

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092120\
 Data File : VU040237.D
 Acq On : 21 Sep 2020 16:35
 Operator : SY/MD
 Sample : L4046-02DL 10X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG0P0DL

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_U\METHOD\SOMUTR083120WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.607	74	83	91	rVB	57660	65997	7.46%	0.943%
2	1.922	173	181	194	rVB	50496	66718	7.54%	0.953%
3	2.388	314	326	346	rBV	163846	253395	28.65%	3.619%
4	2.581	374	386	401	rBV	106088	173532	19.62%	2.478%
5	2.662	401	411	419	rBV2	4964	9399	1.06%	0.134%
6	3.063	523	536	543	rBV3	6319	12339	1.40%	0.176%
7	3.202	565	579	594	rBV3	10644	24151	2.73%	0.345%
8	3.382	623	635	648	rVB3	10533	22795	2.58%	0.326%
9	3.719	727	740	752	rVB5	7376	16862	1.91%	0.241%
10	4.012	809	831	856	rBV	341415	884474	100.00%	12.632%
11	4.552	978	999	1014	rBV2	27714	67535	7.64%	0.965%
12	4.661	1016	1033	1084	rVV3	89105	343790	38.87%	4.910%
13	5.083	1146	1164	1182	rBV2	93772	206733	23.37%	2.953%
14	5.407	1251	1265	1277	rVB7	7510	16721	1.89%	0.239%
15	5.742	1346	1369	1398	rBV3	188048	503370	56.91%	7.189%
16	6.263	1517	1531	1548	rBV	167706	315515	35.67%	4.506%
17	6.703	1655	1668	1683	rBV2	120379	233331	26.38%	3.332%
18	6.774	1683	1690	1699	rVB5	5469	9530	1.08%	0.136%
19	7.574	1927	1939	1956	rBV2	57162	102905	11.63%	1.470%
20	7.722	1972	1985	1996	rVB8	4672	9585	1.08%	0.137%
21	7.906	2021	2042	2056	rBV	219382	384044	43.42%	5.485%
22	8.185	2115	2129	2142	rBV	39987	66584	7.53%	0.951%
23	8.642	2257	2271	2312	rBV	358790	662540	74.91%	9.462%
24	9.420	2497	2513	2516	rBV	251308	377195	42.65%	5.387%
25	9.449	2517	2522	2547	rVB	354780	558267	63.12%	7.973%
26	10.481	2831	2843	2858	rBV	253506	401806	45.43%	5.739%
27	10.754	2908	2928	2946	rBV	99418	163507	18.49%	2.335%
28	10.886	2953	2969	2982	rBV3	29624	51036	5.77%	0.729%
29	11.285	3083	3093	3101	rBV3	9679	14052	1.59%	0.201%
30	11.414	3122	3133	3143	rVB2	13094	19521	2.21%	0.279%
31	11.806	3242	3255	3271	rBV	251233	439085	49.64%	6.271%
32	11.880	3271	3278	3290	rVB4	30837	47733	5.40%	0.682%
33	12.089	3329	3343	3353	rVV3	12722	20133	2.28%	0.288%
34	12.185	3361	3373	3392	rBV	232090	401925	45.44%	5.740%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

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Title : TRACE VOA SOM01.0

35	12.561	3482	3490	3498	rBV2	10379	14429	1.63%	0.206%
36	12.815	3560	3569	3576	rVV4	18415	28101	3.18%	0.401%
37	13.986	3923	3933	3944	rVB7	7479	13129	1.48%	0.188%

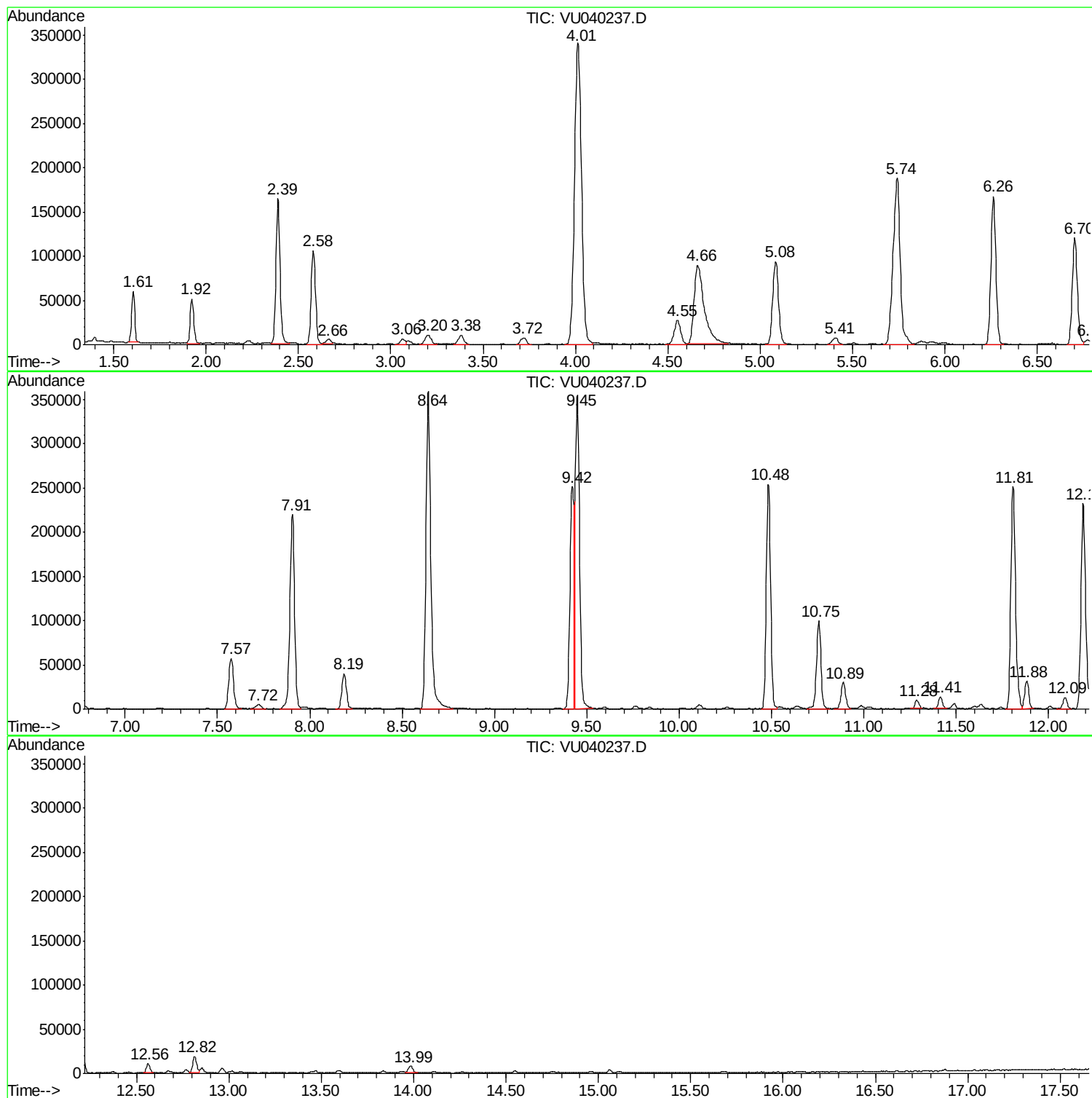
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Quant Title : TRACE VOA SOM01.0

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



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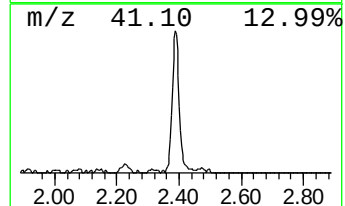
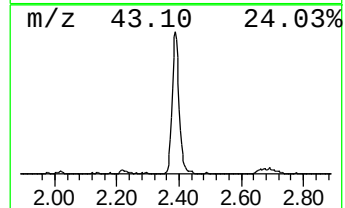
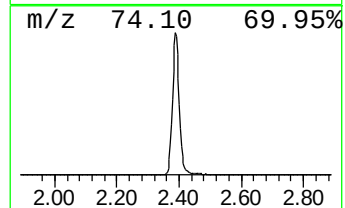
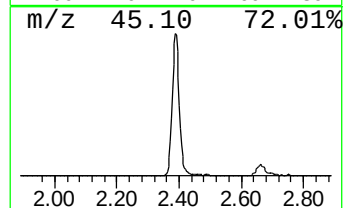
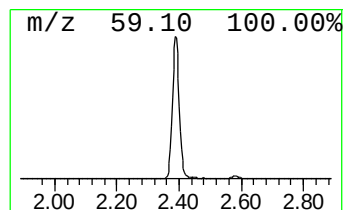
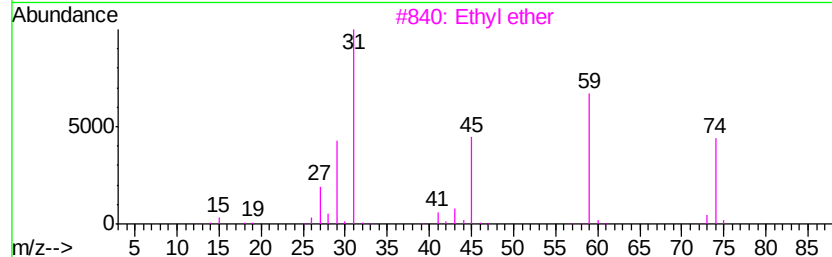
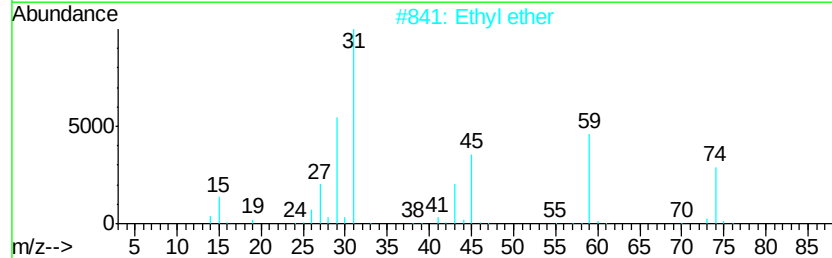
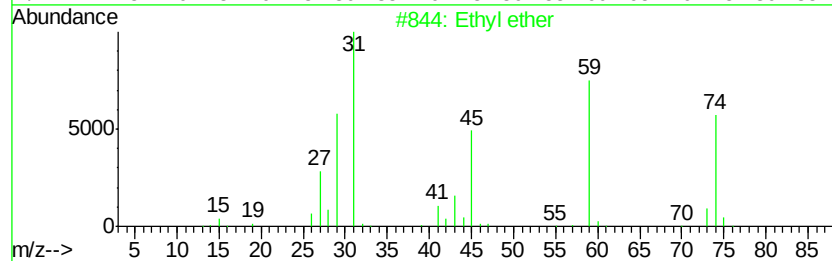
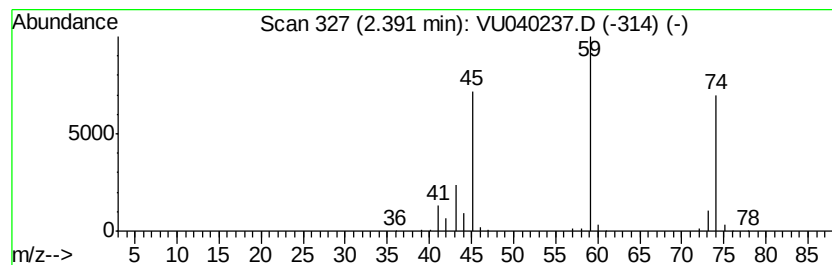
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	4.02 ug/L	253395	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl ether	74	C4H10O	000060-29-7	90
2		Ethyl ether	74	C4H10O	000060-29-7	90
3		Ethyl ether	74	C4H10O	000060-29-7	86
4		Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	83
5		Ethyl ether	74	C4H10O	000060-29-7	78



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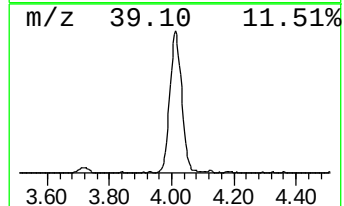
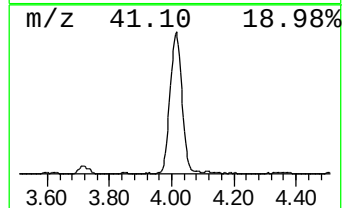
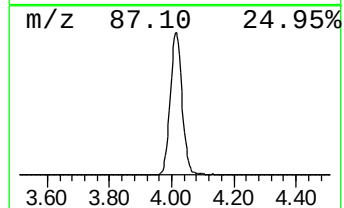
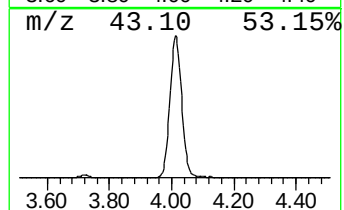
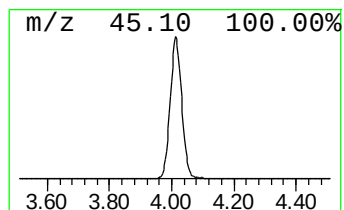
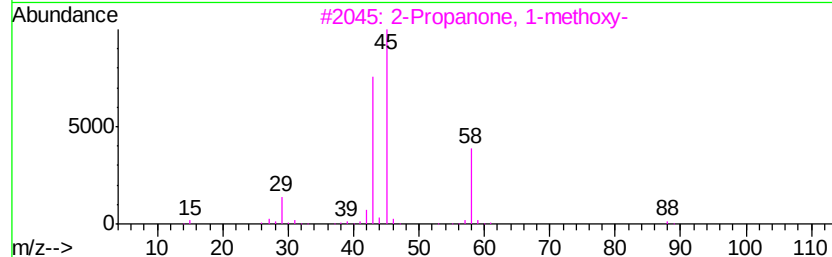
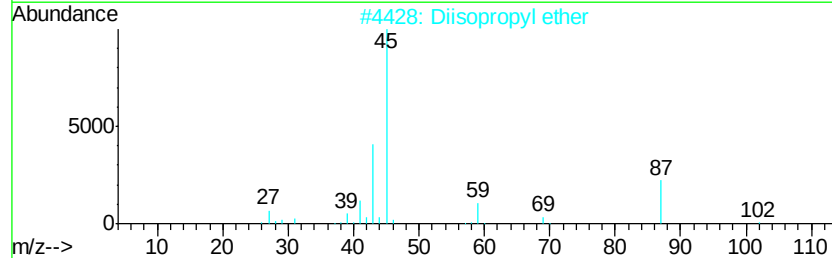
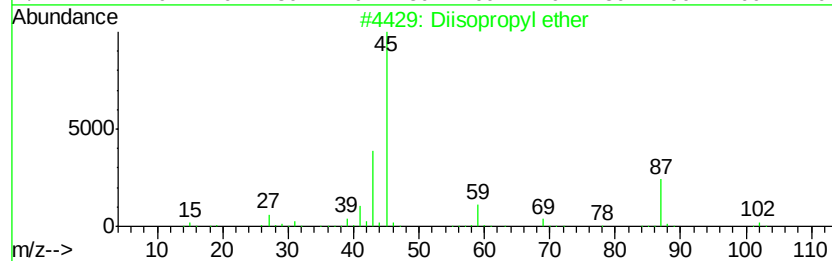
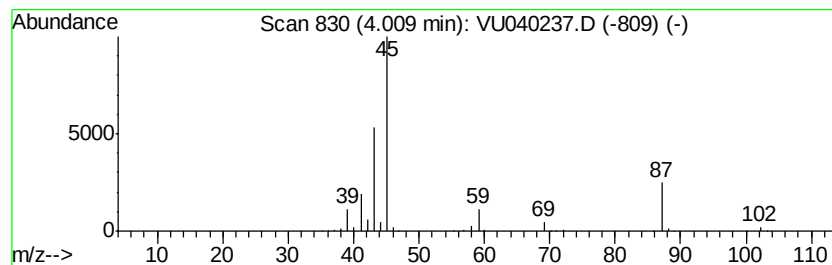
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	14.02 ug/L	884474	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diisopropyl ether	102	C6H14O	000108-20-3	86
2		Diisopropyl ether	102	C6H14O	000108-20-3	83
3		2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	59
4		1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	56
5		Diisopropyl ether	102	C6H14O	000108-20-3	43



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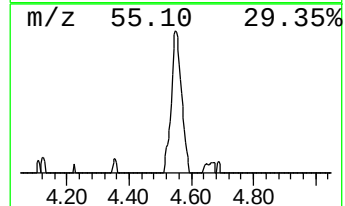
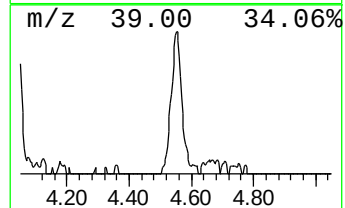
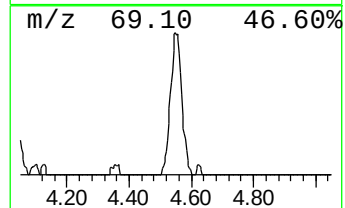
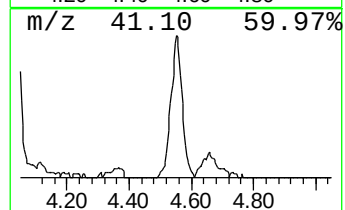
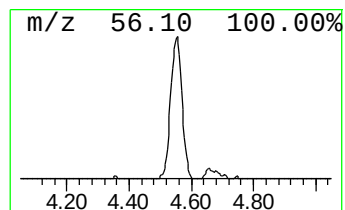
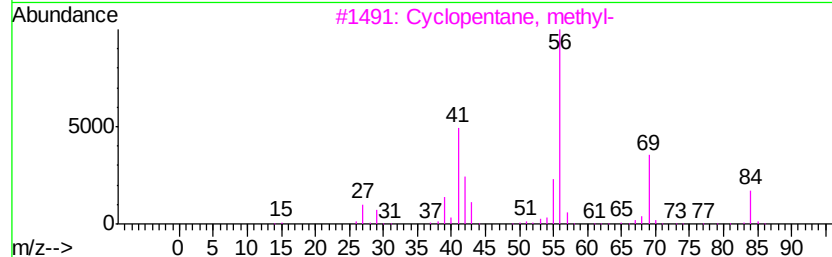
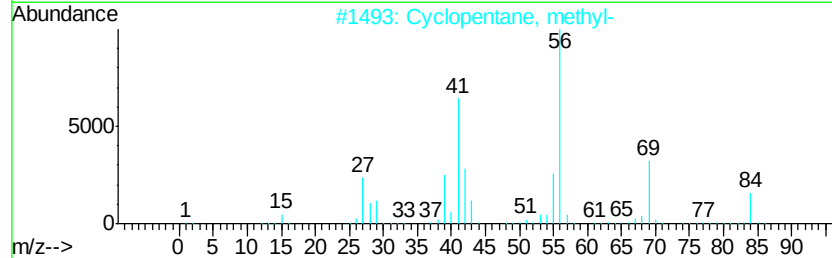
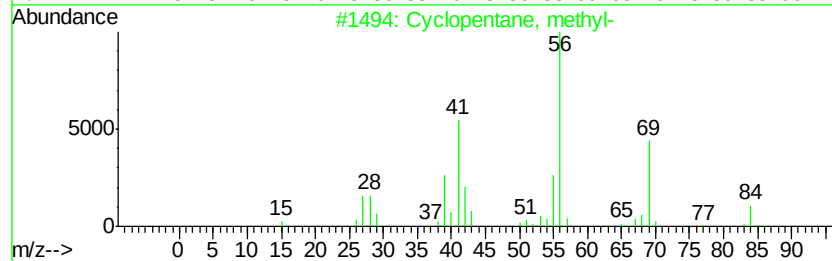
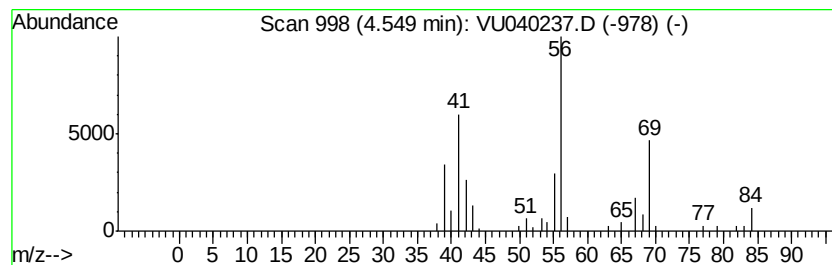
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Cyclic4.55 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.55	1.07 ug/L	67535	1,4-Difluorobenzene	6.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59



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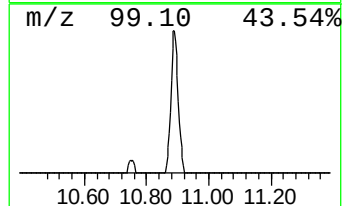
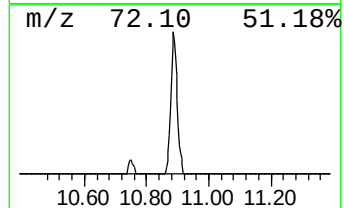
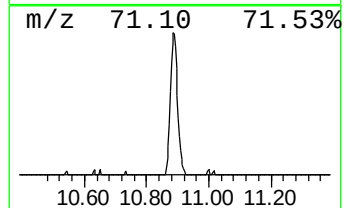
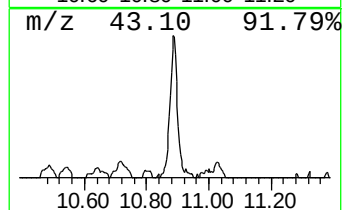
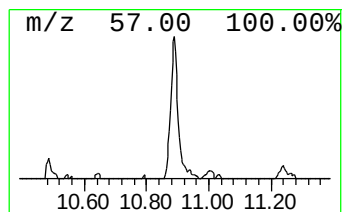
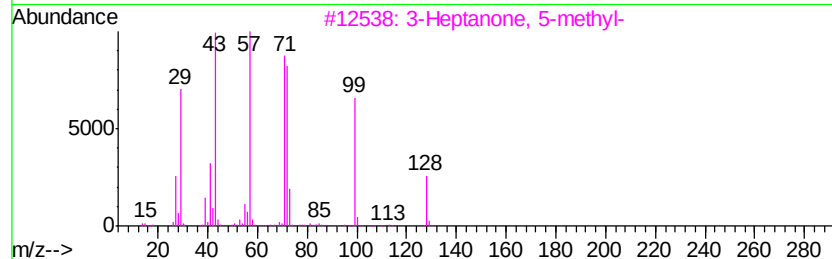
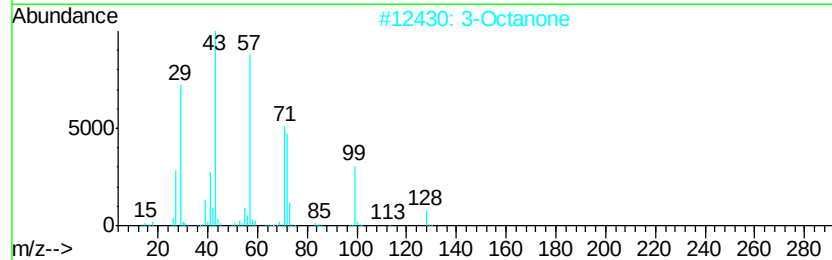
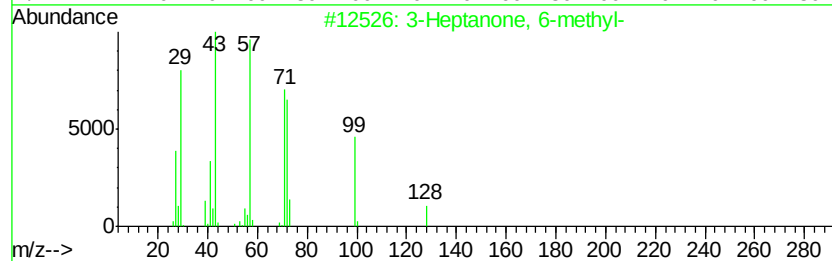
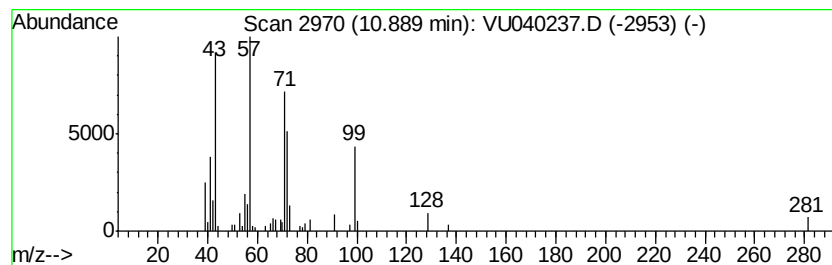
Instrument :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 3-Heptanone, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.89	0.58 ug/L	51036	1,4-Dichlorobenzene-d4	11.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	90
2	3-Octanone	128	C8H16O	000106-68-3	80
3	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	78
4	3-Octanone	128	C8H16O	000106-68-3	72
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl ether	2.39	4.0	ug/L	253395	1	6.26	315515	5.0
Diisopropyl ether	4.01	14.0	ug/L	884474	1	6.26	315515	5.0
(DEL) Alkane: Cyc...	4.55	1.1	ug/L	67535	1	6.26	315515	5.0
3-Heptanone, 6-me...	10.89	0.6	ug/L	51036	3	11.81	439085	5.0