

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
 Data File : BF081068.D
 Acq On : 19 Aug 2015 5:53
 Operator : UM/IZ
 Sample : G3289-11
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3(0-2)-1

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-BF081715.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	3.987	171	175	181	rBV	11356	17585	1.06%	0.102%
2	4.730	237	240	250	rVB	697571	1082603	65.06%	6.262%
3	5.176	276	279	282	rBV	1405002	1536924	92.37%	8.890%
4	6.250	370	373	375	rBV	1612356	1588213	95.45%	9.187%
5	6.364	381	383	386	rBV	1212829	1632888	98.14%	9.445%
6	6.604	402	404	406	rBV	470205	386188	23.21%	2.234%
7	6.765	415	418	420	rBV	974108	1128335	67.81%	6.527%
8	7.176	451	454	456	rBV	1184917	1196849	71.93%	6.923%
9	7.885	514	516	519	rBV	410561	472867	28.42%	2.735%
10	8.970	608	611	613	rBV	1830126	1663898	100.00%	9.624%
11	9.370	643	646	648	rBV	300762	341353	20.52%	1.974%
12	9.633	667	669	671	rBV	664809	561524	33.75%	3.248%
13	10.091	704	709	710	rVB	16052	30074	1.81%	0.174%
14	10.411	735	737	740	rVB2	721335	1007665	60.56%	5.829%
15	10.559	748	750	753	rBV	36771	50717	3.05%	0.293%
16	11.005	786	789	790	rBV	28506	37502	2.25%	0.217%
17	11.108	795	798	800	rBV	588165	608176	36.55%	3.518%
18	11.428	823	826	828	rBV	23849	24094	1.45%	0.139%
19	11.656	844	846	850	rBV	45711	57176	3.44%	0.331%
20	12.537	920	923	924	rBV	65523	79367	4.77%	0.459%
21	12.605	924	929	931	rVB2	27007	35166	2.11%	0.203%
22	12.685	934	936	939	rBV	1178901	1629422	97.93%	9.425%
23	12.937	956	958	966	rVB2	17738	27848	1.67%	0.161%
24	13.234	982	984	987	rBV	76911	74093	4.45%	0.429%
25	13.279	987	988	989	rBV	28764	20864	1.25%	0.121%
26	13.611	1014	1017	1024	rBV	217487	480678	28.89%	2.780%
27	13.725	1024	1027	1029	rVB	562381	629458	37.83%	3.641%
28	13.919	1042	1044	1046	rBV	35968	32824	1.97%	0.190%
29	14.228	1068	1071	1072	rBV	28139	31953	1.92%	0.185%
30	14.262	1072	1074	1080	rVV2	12274	29866	1.79%	0.173%
31	14.514	1095	1096	1098	rVB	31087	28113	1.69%	0.163%
32	14.811	1119	1122	1124	rBV	22135	29699	1.78%	0.172%
33	14.868	1124	1127	1133	rBV2	11303	22380	1.35%	0.129%
34	15.062	1141	1144	1147	rBV	386408	471564	28.34%	2.728%

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COFF-3(0-2)-1

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-BF081715.M
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35	15.120	1147	1149	1153	rVB	16258	25644	1.54%	0.148%
36	15.485	1178	1181	1185	rBV	17435	29934	1.80%	0.173%
37	15.577	1185	1189	1202	rVB2	34820	138885	8.35%	0.803%
38	16.537	1266	1273	1279	rBV5	11206	46038	2.77%	0.266%

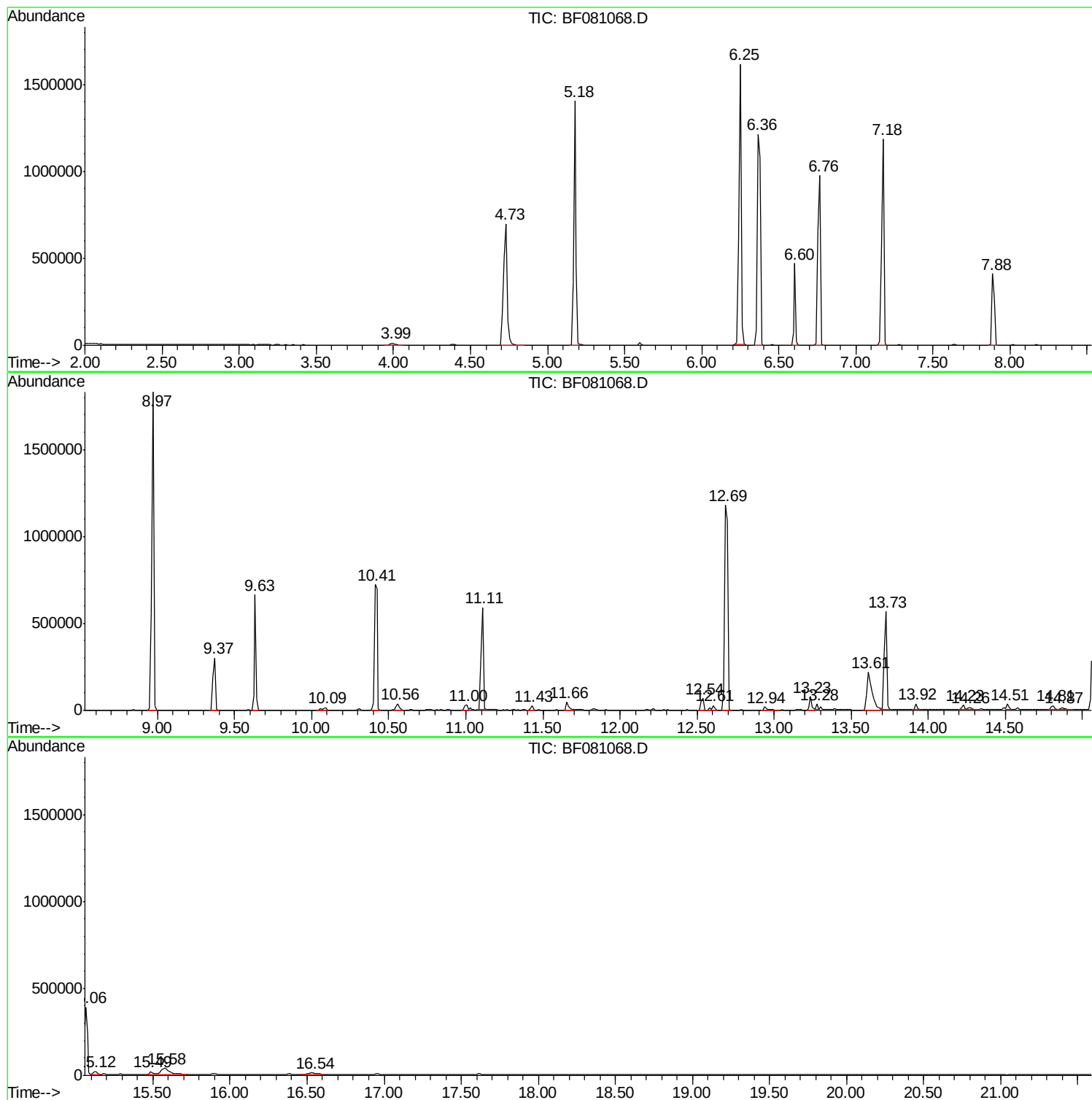
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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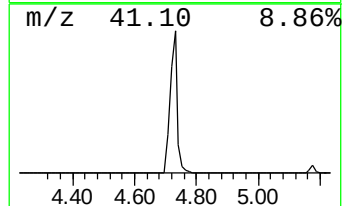
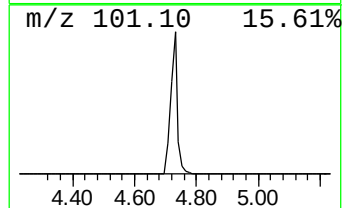
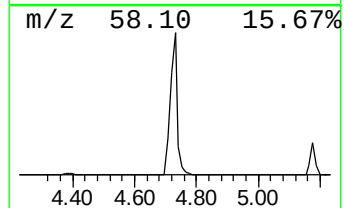
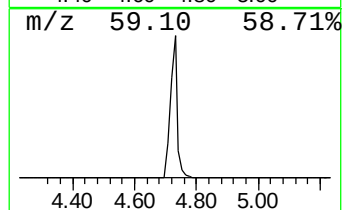
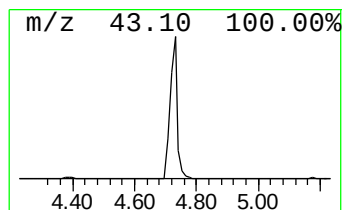
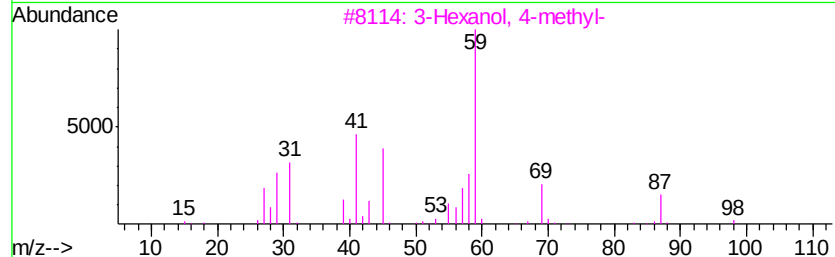
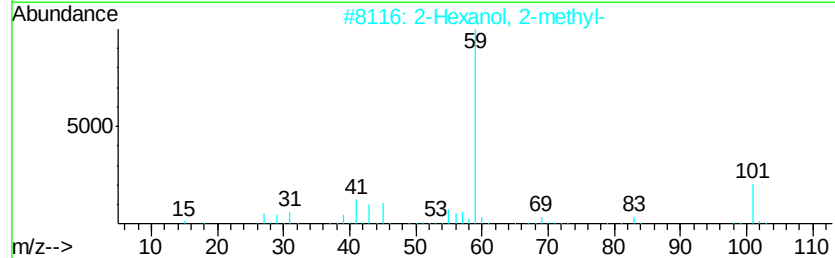
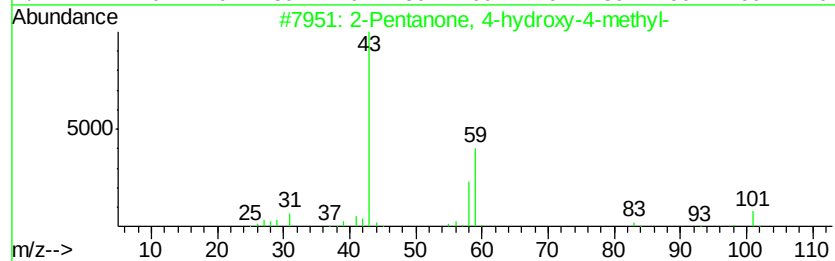
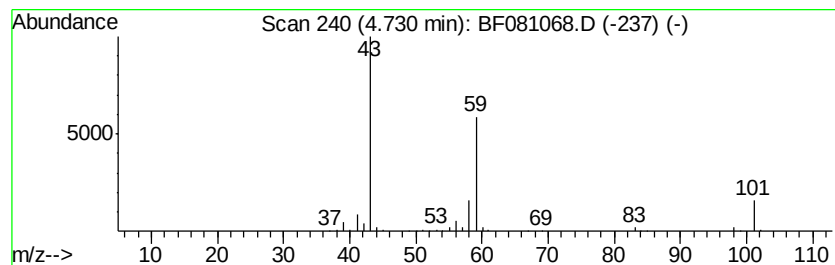
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.73	56.07 ng	1082600	1,4-Dichlorobenzene-d4	6.60

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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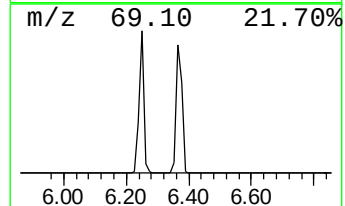
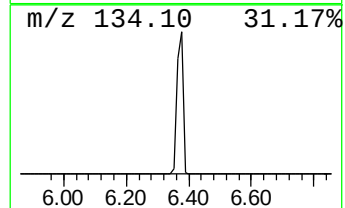
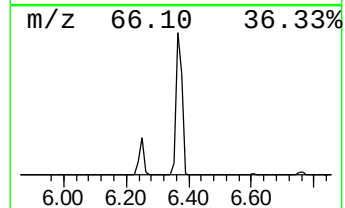
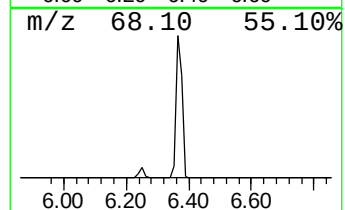
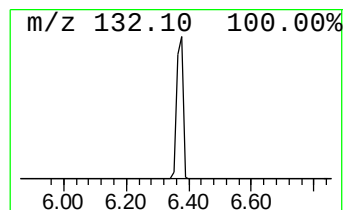
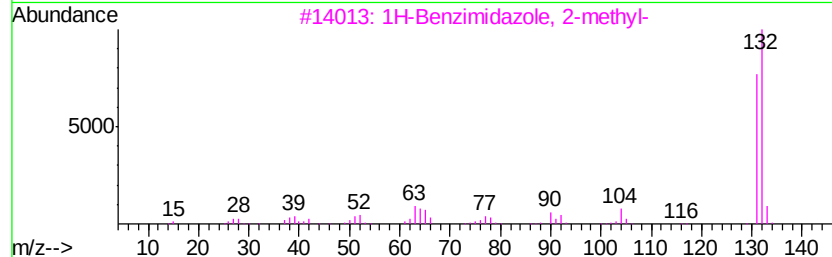
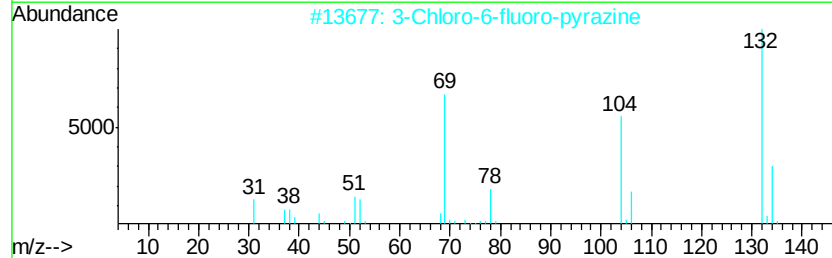
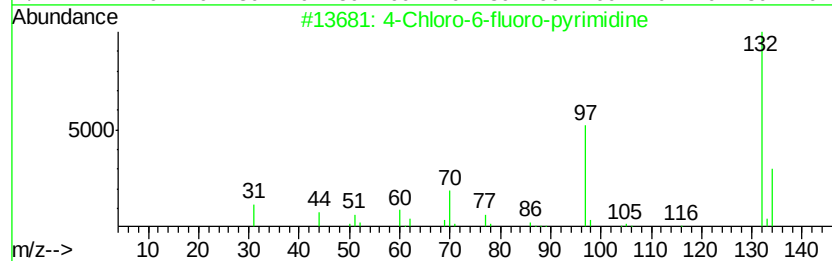
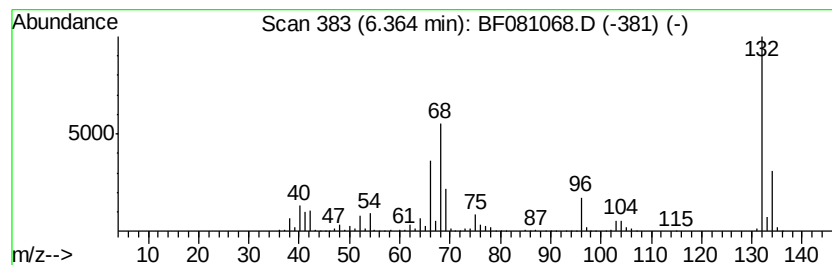
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	84.56 ng	1632890	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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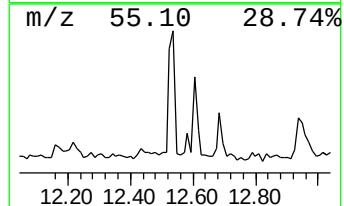
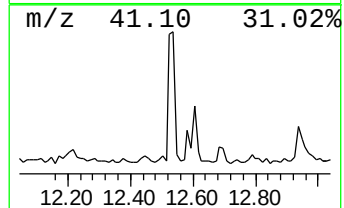
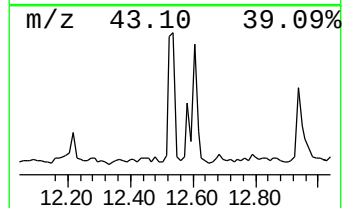
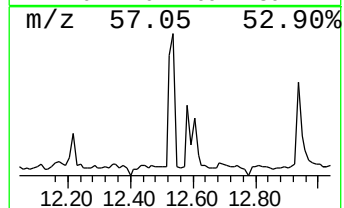
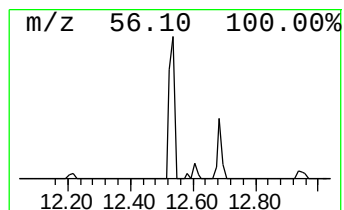
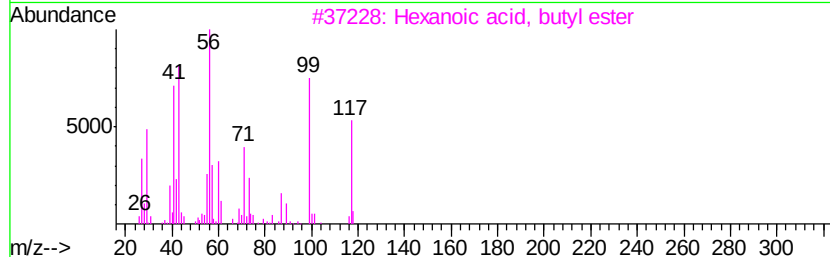
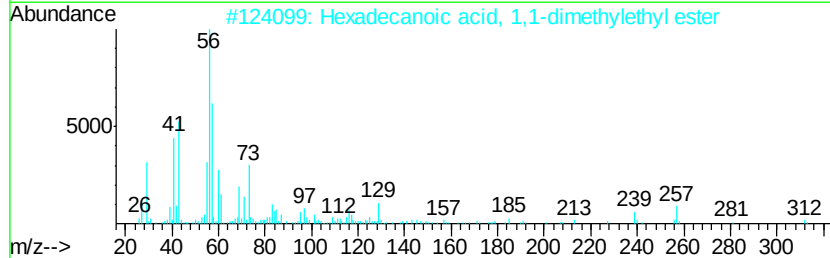
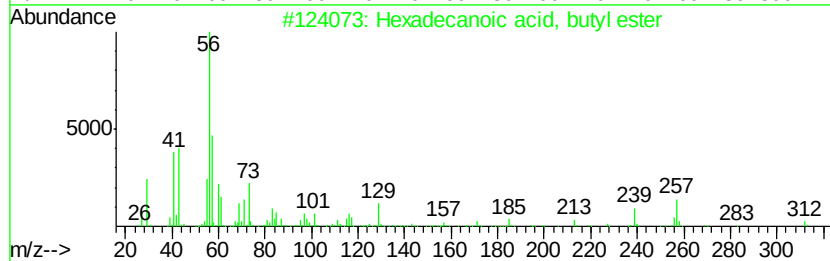
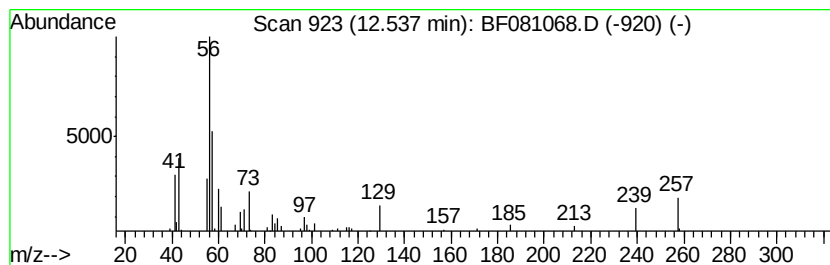
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.52 ng	79367	Chrysene-d12	13.73

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		Hexanoic acid, butyl ester	172	C10H20O2	000626-82-4	40
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38



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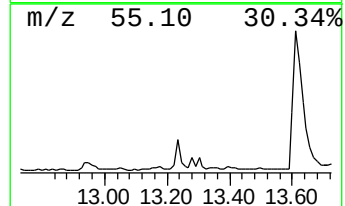
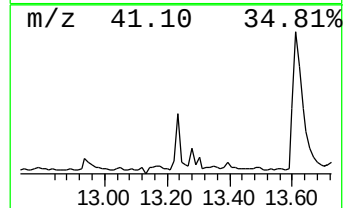
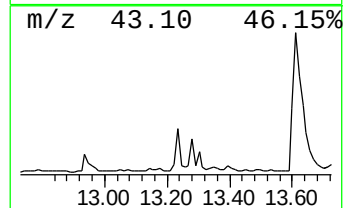
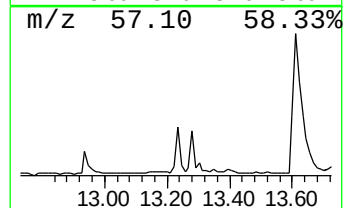
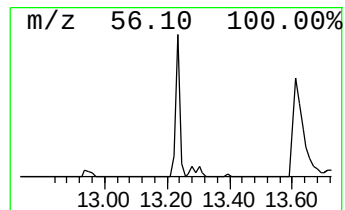
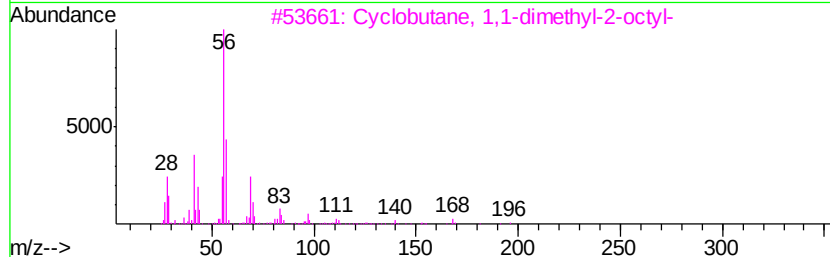
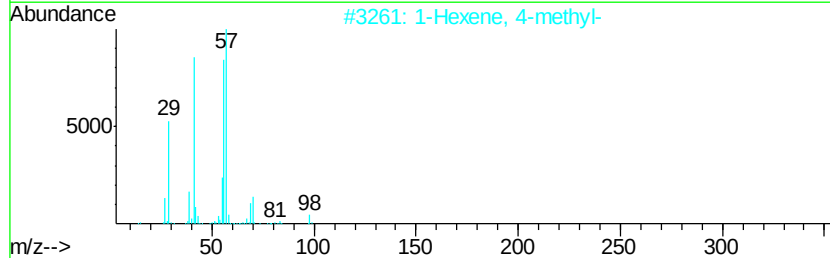
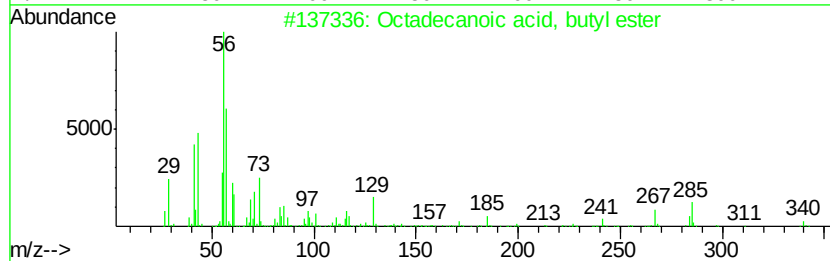
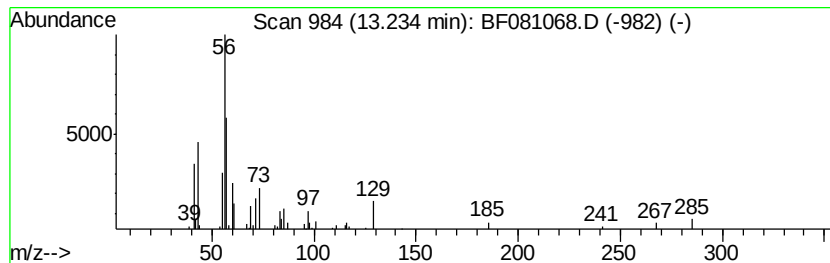
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.23 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	2.35 ng	74093	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
2		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	37
4		2-Methyl-1-octadecene	266	C19H38	061868-20-0	37
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



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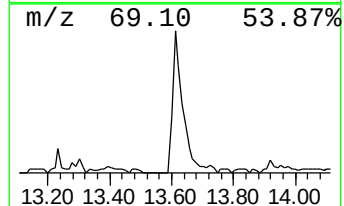
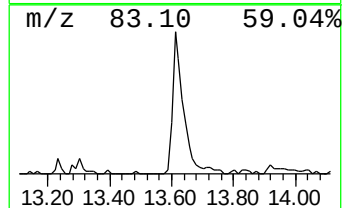
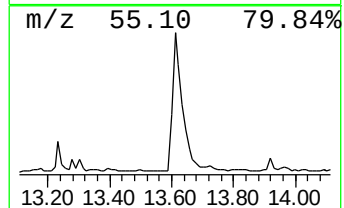
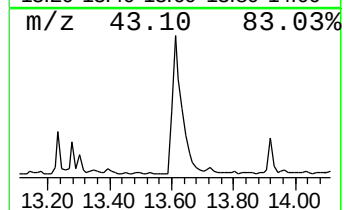
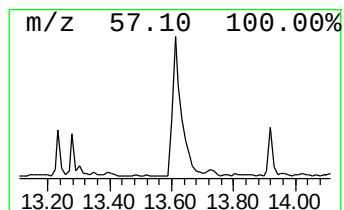
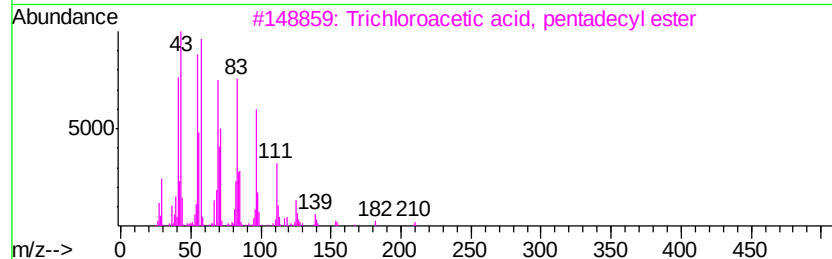
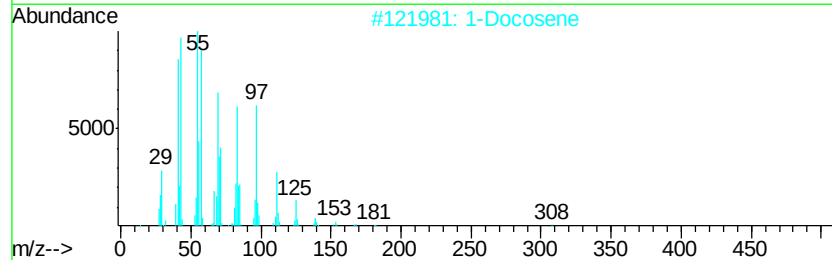
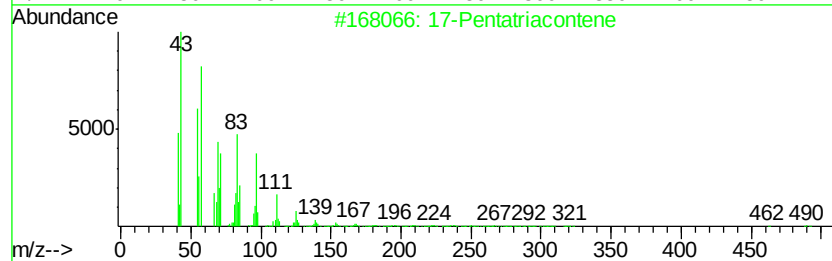
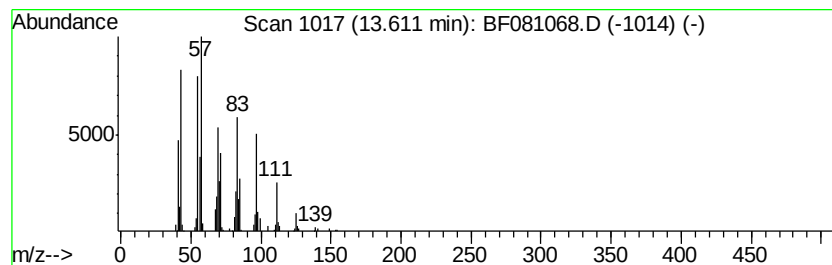
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Peak Number 6 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	15.27 ng	480678	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		1-Docosene	308	C22H44	001599-67-3	87
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	74
4		5-Eicosene, (E)-	280	C20H40	074685-30-6	74
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	68



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Operator : UM/IZ
Sample : G3289-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

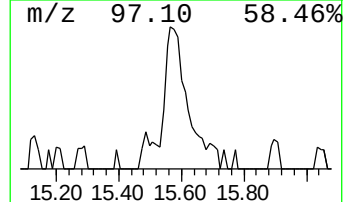
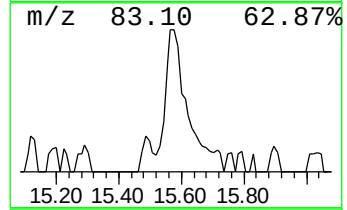
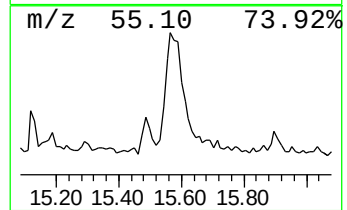
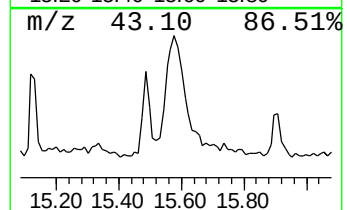
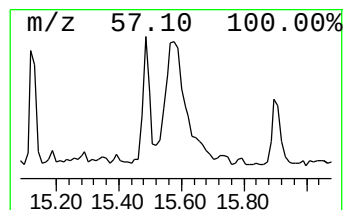
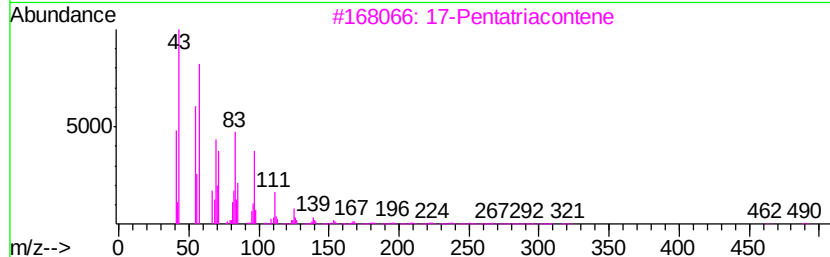
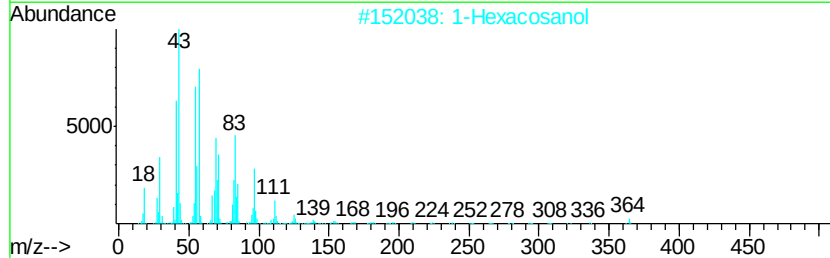
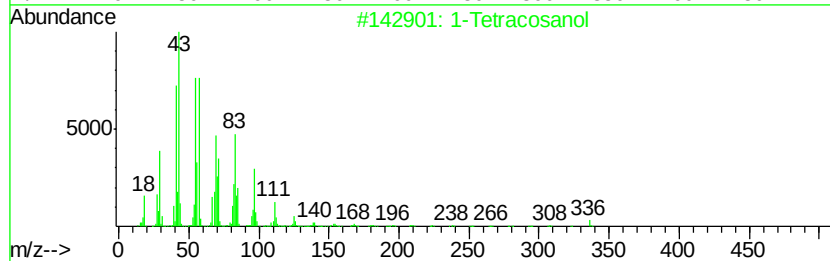
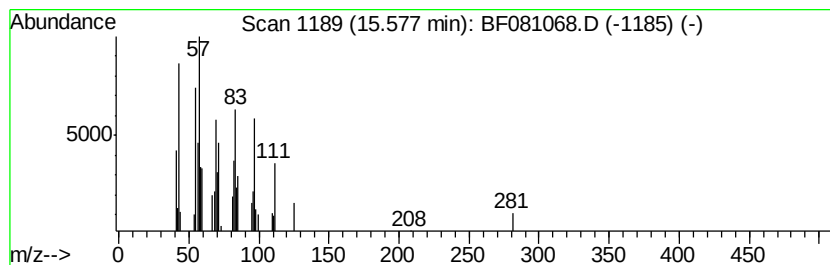
Instrument :
BNA_F
ClientSampleId :
COFF-3(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Tetracosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	5.89 ng	138885	Perylene-d12	15.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Tetracosanol	354 C24H50O	000506-51-4	87
2	1-Hexacosanol	382 C26H54O	000506-52-5	87
3	17-Pentatriacontene	491 C35H70	006971-40-0	81
4	1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1	68
5	Bromoacetic acid, pentadecyl ester	348 C17H33BrO2	131143-01-6	68



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081068.D
Acq On : 19 Aug 2015 5:53
Operator : UM/IZ
Sample : G3289-11
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3(0-2)-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	56.1	ng	1082600	1	6.60	386188	20.0
unknown6.36	6.36	84.6	ng	1632890	1	6.60	386188	20.0
Hexadecanoic acid...	12.54	2.5	ng	79367	5	13.73	629458	20.0
unknown13.23	13.23	2.4	ng	74093	5	13.73	629458	20.0
17-Pentatriacontene	13.61	15.3	ng	480678	5	13.73	629458	20.0
1-Tetracosanol	15.58	5.9	ng	138885	6	15.06	471564	20.0