

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051517\
 Data File : BF095137.D
 Acq On : 15 May 2017 21:23
 Operator : SJ/MA
 Sample : I3147-06
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3COMP

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	5.143	540	545	559	rBV	267591	578515	18.10%	2.257%
2	5.748	644	648	687	rBV	1443293	2552396	79.83%	9.958%
3	6.325	741	746	756	rBV2	19737	39364	1.23%	0.154%
4	7.325	911	916	932	rBV	1672233	2606164	81.52%	10.168%
5	7.442	932	936	951	rVB	2086902	2950721	92.29%	11.512%
6	7.778	989	993	1006	rBV	417515	533698	16.69%	2.082%
7	8.019	1029	1034	1051	rVB	1873589	2227680	69.68%	8.691%
8	8.678	1141	1146	1167	rBV	1230850	1671749	52.29%	6.522%
9	9.795	1332	1336	1353	rBV	504993	704442	22.03%	2.748%
10	11.566	1632	1637	1658	rBV	2357440	3197089	100.00%	12.473%
11	12.260	1751	1755	1766	rBV	212353	328247	10.27%	1.281%
12	12.624	1812	1817	1830	rBV2	548891	767203	24.00%	2.993%
13	13.918	2032	2037	2060	rBV	961592	1491587	46.65%	5.819%
14	14.230	2087	2090	2094	rBV	28934	35127	1.10%	0.137%
15	15.030	2221	2226	2236	rBV	459991	620703	19.41%	2.422%
16	15.983	2384	2388	2399	rBV5	52089	122764	3.84%	0.479%
17	16.818	2526	2530	2537	rBV	45059	64398	2.01%	0.251%
18	17.118	2577	2581	2588	rVB	67294	96348	3.01%	0.376%
19	17.189	2590	2593	2599	rBV2	23351	33809	1.06%	0.132%
20	17.348	2615	2620	2630	rBV2	1939082	2249780	70.37%	8.777%
21	17.553	2650	2655	2657	rBV5	18760	32621	1.02%	0.127%
22	18.042	2734	2738	2747	rVB	727014	874402	27.35%	3.411%
23	18.148	2753	2756	2758	rBV	31578	35819	1.12%	0.140%
24	18.630	2836	2838	2843	rVB6	26900	44846	1.40%	0.175%
25	18.695	2845	2849	2855	rBV	446192	619856	19.39%	2.418%
26	19.718	3020	3023	3031	rBV5	65578	125584	3.93%	0.490%
27	19.971	3063	3066	3069	rBV	75687	96558	3.02%	0.377%
28	20.265	3114	3116	3120	rVB	69639	67444	2.11%	0.263%
29	20.324	3124	3126	3129	rVV	85852	100520	3.14%	0.392%
30	20.377	3131	3135	3147	rVB	342487	540265	16.90%	2.108%
31	20.971	3233	3236	3242	rVB3	83682	139023	4.35%	0.542%
32	21.347	3298	3300	3305	rVB4	60320	82914	2.59%	0.323%

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Misc :
ALS Vial : 15 Sample Multiplier: 1

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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

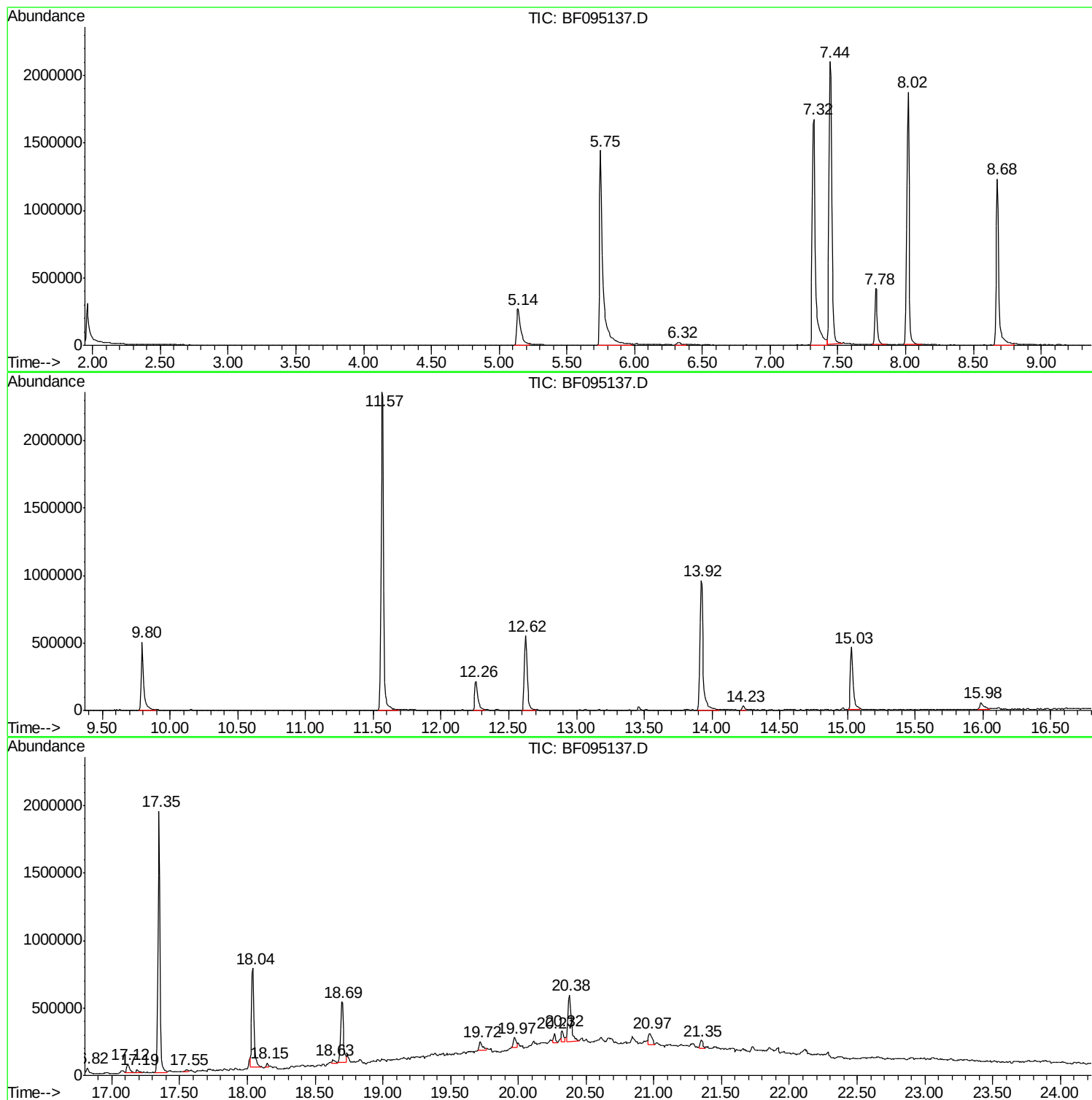
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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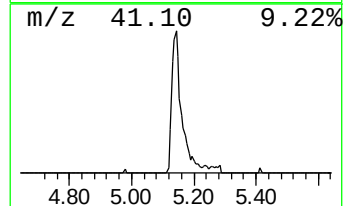
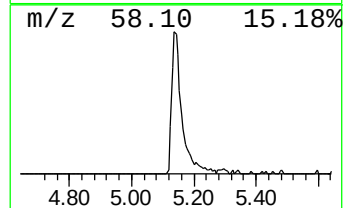
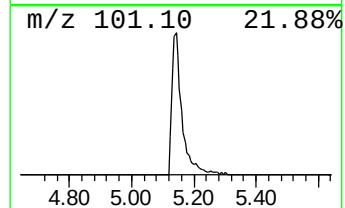
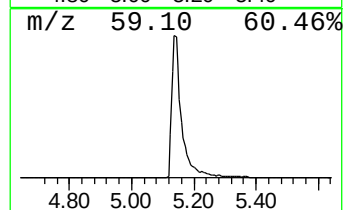
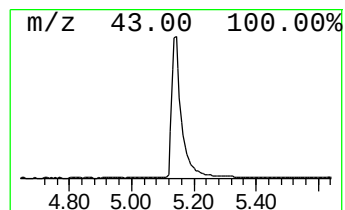
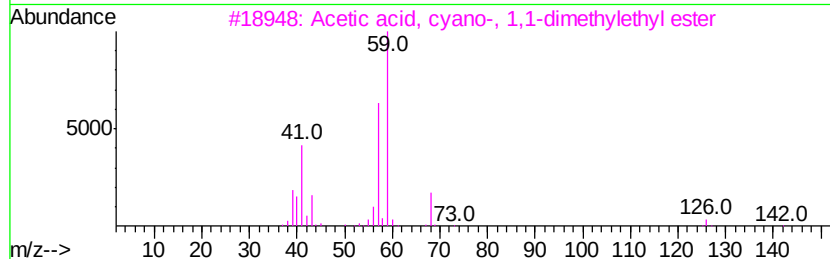
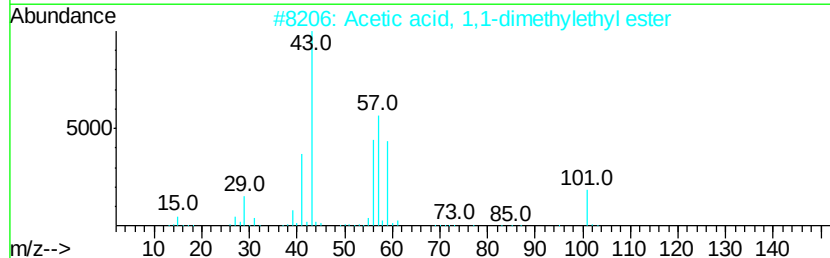
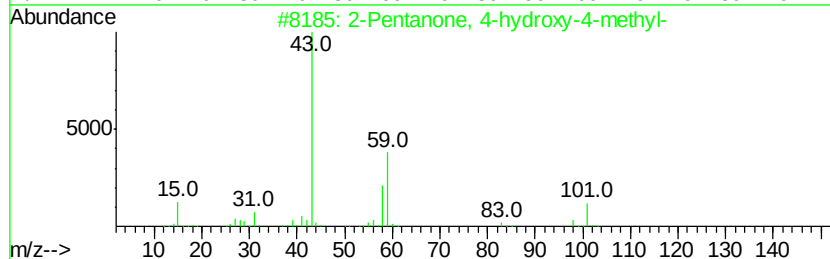
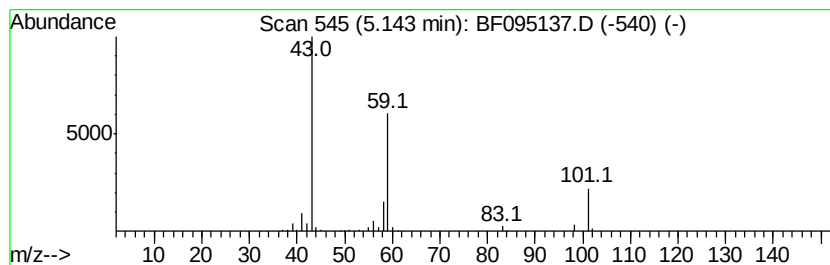
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	21.68 ng	578515	1,4-Dichlorobenzene-d4	7.78

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			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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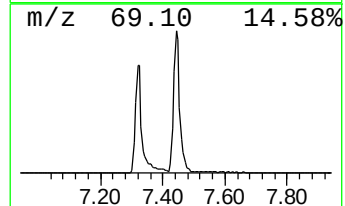
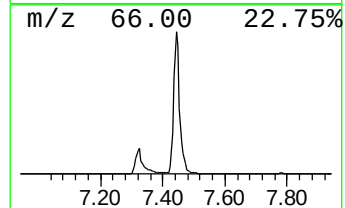
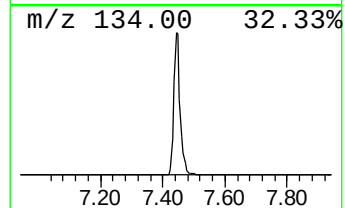
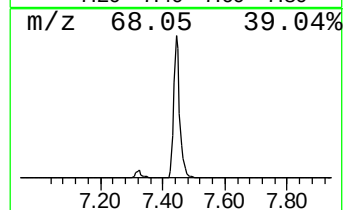
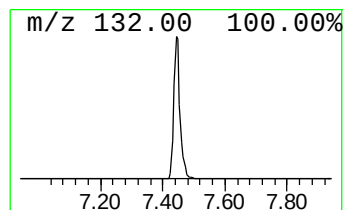
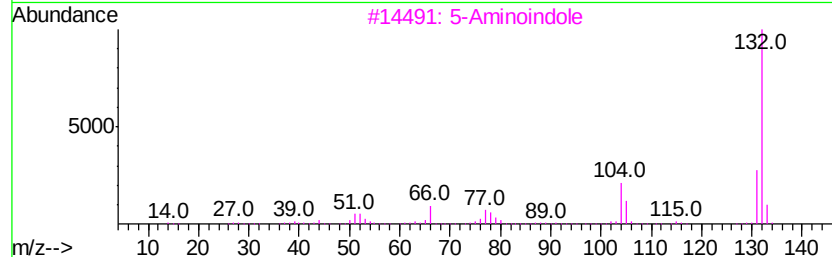
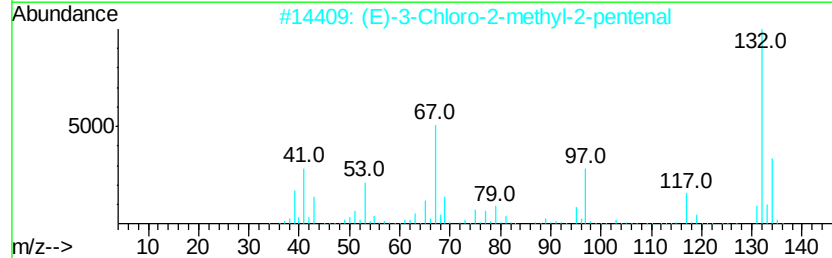
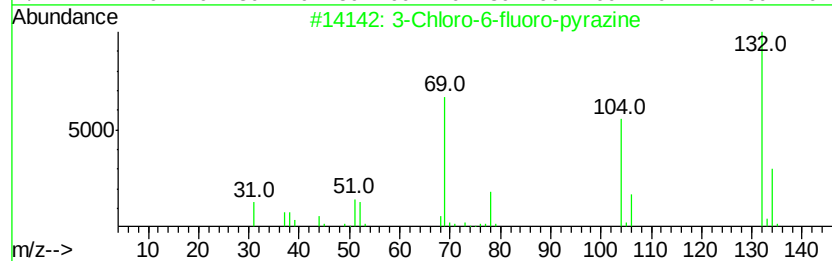
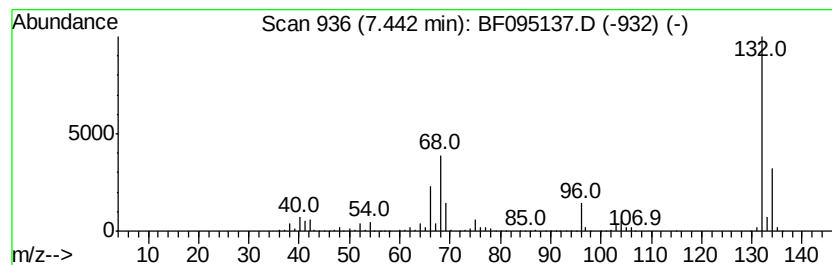
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.44	110.58 ng	2950720	1,4-Dichlorobenzene-d4	7.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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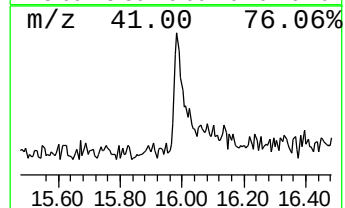
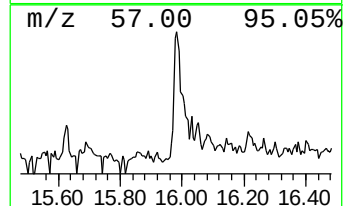
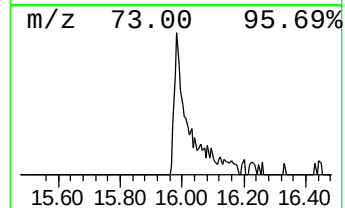
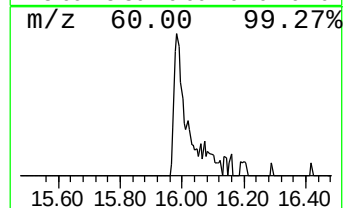
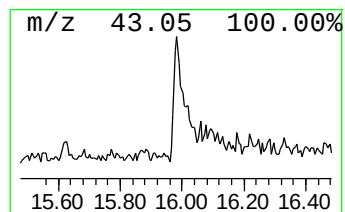
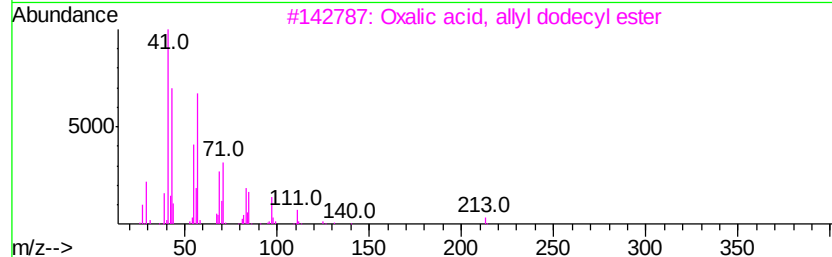
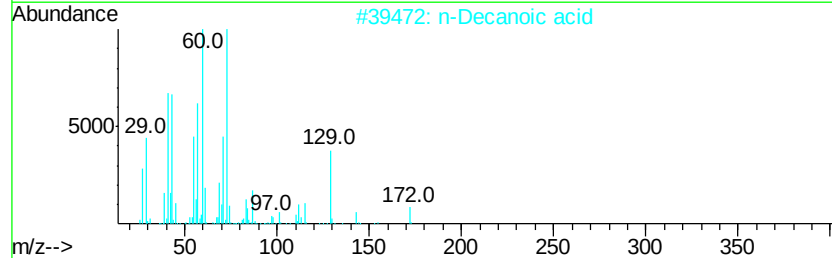
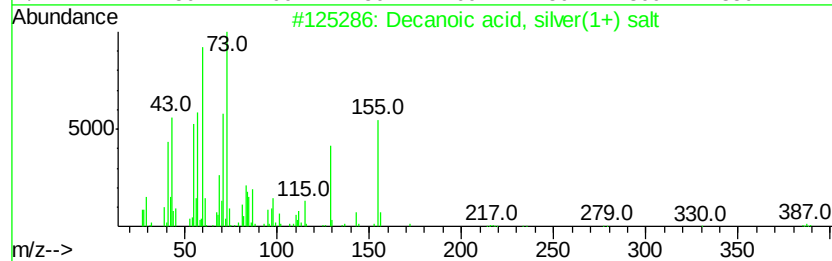
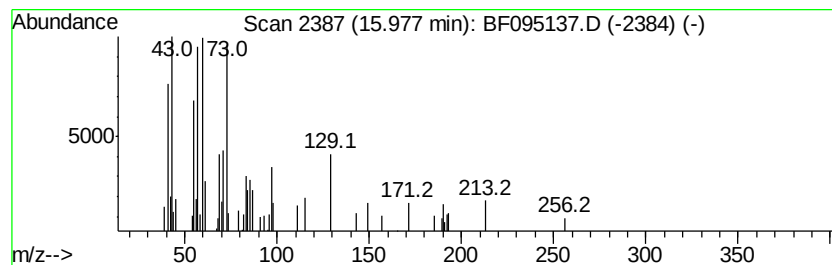
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decanoic acid, silver(1+) salt Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.98	3.96 ng	122764	Phenanthrene-d10		15.03	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
2		n-Decanoic acid	172	C10H20O2	000334-48-5	47
3		Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	25
4		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	18
5		Oxalic acid, cyclobutyl tetradec...	340	C20H36O4	1000309-70-9	14



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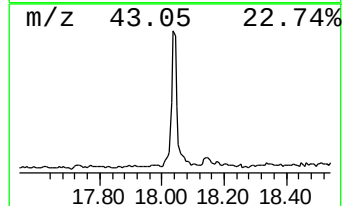
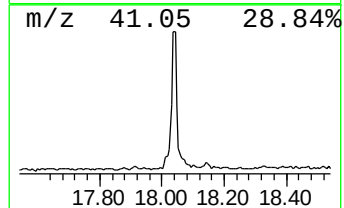
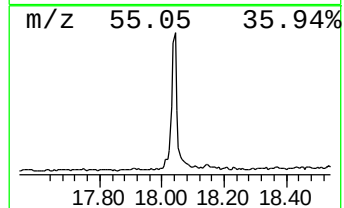
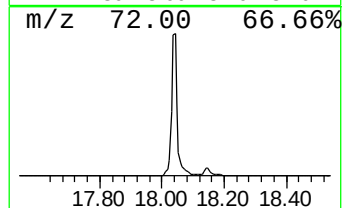
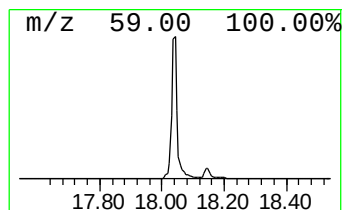
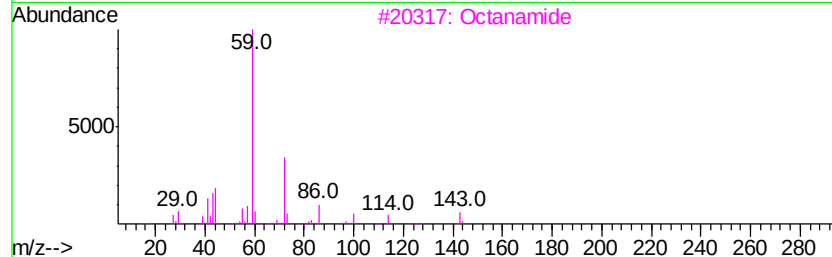
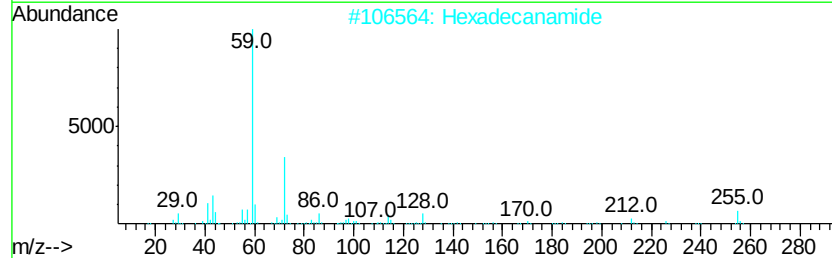
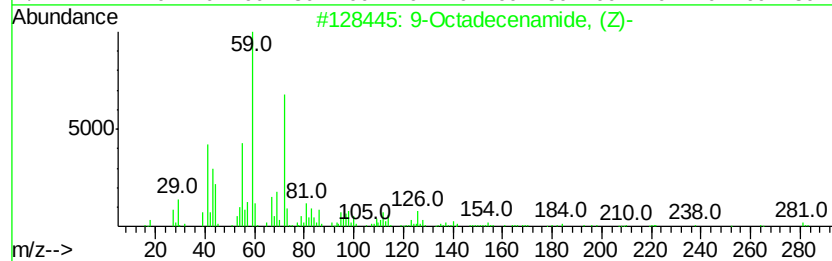
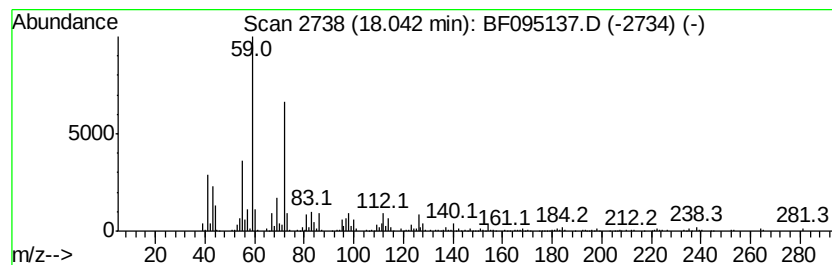
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	28.21 ng	874402	Chrysene-d12	18.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Hexadecanamide	255	C16H33NO	000629-54-9	59
3		Octanamide	143	C8H17NO	000629-01-6	53
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	50
5		Silane, hexyl-	116	C6H16Si	001072-14-6	47



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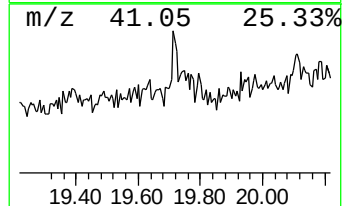
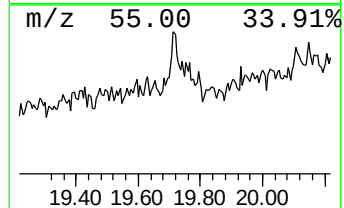
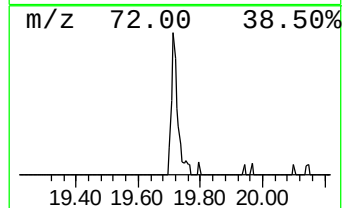
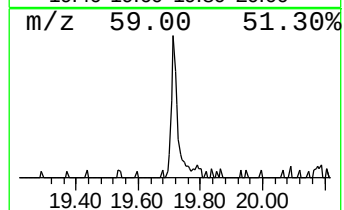
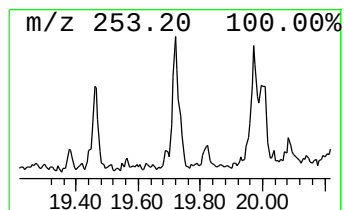
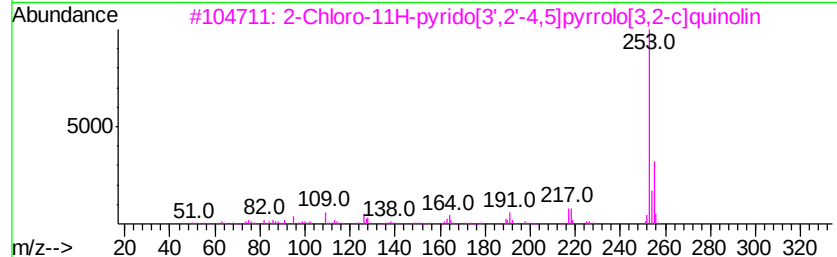
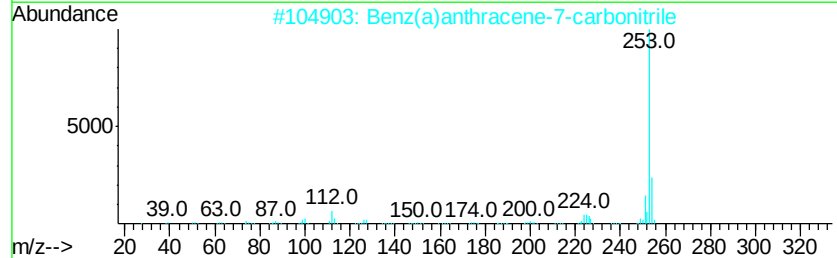
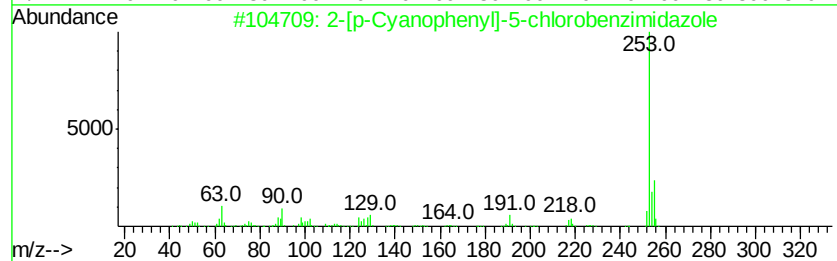
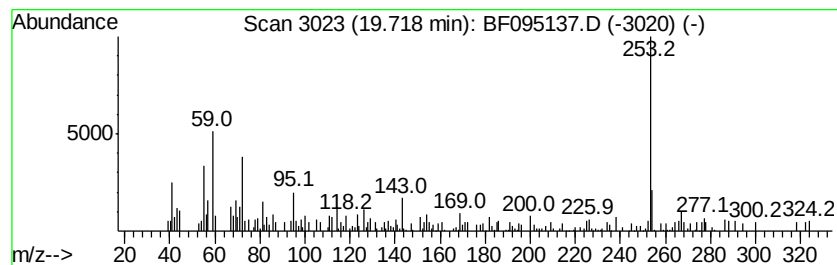
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 unknown19.72 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.72	4.65 ng	125584	Perylene-d12	20.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-[p-Cyanophenyl]-5-chlorobenzim...	253	C14H8ClN3	146132-86-7	38
2		Benz(a)anthracene-7-carbonitrile	253	C19H11N	007476-08-6	38
3		2-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-3	35
4		3-Chloro-11H-pyrido[3',2'-4,5]py...	253	C14H8ClN3	1000212-59-4	35
5		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	30



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TP-3COMP

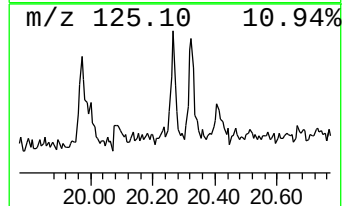
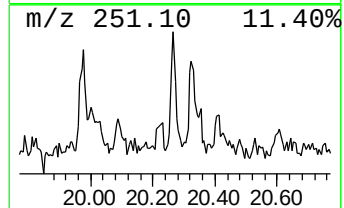
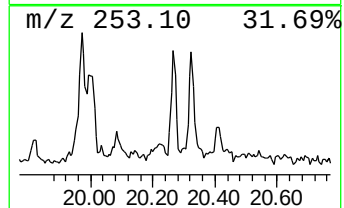
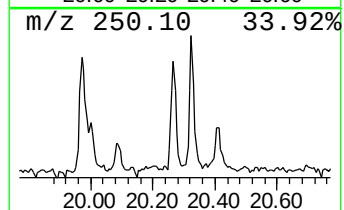
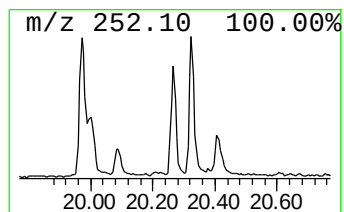
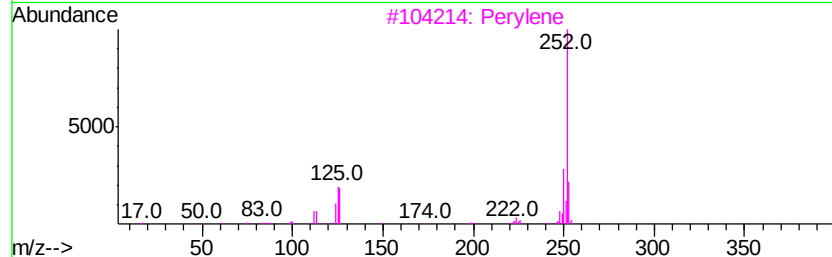
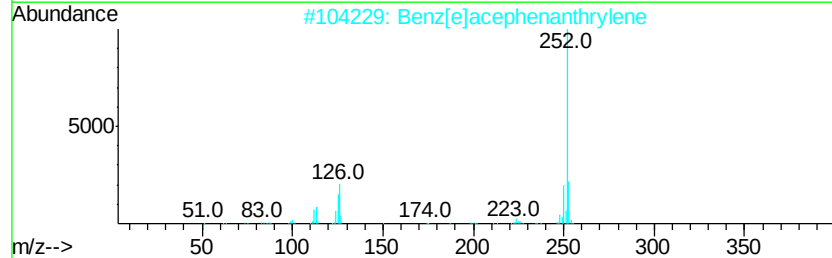
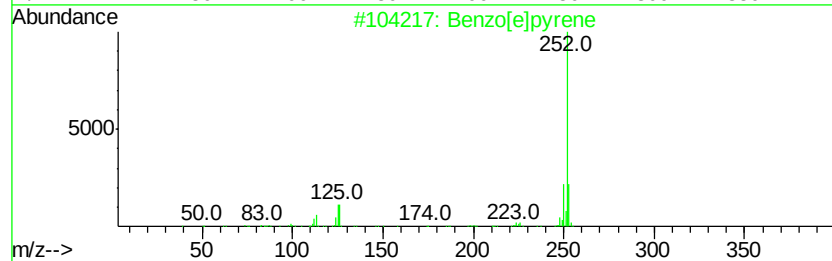
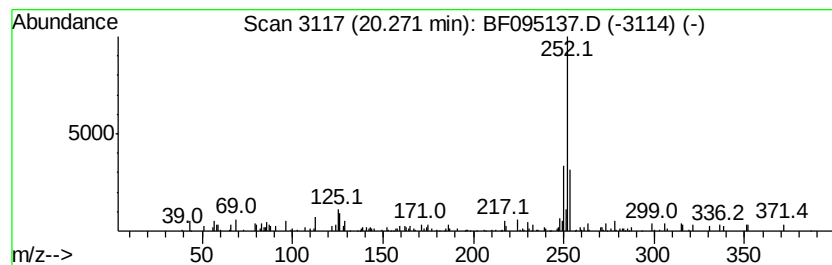
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.50 ng	67444	Perylene-d12	20.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
3		Perylene	252	C20H12	000198-55-0	89
4		Benzo[il]fluoranthene	252	C20H12	000205-82-3	76
5		Benzo[a]pyrene	252	C20H12	000050-32-8	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095137.D
Acq On : 15 May 2017 21:23
Operator : SJ/MA
Sample : I3147-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

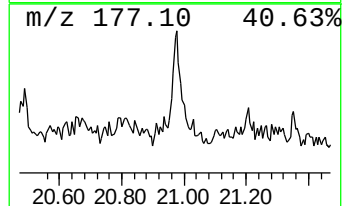
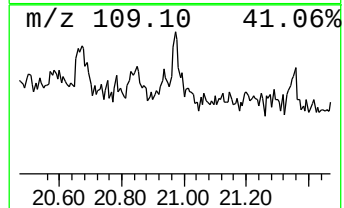
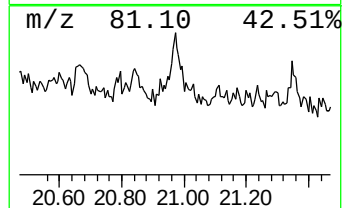
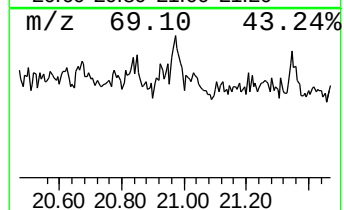
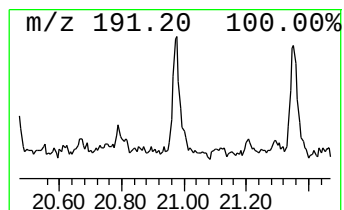
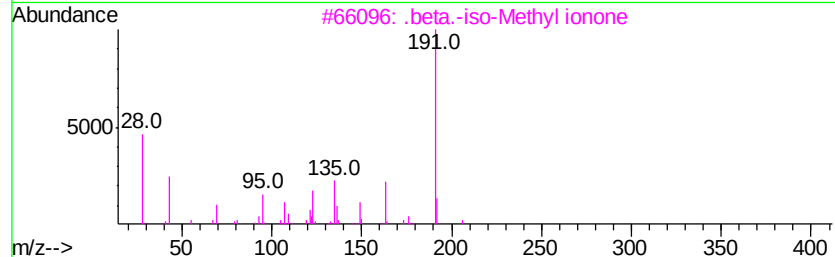
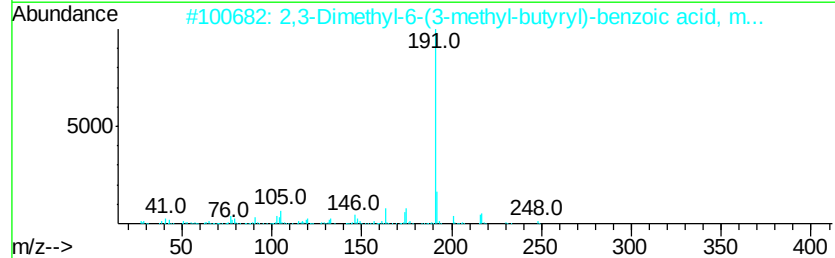
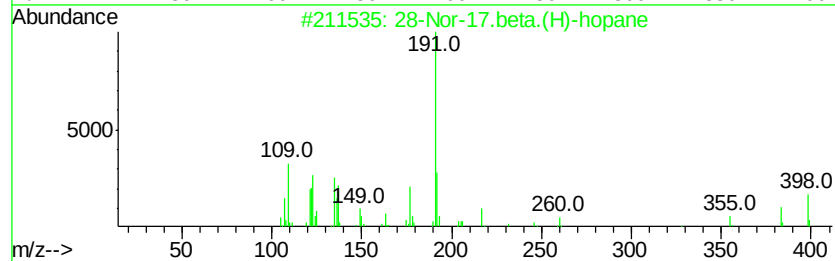
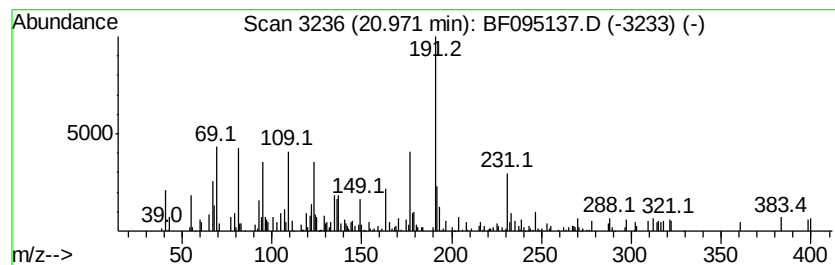
Instrument :
BNA_F
ClientSampleId :
TP-3COMP

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 unknown20.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.97	5.15 ng	139023	Perylene-d12	20.38	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	43
2	2,3-Dimethyl-6-(3-methyl-butyl)-benzoic acid	248	C15H20O3	071940-30-2	38
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
4	2-Fluoro-3-trifluoromethylbenzoic acid	266	C11H10F4O3	1000331-61-6	27
5	Amiphenazole	191	C9H9N3S	000490-55-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095137.D
Acq On : 15 May 2017 21:23
Operator : SJ/MA
Sample : I3147-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

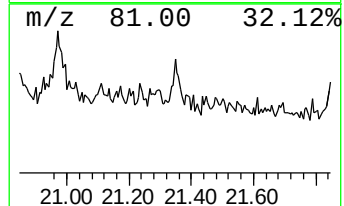
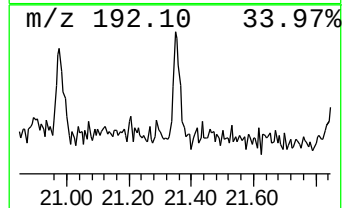
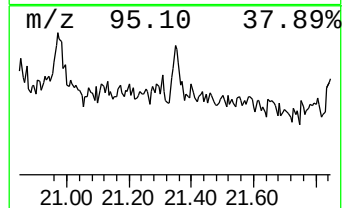
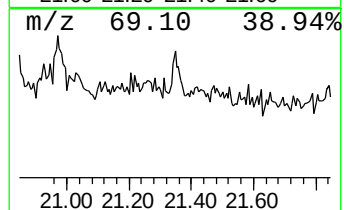
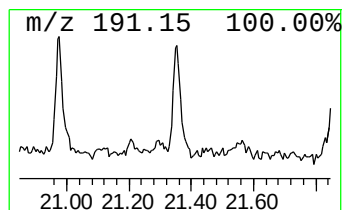
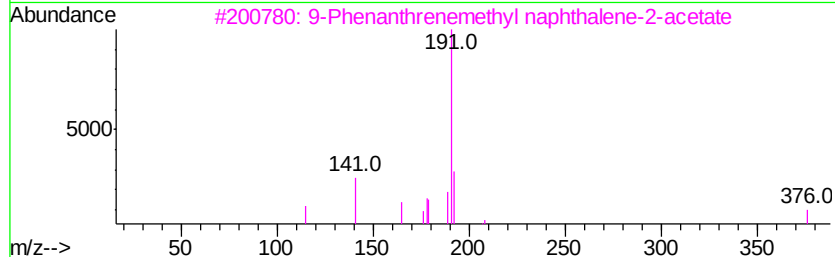
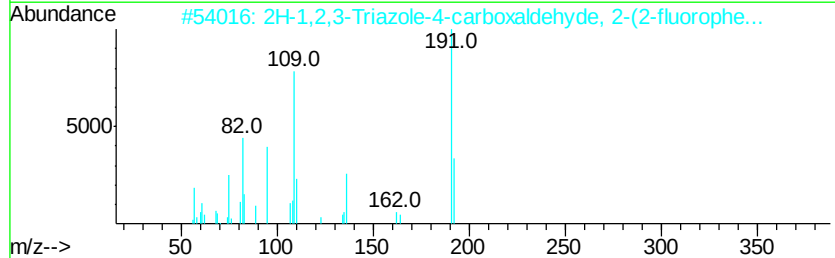
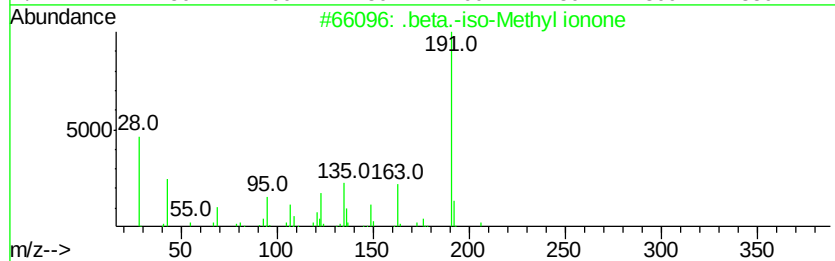
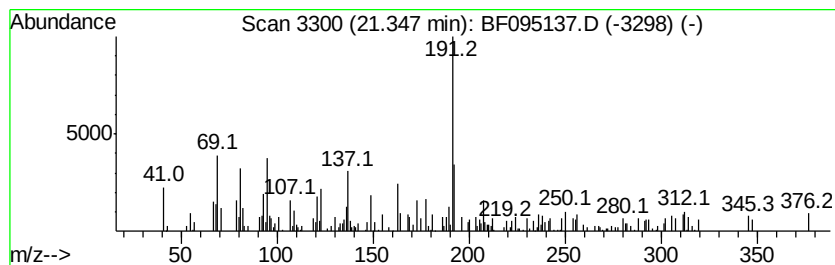
Instrument :
BNA_F
ClientSampleId :
TP-3COMP

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

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

Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	3.07 ng	82914	Perylene-d12	20.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-iso-Methyl ionone	206 C14H22O	1000285-40-2 58
2		2H-1,2,3-Triazole-4-carboxaldehy...	191 C9H6FN3O	051306-43-5 43
3		9-Phenanthrenemethyl naphthalene...	376 C27H20O2	093091-04-4 43
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206 C14H22O	000127-43-5 38
5		N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192 C10H12N2S	003420-40-4 38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051517\
Data File : BF095137.D
Acq On : 15 May 2017 21:23
Operator : SJ/MA
Sample : I3147-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3COMP

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...	5.14	21.7	ng	578515	1	7.78	533698	20.0
unknown7.44	7.44	110.6	ng	2950720	1	7.78	533698	20.0
Decanoic acid, si...	15.98	4.0	ng	122764	4	15.03	620703	20.0
9-Octadecenamamide,...	18.04	28.2	ng	874402	5	18.70	619856	20.0
unknown19.72	19.72	4.7	ng	125584	6	20.38	540265	20.0
Benzo[e]pyrene	20.27	2.5	ng	67444	6	20.38	540265	20.0
unknown20.97	20.97	5.2	ng	139023	6	20.38	540265	20.0
.beta.-iso-Methyl...	21.35	3.1	ng	82914	6	20.38	540265	20.0