

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
 Data File : BF095130.D
 Acq On : 15 May 2017 17:38
 Operator : SJ/MA
 Sample : I3122-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72-11997-72-12002-72-11979-C

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-BF050217.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	1.960	3	4	15	rVB	64926	81730	3.38%	0.423%
2	5.137	540	544	562	rBV	153392	330287	13.66%	1.709%
3	5.748	645	648	675	rBV	838570	1791326	74.10%	9.271%
4	7.319	911	915	932	rBV	1053062	1726943	71.43%	8.938%
5	7.442	932	936	952	rVB	1346857	1953618	80.81%	10.111%
6	7.778	989	993	1005	rBV	386702	509371	21.07%	2.636%
7	8.013	1029	1033	1048	rBV	1301736	1650941	68.29%	8.544%
8	8.677	1141	1146	1163	rBV	675628	974858	40.32%	5.045%
9	9.795	1332	1336	1346	rBV	444759	601380	24.88%	3.112%
10	11.566	1632	1637	1653	rBV	1947870	2417534	100.00%	12.512%
11	11.777	1669	1673	1680	rBV2	40107	54160	2.24%	0.280%
12	12.260	1751	1755	1761	rBV	126479	196419	8.12%	1.017%
13	12.624	1812	1817	1827	rBV2	589222	876557	36.26%	4.537%
14	13.165	1906	1909	1915	rVB2	21028	29306	1.21%	0.152%
15	13.460	1955	1959	1964	rBV	115267	127833	5.29%	0.662%
16	13.818	2012	2020	2024	rBV2	35861	72186	2.99%	0.374%
17	13.918	2030	2037	2051	rBV	760975	1194053	49.39%	6.180%
18	14.236	2087	2091	2093	rBV	128240	160123	6.62%	0.829%
19	14.965	2210	2215	2219	rBV	105898	124160	5.14%	0.643%
20	15.030	2219	2226	2242	rVB	493554	767484	31.75%	3.972%
21	15.624	2323	2327	2332	rVV	89976	100742	4.17%	0.521%
22	15.871	2365	2369	2376	rVB9	12094	26447	1.09%	0.137%
23	15.989	2383	2389	2397	rBV3	44407	98865	4.09%	0.512%
24	16.218	2424	2428	2433	rBV	72257	85268	3.53%	0.441%
25	16.759	2516	2520	2525	rVB	65236	63889	2.64%	0.331%
26	17.259	2601	2605	2609	rVB	44981	49961	2.07%	0.259%
27	17.348	2615	2620	2628	rBV	1606710	1847824	76.43%	9.563%
28	17.730	2681	2685	2688	rBV	33413	36647	1.52%	0.190%
29	18.594	2828	2832	2836	rBV4	29234	40834	1.69%	0.211%
30	18.700	2846	2850	2856	rBV	367773	475778	19.68%	2.462%
31	18.994	2896	2900	2906	rBV5	19382	29494	1.22%	0.153%
32	19.377	2962	2965	2970	rBV3	25585	30466	1.26%	0.158%
33	20.106	3085	3089	3092	rVB2	42888	51035	2.11%	0.264%
34	20.371	3130	3134	3145	rVB	362006	540452	22.36%	2.797%

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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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.836	3211	3213	3216	rVB2	30603	31424	1.30%	0.163%
36	20.971	3234	3236	3242	rBV7	15417	24502	1.01%	0.127%
37	21.247	3278	3283	3284	rBV5	18322	27122	1.12%	0.140%
38	21.271	3284	3287	3292	rVV5	19071	37455	1.55%	0.194%
39	21.783	3370	3374	3379	rVB8	43378	83237	3.44%	0.431%

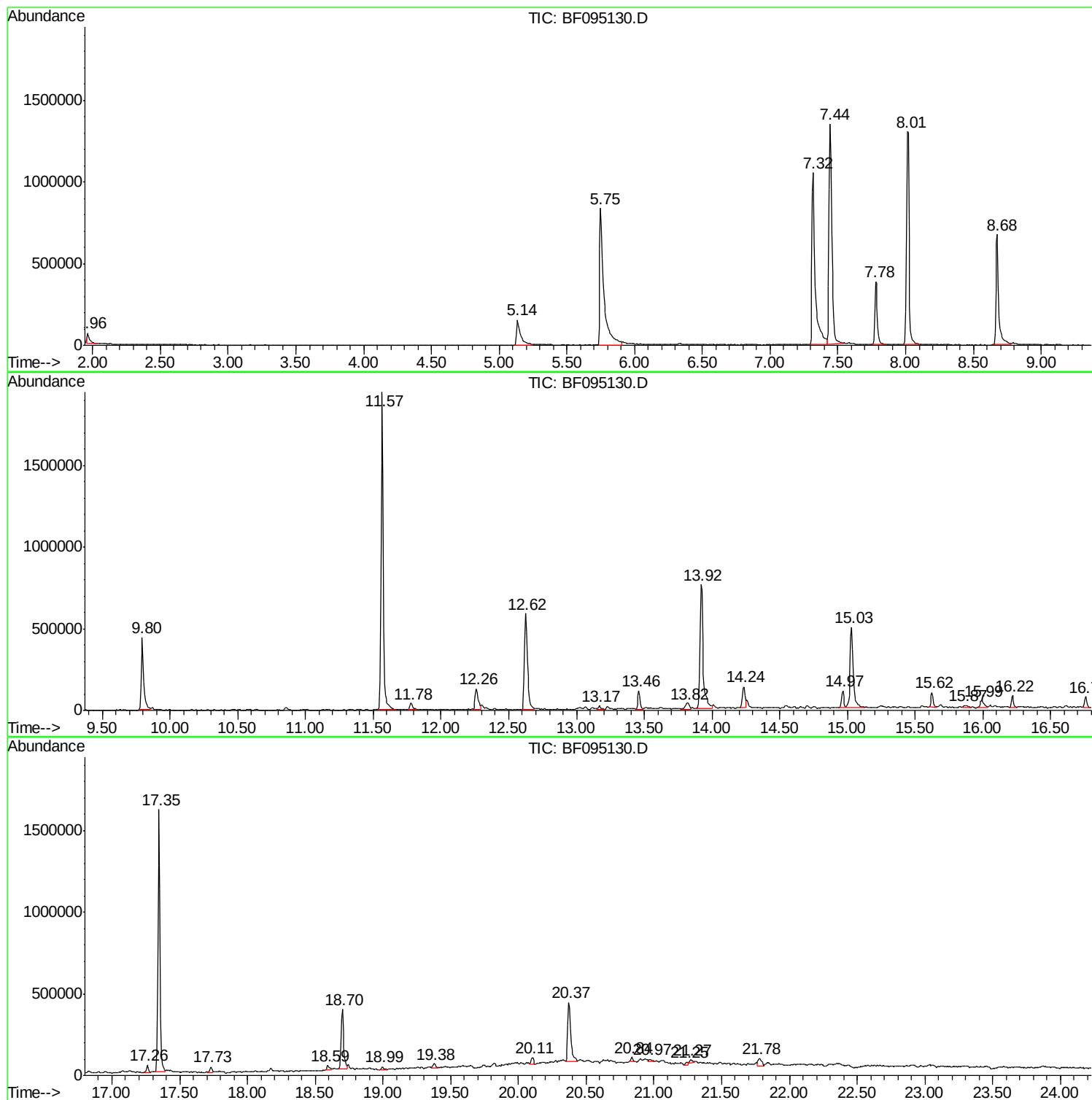
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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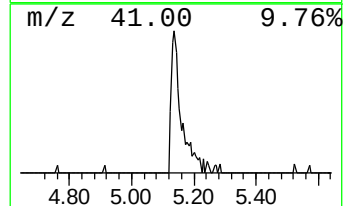
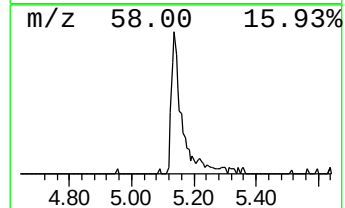
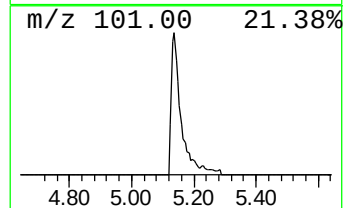
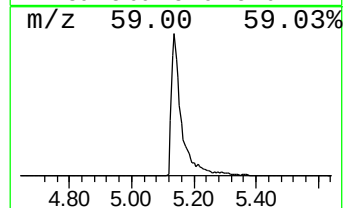
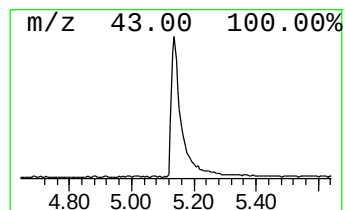
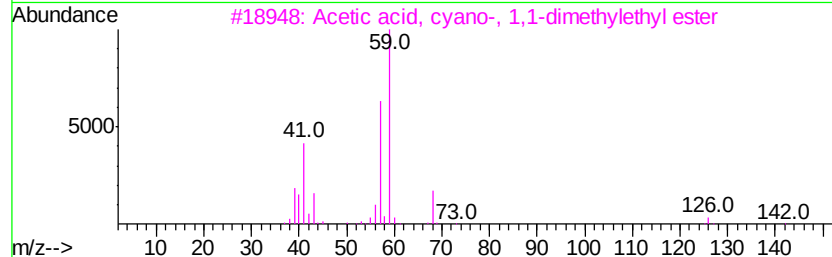
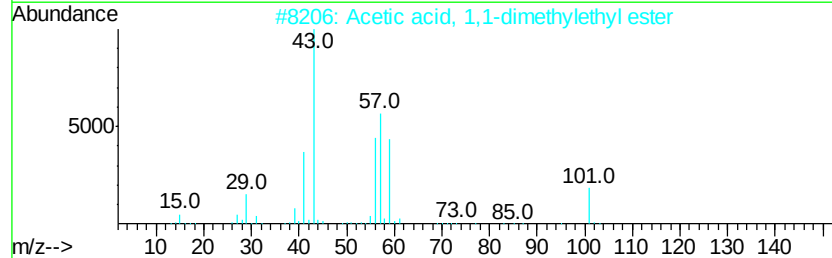
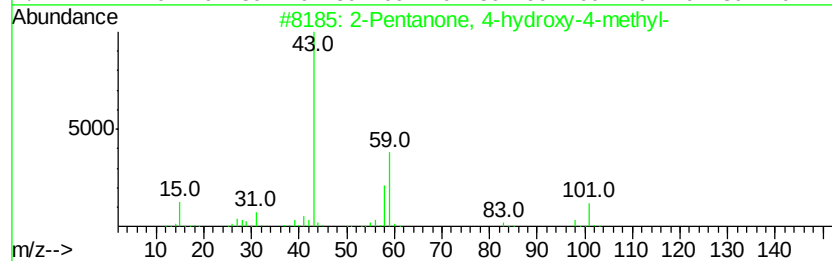
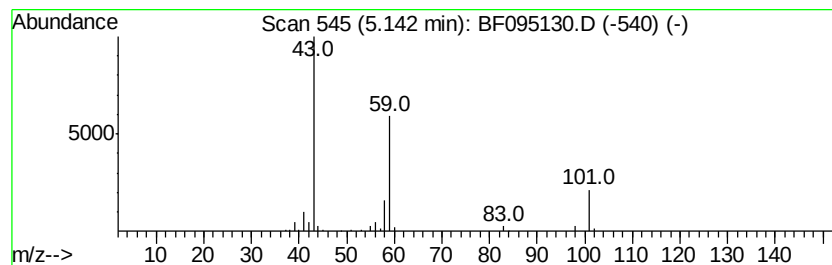
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	12.97 ng	330287	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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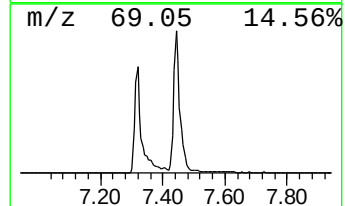
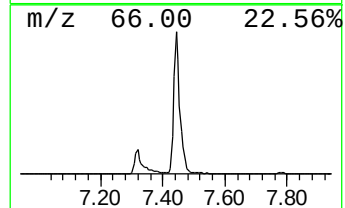
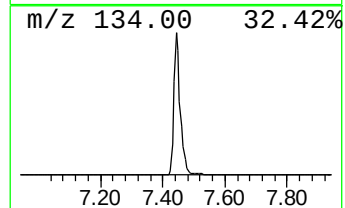
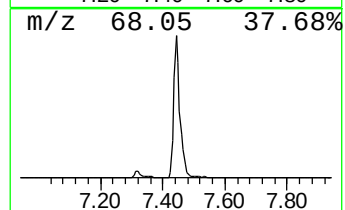
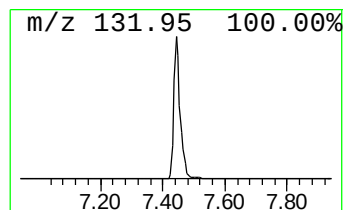
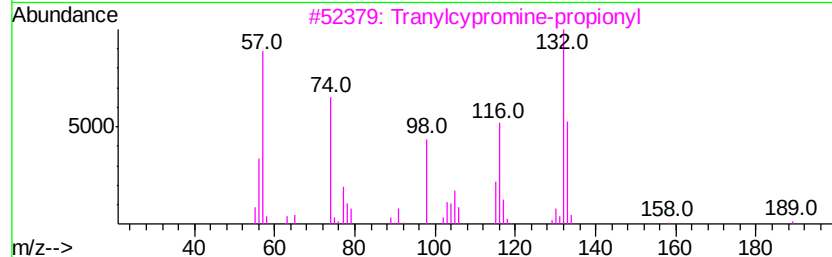
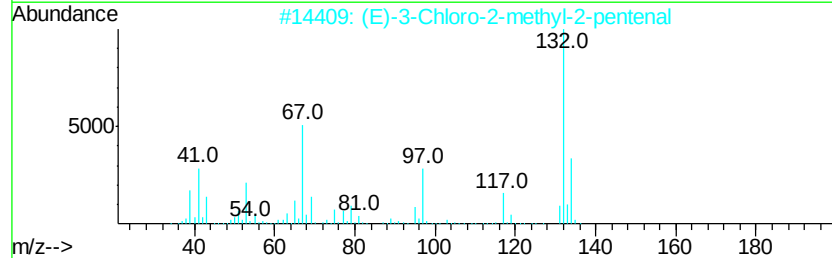
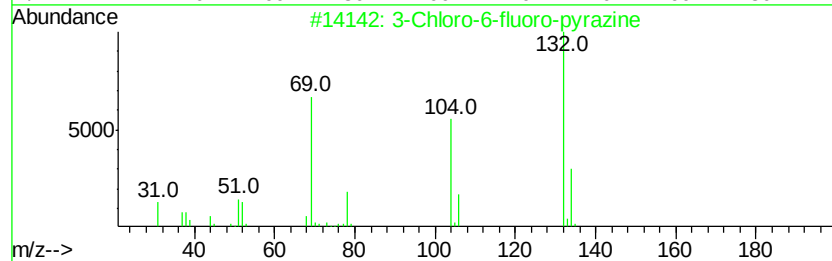
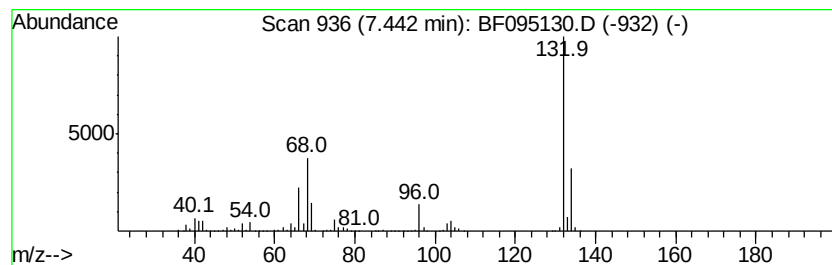
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	76.71 ng	1953620	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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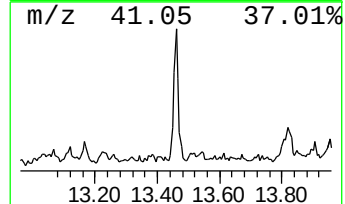
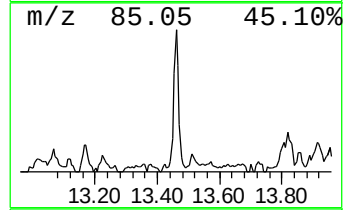
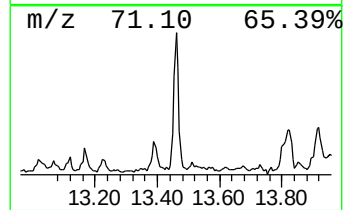
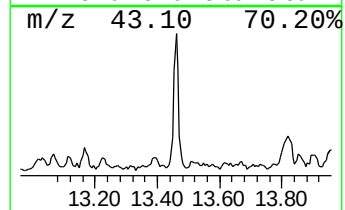
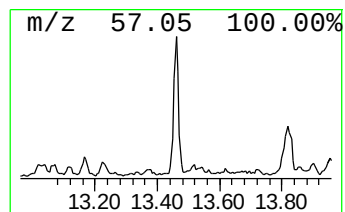
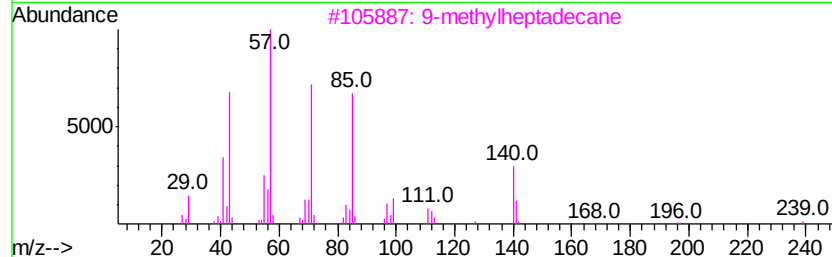
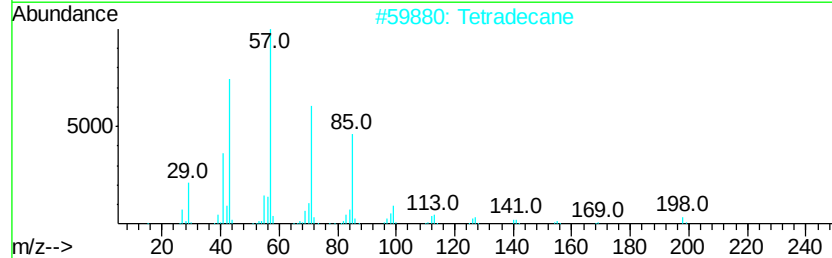
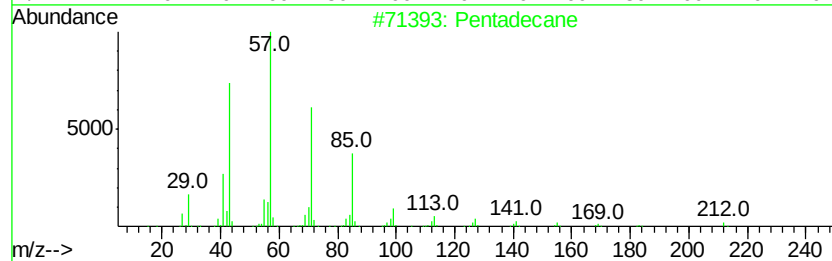
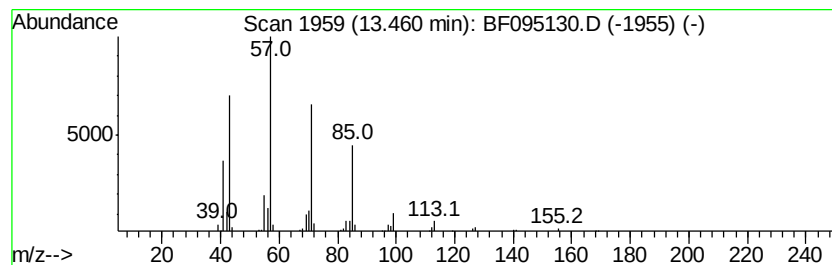
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	2.92 ng	127833	Acenaphthene-d10	12.62
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentadecane	212 C15H32	000629-62-9	87
2	Tetradecane	198 C14H30	000629-59-4	87
3	9-methylheptadecane	254 C18H38	026741-18-4	86
4	Sulfurous acid, 2-propyl tetradec...	320 C17H36O3S	1000309-12-5	86
5	Nonadecane	268 C19H40	000629-92-5	86



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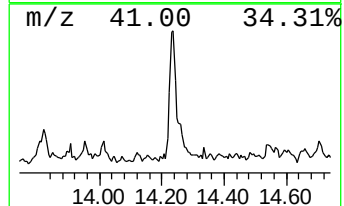
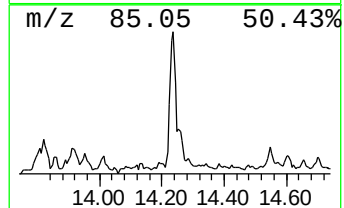
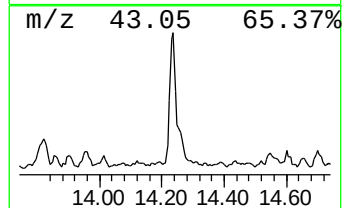
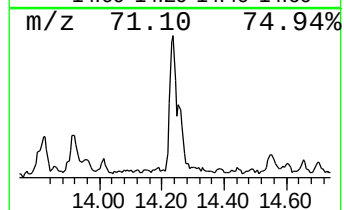
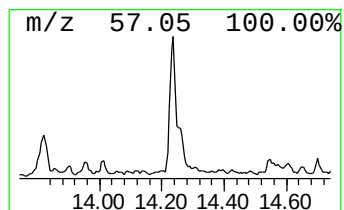
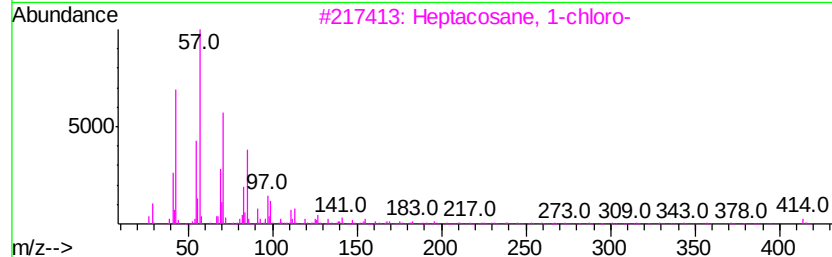
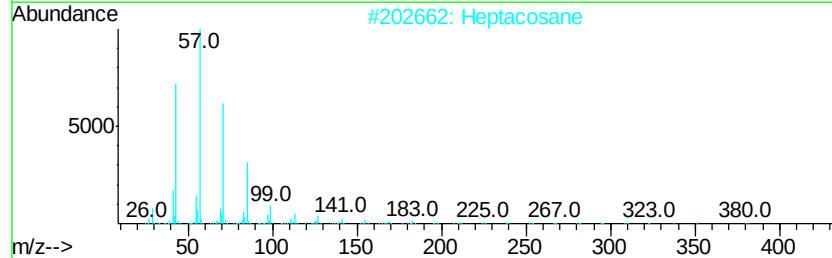
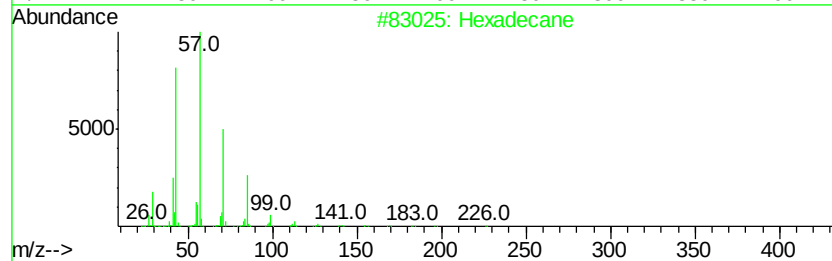
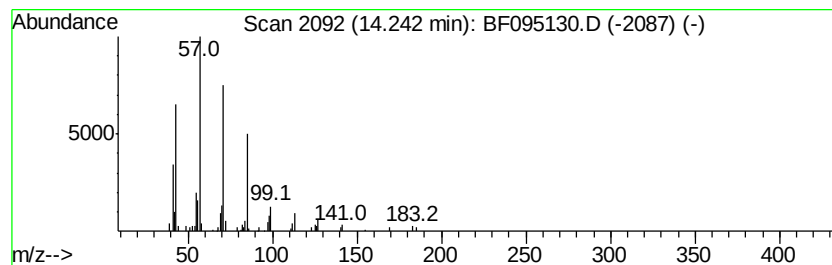
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.24	4.17 ng	160123	Phenanthrene-d10		15.03	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Heptacosane		380	C27H56	000593-49-7	90
3	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	86
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	86
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86



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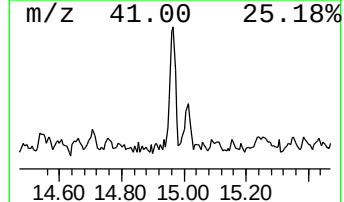
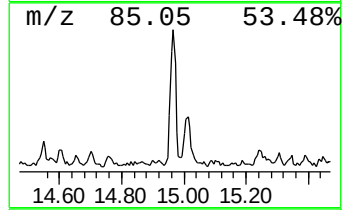
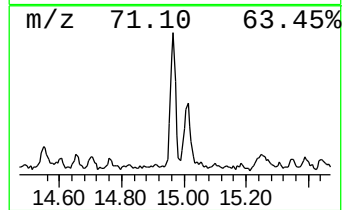
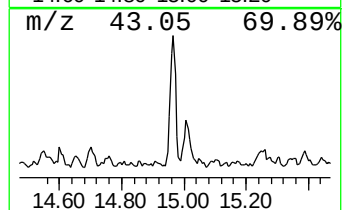
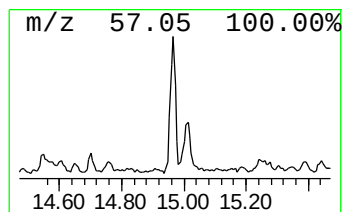
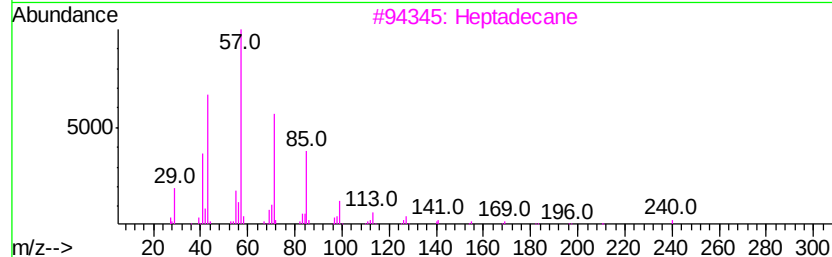
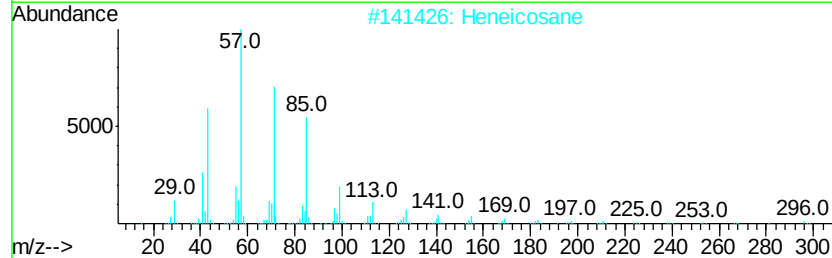
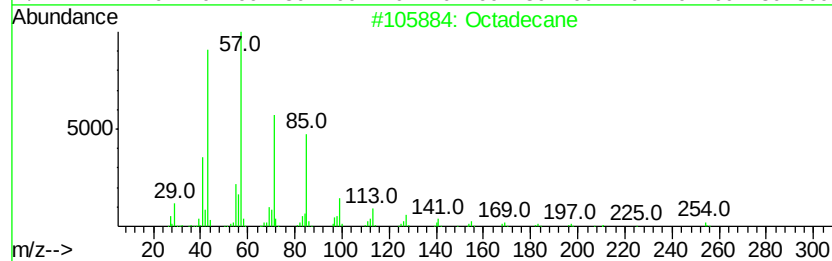
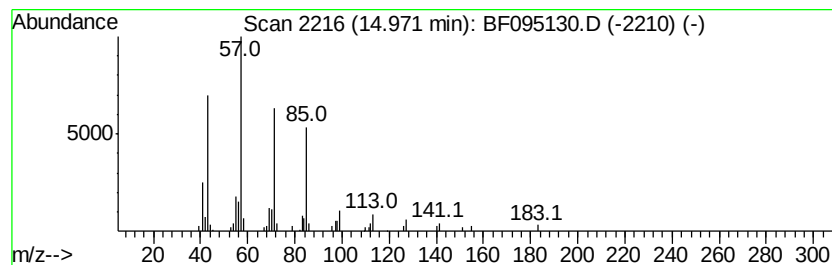
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	3.24 ng	124160	Phenanthrene-d10	15.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Pentadecane	212	C15H32	000629-62-9	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

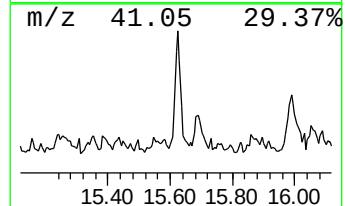
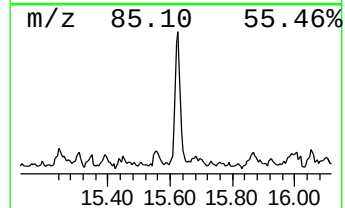
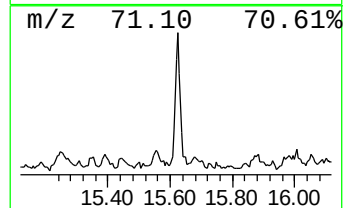
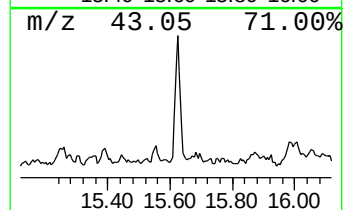
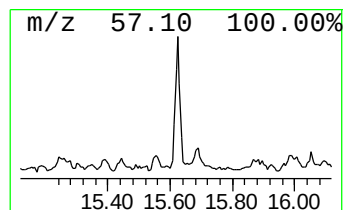
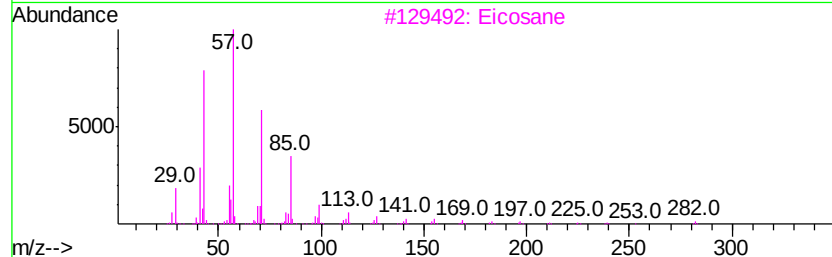
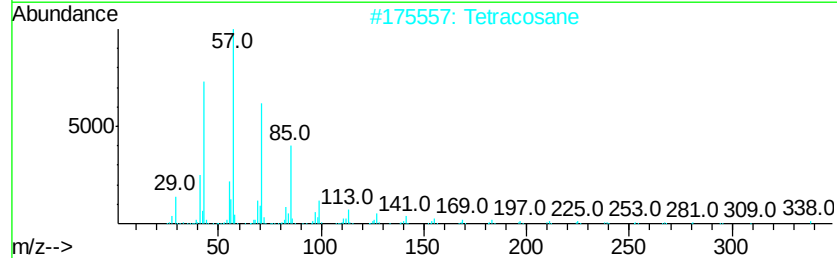
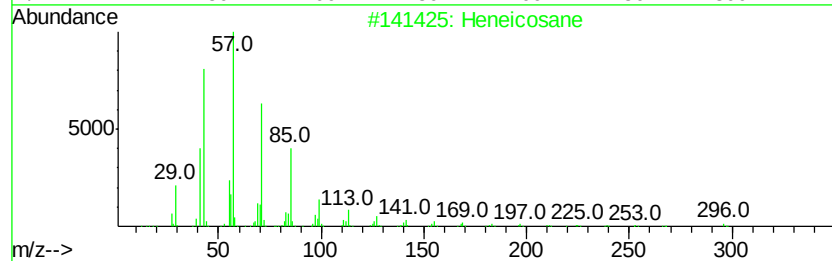
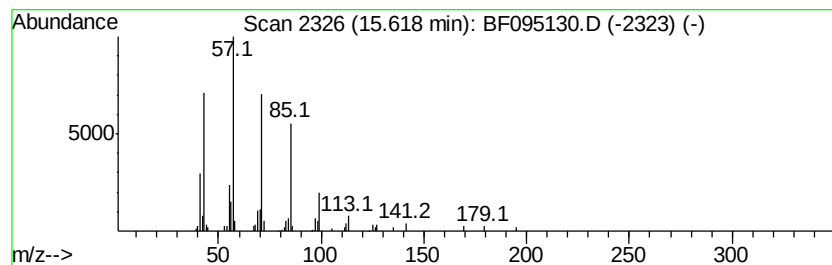
Instrument :
BNA_F
ClientSampleId :
RO-72-11997-72-12002-72-11979-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.62	2.63 ng	100742	Phenanthrene-d10		15.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

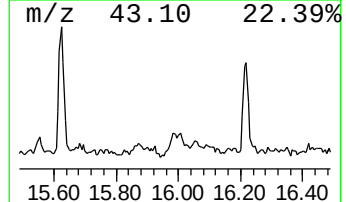
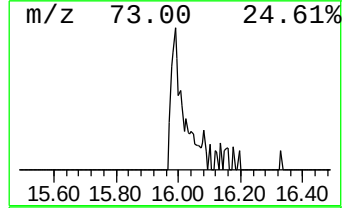
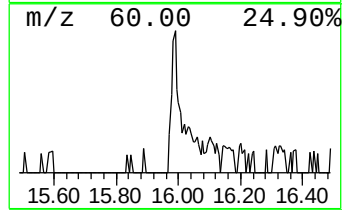
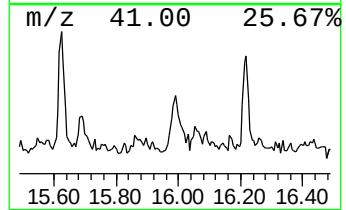
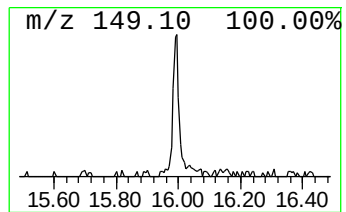
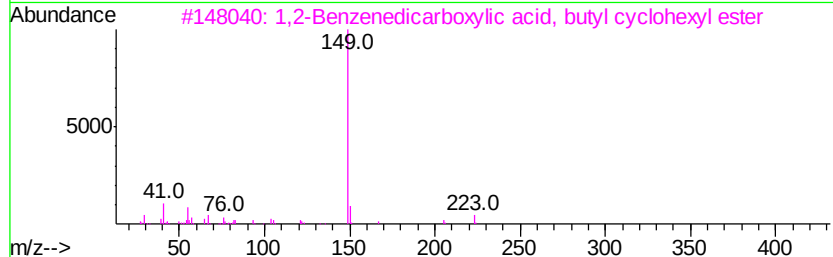
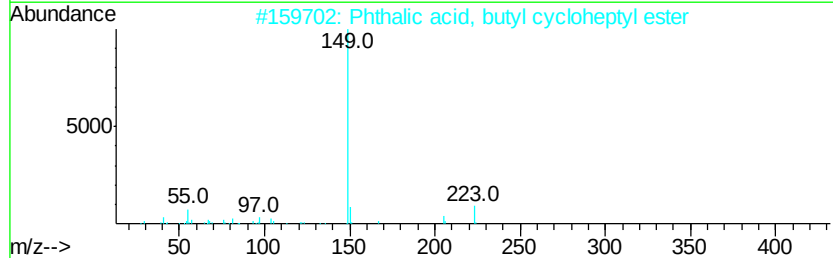
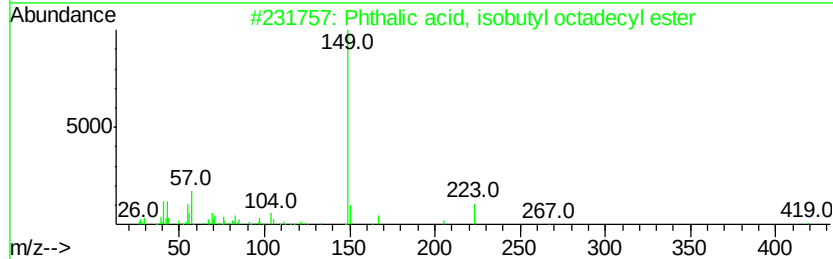
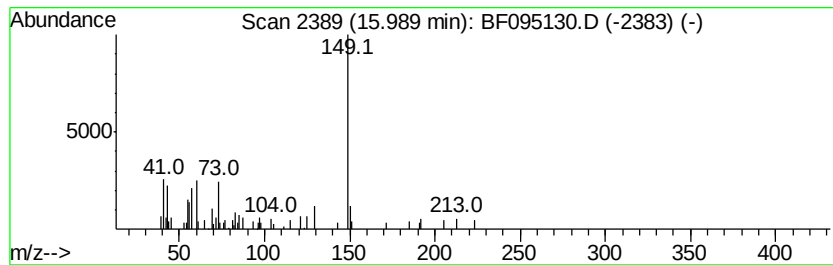
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ClientSampleId :
RO-72-11997-72-12002-72-11979-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.99 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.99	2.58 ng	98865	Phenanthrene-d10	15.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, isobutyl octadecyl...	474	C30H50O4	1000309-06-1	47
2	Phthalic acid, butyl cycloheptyl...	318	C19H26O4	1000322-82-9	47
3	1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	47
4	Phthalic acid, isobutyl 4-methyl...	334	C20H30O4	1000377-93-8	47
5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

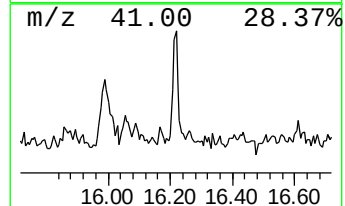
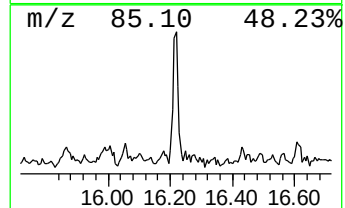
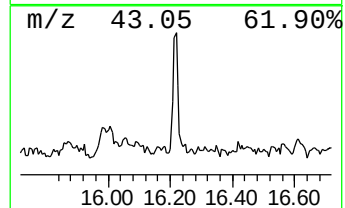
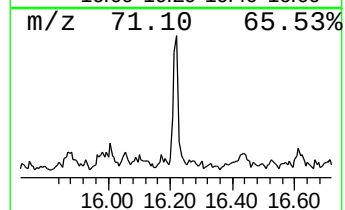
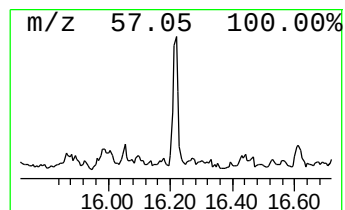
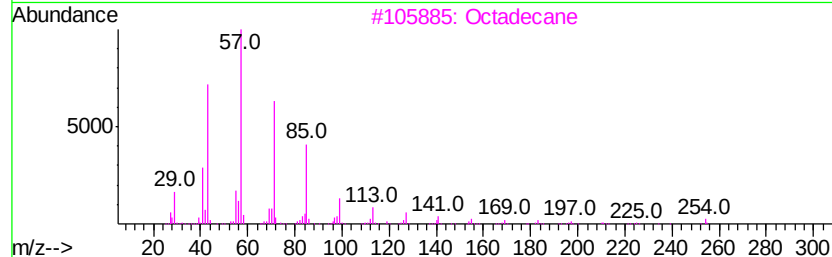
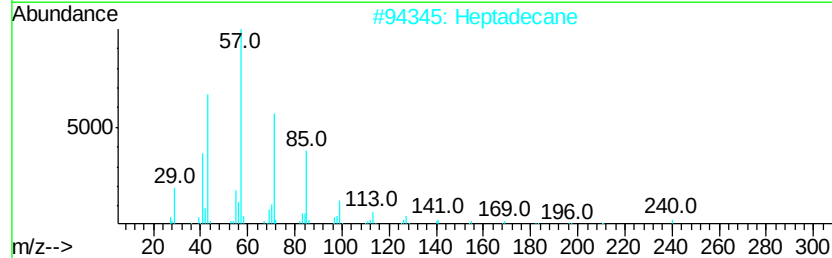
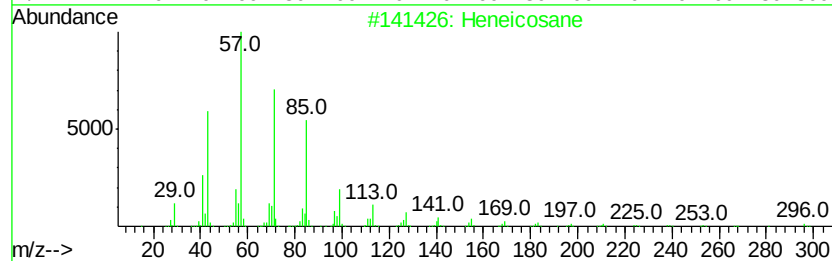
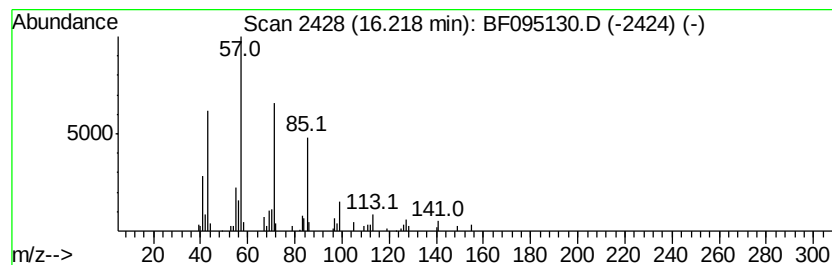
Instrument :
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ClientSampleId :
RO-72-11997-72-12002-72-11979-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.22	2.22 ng	85268	Phenanthrene-d10		15.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11997-72-12002-72-11979-C

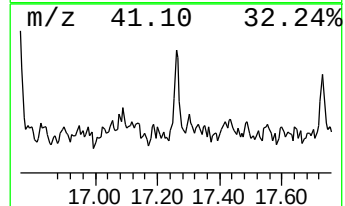
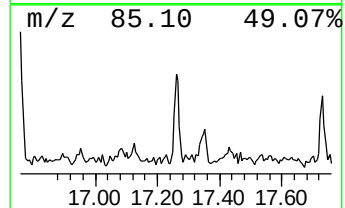
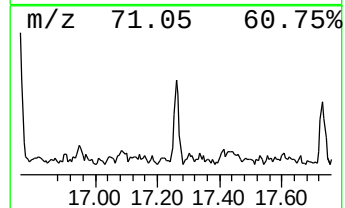
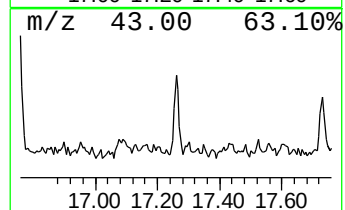
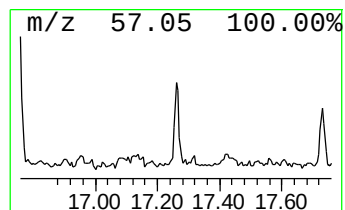
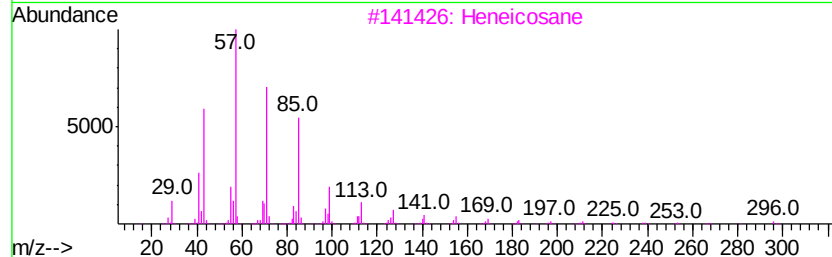
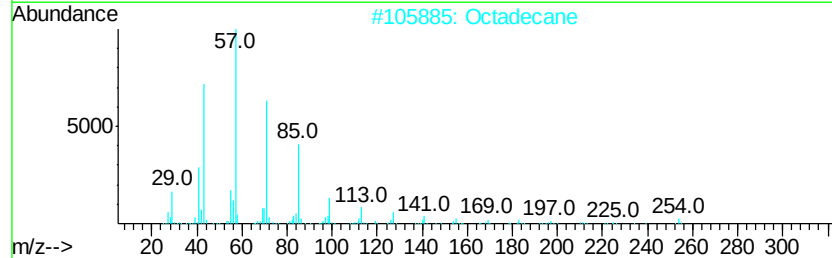
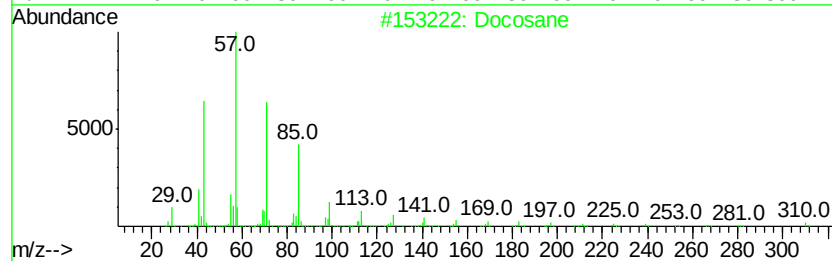
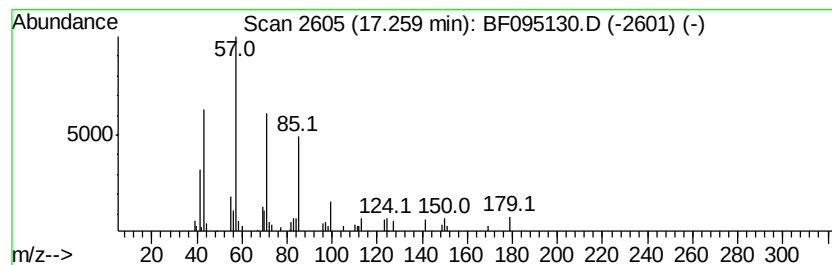
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Docosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.26	2.10 ng	49961	Chrysene-d12	18.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	80
2		Octadecane	254	C18H38	000593-45-3	80
3		Heneicosane	296	C21H44	000629-94-7	74
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	74
5		Tetracosane	338	C24H50	000646-31-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
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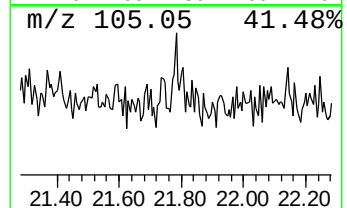
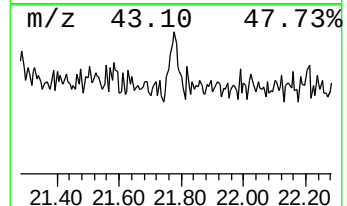
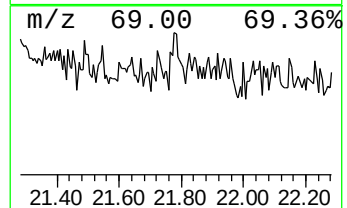
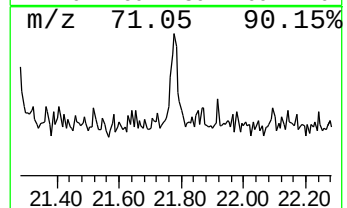
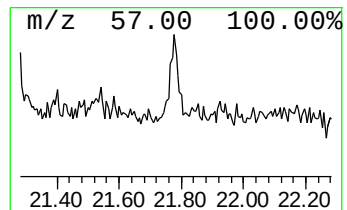
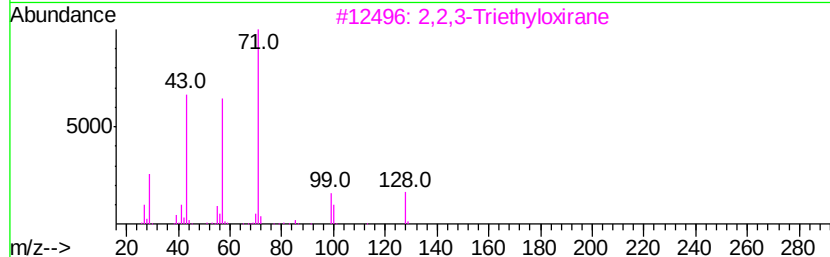
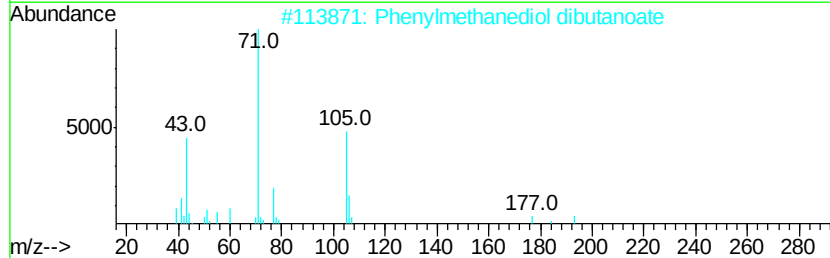
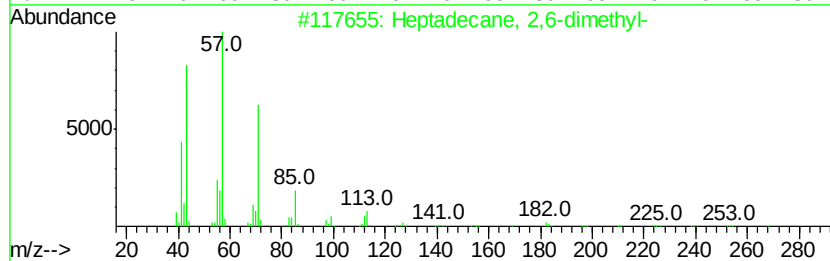
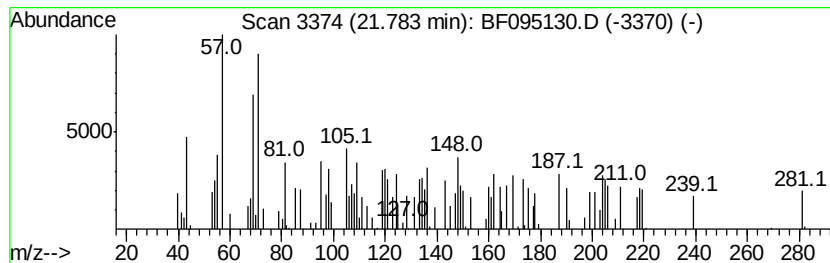
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown21.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.78	3.08 ng	83237	Perylene-d12	20.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	14
2	Phenylmethanediol dibutanoate	264	C15H20O4	002929-77-3	14
3	2,2,3-Triethyloxirane	128	C8H16O	053229-40-6	14
4	2-Ethylbutyryl chloride	134	C6H11ClO	002736-40-5	14
5	11-Methylnonacosane	422	C30H62	007371-99-5	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095130.D
Acq On : 15 May 2017 17:38
Operator : SJ/MA
Sample : I3122-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-72-11997-72-12002-72-11979-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
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unknown7.44	7.44	76.7	ng	1953620	1	7.78	509371	20.0
Pentadecane	13.46	2.9	ng	127833	3	12.62	876557	20.0
Hexadecane	14.24	4.2	ng	160123	4	15.03	767484	20.0
Octadecane	14.97	3.2	ng	124160	4	15.03	767484	20.0
Heneicosane	15.62	2.6	ng	100742	4	15.03	767484	20.0
unknown15.99	15.99	2.6	ng	98865	4	15.03	767484	20.0
Heptadecane	16.22	2.2	ng	85268	4	15.03	767484	20.0
Docosane	17.26	2.1	ng	49961	5	18.70	475778	20.0
unknown21.78	21.78	3.1	ng	83237	6	20.37	540452	20.0