

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY080323\
 Data File : VY014953.D
 Acq On : 03 Aug 2023 17:02
 Operator : SY/MD
 Sample : 03864-01
 Misc : 5.09g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-1

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\82Y071323S.M
 Title : SW846 8260

Signal : TIC: VY014953.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.113	41	48	60	rBV6	26763	124151	9.67%	1.458%
2	2.211	60	64	73	rVB3	21135	48970	3.82%	0.575%
3	3.954	341	350	359	rBV2	10095	30638	2.39%	0.360%
4	4.710	462	474	487	rBV3	39062	121338	9.46%	1.425%
5	5.741	629	643	658	rBV2	36136	111727	8.71%	1.312%
6	6.984	835	847	862	rBV	37081	121069	9.43%	1.422%
7	7.716	955	967	972	rBV	181351	430208	33.53%	5.052%
8	7.789	972	979	990	rVB	299087	692666	53.98%	8.134%
9	8.137	1024	1036	1048	rBV	190845	435572	33.94%	5.115%
10	8.685	1118	1126	1140	rBV	477708	940752	73.31%	11.047%
11	10.179	1363	1371	1377	rBV	740053	1283219	100.00%	15.069%
12	10.240	1377	1381	1388	rVB	22810	43417	3.38%	0.510%
13	10.575	1432	1436	1446	rVB	14912	30353	2.37%	0.356%
14	10.947	1489	1497	1503	rBV4	12388	26386	2.06%	0.310%
15	11.490	1579	1586	1598	rVB	712168	1156842	90.15%	13.585%
16	11.709	1615	1622	1630	rVB5	15349	37457	2.92%	0.440%
17	12.026	1665	1674	1678	rBV4	8442	17206	1.34%	0.202%
18	12.477	1742	1748	1755	rBV	555267	870424	67.83%	10.221%
19	12.733	1786	1790	1793	rBV2	14358	21616	1.68%	0.254%
20	12.806	1797	1802	1807	rVB4	34502	56528	4.41%	0.664%
21	13.117	1848	1853	1858	rVB	29757	47962	3.74%	0.563%
22	13.197	1861	1866	1872	rBV4	26095	51064	3.98%	0.600%
23	13.422	1896	1903	1913	rVB	644701	984525	76.72%	11.561%
24	13.526	1913	1920	1925	rBV5	21263	47249	3.68%	0.555%
25	13.587	1925	1930	1933	rVV2	44626	82525	6.43%	0.969%
26	13.623	1933	1936	1940	rVV2	53142	94520	7.37%	1.110%
27	13.672	1940	1944	1951	rVV4	23277	52707	4.11%	0.619%
28	13.745	1951	1956	1961	rVV2	41820	64059	4.99%	0.752%
29	13.934	1976	1987	1988	rBV4	39427	103736	8.08%	1.218%
30	14.081	2007	2011	2016	rVB7	10858	19431	1.51%	0.228%
31	14.209	2027	2032	2035	rBV6	7207	14966	1.17%	0.176%
32	14.251	2035	2039	2043	rBV6	13778	25880	2.02%	0.304%
33	14.416	2063	2066	2070	rBV5	11383	15695	1.22%	0.184%
34	14.471	2072	2075	2079	rBV6	9788	13603	1.06%	0.160%
35	14.574	2086	2092	2094	rBV4	18350	36658	2.86%	0.430%
36	14.605	2095	2097	2102	rVV2	25583	37768	2.94%	0.444%

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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

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37	14.678	2103	2109	2114	rVV6	29593	70547	5.50%	0.828%
38	14.727	2114	2117	2124	rVB7	20502	35514	2.77%	0.417%
39	14.837	2131	2135	2139	rBV5	22433	42815	3.34%	0.503%
40	14.940	2147	2152	2155	rBV8	16089	27054	2.11%	0.318%
41	15.434	2230	2233	2238	rBV6	26572	46939	3.66%	0.551%

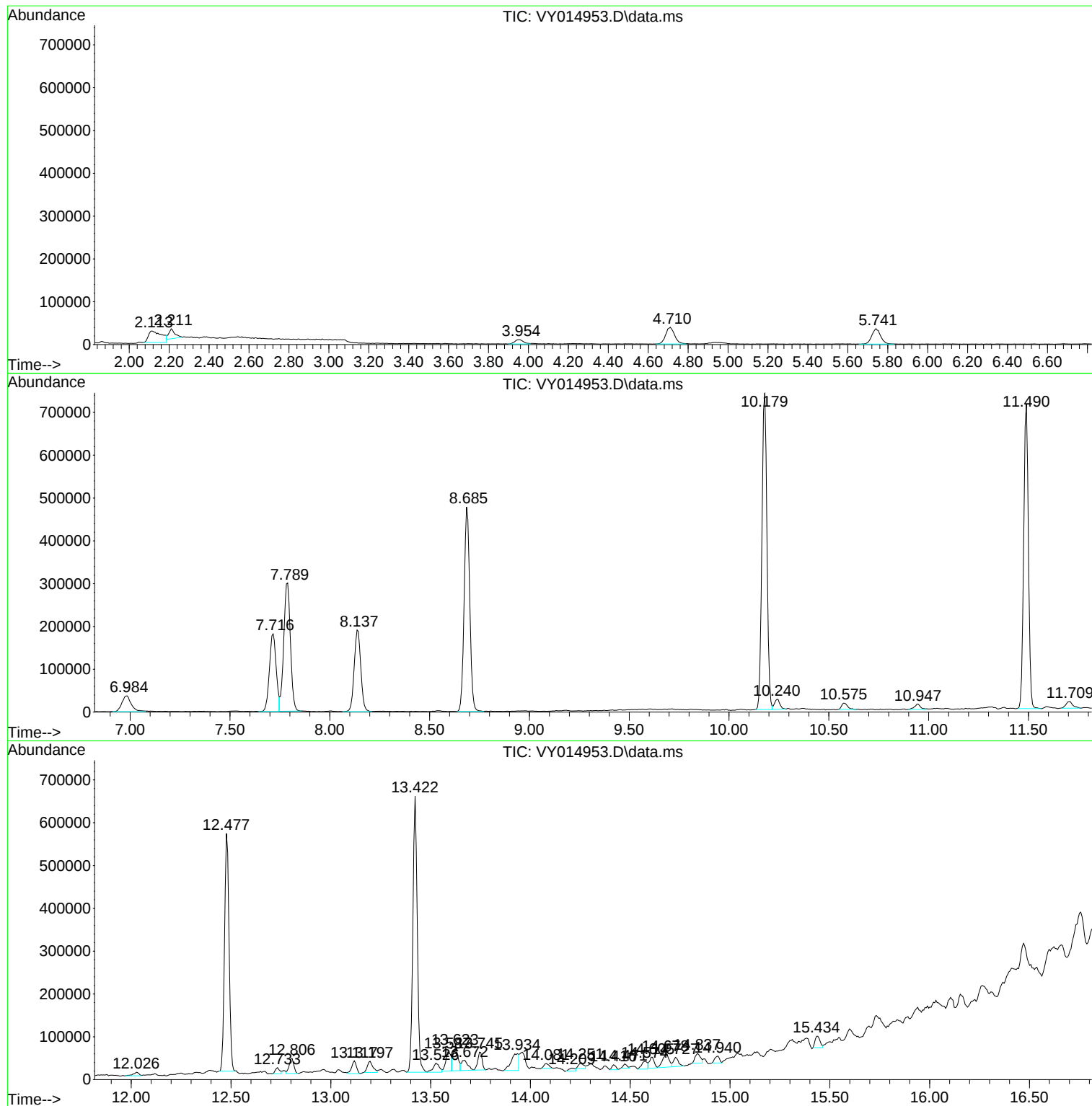
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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



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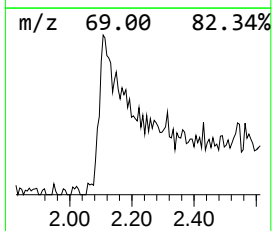
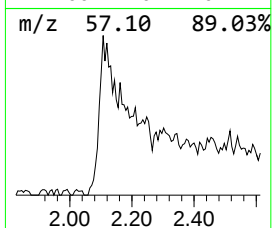
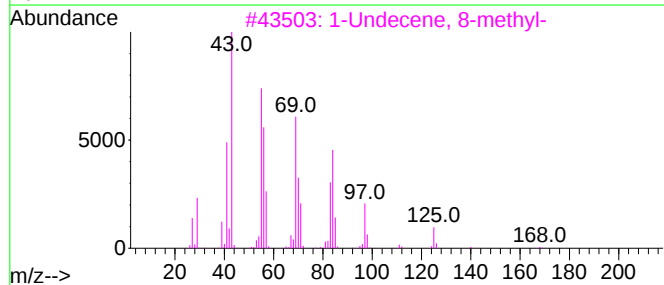
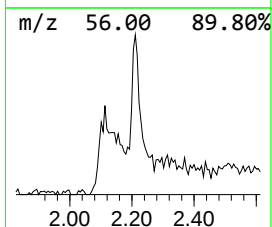
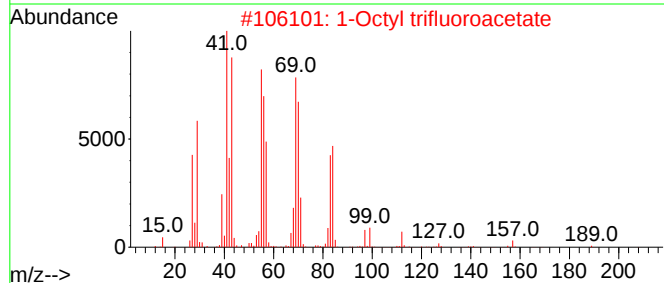
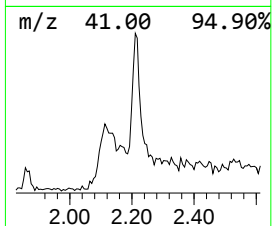
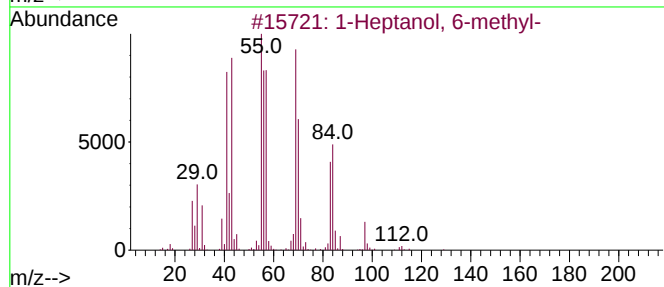
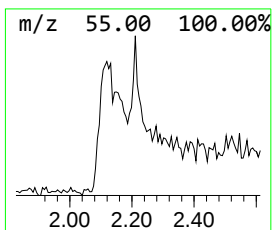
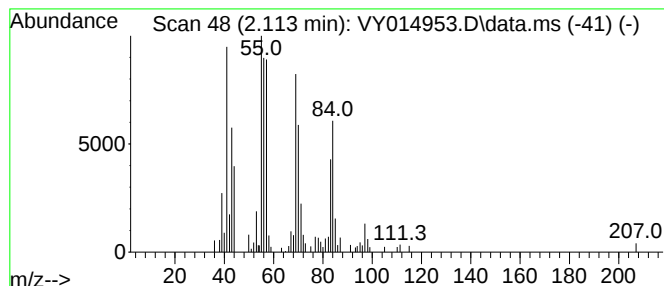
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y071323S.M
Quant Title : SW846 8260

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

Peak Number 1 1-Heptanol, 6-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.113	8.96 ug/l	124151	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-			130	C8H18O	001653-40-3	80
2	1-Octyl trifluoroacetate			226	C10H17F3O2	002561-21-9	72
3	1-Undecene, 8-methyl-			168	C12H24	074630-40-3	52
4	Cyclopentane, 1,1,3-trimethyl-			112	C8H16	004516-69-2	50
5	1-Octanol, 3,7-dimethyl-			158	C10H22O	000106-21-8	38



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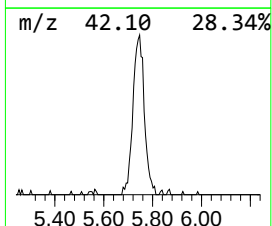
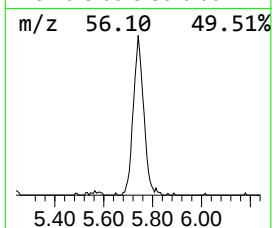
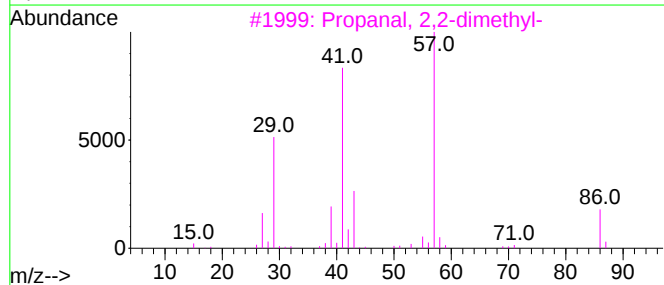
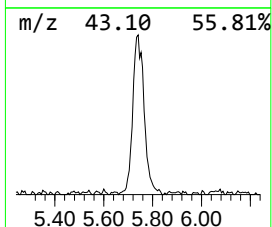
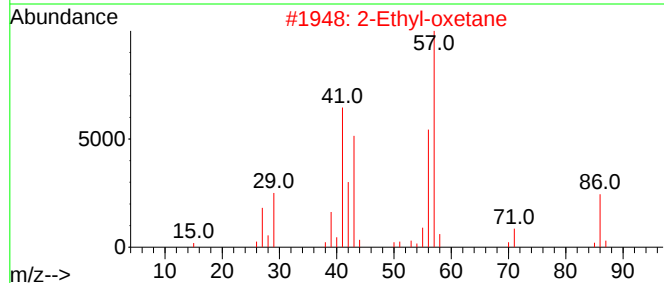
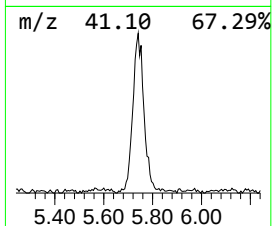
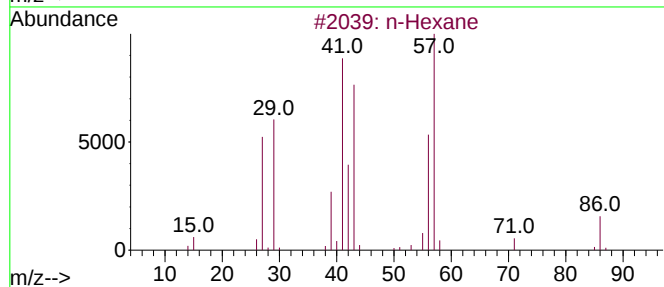
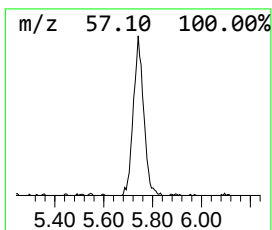
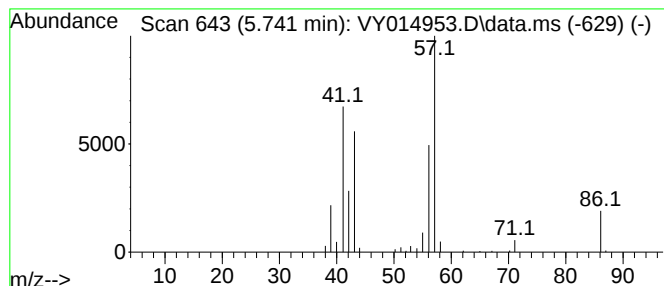
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Peak Number 2 n-Hexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.741	8.06 ug/l	111727	Pentafluorobenzene	7.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	78
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35
4			Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	32
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	32



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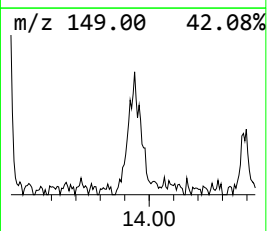
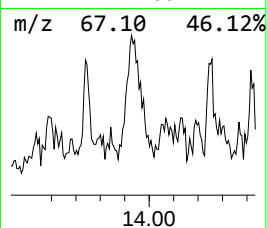
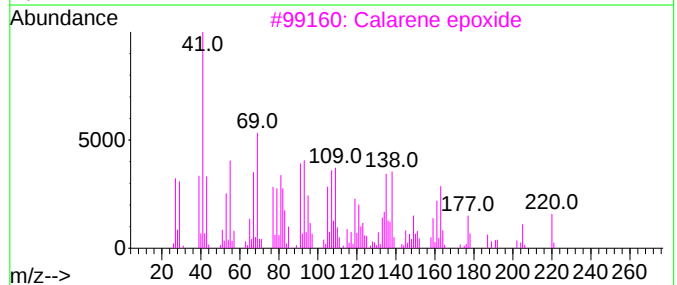
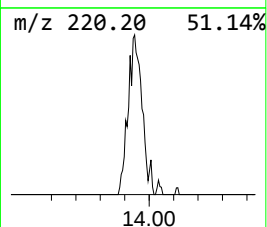
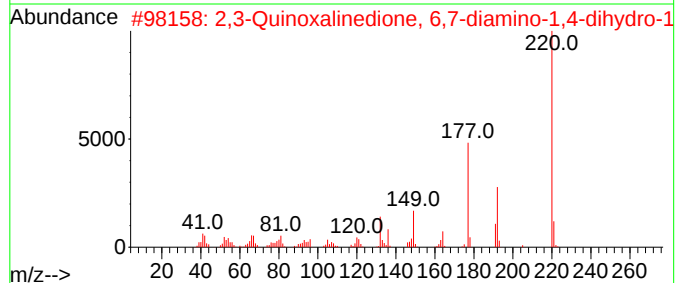
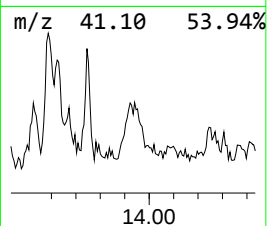
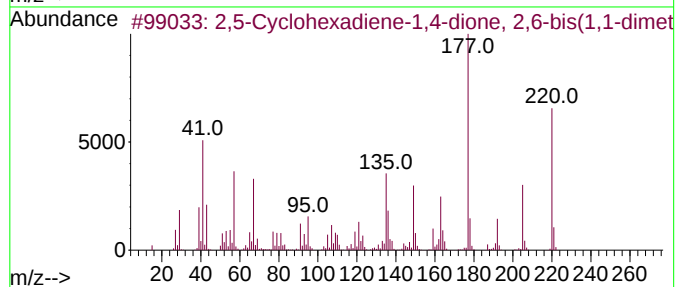
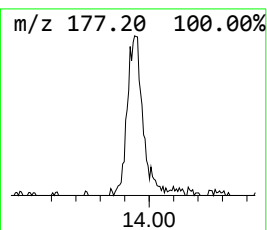
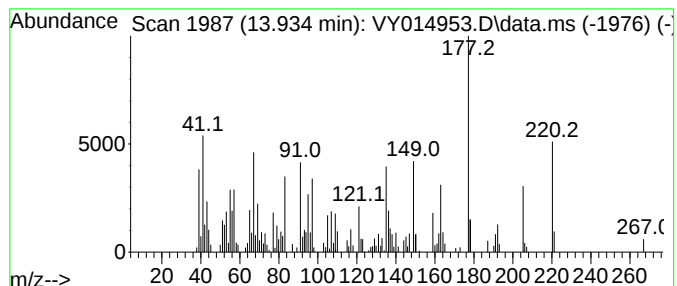
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.934	5.27 ug/l	103736	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2			2,3-Quinoxalinedione, 6,7-diamin...	220	C10H12N4O2	1000338-39-4	53
3			Calarene epoxide	220	C15H24O	1000151-46-0	41
4			2H-1-benzopyran-6-ol, 3,4-dihydr...	220	C14H20O2	1000396-25-4	38
5			1H-indene-4,7-diol, 2,3-dihydro-...	220	C14H20O2	1000396-25-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Heptanol, 6-m...	2.113	9.0	ug/l	124151	1	7.789	692666	50.0
n-Hexane	5.741	8.1	ug/l	111727	1	7.789	692666	50.0
2,5-Cyclohexadi...	13.934	5.3	ug/l	103736	4	13.422	984525	50.0