

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103125\
 Data File : VN088189.D
 Acq On : 31 Oct 2025 15:23
 Operator : JC\MD
 Sample : Q3501-01
 Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 461

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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

Signal : TIC: VN088189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	56	61	70	rBV2	35257	68108	2.87%	0.228%
2	2.877	138	157	158	rBV6	46733	175524	7.39%	0.588%
3	2.924	158	165	168	rVV10	18991	56946	2.40%	0.191%
4	8.147	1039	1053	1057	rBV	309026	771870	32.51%	2.588%
5	8.200	1057	1062	1076	rVB	444805	997468	42.02%	3.344%
6	8.553	1114	1122	1136	rBV	365177	851051	35.85%	2.853%
7	9.077	1202	1211	1223	rBV	799986	1677736	70.67%	5.624%
8	9.577	1286	1296	1300	rBV8	11604	25271	1.06%	0.085%
9	10.541	1452	1460	1469	rBV	1267650	2373902	100.00%	7.958%
10	10.724	1485	1491	1496	rBV4	14247	27509	1.16%	0.092%
11	11.841	1674	1681	1693	rBV	1105481	2079203	87.59%	6.970%
12	12.047	1712	1716	1720	rBV7	16921	30454	1.28%	0.102%
13	12.388	1764	1774	1776	rBV10	21849	56184	2.37%	0.188%
14	12.829	1842	1849	1862	rBV	787734	1533301	64.59%	5.140%
15	13.135	1897	1901	1907	rBV4	35295	72299	3.05%	0.242%
16	13.694	1993	1996	1998	rBV2	24583	27476	1.16%	0.092%
17	13.770	2003	2009	2016	rVV	1100746	1990355	83.84%	6.672%
18	13.829	2016	2019	2026	rVB2	79852	137405	5.79%	0.461%
19	14.082	2055	2062	2076	rVB2	226719	441711	18.61%	1.481%
20	14.235	2084	2088	2096	rBV5	31729	73388	3.09%	0.246%
21	14.406	2113	2117	2123	rBV7	42341	82122	3.46%	0.275%
22	14.559	2138	2143	2147	rBV4	228729	417288	17.58%	1.399%
23	14.600	2147	2150	2153	rVV	220169	328433	13.84%	1.101%
24	14.635	2153	2156	2164	rVB	320799	458039	19.29%	1.535%
25	14.706	2164	2168	2175	rBV	281879	409432	17.25%	1.373%
26	14.811	2184	2186	2188	rBV2	25044	30001	1.26%	0.101%
27	14.935	2201	2207	2214	rVB	553383	852522	35.91%	2.858%
28	15.053	2214	2227	2230	rBV3	186420	585734	24.67%	1.964%
29	15.129	2237	2240	2244	rVB4	63863	90319	3.80%	0.303%
30	15.182	2245	2249	2255	rVB5	74027	165219	6.96%	0.554%
31	15.241	2255	2259	2264	rBV5	101681	159938	6.74%	0.536%
32	15.388	2276	2284	2289	rBV3	674990	1728631	72.82%	5.795%
33	15.441	2289	2293	2296	rVV	506140	831534	35.03%	2.788%
34	15.482	2296	2300	2307	rVV	724760	1148616	48.39%	3.850%
35	15.553	2307	2312	2323	rVV	627469	1103198	46.47%	3.698%
36	15.800	2349	2354	2365	rVB	817223	1453530	61.23%	4.873%

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37	15.917	2366	2374	2379	rBV2	373846	1011769	42.62%	3.392%
38	16.070	2397	2400	2407	rVB5	134639	254258	10.71%	0.852%
39	16.147	2408	2413	2422	rVB5	196427	390358	16.44%	1.309%
40	16.282	2430	2436	2439	rBV	811984	1544287	65.05%	5.177%
41	16.376	2446	2452	2456	rBV	436095	749457	31.57%	2.512%
42	16.423	2456	2460	2466	rVV	583074	1038904	43.76%	3.483%
43	16.511	2470	2475	2482	rVB	623136	1188738	50.08%	3.985%
44	16.676	2498	2503	2509	rBV3	144662	341174	14.37%	1.144%

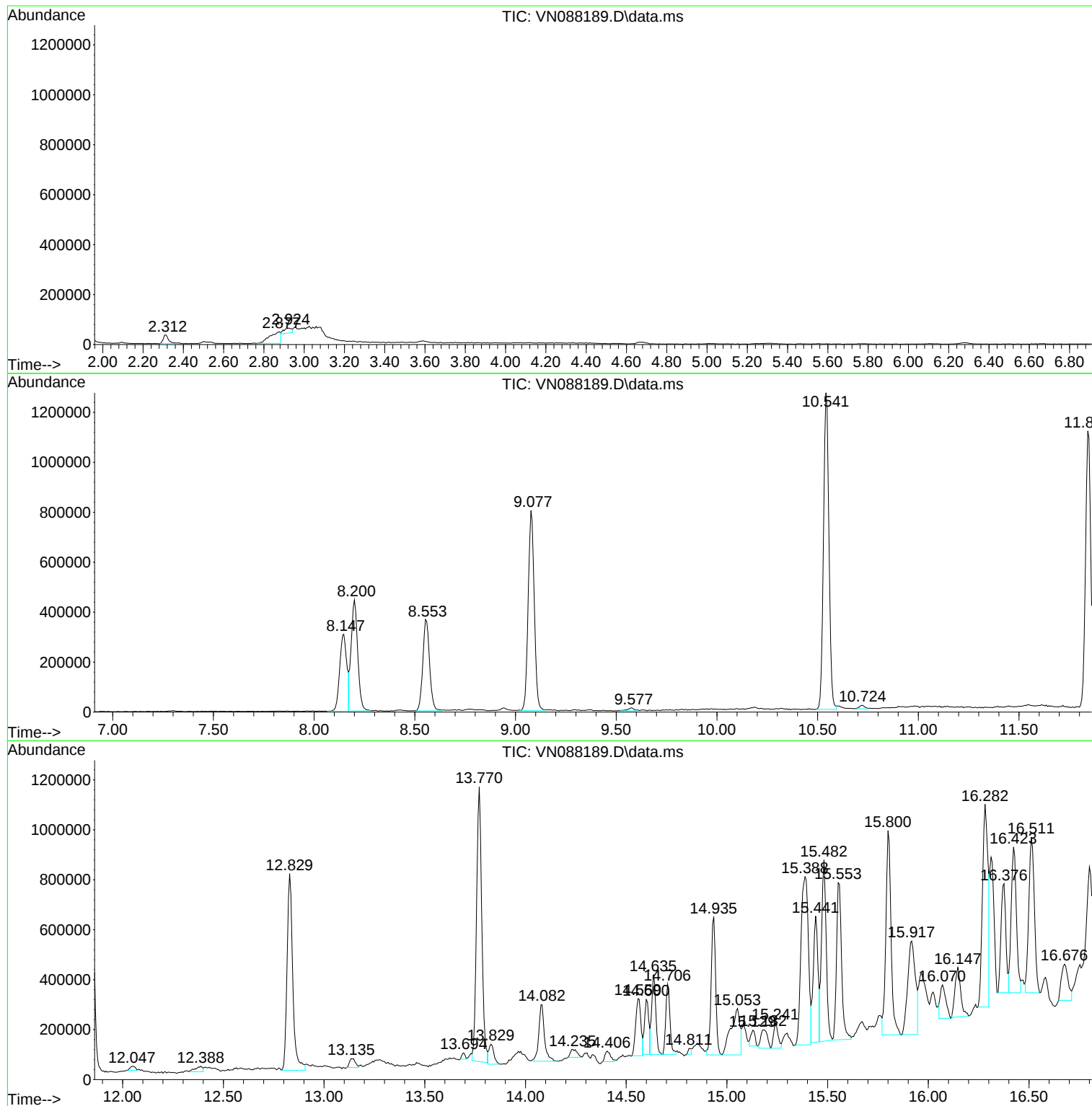
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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



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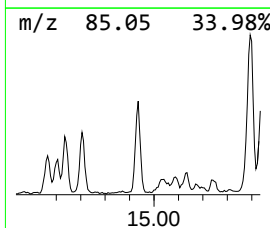
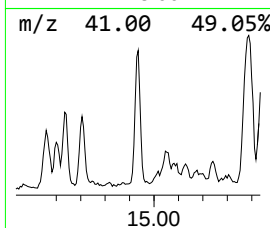
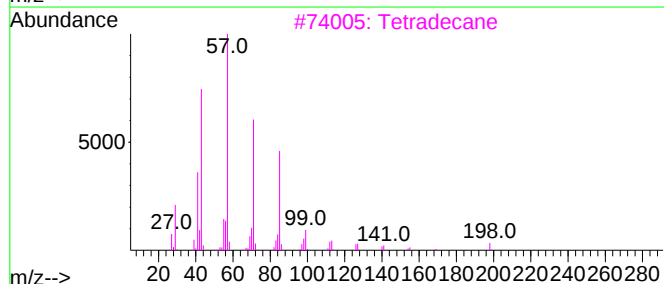
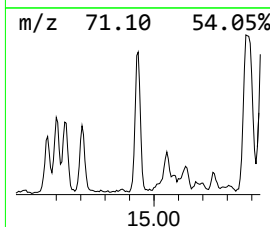
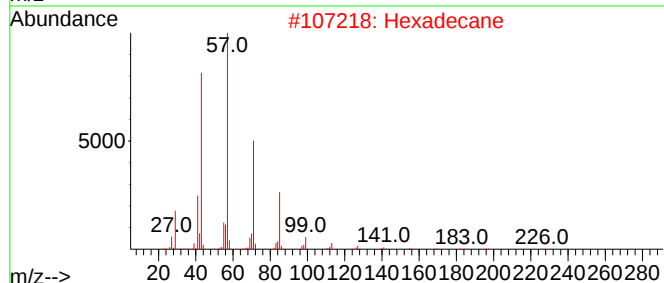
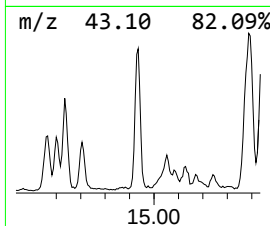
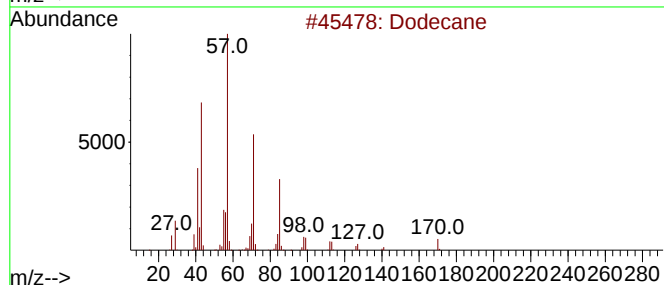
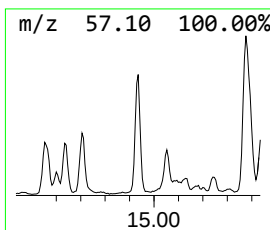
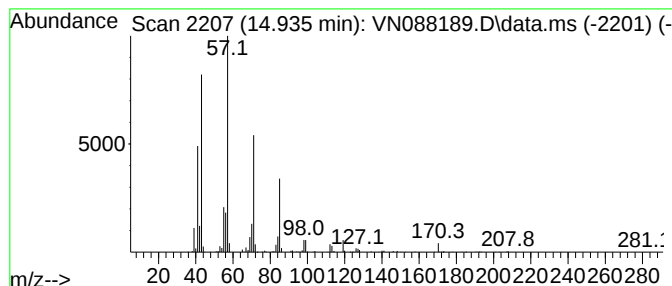
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	21.42 ug/l	852522	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	93
2			Hexadecane	226	C16H34	000544-76-3	80
3			Tetradecane	198	C14H30	000629-59-4	80
4			Tridecane	184	C13H28	000629-50-5	80
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	78



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Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

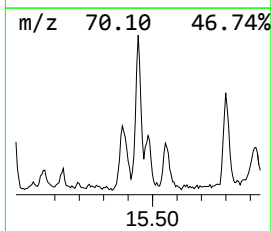
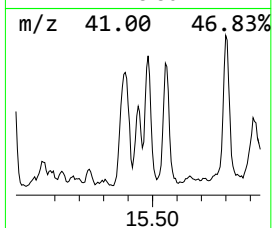
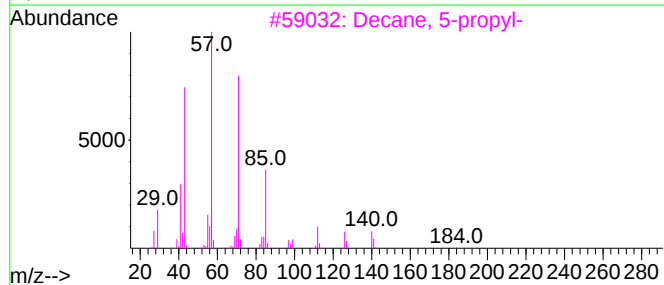
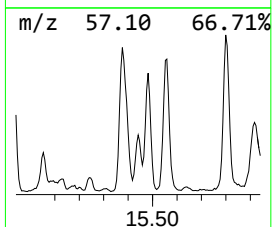
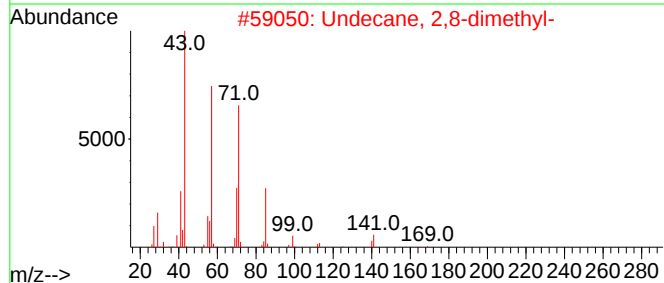
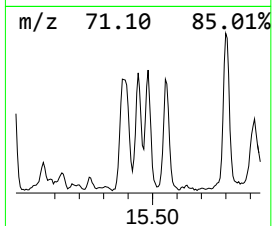
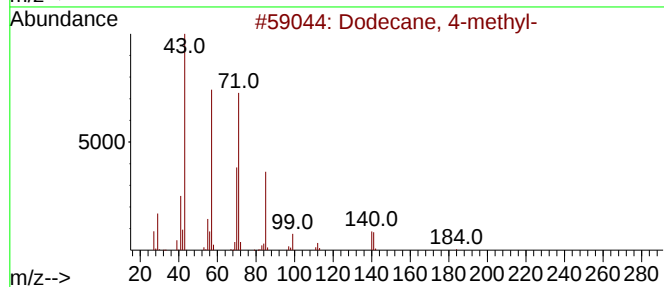
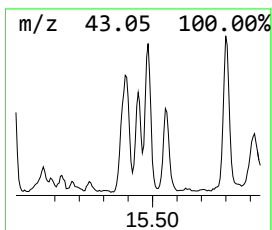
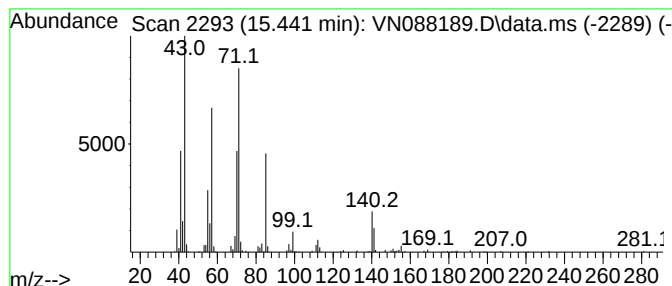
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 3 Dodecane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.441	20.89 ug/l	831534	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4-methyl-	184	C13H28	006117-97-1	94
2			Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	59
3			Decane, 5-propyl-	184	C13H28	017312-62-8	52
4			Hexadecane	226	C16H34	000544-76-3	50
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	50



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Data File : VN088189.D
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Operator : JC\MD
Sample : Q3501-01
Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

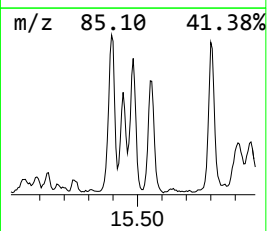
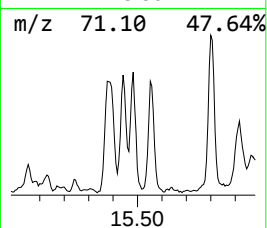
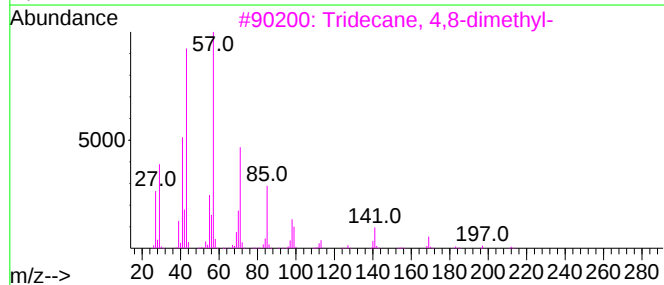
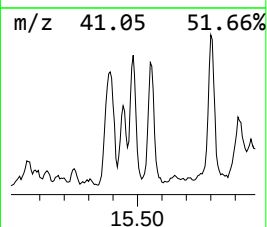
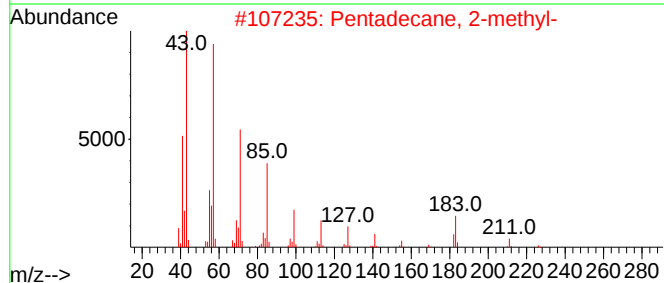
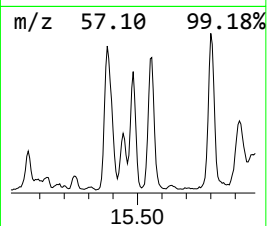
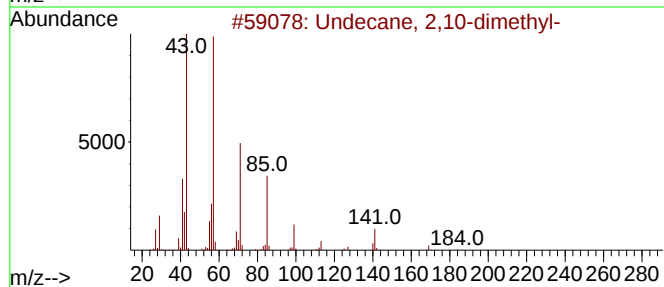
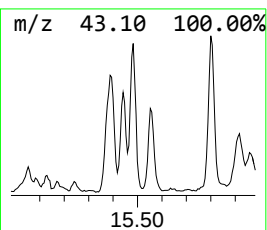
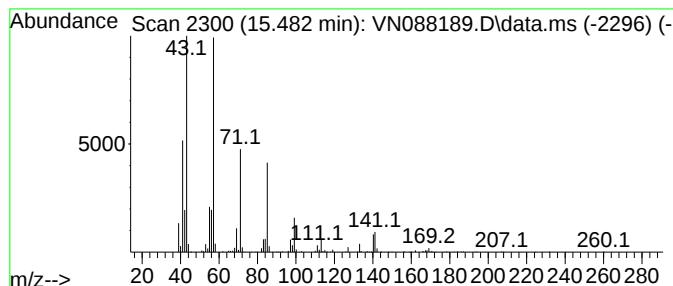
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 4 Undecane, 2,10-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.482	28.85 ug/l	1148620	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	94
2			Pentadecane, 2-methyl-	226	C16H34	001560-93-6	86
3			Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	83
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	78
5			Oxalic acid, 6-ethyloct-3-yl eth...	258	C14H26O4	1000309-33-9	72



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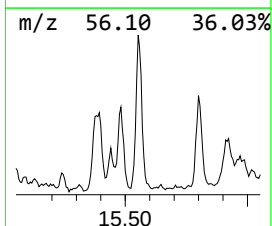
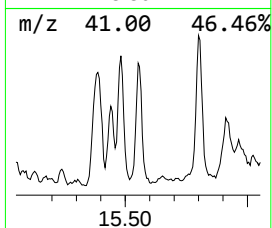
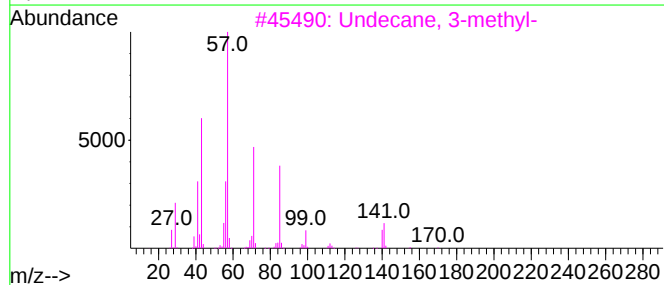
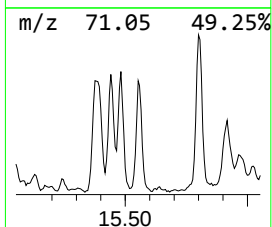
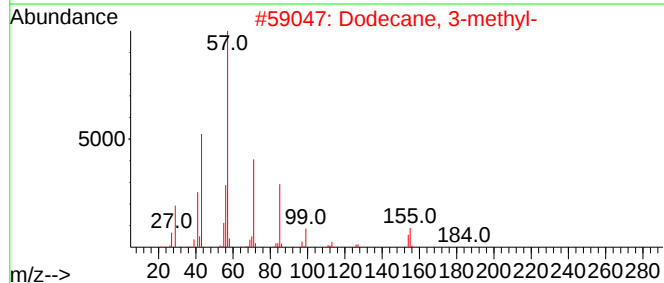
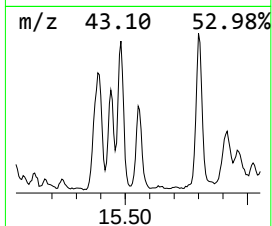
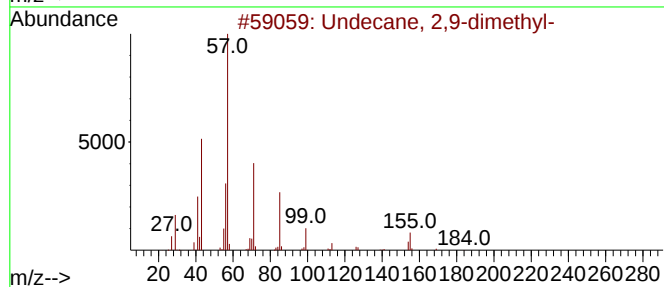
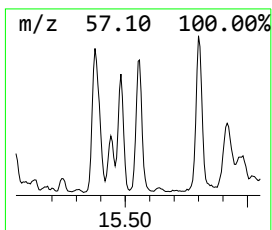
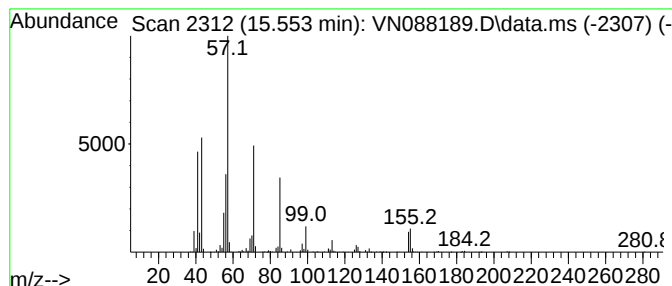
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 5 Undecane, 2,9-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.553	27.71 ug/l	1103200	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	87
2			Dodecane, 3-methyl-	184	C13H28	017312-57-1	83
3			Undecane, 3-methyl-	170	C12H26	001002-43-3	74
4			Pentadecane, 6-methyl-	226	C16H34	010105-38-1	59
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58



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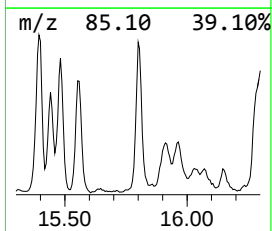
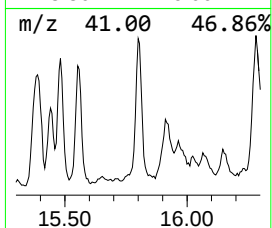
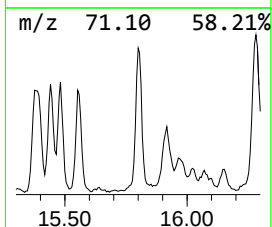
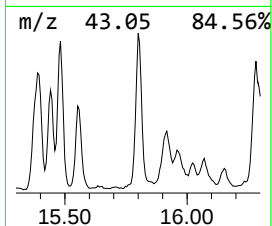
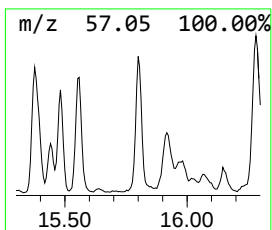
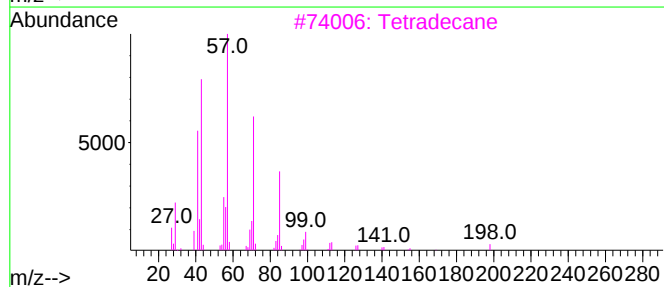
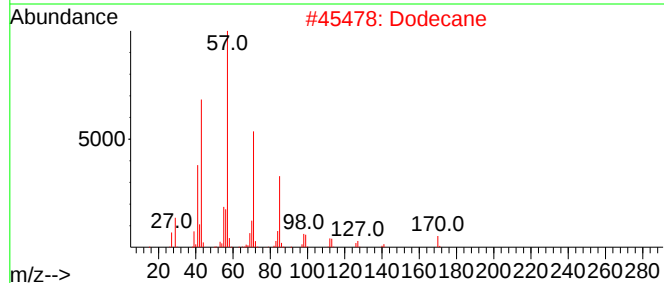
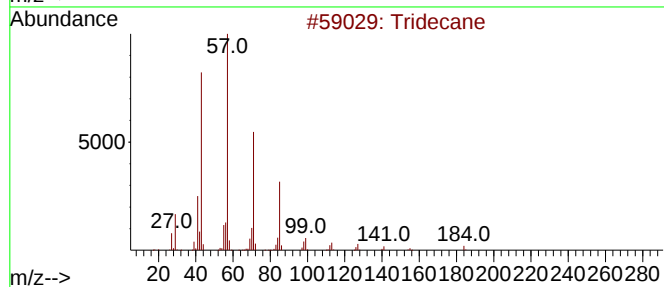
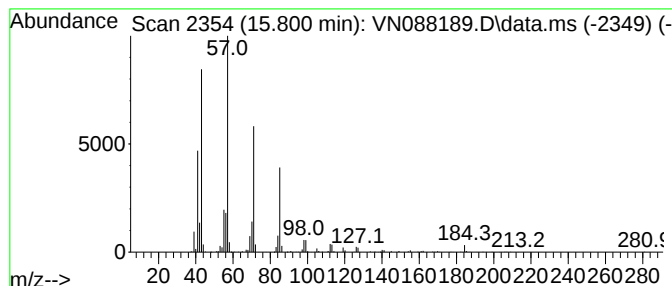
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.800	36.51 ug/l	1453530	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Dodecane	170	C12H26	000112-40-3	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103125\
Data File : VN088189.D
Acq On : 31 Oct 2025 15:23
Operator : JC\MD
Sample : Q3501-01
Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

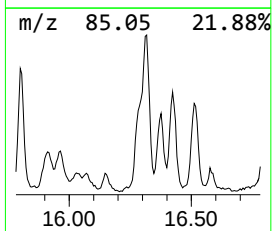
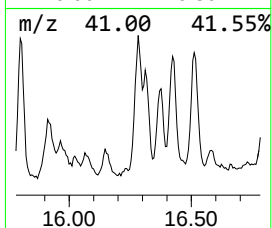
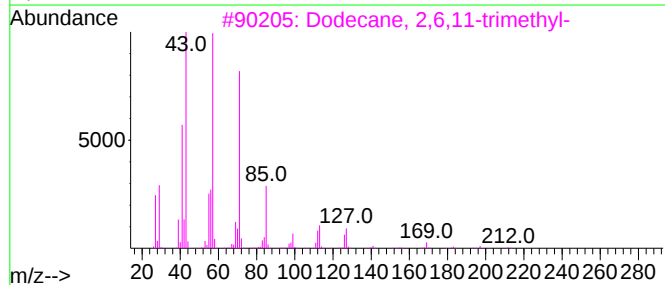
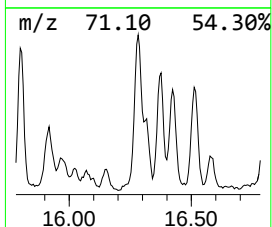
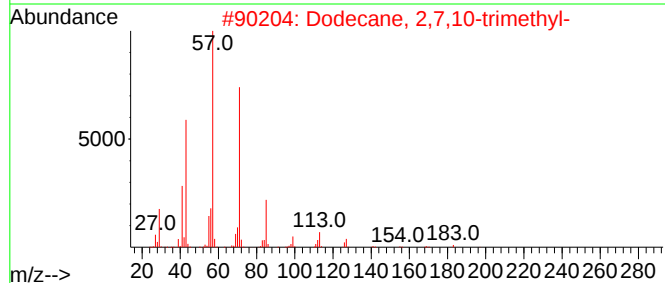
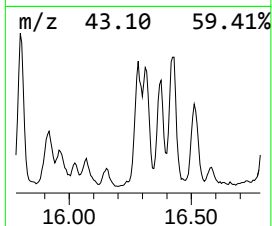
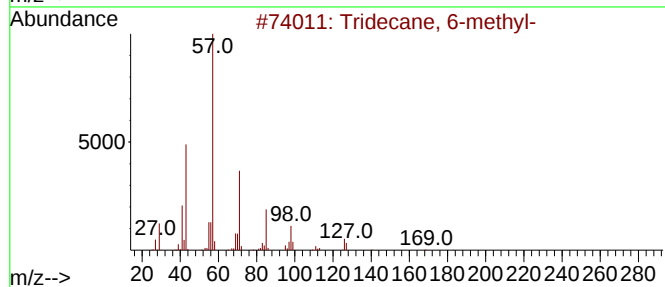
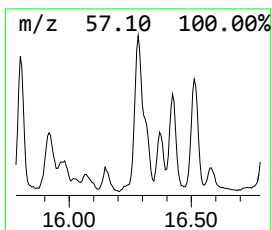
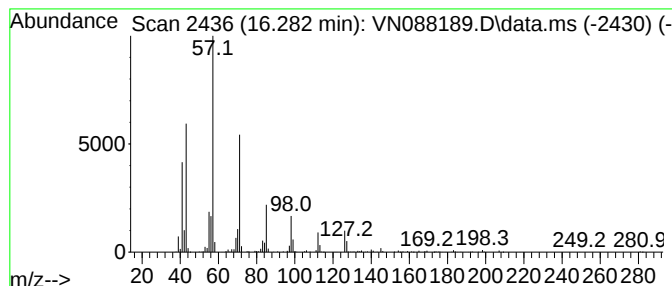
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.282	38.79 ug/l	1544290	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-methyl-	198	C14H30	013287-21-3	86
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
4			Decane, 5-propyl-	184	C13H28	017312-62-8	68
5			Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103125\
Data File : VN088189.D
Acq On : 31 Oct 2025 15:23
Operator : JC\MD
Sample : Q3501-01
Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

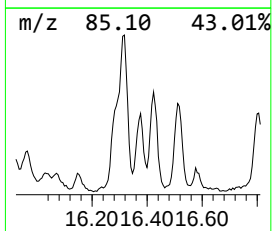
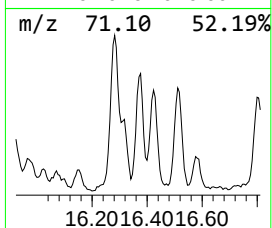
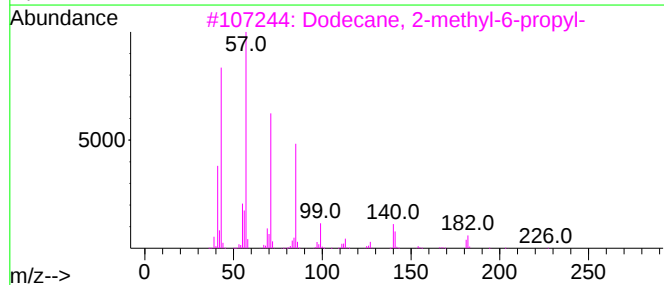
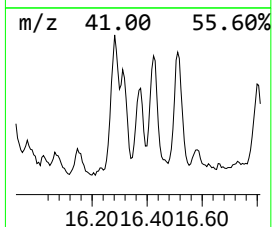
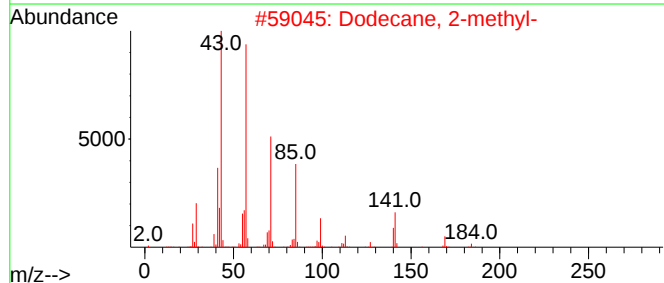
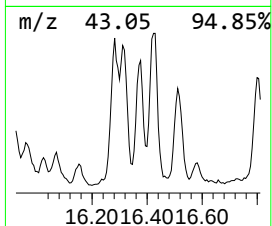
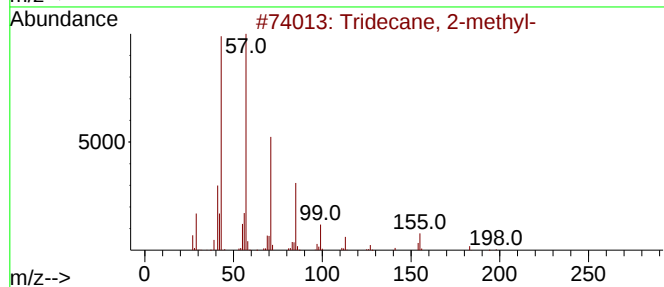
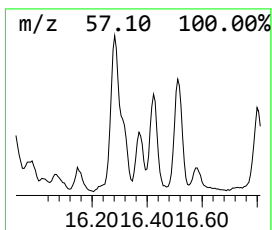
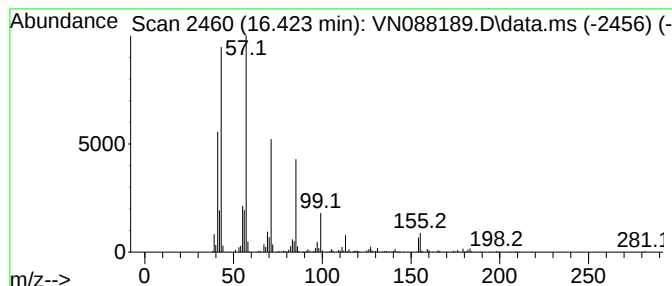
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.423	26.10 ug/l	1038900	1,4-Dichlorobenzene-d4	13.770

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 2-methyl-	198	C14H30	001560-96-9	94
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	78
3			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
4			Undecane, 5-methyl-	170	C12H26	001632-70-8	59
5			3,5-Dimethyldodecane	198	C14H30	107770-99-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103125\
Data File : VN088189.D
Acq On : 31 Oct 2025 15:23
Operator : JC\MD
Sample : Q3501-01
Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

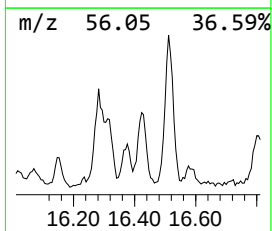
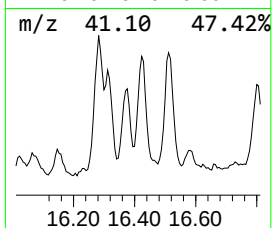
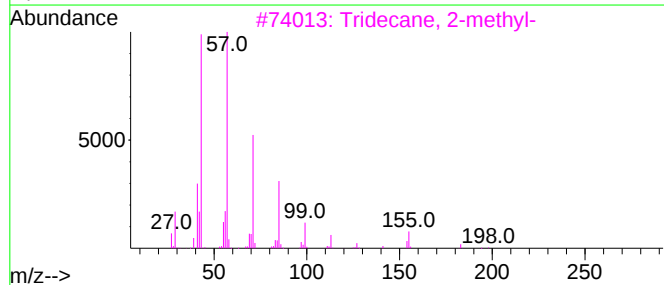
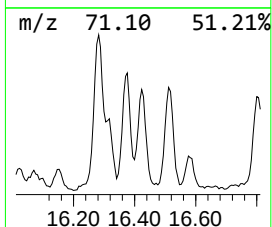
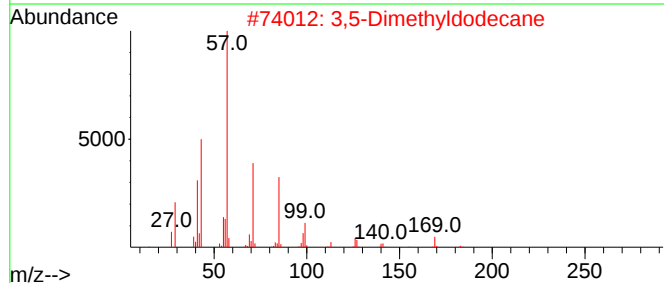
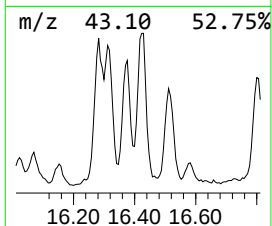
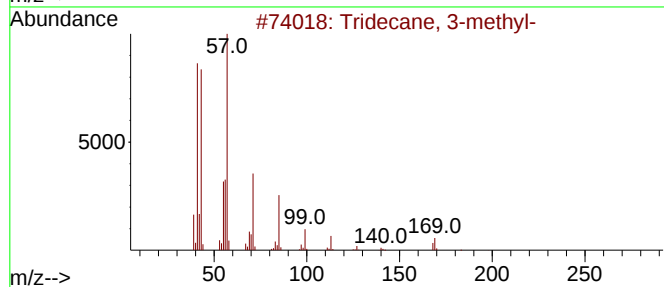
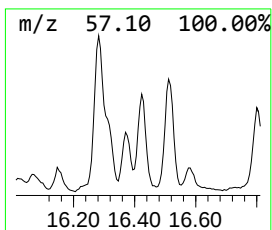
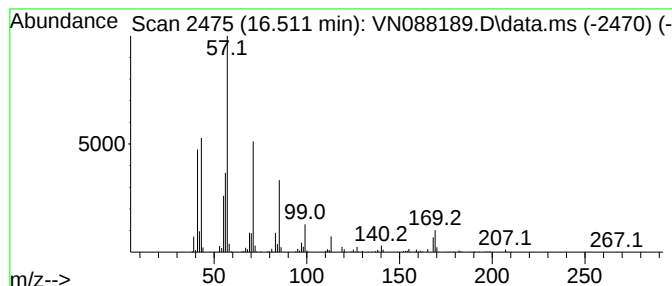
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.M
Quant Title : SW846 8260

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

Peak Number 10 Tridecane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.511	29.86 ug/l	1188740	1,4-Dichlorobenzene-d4	13.770

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 3-methyl-	198	C14H30	006418-41-3	94
2		3,5-Dimethyldodecane	198	C14H30	107770-99-0	87
3		Tridecane, 2-methyl-	198	C14H30	001560-96-9	76
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
5		Heptacosane	380	C27H56	000593-49-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN103125\
Data File : VN088189.D
Acq On : 31 Oct 2025 15:23
Operator : JC\MD
Sample : Q3501-01
Misc : 2.56g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
461

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102325W.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	14.935	21.4	ug/l	852522	4	13.770	1990360	50.0
Dodecane, 4-met...	15.441	20.9	ug/l	831534	4	13.770	1990360	50.0
Undecane, 2,10-...	15.482	28.9	ug/l	1148620	4	13.770	1990360	50.0
Undecane, 2,9-d...	15.553	27.7	ug/l	1103200	4	13.770	1990360	50.0
Tridecane	15.800	36.5	ug/l	1453530	4	13.770	1990360	50.0
Tridecane, 6-me...	16.282	38.8	ug/l	1544290	4	13.770	1990360	50.0
Tridecane, 2-me...	16.423	26.1	ug/l	1038900	4	13.770	1990360	50.0
Tridecane, 3-me...	16.511	29.9	ug/l	1188740	4	13.770	1990360	50.0