

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY110824\
 Data File : VY020230.D
 Acq On : 08 Nov 2024 14:02
 Operator : SY/MD
 Sample : P4722-01
 Misc : 10.39g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-1(5.5)

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\82Y103024S.M

Title : SW846 8260

Signal : TIC: VY020230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.824	11	17	25	rVB	36699	52375	3.44%	0.572%
2	2.025	45	50	55	rBV3	11499	19314	1.27%	0.211%
3	2.196	68	78	89	rBV2	44223	107989	7.10%	1.180%
4	2.842	176	184	192	rBV3	20223	46250	3.04%	0.505%
5	3.184	230	240	250	rVB2	24484	62236	4.09%	0.680%
6	3.873	343	353	366	rBV2	10166	29088	1.91%	0.318%
7	4.623	465	476	487	rBV6	15363	64350	4.23%	0.703%
8	5.141	550	561	568	rBV4	4937	15817	1.04%	0.173%
9	5.641	635	643	644	rBV	9382	16142	1.06%	0.176%
10	6.903	841	850	858	rBV4	5369	16436	1.08%	0.180%
11	7.421	922	935	946	rBV4	7369	22884	1.50%	0.250%
12	7.634	958	970	976	rBV2	213510	514900	33.84%	5.625%
13	7.707	976	982	995	rVB	308039	695002	45.68%	7.593%
14	7.921	1008	1017	1025	rVB6	6303	15947	1.05%	0.174%
15	8.061	1030	1040	1053	rBV2	212726	470380	30.92%	5.139%
16	8.469	1102	1107	1116	rVB5	9786	21166	1.39%	0.231%
17	8.616	1120	1131	1147	rBV	577482	1127668	74.12%	12.319%
18	10.103	1367	1375	1383	rBV	868922	1521503	100.00%	16.622%
19	10.646	1458	1464	1471	rBV2	36544	60246	3.96%	0.658%
20	11.018	1518	1525	1530	rBV3	13475	23669	1.56%	0.259%
21	11.414	1582	1590	1600	rBV	839418	1352526	88.89%	14.776%
22	11.621	1616	1624	1628	rBV7	10261	29172	1.92%	0.319%
23	11.926	1667	1674	1685	rBV7	18302	57074	3.75%	0.624%
24	12.133	1698	1708	1709	rBV4	20409	41012	2.70%	0.448%
25	12.158	1709	1712	1718	rVB2	35047	56021	3.68%	0.612%
26	12.231	1718	1724	1730	rBV8	11251	32549	2.14%	0.356%
27	12.304	1730	1736	1741	rVB8	8769	21049	1.38%	0.230%
28	12.408	1746	1753	1760	rBV	559102	883324	58.06%	9.650%
29	12.566	1773	1779	1786	rVB2	76465	136610	8.98%	1.492%
30	12.658	1786	1794	1799	rBV7	24575	64347	4.23%	0.703%
31	12.731	1799	1806	1821	rVB9	37523	105157	6.91%	1.149%
32	12.871	1825	1829	1833	rVB6	20169	28489	1.87%	0.311%
33	12.926	1833	1838	1841	rBV4	7450	16256	1.07%	0.178%
34	12.963	1841	1844	1847	rBV3	18580	28341	1.86%	0.310%
35	13.048	1854	1858	1862	rBV7	12903	25134	1.65%	0.275%
36	13.219	1882	1886	1887	rBV4	12783	15864	1.04%	0.173%

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ClientSampleId :
WC-1(5.5)

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\82Y103024S.M
Title : SW846 8260

37	13.347	1900	1907	1915	rVB	576189	884762	58.15%	9.666%
38	13.487	1926	1930	1935	rVB6	22967	33095	2.18%	0.362%
39	13.664	1954	1959	1964	rBV3	57147	94270	6.20%	1.030%
40	13.712	1964	1967	1971	rVB5	11038	15488	1.02%	0.169%
41	13.779	1973	1978	1979	rBV4	15533	22227	1.46%	0.243%
42	13.889	1990	1996	2001	rVB	76670	132462	8.71%	1.447%
43	14.176	2037	2043	2050	rBV9	26650	59449	3.91%	0.649%
44	14.340	2065	2070	2075	rVB3	30951	44728	2.94%	0.489%
45	14.596	2109	2112	2117	rVV7	12090	21093	1.39%	0.230%
46	14.651	2117	2121	2129	rVB6	14330	24054	1.58%	0.263%
47	15.133	2193	2200	2206	rBV6	9954	25861	1.70%	0.283%

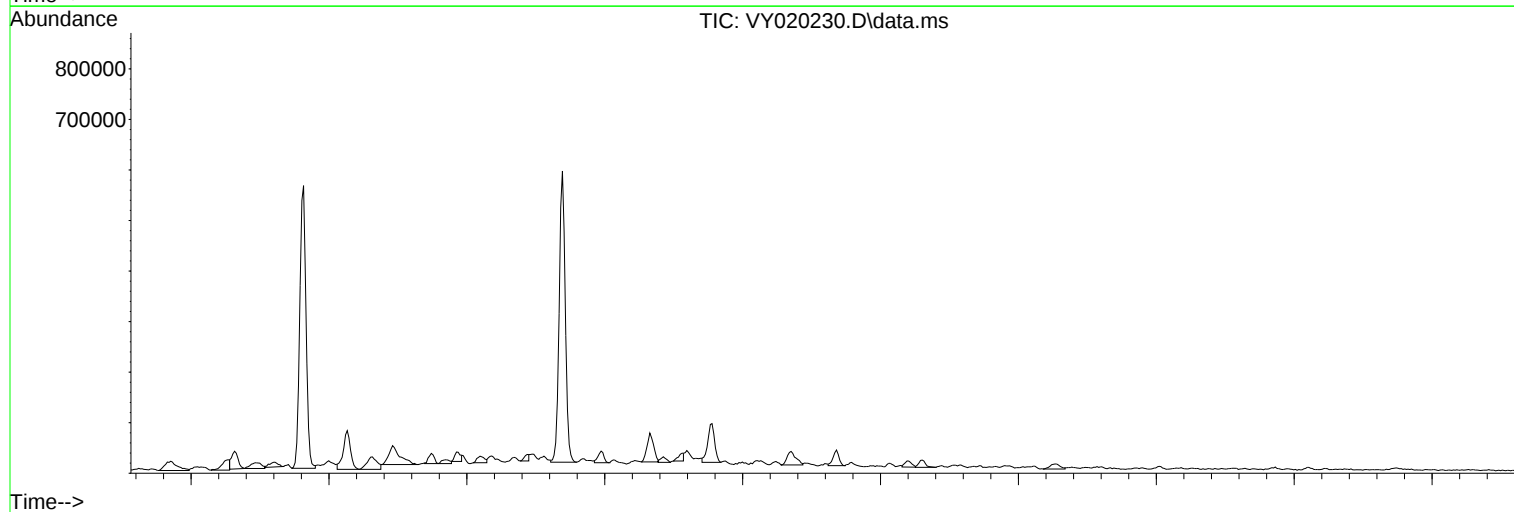
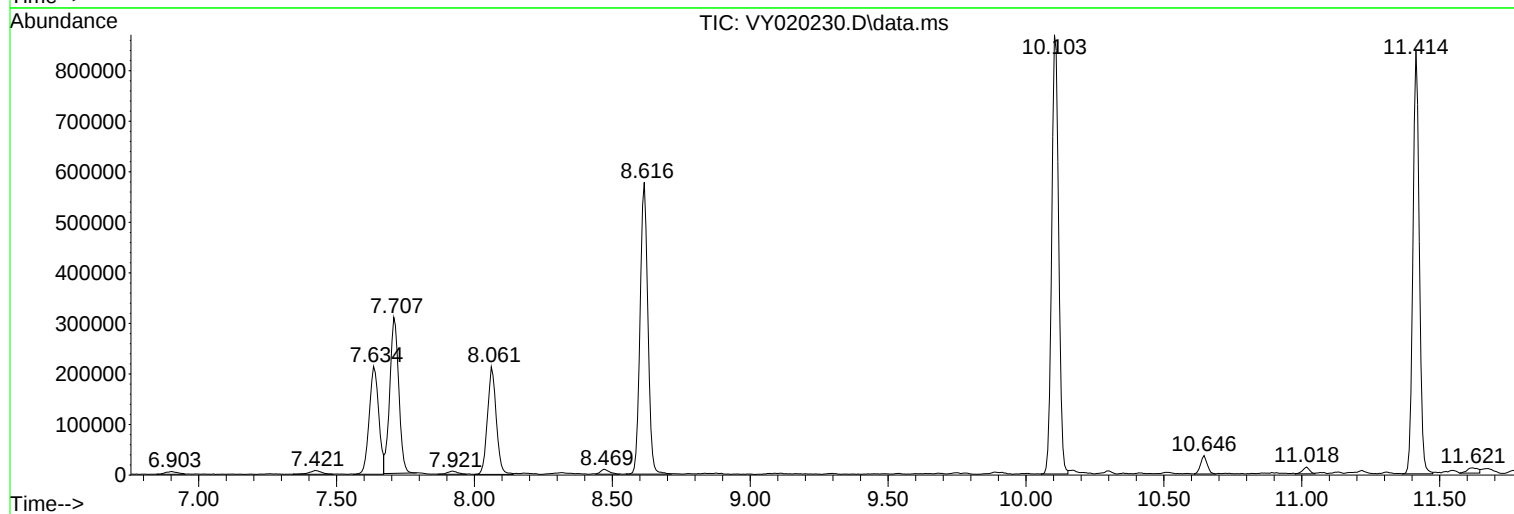
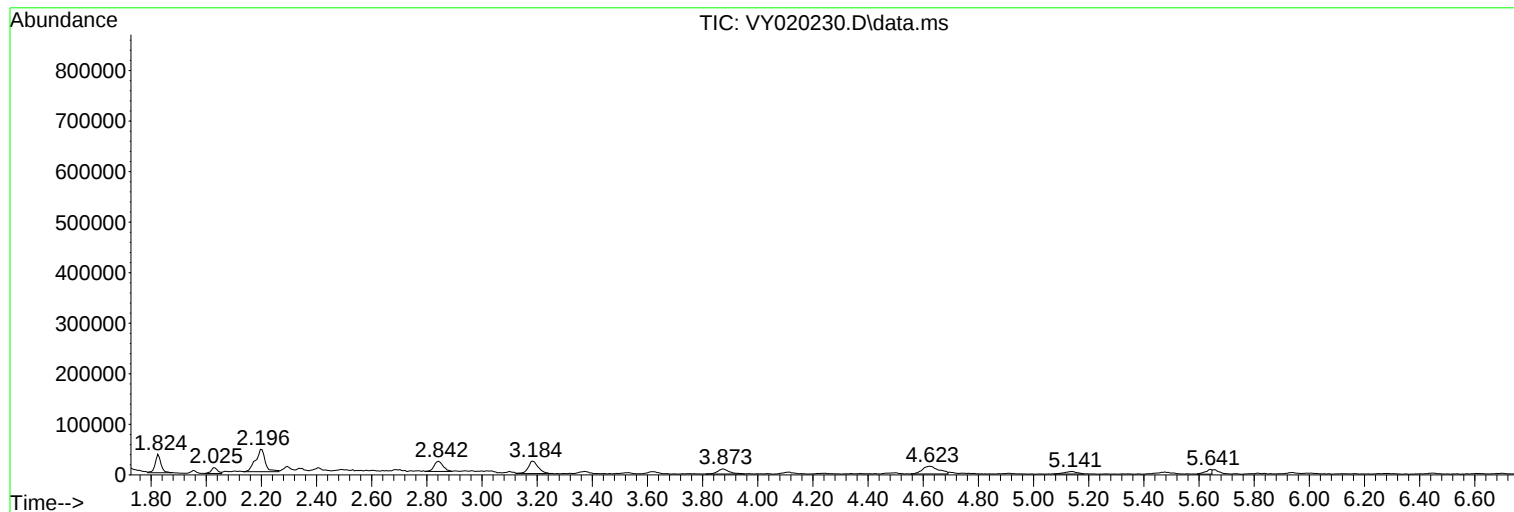
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WC-1(5.5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

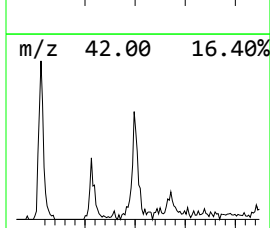
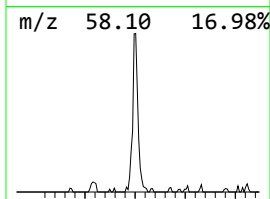
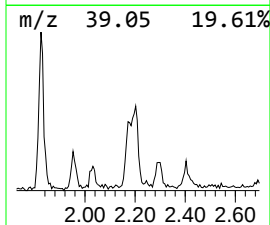
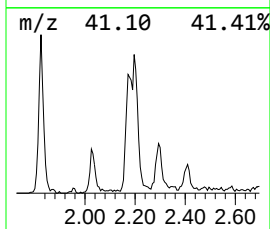
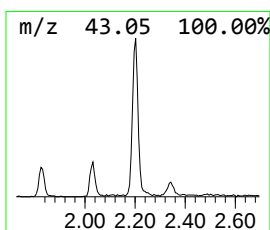
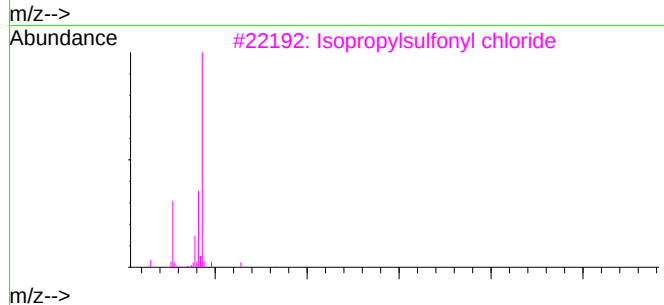
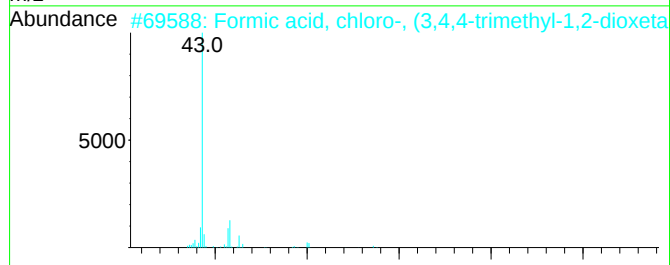
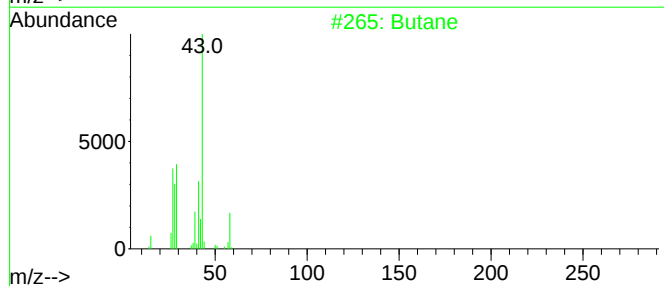
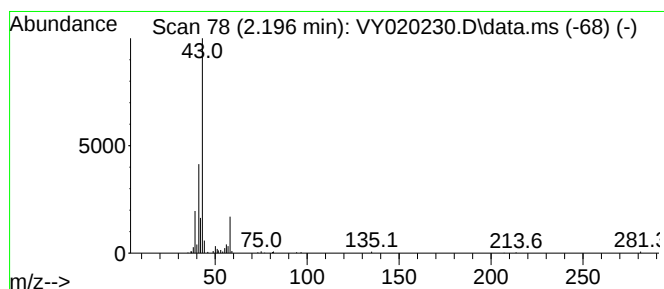
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.196	7.77 ug/l	107989	Pentafluorobenzene	7.707

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	33
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Hydroperoxide, 1-methylethyl	76	C3H8O2	003031-75-2	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-1(5.5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

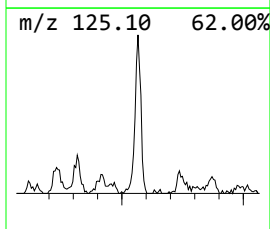
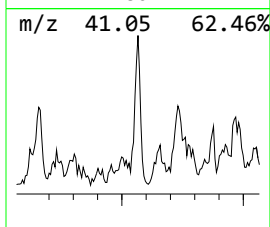
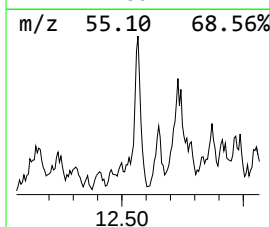
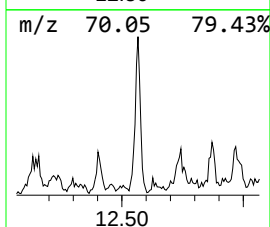
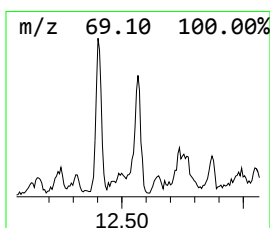
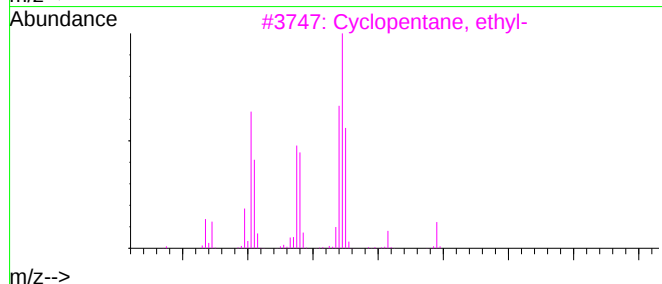
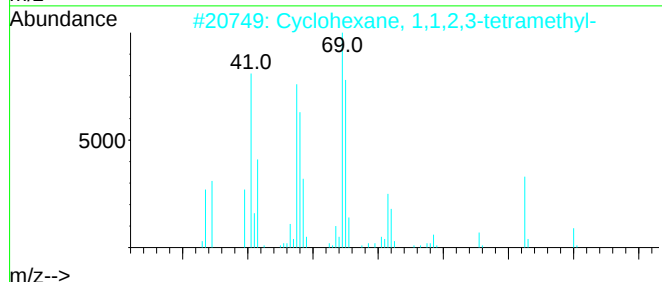
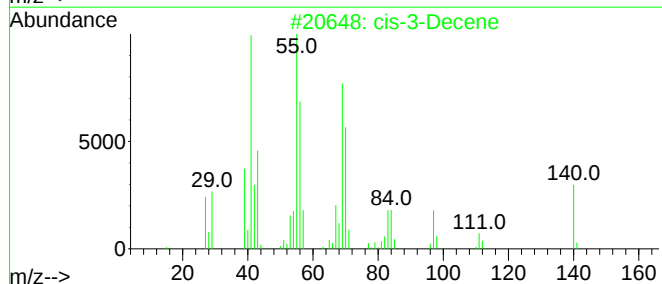
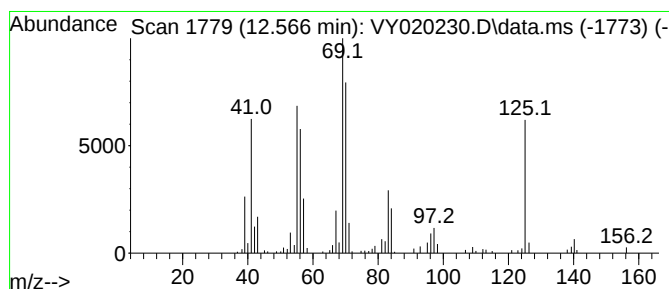
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 cis-3-Decene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.566	7.72 ug/l	136610	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-3-Decene	140	C10H20	019398-86-8	72
2			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	68
3			Cyclopentane, ethyl-	98	C7H14	001640-89-7	50
4			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	50
5			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	43



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WC-1(5.5)

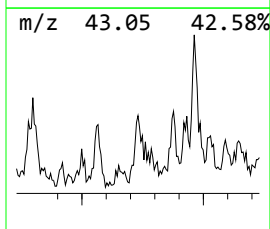
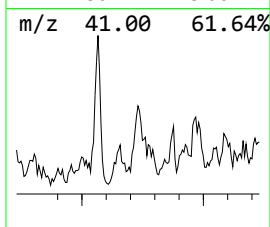
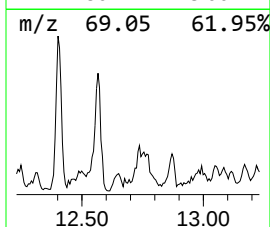
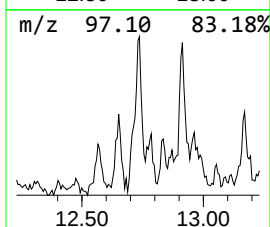
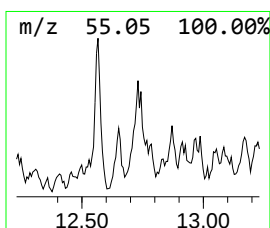
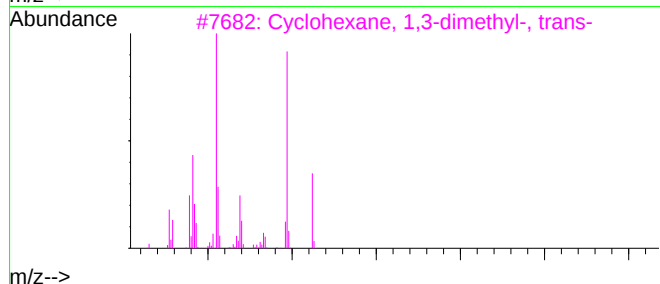
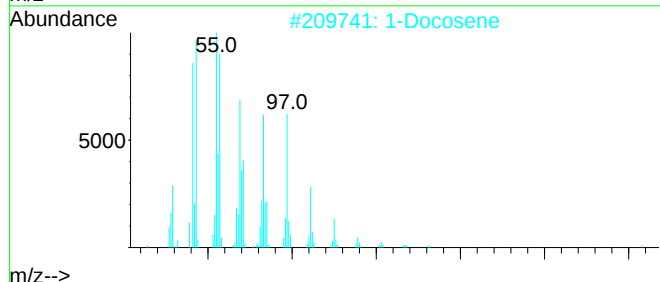
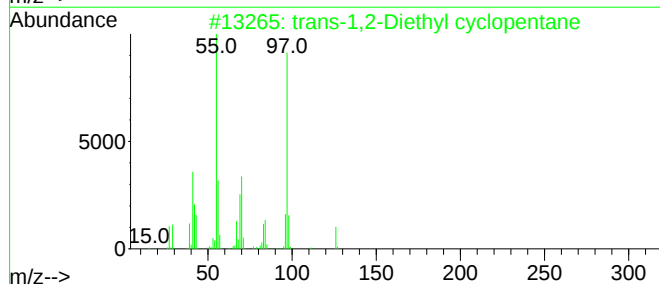
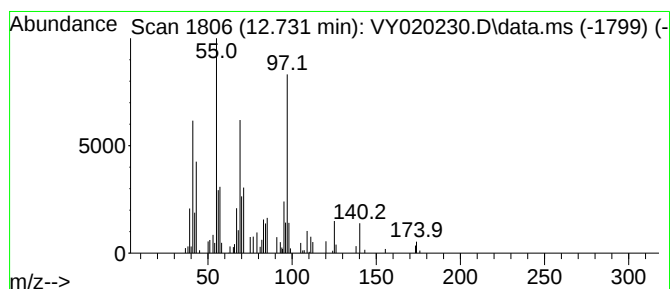
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.731 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.731	5.94 ug/l	105157	1,4-Dichlorobenzene-d4	13.347

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-1,2-Diethyl cyclopentane	126	C9H18	000932-40-1	49
2	1-Docosene	308	C22H44	001599-67-3	47
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	46
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	43
5	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	43



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Instrument :
MSVOA_Y
ClientSampleId :
WC-1(5.5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y103024S.M
Quant Title : SW846 8260

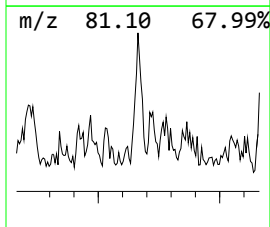
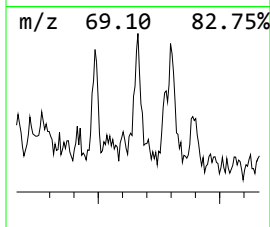
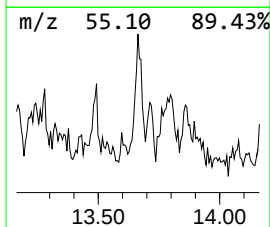
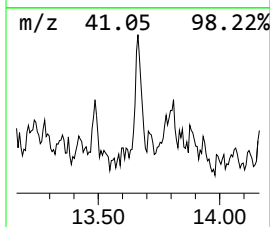
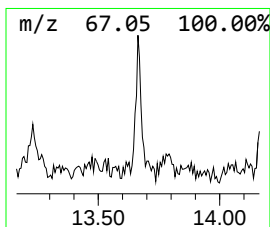
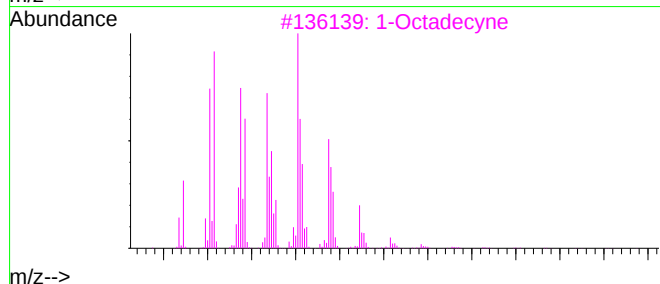
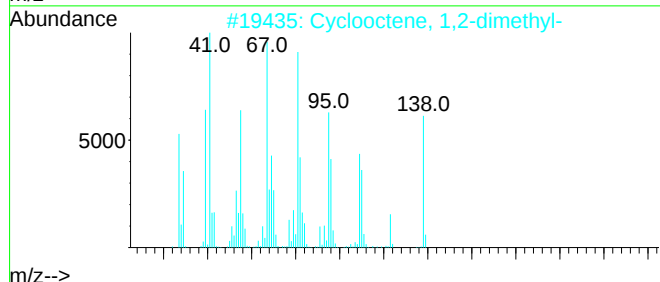
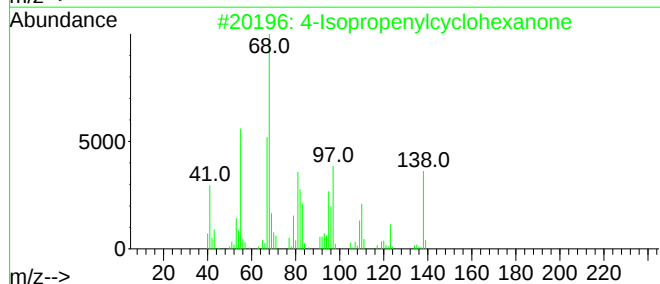
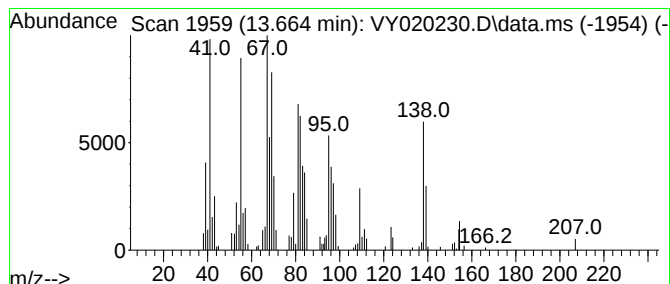
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.664 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.664	5.33 ug/l	94270	1,4-Dichlorobenzene-d4	13.347

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Isopropenylcyclohexanone	138	C9H14O	022460-53-3	49
2			Cyclooctene, 1,2-dimethyl-	138	C10H18	054299-96-6	46
3			1-Octadecyne	250	C18H34	000629-89-0	46
4			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	41
5			Cyclohexanone, 4-ethyl-3,4-dimet...	154	C10H18O	017429-42-4	38



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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
Butane	2.196	7.8	ug/l	107989	1	7.707	695002	50.0
cis-3-Decene	12.566	7.7	ug/l	136610	4	13.347	884762	50.0
unknown12.731	12.731	5.9	ug/l	105157	4	13.347	884762	50.0
unknown13.664	13.664	5.3	ug/l	94270	4	13.347	884762	50.0