

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
 Data File : BF082434.D
 Acq On : 22 Oct 2015 6:32
 Operator : UM/IZ
 Sample : G4116-19
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AB-AC-02(0-2)

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-BF101015.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.948	242	246	255	rVB	846945	1512408	52.16%	6.391%
2	5.371	281	283	286	rBV	2282726	2336740	80.60%	9.875%
3	6.423	372	375	377	rBV	2091159	2530137	87.27%	10.692%
4	6.537	383	385	388	rBV	2173578	2303124	79.44%	9.733%
5	6.766	403	405	408	rBV	618451	609017	21.01%	2.574%
6	6.926	416	419	421	rBV	2252866	1999594	68.97%	8.450%
7	7.349	453	456	458	rBV	1145536	1548767	53.42%	6.545%
8	8.057	516	518	520	rBV	970679	799097	27.56%	3.377%
9	9.143	610	613	615	rBV	2846261	2899359	100.00%	12.253%
10	9.532	645	647	650	rBV	333810	444267	15.32%	1.877%
11	9.818	669	672	674	rBV	868177	852915	29.42%	3.604%
12	10.240	708	709	711	rVB	37293	36308	1.25%	0.153%
13	10.606	738	741	744	rBV	1345471	1276185	44.02%	5.393%
14	10.720	749	751	754	rVV	58871	66711	2.30%	0.282%
15	11.166	788	790	791	rBV	55634	46507	1.60%	0.197%
16	11.303	800	802	804	rBV	803756	719755	24.82%	3.042%
17	11.361	804	807	810	rVB3	16127	32856	1.13%	0.139%
18	11.589	825	827	830	rBV	25024	29934	1.03%	0.126%
19	11.829	846	848	851	rBV2	50097	85549	2.95%	0.362%
20	12.892	939	941	944	rBV	1794508	1637904	56.49%	6.922%
21	13.818	1020	1022	1029	rBV	76698	121652	4.20%	0.514%
22	13.978	1034	1036	1039	rBV	633597	641130	22.11%	2.709%
23	14.492	1077	1081	1089	rBV4	26119	97750	3.37%	0.413%
24	15.487	1165	1168	1171	rBV	430746	673860	23.24%	2.848%
25	15.772	1190	1193	1196	rVB	18441	33641	1.16%	0.142%
26	15.944	1205	1208	1211	rBV	24482	48675	1.68%	0.206%
27	16.310	1237	1240	1245	rVB2	20391	46686	1.61%	0.197%
28	16.961	1294	1297	1304	rVB5	29379	84659	2.92%	0.358%
29	17.738	1361	1365	1370	rVB4	17324	58190	2.01%	0.246%
30	18.161	1399	1402	1412	rVB8	14511	53174	1.83%	0.225%
31	18.378	1418	1421	1427	rVB6	12154	36828	1.27%	0.156%

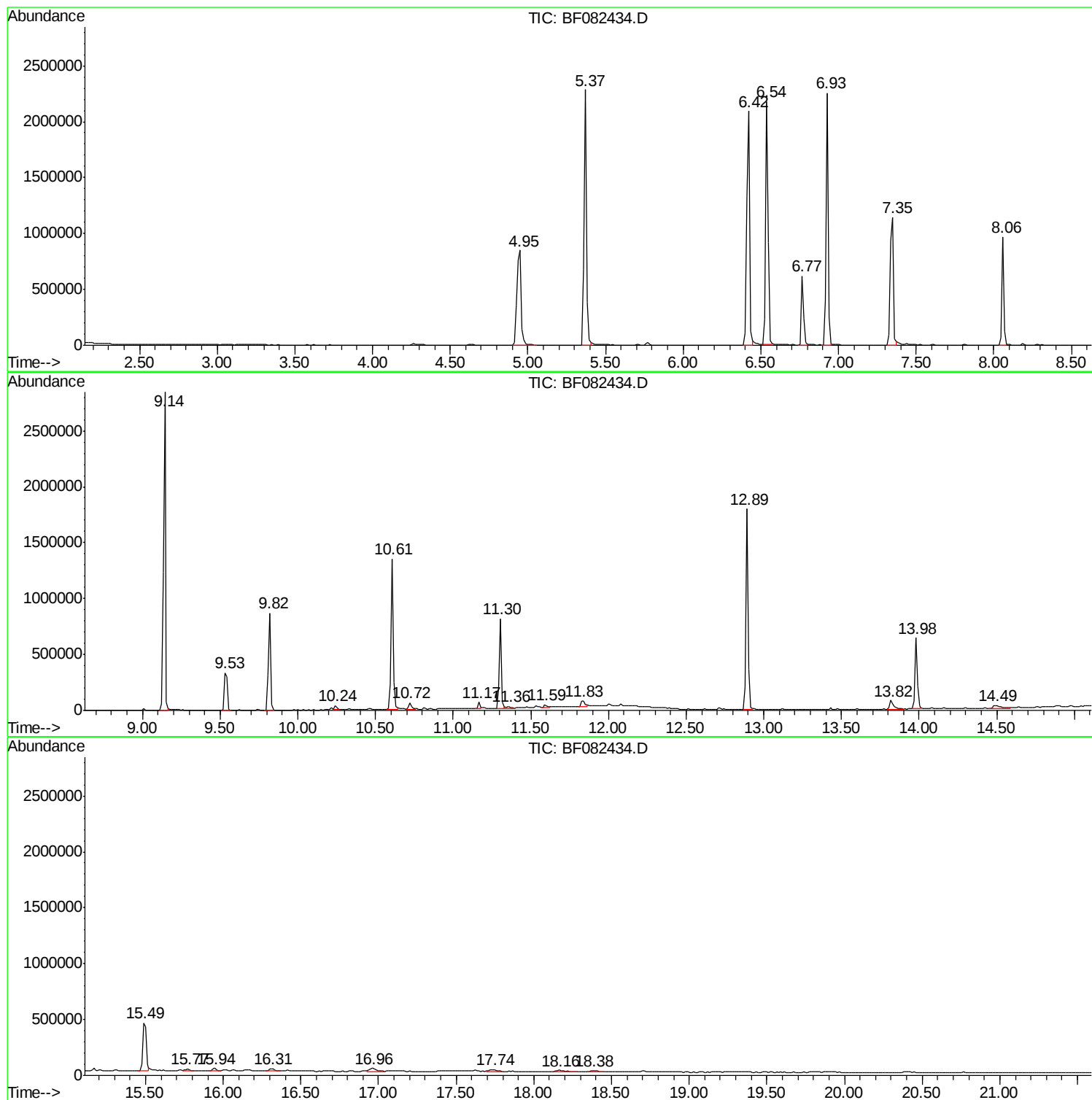
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AB-AC-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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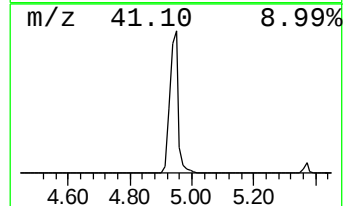
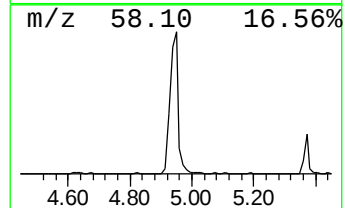
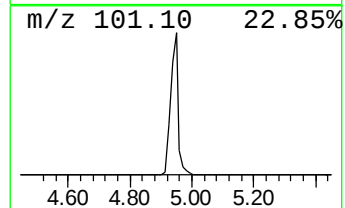
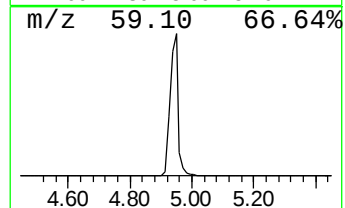
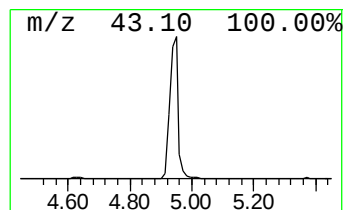
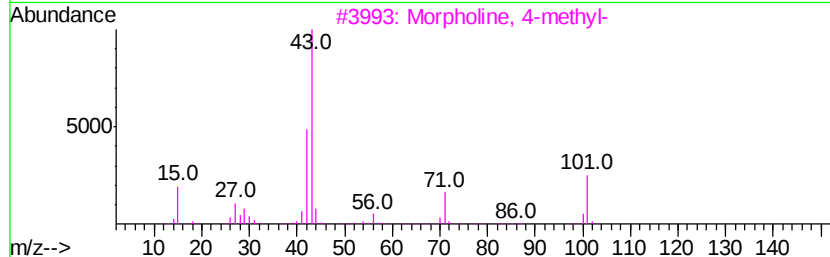
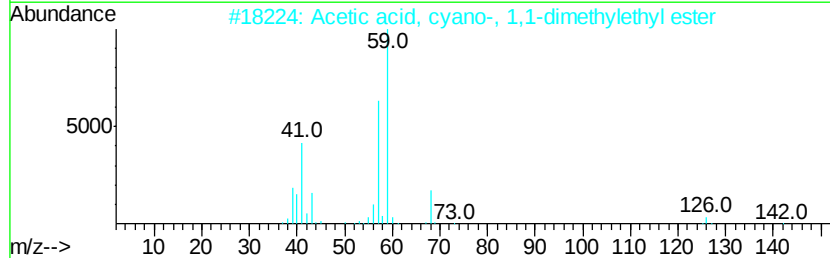
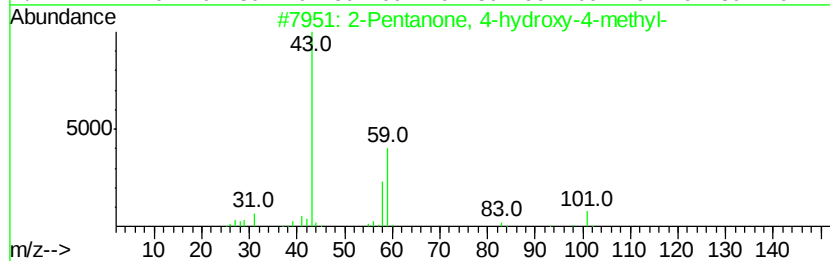
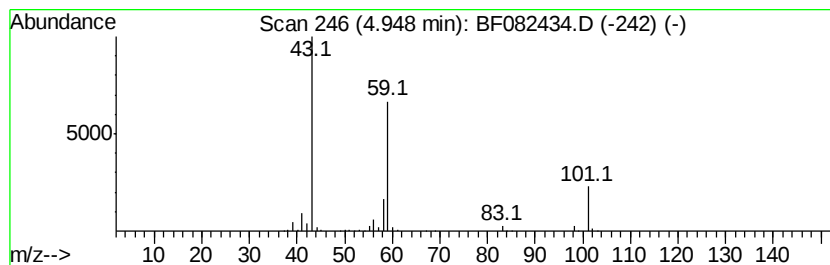
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	49.67 ng	1512410	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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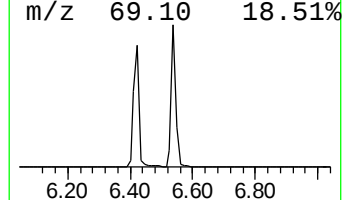
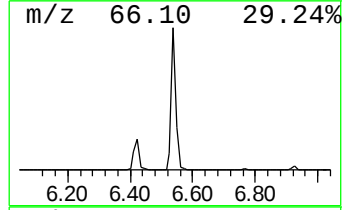
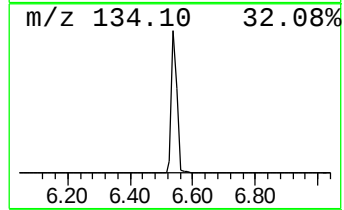
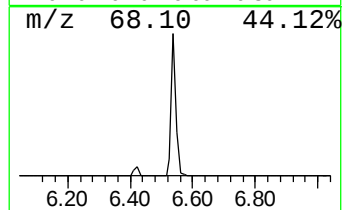
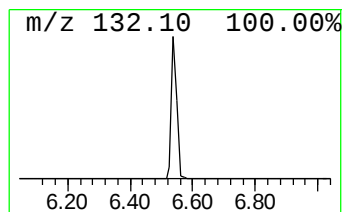
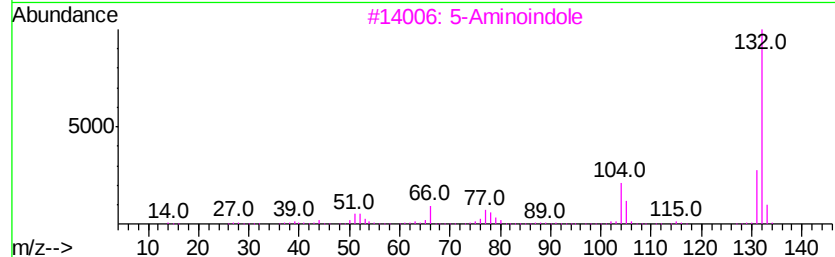
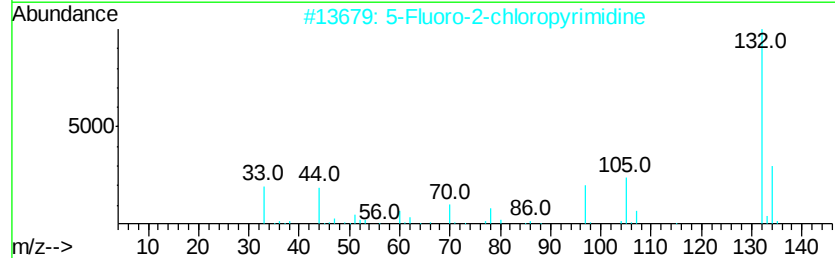
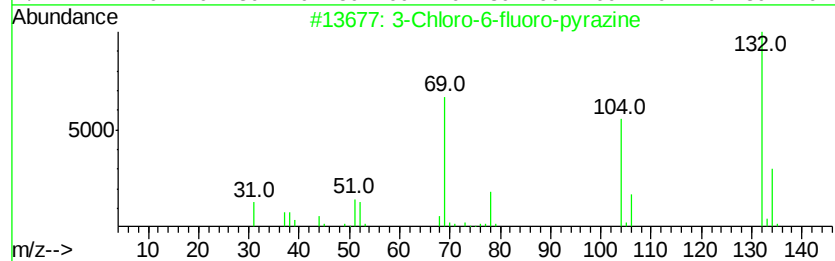
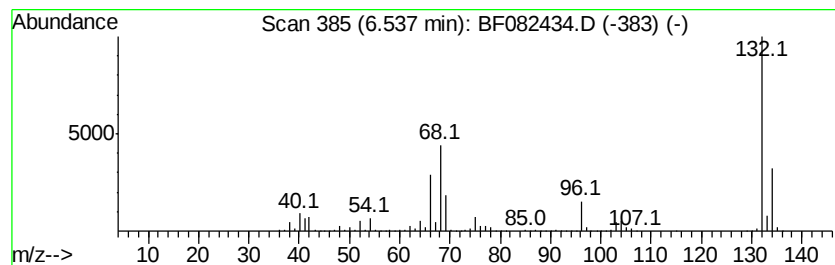
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Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	75.63 ng	2303120	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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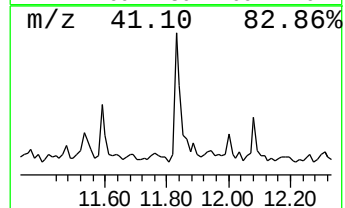
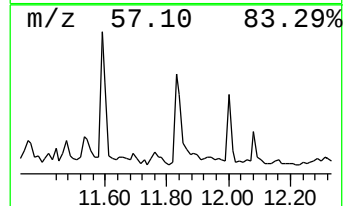
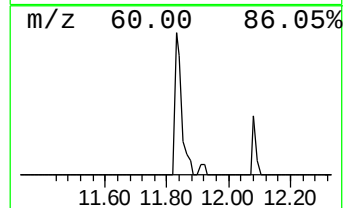
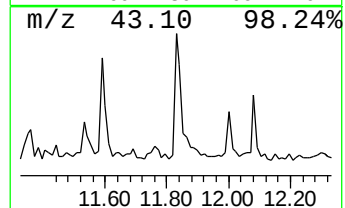
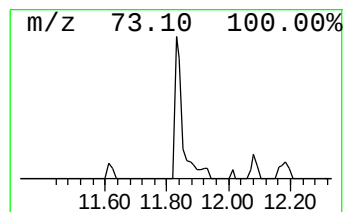
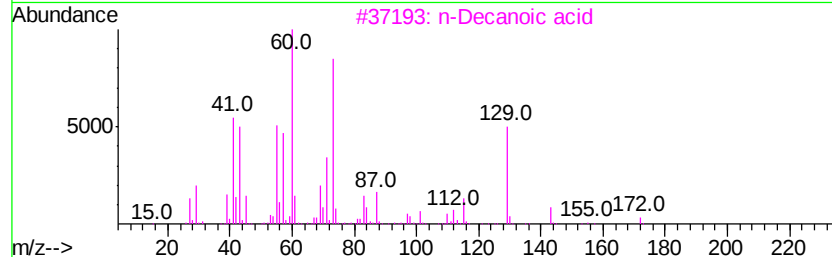
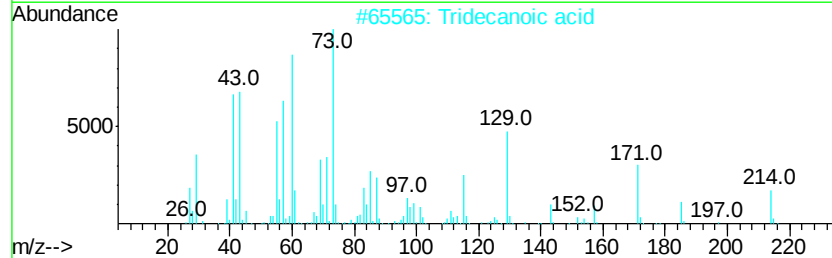
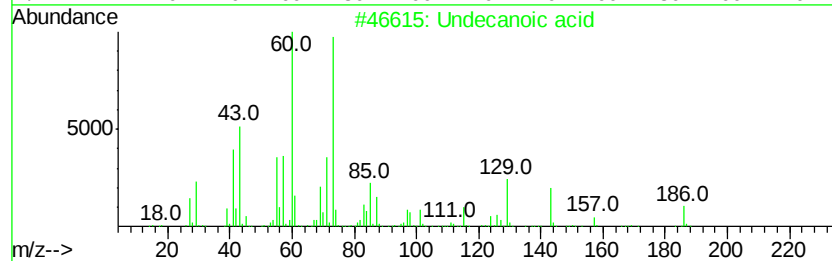
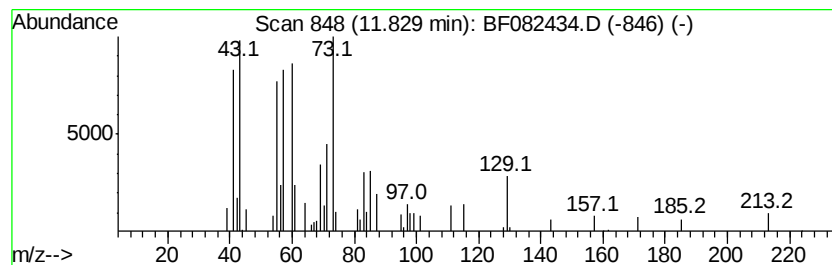
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.83	2.38 ng	85549	Phenanthrene-d10		11.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	72
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			n-Decanoic acid	172	C10H20O2	000334-48-5	59
4			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
5			1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	27



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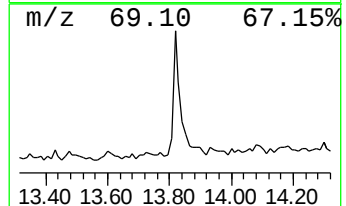
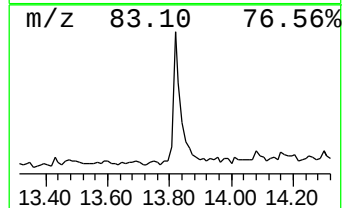
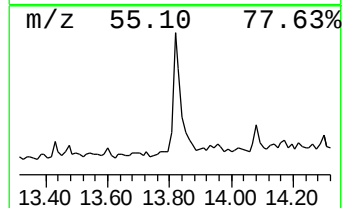
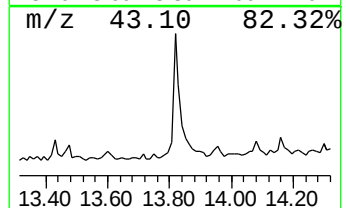
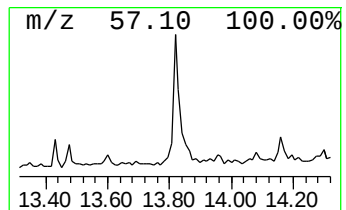
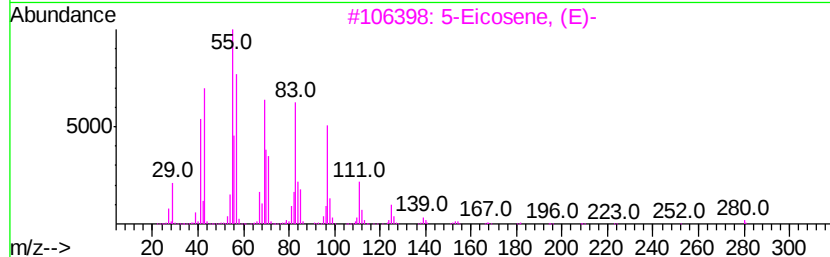
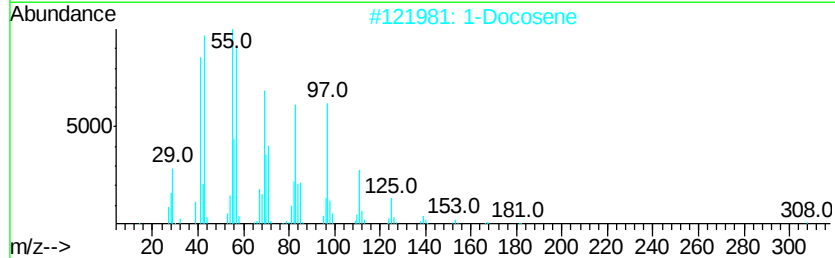
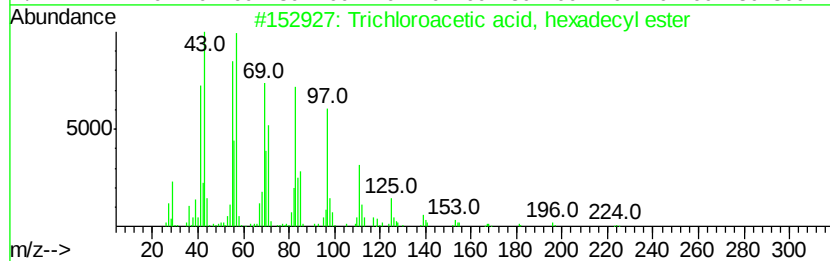
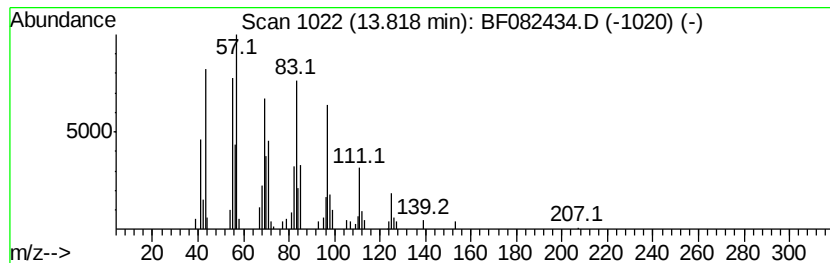
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.79 ng	121652	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4		2-Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	86



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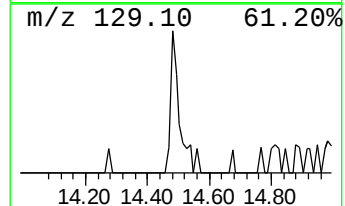
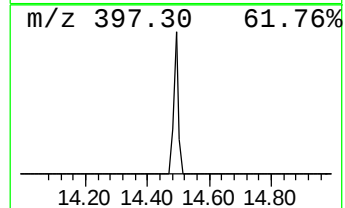
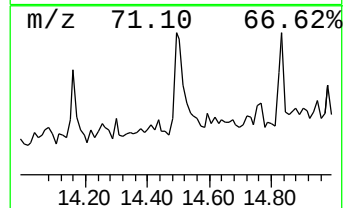
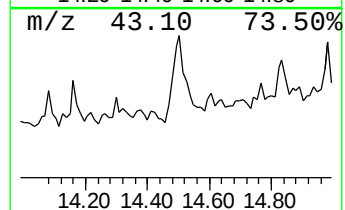
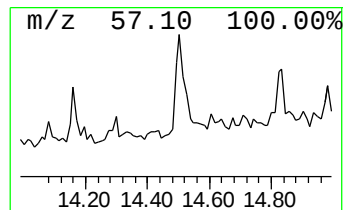
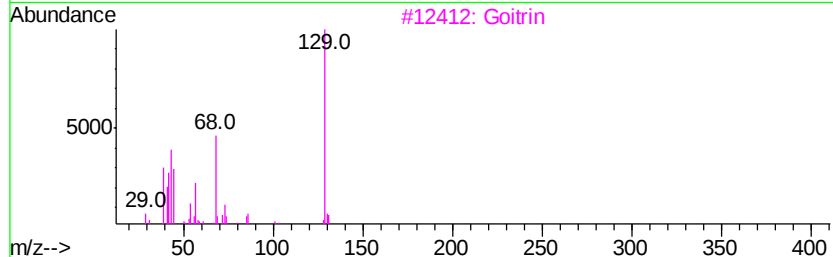
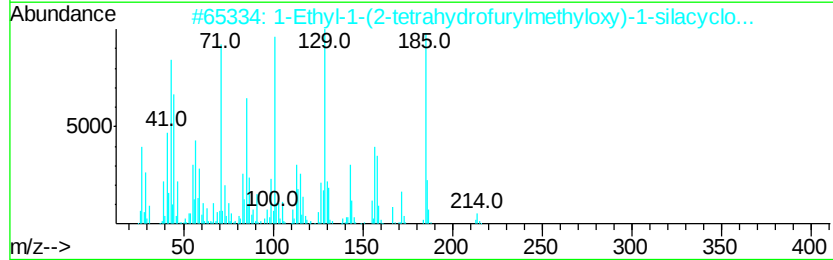
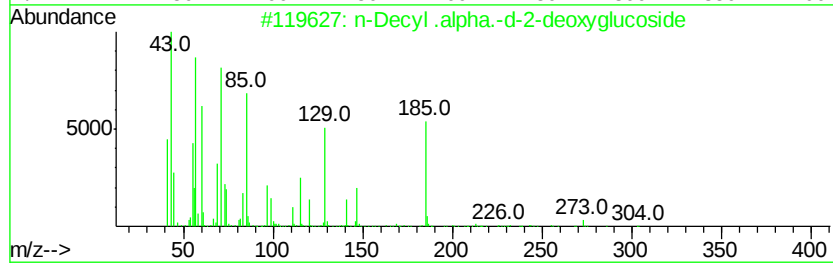
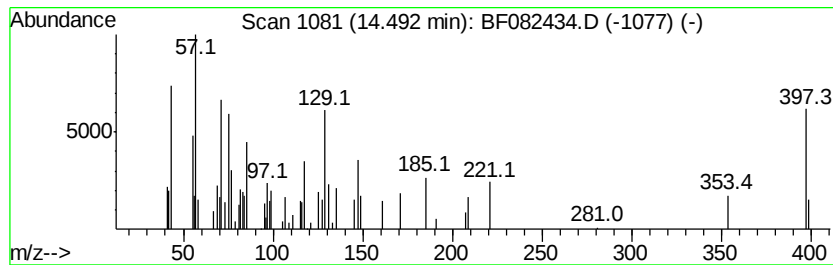
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Peak Number 6 unknown14.49 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	3.05 ng	97750	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	22
2		1-Ethyl-1-(2-tetrahydrofurylmeth...	214	C11H22O2Si	1000279-36-2	14
3		Goitrin	129	C5H7NO5	000500-12-9	9
4		1-Cyano-4-cyclohexylbenzene	185	C13H15N	027634-88-4	9
5		Pyridine, 2-hydroxy-3-chloro-	129	C5H4ClNO	013466-35-8	9



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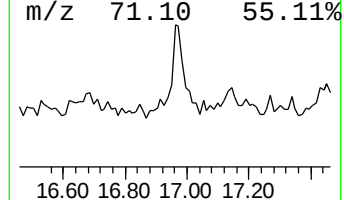
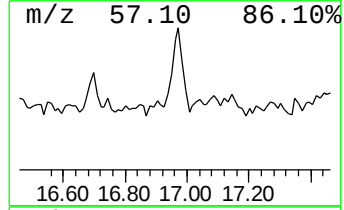
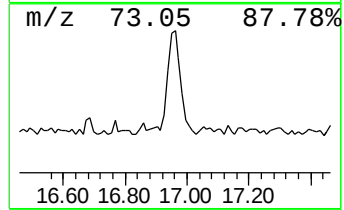
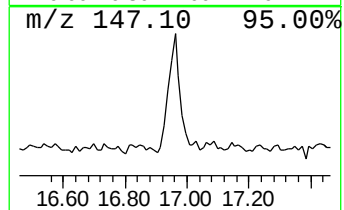
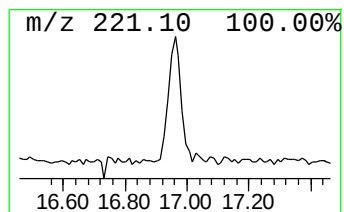
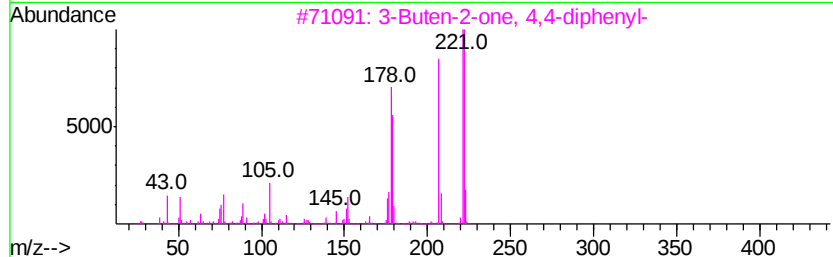
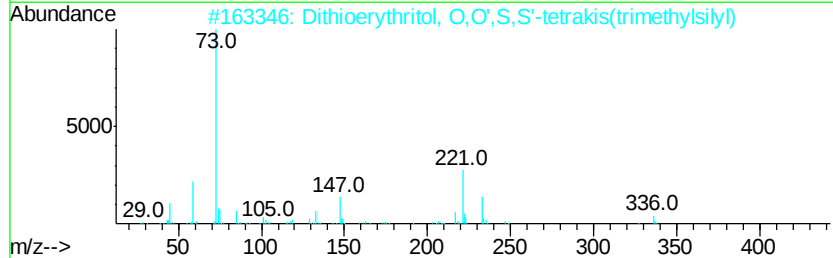
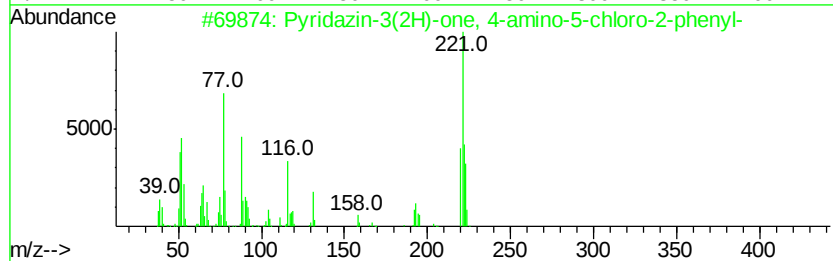
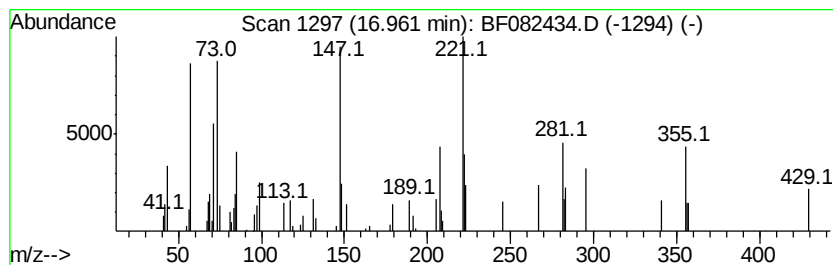
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.51 ng	84659	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridazin-3(2H)-one, 4-amino-5-c...	221	C10H8ClN3O	001698-61-9	14
2		Dithioerythritol, O,O',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	12
3		3-Buten-2-one, 4,4-diphenyl-	222	C16H14O	000837-66-1	10
4		Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	10
5		1,3,5-Triazine-2,4-diamine, 6-(2...	221	C9H8ClN5	029366-77-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082434.D
Acq On : 22 Oct 2015 6:32
Operator : UM/IZ
Sample : G4116-19
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-AC-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.95	49.7	ng	1512410	1	6.77	609017	20.0
unknown6.54	6.54	75.6	ng	2303120	1	6.77	609017	20.0
Undecanoic acid	11.83	2.4	ng	85549	4	11.30	719755	20.0
Trichloroacetic a...	13.82	3.8	ng	121652	5	13.98	641130	20.0
unknown14.49	14.49	3.0	ng	97750	5	13.98	641130	20.0
unknown16.96	16.96	2.5	ng	84659	6	15.50	673860	20.0