

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121124\
Data File : VU062271.D
Acq On : 12 Dec 2024 04:50
Operator : MD/SY
Sample : P5251-10
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7J28

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\SFAMUTR120924WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU062271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.357	15	21	35	rVB3	11434	13451	4.37%	0.387%
2	1.528	57	74	76	rBV	24985	47261	15.34%	1.361%
3	1.592	86	94	121	rVB4	52395	98686	32.04%	2.842%
4	1.907	186	192	204	rVB	26823	36464	11.84%	1.050%
5	2.557	382	394	410	rVB	61672	98462	31.97%	2.835%
6	2.782	455	464	479	rVB	2708	4804	1.56%	0.138%
7	3.685	736	745	759	rVB7	3203	6985	2.27%	0.201%
8	3.843	780	794	816	rBV3	31661	79055	25.67%	2.277%
9	4.418	962	973	987	rBV5	2590	6093	1.98%	0.175%
10	4.653	1033	1046	1063	rBV	24668	68817	22.34%	1.982%
11	5.052	1156	1170	1183	rBV	62305	138441	44.95%	3.987%
12	5.119	1183	1191	1212	rVB2	16348	39363	12.78%	1.134%
13	5.357	1252	1265	1280	rBV3	45643	101139	32.84%	2.913%
14	5.451	1280	1294	1311	rVB2	36102	82448	26.77%	2.374%
15	5.582	1320	1335	1359	rBV	69778	162144	52.64%	4.669%
16	5.714	1359	1376	1402	rVV3	119199	308001	100.00%	8.870%
17	5.840	1402	1415	1427	rVV2	17875	37821	12.28%	1.089%
18	5.910	1428	1437	1447	rVV5	6310	13233	4.30%	0.381%
19	5.978	1449	1458	1473	rVB4	8622	17178	5.58%	0.495%
20	6.126	1497	1504	1515	rBB4	3730	6572	2.13%	0.189%
21	6.242	1528	1540	1570	rBV	115901	230213	74.74%	6.629%
22	6.682	1664	1677	1691	rBV	70100	138571	44.99%	3.990%
23	6.750	1693	1698	1712	rVB7	8313	14607	4.74%	0.421%
24	7.560	1939	1950	1971	rBV	33067	59761	19.40%	1.721%
25	7.891	2040	2053	2066	rBV	139155	247552	80.37%	7.129%
26	7.962	2066	2075	2097	rVB	75444	135294	43.93%	3.896%
27	8.174	2131	2141	2161	rBV	18906	34127	11.08%	0.983%
28	8.634	2273	2284	2323	rBV2	110190	261837	85.01%	7.540%
29	8.791	2323	2333	2344	rVV8	4456	10681	3.47%	0.308%
30	8.852	2344	2352	2360	rVB8	2087	3556	1.15%	0.102%
31	9.155	2439	2446	2454	rBB5	2022	3107	1.01%	0.089%
32	9.409	2514	2525	2549	rBV	164132	281974	91.55%	8.120%
33	9.566	2563	2574	2580	rVB7	2086	3738	1.21%	0.108%
34	9.621	2583	2591	2599	rBV4	3326	4673	1.52%	0.135%
35	9.708	2611	2618	2627	rBV7	2908	4016	1.30%	0.116%
36	10.026	2707	2717	2725	rBV5	5369	9708	3.15%	0.280%

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Title : TRACE VOA SFAM1.0

37	10.267	2784	2792	2799	rVB6	2139	3372	1.09%	0.097%
38	10.357	2809	2820	2833	rBV8	4321	9189	2.98%	0.265%
39	10.746	2931	2941	2953	rBV	53666	87367	28.37%	2.516%
40	10.804	2953	2959	2967	rVB7	2321	3731	1.21%	0.107%
41	11.296	3104	3112	3125	rVB7	6024	11026	3.58%	0.318%
42	11.804	3258	3270	3291	rBV	160807	269199	87.40%	7.752%
43	12.061	3340	3350	3369	rBV2	15083	33368	10.83%	0.961%
44	12.183	3377	3388	3404	rBV	145683	245475	79.70%	7.069%

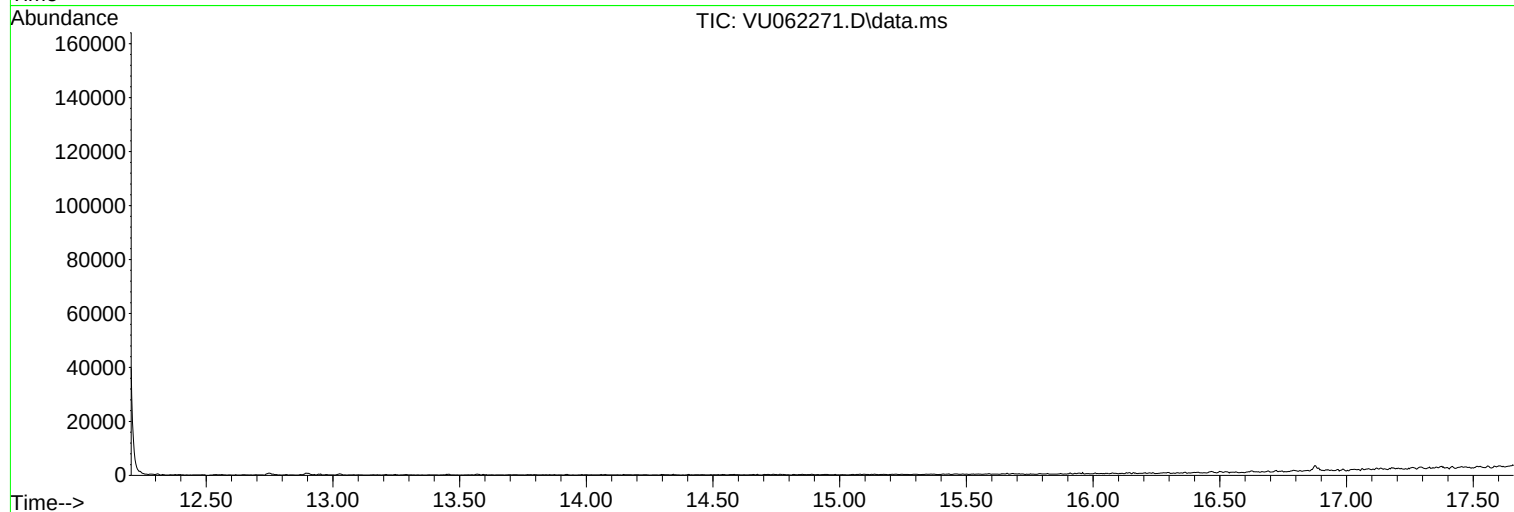
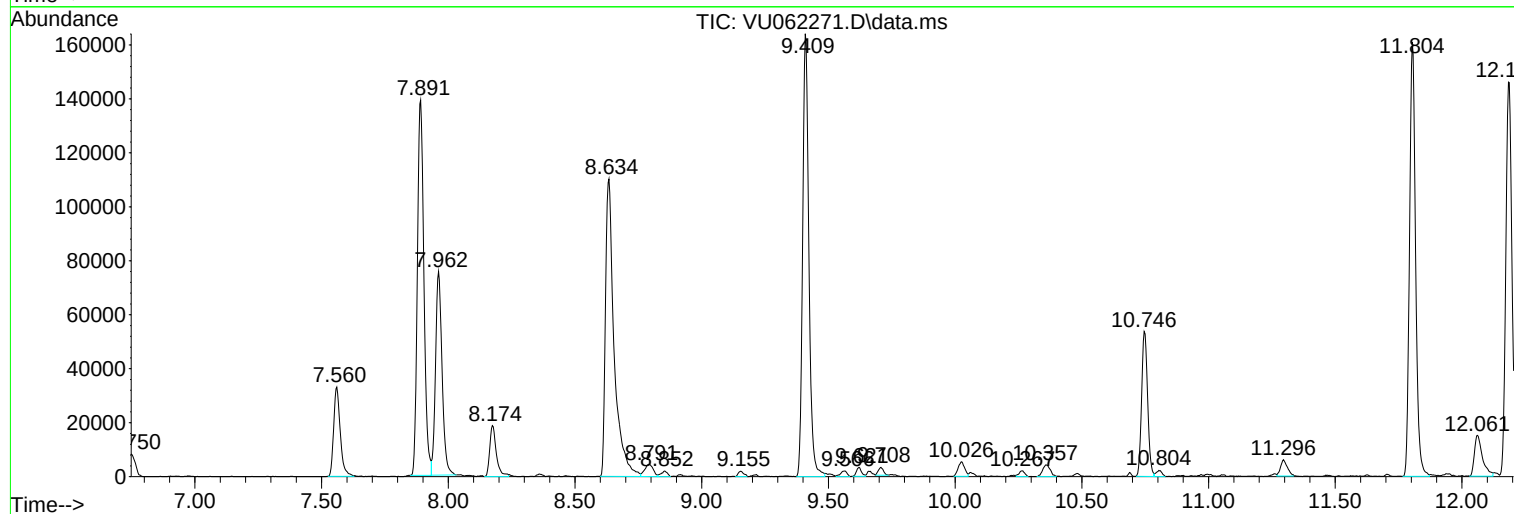
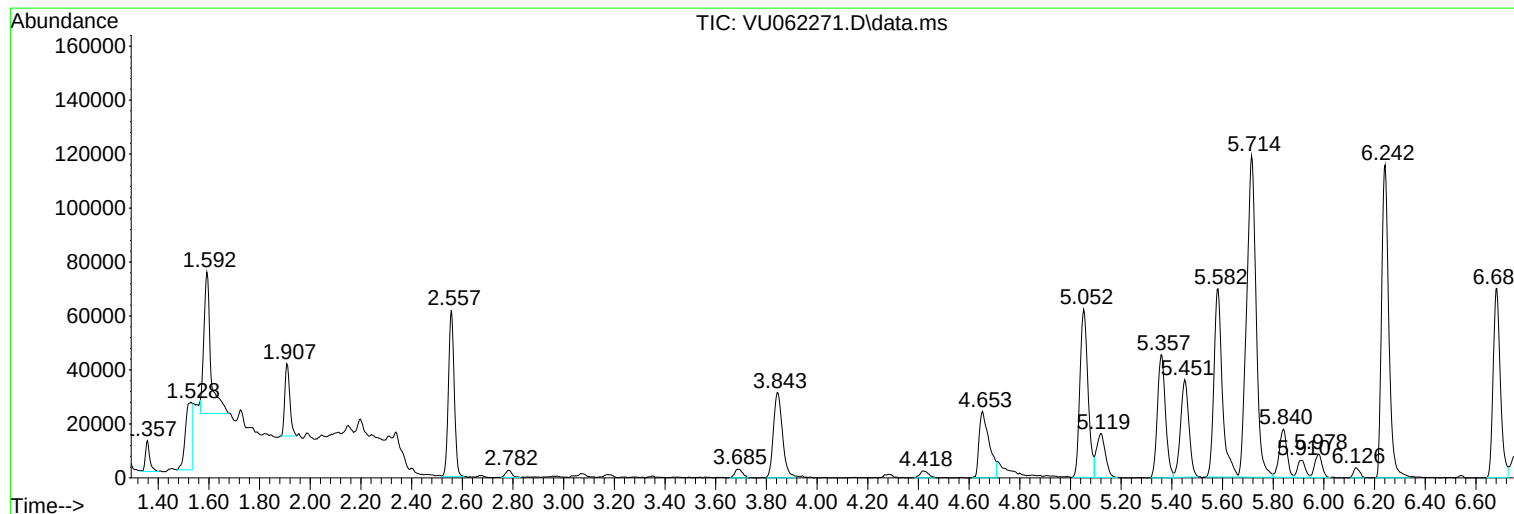
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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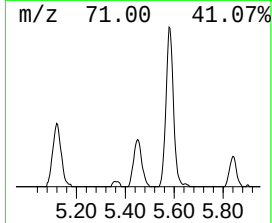
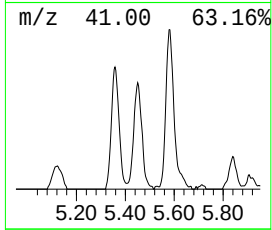
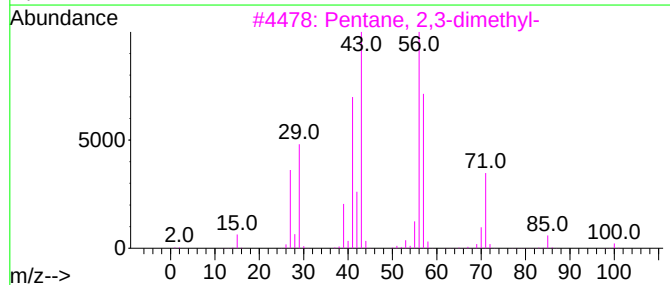
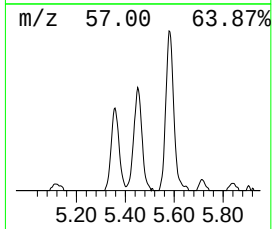
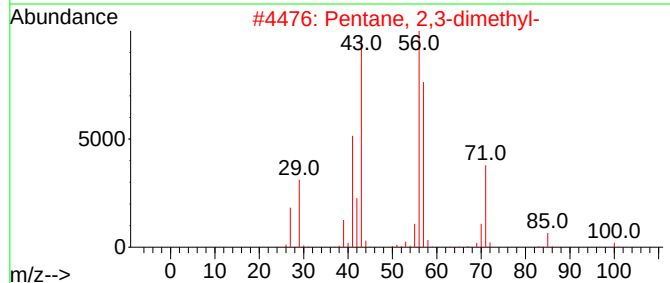
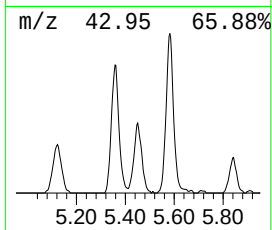
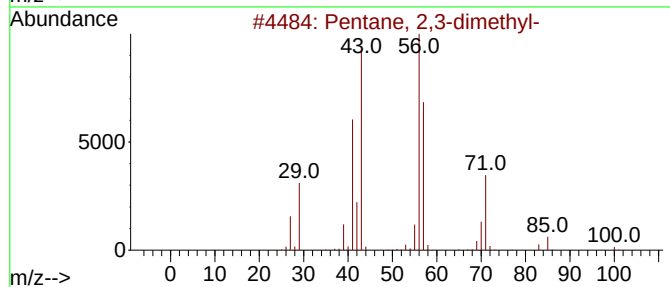
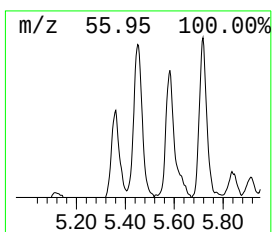
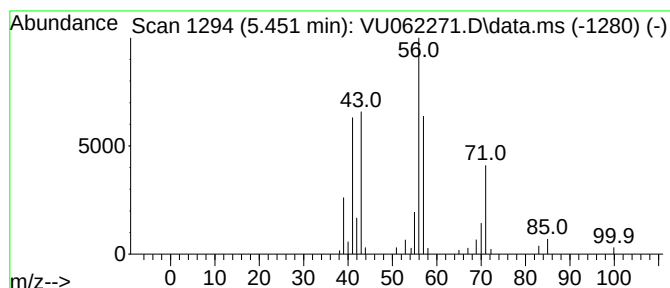
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.451	1.79 ug/L	82448	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	81
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	72



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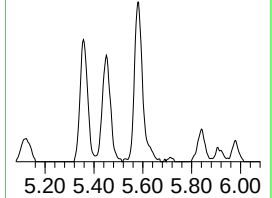
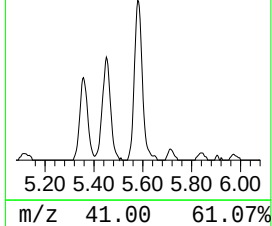
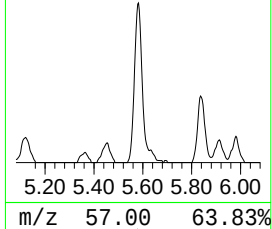
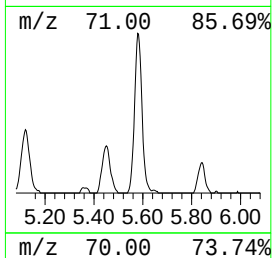
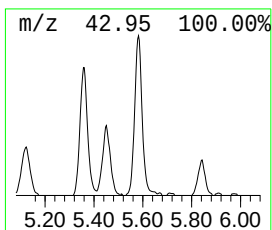
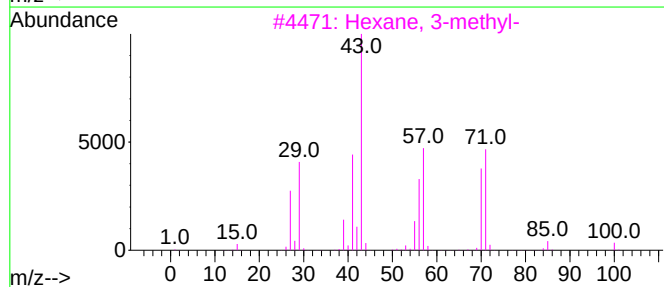
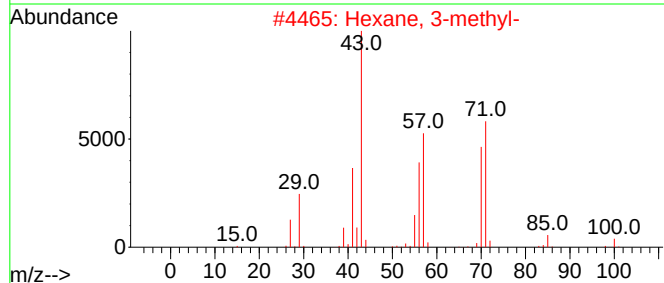
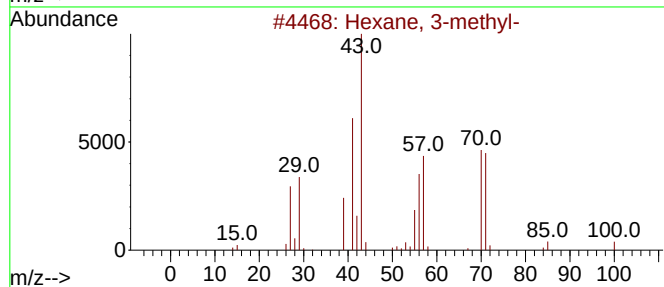
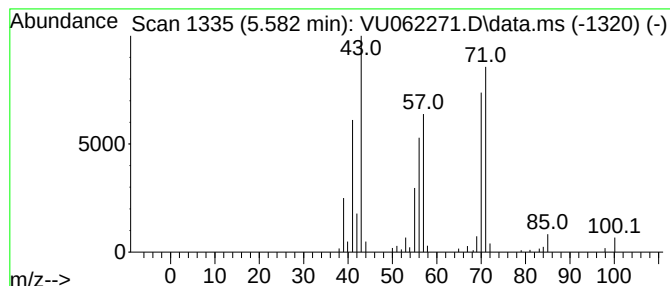
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.582	3.52 ug/L	162144	1,4-Difluorobenzene	6.242

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2		Hexane, 3-methyl-	100	C7H16	000589-34-4	91
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	90
4		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64
5		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	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
(DEL) Alkane: S...	5.451	1.8	ug/L	82448	1	6.242	230213	5.0
(DEL) Alkane: S...	5.582	3.5	ug/L	162144	1	6.242	230213	5.0