

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062123\
 Data File : VU054635.D
 Acq On : 21 Jun 2023 11:52
 Operator : MD/SY
 Sample : 03326-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GCA33

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\SFAMUTR060723WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.361	16	22	41	rVB	245371	271584	24.70%	2.262%
2	1.444	43	48	56	rVB	48315	53455	4.86%	0.445%
3	1.493	56	63	71	rVB	178854	177821	16.18%	1.481%
4	1.599	86	96	111	rBV2	320381	424205	38.59%	3.534%
5	1.689	120	124	131	rBV2	15718	21085	1.92%	0.176%
6	1.914	187	194	210	rVB2	145447	227447	20.69%	1.895%
7	1.994	211	219	230	rVB	143919	199835	18.18%	1.665%
8	2.203	276	284	298	rVB2	65610	96972	8.82%	0.808%
9	2.566	384	397	412	rBV	239821	404103	36.76%	3.366%
10	2.682	426	433	451	rVB2	29469	55950	5.09%	0.466%
11	2.856	479	487	501	rVB2	13087	23248	2.11%	0.194%
12	3.046	532	546	547	rBV8	7476	12651	1.15%	0.105%
13	3.081	548	557	570	rVB	24838	49770	4.53%	0.415%
14	3.357	630	643	664	rVB2	18290	42457	3.86%	0.354%
15	3.698	735	749	761	rBV2	20206	48144	4.38%	0.401%
16	4.531	995	1008	1019	rBV5	7470	17726	1.61%	0.148%
17	4.637	1028	1041	1086	rBV	125405	443375	40.33%	3.693%
18	5.058	1155	1172	1200	rVB	200093	460778	41.91%	3.838%
19	5.377	1258	1271	1284	rVV7	14069	36518	3.32%	0.304%
20	5.454	1285	1295	1309	rVB7	5173	12718	1.16%	0.106%
21	5.589	1325	1337	1353	rVB5	10748	25321	2.30%	0.211%
22	5.721	1357	1378	1409	rBV2	412486	1099342	100.00%	9.158%
23	5.849	1411	1418	1431	rVB2	7140	14646	1.33%	0.122%
24	5.984	1448	1460	1468	rBV9	6272	12918	1.18%	0.108%
25	6.129	1493	1505	1518	rBV4	11808	23069	2.10%	0.192%
26	6.245	1525	1541	1569	rBV	428474	838155	76.24%	6.982%
27	6.541	1614	1633	1652	rBV	190382	366944	33.38%	3.057%
28	6.685	1664	1678	1692	rBV2	254480	504344	45.88%	4.201%
29	6.756	1693	1700	1712	rVB6	23559	48465	4.41%	0.404%
30	7.563	1938	1951	1973	rBV2	128930	233855	21.27%	1.948%
31	7.894	2042	2054	2068	rVV	489478	850714	77.38%	7.087%
32	7.968	2068	2077	2087	rVB2	59602	106272	9.67%	0.885%
33	8.177	2132	2142	2153	rBV	74216	126797	11.53%	1.056%
34	8.235	2157	2160	2173	rVB6	9478	13966	1.27%	0.116%
35	8.631	2270	2283	2317	rBV2	530816	1069544	97.29%	8.909%
36	8.788	2323	2332	2347	rVV7	14930	29952	2.72%	0.250%

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37	8.859	2349	2354	2366	rVB7	7216	11071	1.01%	0.092%
38	9.412	2513	2526	2550	rBV	581035	1011909	92.05%	8.429%
39	9.566	2565	2574	2588	rVB	29270	48309	4.39%	0.402%
40	9.692	2603	2613	2623	rBV	28496	50180	4.56%	0.418%
41	10.100	2730	2740	2747	rBV2	13491	23646	2.15%	0.197%
42	10.341	2809	2815	2827	rVB7	9115	15952	1.45%	0.133%
43	10.466	2843	2854	2864	rBV8	11085	21718	1.98%	0.181%
44	10.749	2931	2942	2957	rBV2	182557	299775	27.27%	2.497%
45	10.891	2975	2986	3000	rBV4	11634	24867	2.26%	0.207%
46	10.997	3010	3019	3023	rBV4	8354	12611	1.15%	0.105%
47	11.463	3155	3164	3178	rBV	23891	39517	3.59%	0.329%
48	11.685	3225	3233	3243	rBV6	19914	31484	2.86%	0.262%
49	11.743	3245	3251	3258	rVV7	8650	11363	1.03%	0.095%
50	11.807	3258	3271	3290	rVV	592899	959293	87.26%	7.991%
51	11.891	3290	3297	3305	rVB4	8274	12126	1.10%	0.101%
52	12.071	3343	3353	3355	rBV5	8747	14476	1.32%	0.121%
53	12.187	3378	3389	3406	rBV	438554	729917	66.40%	6.080%
54	12.325	3421	3432	3445	rBV6	13743	23946	2.18%	0.199%
55	12.881	3596	3605	3621	rBV4	55939	88101	8.01%	0.734%
56	13.203	3698	3705	3715	rBV8	11545	17724	1.61%	0.148%
57	13.978	3937	3946	3960	rVB5	21967	34440	3.13%	0.287%
58	14.142	3988	3997	4006	rVV3	29084	47046	4.28%	0.392%
59	14.370	4061	4068	4078	rVB8	7703	12567	1.14%	0.105%
60	16.338	4671	4680	4692	rBV8	11006	18459	1.68%	0.154%

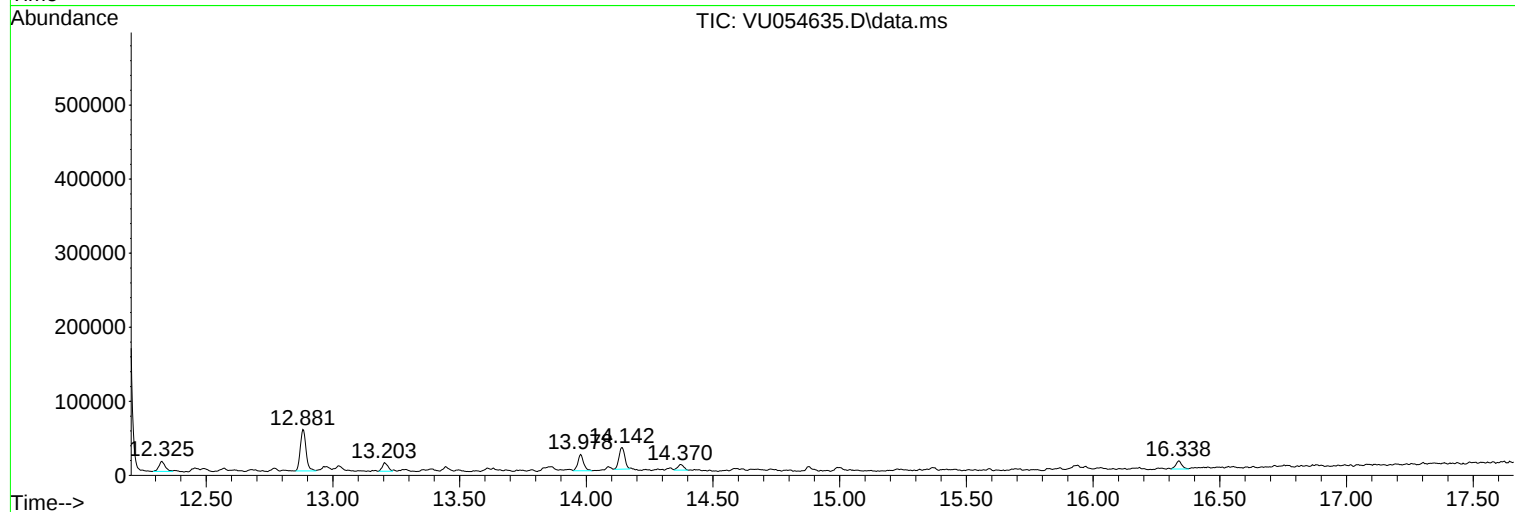
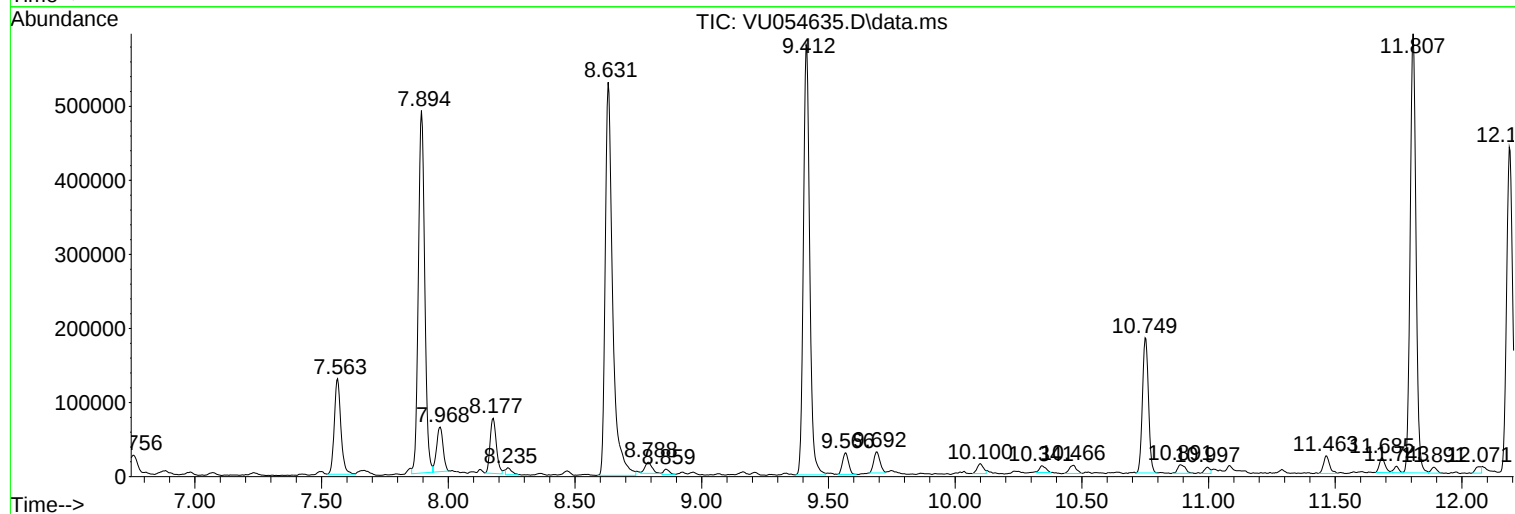
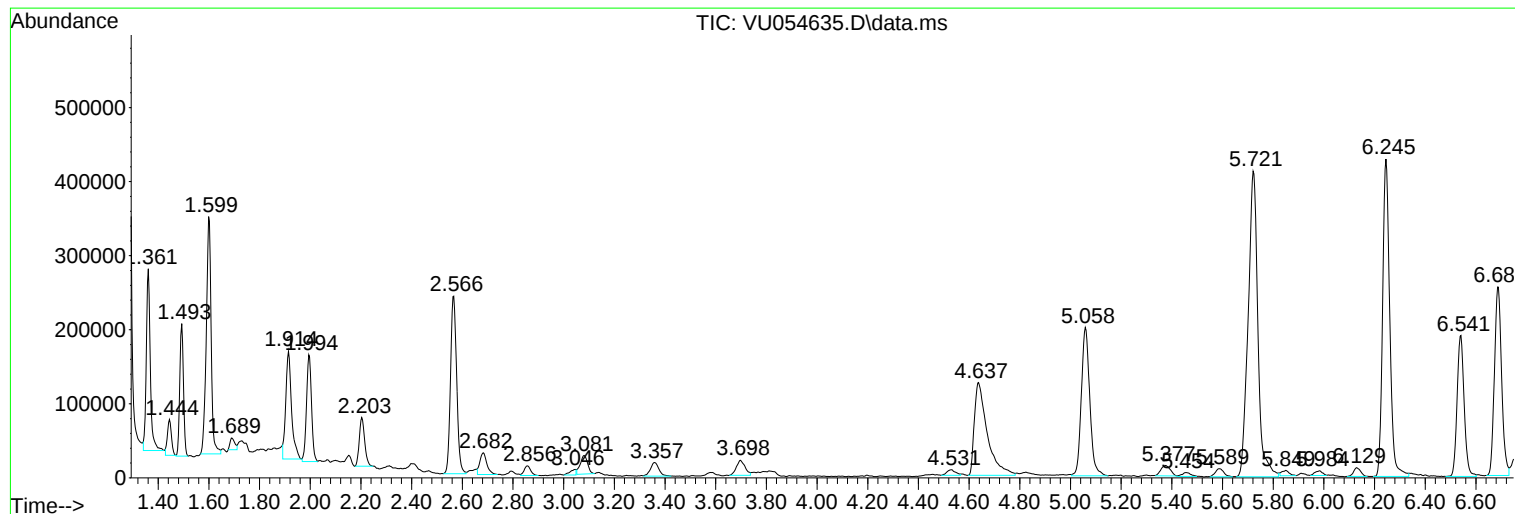
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
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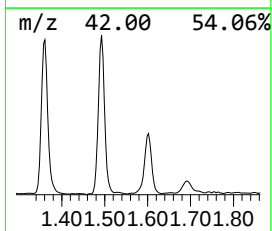
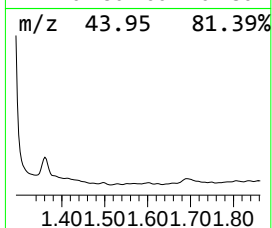
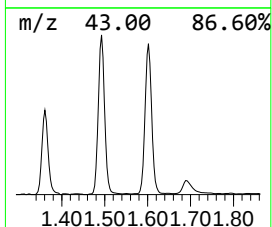
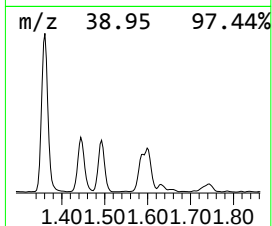
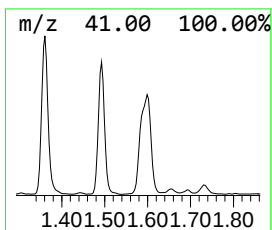
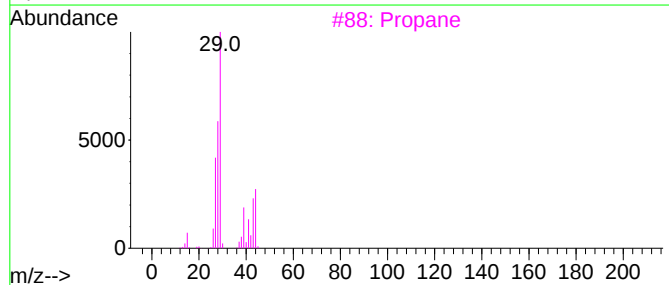
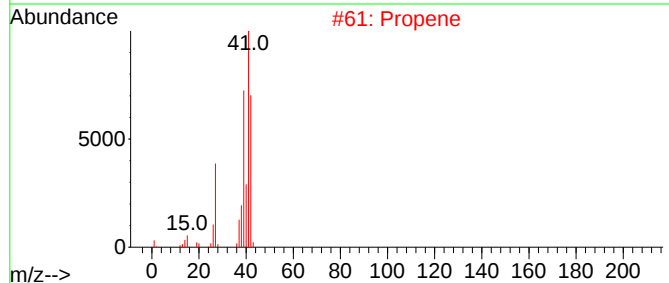
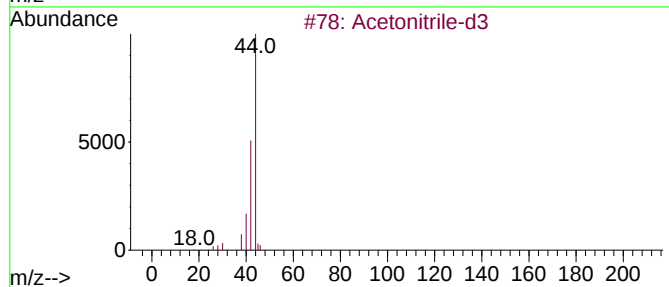
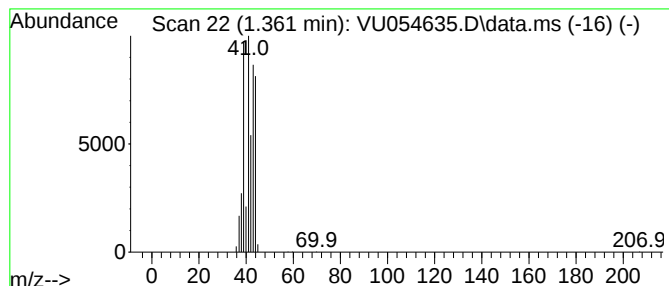
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.361	1.62 ug/L	271584	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile-d3	44	C2D3N	002206-26-0	7
2			Propene	42	C3H6	000115-07-1	7
3			Propane	44	C3H8	000074-98-6	5
4			Cyclopropene	40	C3H4	002781-85-3	4
5			Cyclopropane	42	C3H6	000075-19-4	4



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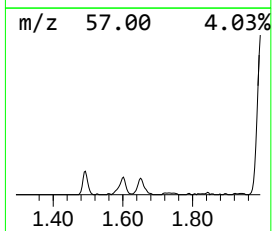
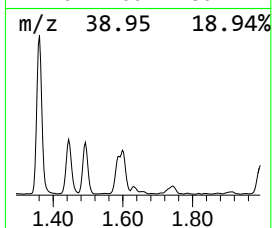
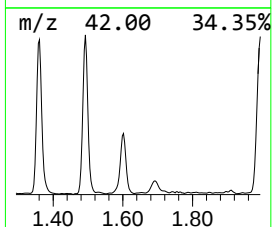
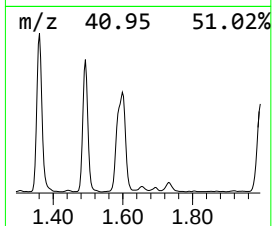
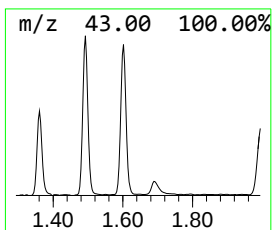
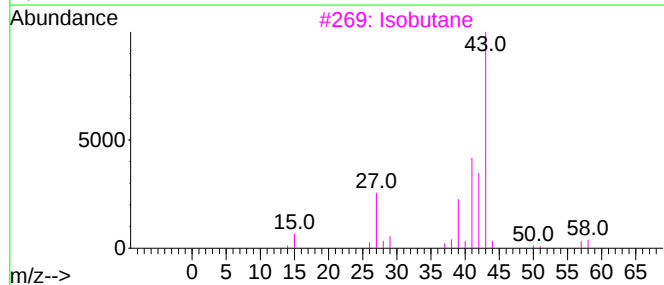
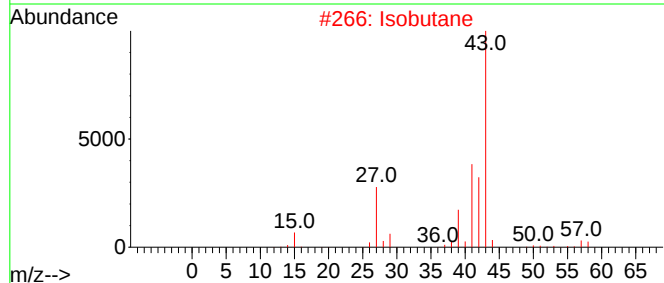
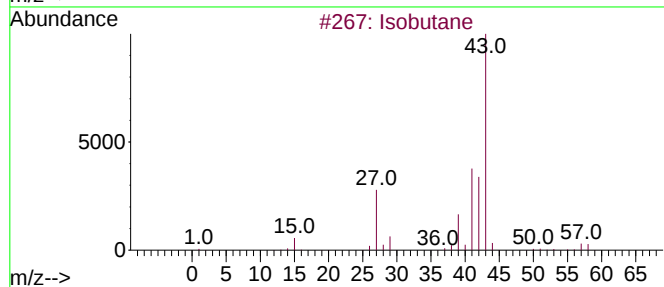
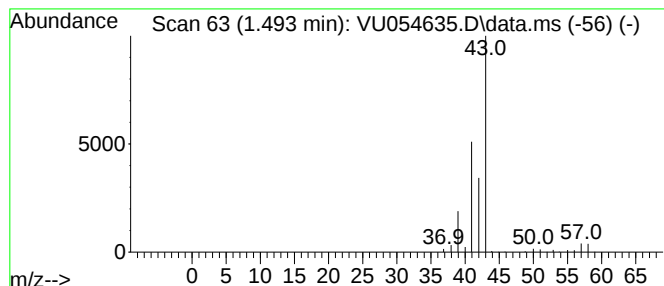
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.493	1.06 ug/L	177821	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	56
4		Isobutane	58	C4H10	000075-28-5	50
5		Isobutane	58	C4H10	000075-28-5	42



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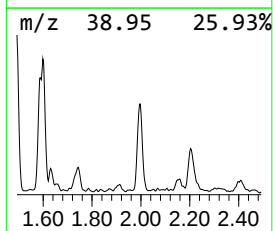
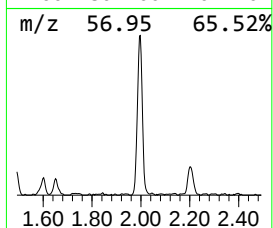
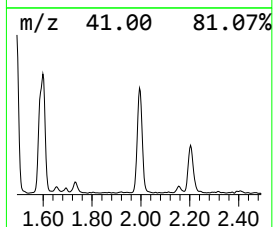
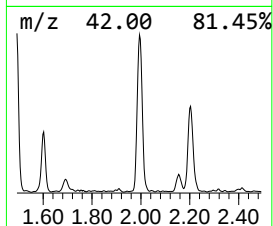
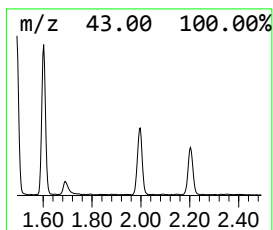
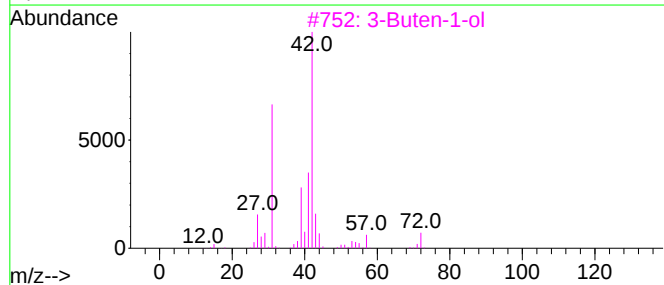
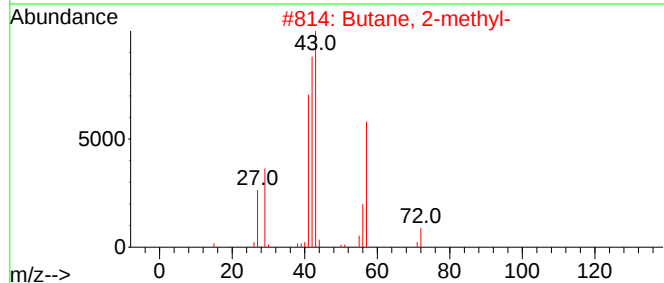
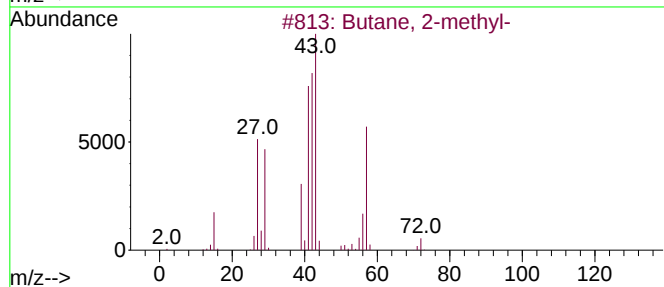
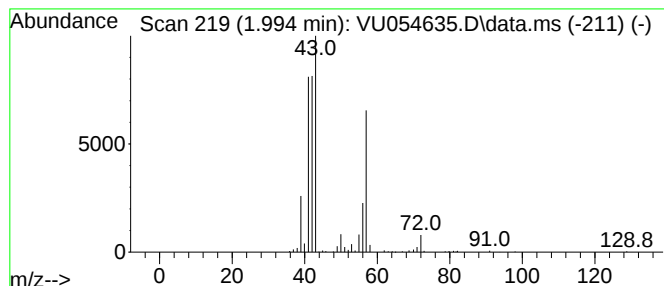
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.994	1.19 ug/L	199835	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	3-Buten-1-ol			72	C4H8O	000627-27-0	38
4	Pentane			72	C5H12	000109-66-0	33
5	Methane, isocyanato-			57	C2H3NO	000624-83-9	9



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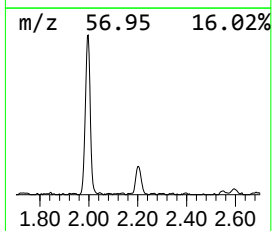
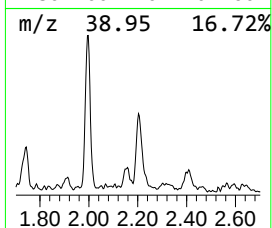
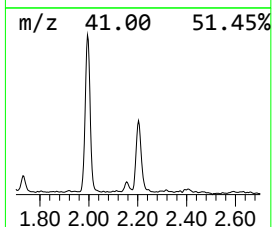
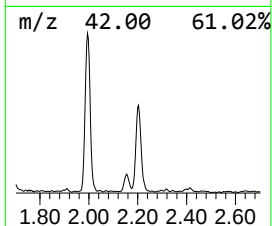
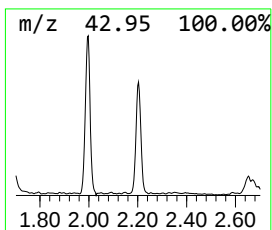
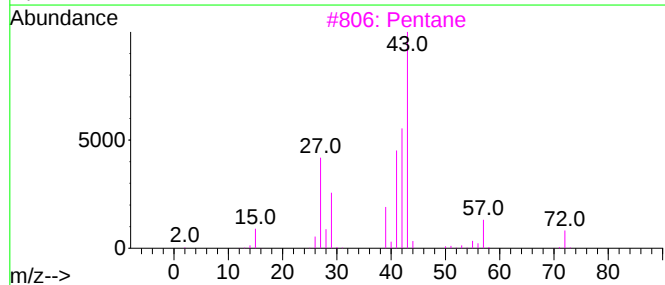
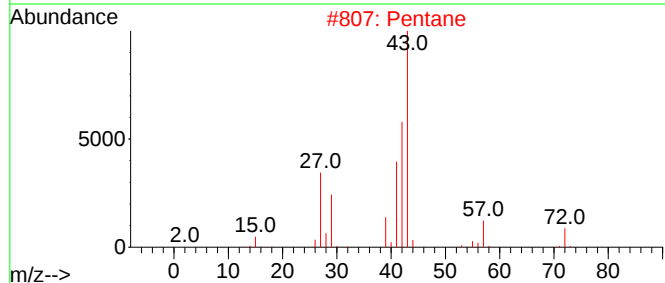
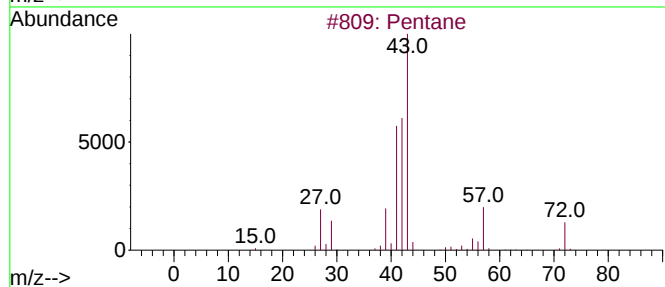
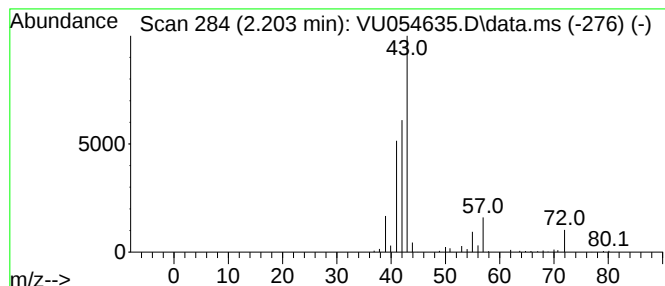
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.203	0.58 ug/L	96972	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	87
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	86
4	Pentane			72	C5H12	000109-66-0	72
5	Butane, 2-methyl-			72	C5H12	000078-78-4	64



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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
unknown-01	1.361	1.6	ug/L	271584	1	6.245	838155	5.0
(DEL) Alkane: S...	1.493	1.1	ug/L	177821	1	6.245	838155	5.0
(DEL) Alkane: S...	1.994	1.2	ug/L	199835	1	6.245	838155	5.0
(DEL) Alkane: S...	2.203	0.6	ug/L	96972	1	6.245	838155	5.0