

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
 Data File : VN086188.D
 Acq On : 31 Mar 2025 22:41
 Operator : JC\MD
 Sample : Q1644-01
 Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 12325-C

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\82N031825W.M
 Title : SW846 8260

Signal : TIC: VN086188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.842	135	151	152	rBV7	20486	59675	4.37%	0.711%
2	8.159	1046	1055	1060	rBV	137494	329425	24.13%	3.922%
3	8.218	1060	1065	1075	rVB	201600	433046	31.72%	5.156%
4	8.571	1116	1125	1132	rBV	136330	305055	22.34%	3.632%
5	8.641	1132	1137	1143	rBV2	17130	40430	2.96%	0.481%
6	8.788	1156	1162	1182	rVB3	35194	120330	8.81%	1.433%
7	9.094	1206	1214	1226	rBV	307230	616618	45.16%	7.342%
8	10.565	1455	1464	1470	rBV	449791	809296	59.28%	9.636%
9	10.630	1470	1475	1481	rVB	46107	84294	6.17%	1.004%
10	11.865	1676	1685	1698	rBV	398931	691133	50.62%	8.229%
11	12.847	1845	1852	1862	rVB	267298	451620	33.08%	5.377%
12	13.159	1901	1905	1912	rVB6	8822	17230	1.26%	0.205%
13	13.482	1955	1960	1965	rBV2	10526	17415	1.28%	0.207%
14	13.788	2006	2012	2021	rBV	328333	571700	41.87%	6.807%
15	13.871	2021	2026	2032	rVB3	7541	13755	1.01%	0.164%
16	14.100	2059	2065	2072	rBV3	16824	28269	2.07%	0.337%
17	14.576	2137	2146	2150	rBV6	6336	15144	1.11%	0.180%
18	14.959	2202	2211	2219	rBV2	53950	99271	7.27%	1.182%
19	15.047	2219	2226	2227	rBV5	14647	28581	2.09%	0.340%
20	15.076	2228	2231	2240	rVB3	19512	39781	2.91%	0.474%
21	15.212	2248	2254	2260	rVB9	9836	20858	1.53%	0.248%
22	15.317	2267	2272	2278	rBV8	8272	15581	1.14%	0.186%
23	15.417	2282	2289	2293	rBV6	25564	71523	5.24%	0.852%
24	15.465	2293	2297	2300	rVV2	37483	62875	4.61%	0.749%
25	15.506	2300	2304	2312	rVB2	52735	89273	6.54%	1.063%
26	15.588	2312	2318	2325	rBV	103738	206092	15.10%	2.454%
27	15.829	2349	2359	2369	rBV	829472	1365281	100.00%	16.255%
28	15.941	2369	2378	2383	rBV6	62038	179642	13.16%	2.139%
29	16.012	2388	2390	2396	rVB2	47746	69509	5.09%	0.828%
30	16.170	2412	2417	2427	rVB9	40446	112179	8.22%	1.336%
31	16.312	2429	2441	2444	rBV2	126820	296443	21.71%	3.530%
32	16.400	2451	2456	2461	rBV	111049	209527	15.35%	2.495%
33	16.453	2461	2465	2475	rVV2	152970	346534	25.38%	4.126%
34	16.541	2475	2480	2486	rVV2	157075	294809	21.59%	3.510%
35	16.612	2486	2492	2500	rVB2	147452	286740	21.00%	3.414%

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M

Title : SW846 8260

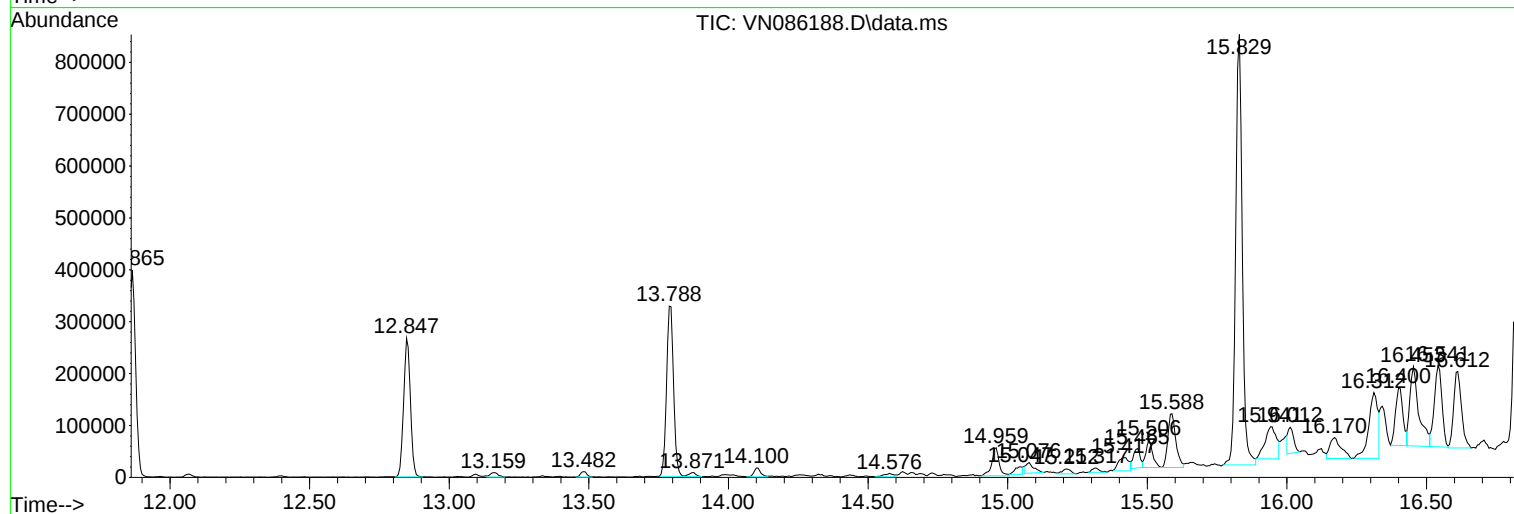
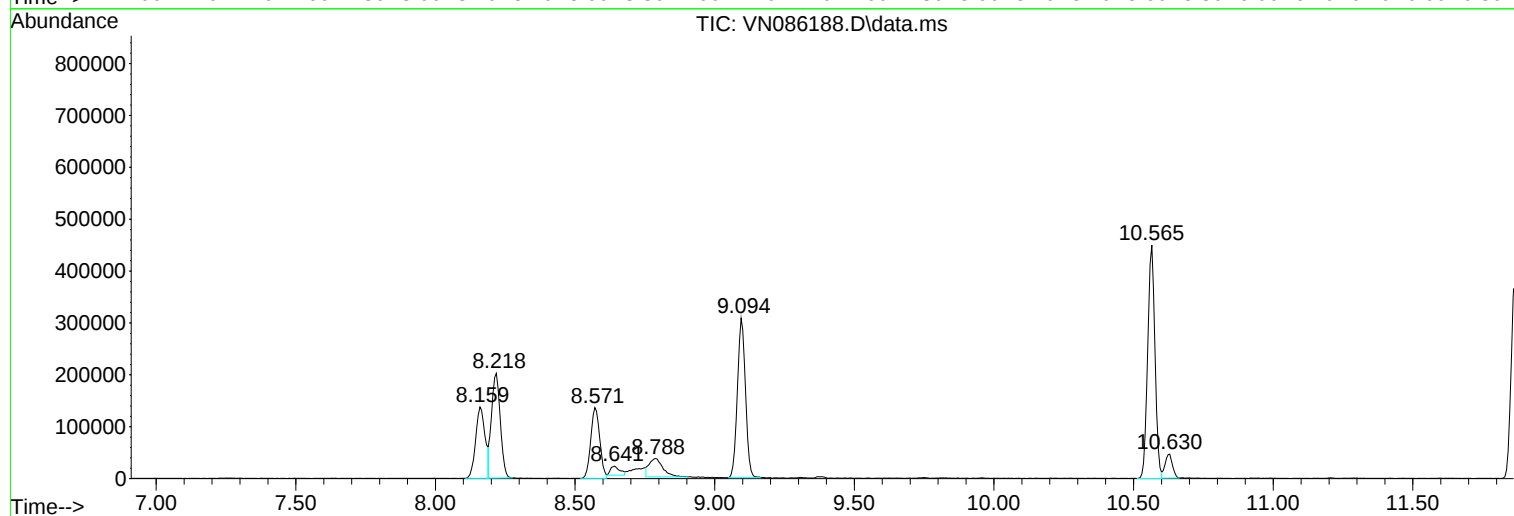
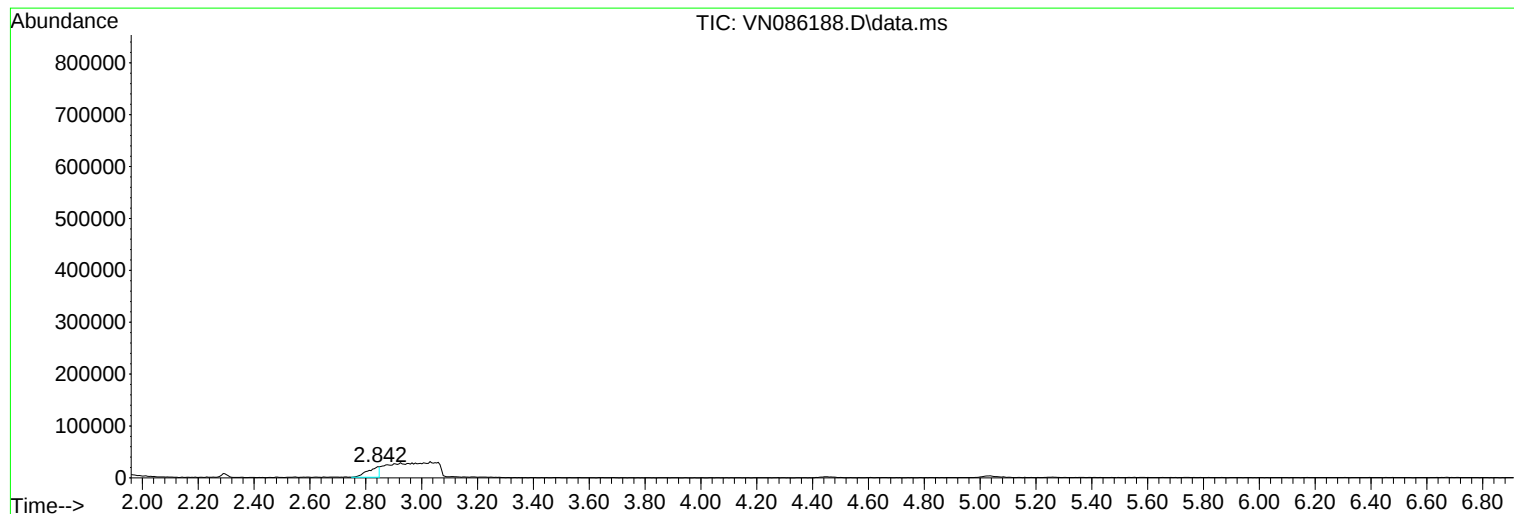
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Quant Title : SW846 8260

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



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Instrument :
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12325-C

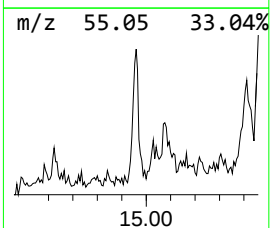
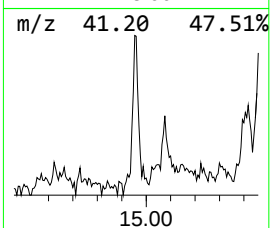
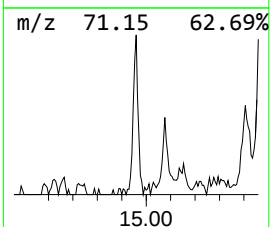
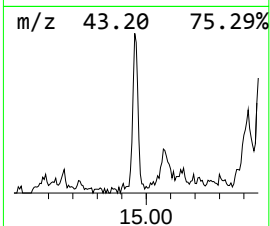
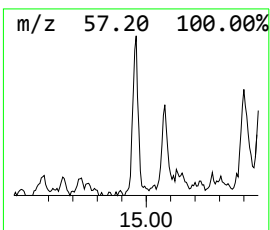
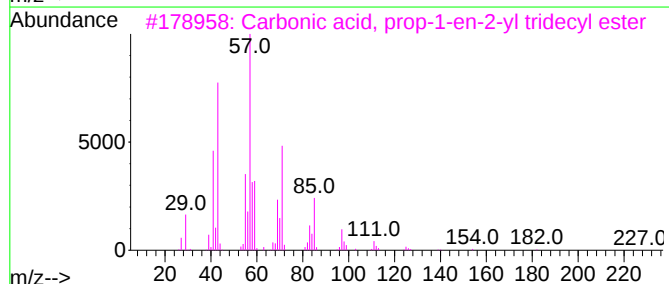
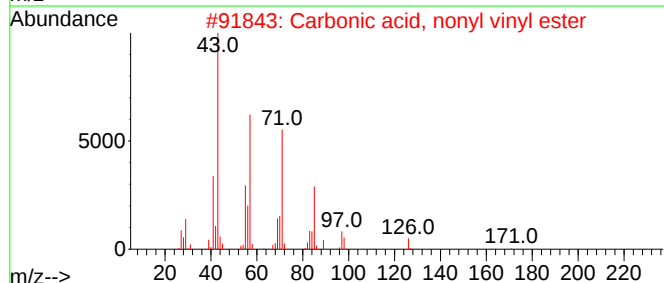
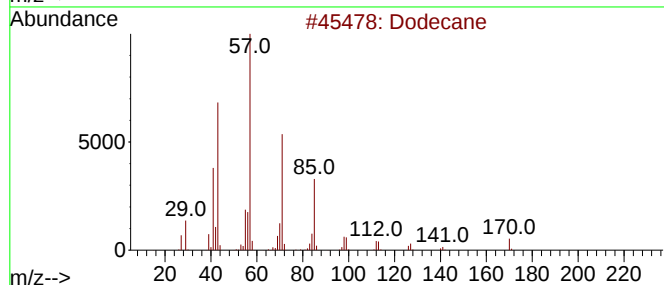
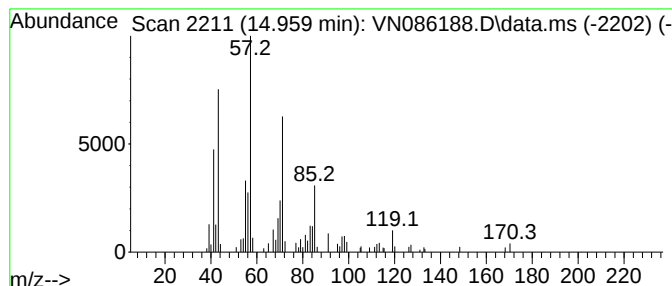
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	8.68 ug/l	99271	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	76
2			Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	64
3			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	58
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	58
5			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	53



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

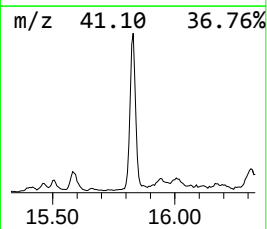
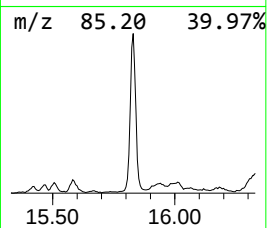
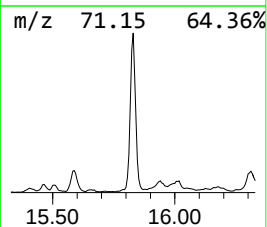
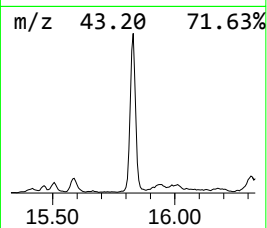
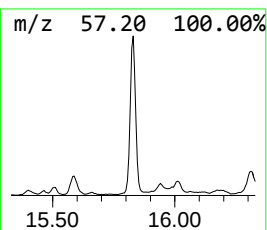
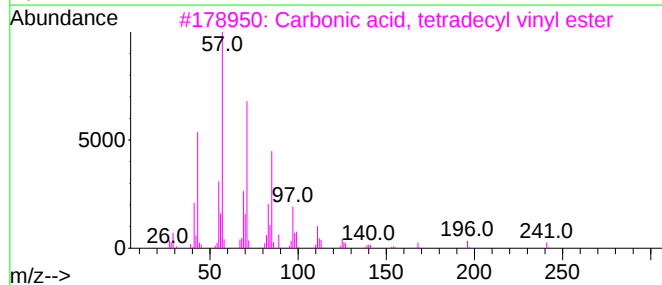
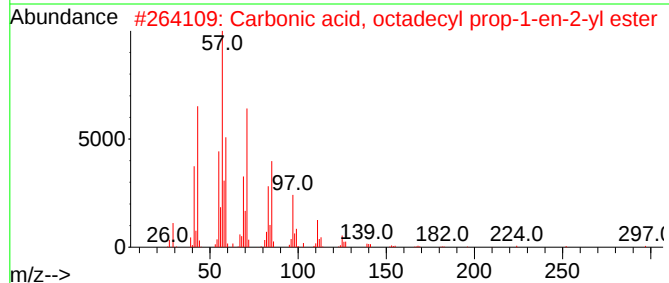
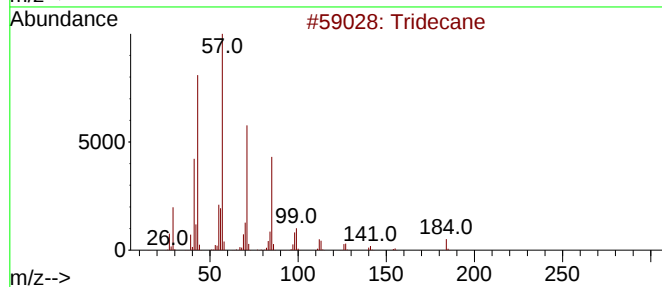
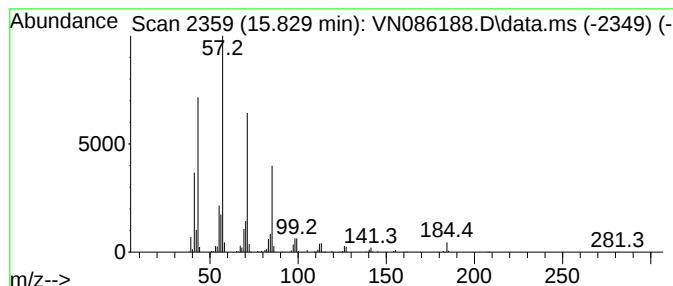
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	119.41 ug/l	1365280	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	86
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	86
4			Dodecane	170	C12H26	000112-40-3	86
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72



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ALS Vial : 23 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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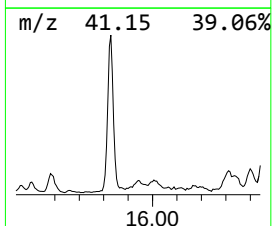
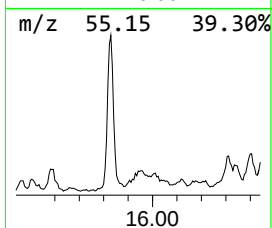
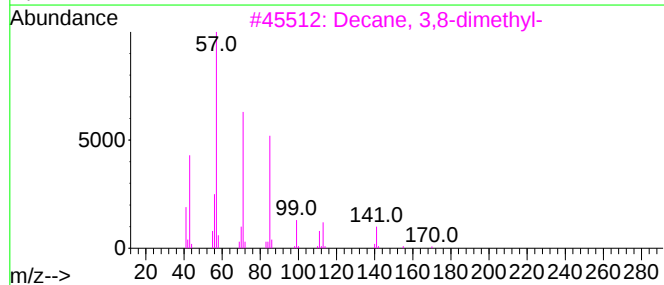
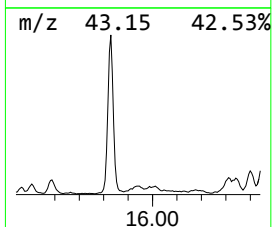
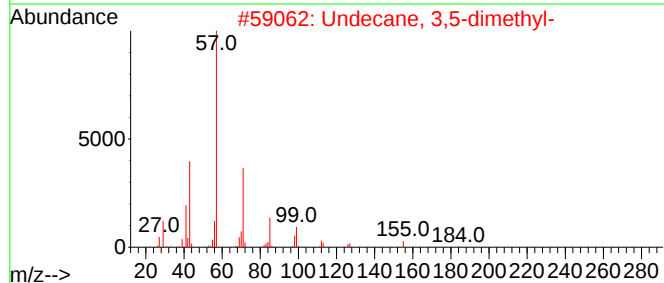
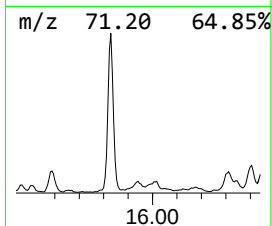
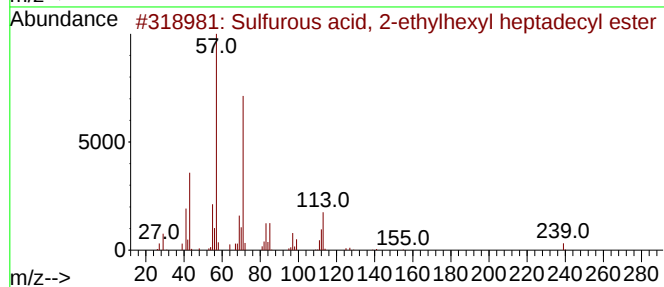
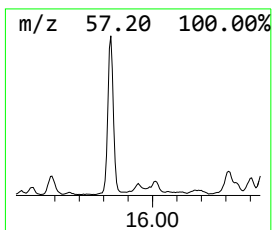
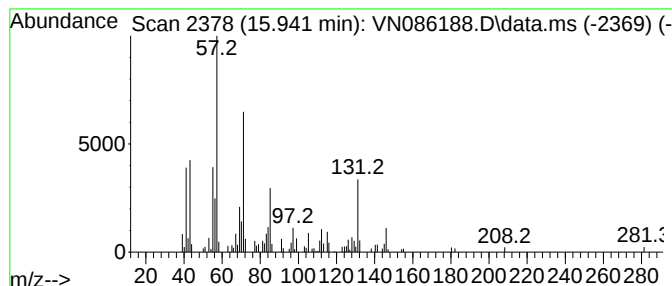
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

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

Peak Number 4 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.941	15.71 ug/l	179642	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	52
2			Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	50
3			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	47
4			Tridecane	184	C13H28	000629-50-5	43
5			Tridecane, 6-methyl-	198	C14H30	013287-21-3	43



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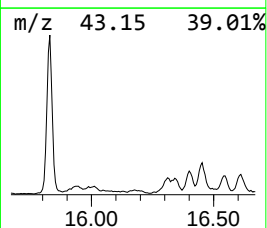
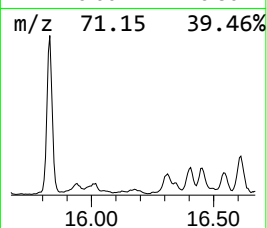
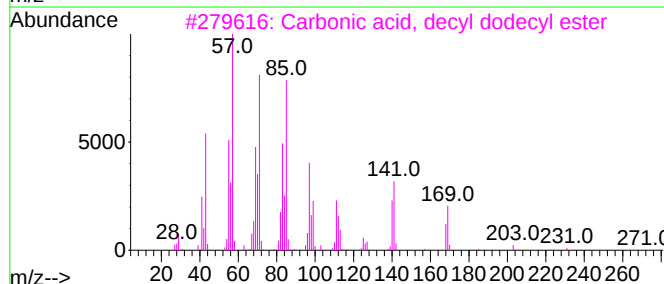
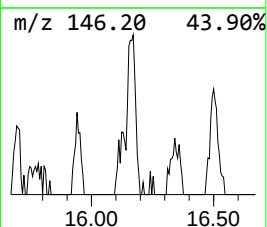
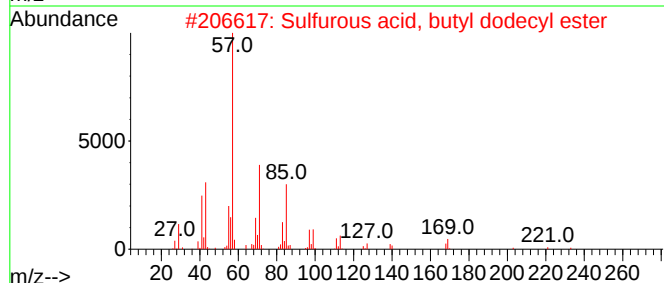
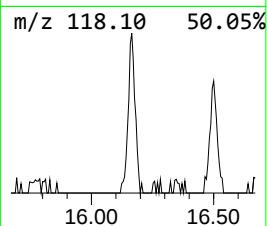
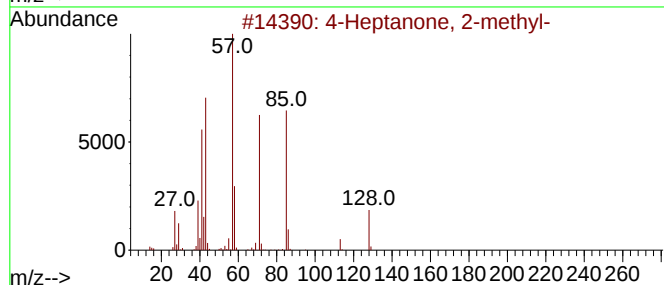
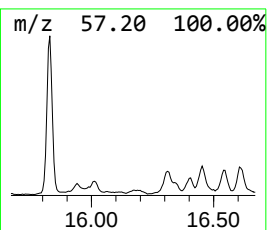
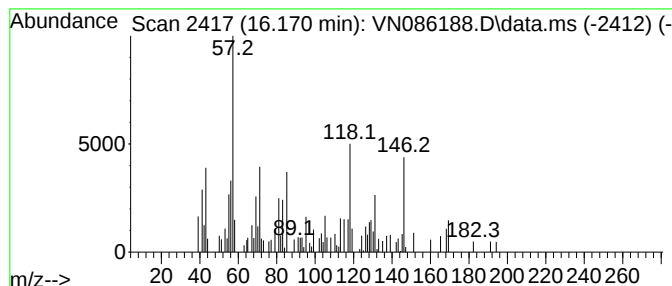
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TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown16.170 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.170	9.81 ug/l	112179	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	18
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	16
3			Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	16
4			Oxalic acid, bis(6-ethyloct-3-yl...)	370	C22H42O4	1000309-34-6	14
5			Dodecane, 3-methyl-	184	C13H28	017312-57-1	14



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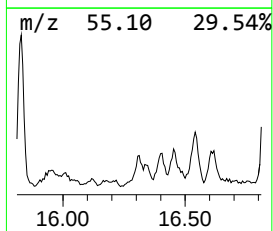
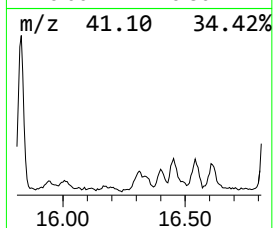
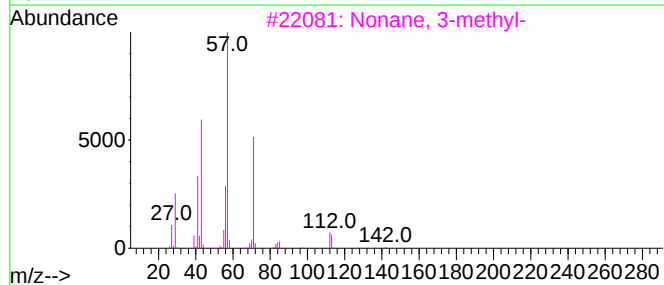
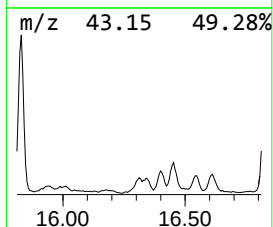
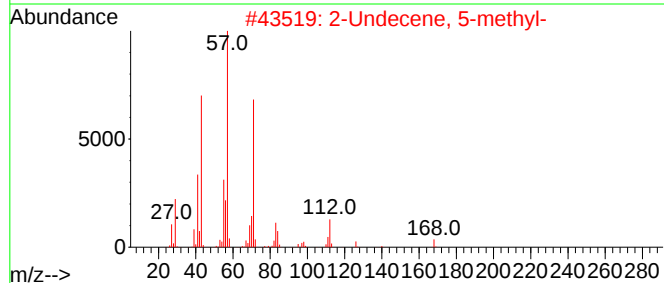
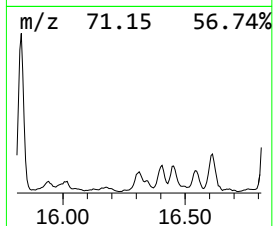
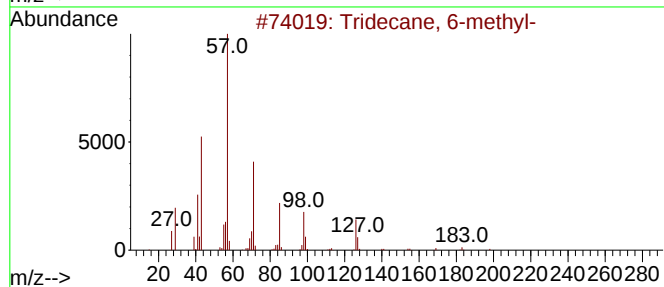
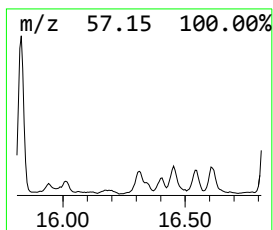
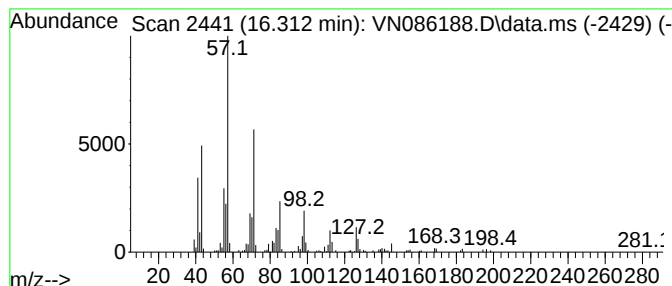
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.311	25.93 ug/l	296443	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-methyl-	198	C14H30	013287-21-3	70
2			2-Undecene, 5-methyl-	168	C12H24	056851-34-4	64
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	53
4			Dodecane	170	C12H26	000112-40-3	53
5			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
Data File : VN086188.D
Acq On : 31 Mar 2025 22:41
Operator : JC\MD
Sample : Q1644-01
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

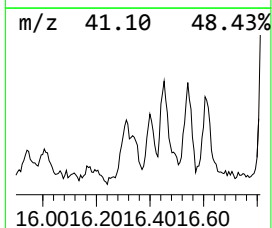
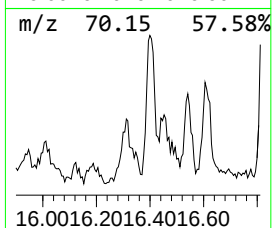
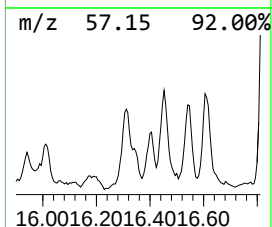
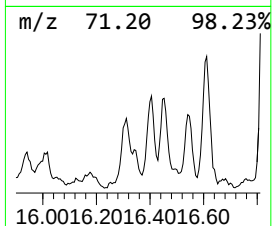
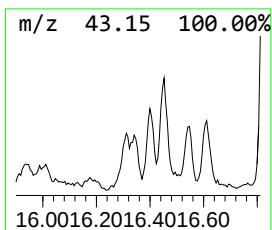
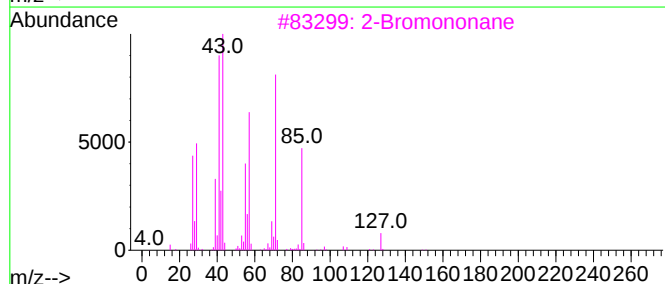
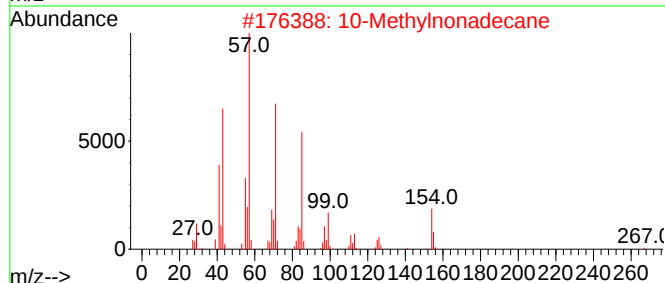
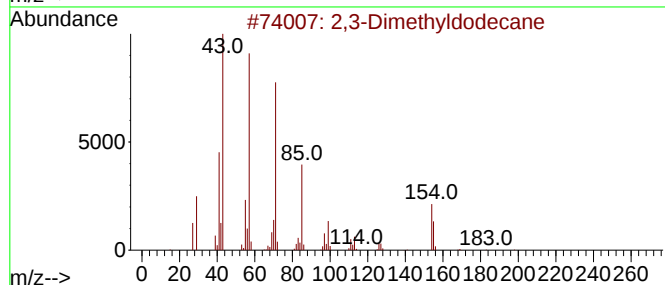
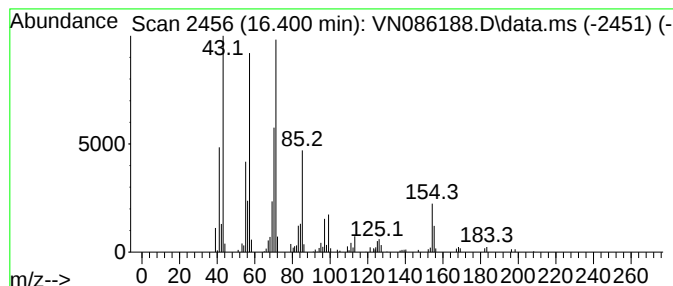
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Quant Title : SW846 8260

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

Peak Number 7 2,3-Dimethyldodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.400	18.32 ug/l	209527	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Dimethyldodecane	198	C14H30	006117-98-2	64
2			10-Methylnonadecane	282	C20H42	056862-62-5	62
3			2-Bromononane	206	C9H19Br	002216-35-5	50
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	49
5			Propanoic acid, 2-methyl-, 2-eth...	200	C12H24O2	035061-61-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
Data File : VN086188.D
Acq On : 31 Mar 2025 22:41
Operator : JC\MD
Sample : Q1644-01
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

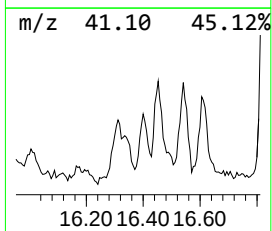
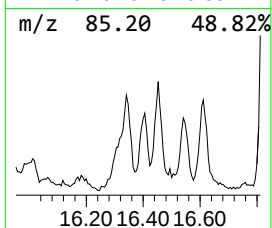
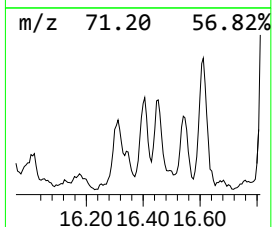
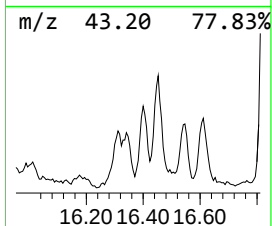
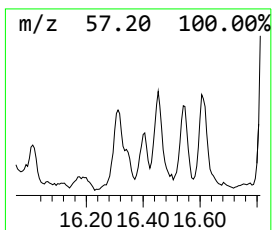
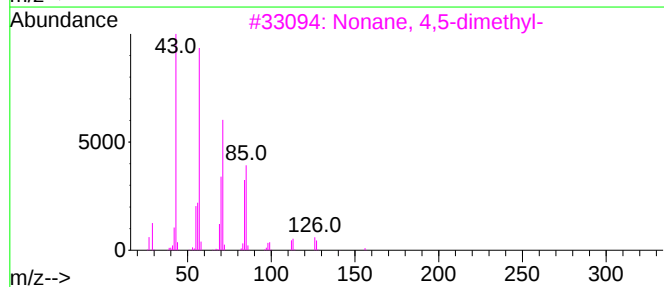
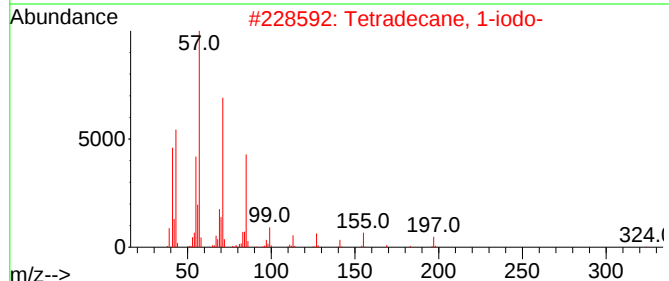
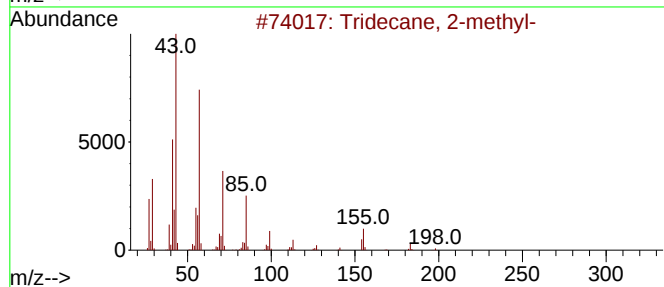
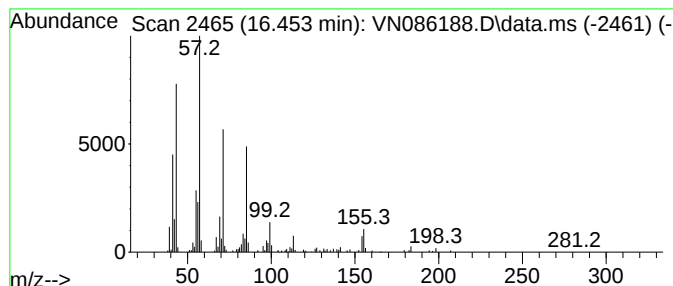
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.453	30.31 ug/l	346534	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 2-methyl-	198	C14H30	001560-96-9	90
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
3			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	72
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	72
5			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
Data File : VN086188.D
Acq On : 31 Mar 2025 22:41
Operator : JC\MD
Sample : Q1644-01
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

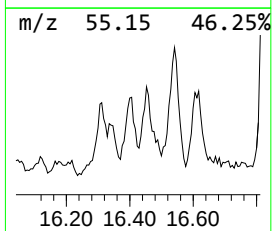
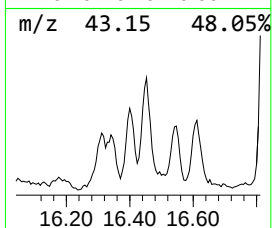
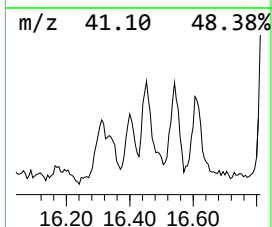
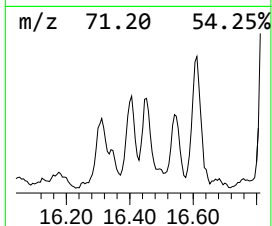
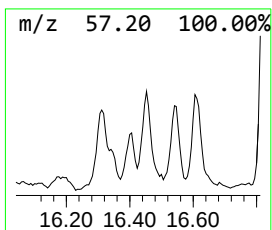
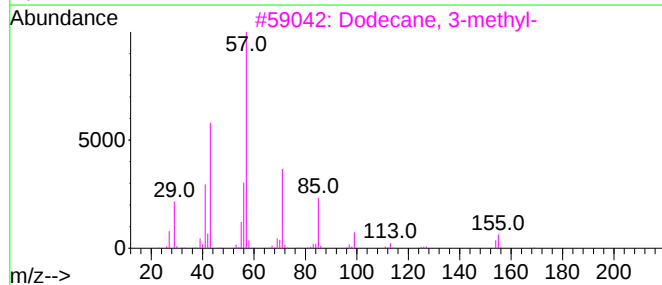
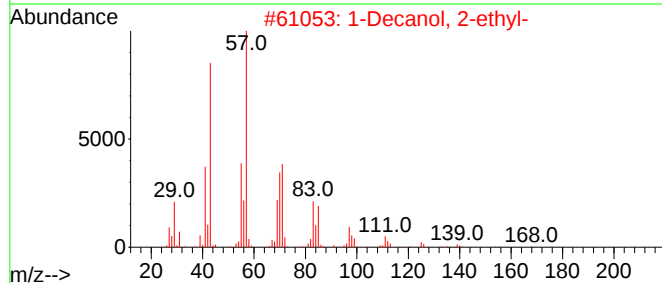
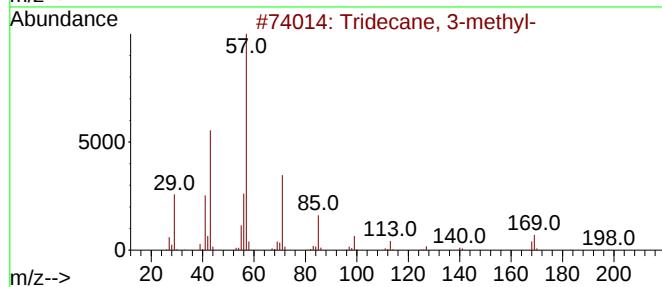
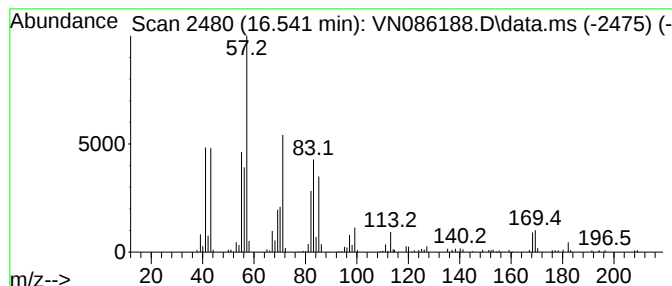
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.541 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.541	25.78 ug/l	294809	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 3-methyl-	198	C14H30	006418-41-3	50
2			1-Decanol, 2-ethyl-	186	C12H26O	021078-65-9	38
3			Dodecane, 3-methyl-	184	C13H28	017312-57-1	38
4			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	35
5			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
Data File : VN086188.D
Acq On : 31 Mar 2025 22:41
Operator : JC\MD
Sample : Q1644-01
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

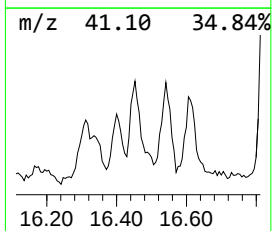
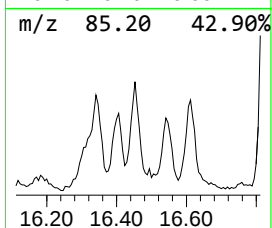
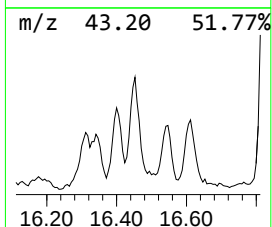
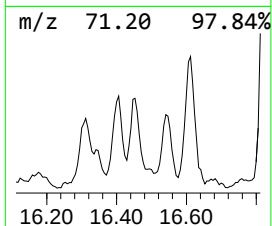
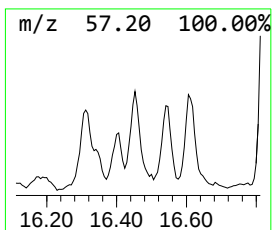
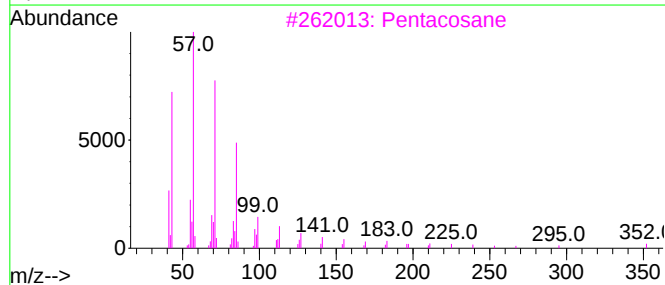
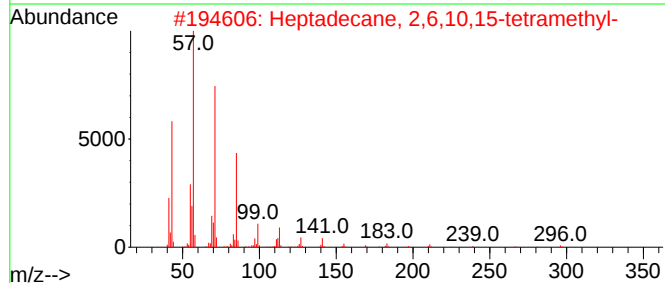
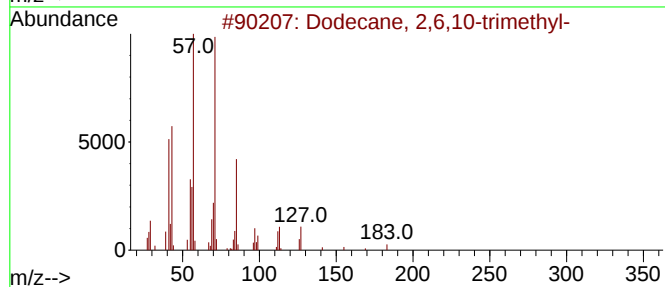
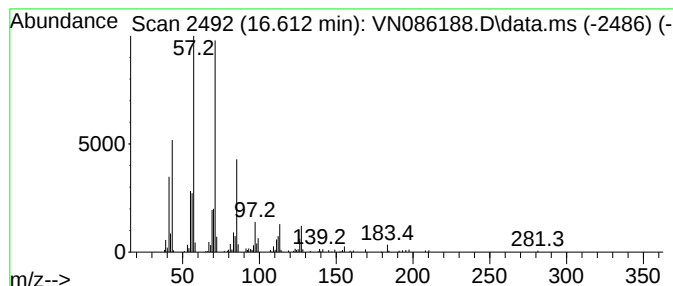
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.611	25.08 ug/l	286740	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	91
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3		Pentacosane	352	C25H52	000629-99-2	80
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	78
5		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN033125\
Data File : VN086188.D
Acq On : 31 Mar 2025 22:41
Operator : JC\MD
Sample : Q1644-01
Misc : 1.12g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
12325-C

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.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	8.7	ug/l	99271	4	13.794	571700	50.0
Tridecane	15.829	119.4	ug/l	1365280	4	13.794	571700	50.0
Sulfurous acid,...	15.941	15.7	ug/l	179642	4	13.794	571700	50.0
unknown16.170	16.170	9.8	ug/l	112179	4	13.794	571700	50.0
Tridecane, 6-me...	16.311	25.9	ug/l	296443	4	13.794	571700	50.0
2,3-Dimethyldod...	16.400	18.3	ug/l	209527	4	13.794	571700	50.0
Tridecane, 2-me...	16.453	30.3	ug/l	346534	4	13.794	571700	50.0
unknown16.541	16.541	25.8	ug/l	294809	4	13.794	571700	50.0
Dodecane, 2,6,1...	16.611	25.1	ug/l	286740	4	13.794	571700	50.0