

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
 Data File : VN072099.D
 Acq On : 21 Apr 2022 00:41
 Operator : JC\MD
 Sample : N2482-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-22R

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\82N033022W.M
 Title : SW846 8260

Signal : TIC: VN072099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	38	46	65	rVB4	55518	177836	5.44%	0.802%
2	2.434	69	76	88	rVB	366925	599827	18.36%	2.705%
3	3.128	184	194	206	rVB	201088	467488	14.31%	2.108%
4	3.510	251	259	275	rVB2	44219	118597	3.63%	0.535%
5	3.993	331	341	356	rBV	170367	470070	14.39%	2.119%
6	4.293	384	392	408	rVB	27586	84249	2.58%	0.380%
7	4.575	429	440	451	rBV	25128	85122	2.61%	0.384%
8	5.192	532	545	564	rVB	91811	331899	10.16%	1.496%
9	6.469	752	762	774	rVB3	22483	67209	2.06%	0.303%
10	6.610	776	786	796	rBV3	11979	37408	1.14%	0.169%
11	7.145	868	877	885	rBV2	43936	122262	3.74%	0.551%
12	7.216	885	889	898	rVB	16853	36871	1.13%	0.166%
13	7.410	914	922	934	rVB3	42488	111485	3.41%	0.503%
14	7.839	986	995	1008	rVB2	32491	78191	2.39%	0.353%
15	8.022	1015	1026	1030	rBV	387080	926379	28.35%	4.177%
16	8.081	1030	1036	1049	rVB	763623	1786305	54.67%	8.054%
17	8.445	1084	1098	1109	rBV3	594945	1820156	55.70%	8.207%
18	8.586	1114	1122	1128	rBV6	20680	56327	1.72%	0.254%
19	8.963	1178	1186	1201	rBV	1120935	2324689	71.14%	10.482%
20	10.439	1429	1437	1444	rBV	1785728	3267563	100.00%	14.733%
21	10.498	1444	1447	1461	rVB	64478	125426	3.84%	0.566%
22	11.739	1650	1658	1669	rBV	1806135	3196821	97.84%	14.414%
23	11.839	1669	1675	1681	rVB	85926	147640	4.52%	0.666%
24	11.951	1688	1694	1706	rVB	44393	87840	2.69%	0.396%
25	12.574	1791	1800	1807	rBV	46416	82673	2.53%	0.373%
26	12.727	1818	1826	1838	rBV	1389107	2358036	72.16%	10.632%
27	12.915	1852	1858	1867	rVB	64141	105007	3.21%	0.473%
28	13.668	1979	1986	1999	rBV	1456817	2508798	76.78%	11.312%
29	13.874	2015	2021	2027	rVB	245072	406769	12.45%	1.834%
30	14.210	2072	2078	2084	rBV2	31267	50653	1.55%	0.228%
31	14.321	2092	2097	2103	rVB	35493	56371	1.73%	0.254%
32	14.927	2192	2200	2206	rBV5	21275	43906	1.34%	0.198%
33	15.498	2290	2297	2305	rVB2	19341	38678	1.18%	0.174%

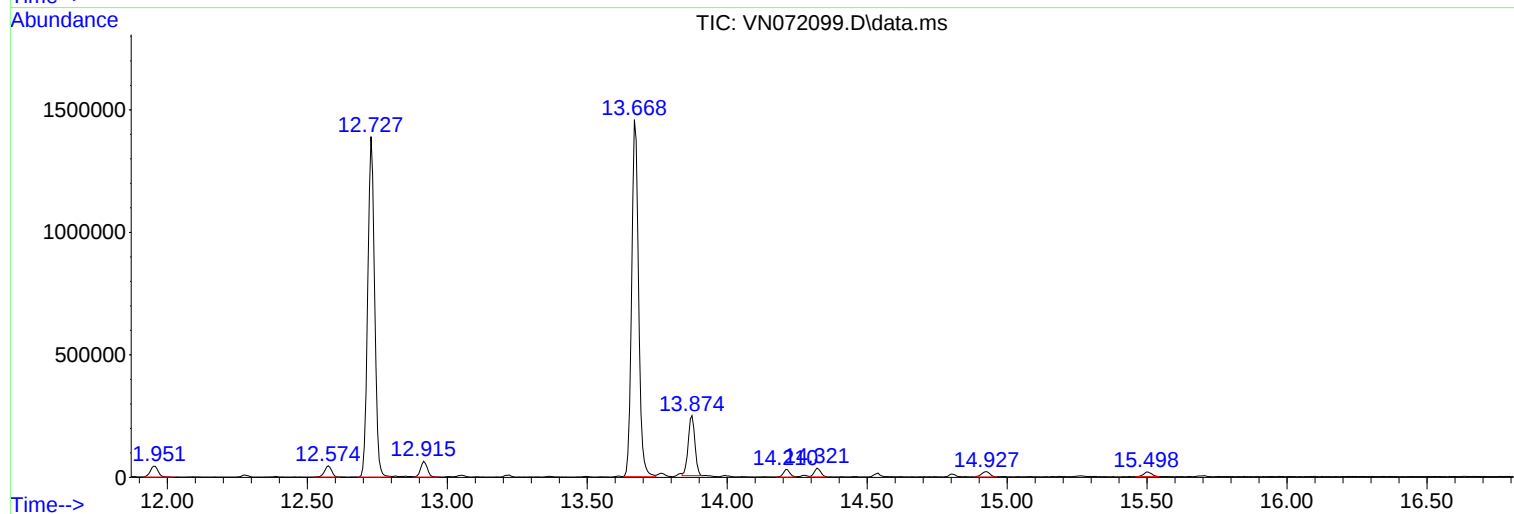
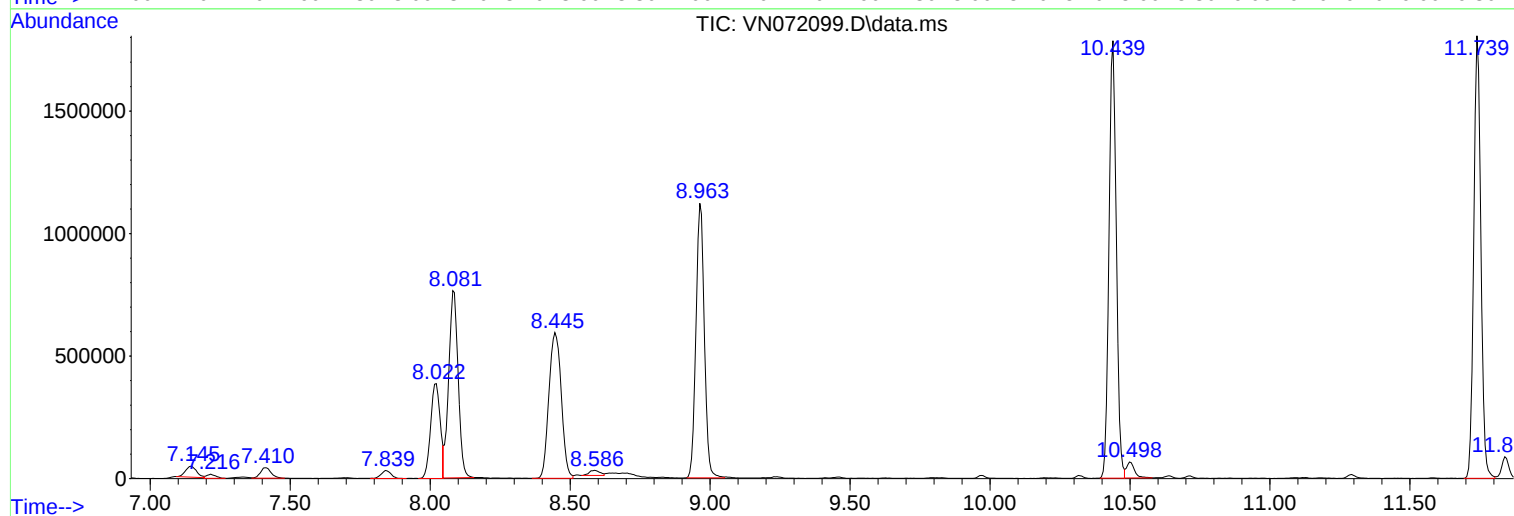
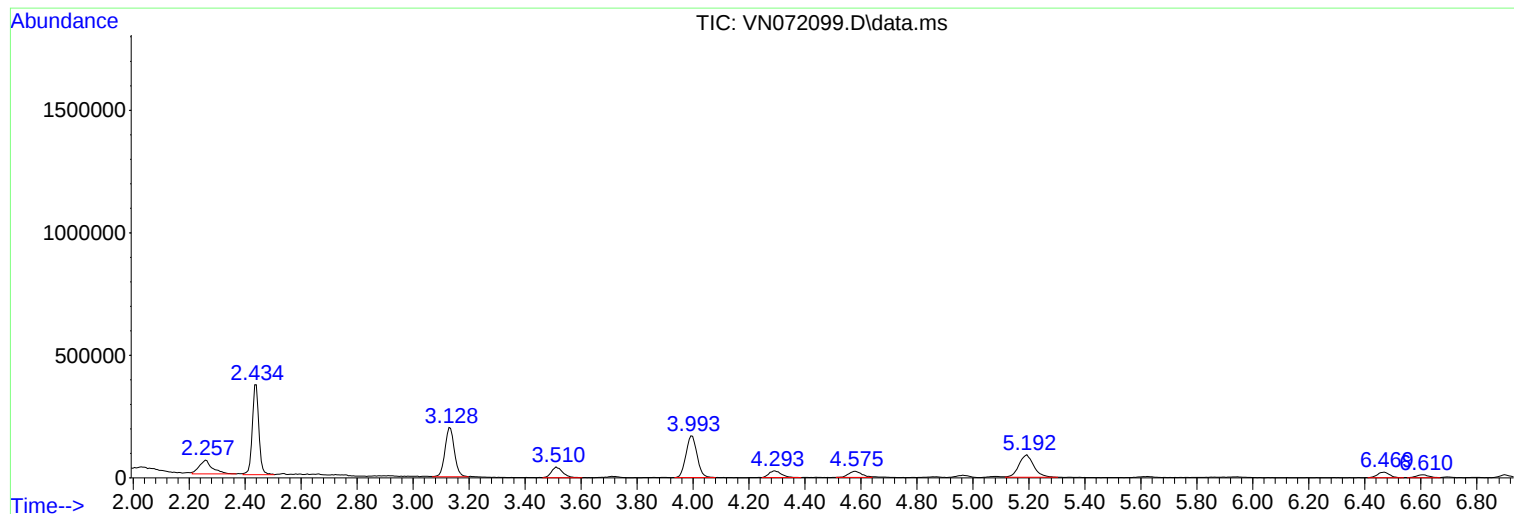
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



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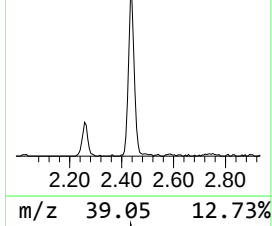
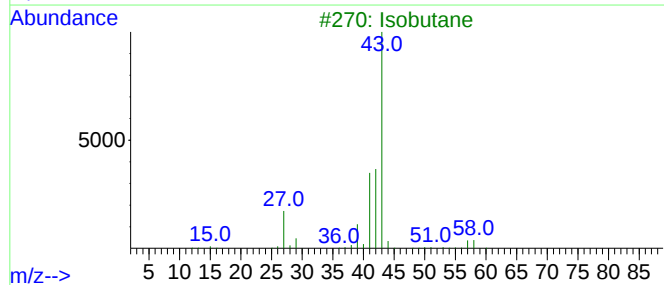
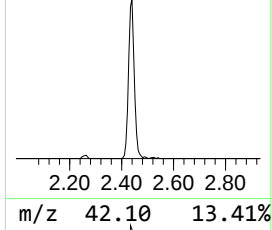
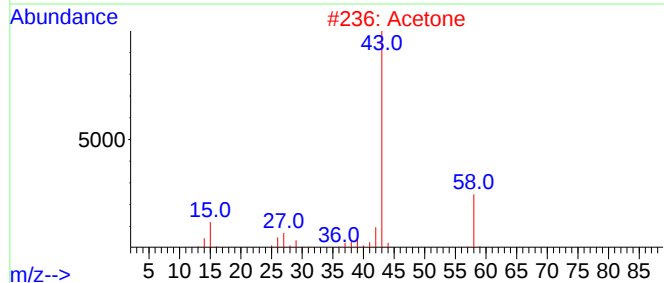
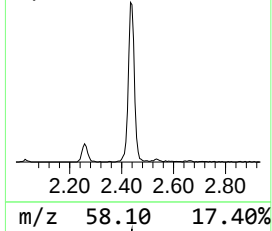
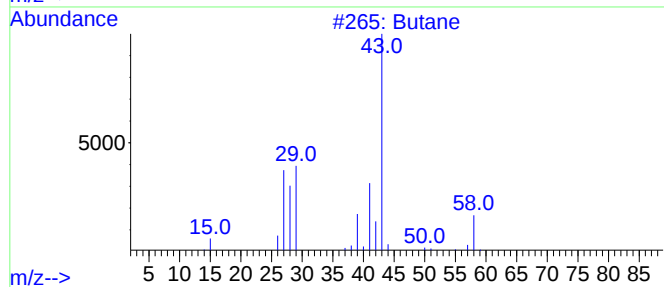
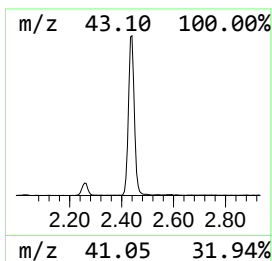
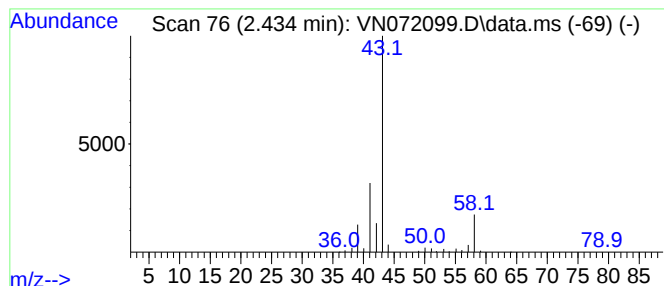
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	16.79 ug/l	599827	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane			58	C4H10	000106-97-8	80
2	Acetone			58	C3H6O	000067-64-1	50
3	Isobutane			58	C4H10	000075-28-5	9
4	Isopropylsulfonyl chloride			142	C3H7ClO2S	010147-37-2	9
5	Cyclobutylamine			71	C4H9N	002516-34-9	4



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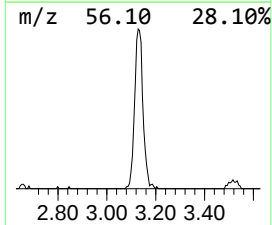
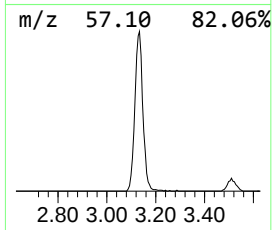
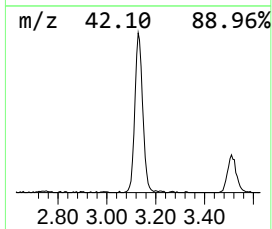
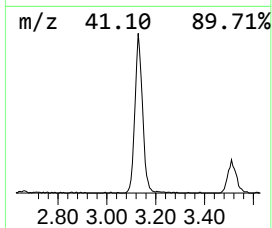
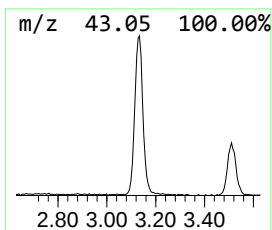
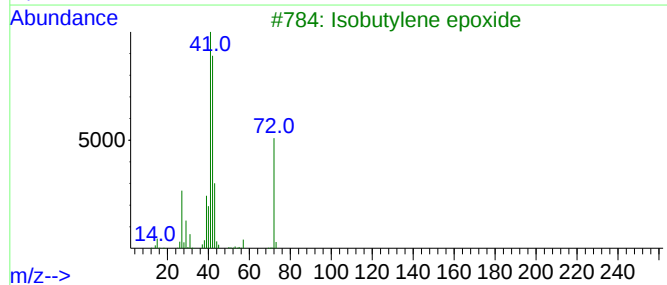
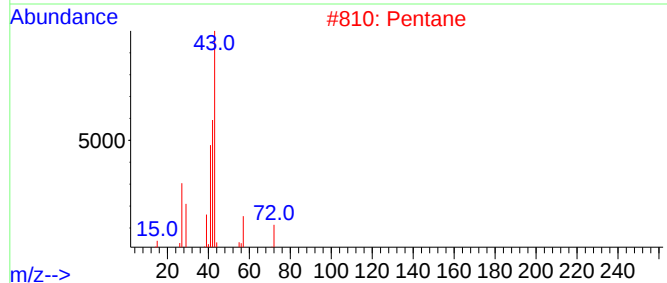
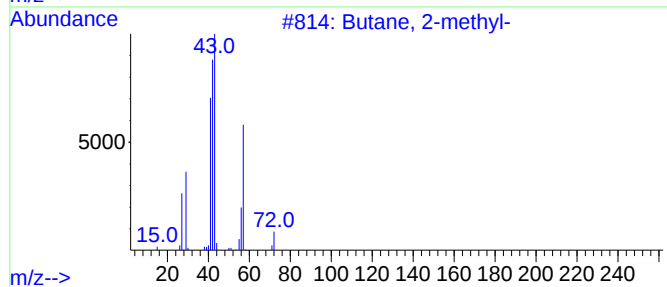
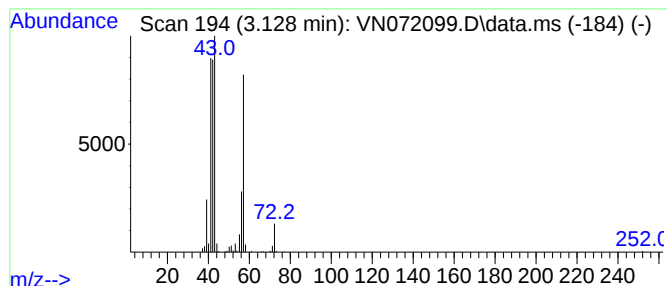
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Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	13.09 ug/l	467488	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	87
2			Pentane	72	C5H12	000109-66-0	59
3			Isobutylene epoxide	72	C4H8O	000558-30-5	38
4			1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
5			Butane, 2-chloro-3-methyl-	106	C5H11Cl	000631-65-2	25



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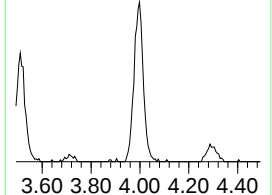
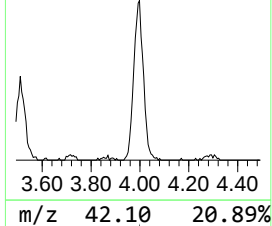
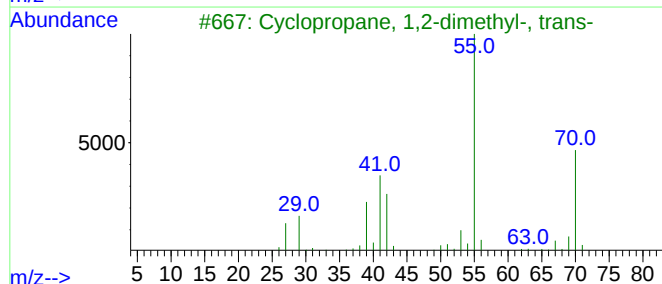
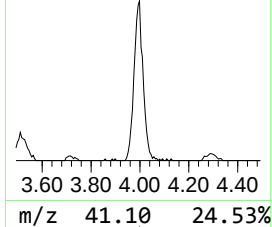
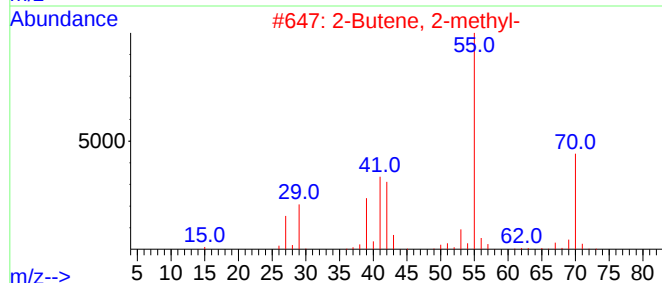
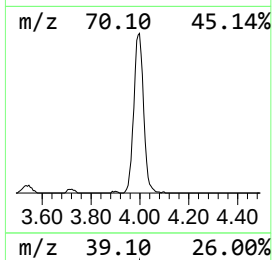
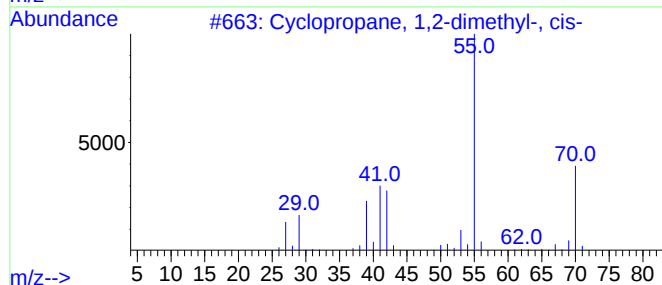
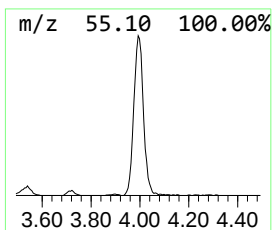
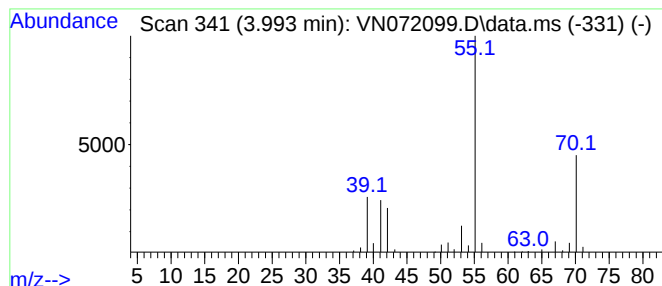
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.993	13.16 ug/l	470070	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2			2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	90
4			2-Pentene, (Z)-	70	C5H10	000627-20-3	78
5			1-Butene, 3-methyl-	70	C5H10	000563-45-1	78



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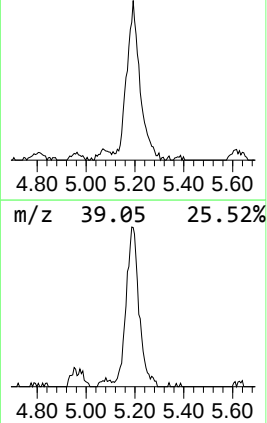
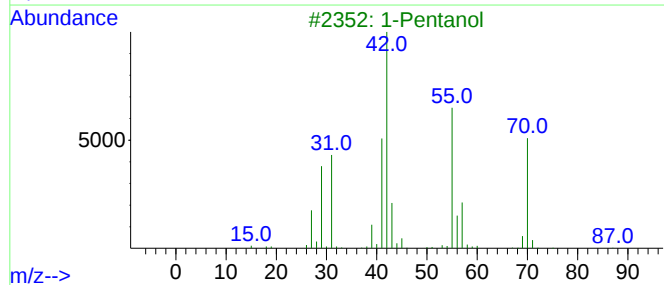
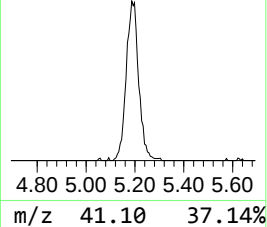
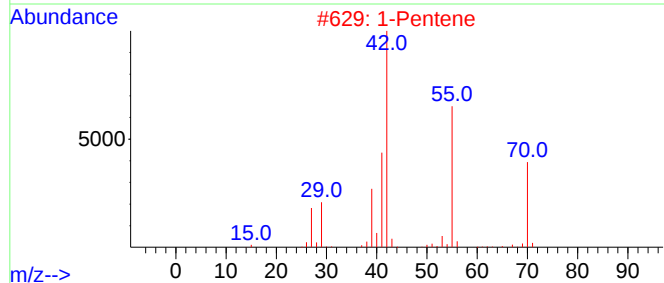
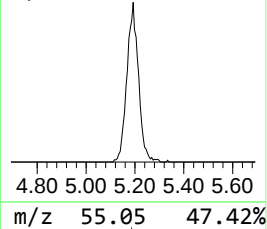
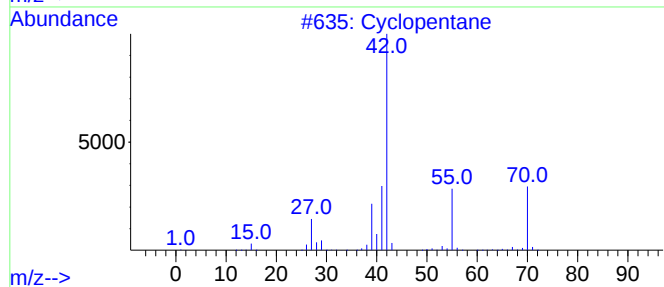
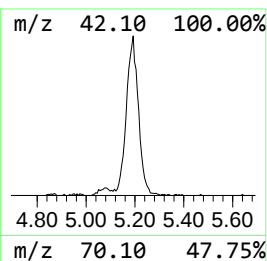
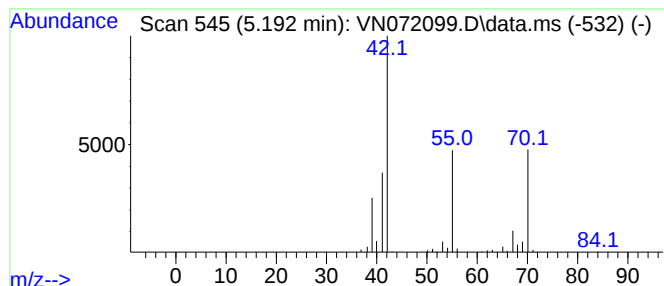
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Quant Title : SW846 8260

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

Peak Number 4 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	9.29 ug/l	331899	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			1-Pentene	70	C5H10	000109-67-1	53
3			1-Pentanol	88	C5H12O	000071-41-0	39
4			3-Buten-1-ol	72	C4H8O	000627-27-0	37
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	17



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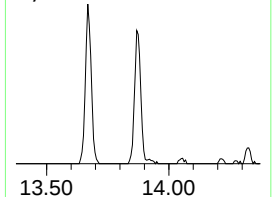
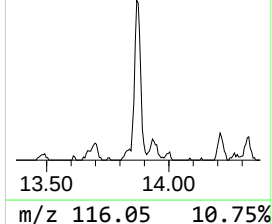
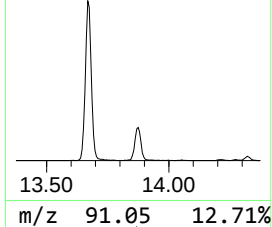
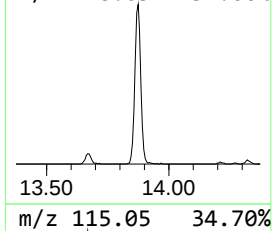
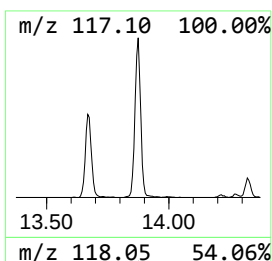
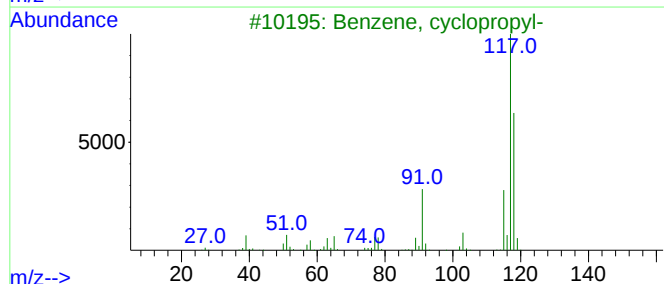
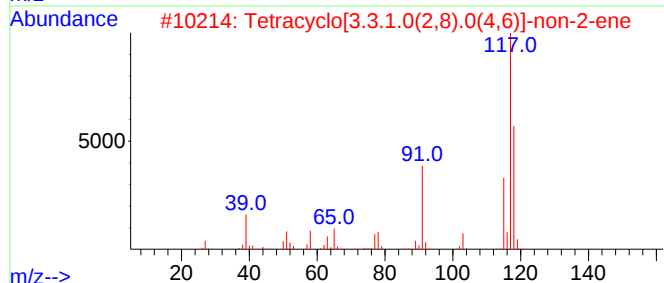
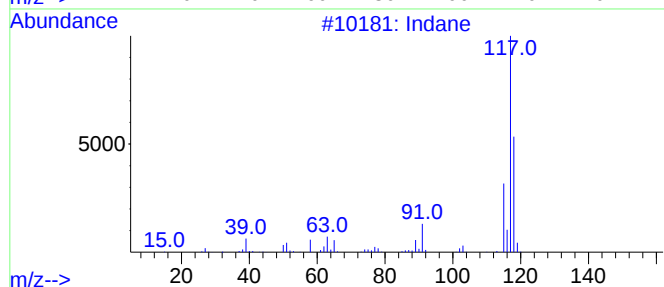
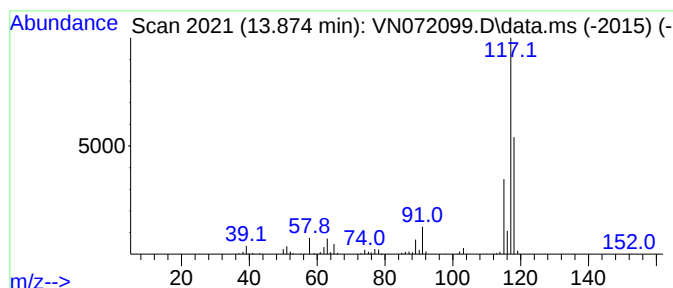
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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

Peak Number 5 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	8.11 ug/l	406769	1,4-Dichlorobenzene-d4	13.668

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	59



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane	2.434	16.8	ug/l	599827	1	8.081	1786310	50.0
Butane, 2-methyl-	3.128	13.1	ug/l	467488	1	8.081	1786310	50.0
Cyclopropane, 1...	3.993	13.2	ug/l	470070	1	8.081	1786310	50.0
Cyclopentane	5.192	9.3	ug/l	331899	1	8.081	1786310	50.0
Indane	13.874	8.1	ug/l	406769	4	13.668	2508800	50.0