

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
 Data File : BF092124.D
 Acq On : 6 Jan 2017 18:35
 Operator : UM/SJ
 Sample : I1025-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP7-8-COMP10

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-BF122116.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	2.790	78	79	95	rBV	170977	420766	7.60%	0.984%
2	4.047	187	189	195	rBV	38567	75905	1.37%	0.178%
3	4.779	250	253	264	rBV	1736245	2414157	43.60%	5.646%
4	5.259	293	295	303	rBV	4197855	4255872	76.86%	9.952%
5	6.322	385	388	390	rBV	3839047	3499396	63.20%	8.183%
6	6.424	394	397	399	rBV	3815691	3651391	65.94%	8.539%
7	6.642	414	416	418	rBV	1449250	1166899	21.07%	2.729%
8	6.802	427	430	432	rBV	2889681	3125923	56.45%	7.310%
9	7.213	463	466	468	rBV	2819973	2572177	46.45%	6.015%
10	7.933	526	529	531	rBV	909010	1139207	20.57%	2.664%
11	9.008	620	623	625	rBV	4095991	3412817	61.63%	7.981%
12	9.408	655	658	660	rVB	1154942	955743	17.26%	2.235%
13	9.670	679	681	683	rBV	1056800	1144094	20.66%	2.675%
14	10.459	748	750	753	rBV2	1293291	1602056	28.93%	3.746%
15	10.596	759	762	765	rBV	58035	98606	1.78%	0.231%
16	11.042	799	801	802	rBV2	44638	56858	1.03%	0.133%
17	11.156	808	811	813	rBV	752028	978378	17.67%	2.288%
18	11.465	836	838	845	rBV2	32078	83175	1.50%	0.195%
19	11.705	856	859	862	rBV3	143261	174722	3.16%	0.409%
20	11.888	873	875	877	rVB	51781	57032	1.03%	0.133%
21	11.979	881	883	886	rVB3	39606	65453	1.18%	0.153%
22	12.219	900	904	906	rBV2	61747	156168	2.82%	0.365%
23	12.356	915	916	918	rBV	74565	71704	1.29%	0.168%
24	12.402	918	920	923	rVB3	32962	62095	1.12%	0.145%
25	12.482	926	927	929	rVV	78120	89011	1.61%	0.208%
26	12.585	933	936	939	rVV	89846	132392	2.39%	0.310%
27	12.734	947	949	952	rBV	1967536	2167476	39.14%	5.069%
28	13.019	972	974	977	rBV3	38440	90883	1.64%	0.213%
29	13.225	990	992	994	rBV3	50638	85353	1.54%	0.200%
30	13.648	1027	1029	1032	rBV3	92737	131055	2.37%	0.306%
31	13.785	1038	1041	1043	rBV	1451189	1701577	30.73%	3.979%
32	14.151	1067	1073	1083	rVB2	1076243	5537182	100.00%	12.949%
33	15.145	1158	1160	1168	rVB	589471	998395	18.03%	2.335%
34	15.751	1211	1213	1218	rVB	177195	317882	5.74%	0.743%

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Instrument :
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ClientSampleId :
TP7-8-COMP10

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.128	1243	1246	1250	rVB	129723	270405	4.88%	0.632%
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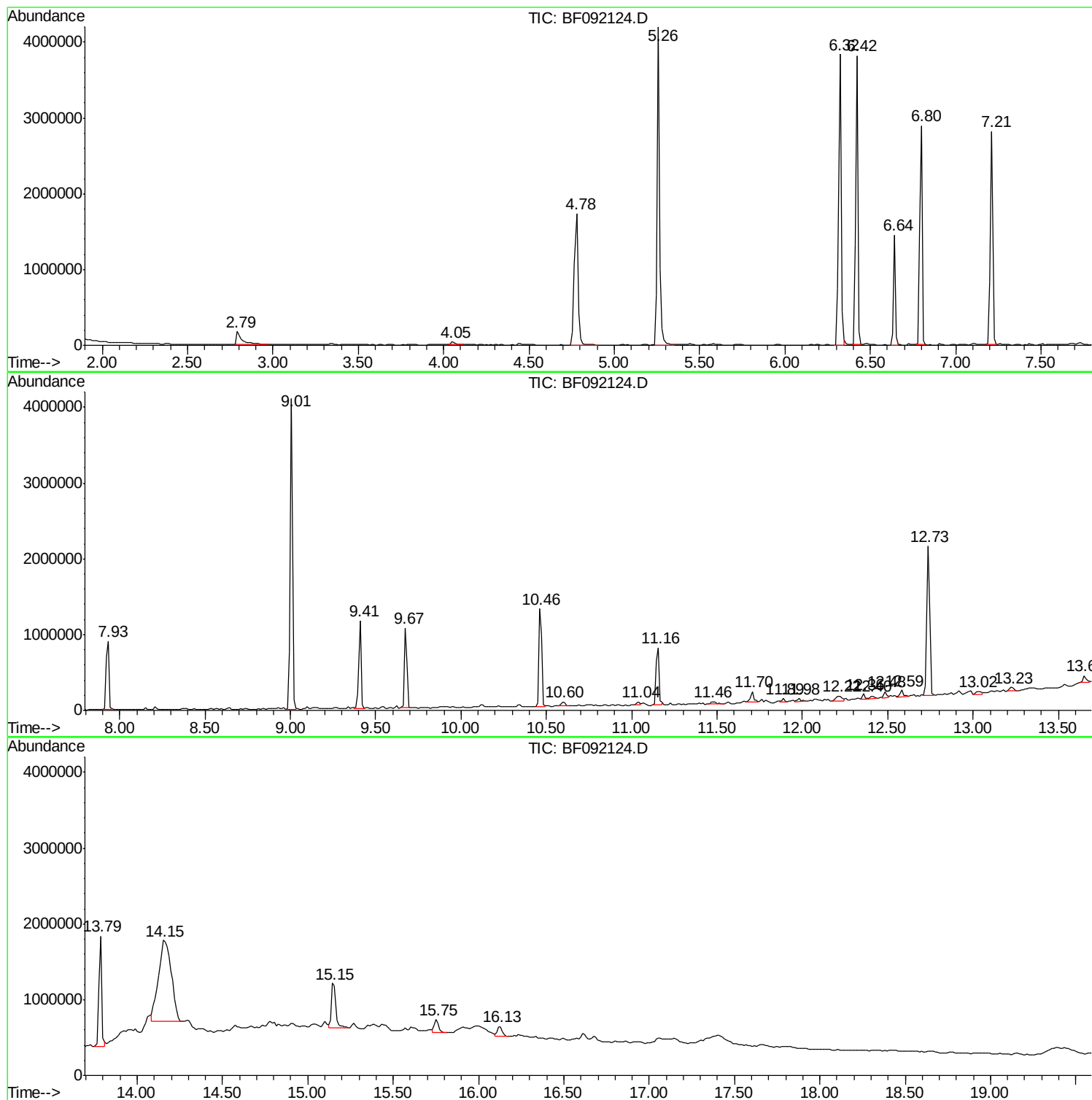
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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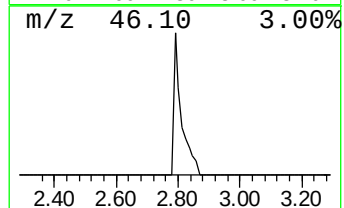
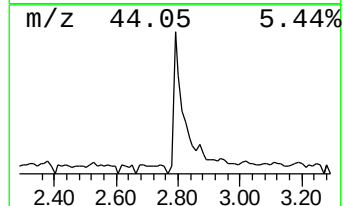
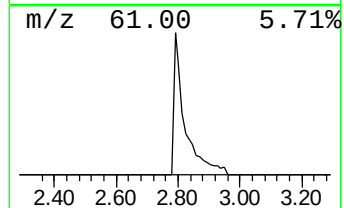
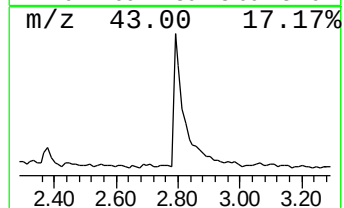
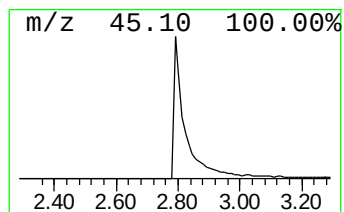
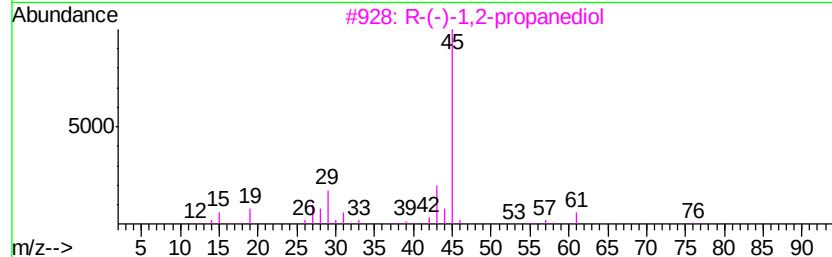
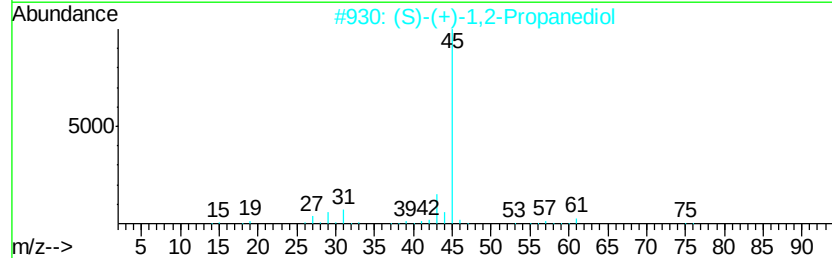
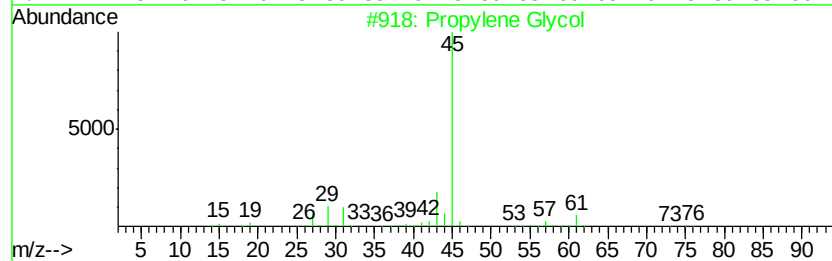
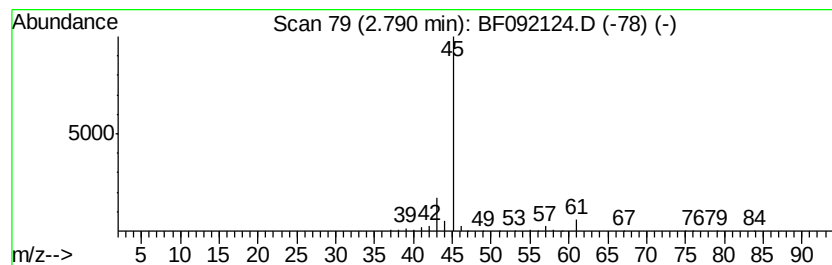
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	7.21 ng	420766	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	90
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9



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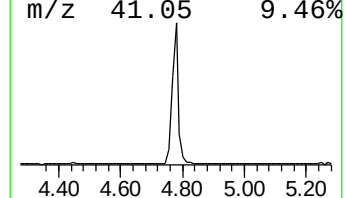
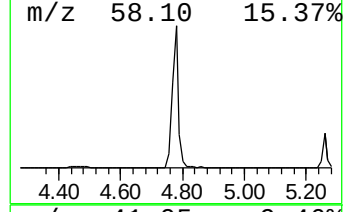
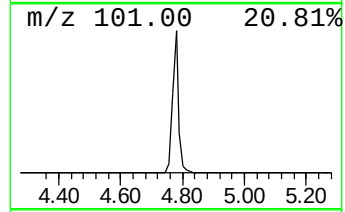
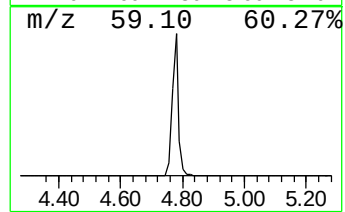
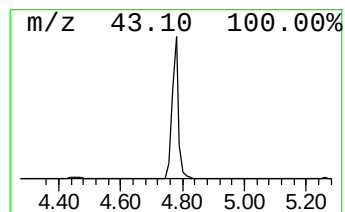
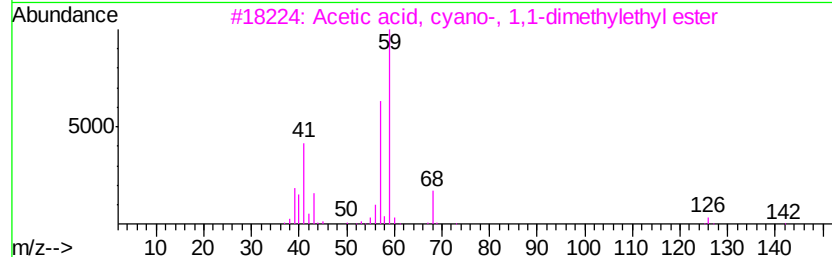
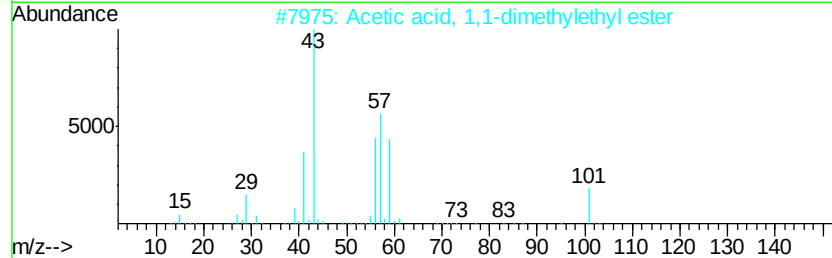
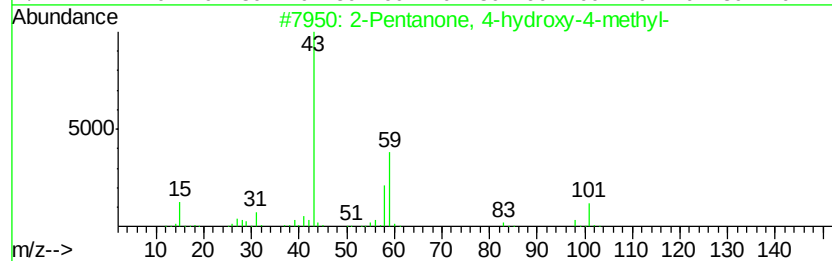
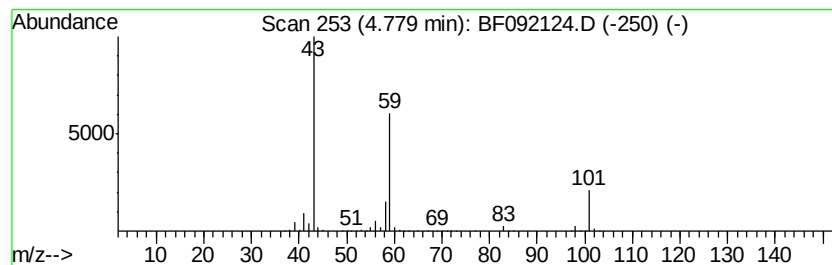
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	41.38 ng	2414160	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
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	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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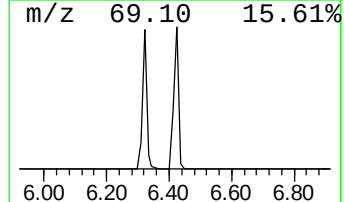
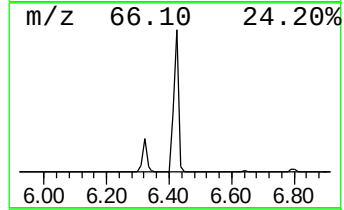
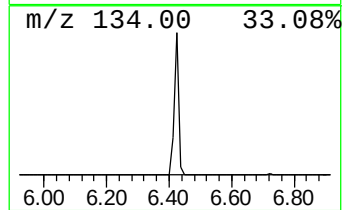
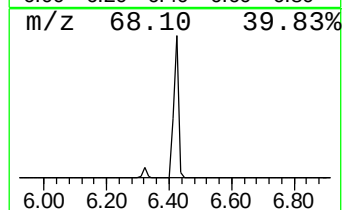
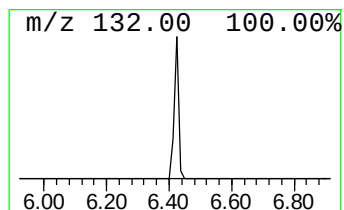
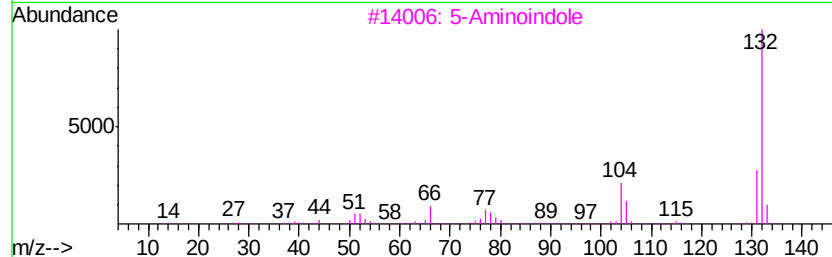
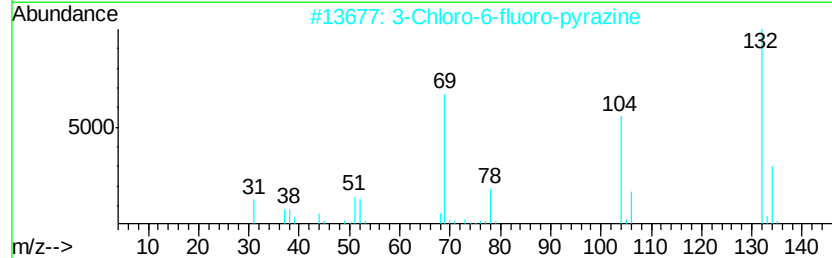
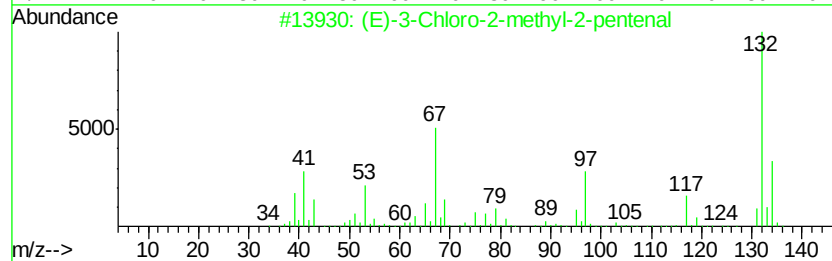
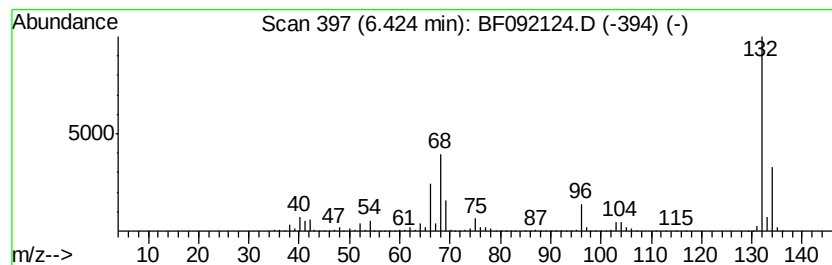
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	62.58 ng	3651390	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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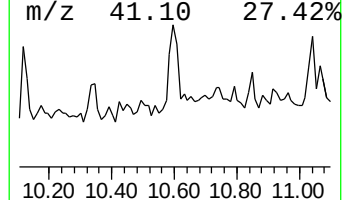
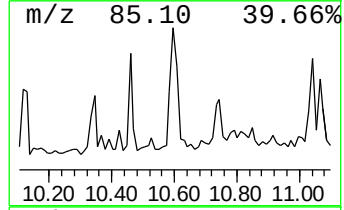
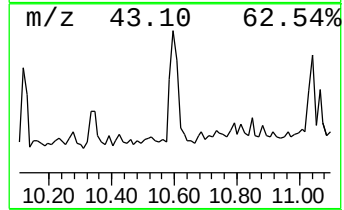
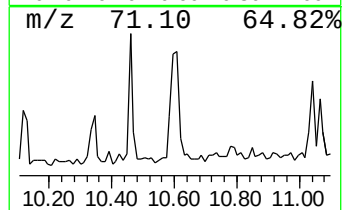
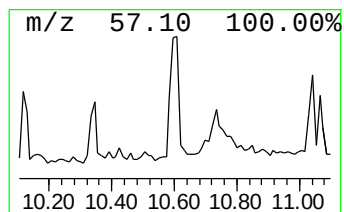
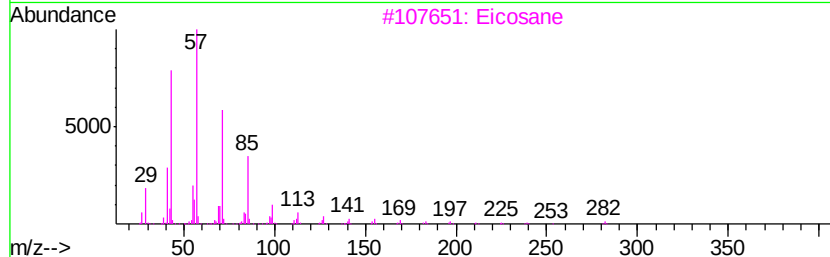
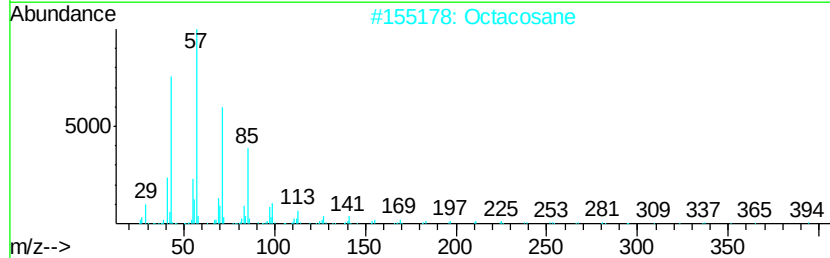
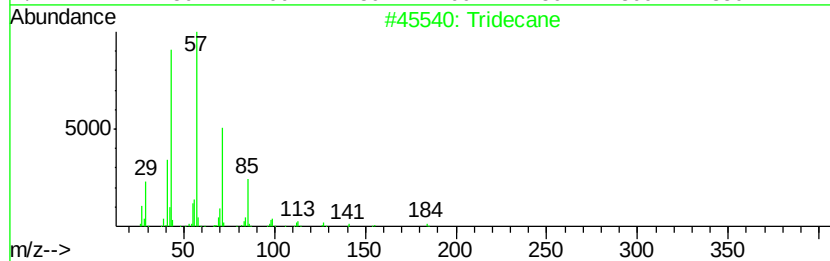
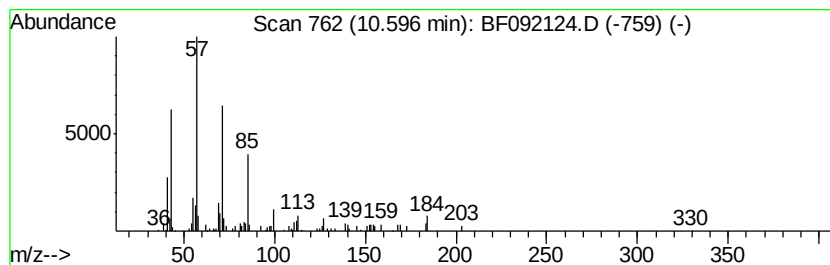
Instrument :
BNA_F
ClientSampleId :
TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.60	2.02 ng	98606	Phenanthrene-d10		11.16
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	81
2	Octacosane	394	C28H58	000630-02-4	72
3	Eicosane	282	C20H42	000112-95-8	72
4	Heptacosane	380	C27H56	000593-49-7	72
5	Tetracosane	338	C24H50	000646-31-1	64



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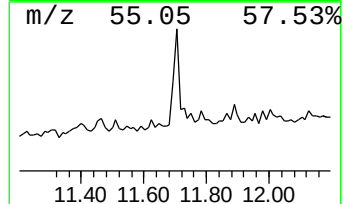
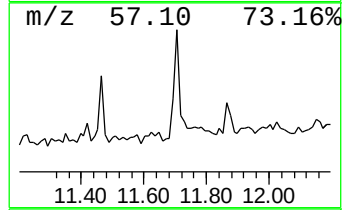
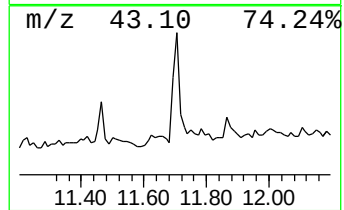
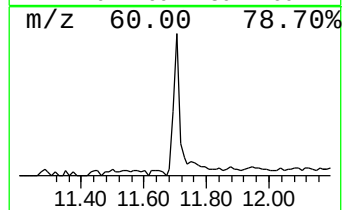
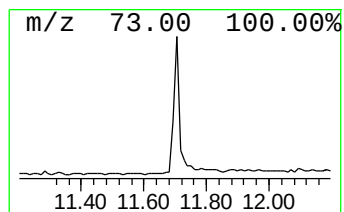
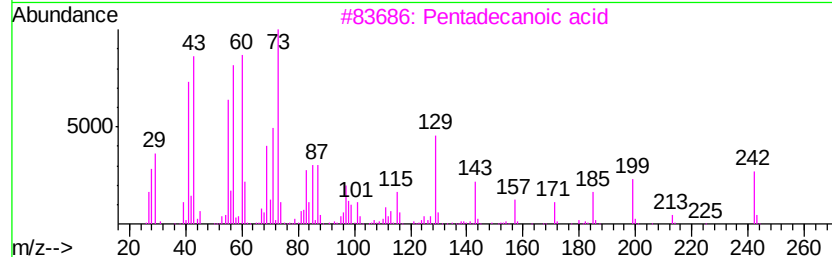
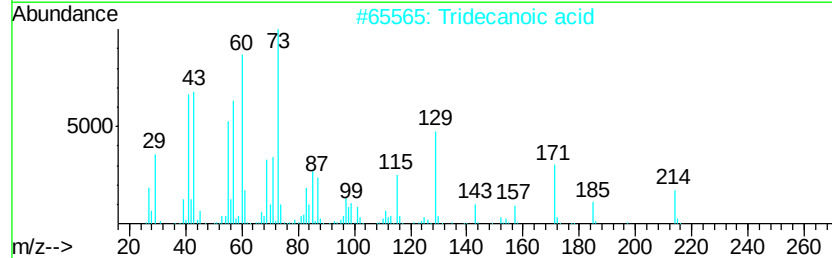
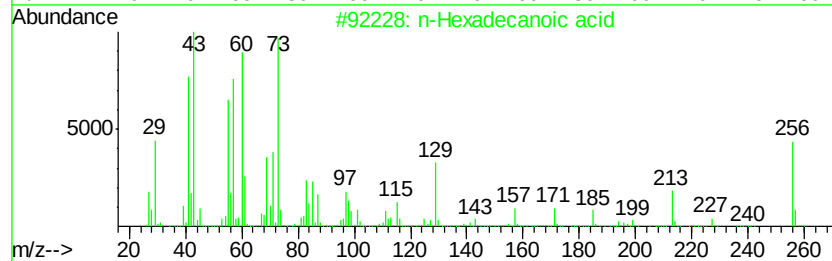
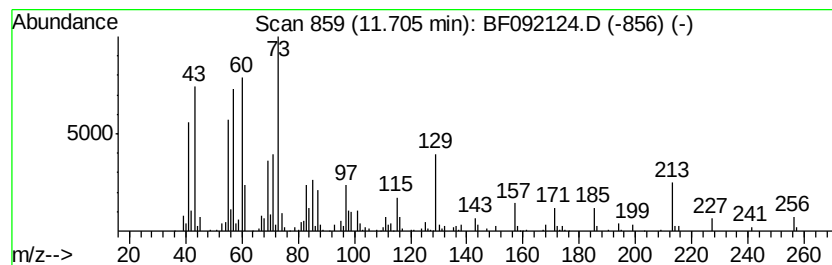
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	3.57 ng	174722	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	11



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ALS Vial : 17 Sample Multiplier: 1

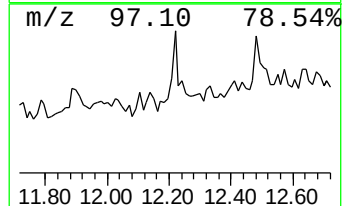
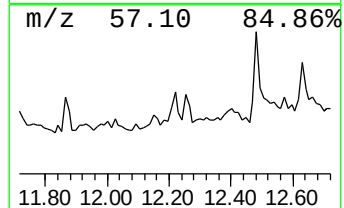
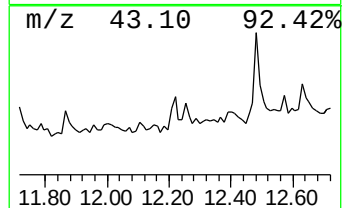
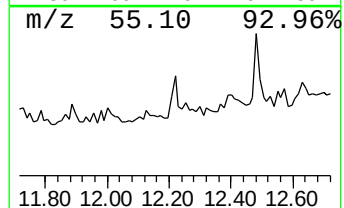
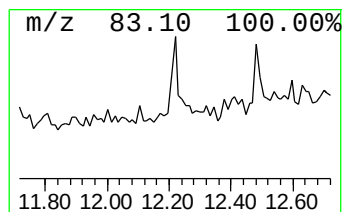
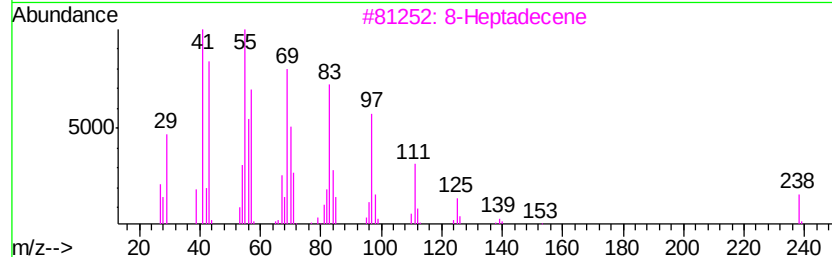
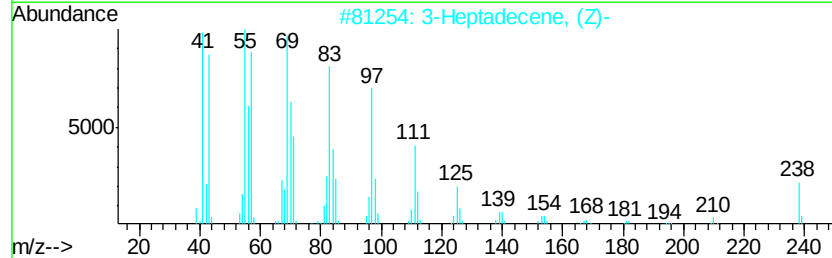
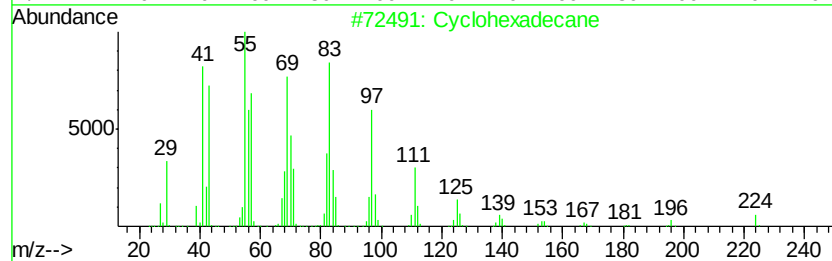
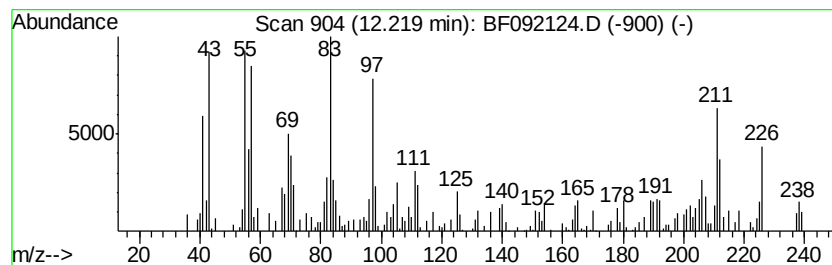
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BNA_F
ClientSampleId :
TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.22	3.19 ng	156168	Phenanthrene-d10	11.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	53
2	3-Heptadecene, (Z)-	238	C17H34	1000141-67-3	53
3	8-Heptadecene	238	C17H34	054290-12-9	44
4	1-Pentadecene	210	C15H30	013360-61-7	43
5	Cyclohexane, 1-(cyclohexylmethyl...)	222	C16H30	054965-61-6	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092124.D
Acq On : 6 Jan 2017 18:35
Operator : UM/SJ
Sample : I1025-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP7-8-COMP10

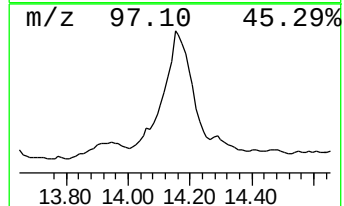
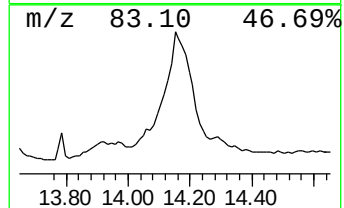
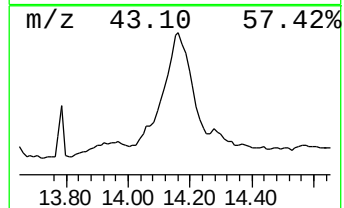
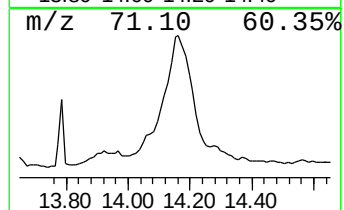
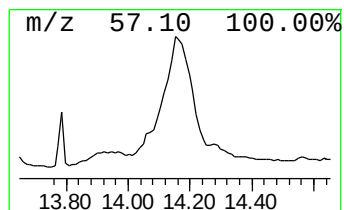
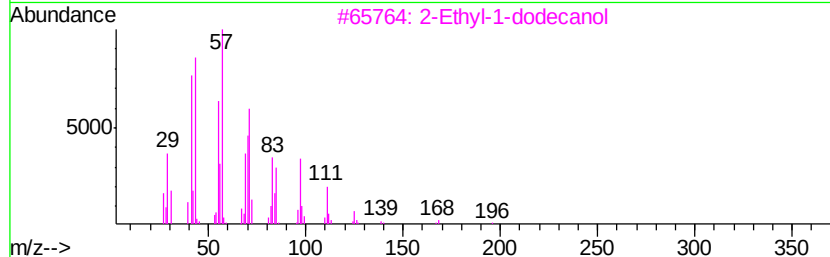
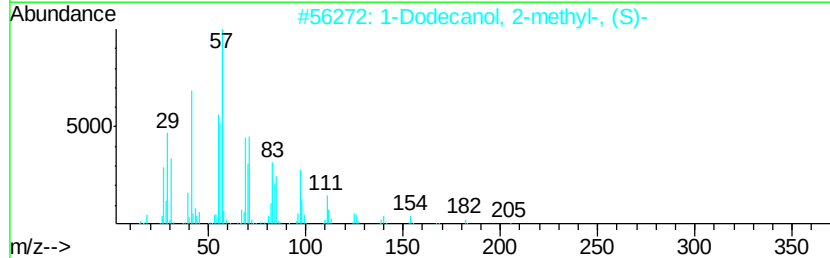
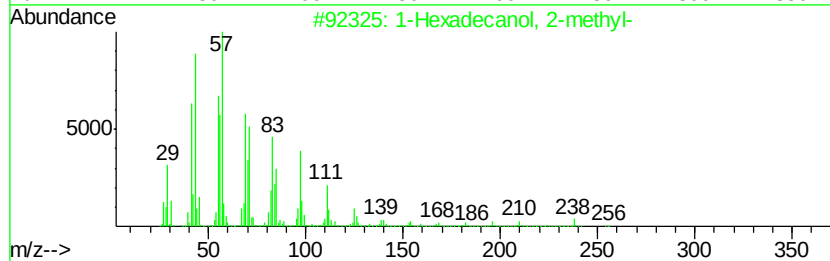
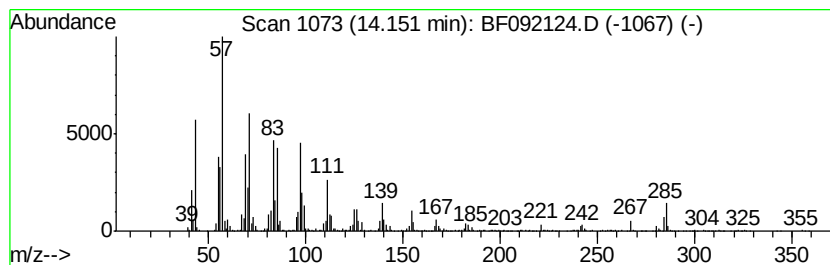
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexadecanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	65.08 ng	5537180	Chrysene-d12	13.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	87
2			1-Dodecanol, 2-methyl-, (S)-	200	C13H28O	057289-26-6	78
3			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	58
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	52
5			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
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Acq On : 6 Jan 2017 18:35
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Sample : I1025-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

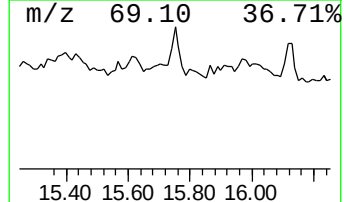
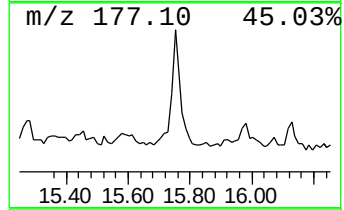
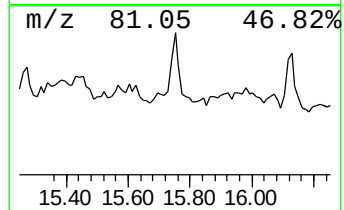
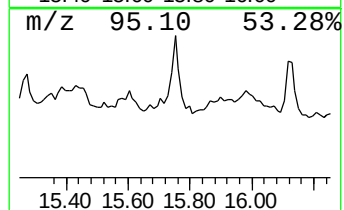
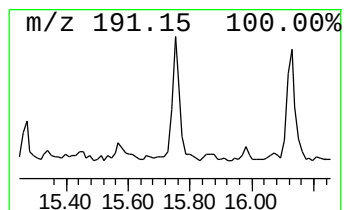
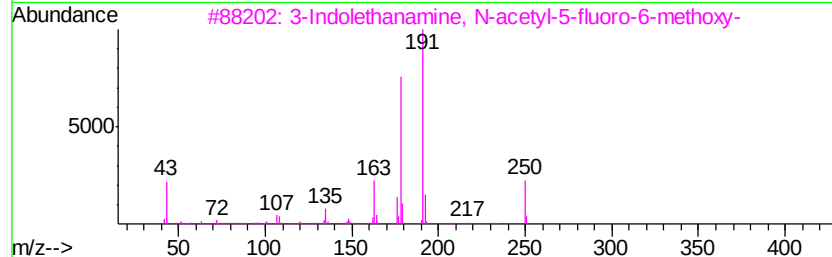
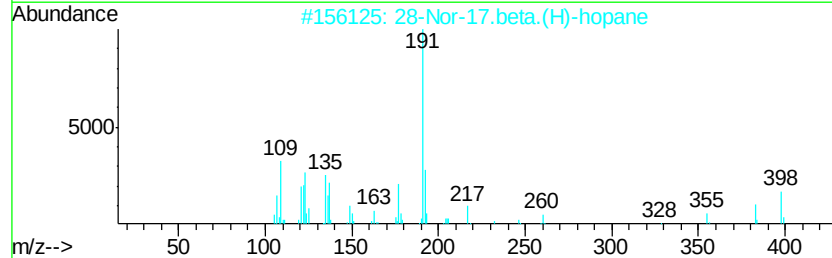
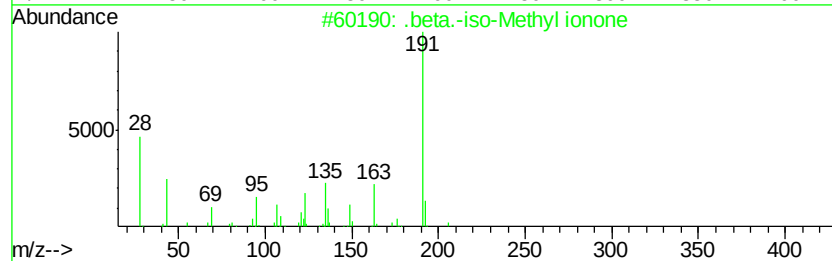
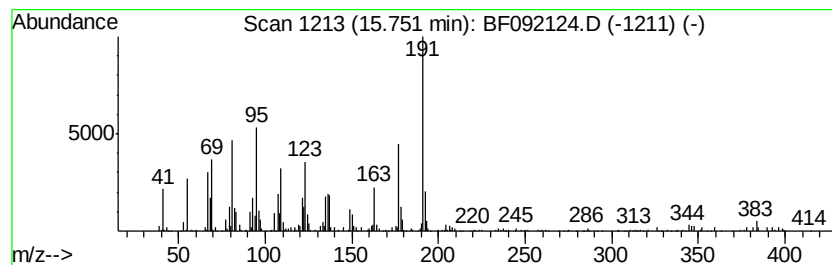
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.75 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.75	6.37 ng	317882	Perylene-d12	15.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	43
2	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	38
3	3-Indolethamine, N-acetyl-5-fl...	250	C13H15FN2O2	1000116-27-1	38
4	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	38
5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010617\
Data File : BF092124.D
Acq On : 6 Jan 2017 18:35
Operator : UM/SJ
Sample : I1025-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

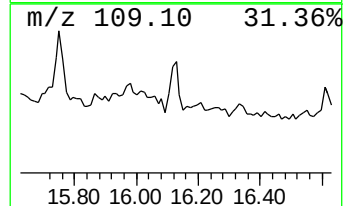
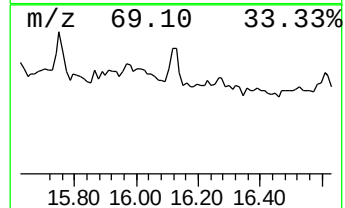
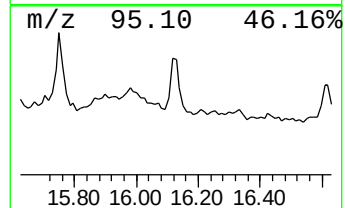
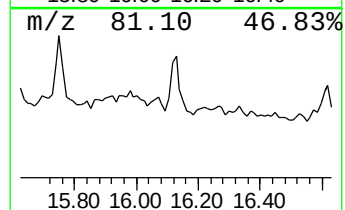
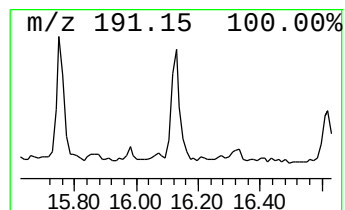
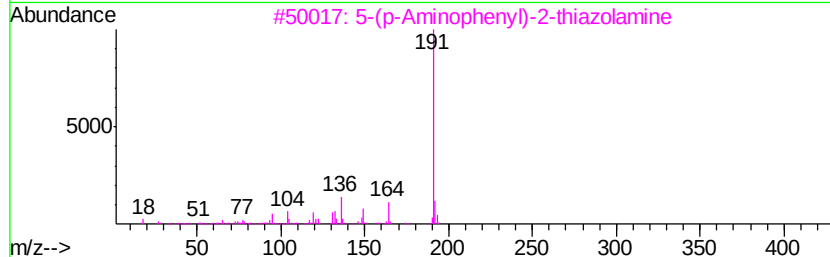
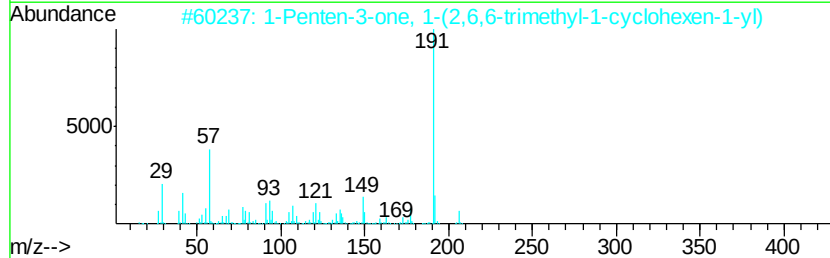
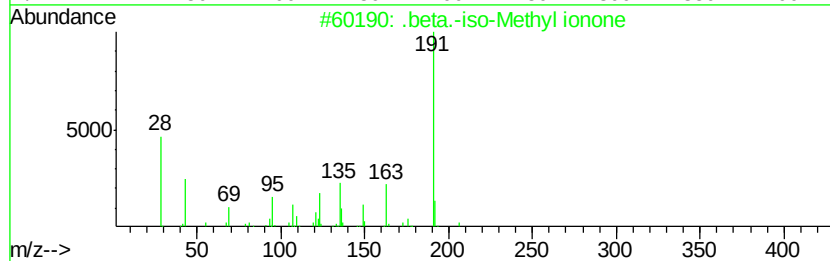
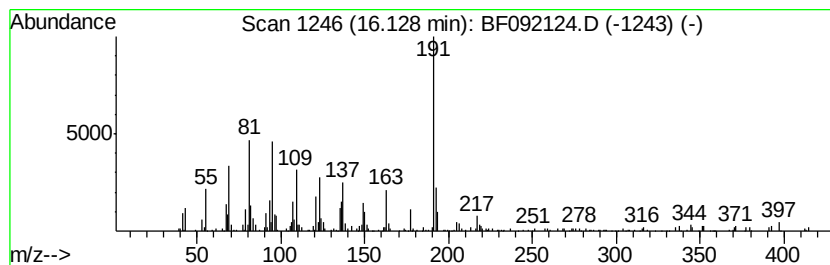
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown16.13 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	5.42 ng	270405	Perylene-d12	15.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-iso-Methyl ionone	206 C14H22O	1000285-40-2 49
2		1-Penten-3-one, 1-(2,6,6-trimeth...	206 C14H22O	000127-43-5 38
3		5-(p-Aminophenyl)-2-thiazolamine	191 C9H9N3S	090349-87-4 38
4		4,5-Dihydrothiazol-4-one, 2-(2-m...	222 C10H10N2O2S	022476-61-5 38
5		1-Cyclohexene, 1,3,3-trimethyl-2...	206 C14H22O	1000197-08-4 37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010617\
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Acq On : 6 Jan 2017 18:35
Operator : UM/SJ
Sample : I1025-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP7-8-COMP10

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
Propylene Glycol	2.79	7.2	ng	420766	1	6.64	1166900	20.0
2-Pentanone, 4-hy...	4.78	41.4	ng	2414160	1	6.64	1166900	20.0
unknown6.42	6.42	62.6	ng	3651390	1	6.64	1166900	20.0
Tridecane	10.60	2.0	ng	98606	4	11.16	978378	20.0
n-Hexadecanoic acid	11.70	3.6	ng	174722	4	11.16	978378	20.0
Cyclohexadecane	12.22	3.2	ng	156168	4	11.16	978378	20.0
1-Hexadecanol, 2-...	14.15	65.1	ng	5537180	5	13.79	1701580	20.0
unknown15.75	15.75	6.4	ng	317882	6	15.16	998395	20.0
unknown16.13	16.13	5.4	ng	270405	6	15.16	998395	20.0