

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
 Data File : VN088164.D
 Acq On : 29 Oct 2025 16:30
 Operator : JC\MD
 Sample : Q3472-14
 Misc : 1.68g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 155

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\82N102325W.M
 Title : SW846 8260

Signal : TIC: VN088164.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	55	61	70	rBV	38429	66627	1.41%	0.242%
2	2.836	139	150	151	rBV4	32521	71804	1.52%	0.260%
3	5.477	585	599	610	rBV3	12807	48945	1.04%	0.178%
4	8.147	1043	1053	1057	rBV	252623	612675	12.98%	2.223%
5	8.200	1057	1062	1074	rVB	359064	814656	17.25%	2.955%
6	8.559	1114	1123	1134	rBV	294801	678091	14.36%	2.460%
7	9.077	1201	1211	1221	rBV	632867	1341586	28.41%	4.867%
8	10.541	1452	1460	1469	rBV	1013572	1908343	40.41%	6.923%
9	10.623	1469	1474	1486	rVB4	38075	102412	2.17%	0.372%
10	11.847	1674	1682	1694	rBV	885262	1656559	35.08%	6.010%
11	12.047	1710	1716	1727	rBV	66945	149106	3.16%	0.541%
12	12.376	1764	1772	1776	rBV4	25074	66236	1.40%	0.240%
13	12.829	1841	1849	1860	rBV	629513	1238441	26.23%	4.493%
14	13.141	1897	1902	1914	rVB4	54986	118523	2.51%	0.430%
15	13.464	1952	1957	1961	rBV2	36441	62466	1.32%	0.227%
16	13.512	1961	1965	1969	rVB2	39360	59104	1.25%	0.214%
17	13.770	2002	2009	2016	rBV	909164	1699286	35.99%	6.165%
18	13.829	2016	2019	2026	rVB	105992	174896	3.70%	0.634%
19	13.911	2029	2033	2036	rBV5	49127	80131	1.70%	0.291%
20	13.994	2038	2047	2048	rBV8	63777	180718	3.83%	0.656%
21	14.082	2056	2062	2067	rBV	2972226	4721924	100.00%	17.130%
22	14.129	2067	2070	2075	rVB2	343046	494573	10.47%	1.794%
23	14.188	2076	2080	2084	rVV2	266372	375770	7.96%	1.363%
24	14.235	2084	2088	2091	rBV3	221323	378789	8.02%	1.374%
25	14.411	2113	2118	2122	rBV5	184679	410853	8.70%	1.490%
26	14.476	2125	2129	2135	rVV4	374494	816835	17.30%	2.963%
27	14.559	2138	2143	2145	rVV2	432943	889082	18.83%	3.225%
28	14.600	2145	2150	2154	rVV4	1371233	2561506	54.25%	9.293%
29	14.635	2154	2156	2164	rVV3	443656	867485	18.37%	3.147%
30	14.706	2164	2168	2172	rVV3	374093	632294	13.39%	2.294%
31	14.764	2175	2178	2183	rVV3	397403	618793	13.10%	2.245%
32	14.817	2183	2187	2193	rVB4	246461	447394	9.47%	1.623%
33	14.935	2198	2207	2216	rBV	1299372	2367976	50.15%	8.590%
34	15.017	2216	2221	2224	rBV4	215076	423111	8.96%	1.535%
35	15.153	2240	2244	2248	rBV5	117401	216852	4.59%	0.787%
36	15.564	2311	2314	2321	rVB4	104678	211448	4.48%	0.767%

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Instrument :
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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\82N102325W.M
Title : SW846 8260

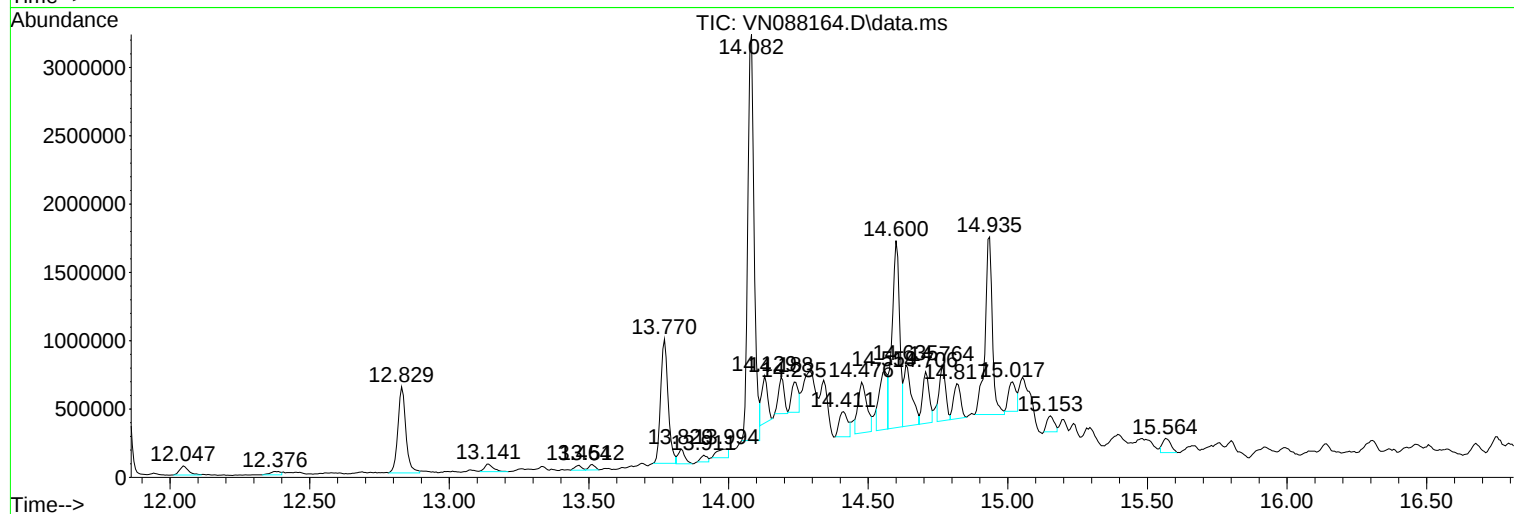
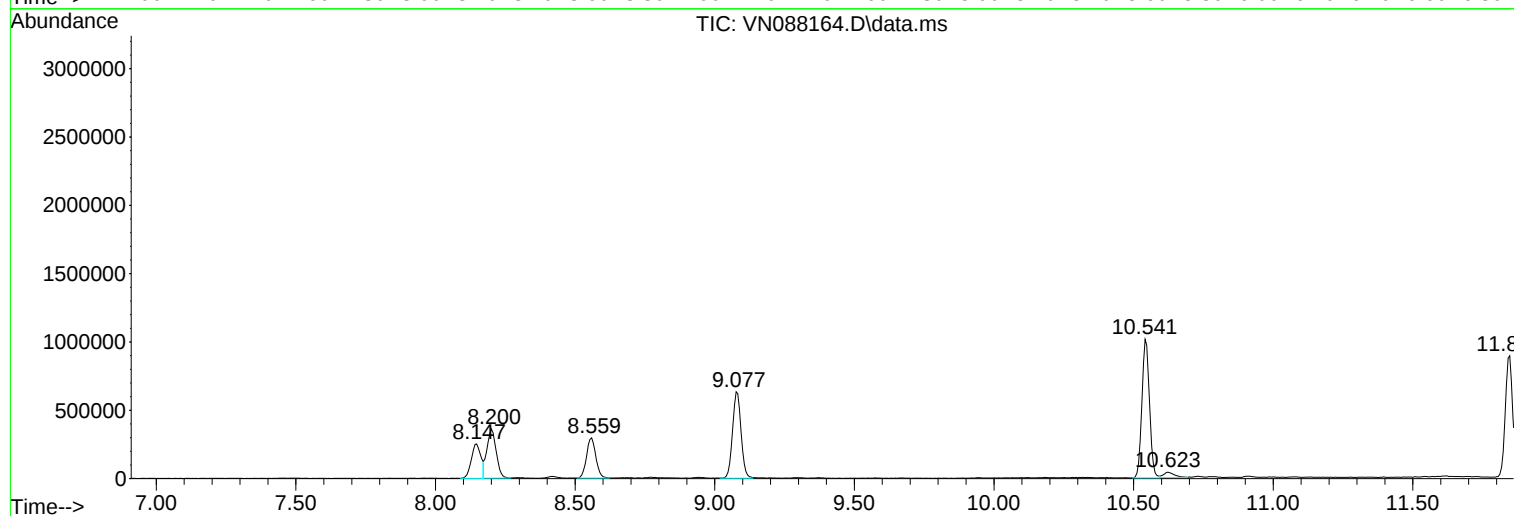
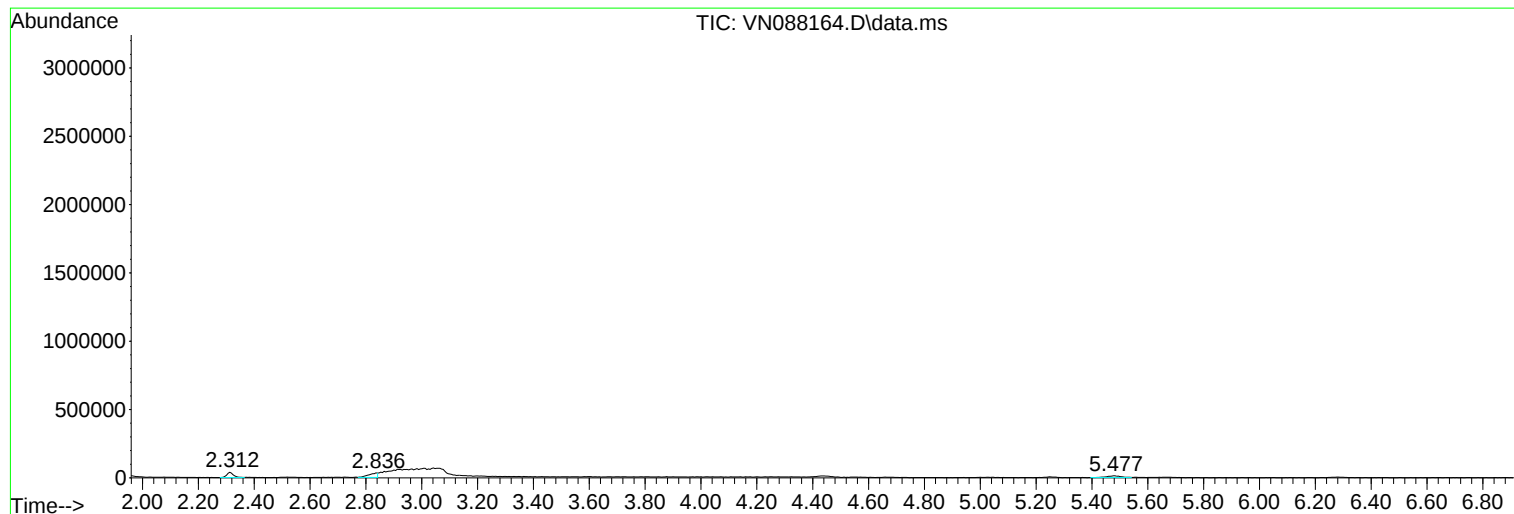
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_N
ClientSampleId :
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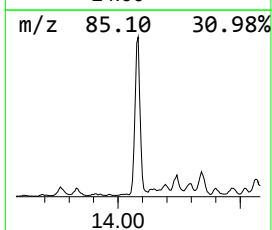
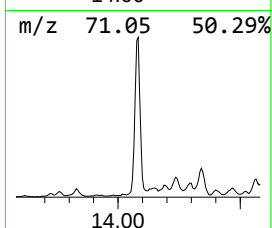
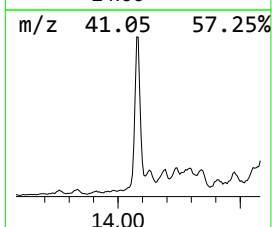
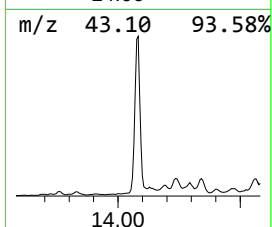
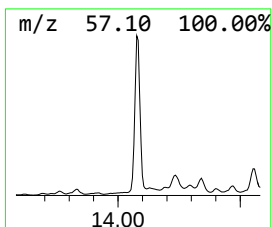
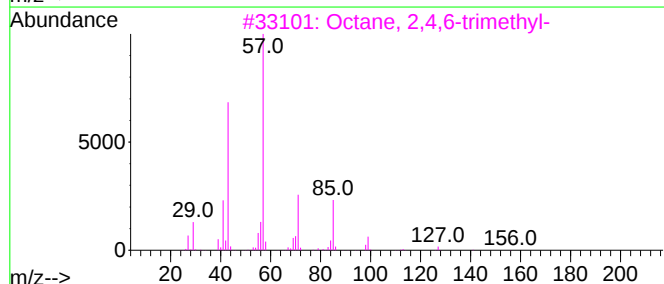
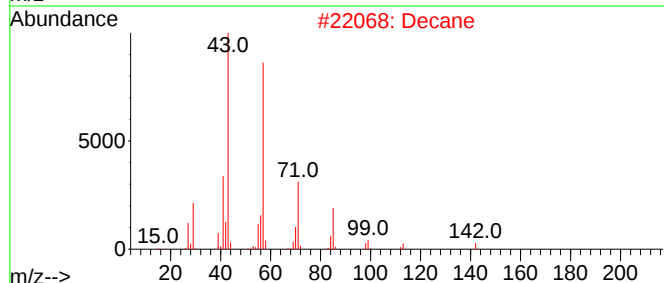
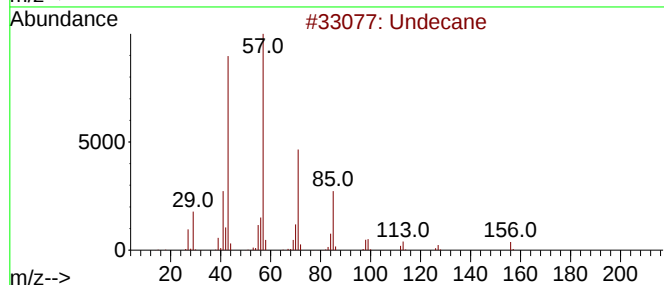
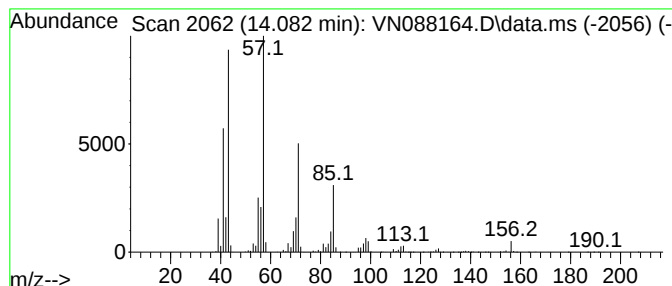
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.082	138.94 ug/l	4721920	1,4-Dichlorobenzene-d4	13.770

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane		156	C11H24	001120-21-4	91
2	Decane		142	C10H22	000124-18-5	78
3	Octane, 2,4,6-trimethyl-		156	C11H24	062016-37-9	72
4	Tridecane		184	C13H28	000629-50-5	72
5	Hexadecane		226	C16H34	000544-76-3	64



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Acq On : 29 Oct 2025 16:30
Operator : JC\MD
Sample : Q3472-14
Misc : 1.68g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
155

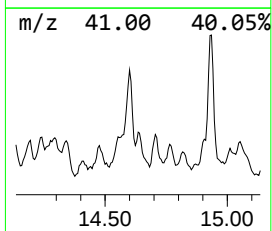
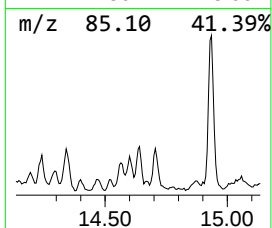
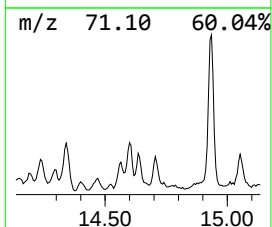
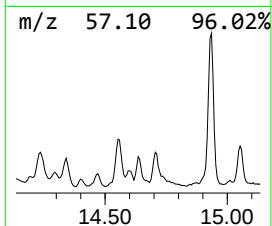
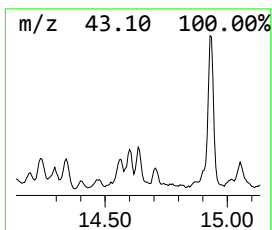
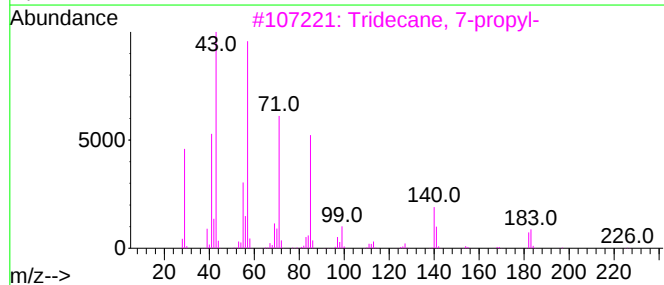
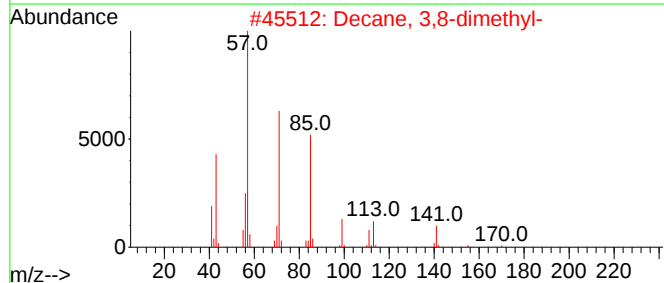
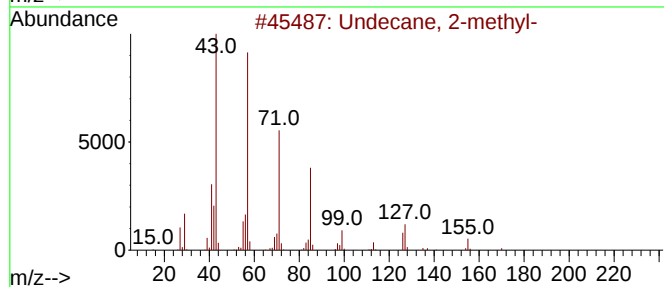
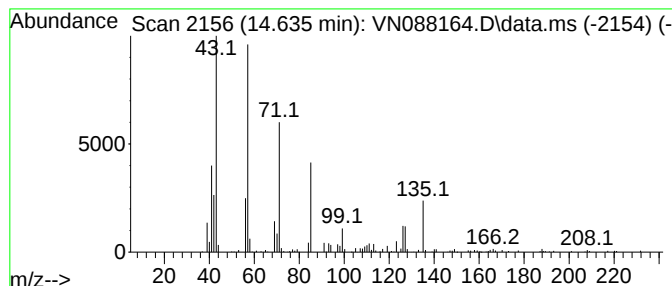
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 6 Undecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.635	25.52 ug/l	867485	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2-methyl-	170	C12H26	007045-71-8	90
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	58
3			Tridecane, 7-propyl-	226	C16H34	055045-09-5	50
4			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	50
5			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	50



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Misc : 1.68g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
155

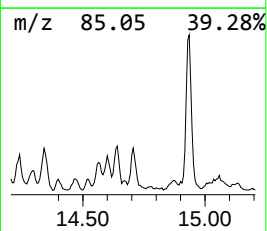
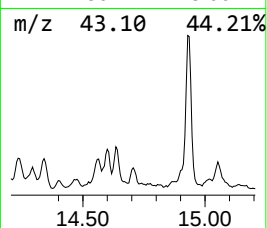
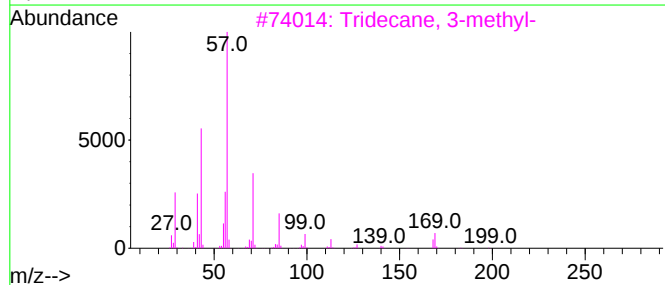
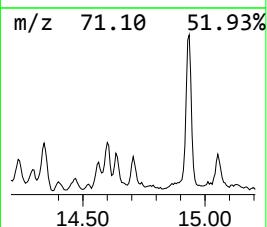
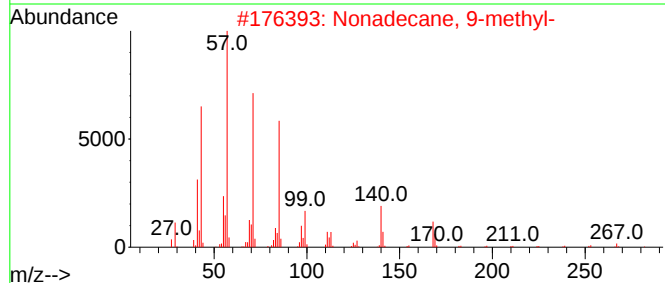
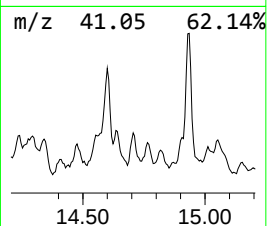
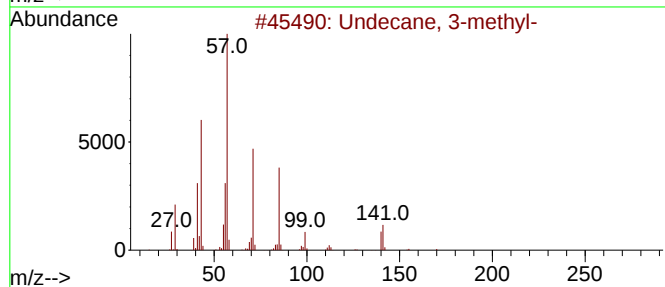
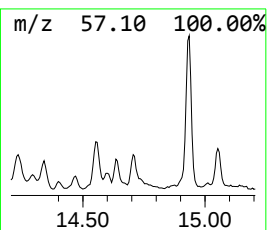
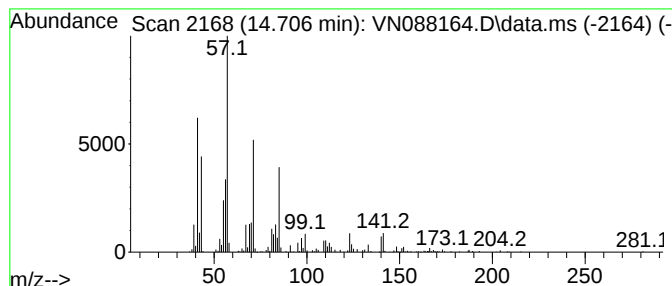
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 7 Undecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.706	18.60 ug/l	632294	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3-methyl-	170	C12H26	001002-43-3	87
2			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64
3			Tridecane, 3-methyl-	198	C14H30	006418-41-3	64
4			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	59
5			9-methylheptadecane	254	C18H38	026741-18-4	53



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Misc : 1.68g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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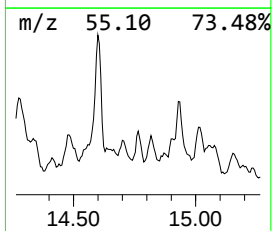
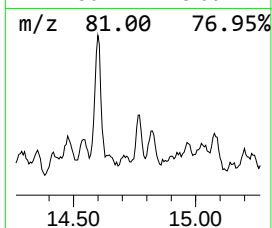
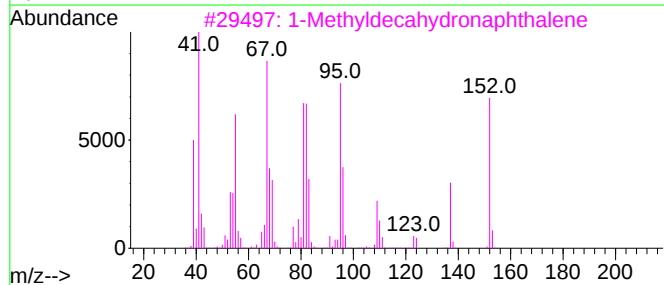
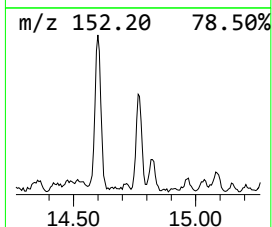
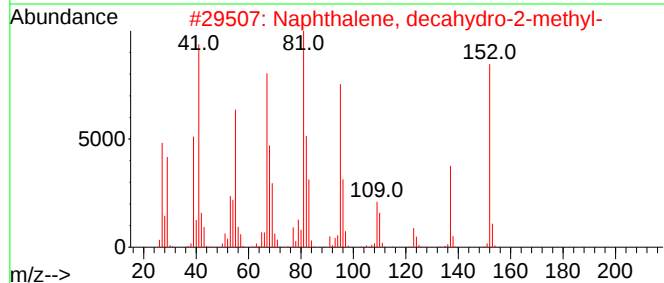
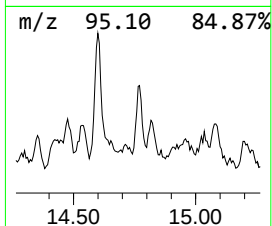
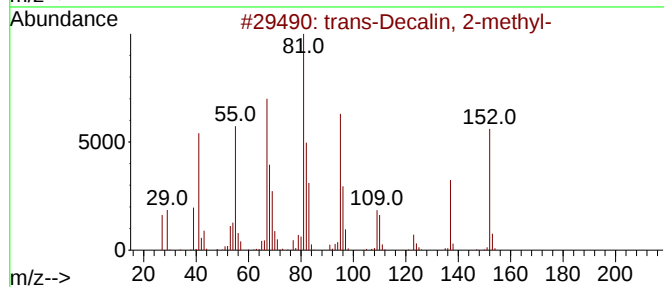
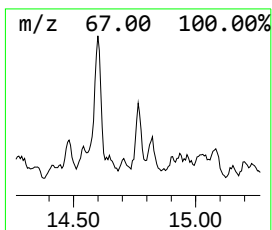
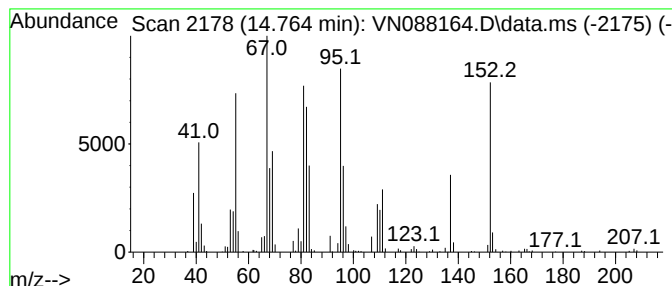
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Quant Title : SW846 8260

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

Peak Number 8 trans-Decalin, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.764	18.21 ug/l	618793	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
3			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	89
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	87
5			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	70



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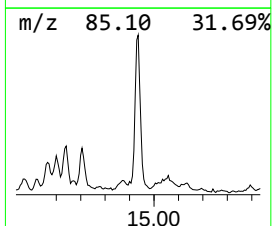
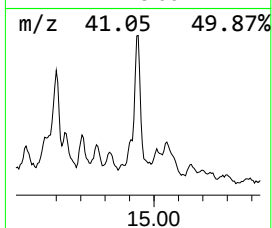
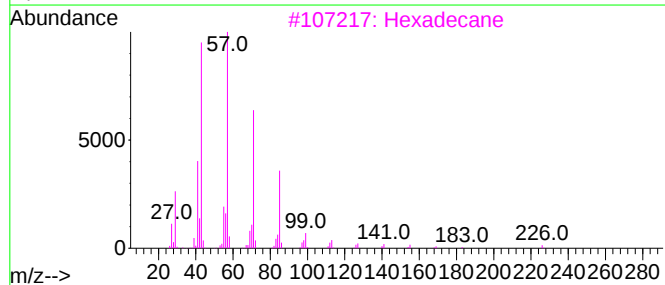
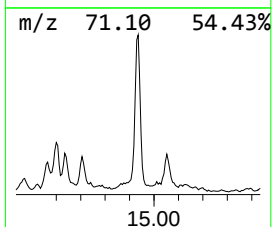
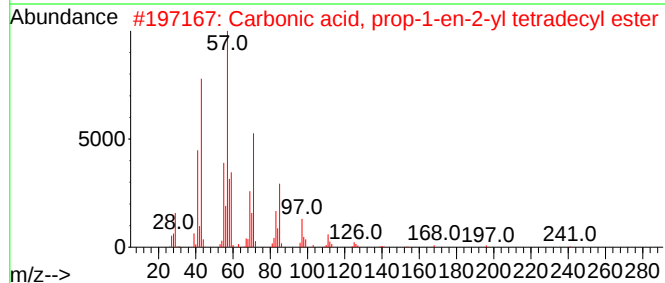
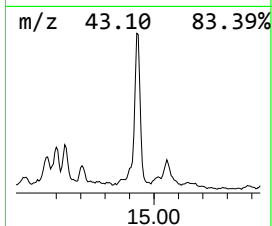
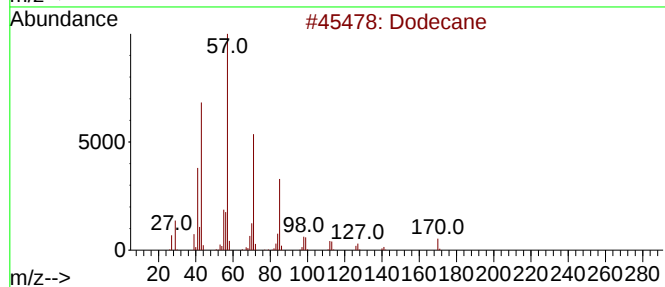
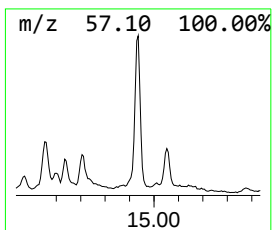
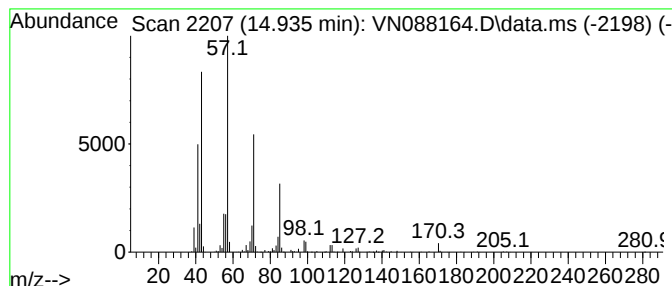
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 10 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	69.68 ug/l	2367980	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	90
3			Hexadecane	226	C16H34	000544-76-3	86
4			Tridecane	184	C13H28	000629-50-5	86
5			Undecane	156	C11H24	001120-21-4	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102925\
Data File : VN088164.D
Acq On : 29 Oct 2025 16:30
Operator : JC\MD
Sample : Q3472-14
Misc : 1.68g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
155

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.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
Undecane	14.082	138.9	ug/l	4721920	4	13.770	1699290	50.0
Undecane, 2-met...	14.635	25.5	ug/l	867485	4	13.770	1699290	50.0
Undecane, 3-met...	14.706	18.6	ug/l	632294	4	13.770	1699290	50.0
trans-Decalin, ...	14.764	18.2	ug/l	618793	4	13.770	1699290	50.0
Dodecane	14.935	69.7	ug/l	2367980	4	13.770	1699290	50.0