

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021623\
 Data File : VN076725.D
 Acq On : 16 Feb 2023 20:41
 Operator : JC\MD
 Sample : 01549-04
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1931

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\82N021323W.M
 Title : SW846 8260

Signal : TIC: VN076725.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.837	143	153	154	rBV6	28437	65669	2.92%	0.460%
2	2.996	177	180	182	rBV4	17907	25227	1.12%	0.177%
3	5.048	517	529	543	rBV3	9132	35589	1.58%	0.250%
4	8.166	1050	1059	1064	rBV2	281096	698551	31.08%	4.897%
5	8.225	1064	1069	1078	rVB2	538131	1172985	52.19%	8.224%
6	8.583	1120	1130	1138	rBV2	329863	757171	33.69%	5.308%
7	8.666	1138	1144	1148	rBV2	32559	74082	3.30%	0.519%
8	9.101	1209	1218	1228	rBV	806617	1641674	73.04%	11.510%
9	10.566	1458	1467	1477	rBV	1171902	2247641	100.00%	15.758%
10	10.742	1491	1497	1504	rVB3	13952	27089	1.21%	0.190%
11	11.648	1645	1651	1662	rVB6	11035	27613	1.23%	0.194%
12	11.866	1680	1688	1699	rBV	988037	1826124	81.25%	12.803%
13	11.966	1701	1705	1710	rVV4	14059	25735	1.14%	0.180%
14	12.071	1713	1723	1730	rVV4	72104	154177	6.86%	1.081%
15	12.407	1766	1780	1786	rBV5	21450	64684	2.88%	0.453%
16	12.854	1849	1856	1865	rVB	715056	1259710	56.05%	8.832%
17	13.101	1891	1898	1902	rVV	35745	59750	2.66%	0.419%
18	13.166	1902	1909	1917	rVV3	130582	256710	11.42%	1.800%
19	13.342	1937	1939	1945	rVV5	13916	28556	1.27%	0.200%
20	13.401	1945	1949	1953	rVV4	26554	40899	1.82%	0.287%
21	13.483	1956	1963	1968	rVV	45989	73170	3.26%	0.513%
22	13.677	1990	1996	2000	rBV7	24503	49350	2.20%	0.346%
23	13.724	2000	2004	2009	rVV5	29601	67699	3.01%	0.475%
24	13.795	2010	2016	2024	rVV	911851	1599245	71.15%	11.212%
25	13.865	2024	2028	2034	rVB4	37250	62668	2.79%	0.439%
26	13.989	2045	2049	2053	rBV5	31007	52020	2.31%	0.365%
27	14.107	2064	2069	2076	rBV	177650	287202	12.78%	2.014%
28	14.330	2101	2107	2111	rBV7	26713	45406	2.02%	0.318%
29	14.442	2121	2126	2132	rBV5	27478	47179	2.10%	0.331%
30	14.536	2137	2142	2144	rBV5	17416	26782	1.19%	0.188%
31	14.583	2146	2150	2154	rVV4	19227	24862	1.11%	0.174%
32	14.630	2154	2158	2161	rBV5	41193	54877	2.44%	0.385%
33	14.665	2161	2164	2168	rVB5	22945	31999	1.42%	0.224%
34	14.736	2172	2176	2180	rBV3	44934	67826	3.02%	0.476%
35	14.883	2199	2201	2206	rVB6	16804	22797	1.01%	0.160%
36	14.960	2206	2214	2221	rVB2	188688	330334	14.70%	2.316%

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37	15.054	2221	2230	2232	rBV6	50786	119554	5.32%	0.838%
38	15.218	2252	2258	2264	rVB9	33585	71429	3.18%	0.501%
39	15.318	2271	2275	2280	rVB8	15648	30055	1.34%	0.211%
40	15.436	2288	2295	2296	rBV7	20559	34920	1.55%	0.245%
41	15.471	2297	2301	2306	rVB	47444	80323	3.57%	0.563%
42	15.595	2317	2322	2326	rBV5	38055	69274	3.08%	0.486%
43	15.836	2358	2363	2374	rVB	86323	172650	7.68%	1.210%
44	15.948	2374	2382	2390	rBV	30672	96115	4.28%	0.674%
45	16.024	2391	2395	2399	rVB6	15130	27427	1.22%	0.192%
46	16.171	2416	2420	2427	rVB9	33495	69908	3.11%	0.490%
47	16.348	2441	2450	2457	rVB9	29161	75434	3.36%	0.529%
48	16.495	2468	2475	2480	rBV10	18437	47521	2.11%	0.333%
49	16.712	2508	2512	2518	rVB8	16981	35972	1.60%	0.252%

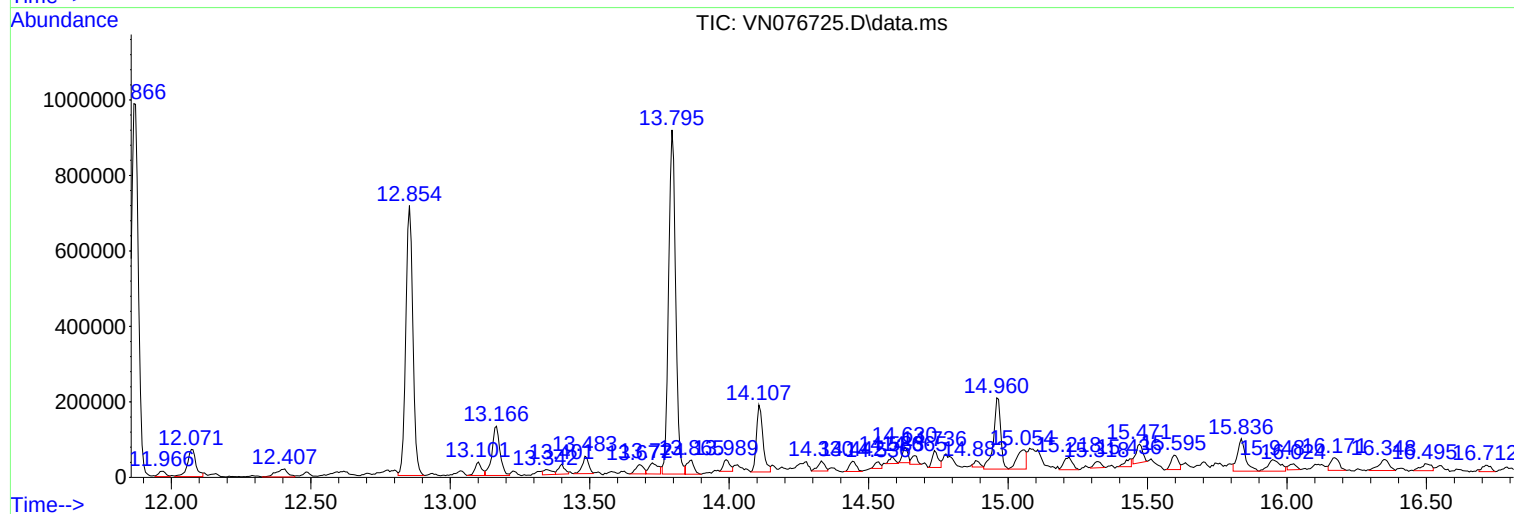
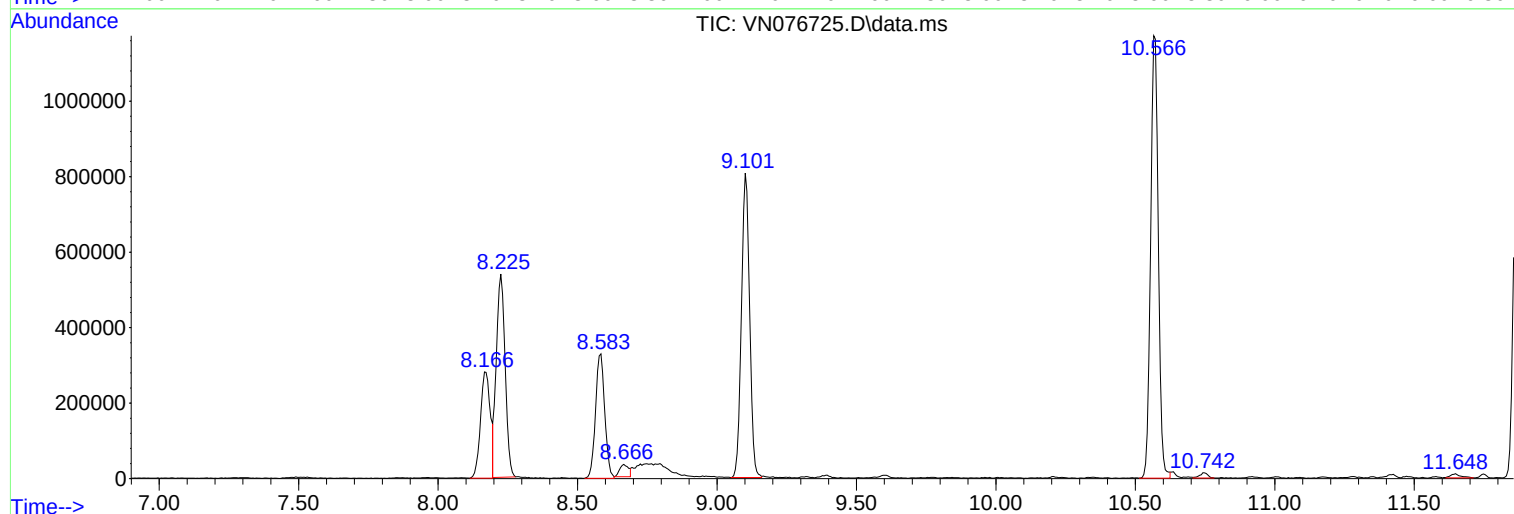
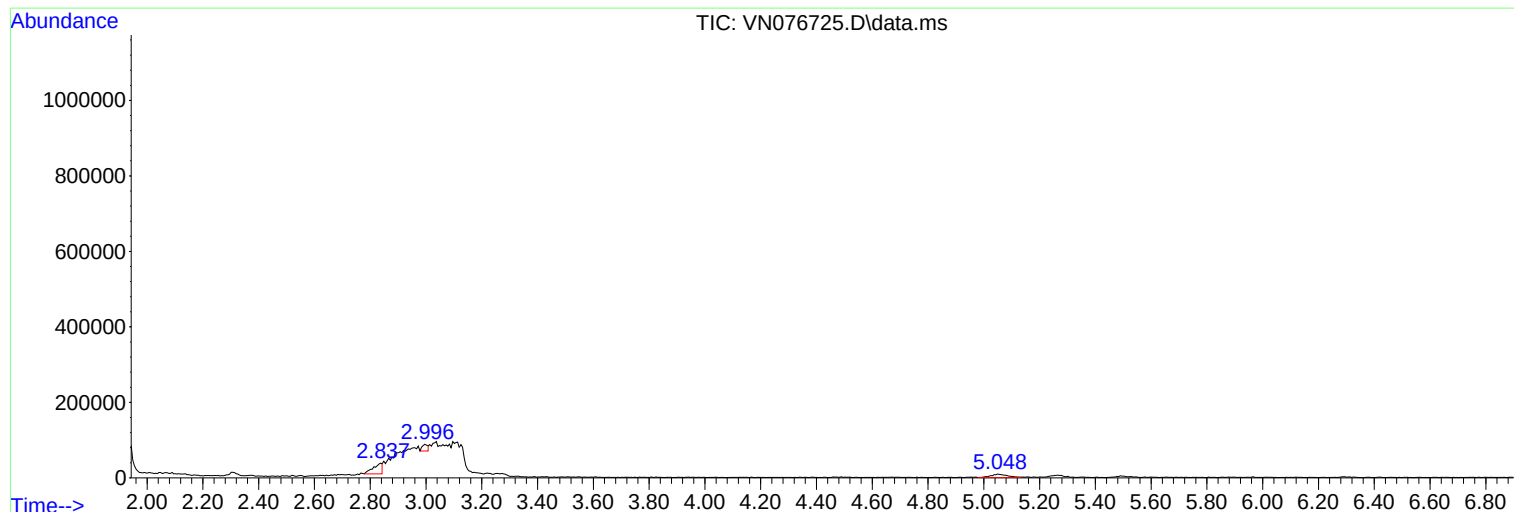
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Quant Title : SW846 8260

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



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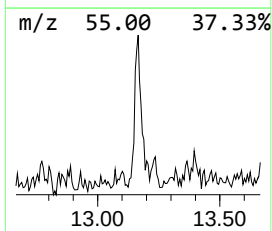
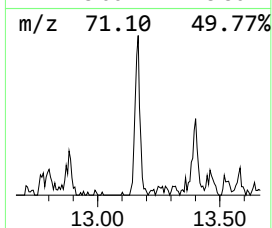
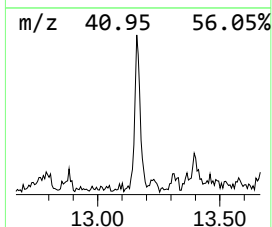
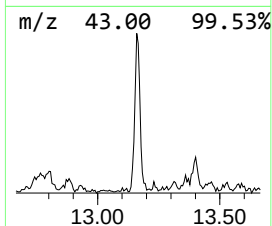
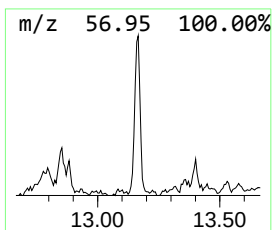
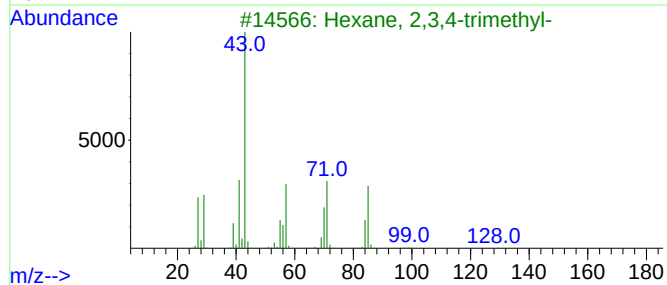
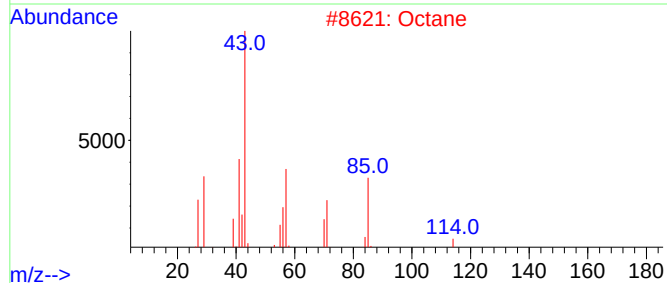
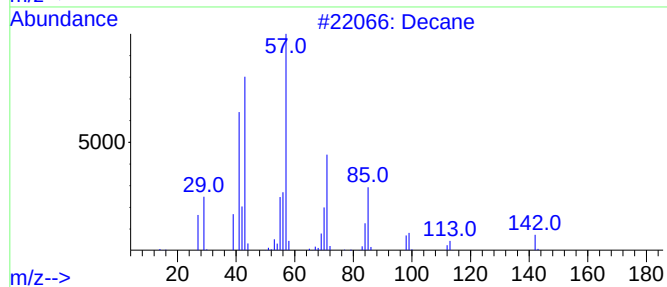
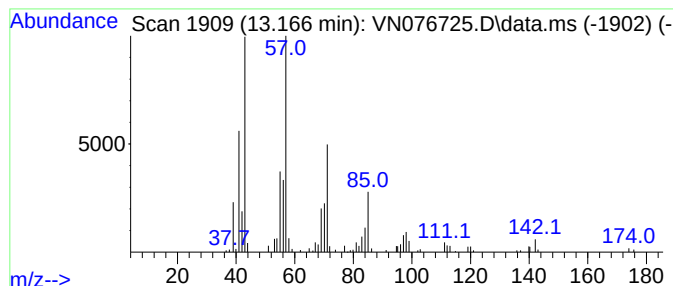
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 1 Decane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.166	8.03 ug/l	256710	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	90
2			Octane	114	C8H18	000111-65-9	50
3			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43
5			cis-3-Decene	140	C10H20	019398-86-8	42



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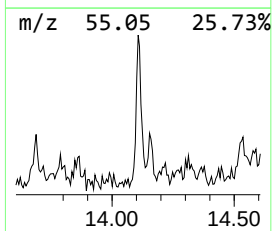
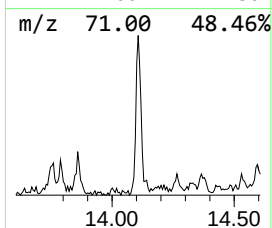
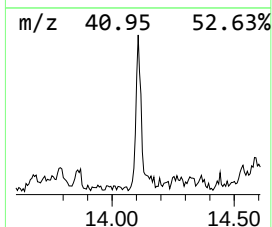
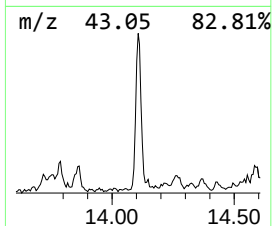
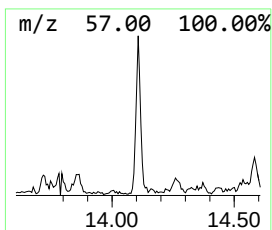
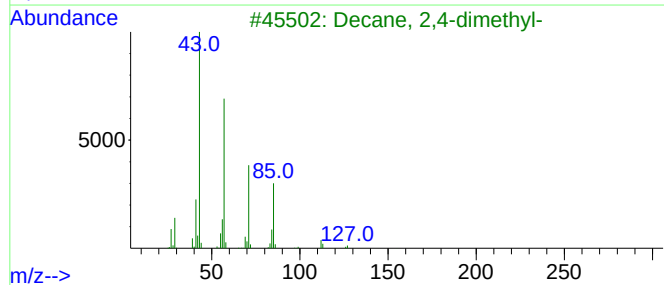
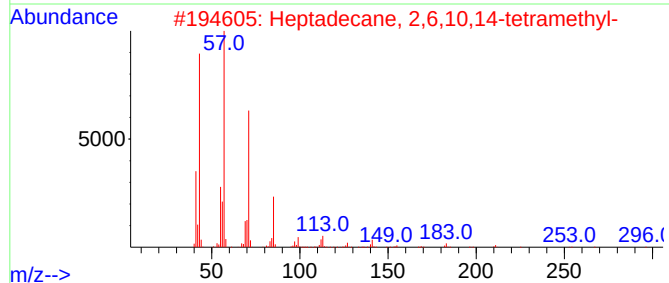
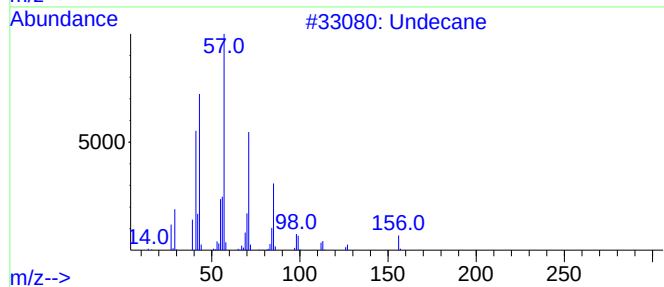
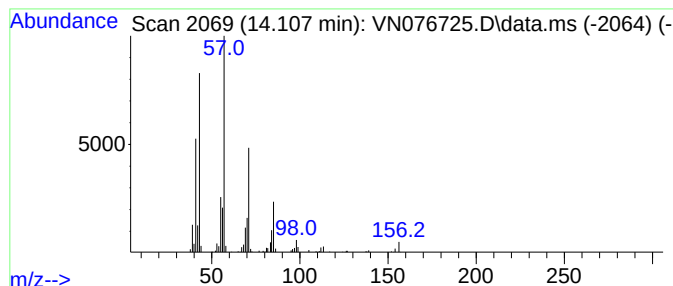
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021323W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.107	8.98 ug/l	287202	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	90
2			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	78
3			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	64
4			Ether, hexyl pentyl	172	C11H24O	032357-83-8	59
5			Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59



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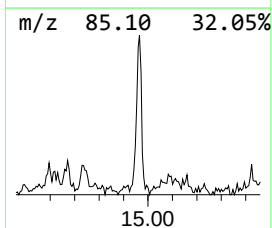
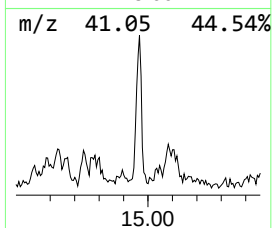
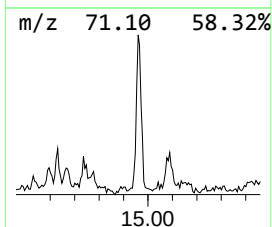
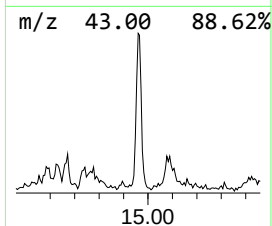
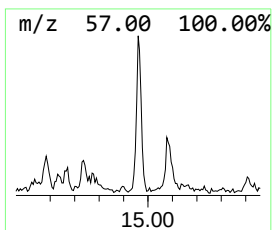
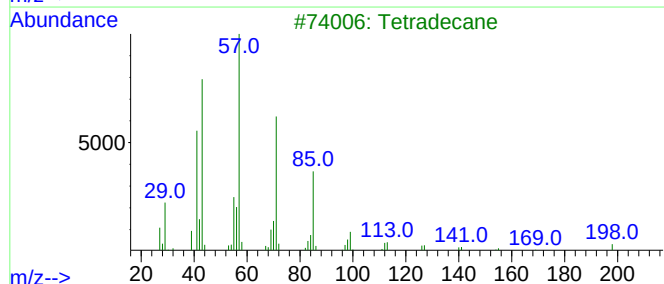
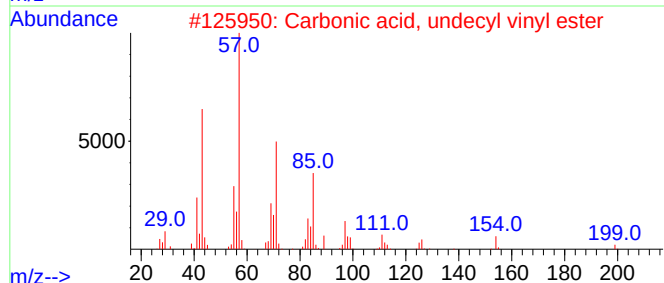
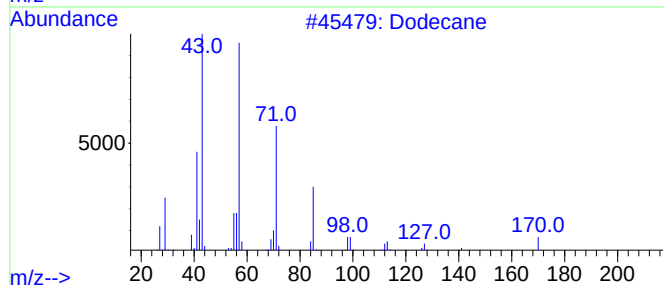
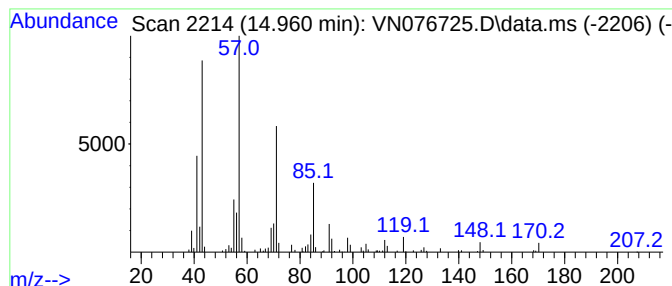
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Carbonic acid, undecyl vinyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.960	10.33 ug/l	330334	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	72
2			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	64
3			Tetradecane	198	C14H30	000629-59-4	64
4			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	59
5			Hexadecane	226	C16H34	000544-76-3	53



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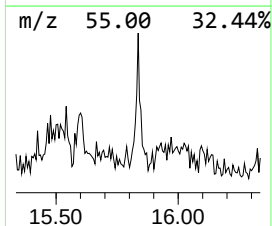
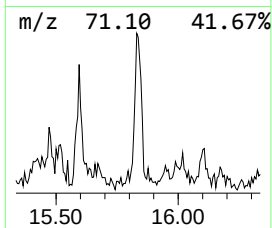
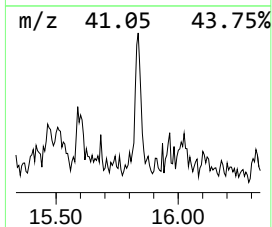
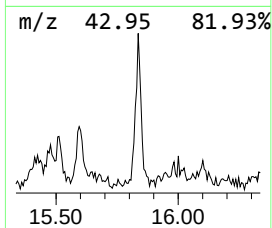
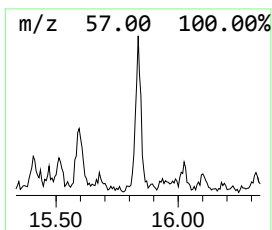
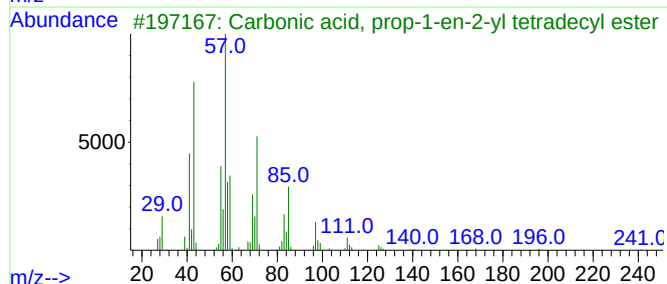
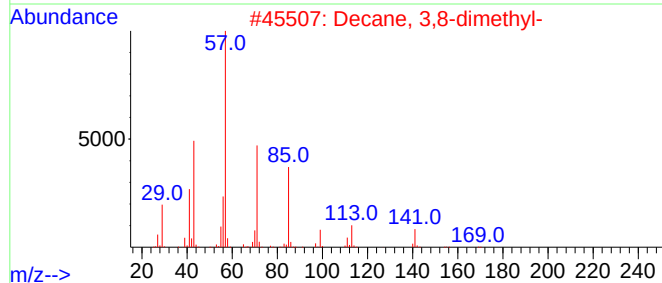
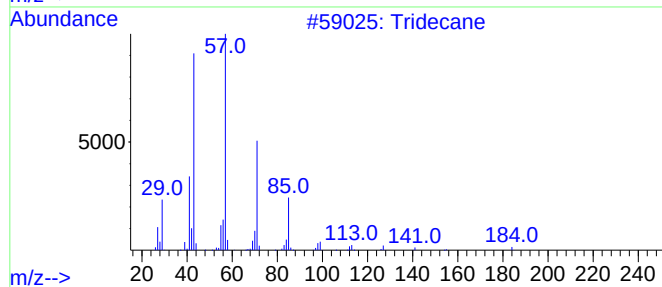
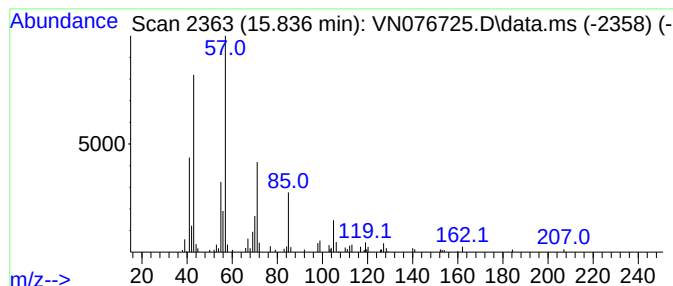
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.836	5.40 ug/l	172650	1,4-Dichlorobenzene-d4	13.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	76
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	64
3			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	64
4			Dodecane	170	C12H26	000112-40-3	59
5			Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decane	13.166	8.0	ug/l	256710	4	13.795	1599250	50.0
Undecane	14.107	9.0	ug/l	287202	4	13.795	1599250	50.0
Carbonic acid, ...	14.960	10.3	ug/l	330334	4	13.795	1599250	50.0
Tridecane	15.836	5.4	ug/l	172650	4	13.795	1599250	50.0