

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
 Data File : VN081786.D
 Acq On : 18 Apr 2024 14:42
 Operator : JC\MD
 Sample : P2121-01 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1348

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\82N041524W.M

Title : SW846 8260

Signal : TIC: VN081786.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.812	140	146	151	rVB7	13197	26905	1.61%	0.224%
2	3.271	223	224	233	rVB4	11003	17050	1.02%	0.142%
3	8.165	1046	1056	1061	rBV	248953	614689	36.68%	5.125%
4	8.224	1061	1066	1079	rVB	457720	1012012	60.39%	8.438%
5	8.577	1118	1126	1139	rBV	238881	552174	32.95%	4.604%
6	9.100	1206	1215	1227	rBV	612266	1266275	75.57%	10.558%
7	10.571	1456	1465	1473	rBV	893145	1675725	100.00%	13.972%
8	11.865	1678	1685	1698	rVB	640035	1140829	68.08%	9.512%
9	12.853	1846	1853	1863	rVB	500149	885697	52.85%	7.385%
10	13.794	2005	2013	2020	rBV	636274	1113473	66.45%	9.284%
11	14.106	2061	2066	2071	rVV	44506	62186	3.71%	0.519%
12	14.335	2097	2105	2107	rBV9	10612	21804	1.30%	0.182%
13	14.370	2107	2111	2117	rVB7	14662	25294	1.51%	0.211%
14	14.588	2143	2148	2151	rBV5	25371	44450	2.65%	0.371%
15	14.623	2151	2154	2158	rVV5	31066	42900	2.56%	0.358%
16	14.664	2158	2161	2166	rVB3	25644	31593	1.89%	0.263%
17	14.729	2169	2172	2176	rBV3	32211	47449	2.83%	0.396%
18	14.782	2176	2181	2182	rBV5	13312	20868	1.25%	0.174%
19	14.958	2205	2211	2217	rBV	278505	433747	25.88%	3.617%
20	15.029	2219	2223	2224	rBV	38218	36124	2.16%	0.301%
21	15.076	2228	2231	2235	rBV2	62862	98925	5.90%	0.825%
22	15.323	2268	2273	2279	rBV7	35651	67724	4.04%	0.565%
23	15.423	2284	2290	2293	rBV8	38128	81694	4.88%	0.681%
24	15.511	2301	2305	2312	rVB7	82211	168598	10.06%	1.406%
25	15.594	2313	2319	2328	rBV	137271	286206	17.08%	2.386%
26	15.829	2353	2359	2370	rVB	532714	1044684	62.34%	8.711%
27	15.953	2371	2380	2385	rBV9	84953	253909	15.15%	2.117%
28	16.017	2389	2391	2397	rVB6	44867	75262	4.49%	0.628%
29	16.170	2412	2417	2420	rBV4	68923	129568	7.73%	1.080%
30	16.317	2437	2442	2445	rBV5	52196	97681	5.83%	0.814%
31	16.464	2462	2467	2470	rBV4	65194	138383	8.26%	1.154%
32	16.547	2477	2481	2487	rVB5	89362	164068	9.79%	1.368%
33	16.611	2488	2492	2500	rVB3	109080	215030	12.83%	1.793%
34	16.705	2505	2508	2514	rVB3	52668	100210	5.98%	0.836%

Sum of corrected areas: 11993186

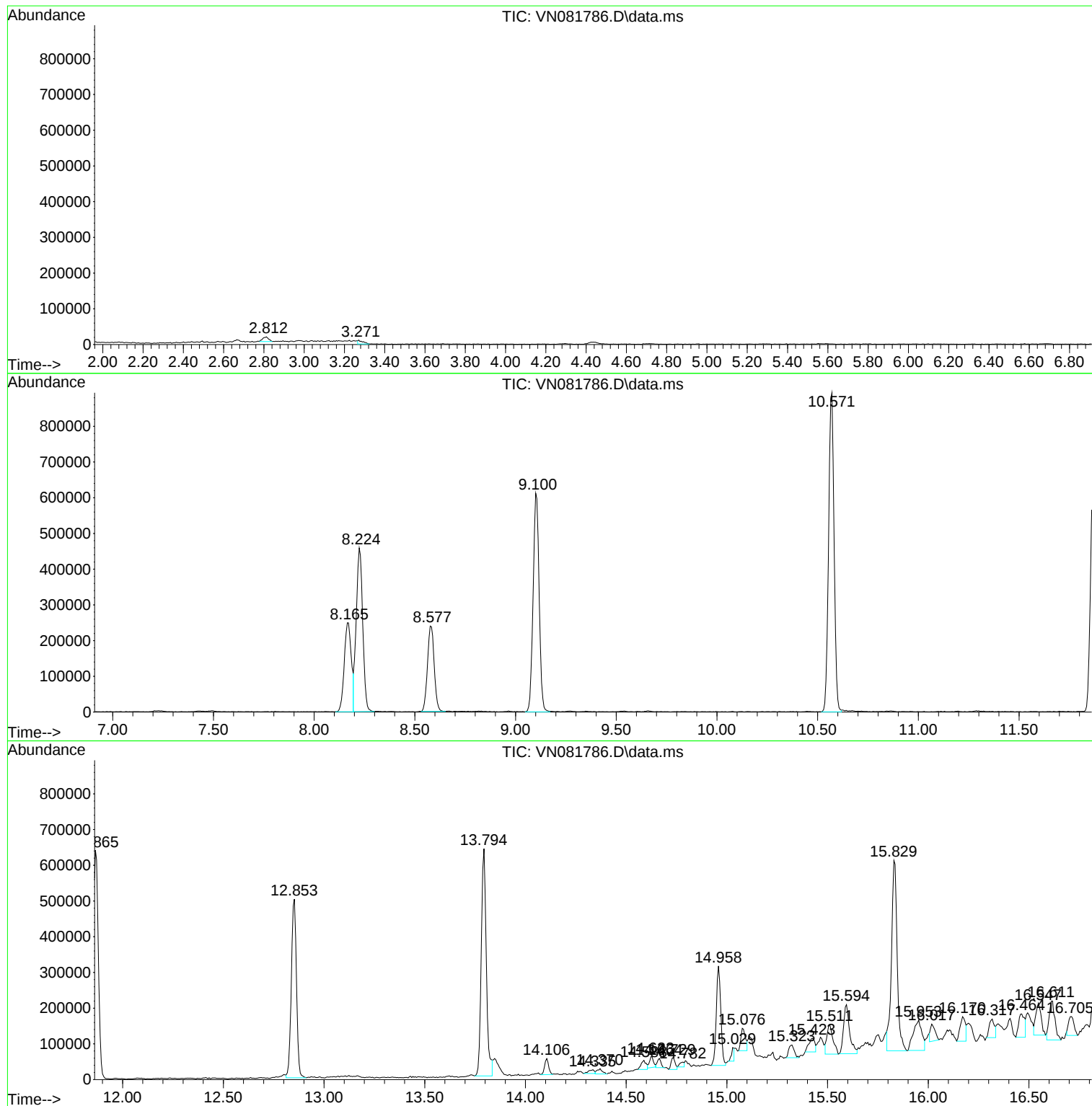
Instrument :
MSVOA_N
ClientSampleId :
1348

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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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



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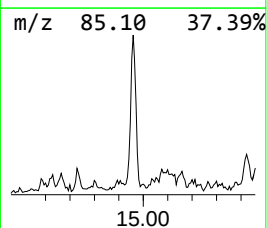
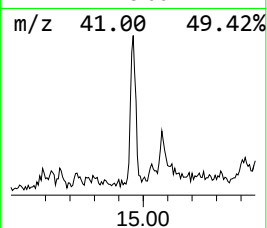
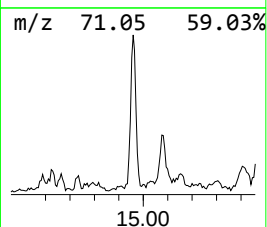
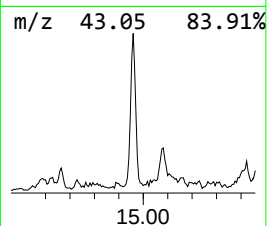
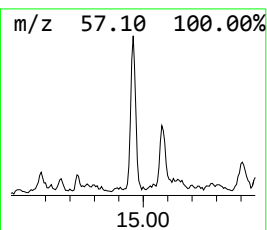
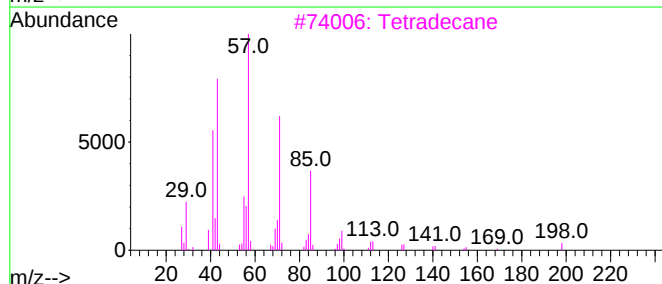
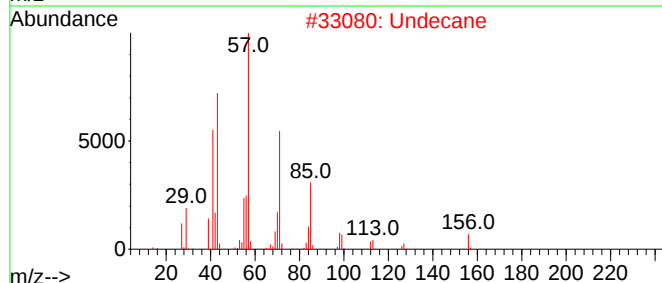
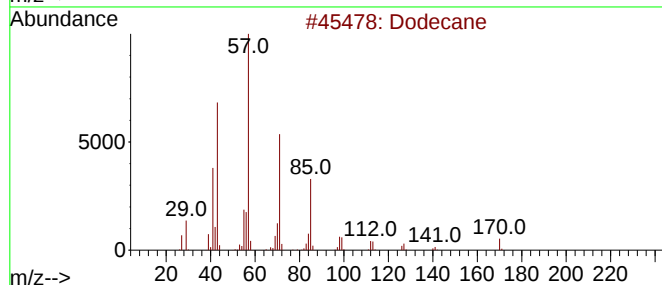
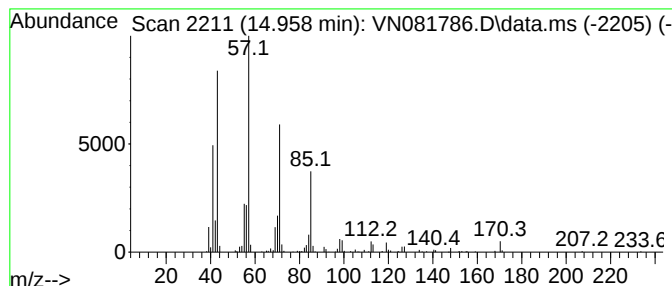
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Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	19.48 ug/l	433747	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Undecane	156	C11H24	001120-21-4	86
3			Tetradecane	198	C14H30	000629-59-4	80
4			Hexadecane	226	C16H34	000544-76-3	80
5			Tridecane	184	C13H28	000629-50-5	72



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ClientSampleId :
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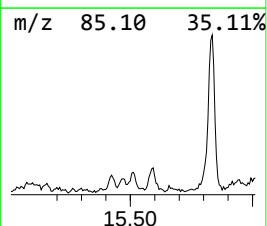
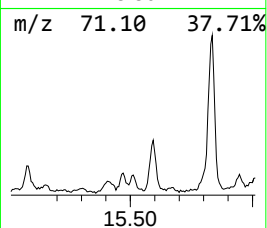
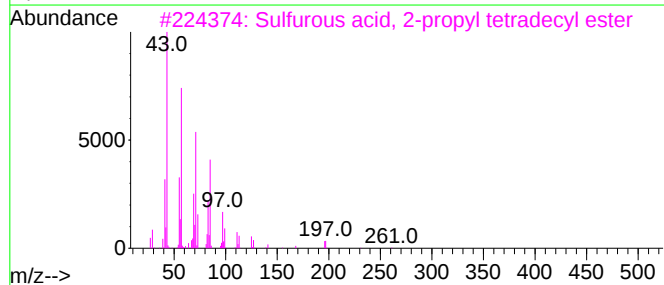
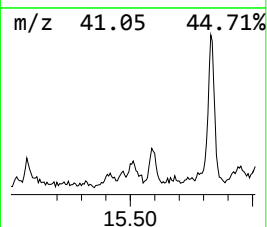
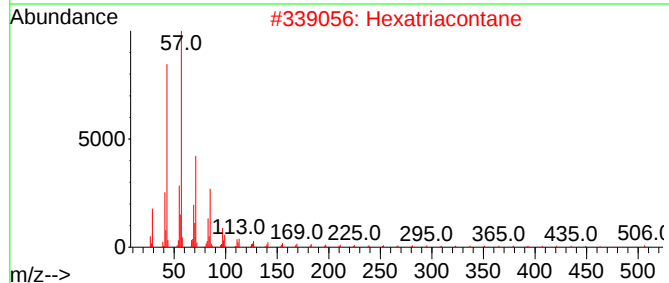
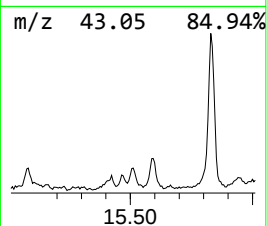
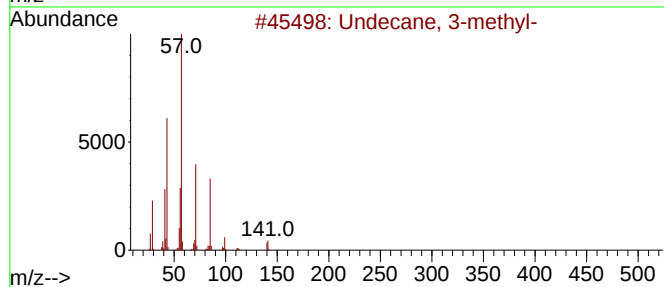
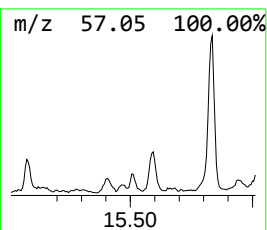
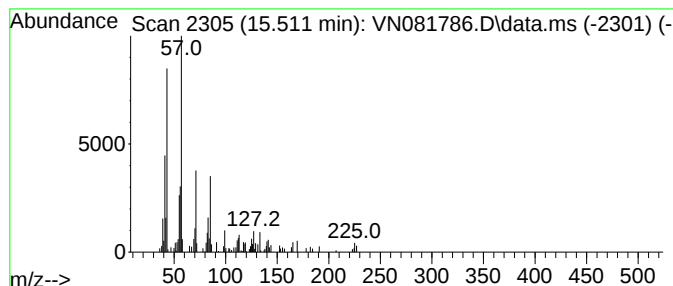
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.511	7.57 ug/l	168598	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3-methyl-	170	C12H26	001002-43-3	59
2			Hexatriacontane	507	C36H74	000630-06-8	50
3			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	49
4			Undecane, 3,4-dimethyl-	184	C13H28	017312-78-6	47
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	46



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

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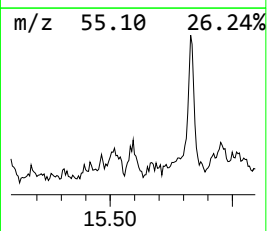
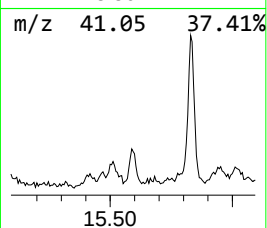
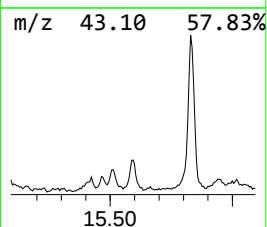
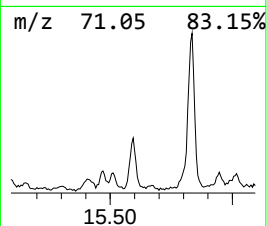
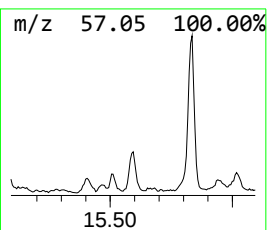
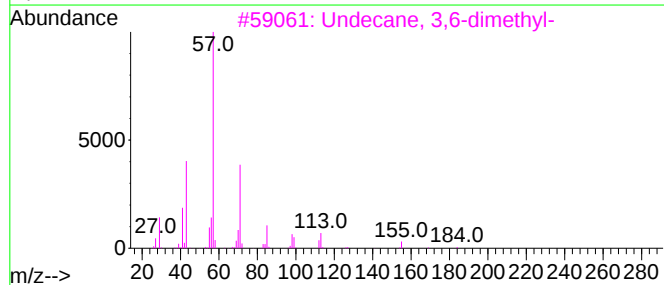
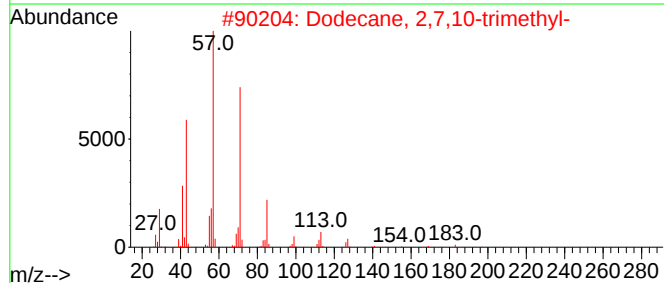
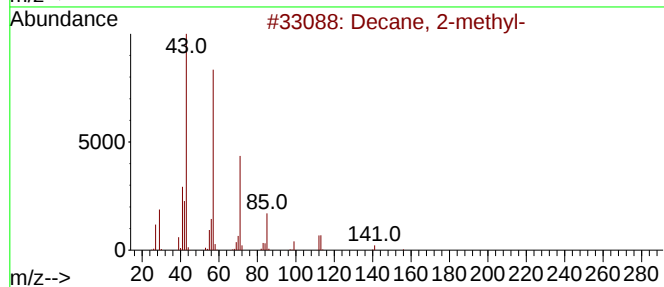
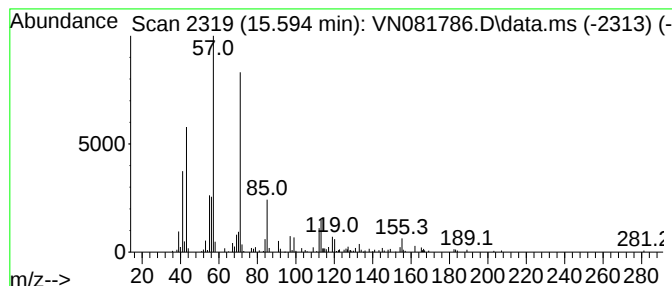
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 3 Decane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.594	12.85 ug/l	286206	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2-methyl-	156	C11H24	006975-98-0	72
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
4			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	59
5			Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
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Acq On : 18 Apr 2024 14:42
Operator : JC\MD
Sample : P2121-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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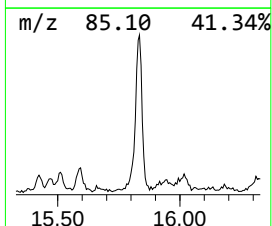
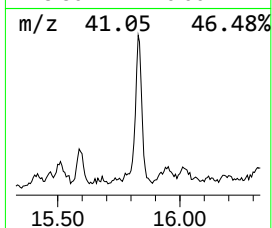
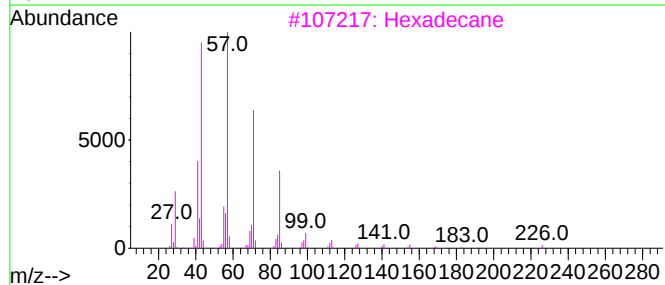
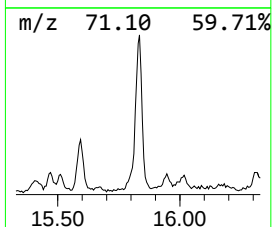
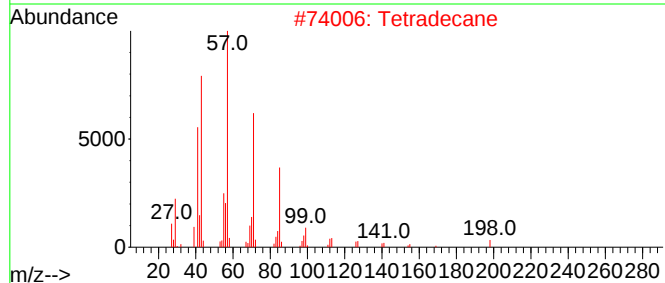
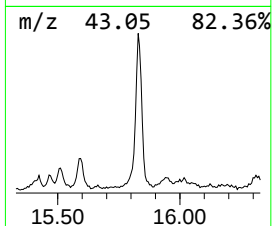
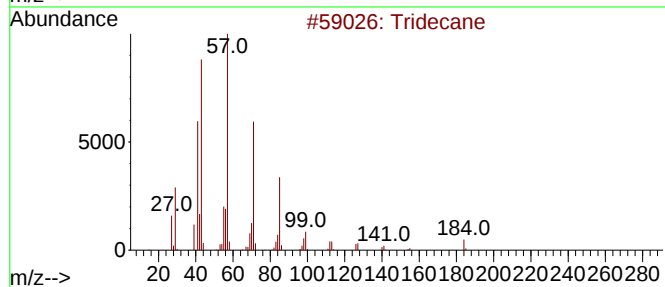
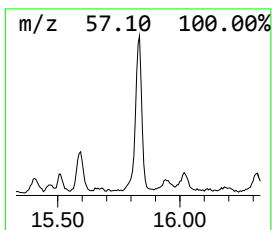
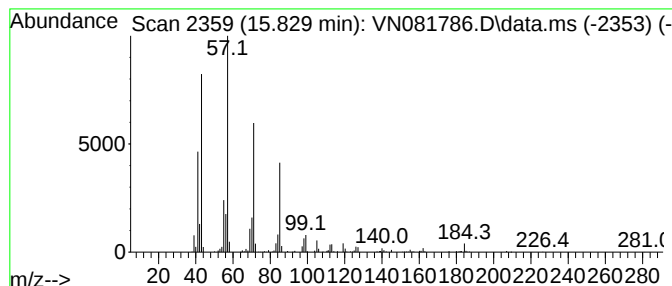
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Quant Title : SW846 8260

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

Peak Number 4 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	46.91 ug/l	1044680	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Tetradecane	198	C14H30	000629-59-4	87
3			Hexadecane	226	C16H34	000544-76-3	80
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
5			Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	80



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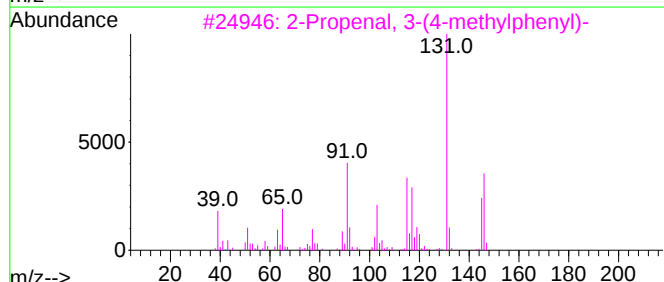
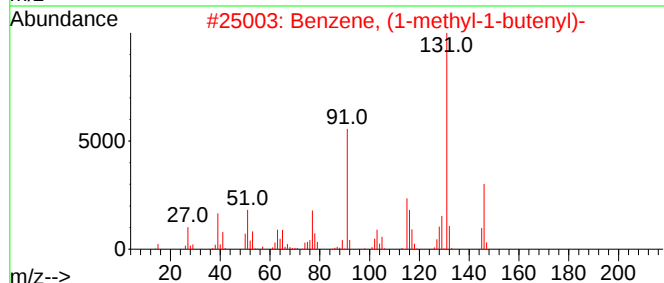
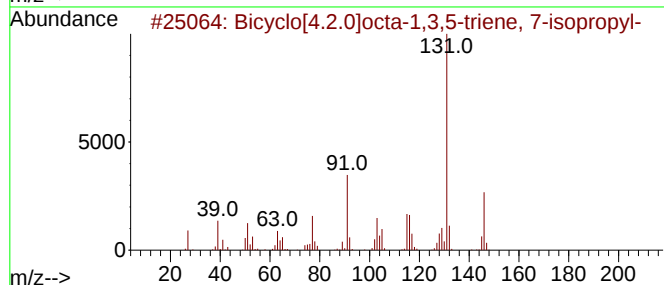
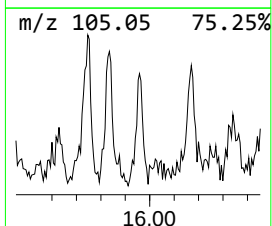
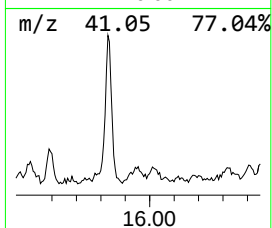
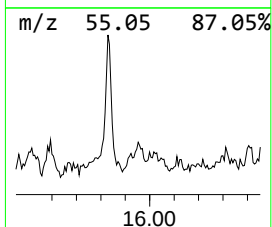
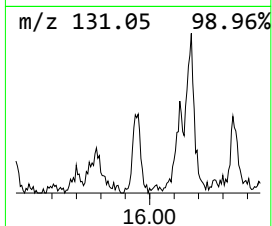
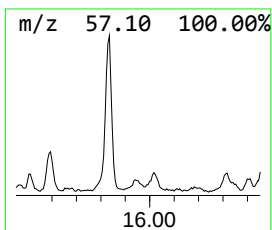
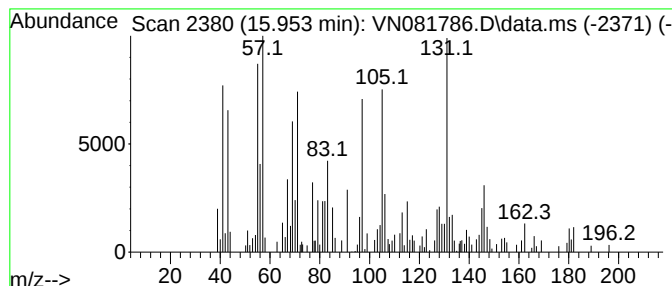
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown15.953 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.953	11.40 ug/l	253909	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.2.0]octa-1,3,5-triene,...	146	C11H14	027087-54-3	20
2			Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	20
3			2-Propenal, 3-(4-methylphenyl)-	146	C10H10O	001504-75-2	20
4			Ethyl-2-benzofuran	146	C10H10O	003131-63-3	18
5			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	18



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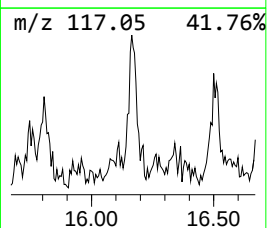
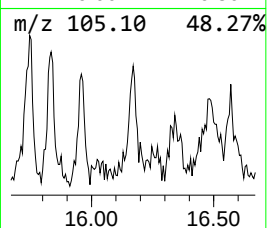
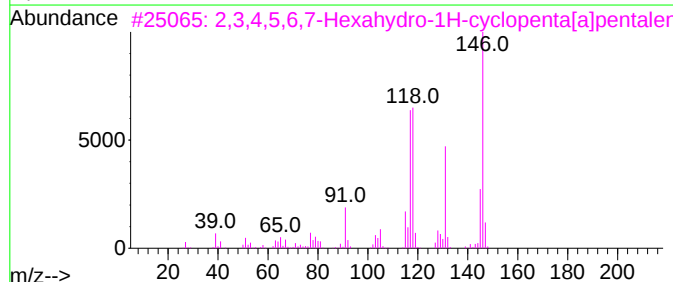
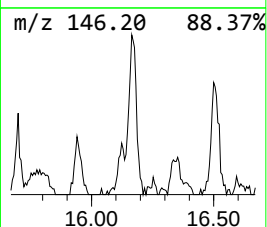
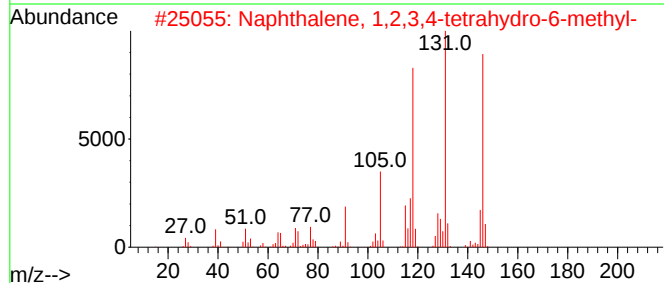
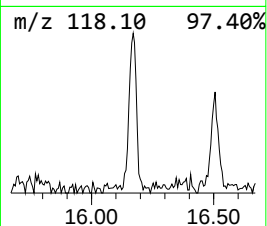
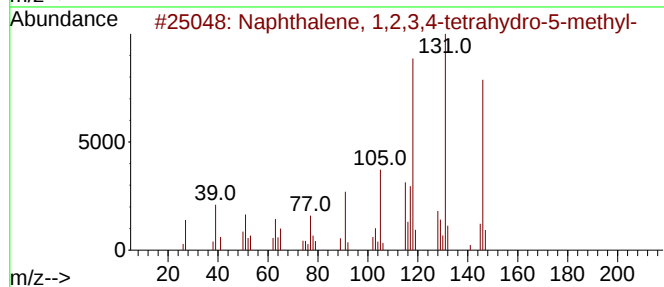
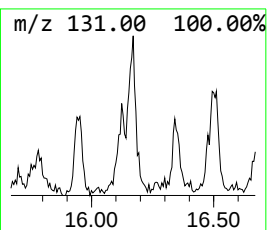
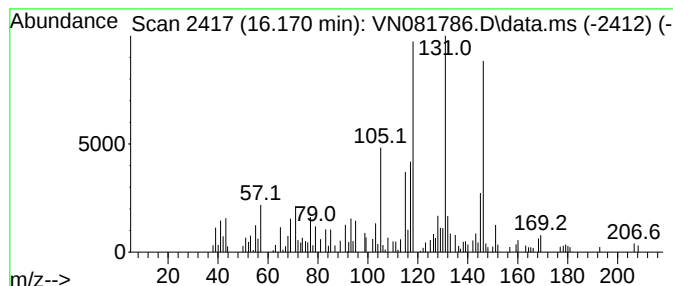
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	5.82 ug/l	129568	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	91
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	87
3			2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1010189-31-0	83
4			1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	80
5			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081786.D
Acq On : 18 Apr 2024 14:42
Operator : JC\MD
Sample : P2121-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1348

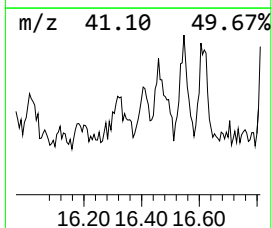
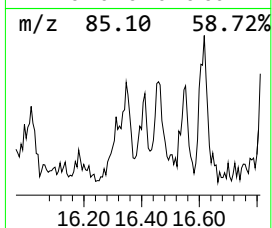
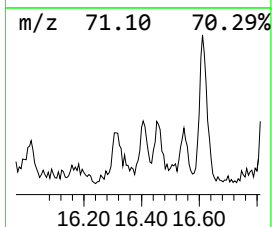
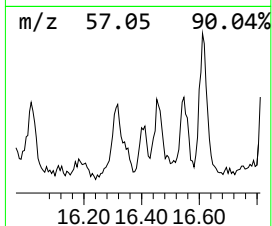
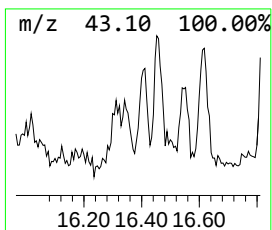
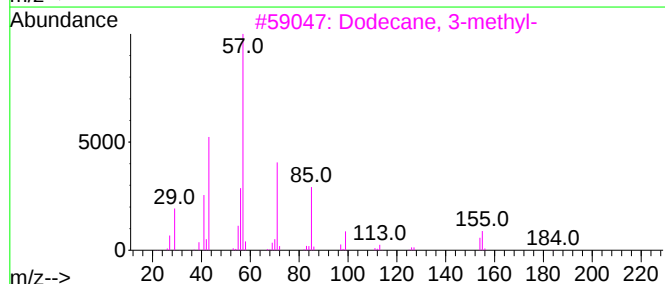
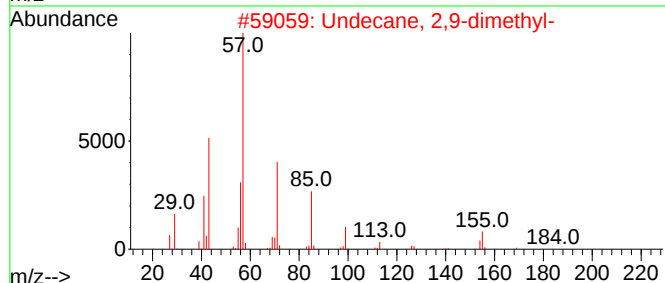
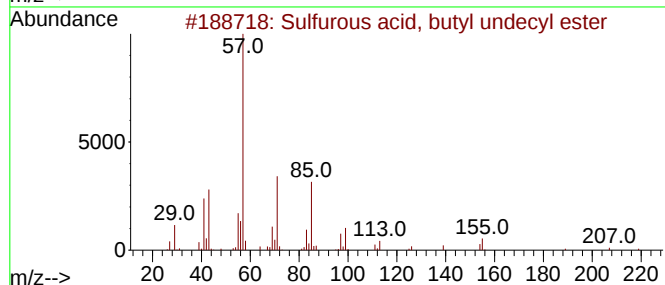
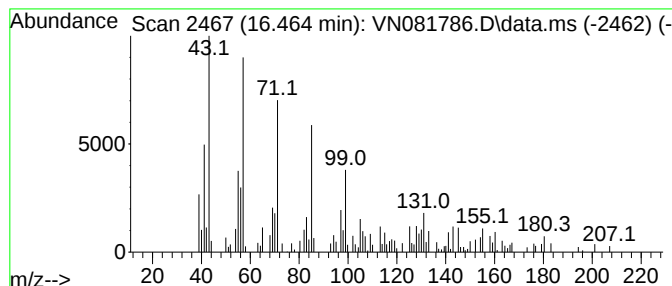
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Quant Title : SW846 8260

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

Peak Number 7 unknown16.464 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.464	6.21 ug/l	138383	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	49
2			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	47
3			Dodecane, 3-methyl-	184	C13H28	017312-57-1	43
4			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	38
5			4-Octanone	128	C8H16O	000589-63-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081786.D
Acq On : 18 Apr 2024 14:42
Operator : JC\MD
Sample : P2121-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1348

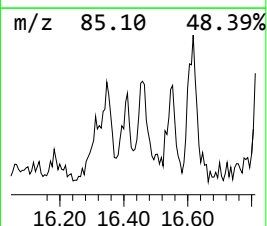
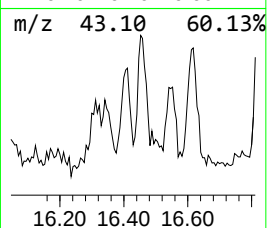
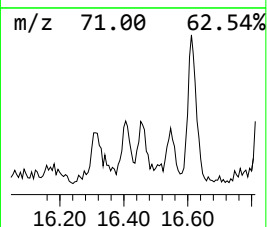
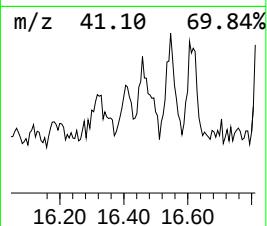
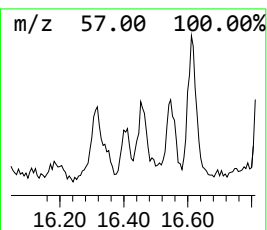
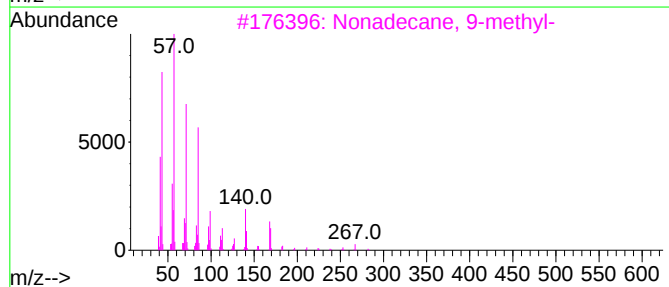
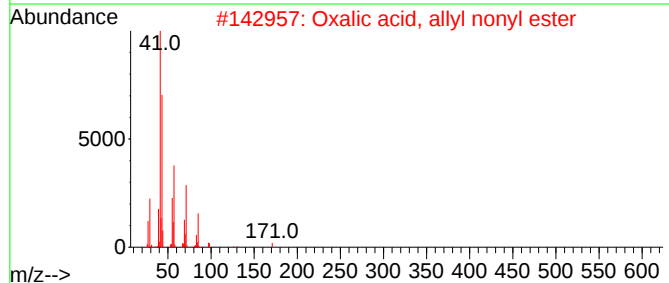
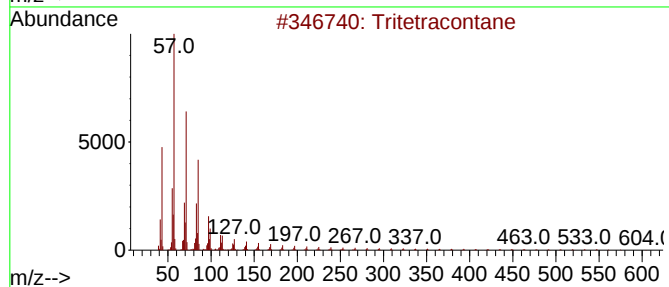
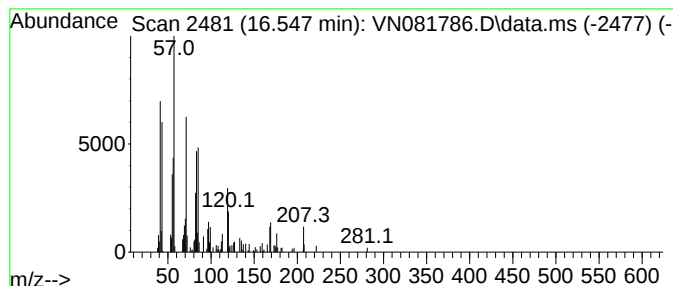
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Quant Title : SW846 8260

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

Peak Number 8 unknown16.547 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.547	7.37 ug/l	164068	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	38
2			Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	38
3			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	38
4			Hexacosane	366	C26H54	000630-01-3	38
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081786.D
Acq On : 18 Apr 2024 14:42
Operator : JC\MD
Sample : P2121-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1348

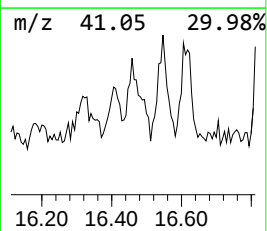
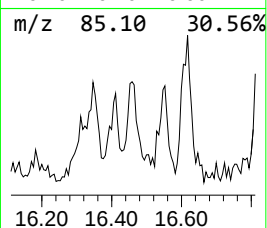
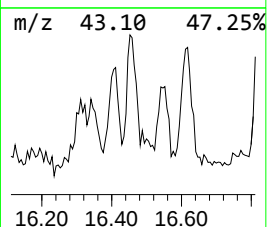
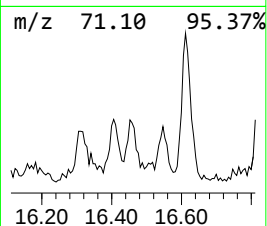
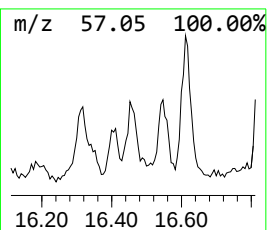
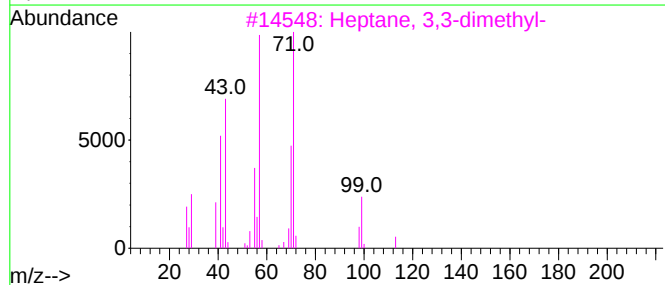
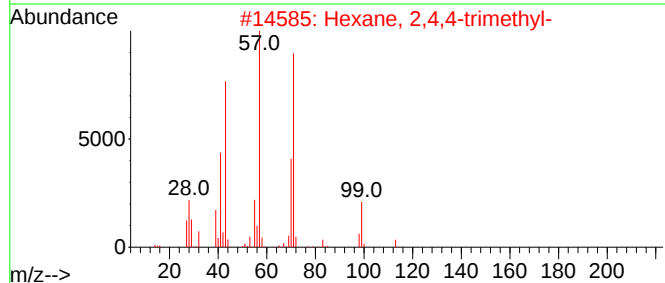
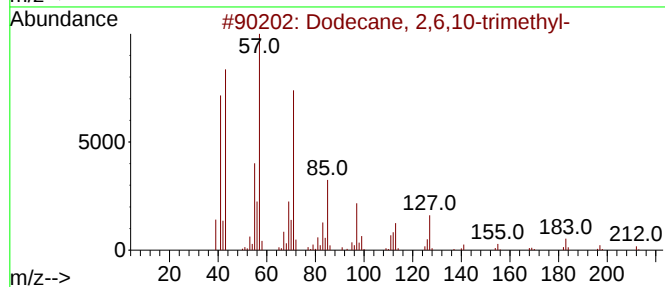
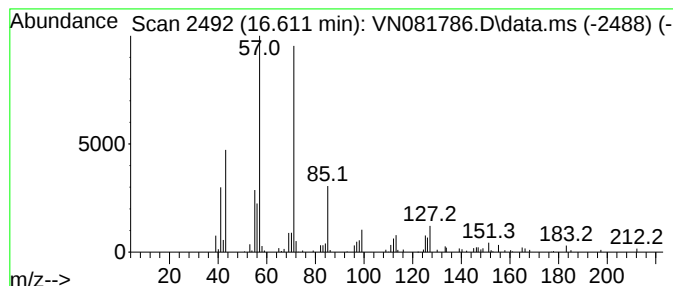
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.M
Quant Title : SW846 8260

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

Peak Number 9 Dodecane, 2,6,10-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.611	9.66 ug/l	215030	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	53
2			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	50
3			Heptane, 3,3-dimethyl-	128	C9H20	004032-86-4	50
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	47
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041824\
Data File : VN081786.D
Acq On : 18 Apr 2024 14:42
Operator : JC\MD
Sample : P2121-01 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1348

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N041524W.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
Dodecane	14.959	19.5	ug/l	433747	4	13.794	1113470	50.0
Undecane, 3-met...	15.511	7.6	ug/l	168598	4	13.794	1113470	50.0
Decane, 2-methyl-	15.594	12.9	ug/l	286206	4	13.794	1113470	50.0
Tridecane	15.829	46.9	ug/l	1044680	4	13.794	1113470	50.0
unknown15.953	15.953	11.4	ug/l	253909	4	13.794	1113470	50.0
Naphthalene, 1,...	16.170	5.8	ug/l	129568	4	13.794	1113470	50.0
unknown16.464	16.464	6.2	ug/l	138383	4	13.794	1113470	50.0
unknown16.547	16.547	7.4	ug/l	164068	4	13.794	1113470	50.0
Dodecane, 2,6,1...	16.611	9.7	ug/l	215030	4	13.794	1113470	50.0