

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN043024\
 Data File : VN081924.D
 Acq On : 30 Apr 2024 12:20
 Operator : JC\MD
 Sample : P2183-04 20X
 Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1241

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\82N042524W.M
 Title : SW846 8260

Signal : TIC: VN081924.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.430	923	931	936	rBV	6603	18094	1.20%	0.174%
2	8.165	1047	1056	1061	rBV2	175776	433751	28.89%	4.162%
3	8.224	1061	1066	1075	rVB	321107	725841	48.34%	6.964%
4	8.577	1117	1126	1138	rBV	221105	488170	32.51%	4.684%
5	9.100	1205	1215	1228	rBV	521731	1070763	71.31%	10.273%
6	10.565	1456	1464	1471	rBV	797311	1501614	100.00%	14.407%
7	10.629	1471	1475	1487	rVB	88997	164592	10.96%	1.579%
8	11.865	1676	1685	1696	rBV	712951	1283587	85.48%	12.315%
9	11.965	1696	1702	1709	rVB2	19766	33912	2.26%	0.325%
10	12.070	1713	1720	1727	rBV2	48694	96921	6.45%	0.930%
11	12.394	1768	1775	1781	rBV2	13625	28167	1.88%	0.270%
12	12.847	1844	1852	1862	rBV	530381	910496	60.63%	8.736%
13	13.794	2002	2013	2022	rBV	652794	1112282	74.07%	10.672%
14	14.106	2060	2066	2072	rBV2	28952	44955	2.99%	0.431%
15	14.582	2138	2147	2150	rBV4	27283	56781	3.78%	0.545%
16	14.629	2150	2155	2158	rVV5	49937	78287	5.21%	0.751%
17	14.664	2158	2161	2165	rVV2	32061	42501	2.83%	0.408%
18	14.729	2168	2172	2179	rBV2	31824	52385	3.49%	0.503%
19	14.794	2179	2183	2187	rVB7	12895	20285	1.35%	0.195%
20	14.841	2188	2191	2196	rVB7	13619	20798	1.39%	0.200%
21	14.906	2196	2202	2205	rBV7	8578	18189	1.21%	0.175%
22	14.959	2205	2211	2220	rBV	323269	509478	33.93%	4.888%
23	15.041	2220	2225	2227	rBV3	32263	52103	3.47%	0.500%
24	15.082	2227	2232	2242	rVB4	82385	199887	13.31%	1.918%
25	15.229	2254	2257	2260	rBV4	18825	24753	1.65%	0.237%
26	15.259	2260	2262	2267	rVB6	21000	32245	2.15%	0.309%
27	15.417	2279	2289	2294	rBV5	61735	185387	12.35%	1.779%
28	15.470	2294	2298	2301	rVV5	41375	63406	4.22%	0.608%
29	15.511	2301	2305	2313	rVB4	71121	184473	12.28%	1.770%
30	15.588	2313	2318	2327	rVB2	107711	234140	15.59%	2.246%
31	15.670	2327	2332	2334	rBV5	35717	53789	3.58%	0.516%
32	15.835	2354	2360	2370	rVB	313102	558800	37.21%	5.361%
33	15.923	2370	2375	2376	rBV5	24086	31927	2.13%	0.306%
34	16.306	2437	2440	2445	rVB7	15224	23489	1.56%	0.225%
35	16.411	2452	2458	2461	rBV8	18857	33053	2.20%	0.317%
36	16.511	2470	2475	2476	rBV4	22422	33357	2.22%	0.320%

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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\82N042524W.M

Title : SW846 8260

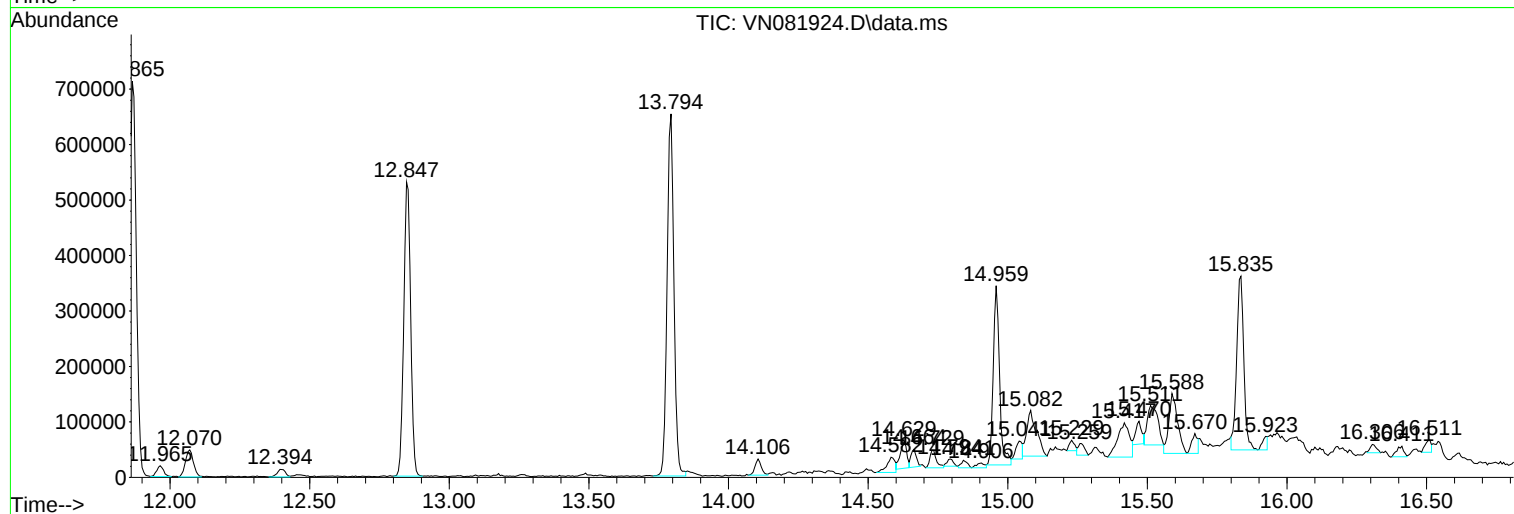
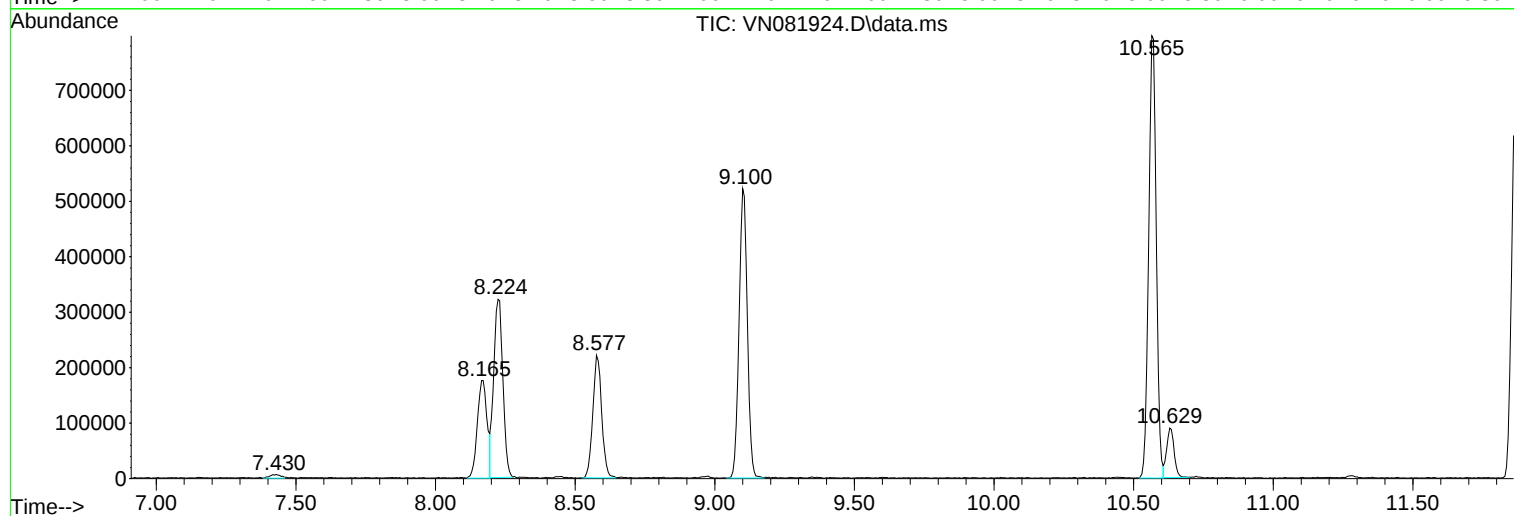
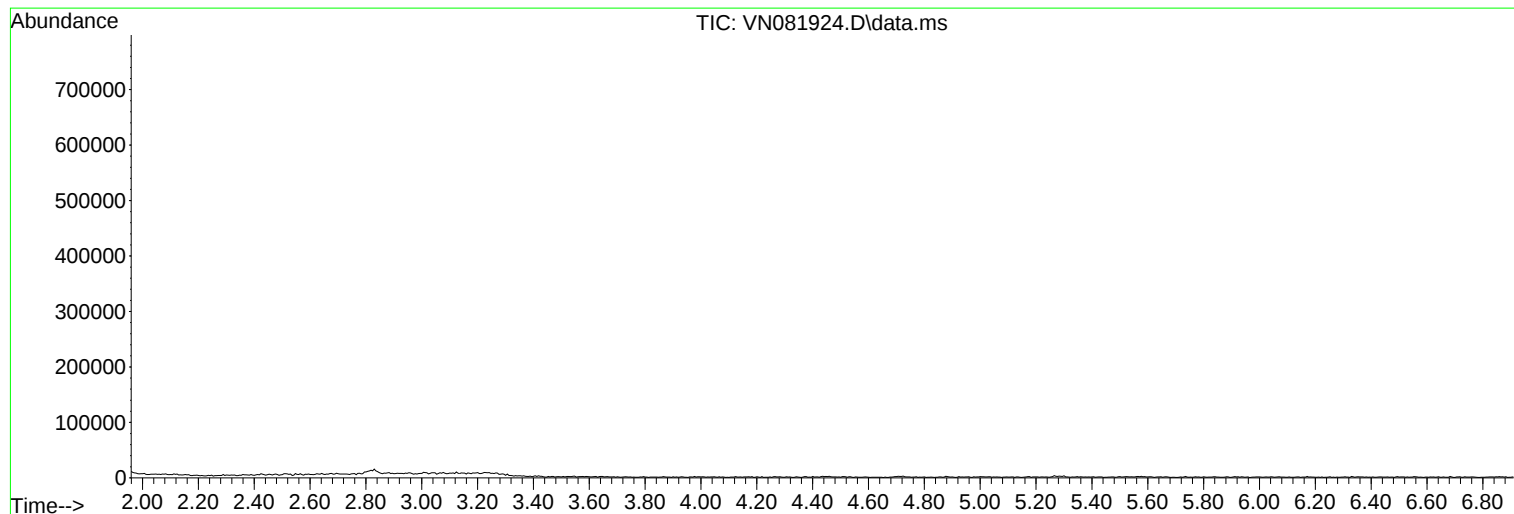
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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



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Instrument :
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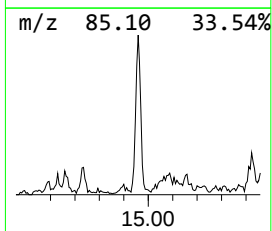
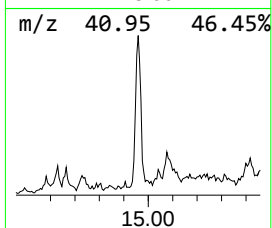
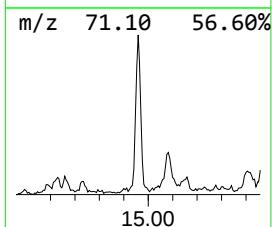
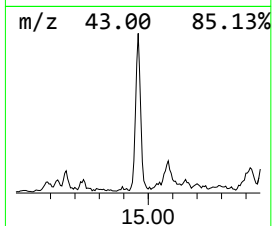
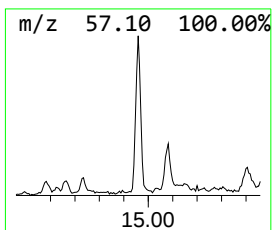
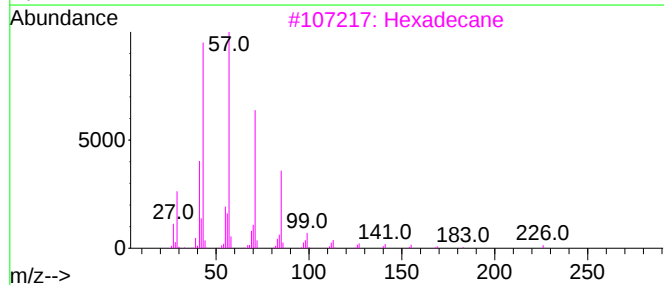
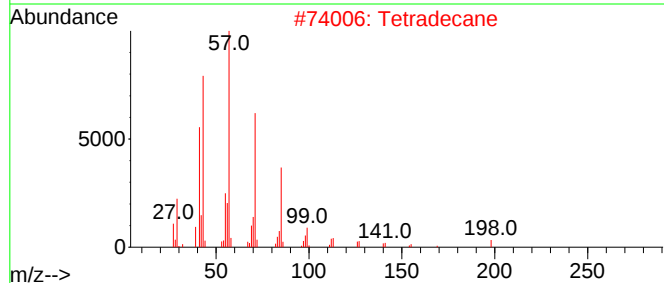
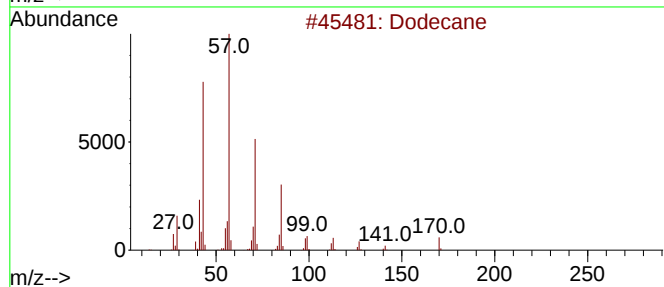
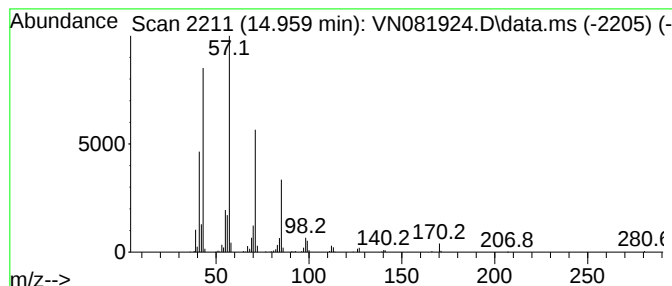
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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	22.90 ug/l	509478	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Tetradecane	198	C14H30	000629-59-4	90
3			Hexadecane	226	C16H34	000544-76-3	90
4			Tridecane	184	C13H28	000629-50-5	90
5			Undecane	156	C11H24	001120-21-4	83



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ALS Vial : 7 Sample Multiplier: 1

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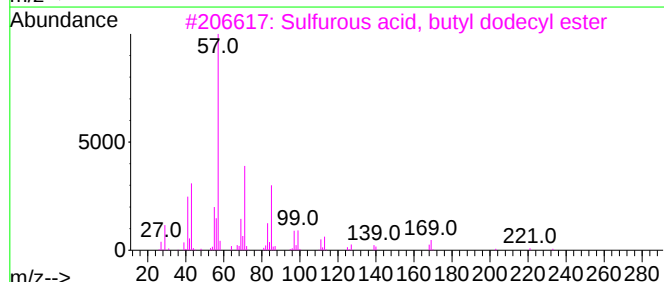
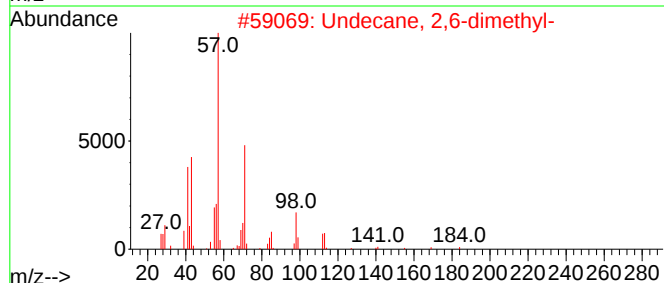
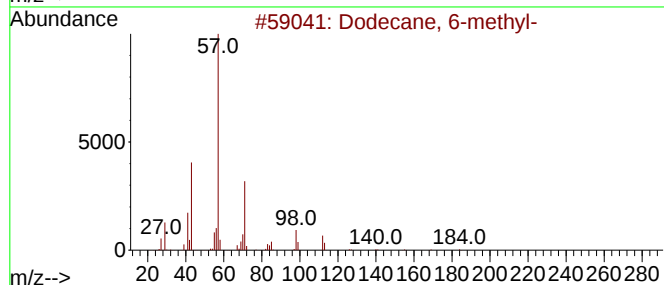
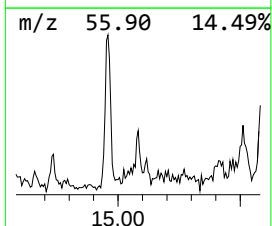
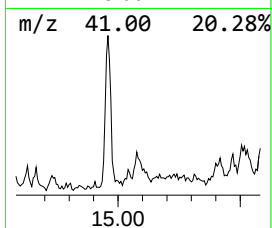
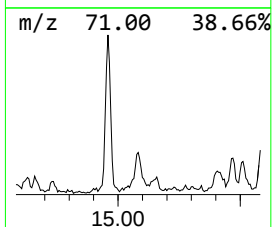
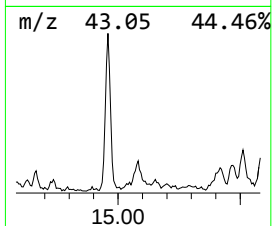
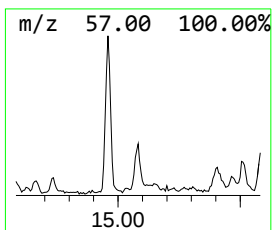
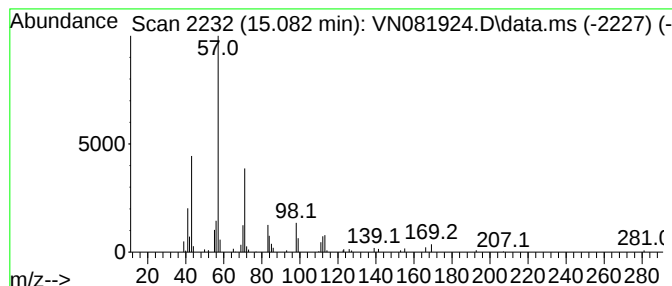
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecane, 6-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.082	8.99 ug/l	199887	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 6-methyl-	184	C13H28	006044-71-9	80
2		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	72
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
4		Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	59
5		Tetratetracontane	619	C44H90	007098-22-8	59



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Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
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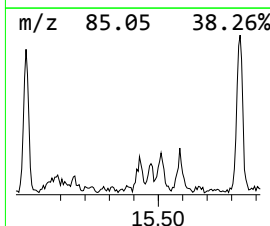
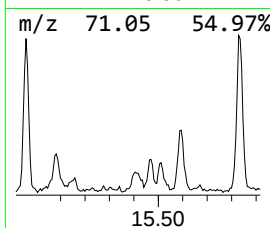
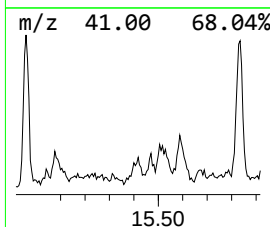
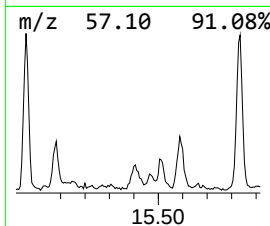
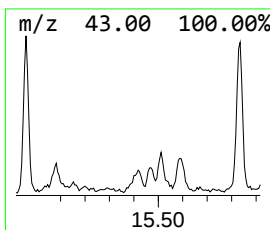
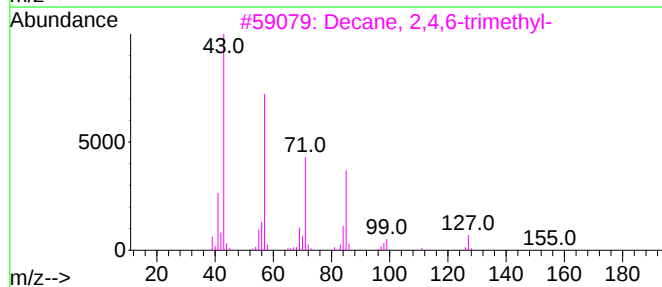
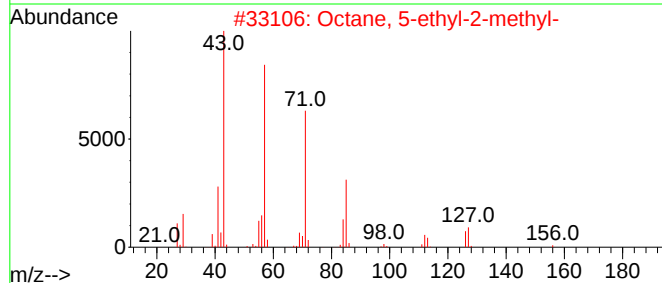
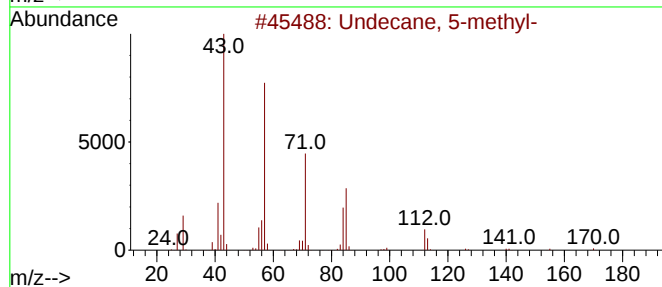
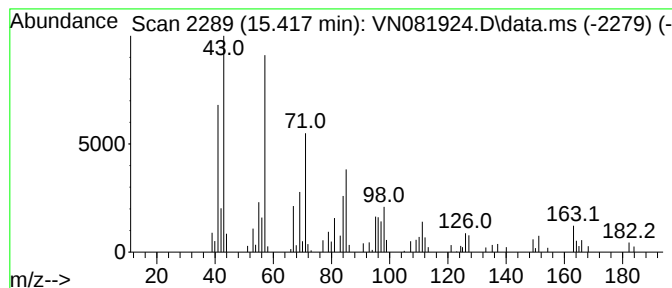
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown15.417 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.417	8.33 ug/l	185387	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5-methyl-	170	C12H26	001632-70-8	38
2			Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	38
3			Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	38
4			Undecane, 3,7-dimethyl-	184	C13H28	017301-29-0	38
5			Tridecane	184	C13H28	000629-50-5	38



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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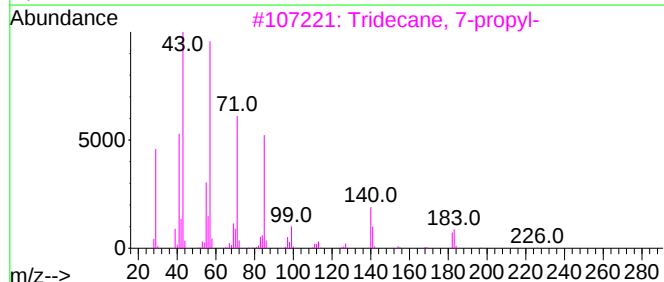
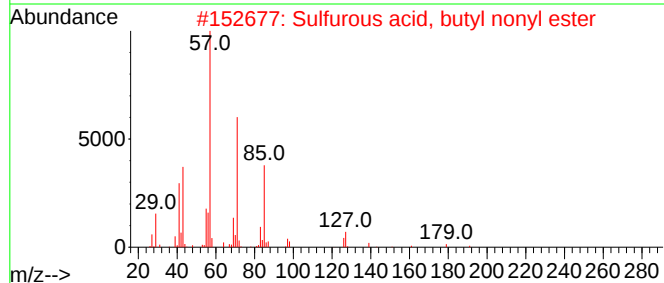
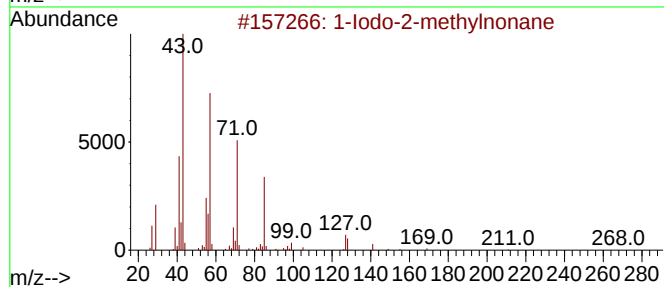
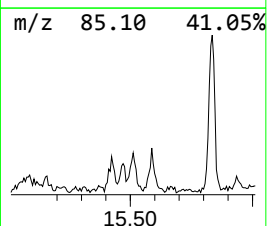
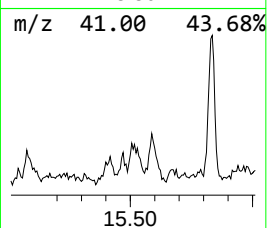
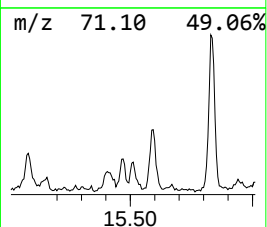
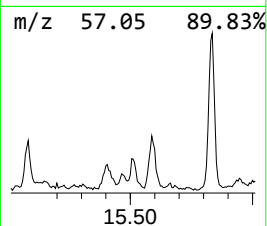
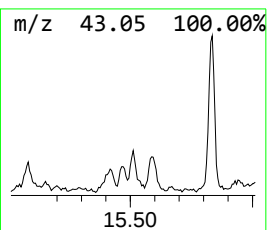
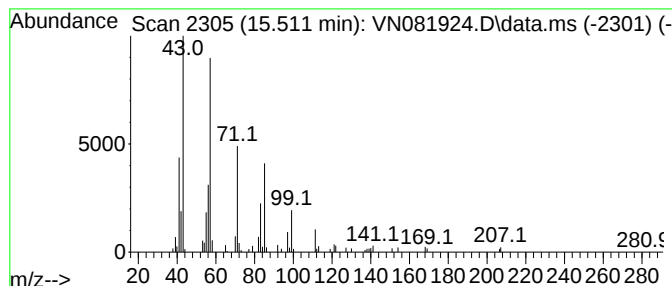
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown15.511 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.511	8.29 ug/l	184473	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	47
2		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47
3		Tridecane, 7-propyl-	226	C16H34	055045-09-5	47
4		Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	47
5		Decane, 1-iodo-	268	C10H21I	002050-77-3	43



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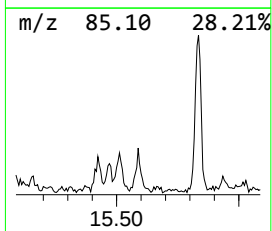
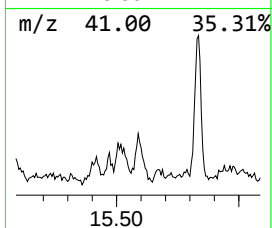
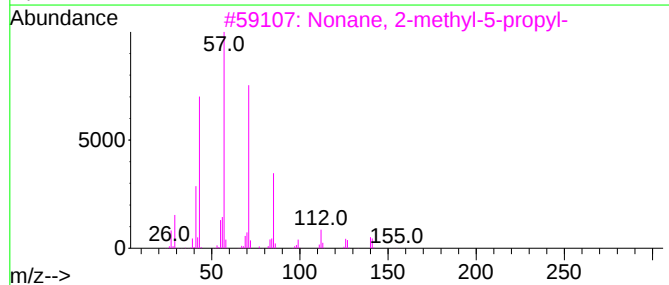
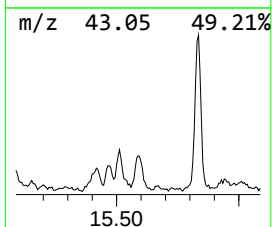
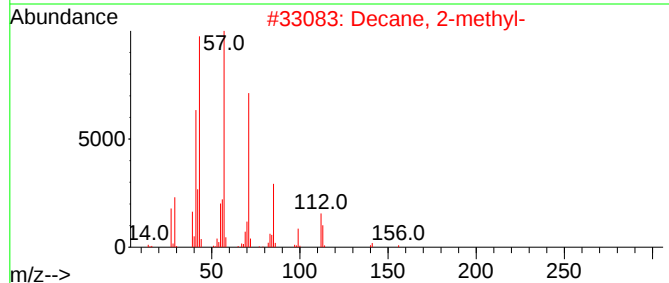
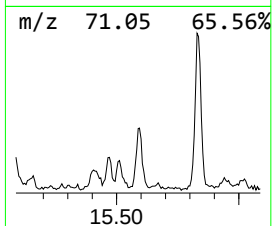
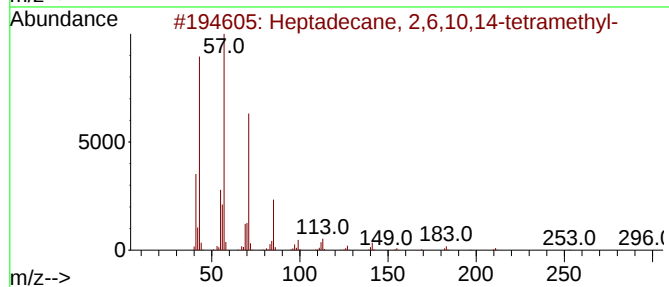
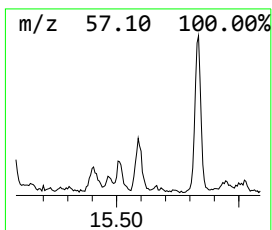
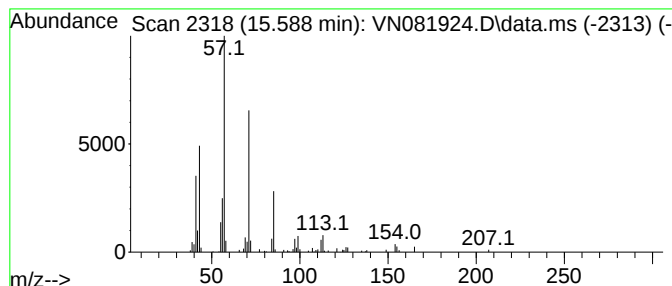
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Quant Title : SW846 8260

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

Peak Number 5 Heptadecane, 2,6,10,14-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.588	10.53 ug/l	234140	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	83
2			Decane, 2-methyl-	156	C11H24	006975-98-0	72
3			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
4			Bacchotricuneatin c	342	C20H22O5	066563-30-2	59
5			Undecane	156	C11H24	001120-21-4	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN043024\
Data File : VN081924.D
Acq On : 30 Apr 2024 12:20
Operator : JC\MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1241

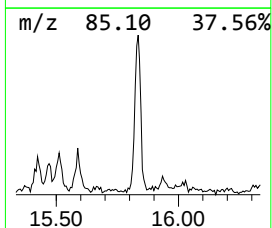
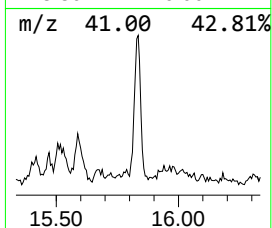
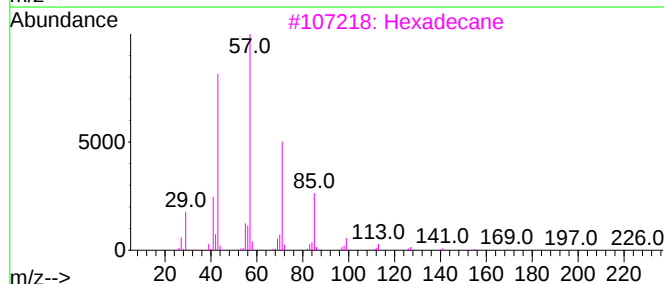
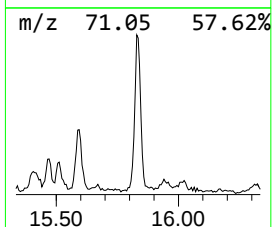
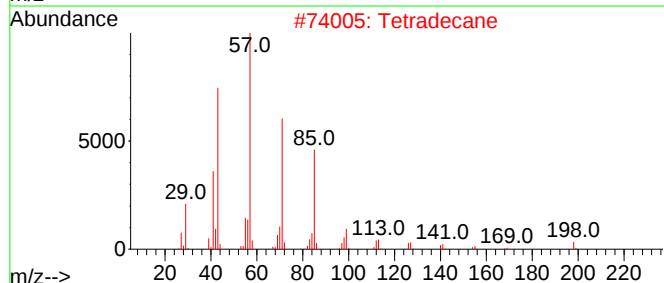
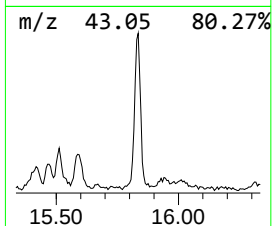
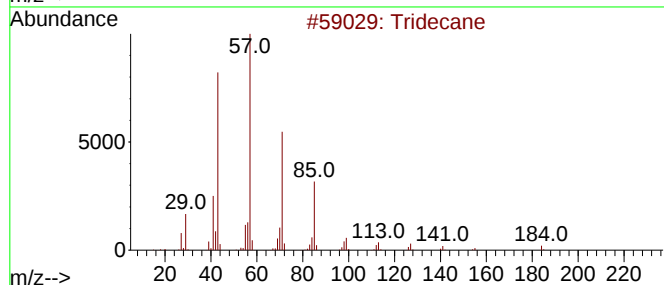
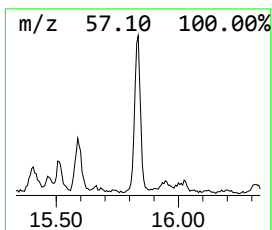
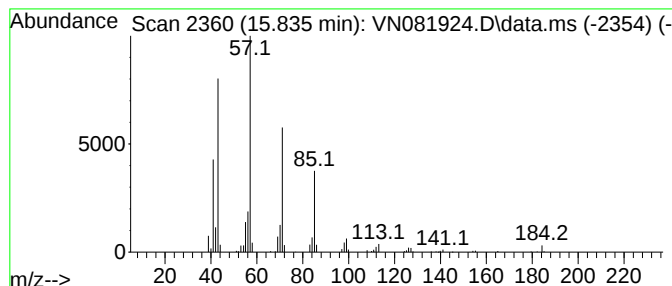
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.M
Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	25.12 ug/l	558800	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	94
2			Tetradecane	198	C14H30	000629-59-4	90
3			Hexadecane	226	C16H34	000544-76-3	90
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5			Dodecane	170	C12H26	000112-40-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN043024\
Data File : VN081924.D
Acq On : 30 Apr 2024 12:20
Operator : JC\MD
Sample : P2183-04 20X
Misc : 1.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042524W.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
Dodecane	14.959	22.9	ug/l	509478	4	13.794	1112280	50.0
Dodecane, 6-met...	15.082	9.0	ug/l	199887	4	13.794	1112280	50.0
unknown15.417	15.417	8.3	ug/l	185387	4	13.794	1112280	50.0
unknown15.511	15.511	8.3	ug/l	184473	4	13.794	1112280	50.0
Heptadecane, 2,...	15.588	10.5	ug/l	234140	4	13.794	1112280	50.0
Tridecane	15.835	25.1	ug/l	558800	4	13.794	1112280	50.0