

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
 Data File : BF081064.D
 Acq On : 19 Aug 2015 3:47
 Operator : UM/IZ
 Sample : G3290-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3(0-2)-6

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	4.730	237	240	251	rBV	734164	1188363	60.56%	6.321%
2	5.176	276	279	282	rBV	1322791	1879892	95.80%	10.000%
3	6.250	370	373	376	rBV	1524602	1744567	88.90%	9.280%
4	6.376	381	384	386	rBV	1589572	1962307	100.00%	10.438%
5	6.604	402	404	406	rBV	460781	379164	19.32%	2.017%
6	6.764	415	418	420	rBV	1213683	1283904	65.43%	6.830%
7	7.176	451	454	456	rBV	1280925	1268659	64.65%	6.748%
8	7.884	514	516	519	rBV	365547	465583	23.73%	2.477%
9	8.970	608	611	613	rBV	1947759	1751465	89.26%	9.317%
10	9.370	643	646	648	rVB	339278	363316	18.51%	1.933%
11	9.633	666	669	672	rVB	661566	574314	29.27%	3.055%
12	10.090	703	709	710	rBB	9569	22524	1.15%	0.120%
13	10.422	735	738	740	rBV	871610	1127068	57.44%	5.995%
14	10.559	748	750	753	rBV	24554	37287	1.90%	0.198%
15	11.005	786	789	790	rBV	25467	29746	1.52%	0.158%
16	11.108	795	798	800	rBV	634280	641266	32.68%	3.411%
17	11.656	844	846	848	rBV	25437	25105	1.28%	0.134%
18	12.536	921	923	925	rBV	160922	167806	8.55%	0.893%
19	12.605	925	929	932	rVB2	40307	62414	3.18%	0.332%
20	12.696	934	937	939	rBV	1328483	1720259	87.67%	9.151%
21	12.936	956	958	965	rBV	25914	36182	1.84%	0.192%
22	13.234	982	984	986	rBV	165253	143296	7.30%	0.762%
23	13.279	986	988	989	rVV	60093	50464	2.57%	0.268%
24	13.302	989	990	992	rVB	27840	22525	1.15%	0.120%
25	13.611	1015	1017	1024	rBV	125516	302119	15.40%	1.607%
26	13.725	1024	1027	1029	rVB	618359	645937	32.92%	3.436%
27	13.919	1042	1044	1047	rBV	67829	61944	3.16%	0.330%
28	14.228	1068	1071	1072	rBV	47186	49065	2.50%	0.261%
29	14.514	1094	1096	1099	rBV	58349	55790	2.84%	0.297%
30	14.582	1099	1102	1104	rBV	35380	41839	2.13%	0.223%
31	14.811	1119	1122	1124	rBV	38733	49826	2.54%	0.265%
32	15.062	1141	1144	1147	rBV	383922	483024	24.62%	2.569%
33	15.119	1147	1149	1152	rVB	26868	40786	2.08%	0.217%
34	15.485	1178	1181	1186	rVB	25335	32941	1.68%	0.175%

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ClientSampleId :
COFF-3(0-2)-6

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

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35	15.588	1186	1190	1197	rBV2	18968	64287	3.28%	0.342%
36	15.897	1214	1217	1221	rBV	13648	24262	1.24%	0.129%

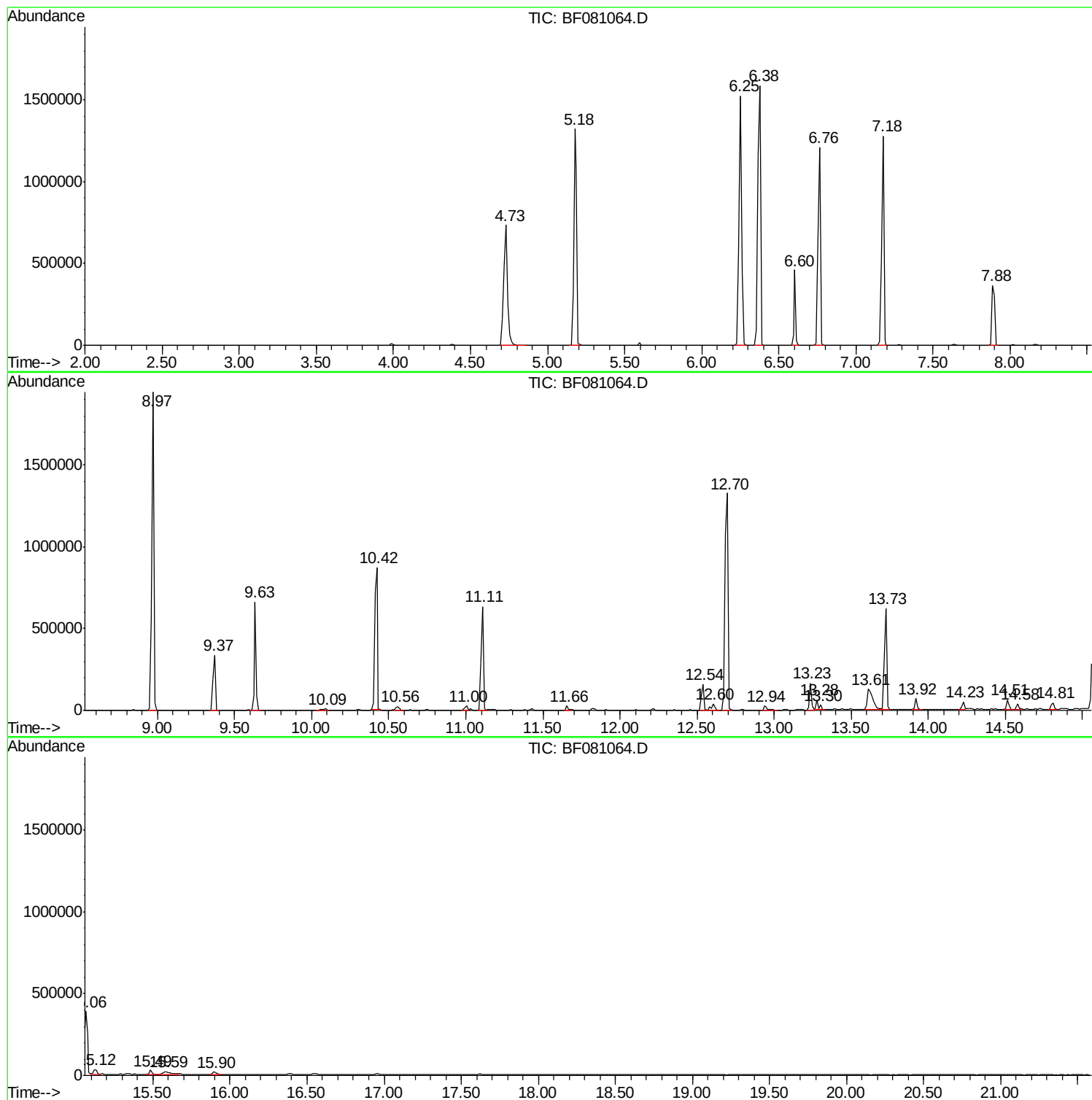
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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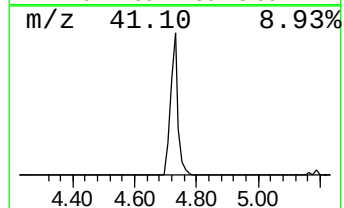
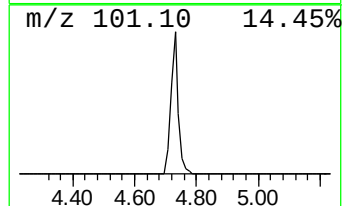
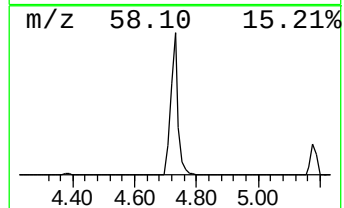
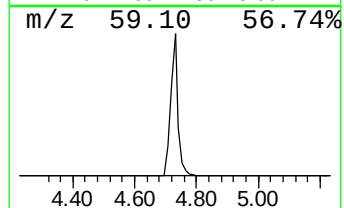
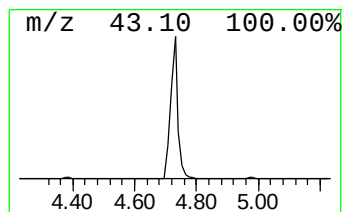
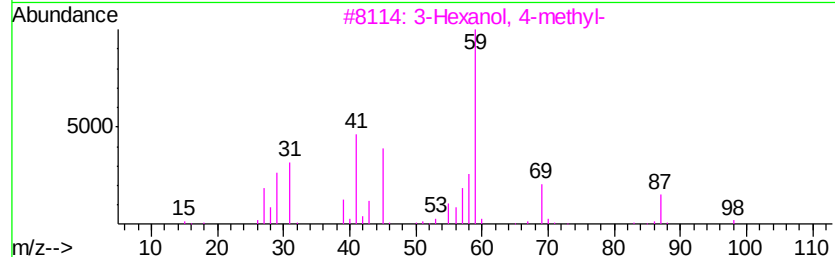
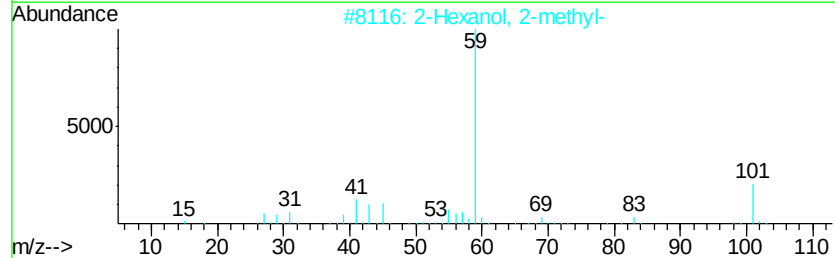
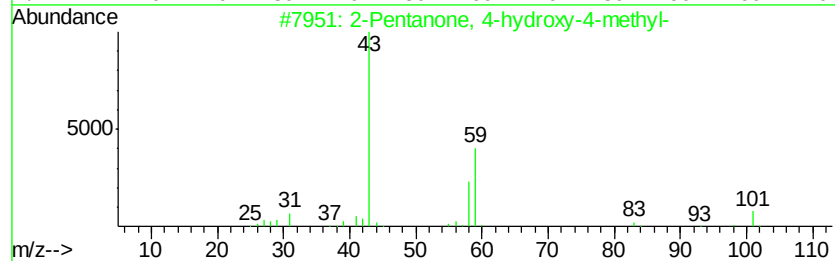
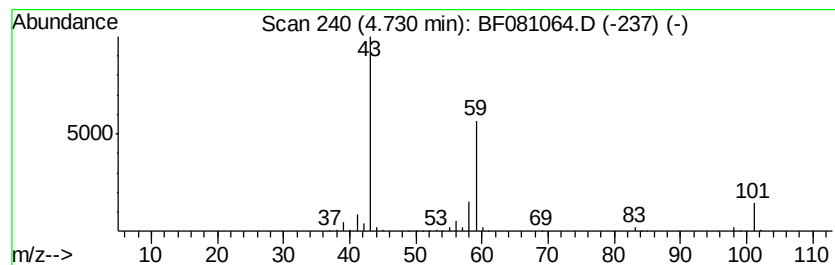
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	62.68 ng	1188360	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	64
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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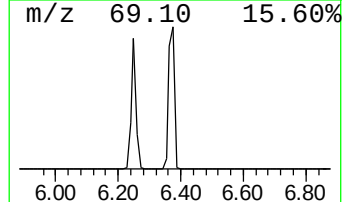
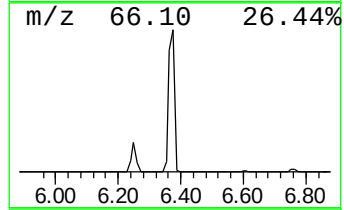
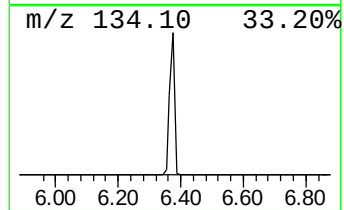
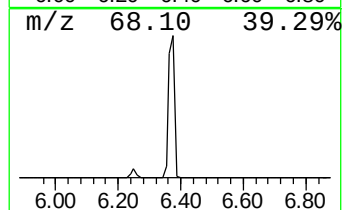
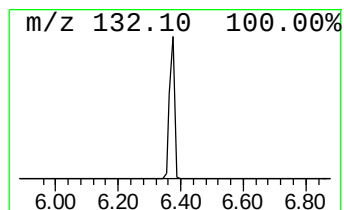
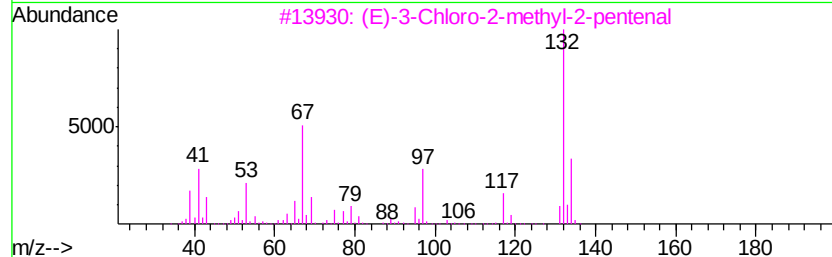
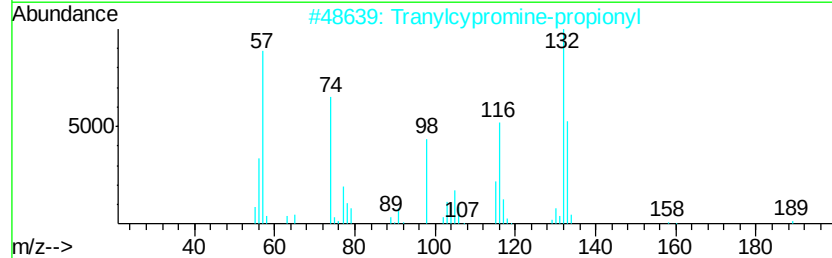
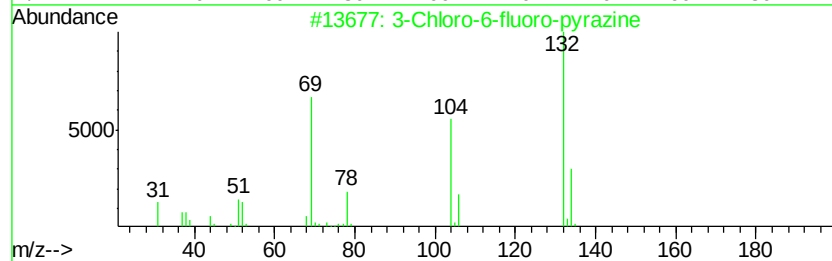
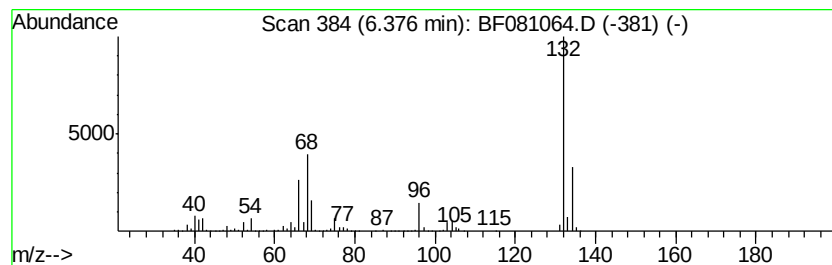
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Peak Number 2 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	103.51 ng	1962310	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Xenon	132	Xe	007440-63-3	9



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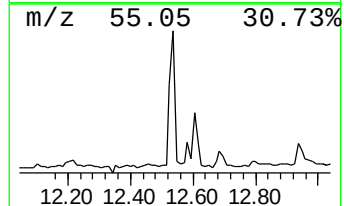
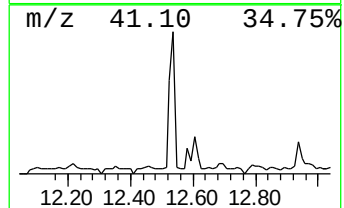
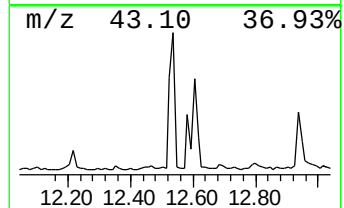
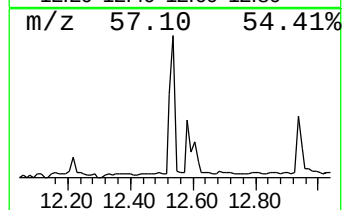
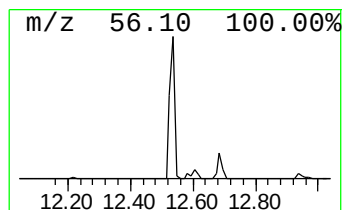
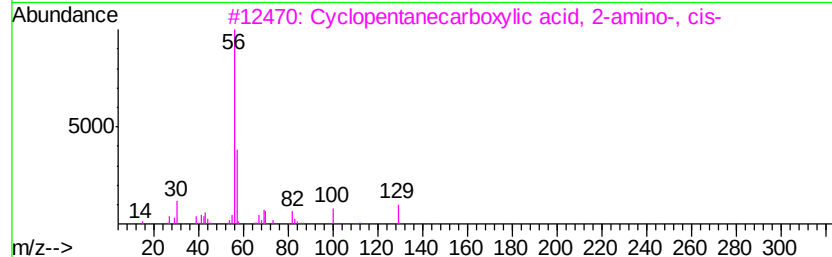
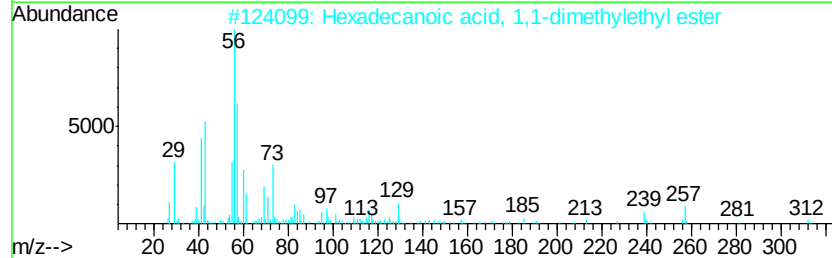
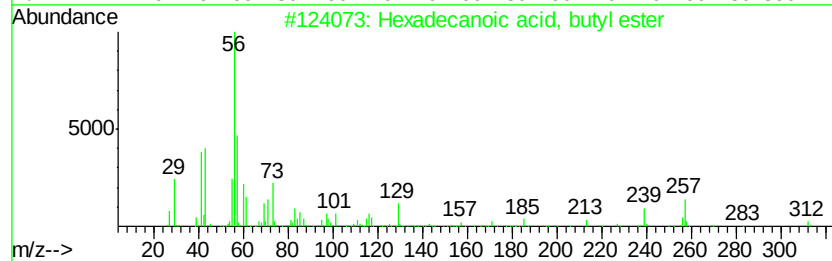
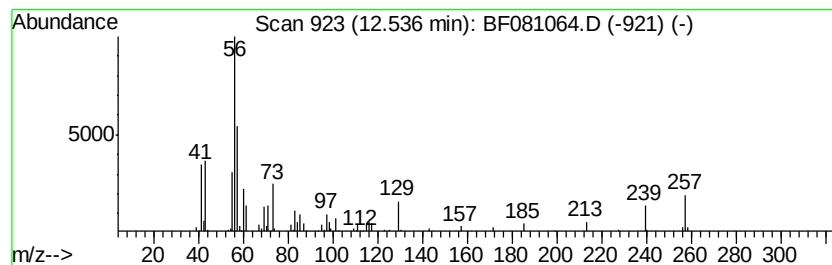
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.54	5.20 ng	167806	Chrysene-d12	13.73		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32



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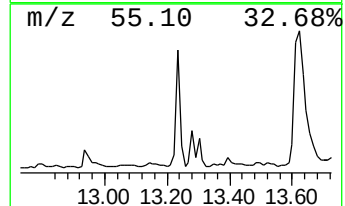
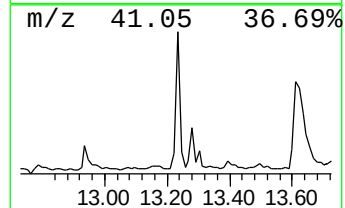
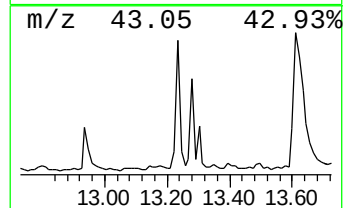
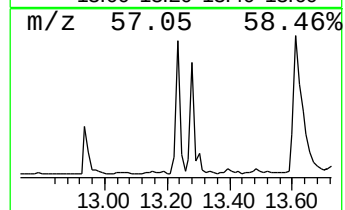
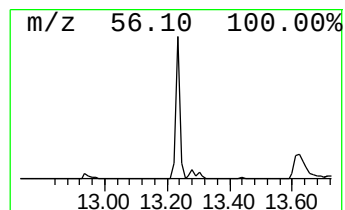
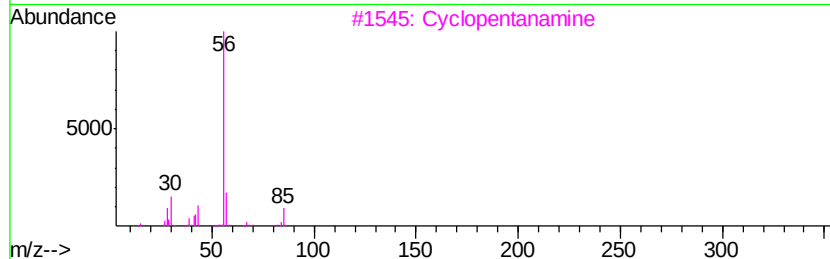
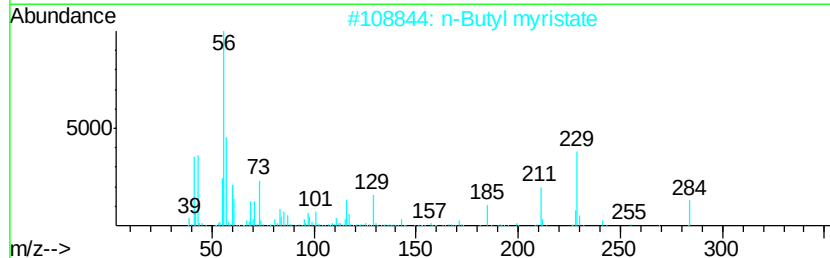
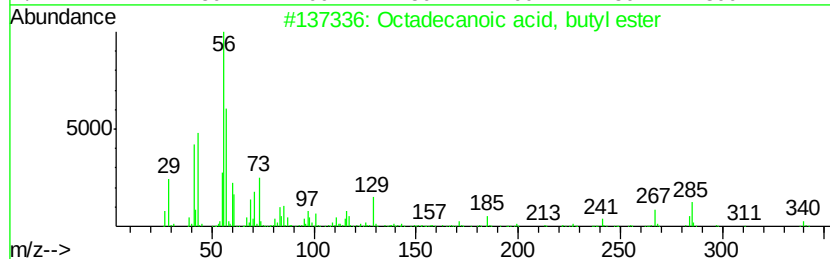
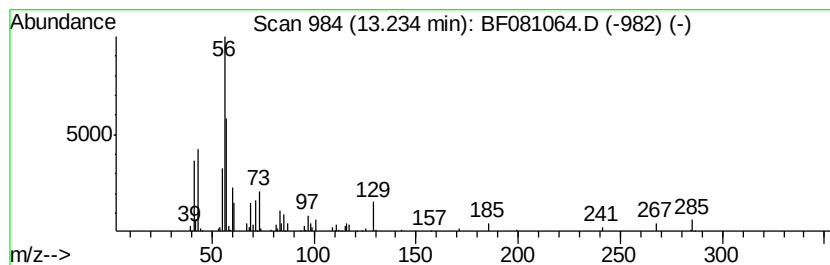
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.23	4.44 ng	143296	Chrysene-d12	13.73	
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	86
3	Cyclopentanamine	85	C5H11N	001003-03-8	37
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	37
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	37



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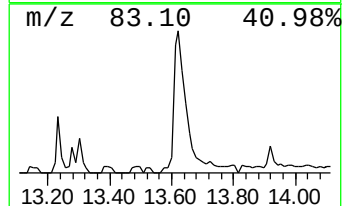
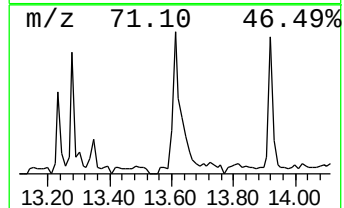
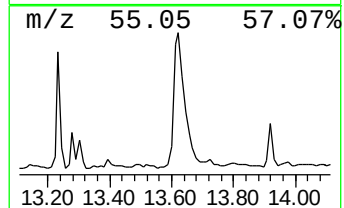
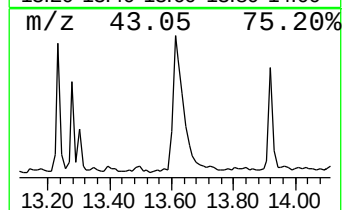
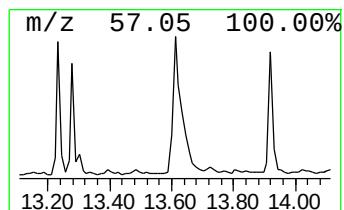
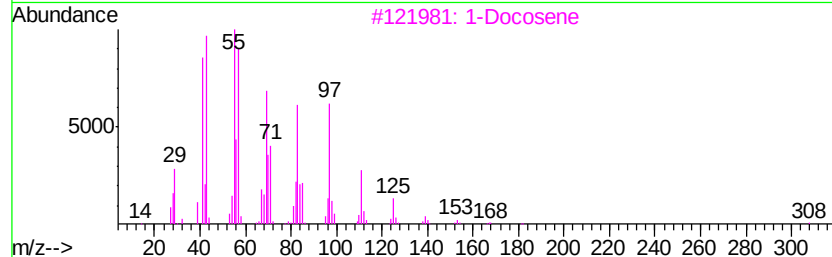
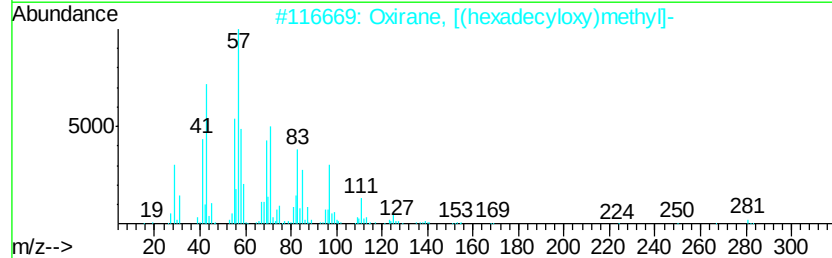
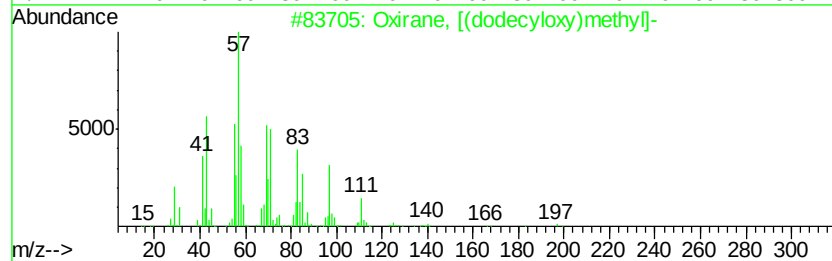
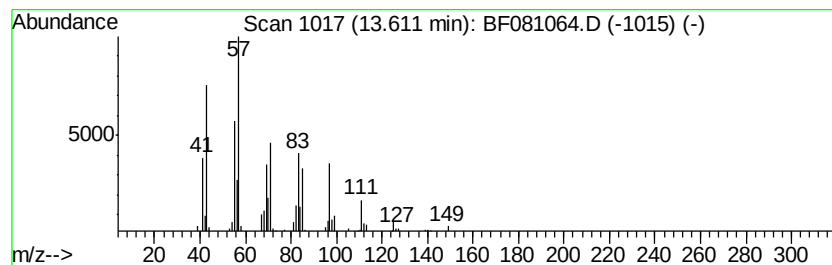
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.61	9.35 ng	302119	Chrysene-d12	13.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	90
2	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	80
3	1-Docosene	308	C22H44	001599-67-3	70
4	Pentafluoropropionic acid, octadecyl...	416	C21H37F5O2	1000280-07-7	64
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	58



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ClientSampleId :
COFF-3(0-2)-6

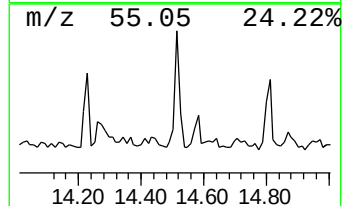
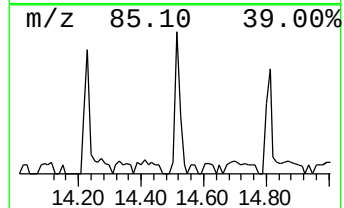
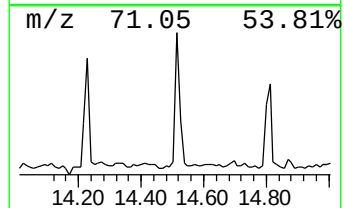
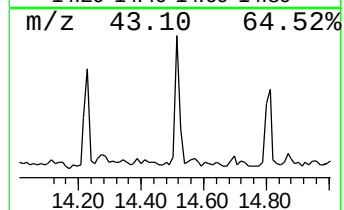
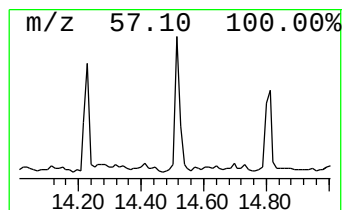
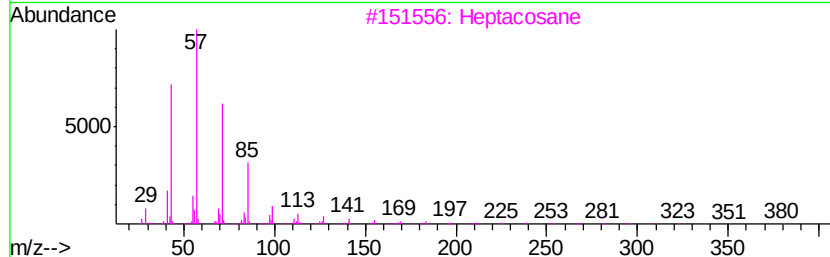
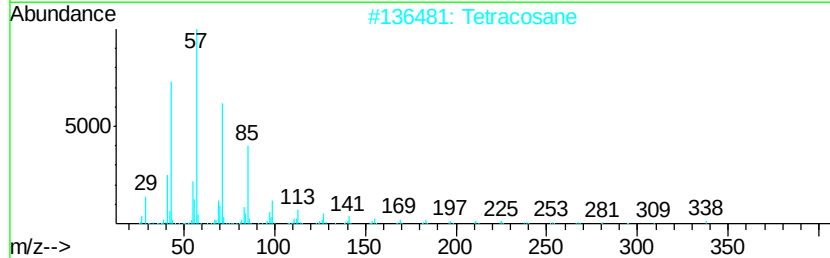
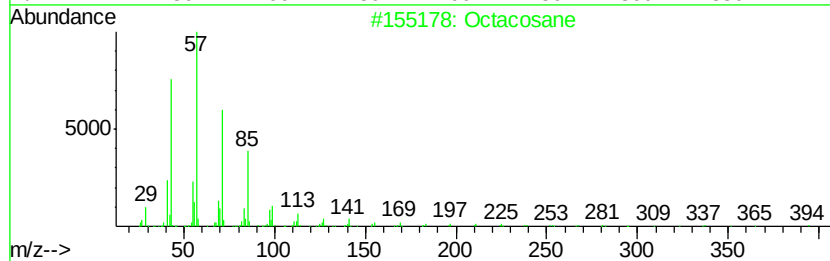
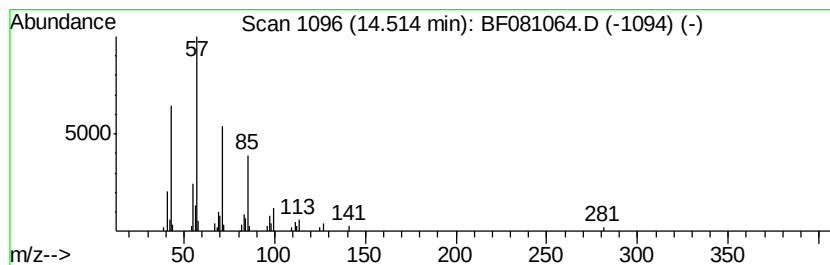
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.31 ng	55790	Perylene-d12	15.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Heptacosane	380	C27H56	000593-49-7	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081064.D
Acq On : 19 Aug 2015 3:47
Operator : UM/IZ
Sample : G3290-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3(0-2)-6

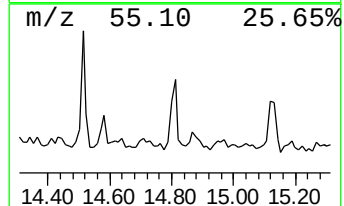
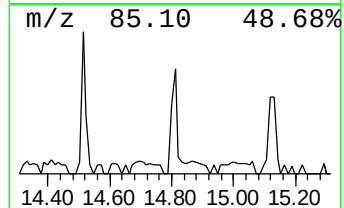
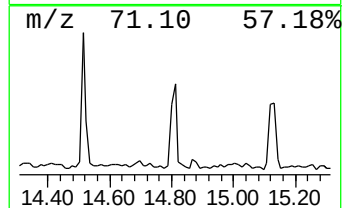
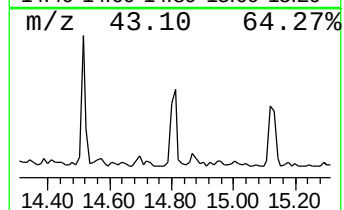
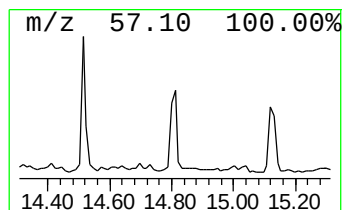
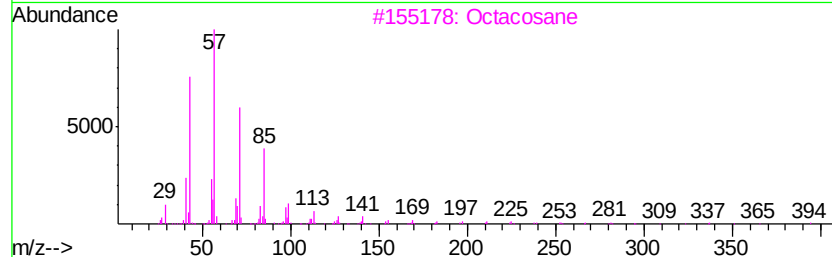
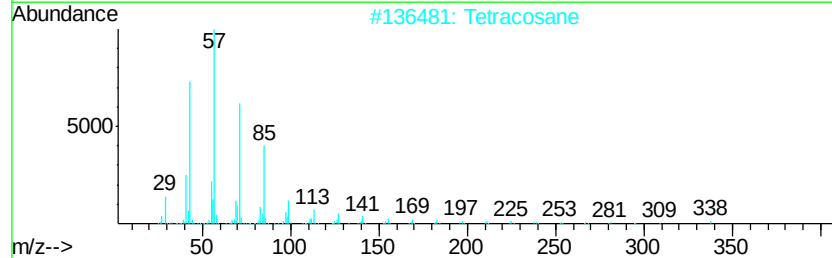
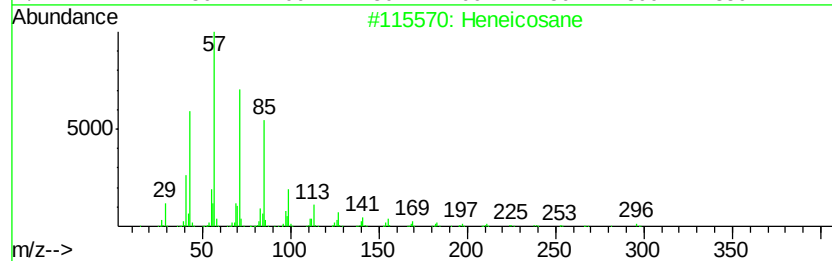
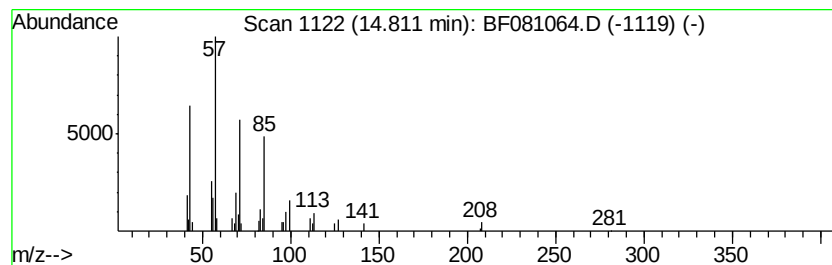
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.06 ng	49826	Perylene-d12	15.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	87
2		Tetracosane	338	C24H50	000646-31-1	86
3		Octacosane	394	C28H58	000630-02-4	86
4		Octadecane	254	C18H38	000593-45-3	86
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081064.D
Acq On : 19 Aug 2015 3:47
Operator : UM/IZ
Sample : G3290-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

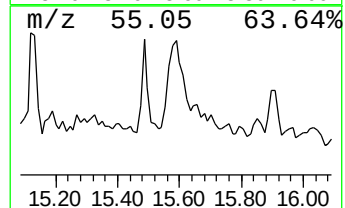
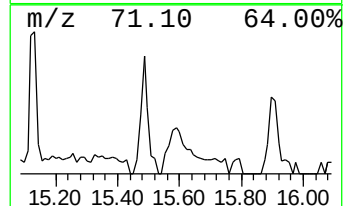
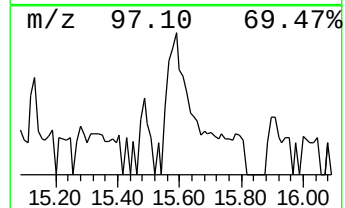
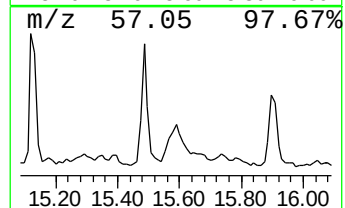
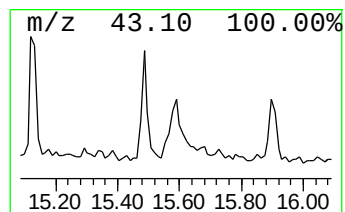
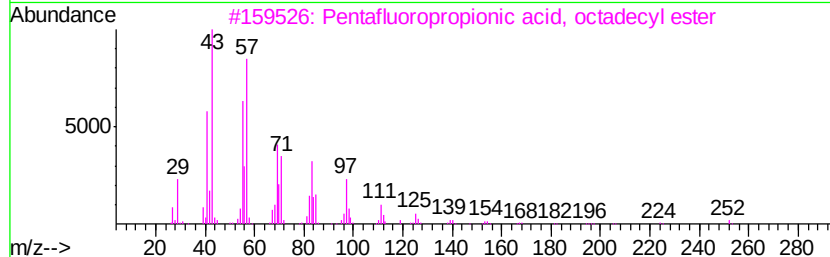
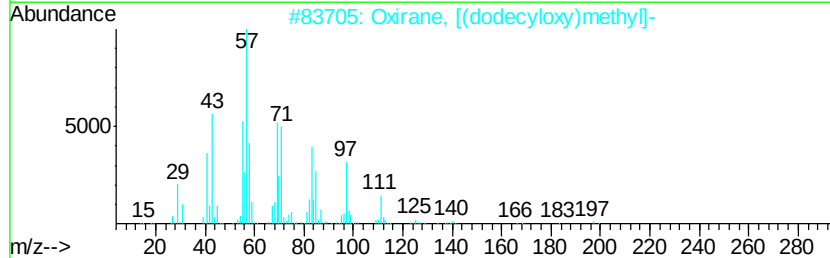
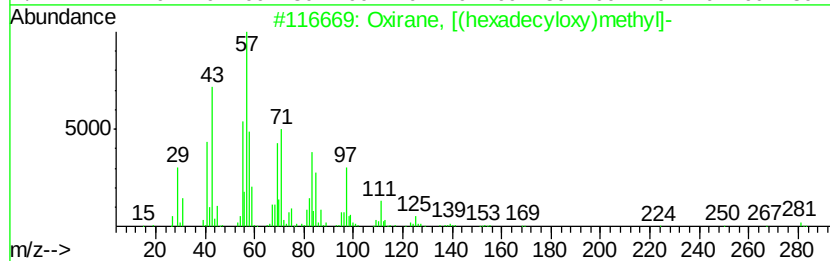
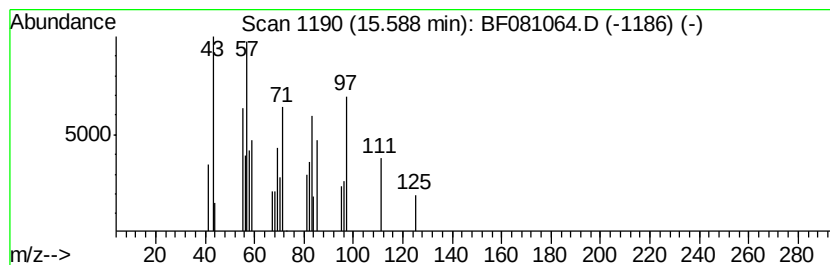
Instrument :
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ClientSampleId :
COFF-3(0-2)-6

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 9 Oxirane, [(hexadecyloxy)met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.59	2.66 ng	64287	Perylene-d12	15.06		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	64	
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	59	
3	Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	1000280-07-7	38	
4	2-Piperidinone, N-[4-bromo-n-butyl]-	233	C9H16BrNO	195194-80-0	38	
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	27	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081064.D
Acq On : 19 Aug 2015 3:47
Operator : UM/IZ
Sample : G3290-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3(0-2)-6

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	62.7	ng	1188360	1	6.60	379164	20.0
unknown6.38	6.38	103.5	ng	1962310	1	6.60	379164	20.0
Hexadecanoic acid...	12.54	5.2	ng	167806	5	13.73	645937	20.0
Octadecanoic acid...	13.23	4.4	ng	143296	5	13.73	645937	20.0
Oxirane, [(dodecy...	13.61	9.3	ng	302119	5	13.73	645937	20.0
Octacosane	14.51	2.3	ng	55790	6	15.06	483024	20.0
Heneicosane	14.81	2.1	ng	49826	6	15.06	483024	20.0
Oxirane, [(hexade...	15.59	2.7	ng	64287	6	15.06	483024	20.0