

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101215\
 Data File : BF082220.D
 Acq On : 12 Oct 2015 15:01
 Operator : UM/IZ
 Sample : PB86065BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB86065BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 1 % 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-BF101015.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	5.006	248	251	259	rBV	196328	252730	8.99%	1.444%
2	5.429	285	288	290	rBV	1132048	1243685	44.25%	7.105%
3	6.469	376	379	381	rBV	1022240	1251750	44.54%	7.151%
4	6.594	388	390	393	rBV	1361670	1265002	45.01%	7.227%
5	6.834	408	411	413	rBV	424002	449038	15.98%	2.565%
6	6.983	422	424	427	rBV	1379986	1449636	51.58%	8.282%
7	7.406	458	461	463	rBV	771828	1113651	39.62%	6.362%
8	8.114	521	523	526	rBV	573714	610667	21.73%	3.489%
9	9.200	615	618	620	rBV	2426303	2442647	86.91%	13.955%
10	9.875	675	677	680	rBV	850997	777322	27.66%	4.441%
11	10.663	744	746	749	rBV	1025376	995245	35.41%	5.686%
12	11.361	805	807	810	rBV	903487	807038	28.71%	4.611%
13	12.766	928	930	933	rVB	240080	203032	7.22%	1.160%
14	12.846	933	937	939	rVB	29699	37597	1.34%	0.215%
15	12.949	943	946	949	rBV	2134140	2810575	100.00%	16.057%
16	13.475	990	992	994	rBV	165200	141478	5.03%	0.808%
17	14.001	1036	1038	1041	rBV	840261	844813	30.06%	4.826%
18	14.161	1050	1052	1055	rVB	33610	30552	1.09%	0.175%
19	14.767	1102	1105	1108	rBV	26716	28783	1.02%	0.164%
20	15.441	1161	1164	1173	rBV	516866	720427	25.63%	4.116%
21	16.344	1239	1243	1246	rBV2	14518	28489	1.01%	0.163%

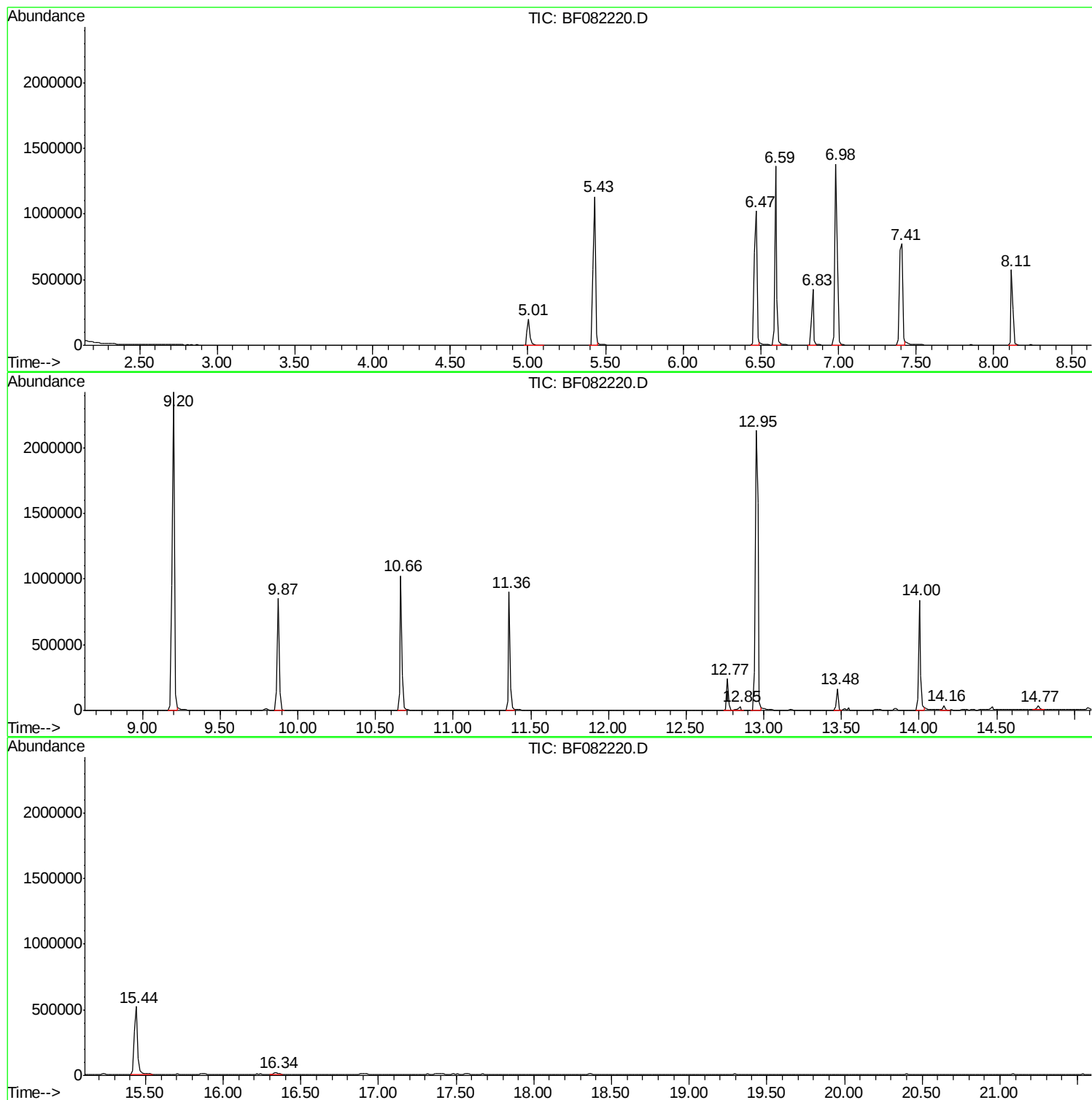
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : UM/IZ
Sample : PB86065BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
PB86065BL

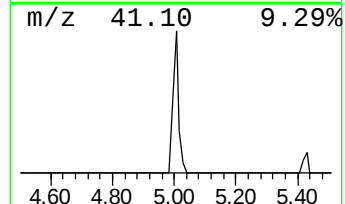
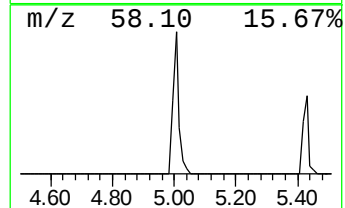
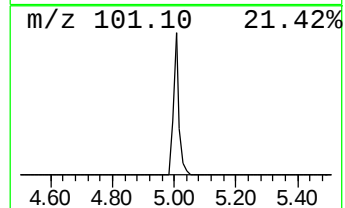
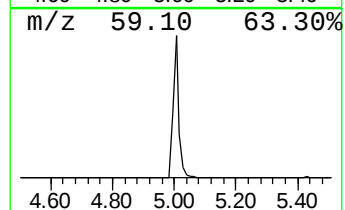
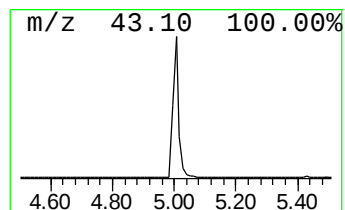
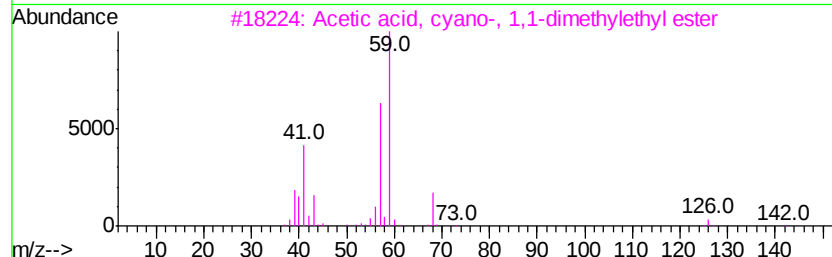
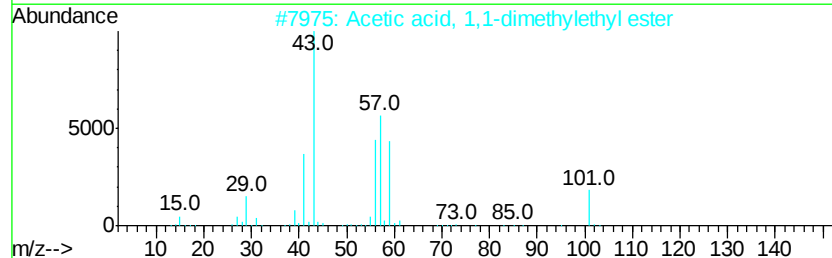
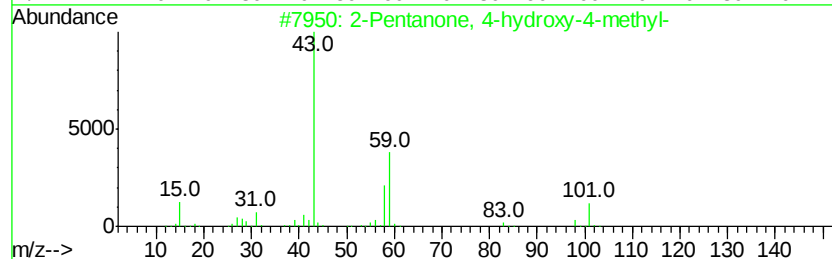
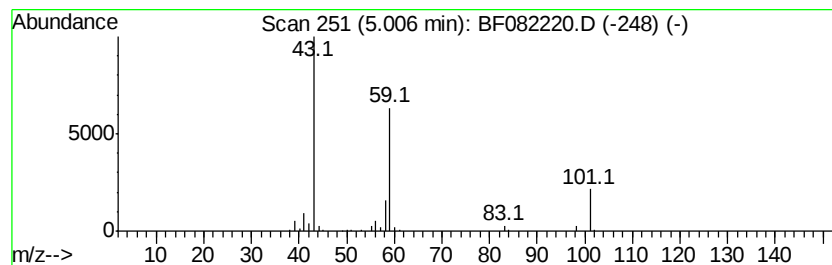
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.01	11.26 ng	252730	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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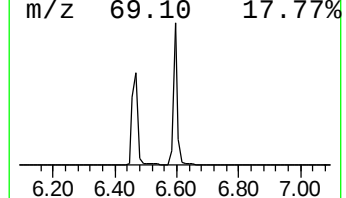
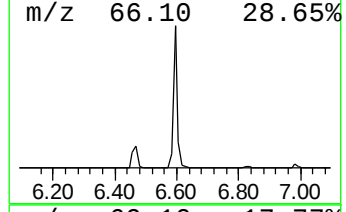
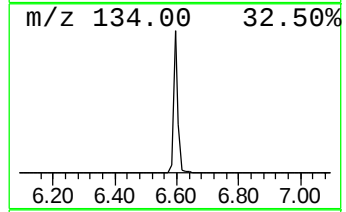
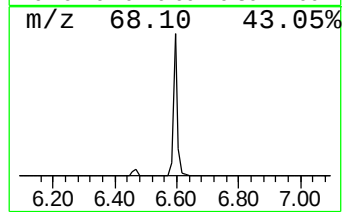
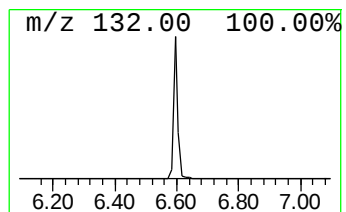
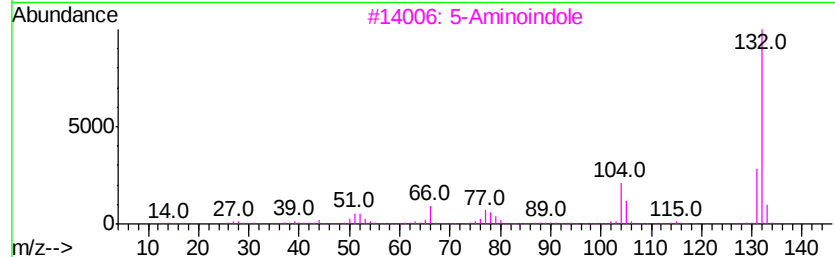
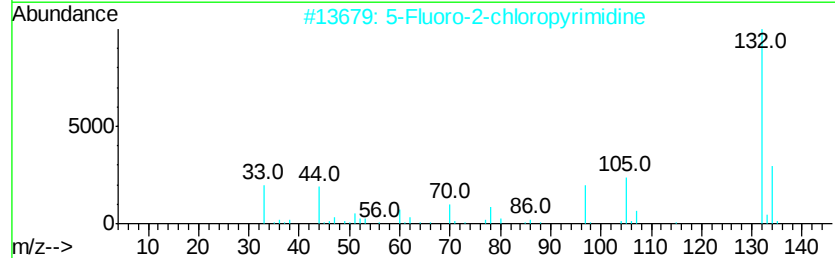
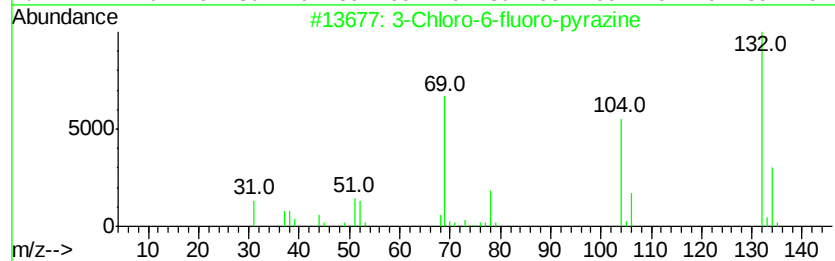
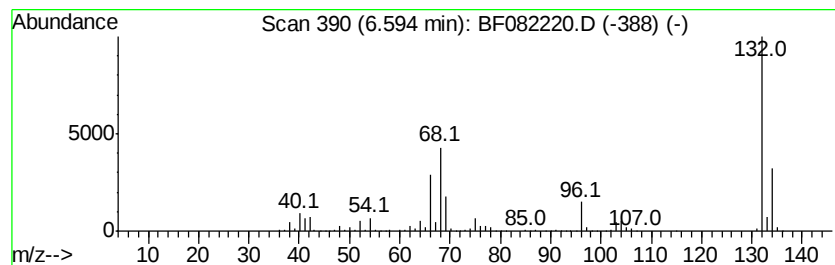
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	56.34 ng	1265000	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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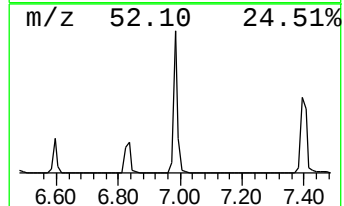
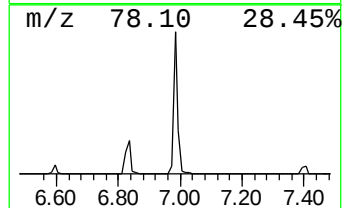
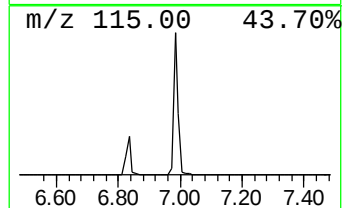
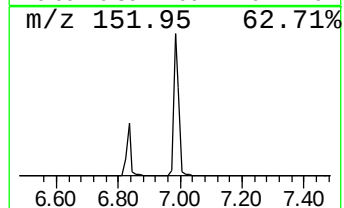
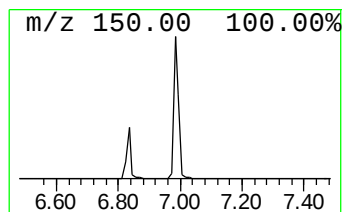
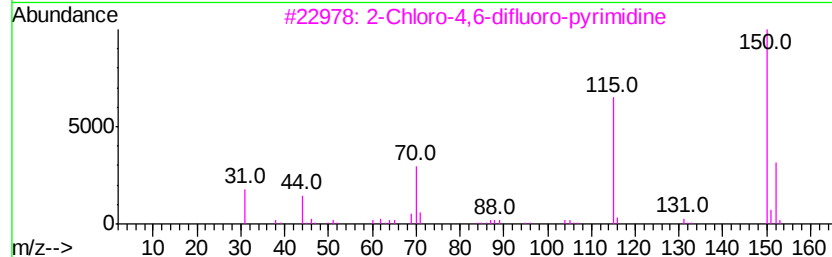
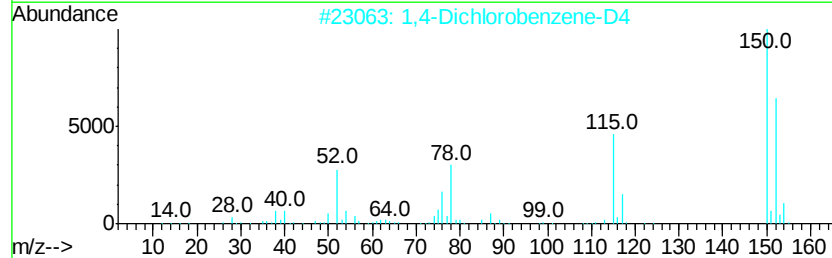
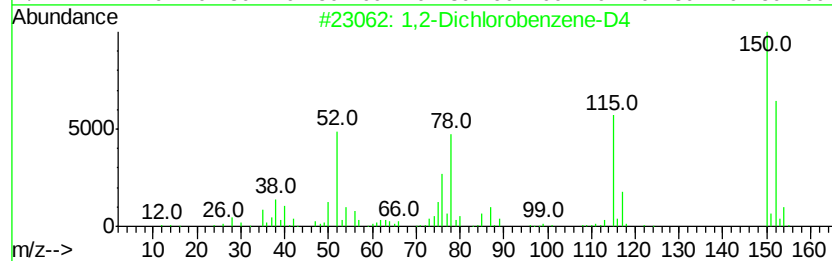
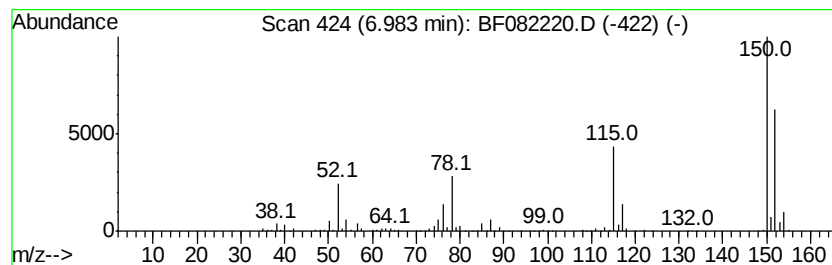
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,2-Dichlorobenzene-D4 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	64.57 ng	1449640	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
2		1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
3		2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	35
4		2-Cyclohexene-1,4-dione, 5,6-dic...	370	C15H12Cl2N2O5	324051-56-1	10
5		3-(4-Nitrobenzoyl)-2-thioxo-4-th...	431	C17H9N3O7S2	329218-74-8	10



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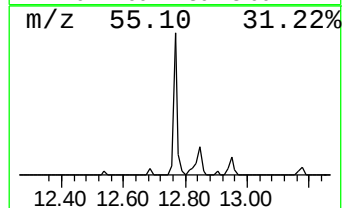
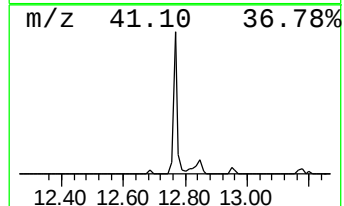
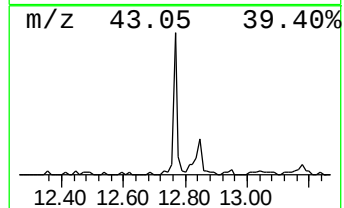
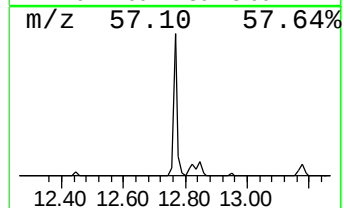
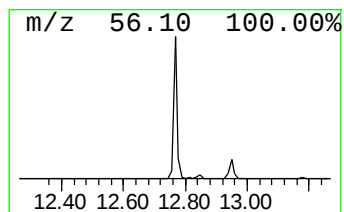
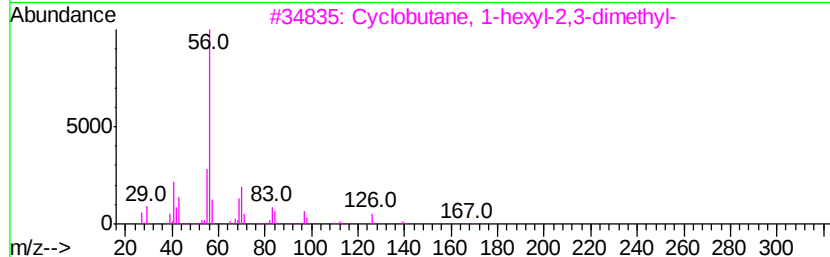
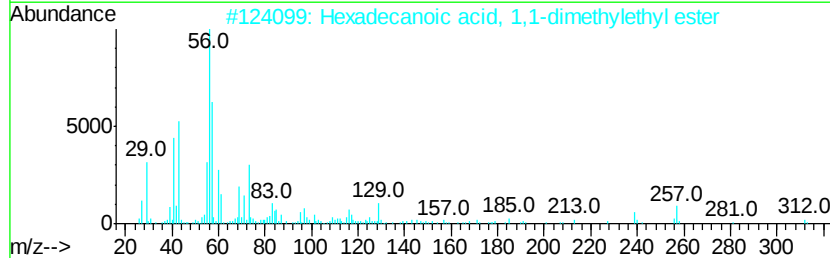
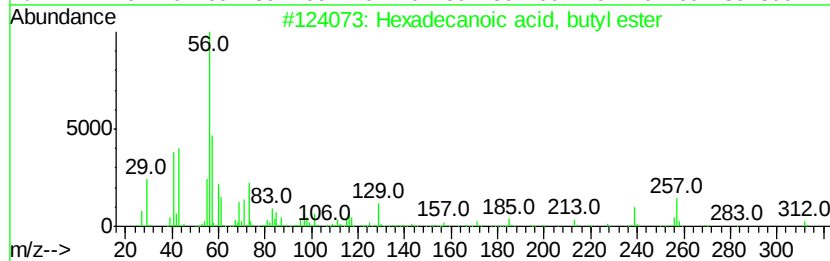
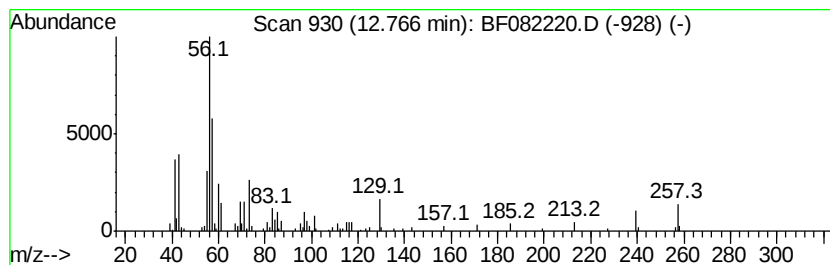
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	4.81 ng	203032	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
4		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
5		1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37



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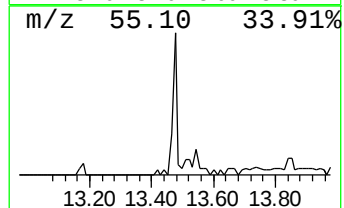
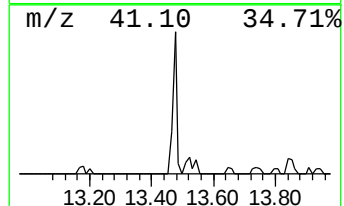
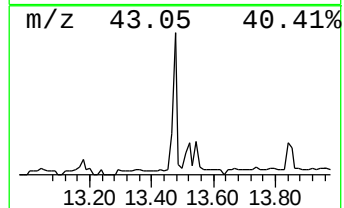
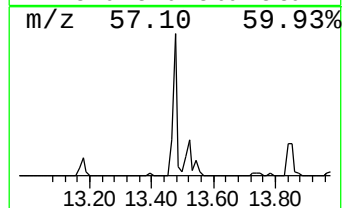
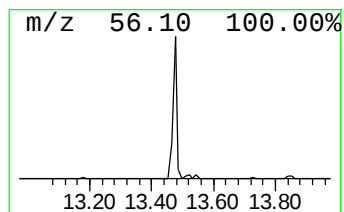
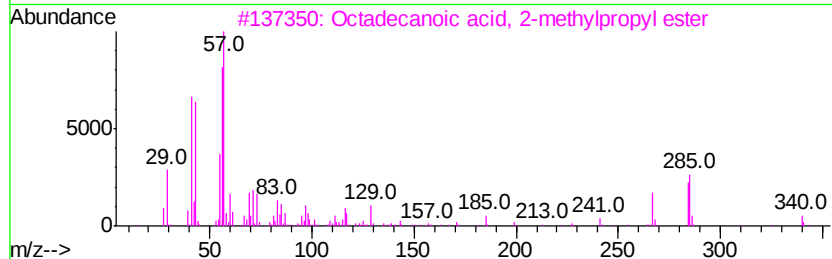
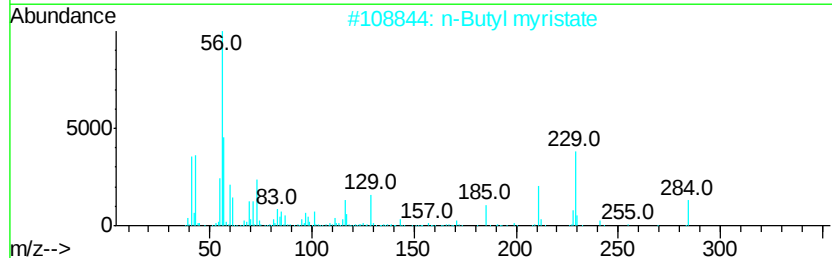
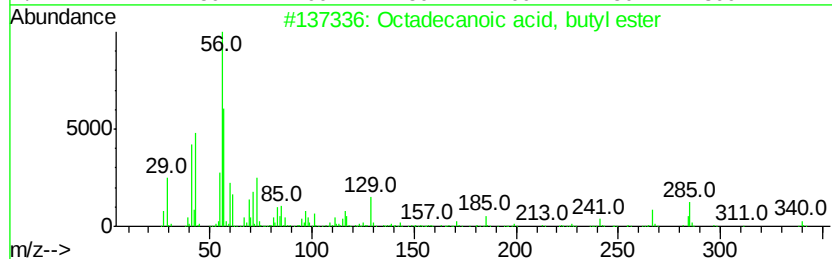
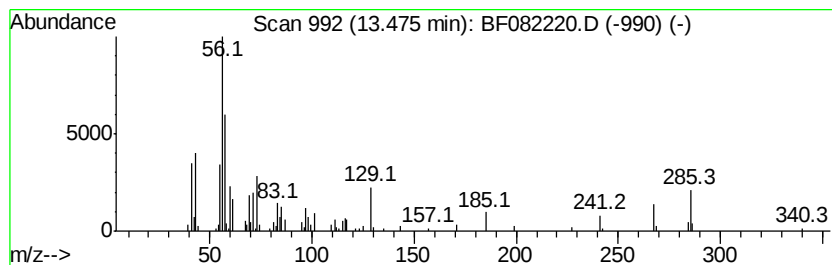
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.48	3.35 ng	141478	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	59
3		Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	38
4		Nipecotic acid	129	C6H11NO2	000498-95-3	38
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	11.3	ng	252730	1	6.83	449038	20.0
3-Chloro-6-fluoro...	6.59	56.3	ng	1265000	1	6.83	449038	20.0
1,2-Dichlorobenze...	6.98	64.6	ng	1449640	1	6.83	449038	20.0
Hexadecanoic acid...	12.77	4.8	ng	203032	5	14.00	844813	20.0
Octadecanoic acid...	13.48	3.3	ng	141478	5	14.00	844813	20.0