

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061316\
 Data File : BF087977.D
 Acq On : 13 Jun 2016 12:13
 Operator : UM/SJ
 Sample : H3438-04
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-11-COMP

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-BF060716.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	1.735	10	13	21	rVV	139614	310663	10.99%	1.133%
2	1.861	21	24	35	rVB	1162884	2194165	77.61%	8.003%
3	3.050	127	128	140	rBV2	15238	46987	1.66%	0.171%
4	4.959	293	295	304	rVB	109662	148118	5.24%	0.540%
5	5.382	329	332	335	rBV	1885129	1981086	70.07%	7.226%
6	6.433	421	424	426	rBV	2085182	2456368	86.88%	8.960%
7	6.559	432	435	437	rBV	2299286	2228988	78.84%	8.130%
8	6.787	453	455	458	rBV	727430	666320	23.57%	2.430%
9	6.947	466	469	471	rBV	2023395	1765351	62.44%	6.439%
10	7.359	502	505	507	rBV	1530074	1566576	55.41%	5.714%
11	8.079	565	568	570	rBV	1155387	978170	34.60%	3.568%
12	9.165	660	663	665	rBV	2372067	2827276	100.00%	10.313%
13	9.553	695	697	699	rBV	763138	655886	23.20%	2.392%
14	9.828	719	721	724	rBV	810043	1107468	39.17%	4.040%
15	10.616	788	790	793	rBV2	1230928	1633286	57.77%	5.957%
16	10.742	799	801	805	rBV	40513	53310	1.89%	0.194%
17	11.188	839	840	842	rBV	44816	50634	1.79%	0.185%
18	11.314	849	851	853	rBV	1309245	1149272	40.65%	4.192%
19	11.622	876	878	880	rBV	41206	43713	1.55%	0.159%
20	11.851	896	898	900	rBV	57331	59878	2.12%	0.218%
21	12.525	955	957	959	rBV	47132	61765	2.18%	0.225%
22	12.731	973	975	978	rVV2	401404	385777	13.64%	1.407%
23	12.811	978	982	984	rVB2	42877	57589	2.04%	0.210%
24	12.902	987	990	993	rVV	2301320	2279216	80.62%	8.314%
25	13.440	1034	1037	1039	rBV	199445	219260	7.76%	0.800%
26	13.485	1039	1041	1044	rVB2	25446	49867	1.76%	0.182%
27	13.817	1067	1070	1078	rBV3	29813	89630	3.17%	0.327%
28	13.942	1079	1081	1084	rBV	1007565	1043698	36.92%	3.807%
29	14.125	1095	1097	1099	rBV	47302	42970	1.52%	0.157%
30	14.434	1122	1124	1125	rBV	32082	36168	1.28%	0.132%
31	14.708	1145	1148	1152	rBV2	77521	148199	5.24%	0.541%
32	14.948	1167	1169	1173	rVB	20913	41316	1.46%	0.151%
33	15.040	1175	1177	1180	rVB	31433	47138	1.67%	0.172%
34	15.360	1202	1205	1207	rBV	568174	765716	27.08%	2.793%

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Instrument :
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ClientSampleId :
SB-11-COMP

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.405	1207	1209	1212	rVB	30496	45935	1.62%	0.168%
36	15.714	1229	1236	1242	rBV	33830	140991	4.99%	0.514%
37	15.805	1242	1244	1249	rVB	24494	36939	1.31%	0.135%

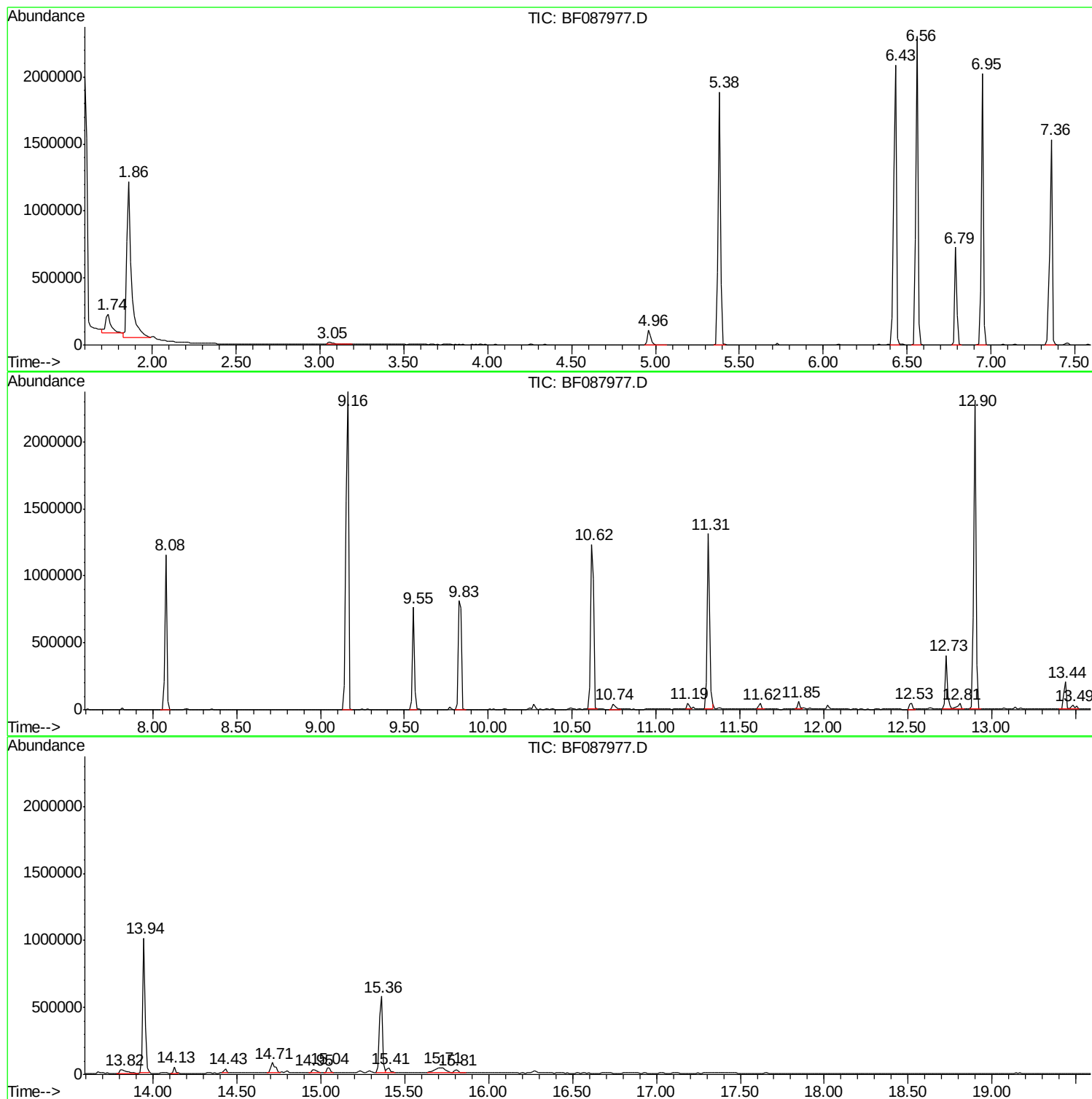
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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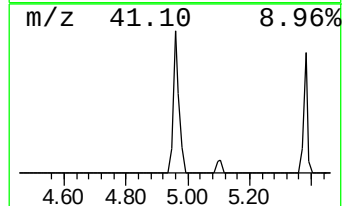
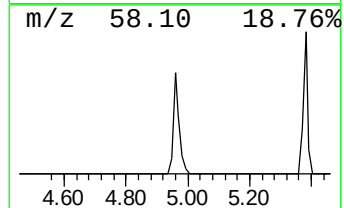
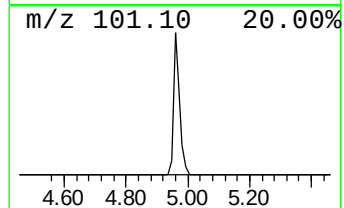
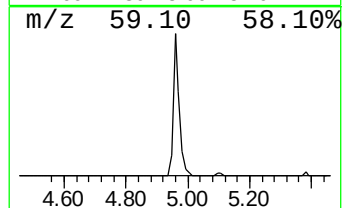
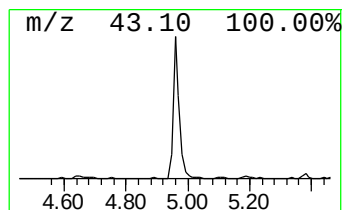
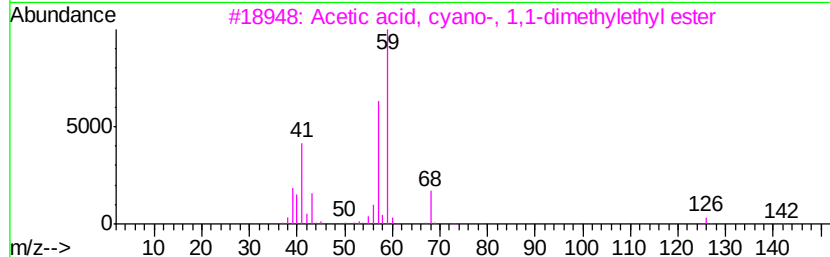
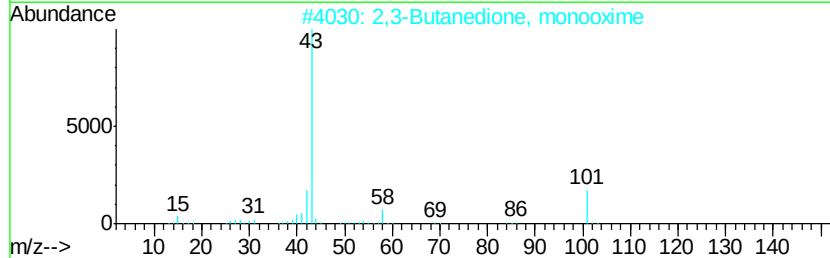
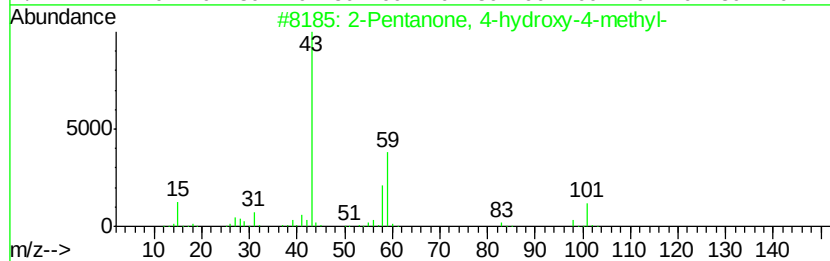
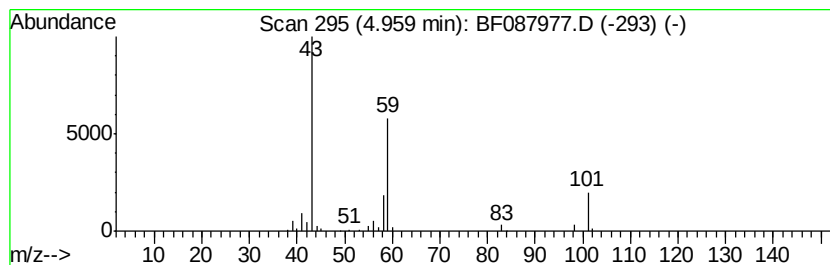
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	4.45 ng	148118	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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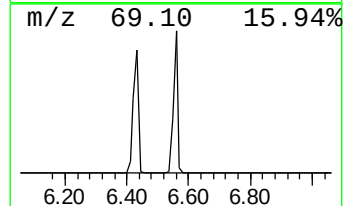
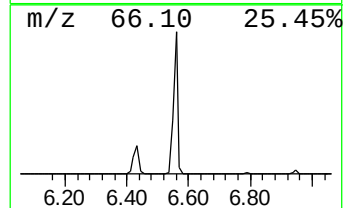
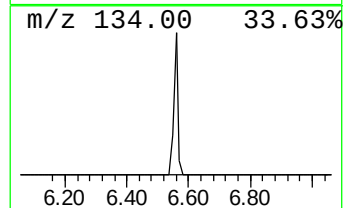
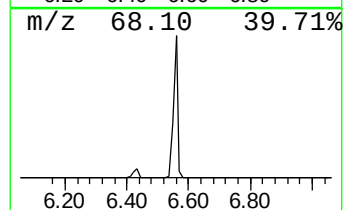
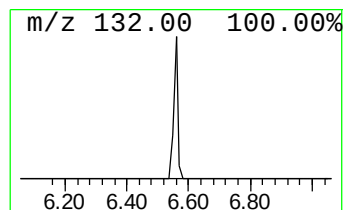
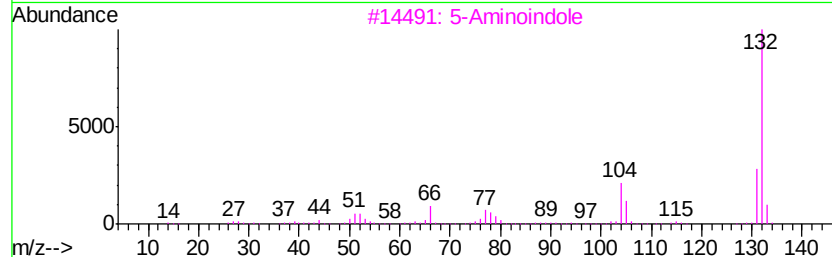
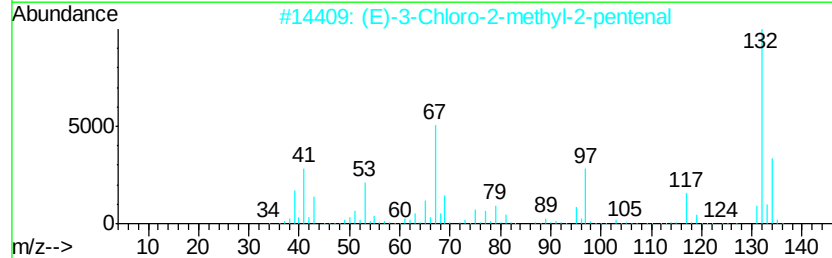
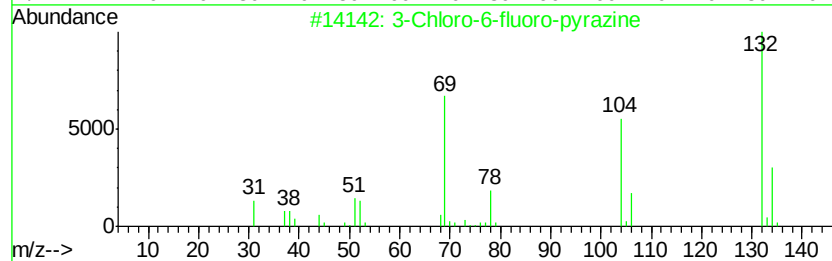
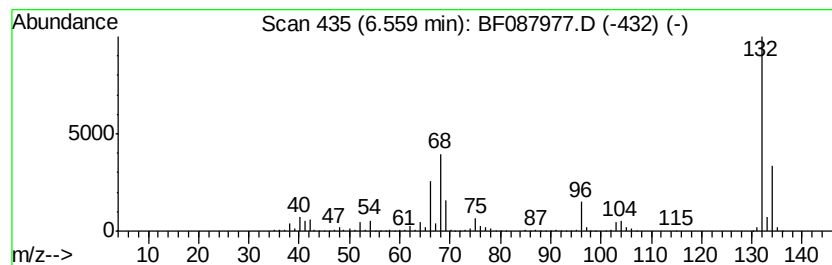
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	66.90 ng	2228990	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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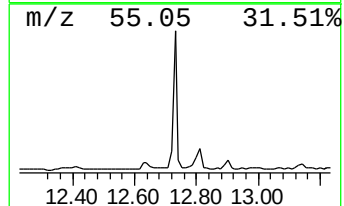
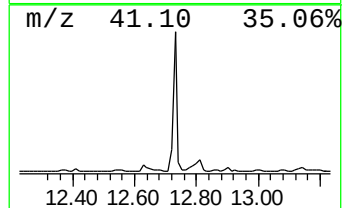
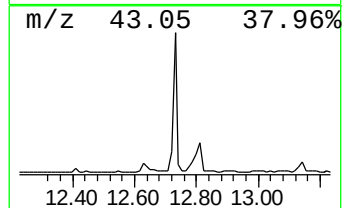
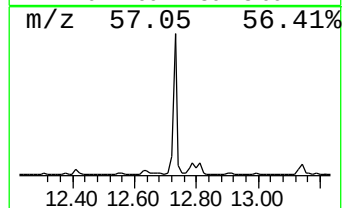
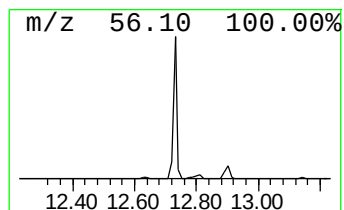
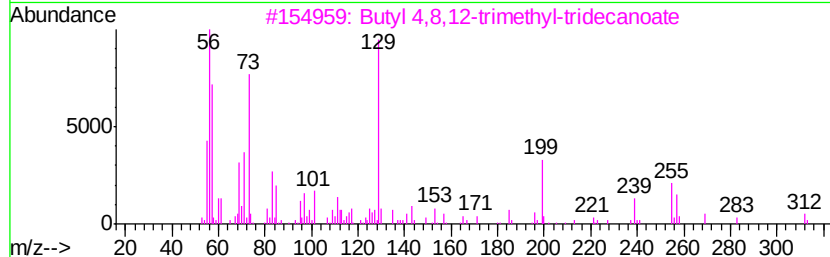
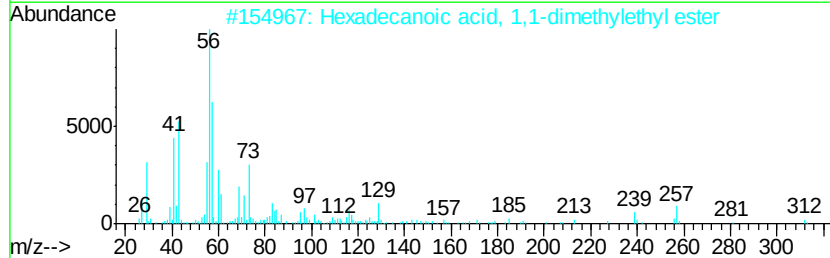
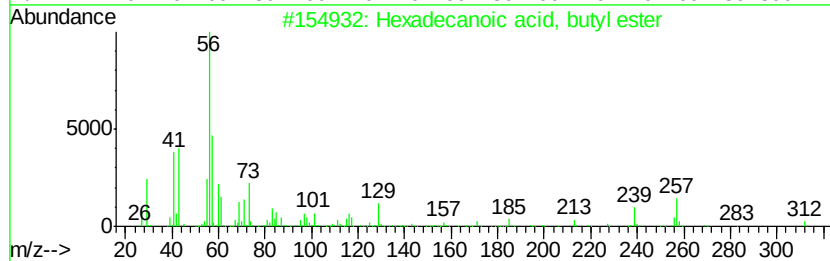
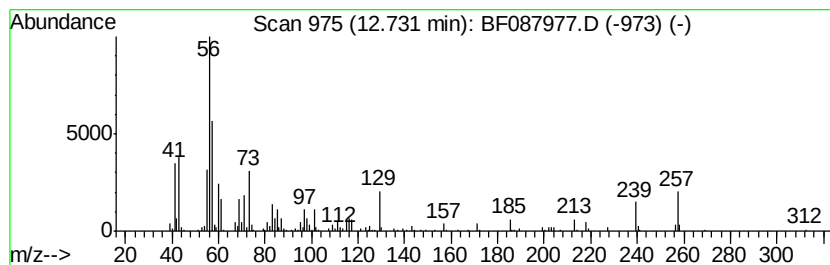
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.73	7.39 ng	385777	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	35



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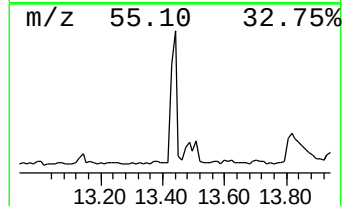
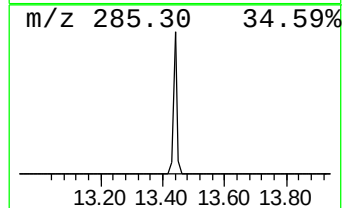
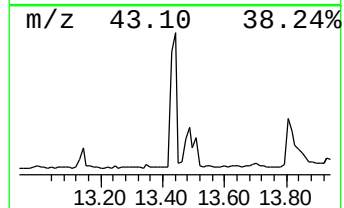
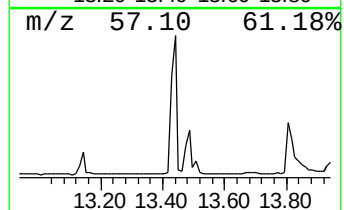
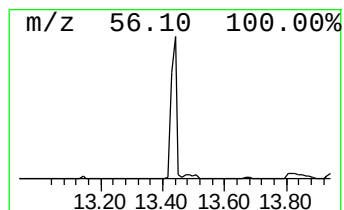
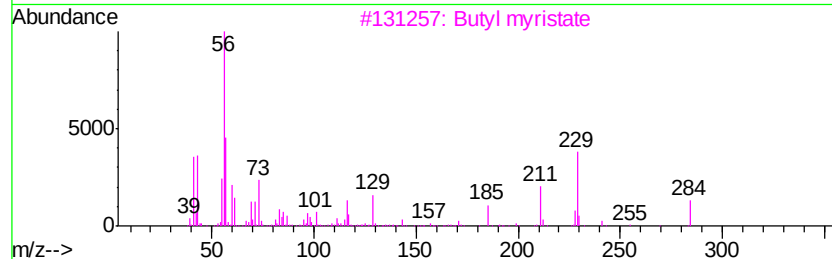
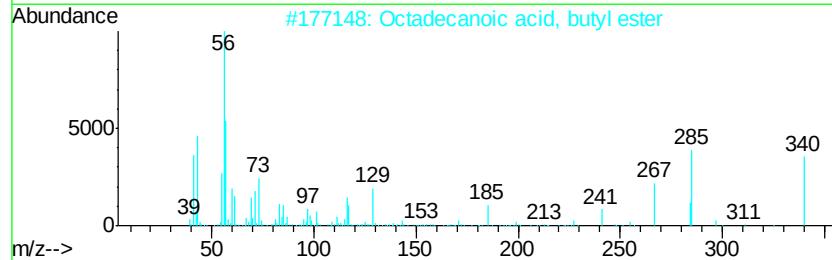
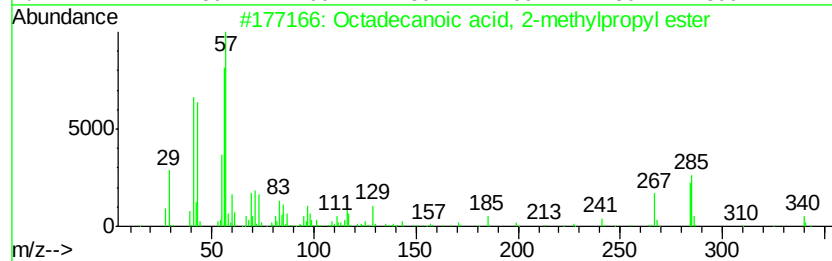
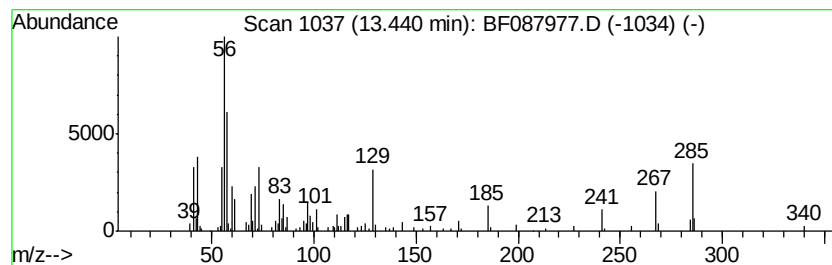
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid, 2-methyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	4.20 ng	219260	Chrysene-d12	13.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	80
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	49
3		Butyl myristate	284	C18H36O2	000110-36-1	47
4		Nipecotic acid	129	C6H11NO2	000498-95-3	43
5		Cyclohexanamine	99	C6H13N	000108-91-8	30



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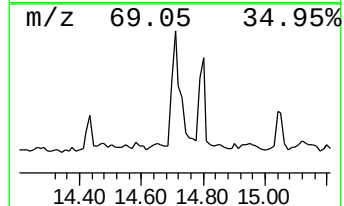
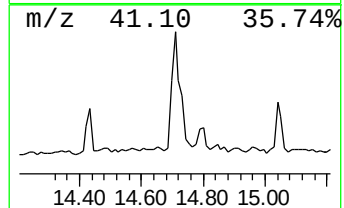
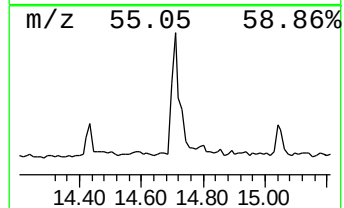
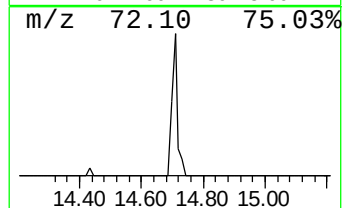
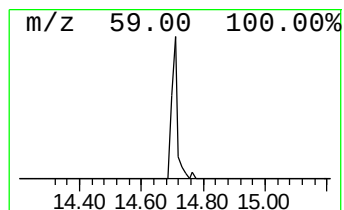
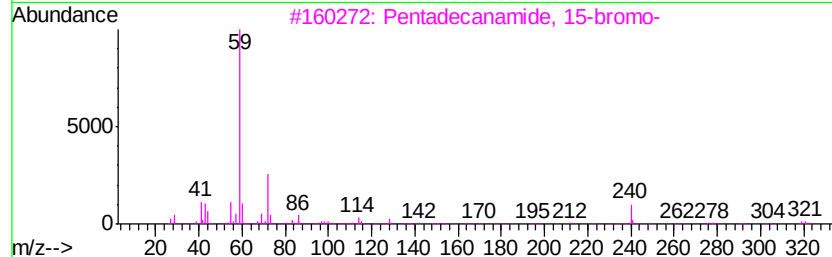
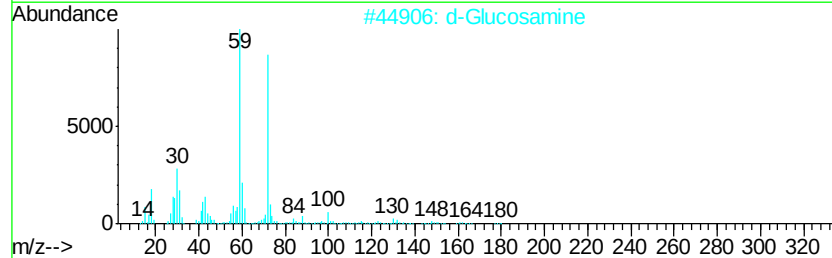
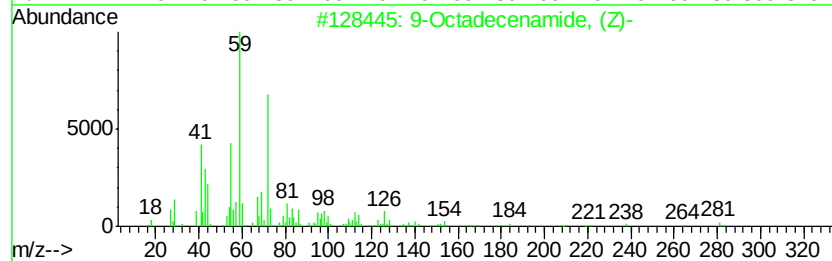
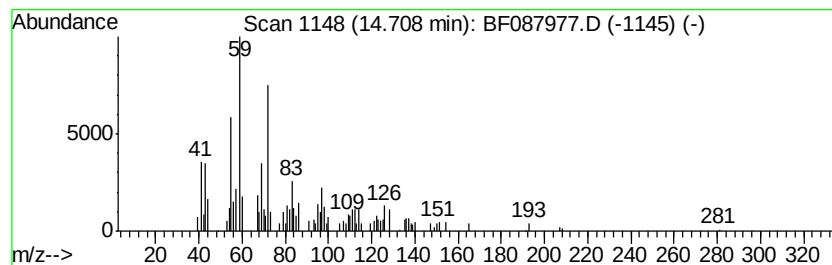
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.87 ng	148199	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		d-Glucosamine	179	C6H13NO5	000090-77-7	47
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	47
4		Hexadecanamide	255	C16H33NO	000629-54-9	43
5		Tetradecanamide	227	C14H29NO	000638-58-4	43



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ClientSampleId :
SB-11-COMP

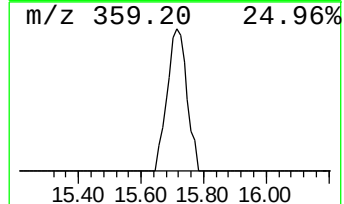
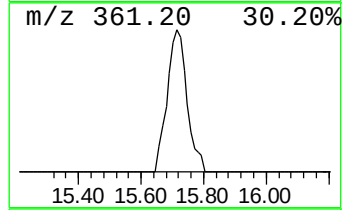
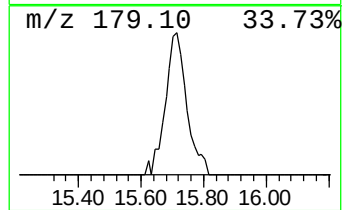
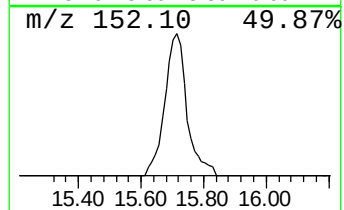
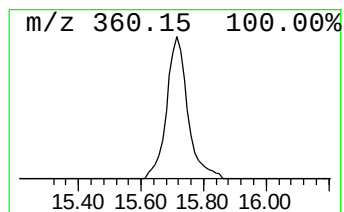
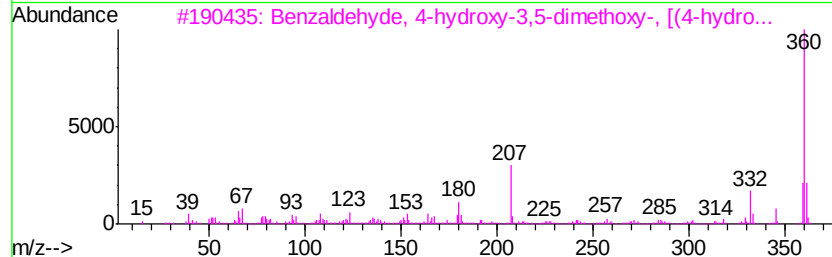
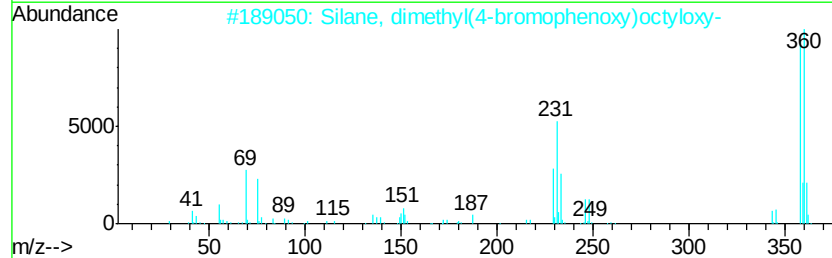
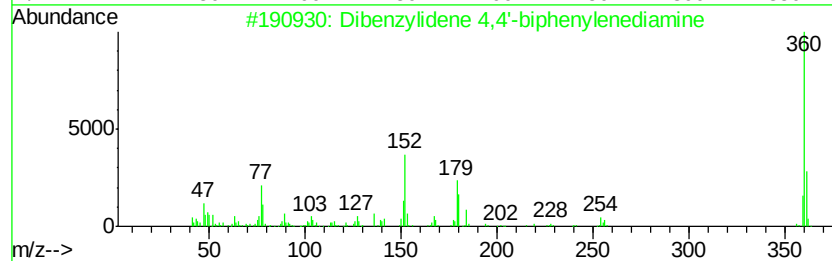
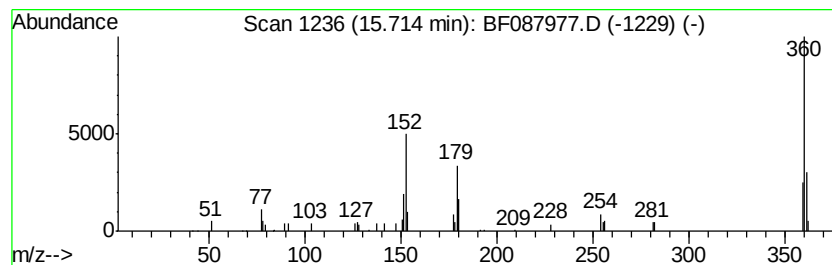
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Dibenzylidene 4,4'-biphenyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.68 ng	140991	Perylene-d12	15.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	93
2		Silane, dimethyl(4-bromophenoxy)...	358	C16H27BrO2Si	1000347-11-2	47
3		Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	46
4		Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	43
5		1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061316\
Data File : BF087977.D
Acq On : 13 Jun 2016 12:13
Operator : UM/SJ
Sample : H3438-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	4.5	ng	148118	1	6.79	666320	20.0
unknown6.56	6.56	66.9	ng	2228990	1	6.79	666320	20.0
Hexadecanoic acid...	12.73	7.4	ng	385777	5	13.94	1043700	20.0
Octadecanoic acid...	13.44	4.2	ng	219260	5	13.94	1043700	20.0
9-Octadecenamide,...	14.71	3.9	ng	148199	6	15.36	765716	20.0
Dibenzylidene 4,4...	15.71	3.7	ng	140991	6	15.36	765716	20.0