

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071374.D
 Acq On : 18 Mar 2022 15:54
 Operator : JC\MD
 Sample : N2009-06 10X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 40453

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\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	37	41	49	rVB4	21205	44370	1.00%	0.152%
2	2.581	95	101	113	rBV	538529	950907	21.52%	3.261%
3	2.816	136	141	148	rVB	49885	100428	2.27%	0.344%
4	3.904	318	326	338	rVB2	16724	45822	1.04%	0.157%
5	4.281	380	390	410	rBV	229652	676910	15.32%	2.322%
6	7.334	899	909	921	rBV	40212	103353	2.34%	0.354%
7	8.022	1013	1026	1031	rBV	529502	1320658	29.88%	4.530%
8	8.081	1031	1036	1050	rVB	1031259	2313744	52.36%	7.936%
9	8.433	1085	1096	1113	rBV	632893	1447514	32.75%	4.965%
10	8.963	1177	1186	1206	rBV	1557614	3176425	71.88%	10.894%
11	10.439	1428	1437	1446	rBV	2433125	4419313	100.00%	15.157%
12	11.180	1553	1563	1574	rVB2	59208	128750	2.91%	0.442%
13	11.739	1648	1658	1672	rBV	2241008	3996984	90.44%	13.709%
14	12.351	1755	1762	1768	rBV	30027	52375	1.19%	0.180%
15	12.527	1784	1792	1797	rBV2	80027	165813	3.75%	0.569%
16	12.580	1797	1801	1811	rVB	72015	129045	2.92%	0.443%
17	12.727	1818	1826	1839	rVB	1868834	3117938	70.55%	10.694%
18	13.045	1866	1880	1888	rBV4	39263	81787	1.85%	0.281%
19	13.527	1953	1962	1966	rBV4	36729	86541	1.96%	0.297%
20	13.592	1966	1973	1978	rVV6	46809	103411	2.34%	0.355%
21	13.674	1978	1987	1992	rBV	1784078	3080024	69.69%	10.564%
22	13.727	1992	1996	2006	rVB2	201475	465091	10.52%	1.595%
23	13.886	2016	2023	2030	rBV2	180399	361989	8.19%	1.242%
24	13.957	2030	2035	2037	rBV3	56923	96038	2.17%	0.329%
25	13.992	2037	2041	2045	rBV	283472	422756	9.57%	1.450%
26	14.198	2071	2076	2079	rBV6	40221	82356	1.86%	0.282%
27	14.380	2103	2107	2115	rVV7	43018	99422	2.25%	0.341%
28	14.504	2123	2128	2133	rVB4	86862	159601	3.61%	0.547%
29	14.621	2143	2148	2151	rBV4	54677	96295	2.18%	0.330%
30	14.662	2153	2155	2161	rVB4	41540	59257	1.34%	0.203%
31	14.845	2181	2186	2194	rVV	88489	137952	3.12%	0.473%
32	14.915	2194	2198	2202	rVV7	26672	48985	1.11%	0.168%
33	14.962	2202	2206	2214	rVB4	45882	108062	2.45%	0.371%
34	15.386	2274	2278	2285	rVB6	40057	82250	1.86%	0.282%
35	15.462	2286	2291	2298	rBV2	75776	137943	3.12%	0.473%
36	15.704	2327	2332	2339	rBV7	25141	63619	1.44%	0.218%

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37	15.815	2347	2351	2356	rVV5	28612	49660	1.12%	0.170%
38	15.880	2358	2362	2370	rVB5	60645	129761	2.94%	0.445%
39	16.033	2383	2388	2391	rBV5	38724	77428	1.75%	0.266%
40	16.251	2422	2425	2430	rBV3	56200	85081	1.93%	0.292%
41	16.309	2430	2435	2437	rBV2	82920	147142	3.33%	0.505%
42	16.386	2443	2448	2455	rVB2	139481	291327	6.59%	0.999%
43	16.456	2455	2460	2469	rVB	200273	412247	9.33%	1.414%

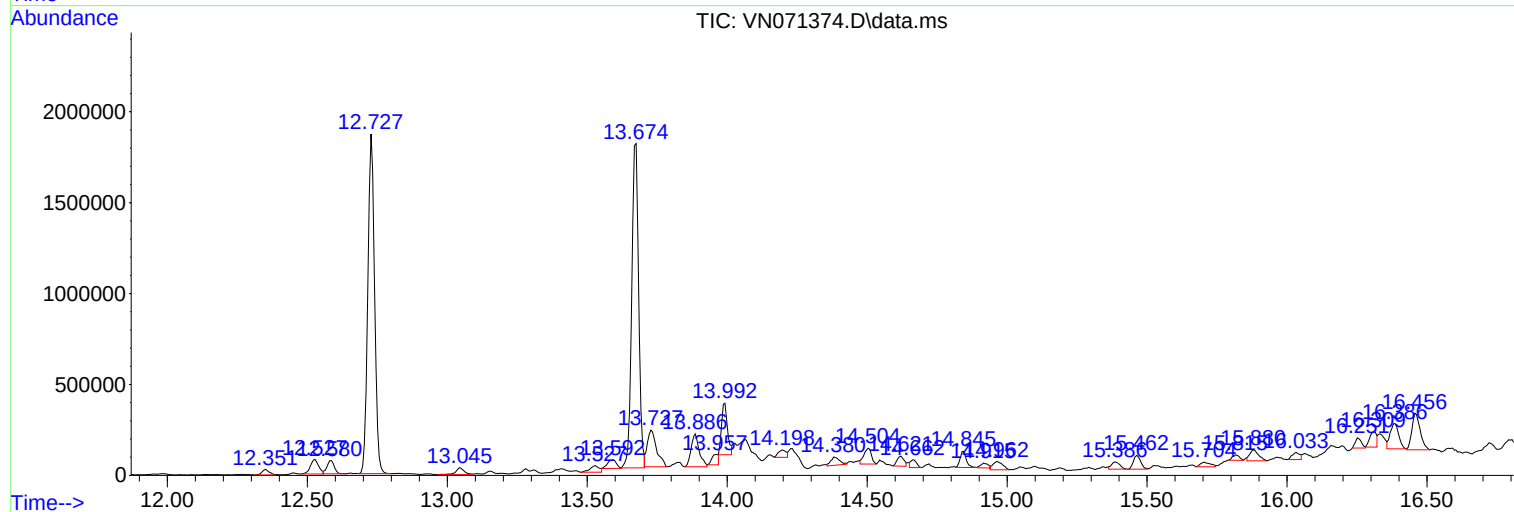
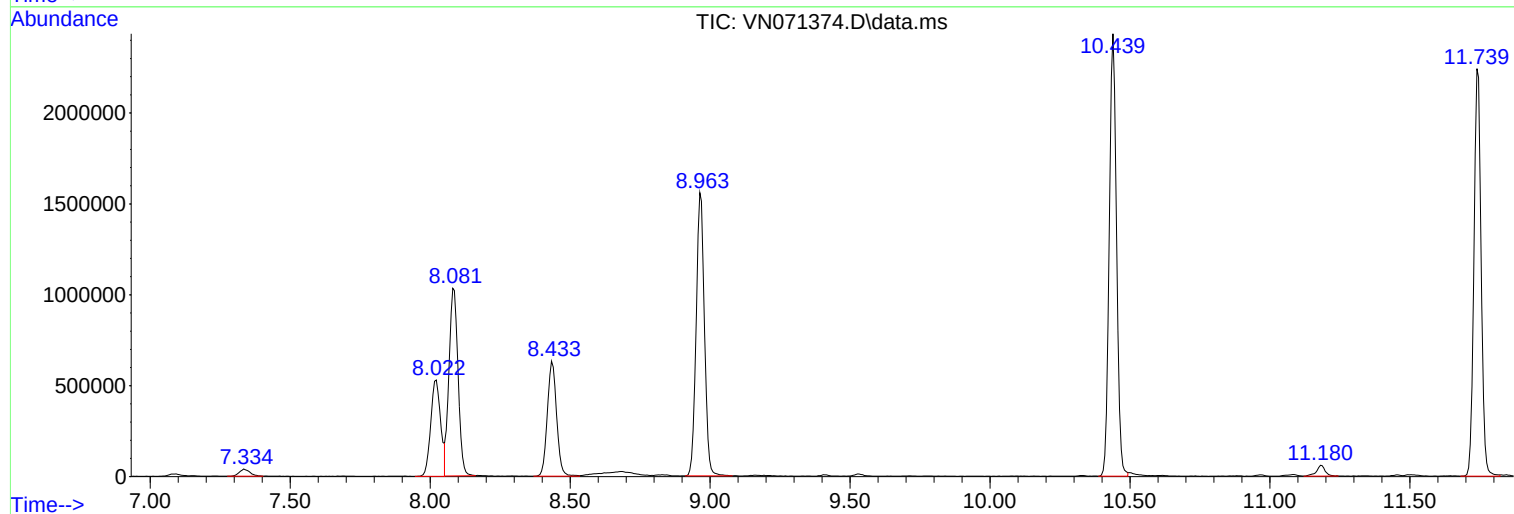
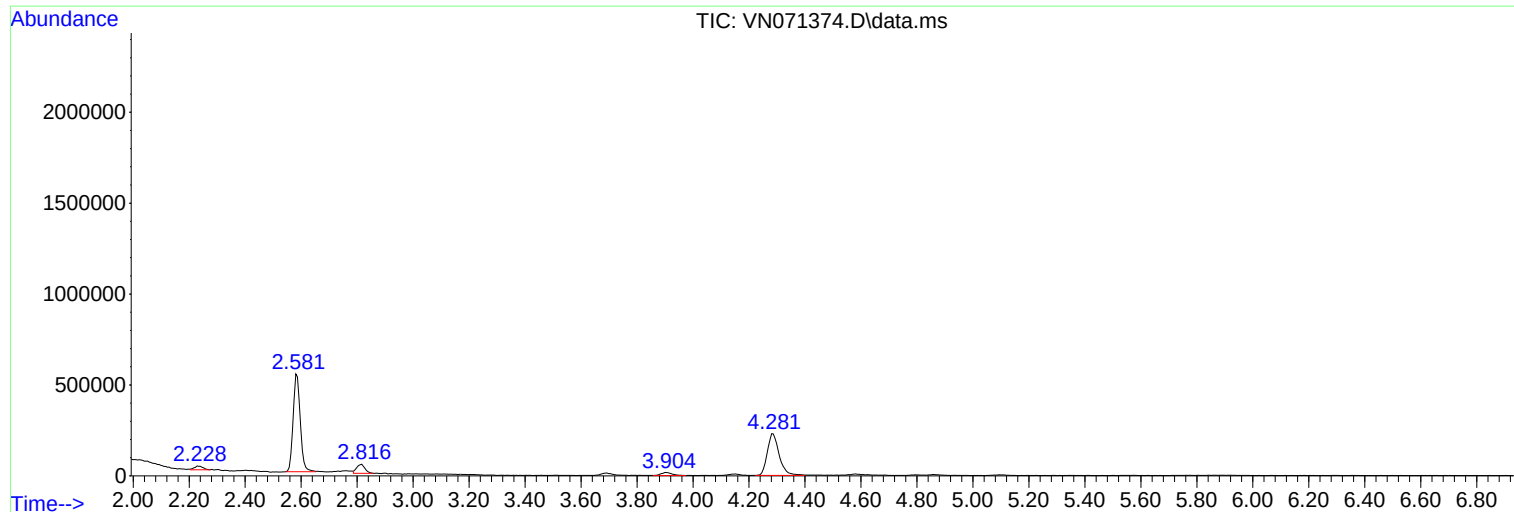
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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40453

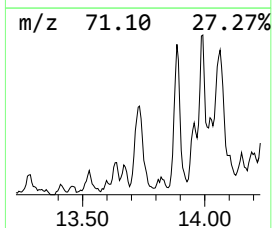
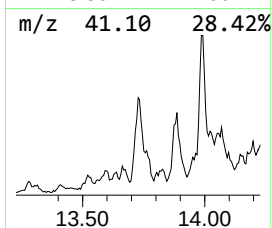
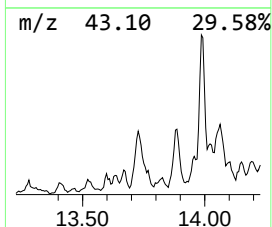
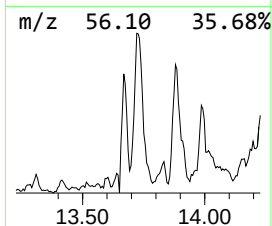
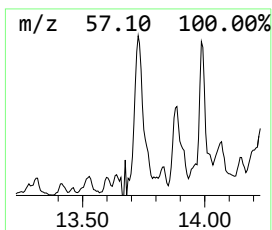
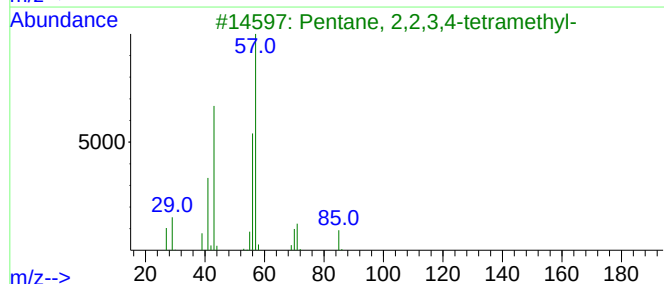
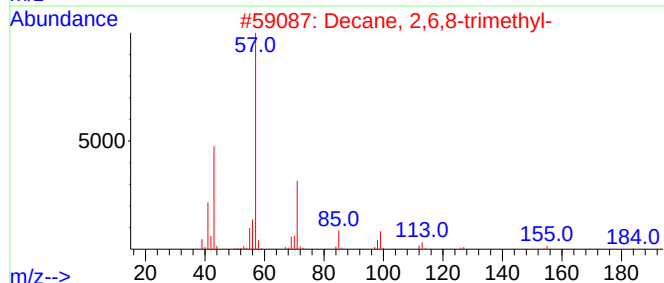
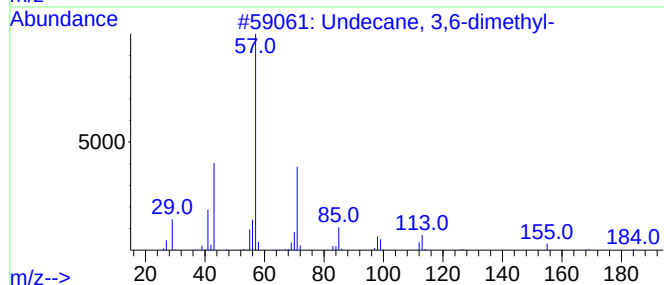
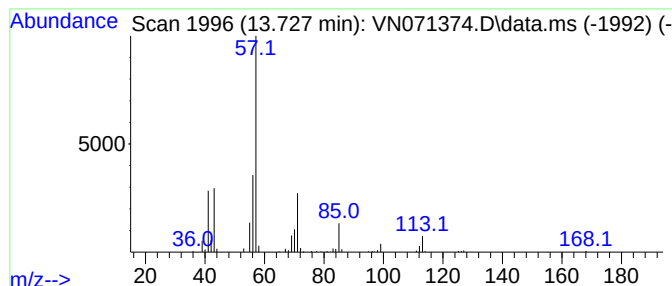
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	7.55 ug/l	465091	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	72
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	59
3			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59
4			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	53
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53



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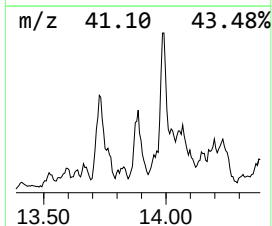
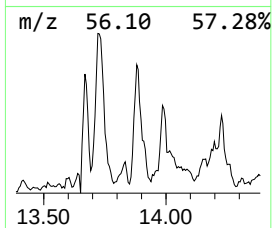
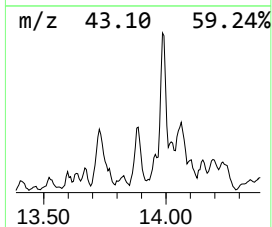
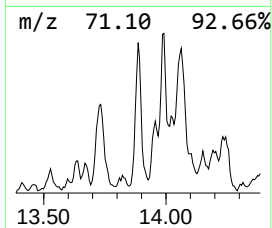
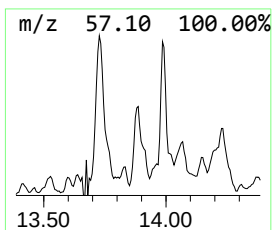
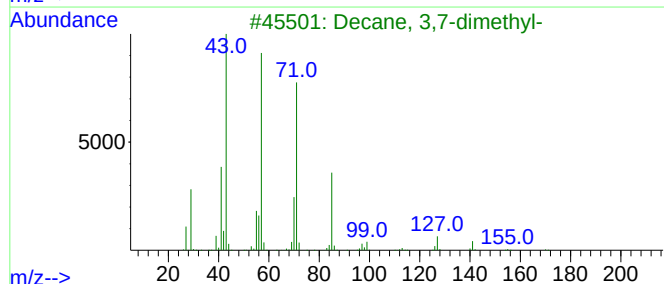
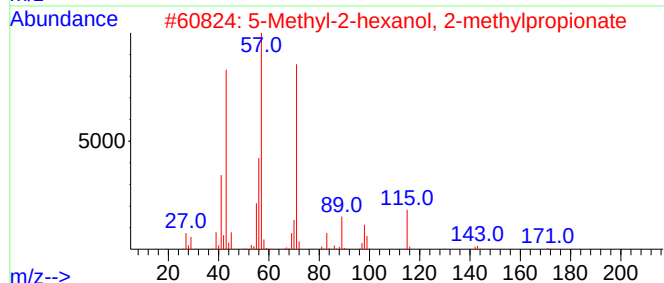
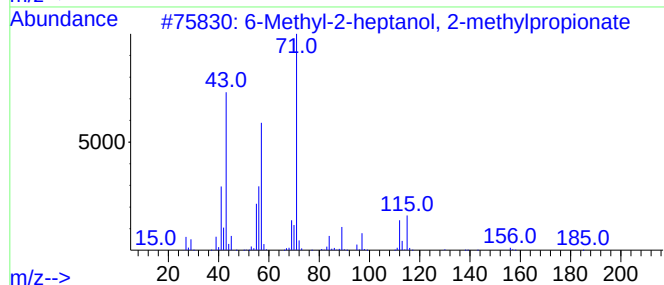
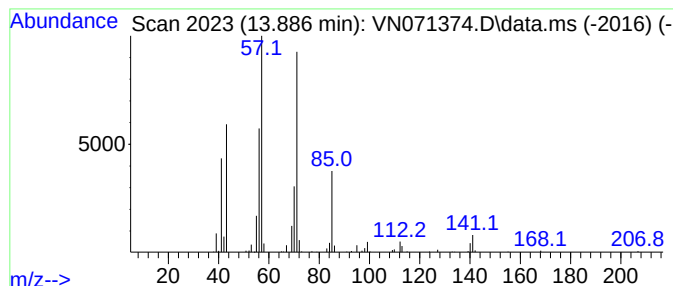
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 6-Methyl-2-heptanol, 2-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.88 ug/l	361989	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Methyl-2-heptanol, 2-methylpro...	200	C12H24O2	1000447-36-7	59
2			5-Methyl-2-hexanol, 2-methylprop...	186	C11H22O2	1000447-34-4	59
3			Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	59
4			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	58
5			Nonane, 3-methyl-	142	C10H22	005911-04-6	47



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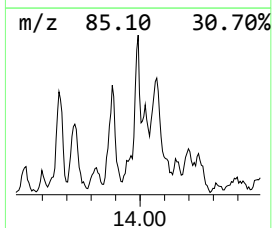
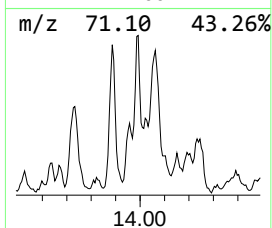
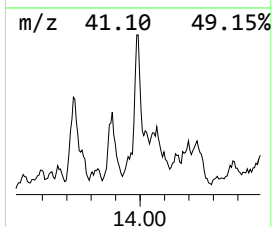
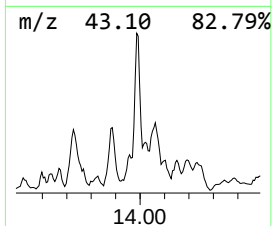
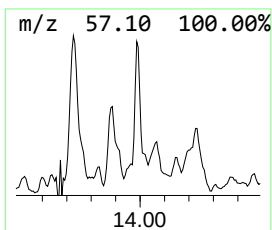
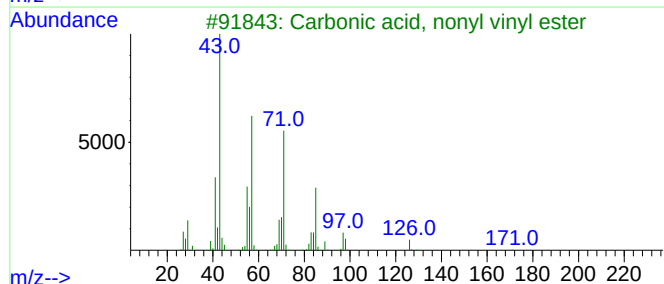
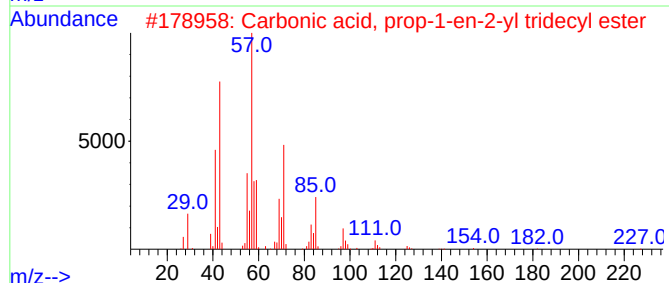
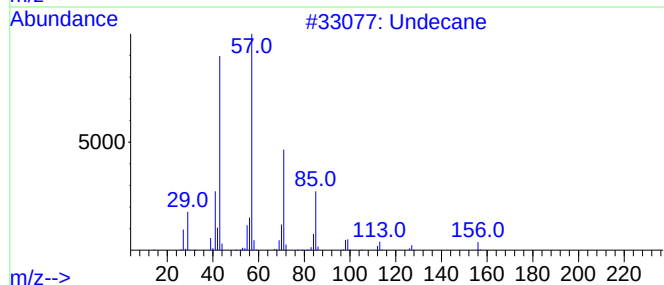
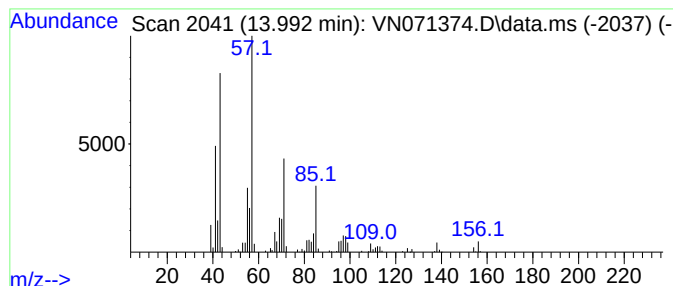
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	6.86 ug/l	422756	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	83
2	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	72
3	Carbonic acid, nonyl vinyl ester			214	C12H22O3	1000383-25-6	64
4	Carbonic acid, nonyl prop-1-en-2...			228	C13H24O3	1000382-53-9	59
5	Tridecane			184	C13H28	000629-50-5	59



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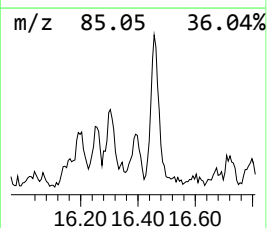
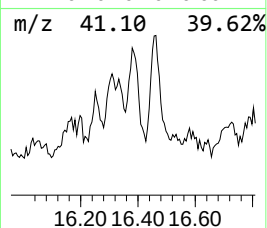
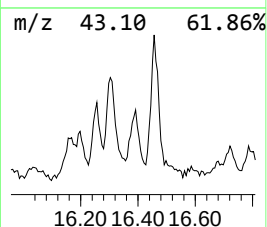
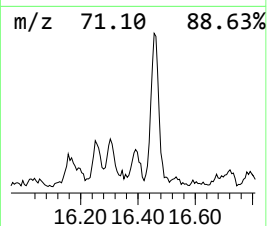
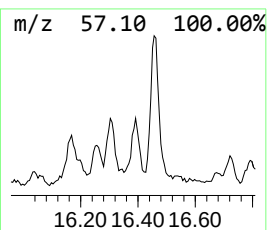
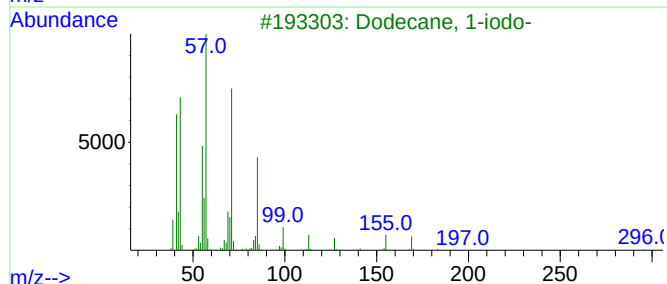
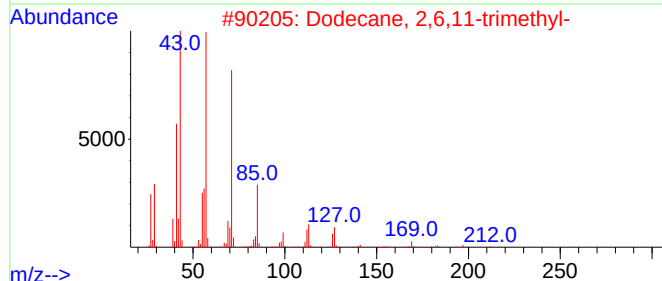
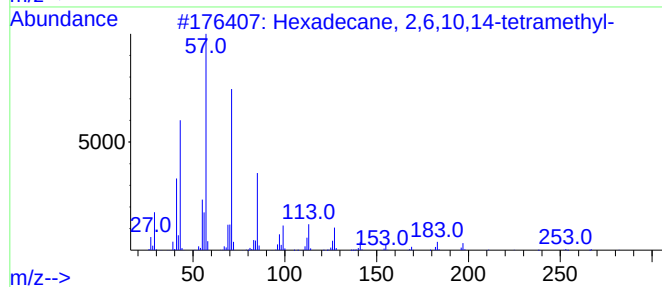
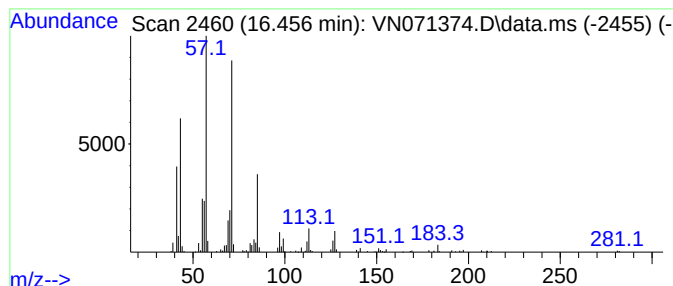
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Quant Title : SW846 8260

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

Peak Number 5 Hexadecane, 2,6,10,14-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.456	6.69 ug/l	412247	1,4-Dichlorobenzene-d4	13.674

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	58
5			Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	53



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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
Undecane, 3,6-d...	13.727	7.5	ug/l	465091	4	13.674	3080020	50.0
6-Methyl-2-hept...	13.886	5.9	ug/l	361989	4	13.674	3080020	50.0
Undecane	13.992	6.9	ug/l	422756	4	13.674	3080020	50.0
Hexadecane, 2,6...	16.456	6.7	ug/l	412247	4	13.674	3080020	50.0