

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100320\
 Data File : VU040498.D
 Acq On : 03 Oct 2020 22:29
 Operator : SY/MD
 Sample : L4240-10 200X
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG3S8

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\SOMUTR092920WMA.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	75	83	97	rVB	47593	52611	2.20%	0.654%
2	1.925	174	182	192	rVB	40938	51430	2.15%	0.640%
3	2.581	373	386	401	rBV	80953	134166	5.60%	1.669%
4	3.099	521	547	569	rBV	313555	704144	29.40%	8.758%
5	3.379	613	634	656	rBV	482277	1078571	45.03%	13.415%
6	3.720	719	740	762	rBV	1079612	2395404	100.00%	29.793%
7	4.318	910	926	944	rVB4	15844	42174	1.76%	0.525%
8	4.453	949	968	984	rBV4	10423	28826	1.20%	0.359%
9	4.552	984	999	1015	rVB2	40084	95611	3.99%	1.189%
10	4.662	1016	1033	1074	rBV	68427	252431	10.54%	3.140%
11	5.083	1148	1164	1185	rBV	76084	173956	7.26%	2.164%
12	5.742	1348	1369	1388	rBV2	154940	405552	16.93%	5.044%
13	6.263	1517	1531	1548	rBV	157876	294135	12.28%	3.658%
14	6.703	1654	1668	1685	rBV	100257	194356	8.11%	2.417%
15	7.575	1926	1939	1958	rBV2	50140	87111	3.64%	1.083%
16	7.906	2018	2042	2061	rBV	176311	304470	12.71%	3.787%
17	8.186	2119	2129	2143	rVB2	33485	53828	2.25%	0.669%
18	8.642	2258	2271	2301	rBV	274739	515588	21.52%	6.413%
19	9.420	2500	2513	2537	rBV	232038	410209	17.12%	5.102%
20	10.755	2916	2928	2946	rVB2	80095	131536	5.49%	1.636%
21	11.809	3243	3256	3272	rBV	213227	348092	14.53%	4.329%
22	12.189	3361	3374	3397	rVB	176035	285993	11.94%	3.557%

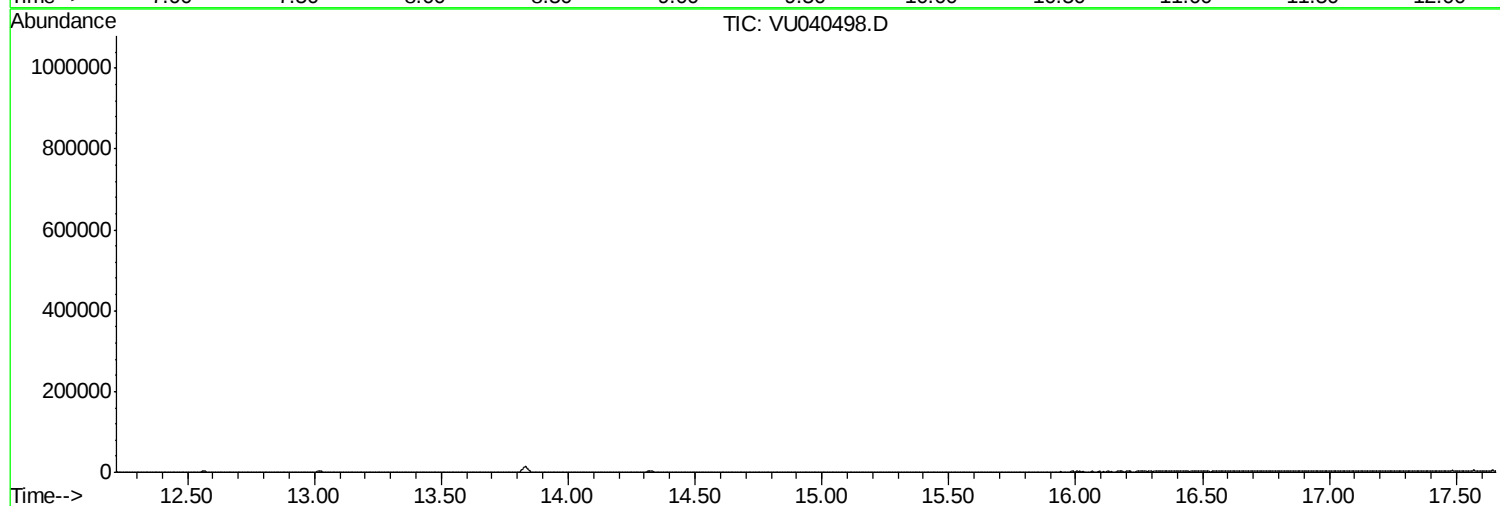
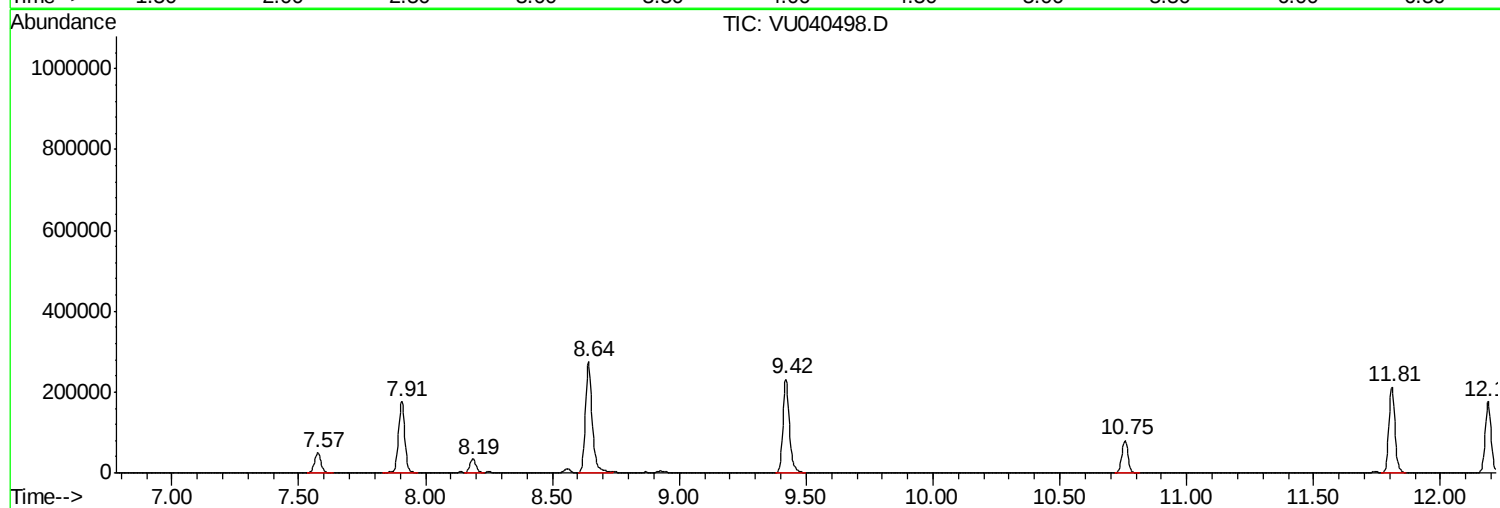
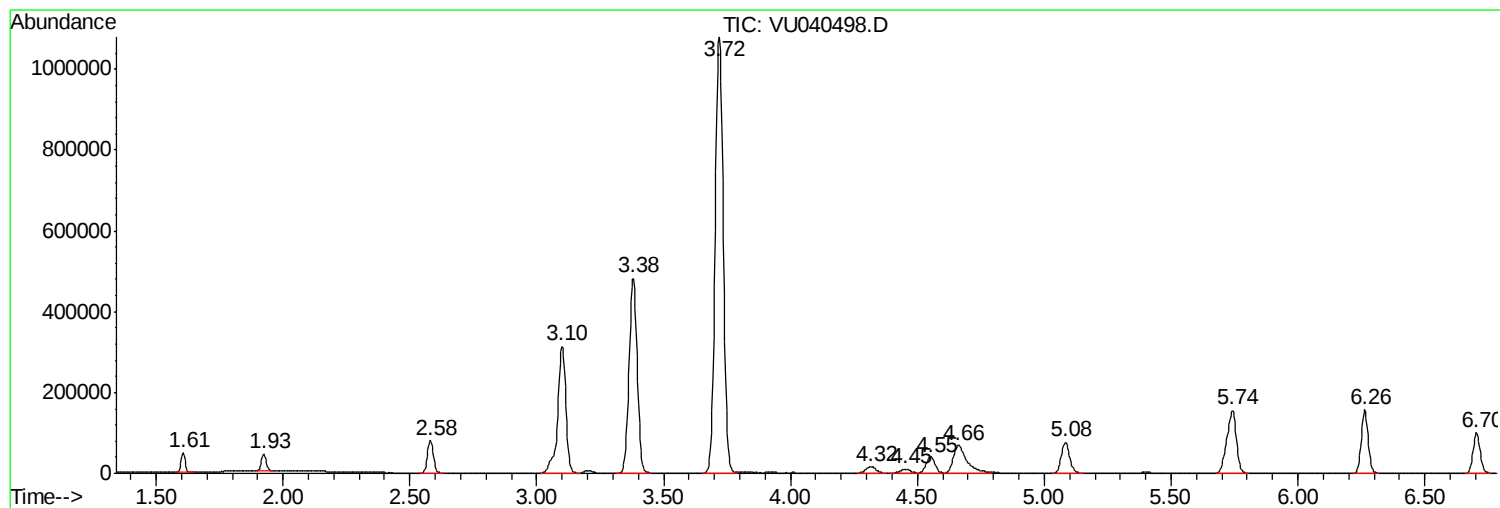
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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



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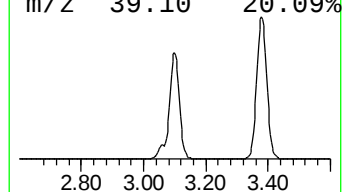
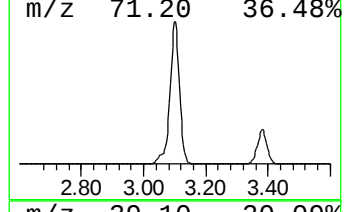
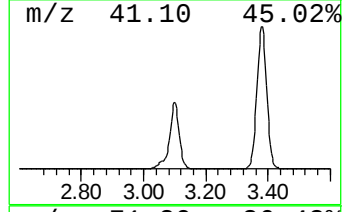
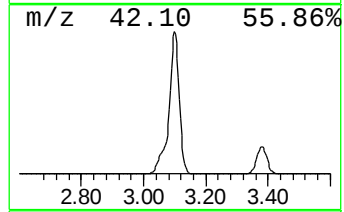
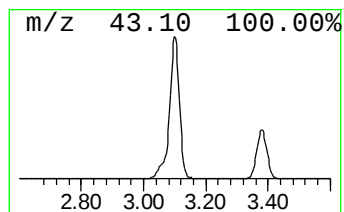
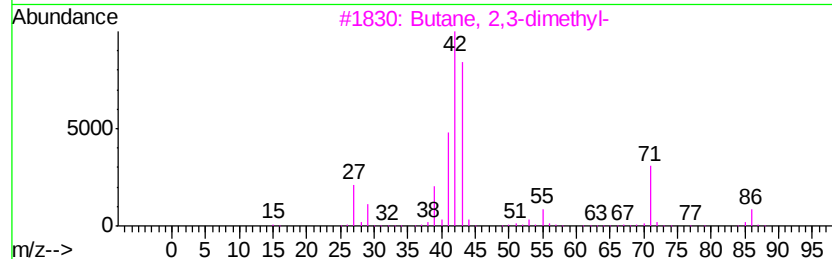
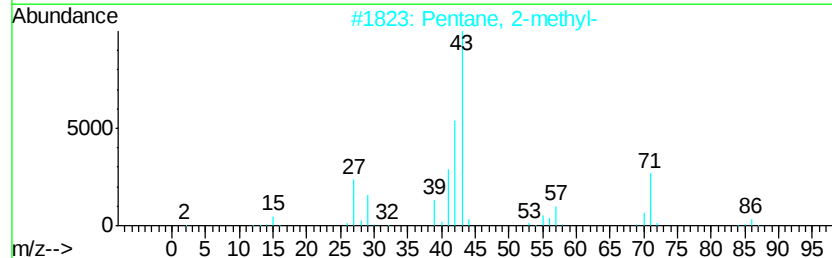
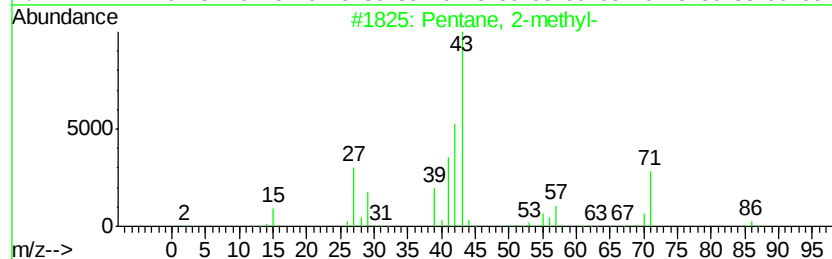
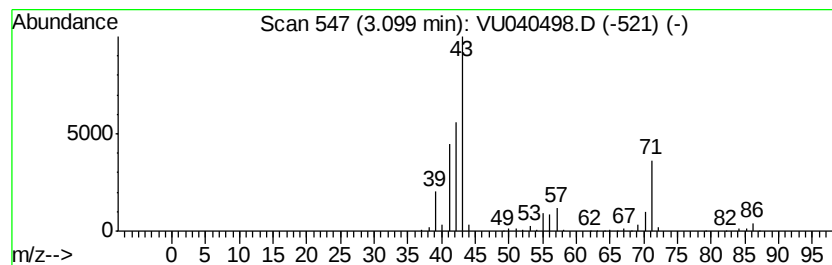
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	11.97 ug/L	704144	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	90
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	90
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	58
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	53
5		1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38



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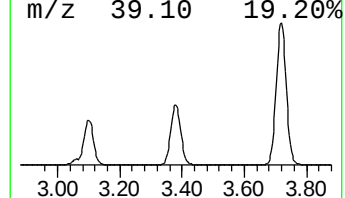
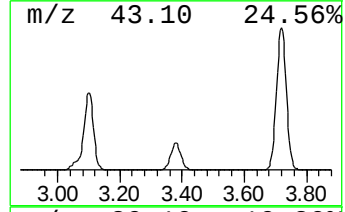
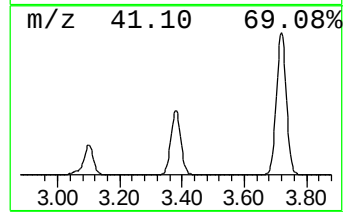
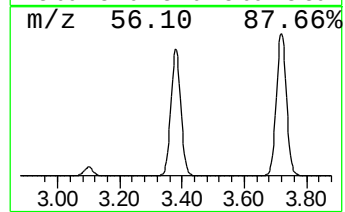
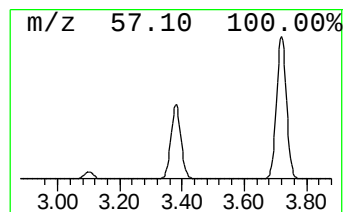
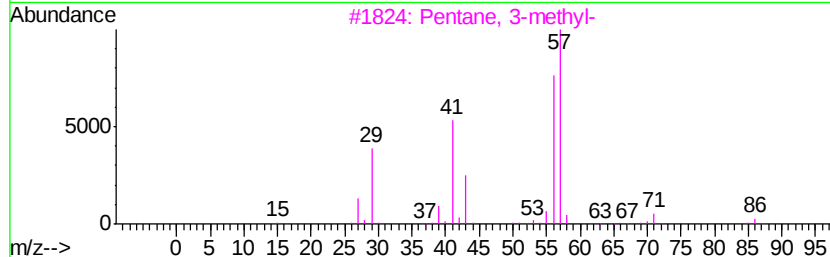
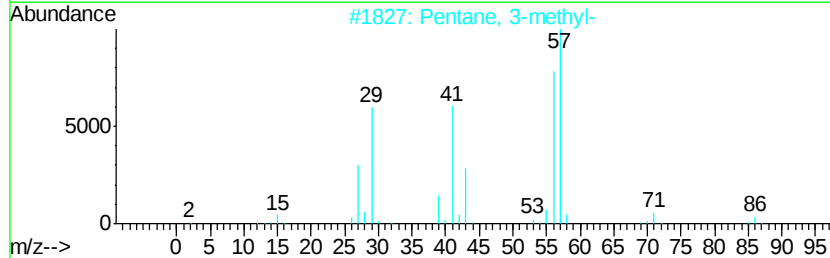
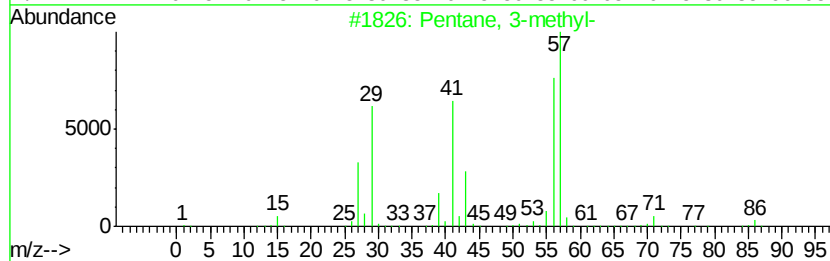
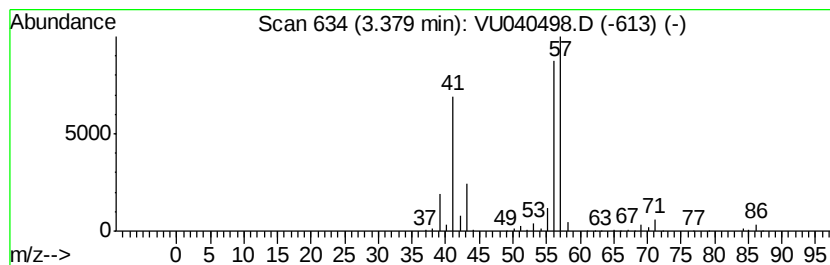
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	18.33 ug/L	1078570	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Pentane, 3-methyl-	86	C6H14	000096-14-0	90
3		Pentane, 3-methyl-	86	C6H14	000096-14-0	86
4		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
5		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43



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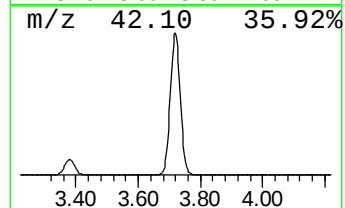
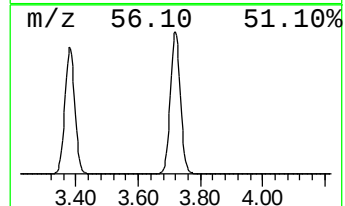
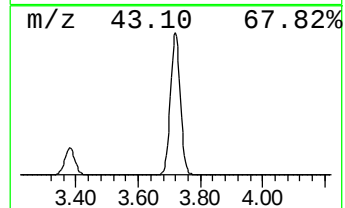
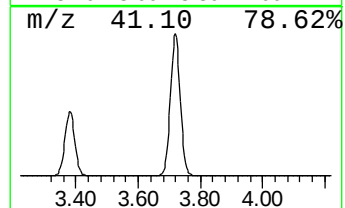
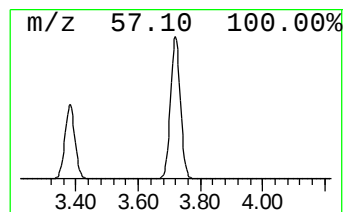
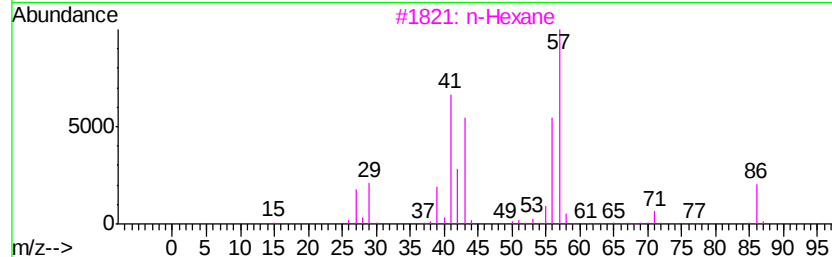
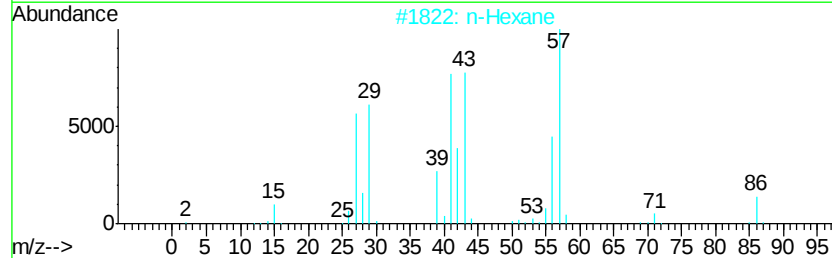
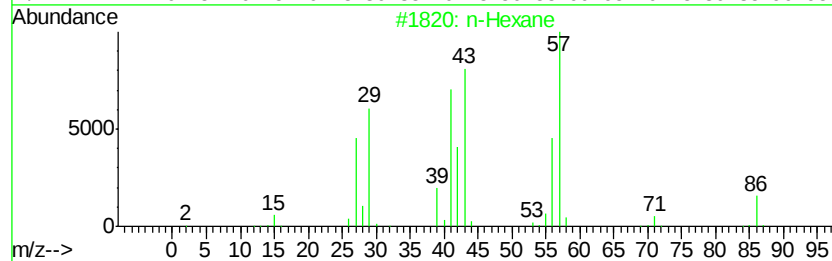
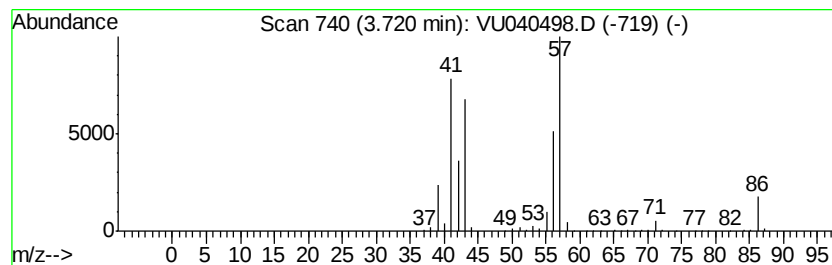
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	40.72 ug/L	2395400	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	91
2		n-Hexane	86	C6H14	000110-54-3	91
3		n-Hexane	86	C6H14	000110-54-3	91
4		Butanal, 2-methyl-	86	C5H10O	000096-17-3	35
5		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35



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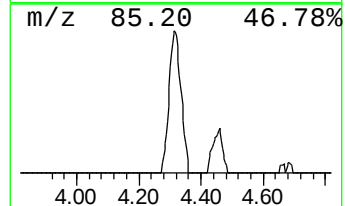
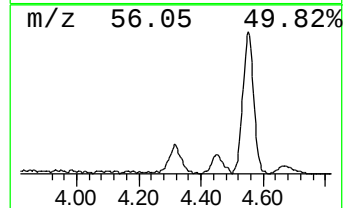
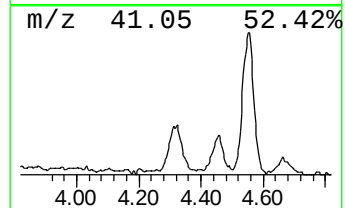
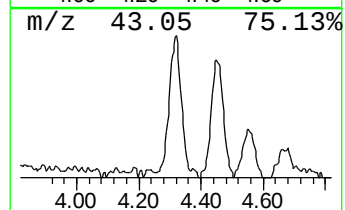
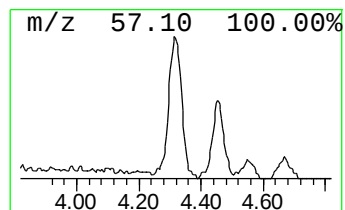
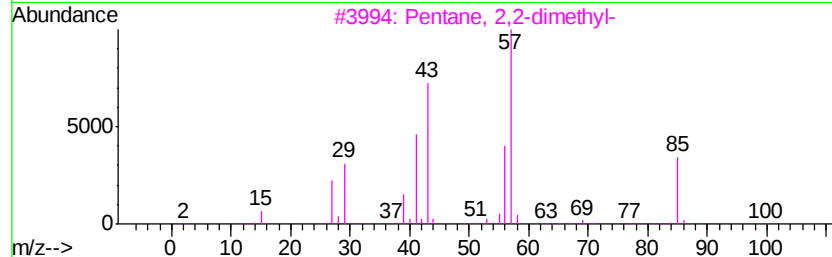
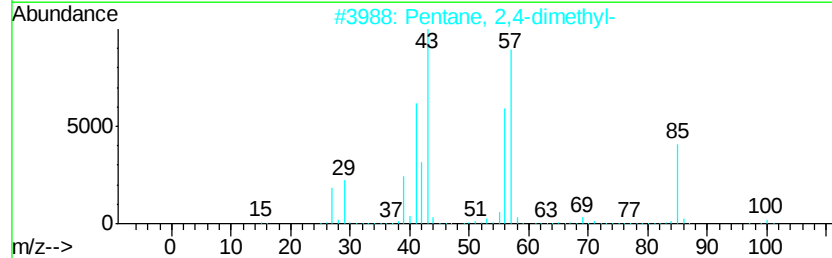
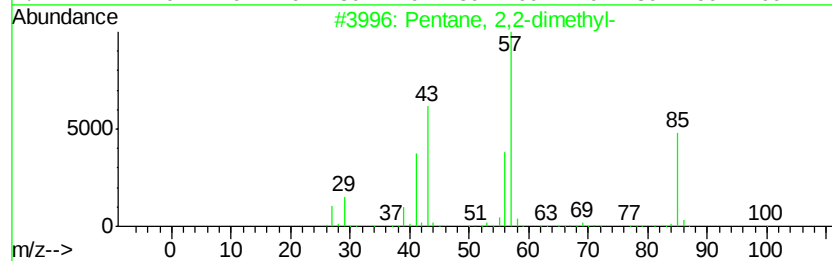
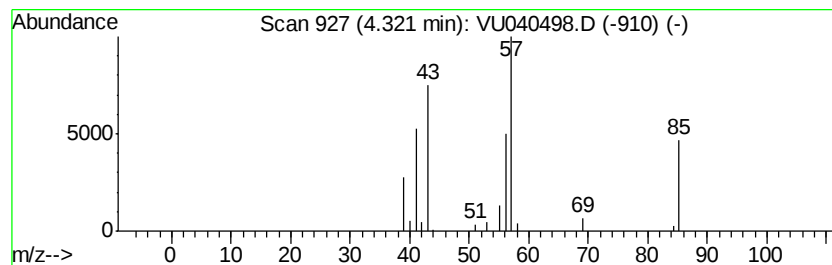
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	0.72 ug/L	42174	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	83
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	83
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	78
5		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	78



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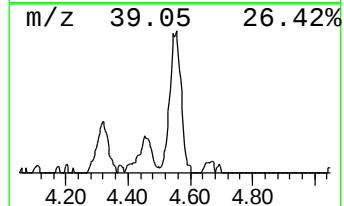
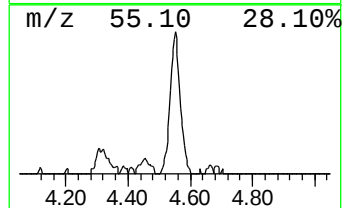
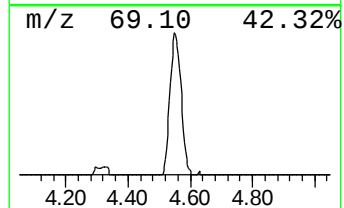
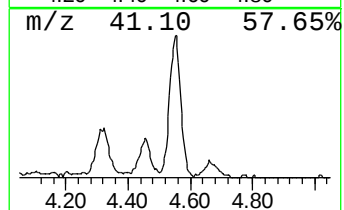
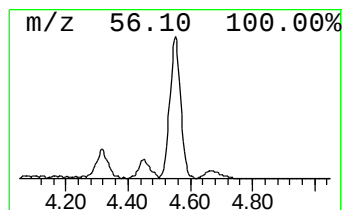
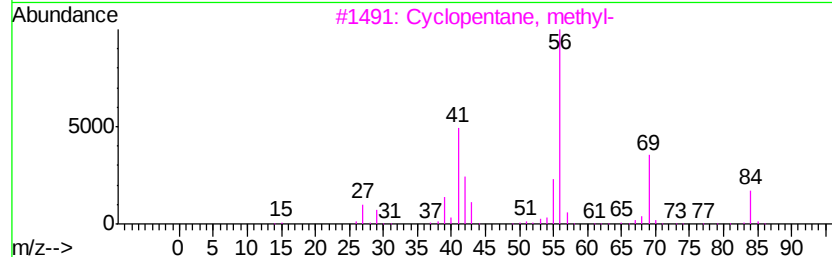
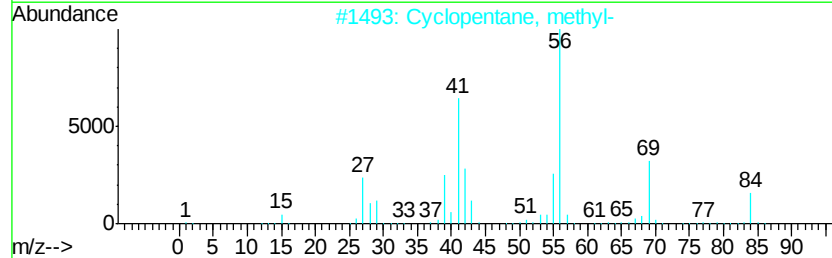
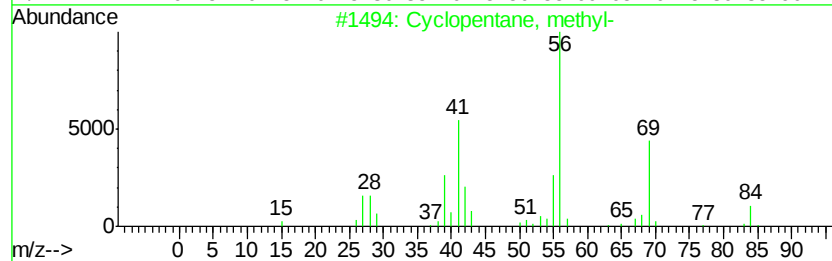
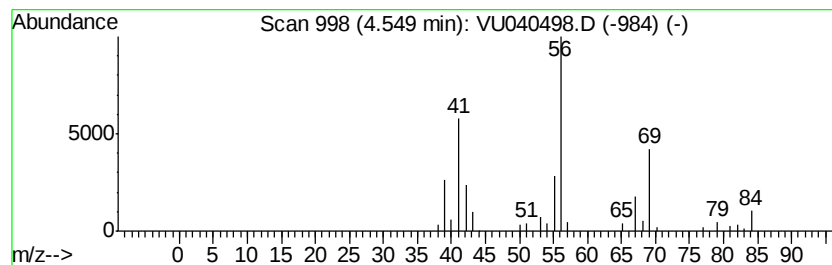
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Cyclic4.55 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	1.63 ug/L	95611	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59



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					--Internal Standard--				
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc	
(DEL) Alkane: Str...	3.10	12.0	ug/L	704144	1	6.26	294135	5.0	
(DEL) Alkane: Str...	3.38	18.3	ug/L	1078570	1	6.26	294135	5.0	
(DEL) Alkane: Str...	3.72	40.7	ug/L	2395400	1	6.26	294135	5.0	
(DEL) Alkane: Str...	4.32	0.7	ug/L	42174	1	6.26	294135	5.0	
(DEL) Alkane: Cyc...	4.55	1.6	ug/L	95611	1	6.26	294135	5.0	