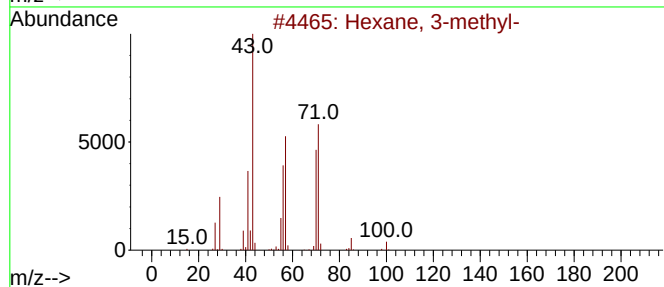
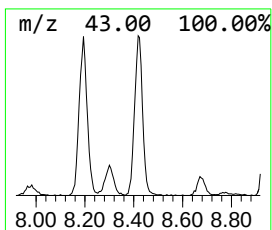
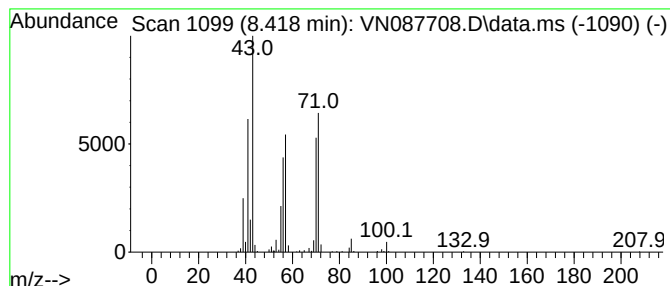
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.418	29.37 ug/l	659563	Pentafluorobenzene	8.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	91
2			Heptane	100	C7H16	000142-82-5	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



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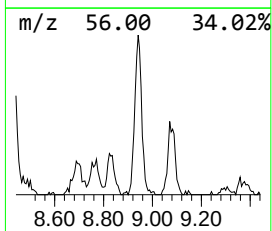
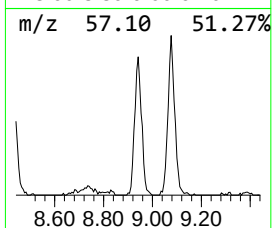
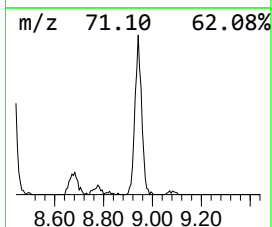
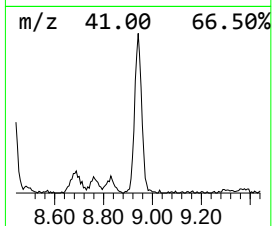
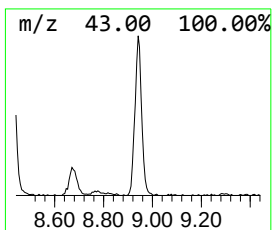
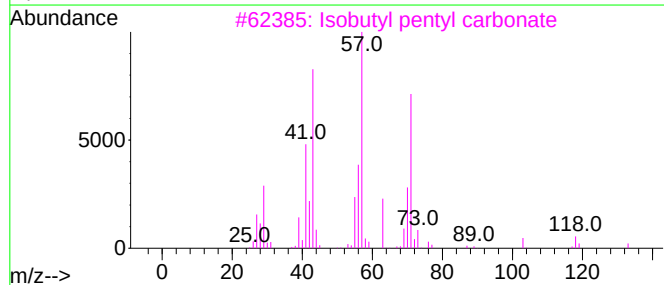
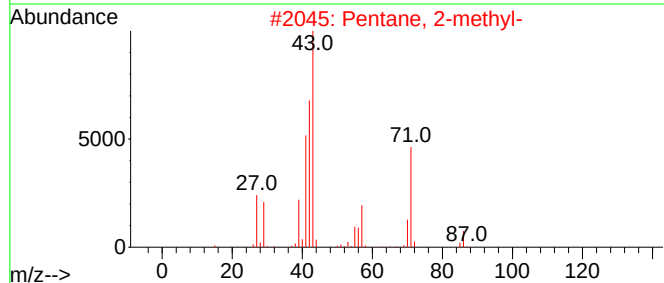
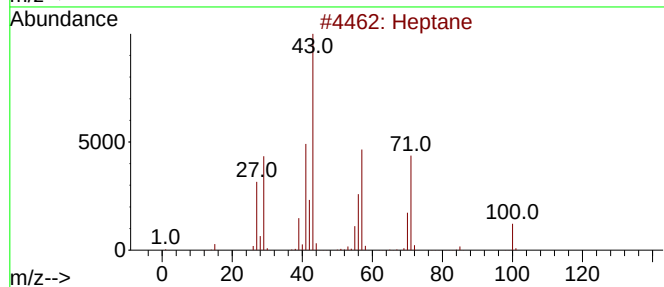
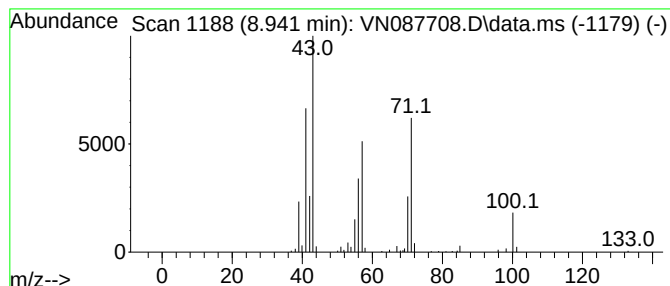
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.941	18.04 ug/l	361487	1,4-Difluorobenzene	9.077

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	50
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	45



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ClientSampleId :
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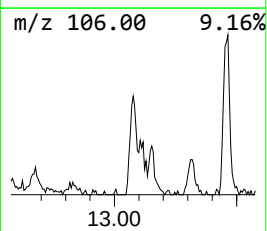
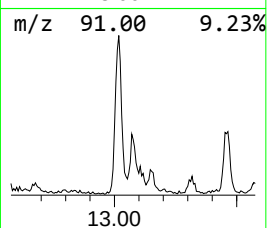
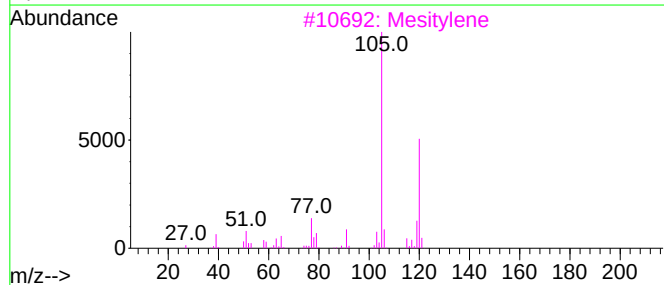
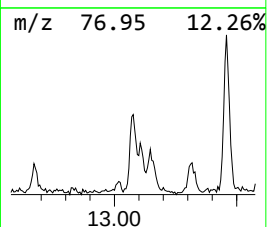
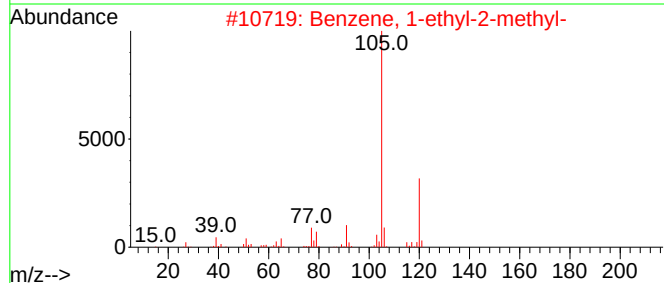
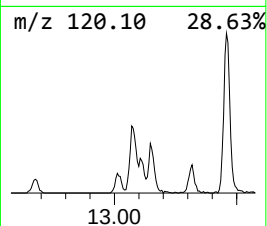
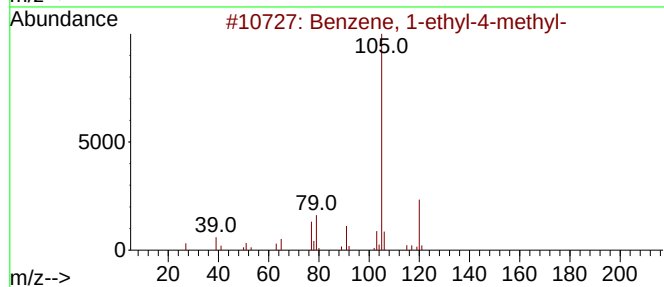
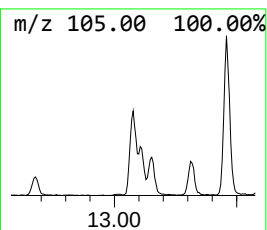
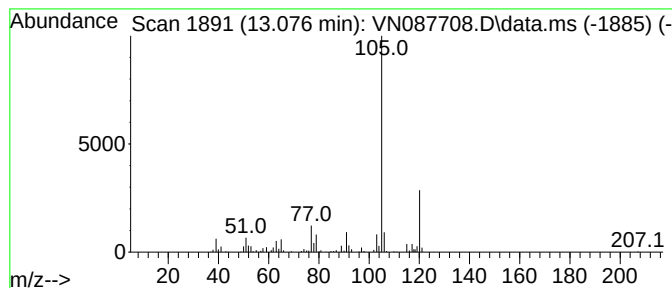
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.076	13.49 ug/l	352850	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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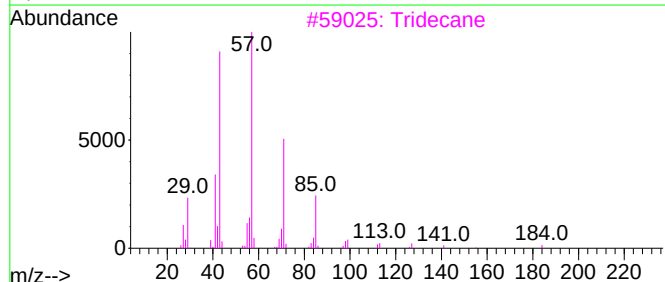
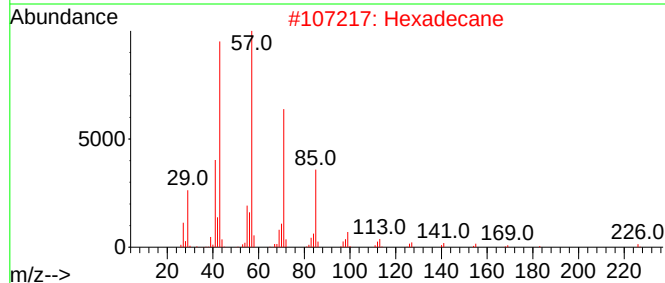
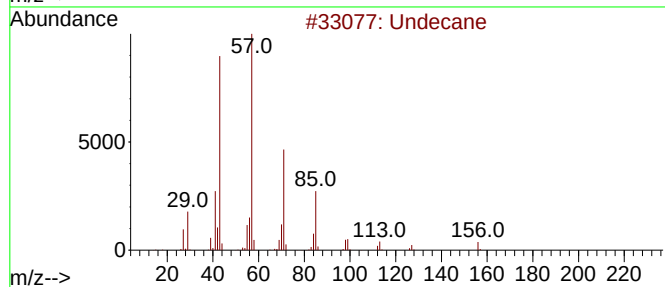
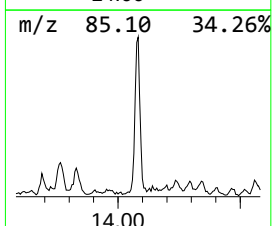
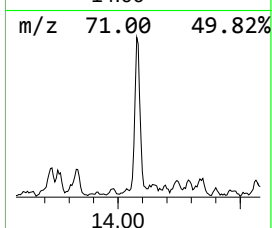
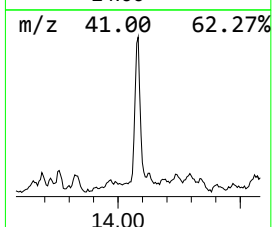
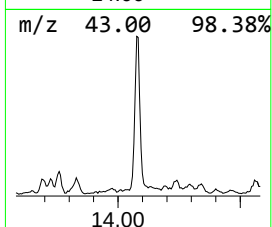
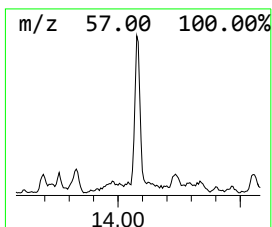
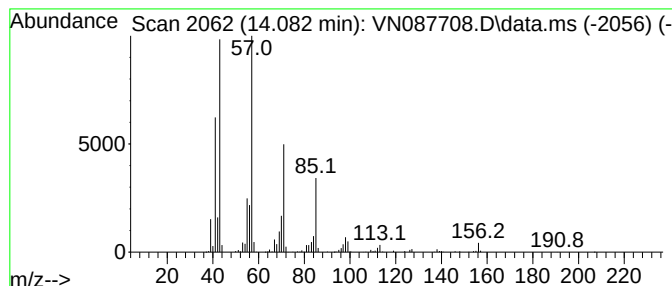
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Quant Title : SW846 8260

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

Peak Number 4 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.082	36.23 ug/l	947393	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	83
2	Hexadecane			226	C16H34	000544-76-3	72
3	Tridecane			184	C13H28	000629-50-5	72
4	Decane, 2,3,7-trimethyl-			184	C13H28	062238-13-5	59
5	Decane			142	C10H22	000124-18-5	53



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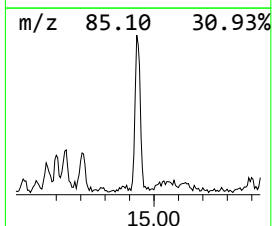
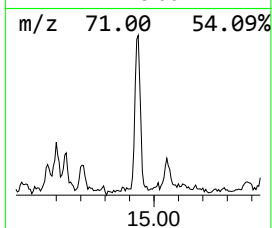
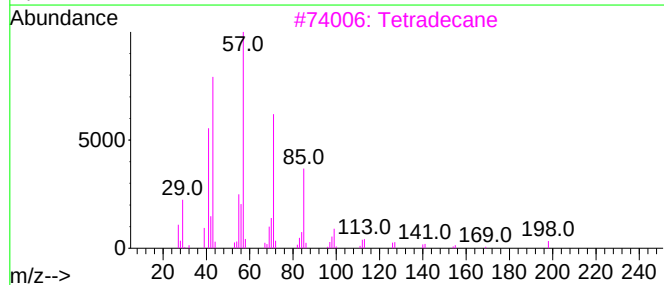
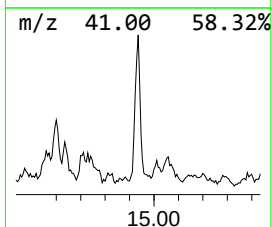
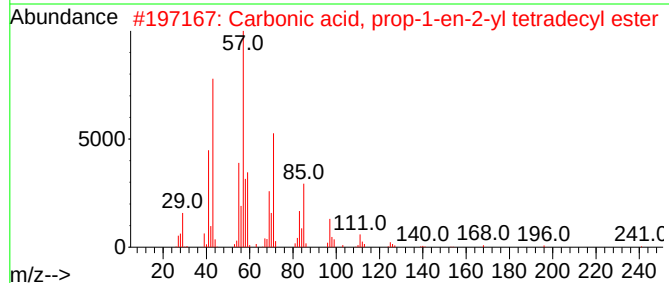
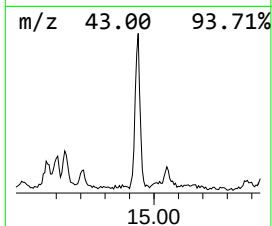
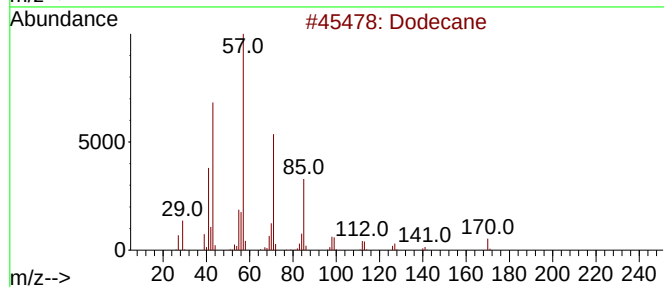
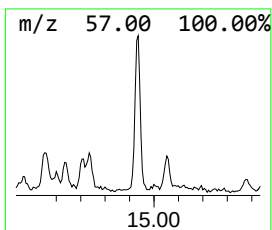
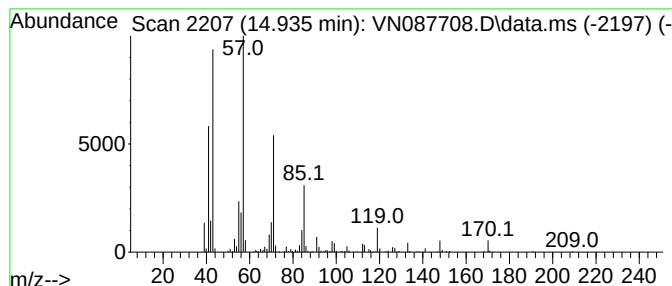
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.M
Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	23.34 ug/l	610500	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	72
3			Tetradecane	198	C14H30	000629-59-4	64
4			Tridecane	184	C13H28	000629-50-5	64
5			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	59



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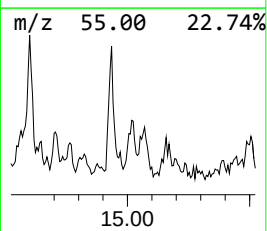
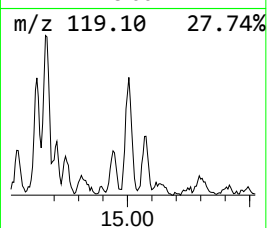
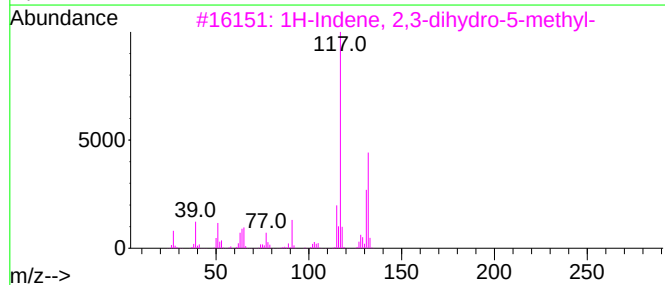
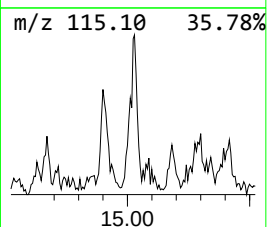
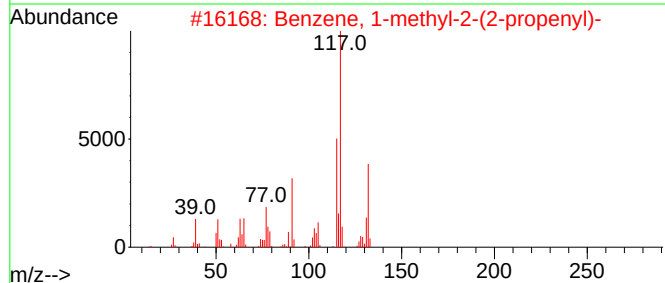
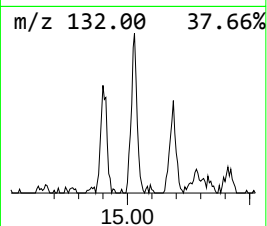
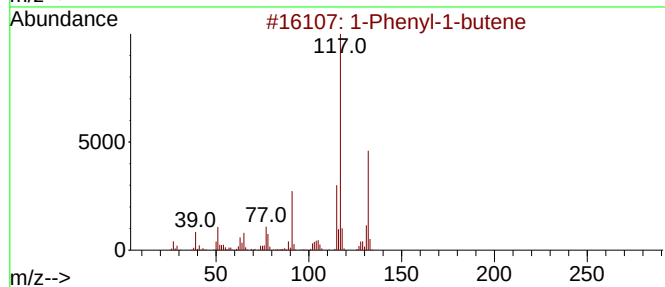
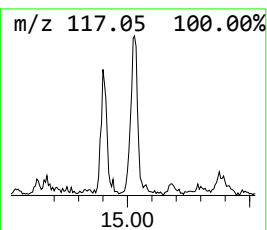
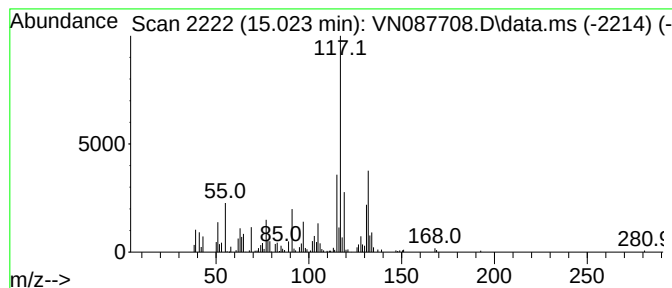
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Quant Title : SW846 8260

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

Peak Number 6 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.023	15.10 ug/l	394892	1,4-Dichlorobenzene-d4	13.770

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenyl-1-butene	132	C10H12	000824-90-8	89
2		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	86
3		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
4		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090225\
Data File : VN087708.D
Acq On : 02 Sep 2025 12:49
Operator : JC\MD
Sample : Q2991-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
309

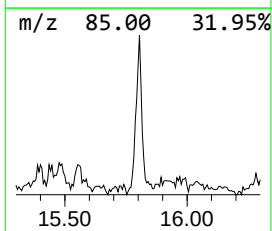
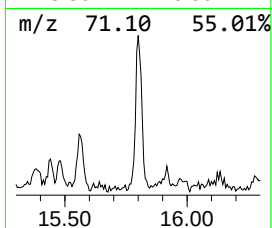
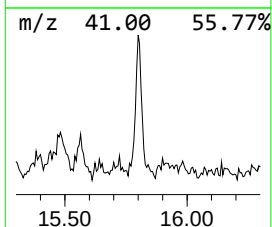
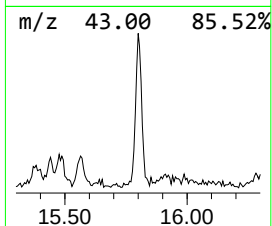
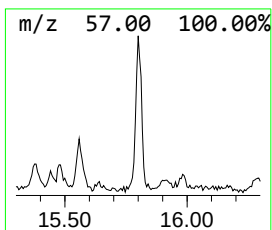
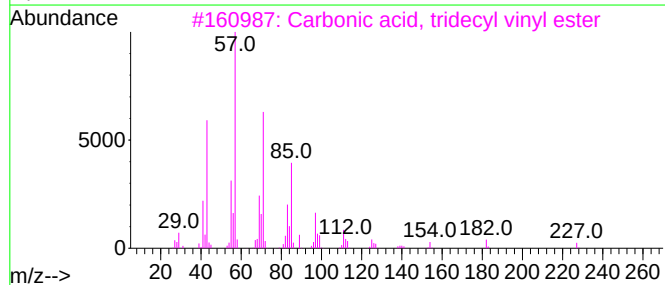
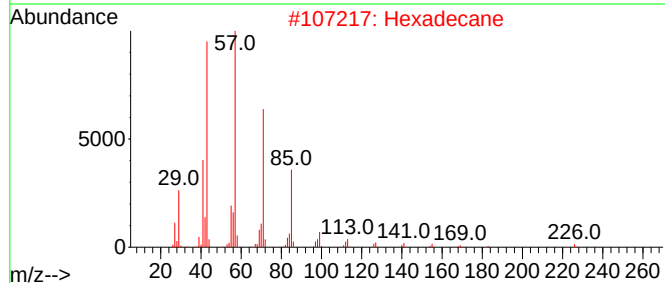
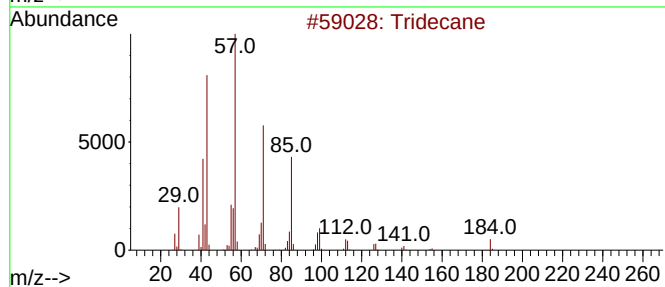
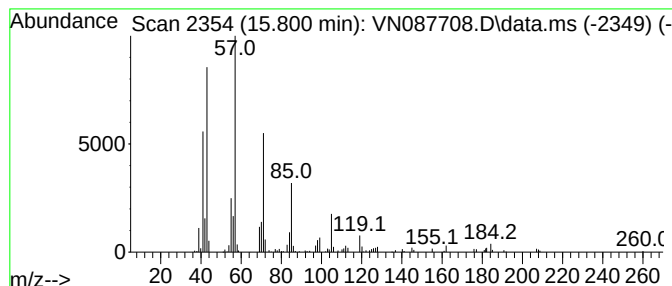
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.800	15.02 ug/l	392688	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Hexadecane	226	C16H34	000544-76-3	64
3			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	64
4			Tetradecane	198	C14H30	000629-59-4	64
5			Undecane	156	C11H24	001120-21-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090225\
Data File : VN087708.D
Acq On : 02 Sep 2025 12:49
Operator : JC\MD
Sample : Q2991-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
309

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N082125W.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
Hexane, 3-methyl-	8.418	29.4	ug/l	659563	1	8.200	1122770	50.0
Heptane	8.941	18.0	ug/l	361487	2	9.077	1001880	50.0
Benzene, 1-ethy...	13.076	13.5	ug/l	352850	4	13.770	1307580	50.0
Undecane	14.082	36.2	ug/l	947393	4	13.770	1307580	50.0
Dodecane	14.935	23.3	ug/l	610500	4	13.770	1307580	50.0
1-Phenyl-1-butene	15.023	15.1	ug/l	394892	4	13.770	1307580	50.0
Tridecane	15.800	15.0	ug/l	392688	4	13.770	1307580	50.0