

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
 Data File : VN087587.D
 Acq On : 15 Aug 2025 17:07
 Operator : JC\MD
 Sample : Q2844-09
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MOO-25-0226

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\82N071625W.M
 Title : SW846 8260

Signal : TIC: VN087587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.147	1042	1053	1057	rBV	227747	550040	3.21%	1.483%
2	8.200	1057	1062	1073	rVV2	476899	1129986	6.59%	3.046%
3	8.424	1091	1100	1111	rBV	234264	536555	3.13%	1.447%
4	8.559	1114	1123	1135	rVB	262107	602485	3.52%	1.624%
5	8.947	1178	1189	1198	rBV	354711	719932	4.20%	1.941%
6	9.082	1202	1212	1226	rBV	627415	1319558	7.70%	3.557%
7	9.576	1283	1296	1302	rBV3	81771	232000	1.35%	0.625%
8	10.547	1453	1461	1465	rBV	917367	1689281	9.86%	4.554%
9	10.612	1465	1472	1485	rVV	9338549	17135842	100.00%	46.197%
10	11.847	1673	1682	1692	rBV	827158	1546214	9.02%	4.168%
11	11.947	1692	1699	1707	rBV	459352	825438	4.82%	2.225%
12	12.047	1707	1716	1728	rBV	2123192	4195729	24.49%	11.311%
13	12.376	1760	1772	1781	rBV	716320	1378075	8.04%	3.715%
14	12.829	1843	1849	1859	rVB2	543351	1043602	6.09%	2.813%
15	13.076	1885	1891	1895	rBV	100618	189782	1.11%	0.512%
16	13.141	1895	1902	1909	rVB3	373218	720868	4.21%	1.943%
17	13.464	1951	1957	1968	rVB	132420	257130	1.50%	0.693%
18	13.770	2003	2009	2017	rVB	798847	1406832	8.21%	3.793%
19	14.082	2057	2062	2074	rBV2	263503	479113	2.80%	1.292%
20	14.935	2197	2207	2214	rBV3	194255	363334	2.12%	0.980%
21	15.023	2215	2222	2237	rVB9	68721	308791	1.80%	0.832%
22	15.617	2318	2323	2329	rVB	100443	187676	1.10%	0.506%
23	15.805	2350	2355	2366	rVB	129730	274640	1.60%	0.740%

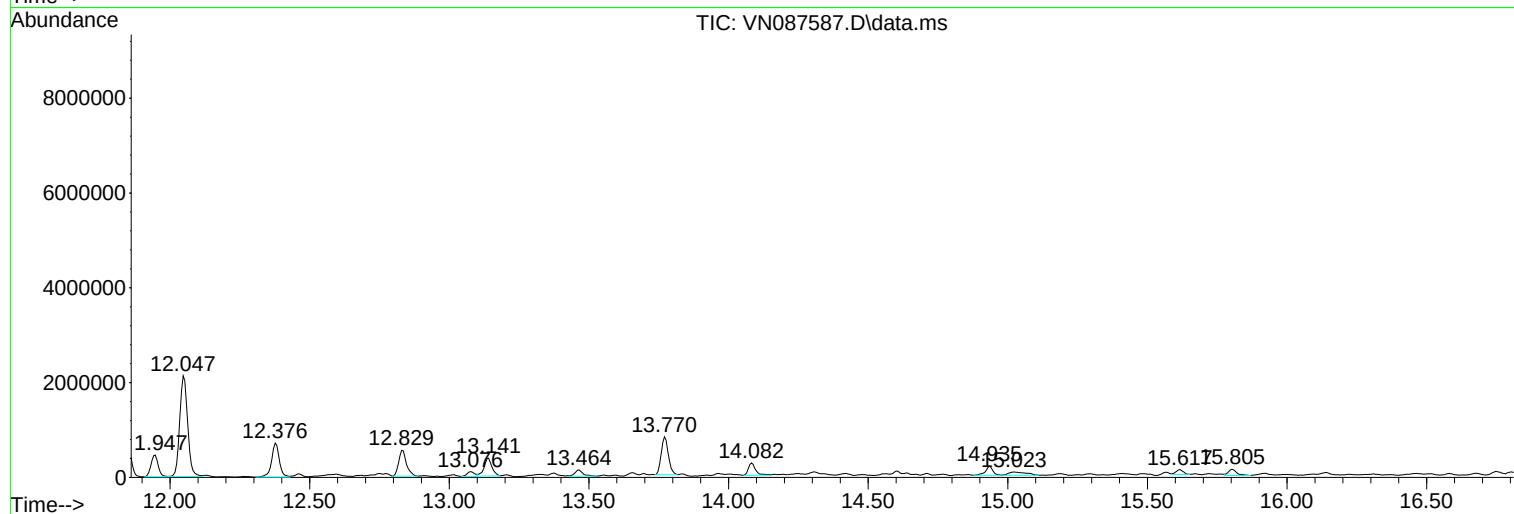
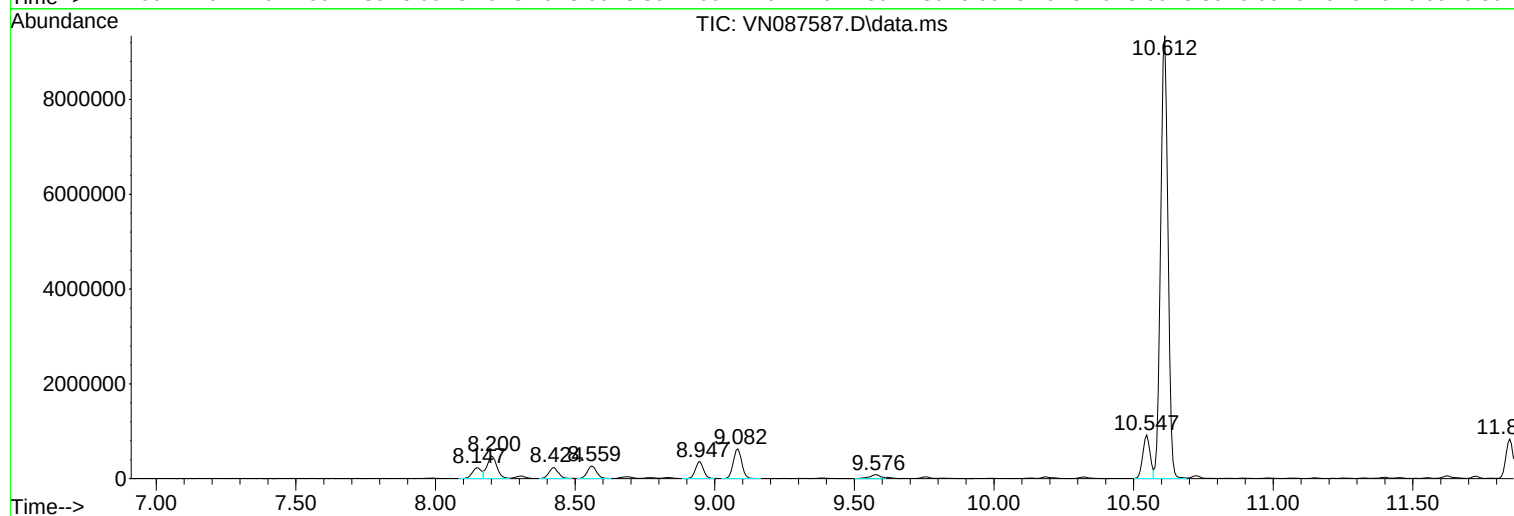
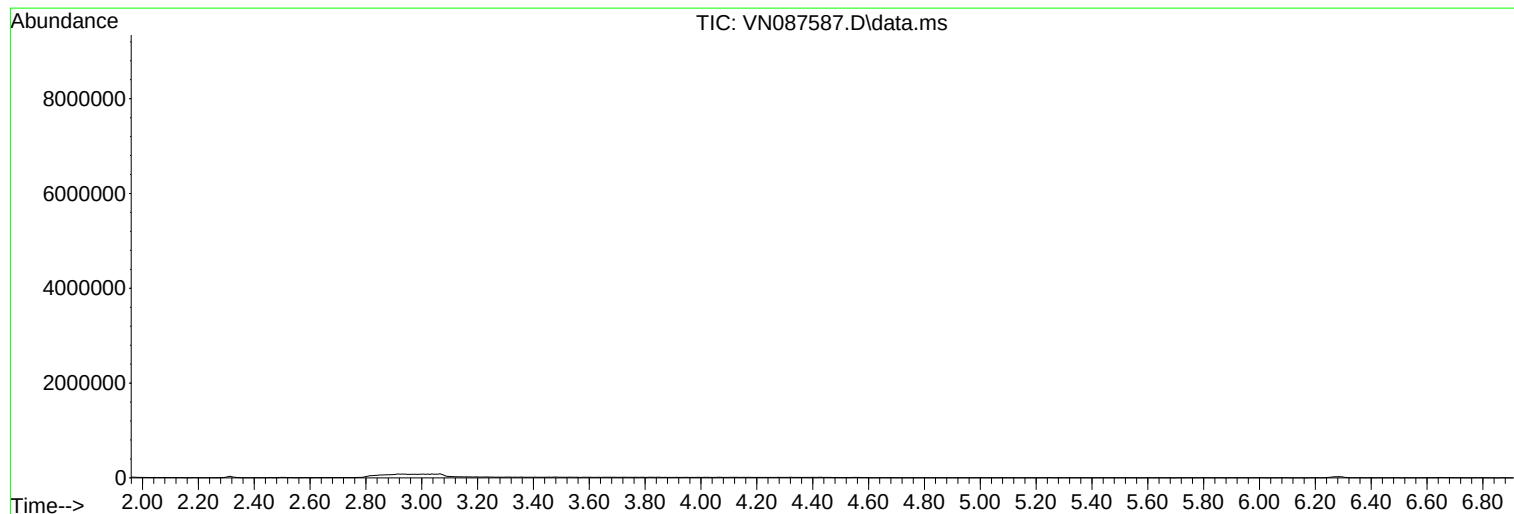
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Instrument :
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ClientSampleId :
MOO-25-0226

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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



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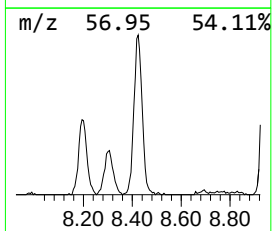
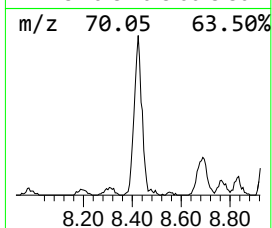
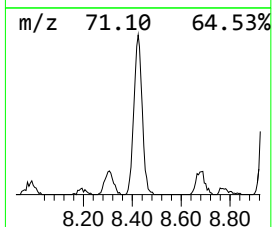
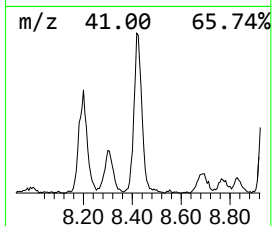
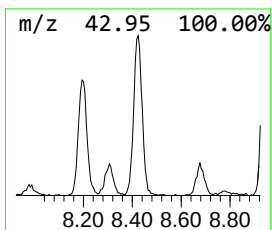
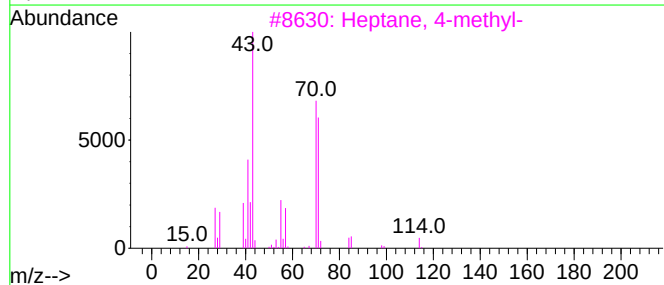
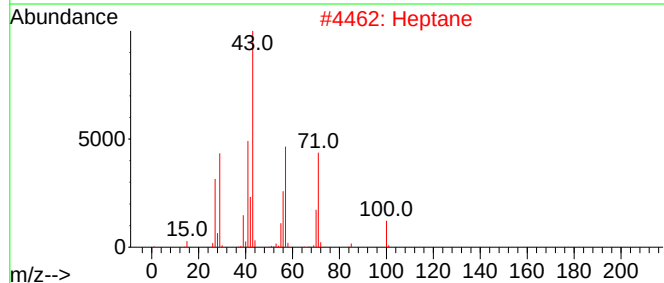
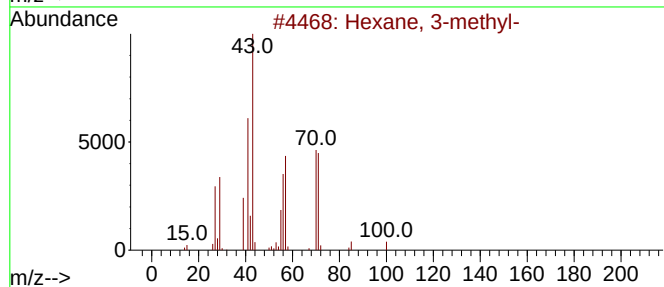
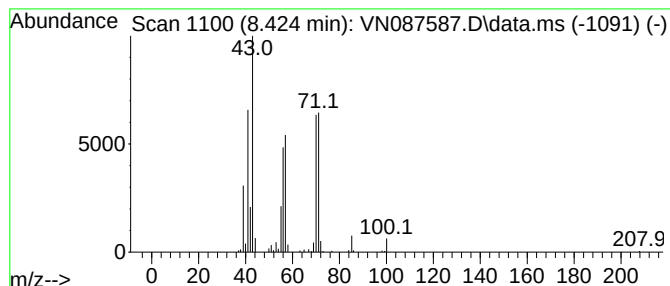
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.424	23.74 ug/l	536555	Pentafluorobenzene	8.206

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	64
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	53
5		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	53



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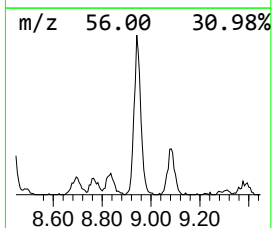
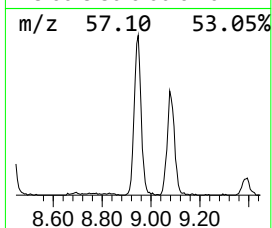
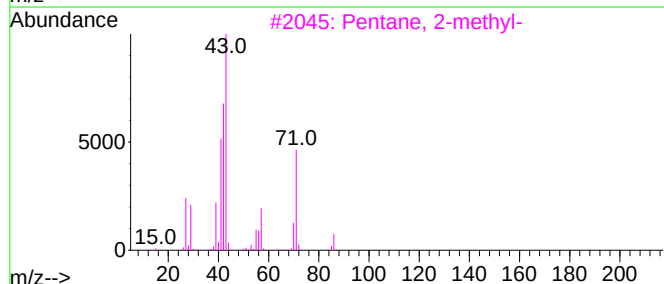
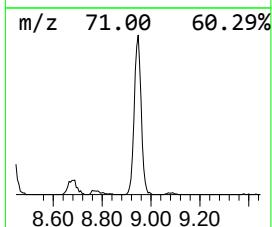
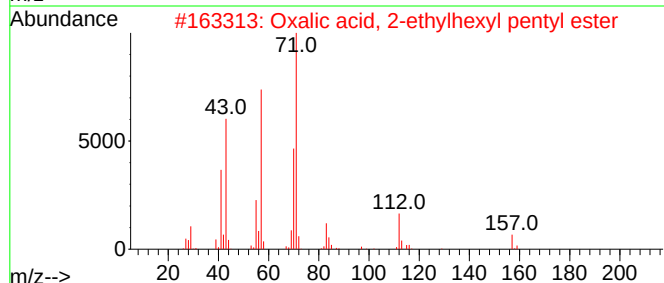
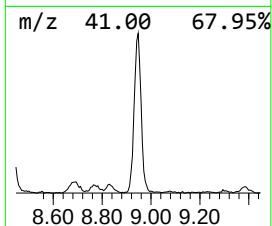
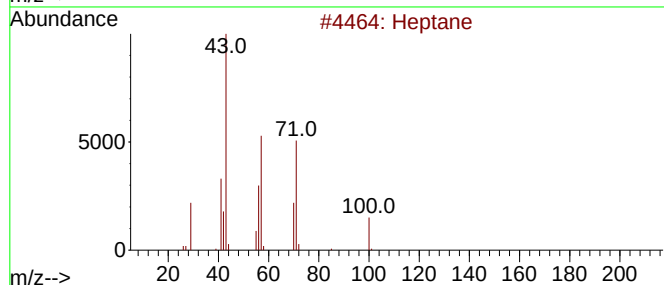
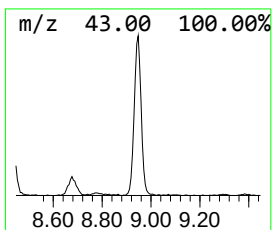
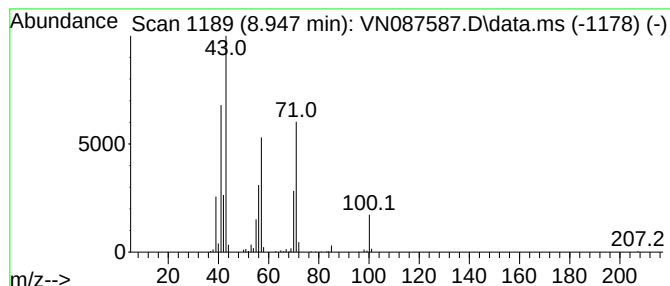
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Quant Title : SW846 8260

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

Peak Number 2 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.947	27.28 ug/l	719932	1,4-Difluorobenzene	9.082

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	91
2			Oxalic acid, 2-ethylhexyl pentyl...	272	C15H28O4	1000309-38-7	47
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
4			Decane, 4-methyl-	156	C11H24	002847-72-5	45
5			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	43



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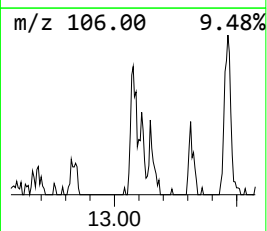
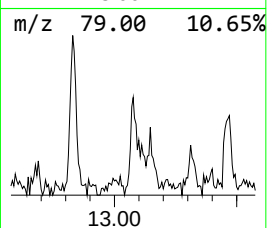
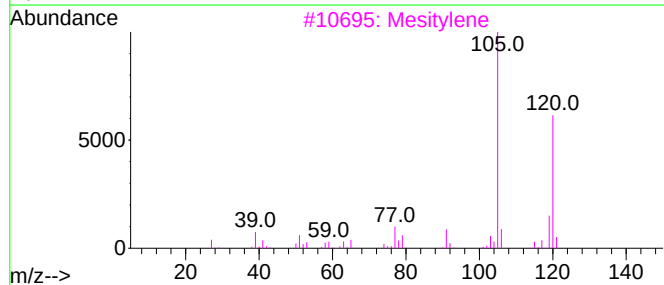
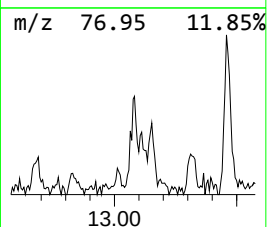
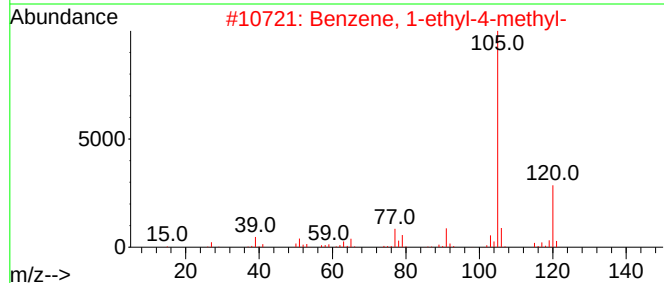
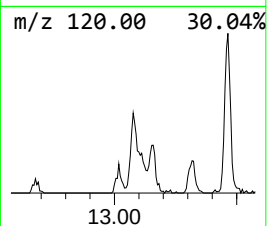
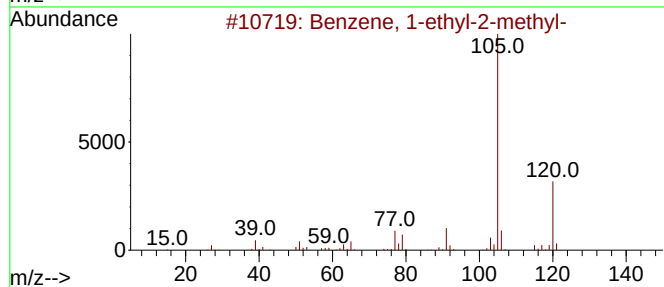
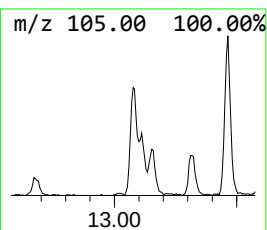
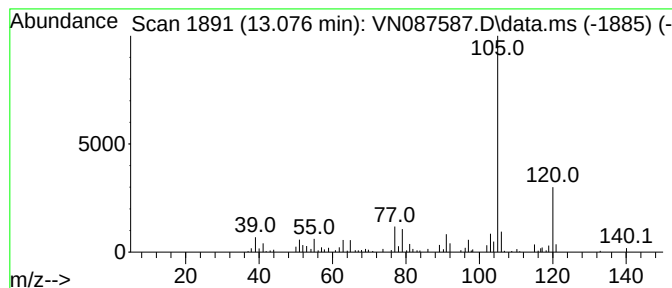
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.076	6.75 ug/l	189782	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3			Mesitylene	120	C9H12	000108-67-8	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	80



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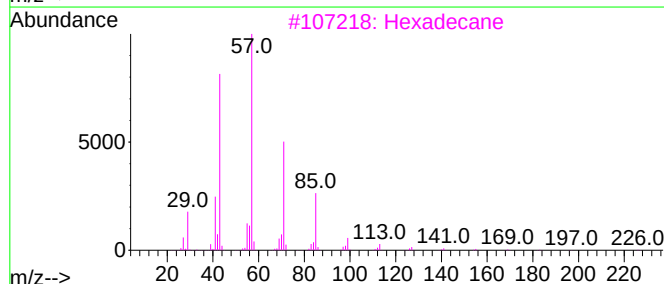
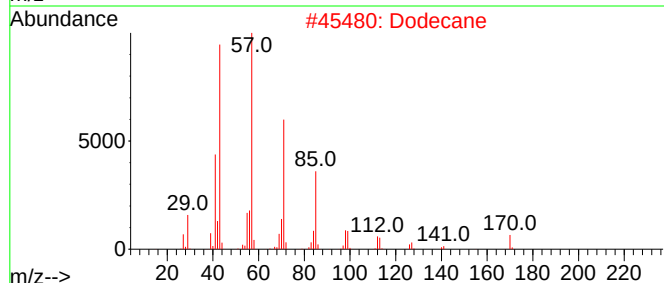
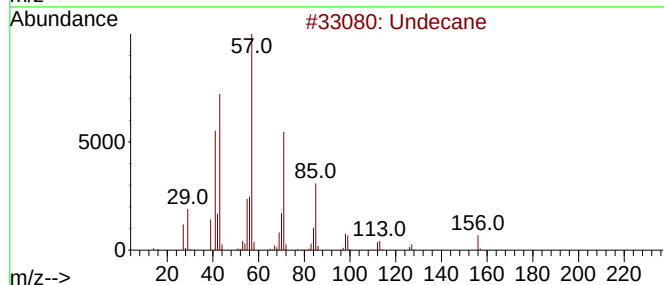
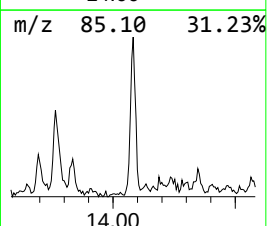
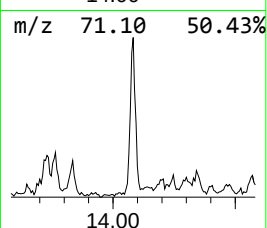
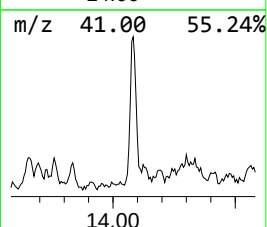
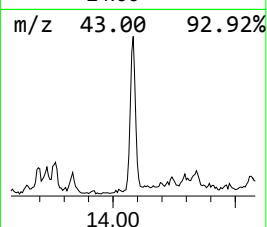
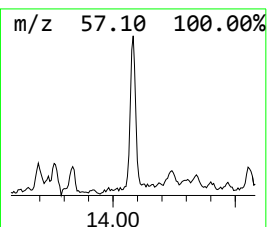
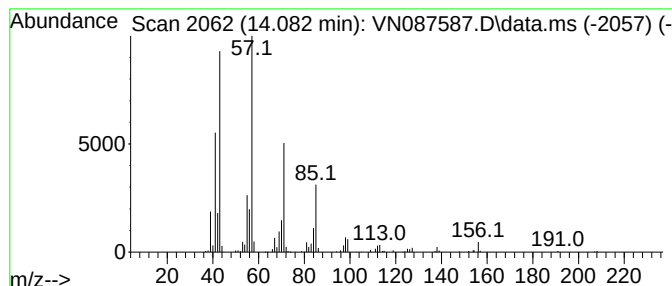
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.082	17.03 ug/l	479113	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	94
2	Dodecane			170	C12H26	000112-40-3	86
3	Hexadecane			226	C16H34	000544-76-3	80
4	Decane			142	C10H22	000124-18-5	78
5	Tridecane			184	C13H28	000629-50-5	72



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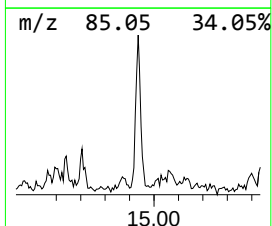
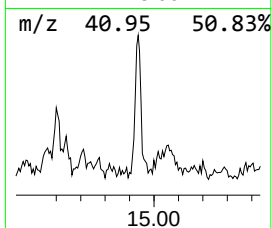
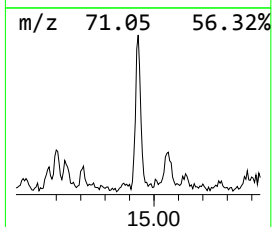
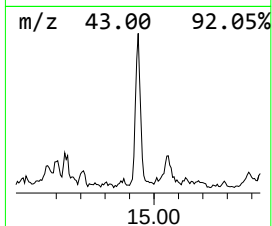
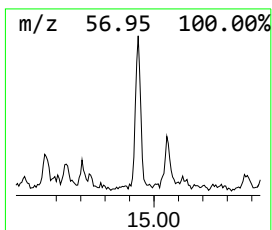
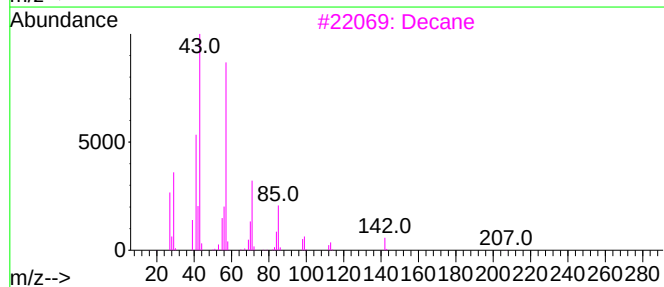
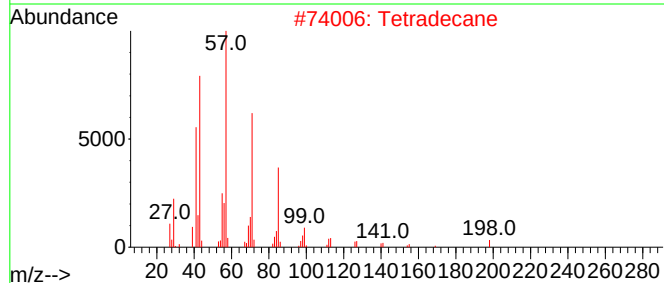
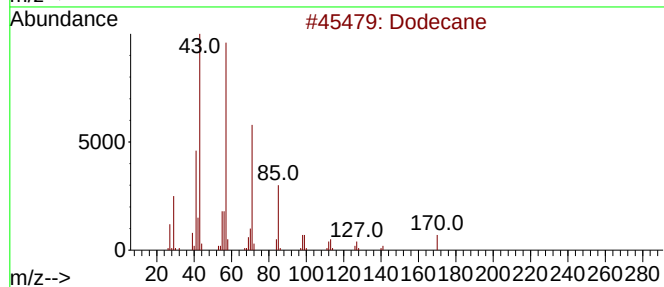
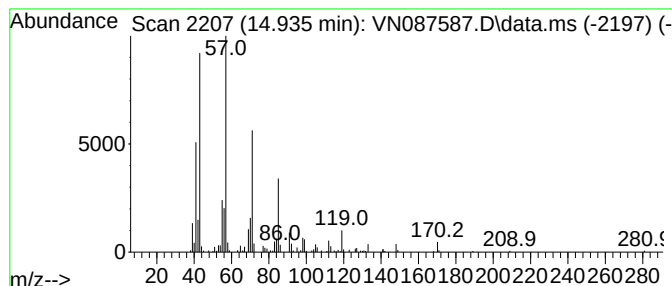
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	12.91 ug/l	363334	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	87
2			Tetradecane	198	C14H30	000629-59-4	72
3			Decane	142	C10H22	000124-18-5	64
4			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	58
5			Hexadecane	226	C16H34	000544-76-3	58



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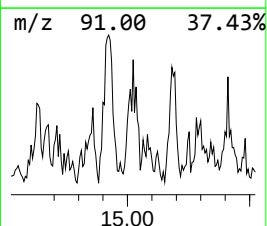
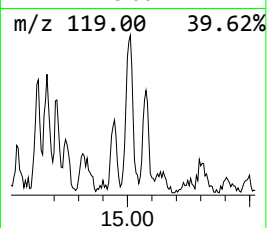
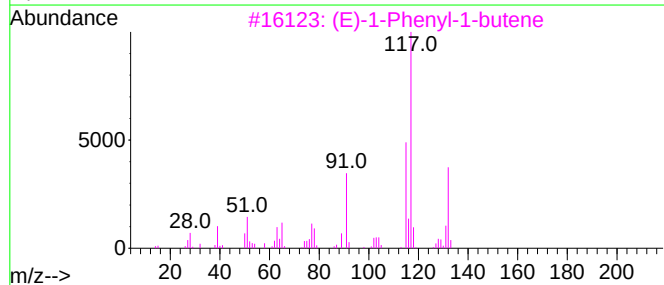
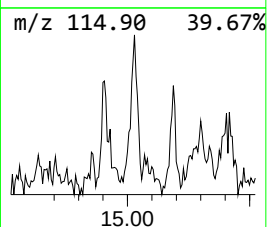
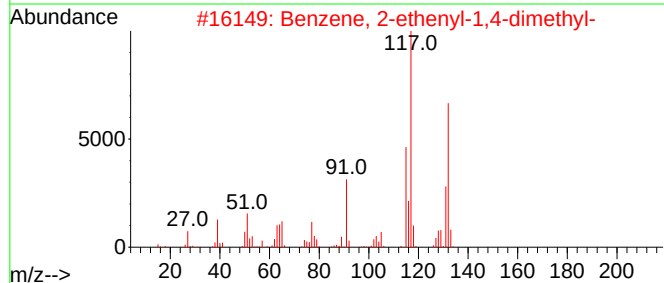
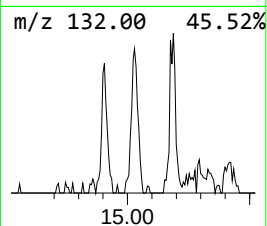
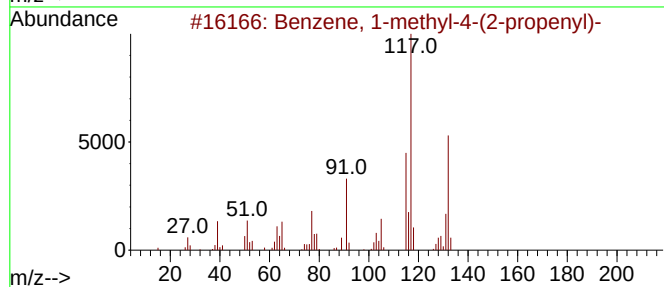
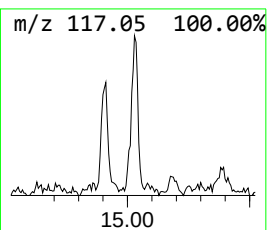
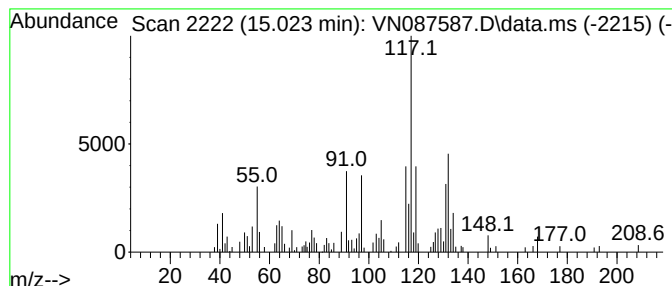
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Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-4-(2-prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.023	10.97 ug/l	308791	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	70
3			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	64
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	64
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087587.D
Acq On : 15 Aug 2025 17:07
Operator : JC\MD
Sample : Q2844-09
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MOO-25-0226

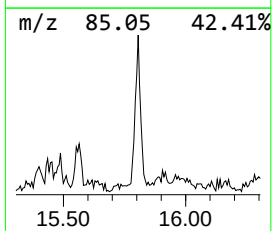
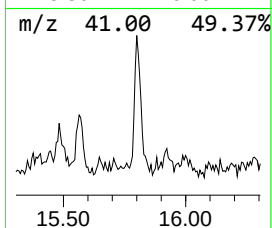
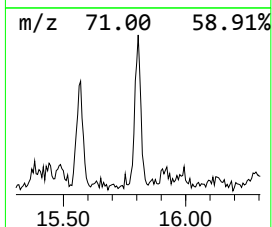
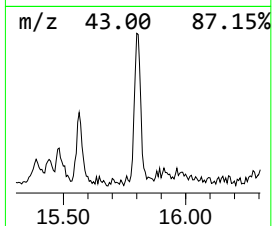
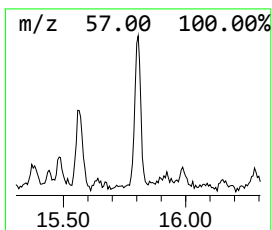
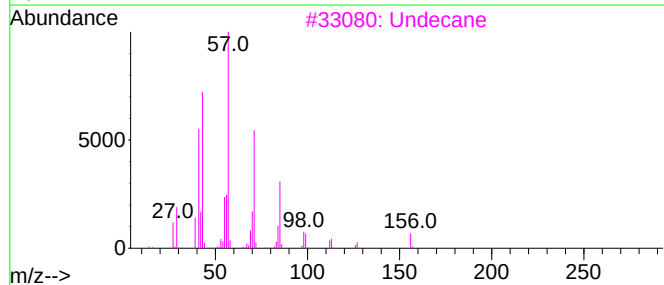
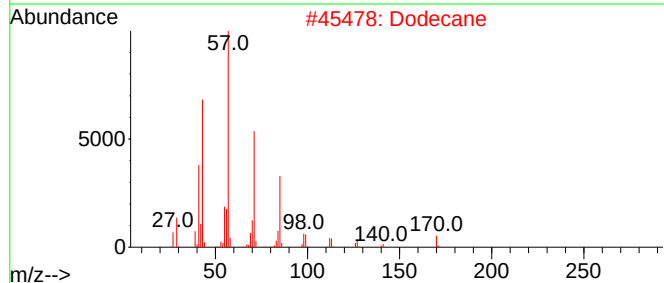
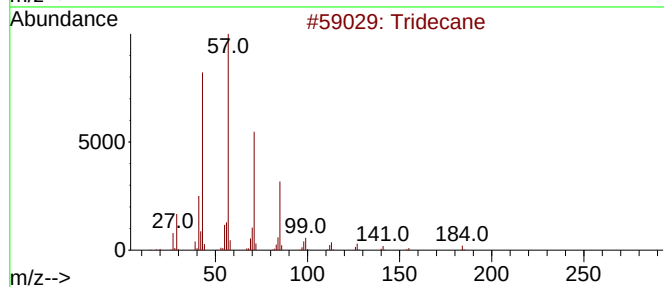
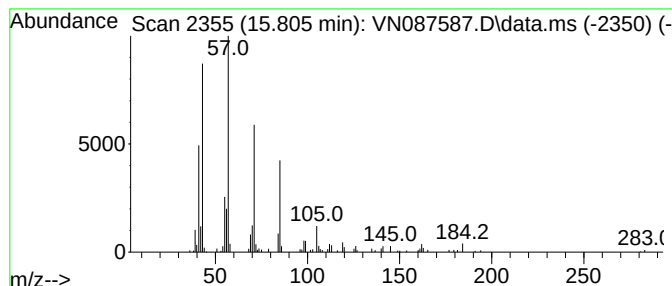
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.806	9.76 ug/l	274640	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	91
2			Dodecane	170	C12H26	000112-40-3	53
3			Undecane	156	C11H24	001120-21-4	53
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53
5			Hexadecane	226	C16H34	000544-76-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087587.D
Acq On : 15 Aug 2025 17:07
Operator : JC\MD
Sample : Q2844-09
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MOO-25-0226

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	8.424	23.7	ug/l	536555	1	8.206	1129990	50.0
Heptane	8.947	27.3	ug/l	719932	2	9.082	1319560	50.0
Benzene, 1-ethy...	13.076	6.8	ug/l	189782	4	13.770	1406830	50.0
Undecane	14.082	17.0	ug/l	479113	4	13.770	1406830	50.0
Dodecane	14.935	12.9	ug/l	363334	4	13.770	1406830	50.0
Benzene, 1-meth...	15.023	11.0	ug/l	308791	4	13.770	1406830	50.0
Tridecane	15.806	9.8	ug/l	274640	4	13.770	1406830	50.0