

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102723\
 Data File : VU055931.D
 Acq On : 27 Oct 2023 18:20
 Operator : MD/SY
 Sample : 04995-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4935

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\SFAMUTR102423WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU055931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	105	rBV	101904	113769	8.15%	1.015%
2	1.914	186	194	208	rVB	88871	118075	8.46%	1.054%
3	2.566	384	397	408	rBV	166034	275773	19.76%	2.461%
4	2.631	408	417	448	rVB	127789	294514	21.11%	2.628%
5	3.184	579	589	608	rVB2	18230	42517	3.05%	0.379%
6	4.457	974	985	1002	rBV6	12918	38902	2.79%	0.347%
7	4.624	1023	1037	1058	rBV2	194925	550015	39.42%	4.909%
8	5.058	1154	1172	1196	rBV	201975	460501	33.00%	4.110%
9	5.721	1358	1378	1409	rBV2	362719	977988	70.09%	8.728%
10	6.245	1525	1541	1566	rBV	438894	894964	64.14%	7.987%
11	6.689	1665	1679	1696	rBV	236413	475483	34.08%	4.244%
12	6.881	1729	1739	1754	rBV4	35523	73019	5.23%	0.652%
13	7.563	1937	1951	1973	rBV2	108415	205489	14.73%	1.834%
14	7.791	2010	2022	2038	rBV2	20009	41252	2.96%	0.368%
15	7.894	2043	2054	2070	rVV	411451	740204	53.05%	6.606%
16	7.968	2070	2077	2092	rVB	29408	54845	3.93%	0.489%
17	8.177	2132	2142	2163	rBV	64908	118478	8.49%	1.057%
18	8.473	2219	2234	2247	rBV5	7210	16497	1.18%	0.147%
19	8.631	2271	2283	2320	rBV2	652315	1395308	100.00%	12.453%
20	8.785	2321	2331	2359	rVB	160808	303215	21.73%	2.706%
21	9.415	2513	2527	2553	rBV	600442	1058217	75.84%	9.444%
22	9.695	2604	2614	2628	rBV2	15742	28916	2.07%	0.258%
23	10.103	2733	2741	2763	rVB6	12324	32865	2.36%	0.293%
24	10.238	2770	2783	2799	rBV	30302	55469	3.98%	0.495%
25	10.344	2804	2816	2828	rBV3	42955	76342	5.47%	0.681%
26	10.569	2873	2886	2896	rBV4	16040	30979	2.22%	0.276%
27	10.753	2931	2943	2961	rVB	217955	356118	25.52%	3.178%
28	10.894	2974	2987	2998	rBV3	11263	20065	1.44%	0.179%
29	11.473	3159	3167	3181	rVB4	10443	20423	1.46%	0.182%
30	11.685	3224	3233	3247	rBV2	55889	94936	6.80%	0.847%
31	11.810	3260	3272	3292	rVV	646673	1061705	76.09%	9.475%
32	12.065	3337	3351	3369	rBV2	44882	116282	8.33%	1.038%
33	12.190	3378	3390	3417	rVB	467888	794753	56.96%	7.093%
34	12.528	3486	3495	3503	rBV5	10264	21048	1.51%	0.188%
35	12.884	3597	3606	3628	rVB2	153356	245918	17.62%	2.195%

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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\SFAMUTR102423WMA.M
Title : TRACE VOA SFAM1.0

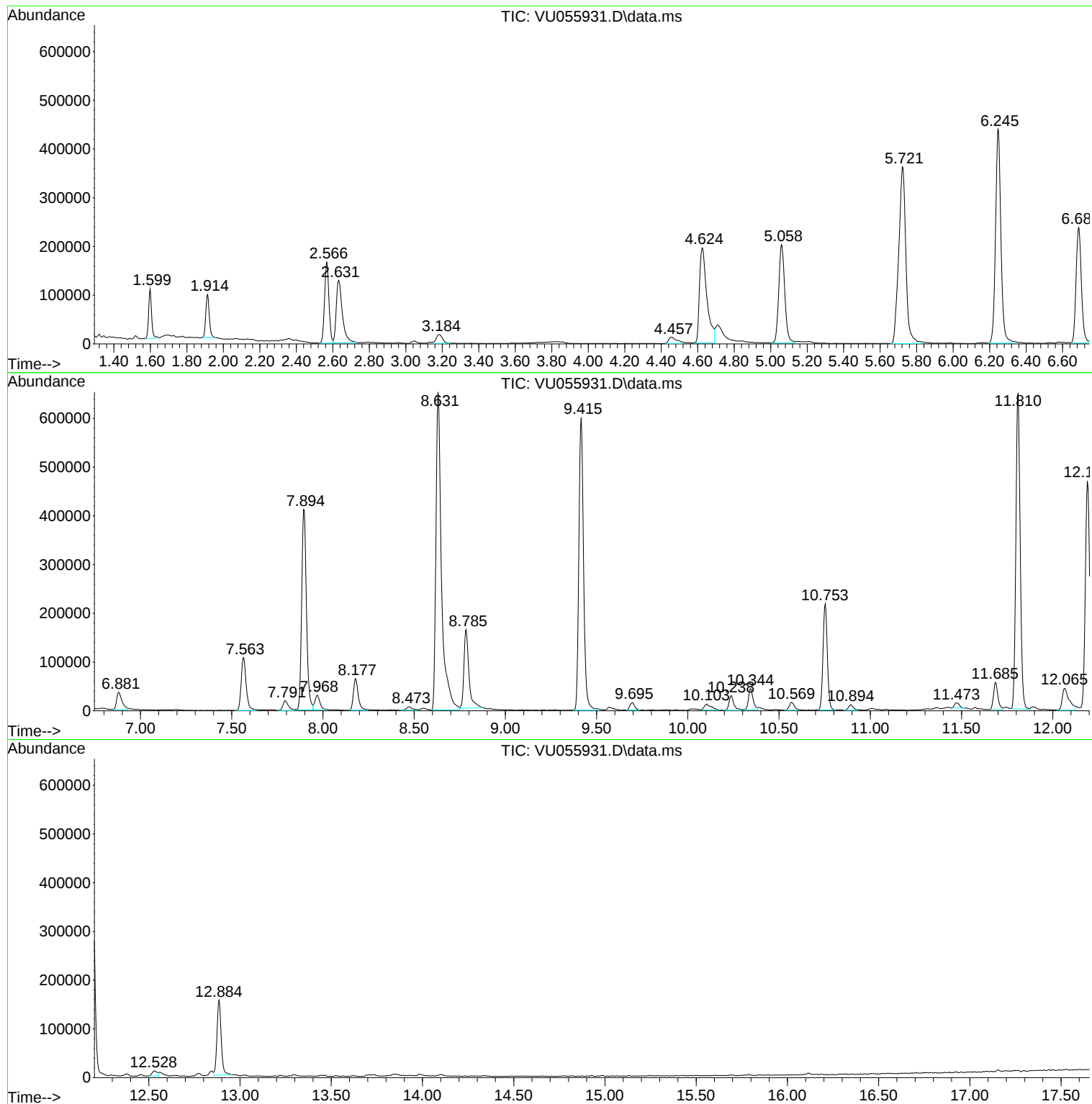
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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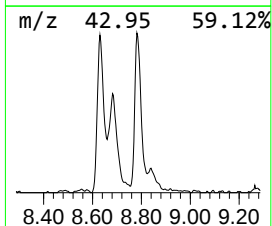
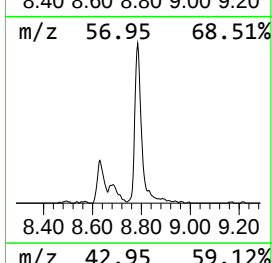
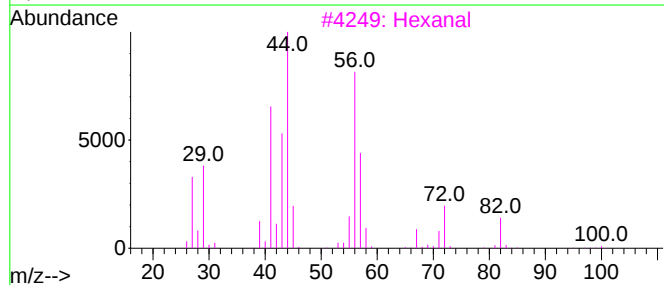
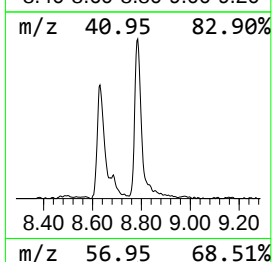
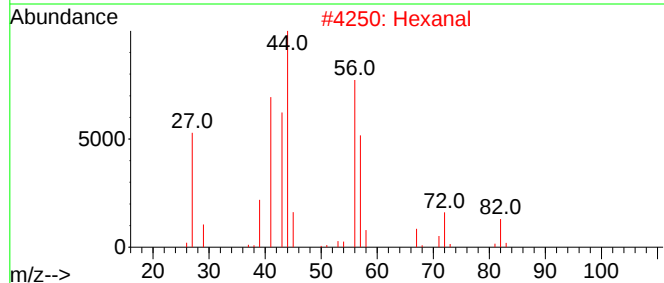
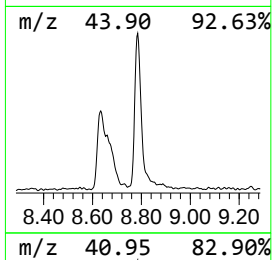
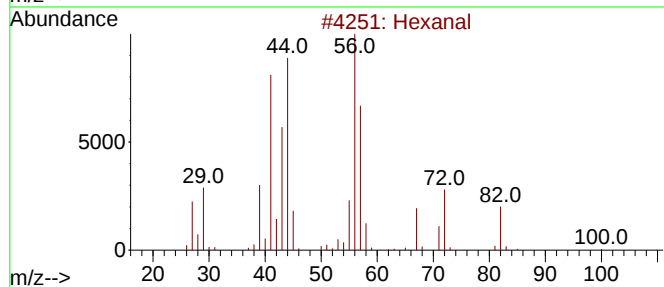
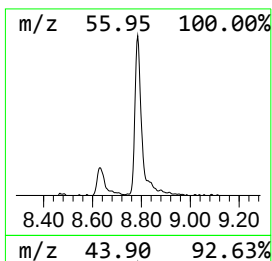
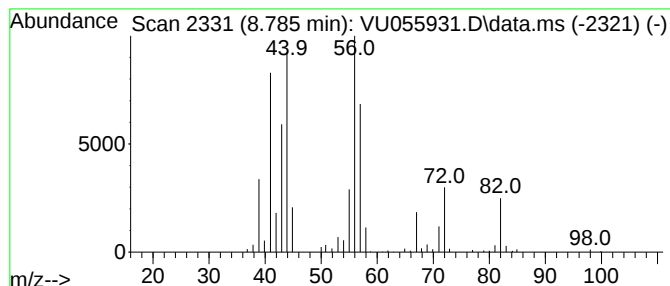
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	1.43 ug/L	303215	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	96
2	Hexanal			100	C6H12O	000066-25-1	90
3	Hexanal			100	C6H12O	000066-25-1	83
4	Hexanal			100	C6H12O	000066-25-1	80
5	Hexanal			100	C6H12O	000066-25-1	72



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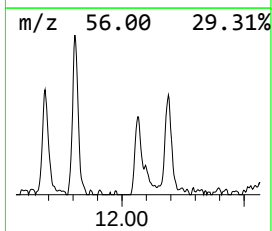
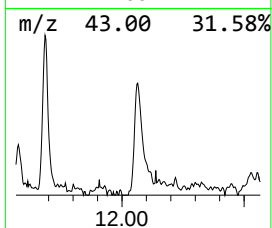
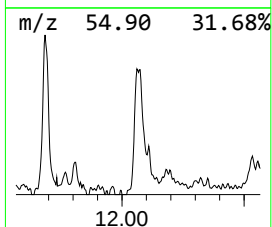
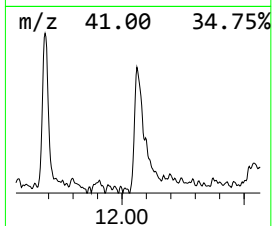
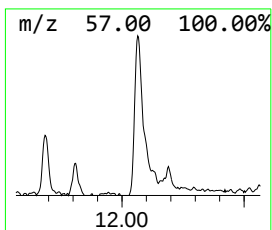
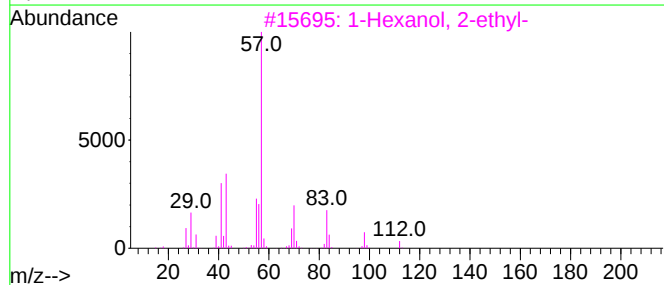
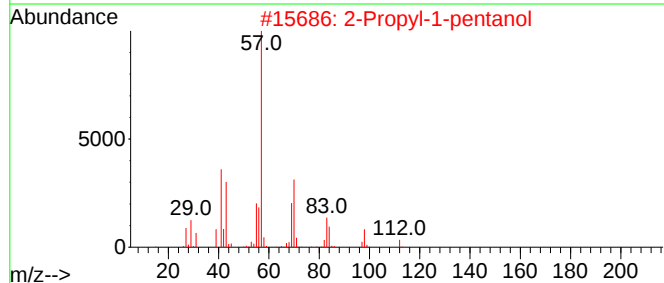
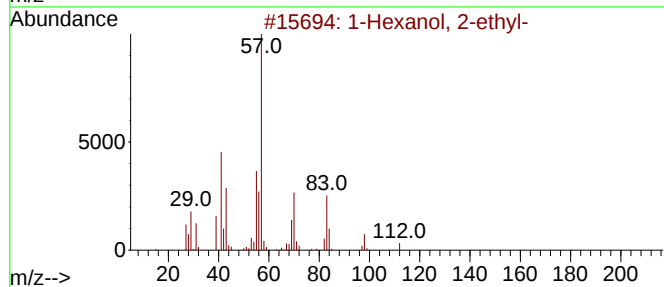
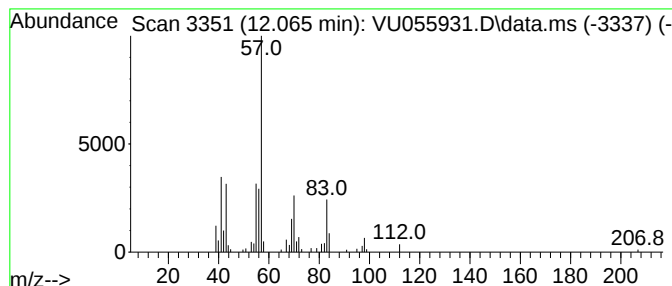
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.065	0.55 ug/L	116282	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	64
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



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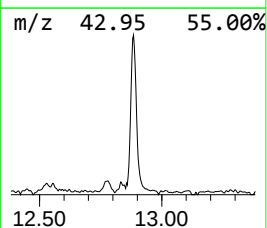
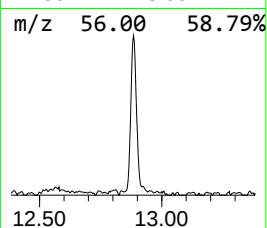
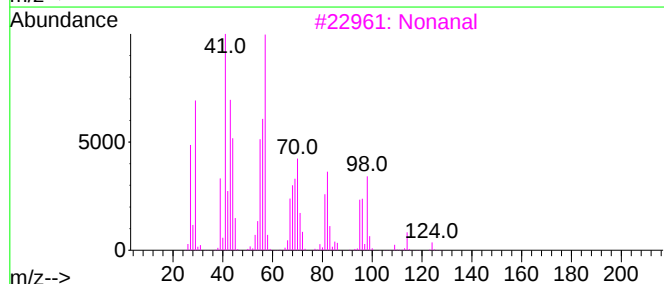
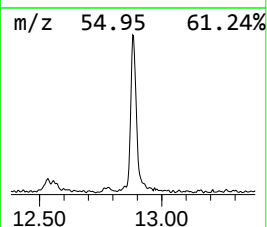
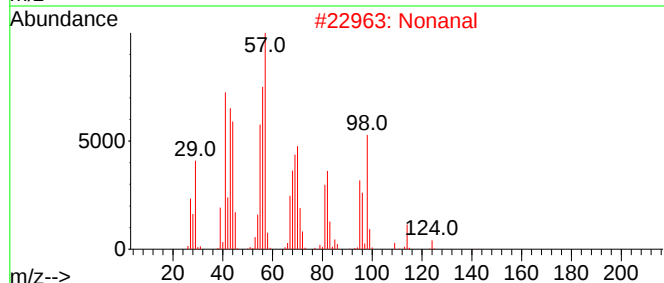
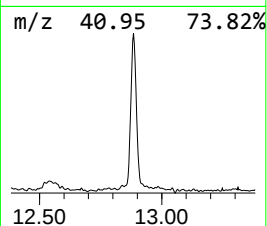
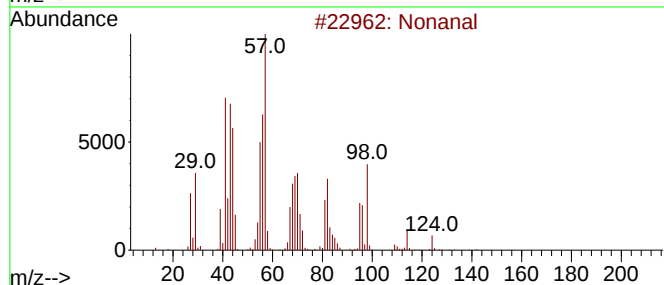
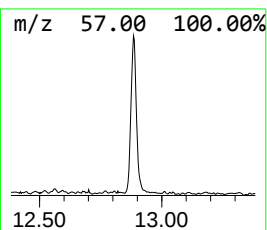
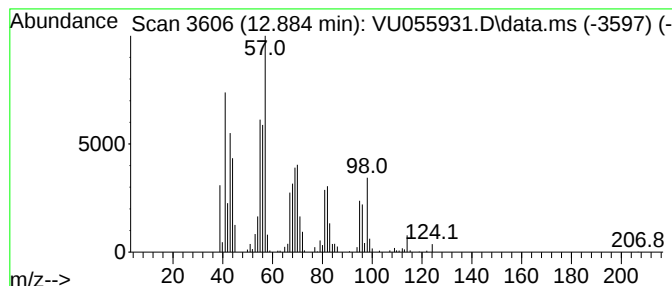
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	1.16 ug/L	245918	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	91
3			Nonanal	142	C9H18O	000124-19-6	91
4			Cycloheptane	98	C7H14	000291-64-5	38
5			Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.785	1.4	ug/L	303215	2	9.415	1058220	5.0
1-Hexanol, 2-et...	12.065	0.6	ug/L	116282	3	11.810	1061710	5.0
Nonanal	12.884	1.2	ug/L	245918	3	11.810	1061710	5.0