

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
 Data File : BF097499.D
 Acq On : 9 Aug 2017 5:34
 Operator : SJ/JU
 Sample : I4604-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PMW-1A-080217

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-BF072517.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	4.534	464	467	481	rBV	44857	86662	3.95%	0.526%
2	5.004	544	547	578	rBV	933764	1347242	61.41%	8.172%
3	6.081	727	730	743	rBV	614611	809500	36.90%	4.910%
4	6.181	743	747	764	rVB	2193462	2193823	100.00%	13.307%
5	6.404	782	785	798	rVB	489760	472365	21.53%	2.865%
6	6.563	808	812	826	rBV	1984022	1897863	86.51%	11.512%
7	6.981	879	883	901	rBV	1643779	1619110	73.80%	9.821%
8	7.686	1000	1003	1016	rBV	529298	564622	25.74%	3.425%
9	8.098	1069	1073	1077	rBV3	33691	51098	2.33%	0.310%
10	8.769	1183	1187	1190	rBV	2296500	2053914	93.62%	12.458%
11	9.169	1252	1255	1262	rBV	88472	80339	3.66%	0.487%
12	9.433	1296	1300	1309	rVB	606022	544599	24.82%	3.303%
13	10.222	1430	1434	1448	rBV	1063281	1019712	46.48%	6.185%
14	10.904	1547	1550	1560	rVB	501024	470352	21.44%	2.853%
15	11.145	1586	1591	1599	rBV	41750	74874	3.41%	0.454%
16	12.292	1782	1786	1797	rBV	99393	147906	6.74%	0.897%
17	12.492	1815	1820	1823	rBV	1664466	1734480	79.06%	10.521%
18	13.292	1950	1956	1962	rBV	55017	91625	4.18%	0.556%
19	13.439	1975	1981	1986	rVB5	16634	29364	1.34%	0.178%
20	13.533	1993	1997	2004	rVB	453835	453646	20.68%	2.752%
21	14.174	2102	2106	2113	rVB2	30519	50453	2.30%	0.306%
22	14.315	2124	2130	2134	rVB6	16811	30142	1.37%	0.183%
23	14.604	2176	2179	2182	rBV	29779	27842	1.27%	0.169%
24	14.868	2221	2224	2228	rBV	308327	348212	15.87%	2.112%
25	14.904	2228	2230	2235	rVB2	45793	49509	2.26%	0.300%
26	15.251	2285	2289	2293	rVB	36848	53368	2.43%	0.324%
27	15.639	2351	2355	2361	rVB2	51068	88010	4.01%	0.534%
28	16.092	2430	2432	2437	rVB3	18909	31451	1.43%	0.191%
29	16.633	2520	2524	2530	rVB4	30111	41474	1.89%	0.252%
30	19.268	2969	2972	2977	rVB6	14432	22924	1.04%	0.139%

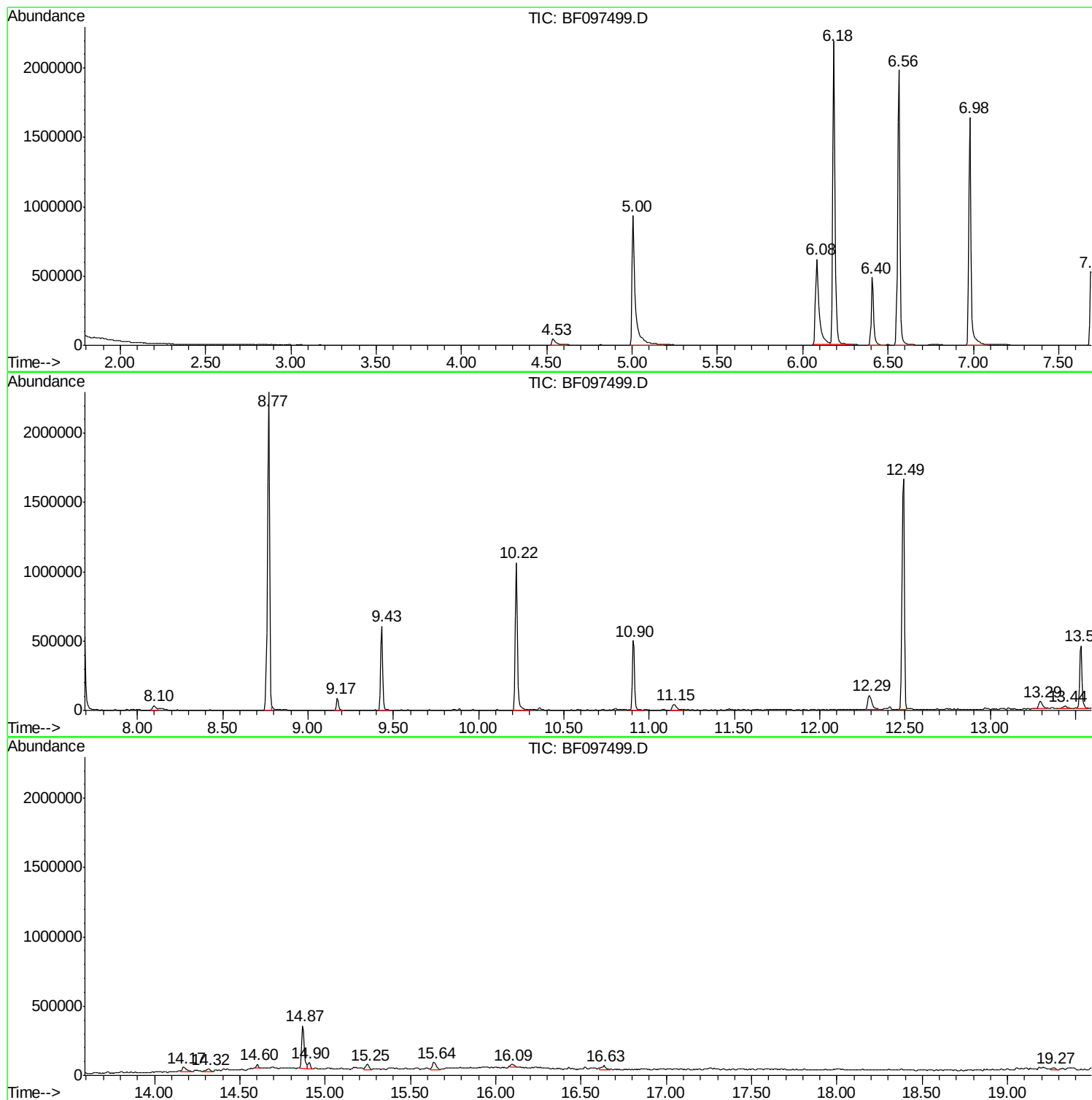
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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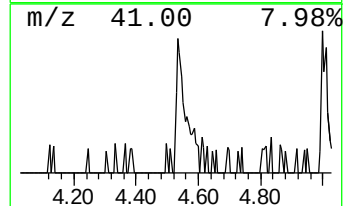
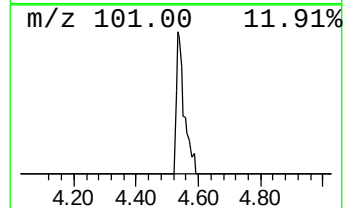
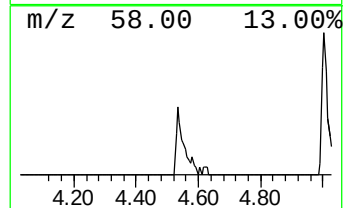
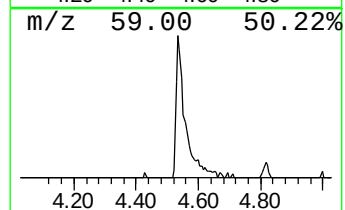
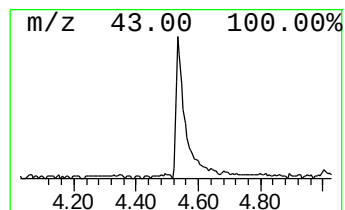
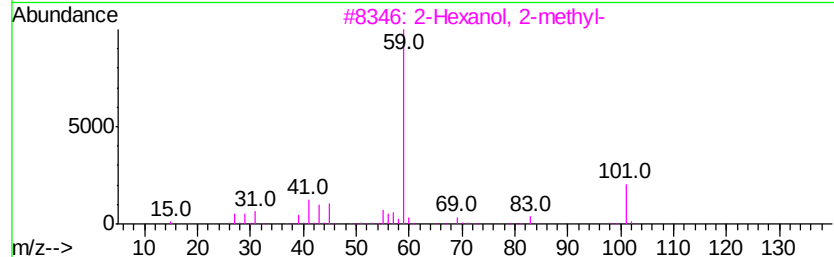
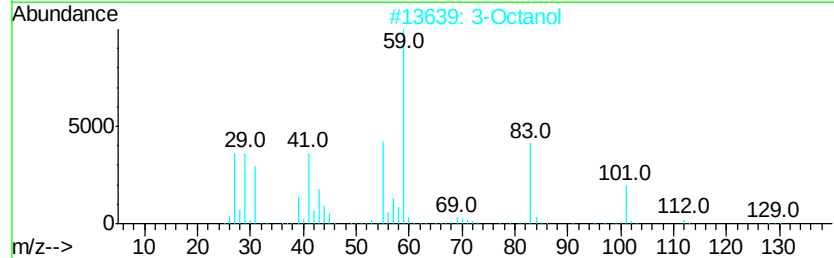
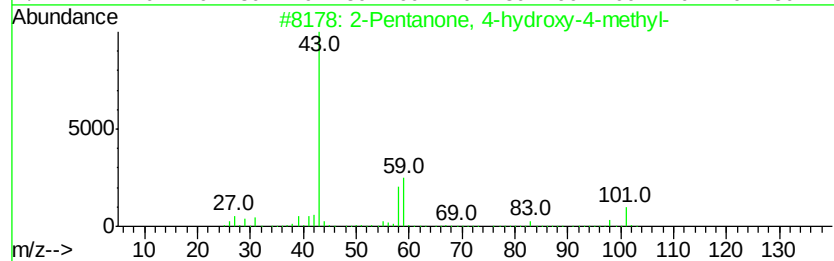
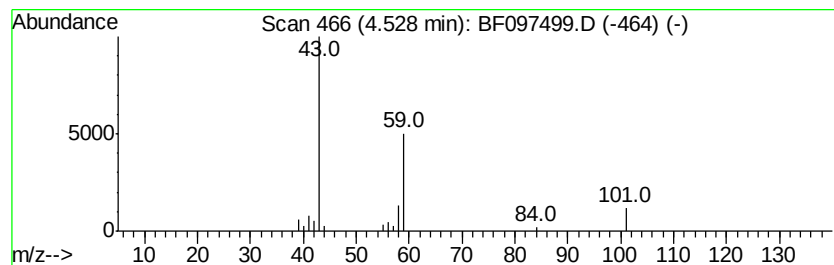
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.67 ng	86662	1,4-Dichlorobenzene-d4	6.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Octanol	130	C8H18O	000589-98-0	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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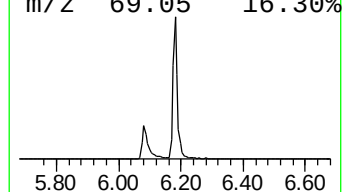
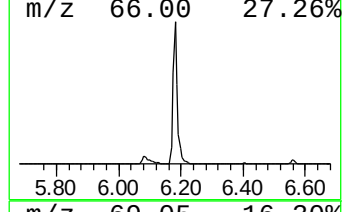
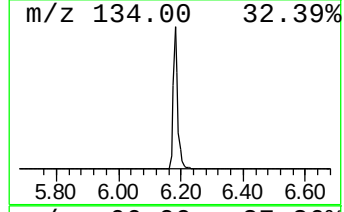
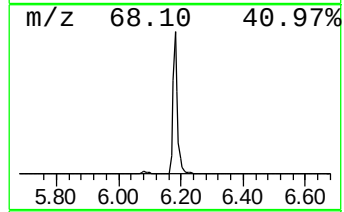
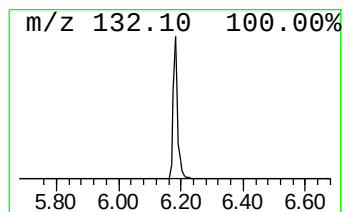
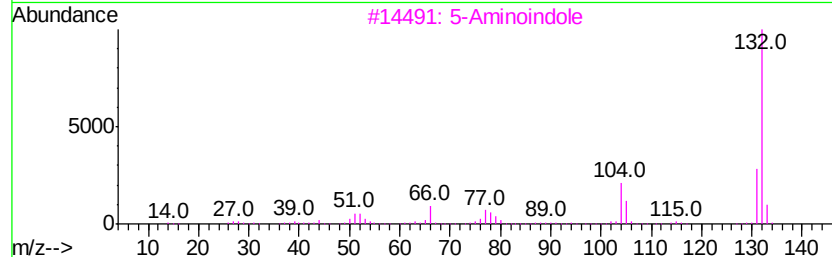
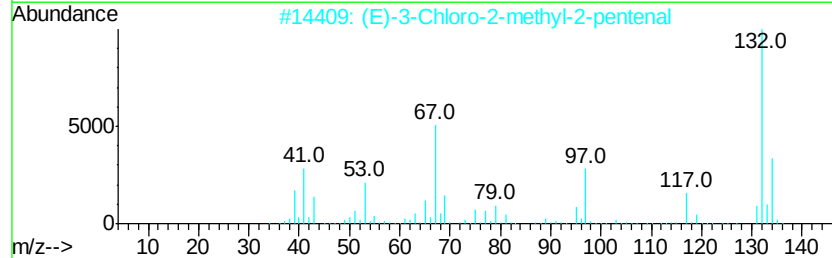
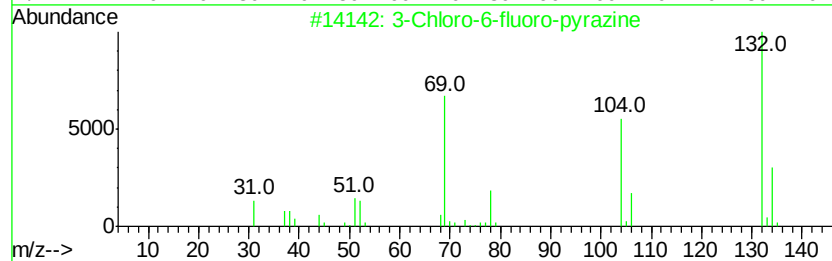
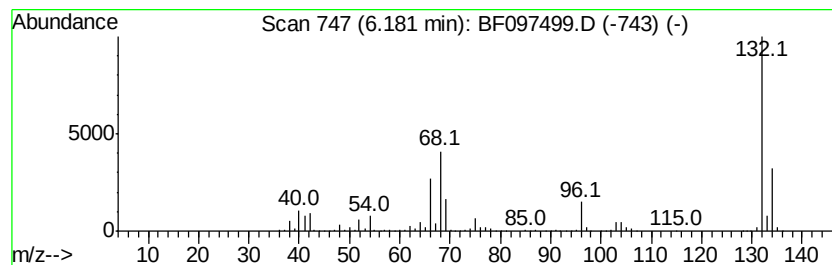
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Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	92.89 ng	2193820	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
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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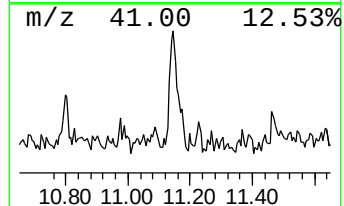
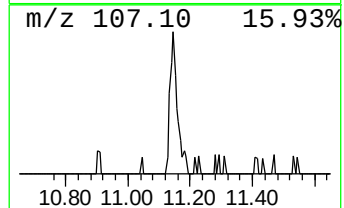
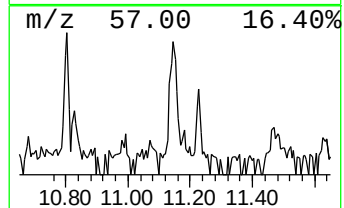
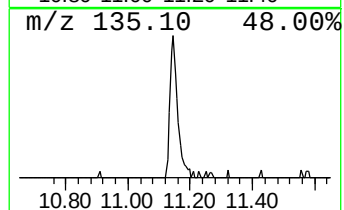
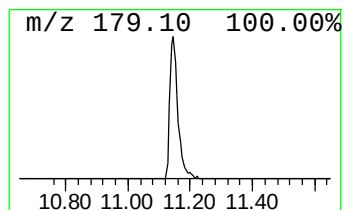
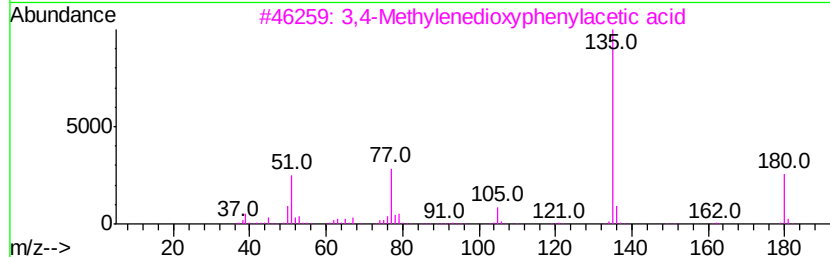
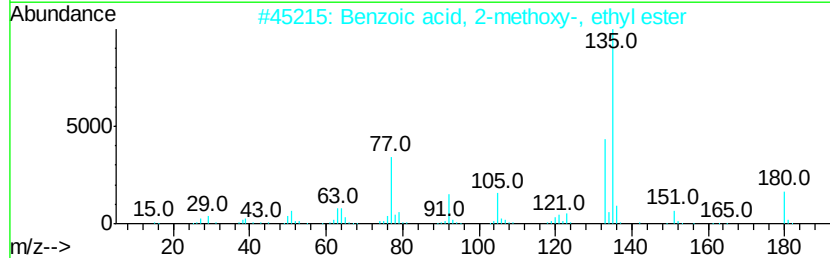
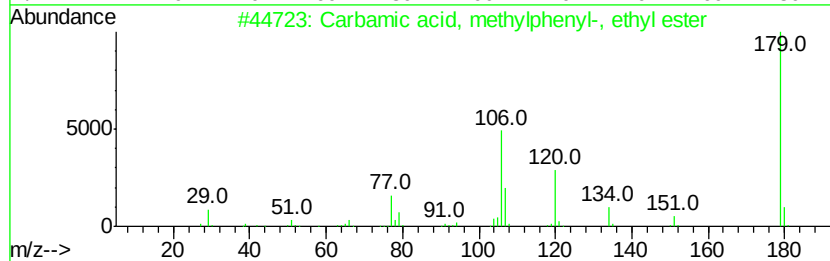
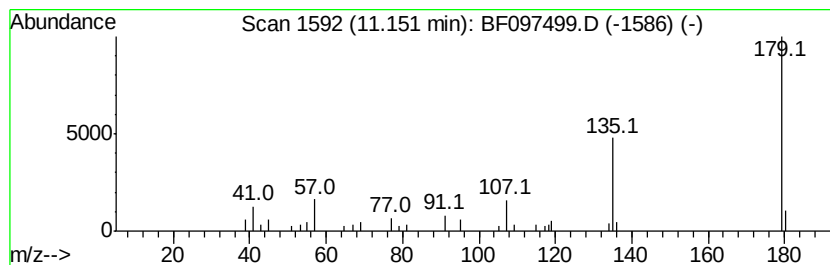
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Peak Number 4 unknown11.15 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	3.18 ng	74874	Phenanthrene-d10	10.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbamic acid, methylphenyl-, et...	179	C10H13NO2	002621-79-6	38
2		Benzoic acid, 2-methoxy-, ethyl ...	180	C10H12O3	007335-26-4	22
3		3,4-Methylenedioxyphenylacetic acid	180	C9H8O4	002861-28-1	14
4		4-Methoxy-3-methylphenylacetic acid	180	C10H12O3	004513-73-9	14
5		Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	000501-00-8	12



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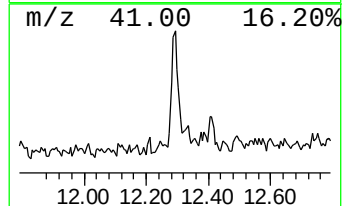
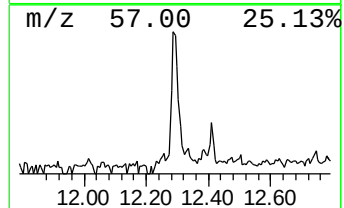
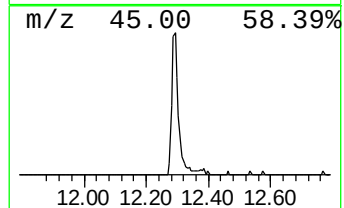
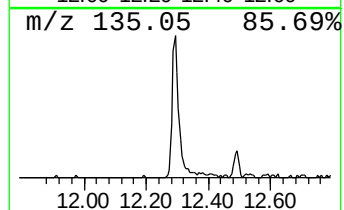
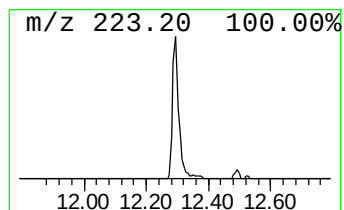
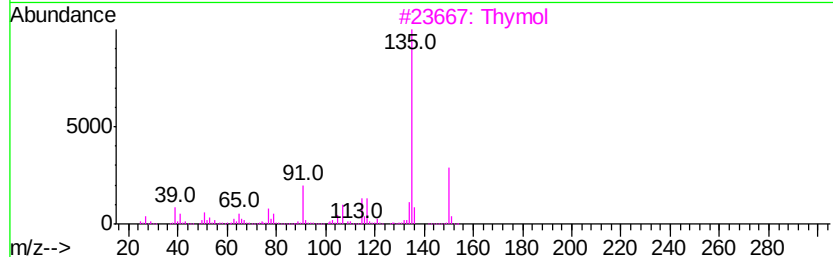
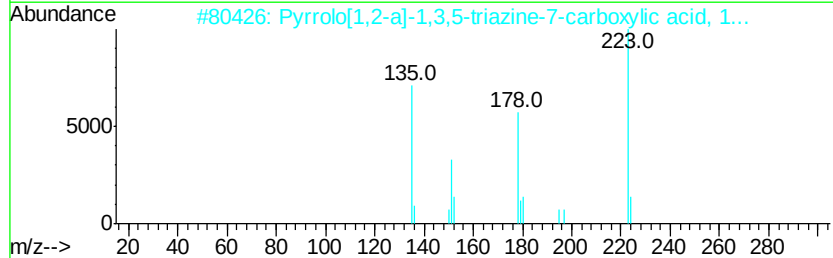
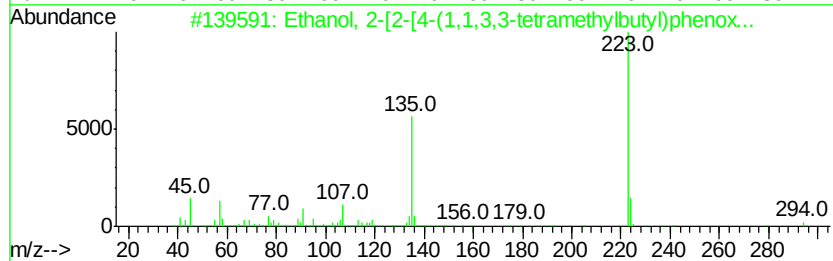
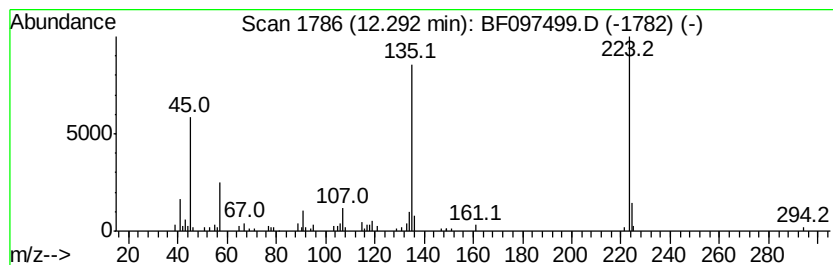
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Peak Number 5 Ethanol, 2-[2-[4-(1,1,3,3-t... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.29	6.52 ng	147906	Chrysene-d12	13.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	92
2	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	83
3	Thymol	150	C10H14O	000089-83-8	35
4	((1,2-Diethylethylene)bis(p-phen...	354	C22H26O4	004547-76-6	35
5	4-Cyanobenzoic acid, 2-(1-adaman...	309	C20H23NO2	1000292-45-1	27



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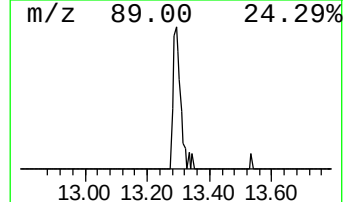
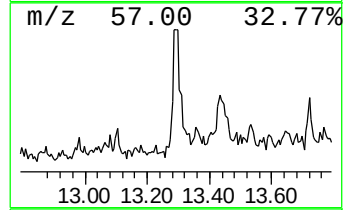
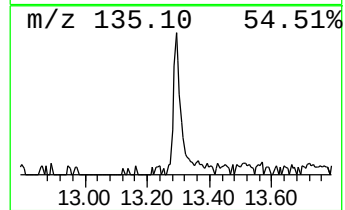
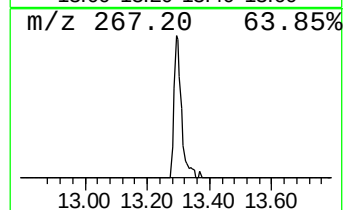
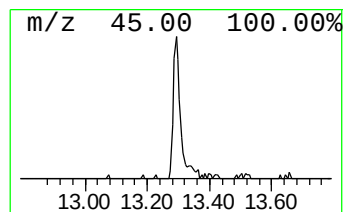
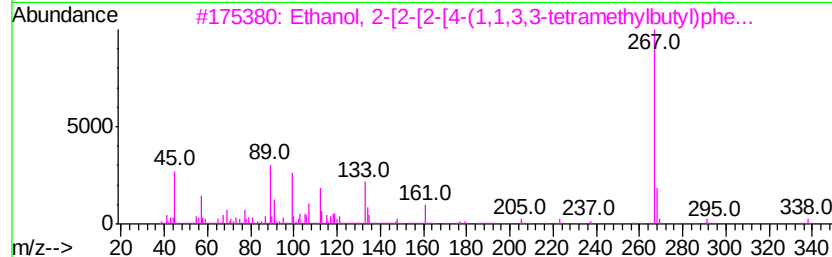
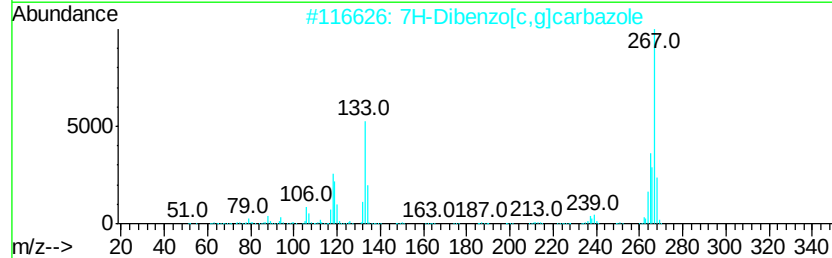
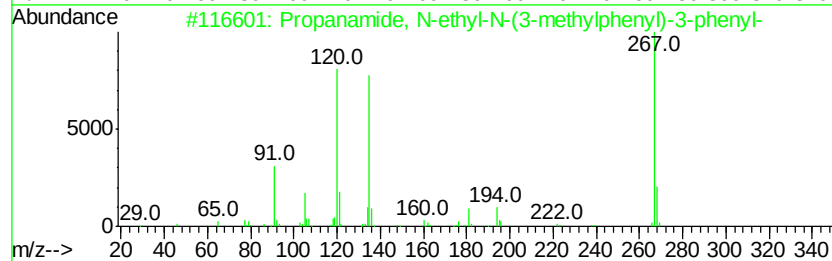
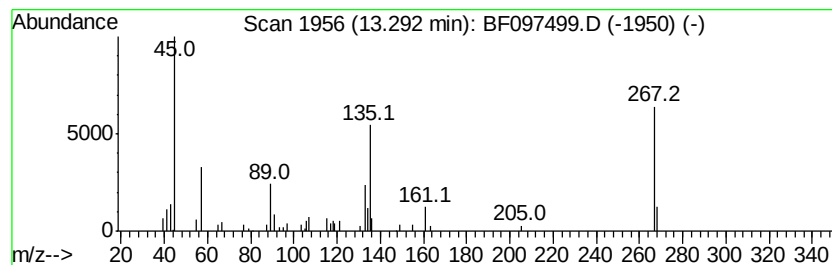
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Peak Number 6 Propanamide, N-ethyl-N-(3-m... Concentration Rank 5

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13.29	4.04 ng	91625	Chrysene-d12	13.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1000308-21-3	52
2	7H-Dibenzo[c,q]carbazole	267	C20H13N	000194-59-2	32
3	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	27
4	N-(1-Methyl-2-benzovlethylidene)...	267	C17H17NO2	039137-44-5	12
5	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	10



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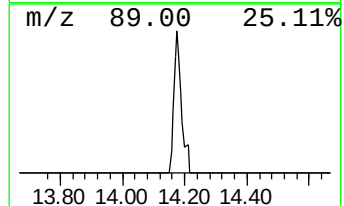
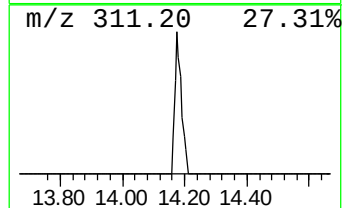
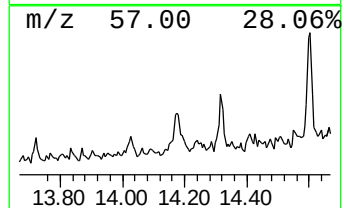
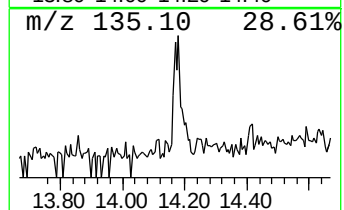
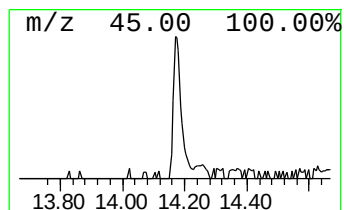
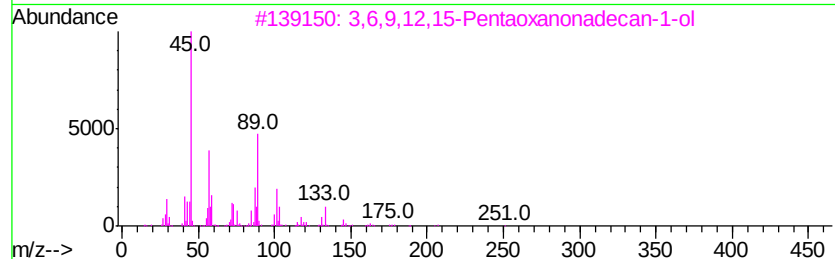
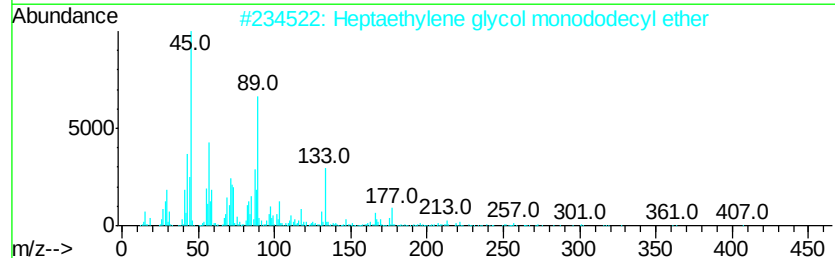
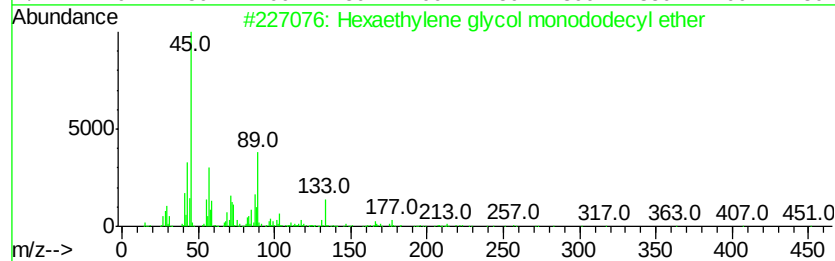
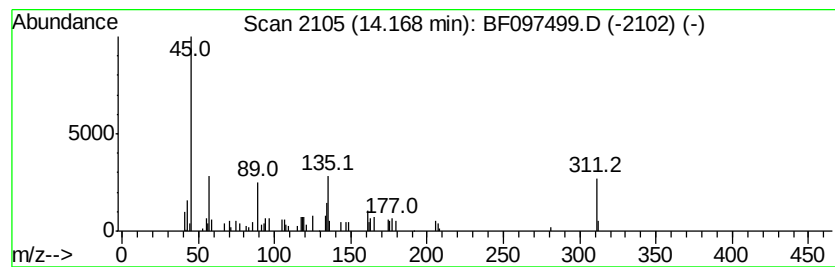
Instrument :
BNA_F
ClientSampleId :
PMW-1A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.17 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	2.22 ng	50453	Chrysene-d12	13.53
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexaethylene glycol monododecyl ...	450 C24H50O7	003055-96-7	38
2	Heptaethylene glycol monododecyl...	494 C26H54O8	003055-97-8	32
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294 C14H30O6	001786-94-3	32
4	1-Methoxy-3-(2-trimethylsilyloxy...	274 C15H34O2Si	1000216-82-7	25
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370 C16H34O9	005117-19-1	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097499.D
Acq On : 9 Aug 2017 5:34
Operator : SJ/JU
Sample : I4604-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

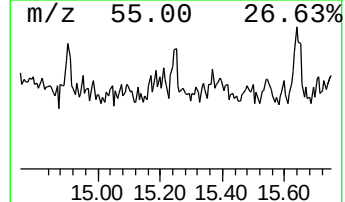
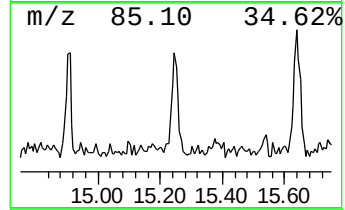
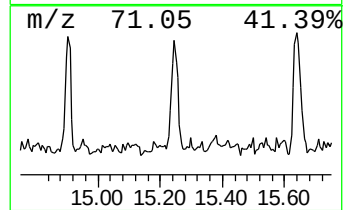
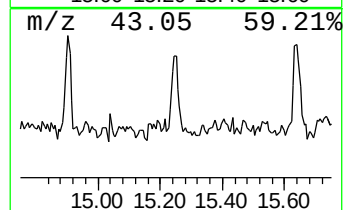
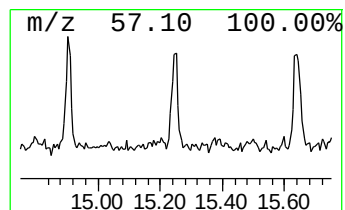
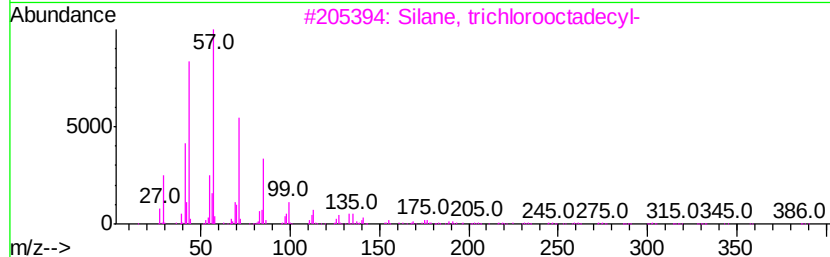
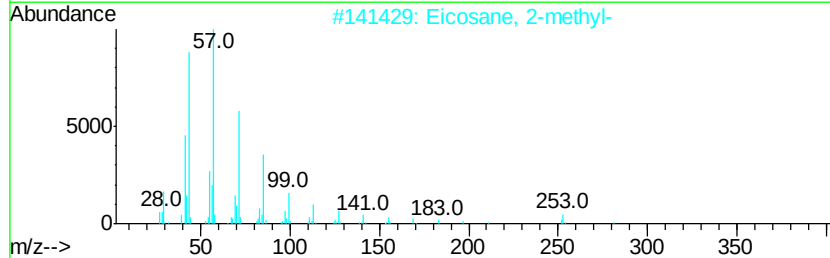
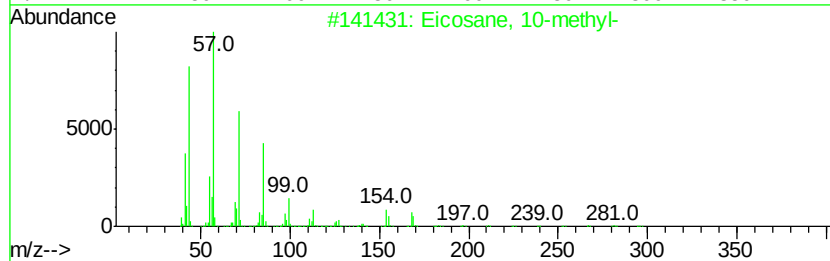
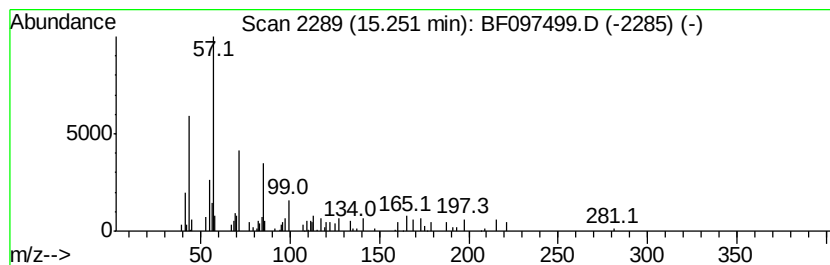
Instrument :
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ClientSampleId :
PMW-1A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Eicosane, 10-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.07 ng	53368	Perylene-d12	14.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane, 10-methyl-	296 C21H44	054833-23-7	64
2	Eicosane, 2-methyl-	296 C21H44	001560-84-5	64
3	Silane, trichlorooctadecyl-	386 C18H37Cl3Si	000112-04-9	64
4	Tetracosane	338 C24H50	000646-31-1	64
5	5-Ethylnonadecane	296 C21H44	1000360-43-1	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097499.D
Acq On : 9 Aug 2017 5:34
Operator : SJ/JU
Sample : I4604-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

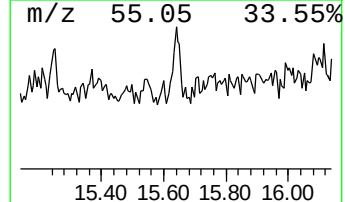
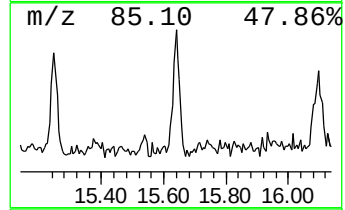
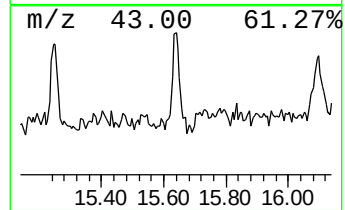
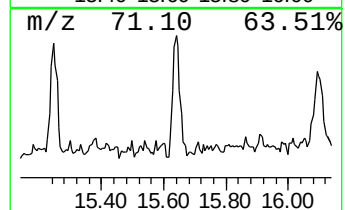
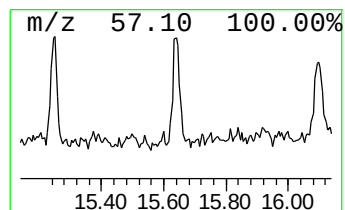
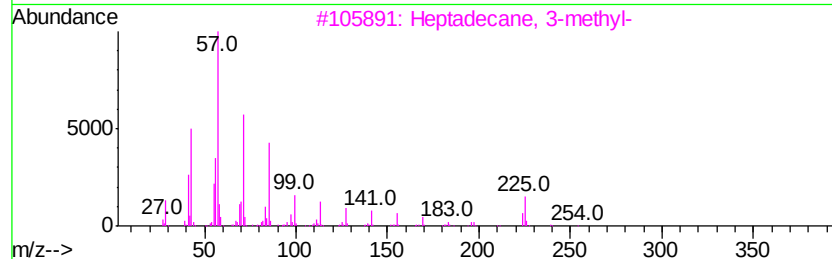
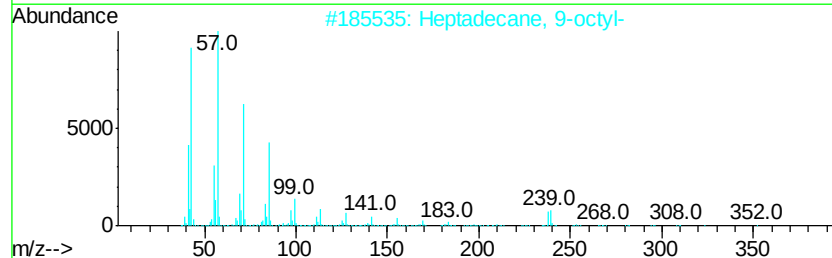
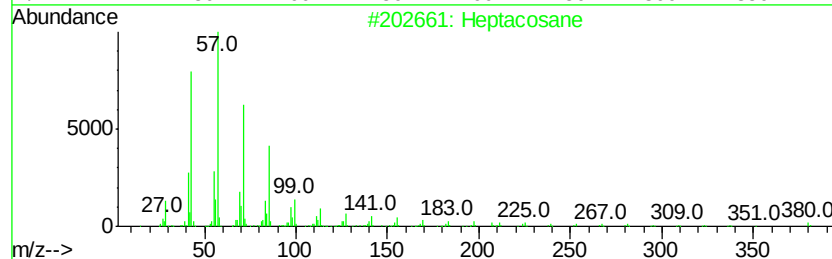
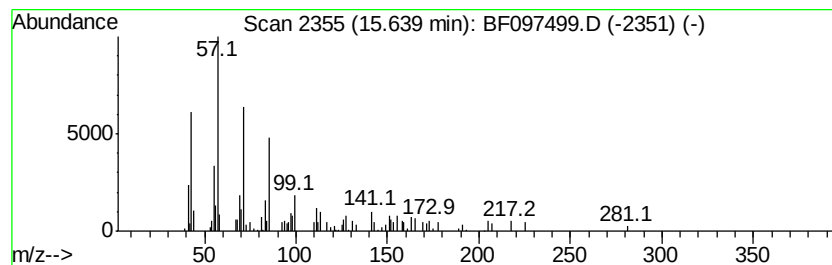
Instrument :
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ClientSampleId :
PMW-1A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	5.05 ng	88010	Perylene-d12	14.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptacosane	380 C27H56	000593-49-7	87
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
3	Heptadecane, 3-methyl-	254 C18H38	006418-44-6	86
4	triacontane	422 C30H62	000638-68-6	86
5	Pentacosane	352 C25H52	000629-99-2	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097499.D
Acq On : 9 Aug 2017 5:34
Operator : SJ/JU
Sample : I4604-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PMW-1A-080217

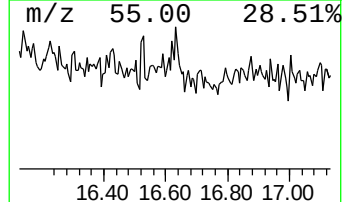
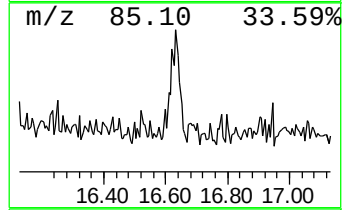
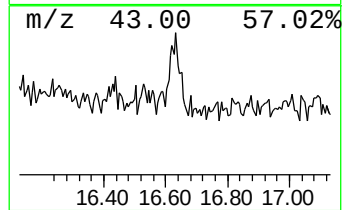
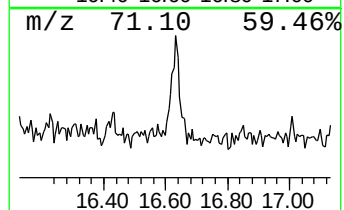
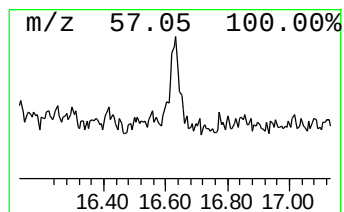
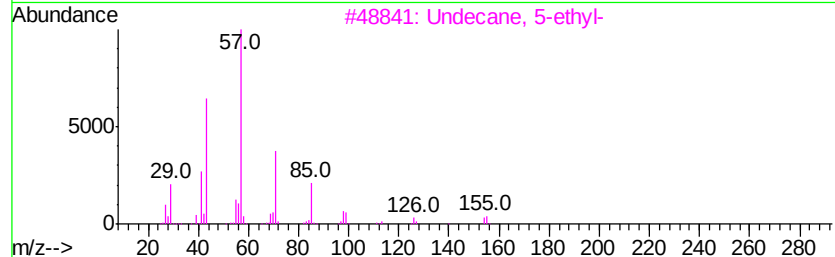
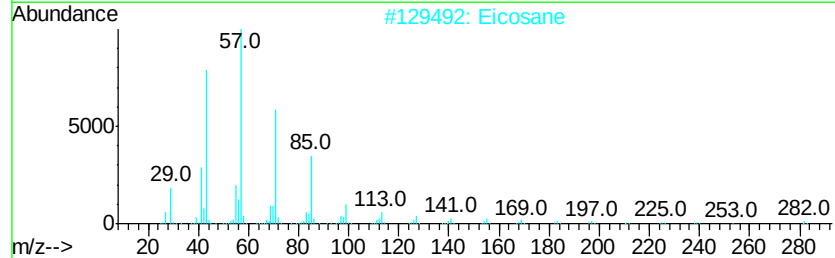
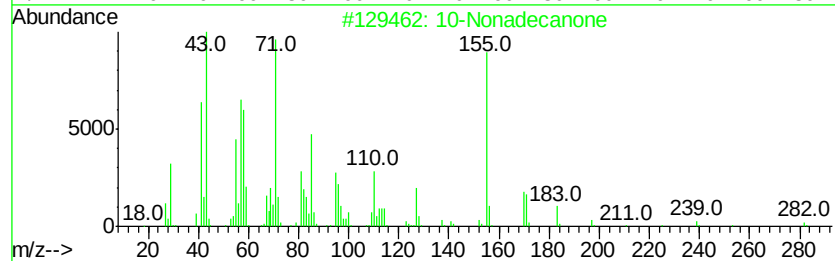
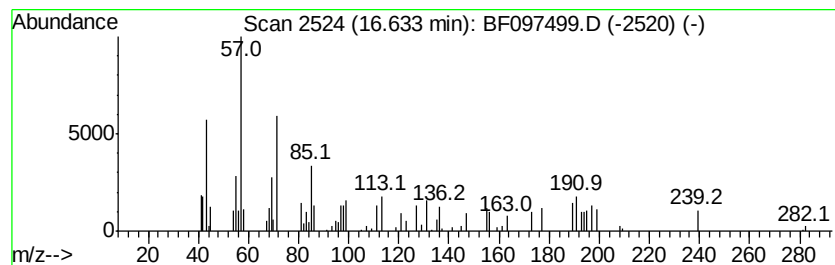
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.63 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.38 ng	41474	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	10-Nonadecanone	282	C19H38O	000504-57-4	38
2		Eicosane	282	C20H42	000112-95-8	30
3		Undecane, 5-ethyl-	184	C13H28	017453-94-0	27
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	27
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097499.D
Acq On : 9 Aug 2017 5:34
Operator : SJ/JU
Sample : I4604-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PMW-1A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.53	3.7	ng	86662	1	6.40	472365	20.0
unknown6.18	6.18	92.9	ng	2193820	1	6.40	472365	20.0
unknown11.15	11.15	3.2	ng	74874	4	10.90	470352	20.0
Ethanol, 2-[2-[4-...	12.29	6.5	ng	147906	5	13.53	453646	20.0
Propanamide, N-et...	13.29	4.0	ng	91625	5	13.53	453646	20.0
unknown14.17	14.17	2.2	ng	50453	5	13.53	453646	20.0
Eicosane, 10-methyl-	15.25	3.1	ng	53368	6	14.87	348212	20.0
Heptacosane	15.64	5.0	ng	88010	6	14.87	348212	20.0
unknown16.63	16.63	2.4	ng	41474	6	14.87	348212	20.0