

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
 Data File : BF095131.D
 Acq On : 15 May 2017 18:10
 Operator : SJ/MA
 Sample : I3141-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01_002

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.131	538	543	560	rBV	241052	499195	21.61%	2.803%
2	5.742	644	647	671	rBV	877147	1748941	75.72%	9.820%
3	7.319	910	915	932	rBV	1111654	1732653	75.02%	9.728%
4	7.442	932	936	950	rVB	1485689	2033280	88.04%	11.416%
5	7.778	989	993	1006	rBV	353396	436365	18.89%	2.450%
6	8.013	1029	1033	1047	rBV	1240490	1519203	65.78%	8.530%
7	8.677	1141	1146	1167	rBV	793017	1100653	47.66%	6.180%
8	9.795	1332	1336	1349	rBV	394030	552230	23.91%	3.101%
9	11.566	1632	1637	1658	rBV	1857545	2309605	100.00%	12.968%
10	12.260	1751	1755	1766	rBV	125550	208484	9.03%	1.171%
11	12.624	1812	1817	1829	rBV2	460308	634841	27.49%	3.564%
12	13.460	1956	1959	1965	rVB	22315	23597	1.02%	0.132%
13	13.918	2033	2037	2051	rBV	735641	1099855	47.62%	6.175%
14	14.230	2086	2090	2093	rBV	22049	27475	1.19%	0.154%
15	15.030	2221	2226	2243	rBV	370001	528857	22.90%	2.969%
16	15.983	2384	2388	2398	rBV2	42200	84283	3.65%	0.473%
17	17.347	2615	2620	2630	rBV	1449812	1612294	69.81%	9.053%
18	18.624	2827	2837	2841	rBV7	19300	62859	2.72%	0.353%
19	18.700	2846	2850	2865	rVB	281044	402678	17.43%	2.261%
20	20.106	3085	3089	3092	rBV	40073	43530	1.88%	0.244%
21	20.371	3130	3134	3145	rBV	285148	430498	18.64%	2.417%
22	20.836	3210	3213	3218	rVB2	23329	28207	1.22%	0.158%
23	21.053	3246	3250	3257	rVB5	20080	41823	1.81%	0.235%
24	21.677	3353	3356	3361	rVB7	20349	32186	1.39%	0.181%
25	22.000	3406	3411	3418	rVB5	61045	112447	4.87%	0.631%
26	22.200	3438	3445	3455	rBV5	28542	81407	3.52%	0.457%
27	23.035	3582	3587	3594	rVB6	36898	78112	3.38%	0.439%
28	23.765	3704	3711	3713	rBV8	22794	49592	2.15%	0.278%
29	23.888	3723	3732	3744	rVB7	97525	295199	12.78%	1.657%

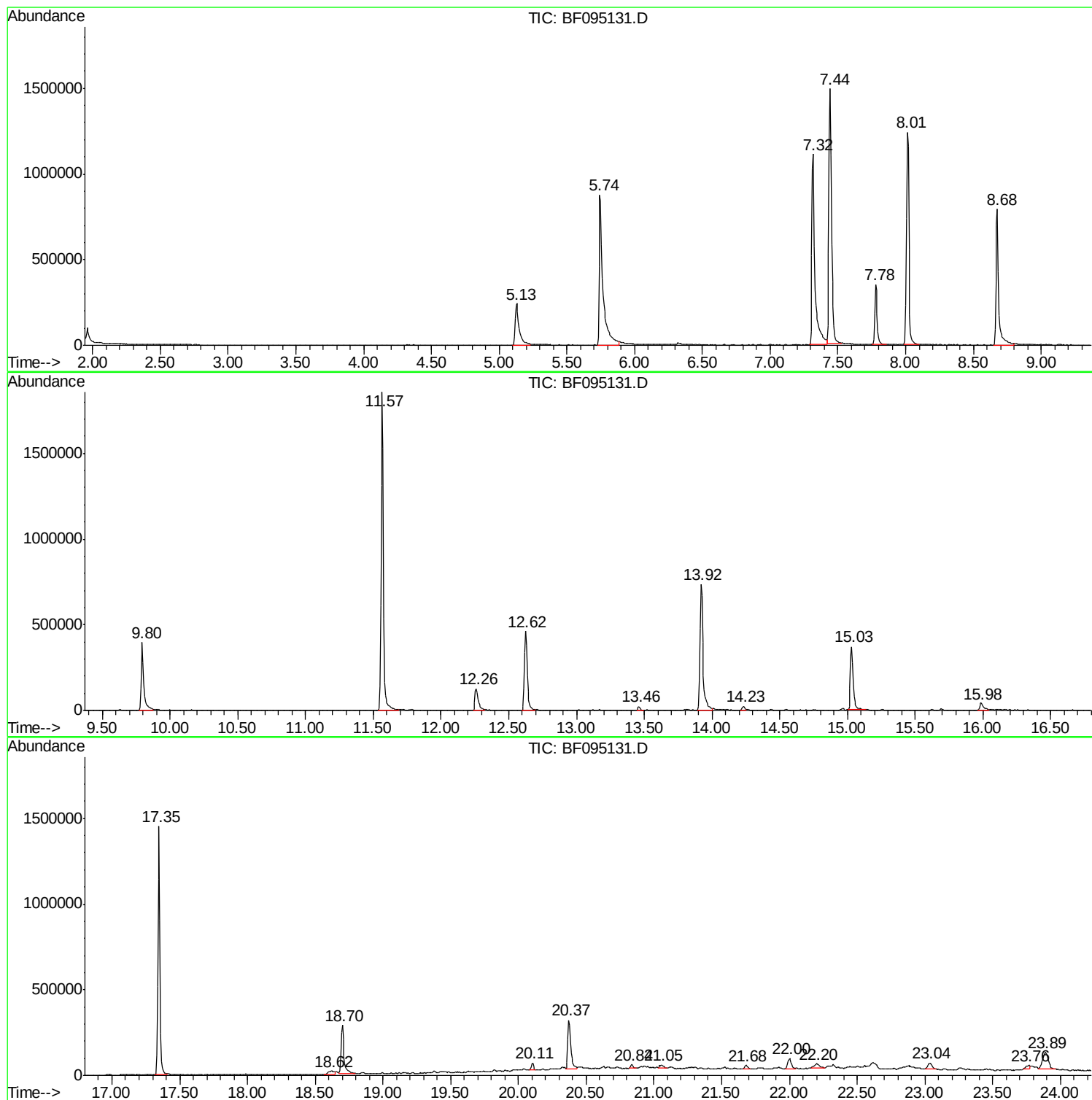
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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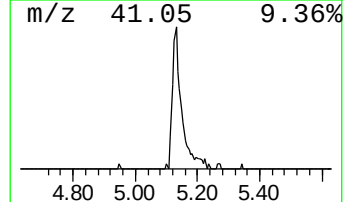
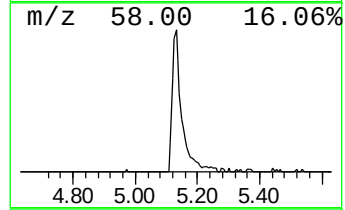
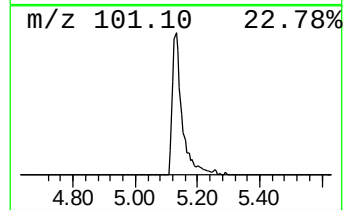
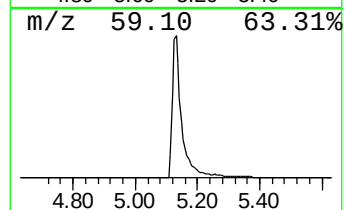
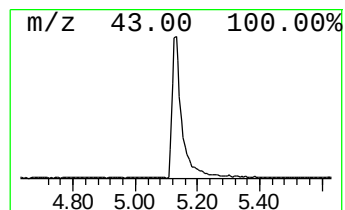
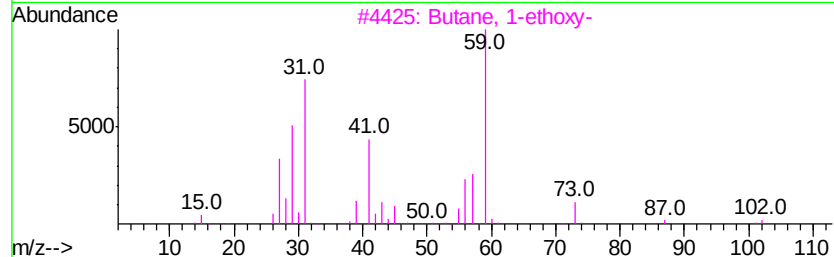
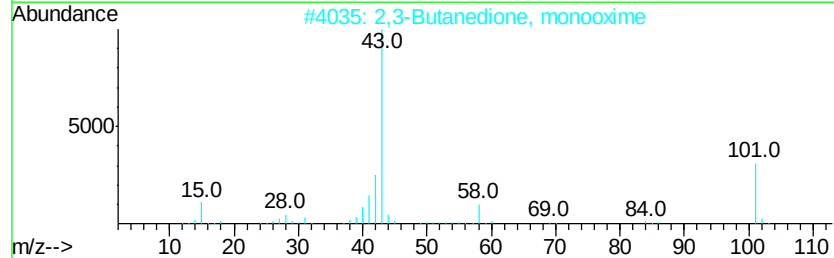
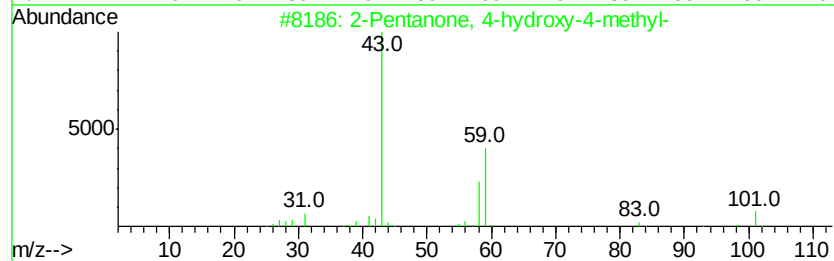
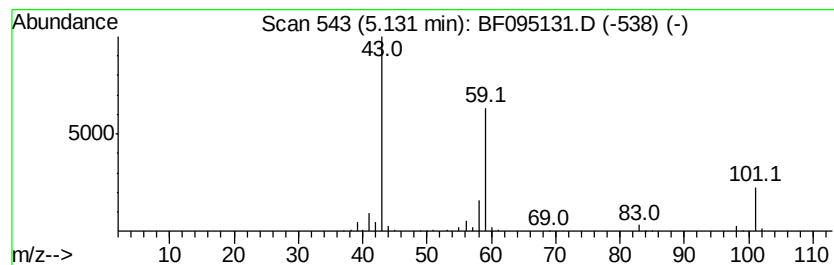
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	22.88 ng	499195	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	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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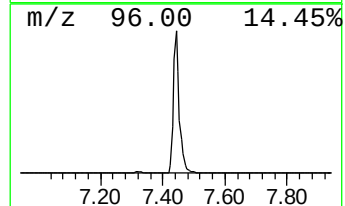
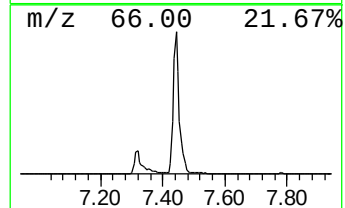
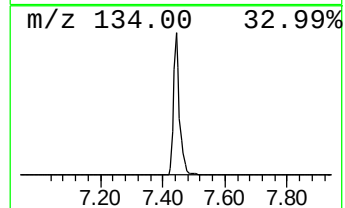
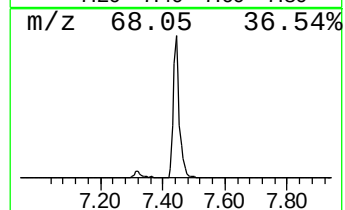
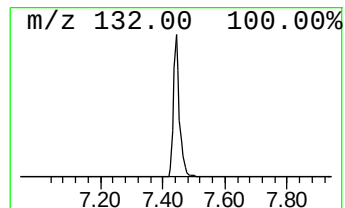
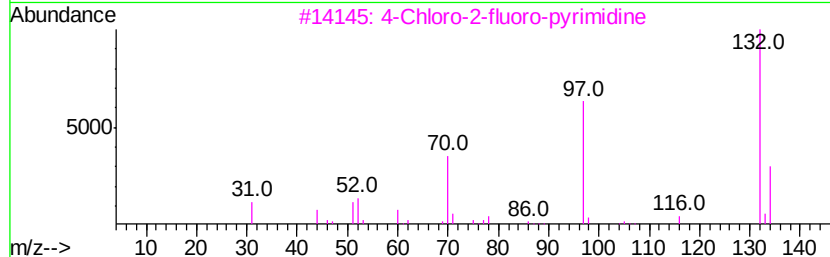
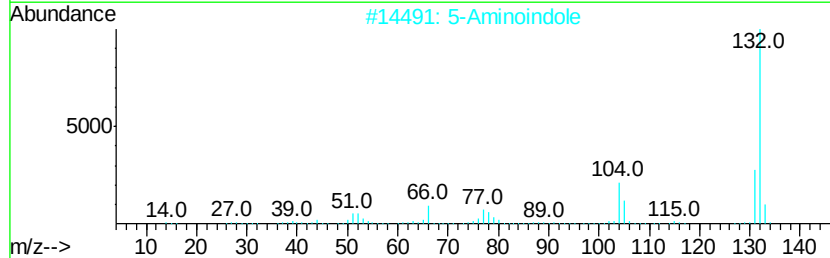
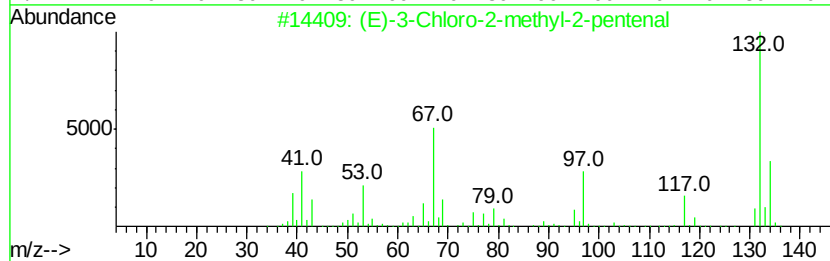
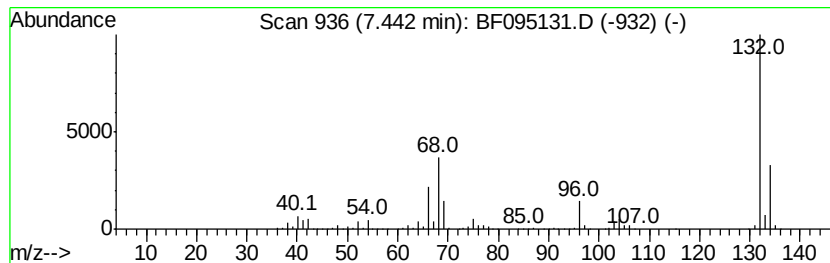
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Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	93.19 ng	2033280	1,4-Dichlorobenzene-d4	7.78

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	Xenon	132	Xe	007440-63-3	9	



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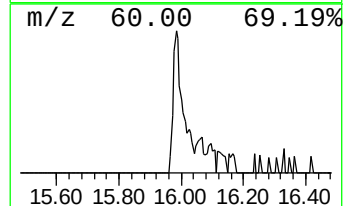
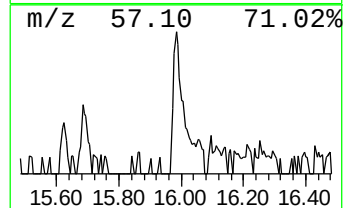
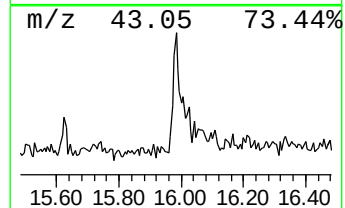
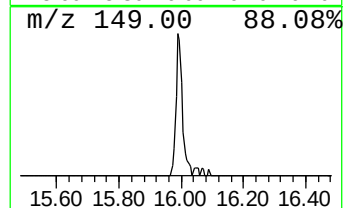
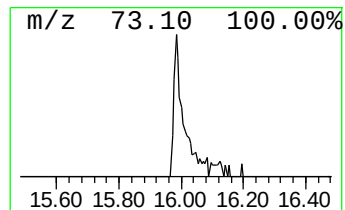
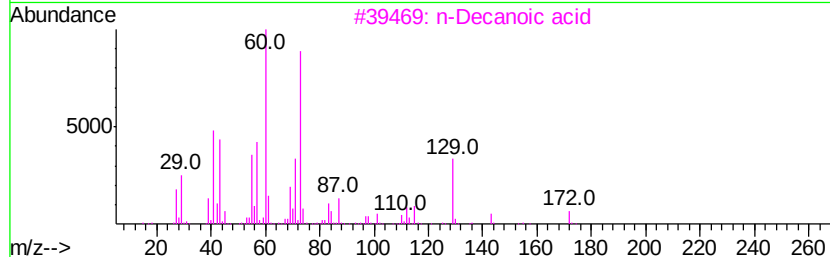
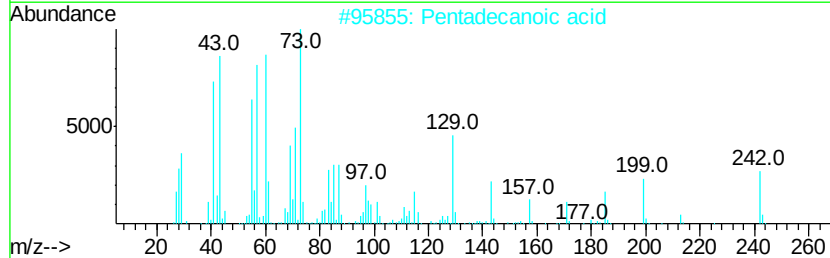
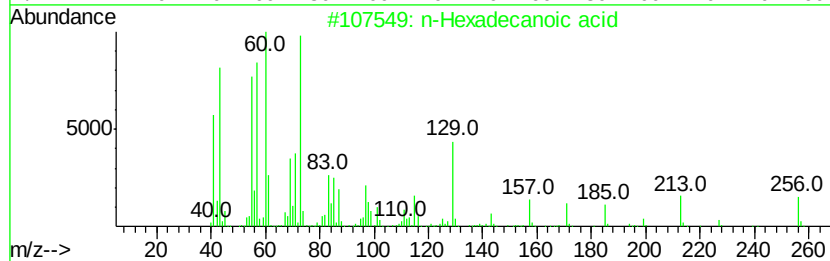
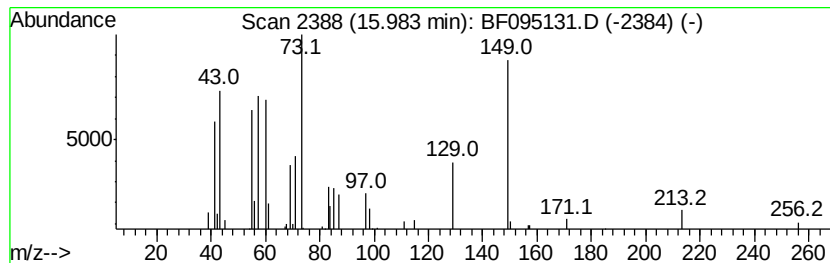
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.98	3.19 ng	84283	Phenanthrene-d10	15.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	14
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	11



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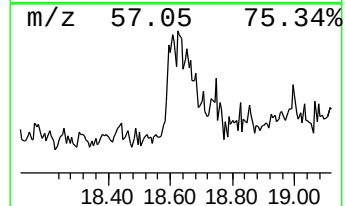
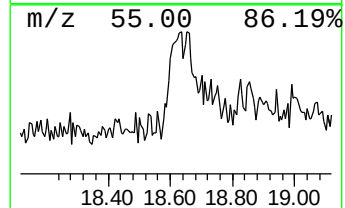
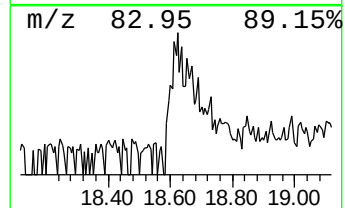
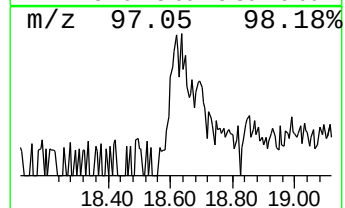
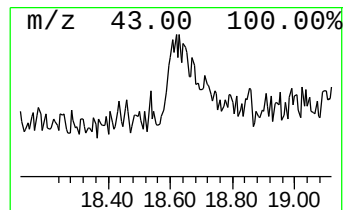
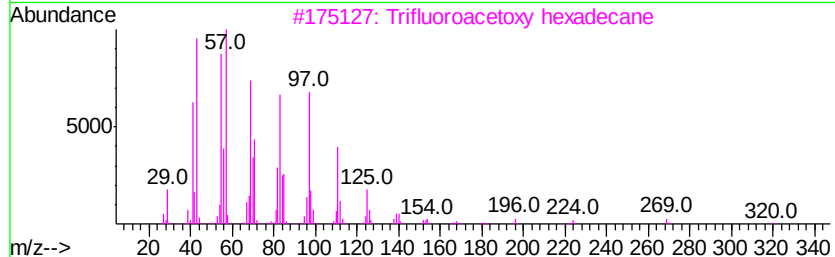
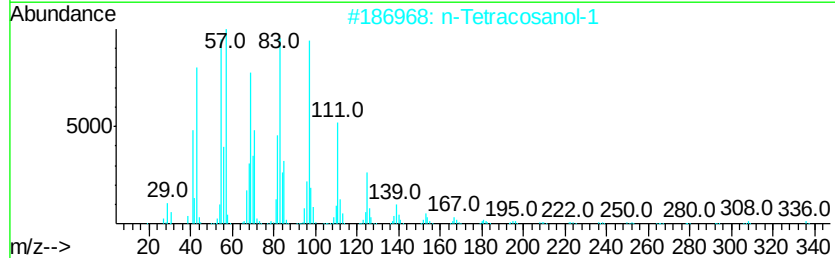
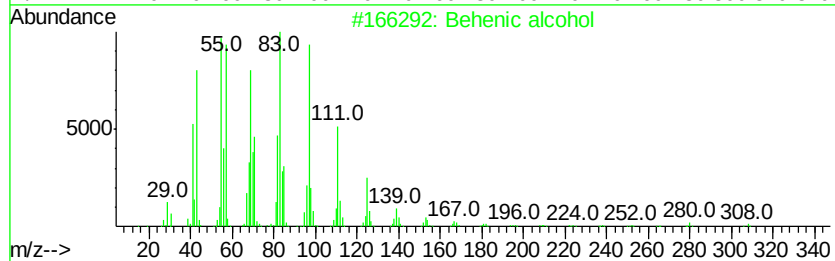
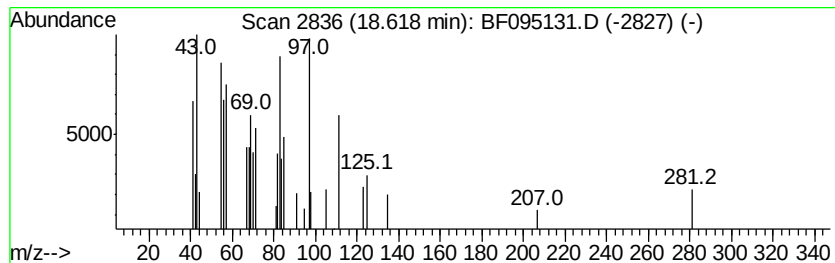
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Peak Number 5 Behenic alcohol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.62	3.12 ng	62859	Chrysene-d12	18.70	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	80
4	11-Methyldodecanol	200	C13H28O	085763-57-1	80
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	68



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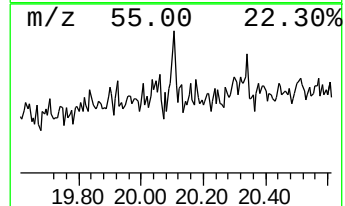
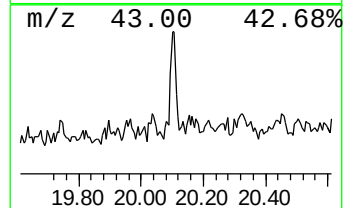
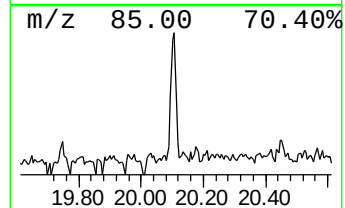
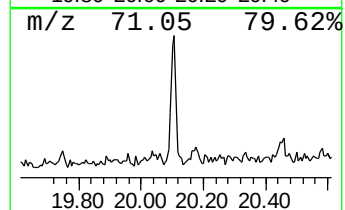
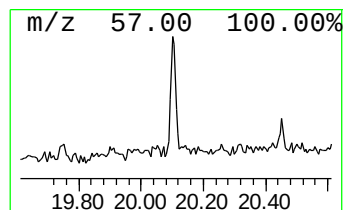
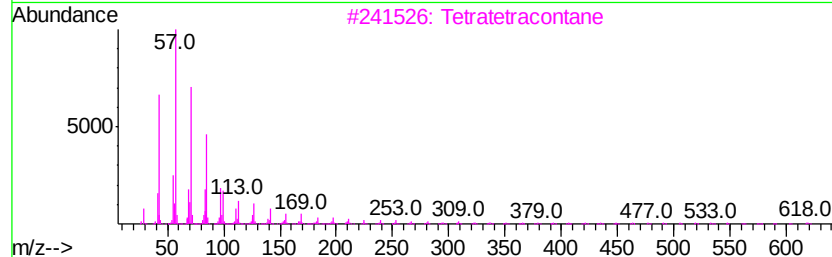
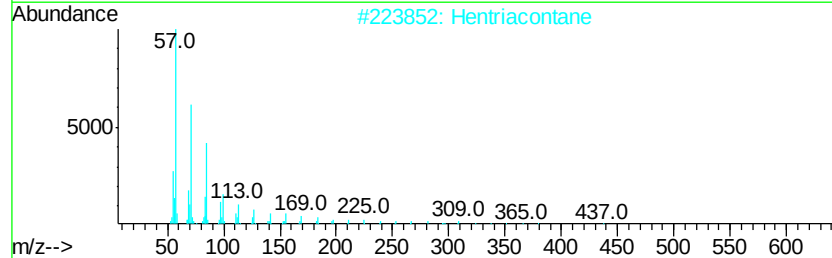
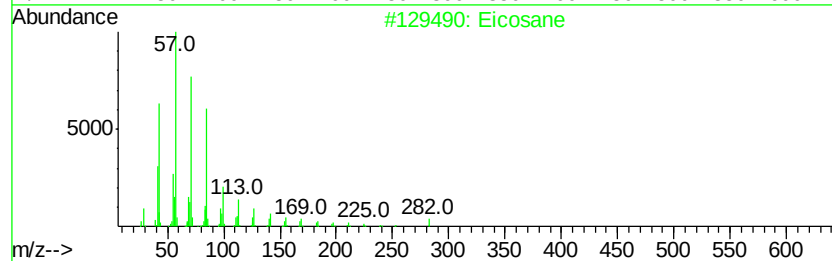
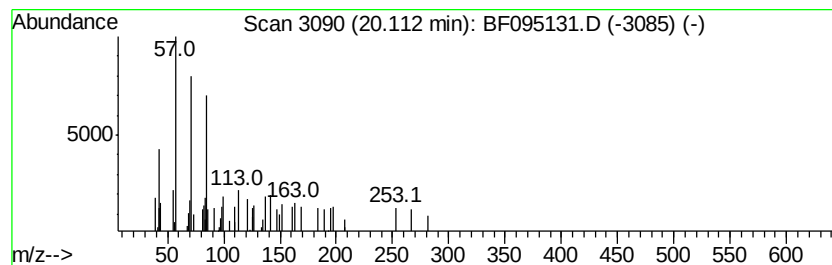
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Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.11	2.02 ng	43530	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Tetratetracontane	619	C44H90	007098-22-8	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Heneicosane	296	C21H44	000629-94-7	87



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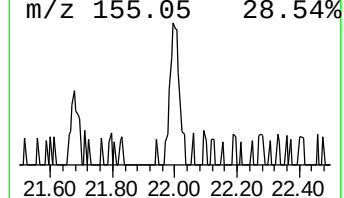
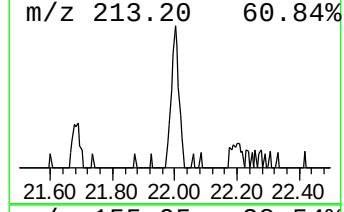
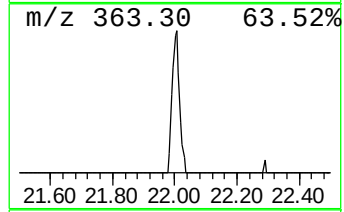
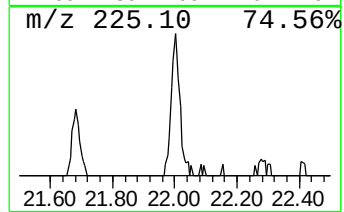
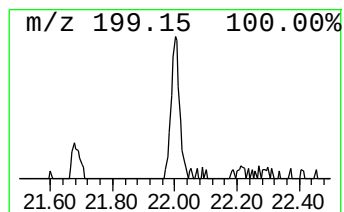
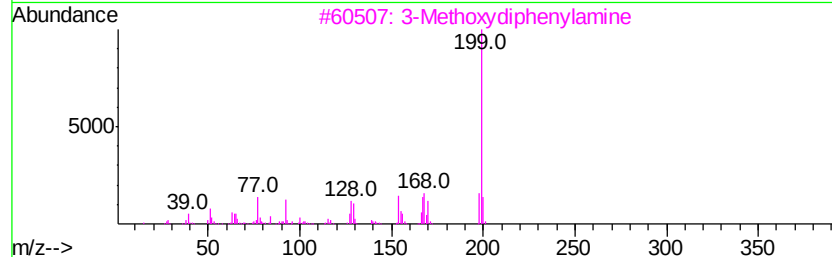
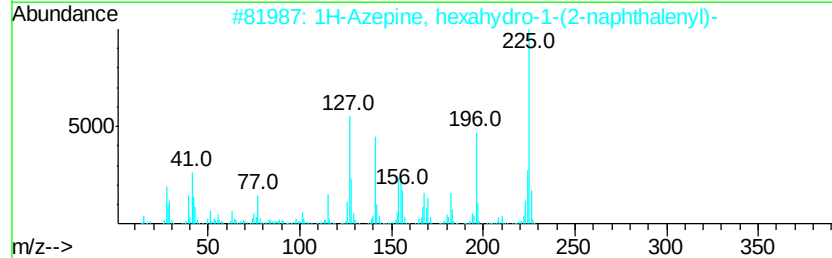
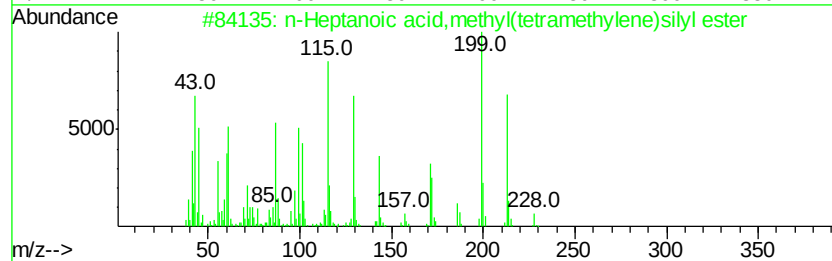
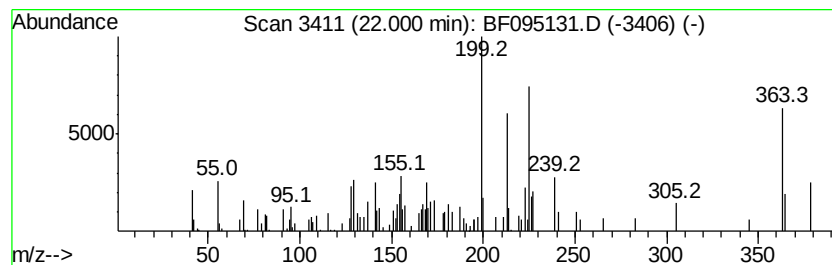
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown22.0 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.00	5.22 ng	112447	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Heptanoic acid,methyl(tetramet...	228	C12H24O2Si	1000217-03-6	22
2		1H-Azepine, hexahydro-1-(2-napht...	225	C16H19N	055045-05-1	15
3		3-Methoxydiphenylamine	199	C13H13NO	000101-16-6	15
4		2-Fluoro-9-formylacridine	225	C14H8FNO	024986-45-6	11
5		2,2,5-Trimethyl-1-phenylhexa-3,4...	214	C15H18O	261786-81-6	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
Data File : BF095131.D
Acq On : 15 May 2017 18:10
Operator : SJ/MA
Sample : I3141-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

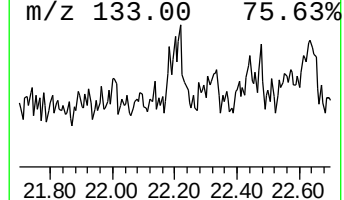
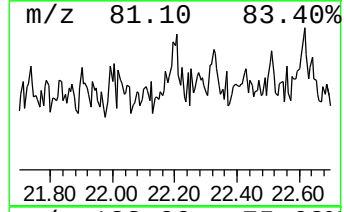
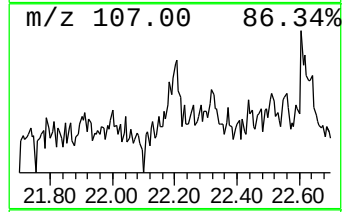
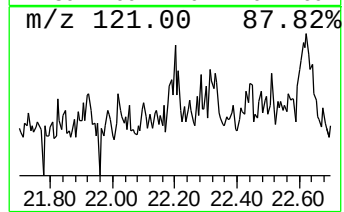
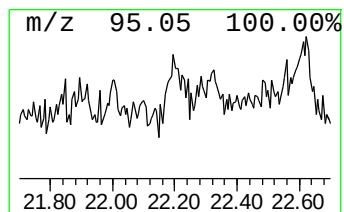
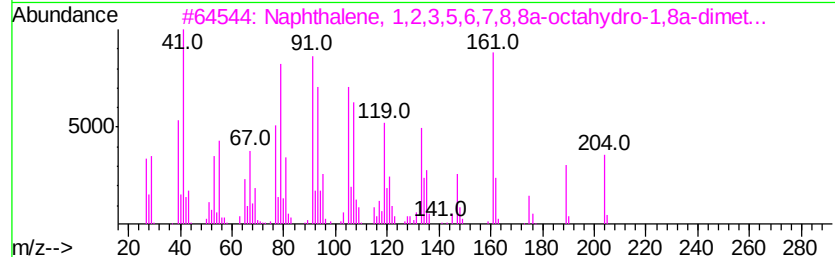
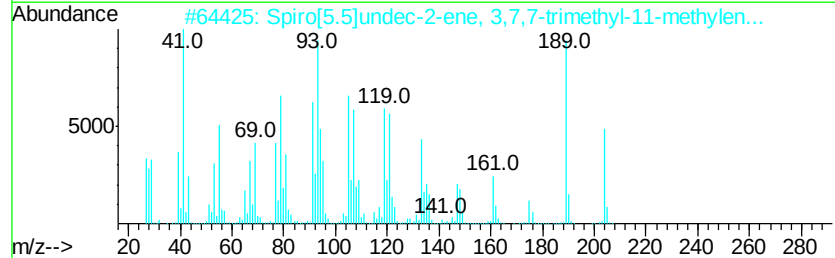
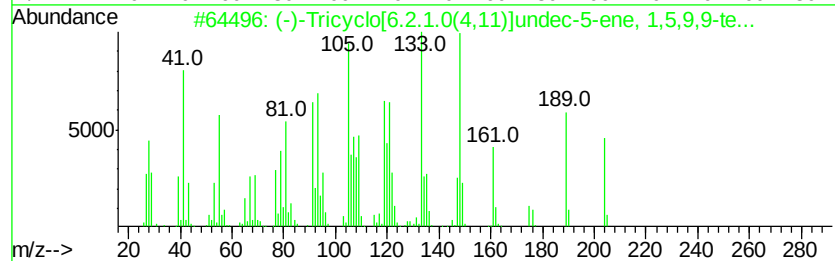
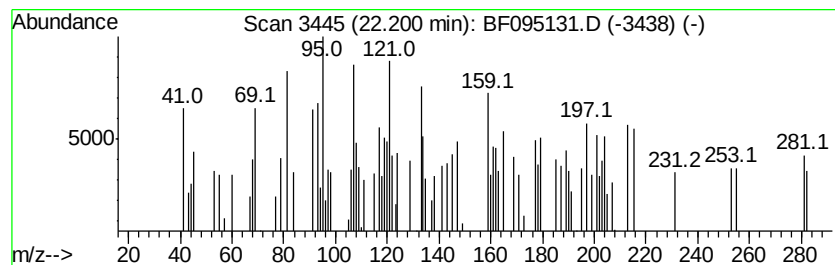
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 (-)-Tricyclo[6.2.1.0(4,11)]... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.20	3.78 ng	81407	Perylene-d12	20.37	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Tricyclo[6.2.1.0(4,11)]undec...	204	C15H24	1000154-06-7	60
2	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	41
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	38
4	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	38
5	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
Data File : BF095131.D
Acq On : 15 May 2017 18:10
Operator : SJ/MA
Sample : I3141-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_002

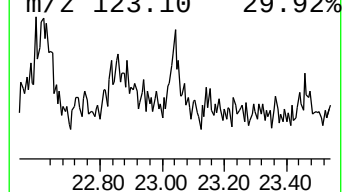
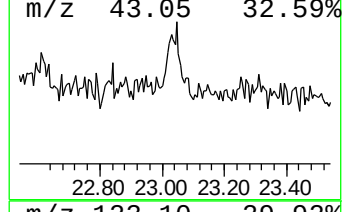
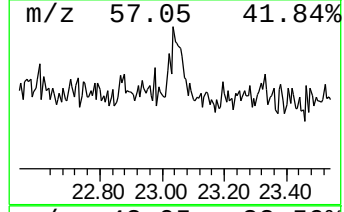
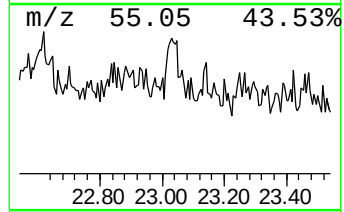
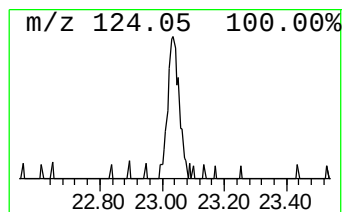
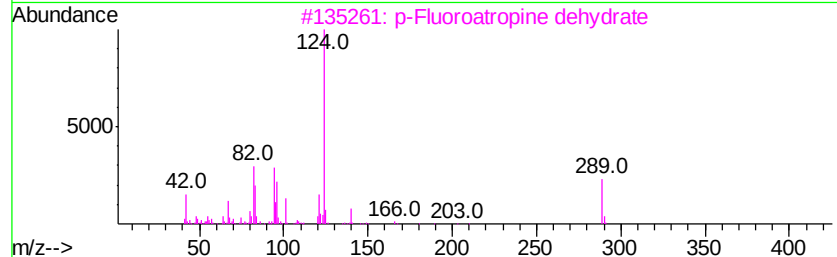
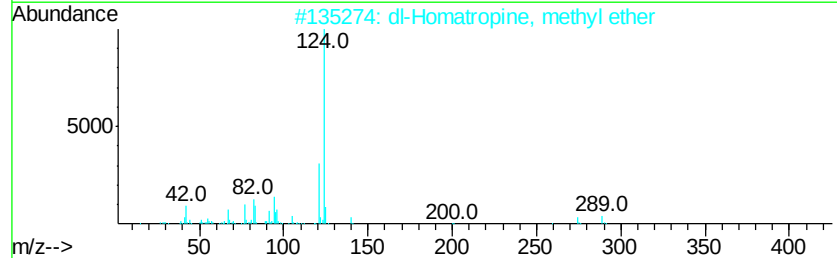
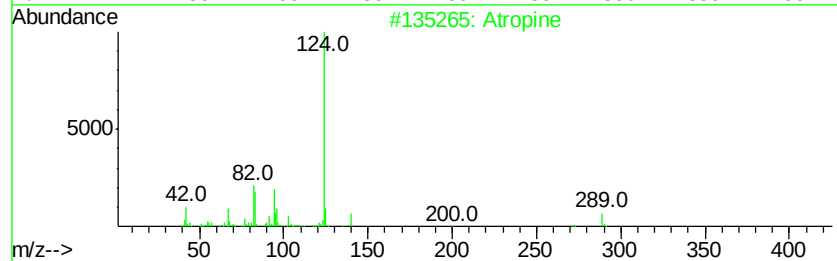
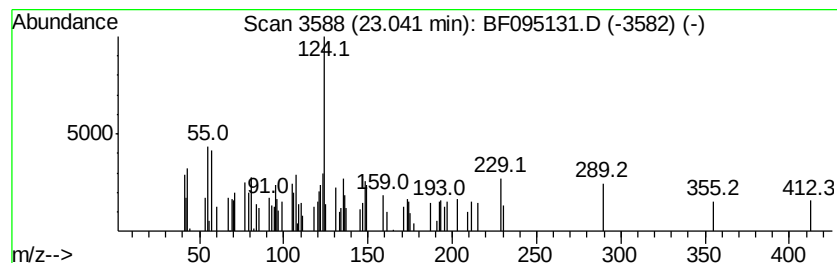
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.04 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.04	3.63 ng	78112	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Atropine	289	C17H23NO3	000051-55-8	30
2		dl-Homatropine, methyl ether	289	C17H23NO3	1000333-83-4	27
3		p-Fluoroatropine dehydrate	289	C17H20FN02	1000212-74-8	27
4		Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	25
5		4-(Bromomethyl)-1-azabicyclo[2.2...	203	C8H14BrN	026458-73-1	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
Data File : BF095131.D
Acq On : 15 May 2017 18:10
Operator : SJ/MA
Sample : I3141-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_002

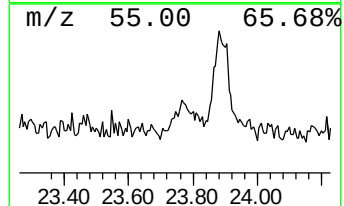
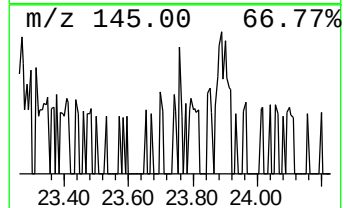
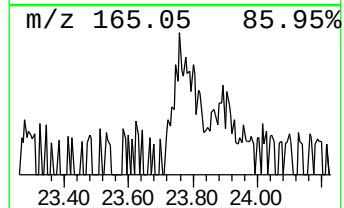
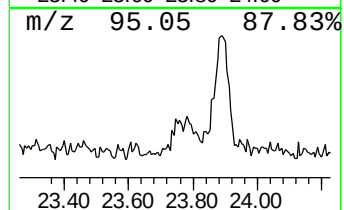
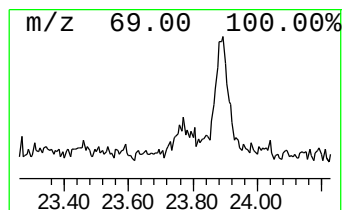
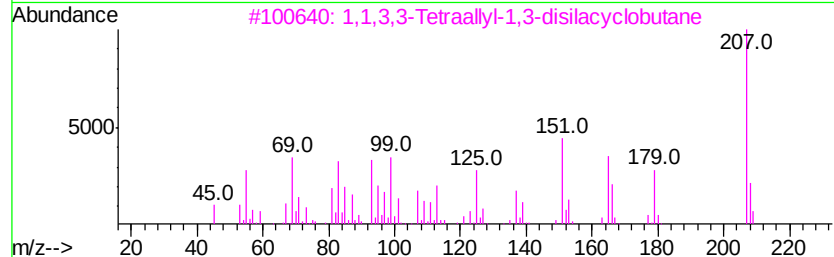
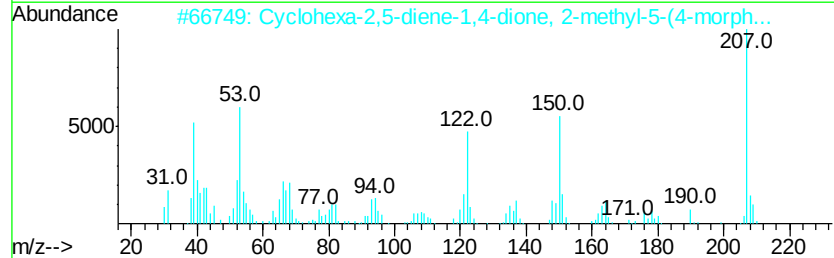
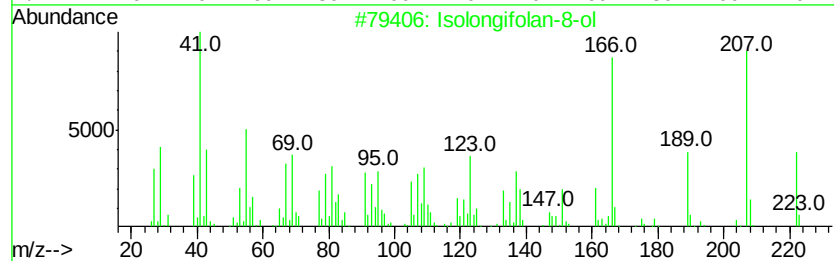
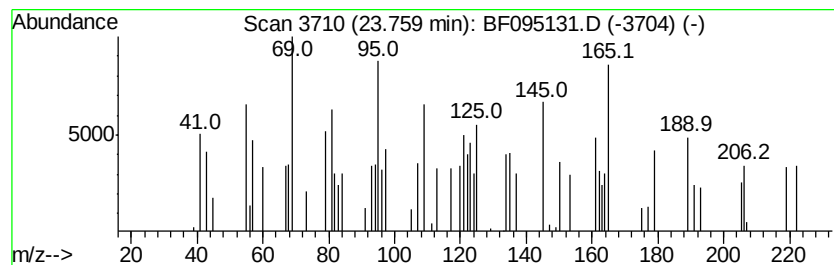
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown23.76 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	2.30 ng	49592	Perylene-d12	20.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isolongifolan-8-ol	222	C15H26O	001139-08-8	12
2		Cyclohexa-2,5-diene-1,4-dione, 2...	207	C11H13NO3	002158-89-6	11
3		1,1,3,3-Tetraallyl-1,3-disilacyc...	248	C14H24Si2	1000302-02-9	10
4		2-Pyridinamine, N-(4,5-dihydro-5...	207	C10H13N3S	1000362-45-9	9
5		Corydaldine	207	C11H13NO3	000493-49-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
Data File : BF095131.D
Acq On : 15 May 2017 18:10
Operator : SJ/MA
Sample : I3141-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

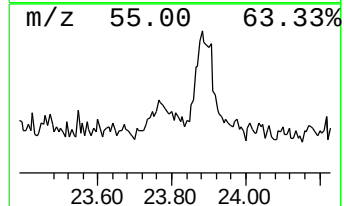
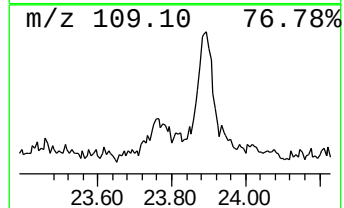
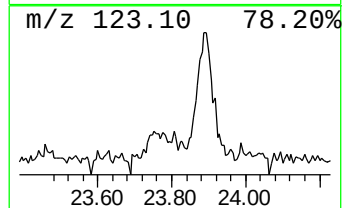
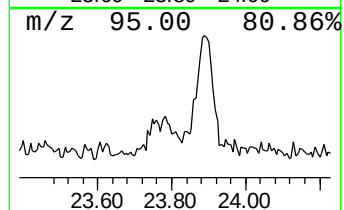
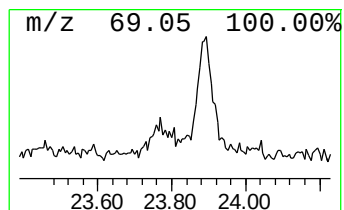
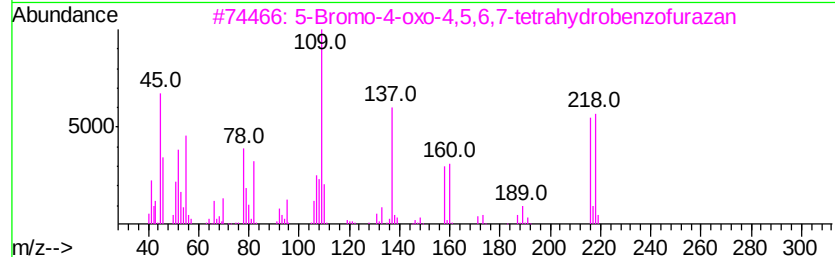
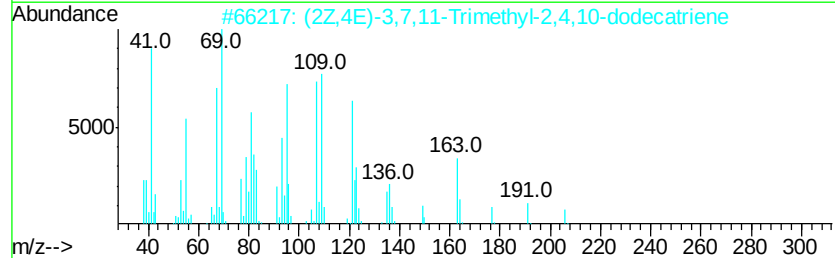
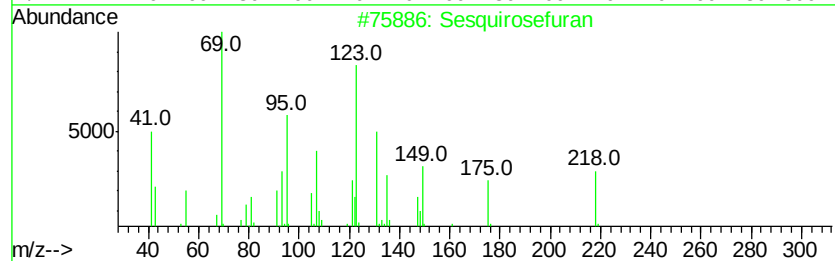
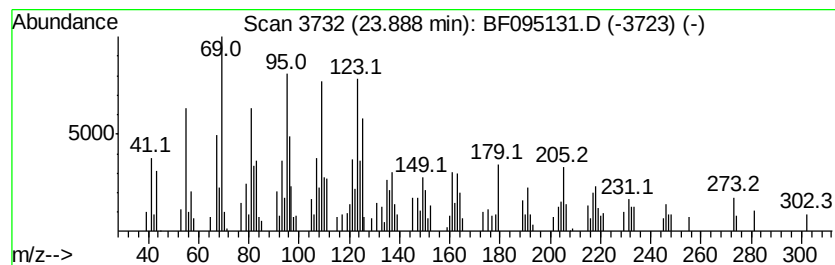
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Sesquirosefuran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
23.89	13.71 ng	295199	Perylene-d12	20.37		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sesquirosefuran	218	C15H22O	039007-93-7	70
2		(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	60
3		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
4		7-Octadecyne, 2-methyl-	264	C19H36	035354-38-2	49
5		Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095131.D
Acq On : 15 May 2017 18:10
Operator : SJ/MA
Sample : I3141-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01_002

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
2-Pentanone, 4-hy...	5.13	22.9	ng	499195	1	7.78	436365	20.0
unknown7.44	7.44	93.2	ng	2033280	1	7.78	436365	20.0
n-Hexadecanoic acid	15.98	3.2	ng	84283	4	15.03	528857	20.0
Behenic alcohol	18.62	3.1	ng	62859	5	18.70	402678	20.0
Eicosane	20.11	2.0	ng	43530	6	20.37	430498	20.0
unknown22.0	22.00	5.2	ng	112447	6	20.37	430498	20.0
(-)-Tricyclo[6.2....	22.20	3.8	ng	81407	6	20.37	430498	20.0
unknown23.04	23.04	3.6	ng	78112	6	20.37	430498	20.0
unknown23.76	23.76	2.3	ng	49592	6	20.37	430498	20.0
Sesquirosefuran	23.89	13.7	ng	295199	6	20.37	430498	20.0