

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY032421\
 Data File : VY004183.D
 Acq On : 24 Mar 2021 13:15
 Operator : SY/MD
 Sample : M1777-01
 Misc : 5.05g/5mL/MSVOA_Y/SOIL
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 244

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_Y\methods\82Y030821S.M
 Title : SW846 8260

Signal : TIC: VY004183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.960	343	351	361	rBV	4444	12633	1.25%	0.164%
2	4.424	416	427	443	rBV	8602	30860	3.06%	0.400%
3	4.735	465	478	491	rBV	12166	36766	3.65%	0.476%
4	4.972	504	517	526	rBV3	4917	17811	1.77%	0.231%
5	7.728	958	969	975	rBV	138125	332776	33.03%	4.309%
6	7.801	975	981	995	rVB	236417	537479	53.35%	6.959%
7	8.155	1029	1039	1052	rBV	139113	318544	31.62%	4.124%
8	8.697	1120	1128	1141	rBV	374636	724567	71.92%	9.381%
9	10.185	1364	1372	1379	rBV	586450	1007409	100.00%	13.043%
10	10.246	1379	1382	1388	rVB	12944	20131	2.00%	0.261%
11	11.496	1579	1587	1598	rVB	532172	871683	86.53%	11.286%
12	11.703	1616	1621	1627	rBV	14215	25728	2.55%	0.333%
13	12.032	1668	1675	1684	rVB4	6101	11508	1.14%	0.149%
14	12.483	1742	1749	1760	rVB	455559	710422	70.52%	9.198%
15	12.806	1798	1802	1808	rVB3	14461	22367	2.22%	0.290%
16	13.038	1836	1840	1845	rVB2	12907	18327	1.82%	0.237%
17	13.123	1845	1854	1858	rBV2	8883	15549	1.54%	0.201%
18	13.318	1878	1886	1890	rBV6	13412	30534	3.03%	0.395%
19	13.367	1890	1894	1896	rVV	24575	36621	3.64%	0.474%
20	13.428	1896	1904	1913	rVV	588921	934595	92.77%	12.101%
21	13.501	1913	1916	1923	rVV	35724	51467	5.11%	0.666%
22	13.568	1923	1927	1931	rVV5	6835	12665	1.26%	0.164%
23	13.623	1931	1936	1940	rVV6	7210	16607	1.65%	0.215%
24	13.672	1940	1944	1950	rVV6	9855	22987	2.28%	0.298%
25	13.751	1951	1957	1962	rVV	363054	534608	53.07%	6.922%
26	13.794	1962	1964	1968	rVV	32981	53557	5.32%	0.693%
27	13.855	1971	1974	1978	rVV6	25043	55128	5.47%	0.714%
28	13.916	1980	1984	1990	rVV4	42287	106753	10.60%	1.382%
29	13.971	1990	1993	1997	rVV2	34658	60740	6.03%	0.786%
30	14.019	1997	2001	2006	rVV	25640	38998	3.87%	0.505%
31	14.080	2006	2011	2016	rVV4	27222	45702	4.54%	0.592%
32	14.147	2016	2022	2027	rVV5	17102	43609	4.33%	0.565%
33	14.196	2027	2030	2032	rVV3	9703	14437	1.43%	0.187%
34	14.263	2032	2041	2046	rVV9	51192	161831	16.06%	2.095%
35	14.312	2046	2049	2056	rVV4	25726	54641	5.42%	0.707%
36	14.385	2056	2061	2064	rVV3	27380	39635	3.93%	0.513%

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37	14.422	2064	2067	2072	rVB4	26098	34918	3.47%	0.452%
38	14.519	2080	2083	2088	rVB	11937	17639	1.75%	0.228%
39	14.611	2088	2098	2103	rVV4	63803	107483	10.67%	1.392%
40	14.678	2103	2109	2115	rVV5	28045	64512	6.40%	0.835%
41	14.733	2115	2118	2125	rVB3	22382	36792	3.65%	0.476%
42	14.836	2131	2135	2140	rVB2	12384	18235	1.81%	0.236%
43	14.946	2149	2153	2157	rBV6	8776	12764	1.27%	0.165%
44	15.007	2157	2163	2168	rBV	107260	171429	17.02%	2.220%
45	15.135	2182	2184	2191	rVB6	8687	14340	1.42%	0.186%
46	15.214	2191	2197	2205	rBV4	11814	38942	3.87%	0.504%
47	15.294	2206	2210	2214	rBV5	8049	16075	1.60%	0.208%
48	15.428	2228	2232	2241	rVB4	34680	64548	6.41%	0.836%
49	15.525	2244	2248	2254	rBV6	7808	18914	1.88%	0.245%
50	15.726	2277	2281	2286	rVB2	17391	28900	2.87%	0.374%
51	16.159	2349	2352	2357	rBV6	7634	14297	1.42%	0.185%
52	16.476	2401	2404	2411	rVB8	18665	34039	3.38%	0.441%

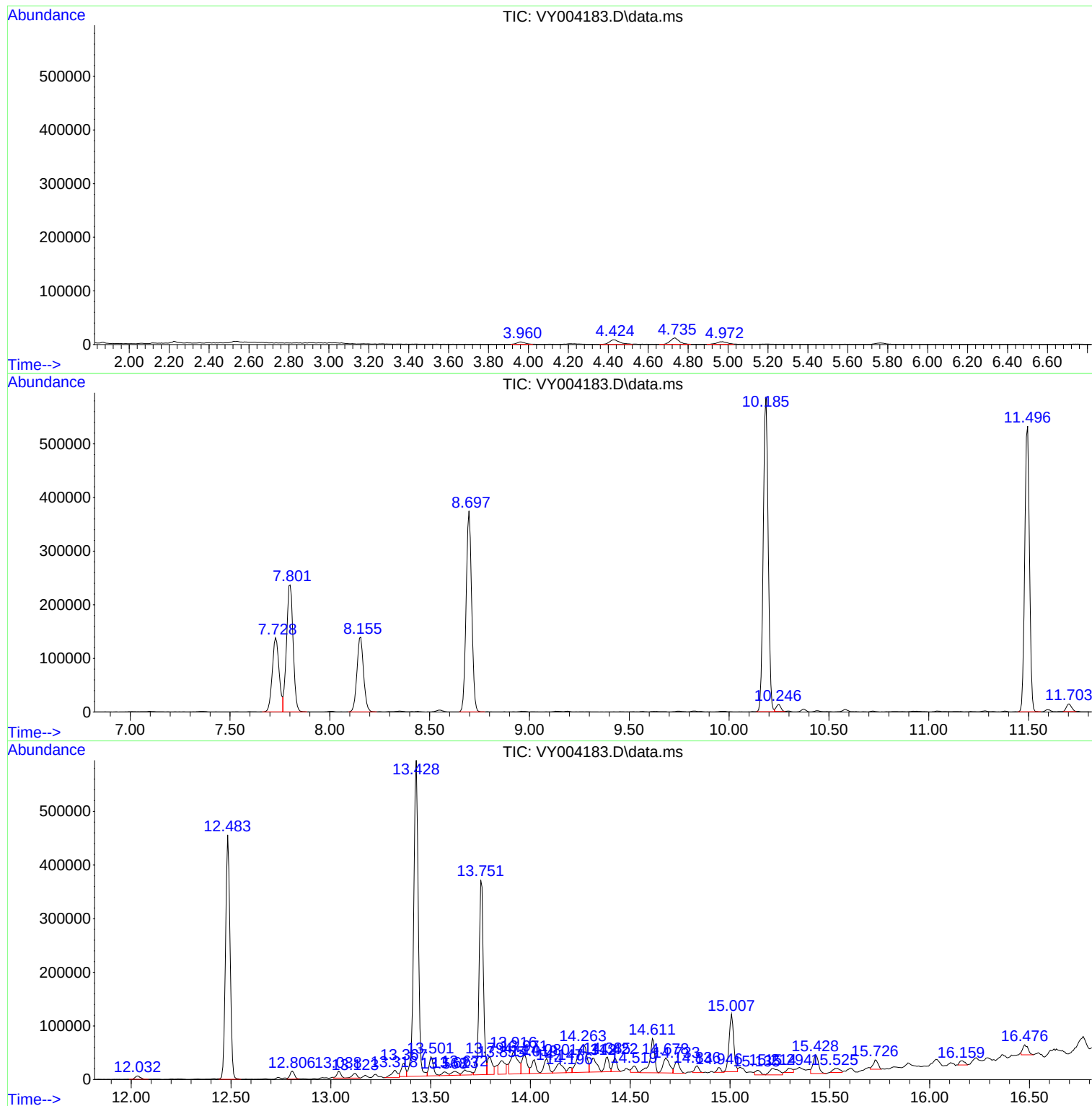
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030821S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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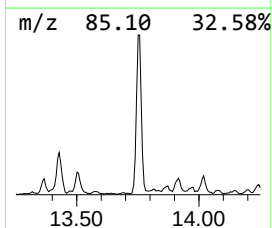
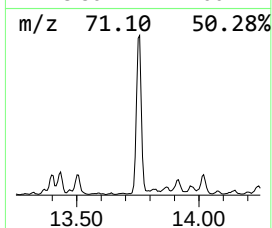
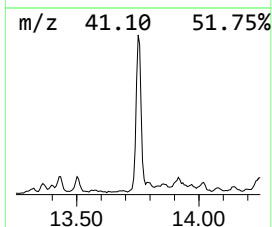
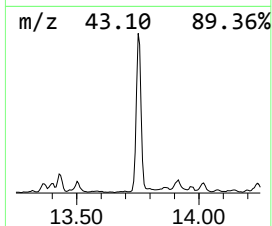
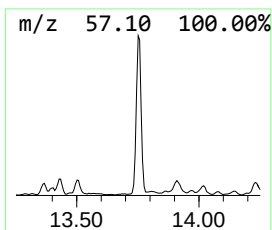
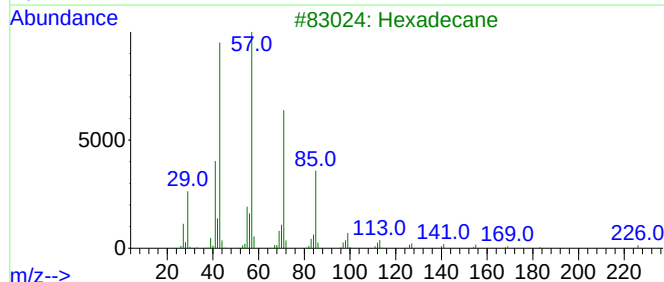
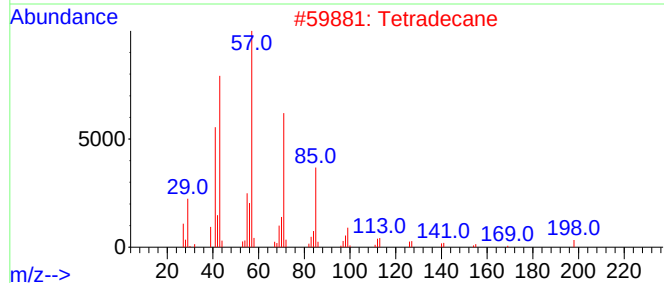
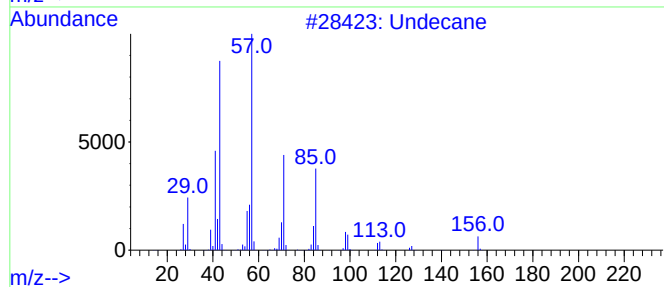
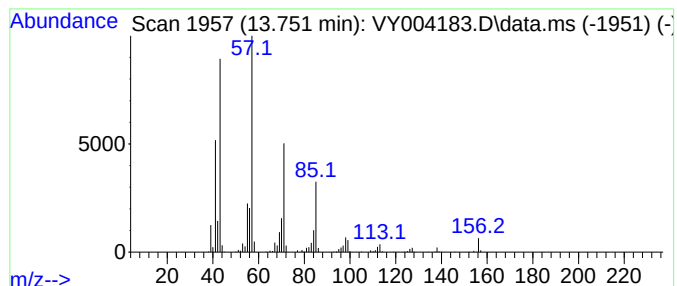
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030821S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	28.60 ug/l	534608	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	95
2	Tetradecane			198	C14H30	000629-59-4	90
3	Hexadecane			226	C16H34	000544-76-3	80
4	Decane, 2,3,5-trimethyl-			184	C13H28	062238-11-3	64
5	Oxalic acid, allyl octyl ester			242	C13H22O4	1000309-23-6	53



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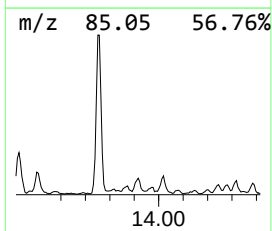
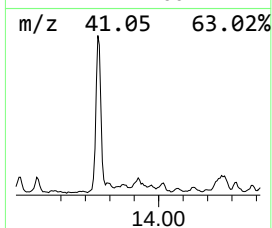
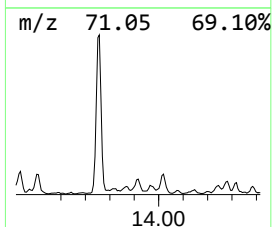
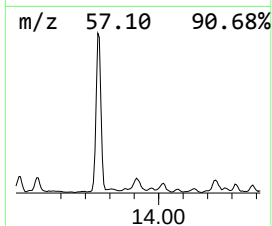
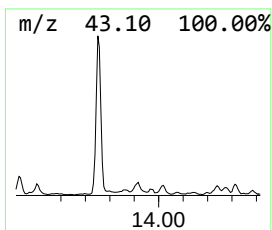
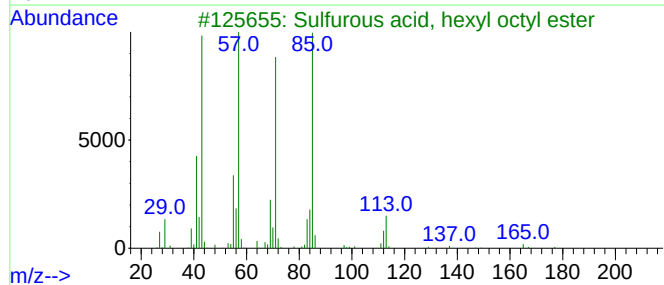
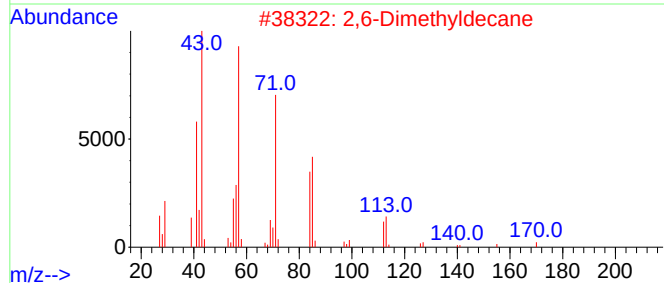
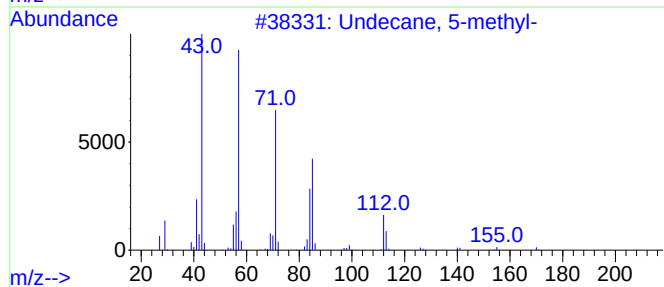
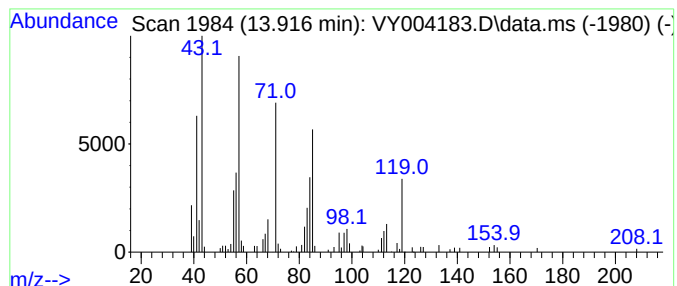
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y030821S.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Undecane, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	5.71 ug/l	106753	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5-methyl-	170	C12H26	001632-70-8	83
2			2,6-Dimethyldecane	170	C12H26	013150-81-7	60
3			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	47
4			Dodecane, 5-methyl-	184	C13H28	017453-93-9	47
5			Hexyl octyl ether	214	C14H30O	017071-54-4	47



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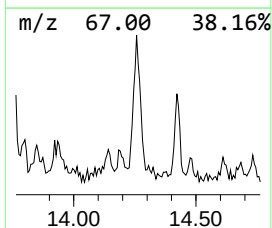
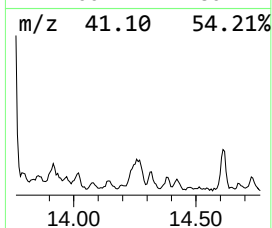
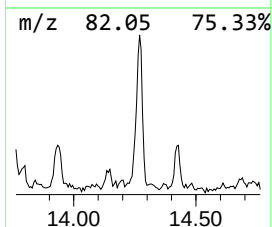
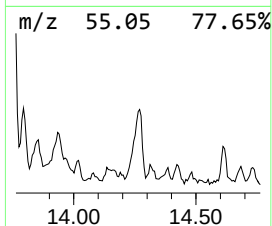
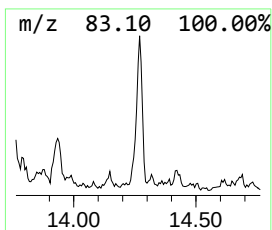
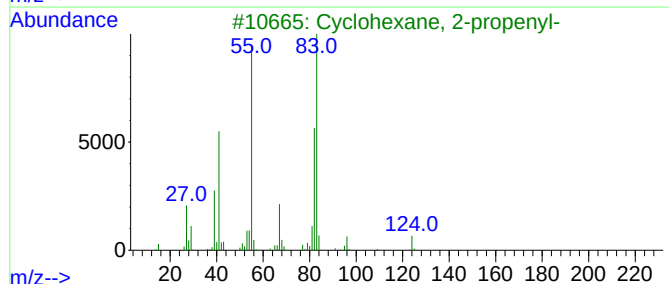
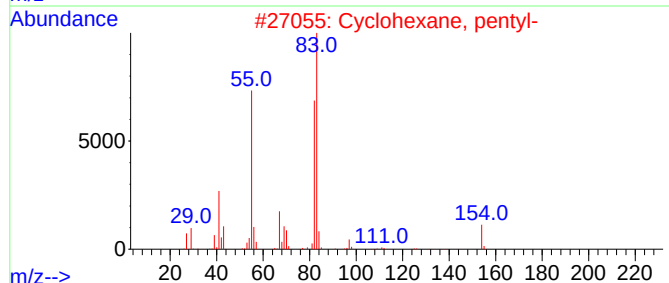
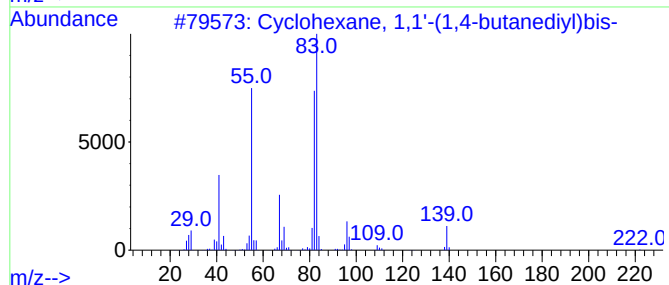
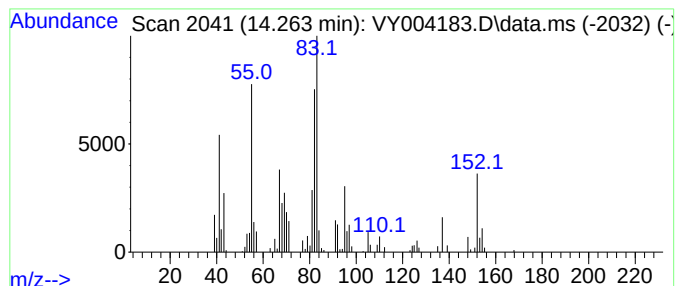
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclohexane, 1,1'-(1,4-buta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.263	8.66 ug/l	161831	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1'-(1,4-butanediyl)bis-	222	C16H30	006165-44-2	53
2			Cyclohexane, pentyl-	154	C11H22	004292-92-6	53
3			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	50
4			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	49
5			Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	49



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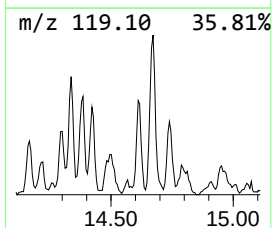
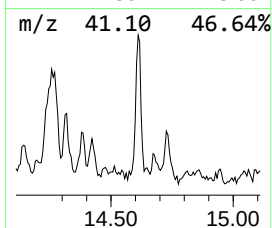
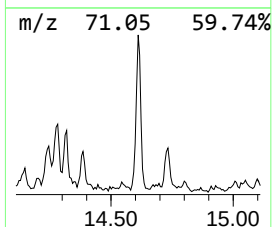
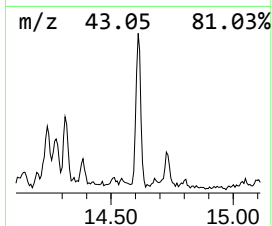
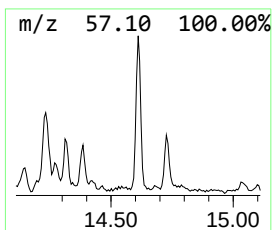
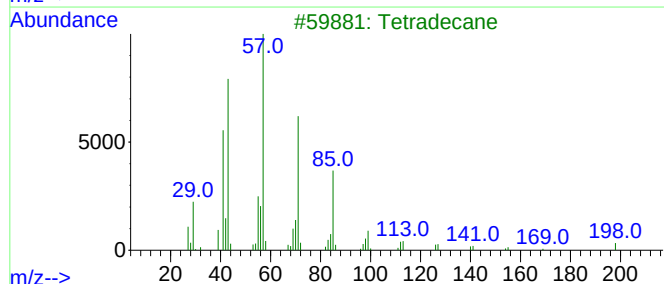
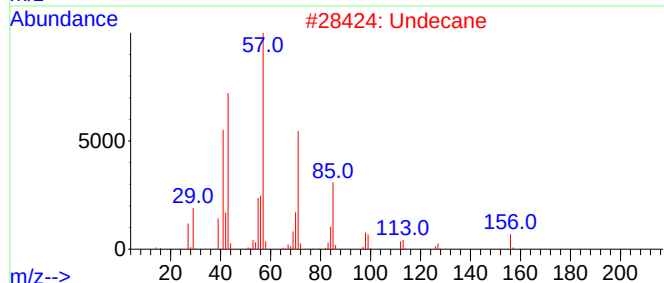
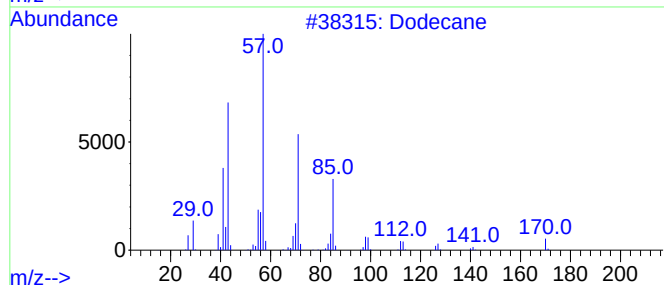
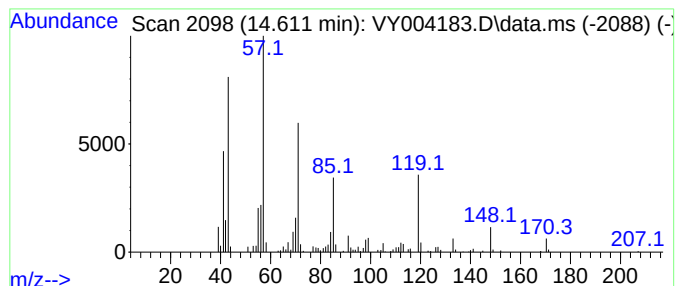
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dodecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.611	5.75 ug/l	107483	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Undecane	156	C11H24	001120-21-4	58
3			Tetradecane	198	C14H30	000629-59-4	58
4			Pentadecane	212	C15H32	000629-62-9	52
5			Tridecane	184	C13H28	000629-50-5	52



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	13.751	28.6	ug/l	534608	4	13.428	934595	50.0
Undecane, 5-met...	13.916	5.7	ug/l	106753	4	13.428	934595	50.0
Cyclohexane, 1,...	14.263	8.7	ug/l	161831	4	13.428	934595	50.0
Dodecane	14.611	5.8	ug/l	107483	4	13.428	934595	50.0