

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
 Data File : BF090771.D
 Acq On : 22 Oct 2016 19:16
 Operator : UM/SJ
 Sample : H5343-02
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RMAB-SB01-19.5-20.0

Integration Parameters: rteint.p
 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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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	5.057	235	238	246	rBV	730487	1170264	20.68%	2.448%
2	5.469	271	274	277	rBV	3939537	4450978	78.65%	9.310%
3	6.497	361	364	366	rBV	3814183	4611852	81.50%	9.646%
4	6.623	372	375	378	rBV	4267331	4665485	82.44%	9.759%
5	6.852	393	395	400	rBV	1236037	1297390	22.93%	2.714%
6	7.012	406	409	411	rBV	3775762	3912885	69.14%	8.184%
7	7.423	442	445	447	rBV	2271554	3037874	53.68%	6.354%
8	7.526	451	454	461	rVB	80119	195247	3.45%	0.408%
9	8.143	505	508	510	rBV	1252987	1692250	29.90%	3.540%
10	9.218	599	602	604	rBV	5436977	5659017	100.00%	11.837%
11	9.618	633	637	639	rBV	1314404	1837129	32.46%	3.843%
12	9.892	658	661	664	rBV	2227668	2101275	37.13%	4.395%
13	10.326	698	699	701	rVB	88372	66320	1.17%	0.139%
14	10.543	715	718	722	rBV	36453	66144	1.17%	0.138%
15	10.681	727	730	733	rBV	3018574	3538511	62.53%	7.401%
16	10.795	739	740	747	rVB	101214	174196	3.08%	0.364%
17	11.252	777	780	781	rBV	56341	79173	1.40%	0.166%
18	11.378	788	791	793	rBV	2037801	1872904	33.10%	3.917%
19	12.967	927	930	932	rBV	5275651	5068652	89.57%	10.602%
20	13.858	1006	1008	1014	rBV	116033	160201	2.83%	0.335%
21	14.018	1019	1022	1024	rBV	926150	1169755	20.67%	2.447%
22	15.447	1144	1147	1160	rBV	734704	981589	17.35%	2.053%

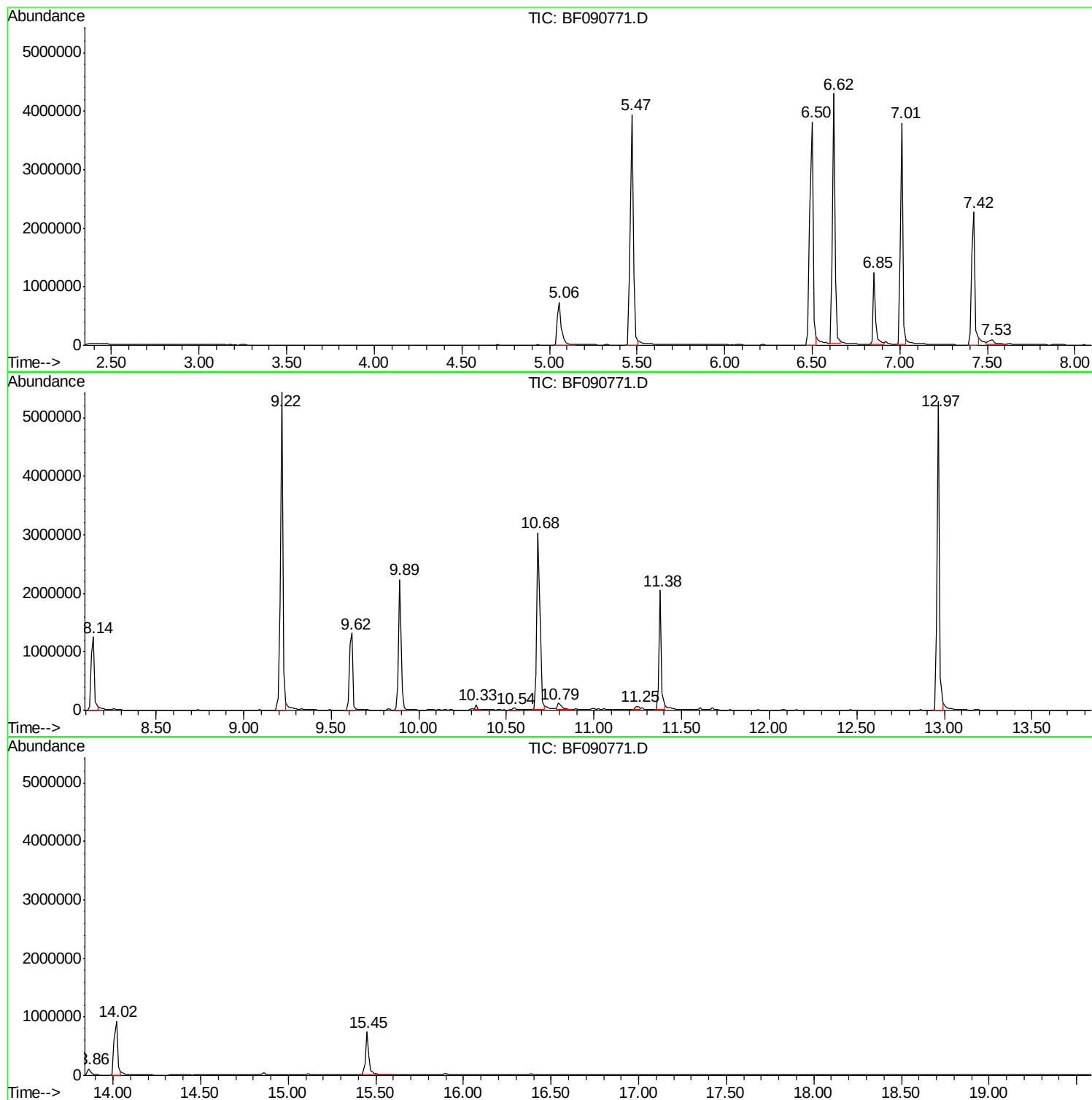
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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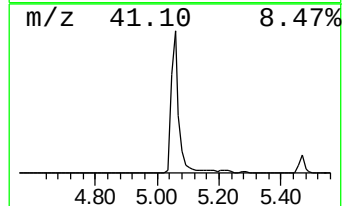
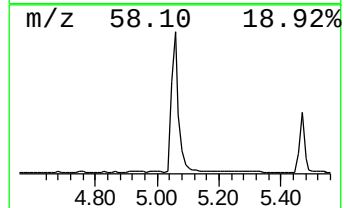
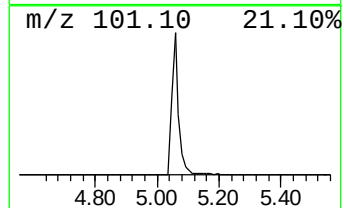
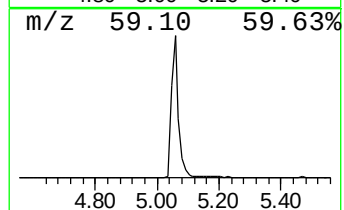
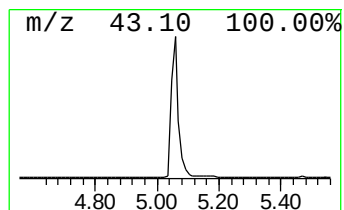
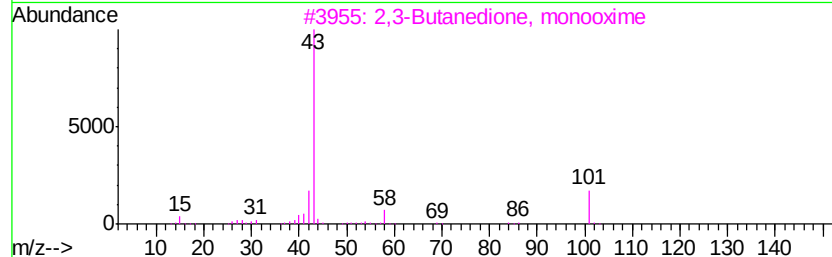
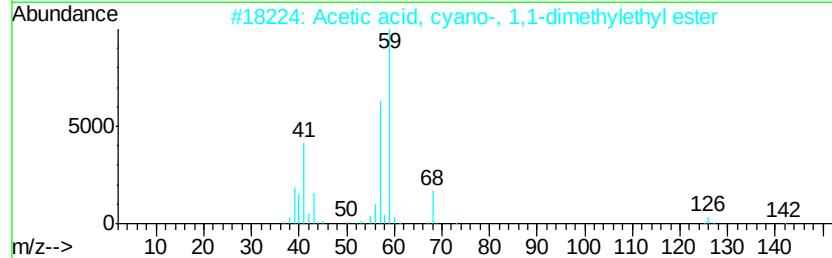
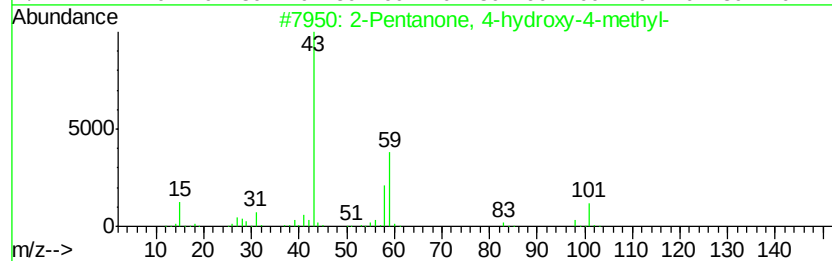
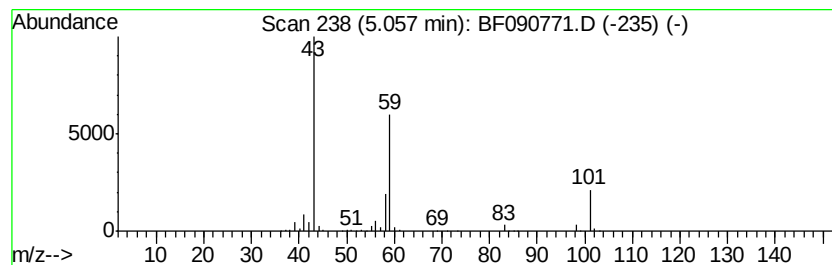
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	18.04 ng	1170260	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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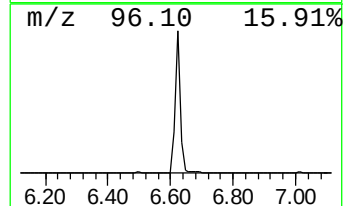
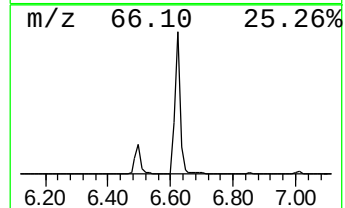
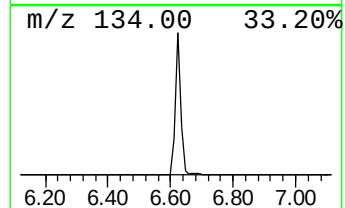
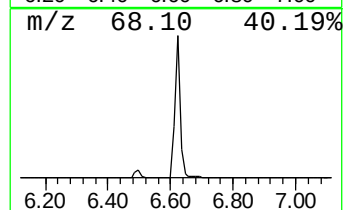
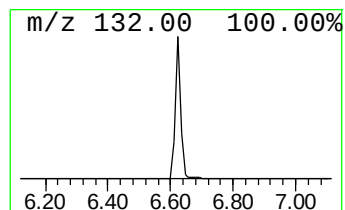
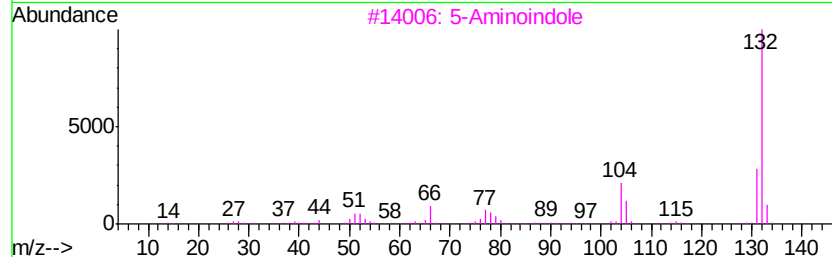
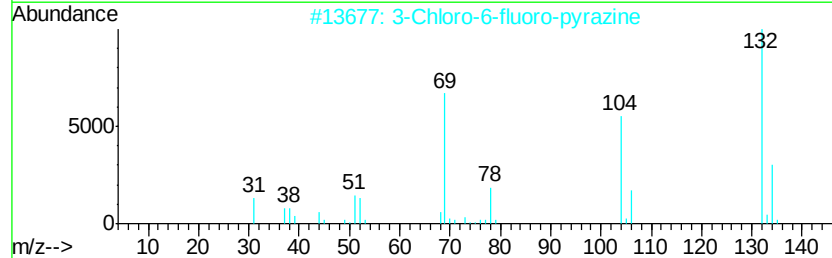
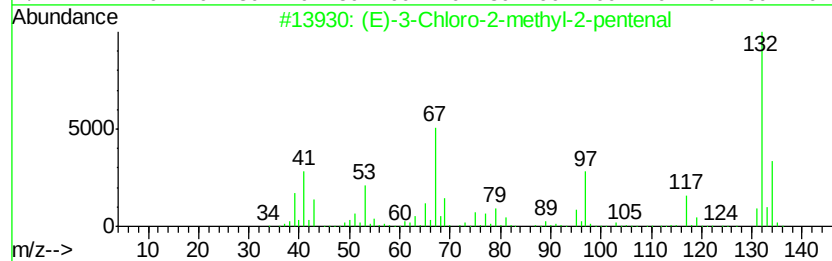
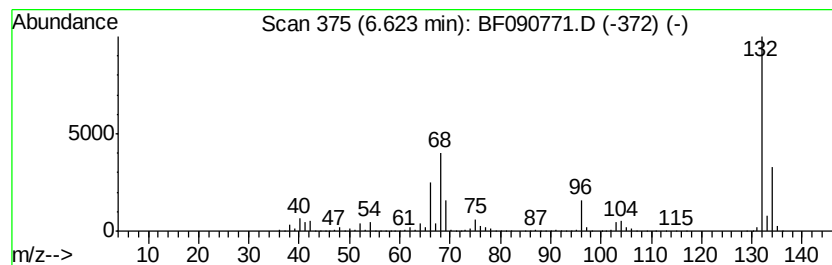
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Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	71.92 ng	4665490	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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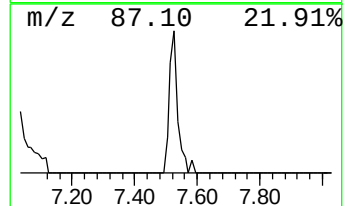
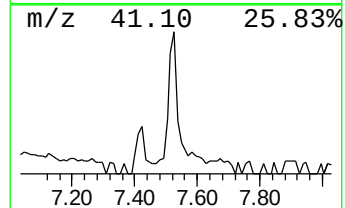
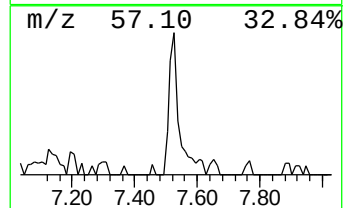
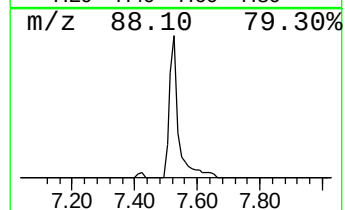
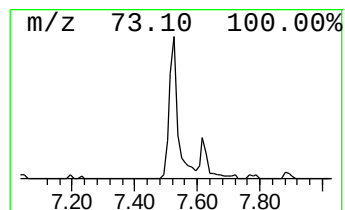
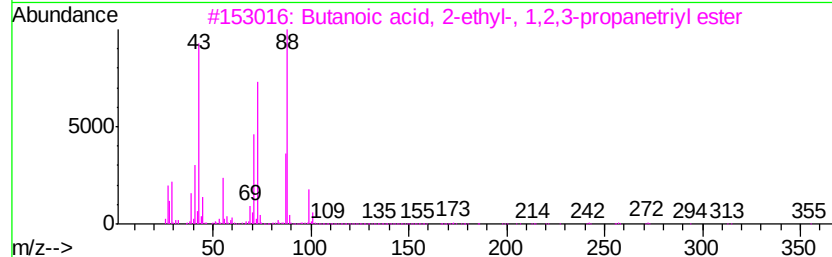
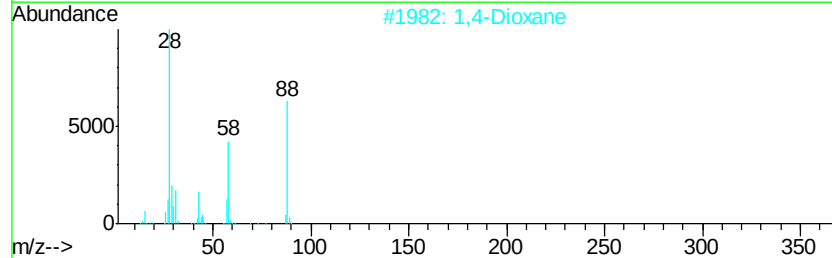
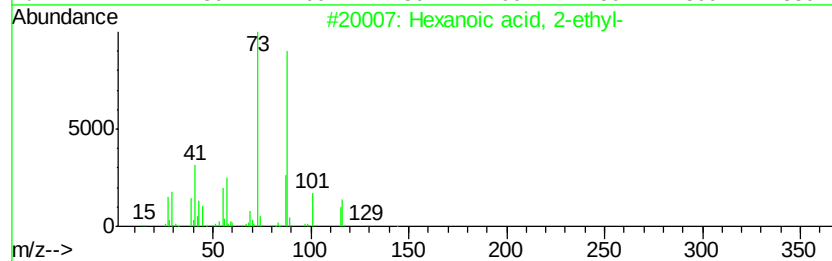
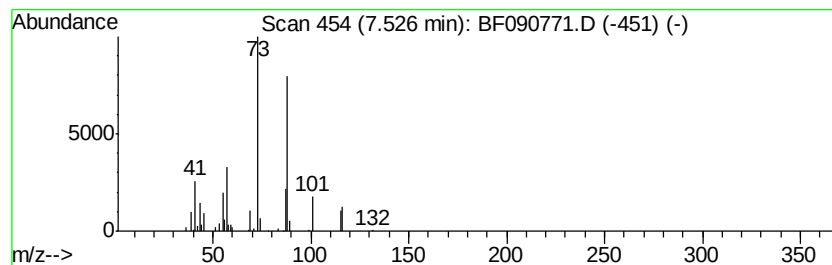
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Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	2.31 ng	195247	Naphthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		1,4-Dioxane	88	C4H8O2	000123-91-1	43
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	40
4		Acetic acid, diethyl-	116	C6H12O2	000088-09-5	33
5		Methyl 4-O-acetyl-2,3-di-O-methy...	248	C11H20O6	072945-56-3	28



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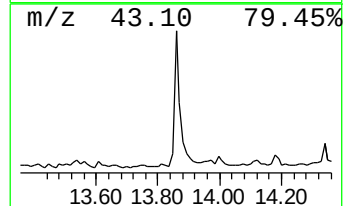
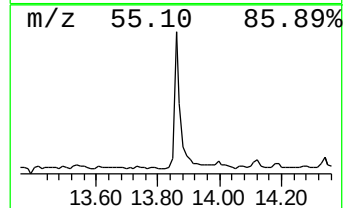
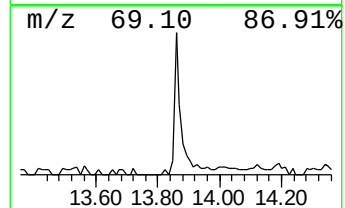
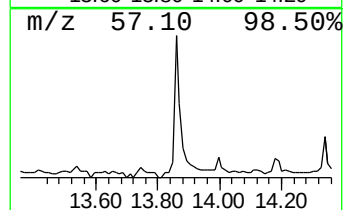
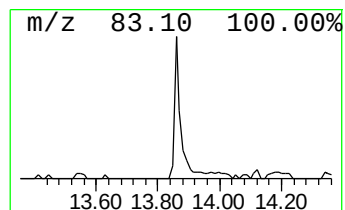
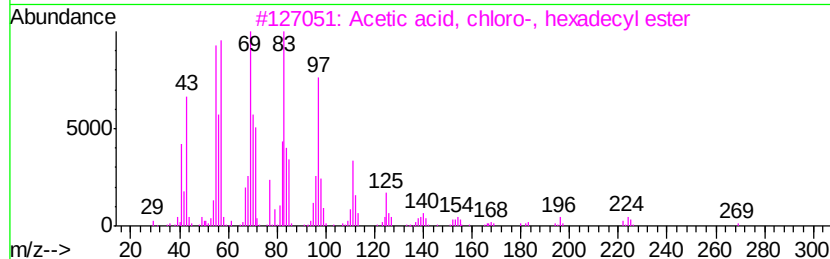
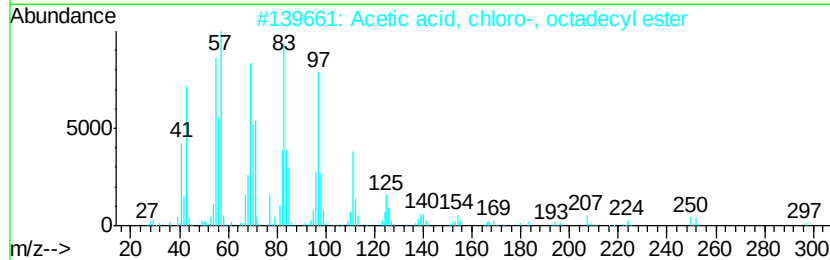
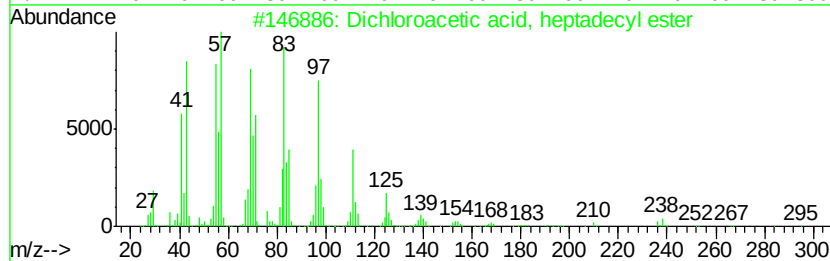
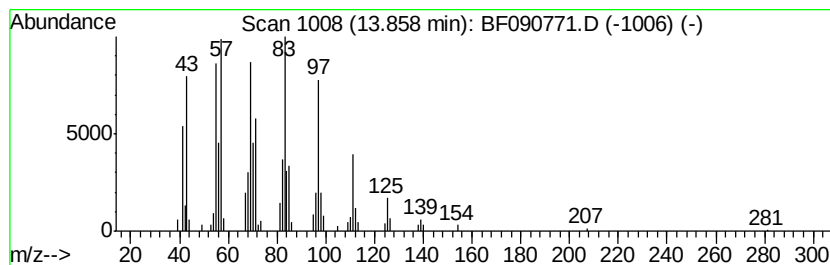
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.74 ng	160201	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	94
3		Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	93
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	18.0	ng	1170260	1	6.85	1297390	20.0
unknown6.62	6.62	71.9	ng	4665490	1	6.85	1297390	20.0
Hexanoic acid, 2-...	7.53	2.3	ng	195247	2	8.14	1692250	20.0
Dichloroacetic ac...	13.86	2.7	ng	160201	5	14.02	1169760	20.0