

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY041620\
 Data File : VY002364.D
 Acq On : 16 Apr 2020 14:10
 Operator : SY/MD
 Sample : L2279-02
 Misc : 5.03G/5ML/MSVOA Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OILY-STONE-POTHEAD

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_Y\METHODS\82Y040820S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.730	481	491	504	rBV2	19901	60786	8.86%	1.365%
2	5.761	651	660	672	rBV4	5220	16621	2.42%	0.373%
3	6.992	852	862	874	rBV	10908	32872	4.79%	0.738%
4	7.730	973	983	989	rBV2	86409	209055	30.46%	4.695%
5	7.803	989	995	1008	rVB	149959	339794	49.51%	7.631%
6	8.150	1041	1052	1064	rVB	85227	198182	28.87%	4.451%
7	8.699	1131	1142	1151	rBV	256690	500199	72.88%	11.233%
8	10.181	1378	1385	1392	rBV	398704	686360	100.00%	15.413%
9	10.248	1392	1396	1401	rVB	6699	10583	1.54%	0.238%
10	10.370	1409	1416	1421	rBV5	3718	7262	1.06%	0.163%
11	10.583	1444	1451	1459	rVB3	19032	35306	5.14%	0.793%
12	10.949	1506	1511	1516	rBV3	13862	23189	3.38%	0.521%
13	11.321	1568	1572	1577	rVB2	5464	7746	1.13%	0.174%
14	11.491	1593	1600	1609	rBV	356395	571275	83.23%	12.829%
15	11.595	1611	1617	1623	rBV	19333	29815	4.34%	0.670%
16	11.699	1628	1634	1645	rVB	52946	97445	14.20%	2.188%
17	12.028	1678	1688	1698	rVB3	22445	42799	6.24%	0.961%
18	12.381	1742	1746	1755	rBV8	3389	7470	1.09%	0.168%
19	12.485	1755	1763	1774	rBV	255201	422676	61.58%	9.492%
20	12.735	1799	1804	1808	rBV3	5732	8253	1.20%	0.185%
21	12.808	1810	1816	1822	rVB6	8627	16067	2.34%	0.361%
22	13.174	1873	1876	1882	rVB6	4879	8310	1.21%	0.187%
23	13.247	1882	1888	1892	rBV7	7156	15481	2.26%	0.348%
24	13.345	1897	1904	1912	rBV7	30253	77046	11.23%	1.730%
25	13.430	1912	1918	1924	rVB	248269	390307	56.87%	8.765%
26	13.491	1924	1928	1936	rVB9	6484	13020	1.90%	0.292%
27	13.753	1967	1971	1973	rBV4	13437	19490	2.84%	0.438%
28	13.790	1973	1977	1984	rVB2	36928	57974	8.45%	1.302%
29	13.857	1984	1988	1995	rBV3	15610	39036	5.69%	0.877%
30	14.040	2011	2018	2022	rVB6	12308	28229	4.11%	0.634%
31	14.137	2028	2034	2039	rVB6	12468	26566	3.87%	0.597%
32	14.186	2040	2042	2048	rVB7	4563	8074	1.18%	0.181%
33	14.271	2050	2056	2059	rBV5	11960	23633	3.44%	0.531%
34	14.375	2070	2073	2078	rVV7	8379	13589	1.98%	0.305%

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Sampling : 1
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35	14.424	2078	2081	2085	rVB6	6657	10064	1.47%	0.226%
36	14.540	2095	2100	2105	rVV	17641	25000	3.64%	0.561%
37	14.613	2108	2112	2118	rBV4	17582	31527	4.59%	0.708%
38	14.680	2118	2123	2129	rVV5	15971	34787	5.07%	0.781%
39	14.741	2129	2133	2139	rVB6	13065	25158	3.67%	0.565%
40	14.863	2148	2153	2156	rBV6	6562	13678	1.99%	0.307%
41	14.948	2163	2167	2170	rBV4	6538	9451	1.38%	0.212%
42	15.216	2207	2211	2216	rBV5	11373	19813	2.89%	0.445%
43	15.503	2254	2258	2264	rBV	20210	36017	5.25%	0.809%
44	15.680	2284	2287	2293	rBV8	5575	10586	1.54%	0.238%
45	16.167	2364	2367	2371	rBV5	8970	15239	2.22%	0.342%
46	16.295	2383	2388	2394	rVB4	27041	53824	7.84%	1.209%
47	16.497	2417	2421	2424	rBV6	7294	14881	2.17%	0.334%
48	16.643	2443	2445	2453	rVB5	10042	19333	2.82%	0.434%
49	16.856	2475	2480	2488	rVB3	27320	61413	8.95%	1.379%
50	16.972	2490	2499	2501	rBV6	10563	27706	4.04%	0.622%

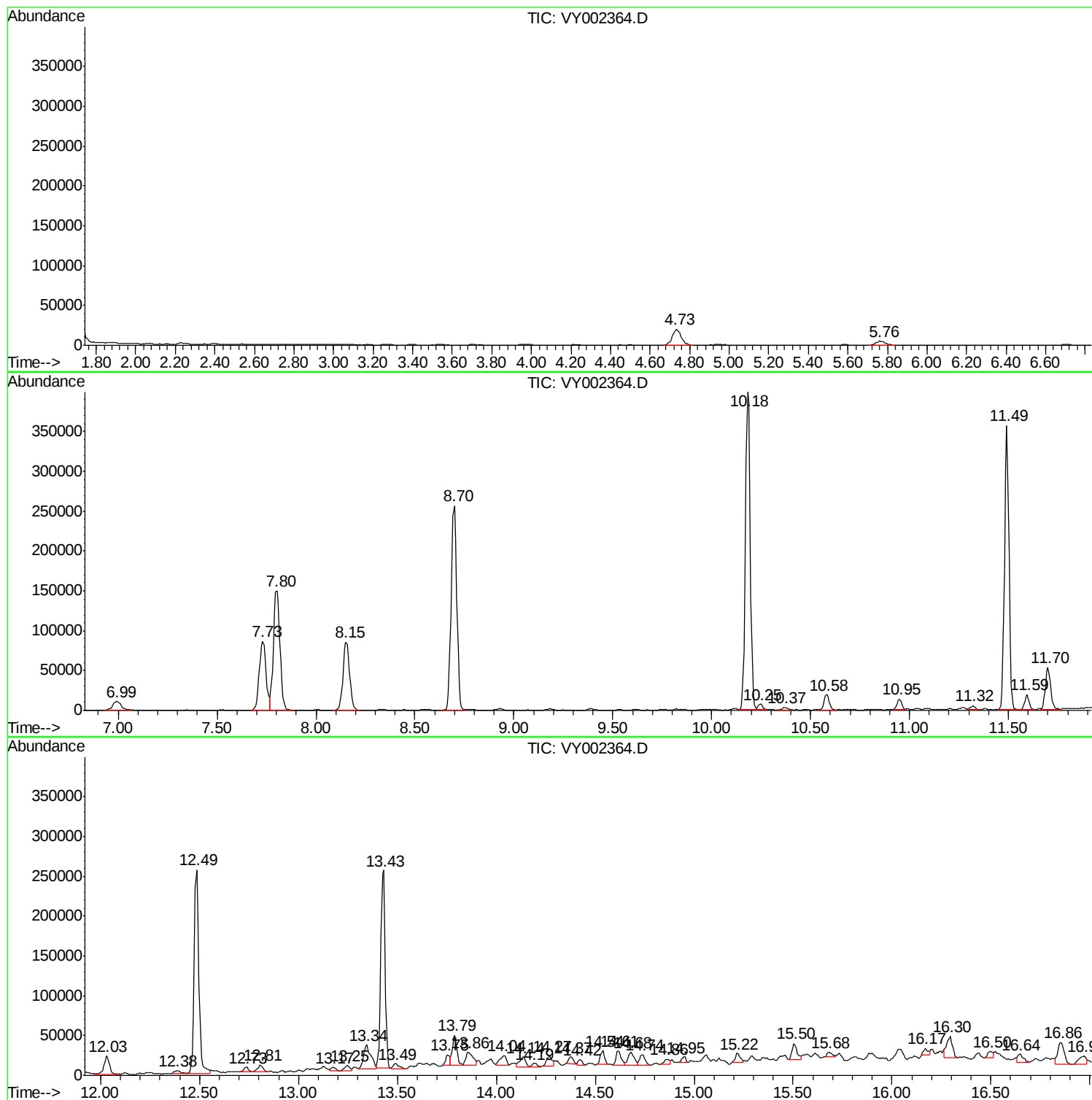
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y040820S.M
Quant Title : SW846 8260

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



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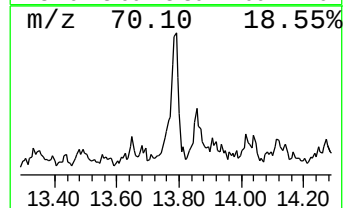
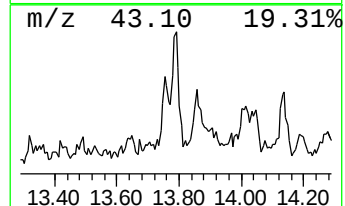
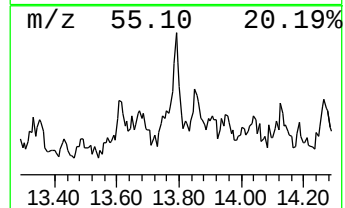
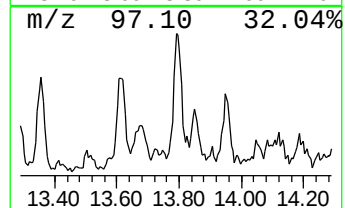
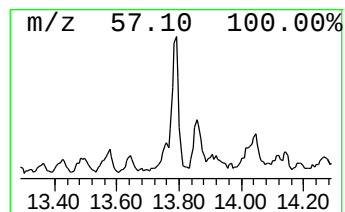
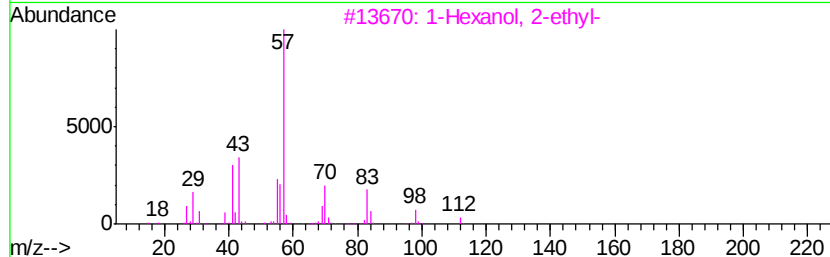
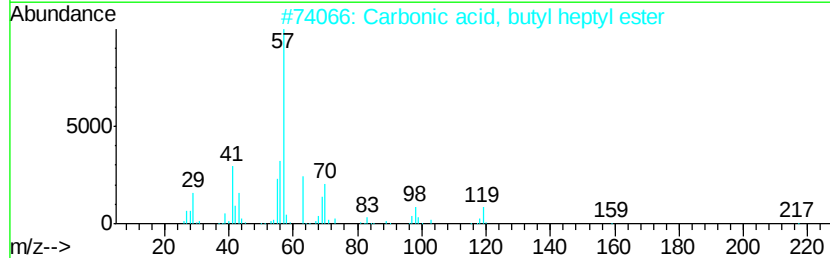
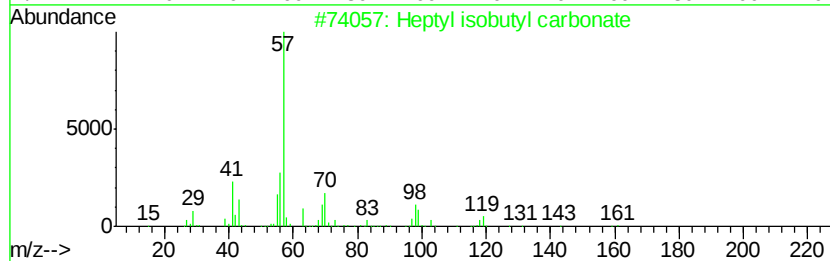
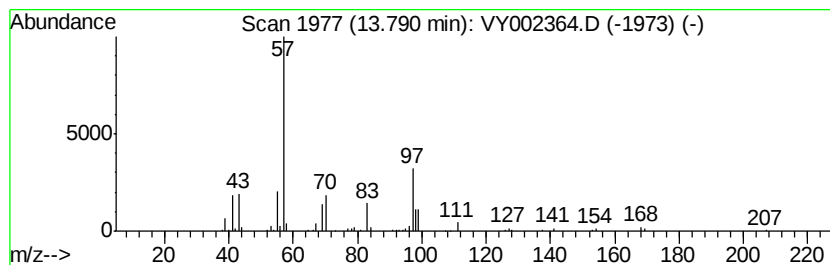
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 ClientSampleId :
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 Quant Title : SW846 8260

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

 Peak Number 1 Heptyl isobutyl carbonate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.79	7.43 ug/l	57974	1,4-Dichlorobenzene-d4	13.43		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
2		Carbonic acid, butyl heptyl ester	216	C12H24O3	1000314-63-4	38
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	38
4		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	37
5		Isobutyl undecyl carbonate	272	C16H32O3	1000372-78-8	36



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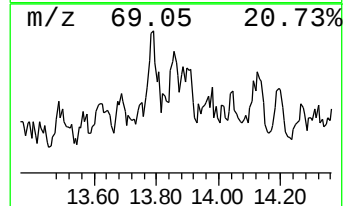
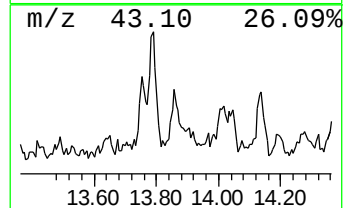
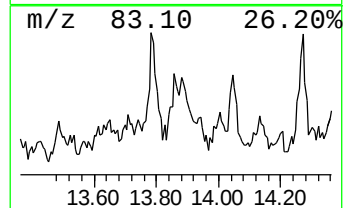
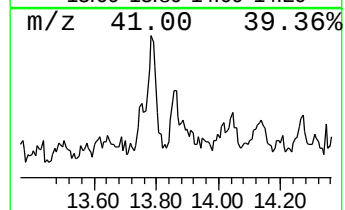
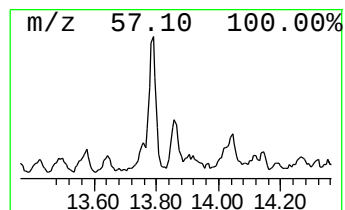
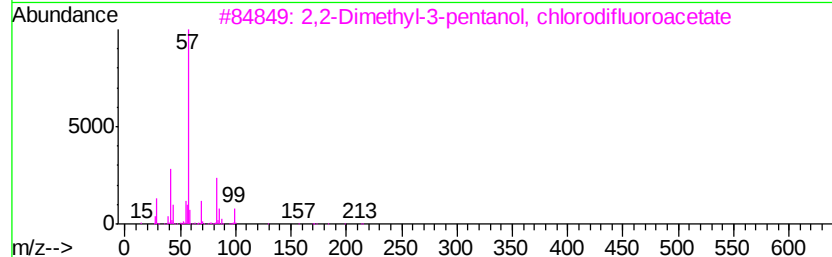
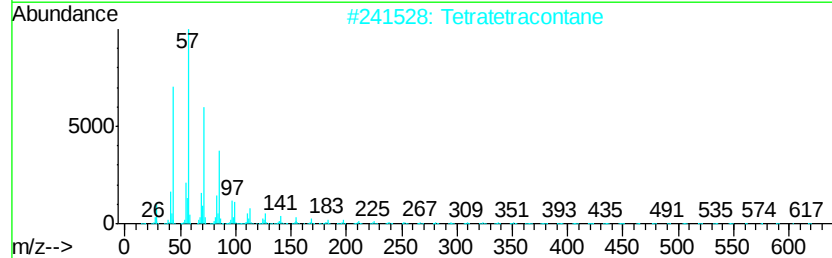
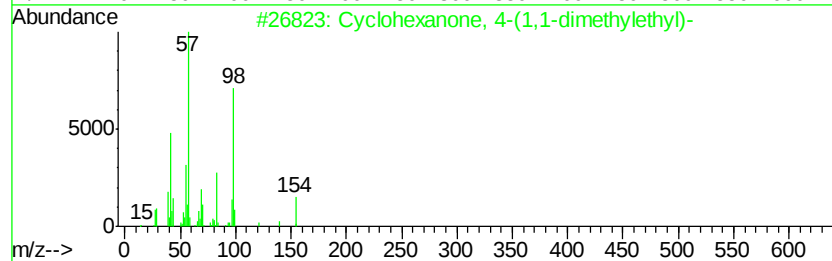
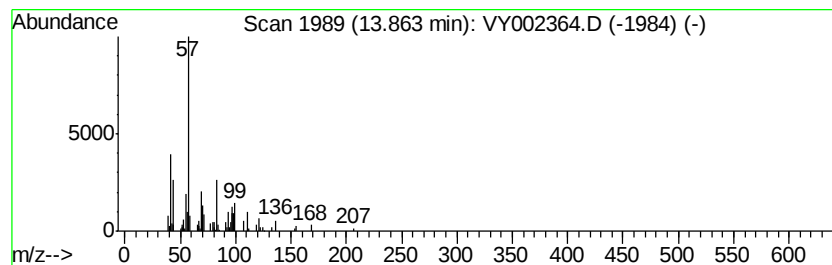
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Quant Title : SW846 8260

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

Peak Number 2 Cyclohexanone, 4-(1,1-dimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	5.00 ug/l	39036	1,4-Dichlorobenzene-d4	13.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclohexanone, 4-(1,1-dimethylet...	154	C10H18O	000098-53-3	50
2	Tetratetracontane	619	C44H90	007098-22-8	50
3	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	43
4	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	38
5	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	38



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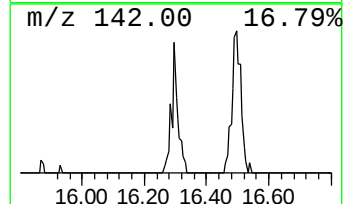
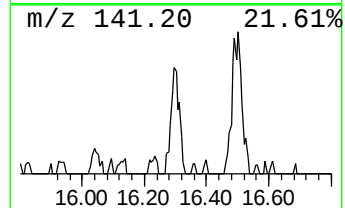
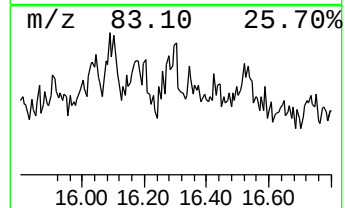
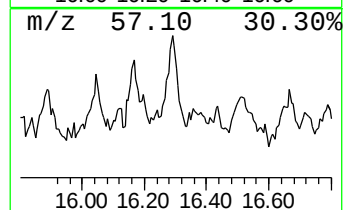
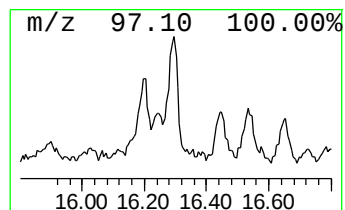
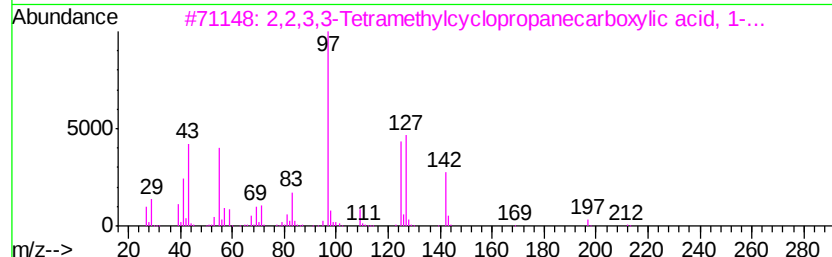
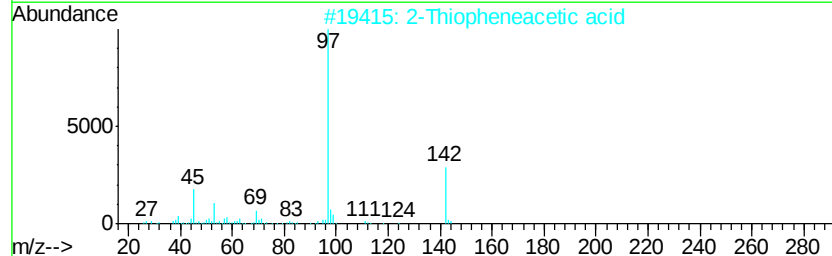
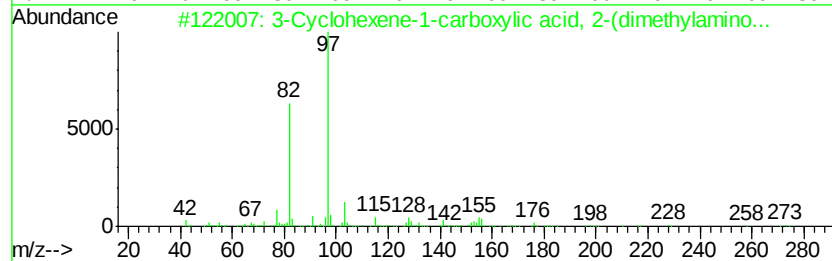
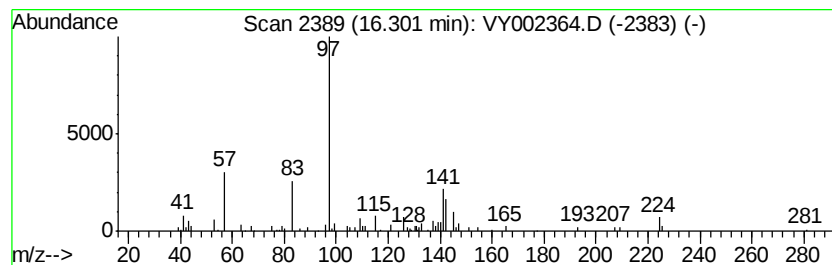
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown16.30 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.30	6.90 ug/l	53824	1,4-Dichlorobenzene-d4	13.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxylic acid,...	273	C17H23NO2	051931-66-9	43
2	2-Thiopheneacetic acid	142	C6H6O2S	001918-77-0	40
3	2,2,3,3-Tetramethylcyclopropanec...	212	C13H24O2	1000221-98-7	40
4	2,2,3,3-Tetramethylcyclopropanec...	238	C15H26O2	1000221-97-5	40
5	Cyclopentanecarboxylic acid, 2,2...	184	C11H20O2	1000282-42-6	38



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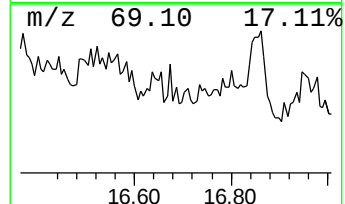
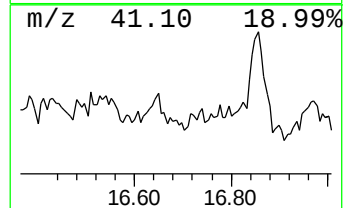
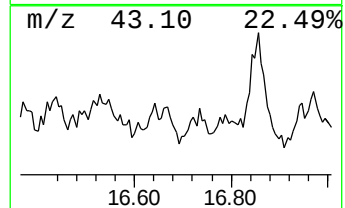
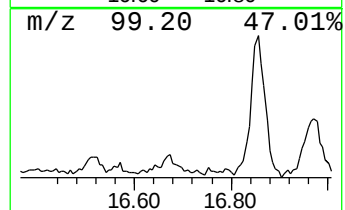
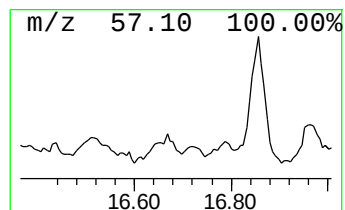
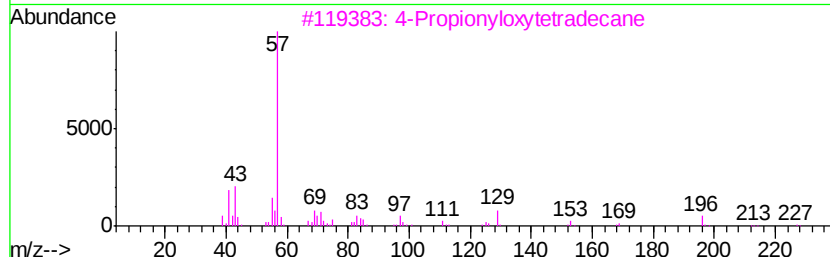
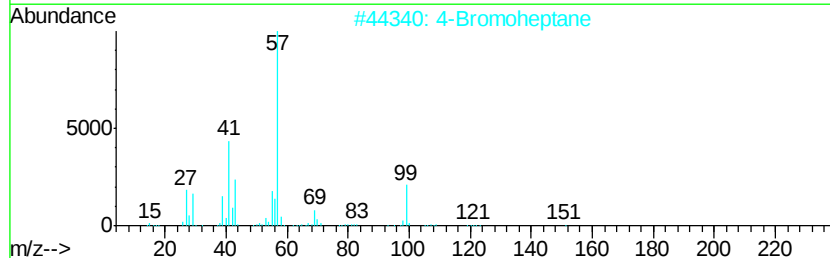
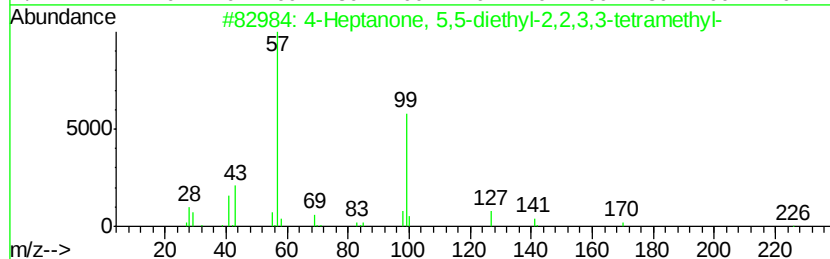
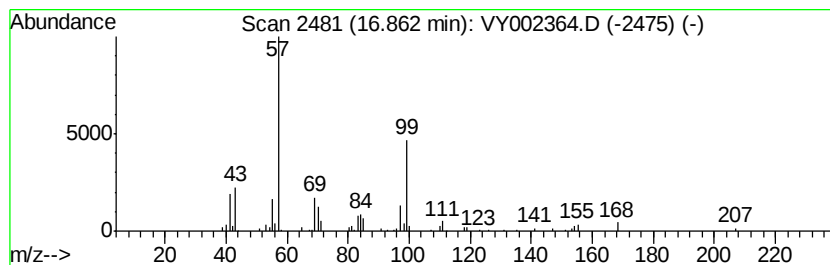
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Heptanone, 5,5-diethyl-2,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	7.87 ug/l	61413	1,4-Dichlorobenzene-d4	13.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone, 5,5-diethyl-2,2,3,3...	226	C15H30O	016424-67-2	59
2		4-Bromoheptane	178	C7H15Br	000998-93-6	59
3		4-Propionyloxvtetradecane	270	C17H34O2	1000245-62-9	43
4		Heptane, 2-iodo-	226	C7H15I	018589-29-2	40
5		2-Pyrrolidinone, 4-methyl-	99	C5H9NO	1000197-00-3	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Heptyl isobutyl c...	13.79	7.4	ug/l	57974	4	13.43	390307	50.0
Cyclohexanone, 4-...	13.86	5.0	ug/l	39036	4	13.43	390307	50.0
unknown16.30	16.30	6.9	ug/l	53824	4	13.43	390307	50.0
4-Heptanone, 5,5-...	16.86	7.9	ug/l	61413	4	13.43	390307	50.0