

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121118\
 Data File : VX006422.D
 Acq On : 11 Dec 2018 15:58
 Operator : JC/MD
 Sample : J6334-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B1-121018

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_X\METHOD\82X112918W.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	1.300	18	24	26	rBV4	28850	39226	1.09%	0.153%
2	1.342	26	31	34	rVV	17517	40324	1.12%	0.157%
3	1.403	36	41	47	rVV	87049	129828	3.60%	0.505%
4	1.617	67	76	80	rVB5	44063	104321	2.89%	0.406%
5	1.788	100	104	115	rVB	205720	310809	8.62%	1.210%
6	2.007	134	140	151	rVV3	137953	269526	7.47%	1.049%
7	2.269	178	183	192	rVB	163295	260562	7.23%	1.014%
8	2.446	207	212	219	rVB	47280	77387	2.15%	0.301%
9	2.611	234	239	244	rBV	34913	70628	1.96%	0.275%
10	2.934	288	292	301	rVB2	84042	169956	4.71%	0.662%
11	3.165	325	330	339	rVB2	34724	88891	2.47%	0.346%
12	3.525	382	389	396	rVB4	14558	39154	1.09%	0.152%
13	3.812	429	436	444	rVV	20270	43479	1.21%	0.169%
14	4.397	522	532	545	rVB2	97532	296293	8.22%	1.153%
15	4.702	573	582	587	rBV2	19308	50428	1.40%	0.196%
16	5.177	653	660	670	rBV3	12448	37814	1.05%	0.147%
17	5.305	670	681	690	rVB3	27212	80813	2.24%	0.315%
18	5.506	702	714	721	rBV	442909	1269713	35.21%	4.942%
19	5.580	721	726	732	rVV3	108781	312038	8.65%	1.215%
20	5.665	732	740	759	rVB	787360	2202954	61.10%	8.575%
21	6.067	795	806	814	rBV	432876	1117621	31.00%	4.350%
22	6.146	814	819	828	rVB2	57587	146239	4.06%	0.569%
23	6.372	849	856	862	rVB5	13745	37411	1.04%	0.146%
24	6.860	926	936	947	rBV	1109581	2614977	72.52%	10.178%
25	7.463	1026	1035	1044	rBV2	122231	278761	7.73%	1.085%
26	8.573	1211	1217	1222	rBV2	34961	61706	1.71%	0.240%
27	8.646	1222	1229	1234	rVV	73337	136082	3.77%	0.530%
28	8.713	1234	1240	1248	rVV	2308225	3605723	100.00%	14.035%
29	8.786	1248	1252	1257	rVB2	45464	69485	1.93%	0.270%
30	8.878	1263	1267	1271	rBV	31115	46812	1.30%	0.182%
31	9.097	1299	1303	1310	rBV3	31855	56451	1.57%	0.220%
32	9.518	1363	1372	1376	rBV	44750	71779	1.99%	0.279%
33	10.115	1460	1470	1480	rBV	2240977	3120507	86.54%	12.146%
34	10.274	1489	1496	1502	rBV3	41057	84314	2.34%	0.328%

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Integration Parameters: RTEINT.P

Integrator: RTE
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35	10.359	1502	1510	1516	rVB	224370	332347	9.22%	1.294%
36	10.701	1561	1566	1570	rBV	61868	81383	2.26%	0.317%
37	10.926	1595	1603	1606	rBV4	23102	42293	1.17%	0.165%
38	11.139	1632	1638	1645	rBV	1924787	2525368	70.04%	9.829%
39	11.225	1648	1652	1658	rVB3	31793	47545	1.32%	0.185%
40	11.359	1670	1674	1682	rBV6	22554	55918	1.55%	0.218%
41	11.432	1682	1686	1688	rBV	95573	116450	3.23%	0.453%
42	11.505	1693	1698	1702	rVV	87255	119215	3.31%	0.464%
43	11.670	1721	1725	1733	rBV	55276	85124	2.36%	0.331%
44	11.804	1743	1747	1752	rVB	220383	276866	7.68%	1.078%
45	12.078	1786	1792	1798	rVV	2516435	3095146	85.84%	12.047%
46	12.139	1798	1802	1806	rVB	115051	140098	3.89%	0.545%
47	12.298	1823	1828	1837	rBV3	117571	183511	5.09%	0.714%
48	12.377	1837	1841	1849	rVB4	63280	107003	2.97%	0.416%
49	12.584	1870	1875	1877	rBV	37640	51512	1.43%	0.200%
50	12.609	1877	1879	1884	rVB	37583	41501	1.15%	0.162%
51	12.670	1884	1889	1892	rBV	80256	97393	2.70%	0.379%
52	12.755	1897	1903	1910	rVB2	63427	95161	2.64%	0.370%
53	12.975	1934	1939	1943	rVV2	53551	76768	2.13%	0.299%
54	13.017	1943	1946	1951	rVB	57683	63880	1.77%	0.249%
55	13.224	1976	1980	1984	rVB	42598	46252	1.28%	0.180%
56	13.346	1996	2000	2005	rVB2	111991	152768	4.24%	0.595%
57	13.481	2017	2022	2028	rVB2	34647	50323	1.40%	0.196%
58	13.639	2045	2048	2055	rVV6	22677	37847	1.05%	0.147%
59	13.718	2055	2061	2068	rVB2	22192	48936	1.36%	0.190%
60	13.834	2074	2080	2088	rVB	120590	165331	4.59%	0.644%
61	14.700	2218	2222	2231	rVB	90618	130538	3.62%	0.508%
62	14.840	2240	2245	2251	rVB2	54519	83291	2.31%	0.324%

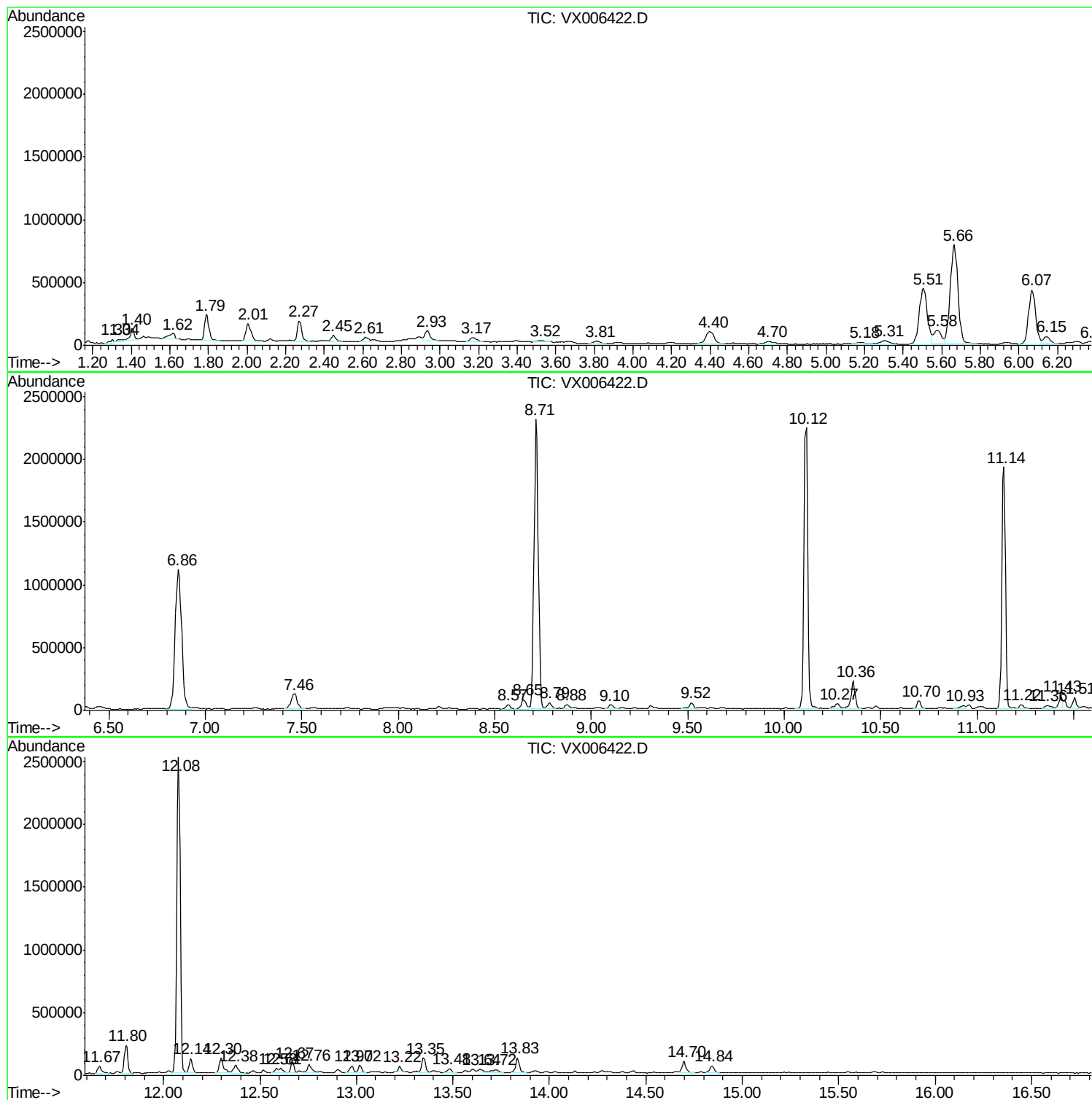
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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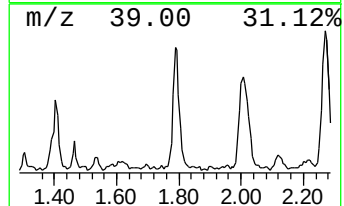
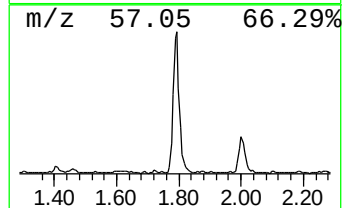
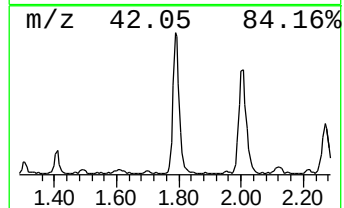
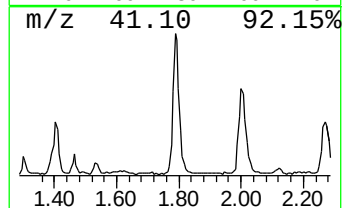
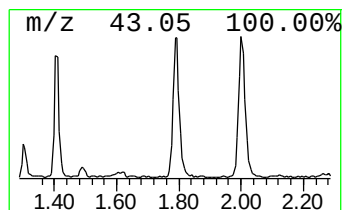
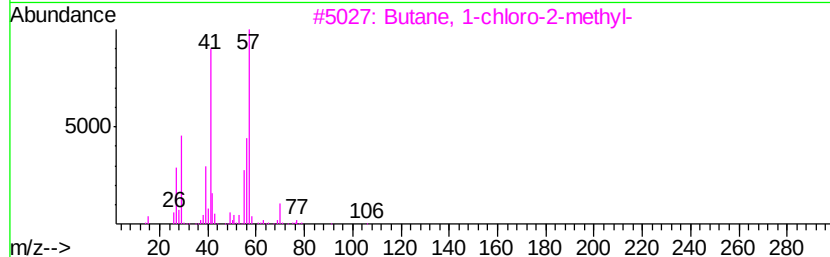
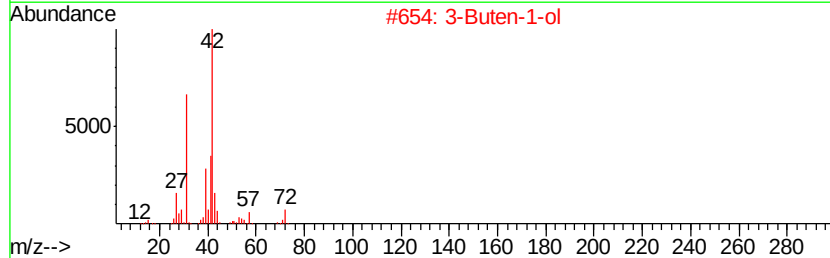
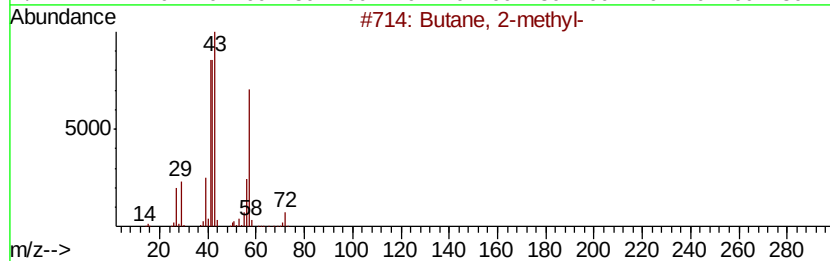
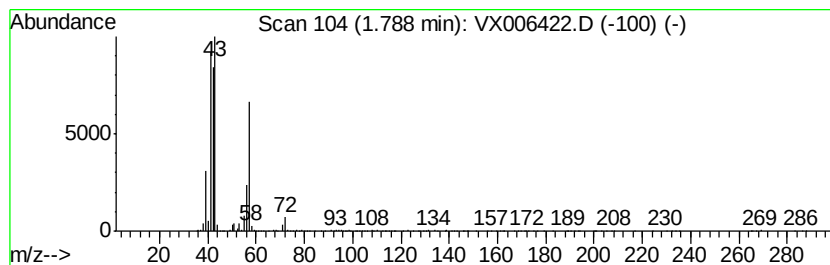
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	7.05 ug/l	310809	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5		Azetidine	57	C3H7N	000503-29-7	9



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Instrument :
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ClientSampled :
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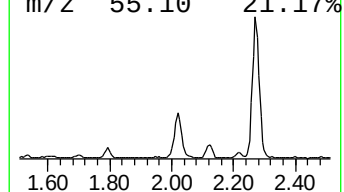
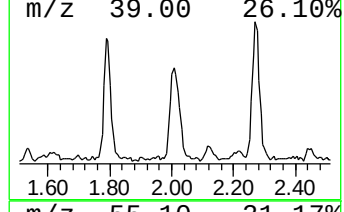
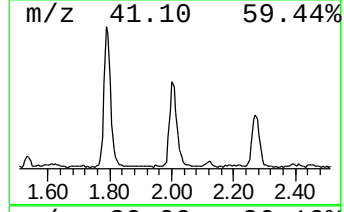
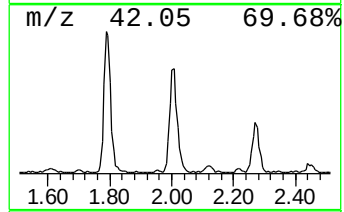
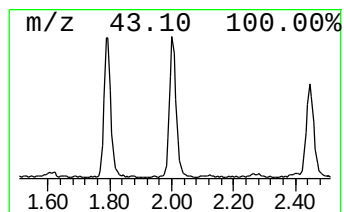
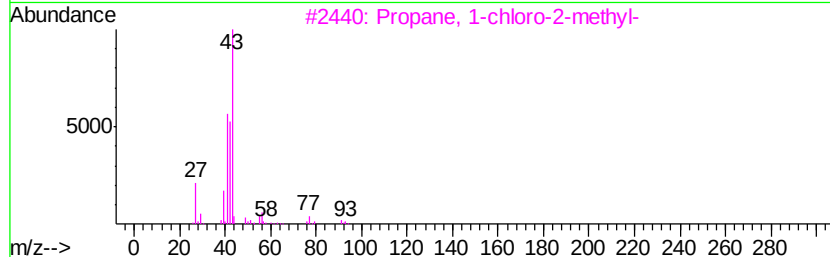
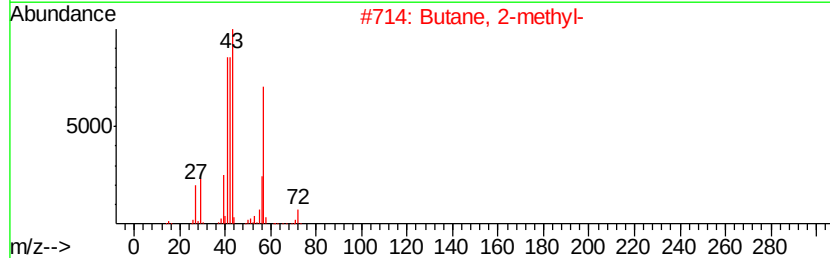
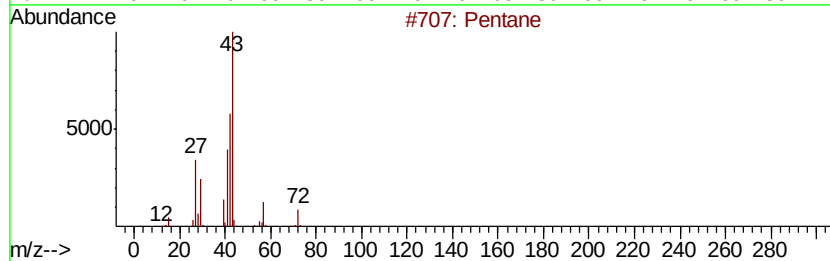
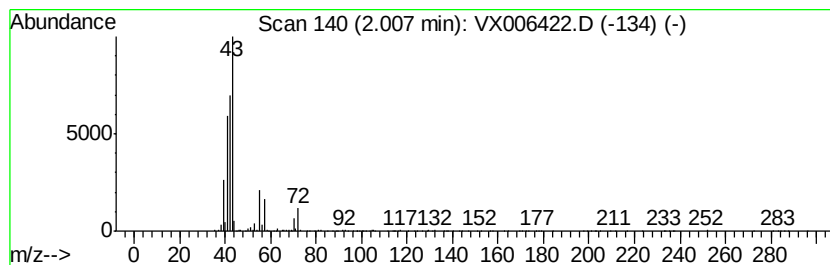
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	6.12 ug/l	269526	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	80
2		Butane, 2-methyl-	72	C5H12	000078-78-4	42
3		Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	40
4		3-Methyl-3-isopropylidiaziridine	100	C5H12N2	024476-95-7	38
5		Oxirane, ethyl-	72	C4H8O	000106-88-7	38



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ClientSampleId :
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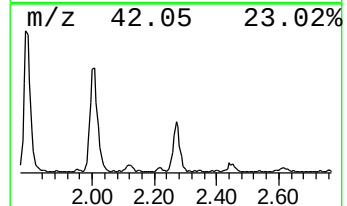
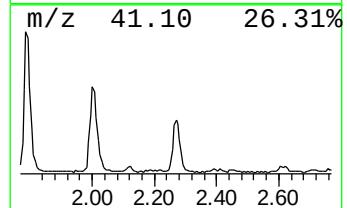
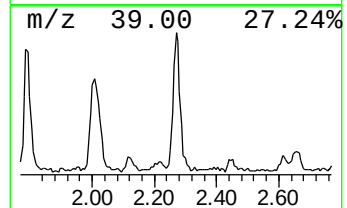
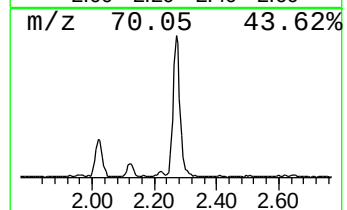
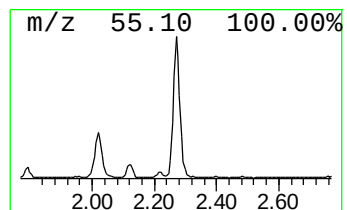
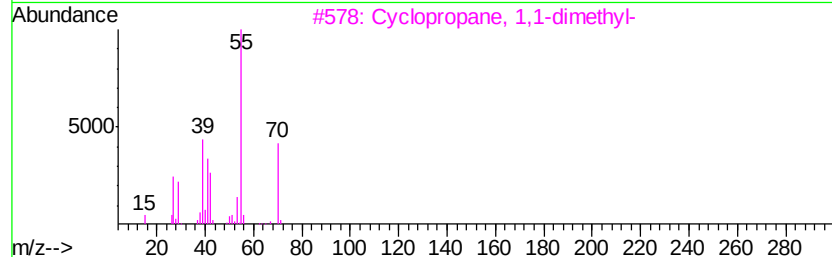
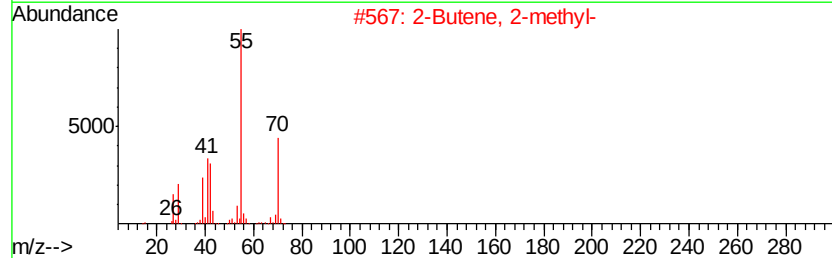
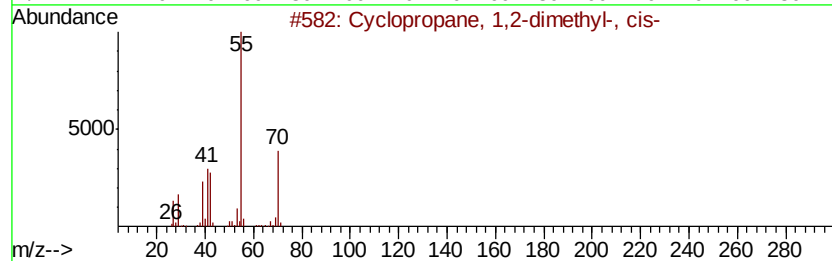
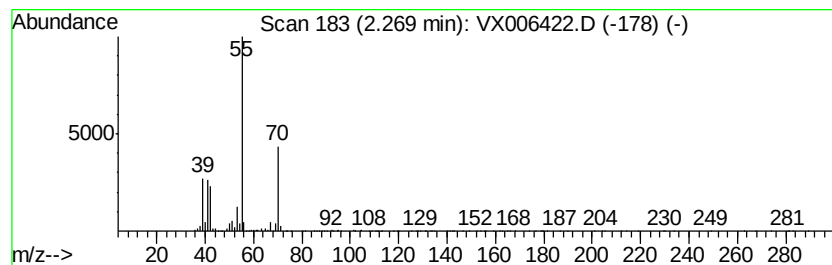
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	5.91 ug/l	260562	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2		2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3		Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86
4		2-Pentene, (E)-	70	C5H10	000646-04-8	86
5		Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86



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ClientSampleId :
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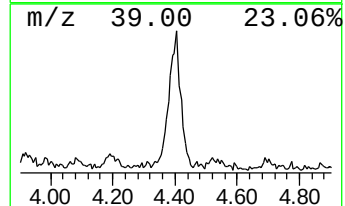
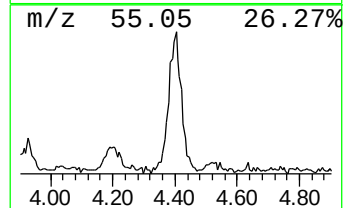
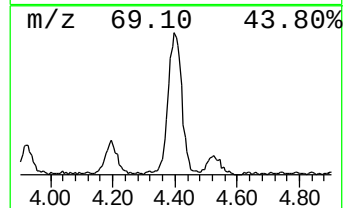
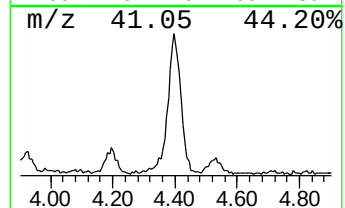
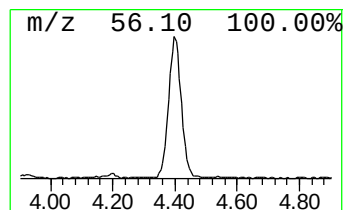
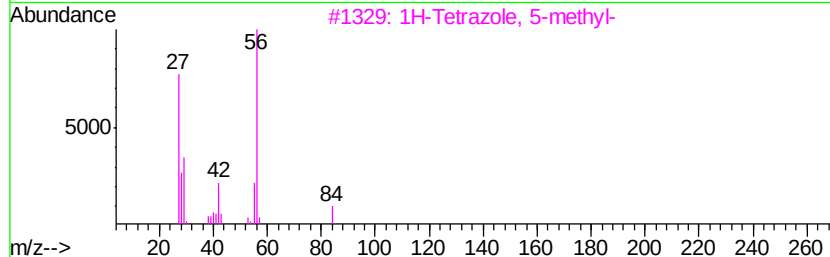
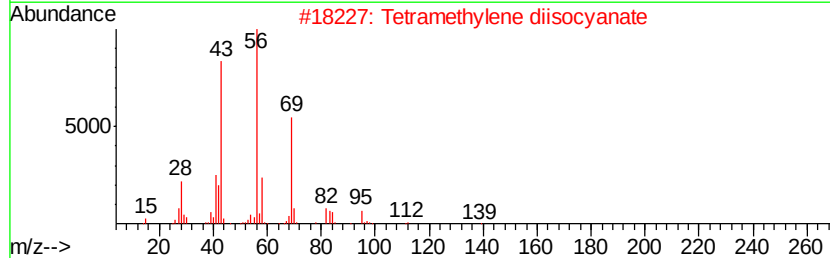
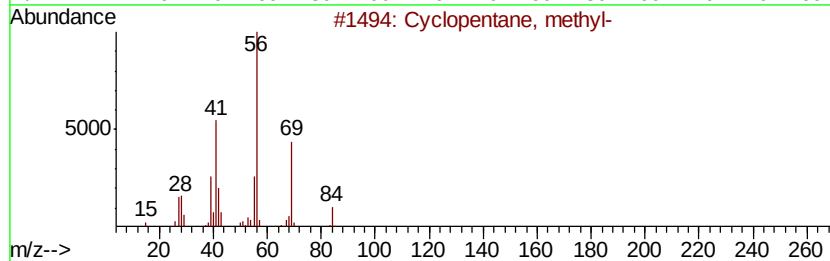
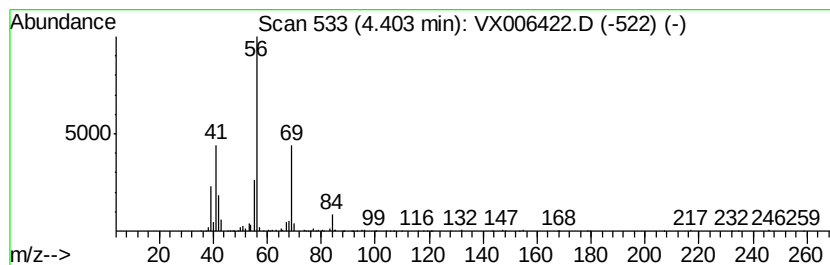
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	6.72 ug/l	296293	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Tetramethylene diisocyanate	140	C6H8N2O2	004538-37-8	72
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
5		Cyclohexane	84	C6H12	000110-82-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	1.79	7.0	ug/l	310809	1	5.66	2202950	50.0
Pentane	2.01	6.1	ug/l	269526	1	5.66	2202950	50.0
Cyclopropane, 1,2...	2.27	5.9	ug/l	260562	1	5.66	2202950	50.0
Cyclopentane, met...	4.40	6.7	ug/l	296293	1	5.66	2202950	50.0