

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102822\
 Data File : VU051579.D
 Acq On : 28 Oct 2022 20:01
 Operator : JC/MD
 Sample : N5300-12DL2 400X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA78DL2

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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	89	rBV	99499	124683	6.22%	1.084%
2	1.913	170	178	196	rVB	105629	141761	7.07%	1.233%
3	2.565	367	381	394	rBV	147628	238936	11.92%	2.078%
4	3.044	518	530	555	rBV3	46058	110345	5.51%	0.960%
5	3.359	613	628	642	rBV3	25437	54709	2.73%	0.476%
6	3.697	720	733	746	rVB4	14668	30912	1.54%	0.269%
7	3.864	756	785	800	rBV3	14637	51337	2.56%	0.446%
8	4.527	973	991	1009	rBV2	24040	58802	2.93%	0.511%
9	4.633	1009	1024	1068	rBV3	193021	720542	35.95%	6.266%
10	5.064	1142	1158	1187	rBV	186622	428005	21.35%	3.722%
11	5.723	1343	1363	1372	rBV2	341909	918144	45.81%	7.985%
12	5.771	1373	1378	1406	rVB	184877	358233	17.87%	3.115%
13	6.247	1508	1526	1544	rBV	249494	484831	24.19%	4.216%
14	6.690	1650	1664	1682	rBV	238814	467031	23.30%	4.062%
15	7.565	1921	1936	1957	rBV	87711	158070	7.89%	1.375%
16	7.896	2023	2039	2050	rBV	326796	563469	28.11%	4.900%
17	7.967	2050	2061	2090	rVB	1170515	2004258	100.00%	17.431%
18	8.179	2117	2127	2145	rVB	57509	97603	4.87%	0.849%
19	8.633	2256	2268	2306	rBV	626760	1200244	59.88%	10.438%
20	9.417	2498	2512	2538	rBV	375456	651695	32.52%	5.668%
21	9.568	2547	2559	2575	rBV	113902	185612	9.26%	1.614%
22	9.690	2584	2597	2616	rBV	234101	395849	19.75%	3.443%
23	10.099	2711	2724	2746	rBV	88395	147052	7.34%	1.279%
24	10.755	2916	2928	2944	rVB	210262	335480	16.74%	2.918%
25	10.906	2963	2975	2991	rBV2	23206	39138	1.95%	0.340%
26	10.996	2991	3003	3009	rBV	44672	76463	3.82%	0.665%
27	11.086	3022	3031	3044	rVB	28696	44281	2.21%	0.385%
28	11.292	3086	3095	3110	rVB2	25199	38935	1.94%	0.339%
29	11.465	3139	3149	3167	rBV	97778	155667	7.77%	1.354%
30	11.809	3243	3256	3274	rBV	362532	591622	29.52%	5.145%
31	11.893	3274	3282	3296	rVB	25267	40082	2.00%	0.349%
32	12.192	3362	3375	3395	rBV	349206	584769	29.18%	5.086%

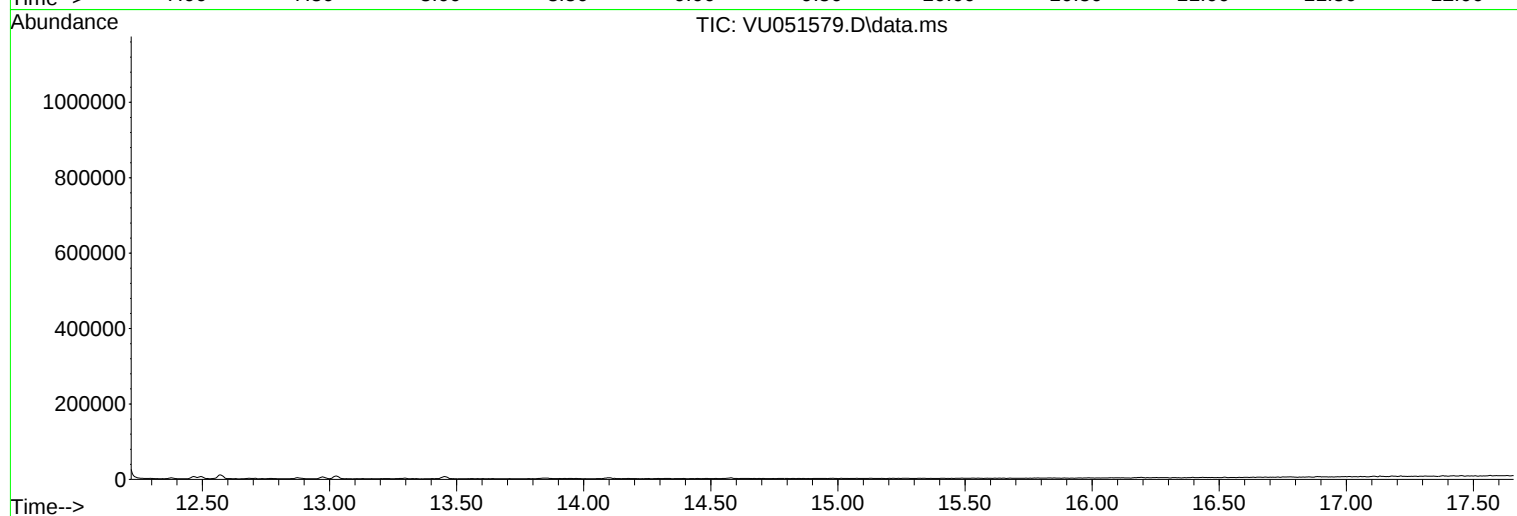
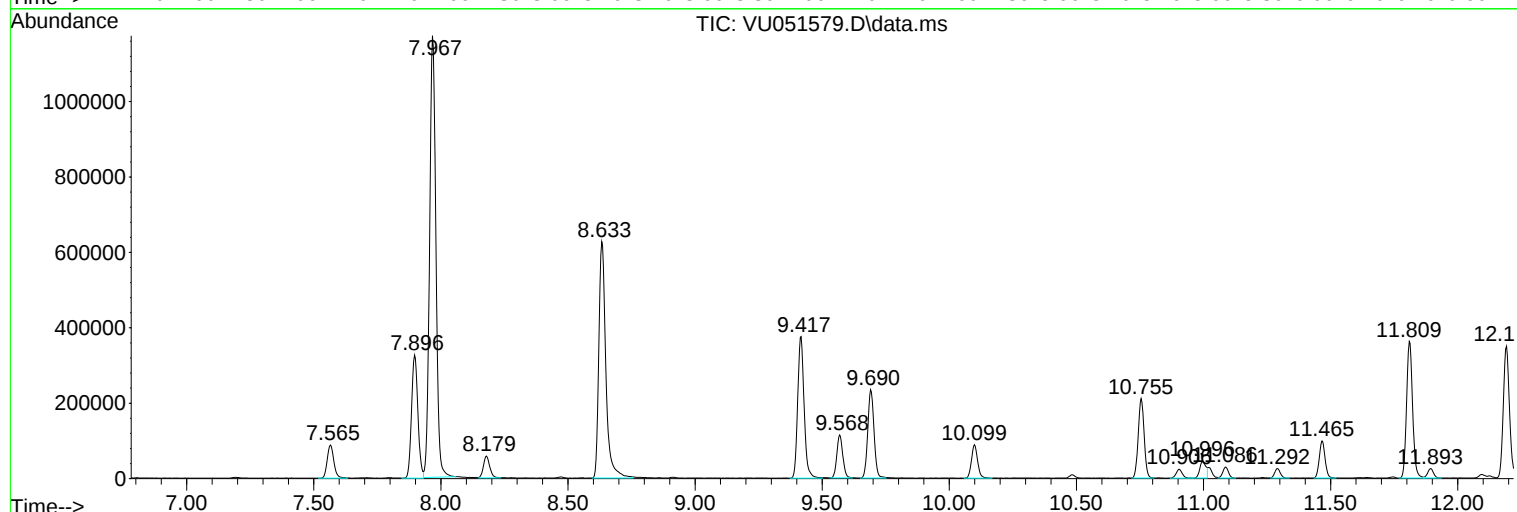
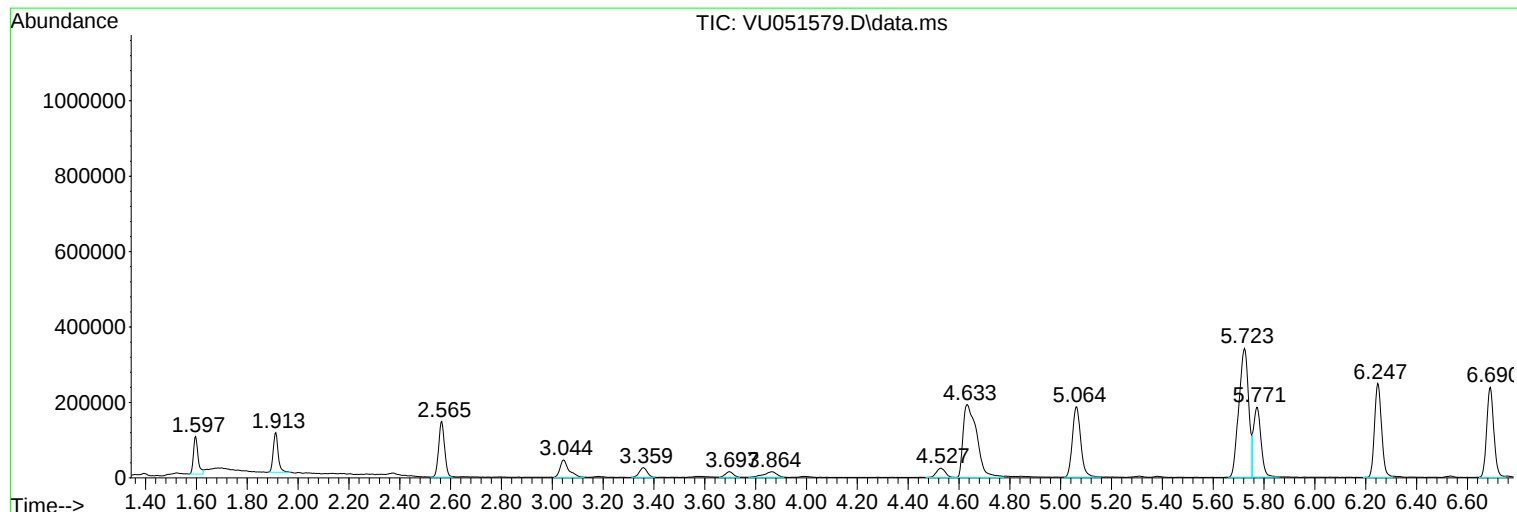
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA78DL2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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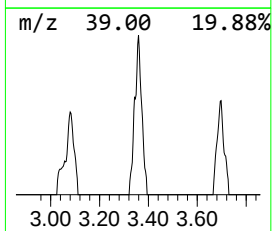
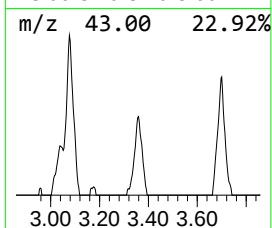
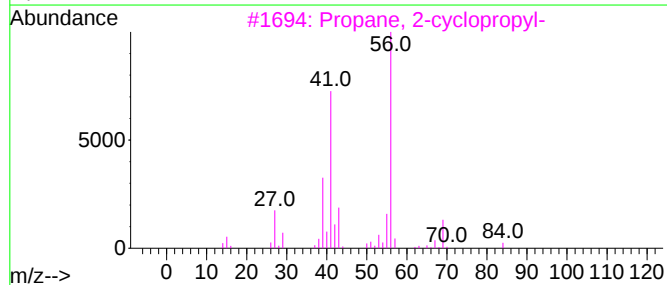
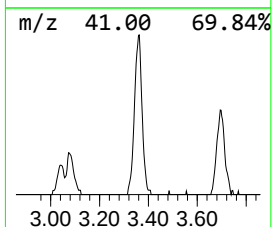
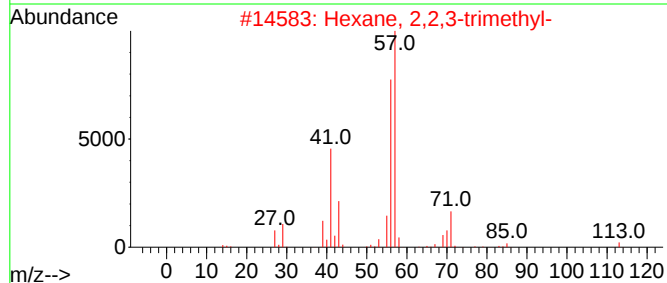
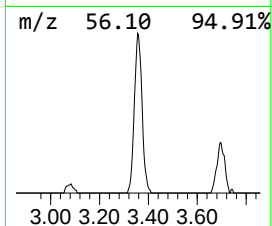
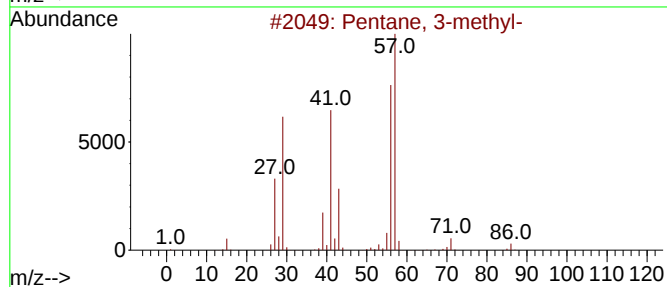
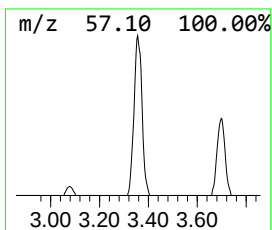
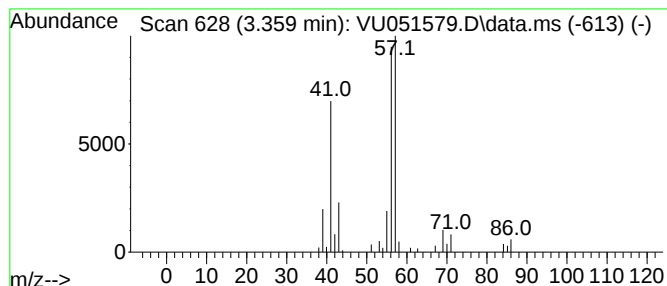
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.359	0.56 ug/L	54709	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 3-methyl-	86	C6H14	000096-14-0	72
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	58
4		Pentane, 3-methyl-	86	C6H14	000096-14-0	53
5		Cyclobutane, ethyl-	84	C6H12	004806-61-5	53



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Instrument :
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ClientSampleId :
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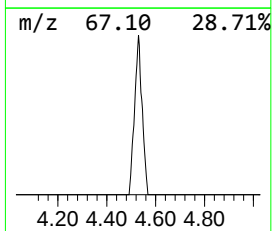
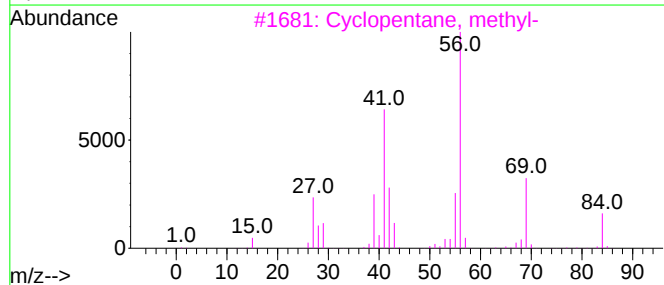
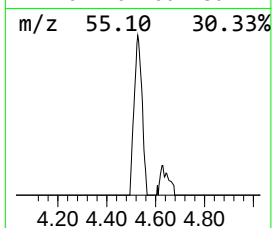
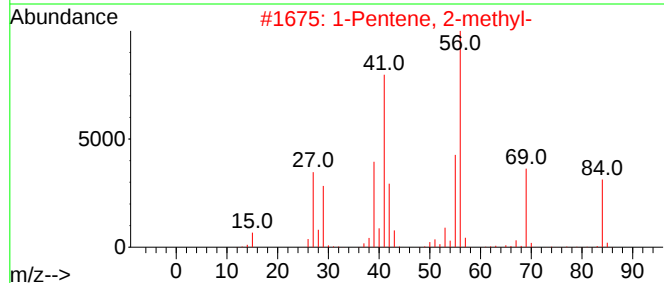
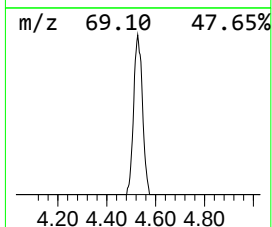
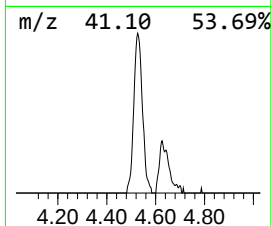
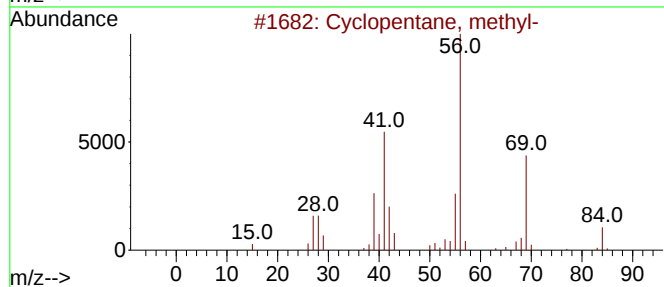
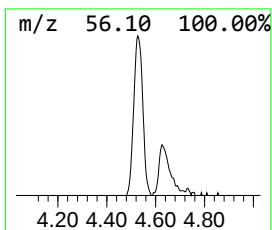
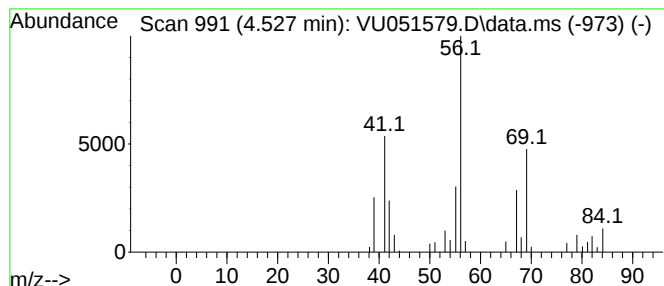
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Cyclic4.527 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.527	0.61 ug/L	58802	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	59
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	58
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	53
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



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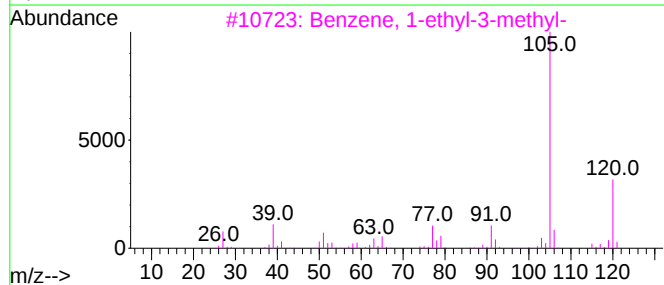
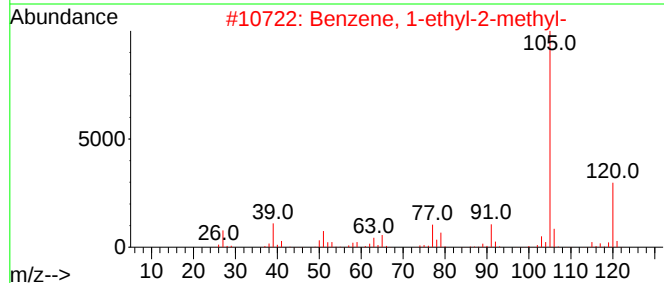
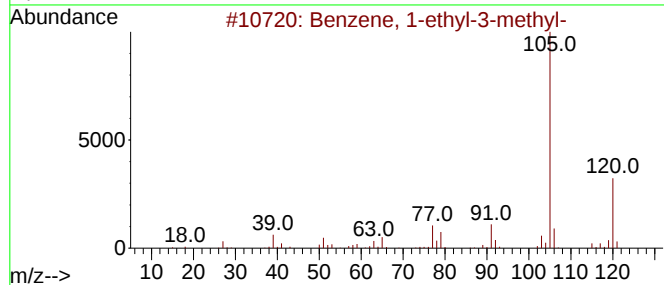
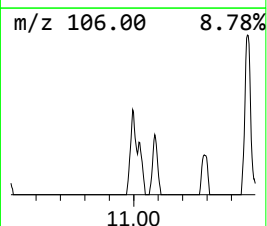
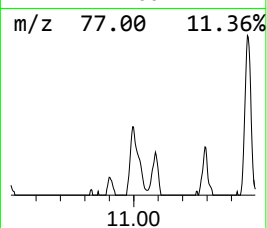
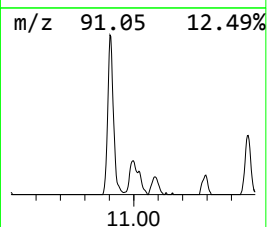
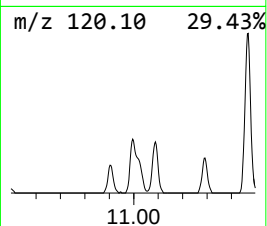
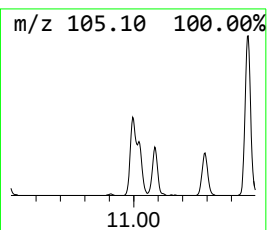
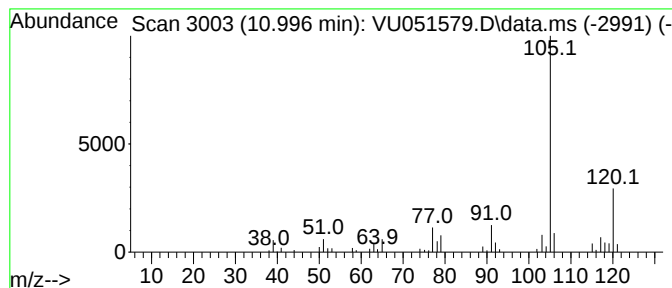
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.996	0.65 ug/L	76463	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	93
4			Mesitylene	120	C9H12	000108-67-8	87
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	3.359	0.6	ug/L	54709	1	6.247	484831	5.0
(DEL) Alkane: C...	4.527	0.6	ug/L	58802	1	6.247	484831	5.0
Benzene, 1-ethy...	10.996	0.7	ug/L	76463	3	11.813	591622	5.0