

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
 Data File : BF095095.D
 Acq On : 11 May 2017 23:21
 Operator : SJ/MA
 Sample : I3084-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-001

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	5.007	517	522	549	rBV	387360	828170	26.65%	3.208%
2	5.648	627	631	660	rBV	1340949	2313222	74.44%	8.962%
3	6.225	726	729	736	rBV	21037	36769	1.18%	0.142%
4	7.248	899	903	918	rBV	1438861	2235598	71.94%	8.661%
5	7.366	918	923	945	rVB	1780776	2635533	84.81%	10.211%
6	7.701	976	980	989	rBV	466079	537635	17.30%	2.083%
7	7.936	1015	1020	1040	rBV	1575012	1991889	64.10%	7.717%
8	8.601	1128	1133	1158	rBV	1049779	1535934	49.42%	5.951%
9	9.725	1319	1324	1339	rBV	501771	757909	24.39%	2.936%
10	11.495	1620	1625	1639	rBV	2461713	3107648	100.00%	12.040%
11	12.189	1739	1743	1755	rBV	237551	339644	10.93%	1.316%
12	12.554	1800	1805	1817	rBV2	601057	883356	28.43%	3.422%
13	13.395	1942	1948	1952	rBV	39380	44283	1.42%	0.172%
14	13.848	2020	2025	2040	rBV	1108659	1705689	54.89%	6.608%
15	14.165	2074	2079	2089	rBV	38402	55345	1.78%	0.214%
16	14.954	2208	2213	2230	rVB2	547203	824842	26.54%	3.196%
17	15.924	2373	2378	2388	rBV2	142468	195957	6.31%	0.759%
18	16.589	2486	2491	2495	rBV	25778	31321	1.01%	0.121%
19	17.006	2558	2562	2570	rBV3	48887	81161	2.61%	0.314%
20	17.283	2603	2609	2623	rBV	2349383	2777082	89.36%	10.759%
21	18.553	2810	2825	2833	rBV9	37582	150142	4.83%	0.582%
22	18.624	2833	2837	2844	rVV	486867	658251	21.18%	2.550%
23	18.677	2844	2846	2855	rVB	27800	34360	1.11%	0.133%
24	19.165	2918	2929	2930	rBV7	14406	33788	1.09%	0.131%
25	19.747	3024	3028	3032	rVB	56898	64124	2.06%	0.248%
26	19.895	3047	3053	3060	rBV7	20779	47064	1.51%	0.182%
27	19.971	3062	3066	3072	rVB7	20331	33892	1.09%	0.131%
28	20.036	3072	3077	3083	rBV	74756	89721	2.89%	0.348%
29	20.294	3117	3121	3132	rVB	400732	535439	17.23%	2.074%
30	20.753	3195	3199	3204	rBV2	24724	33531	1.08%	0.130%
31	22.065	3412	3422	3432	rBV9	53015	168037	5.41%	0.651%
32	22.183	3438	3442	3447	rVB5	26738	45425	1.46%	0.176%
33	22.306	3457	3463	3467	rBV7	14589	39009	1.26%	0.151%
34	22.465	3485	3490	3501	rVB7	59471	184193	5.93%	0.714%

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ClientSampleId :
FK-PS-01-001

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	22.712	3522	3532	3541	rBV10	39601	151662	4.88%	0.588%
36	22.877	3554	3560	3566	rVB7	44301	104944	3.38%	0.407%
37	23.588	3670	3681	3692	rBV7	48078	227939	7.33%	0.883%
38	23.694	3692	3699	3709	rVB5	101419	291300	9.37%	1.129%

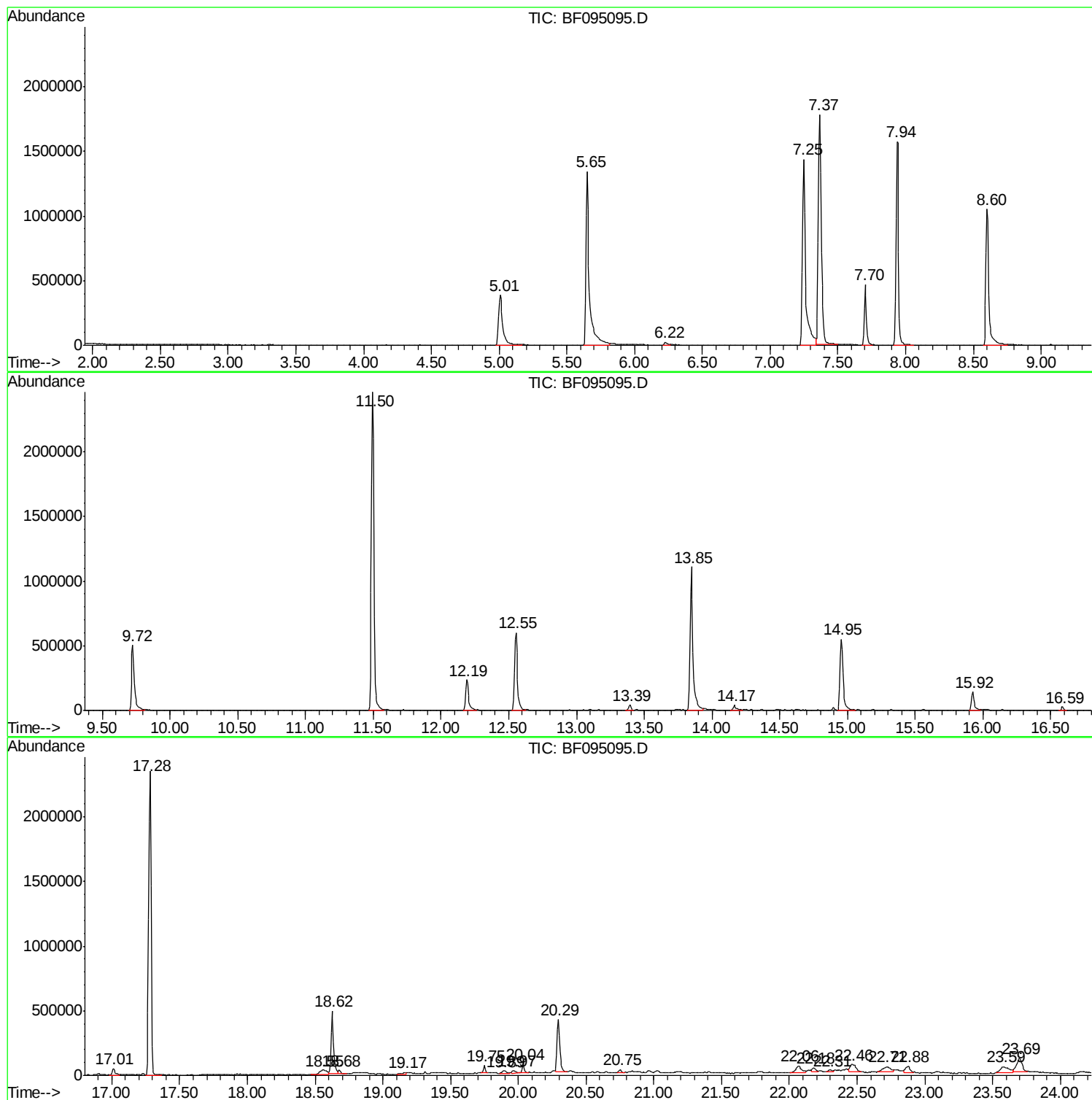
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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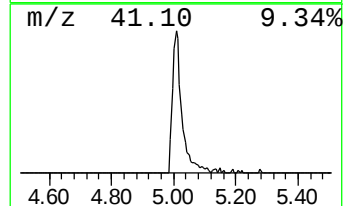
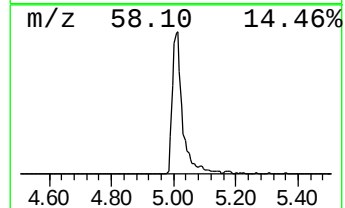
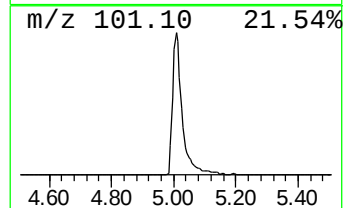
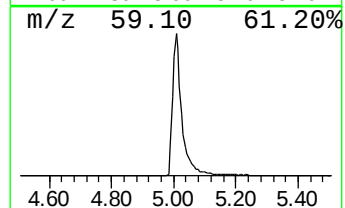
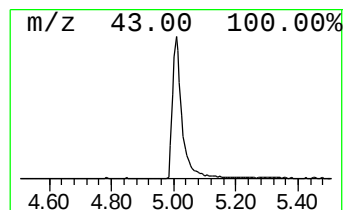
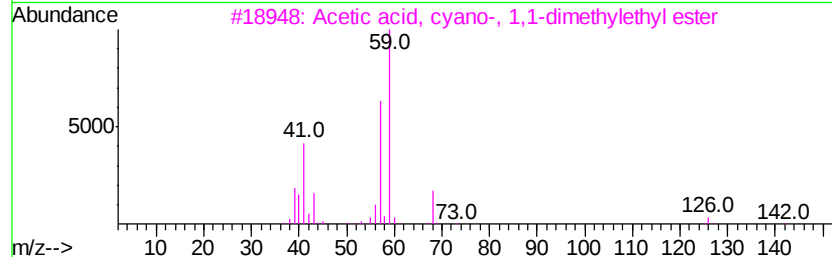
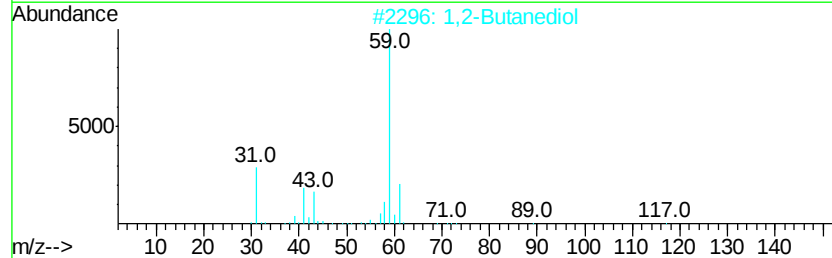
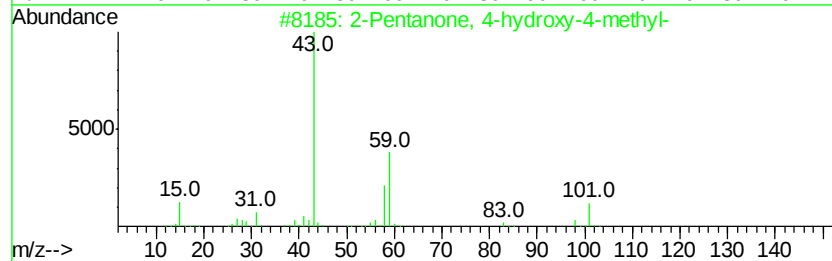
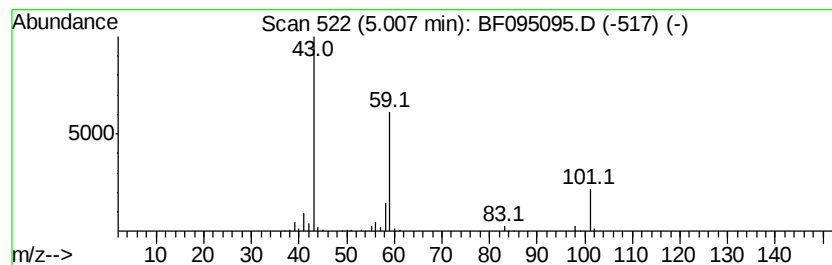
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	30.81 ng	828170	1,4-Dichlorobenzene-d4	7.70

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,2-Butanediol	90	C4H10O2	000584-03-2	23
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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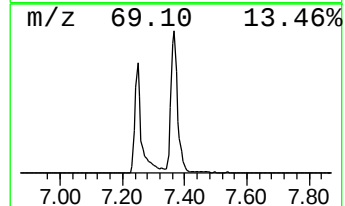
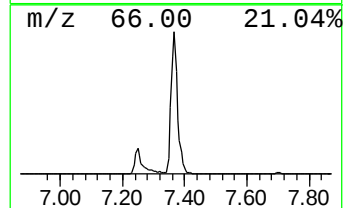
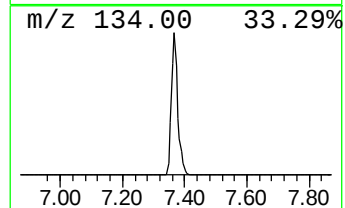
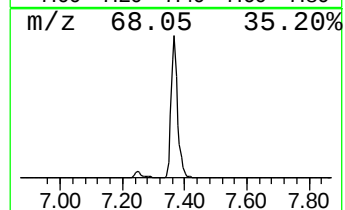
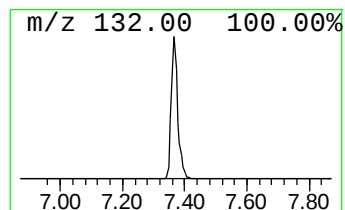
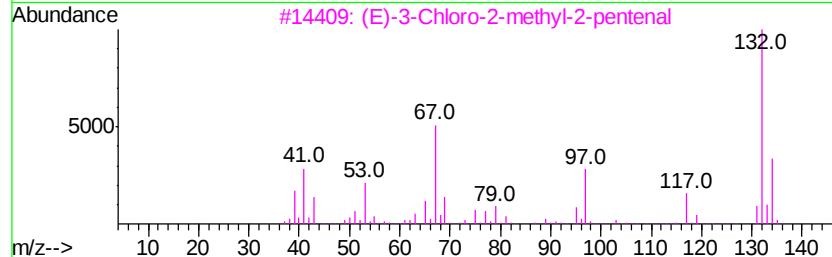
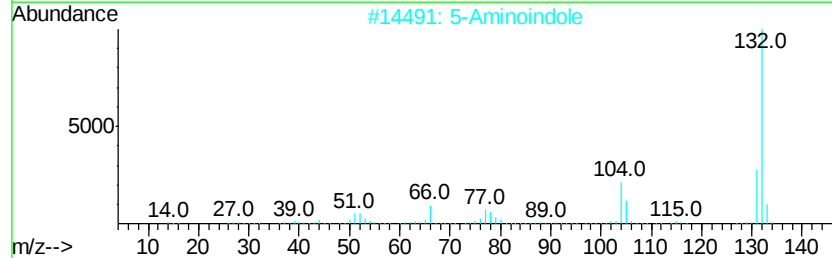
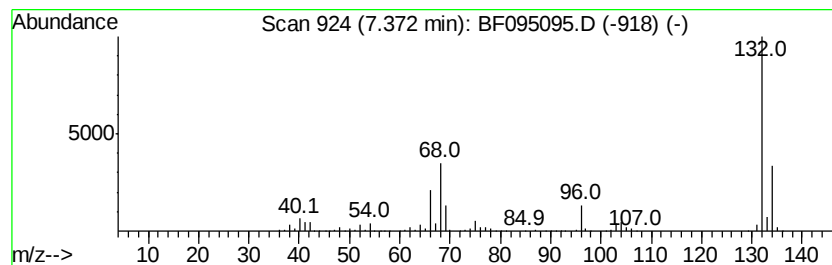
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	98.04 ng	2635530	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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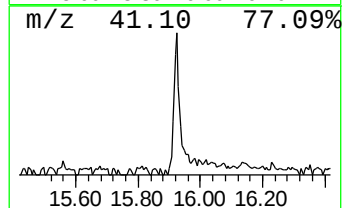
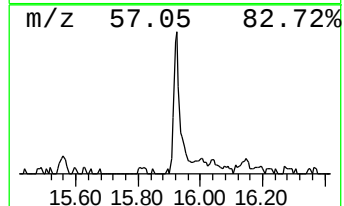
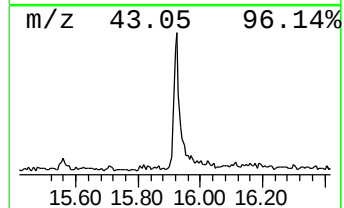
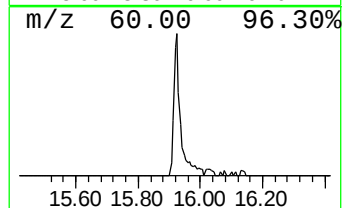
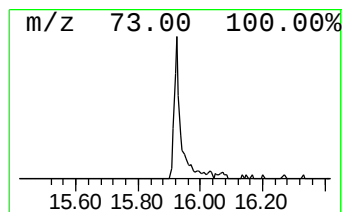
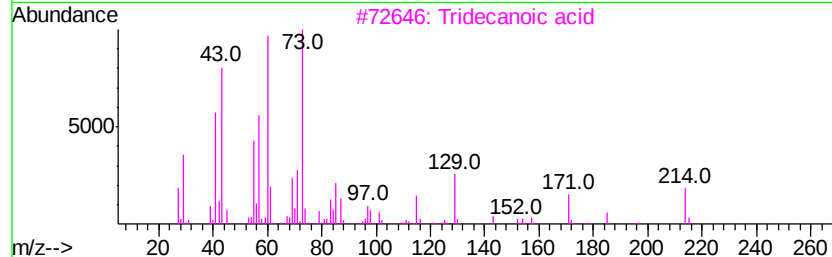
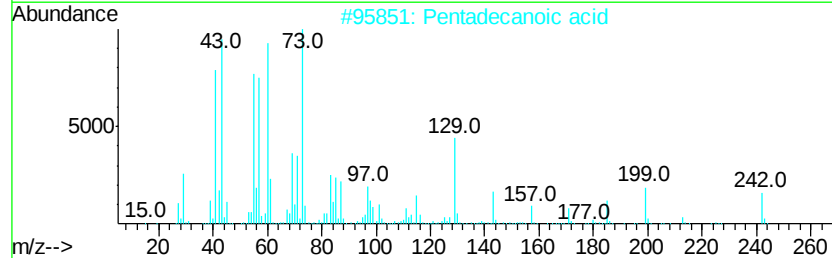
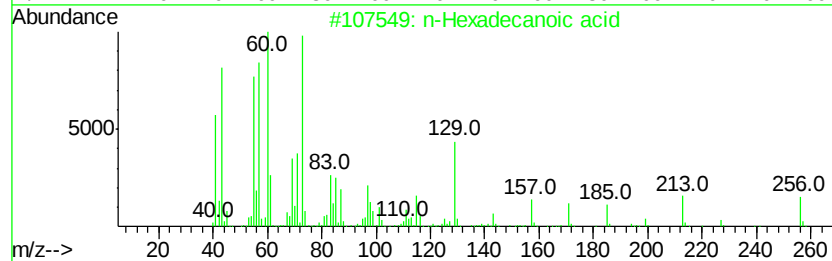
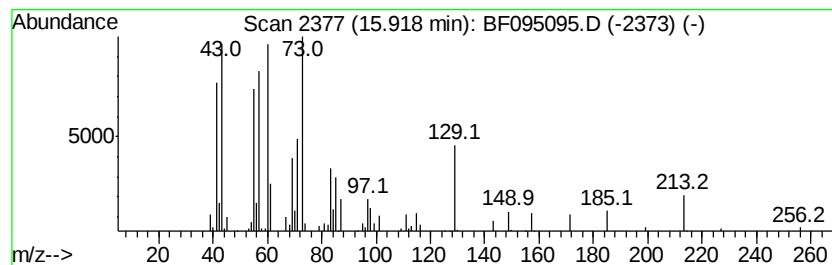
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	4.75 ng	195957	Phenanthrene-d10	14.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30



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Misc :
ALS Vial : 19 Sample Multiplier: 1

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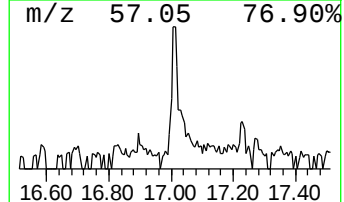
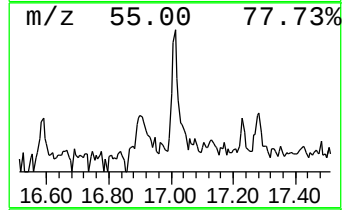
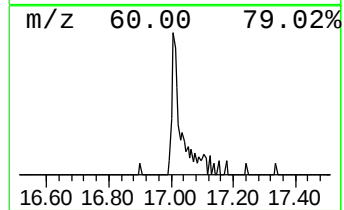
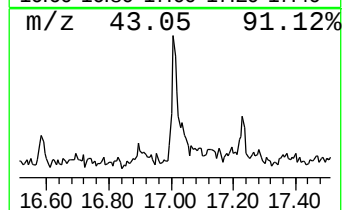
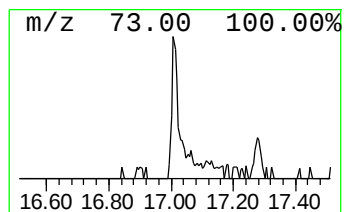
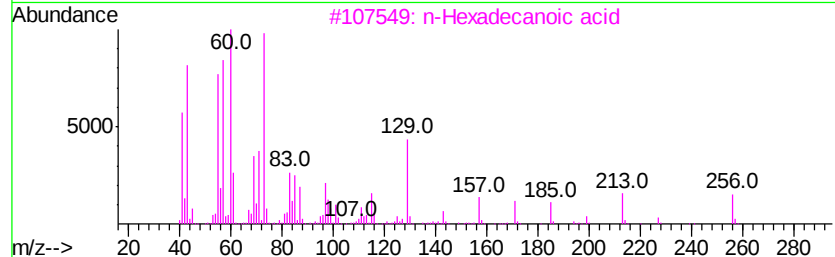
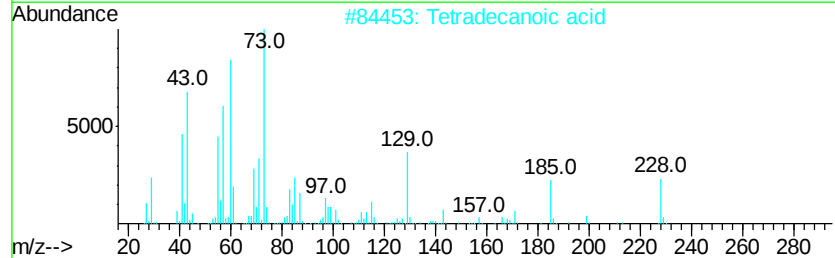
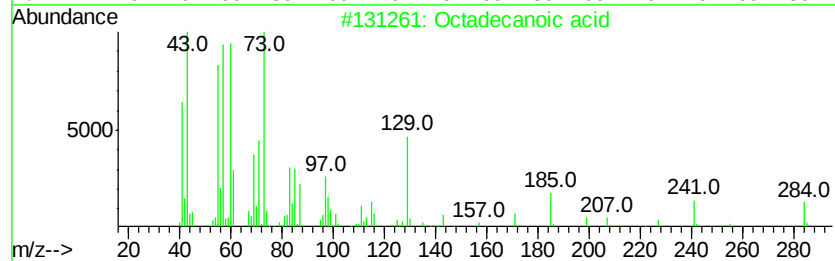
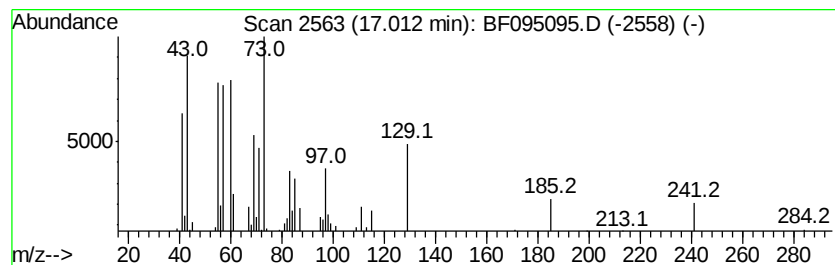
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	2.47 ng	81161	Chrysene-d12	18.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	59
5		Tridecanoic acid	214	C13H26O2	000638-53-9	59



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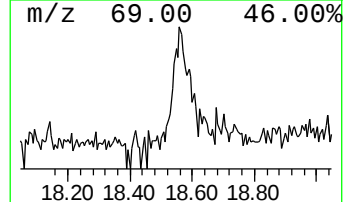
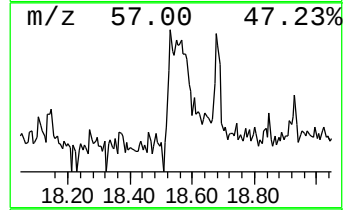
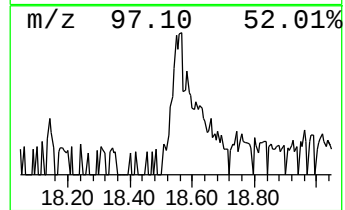
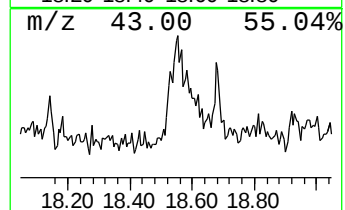
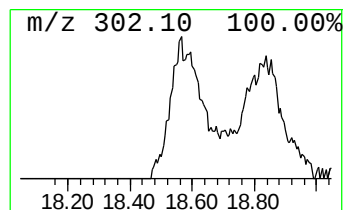
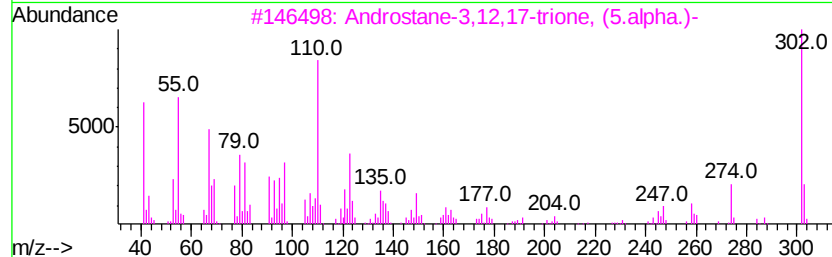
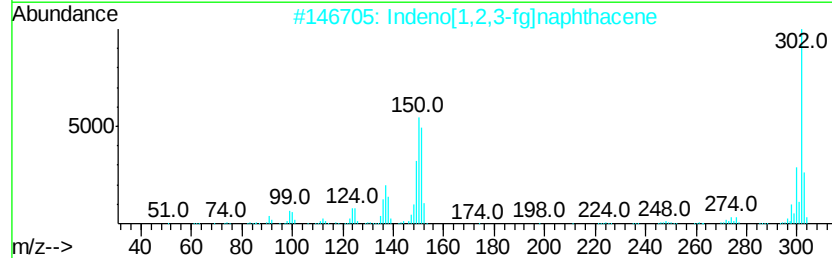
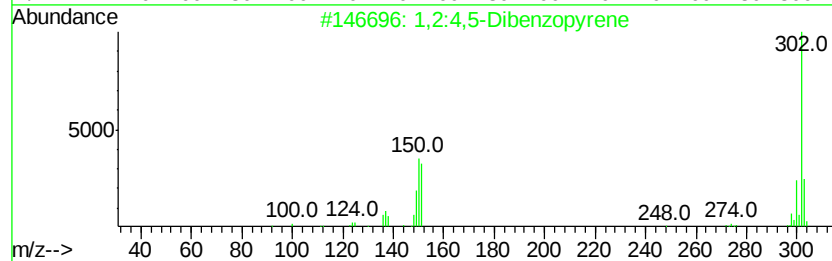
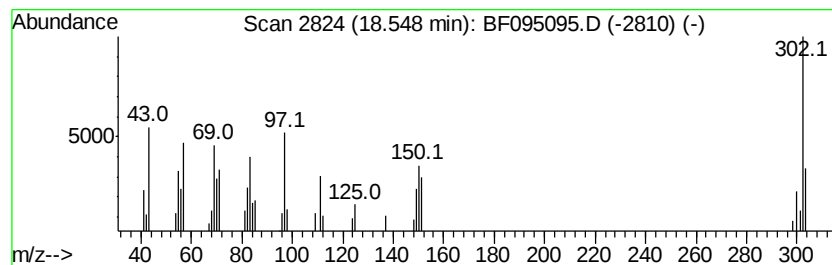
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,2:4,5-Dibenzopyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.55	4.56 ng	150142	Chrysene-d12	18.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopvrene	302	C24H14	000192-65-4	64
2	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	58
3	Androstane-3,12,17-trione, (5.alpha.)-	302	C19H26O3	004171-01-1	47
4	3,4:8,9-Dibenzopvrene	302	C24H14	000189-64-0	46
5	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	38



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Operator : SJ/MA
Sample : I3084-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-001

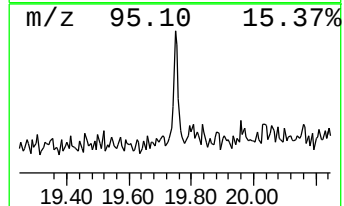
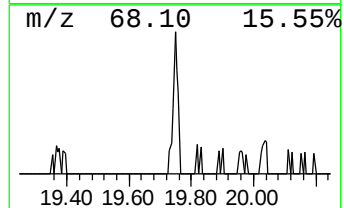
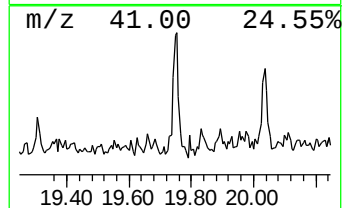
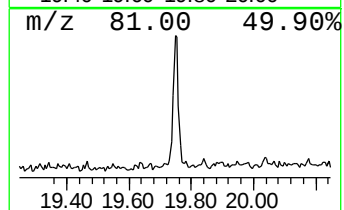
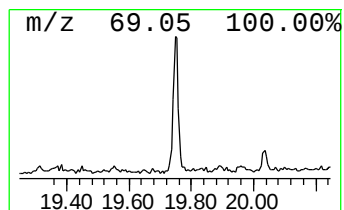
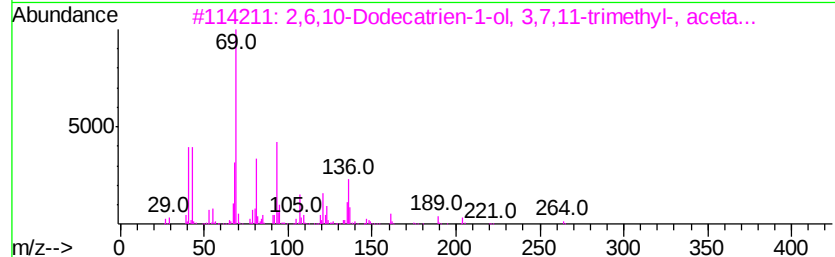
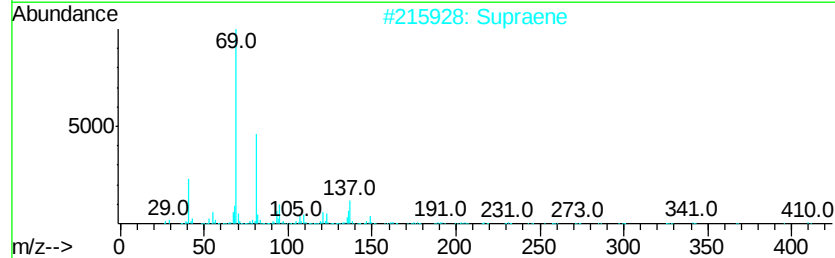
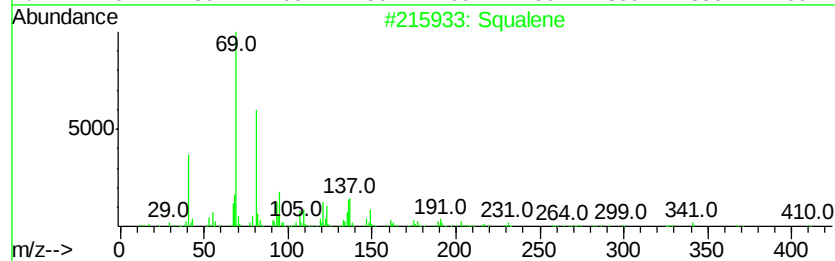
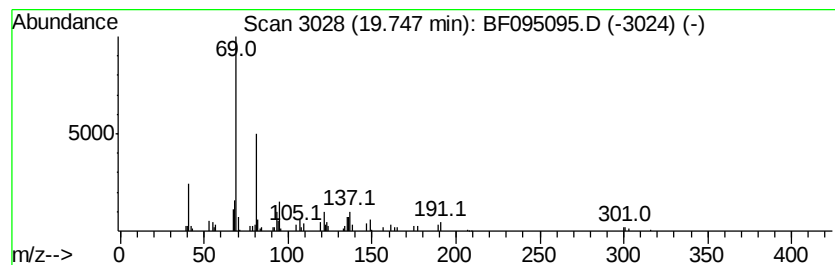
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	2.40 ng	64124	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Supraene	410	C30H50	007683-64-9	72
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	59
4		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
Data File : BF095095.D
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Sample : I3084-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

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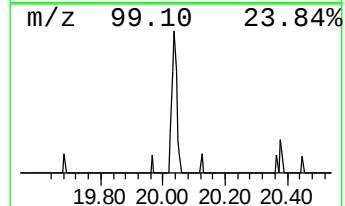
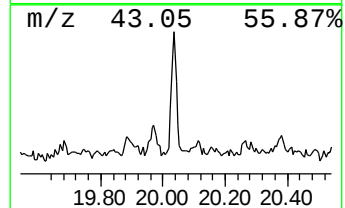
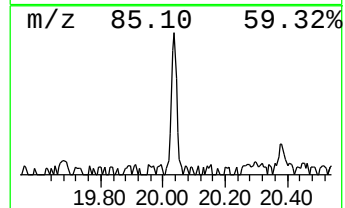
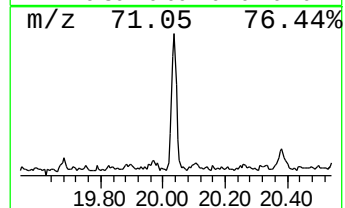
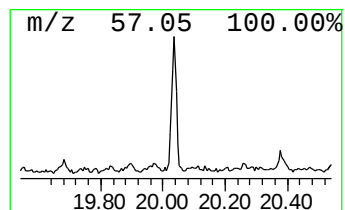
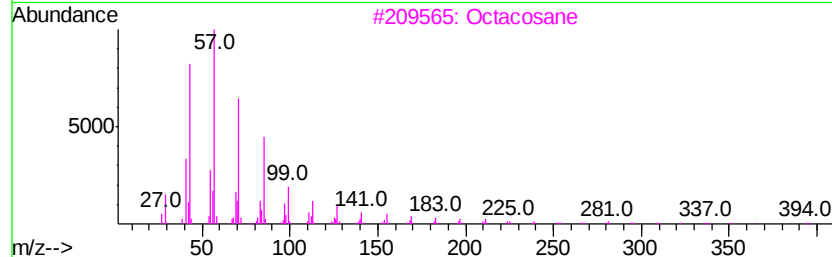
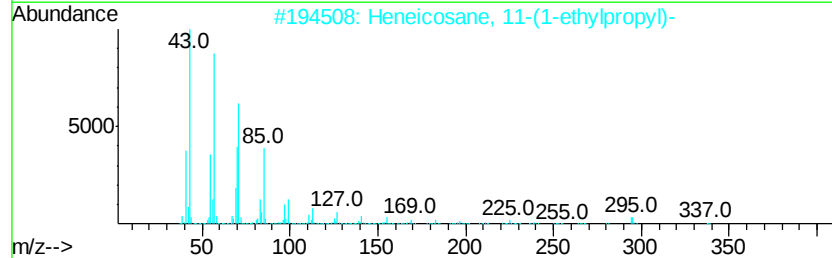
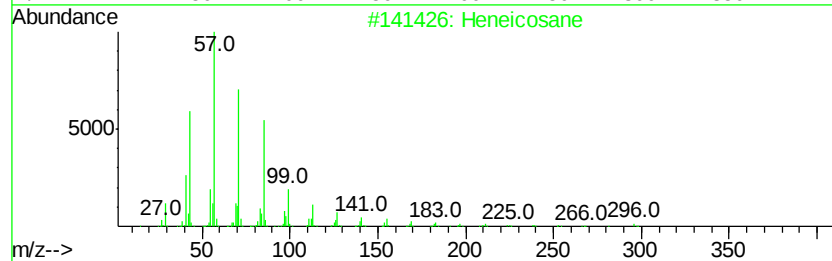
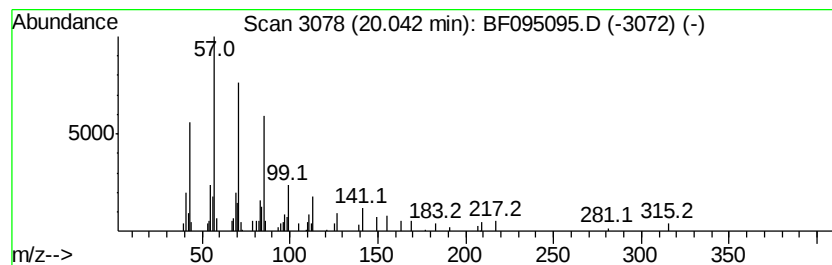
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.04	3.35 ng	89721	Perylene-d12	20.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	90
3	Octacosane		394	C28H58	000630-02-4	87
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Tetratetracontane		619	C44H90	007098-22-8	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
Data File : BF095095.D
Acq On : 11 May 2017 23:21
Operator : SJ/MA
Sample : I3084-01
Misc :
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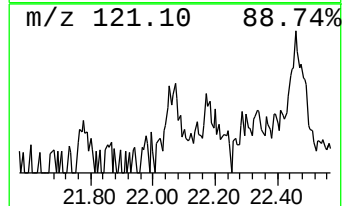
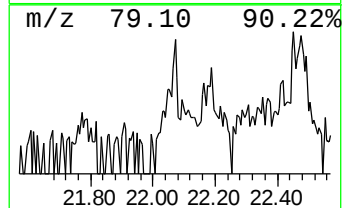
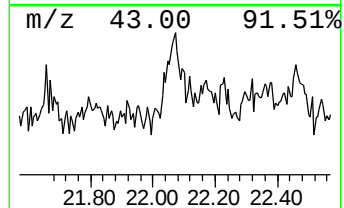
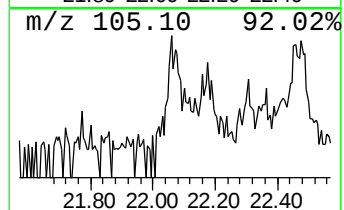
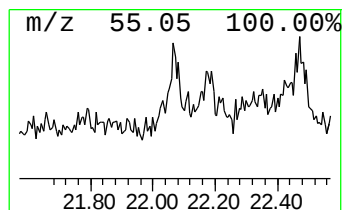
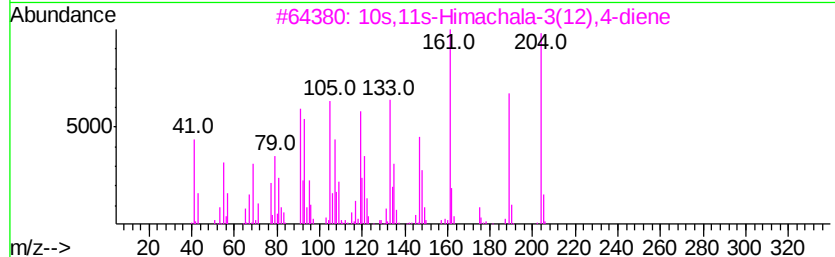
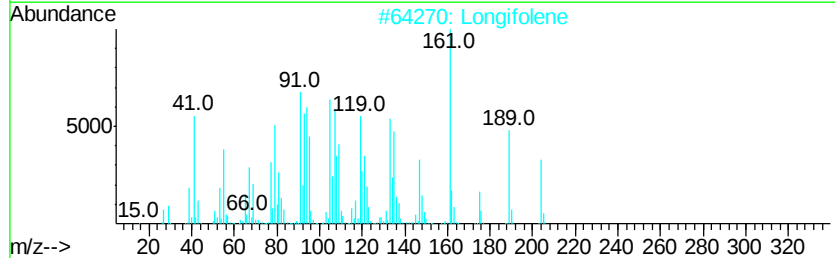
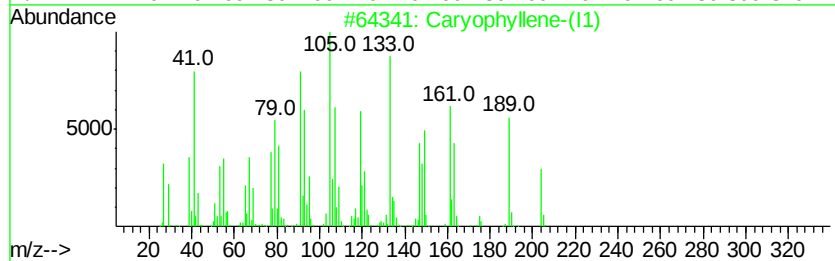
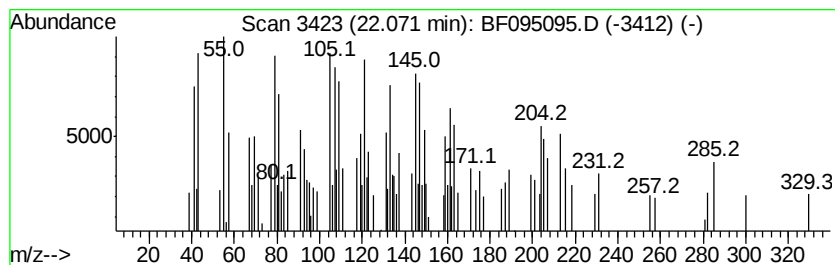
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Caryophyllene-(I1) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	6.28 ng	168037	Perylene-d12	20.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Caryophyllene-(I1)	204 C15H24	1000158-18-5 78
2		Longifolene	204 C15H24	000475-20-7 56
3		10s,11s-Himachala-3(12),4-diene	204 C15H24	060909-28-6 53
4		Azulene, 1,2,3,3a,4,5,6,7-octahv...	204 C15H24	022567-17-5 49
5		Aromandendrene	204 C15H24	000489-39-4 45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
Data File : BF095095.D
Acq On : 11 May 2017 23:21
Operator : SJ/MA
Sample : I3084-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

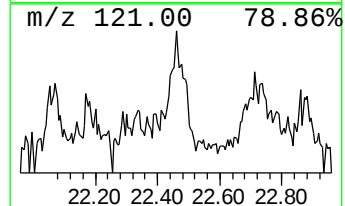
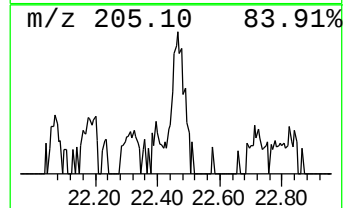
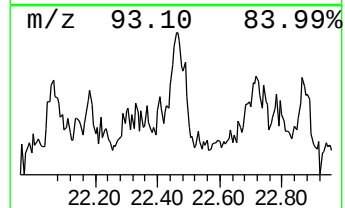
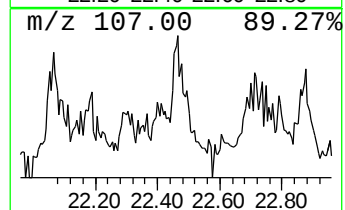
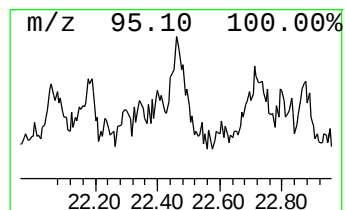
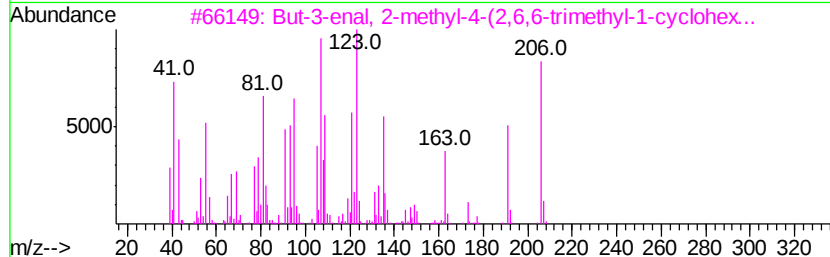
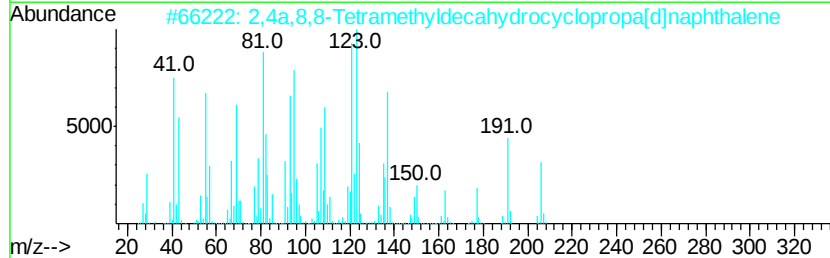
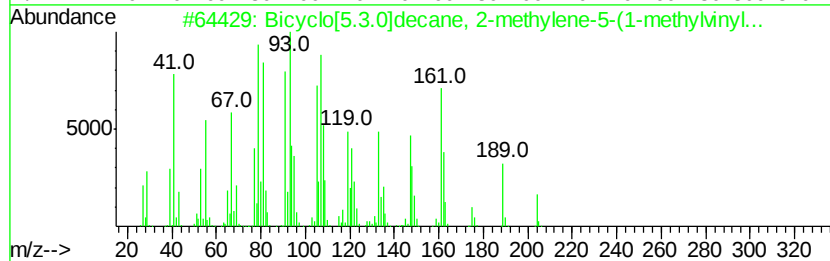
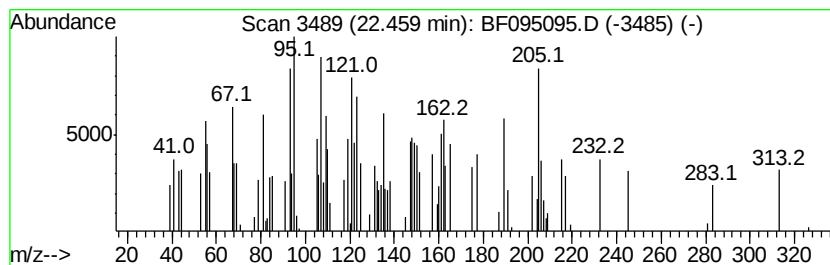
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown22.46 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.46	6.88 ng	184193	Perylene-d12	20.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicvclo[5.3.0]decane, 2-methylen...	204	C15H24	1000159-39-3	45
2	2,4a,8,8-Tetramethyldecahydrocvc...	206	C15H26	074022-04-1	41
3	But-3-enal, 2-methyl-4-(2,6,6-tr...	206	C14H22O	104900-59-6	38
4	1-Oxaspiro[2.5]octane, 5,5-dimet...	206	C14H22O	1000195-92-1	38
5	2-Butenal, 2-methyl-4-(2,6,6-tri...	206	C14H22O	003155-71-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
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ALS Vial : 19 Sample Multiplier: 1

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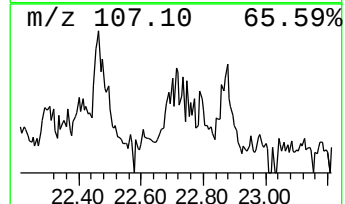
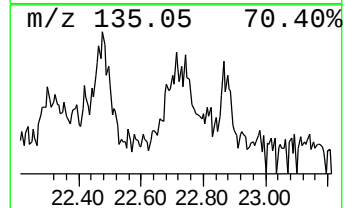
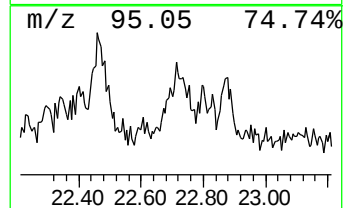
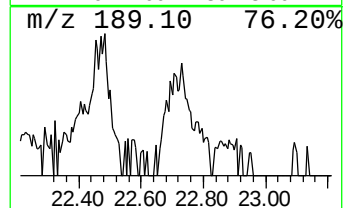
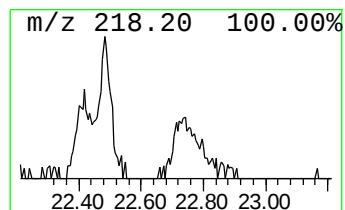
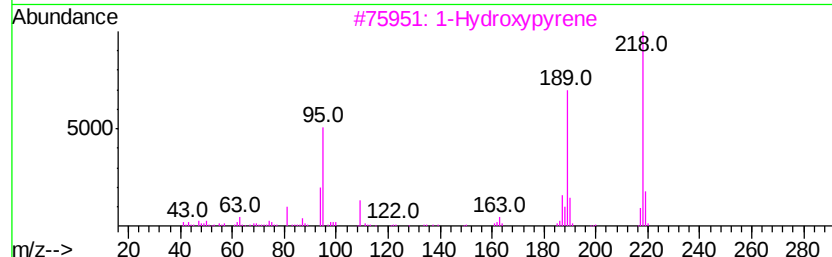
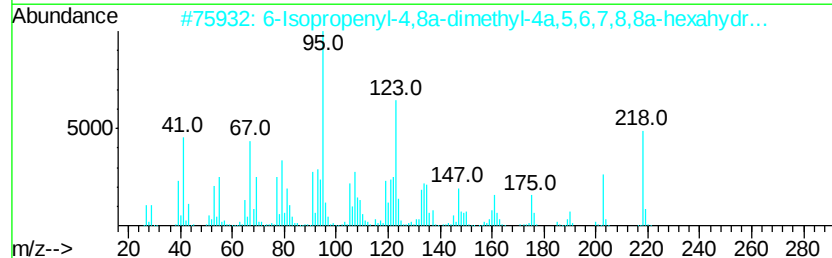
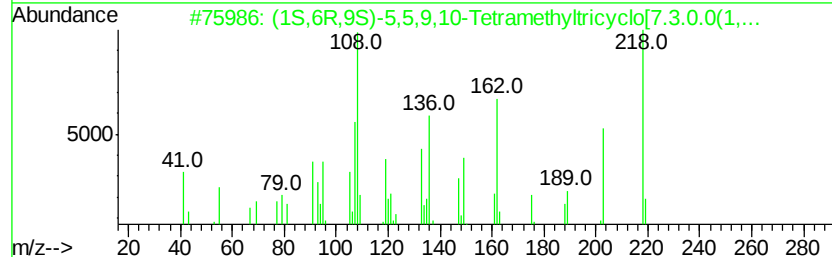
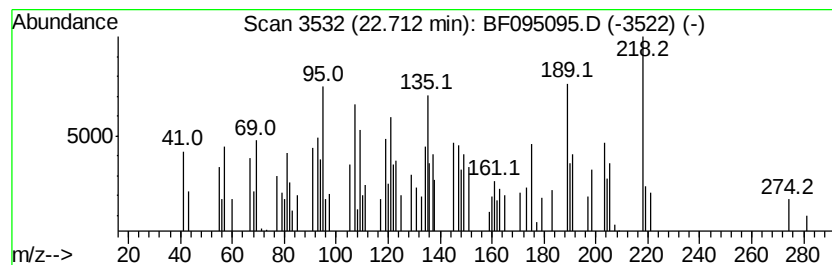
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown22.71 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.71	5.66 ng	151662	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	38
2		6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	35
3		1-Hydroxypvrene	218	C16H10O	005315-79-7	35
4		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	25
5		Benzenamine, 2-bromo-4-nitro-	216	C6H5BrN2O2	013296-94-1	25



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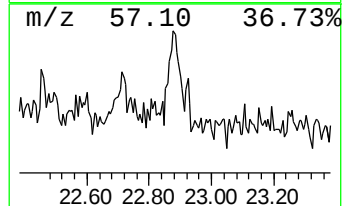
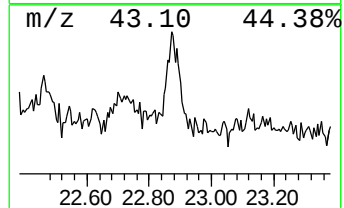
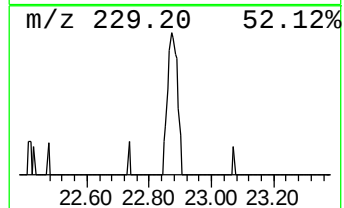
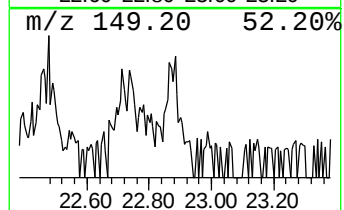
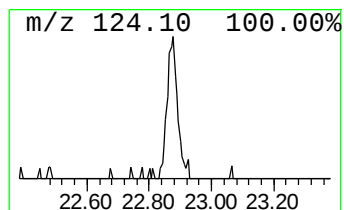
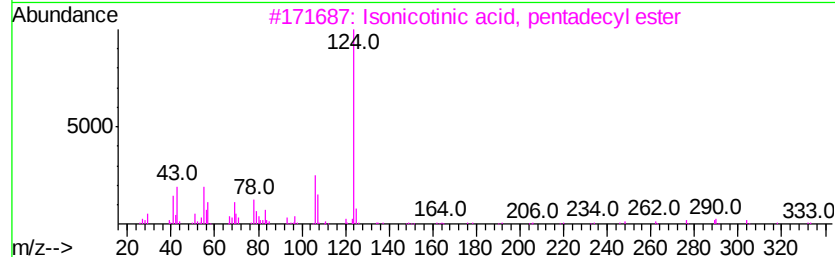
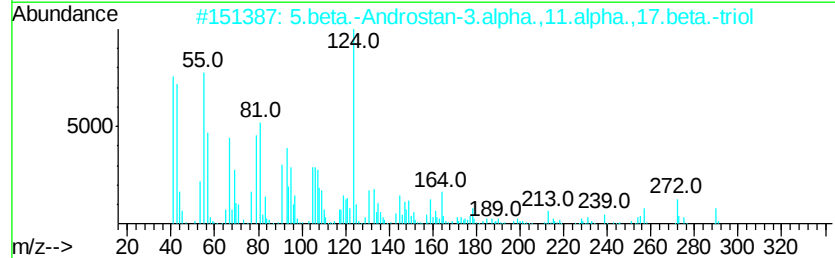
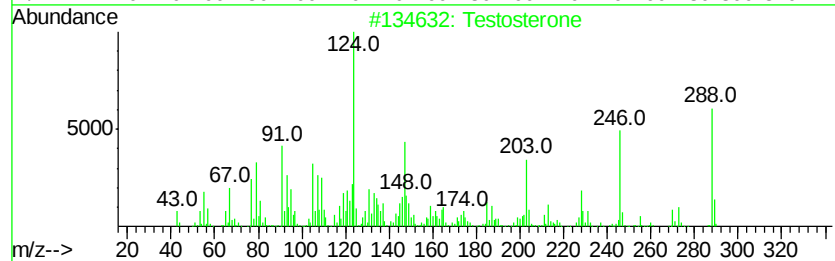
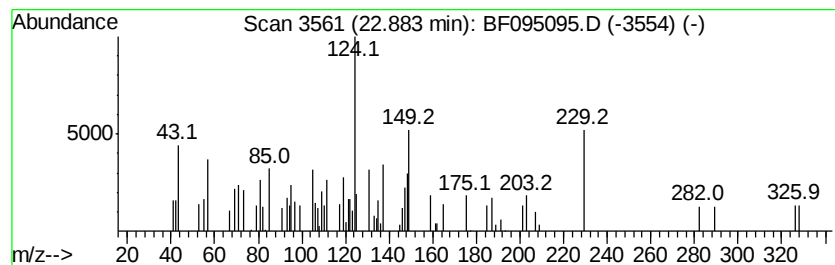
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown22.88 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.88	3.92 ng	104944	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Testosterone	288	C19H28O2	000058-22-0	43
2		5.beta.-Androstan-3.alpha.,11.al...	308	C19H32O3	032212-61-6	27
3		Isonicotinic acid, pentadecyl ester	333	C21H35NO2	1000299-89-0	27
4		Cyclobuta[1,2:3,4]dicyclooctene-...	248	C16H24O2	069926-83-6	25
5		Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000481-30-1	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051117\
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ALS Vial : 19 Sample Multiplier: 1

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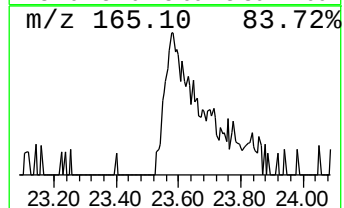
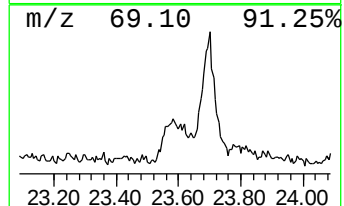
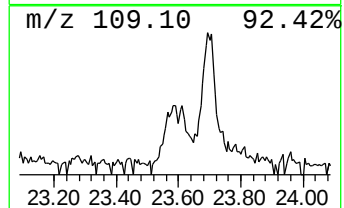
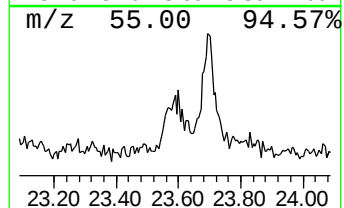
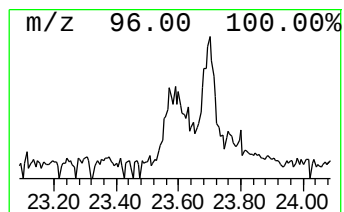
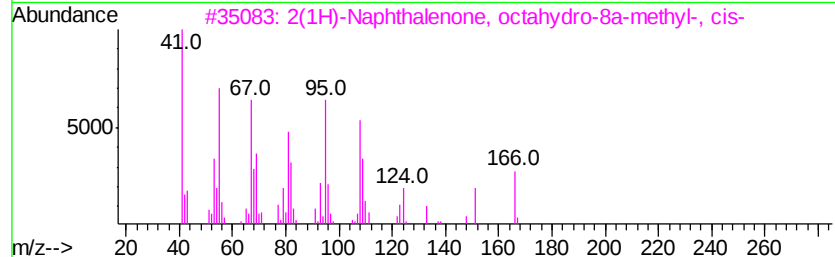
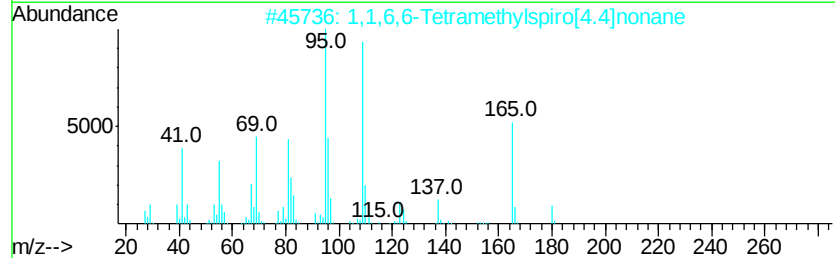
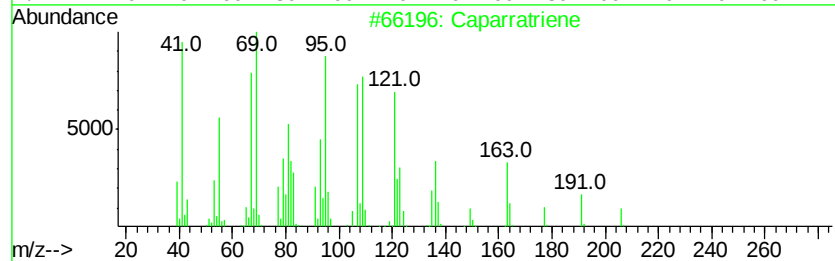
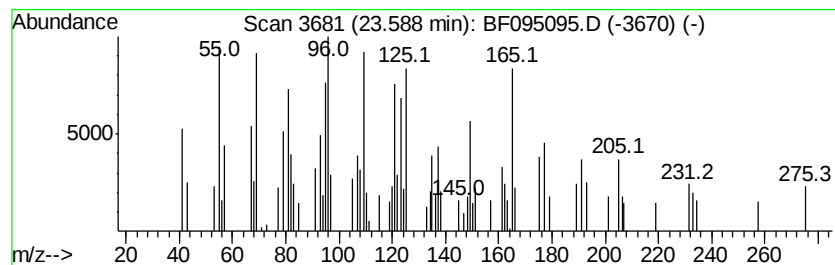
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown23.59 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.59	8.51 ng	227939	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Caparratriene	206	C15H26	1000374-08-7	42
2		1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	27
3		2(1H)-Naphthalenone, octahydro-8...	166	C11H18O	002530-17-8	25
4		1,E-11,Z-13-Heptadecatriene	234	C17H30	080625-35-0	25
5		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
Data File : BF095095.D
Acq On : 11 May 2017 23:21
Operator : SJ/MA
Sample : I3084-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-PS-01-001

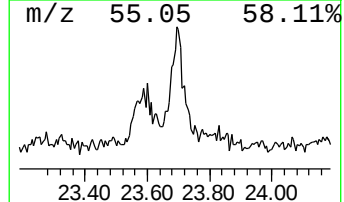
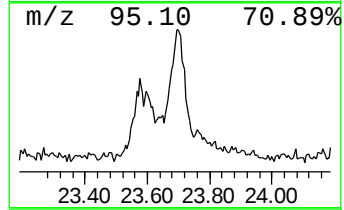
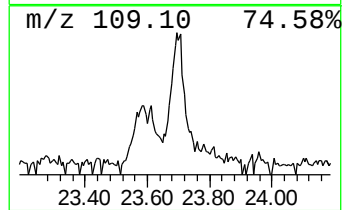
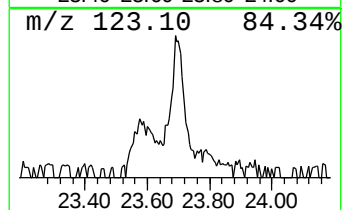
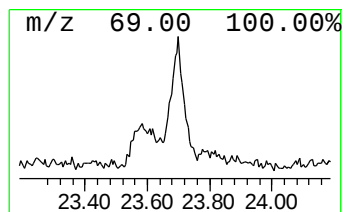
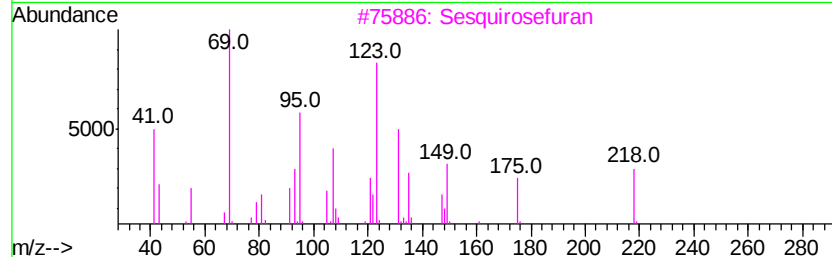
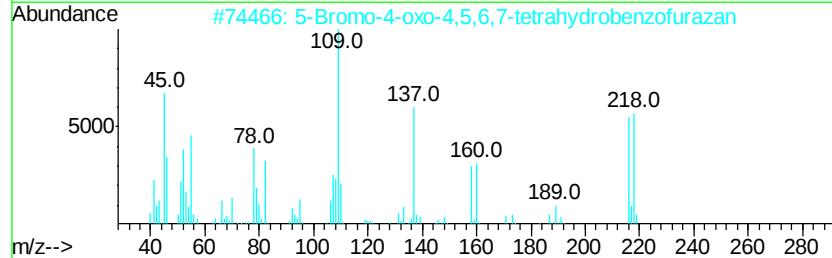
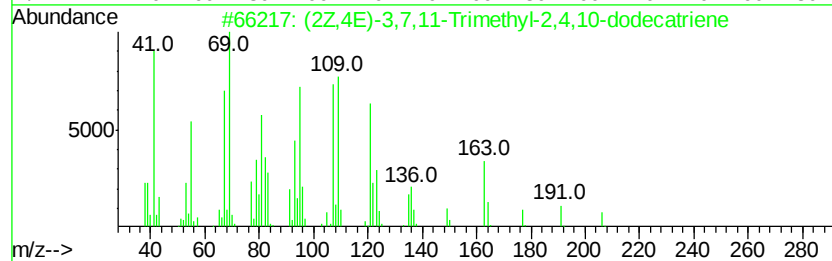
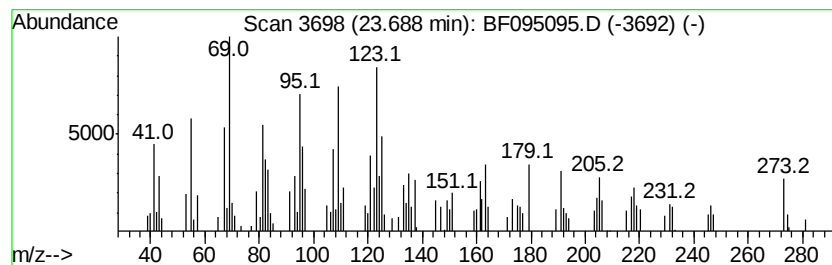
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 (2Z,4E)-3,7,11-Trimethyl-2,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.69	10.88 ng	291300	Perylene-d12	20.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	78
2		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	70
3		Sesquirosefuran	218	C15H22O	039007-93-7	50
4		Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	42
5		Longifolenaldehyde	220	C15H24O	019890-84-7	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051117\
 Data File : BF095095.D
 Acq On : 11 May 2017 23:21
 Operator : SJ/MA
 Sample : I3084-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-001

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...	5.01	30.8	ng	828170	1	7.70	537635	20.0
unknown7.37	7.37	98.0	ng	2635530	1	7.70	537635	20.0
n-Hexadecanoic acid	15.92	4.8	ng	195957	4	14.95	824842	20.0
Octadecanoic acid	17.01	2.5	ng	81161	5	18.62	658251	20.0
1,2:4,5-Dibenzopy...	18.55	4.6	ng	150142	5	18.62	658251	20.0
Squalene	19.75	2.4	ng	64124	6	20.29	535439	20.0
Heneicosane	20.04	3.4	ng	89721	6	20.29	535439	20.0
Caryophyllene-(I1)	22.07	6.3	ng	168037	6	20.29	535439	20.0
unknown22.46	22.46	6.9	ng	184193	6	20.29	535439	20.0
unknown22.71	22.71	5.7	ng	151662	6	20.29	535439	20.0
unknown22.88	22.88	3.9	ng	104944	6	20.29	535439	20.0
unknown23.59	23.59	8.5	ng	227939	6	20.29	535439	20.0
(2Z,4E)-3,7,11-Tr...	23.69	10.9	ng	291300	6	20.29	535439	20.0