

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
 Data File : BF099246.D
 Acq On : 8 Oct 2017 21:49
 Operator : SJ/JU
 Sample : I5707-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2AVE-06

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-BF092317.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	2.169	9	14	33	rVB	571960	806767	20.50%	2.801%
2	4.598	423	427	432	rVB	206851	232793	5.91%	0.808%
3	5.081	506	509	522	rVB	204238	238022	6.05%	0.826%
4	5.487	574	578	589	rBV	1203707	1165645	29.62%	4.046%
5	6.487	744	748	753	rBV	862449	740574	18.82%	2.571%
6	6.634	769	773	776	rBV	2357982	2049159	52.07%	7.113%
7	6.863	804	812	820	rBV	889818	817801	20.78%	2.839%
8	7.022	834	839	842	rBV	2948015	2730190	69.37%	9.478%
9	7.434	901	909	912	rBV	1996506	2276143	57.83%	7.901%
10	7.669	942	949	959	rVB2	50852	74736	1.90%	0.259%
11	7.763	959	965	967	rBV	50652	47737	1.21%	0.166%
12	7.881	980	985	988	rBV2	34065	50680	1.29%	0.176%
13	7.981	992	1002	1005	rBV2	112427	249200	6.33%	0.865%
14	8.098	1010	1022	1024	rVV5	222208	590294	15.00%	2.049%
15	8.145	1024	1030	1033	rVV	1257268	1479492	37.59%	5.136%
16	8.175	1033	1035	1039	rVB	100669	99838	2.54%	0.347%
17	8.275	1046	1052	1055	rBV3	199625	304964	7.75%	1.059%
18	8.310	1055	1058	1062	rVV2	169322	165283	4.20%	0.574%
19	8.363	1062	1067	1072	rVB4	59091	102683	2.61%	0.356%
20	8.410	1072	1075	1076	rBV2	64477	62824	1.60%	0.218%
21	8.428	1076	1078	1085	rVV3	122825	159869	4.06%	0.555%
22	8.545	1087	1098	1101	rVV2	347419	705219	17.92%	2.448%
23	8.575	1101	1103	1104	rVV	148873	140352	3.57%	0.487%
24	8.592	1104	1106	1113	rVB2	242836	291674	7.41%	1.013%
25	9.222	1207	1213	1216	rBV	3862842	3935698	100.00%	13.662%
26	9.328	1227	1231	1236	rBV2	85979	88354	2.24%	0.307%
27	9.610	1275	1279	1283	rBV	55693	45796	1.16%	0.159%
28	9.816	1311	1314	1317	rVB3	37161	42526	1.08%	0.148%
29	9.898	1324	1328	1338	rVB	1185577	1123839	28.56%	3.901%
30	10.275	1388	1392	1395	rBV	315130	245550	6.24%	0.852%
31	10.692	1458	1463	1466	rBV	1595594	1531629	38.92%	5.317%
32	10.792	1476	1480	1487	rVB2	45455	57442	1.46%	0.199%
33	11.386	1577	1581	1585	rBV	1205250	1065763	27.08%	3.700%
34	12.974	1846	1851	1854	rBV	3331092	3570905	90.73%	12.396%

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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.027	2026	2030	2037	rVB	964995	857887	21.80%	2.978%
36	15.498	2275	2280	2288	rBV	509683	659614	16.76%	2.290%

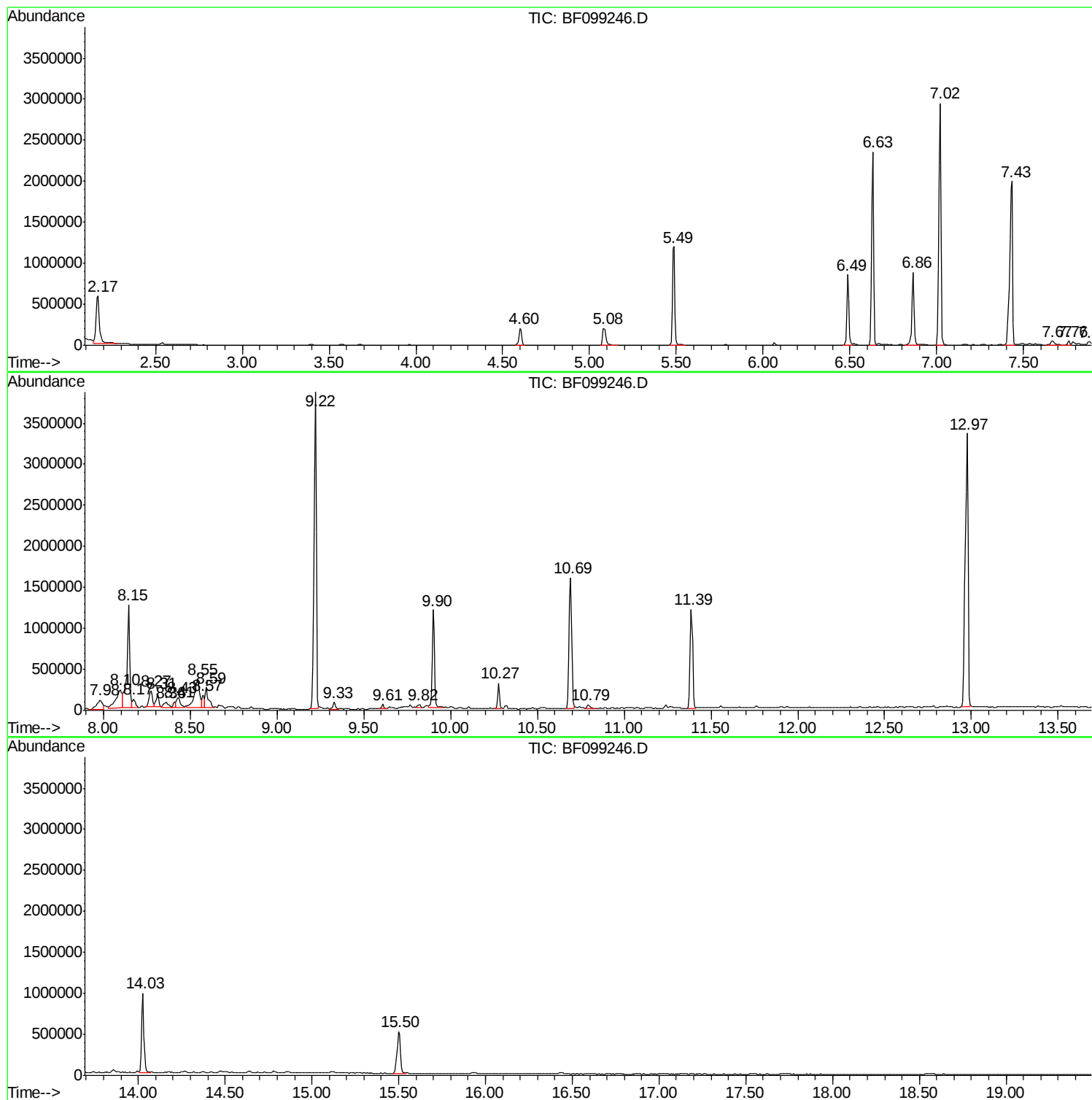
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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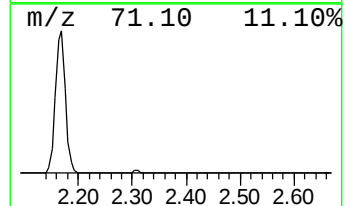
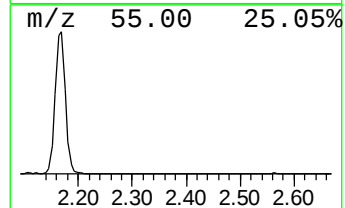
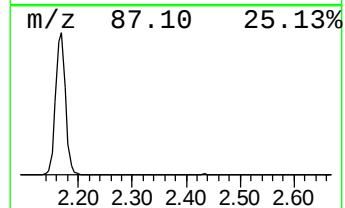
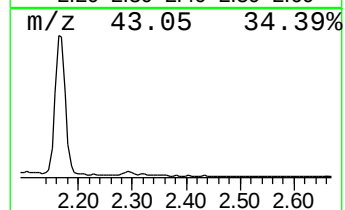
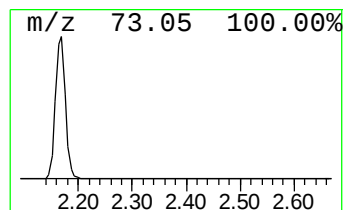
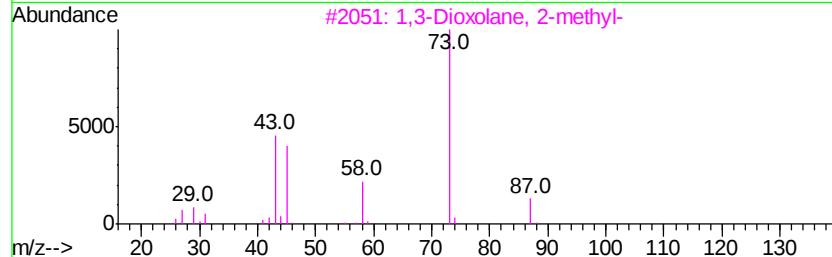
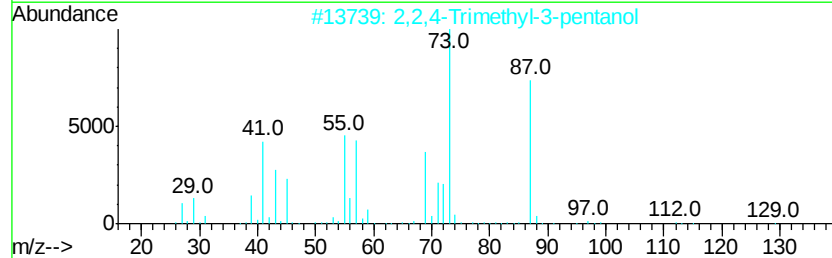
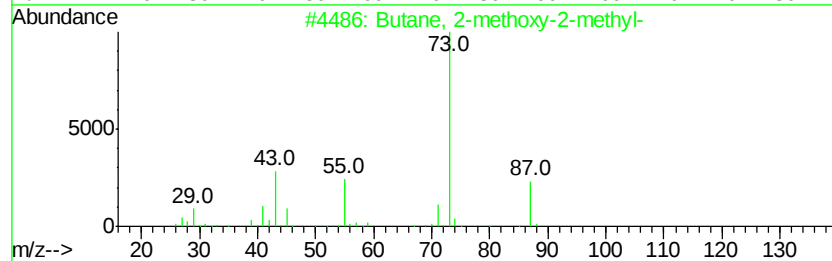
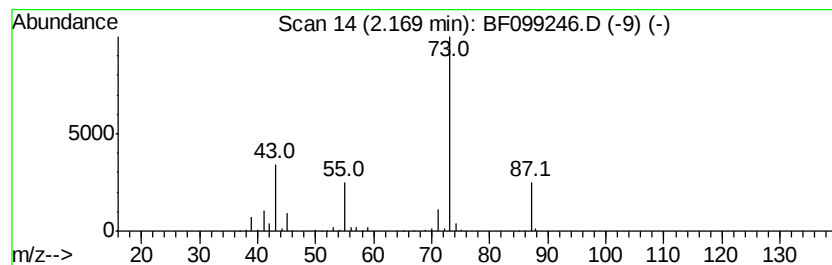
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	19.73 ng	806767	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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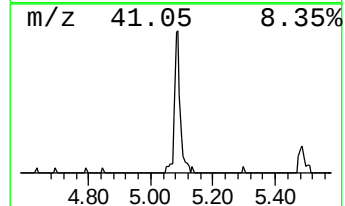
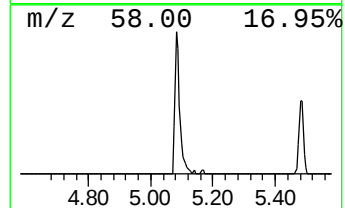
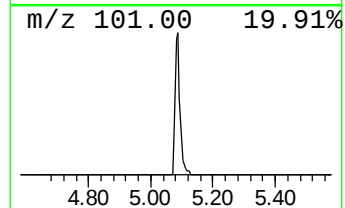
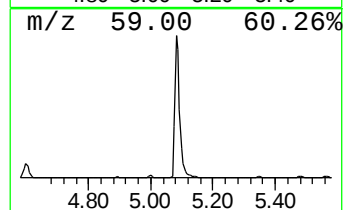
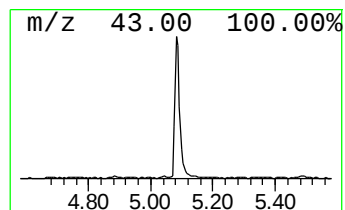
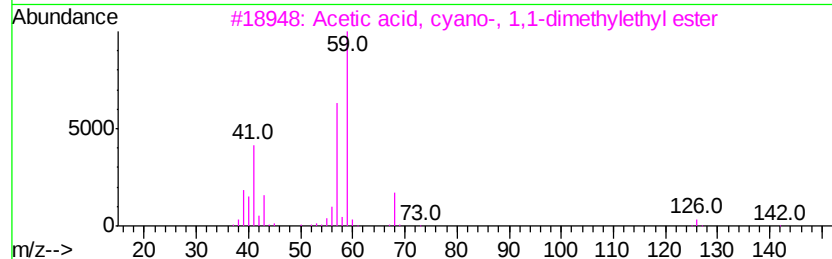
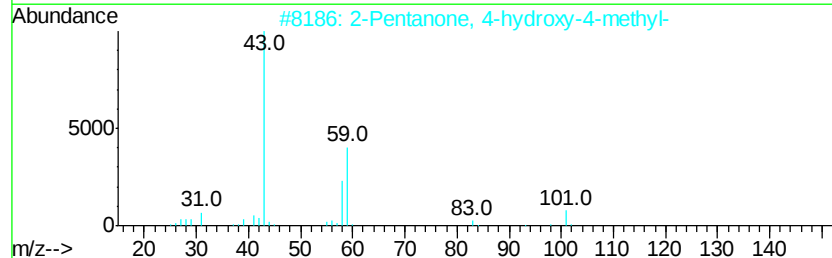
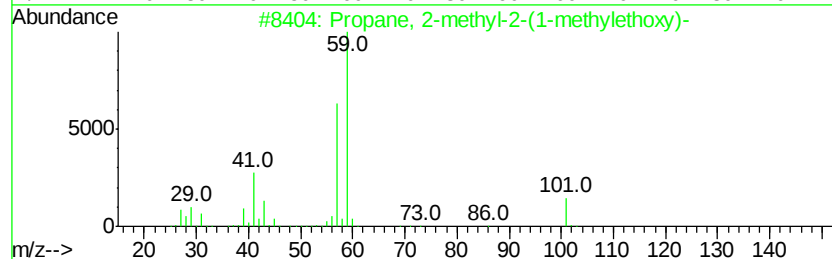
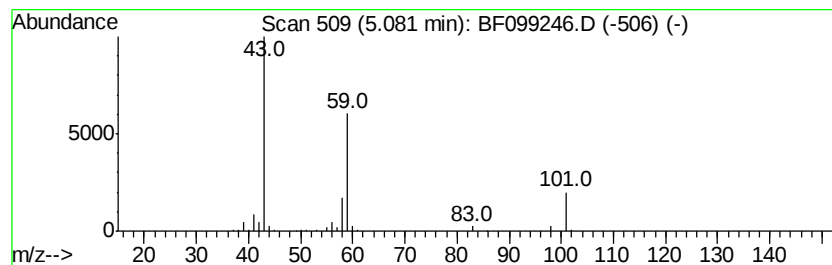
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.08 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	5.82 ng	238022	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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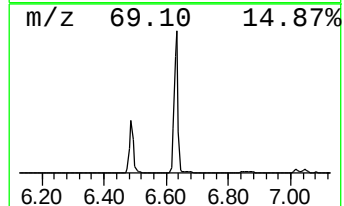
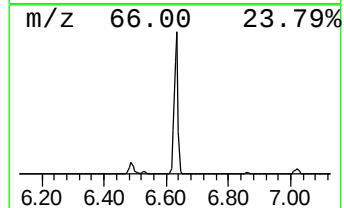
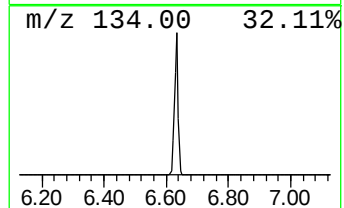
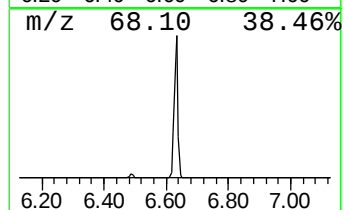
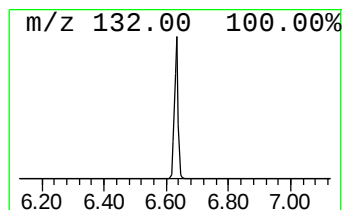
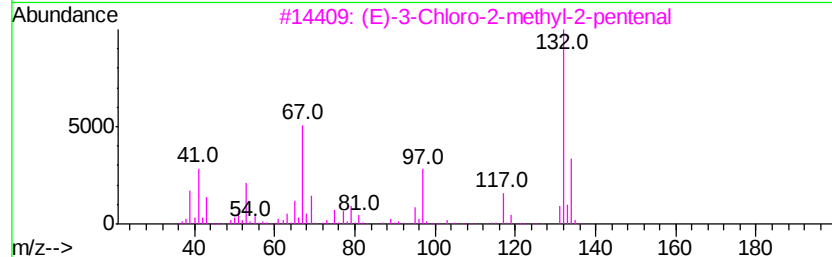
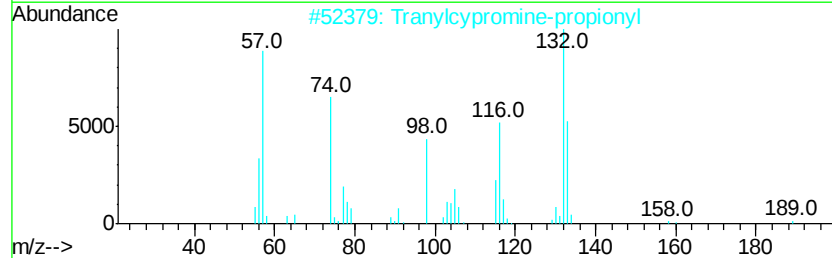
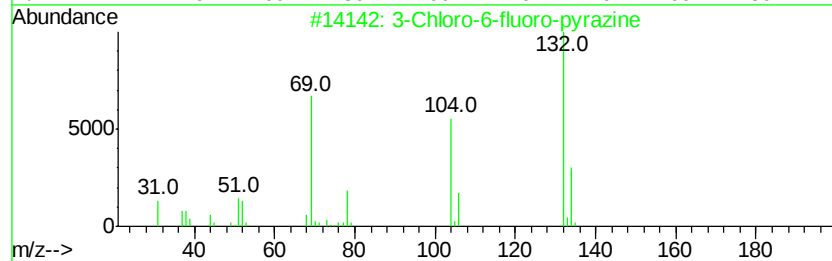
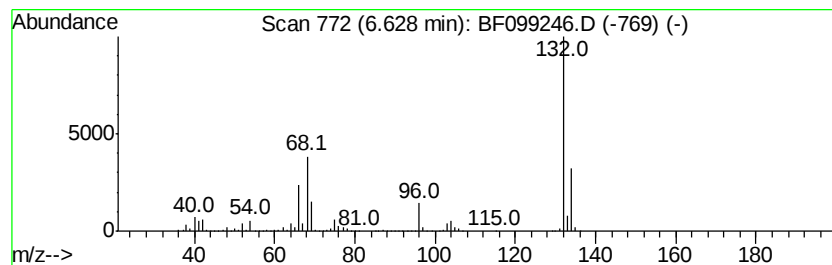
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	50.11 ng	2049160	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
4	5-Aminoindole	132	C8H8N2	005192-03-0	12	
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9	



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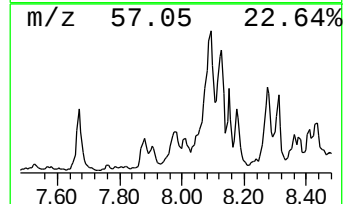
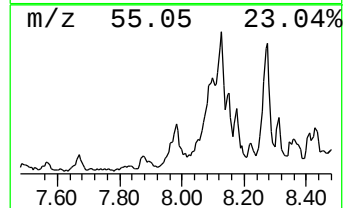
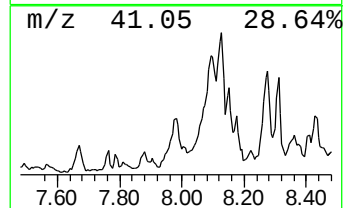
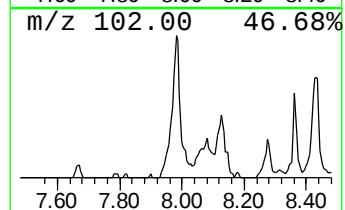
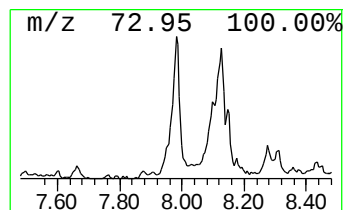
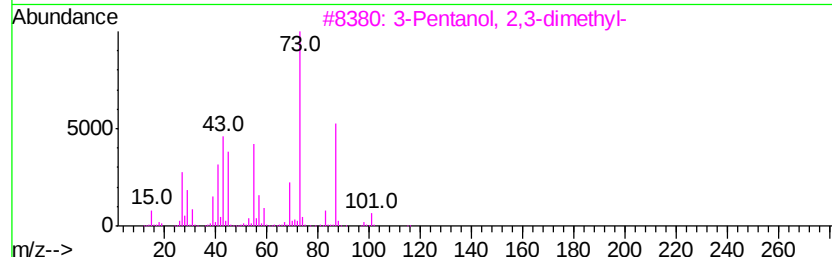
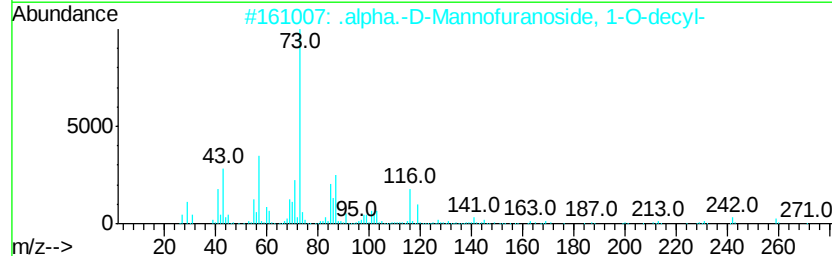
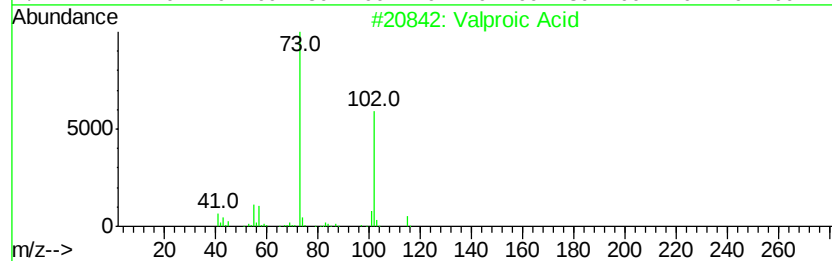
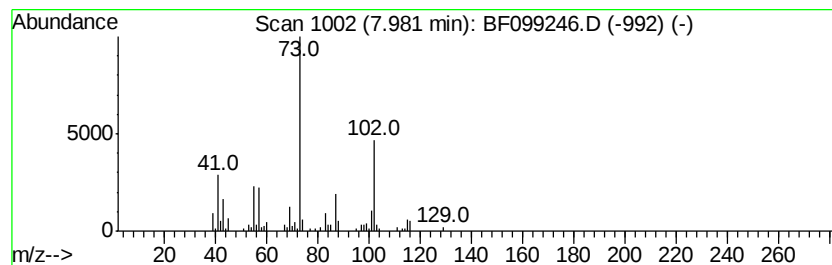
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown7.98 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.98	3.37 ng	249200	Napthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Valproic Acid	144	C8H16O2	000099-66-1	49
2		.alpha.-D-Mannofuranoside, 1-O-d...	320	C16H32O6	1000160-04-7	12
3		3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	12
4		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	12
5		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	12



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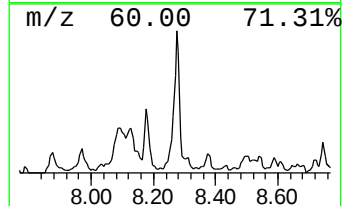
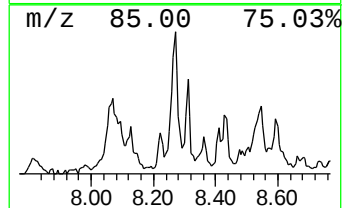
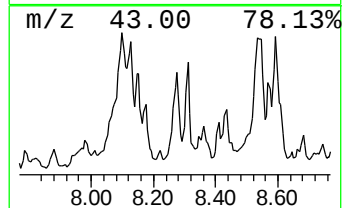
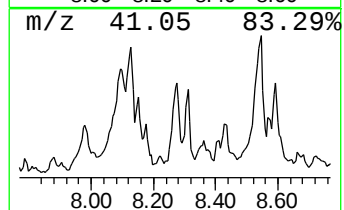
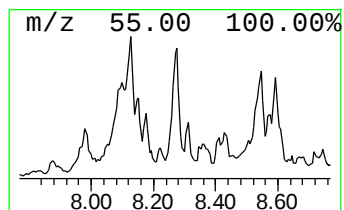
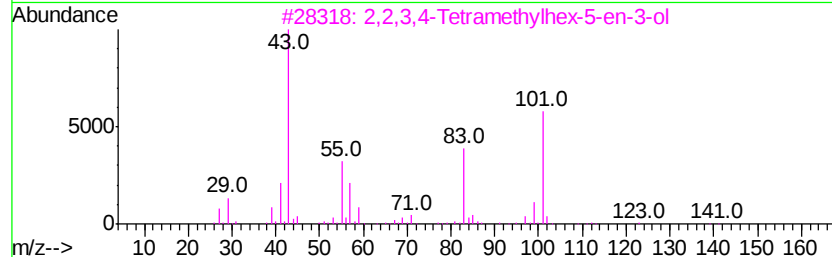
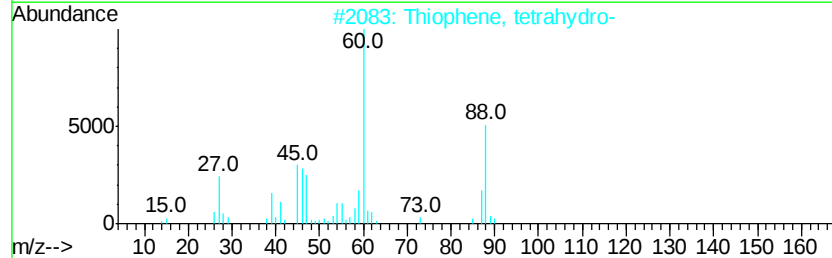
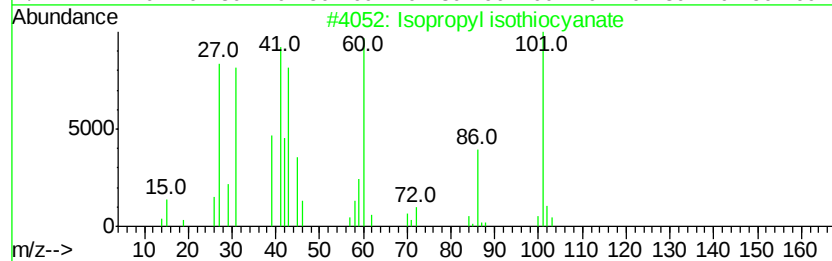
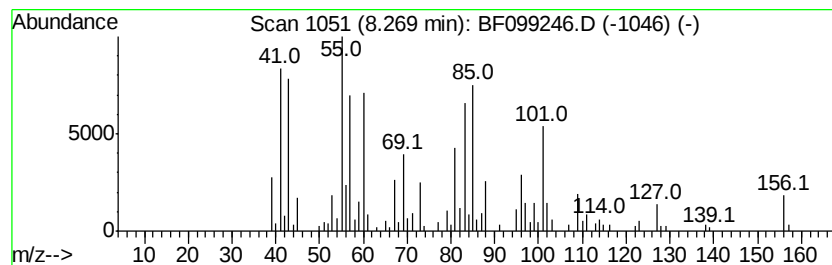
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 unknown8.27 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	4.12 ng	304964	Naphthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	35
2		Thiophene, tetrahydro-	88	C4H8S	000110-01-0	22
3		2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1000191-06-9	22
4		Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	14
5		2-Butenoic acid, 2-methyl-, 2-me...	156	C9H16O2	061692-84-0	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099246.D
Acq On : 8 Oct 2017 21:49
Operator : SJ/JU
Sample : I5707-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
2AVE-06

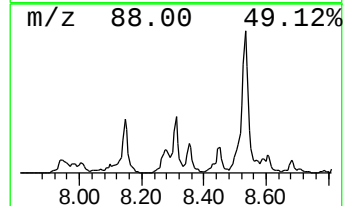
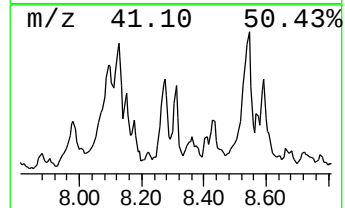
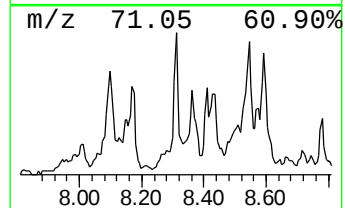
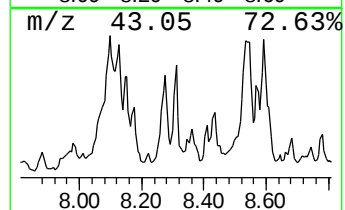
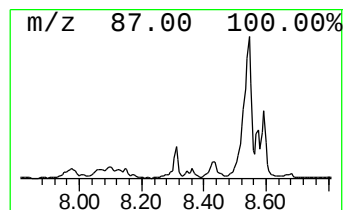
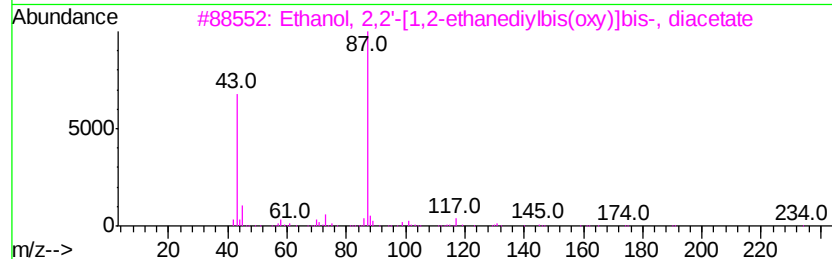
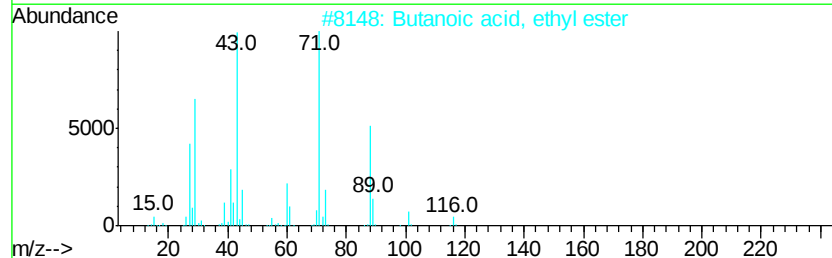
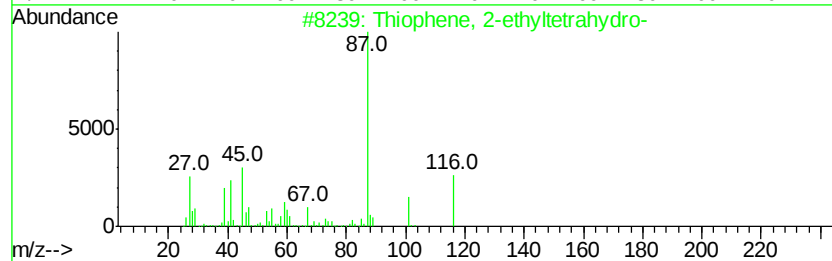
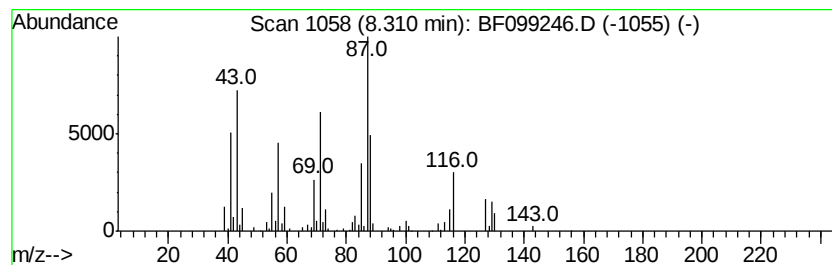
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.31 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.31	2.23 ng	165283	Naphthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	35
2		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	22
3		Ethanol, 2,2'-[1,2-ethanedivlbis...	234	C10H18O6	000111-21-7	22
4		2-[2-[2-[2-[2-[2-[2-(2-Acetyl...	498	C22H42O12	1000351-90-5	16
5		2-[2-[2-[2-[2-[2-[2-(2-Ace...	542	C24H46O13	1000351-90-4	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
Data File : BF099246.D
Acq On : 8 Oct 2017 21:49
Operator : SJ/JU
Sample : I5707-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2AVE-06

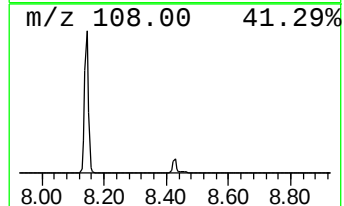
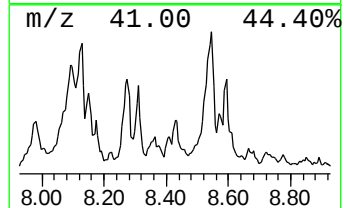
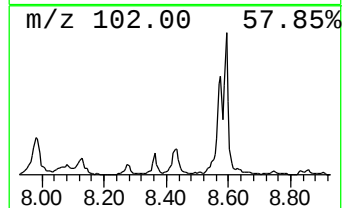
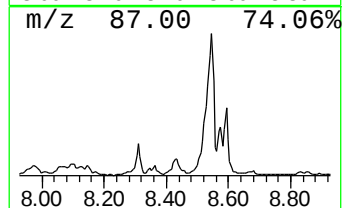
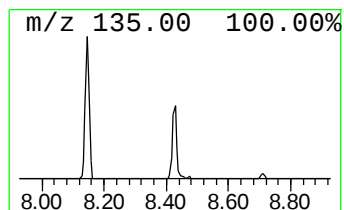
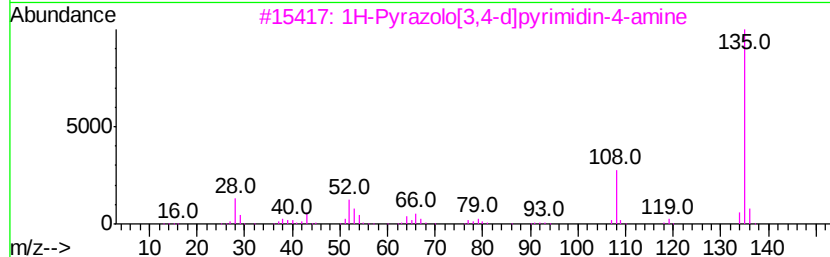
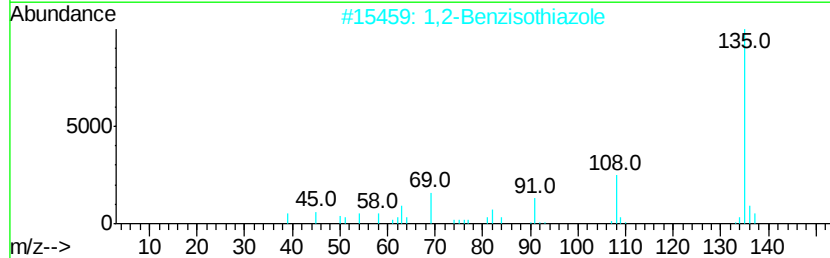
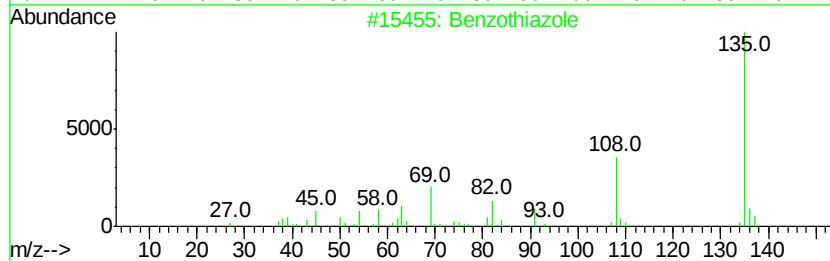
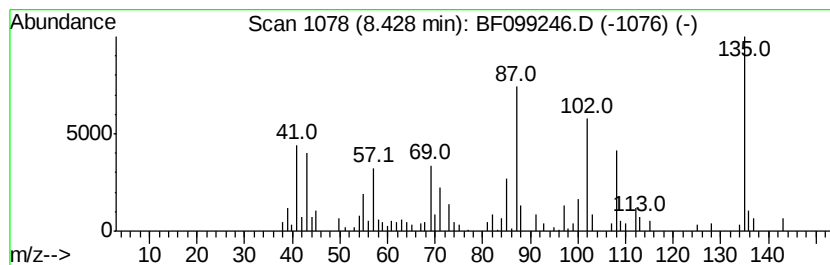
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.43 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.43	2.16 ng	159869	Naphthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole	135	C7H5NS	000095-16-9	38
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	38
3		1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	27
4		1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	27
5		Septacidin aminonucleoside	326	C12H18N6O5	003059-05-0	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099246.D
Acq On : 8 Oct 2017 21:49
Operator : SJ/JU
Sample : I5707-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2AVE-06

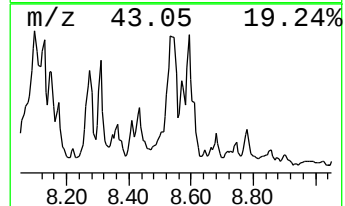
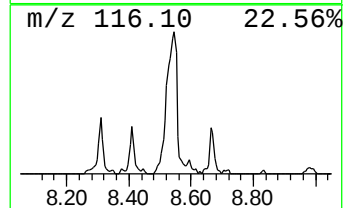
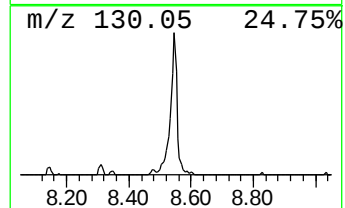
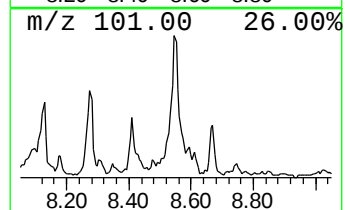
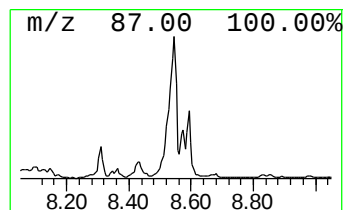
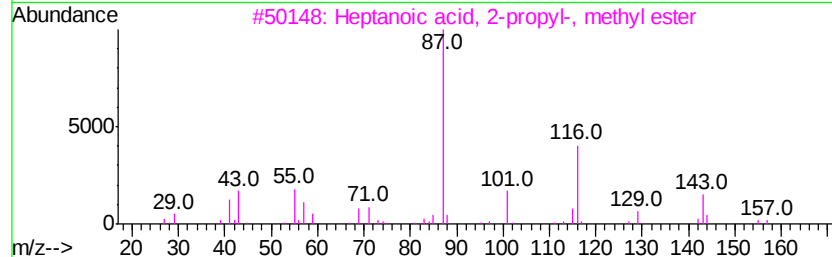
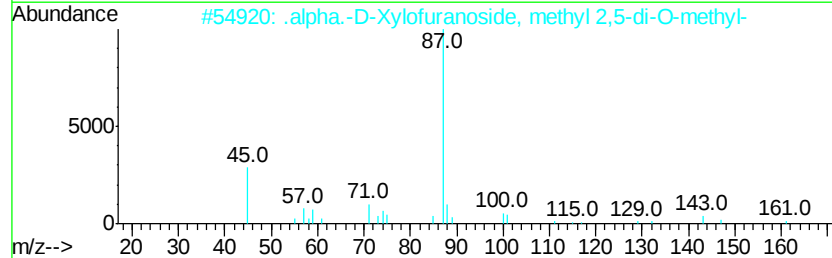
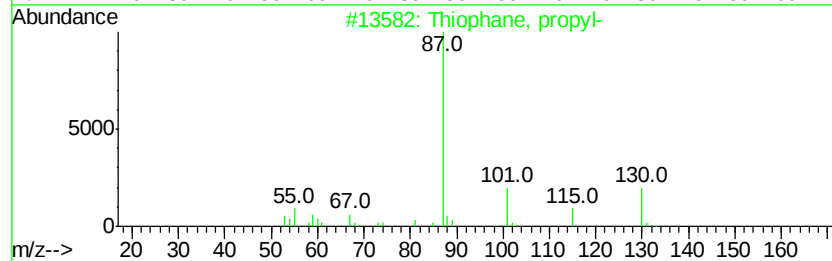
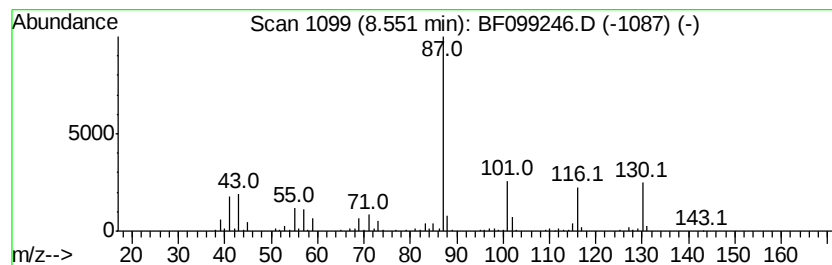
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Thiophane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	9.53 ng	705219	Napthalene-d8	8.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	72
2			.alpha.-D-Xylofuranoside, methyl...	192	C8H16O5	035007-52-4	59
3			Heptanoic acid, 2-propyl-, methv...	186	C11H22O2	056247-53-1	53
4			2-[2-[2-[2-[2-(2-Acetyloxveth...	410	C18H34O10	1000351-90-7	47
5			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF100817\
Data File : BF099246.D
Acq On : 8 Oct 2017 21:49
Operator : SJ/JU
Sample : I5707-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2AVE-06

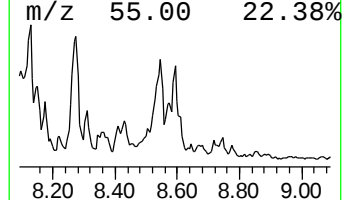
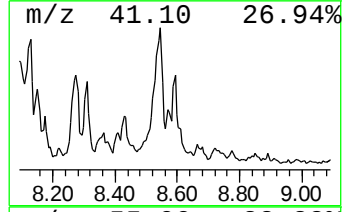
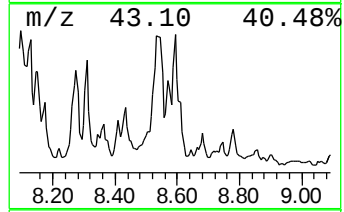
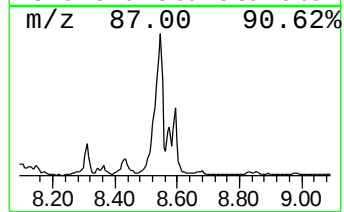
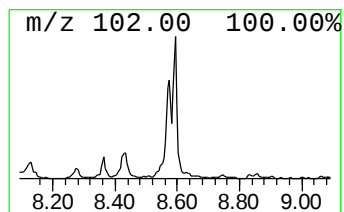
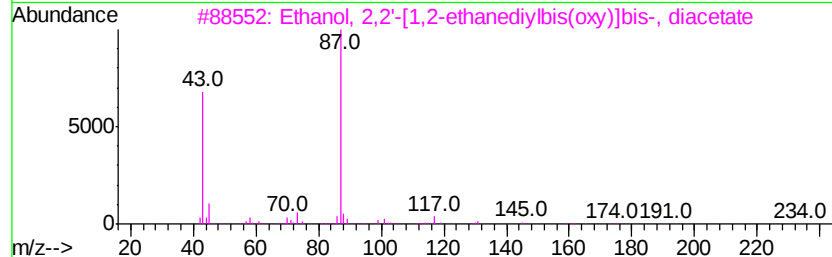
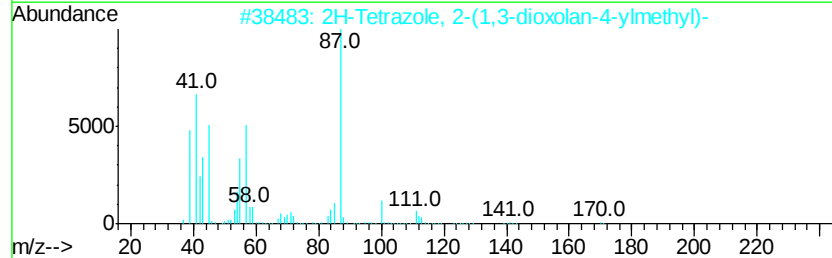
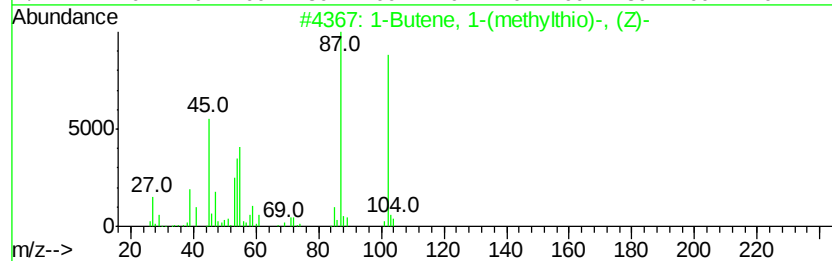
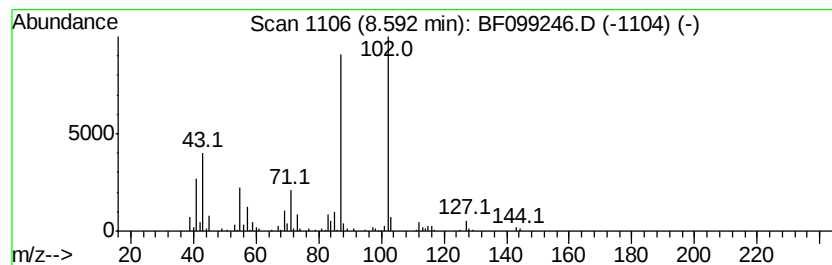
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Butene, 1-(methylthio)-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.59	3.94 ng	291674	Naphthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	50
2		2H-Tetrazole, 2-(1,3-dioxolan-4-ylmethyl)-	170	C6H10N4O2	339292-86-3	38
3		Ethanol, 2,2'-[1,2-ethanedivylbis(oxy)]bis-, diacetate	234	C10H18O6	000111-21-7	27
4		4,4-(Ethylenedioxy)-2-pentanone	144	C7H12O3	014255-36-8	27
5		Phenylethyne	102	C8H6	000536-74-3	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
Data File : BF099246.D
Acq On : 8 Oct 2017 21:49
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Sample : I5707-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
2AVE-06

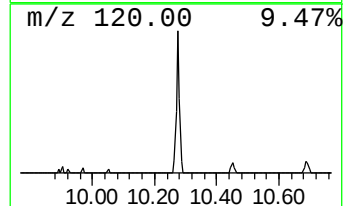
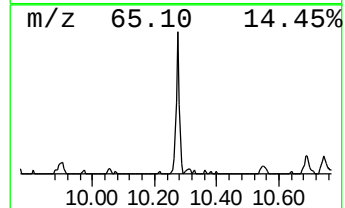
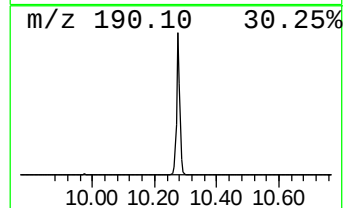
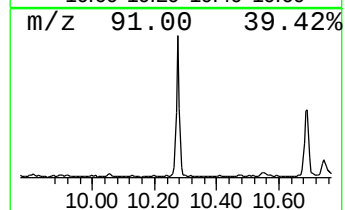
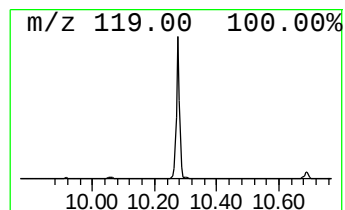
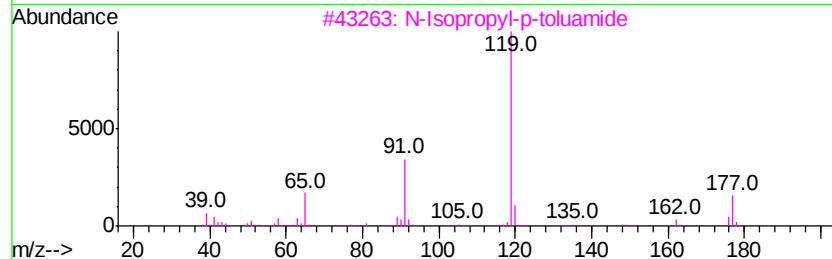
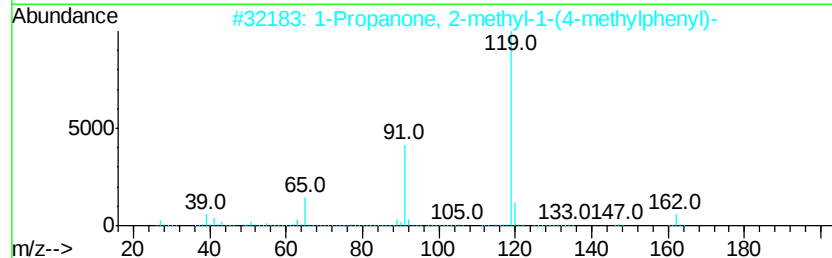
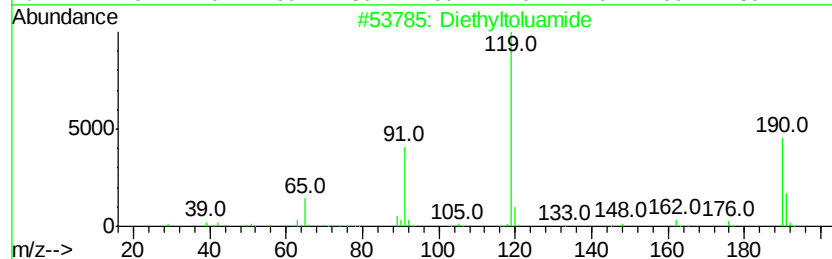
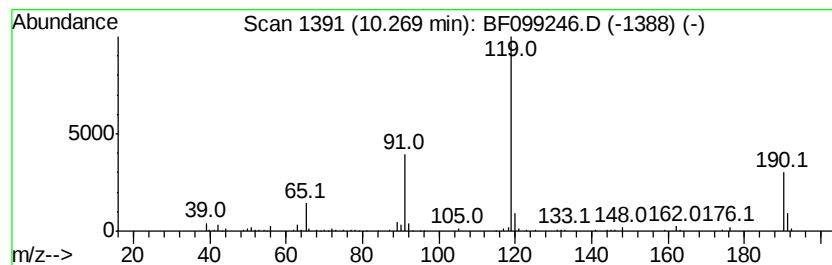
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Diethyltoluamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	4.37 ng	245550	Acenaphthene-d10	9.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2		1-Propanone, 2-methyl-1-(4-methylphenyl)-	162	C11H14O	050390-51-7	68
3		N-Isopropyl-p-toluamide	177	C11H15NO	002144-17-4	59
4		Benzoyl chloride, 3-methyl-	154	C8H7ClO	001711-06-4	53
5		p-Toluic acid, cyclobutyl ester	190	C12H14O2	1000292-21-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100817\
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
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unknown5.08	5.08	5.8	ng	238022	1	6.86	817801	20.0
unknown6.63	6.63	50.1	ng	2049160	1	6.86	817801	20.0
unknown7.98	7.98	3.4	ng	249200	2	8.15	1479490	20.0
unknown8.27	8.27	4.1	ng	304964	2	8.15	1479490	20.0
unknown8.31	8.31	2.2	ng	165283	2	8.15	1479490	20.0
unknown8.43	8.43	2.2	ng	159869	2	8.15	1479490	20.0
Thiophane, propyl-	8.55	9.5	ng	705219	2	8.15	1479490	20.0
1-Butene, 1-(meth...	8.59	3.9	ng	291674	2	8.15	1479490	20.0
Diethyltoluamide	10.27	4.4	ng	245550	3	9.90	1123840	20.0