

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
 Data File : VX048335.D
 Acq On : 23 Oct 2025 18:32
 Operator : JC/MD
 Sample : Q3388-01
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 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_X\Method\82X102025W.M
 Title : SW846 8260

Signal : TIC: VX048335.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	27	30	42	rVB2	15212	28863	4.62%	0.347%
2	1.629	70	89	90	rBV5	12367	51910	8.32%	0.624%
3	1.934	135	139	146	rVB4	6720	11768	1.89%	0.142%
4	2.446	217	223	229	rBV3	9620	17870	2.86%	0.215%
5	3.428	378	384	395	rBV2	6042	14809	2.37%	0.178%
6	4.580	561	573	579	rBV5	2026	6887	1.10%	0.083%
7	5.373	692	703	719	rBV	48906	168620	27.01%	2.029%
8	5.531	720	729	753	rVB2	81552	268162	42.96%	3.226%
9	5.940	783	796	818	rBV	62175	196132	31.42%	2.360%
10	6.592	894	903	914	rBV3	4720	12088	1.94%	0.145%
11	6.744	919	928	947	rBV	151058	414862	66.46%	4.991%
12	7.360	1022	1029	1037	rBV8	3699	9267	1.48%	0.111%
13	8.256	1171	1176	1182	rBV4	3686	6499	1.04%	0.078%
14	8.634	1231	1238	1254	rBV	343547	589369	94.42%	7.090%
15	8.896	1275	1281	1288	rBV	8993	13750	2.20%	0.165%
16	10.036	1463	1468	1484	rVB	385752	572543	91.72%	6.888%
17	10.286	1504	1509	1514	rVV4	4717	7629	1.22%	0.092%
18	10.341	1514	1518	1526	rVB	8613	12217	1.96%	0.147%
19	11.067	1631	1637	1648	rVV	326345	474138	75.96%	5.704%
20	11.170	1651	1654	1663	rVB4	5345	7617	1.22%	0.092%
21	11.463	1697	1702	1708	rVB	22055	30185	4.84%	0.363%
22	11.737	1743	1747	1756	rVB3	8115	13965	2.24%	0.168%
23	12.006	1785	1791	1797	rVV	461858	624224	100.00%	7.510%
24	12.054	1797	1799	1801	rVV2	19900	22739	3.64%	0.274%
25	12.085	1801	1804	1809	rVV	38571	45692	7.32%	0.550%
26	12.152	1811	1815	1820	rVB3	29789	36127	5.79%	0.435%
27	12.298	1835	1839	1845	rBV6	4730	8551	1.37%	0.103%
28	12.408	1852	1857	1861	rBV	92472	108291	17.35%	1.303%
29	12.444	1861	1863	1869	rVB3	7872	9293	1.49%	0.112%
30	12.530	1873	1877	1879	rVV3	5750	8999	1.44%	0.108%
31	12.566	1879	1883	1888	rVV3	12794	21630	3.47%	0.260%
32	12.621	1888	1892	1895	rVV2	6791	7754	1.24%	0.093%
33	12.658	1895	1898	1903	rVB4	9242	11287	1.81%	0.136%
34	12.719	1903	1908	1911	rBV3	11508	13778	2.21%	0.166%
35	12.792	1916	1920	1925	rVB7	7347	11587	1.86%	0.139%
36	12.890	1929	1936	1939	rBV2	101959	160323	25.68%	1.929%

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

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37	12.926	1939	1942	1944	rVV	81198	92449	14.81%	1.112%
38	12.957	1944	1947	1951	rVV	139104	154716	24.79%	1.861%
39	13.024	1953	1958	1962	rVV	129376	142968	22.90%	1.720%
40	13.146	1975	1978	1983	rVB5	7090	9011	1.44%	0.108%
41	13.249	1988	1995	1998	rBV	252849	287155	46.00%	3.455%
42	13.365	2011	2014	2017	rBV	41391	41725	6.68%	0.502%
43	13.396	2017	2019	2022	rVV3	28036	30639	4.91%	0.369%
44	13.432	2023	2025	2029	rVB	36225	42612	6.83%	0.513%
45	13.469	2029	2031	2034	rBV3	18812	22124	3.54%	0.266%
46	13.536	2038	2042	2045	rBV2	29714	31411	5.03%	0.378%
47	13.591	2045	2051	2057	rVB9	9682	21950	3.52%	0.264%
48	13.676	2058	2065	2069	rBV2	234173	485450	77.77%	5.840%
49	13.719	2069	2072	2074	rVV	193090	207127	33.18%	2.492%
50	13.749	2074	2077	2081	rVV	280586	285656	45.76%	3.437%
51	13.810	2084	2087	2096	rVB	249044	294595	47.19%	3.544%
52	13.889	2097	2100	2102	rBV3	11435	15519	2.49%	0.187%
53	14.017	2117	2121	2125	rBV	260873	282898	45.32%	3.403%
54	14.115	2132	2137	2140	rBV	72585	114355	18.32%	1.376%
55	14.145	2140	2142	2147	rVB3	46945	60874	9.75%	0.732%
56	14.194	2147	2150	2151	rBV2	29714	31272	5.01%	0.376%
57	14.286	2161	2165	2171	rVB	30757	34593	5.54%	0.416%
58	14.347	2172	2175	2178	rVB4	10354	11100	1.78%	0.134%
59	14.389	2178	2182	2184	rBV	206249	254585	40.78%	3.063%
60	14.414	2184	2186	2189	rVV	145881	151879	24.33%	1.827%
61	14.450	2189	2192	2195	rVV	133360	168462	26.99%	2.027%
62	14.481	2195	2197	2203	rVB	164062	178374	28.58%	2.146%
63	14.542	2203	2207	2213	rVB	143485	174709	27.99%	2.102%
64	14.597	2213	2216	2222	rBV2	27785	47127	7.55%	0.567%
65	14.651	2222	2225	2228	rVB2	20309	23031	3.69%	0.277%
66	14.737	2235	2239	2242	rBV	95316	106902	17.13%	1.286%
67	14.816	2247	2252	2256	rBV2	55635	97509	15.62%	1.173%
68	14.853	2256	2258	2262	rVB	24058	25686	4.11%	0.309%
69	14.889	2262	2264	2267	rBV4	10247	16489	2.64%	0.198%
70	15.078	2290	2295	2298	rBV4	37223	65076	10.43%	0.783%
71	15.109	2298	2300	2303	rVB2	21945	23678	3.79%	0.285%
72	15.157	2304	2308	2311	rVV4	25369	38536	6.17%	0.464%
73	15.188	2311	2313	2317	rVV3	22920	25237	4.04%	0.304%
74	15.255	2321	2324	2327	rVB4	14869	17135	2.75%	0.206%
75	15.389	2343	2346	2354	rVB3	22316	33195	5.32%	0.399%
76	15.468	2354	2359	2366	rBV9	11848	27314	4.38%	0.329%

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ClientSampleId :
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Integration Parameters: RTEINT.P

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77	15.712	2396	2399	2408	rVB9	15718	26387	4.23%	0.317%
78	15.834	2416	2419	2430	rVB9	9715	24376	3.91%	0.293%
79	16.066	2451	2457	2464	rVB2	37548	66944	10.72%	0.805%

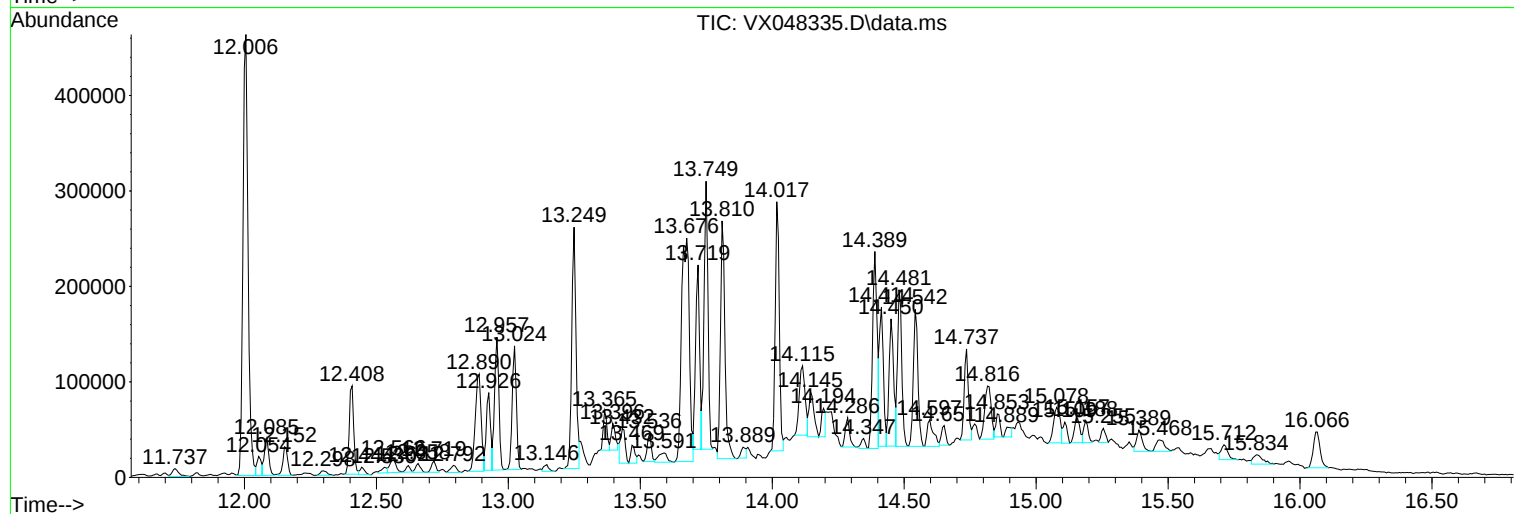
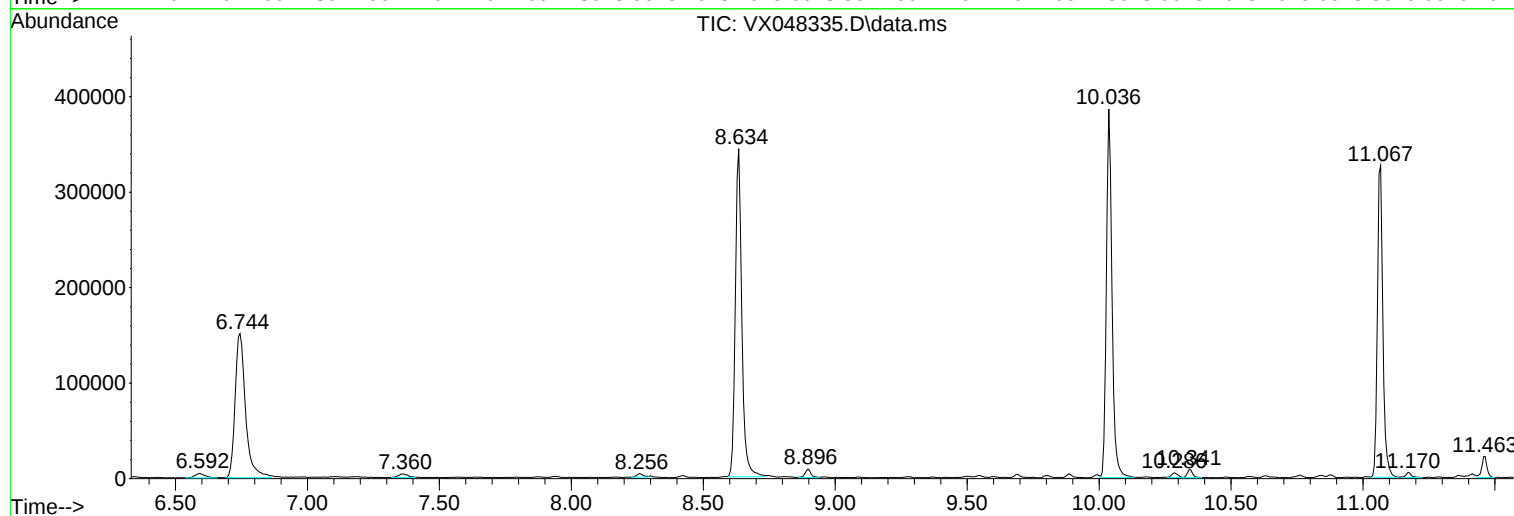
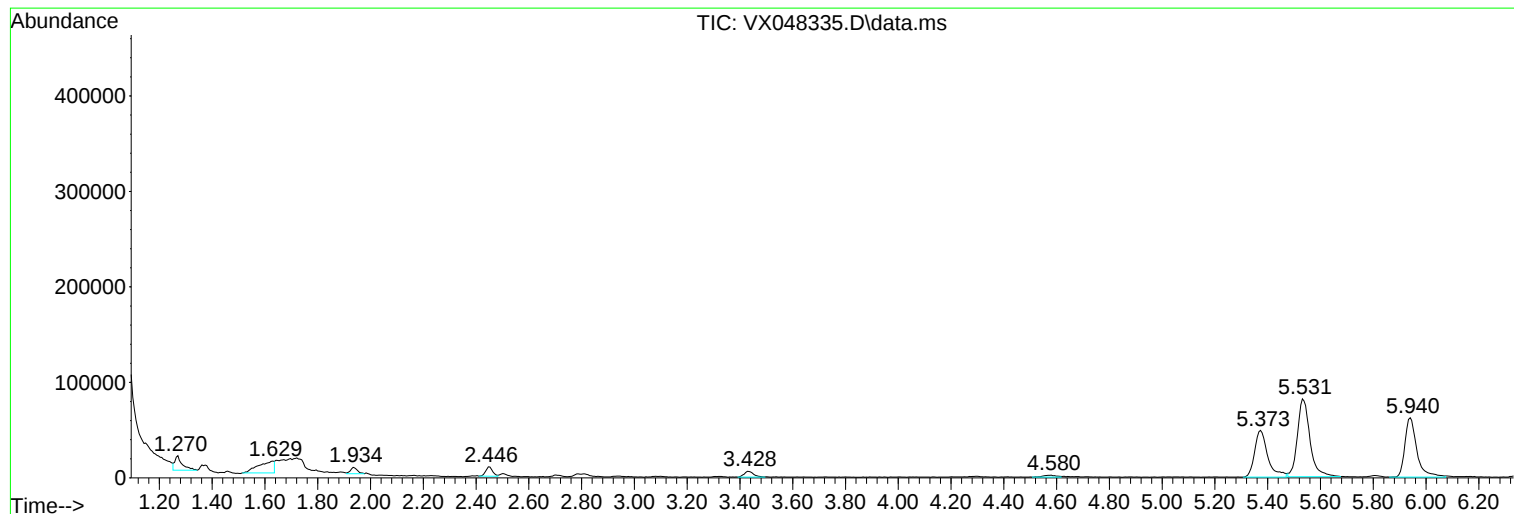
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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



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Instrument :
MSVOA_X
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461

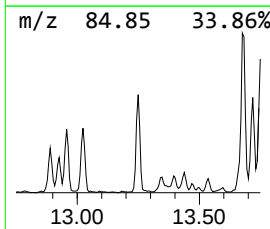
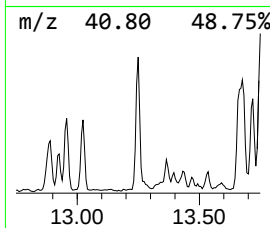
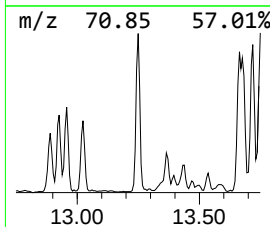
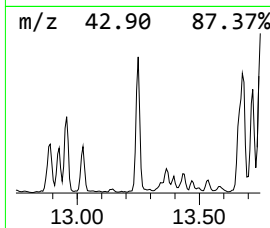
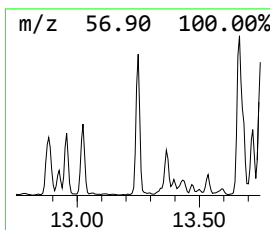
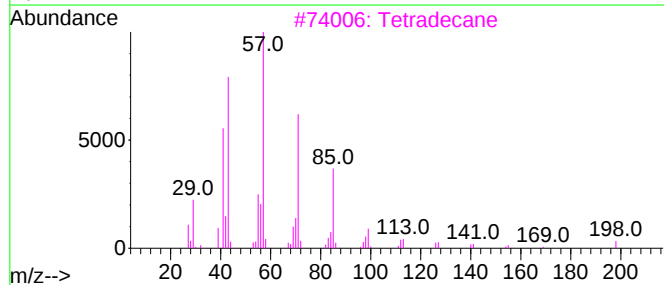
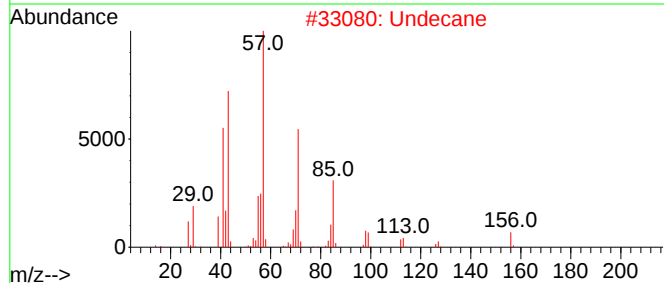
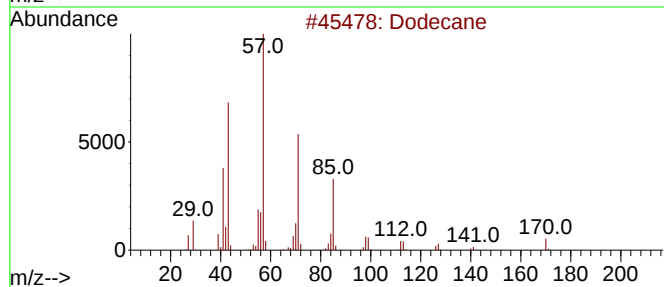
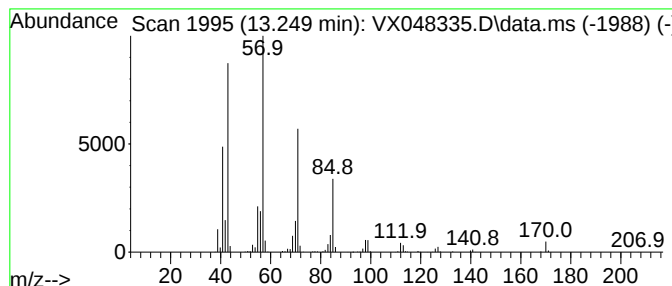
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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

Peak Number 1 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.249	23.00 ug/l	287155	1,4-Dichlorobenzene-d4	12.006

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane	170	C12H26	000112-40-3	96
2		Undecane	156	C11H24	001120-21-4	90
3		Tetradecane	198	C14H30	000629-59-4	90
4		Hexadecane	226	C16H34	000544-76-3	86
5		Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	83



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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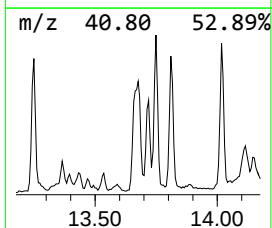
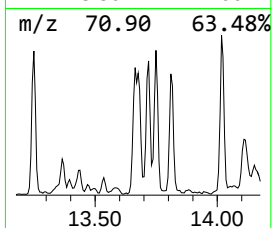
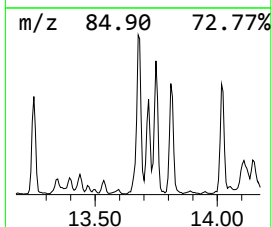
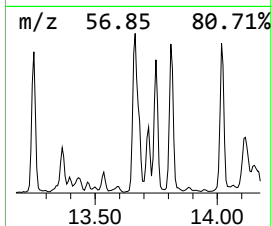
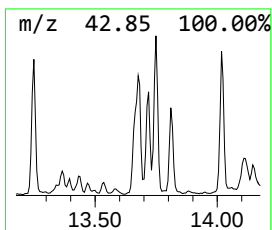
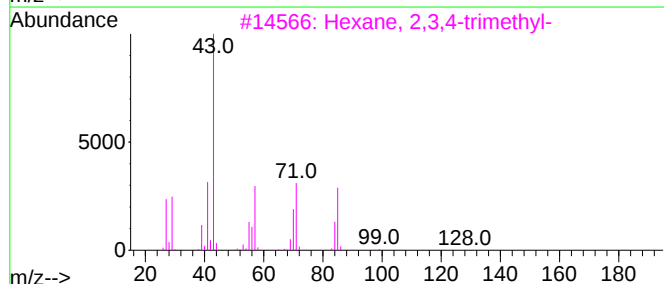
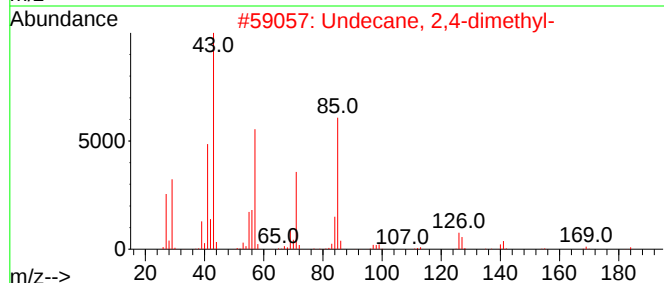
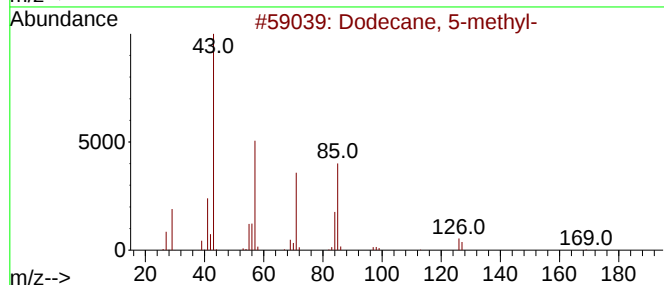
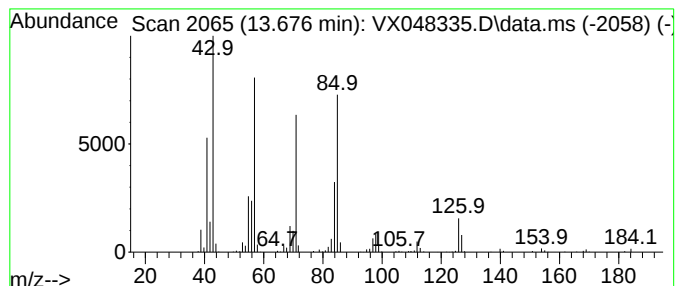
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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

Peak Number 2 Dodecane, 5-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	38.88 ug/l	485450	1,4-Dichlorobenzene-d4	12.006

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 5-methyl-	184	C13H28	017453-93-9	86
2		Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	81
3		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	68
4		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	52
5		Tridecane	184	C13H28	000629-50-5	50



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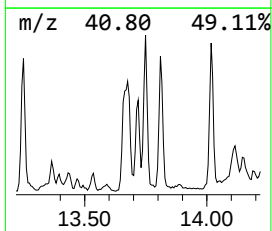
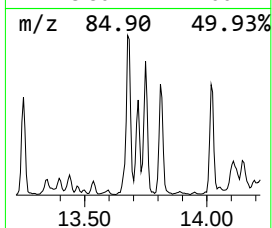
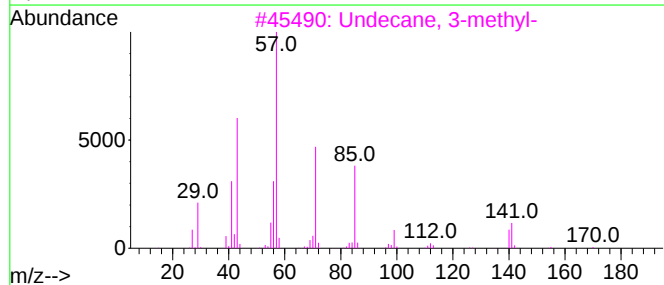
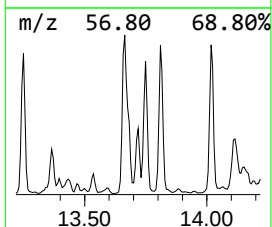
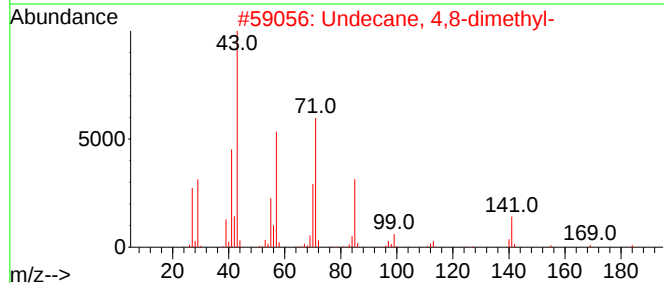
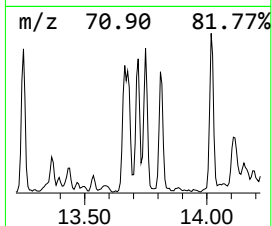
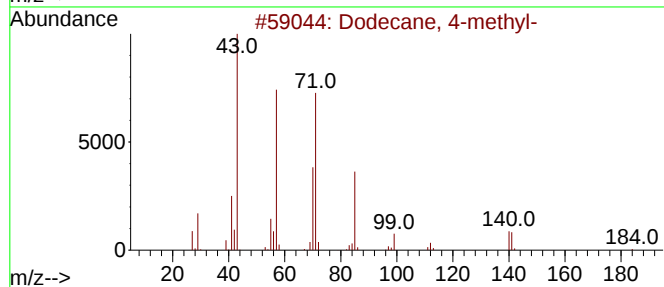
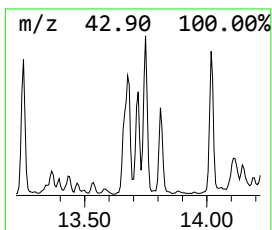
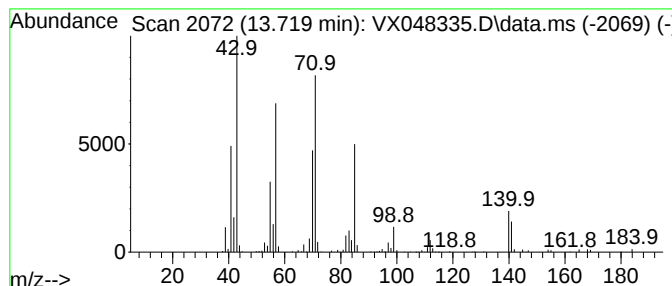
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.M
Quant Title : SW846 8260

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

Peak Number 3 Dodecane, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.719	16.59 ug/l	207127	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4-methyl-	184	C13H28	006117-97-1	95
2			Undecane, 4,8-dimethyl-	184	C13H28	017301-33-6	76
3			Undecane, 3-methyl-	170	C12H26	001002-43-3	59
4			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	50
5			Decane, 2,8,8-trimethyl-	184	C13H28	1000060-81-2	50



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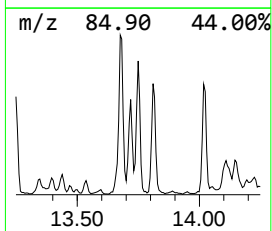
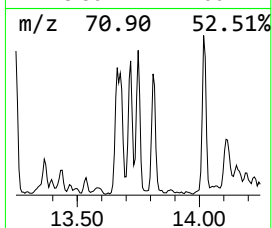
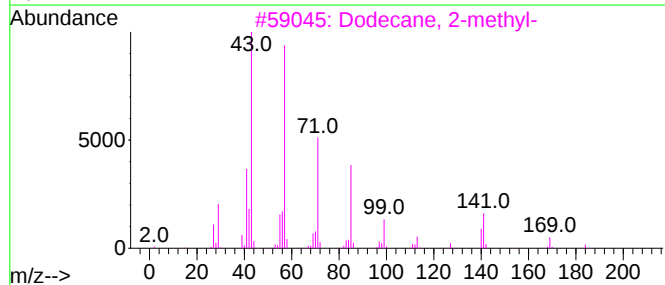
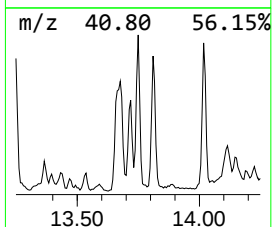
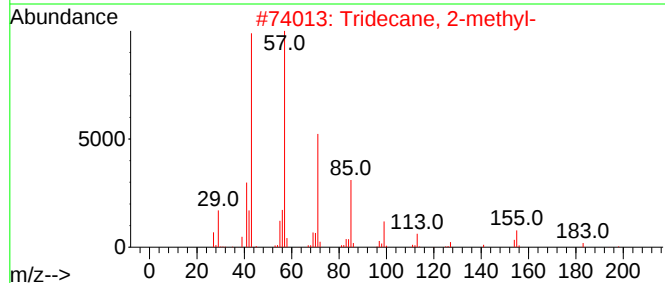
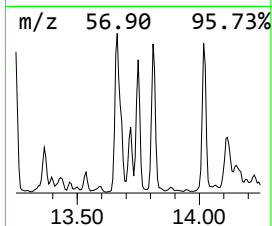
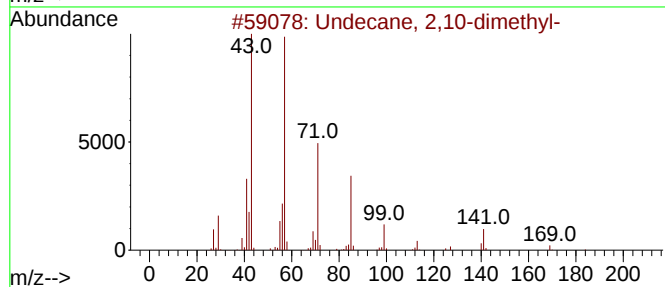
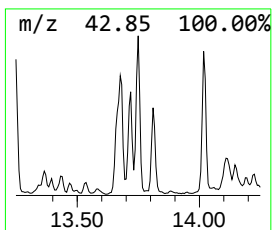
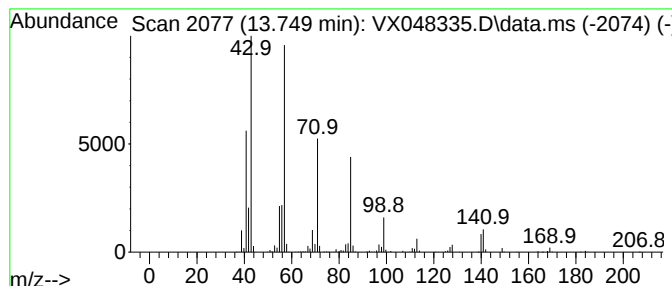
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.749	22.88 ug/l	285656	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	97
2			Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	83
4			Decane	142	C10H22	000124-18-5	59
5			Tetradecane, 5-methyl-	212	C15H32	025117-32-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

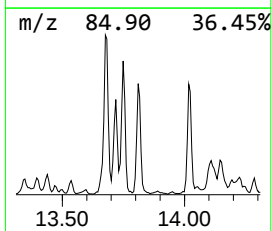
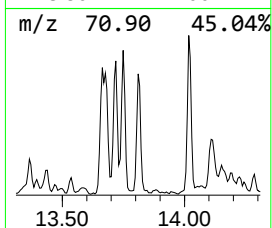
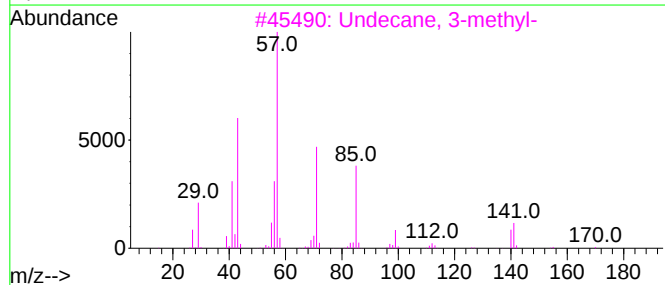
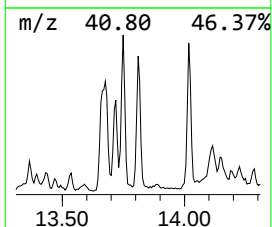
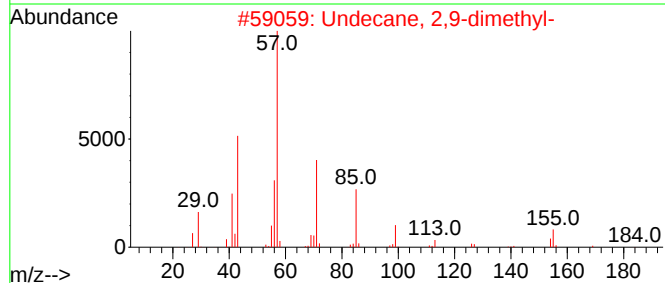
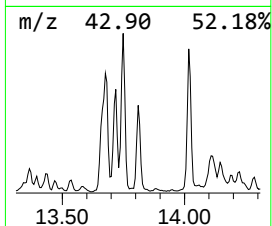
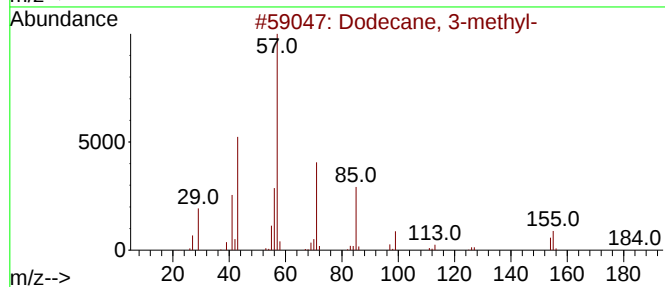
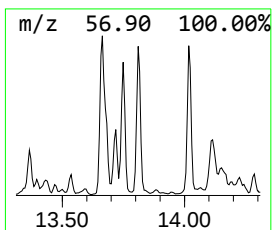
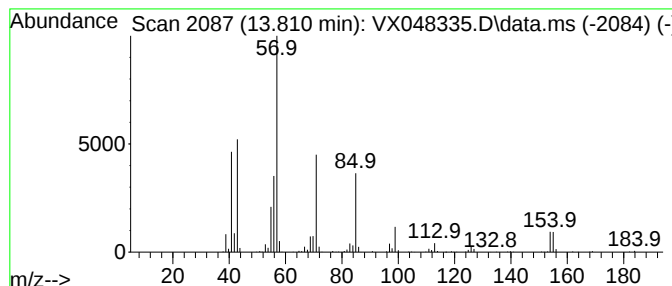
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Quant Title : SW846 8260

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

Peak Number 5 Dodecane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	23.60 ug/l	294595	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 3-methyl-	184	C13H28	017312-57-1	91
2			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	87
3			Undecane, 3-methyl-	170	C12H26	001002-43-3	64
4			1-Iodoundecane	282	C11H23I	004282-44-4	64
5			Decane, 3-methyl-	156	C11H24	013151-34-3	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

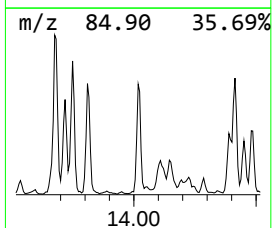
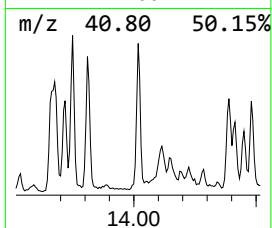
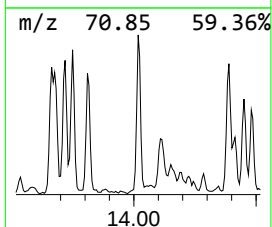
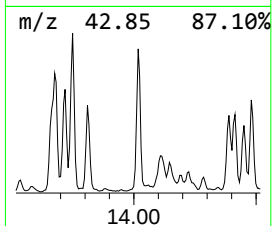
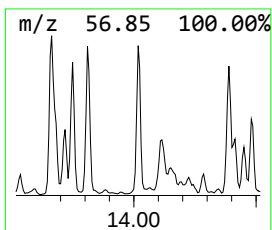
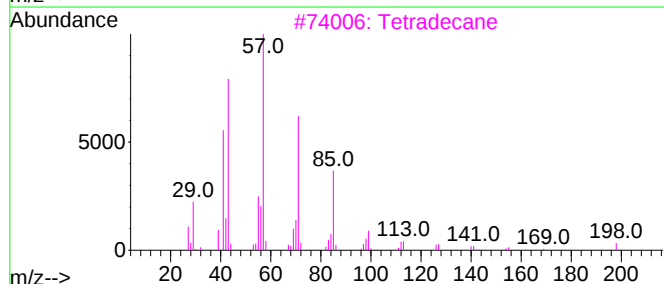
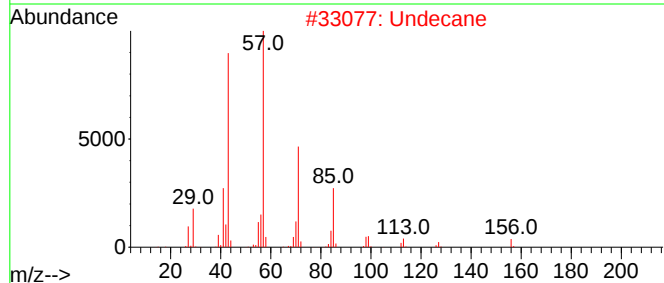
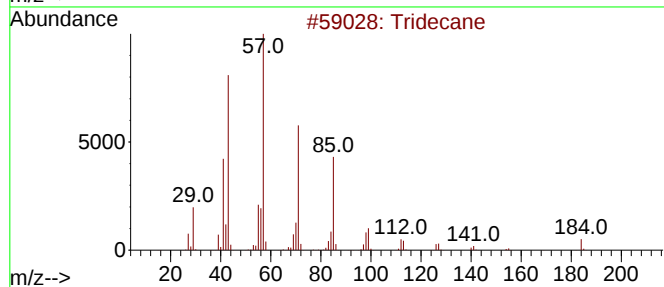
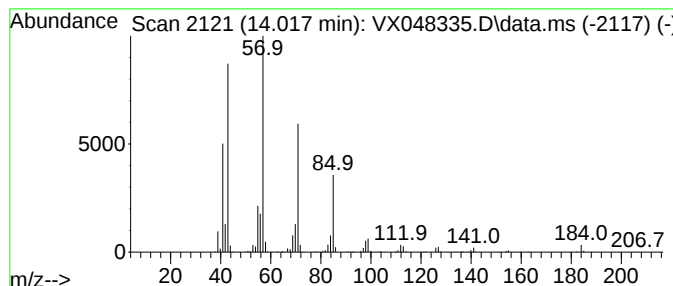
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Quant Title : SW846 8260

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

Peak Number 6 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.017	22.66 ug/l	282898	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	97
2			Undecane	156	C11H24	001120-21-4	90
3			Tetradecane	198	C14H30	000629-59-4	90
4			Hexadecane	226	C16H34	000544-76-3	90
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

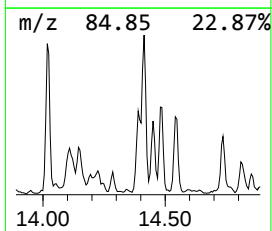
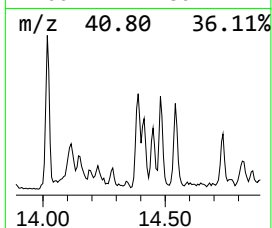
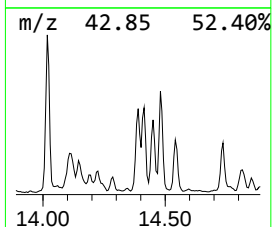
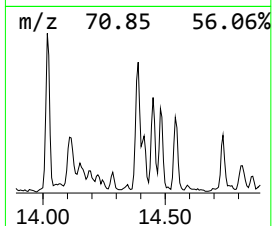
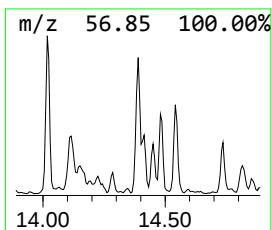
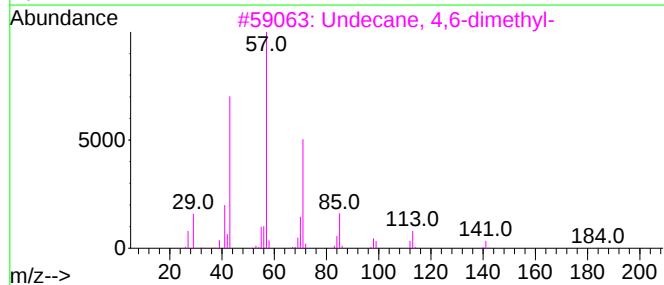
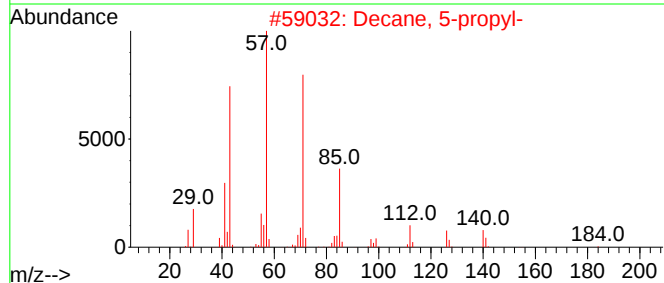
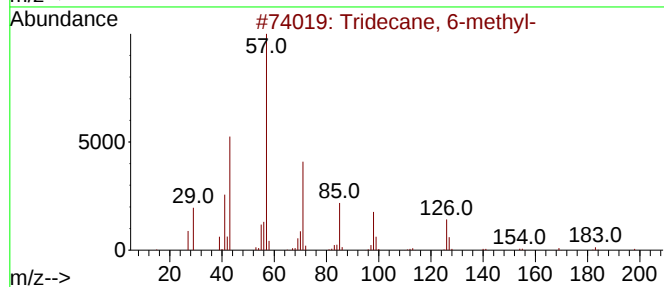
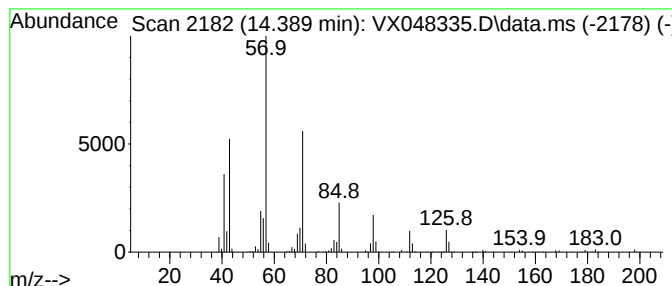
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane, 6-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.389	20.39 ug/l	254585	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-methyl-	198	C14H30	013287-21-3	86
2			Decane, 5-propyl-	184	C13H28	017312-62-8	76
3			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	64
4			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	59
5			Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

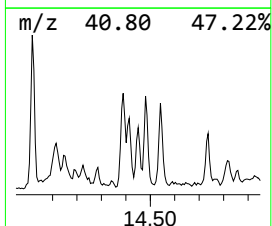
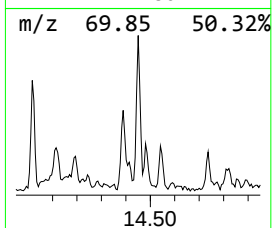
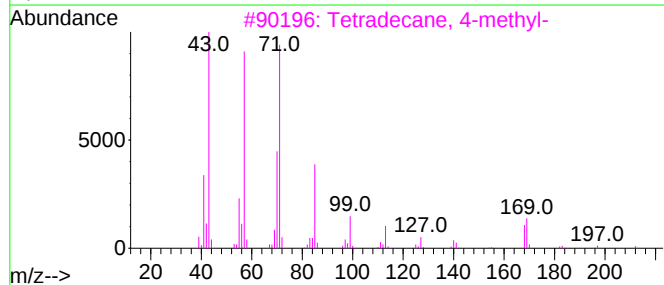
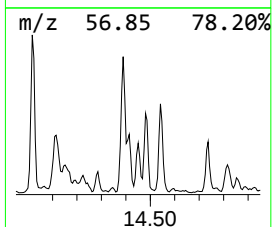
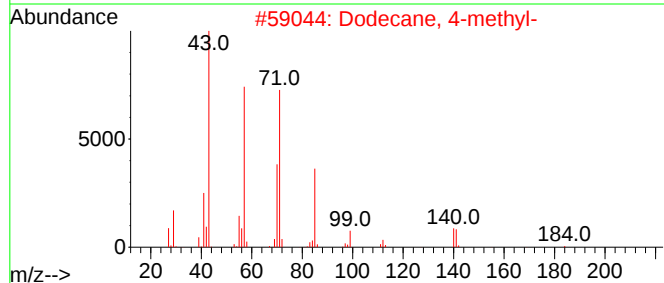
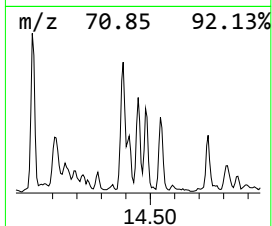
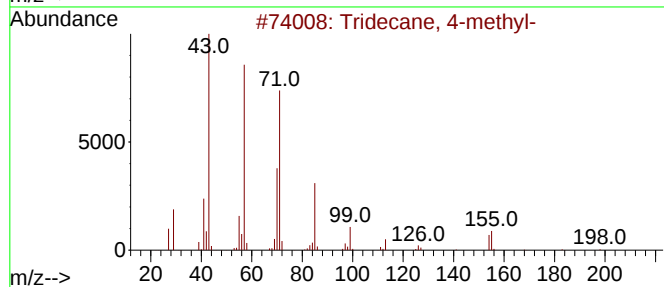
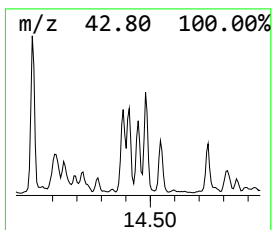
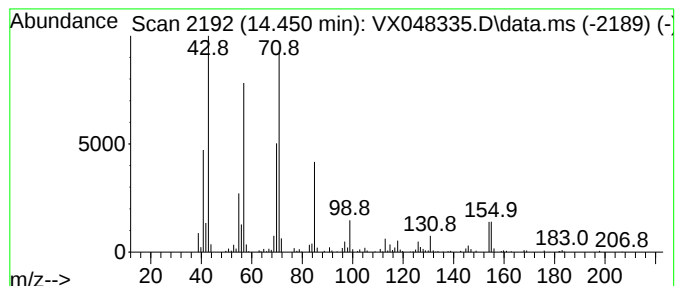
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.450	13.49 ug/l	168462	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 4-methyl-	198	C14H30	026730-12-1	94
2			Dodecane, 4-methyl-	184	C13H28	006117-97-1	80
3			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72
4			Decane, 3,3,5-trimethyl-	184	C13H28	062338-13-0	64
5			Decane, 2,8,8-trimethyl-	184	C13H28	1000060-81-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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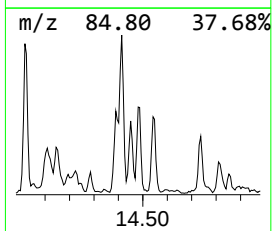
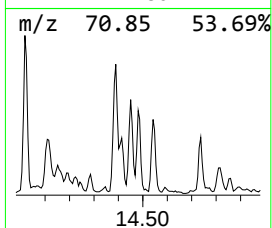
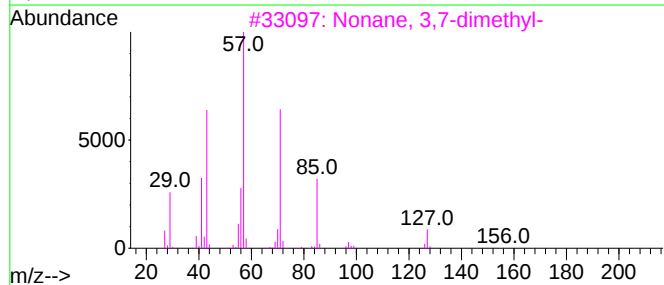
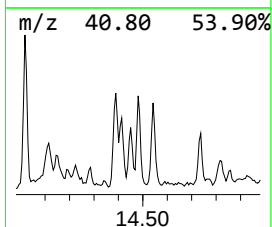
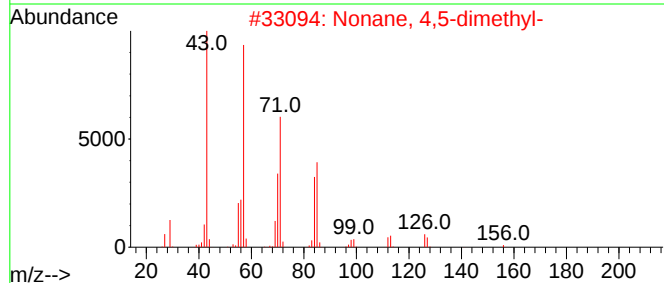
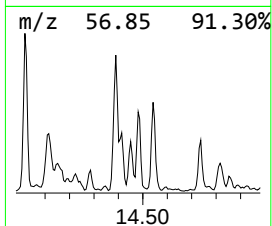
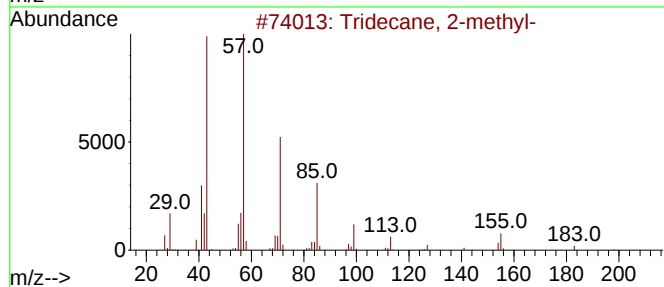
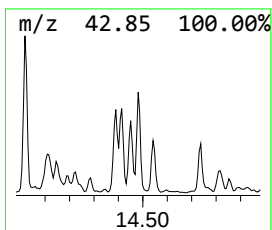
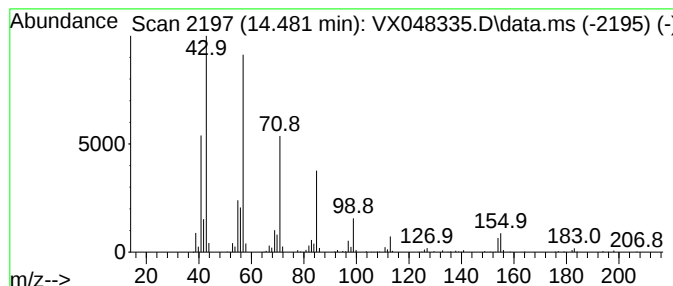
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.481	14.29 ug/l	178374	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 2-methyl-	198	C14H30	001560-96-9	90
2			Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	81
3			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	74
4			Heptacosane	380	C27H56	000593-49-7	74
5			Tridecane, 6-methyl-	198	C14H30	013287-21-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

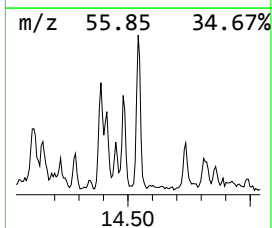
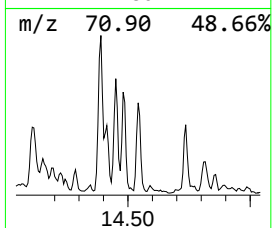
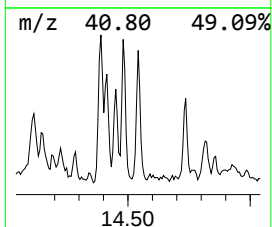
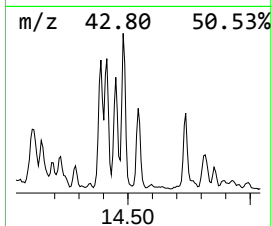
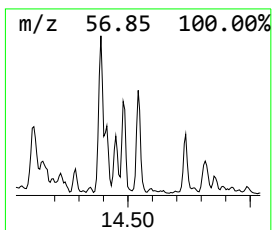
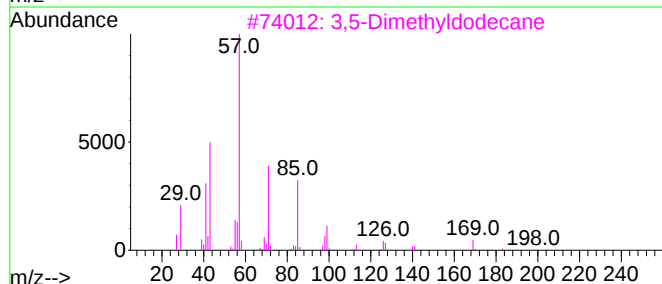
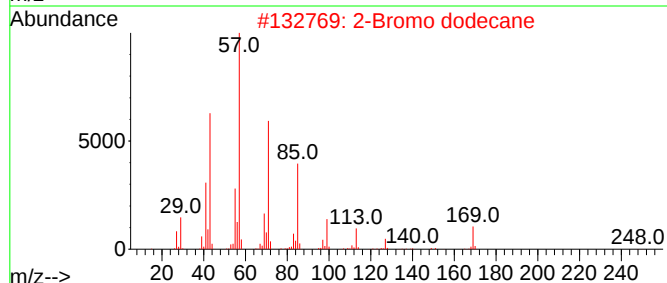
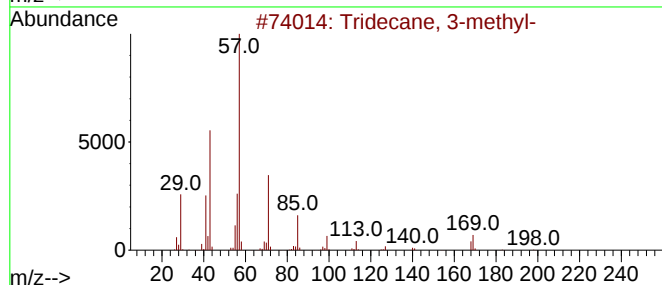
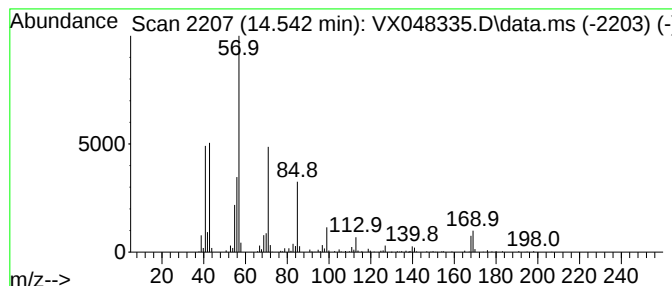
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Quant Title : SW846 8260

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

Peak Number 10 Tridecane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.542	13.99 ug/l	174709	1,4-Dichlorobenzene-d4	12.006

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 3-methyl-	198	C14H30	006418-41-3	89
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	86
3			3,5-Dimethyldodecane	198	C14H30	107770-99-0	74
4			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	72
5			Tetradecane, 4-methyl-	212	C15H32	025117-24-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102325\
Data File : VX048335.D
Acq On : 23 Oct 2025 18:32
Operator : JC/MD
Sample : Q3388-01
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
461

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102025W.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	13.249	23.0	ug/l	287155	4	12.006	624224	50.0
Dodecane, 5-met...	13.676	38.9	ug/l	485450	4	12.006	624224	50.0
Dodecane, 4-met...	13.719	16.6	ug/l	207127	4	12.006	624224	50.0
Undecane, 2,10-...	13.749	22.9	ug/l	285656	4	12.006	624224	50.0
Dodecane, 3-met...	13.810	23.6	ug/l	294595	4	12.006	624224	50.0
Tridecane	14.017	22.7	ug/l	282898	4	12.006	624224	50.0
Tridecane, 6-me...	14.389	20.4	ug/l	254585	4	12.006	624224	50.0
Tridecane, 4-me...	14.450	13.5	ug/l	168462	4	12.006	624224	50.0
Tridecane, 2-me...	14.481	14.3	ug/l	178374	4	12.006	624224	50.0
Tridecane, 3-me...	14.542	14.0	ug/l	174709	4	12.006	624224	50.0