

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
 Data File : VN086305.D
 Acq On : 16 Apr 2025 18:27
 Operator : JC\MD
 Sample : Q1791-14 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VB16164

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\82N041525W.M
 Title : SW846 8260

Signal : TIC: VN086305.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.165	1046	1056	1060	rBV	128673	303149	24.43%	2.879%
2	8.218	1060	1065	1076	rVB	261366	590066	47.55%	5.603%
3	8.577	1117	1126	1135	rBV	170164	377302	30.40%	3.583%
4	9.100	1205	1215	1225	rBV	417854	864061	69.63%	8.205%
5	10.565	1455	1464	1472	rBV	672486	1241020	100.00%	11.784%
6	11.865	1675	1685	1696	rBV	594171	1061761	85.56%	10.082%
7	12.847	1841	1852	1859	rBV2	460743	928045	74.78%	8.812%
8	12.912	1859	1863	1865	rBV3	9508	13908	1.12%	0.132%
9	12.988	1870	1876	1886	rVB3	39628	93716	7.55%	0.890%
10	13.194	1900	1911	1916	rBV2	40121	100930	8.13%	0.958%
11	13.241	1916	1919	1927	rVB2	12406	20550	1.66%	0.195%
12	13.359	1935	1939	1941	rVV3	11592	20049	1.62%	0.190%
13	13.417	1941	1949	1962	rVB	190076	371308	29.92%	3.526%
14	13.529	1962	1968	1976	rBV	85714	136586	11.01%	1.297%
15	13.641	1976	1987	1993	rBV	315493	599859	48.34%	5.696%
16	13.712	1995	1999	2001	rVV	30762	51670	4.16%	0.491%
17	13.753	2001	2006	2007	rVV2	72386	115140	9.28%	1.093%
18	13.788	2007	2012	2016	rVV	608523	1036000	83.48%	9.837%
19	13.835	2016	2020	2030	rVV	474362	979606	78.94%	9.302%
20	13.935	2030	2037	2041	rVV2	28492	77796	6.27%	0.739%
21	13.994	2041	2047	2055	rVV2	216914	476894	38.43%	4.528%
22	14.070	2055	2060	2064	rVV2	53284	115279	9.29%	1.095%
23	14.135	2065	2071	2074	rVV2	62322	148569	11.97%	1.411%
24	14.182	2074	2079	2090	rVV2	79812	217106	17.49%	2.062%
25	14.270	2090	2094	2095	rVV3	15193	22686	1.83%	0.215%
26	14.306	2095	2100	2102	rVV2	38577	74442	6.00%	0.707%
27	14.341	2102	2106	2115	rVB2	59732	123337	9.94%	1.171%
28	14.506	2123	2134	2135	rBV6	20360	49071	3.95%	0.466%
29	14.735	2167	2173	2184	rVB2	80685	180888	14.58%	1.718%
30	14.876	2192	2197	2201	rBV2	14322	23232	1.87%	0.221%
31	15.223	2251	2256	2260	rBV5	6837	12597	1.02%	0.120%
32	15.588	2314	2318	2324	rBV3	11873	22261	1.79%	0.211%
33	15.829	2354	2359	2369	rVB3	21850	46494	3.75%	0.441%
34	16.017	2387	2391	2399	rVB9	6907	15804	1.27%	0.150%
35	16.611	2486	2492	2498	rBV3	10311	20032	1.61%	0.190%

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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\82N041525W.M
Title : SW846 8260

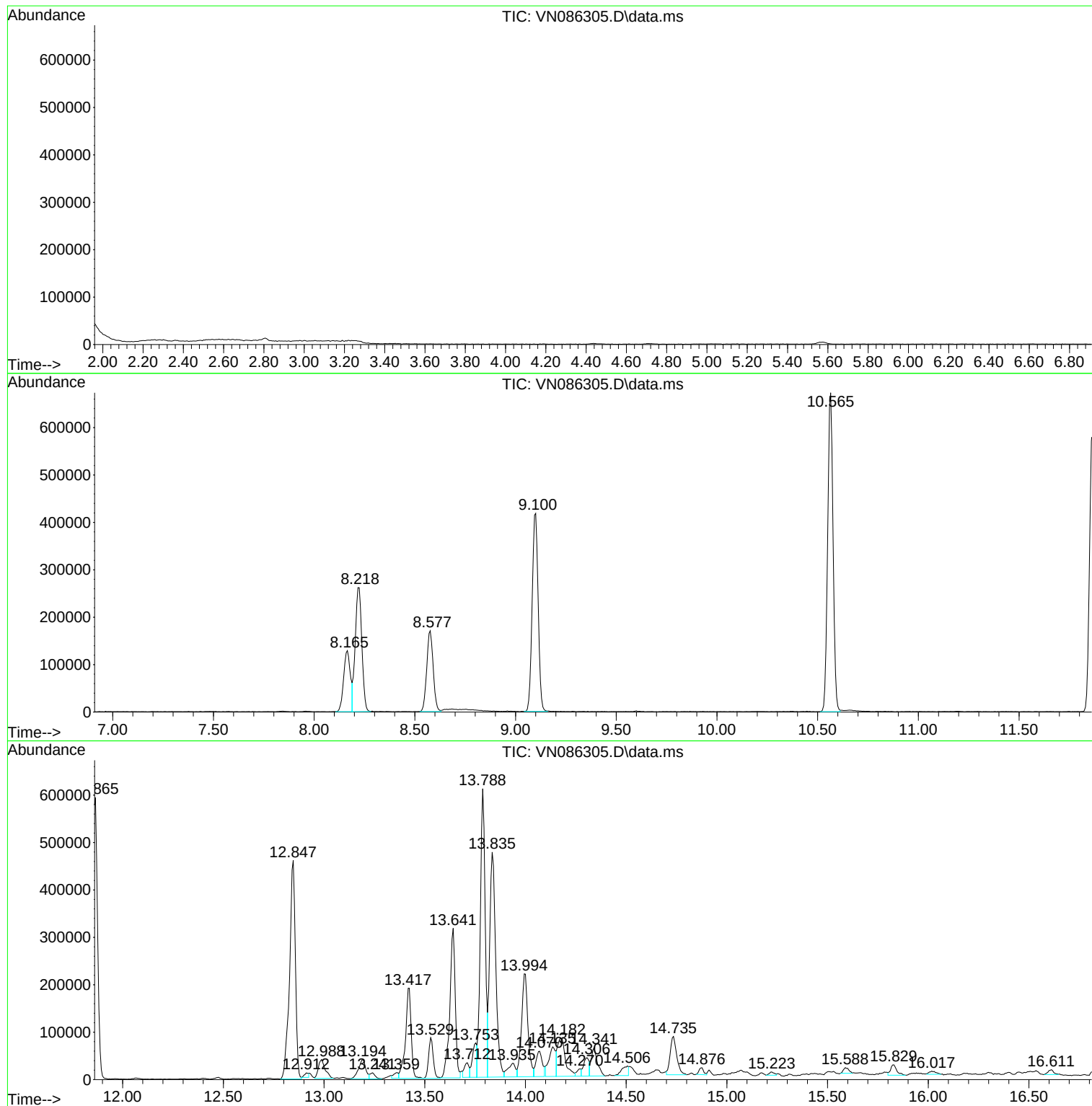
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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



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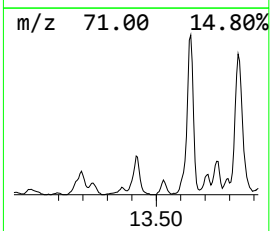
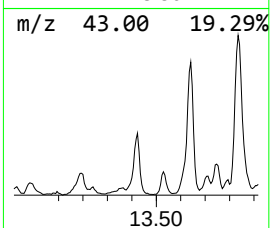
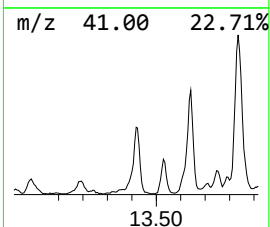
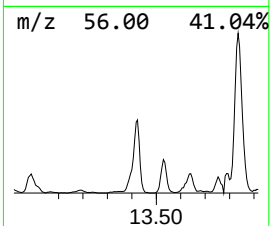
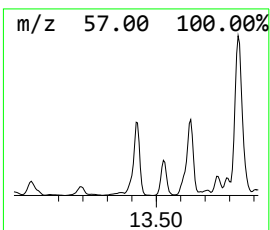
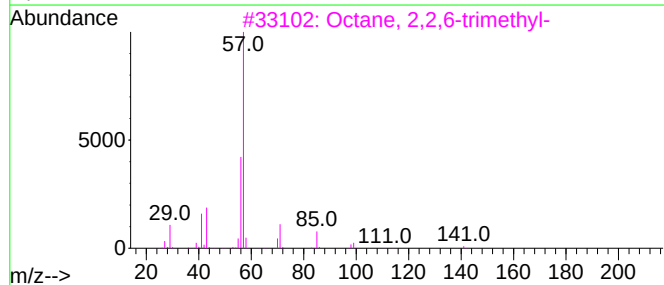
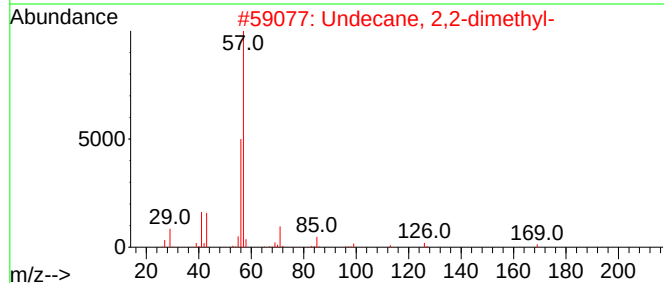
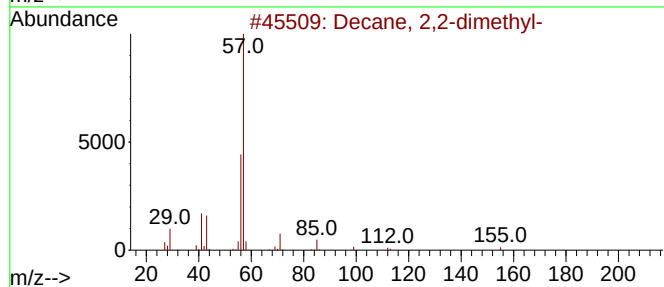
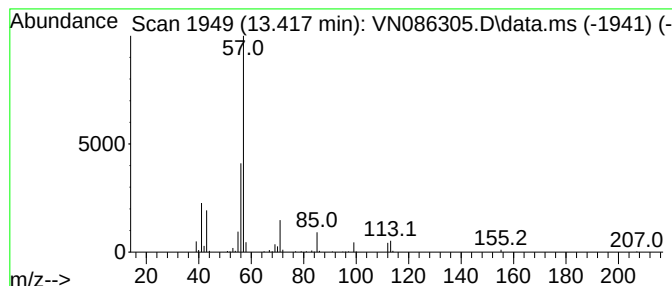
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.418	17.92 ug/l	371308	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	78
2			Undecane, 2,2-dimethyl-	184	C13H28	017312-64-0	72
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
4			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72
5			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72



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Instrument :
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ClientSampleId :
VB16164

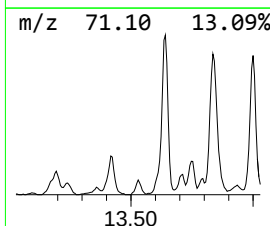
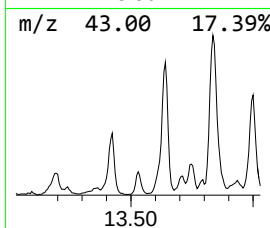
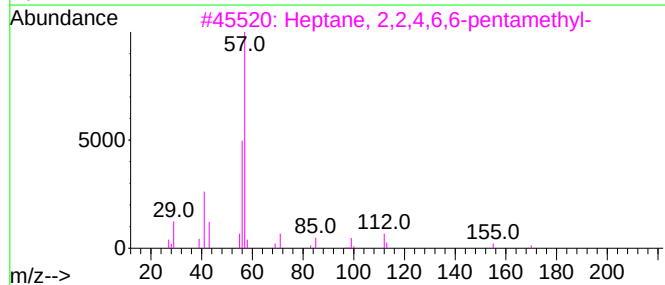
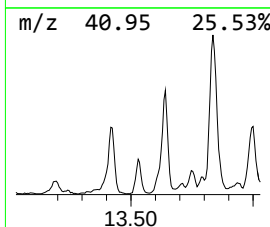
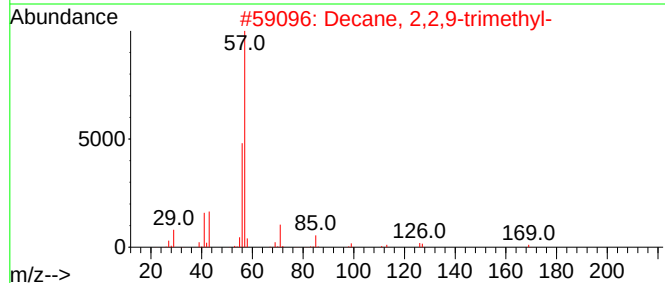
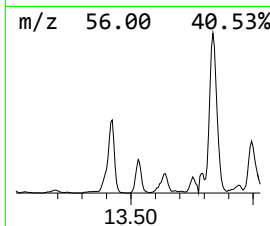
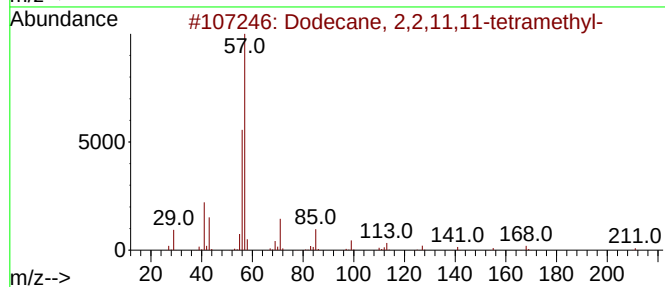
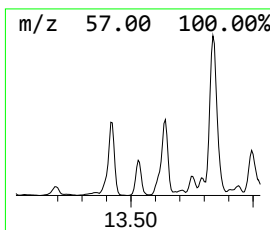
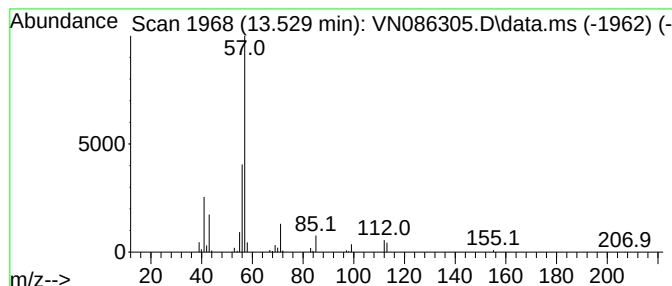
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane, 2,2,11,11-tetrame... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.529	6.59 ug/l	136586	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	78
2			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	78
3			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	78
4			Decane, 2,2,5-trimethyl-	184	C13H28	062237-96-1	72
5			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	72



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Instrument :
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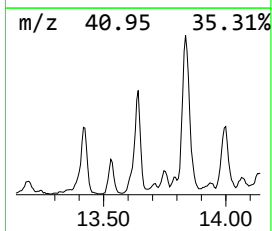
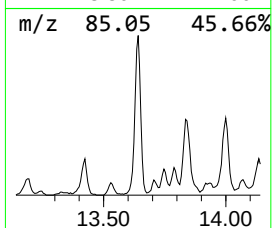
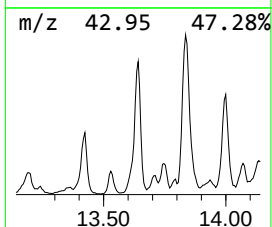
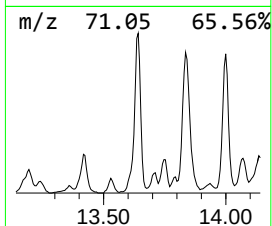
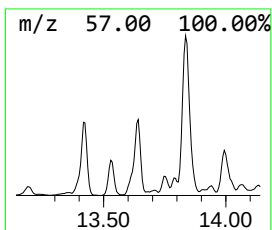
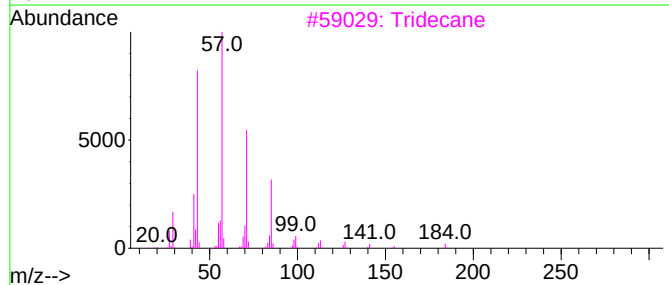
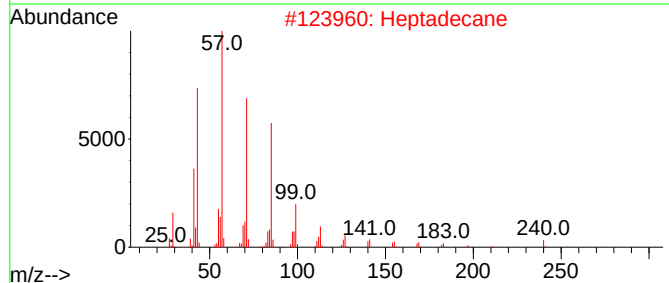
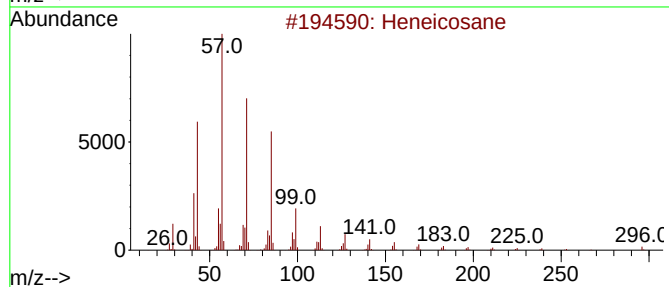
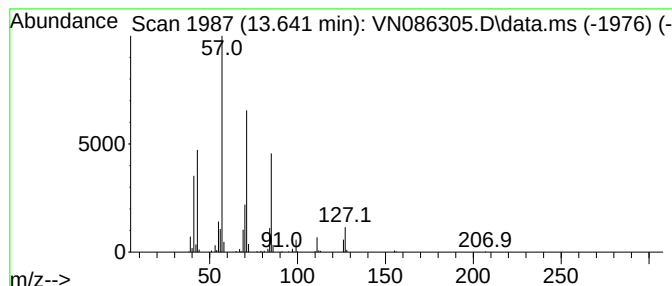
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 3 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	28.95 ug/l	599859	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	72
2			Heptadecane	240	C17H36	000629-78-7	72
3			Tridecane	184	C13H28	000629-50-5	64
4			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	59



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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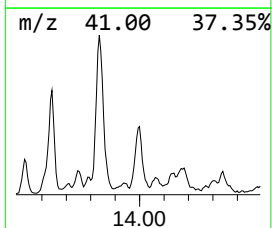
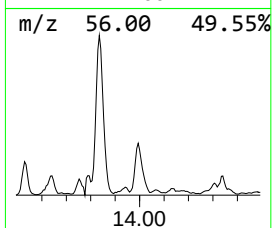
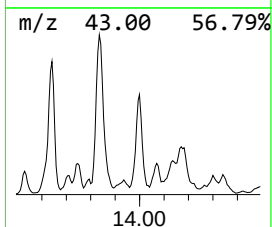
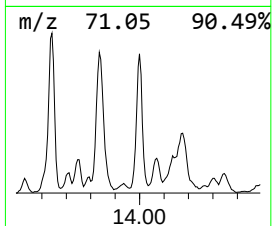
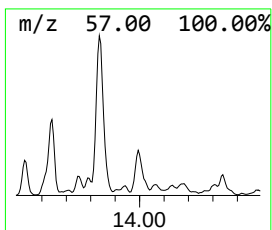
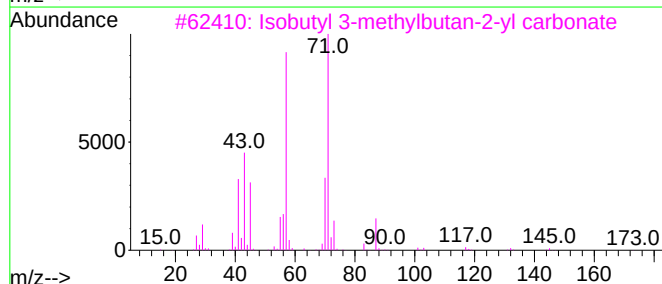
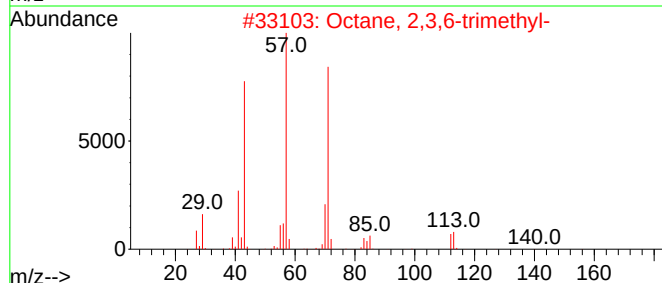
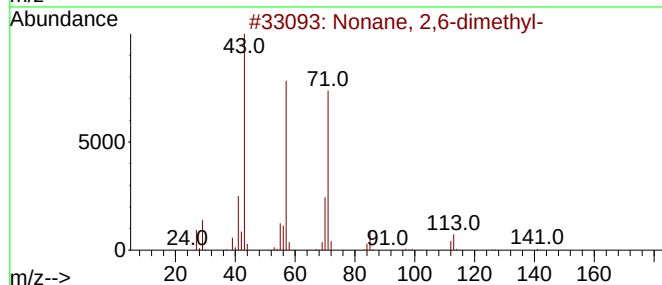
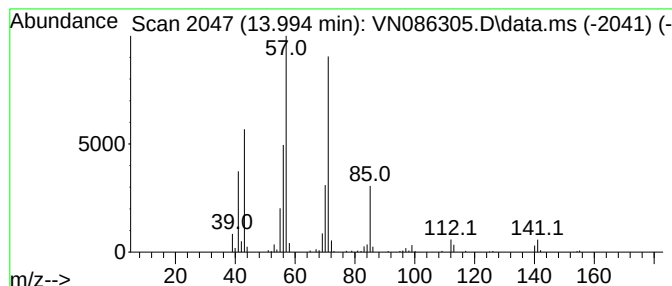
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 4 Nonane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	23.02 ug/l	476894	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	59
2			Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	50
3			Isobutyl 3-methylbutan-2-yl carb...	188	C10H20O3	1000372-77-0	50
4			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	50
5			Oxalic acid, hexyl neopentyl ester	244	C13H24O4	1000309-73-1	50



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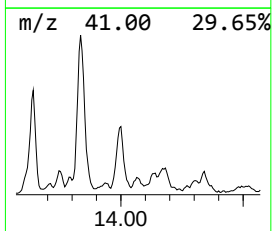
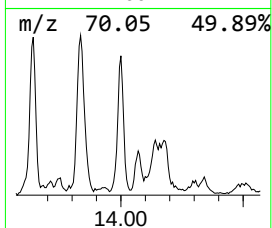
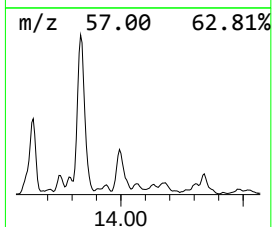
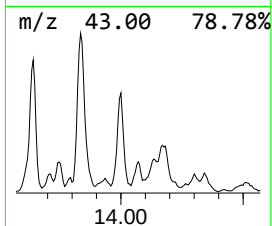
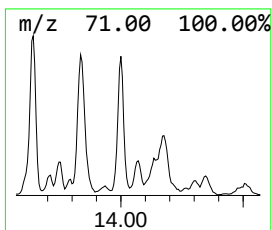
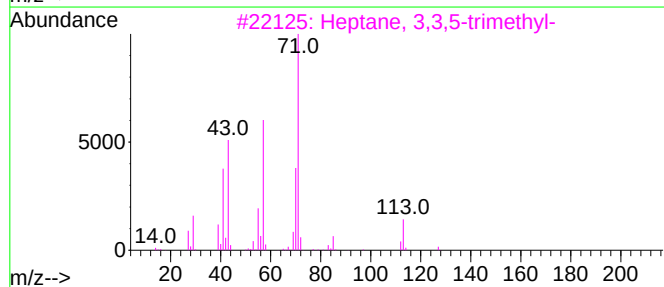
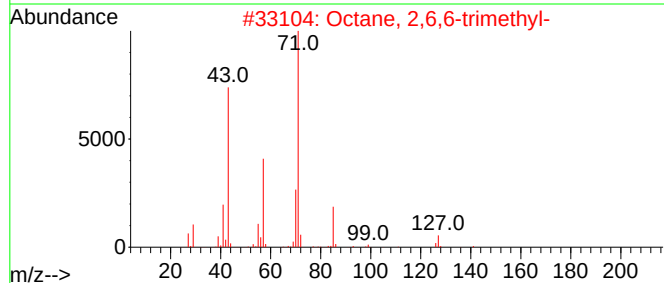
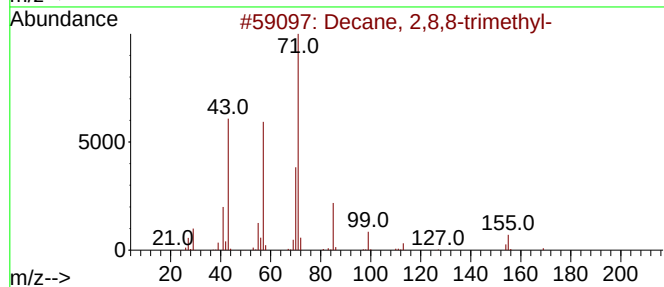
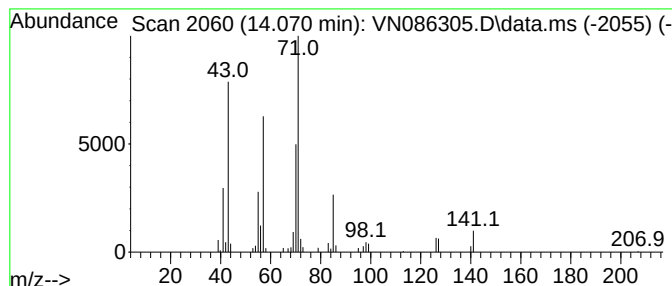
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 5 Decane, 2,8,8-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.070	5.56 ug/l	115279	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,8,8-trimethyl-	184	C13H28	1000060-81-2	64
2			Octane, 2,6,6-trimethyl-	156	C11H24	054166-32-4	59
3			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
4			Oxalic acid, 2-ethylhexyl ethyl ...	230	C12H22O4	1000309-38-4	53
5			Hexanoic acid, 1,1-dimethylpropyl...	186	C11H22O2	116423-69-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086305.D
Acq On : 16 Apr 2025 18:27
Operator : JC\MD
Sample : Q1791-14 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16164

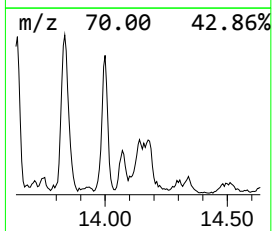
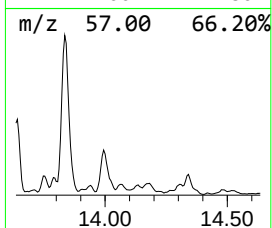
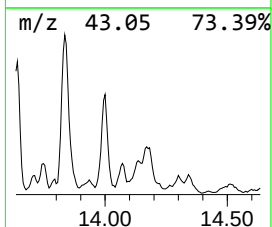
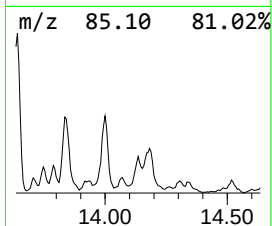
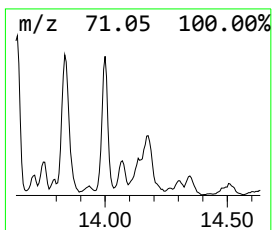
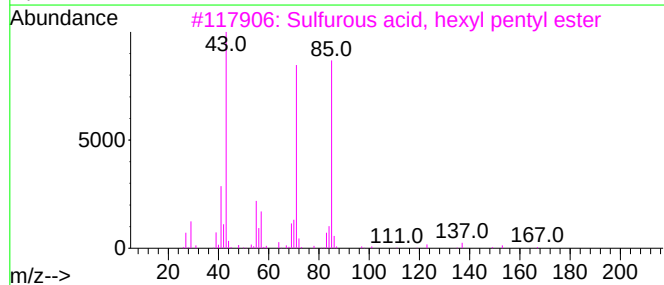
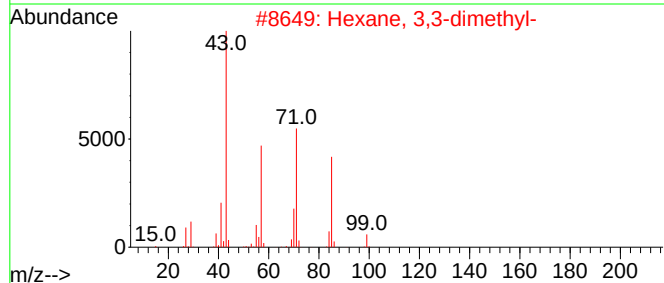
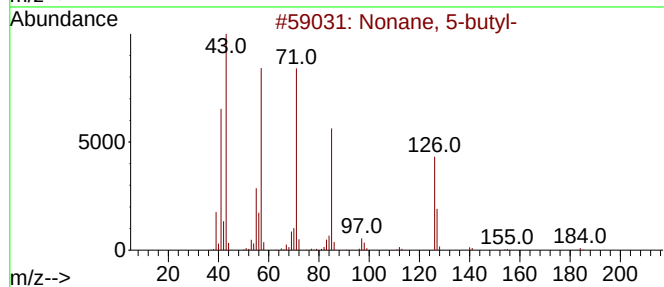
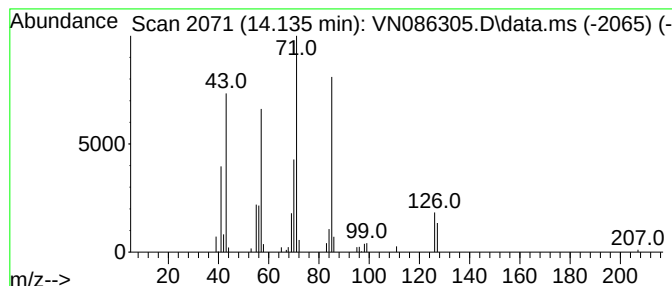
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Quant Title : SW846 8260

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

Peak Number 6 Nonane, 5-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.135	7.17 ug/l	148569	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane, 5-butyl-	184	C13H28	017312-63-9	64
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
3			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	53
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	53
5			Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086305.D
Acq On : 16 Apr 2025 18:27
Operator : JC\MD
Sample : Q1791-14 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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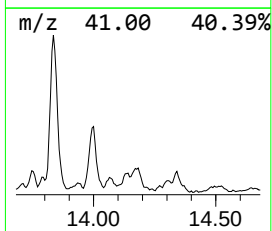
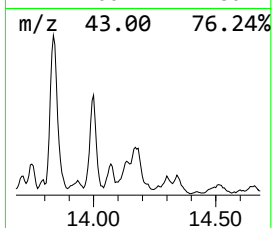
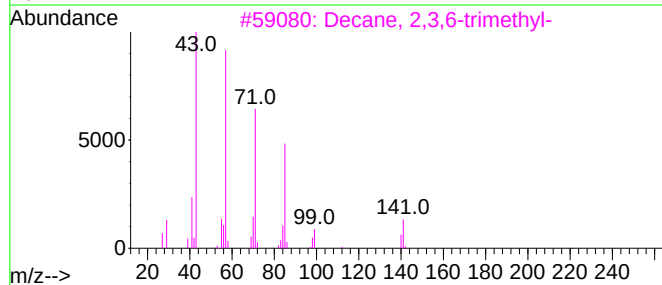
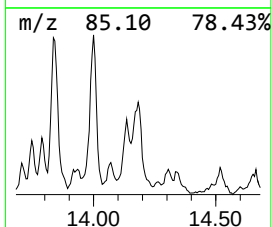
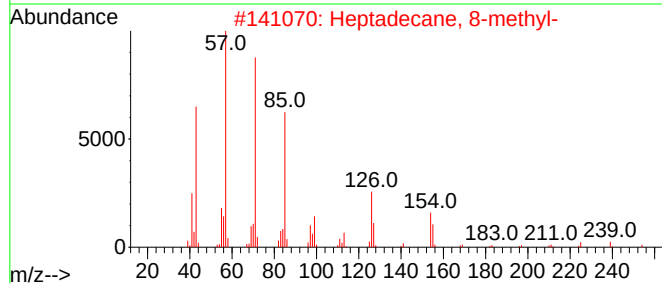
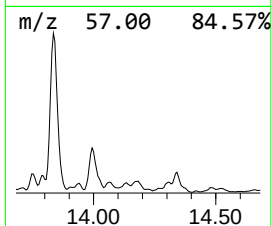
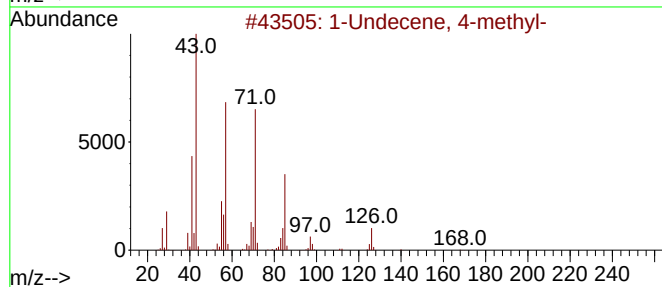
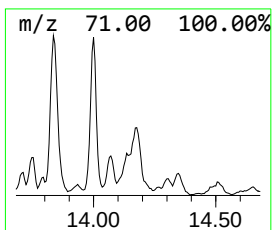
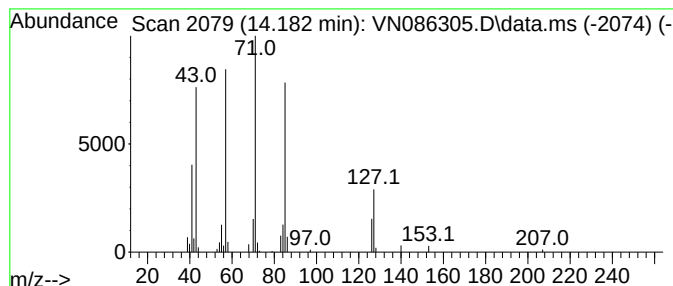
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Quant Title : SW846 8260

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

Peak Number 7 1-Undecene, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.182	10.48 ug/l	217106	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Undecene, 4-methyl-	168	C12H24	074630-39-0	72
2			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	72
3			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	72
4			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086305.D
Acq On : 16 Apr 2025 18:27
Operator : JC\MD
Sample : Q1791-14 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16164

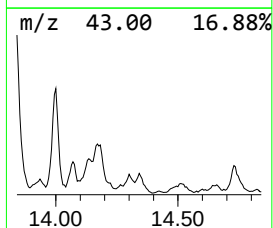
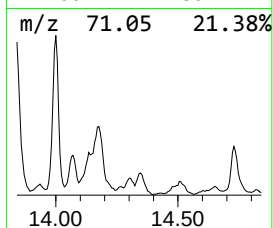
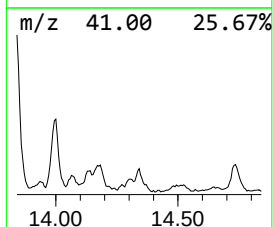
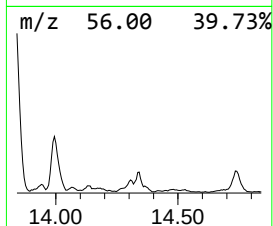
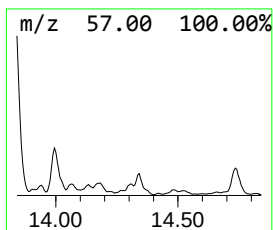
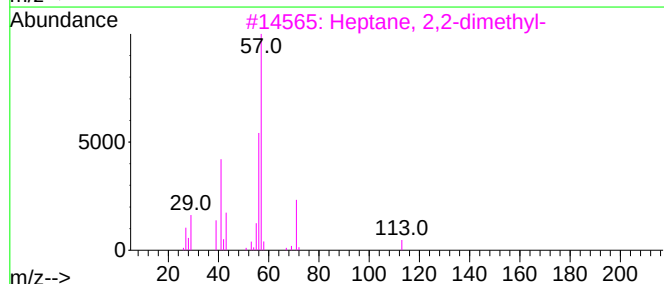
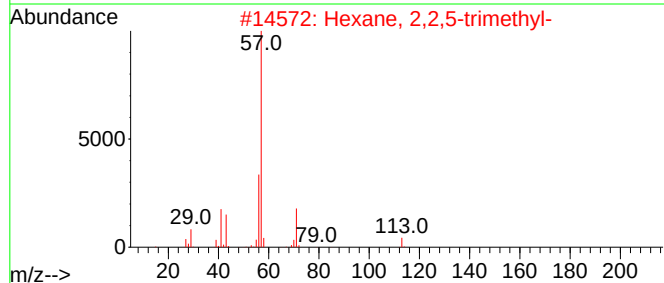
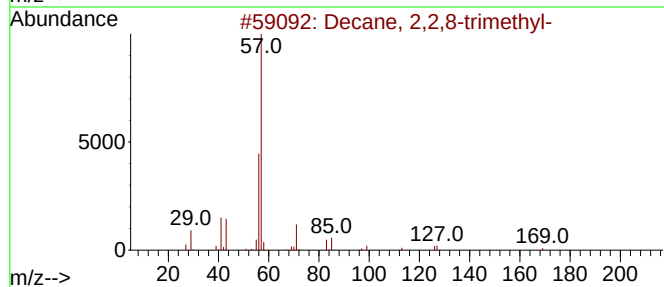
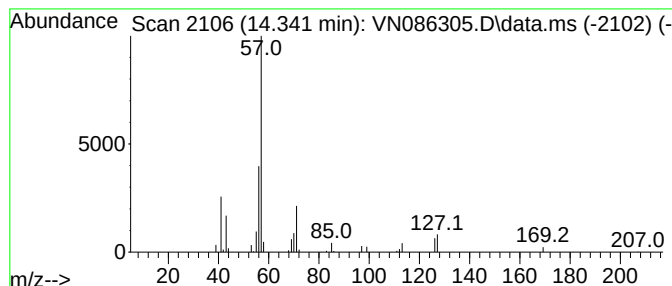
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Quant Title : SW846 8260

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

Peak Number 8 Decane, 2,2,8-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.341	5.95 ug/l	123337	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	72
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	64
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086305.D
Acq On : 16 Apr 2025 18:27
Operator : JC\MD
Sample : Q1791-14 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16164

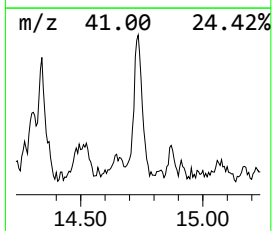
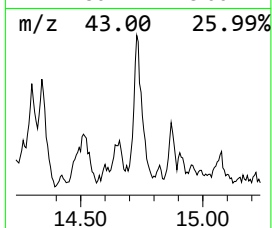
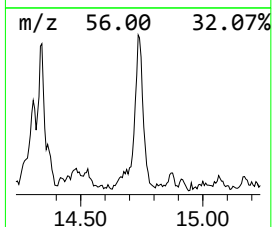
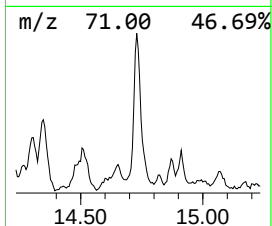
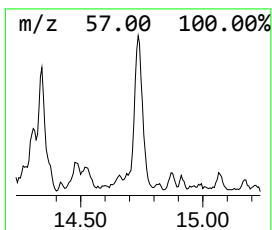
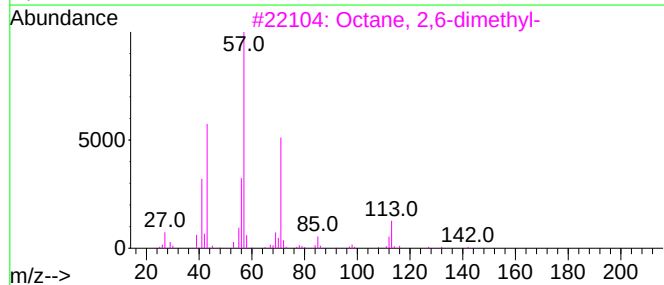
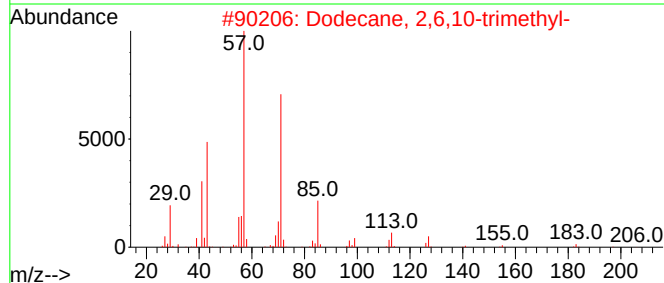
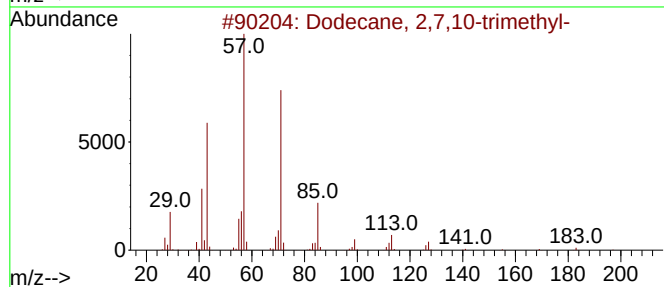
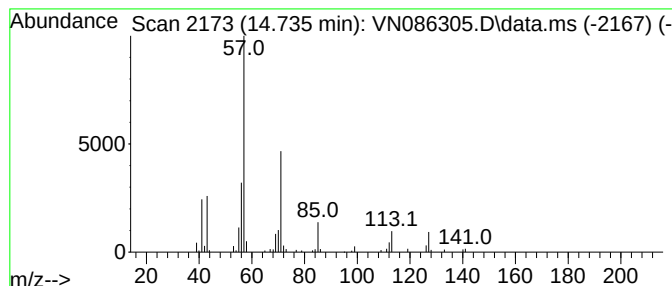
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.M
Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,7,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	8.73 ug/l	180888	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
2			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	72
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
4			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041625\
Data File : VN086305.D
Acq On : 16 Apr 2025 18:27
Operator : JC\MD
Sample : Q1791-14 10X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
VB16164

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041525W.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
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Dodecane, 2,2,1...	13.529	6.6	ug/l	136586	4	13.788	1036000	50.0
Heneicosane	13.641	28.9	ug/l	599859	4	13.788	1036000	50.0
Nonane, 2,6-dim...	13.994	23.0	ug/l	476894	4	13.788	1036000	50.0
Decane, 2,8,8-t...	14.070	5.6	ug/l	115279	4	13.788	1036000	50.0
Nonane, 5-butyl-	14.135	7.2	ug/l	148569	4	13.788	1036000	50.0
1-Undecene, 4-m...	14.182	10.5	ug/l	217106	4	13.788	1036000	50.0
Decane, 2,2,8-t...	14.341	6.0	ug/l	123337	4	13.788	1036000	50.0
Dodecane, 2,7,1...	14.735	8.7	ug/l	180888	4	13.788	1036000	50.0