

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012324\
 Data File : VU057608.D
 Acq On : 24 Jan 2024 08:02
 Operator : MD/SY
 Sample : P1227-20
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0BF3

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\SFAMUTR012324WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU057608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	85	95	107	rVB	25030	31157	17.21%	1.688%
2	1.698	119	127	130	rBV2	1443	1953	1.08%	0.106%
3	1.731	132	137	146	rVB	3295	4021	2.22%	0.218%
4	1.914	185	194	204	rBV	18512	24620	13.60%	1.334%
5	2.515	363	381	382	rBV4	2472	5109	2.82%	0.277%
6	2.563	386	396	410	rVV	42793	74398	41.09%	4.030%
7	3.177	573	587	602	rBV	8113	18644	10.30%	1.010%
8	3.277	602	618	619	rBV3	1299	1887	1.04%	0.102%
9	4.435	961	978	988	rBV2	4672	12377	6.84%	0.671%
10	4.640	1024	1042	1086	rBV2	27844	98070	54.17%	5.313%
11	5.055	1157	1171	1195	rVB	36429	80912	44.69%	4.383%
12	5.721	1356	1378	1401	rBV3	71466	181045	100.00%	9.808%
13	6.242	1526	1540	1562	rBV	71405	138770	76.65%	7.518%
14	6.685	1665	1678	1696	rBV	43188	82997	45.84%	4.496%
15	7.119	1802	1813	1837	rBV2	15261	34375	18.99%	1.862%
16	7.563	1939	1951	1967	rBV	22131	39310	21.71%	2.130%
17	7.894	2041	2054	2069	rBV	91775	161515	89.21%	8.750%
18	7.968	2072	2077	2088	rVB2	2533	4155	2.30%	0.225%
19	8.177	2132	2142	2165	rBV	11600	20755	11.46%	1.124%
20	8.547	2248	2257	2270	rVB2	19089	32036	17.70%	1.735%
21	8.634	2272	2284	2321	rBV3	71021	160780	88.81%	8.710%
22	8.785	2321	2331	2346	rBV2	16032	29518	16.30%	1.599%
23	9.412	2514	2526	2553	rBV	97855	168518	93.08%	9.129%
24	9.569	2567	2575	2584	rBV	2042	2922	1.61%	0.158%
25	9.692	2603	2613	2627	rBV	6389	10224	5.65%	0.554%
26	10.097	2730	2739	2751	rBV3	2847	5240	2.89%	0.284%
27	10.344	2799	2816	2829	rBV4	3118	6742	3.72%	0.365%
28	10.749	2931	2942	2958	rVB	26873	43260	23.89%	2.344%
29	11.531	3177	3185	3197	rVB3	4567	7048	3.89%	0.382%
30	11.688	3226	3234	3243	rVB5	1969	2725	1.51%	0.148%
31	11.807	3259	3271	3289	rBV	101062	163878	90.52%	8.878%
32	12.065	3342	3351	3360	rBV2	4962	9547	5.27%	0.517%
33	12.187	3378	3389	3414	rVB	76721	126119	69.66%	6.832%
34	12.524	3483	3494	3509	rBV	18289	29903	16.52%	1.620%
35	12.769	3558	3570	3579	rBV2	4432	6991	3.86%	0.379%
36	12.884	3597	3606	3620	rBV3	7518	11675	6.45%	0.632%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Title : TRACE VOA SFAM1.0

37	12.965	3624	3631	3641	rBV4	1434	2220	1.23%	0.120%
38	14.309	4039	4049	4060	rVB4	2421	3786	2.09%	0.205%
39	14.479	4095	4102	4114	rVB3	1383	2251	1.24%	0.122%
40	15.685	4471	4477	4485	rVB3	3422	4471	2.47%	0.242%

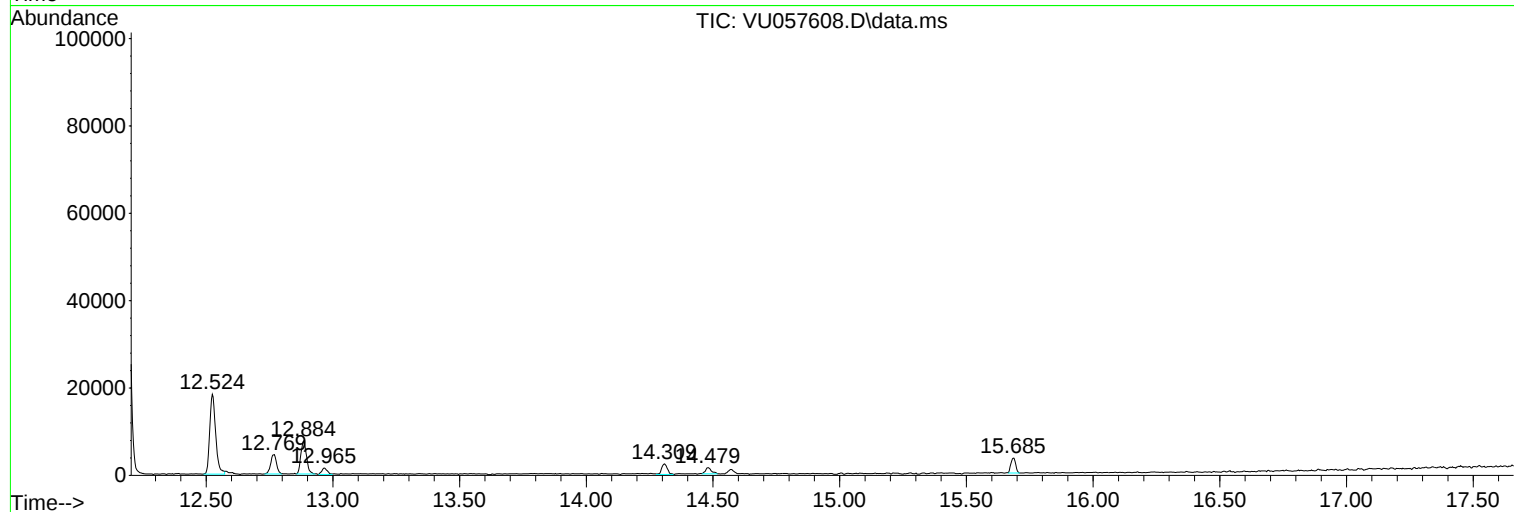
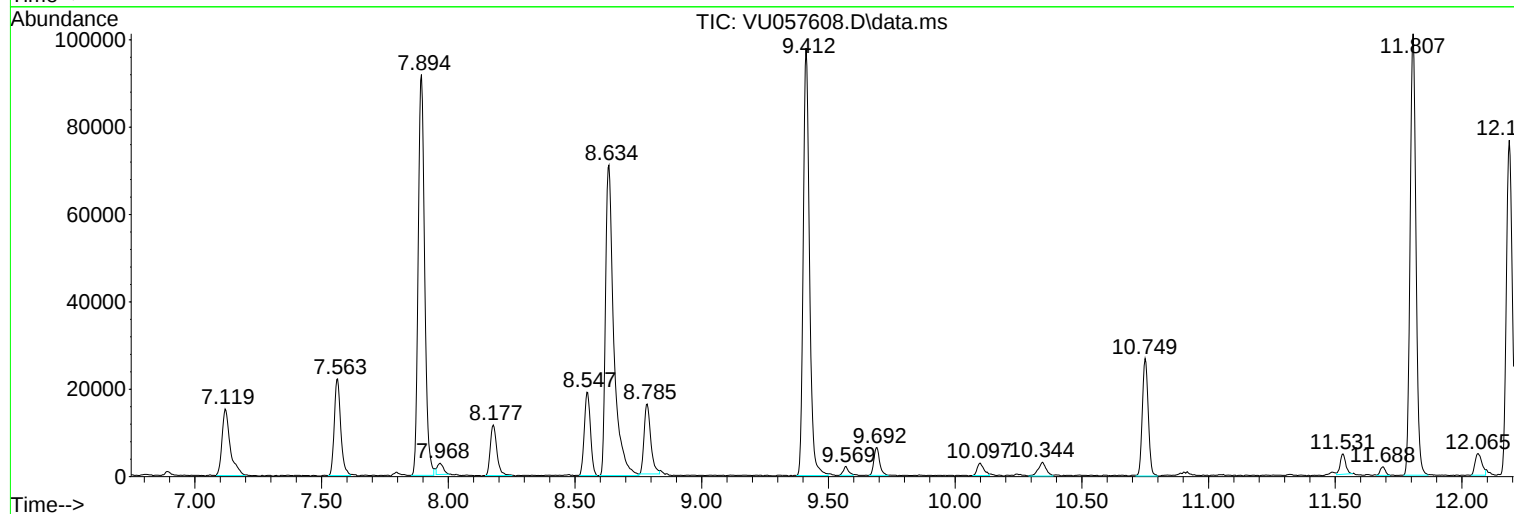
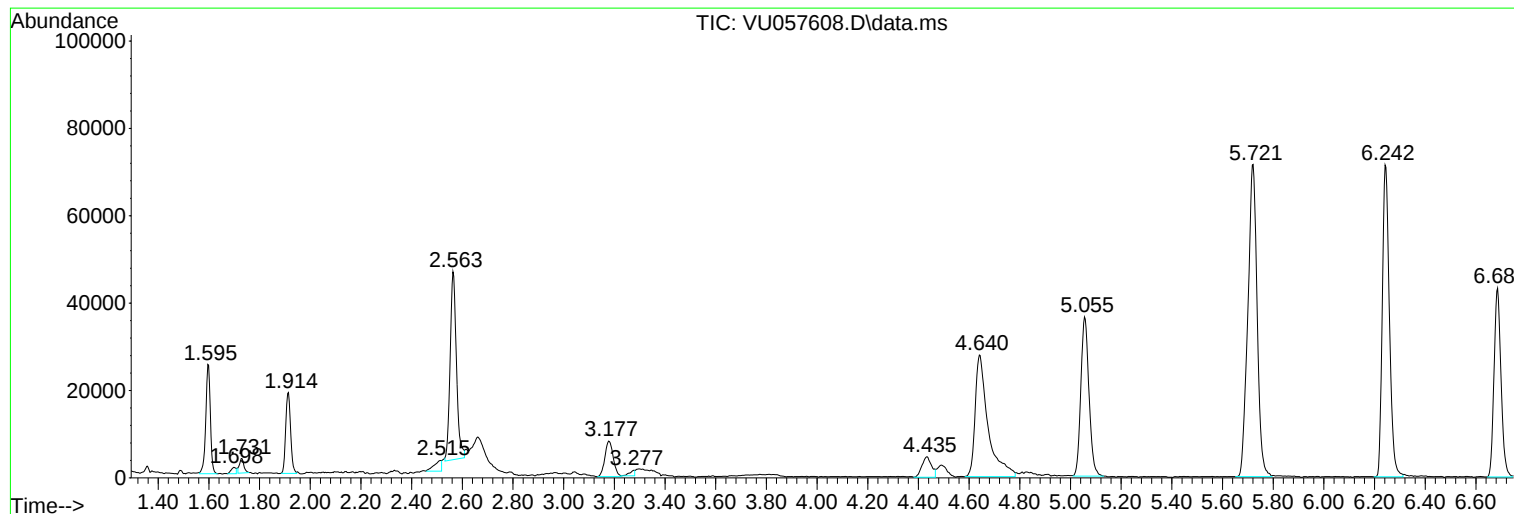
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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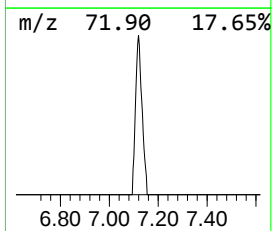
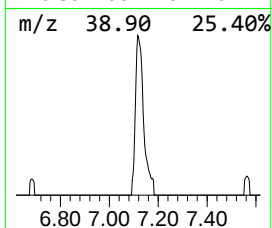
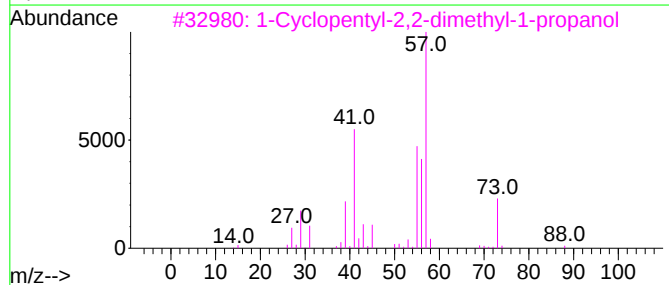
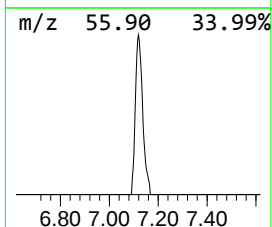
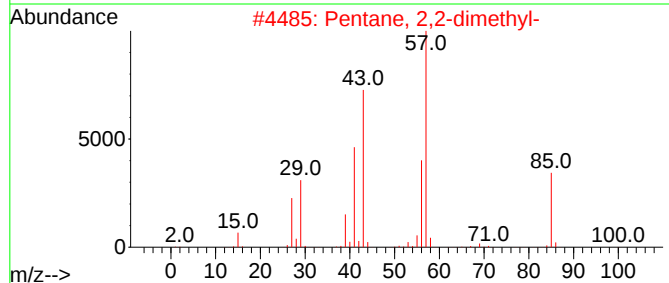
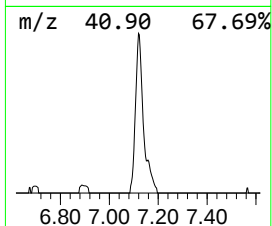
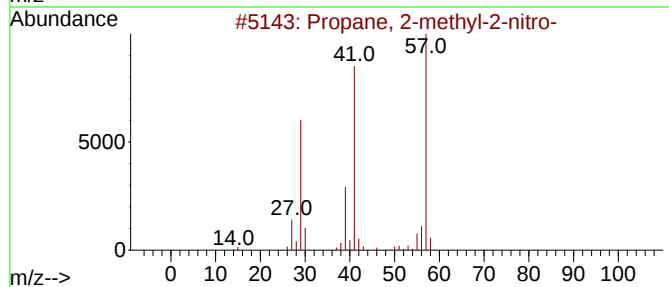
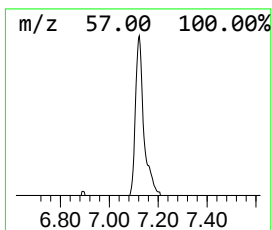
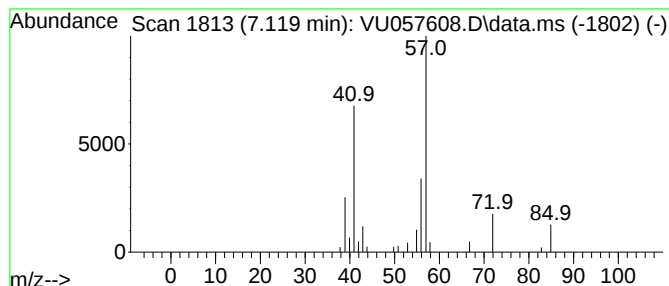
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.119	1.24 ug/L	34375	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
2			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	42
3			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	36
4			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	33
5			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	33



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Instrument :
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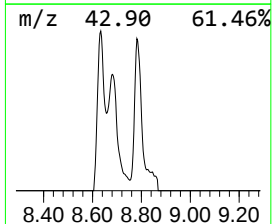
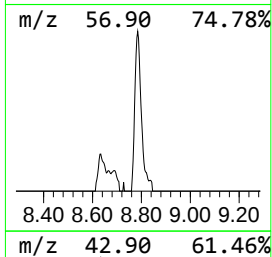
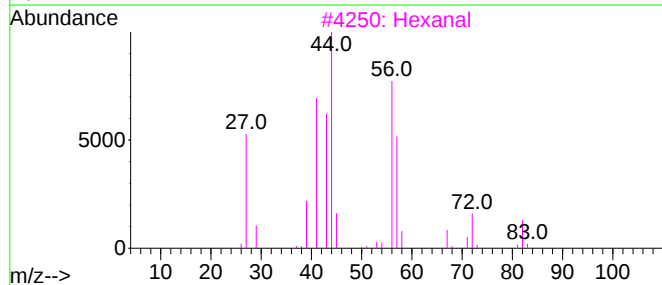
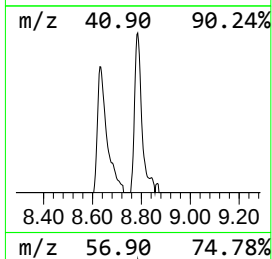
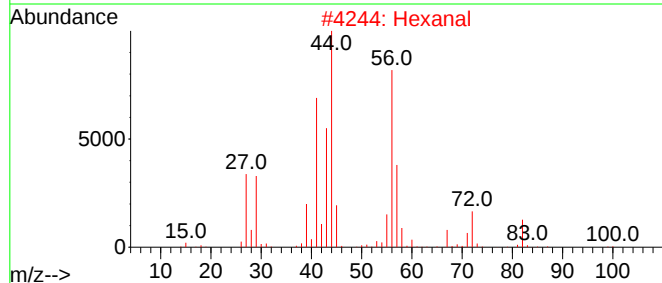
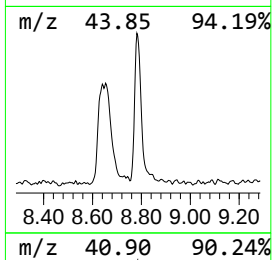
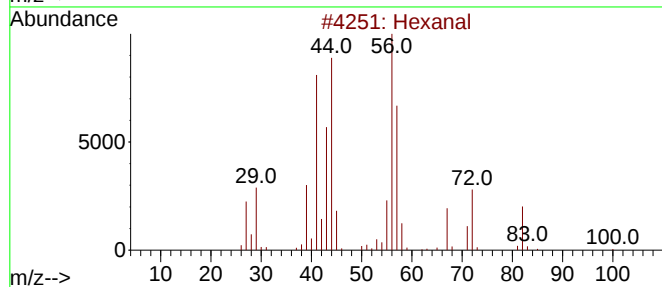
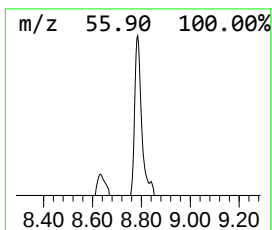
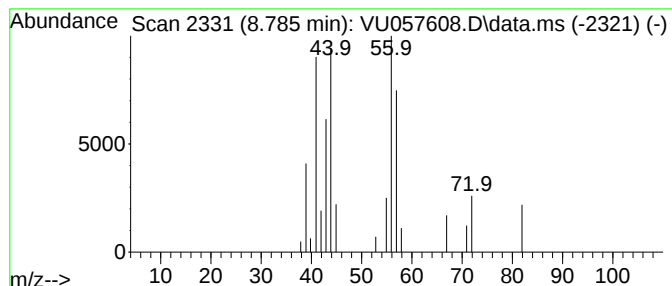
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	0.88 ug/L	29518	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	80
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	53



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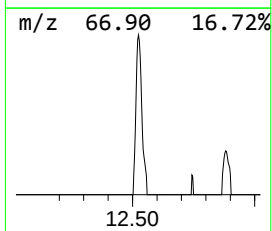
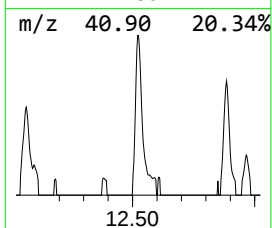
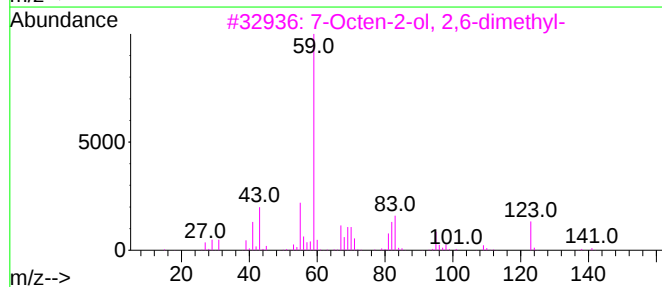
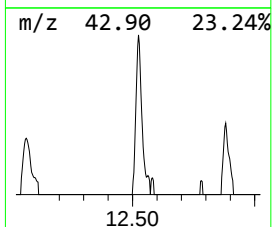
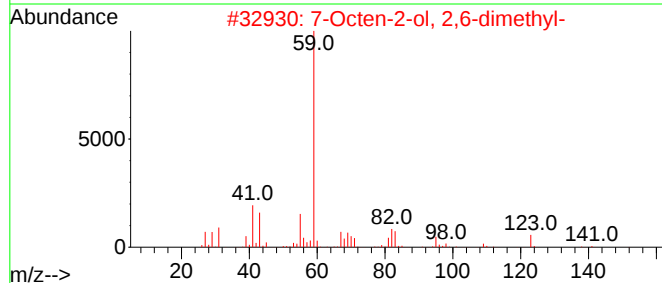
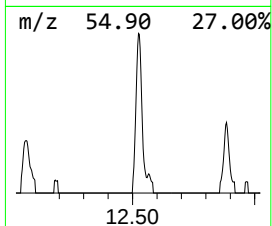
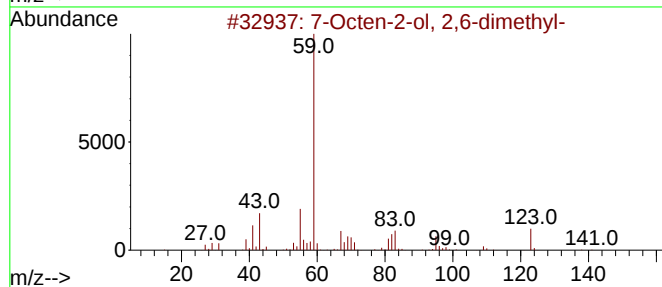
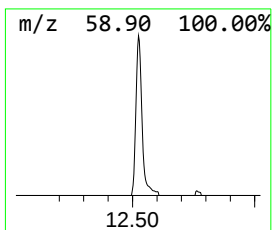
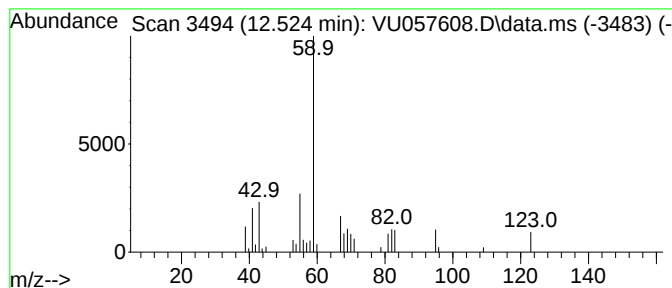
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.524	0.91 ug/L	29903	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	83
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	74
4			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	72
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	53



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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	7.119	1.2	ug/L	34375	1	6.245	138770	5.0
Hexanal	8.785	0.9	ug/L	29518	2	9.412	168518	5.0
7-Octen-2-ol, 2...	12.524	0.9	ug/L	29903	3	11.807	163878	5.0