

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
 Data File : BF093252.D
 Acq On : 28 Feb 2017 16:55
 Operator : SJ/MA
 Sample : I2017-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TK3-4-20170227

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-BF013017.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	4.967	249	252	260	rBV	894586	1283169	38.40%	4.173%
2	5.402	288	290	293	rBV	2108850	3022238	90.44%	9.829%
3	6.464	380	383	391	rBV	2155536	3341701	100.00%	10.868%
4	6.579	391	393	395	rBV	3227082	3103045	92.86%	10.092%
5	6.807	410	413	415	rBV	698945	795005	23.79%	2.585%
6	6.956	424	426	429	rBV	2160084	2252367	67.40%	7.325%
7	7.379	460	463	465	rBV	1347824	1924448	57.59%	6.259%
8	7.459	468	470	477	rVB	23394	51704	1.55%	0.168%
9	7.847	502	504	508	rBV	21242	35332	1.06%	0.115%
10	8.087	523	525	528	rBV	1082699	1011274	30.26%	3.289%
11	8.453	555	557	561	rBV	20765	37028	1.11%	0.120%
12	9.162	617	619	622	rBV	2225249	2743848	82.11%	8.923%
13	9.562	652	654	656	rBV	239381	194592	5.82%	0.633%
14	9.699	665	666	668	rBV	28899	40121	1.20%	0.130%
15	9.779	671	673	675	rBV	27203	34257	1.03%	0.111%
16	9.848	676	679	681	rVV	759554	932272	27.90%	3.032%
17	10.053	694	697	699	rBV	24471	33418	1.00%	0.109%
18	10.271	715	716	718	rVB	56328	38808	1.16%	0.126%
19	10.488	733	735	738	rBV	22523	36635	1.10%	0.119%
20	10.636	745	748	750	rBV	1297233	1371740	41.05%	4.461%
21	10.739	756	757	761	rBV	55959	88581	2.65%	0.288%
22	11.196	794	797	798	rBV	38294	47890	1.43%	0.156%
23	11.322	806	808	812	rBV	620791	881235	26.37%	2.866%
24	11.562	825	829	832	rBV2	17889	33922	1.02%	0.110%
25	11.619	832	834	837	rVV	51173	49956	1.49%	0.162%
26	11.825	850	852	854	rBV2	23620	35621	1.07%	0.116%
27	11.859	854	855	857	rVV	58382	52894	1.58%	0.172%
28	11.939	860	862	866	rVB	30759	55287	1.65%	0.180%
29	12.385	899	901	902	rBV	26902	46342	1.39%	0.151%
30	12.465	907	908	912	rVV3	23849	40155	1.20%	0.131%
31	12.545	912	915	917	rVV	91159	115225	3.45%	0.375%
32	12.602	917	920	921	rVV3	23114	39403	1.18%	0.128%
33	12.625	921	922	924	rVB2	43362	49479	1.48%	0.161%
34	12.728	929	931	932	rBV2	46038	49391	1.48%	0.161%

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35	12.774	932	935	937 rBV	100558	139684	4.18%	0.454%
36	12.854	940	942	944 rBV	340658	379872	11.37%	1.235%
37	12.911	945	947	950 rBV	2133222	2004144	59.97%	6.518%
38	13.082	960	962	965 rBV3	45561	80956	2.42%	0.263%
39	13.185	969	971	976 rVV	313079	422149	12.63%	1.373%
40	13.482	995	997	999 rBV	115460	125996	3.77%	0.410%
41	13.814	1023	1026	1028 rBV2	108138	170275	5.10%	0.554%
42	13.974	1037	1040	1043 rVB2	674145	1125635	33.68%	3.661%
43	15.391	1162	1164	1167 rVB	509376	721676	21.60%	2.347%
44	15.505	1172	1174	1177 rVB	155592	200814	6.01%	0.653%
45	16.020	1217	1219	1227 rVB	353741	821261	24.58%	2.671%
46	16.431	1252	1255	1263 rVB	222215	456611	13.66%	1.485%
47	16.968	1299	1302	1305 rBV	128094	231544	6.93%	0.753%

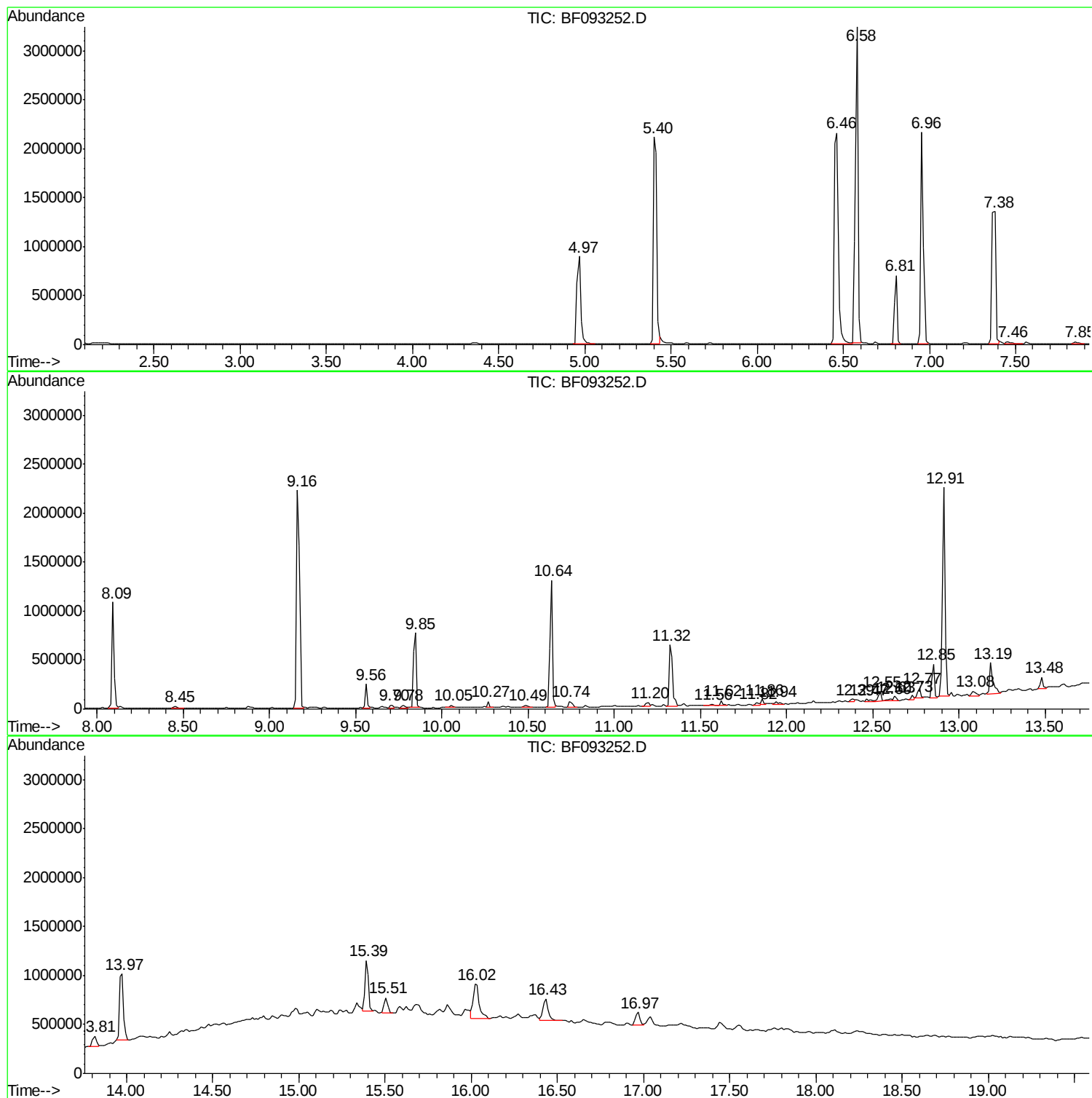
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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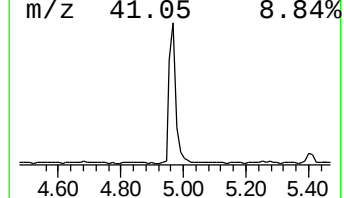
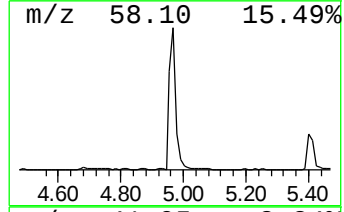
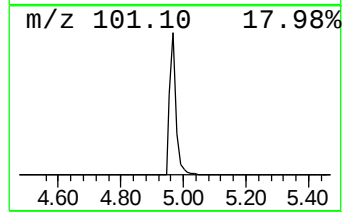
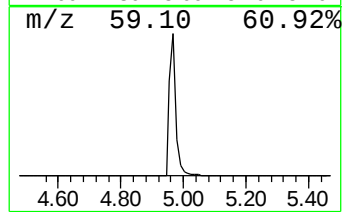
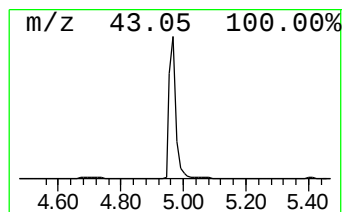
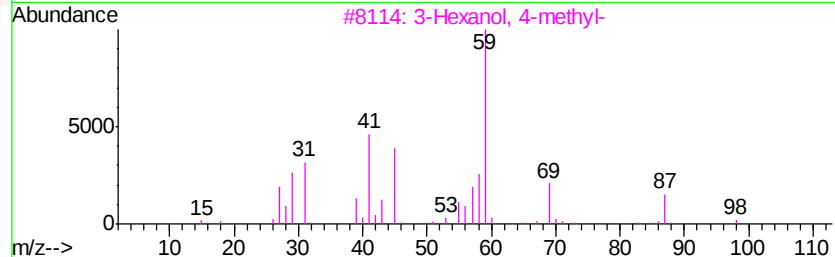
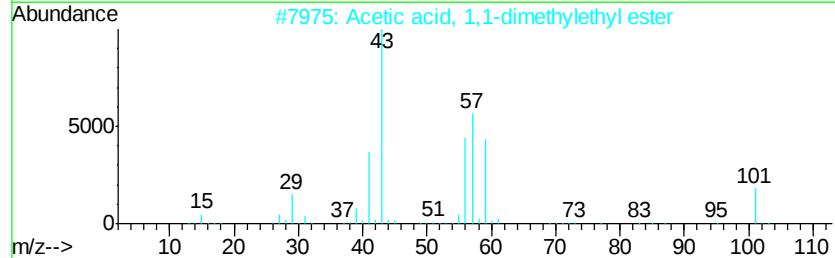
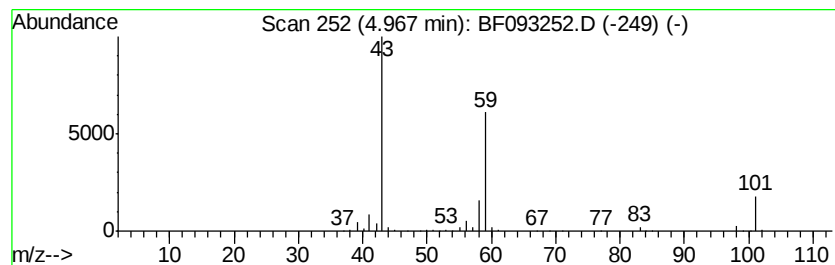
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	32.28 ng	1283170	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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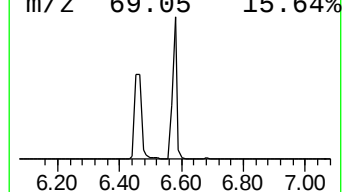
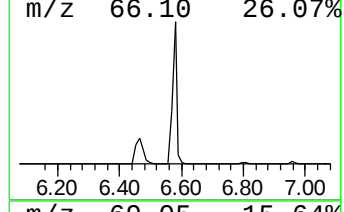
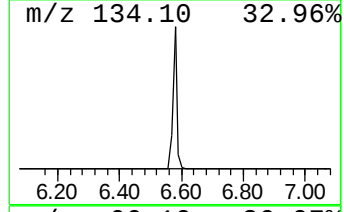
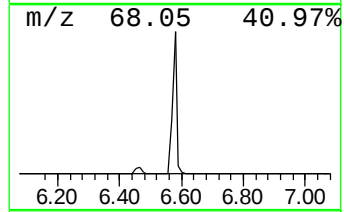
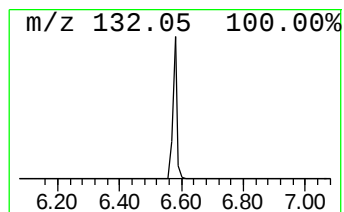
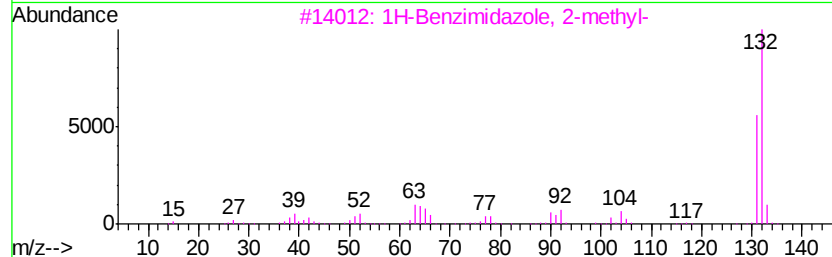
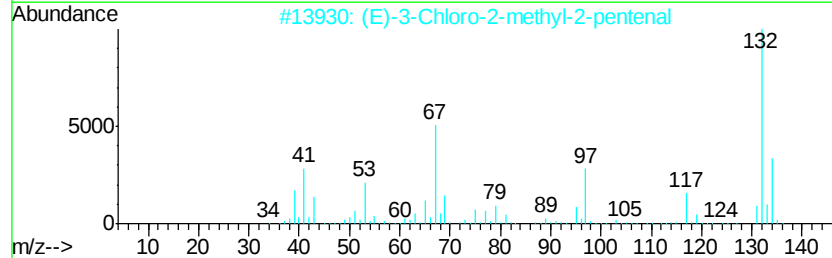
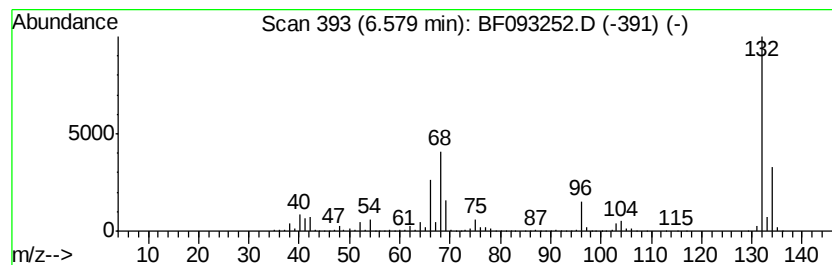
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	78.06 ng	3103050	1,4-Dichlorobenzene-d4	6.81

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	16
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		5-Aminoindole	132	C8H8N2	005192-03-0	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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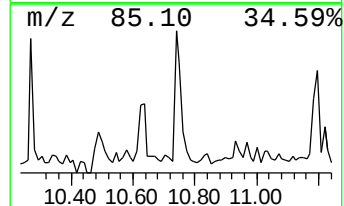
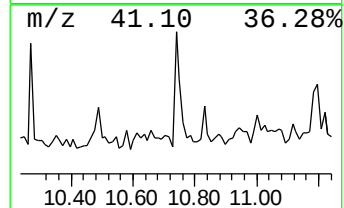
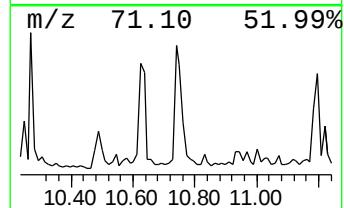
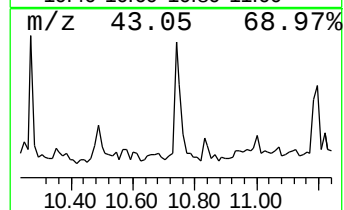
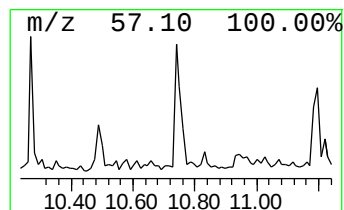
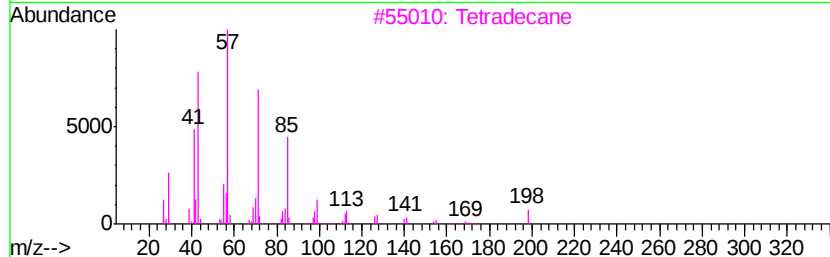
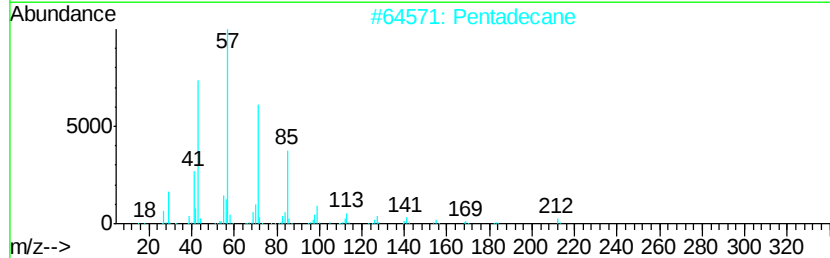
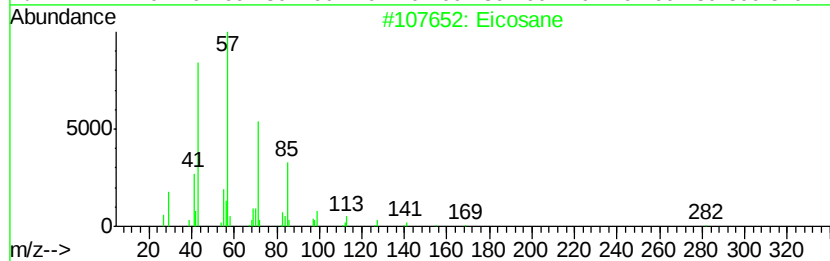
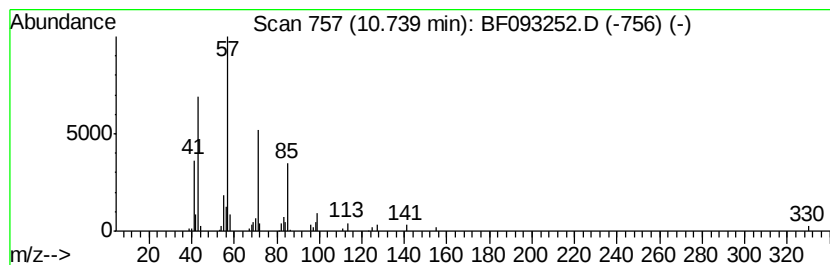
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.01 ng	88581	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	90
2	Pentadecane		212	C15H32	000629-62-9	90
3	Tetradecane		198	C14H30	000629-59-4	86
4	Hexadecane		226	C16H34	000544-76-3	86
5	Heptadecane		240	C17H36	000629-78-7	80



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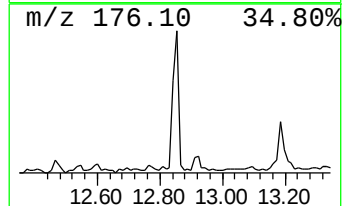
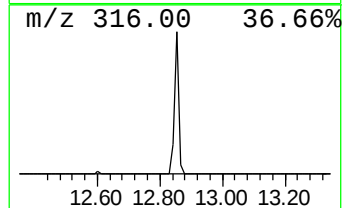
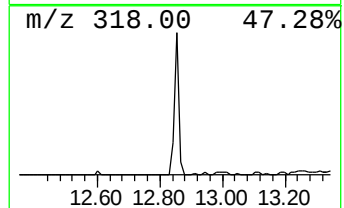
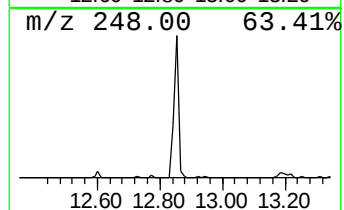
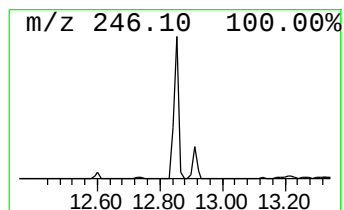
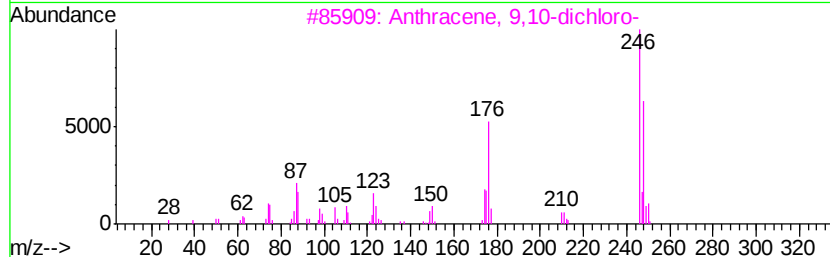
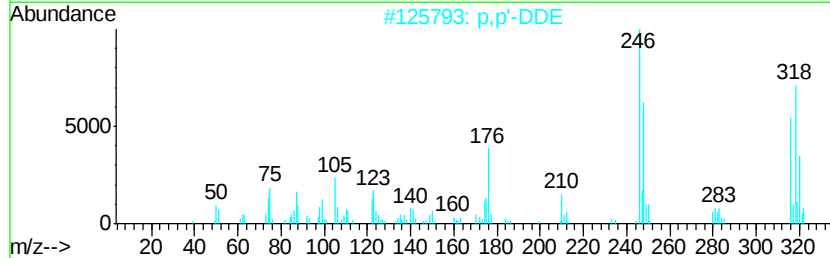
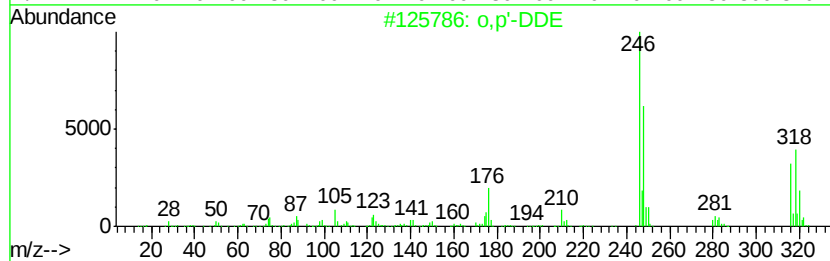
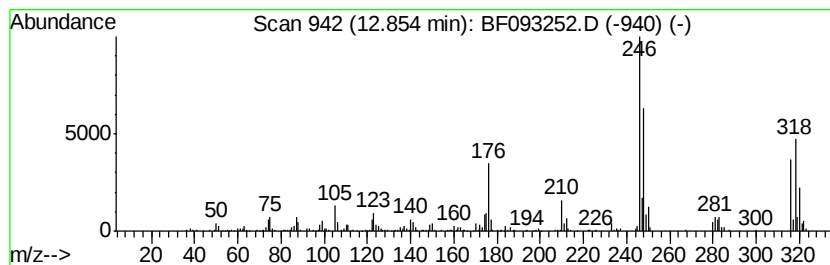
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 o,p'-DDE Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	6.75 ng	379872	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o,p'-DDE	316	C14H8Cl4	003424-82-6	99
2		p,p'-DDE	316	C14H8Cl4	000072-55-9	99
3		Anthracene, 9,10-dichloro-	246	C14H8Cl2	000605-48-1	98
4		Benzene, 1,1'-(1,2-dichloro-1,2-...	316	C14H8Cl4	088970-69-8	91
5		Anthracene, 1,8-dichloro-	246	C14H8Cl2	014381-66-9	91



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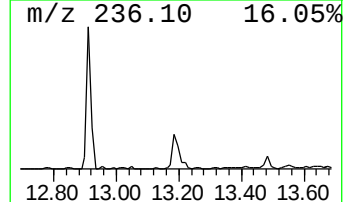
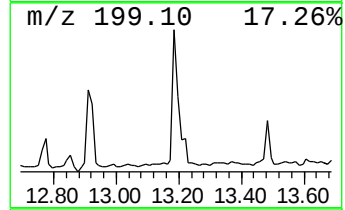
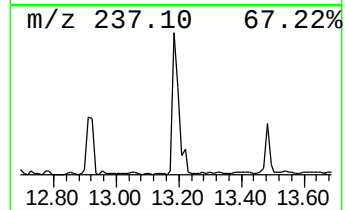
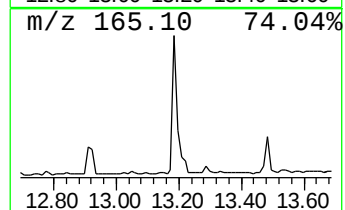
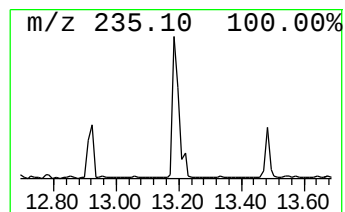
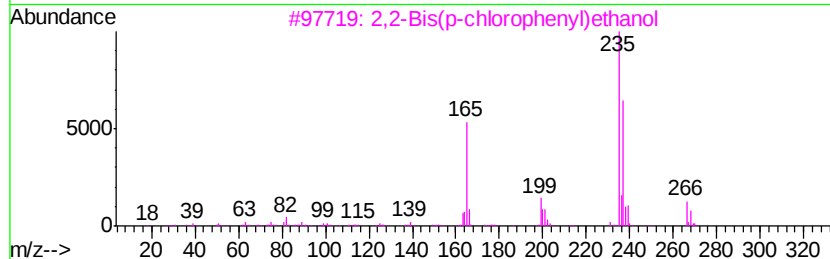
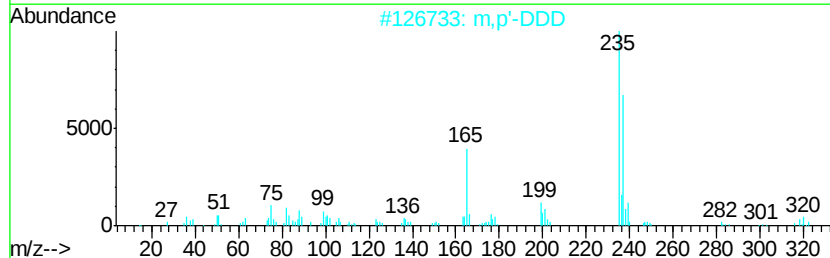
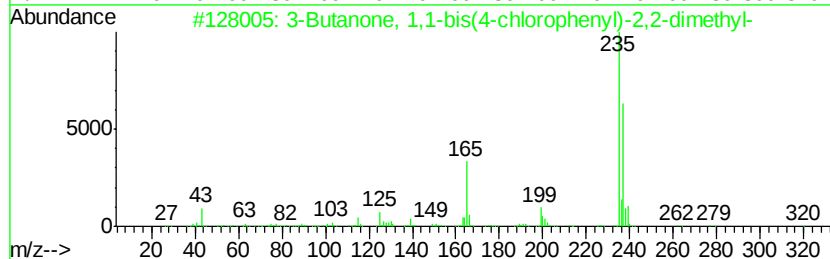
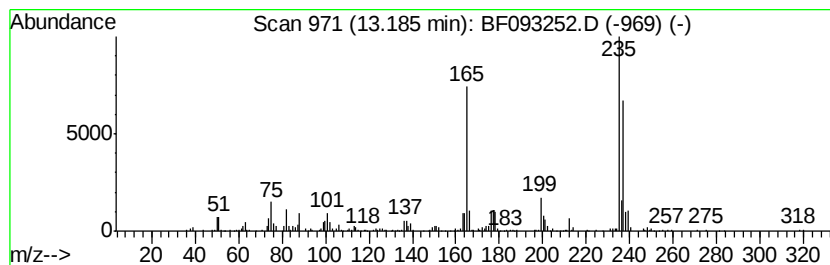
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Peak Number 6 3-Butanone, 1,1-bis(4-chlor... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	7.50 ng	422149	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	91
2		m,p'-DDD	318	C14H10Cl4	004329-12-8	90
3		2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	86
4		1-Chloro-2,2-Bis(p-chlorophenyl)...	284	C14H11Cl3	002642-80-0	86
5		Benzene, 1,1'-(chloromethylene)b...	270	C13H9Cl3	000782-08-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

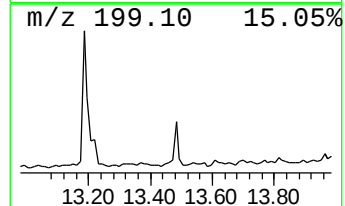
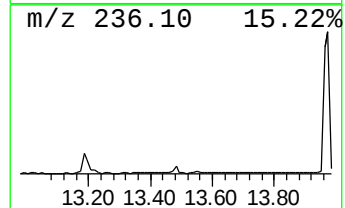
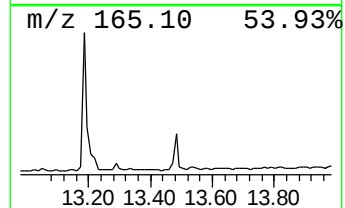
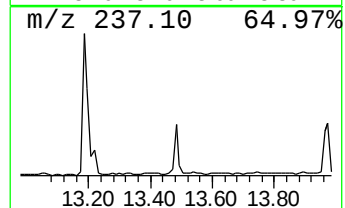
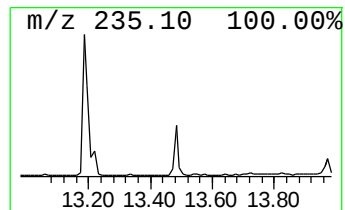
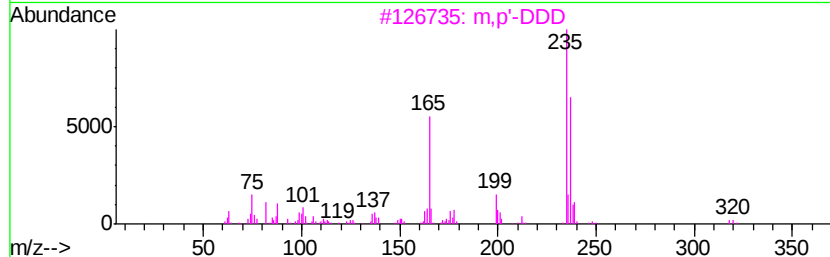
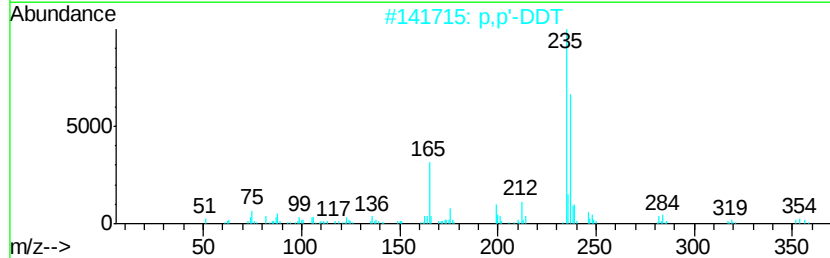
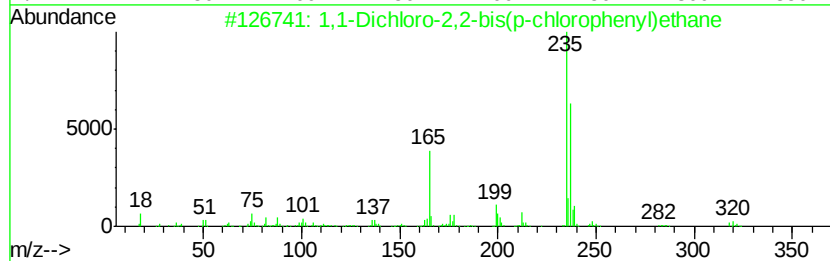
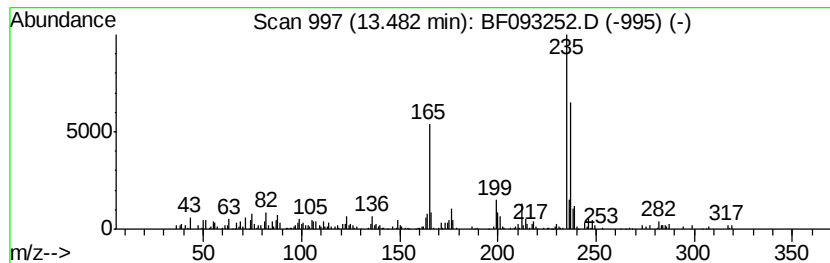
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ClientSampleID :
TK3-4-20170227

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,1-Dichloro-2,2-bis(p-chlo... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.48	2.24 ng	125996	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	91	
2	p,p'-DDT	352	C14H9Cl5	000050-29-3	87	
3	m,p'-DDD	318	C14H10Cl4	004329-12-8	86	
4	2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	83	
5	3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	74	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

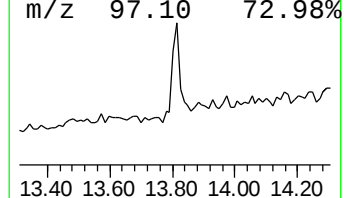
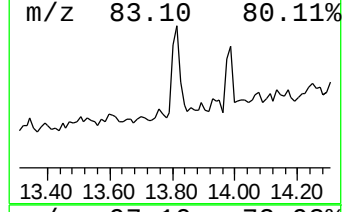
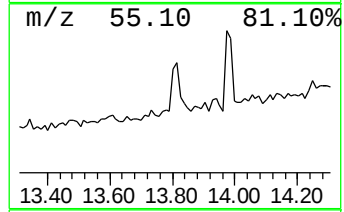
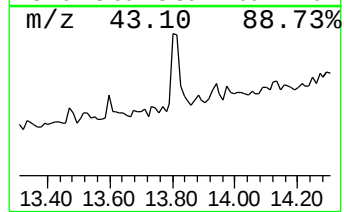
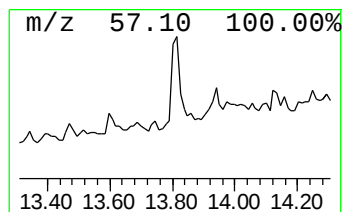
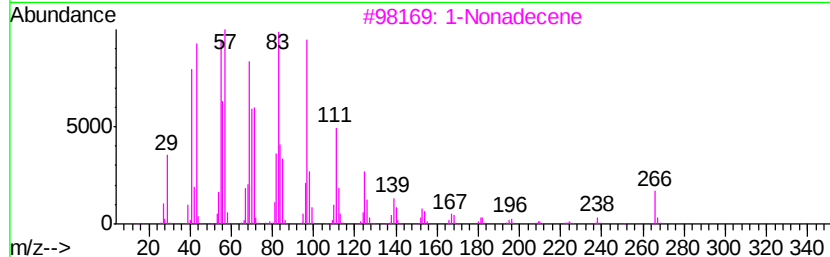
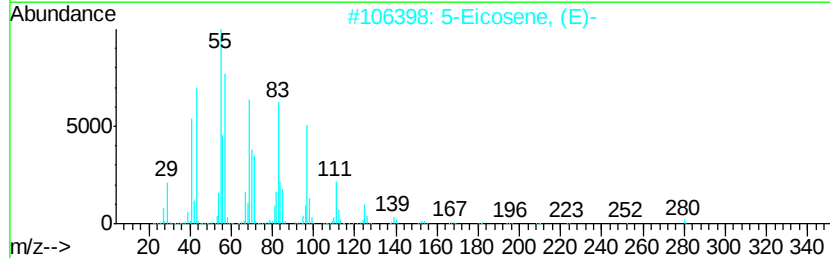
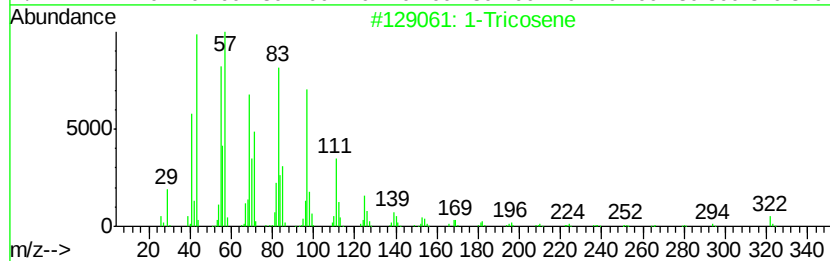
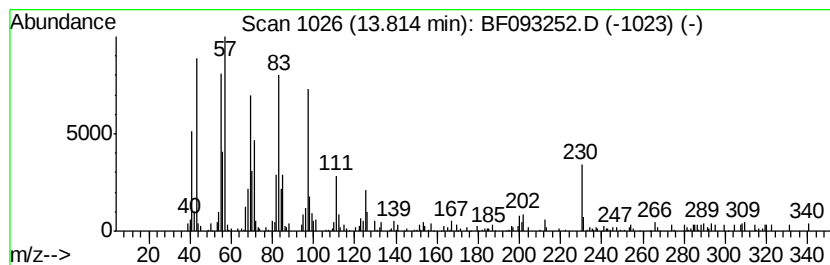
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ClientSampleId :
TK3-4-20170227

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Tricosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.81	3.03 ng	170275	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3	1-Nonadecene	266	C19H38	018435-45-5	93
4	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TK3-4-20170227

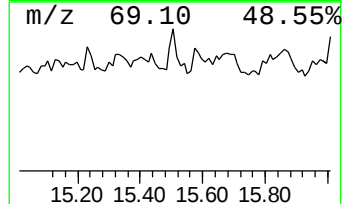
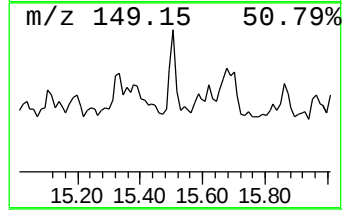
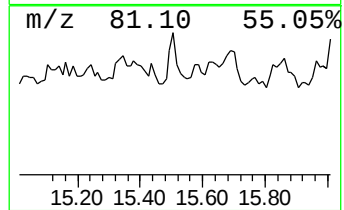
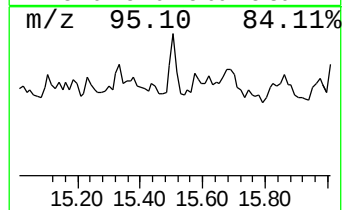
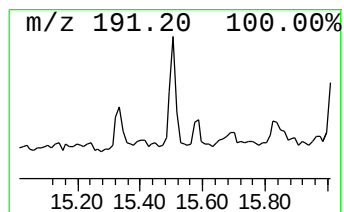
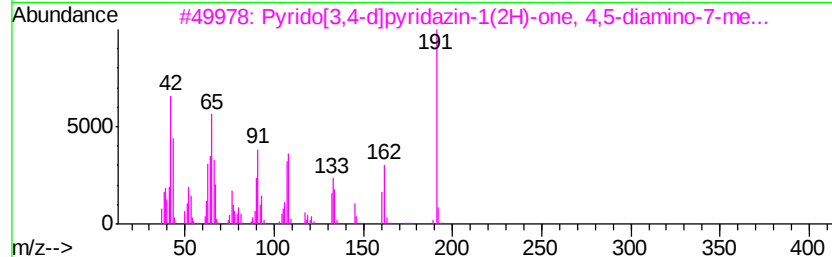
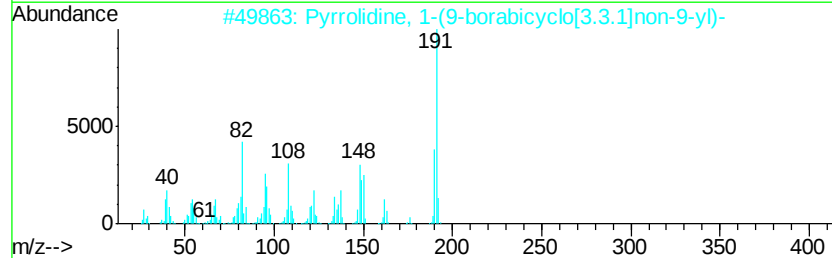
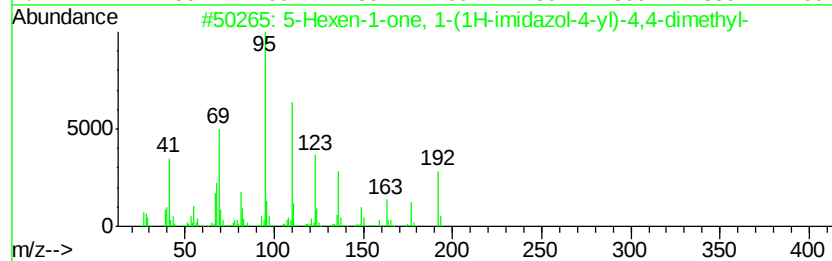
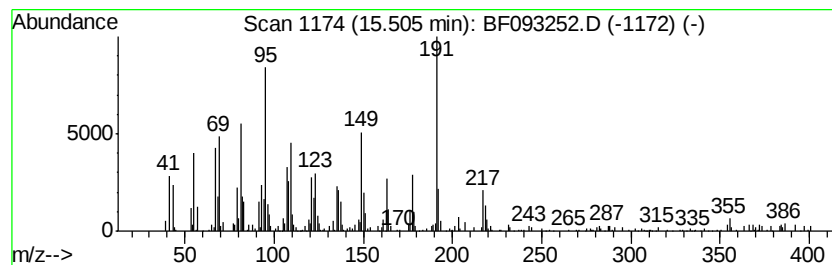
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown15.51 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	5.57 ng	200814	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	42
2		Pyrrolidine, 1-(9-borabicyclo[3....	191	C12H22BN	022516-41-2	25
3		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	25
4		1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	22
5		Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TK3-4-20170227

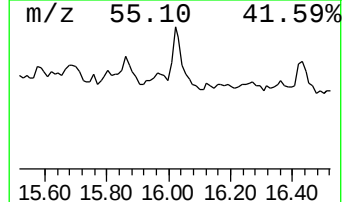
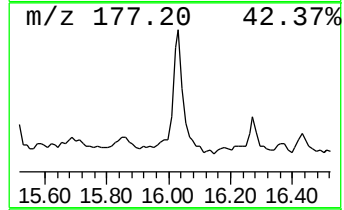
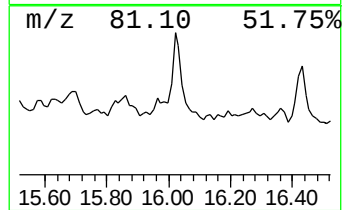
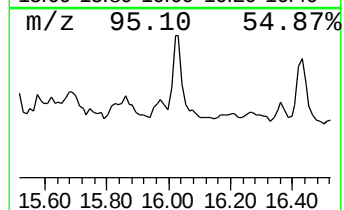
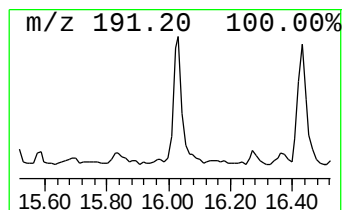
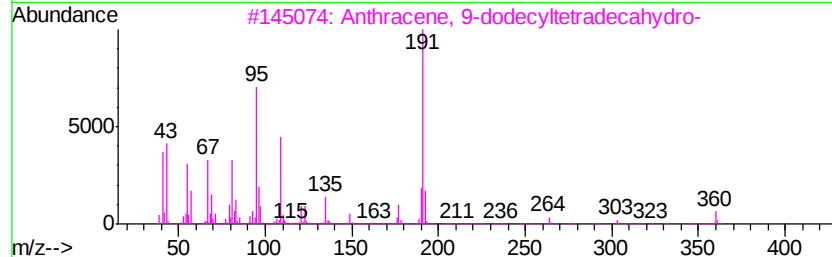
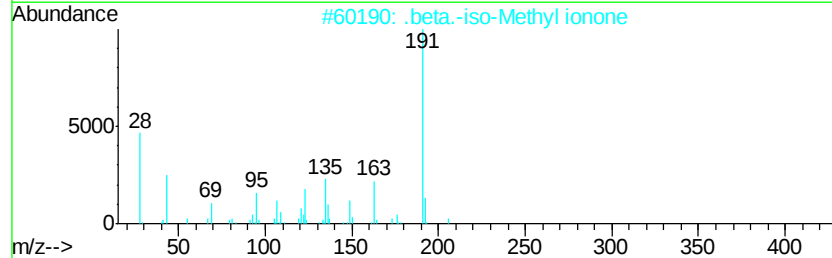
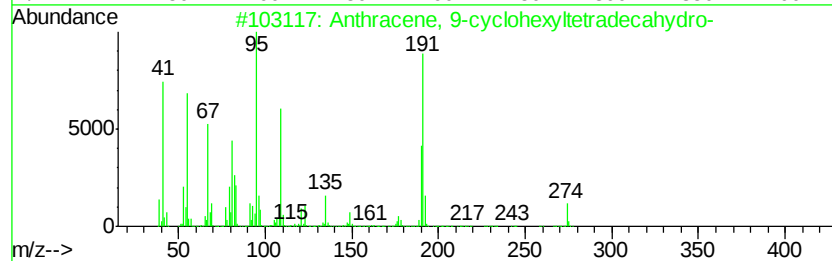
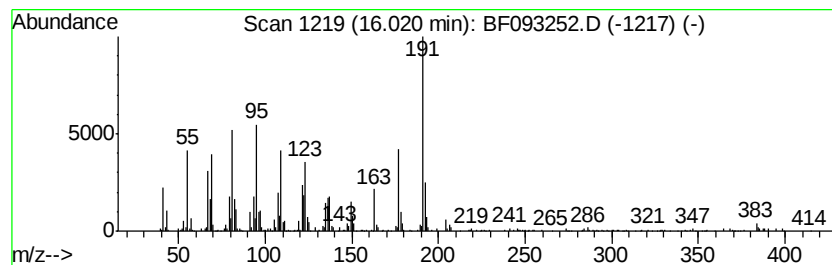
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	22.76 ng	821261	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	47
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
3		Anthracene, 9-dodecyltetradeca...	360	C26H48	055401-75-7	38
4		2H-1,2,3-Triazole-4-carboxalde...	191	C9H6FN3O	051306-43-5	38
5		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

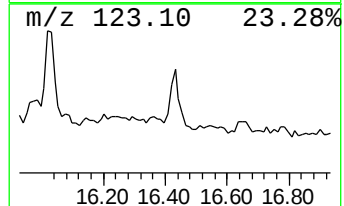
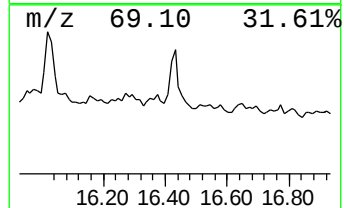
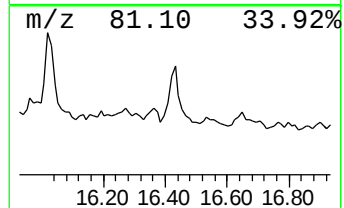
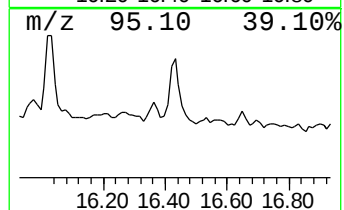
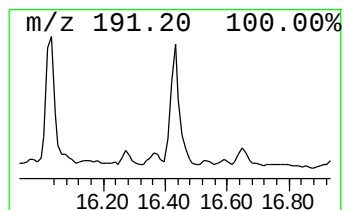
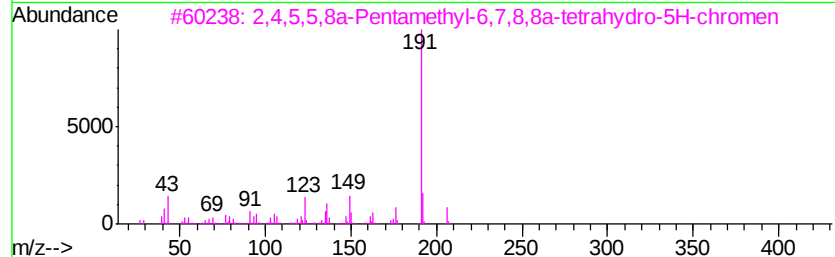
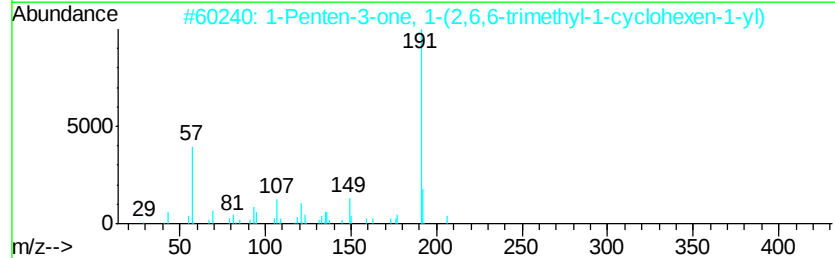
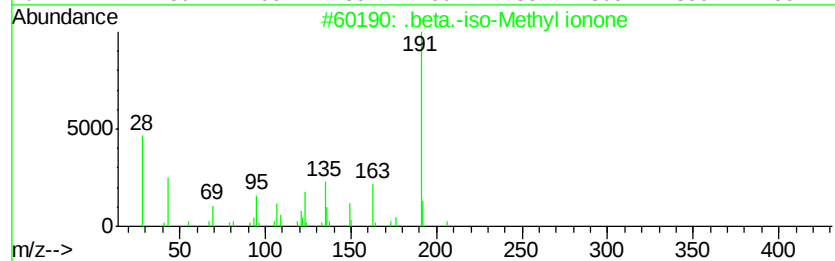
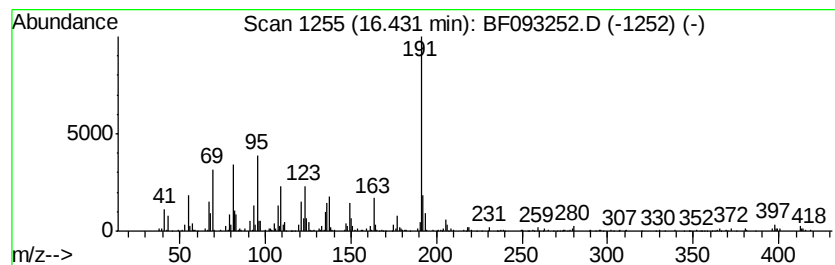
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.43	12.65 ng	456611	Perylene-d12	15.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	86
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	55
3		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	50
4		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	43
5		3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
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Acq On : 28 Feb 2017 16:55
Operator : SJ/MA
Sample : I2017-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TK3-4-20170227

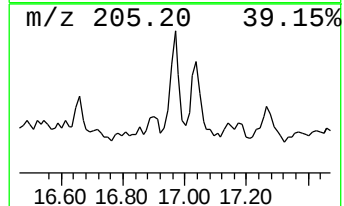
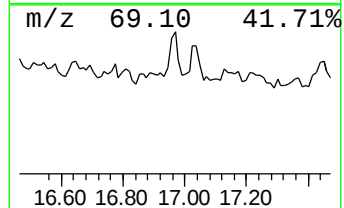
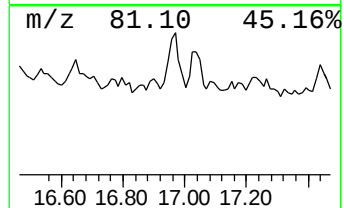
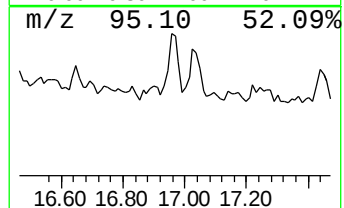
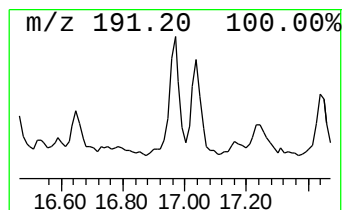
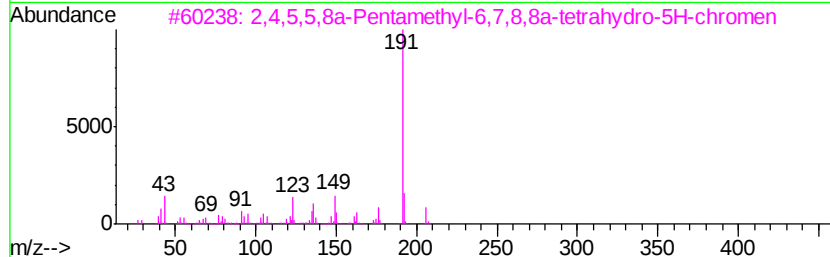
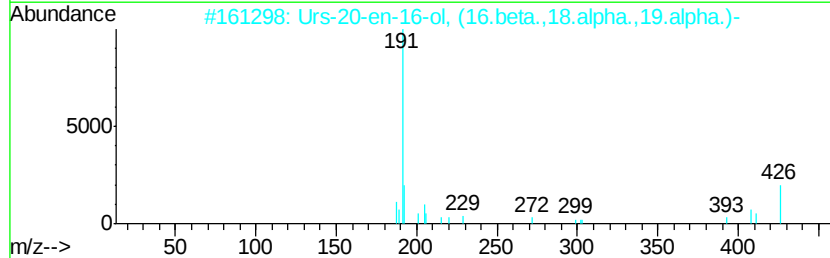
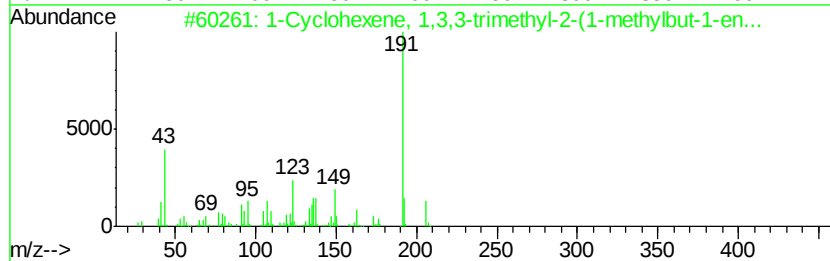
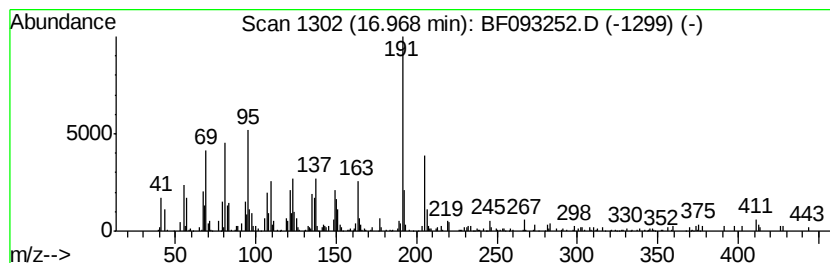
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown16.97 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	6.42 ng	231544	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	46
2		Urs-20-en-16-ol, (16.beta.,18.al...	426	C30H50O	066394-74-9	45
3		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	43
4		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	35
5		3-Indolethanamine, N-acetyl-5-fl...	250	C13H15FN2O2	1000116-27-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022817\
Data File : BF093252.D
Acq On : 28 Feb 2017 16:55
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TK3-4-20170227

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	32.3	ng	1283170	1	6.81	795005	20.0
unknown6.58	6.58	78.1	ng	3103050	1	6.81	795005	20.0
Eicosane	10.74	2.0	ng	88581	4	11.32	881235	20.0
o,p'-DDE	12.85	6.8	ng	379872	5	13.97	1125640	20.0
3-Butanone, 1,1-b...	13.19	7.5	ng	422149	5	13.97	1125640	20.0
1,1-Dichloro-2,2-...	13.48	2.2	ng	125996	5	13.97	1125640	20.0
1-Tricosene	13.81	3.0	ng	170275	5	13.97	1125640	20.0
unknown15.51	15.51	5.6	ng	200814	6	15.39	721676	20.0
unknown16.02	16.02	22.8	ng	821261	6	15.39	721676	20.0
.beta.-iso-Methyl...	16.43	12.7	ng	456611	6	15.39	721676	20.0
unknown16.97	16.97	6.4	ng	231544	6	15.39	721676	20.0