

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
 Data File : BF093491.D
 Acq On : 9 Mar 2017 22:34
 Operator : SJ/MA
 Sample : I2195-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-7-TP-6-COMP-0-12FT

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 : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.955	5	6	11	rVB	77417	111631	1.84%	0.210%
2	4.916	263	265	281	rBV	695562	1399233	23.02%	2.637%
3	5.350	301	303	321	rBV	4946786	5618126	92.43%	10.589%
4	5.750	336	338	347	rVB	41843	66668	1.10%	0.126%
5	6.413	393	396	398	rBV	4194713	6078120	100.00%	11.456%
6	6.527	403	406	408	rBV	4527685	5570825	91.65%	10.500%
7	6.744	423	425	428	rBV	915779	1102151	18.13%	2.077%
8	6.904	437	439	442	rBV	4359712	4109528	67.61%	7.746%
9	7.327	473	476	478	rBV	3463651	4058612	66.77%	7.650%
10	8.036	535	538	540	rBV	1596380	1449321	23.84%	2.732%
11	9.110	629	632	634	rBV	5396905	5430378	89.34%	10.235%
12	9.510	664	667	669	rBV	706483	632677	10.41%	1.192%
13	9.785	689	691	693	rBV	1727499	1580234	26.00%	2.978%
14	10.208	727	728	730	rVB	70277	76770	1.26%	0.145%
15	10.573	758	760	763	rBV2	2351942	3046494	50.12%	5.742%
16	10.688	768	770	777	rVB2	104353	168339	2.77%	0.317%
17	11.088	804	805	807	rBV	75681	79732	1.31%	0.150%
18	11.133	807	809	810	rVV	100020	96032	1.58%	0.181%
19	11.271	819	821	822	rBV	1804246	1685617	27.73%	3.177%
20	11.522	840	843	845	rBV2	44340	64061	1.05%	0.121%
21	11.556	845	846	849	rVB	80628	65809	1.08%	0.124%
22	11.808	866	868	873	rVB2	58169	78385	1.29%	0.148%
23	11.888	873	875	879	rVB2	34862	62881	1.03%	0.119%
24	12.116	893	895	899	rBV	98093	129116	2.12%	0.243%
25	12.425	920	922	925	rVB	56461	67041	1.10%	0.126%
26	12.482	925	927	930	rBV	708874	622082	10.23%	1.172%
27	12.711	942	947	950	rBV	440514	479228	7.88%	0.903%
28	12.859	957	960	962	rBV	4292366	5412478	89.05%	10.201%
29	13.568	1019	1022	1024	rBV	54227	63282	1.04%	0.119%
30	13.751	1036	1038	1047	rBV3	247683	542591	8.93%	1.023%
31	13.911	1050	1052	1054	rBV	1528945	1654556	27.22%	3.118%
32	14.928	1139	1141	1142	rBV	59858	73866	1.22%	0.139%
33	14.962	1142	1144	1146	rVB2	56223	77570	1.28%	0.146%
34	15.317	1172	1175	1180	rBV	932057	1209292	19.90%	2.279%

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Sampling : 1 Min Area: 3 % of largest Peak
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35	15.797	1212	1217	1224	rVB7	23595	93689	1.54%	0.177%
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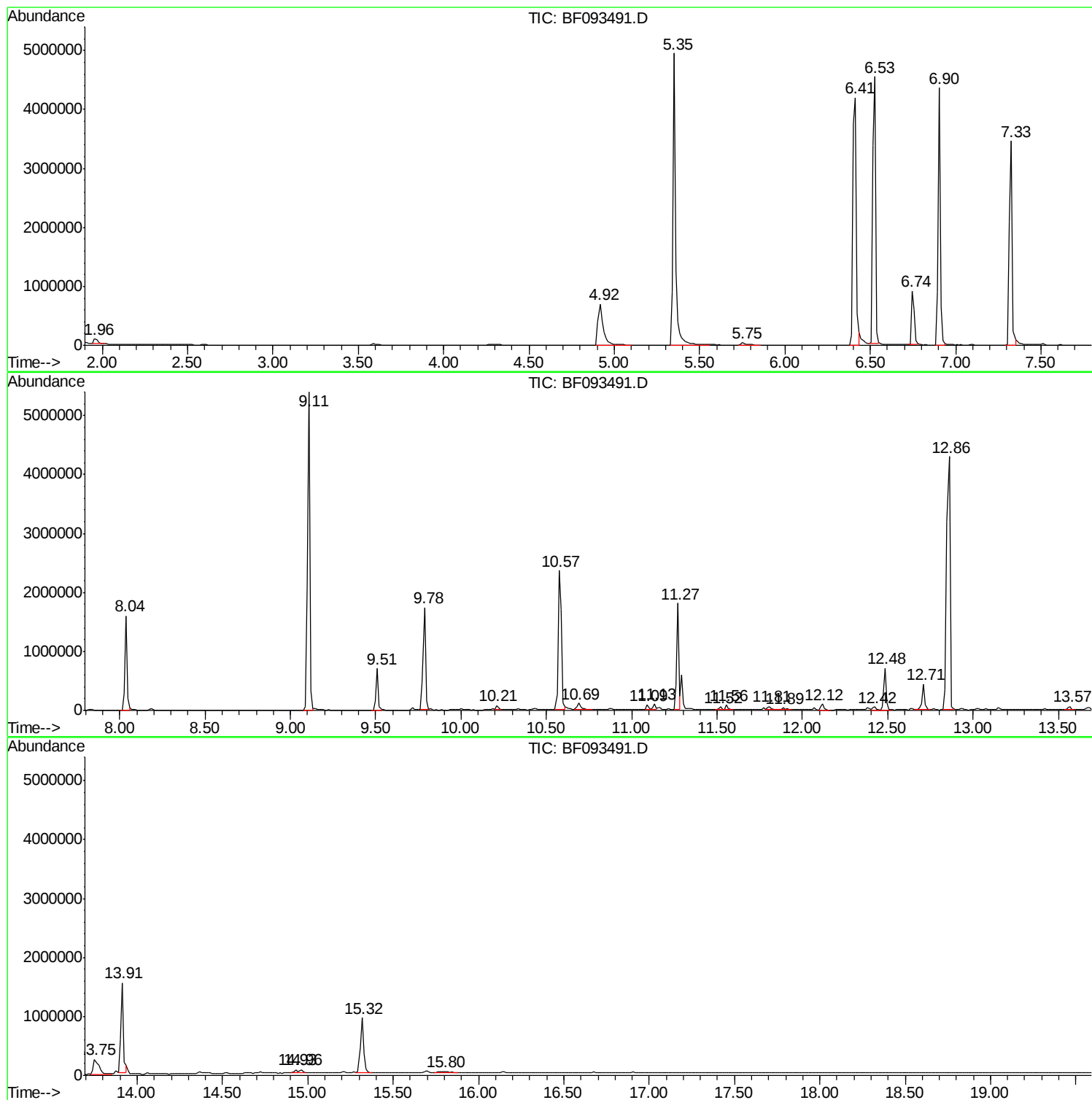
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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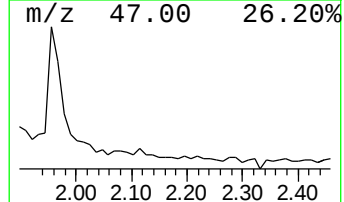
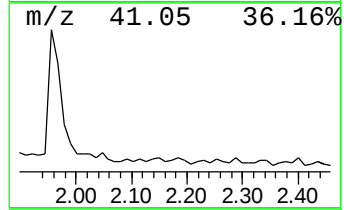
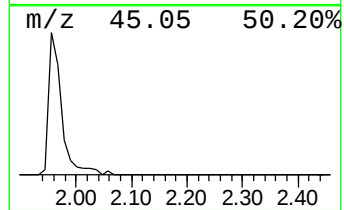
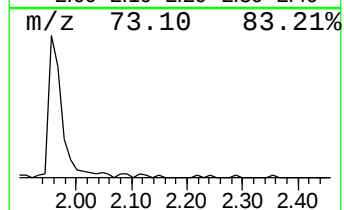
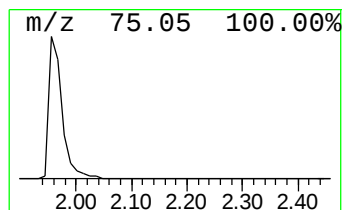
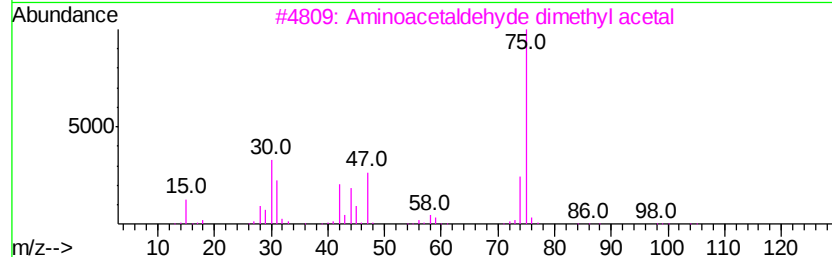
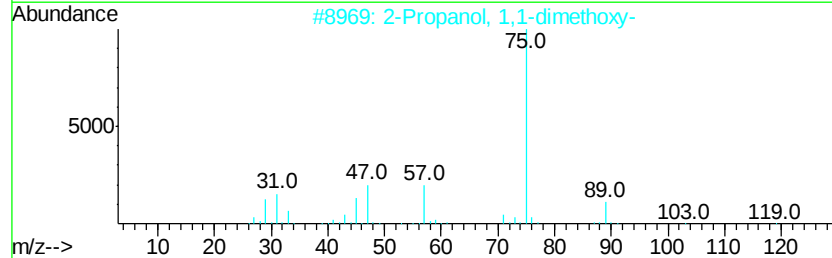
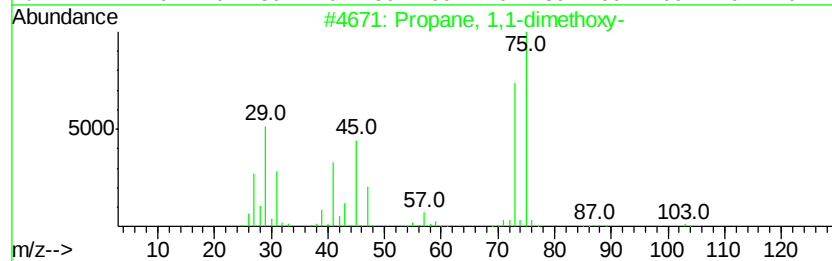
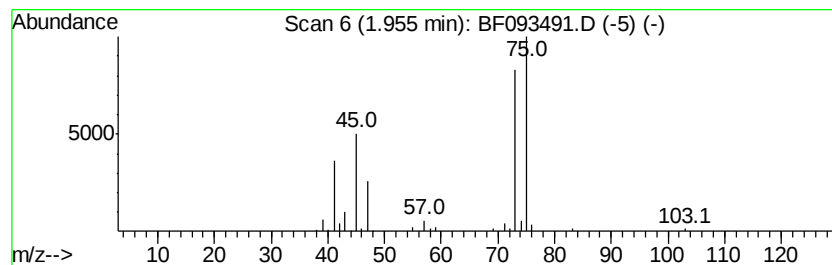
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	2.03 ng	111631	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	40
3		Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	33
4		1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	10
5		Ethanethioamide	75	C2H5NS	000062-55-5	9



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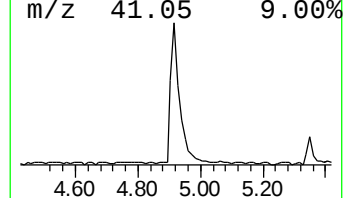
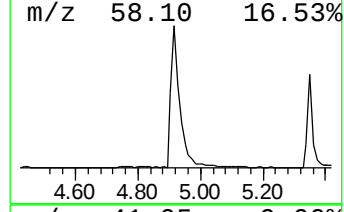
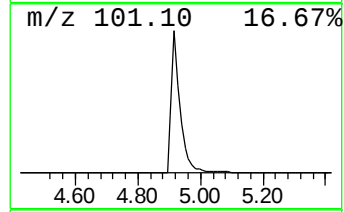
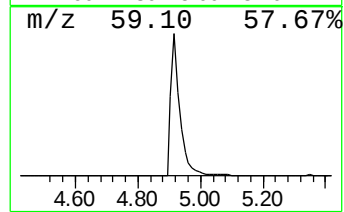
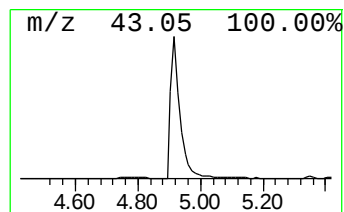
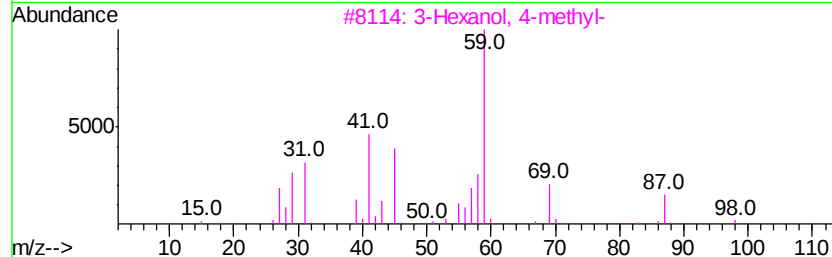
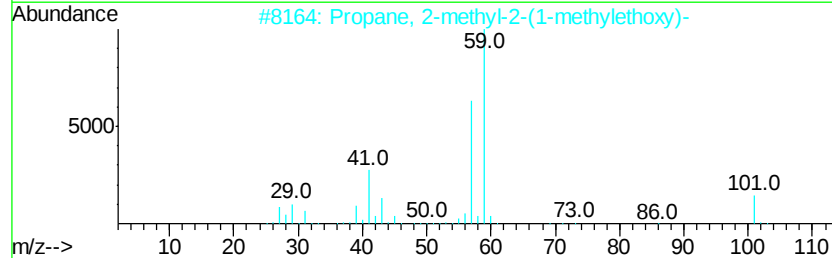
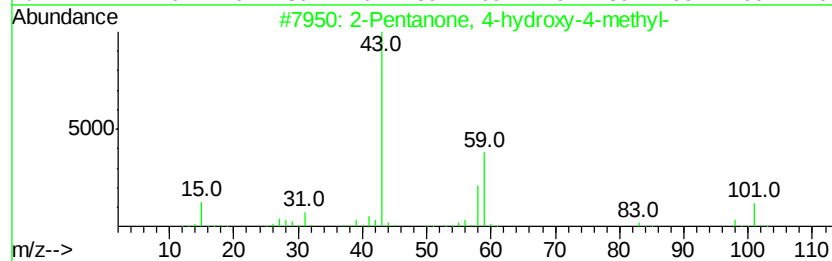
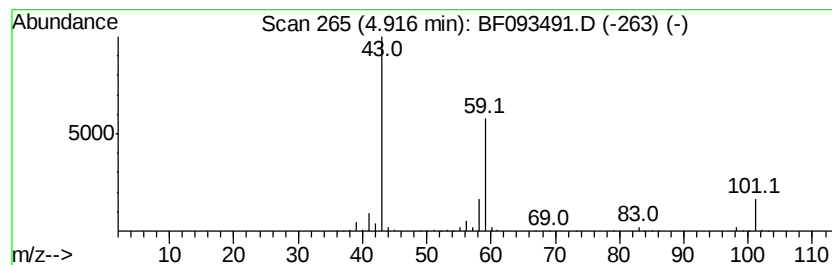
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	25.39 ng	1399230	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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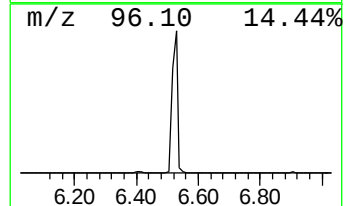
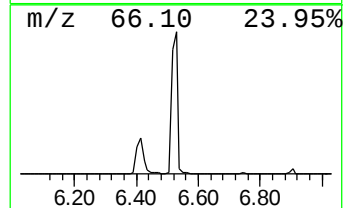
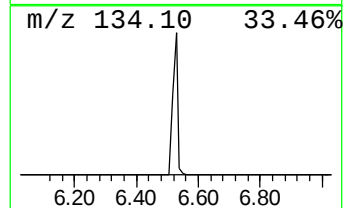
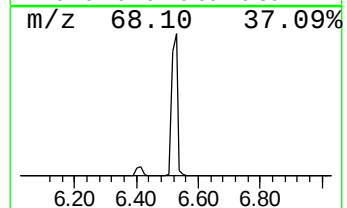
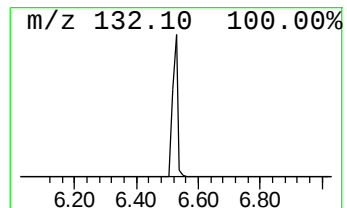
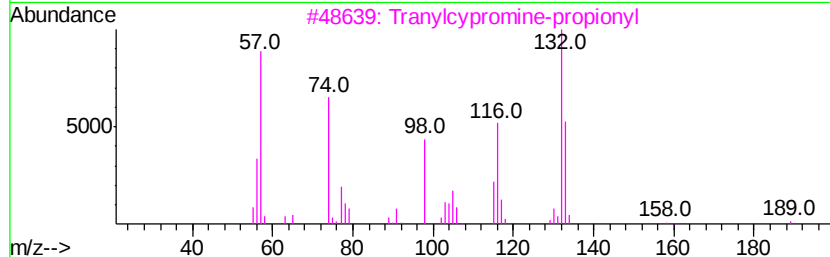
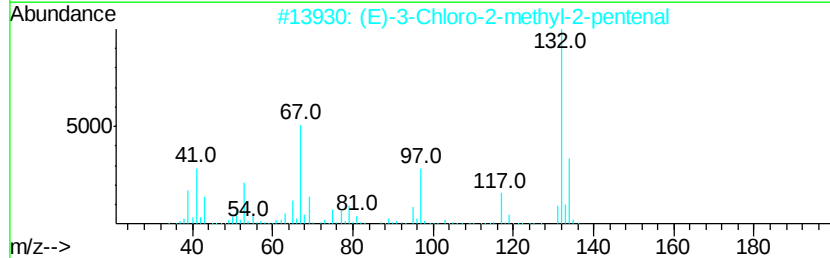
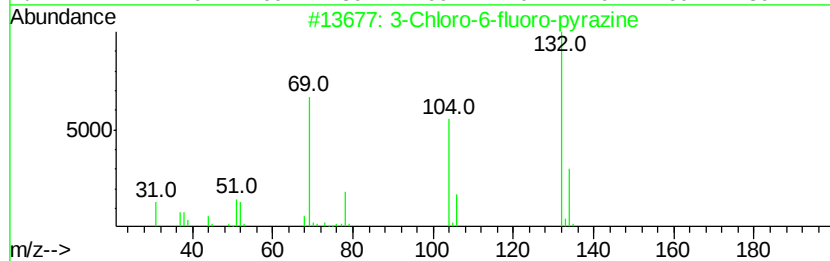
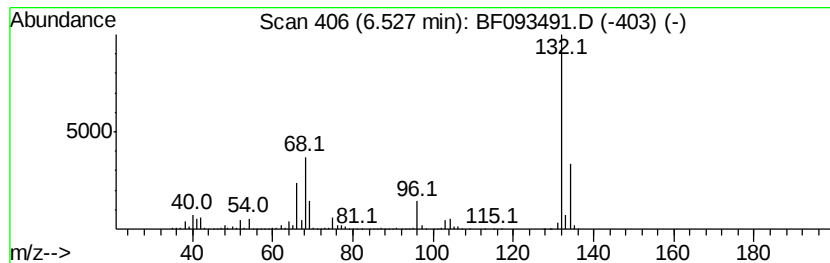
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	101.09 ng	5570830	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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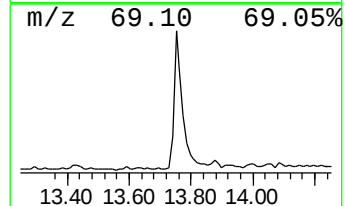
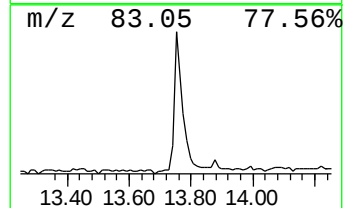
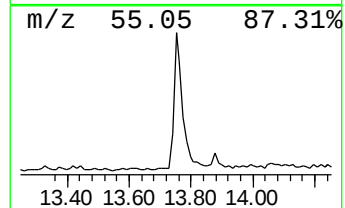
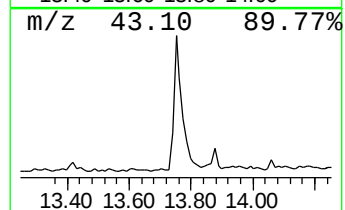
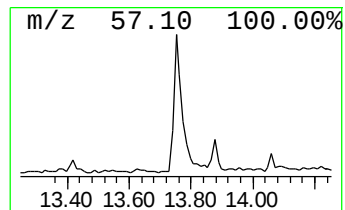
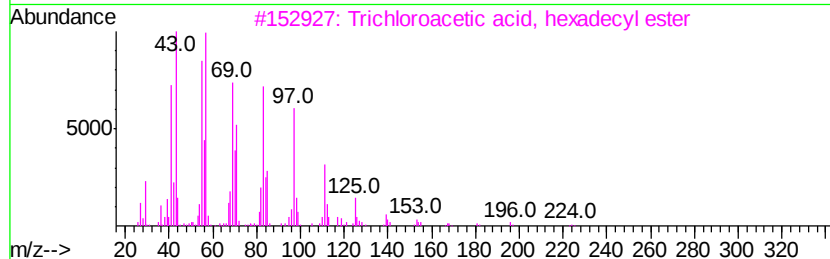
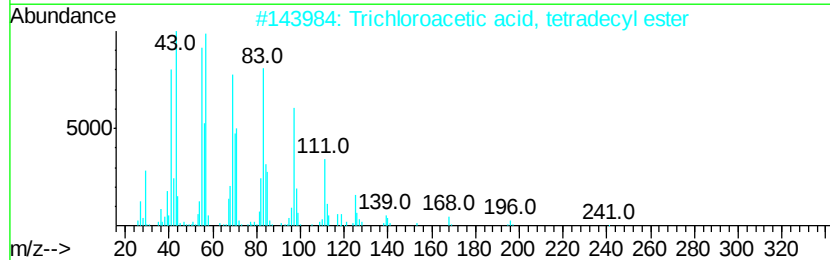
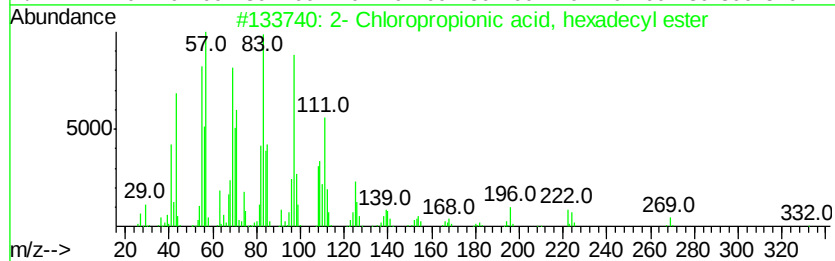
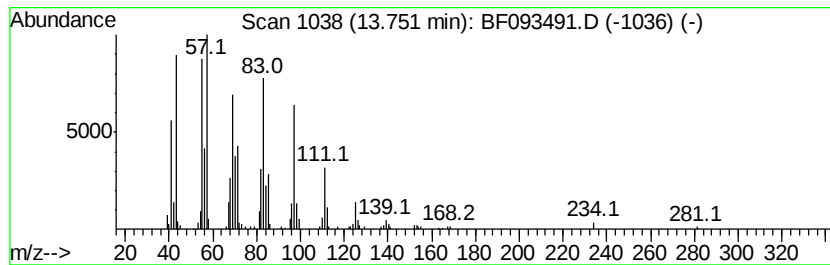
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Peak Number 5 2- Chloropropionic acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	6.56 ng	542591	Chrysene-d12	13.91

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-		Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
2			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4			1-Docosene	308	C22H44	001599-67-3	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.96	2.0	ng	111631	1	6.74	1102150	20.0
2-Pentanone, 4-hy...	4.92	25.4	ng	1399230	1	6.74	1102150	20.0
unknown6.53	6.53	101.1	ng	5570830	1	6.74	1102150	20.0
2- Chloropropioni...	13.75	6.6	ng	542591	5	13.91	1654560	20.0