

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120415\
 Data File : BF083519.D
 Acq On : 5 Dec 2015 17:25
 Operator : UM/IZ
 Sample : G4588-16
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-10

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-BF120415.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	3.584	164	166	177	rBV	263409	498455	9.26%	1.349%
2	4.030	203	205	219	rBV	1681998	2388421	44.35%	6.465%
3	5.322	315	318	327	rBV	871190	1615098	29.99%	4.372%
4	5.459	327	330	338	rVB	3454240	4043956	75.09%	10.946%
5	5.767	354	357	365	rBV	691404	867221	16.10%	2.347%
6	5.984	373	376	379	rBV	2984077	3571038	66.31%	9.666%
7	6.590	426	429	432	rBV	2094833	3300533	61.29%	8.934%
8	7.596	513	517	521	rBV	67240	100643	1.87%	0.272%
9	7.665	521	523	531	rVV	769902	1128749	20.96%	3.055%
10	9.230	655	660	665	rBV3	22271	62114	1.15%	0.168%
11	9.413	673	676	679	rBV	3697871	5385421	100.00%	14.577%
12	10.099	733	736	739	rBV	64641	79585	1.48%	0.215%
13	10.453	765	767	773	rBV	848185	1347436	25.02%	3.647%
14	11.299	839	841	844	rVB	74127	102905	1.91%	0.279%
15	11.745	877	880	883	rBV	2299225	3188569	59.21%	8.631%
16	12.076	906	909	913	rBV	62455	124848	2.32%	0.338%
17	12.854	974	977	984	rVB	918381	1227408	22.79%	3.322%
18	13.905	1066	1069	1078	rBV	133584	242511	4.50%	0.656%
19	14.637	1130	1133	1136	rBV	43277	75318	1.40%	0.204%
20	14.820	1148	1149	1155	rVB2	39879	81955	1.52%	0.222%
21	15.185	1178	1181	1185	rBV	174148	288026	5.35%	0.780%
22	15.323	1191	1193	1199	rVB	138557	213001	3.96%	0.577%
23	15.483	1203	1207	1210	rBV	3032423	4879411	90.60%	13.207%
24	16.465	1291	1293	1297	rBV	114943	164296	3.05%	0.445%
25	16.980	1336	1338	1341	rBV2	44188	100870	1.87%	0.273%
26	17.037	1341	1343	1349	rVB	715894	1005463	18.67%	2.722%
27	17.414	1374	1376	1379	rVB	50074	60876	1.13%	0.165%
28	18.671	1483	1486	1493	rBV	649195	800202	14.86%	2.166%

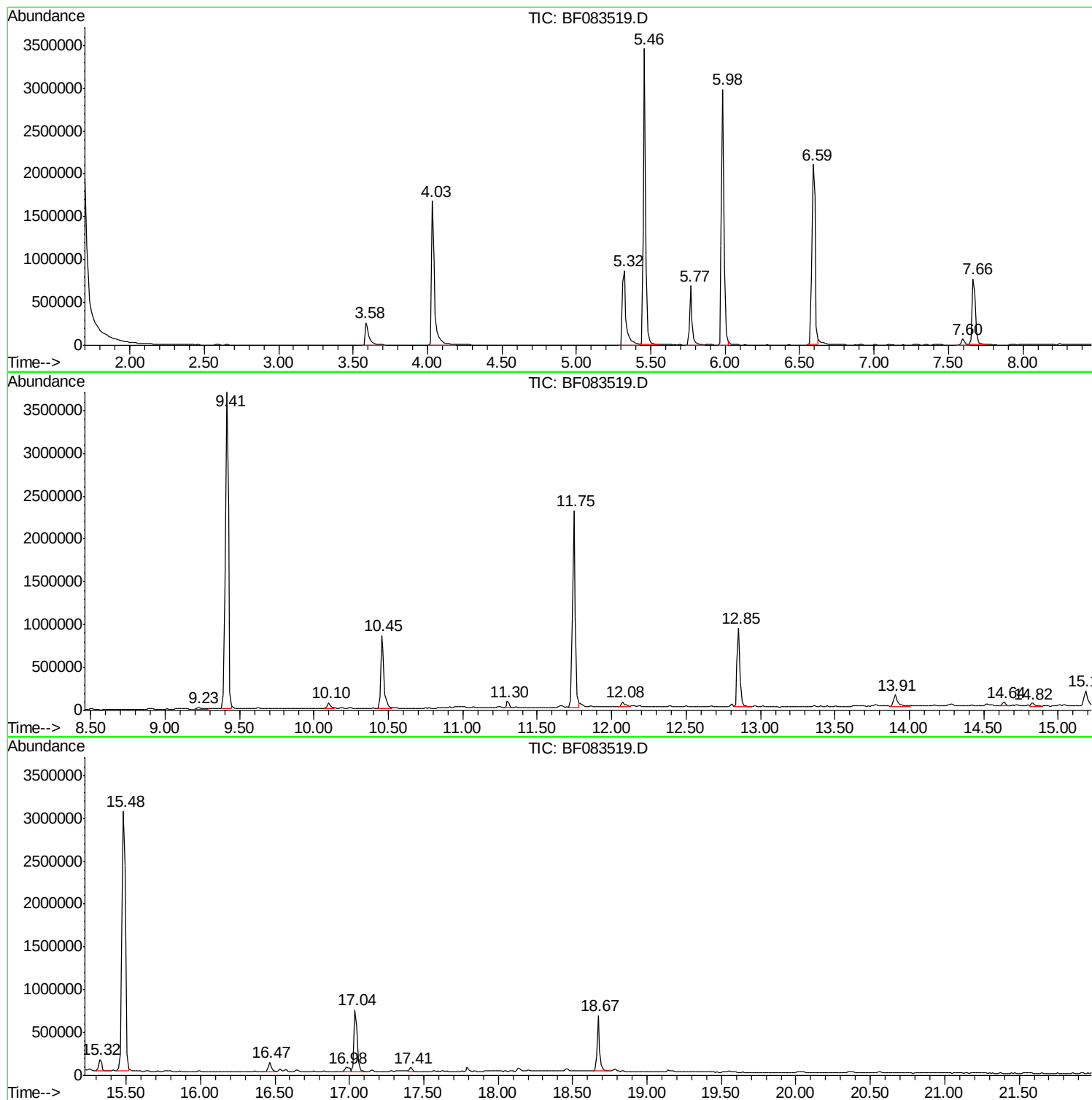
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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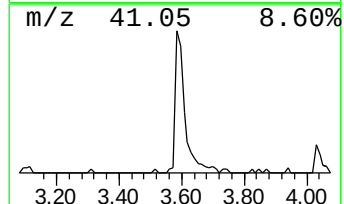
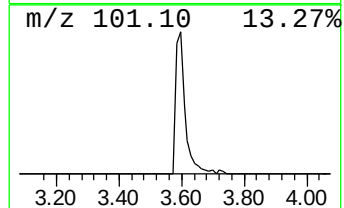
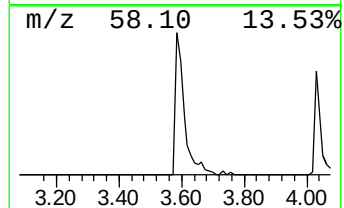
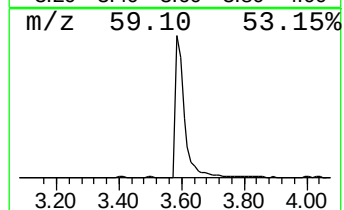
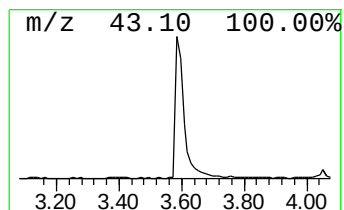
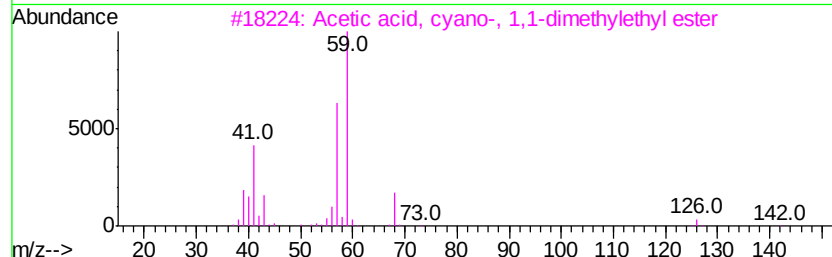
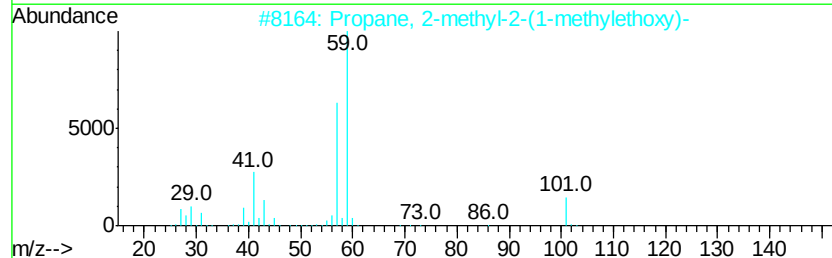
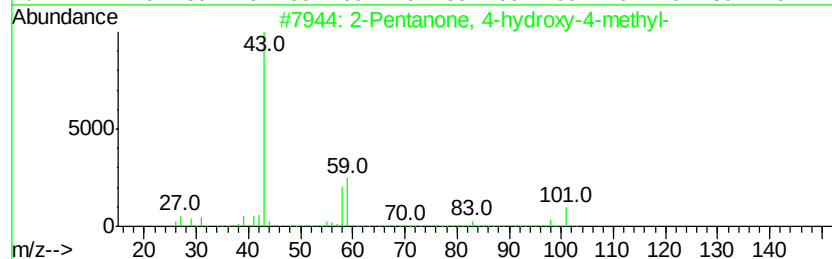
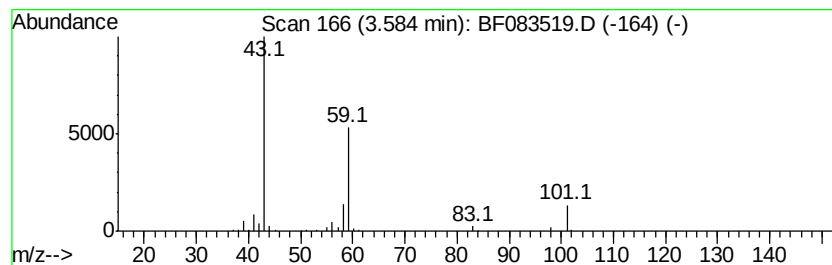
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.58	11.50 ng	498455	1,4-Dichlorobenzene-d4	5.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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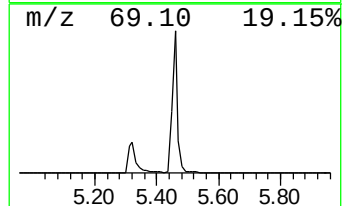
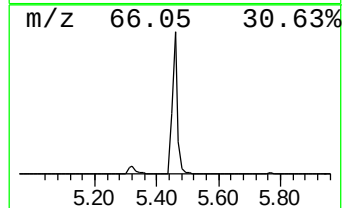
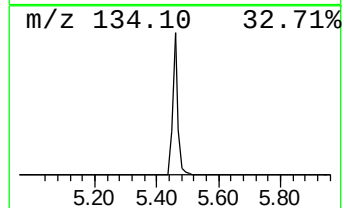
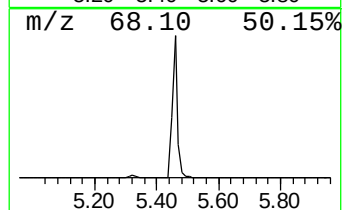
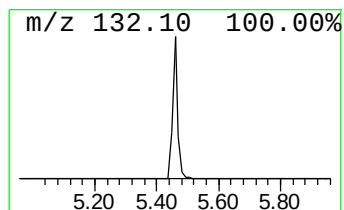
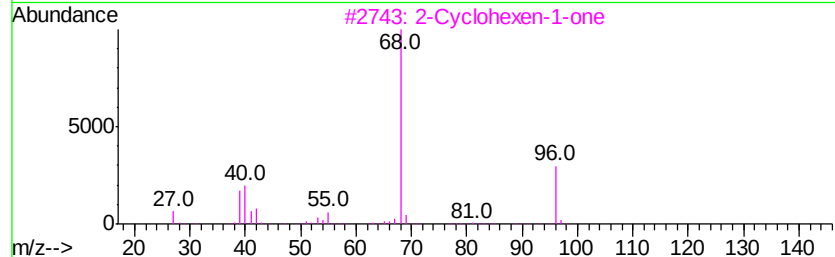
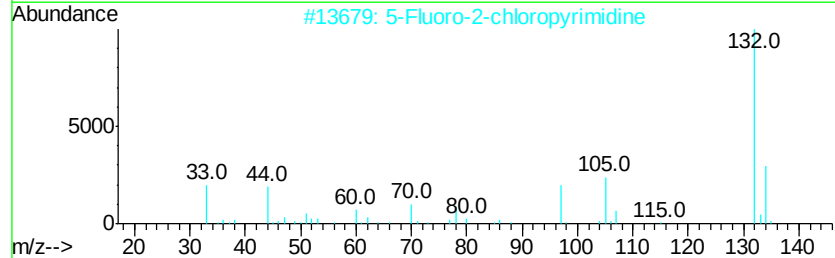
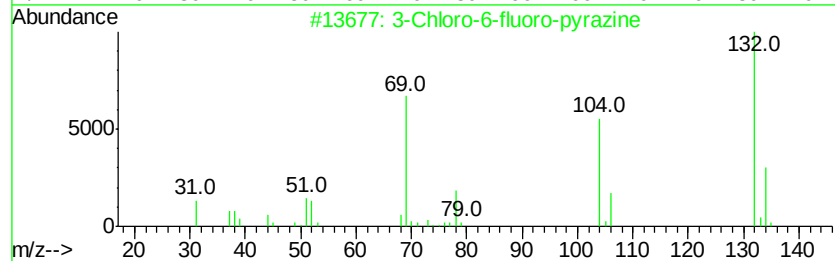
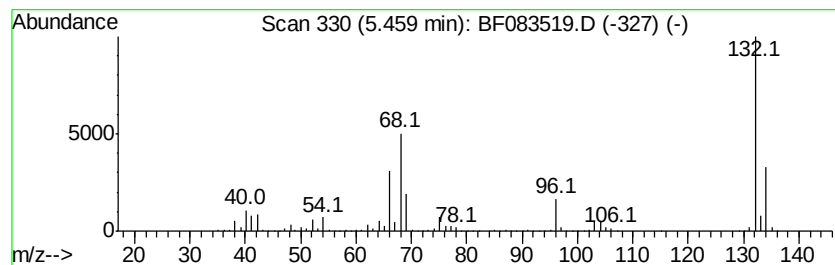
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown5.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.46	93.26 ng	4043960	1,4-Dichlorobenzene-d4	5.77

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	16
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1-Aminoindan	133	C9H11N	034698-41-4	9



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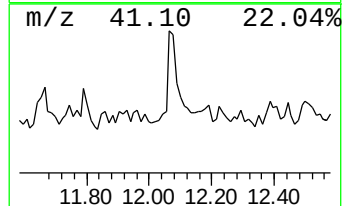
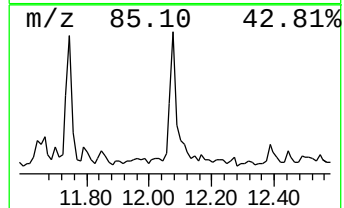
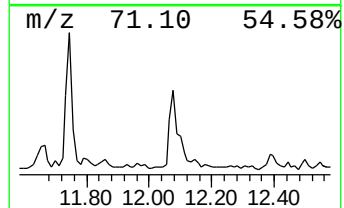
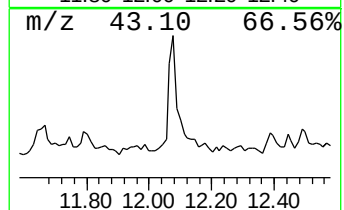
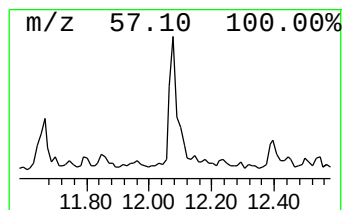
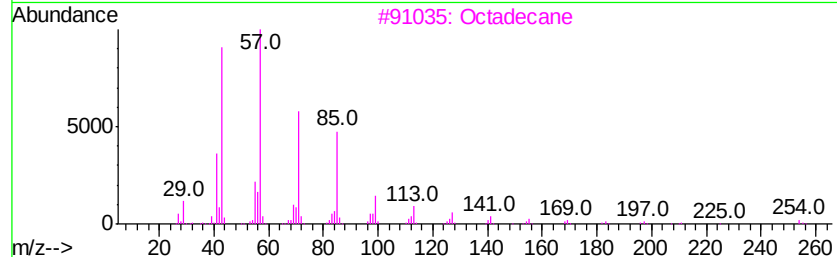
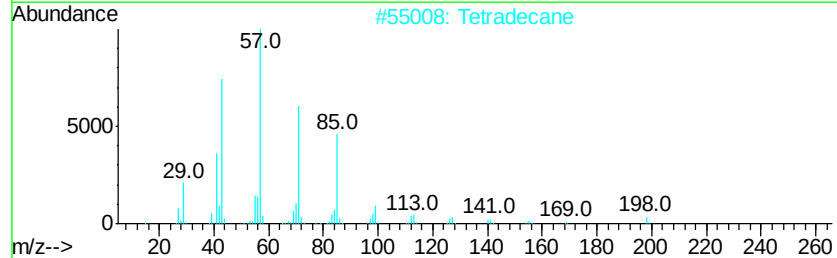
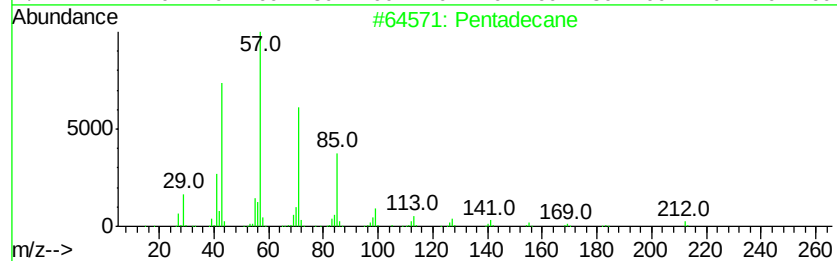
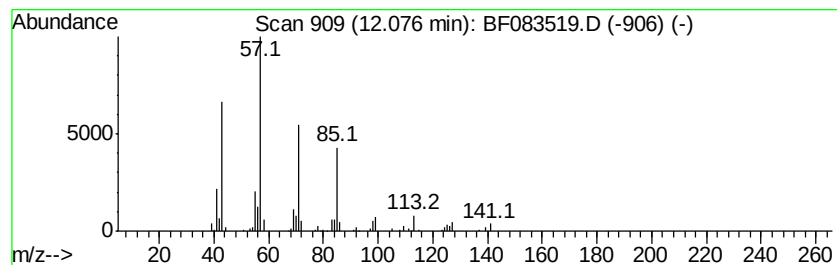
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Peak Number 4 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.03 ng	124848	Phenanthrene-d10	12.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	90
2	Tetradecane		198	C14H30	000629-59-4	86
3	Octadecane		254	C18H38	000593-45-3	86
4	Heptadecane		240	C17H36	000629-78-7	80
5	Undecane, 5,7-dimethyl-		184	C13H28	017312-83-3	72



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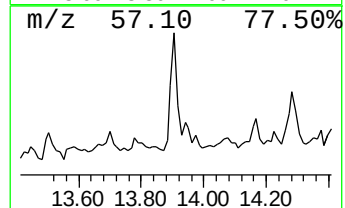
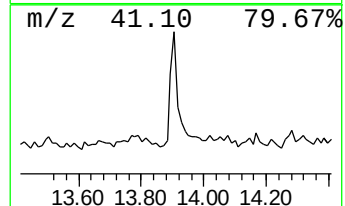
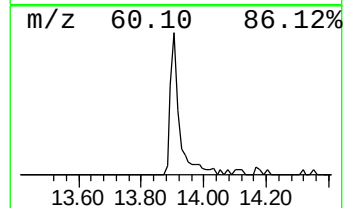
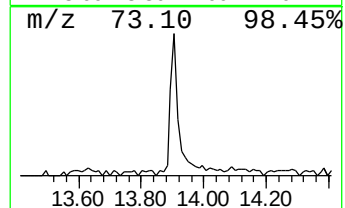
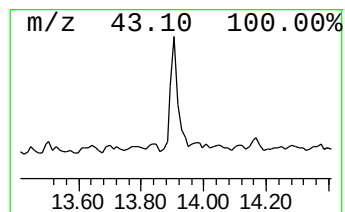
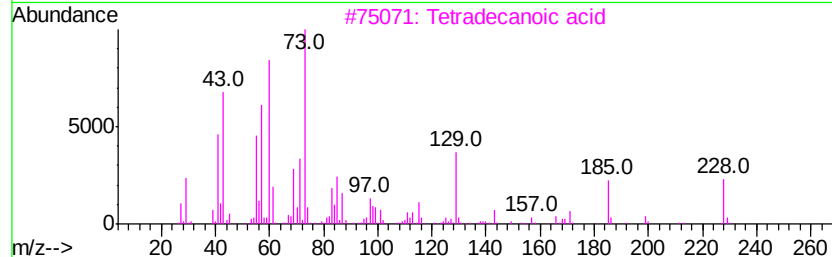
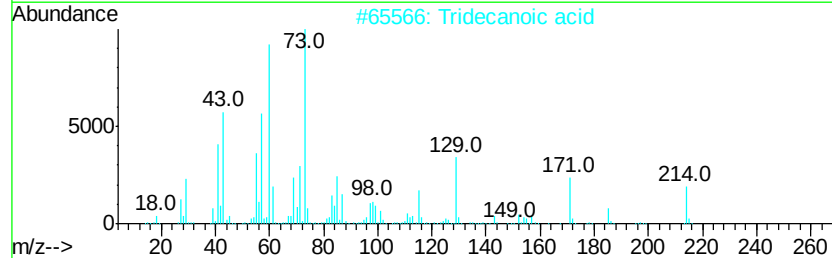
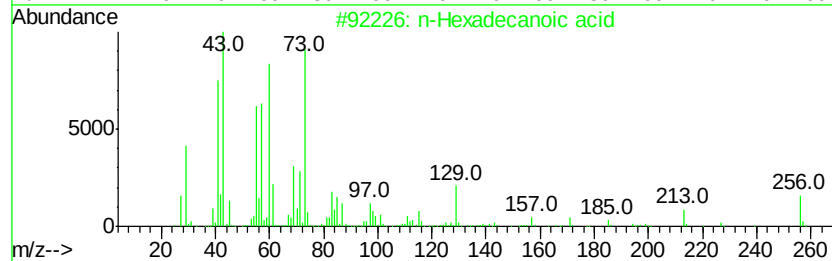
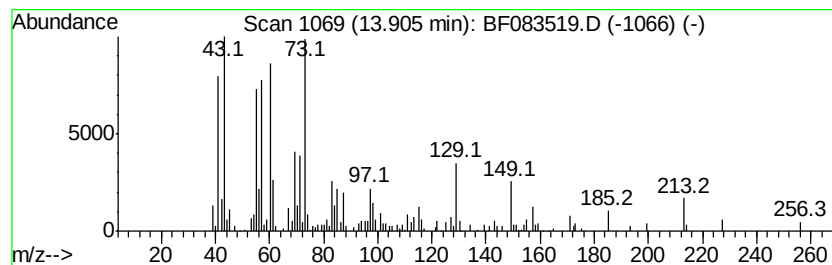
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.95 ng	242511	Phenanthrene-d10	12.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
2		Tridecanoic acid	214	C13H26O2	000638-53-9	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Dodecanoic acid	200	C12H24O2	000143-07-7	50
5		1,2,3,4,5-Cyclopentanepentol	150	C5H10O5	056772-25-9	43



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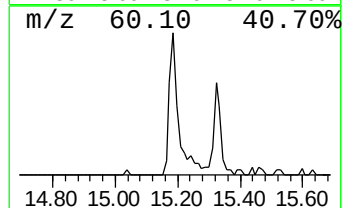
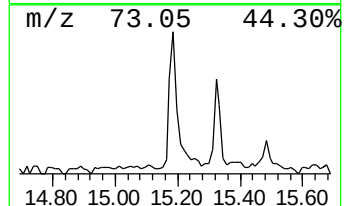
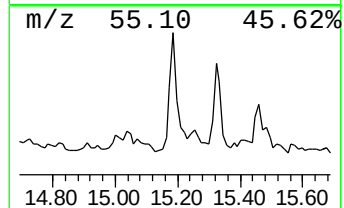
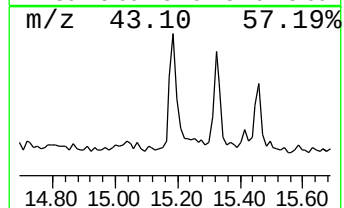
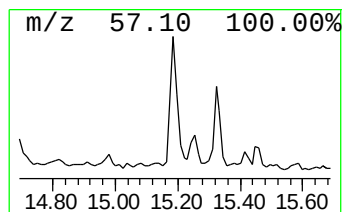
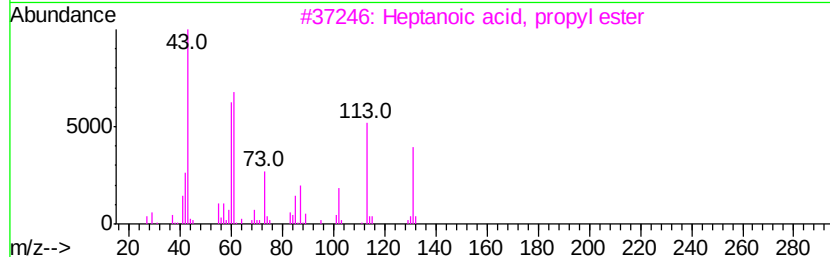
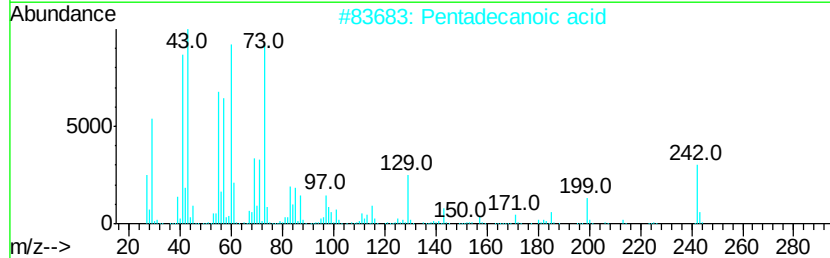
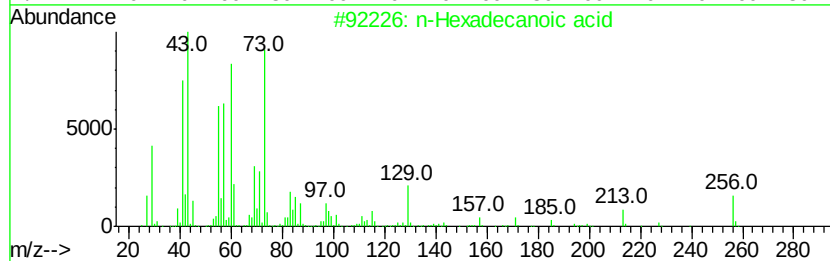
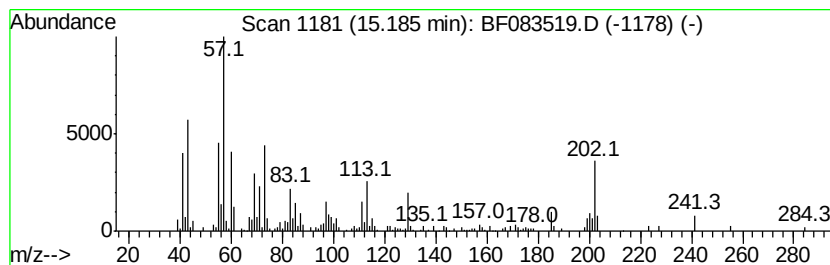
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown15.19 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.19	5.73 ng	288026	Chrysene-d12	17.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	32
3	Heptanoic acid, propyl ester	172	C10H20O2	007778-87-2	32
4	N-Acetyl-d-serine	147	C5H9NO4	1000126-44-0	27
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27



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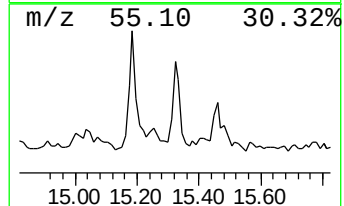
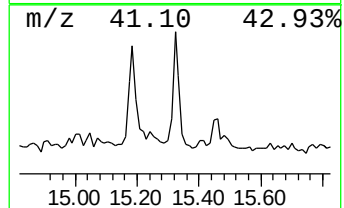
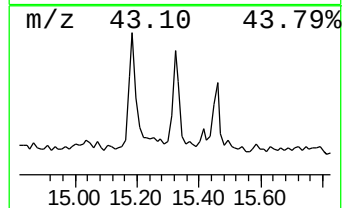
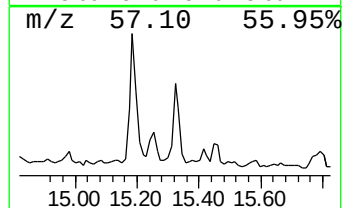
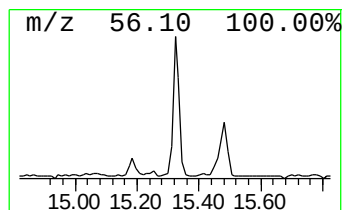
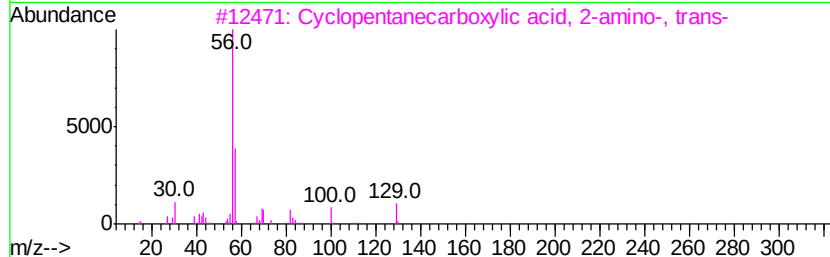
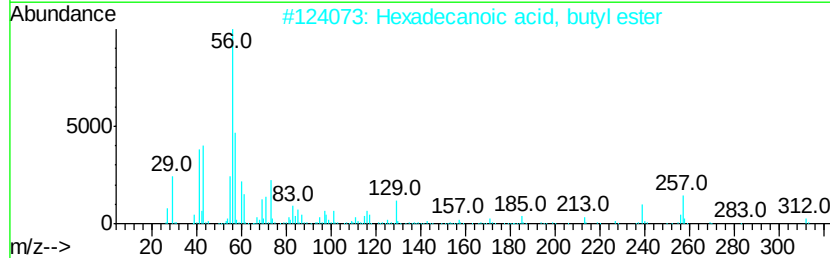
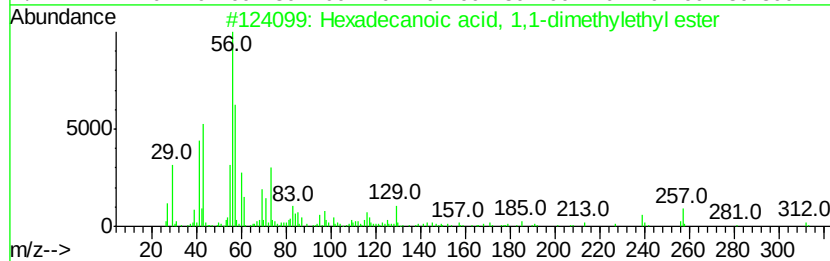
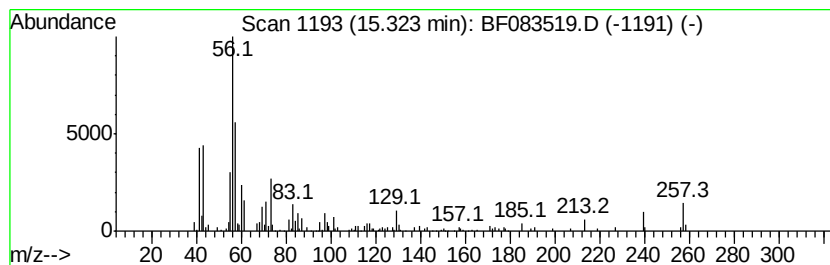
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.24 ng	213001	Chrysene-d12	17.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
5		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120415\
Data File : BF083519.D
Acq On : 5 Dec 2015 17:25
Operator : UM/IZ
Sample : G4588-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-10

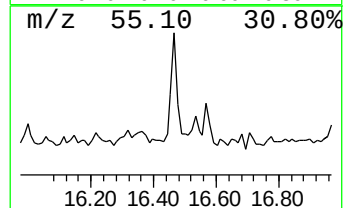
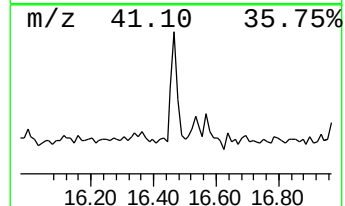
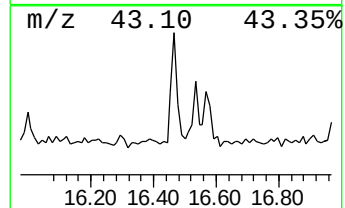
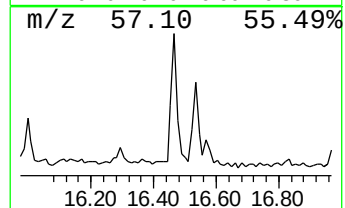
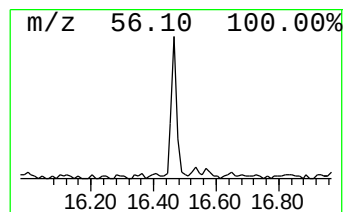
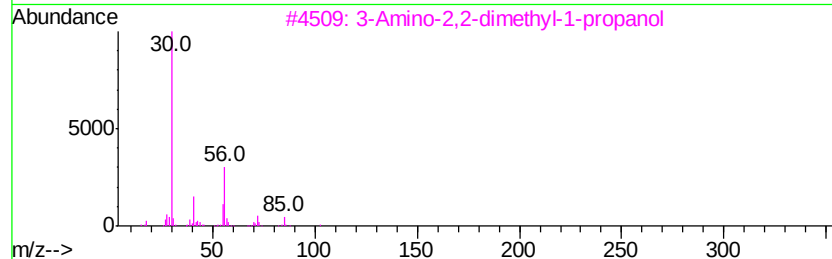
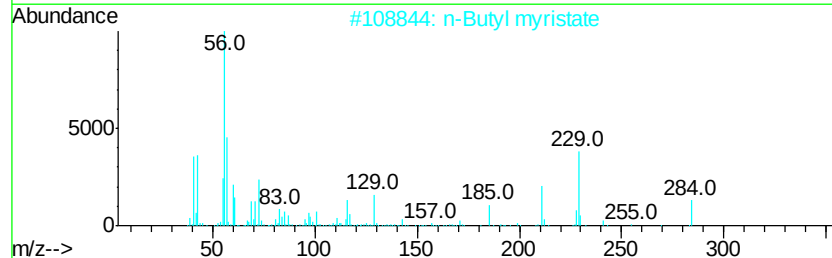
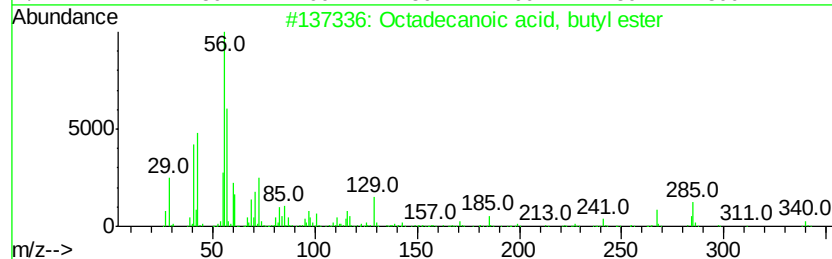
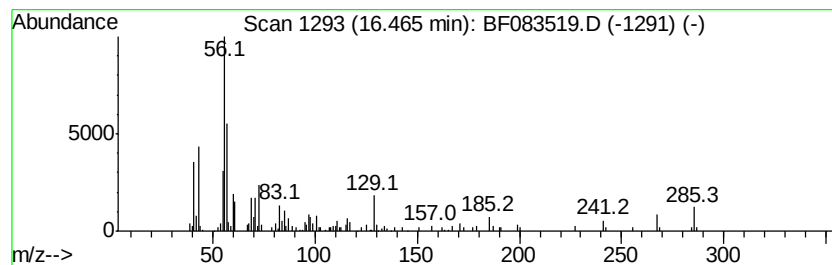
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	3.27 ng	164296	Chrysene-d12	17.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	43
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120415\
Data File : BF083519.D
Acq On : 5 Dec 2015 17:25
Operator : UM/IZ
Sample : G4588-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-10

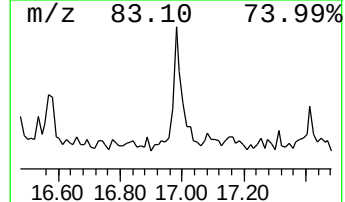
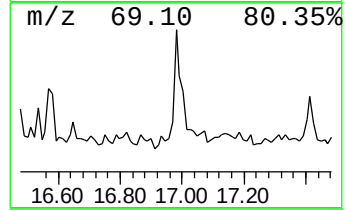
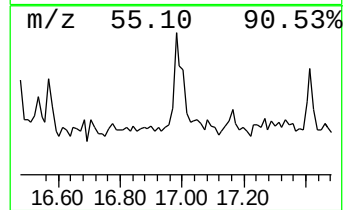
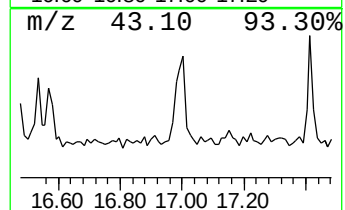
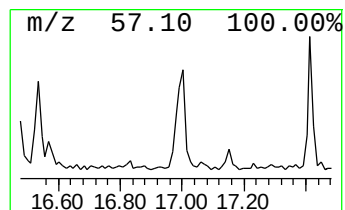
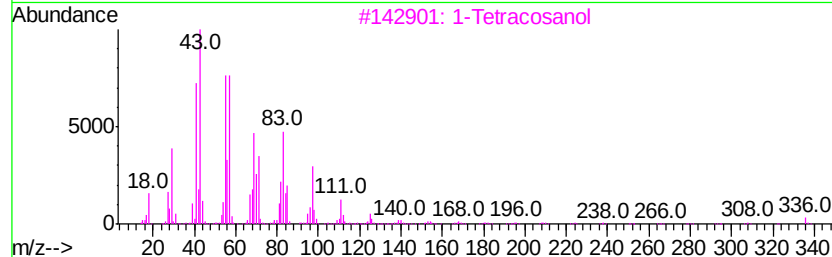
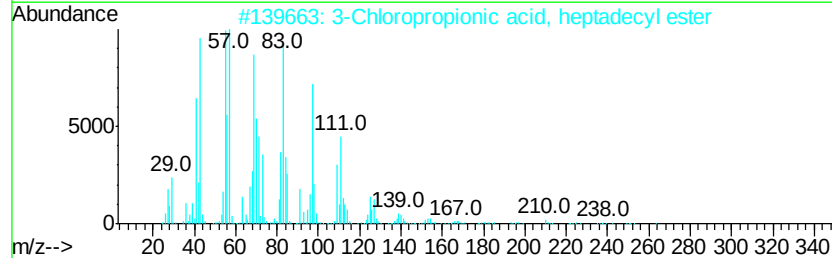
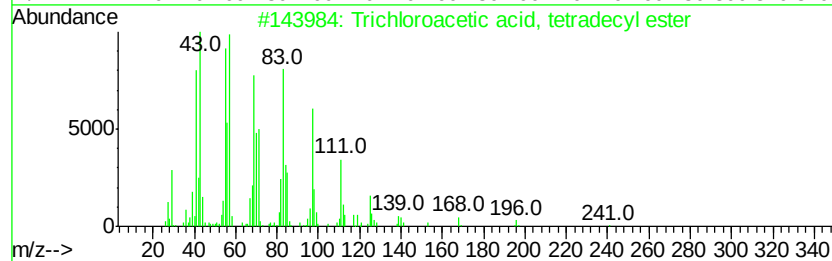
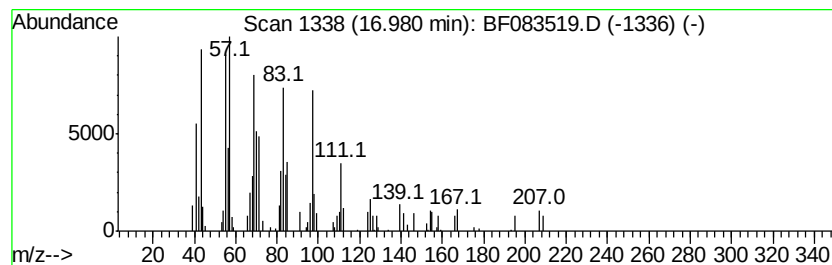
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.98	2.01 ng	100870	Chrysene-d12	17.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	93
2		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3		1-Tetracosanol	354	C24H50O	000506-51-4	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120415\
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Acq On : 5 Dec 2015 17:25
Operator : UM/IZ
Sample : G4588-16
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120415.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...	3.58	11.5	ng	498455	1	5.77	867221	20.0
unknown5.46	5.46	93.3	ng	4043960	1	5.77	867221	20.0
Pentadecane	12.08	2.0	ng	124848	4	12.85	1227410	20.0
n-Hexadecanoic acid	13.91	4.0	ng	242511	4	12.85	1227410	20.0
unknown15.19	15.19	5.7	ng	288026	5	17.04	1005460	20.0
Hexadecanoic acid...	15.32	4.2	ng	213001	5	17.04	1005460	20.0
Octadecanoic acid...	16.47	3.3	ng	164296	5	17.04	1005460	20.0
Trichloroacetic a...	16.98	2.0	ng	100870	5	17.04	1005460	20.0