

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102738.D
 Acq On : 5 Feb 2018 15:23
 Operator : SJ/JU
 Sample : J1437-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-148-20

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-BF020318.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	8	14	21	rVB	506932	659410	12.70%	1.664%
2	5.116	512	515	523	rVB	141471	191192	3.68%	0.483%
3	5.498	575	580	583	rBV	4732604	5192247	100.00%	13.104%
4	6.510	745	752	755	rBV	4430896	5153709	99.26%	13.007%
5	6.651	771	776	779	rBV	5100679	5039193	97.05%	12.718%
6	6.704	782	785	790	rVB	228671	166580	3.21%	0.420%
7	6.881	811	815	818	rBV	1627612	1272924	24.52%	3.213%
8	7.039	837	842	845	rVB	4227828	3843870	74.03%	9.701%
9	7.445	905	911	914	rBV	3347824	3291707	63.40%	8.308%
10	7.851	975	980	983	rBV	69895	91437	1.76%	0.231%
11	8.163	1027	1033	1036	rBV	2030465	1671871	32.20%	4.220%
12	8.833	1141	1147	1149	rBV7	54691	92807	1.79%	0.234%
13	8.939	1156	1165	1168	rBV9	97531	291087	5.61%	0.735%
14	8.992	1168	1174	1175	rBV5	76995	128557	2.48%	0.324%
15	9.039	1179	1182	1185	rVB3	189624	187547	3.61%	0.473%
16	9.081	1185	1189	1191	rBV5	110028	167263	3.22%	0.422%
17	9.239	1211	1216	1219	rBV	4773418	4714704	90.80%	11.899%
18	9.275	1220	1222	1225	rBV3	181320	252088	4.86%	0.636%
19	9.322	1226	1230	1233	rBV5	362562	565266	10.89%	1.427%
20	9.492	1257	1259	1261	rBV2	276221	222620	4.29%	0.562%
21	9.557	1267	1270	1272	rBV3	572778	641439	12.35%	1.619%
22	9.633	1280	1283	1286	rBV2	716966	1026568	19.77%	2.591%
23	13.004	1853	1856	1860	rVB	2029308	2154780	41.50%	5.438%
24	13.874	2002	2004	2017	rVB	674468	843389	16.24%	2.129%
25	14.045	2030	2033	2037	rVB	964499	944754	18.20%	2.384%
26	15.521	2280	2284	2294	rVB2	629010	814954	15.70%	2.057%

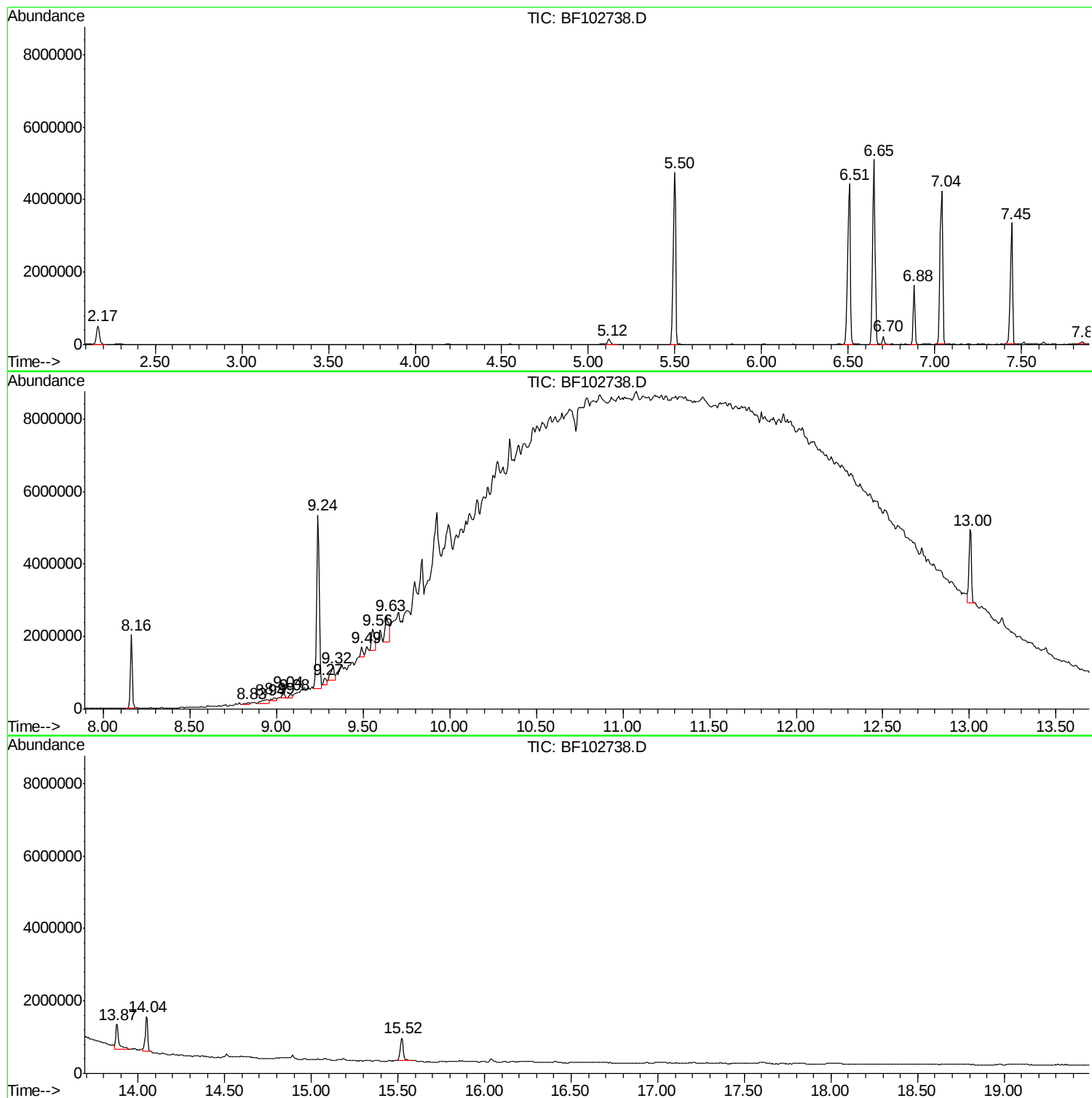
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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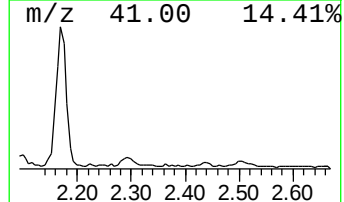
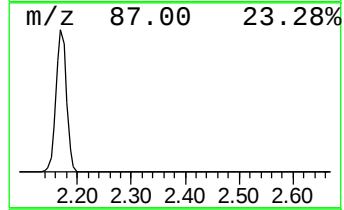
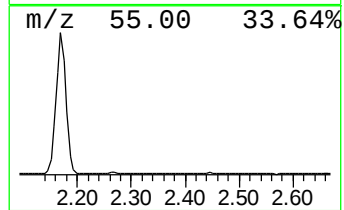
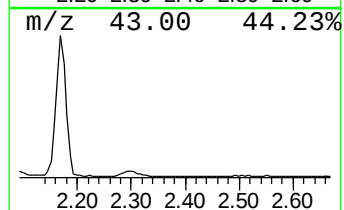
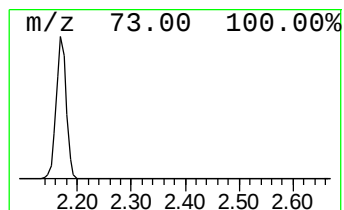
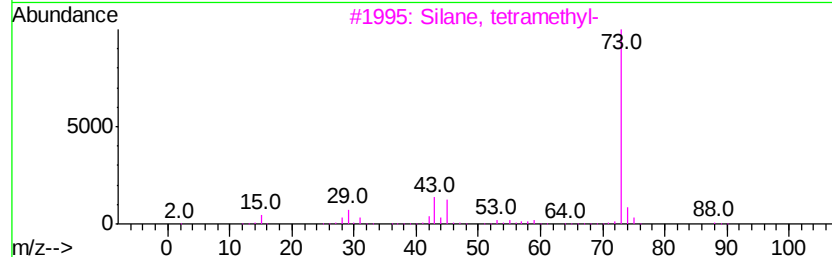
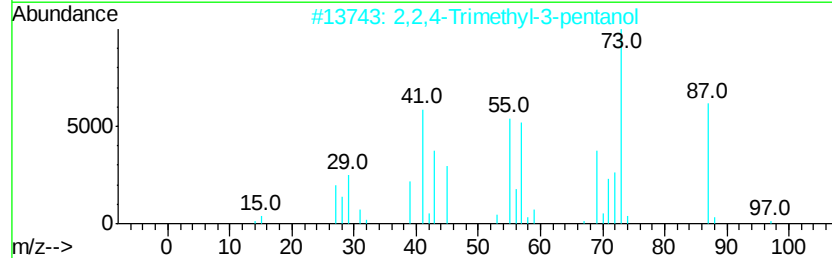
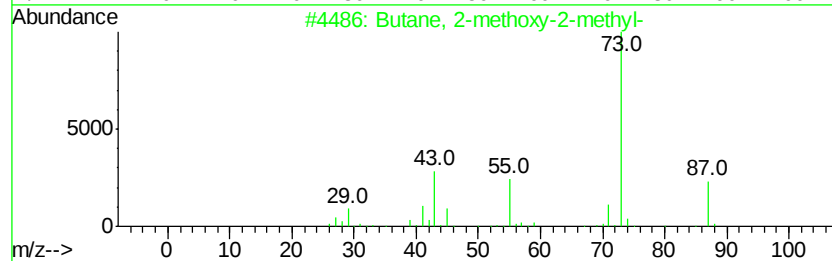
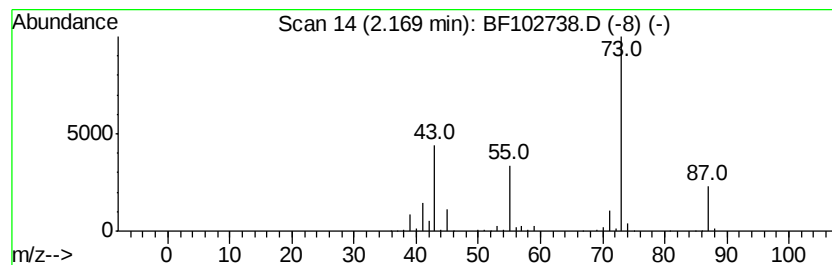
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	10.36 ng	659410	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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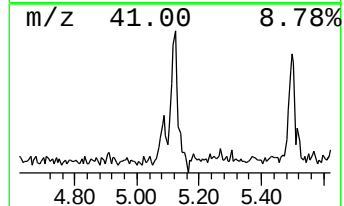
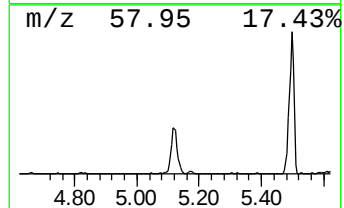
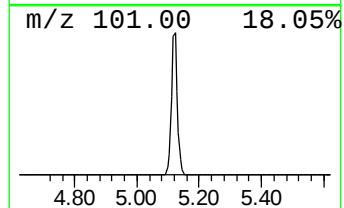
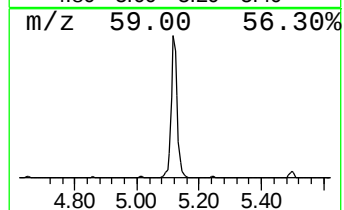
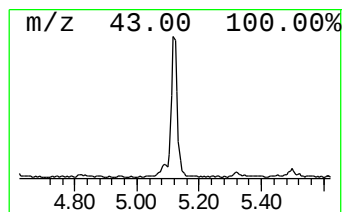
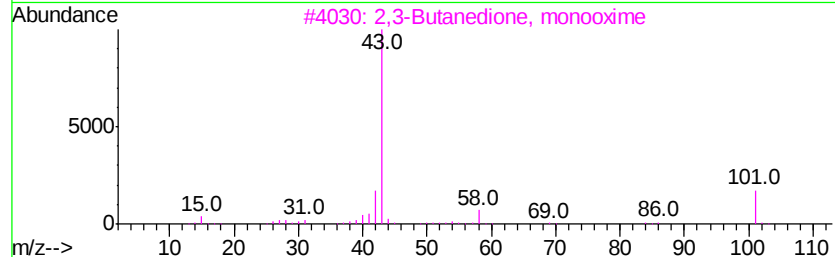
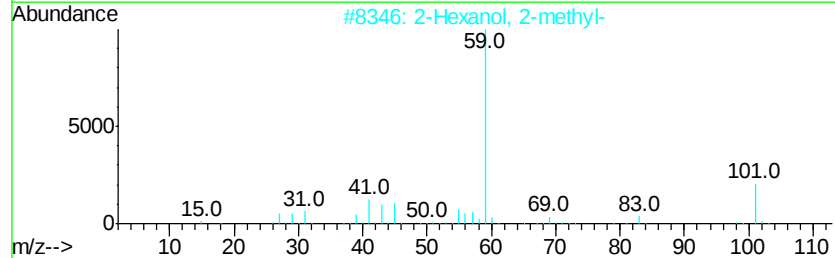
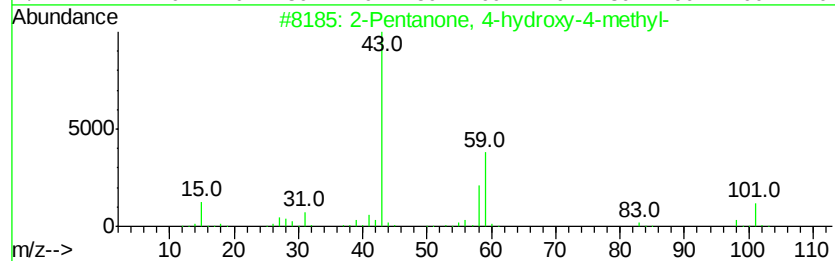
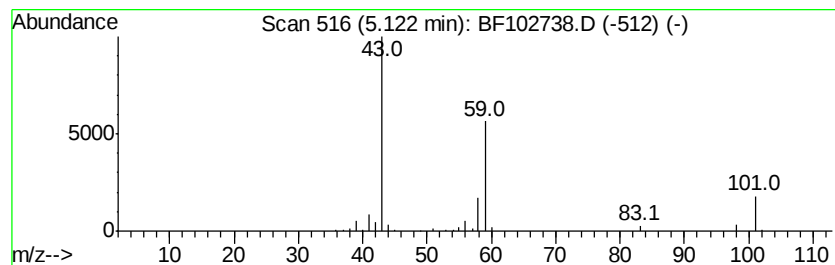
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.00 ng	191192	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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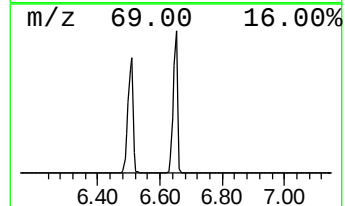
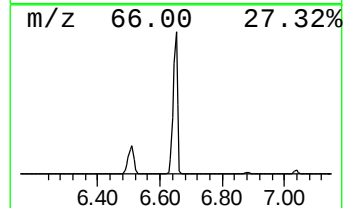
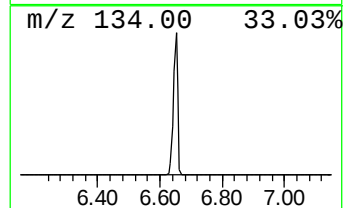
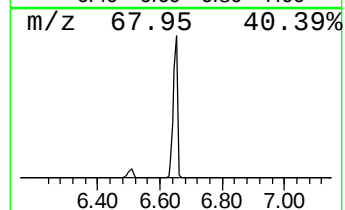
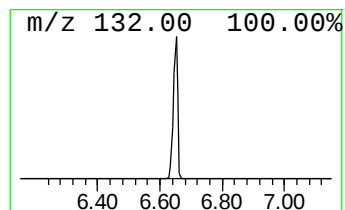
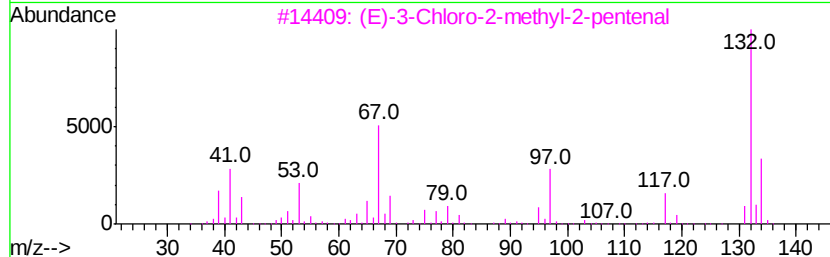
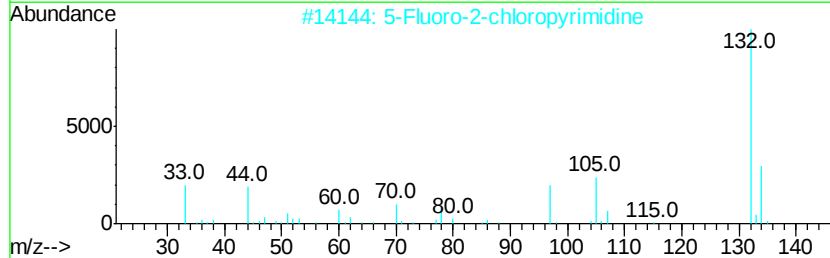
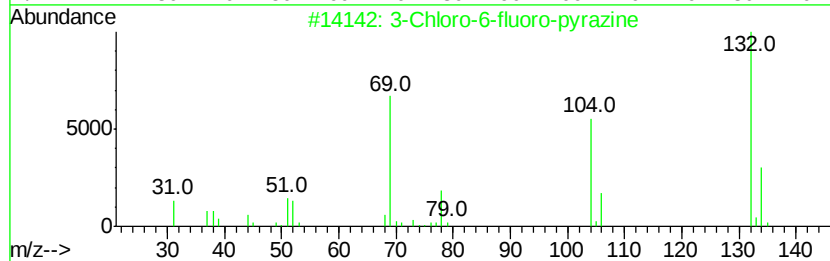
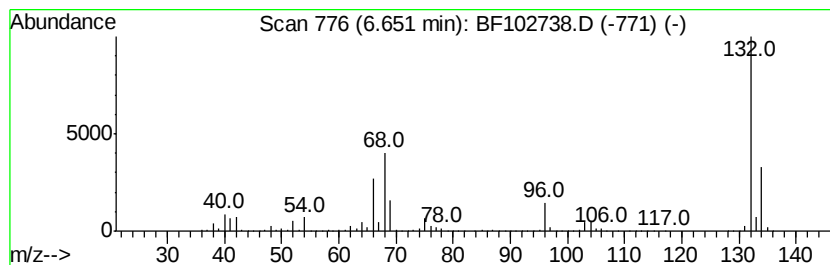
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Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	79.18 ng	5039190	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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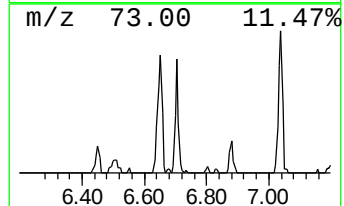
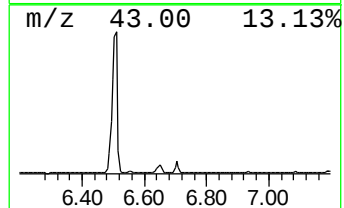
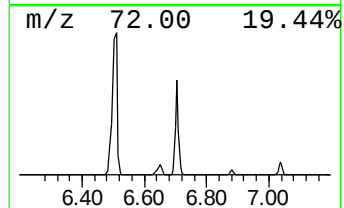
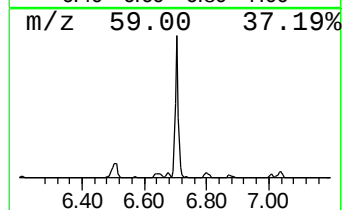
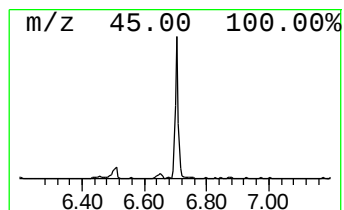
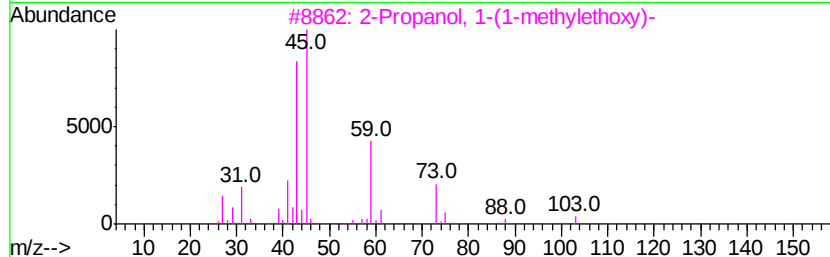
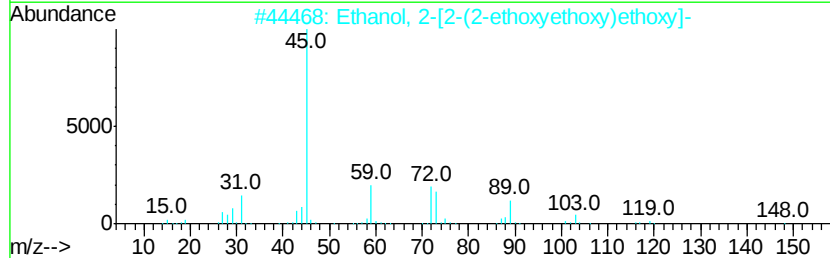
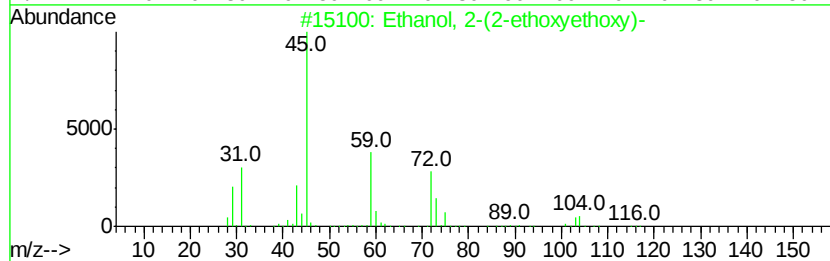
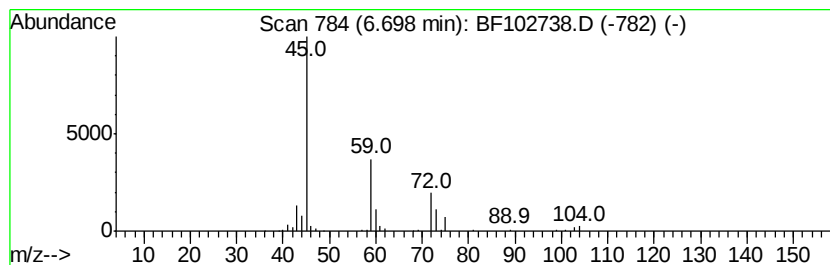
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Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	2.62 ng	166580	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	64
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	36
4			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	36
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	32



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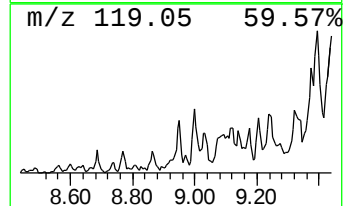
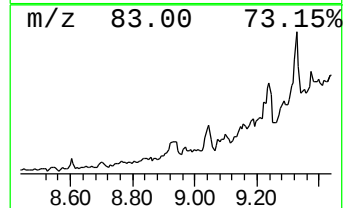
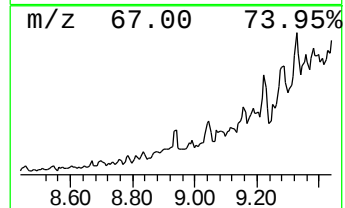
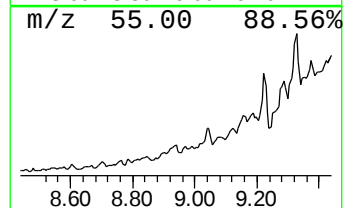
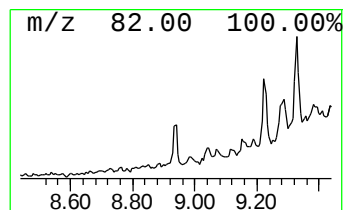
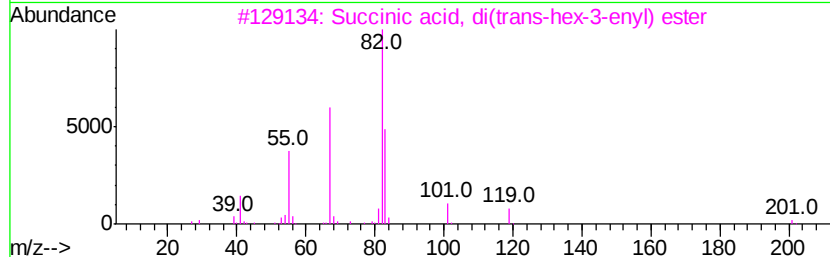
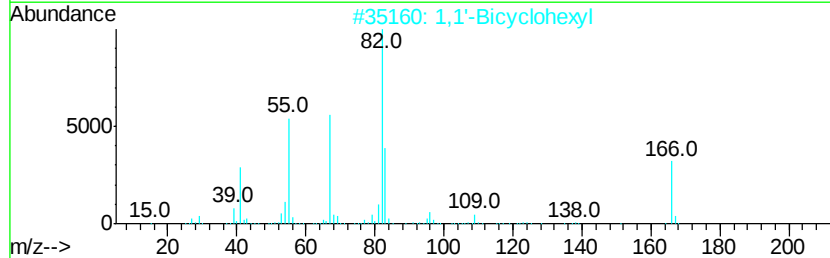
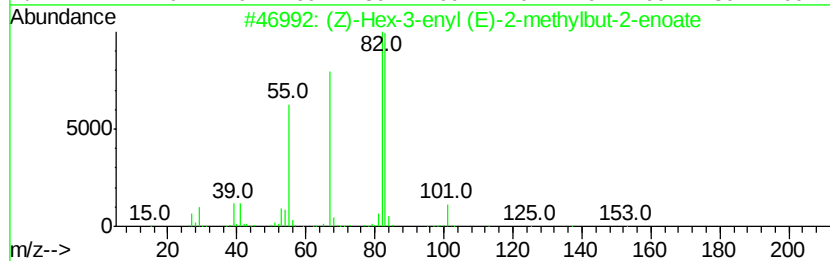
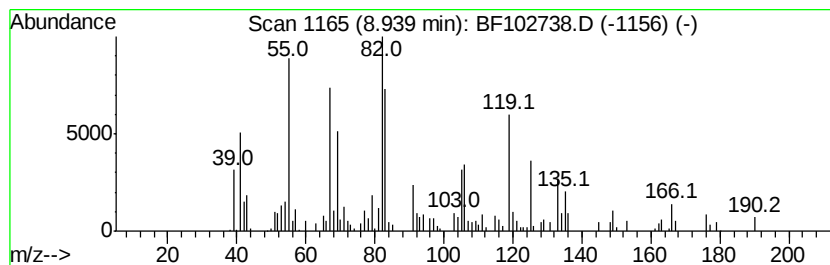
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown8.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	3.48 ng	291087	Napthalene-d8	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Z)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	1000373-73-0	47
2			1,1'-Bicyclohexyl	166	C12H22	000092-51-3	43
3			Succinic acid, di(trans-hex-3-en...	282	C16H26O4	1000353-43-7	43
4			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	35
5			Fumaric acid, decyl trans-hex-3-...	338	C20H34O4	1000348-89-0	35



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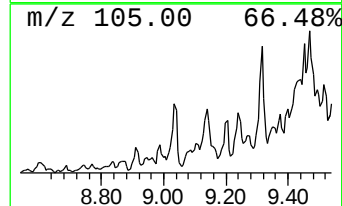
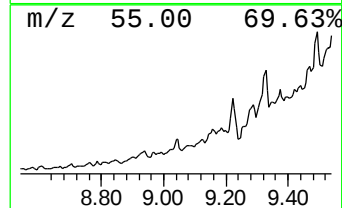
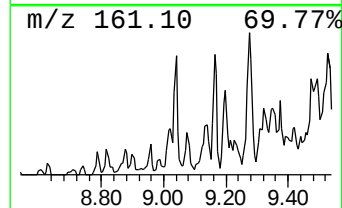
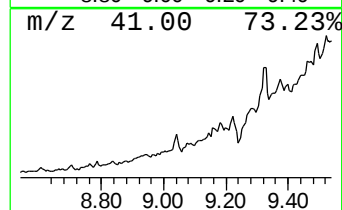
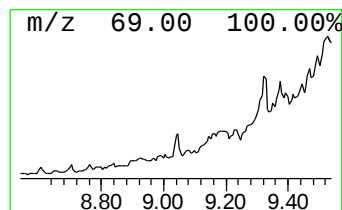
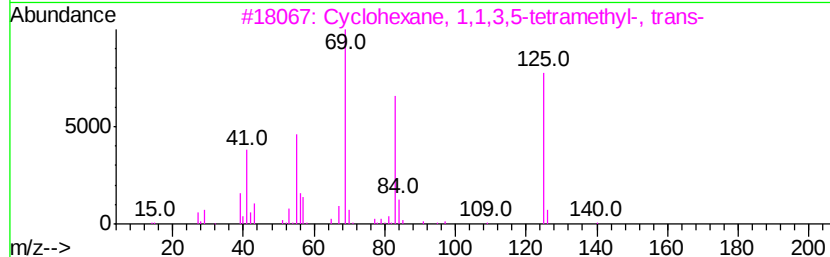
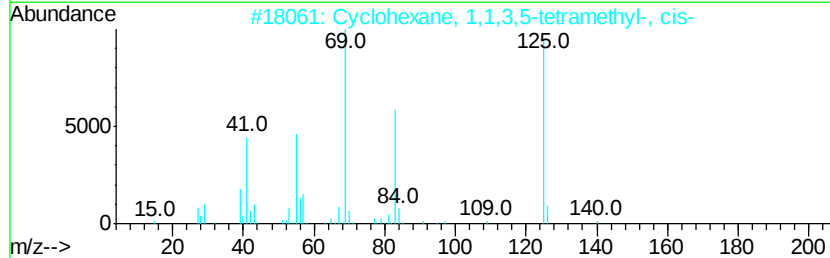
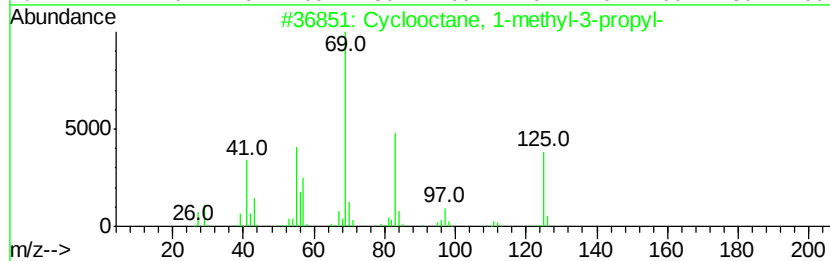
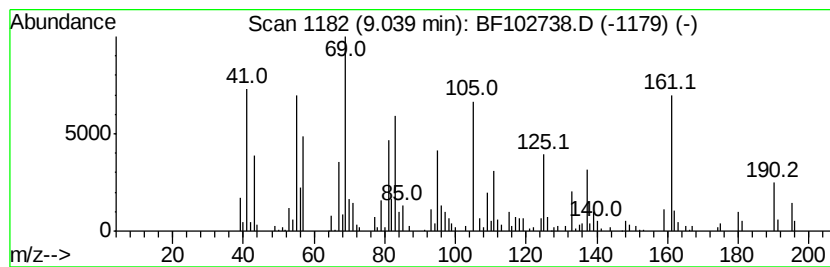
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.04 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	2.24 ng	187547	Naphthalene-d8	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	35
2		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	35
3		Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-31-8	35
4		3-Heptene, 2,2,3,5,6-pentamethyl-	168	C12H24	116164-06-8	32
5		1,5-Heptadiene, 2,3,6-trimethyl-	138	C10H18	033501-88-1	22



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102738.D
Acq On : 5 Feb 2018 15:23
Operator : SJ/JU
Sample : J1437-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-148-20

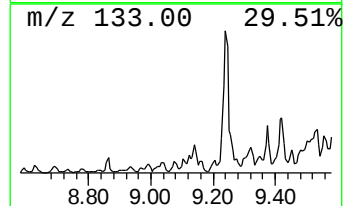
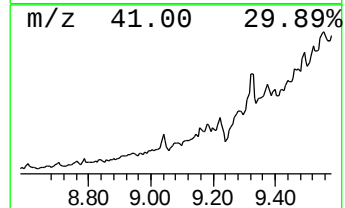
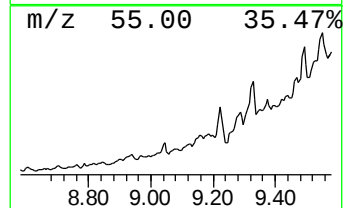
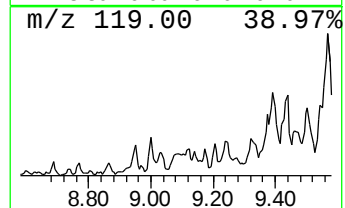
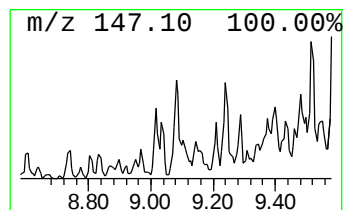
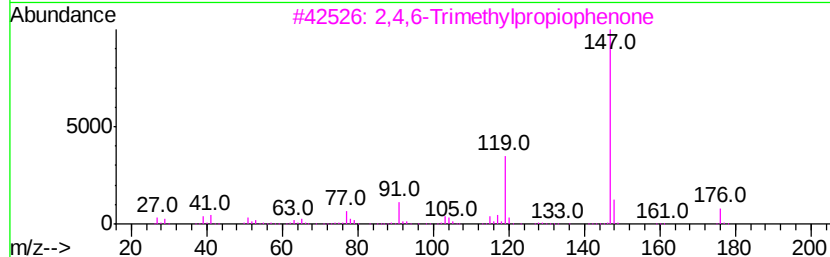
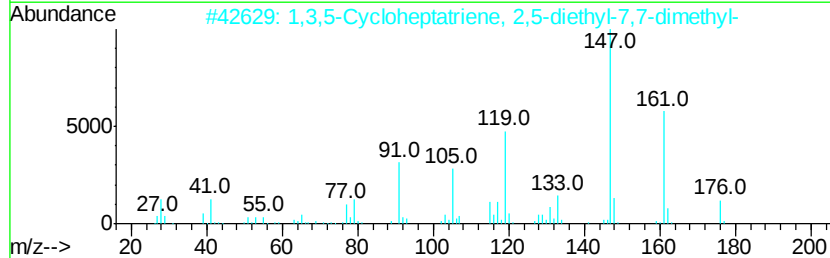
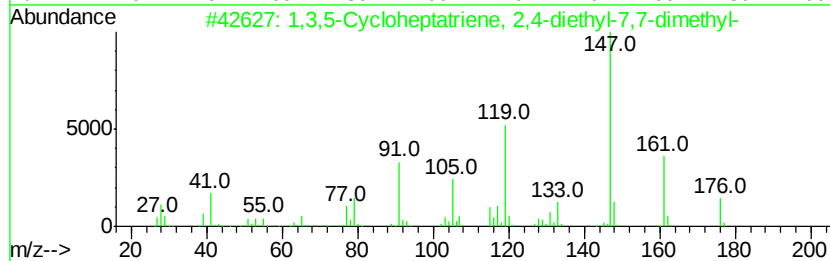
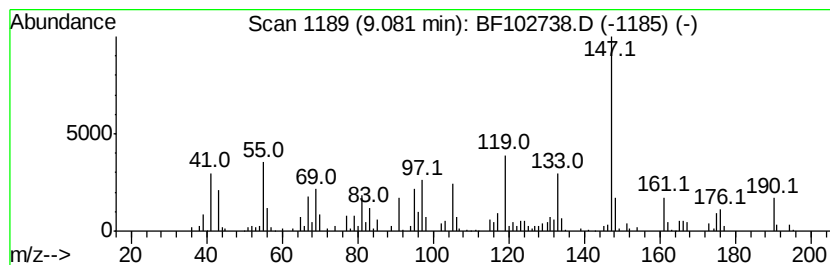
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.08 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.08	3.26 ng	167263	Acenaphthene-d10	9.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Cycloheptatriene, 2,4-diet...	176	C13H20	1000156-99-6	49
2		1,3,5-Cycloheptatriene, 2,5-diet...	176	C13H20	1000156-99-5	47
3		2,4,6-Trimethylpropiofenone	176	C12H16O	002040-15-5	46
4		Benzene, 1,2-diethyl-3,4-dimethyl-	162	C12H18	054410-75-2	46
5		Benzimidazole, 2-amino-1-methyl-	147	C8H9N3	001622-57-7	43



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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Acq On : 5 Feb 2018 15:23
Operator : SJ/JU
Sample : J1437-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

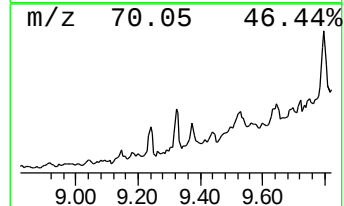
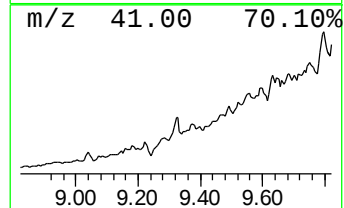
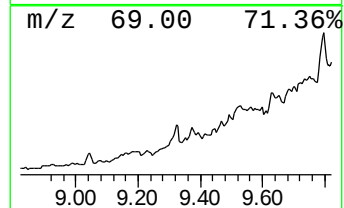
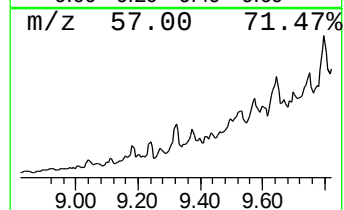
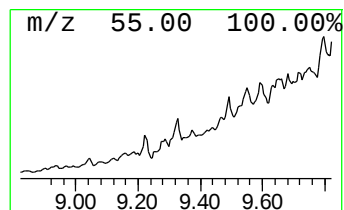
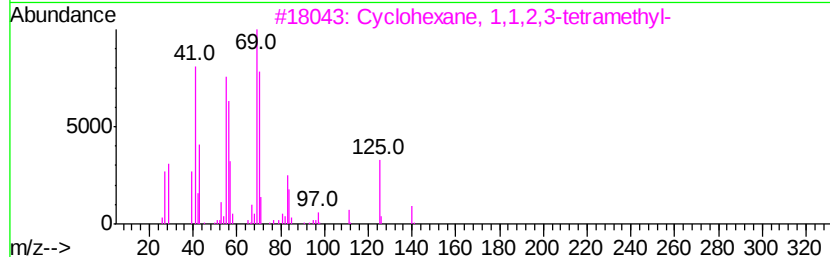
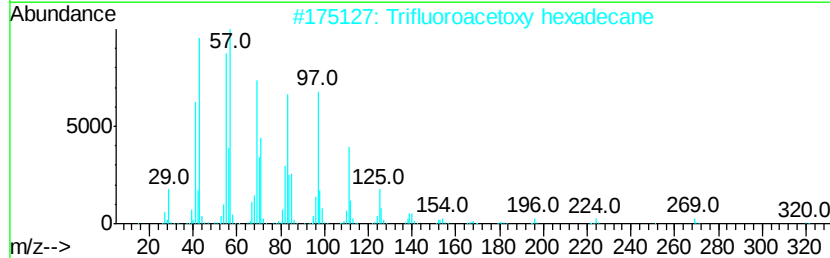
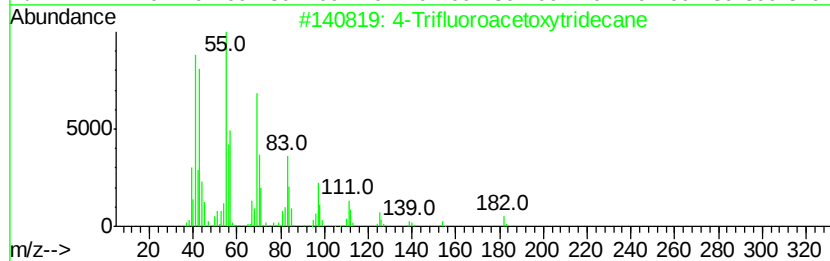
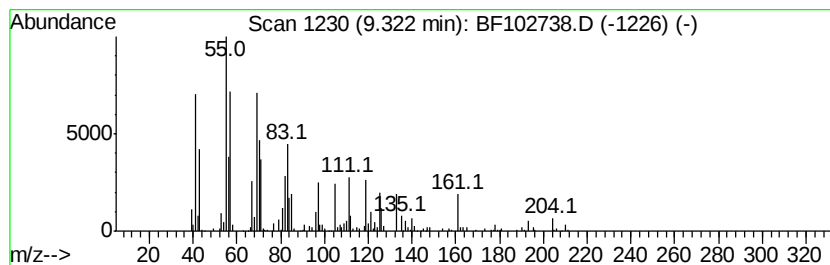
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ClientSampleId :
RO-148-20

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4-Trifluoroacetoxytridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.32	11.01 ng	565266	Acenaphthene-d10		9.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Trifluoroacetoxytridecane	296	C15H27F3O2	1000245-47-3	50
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	49
3		Cvclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	43
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	43
5		1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	43



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102738.D
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Operator : SJ/JU
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Misc :
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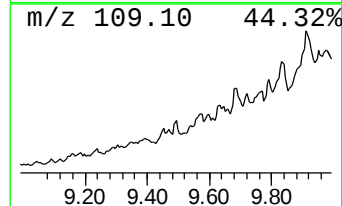
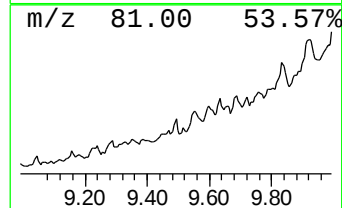
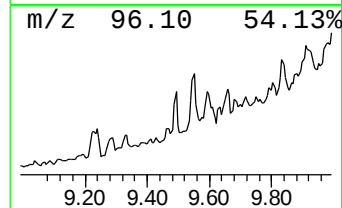
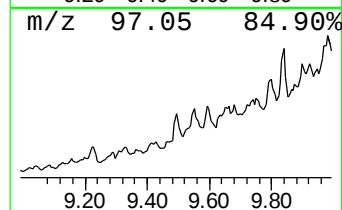
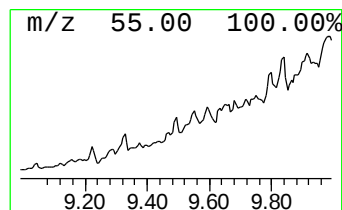
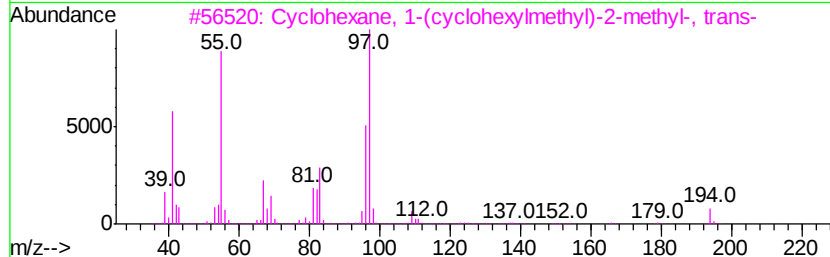
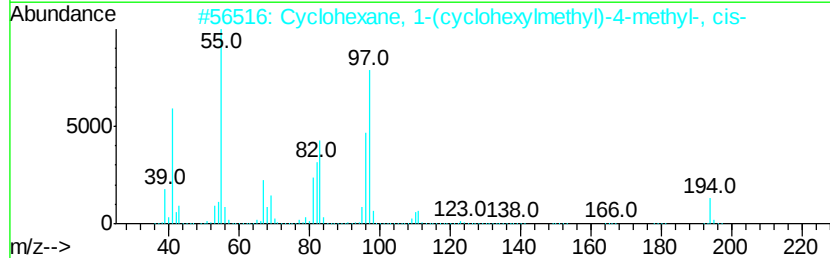
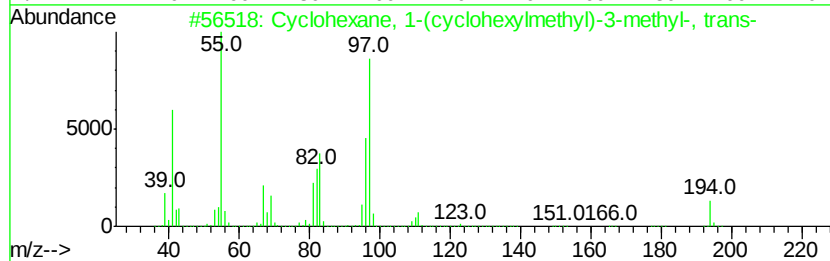
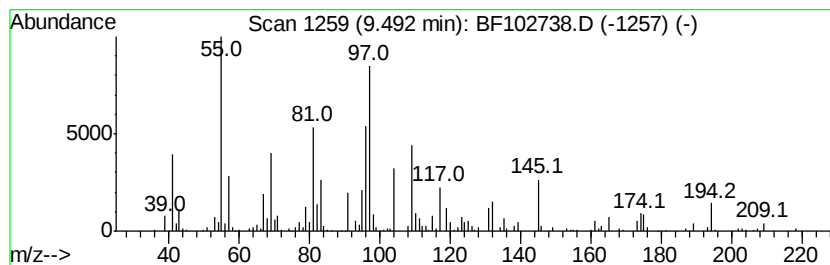
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.49 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.49	4.34 ng	222620	Acenaphthene-d10	9.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-95-9	43
2			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-97-1	43
3			Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-94-8	43
4			Cyclohexane, 1-isopropyl-1-methyl-	140	C10H20	016580-26-0	35
5			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	35



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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Operator : SJ/JU
Sample : J1437-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

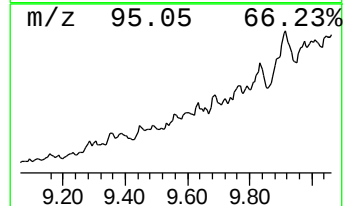
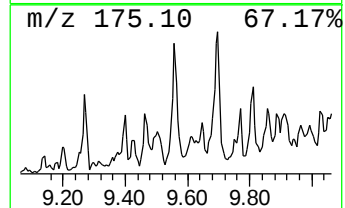
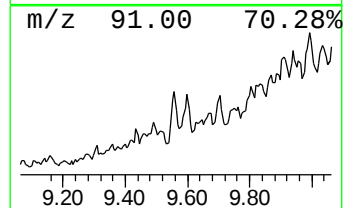
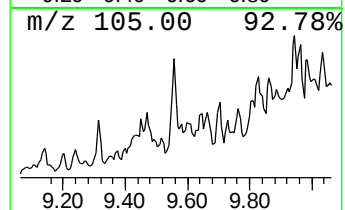
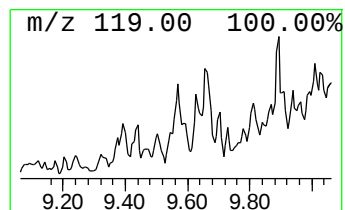
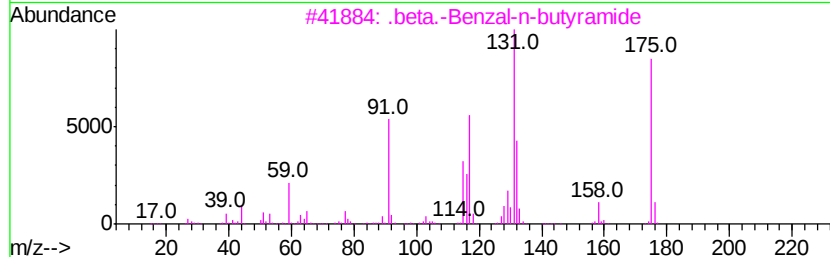
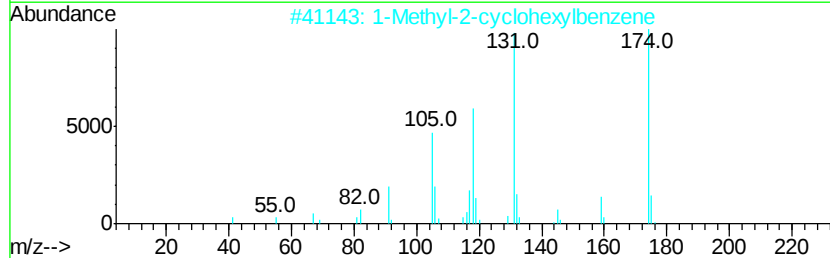
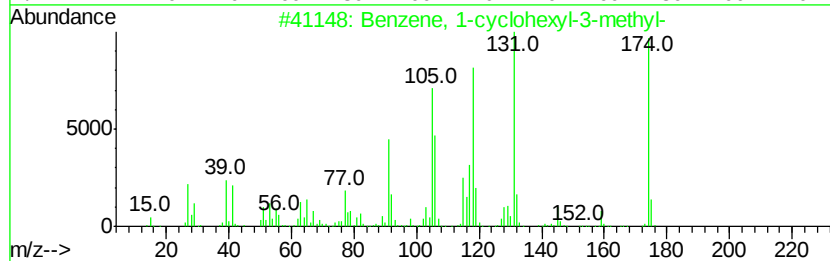
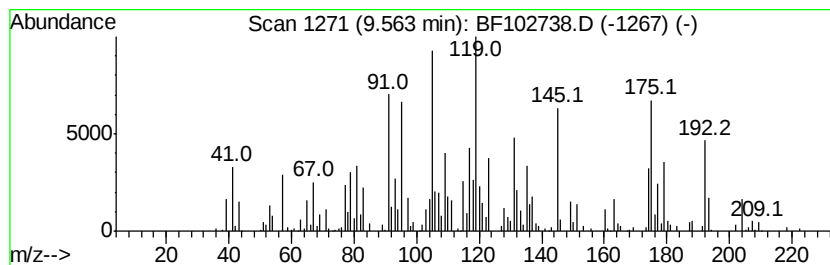
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 1-cyclohexyl-3-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.56	12.50 ng	641439	Acenaphthene-d10	9.93		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 1-cvclohexyl-3-methyl-	174	C13H18	004575-46-6	60
2		1-Methyl-2-cvclohexylbenzene	174	C13H18	004501-35-3	49
3		.beta.-Benzal-n-butvramide	175	C11H13NO	007236-47-7	41
4		2H-1-Benzopyran-2-one 3,4-dimethyl-	174	C11H10O2	004281-39-4	38
5		4-Pyrrolidinobenzaldehyde	175	C11H13NO	051980-54-2	35



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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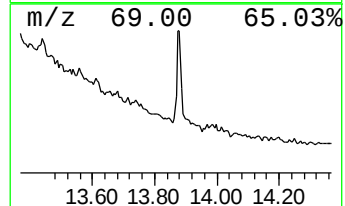
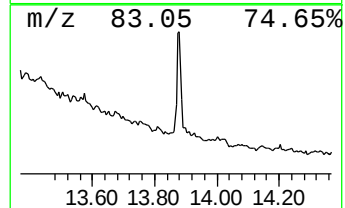
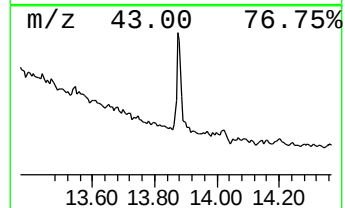
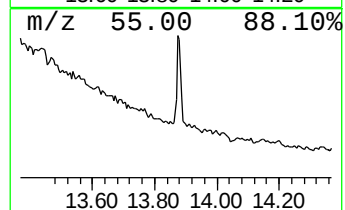
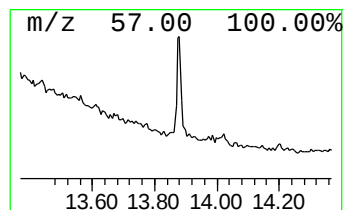
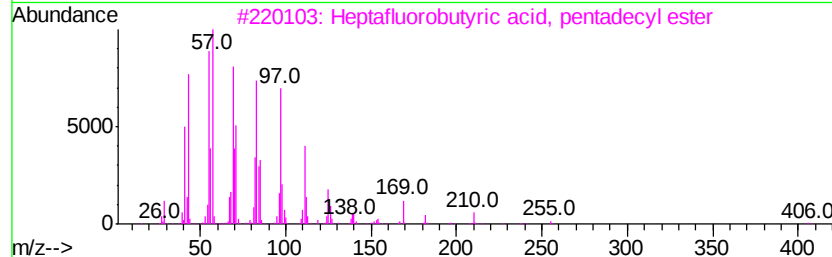
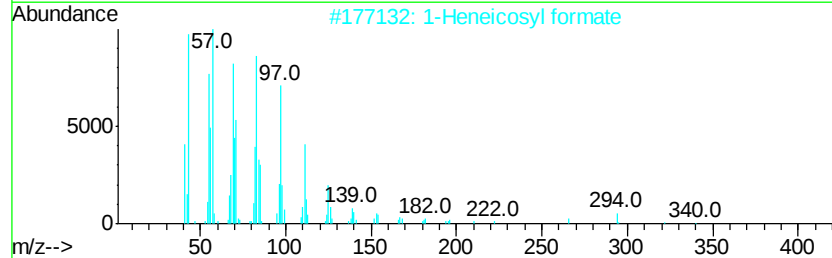
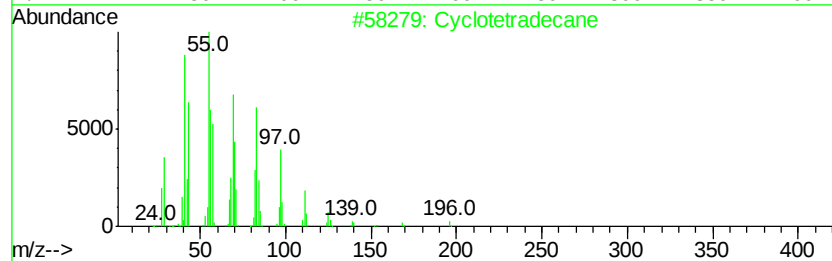
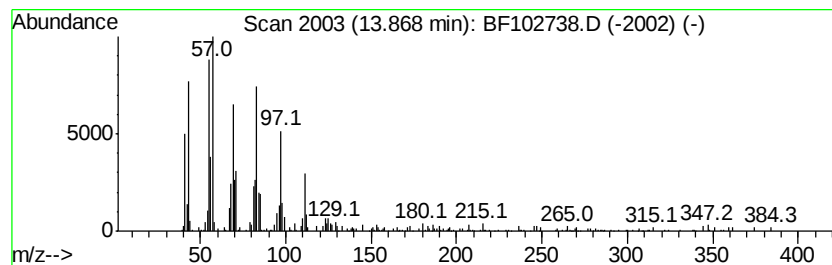
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.87	17.85 ng	843389	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	Heptafluorobutyric acid, pentadecyl ...	424	C19H31F7O2	959261-23-5	94
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
 Data File : BF102738.D
 Acq On : 5 Feb 2018 15:23
 Operator : SJ/JU
 Sample : J1437-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.17	10.4	ng	659410	1	6.88	1272920	20.0
2-Pentanone, 4-hy...	5.12	3.0	ng	191192	1	6.88	1272920	20.0
unknown6.65	6.65	79.2	ng	5039190	1	6.88	1272920	20.0
Ethanol, 2-(2-eth...	6.70	2.6	ng	166580	1	6.88	1272920	20.0
unknown8.94	8.94	3.5	ng	291087	2	8.16	1671870	20.0
unknown9.04	9.04	2.2	ng	187547	2	8.16	1671870	20.0
unknown9.08	9.08	3.3	ng	167263	3	9.93	1026570	20.0
4-Trifluoroacetox...	9.32	11.0	ng	565266	3	9.93	1026570	20.0
unknown9.49	9.49	4.3	ng	222620	3	9.93	1026570	20.0
Benzene, 1-cycloh...	9.56	12.5	ng	641439	3	9.93	1026570	20.0
Cyclotetradecane	13.87	17.9	ng	843389	5	14.04	944754	20.0