

Data Path : W:\HPCHEM1\MSVOA F\DATA\VF091715\
 Data File : VF045413.D
 Acq On : 17 Sep 2015 18:23
 Operator : FY/SY
 Sample : G3708-02
 Misc : 12.20g/5mL/MSVOA F/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_F
 ClientSampleId :
 MGP2090BR-15-17

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : W:\HPCHEM1\MSVOA_F\METHODS\82F091615S.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.036	49	51	59	rVB2	100699	192738	4.52%	0.659%
2	1.400	83	88	93	rBV2	130480	294263	6.90%	1.006%
3	1.971	143	146	157	rVB5	43800	121622	2.85%	0.416%
4	2.139	159	163	166	rBV3	54381	118245	2.77%	0.404%
5	2.188	166	168	173	rVB2	39804	83914	1.97%	0.287%
6	2.346	178	184	191	rVB	158001	385734	9.05%	1.319%
7	4.050	350	357	371	rVB2	569477	1781423	41.80%	6.093%
8	4.582	404	411	412	rBV5	21198	43949	1.03%	0.150%
9	4.631	412	416	423	rVB4	65111	201200	4.72%	0.688%
10	4.818	423	435	451	rBV3	1128810	4261789	100.00%	14.576%
11	5.547	503	509	519	rBV	1304896	3613950	84.80%	12.361%
12	6.818	630	638	642	rBV3	28250	92210	2.16%	0.315%
13	7.340	688	691	695	rBV2	52272	100900	2.37%	0.345%
14	7.448	695	702	703	rBV	97576	180746	4.24%	0.618%
15	7.507	703	708	715	rVV	1728595	3932881	92.28%	13.451%
16	7.704	725	728	732	rVV4	23053	50655	1.19%	0.173%
17	7.813	735	739	743	rVB3	33290	71551	1.68%	0.245%
18	7.980	753	756	761	rVB2	30569	65293	1.53%	0.223%
19	9.428	897	903	915	rBV	164555	427282	10.03%	1.461%
20	9.714	927	932	941	rBV	1751886	4013300	94.17%	13.727%
21	9.852	941	946	949	rVB2	72744	172508	4.05%	0.590%
22	10.078	965	969	972	rBV3	23774	47351	1.11%	0.162%
23	10.738	1031	1036	1039	rBV4	18926	46778	1.10%	0.160%
24	11.241	1084	1087	1092	rBV	31678	62331	1.46%	0.213%
25	11.359	1095	1099	1104	rVV	1584245	2951306	69.25%	10.094%
26	11.438	1104	1107	1114	rVV	267793	563474	13.22%	1.927%
27	11.526	1114	1116	1121	rVV4	18482	47133	1.11%	0.161%
28	11.615	1121	1125	1128	rVV	40946	71375	1.67%	0.244%
29	12.107	1171	1175	1178	rBV	246806	379257	8.90%	1.297%
30	12.501	1211	1215	1225	rVB	2106110	3613207	84.78%	12.358%
31	12.679	1229	1233	1235	rBV	150868	251505	5.90%	0.860%
32	12.895	1250	1255	1259	rBV	371541	692470	16.25%	2.368%
33	12.954	1259	1261	1266	rVB	40338	64670	1.52%	0.221%
34	13.664	1330	1333	1339	rVB2	68270	110866	2.60%	0.379%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	14.393	1403	1407	1412	rBV	67306	129695	3.04%	0.444%
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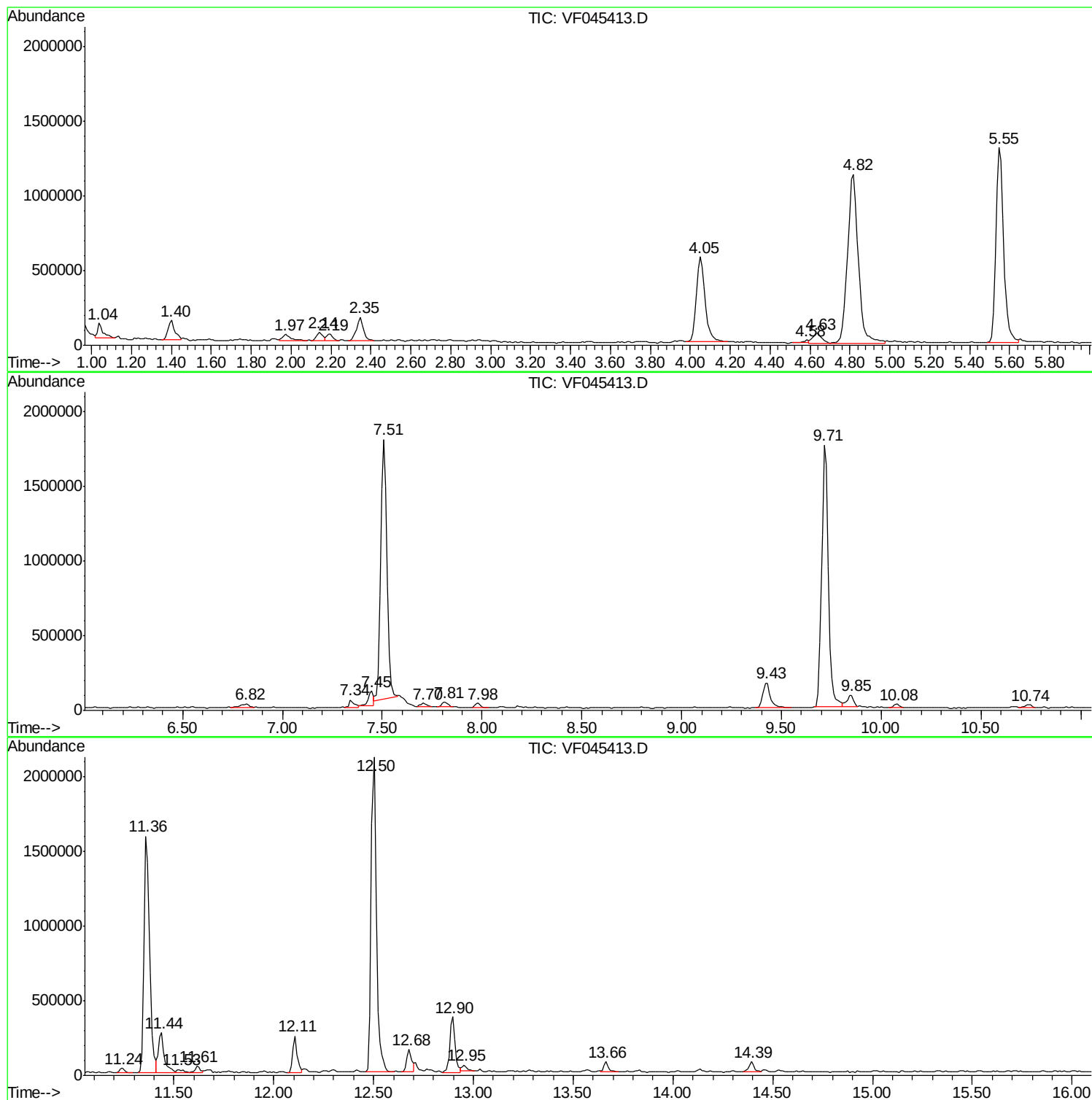
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TIC Library : C:\DATABASE\NIST02.L
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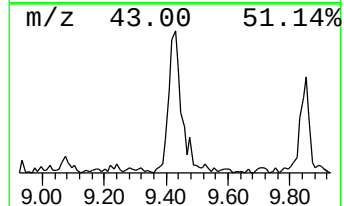
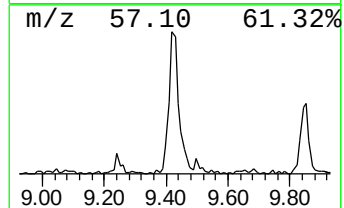
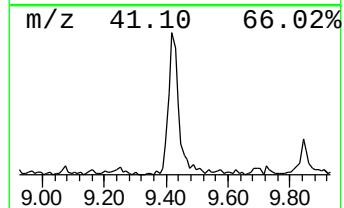
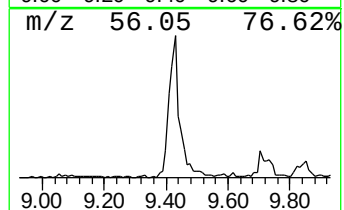
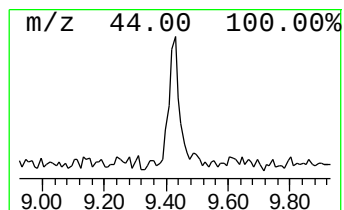
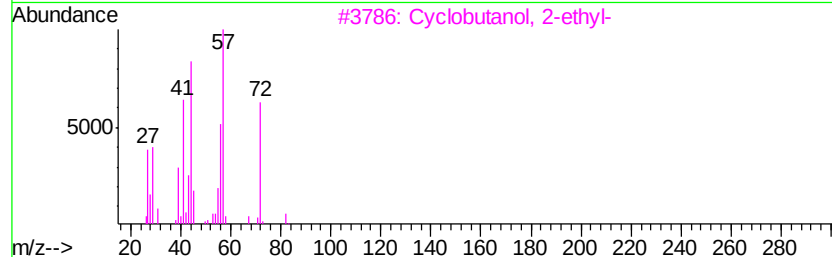
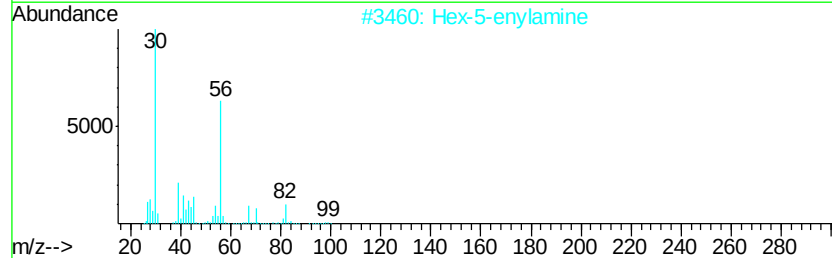
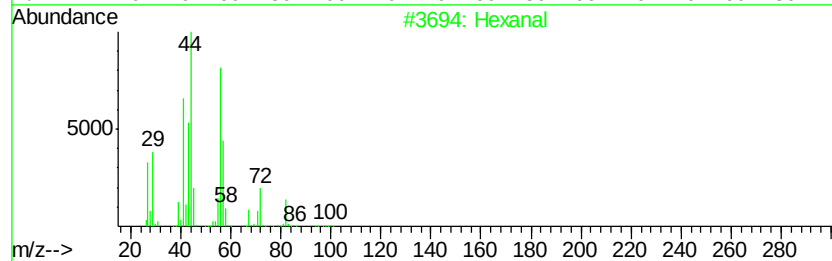
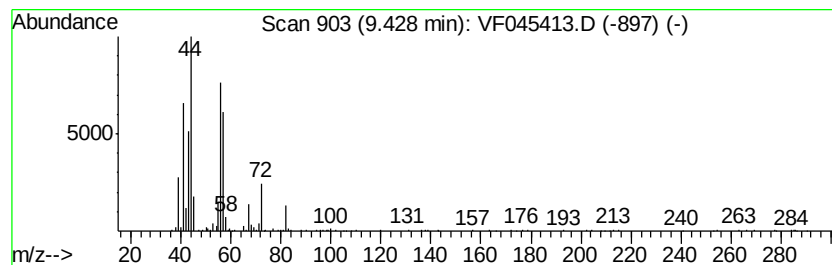
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	5.32 ug/l	427282	Chlorobenzene-d5	9.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	90
2		Hex-5-enylamine	99	C6H13N	034825-70-2	43
3		Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	42
4		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
5		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	23



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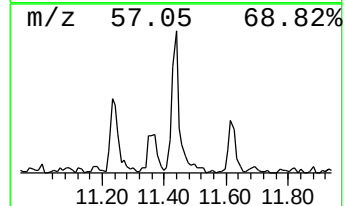
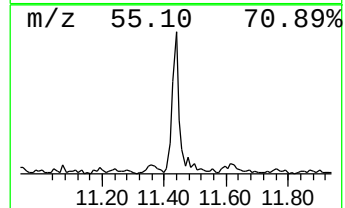
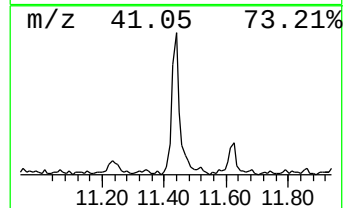
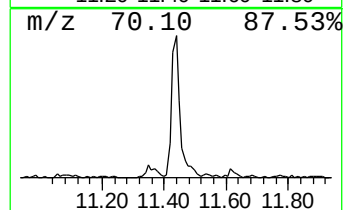
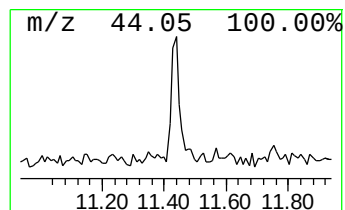
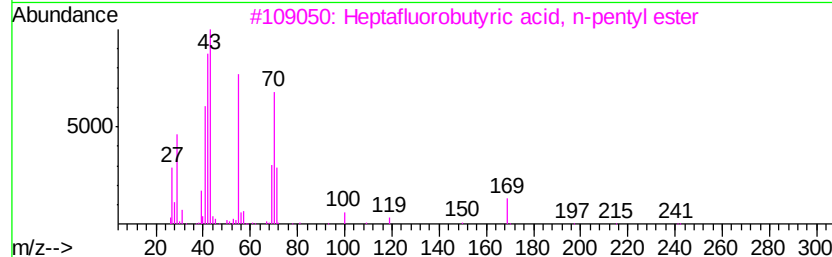
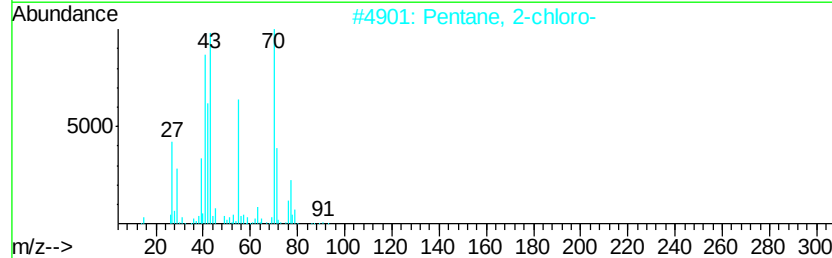
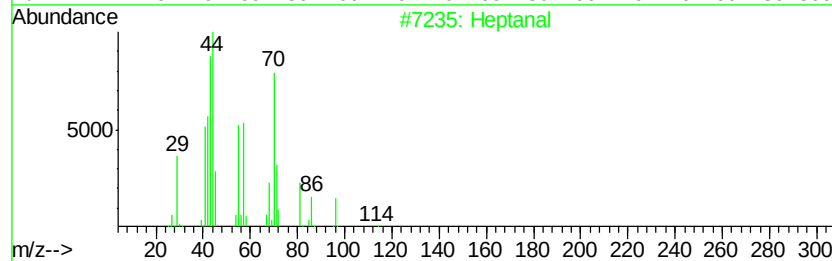
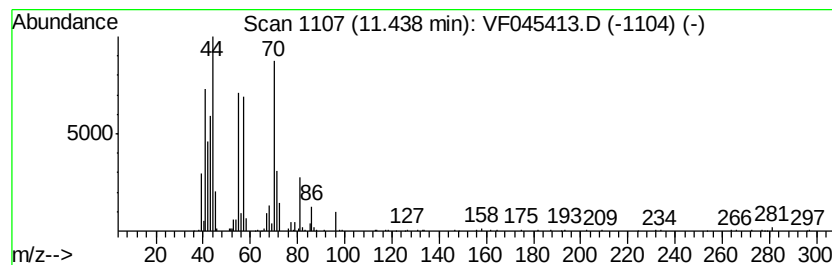
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Peak Number 2 Heptanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.44	7.80 ug/l	563474	1,4-Dichlorobenzene-d4	12.50		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptanal	114	C7H14O	000111-71-7	83
2		Pentane, 2-chloro-	106	C5H11Cl	000625-29-6	38
3		Heptafluorobutyric acid, n-pentyl-	284	C9H11F7O2	000425-26-3	38
4		1-Butanol, 2-methyl-, (+/-)-	88	C5H12O	034713-94-5	32
5		1-(2-Methylallyl)azetidine	111	C7H13N	1000194-99-1	25



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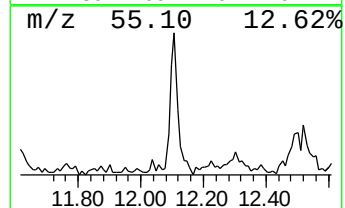
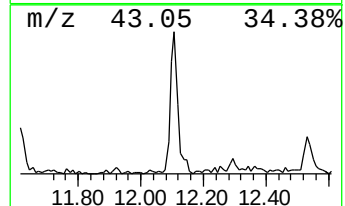
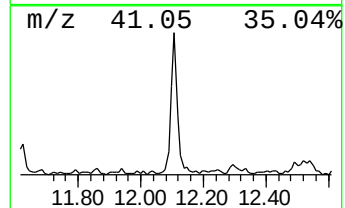
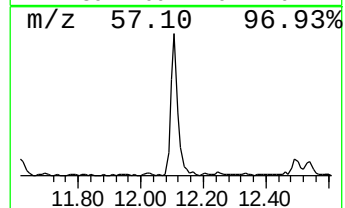
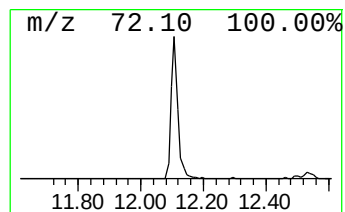
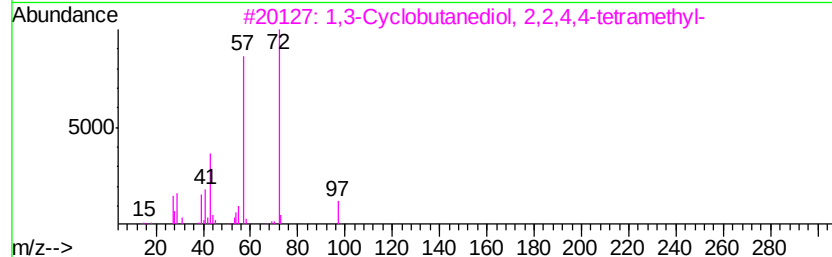
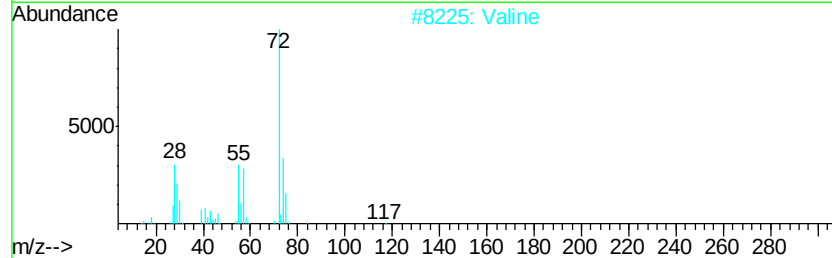
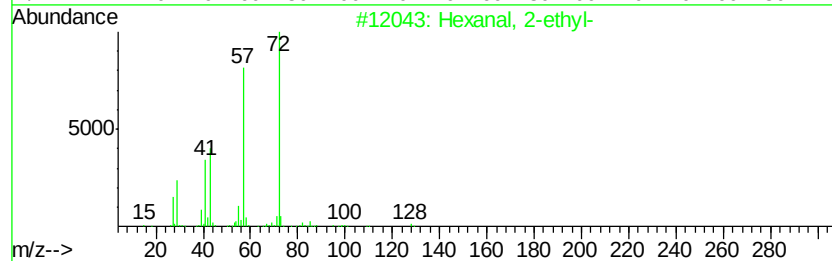
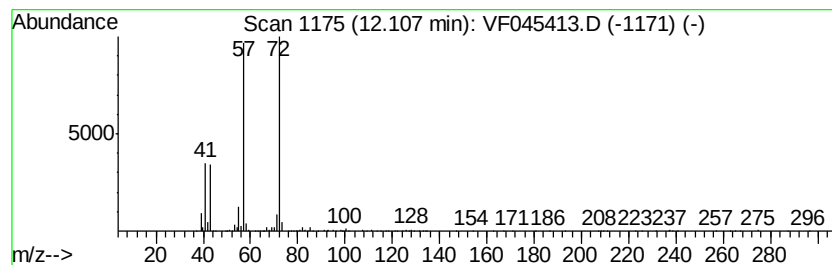
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Peak Number 3 Hexanal, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	5.25 ug/l	379257	1,4-Dichlorobenzene-d4	12.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexanal, 2-ethyl-	128 C8H16O	000123-05-7	74
2	Valine	117 C5H11NO2	000072-18-4	53
3	1,3-Cyclobutanediol, 2,2,4,4-tet...	144 C8H16O2	003010-96-6	50
4	2-Propenoic acid	72 C3H4O2	000079-10-7	42
5	6-Chloro-4-methyl-2-oxo-2H-chrom...	281 C13H12ClNO4	283170-70-7	40



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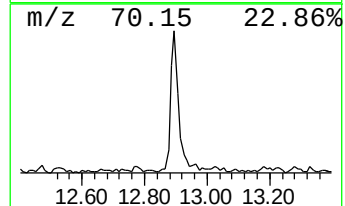
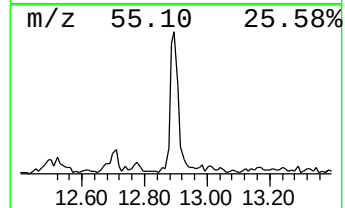
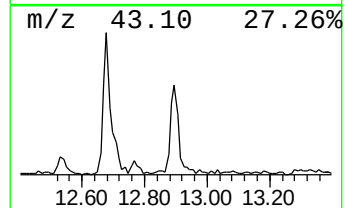
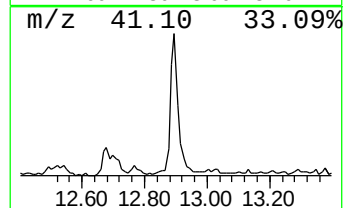
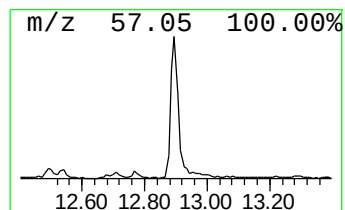
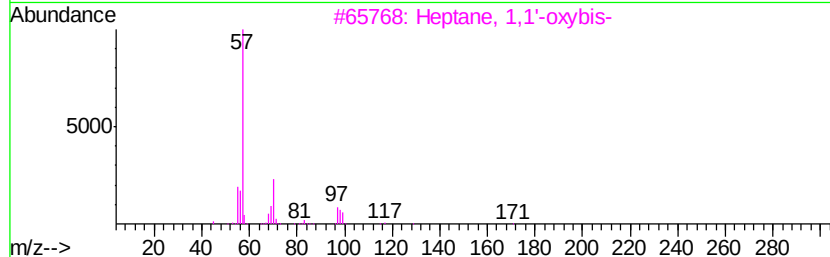
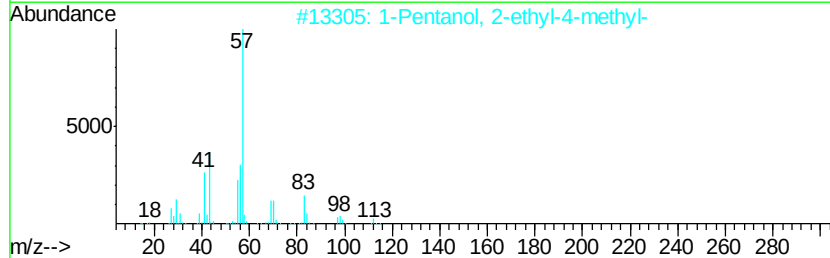
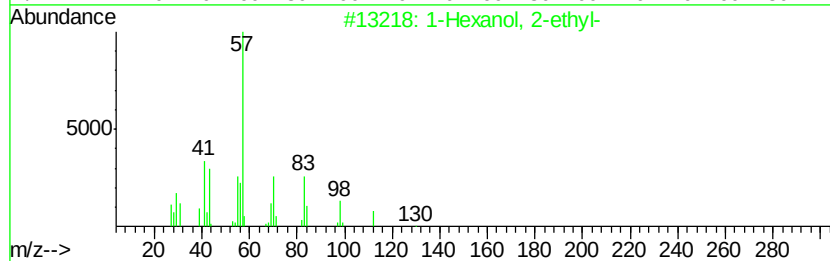
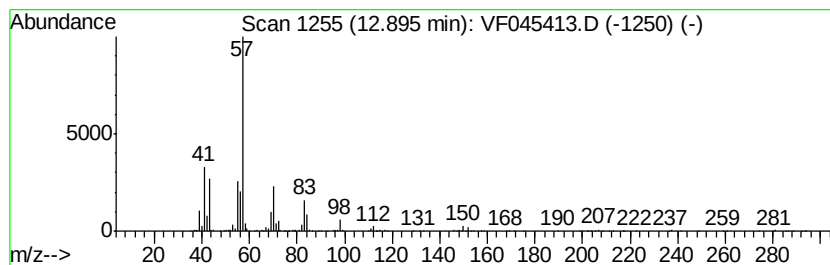
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.90	9.58 ug/l	692470	1,4-Dichlorobenzene-d4	12.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	1-Decene, 3,4-dimethyl-	168	C12H24	050871-03-9	56
5	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	9.43	5.3	ug/l	427282	3	9.71	4013300	50.0
Heptanal	11.44	7.8	ug/l	563474	4	12.50	3613210	50.0
Hexanal, 2-ethyl-	12.11	5.3	ug/l	379257	4	12.50	3613210	50.0
1-Hexanol, 2-ethyl-	12.90	9.6	ug/l	692470	4	12.50	3613210	50.0