

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
 Data File : BF095793.D
 Acq On : 8 Jun 2017 20:30
 Operator : SJ/MA
 Sample : I3541-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-4215

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-BF060517.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	4.581	506	509	527	rBV	58564	165180	8.81%	0.965%
2	5.263	621	625	655	rBV	951662	1635638	87.26%	9.552%
3	5.522	664	669	676	rVB	20172	35586	1.90%	0.208%
4	6.928	903	908	920	rBV	1047283	1601414	85.43%	9.352%
5	7.022	920	924	937	rVB	1262229	1806650	96.38%	10.550%
6	7.369	978	983	996	rBV	304240	417026	22.25%	2.435%
7	7.604	1018	1023	1037	rBV	993147	1319551	70.39%	7.706%
8	8.286	1133	1139	1161	rBV	675787	994030	53.03%	5.805%
9	9.398	1324	1328	1344	rBV	423873	569569	30.39%	3.326%
10	11.180	1624	1631	1645	rBV	1475521	1874497	100.00%	10.946%
11	11.874	1744	1749	1760	rBV	267389	339087	18.09%	1.980%
12	12.222	1802	1808	1813	rBV2	489252	611287	32.61%	3.570%
13	12.269	1813	1816	1823	rVB	19821	23479	1.25%	0.137%
14	13.080	1948	1954	1959	rBB	24148	29541	1.58%	0.173%
15	13.516	2023	2028	2045	rBV	725236	966275	51.55%	5.643%
16	13.851	2080	2085	2092	rBV	23564	34335	1.83%	0.201%
17	14.304	2158	2162	2168	rBV	63048	74526	3.98%	0.435%
18	14.615	2210	2215	2228	rVB	420806	585330	31.23%	3.418%
19	15.633	2383	2388	2400	rBV2	54944	73863	3.94%	0.431%
20	16.439	2522	2525	2532	rVB	26091	31941	1.70%	0.187%
21	16.739	2570	2576	2583	rBV2	38581	59154	3.16%	0.345%
22	16.992	2613	2619	2623	rBV	1266588	1506799	80.38%	8.799%
23	18.115	2802	2810	2815	rBV	235920	245771	13.11%	1.435%
24	18.245	2828	2832	2842	rBV	80521	120567	6.43%	0.704%
25	18.327	2842	2846	2857	rVV	372771	480819	25.65%	2.808%
26	18.515	2873	2878	2882	rVB	172552	187137	9.98%	1.093%
27	18.568	2882	2887	2890	rBV	268345	291927	15.57%	1.705%
28	18.598	2890	2892	2896	rVV	81427	85149	4.54%	0.497%
29	18.639	2896	2899	2905	rVB	99780	111714	5.96%	0.652%
30	19.015	2959	2963	2965	rBV	34186	34497	1.84%	0.201%
31	19.045	2965	2968	2974	rVB3	21640	26570	1.42%	0.155%
32	19.768	3086	3091	3099	rBV	196699	223347	11.92%	1.304%
33	19.997	3126	3130	3138	rBV	310778	391370	20.88%	2.285%
34	20.445	3202	3206	3210	rBV	43324	55865	2.98%	0.326%

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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

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35	20.815	3262	3269	3273	rBV5	13877	24333	1.30%	0.142%
36	21.027	3301	3305	3311	rVB5	28677	46199	2.46%	0.270%
37	23.021	3636	3644	3655	rVB10	14858	44271	2.36%	0.259%

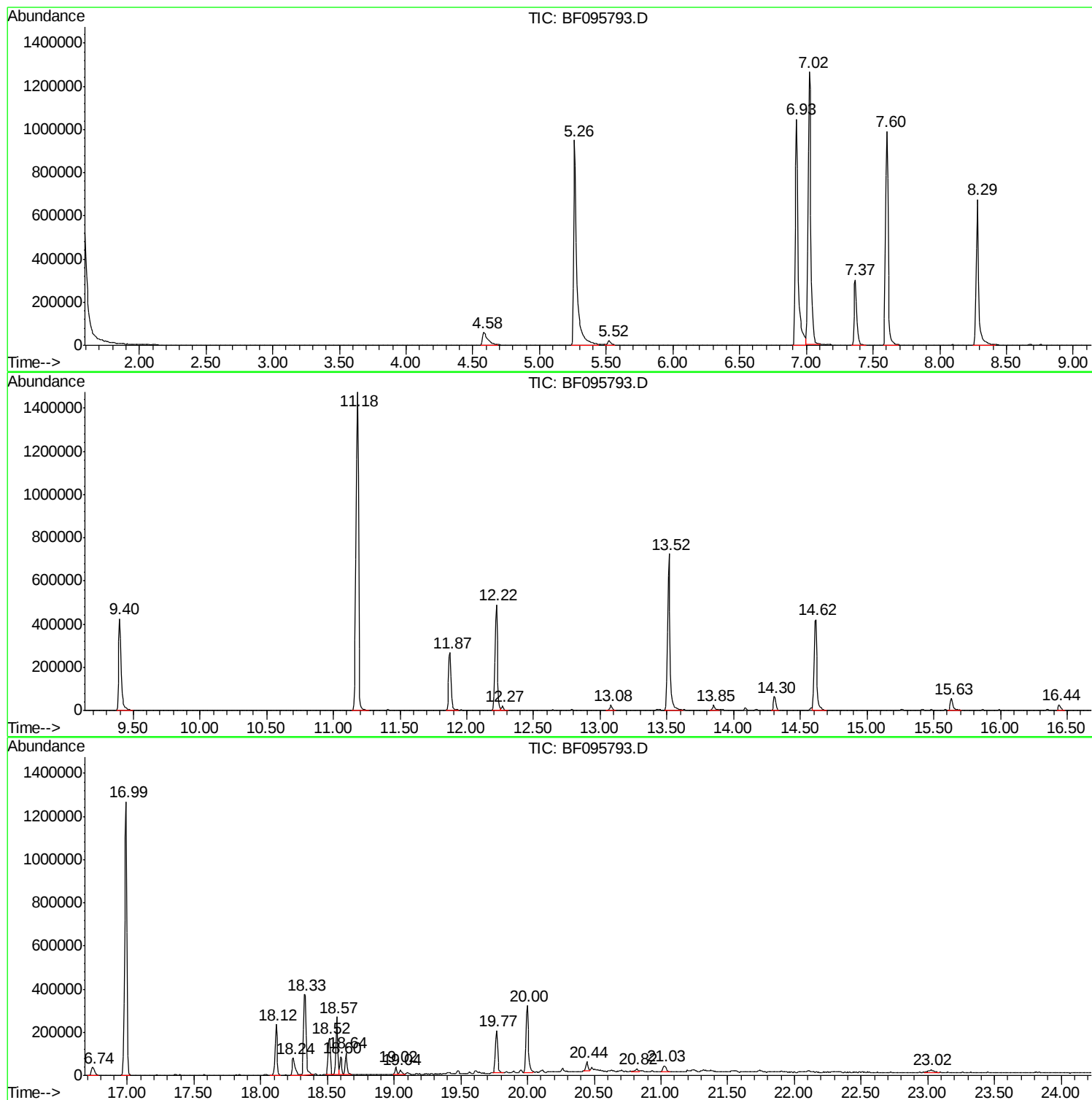
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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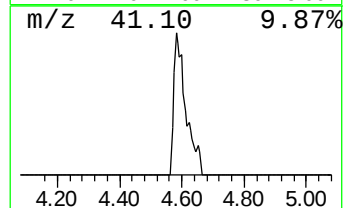
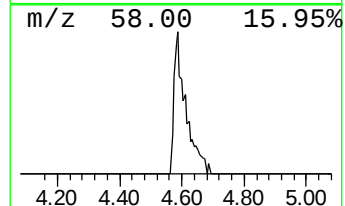
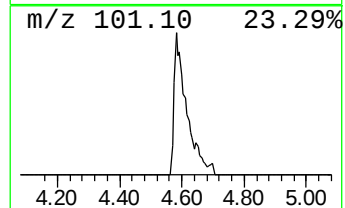
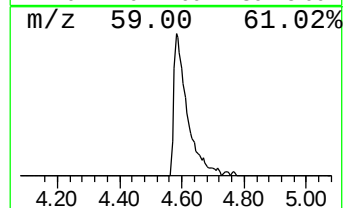
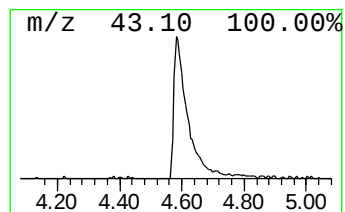
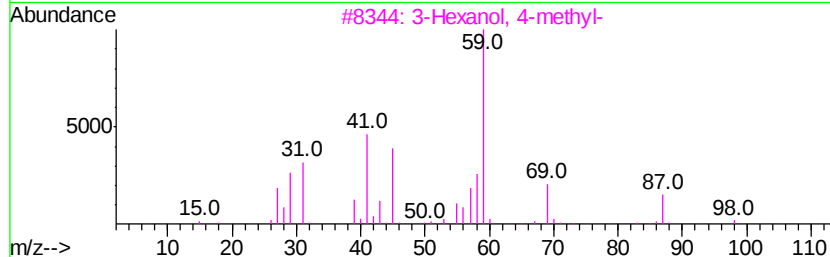
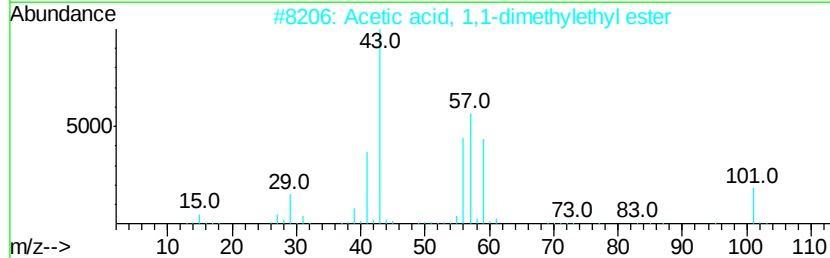
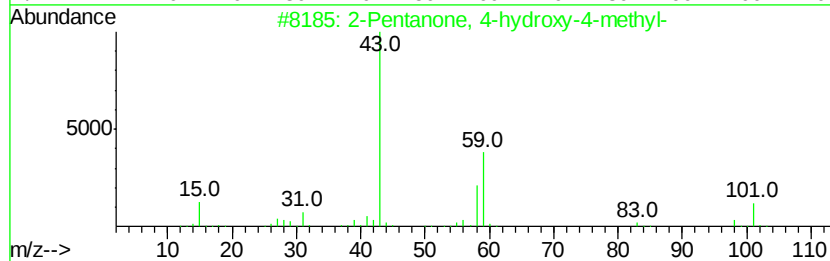
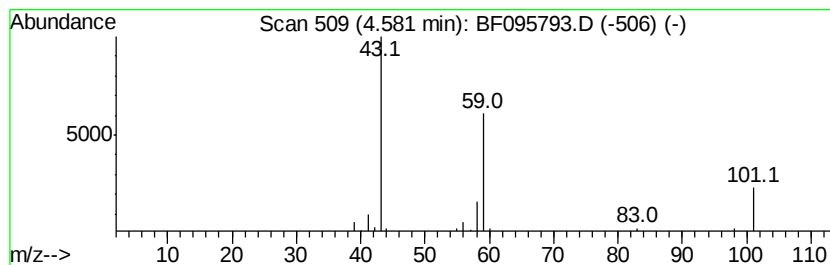
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	7.92 ng	165180	1,4-Dichlorobenzene-d4	7.37

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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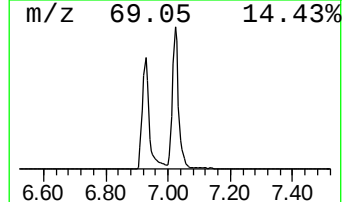
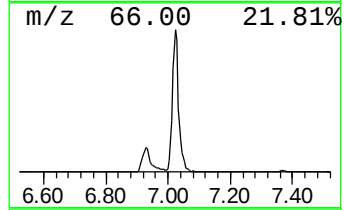
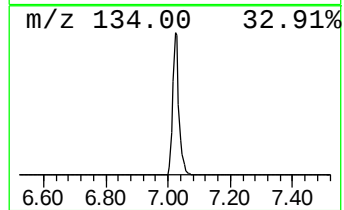
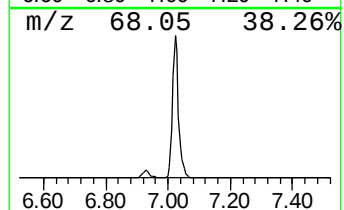
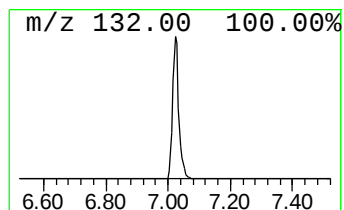
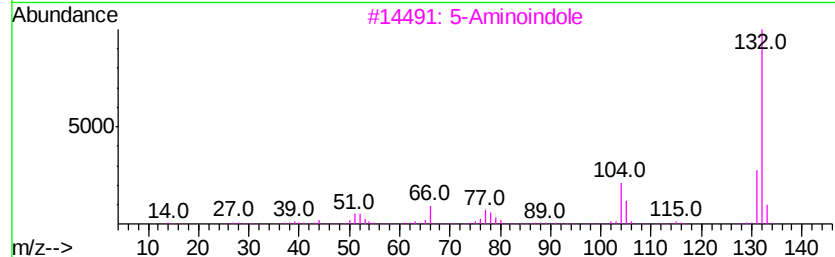
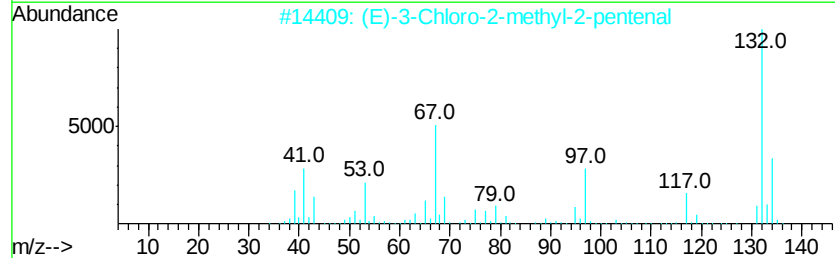
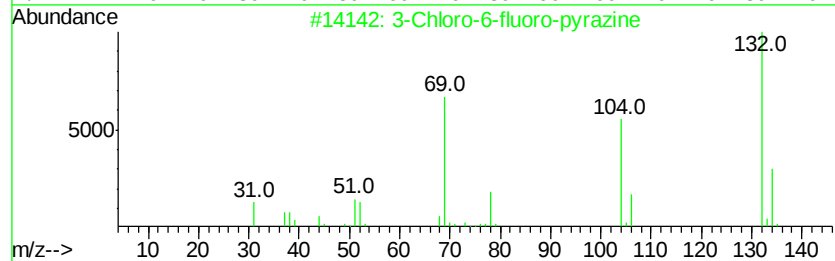
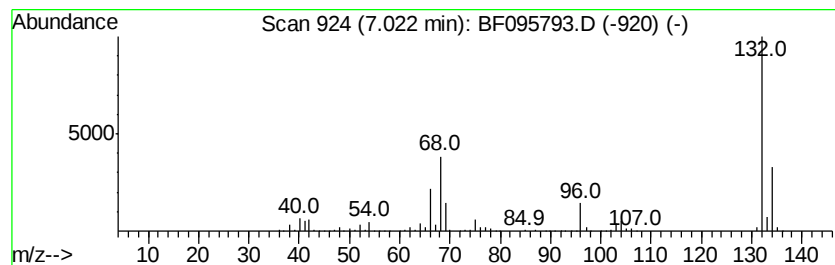
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	86.64 ng	1806650	1,4-Dichlorobenzene-d4	7.37

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		1-Aminoindan	133	C9H11N	034698-41-4	9



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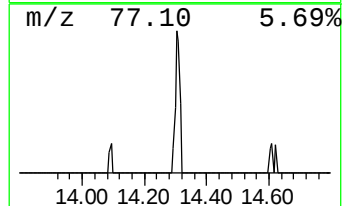
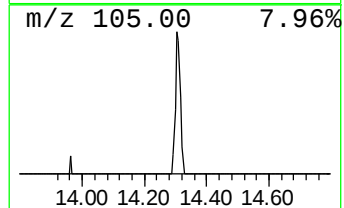
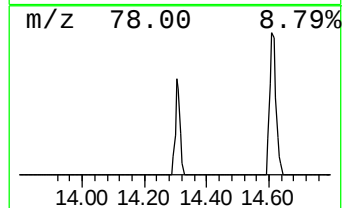
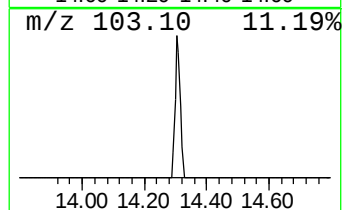
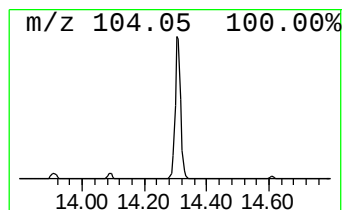
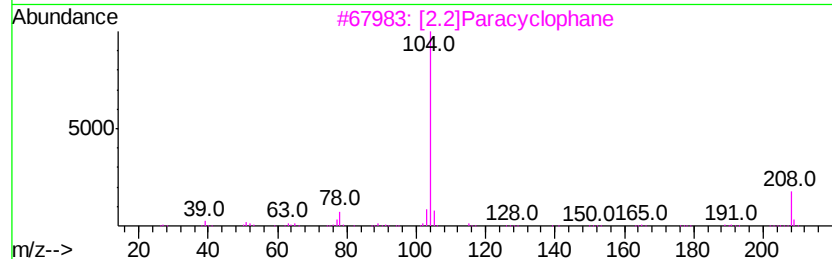
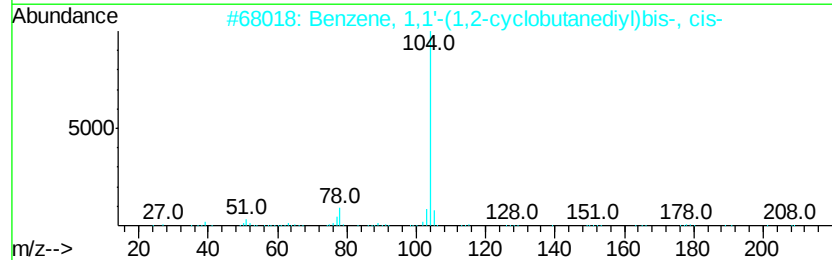
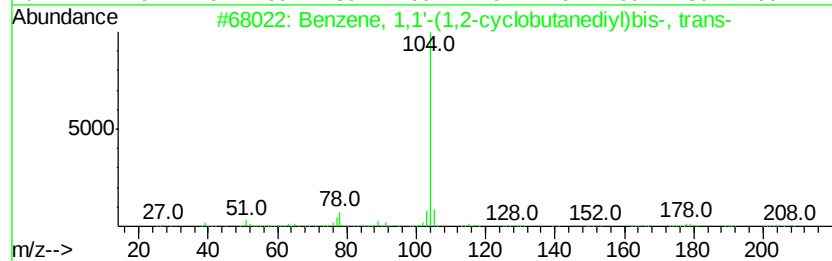
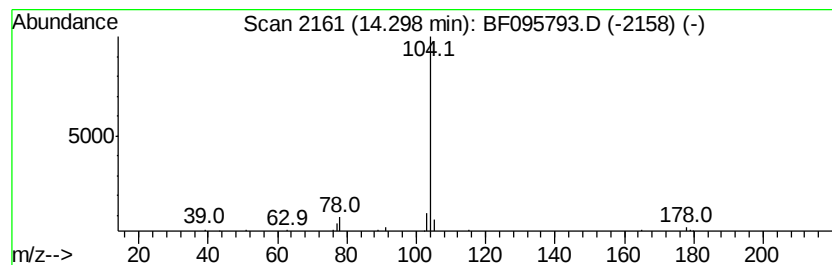
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,1'-(1,2-cyclobut... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.55 ng	74526	Phenanthrene-d10	14.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	90
2		Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	83
3		[2.2]Paracyclophane	208	C16H16	001633-22-3	72
4		Cyclobutane, 1,3-diphenyl-, trans-	208	C16H16	025558-23-0	72
5		Cyclobutane, 1,2-diphenyl-	208	C16H16	003018-21-1	56



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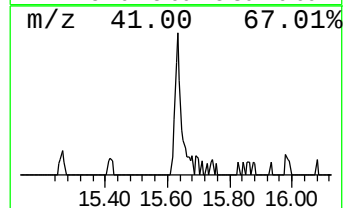
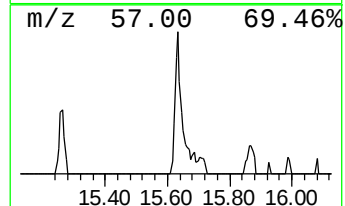
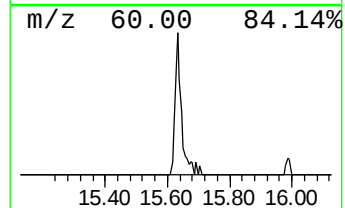
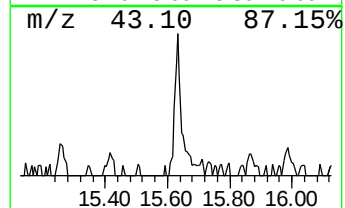
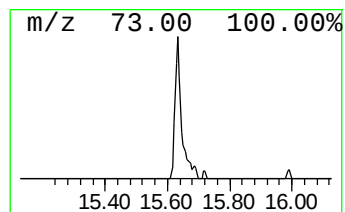
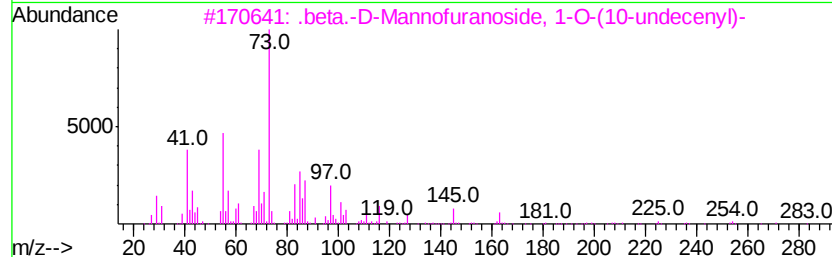
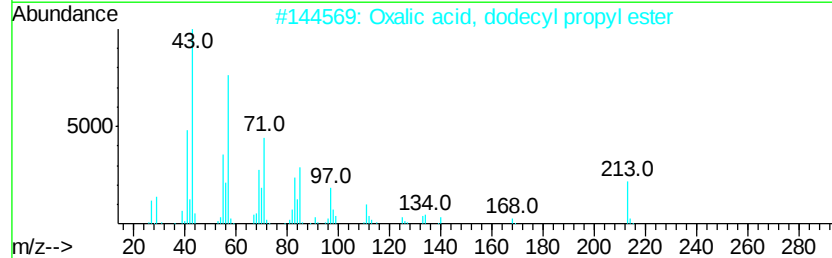
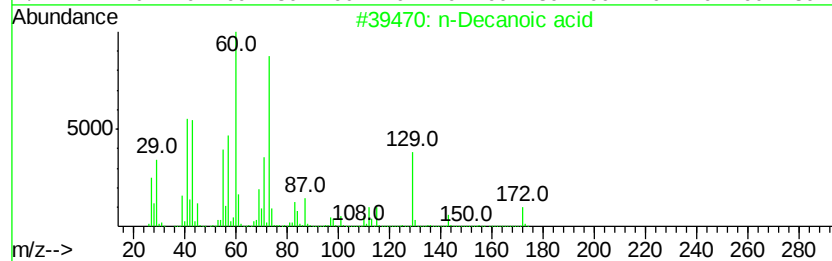
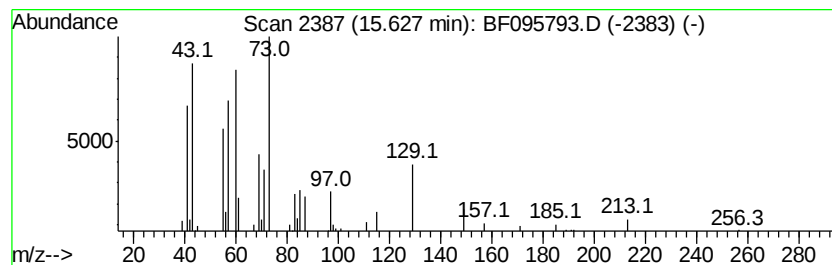
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Decanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.63	2.52 ng	73863	Phenanthrene-d10	14.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	53
2	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18
3	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	10
4	10-Methylnonadecane	282	C20H42	056862-62-5	10
5	Undecane, 5-ethyl-	184	C13H28	017453-94-0	10



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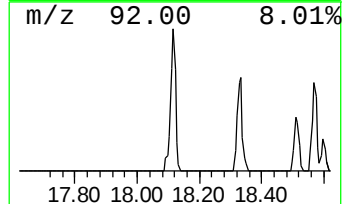
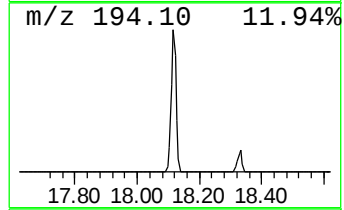
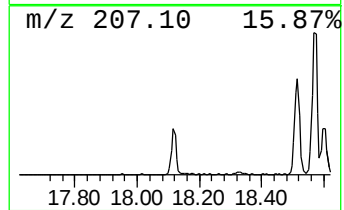
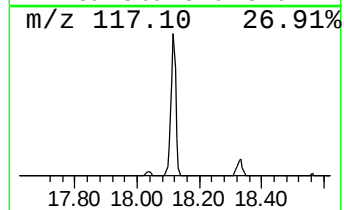
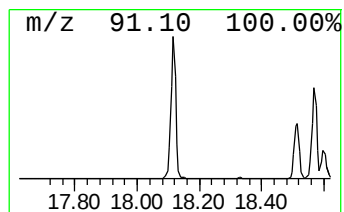
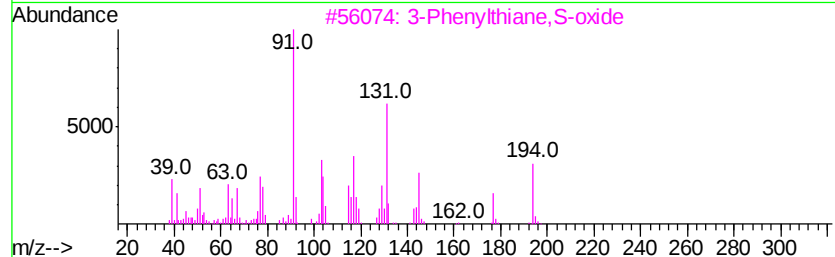
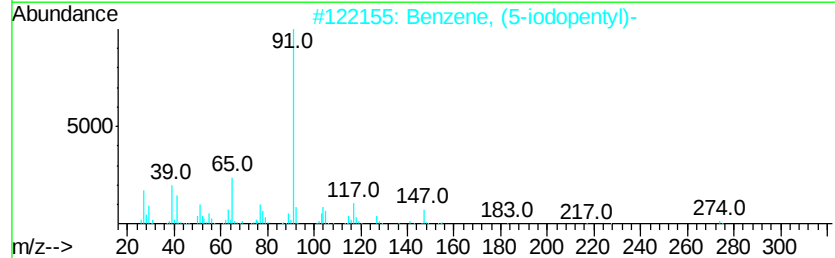
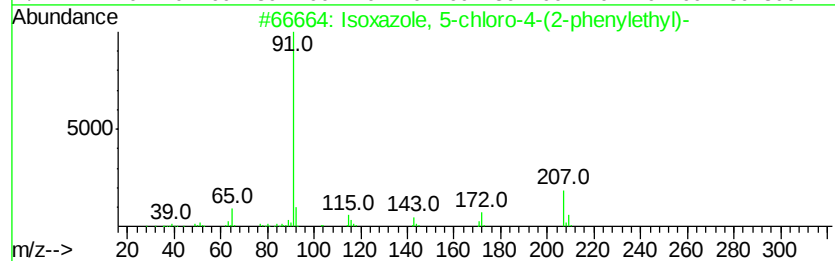
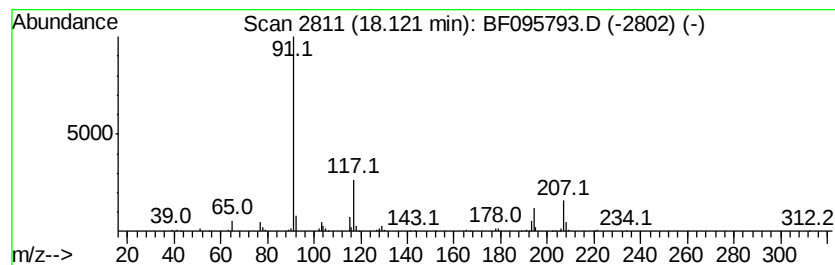
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown18.12 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.12	10.22 ng	245771	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoxazole, 5-chloro-4-(2-phenyle...	207	C11H10ClNO	1000362-09-0	25
2	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
3	3-Phenylthiane,S-oxide	194	C11H14OS	058121-26-9	10
4	2-Pentenal, 5-phenyl-	160	C11H12O	033046-84-3	10
5	Dichloroacetic acid, 4-benzyloxy...	310	C15H12Cl2O3	1000307-59-1	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
Operator : SJ/MA
Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

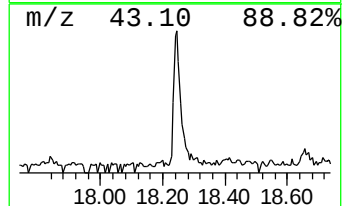
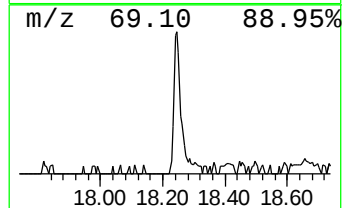
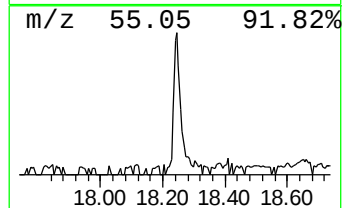
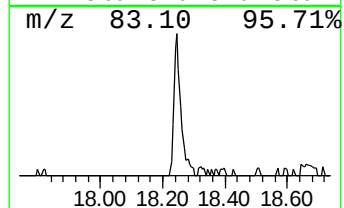
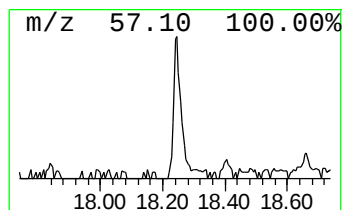
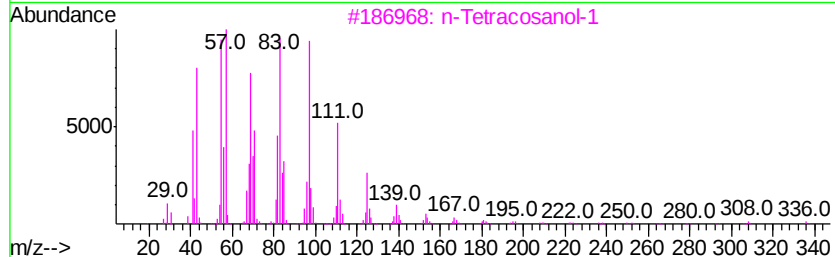
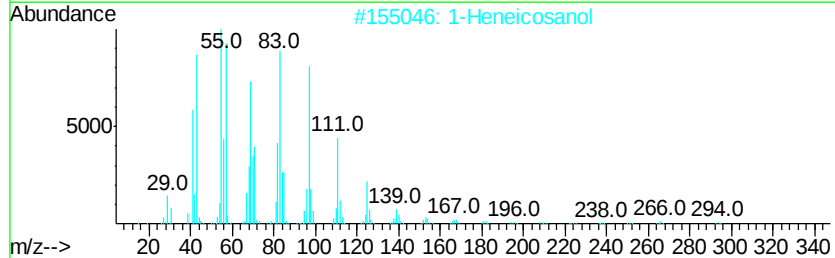
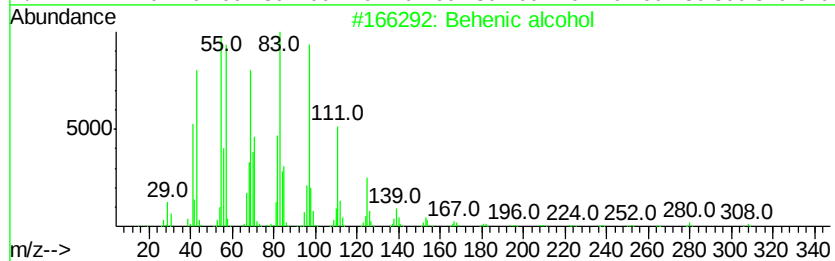
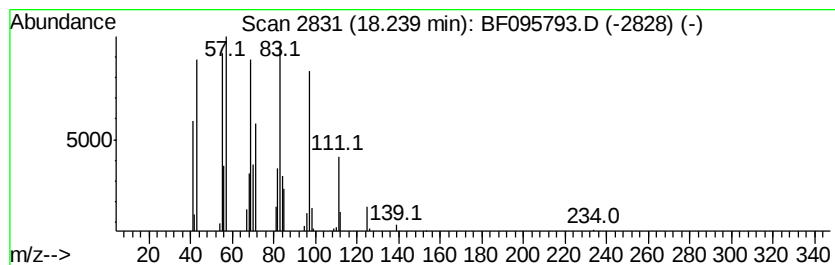
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.24	5.02 ng	120567	Chrysene-d12	18.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
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Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleID :
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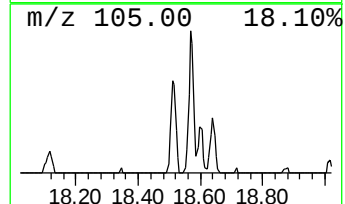
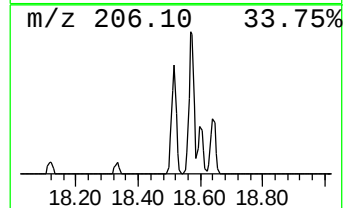
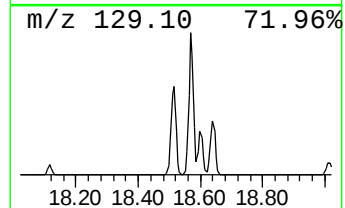
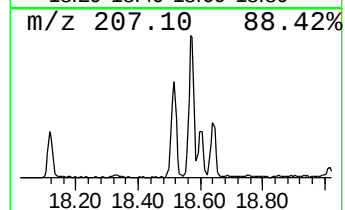
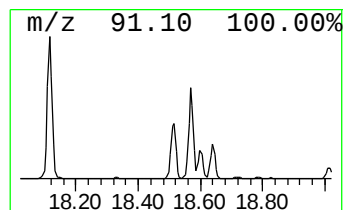
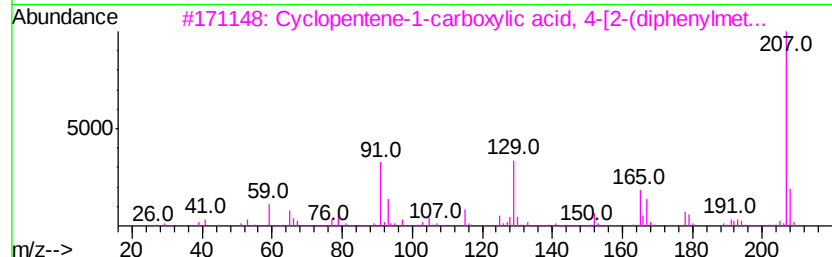
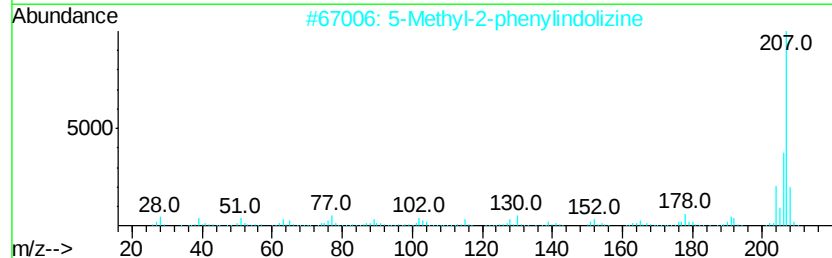
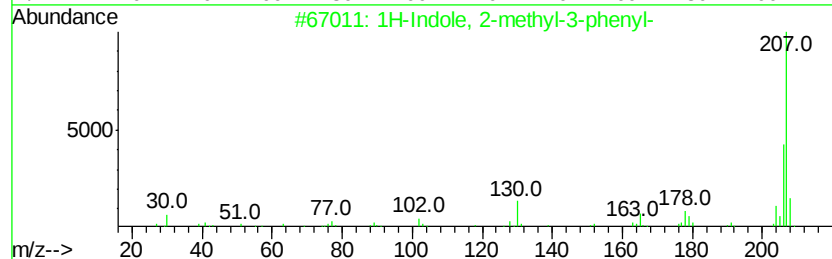
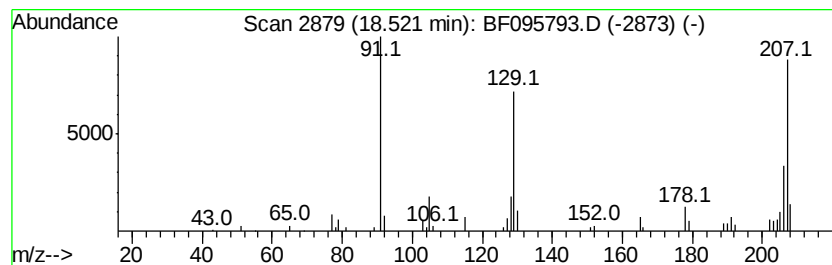
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown18.52 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.52	7.78 ng	187137	Chrysene-d12	18.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	49
2		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	45
3		Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	42
4		1-benzylindole	207	C15H13N	1000334-31-3	38
5		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20O5	131758-71-9	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
Operator : SJ/MA
Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4215

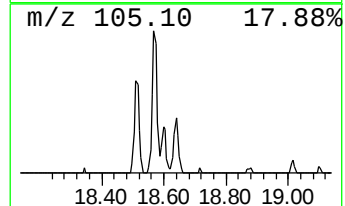
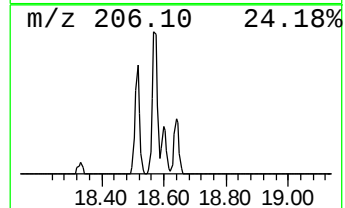
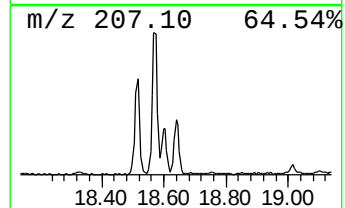
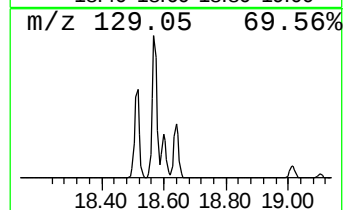
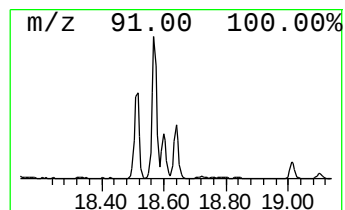
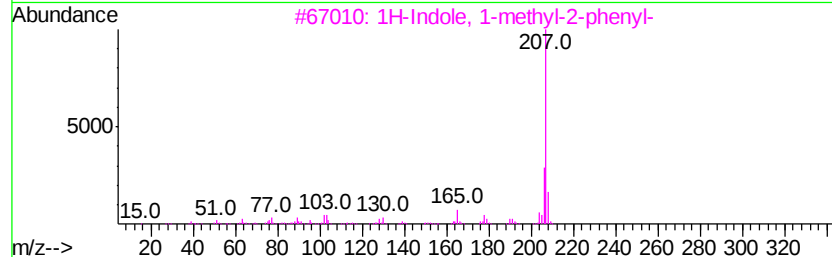
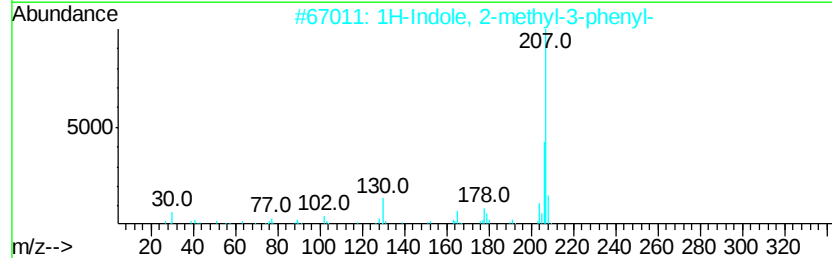
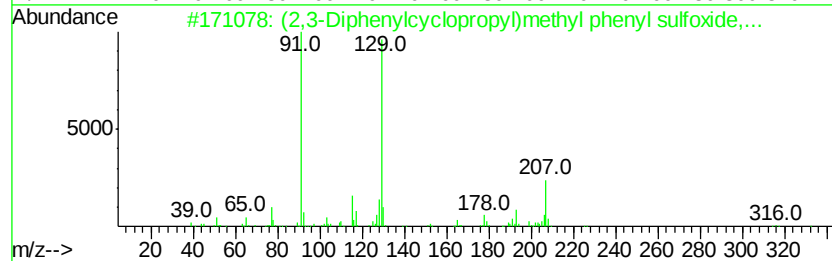
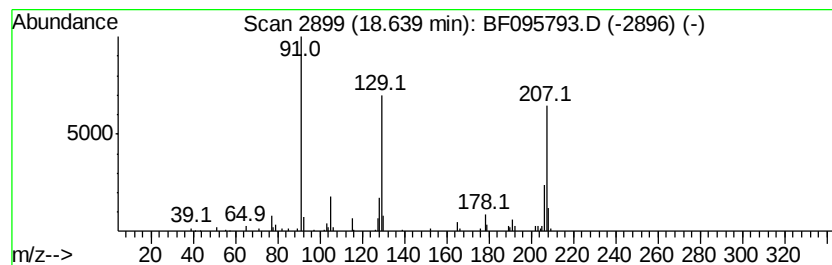
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 (2,3-Diphenylcyclopropyl)me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.64	4.65 ng	111714	Chrysene-d12	18.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	78
2		1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
3		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	45
4		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	43
5		Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
Operator : SJ/MA
Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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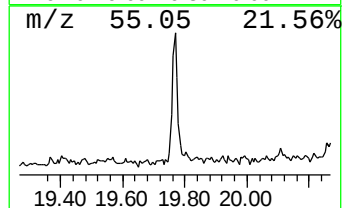
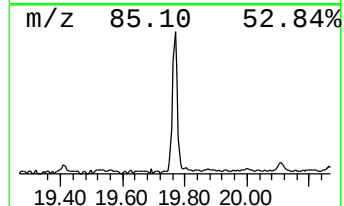
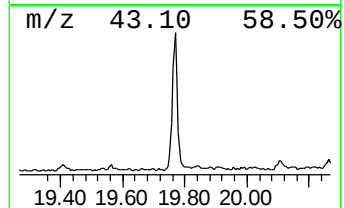
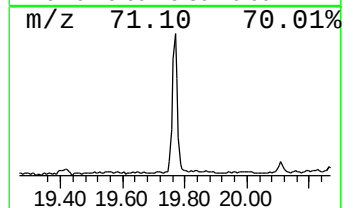
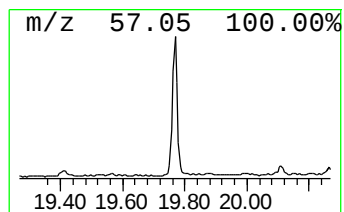
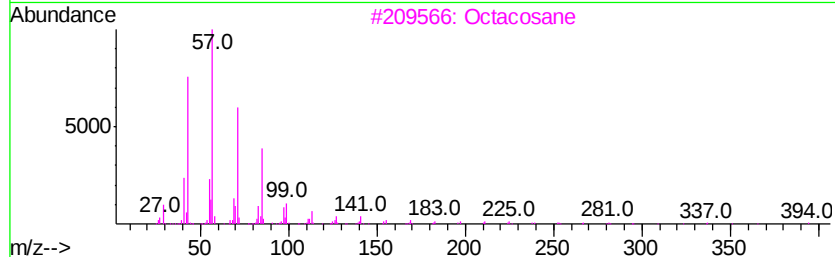
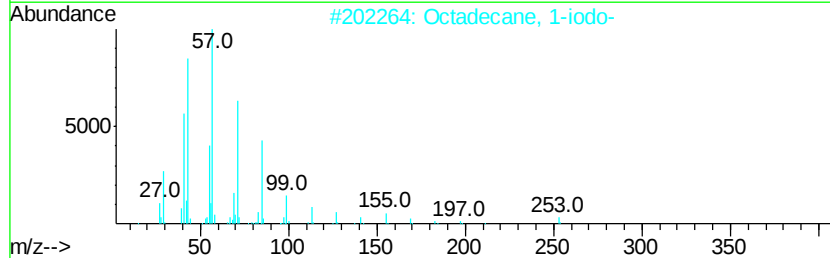
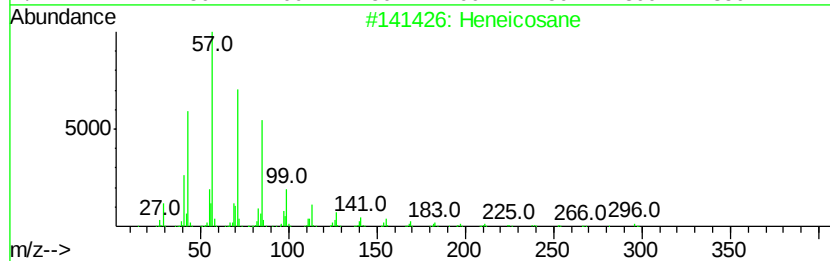
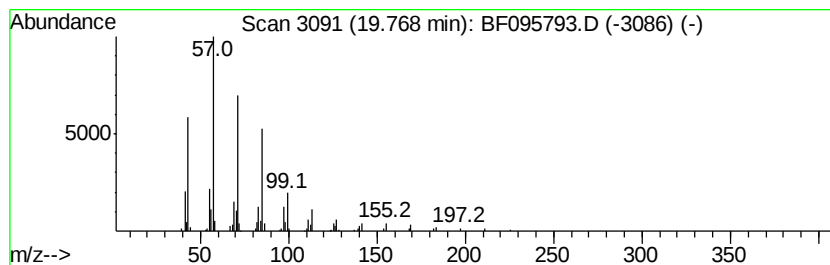
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	11.41 ng	223347	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Octadecane	254	C18H38	000593-45-3	83
5		Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
Operator : SJ/MA
Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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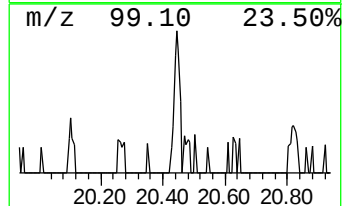
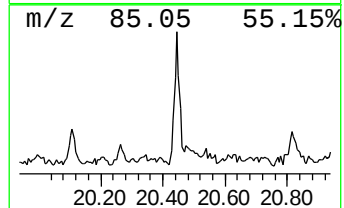
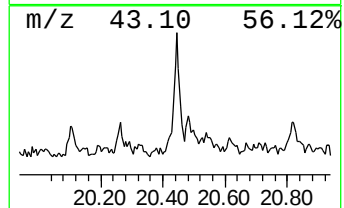
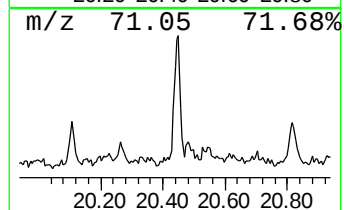
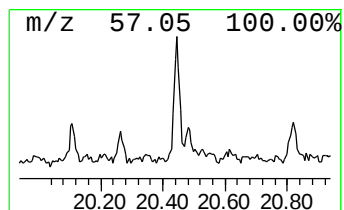
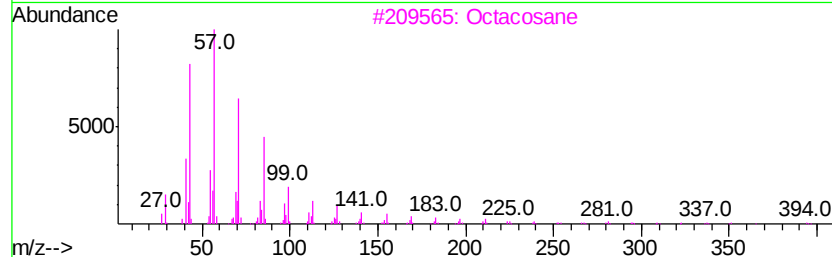
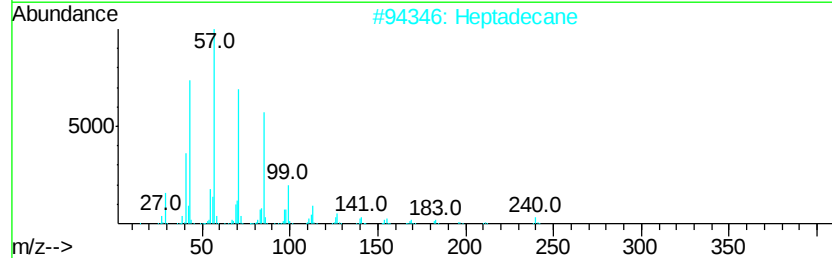
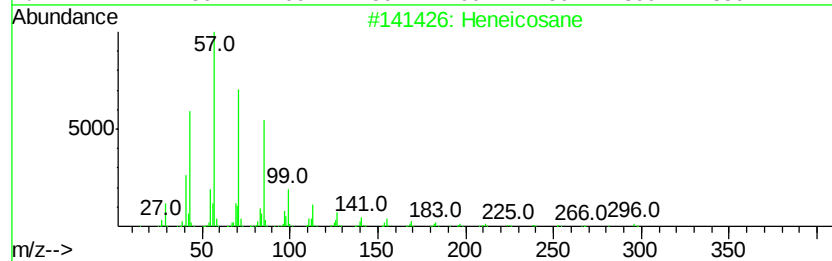
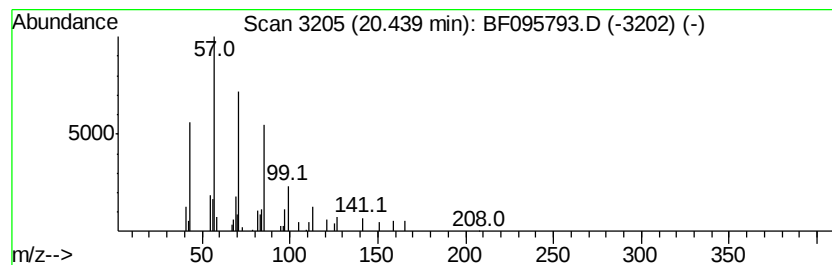
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	2.85 ng	55865	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Heptadecane	240	C17H36	000629-78-7	86
3		Octacosane	394	C28H58	000630-02-4	86
4		triacontane	422	C30H62	000638-68-6	86
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
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Misc :
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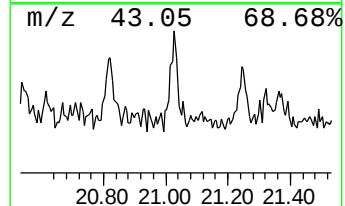
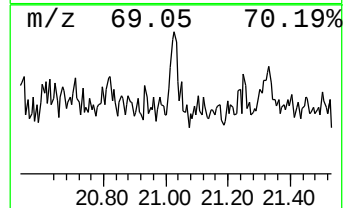
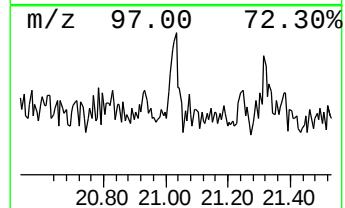
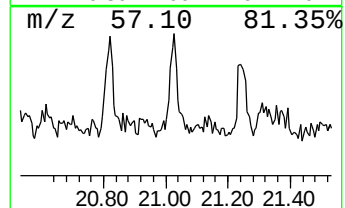
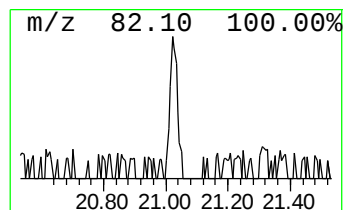
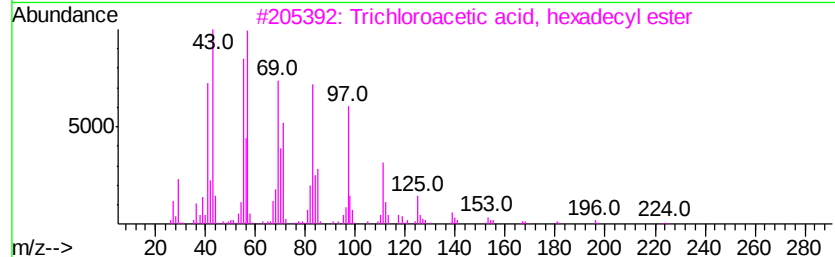
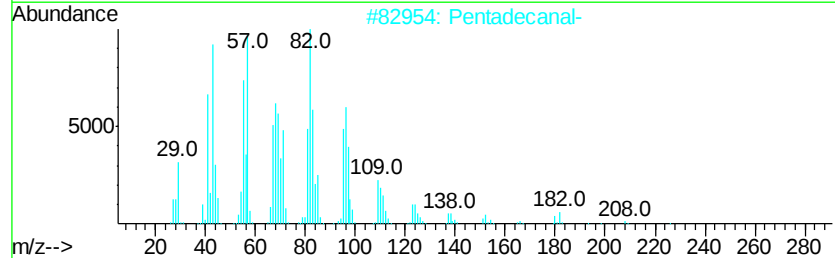
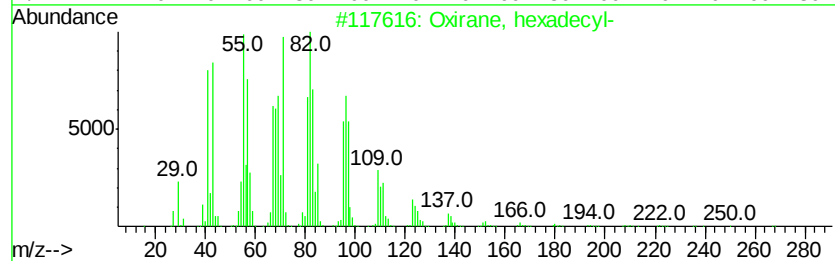
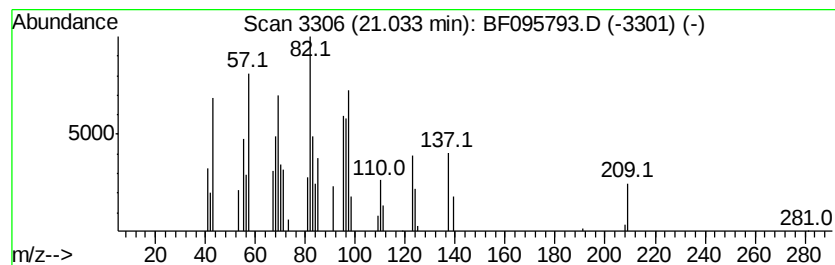
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	2.36 ng	46199	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	59
2		Pentadecanal-	226	C15H30O	002765-11-9	53
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	41
4		1-Hentetracontanol	593	C41H84O	040710-42-7	38
5		1-Hexacosanol	382	C26H54O	000506-52-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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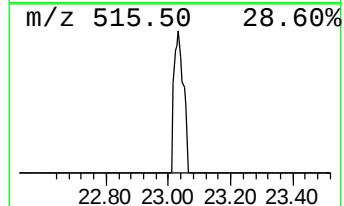
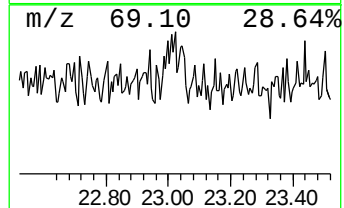
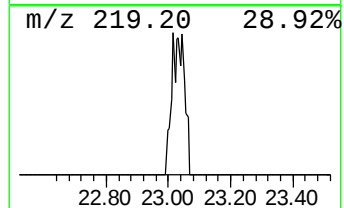
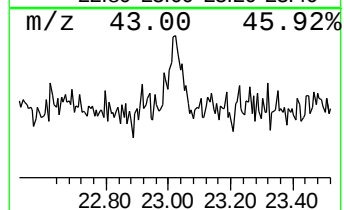
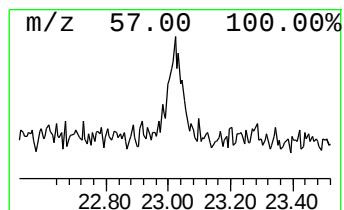
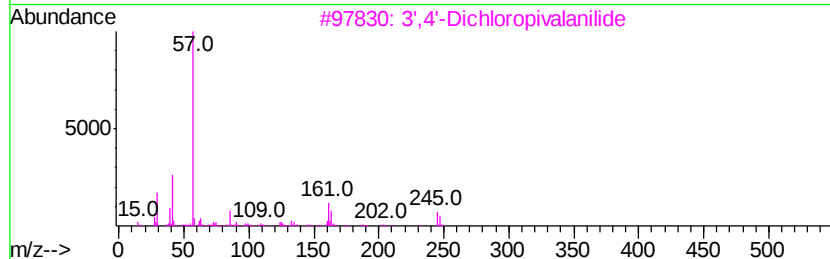
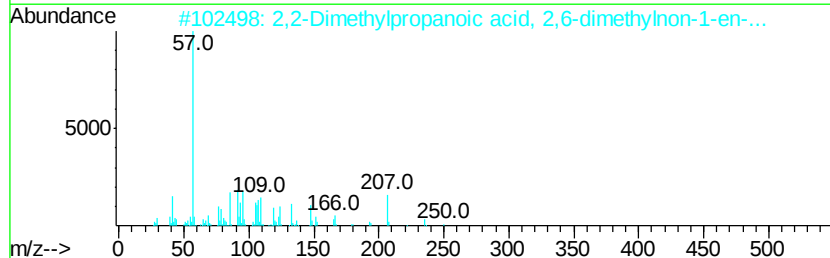
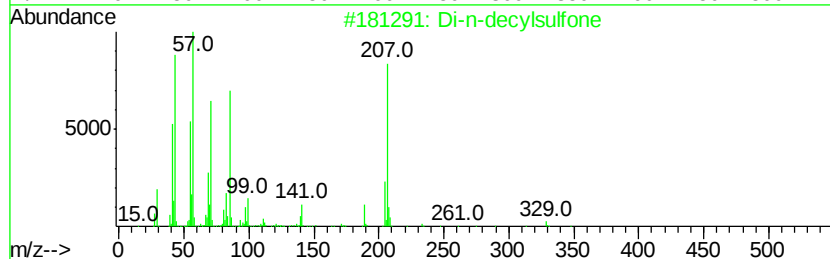
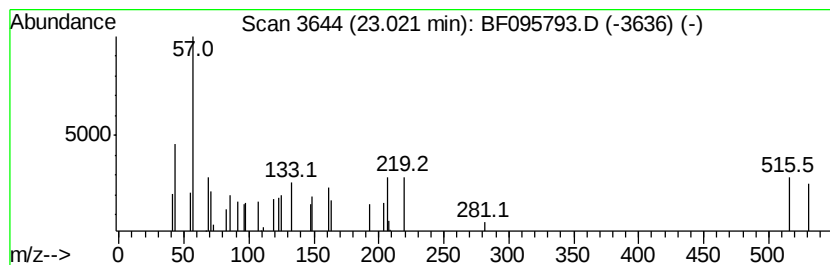
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown23.02 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.02	2.26 ng	44271	Perylene-d12	20.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Di-n-decylsulfone	346	C20H42O2S	111530-37-1	9
2		2,2-Dimethylpropanoic acid, 2,6-...	250	C16H26O2	1000299-33-6	7
3		3',4'-Dichloropivalanilide	245	C11H13Cl2NO	007160-22-7	4
4		.beta.-D-Lyxofuranoside, 5-O-(.b...	422	C20H38O9	1000154-98-4	4
5		(Z)-5-(4-tert-Butyl-1-hydroxycyc...	264	C16H24O3	1000280-72-0	2



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060817\
Data File : BF095793.D
Acq On : 8 Jun 2017 20:30
Operator : SJ/MA
Sample : I3541-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RT-4215

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.58	7.9	ng	165180	1	7.37	417026	20.0
unknown7.02	7.02	86.6	ng	1806650	1	7.37	417026	20.0
Benzene, 1,1'-(1,...	14.30	2.5	ng	74526	4	14.62	585330	20.0
n-Decanoic acid	15.63	2.5	ng	73863	4	14.62	585330	20.0
unknown18.12	18.12	10.2	ng	245771	5	18.33	480819	20.0
Behenic alcohol	18.24	5.0	ng	120567	5	18.33	480819	20.0
unknown18.52	18.52	7.8	ng	187137	5	18.33	480819	20.0
(2,3-Diphenylcycl...	18.64	4.7	ng	111714	5	18.33	480819	20.0
Heneicosane	19.77	11.4	ng	223347	6	20.00	391370	20.0
Octacosane	20.44	2.9	ng	55865	6	20.00	391370	20.0
Oxirane, hexadecyl-	21.03	2.4	ng	46199	6	20.00	391370	20.0
unknown23.02	23.02	2.3	ng	44271	6	20.00	391370	20.0