

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
 Data File : BF092244.D
 Acq On : 13 Jan 2017 12:49
 Operator : UM/SJ
 Sample : I1131-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-002

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.713	253	256	271	rBV	1638093	3159833	48.38%	5.451%
2	5.181	295	297	300	rBV	4719461	6531369	100.00%	11.267%
3	6.256	388	391	398	rBV	5137220	5994295	91.78%	10.341%
4	6.359	398	400	403	rVB	5734886	5978853	91.54%	10.314%
5	6.587	418	420	422	rBV	1240045	1251902	19.17%	2.160%
6	6.747	431	434	436	rBV	3526750	4879585	74.71%	8.418%
7	7.159	467	470	472	rBV	3442584	3567356	54.62%	6.154%
8	7.296	480	482	487	rBV	54346	87948	1.35%	0.152%
9	7.867	530	532	535	rBV	1185918	1445055	22.12%	2.493%
10	8.953	624	627	630	rBV	5587378	5587119	85.54%	9.638%
11	9.353	660	662	664	rBV	1226232	1019150	15.60%	1.758%
12	9.616	683	685	687	rBV	1454365	1539524	23.57%	2.656%
13	10.073	723	725	726	rVB	85579	82434	1.26%	0.142%
14	10.416	752	755	757	rBV	2681504	3593467	55.02%	6.199%
15	10.542	764	766	770	rBV	162211	192080	2.94%	0.331%
16	10.988	803	805	806	rBV2	103016	101981	1.56%	0.176%
17	11.091	812	814	819	rVV2	1260149	1956788	29.96%	3.376%
18	11.171	819	821	823	rVB	106506	103116	1.58%	0.178%
19	11.342	833	836	840	rBV3	52702	114806	1.76%	0.198%
20	11.651	862	863	866	rVV2	297552	324595	4.97%	0.560%
21	11.708	866	868	873	rVB2	79925	119608	1.83%	0.206%
22	12.302	918	920	922	rVB	482247	423917	6.49%	0.731%
23	12.531	937	940	942	rVV	354830	492415	7.54%	0.849%
24	12.679	951	953	956	rVB	3472166	4811016	73.66%	8.300%
25	12.931	971	975	976	rBV2	45844	68732	1.05%	0.119%
26	13.228	998	1001	1002	rBV	63535	66997	1.03%	0.116%
27	13.594	1030	1033	1040	rBV2	261350	488182	7.47%	0.842%
28	13.719	1041	1044	1049	rBV2	1127089	1609834	24.65%	2.777%
29	14.199	1083	1086	1088	rBV4	30920	75917	1.16%	0.131%
30	14.577	1116	1119	1123	rBV	133369	154774	2.37%	0.267%
31	14.714	1129	1131	1135	rBV	138196	288038	4.41%	0.497%
32	14.977	1152	1154	1157	rBV	86544	99163	1.52%	0.171%
33	15.034	1157	1159	1161	rBV	108515	142421	2.18%	0.246%
34	15.080	1161	1163	1166	rBV	1015234	1277794	19.56%	2.204%

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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

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35	15.560	1201	1205	1213	rBV7	43549	148097	2.27%	0.255%
36	15.903	1233	1235	1241	rBV4	28358	91111	1.39%	0.157%
37	16.325	1269	1272	1275	rVB	53850	97997	1.50%	0.169%

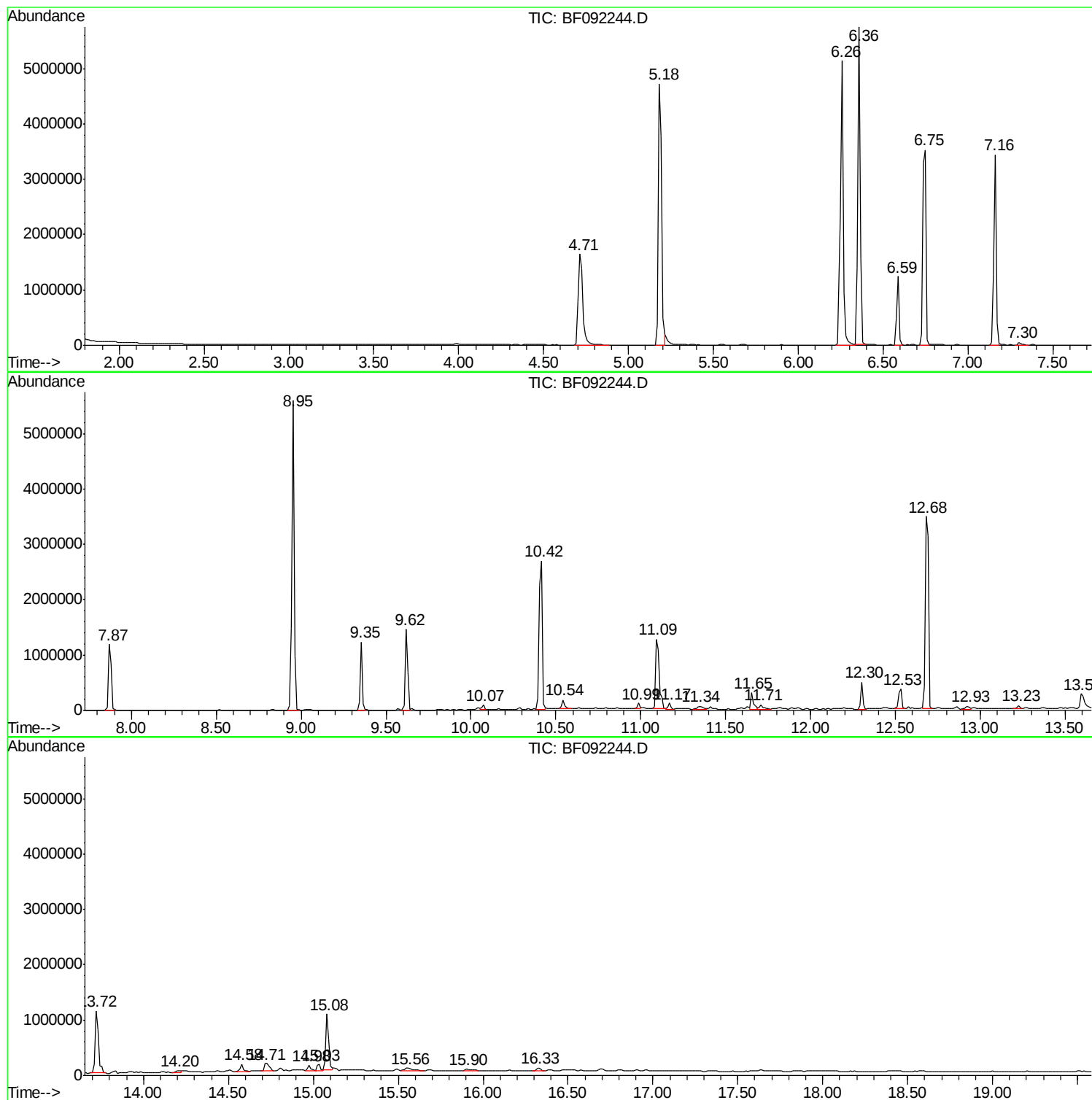
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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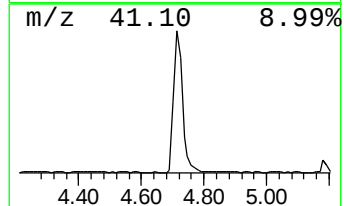
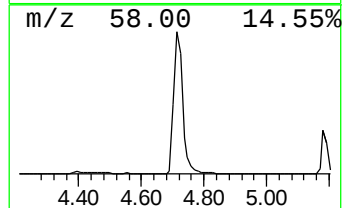
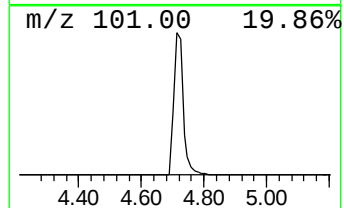
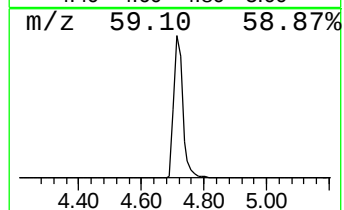
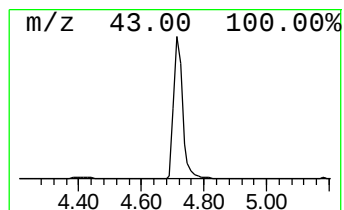
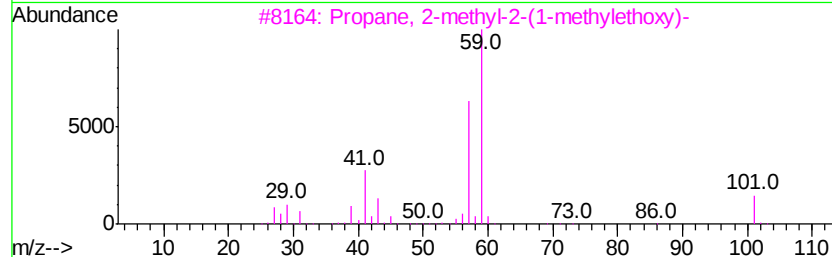
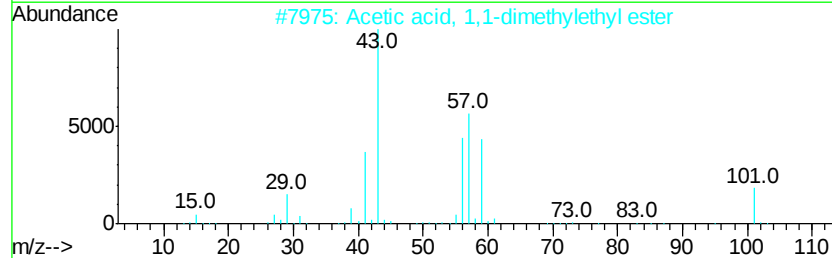
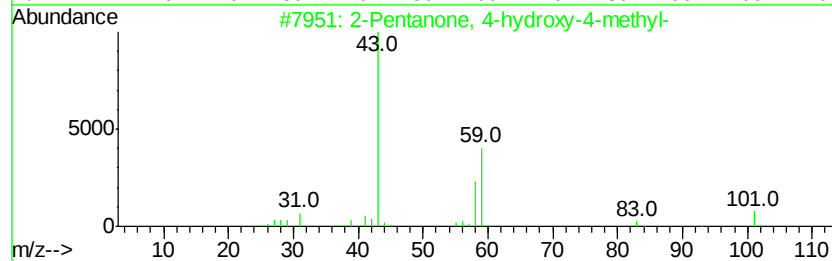
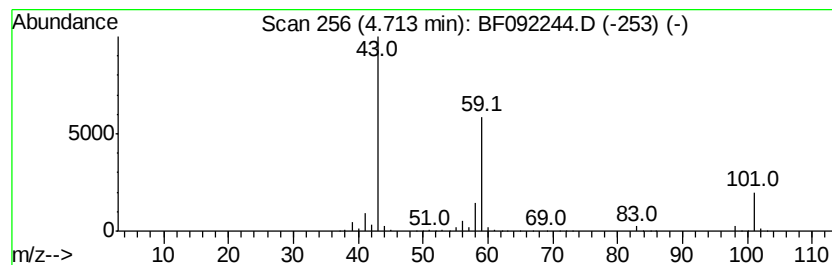
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	50.48 ng	3159830	1,4-Dichlorobenzene-d4	6.59

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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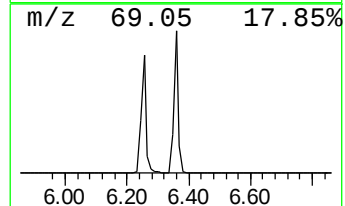
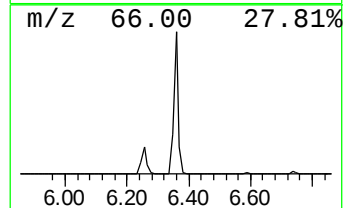
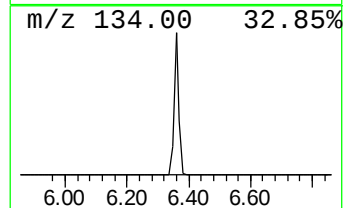
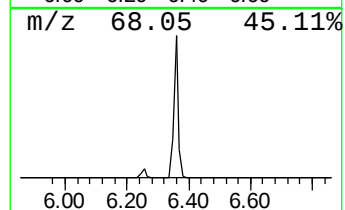
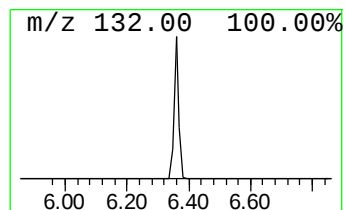
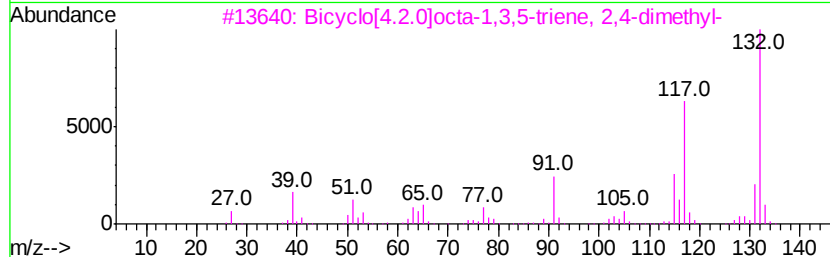
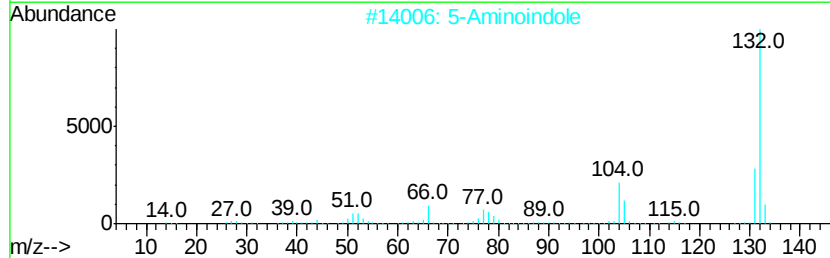
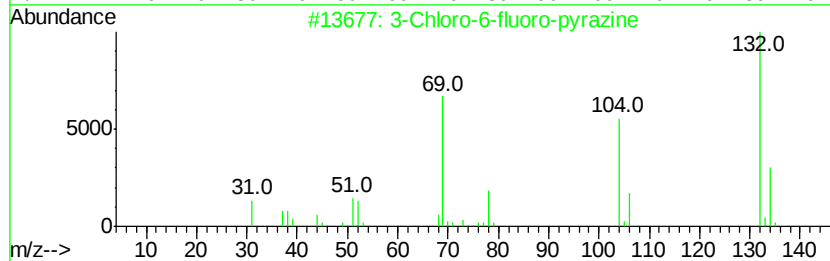
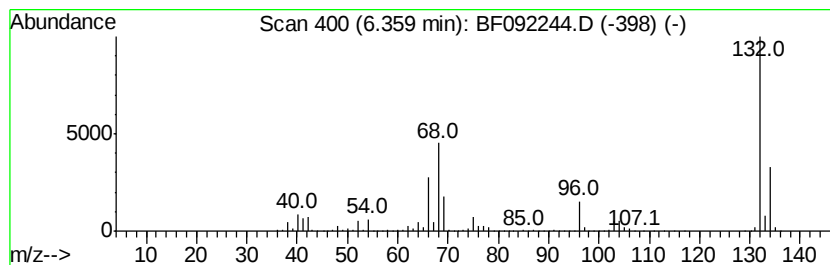
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	95.52 ng	5978850	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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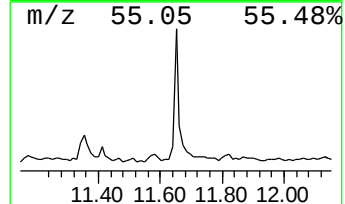
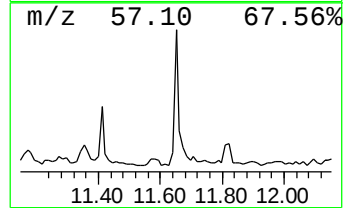
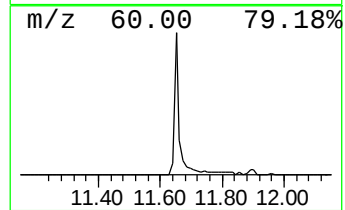
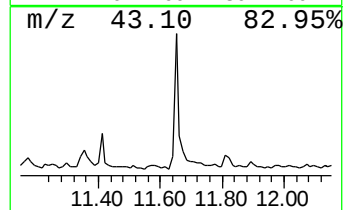
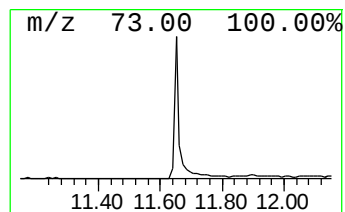
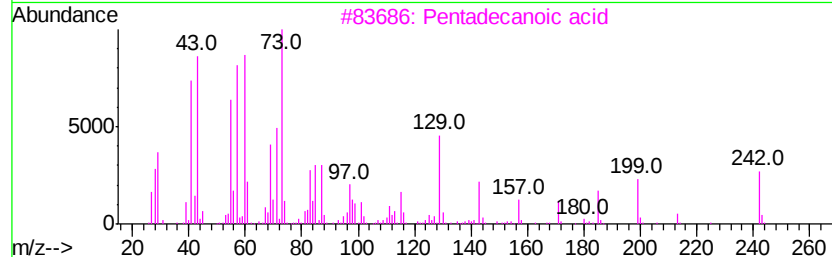
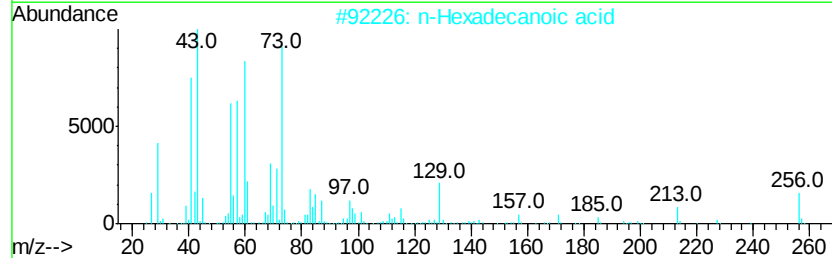
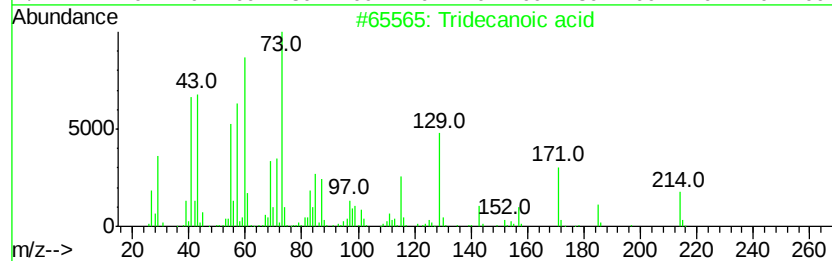
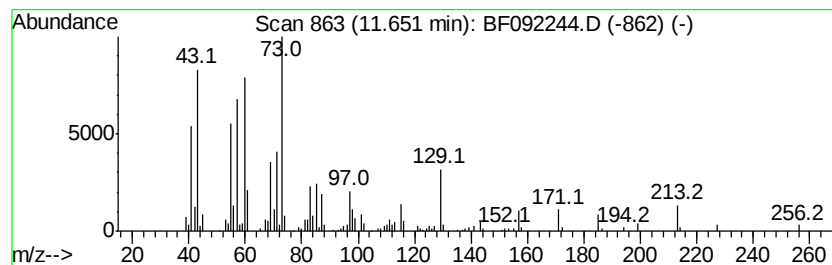
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	3.32 ng	324595	Phenanthrene-d10	11.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		N-Acetylisoaxazolidine	115	C5H9NO2	115615-36-6	30



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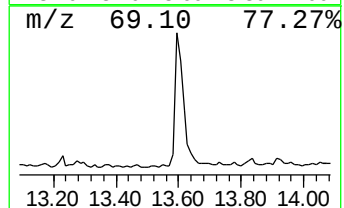
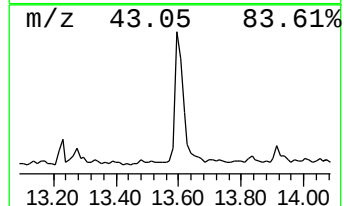
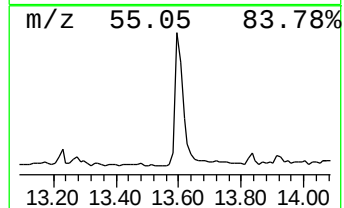
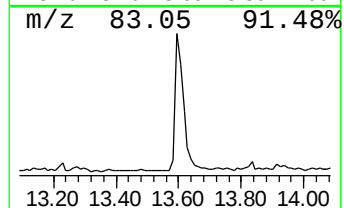
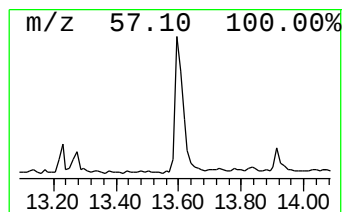
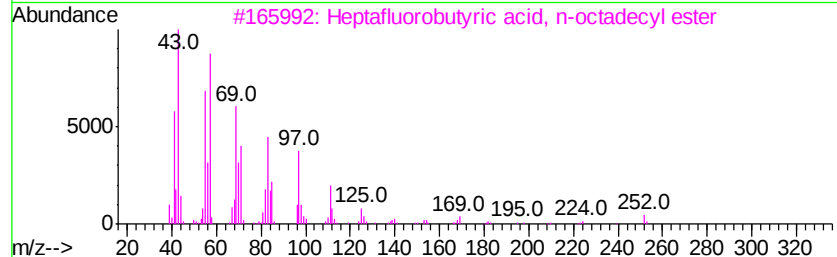
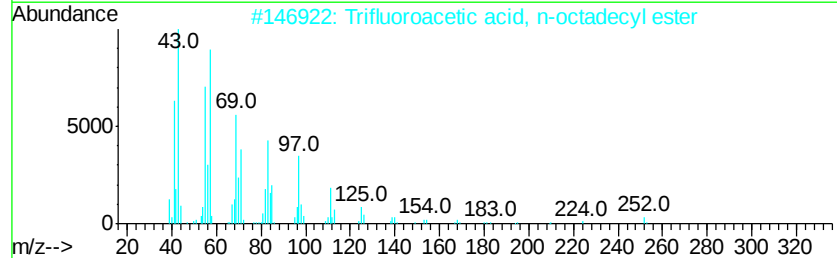
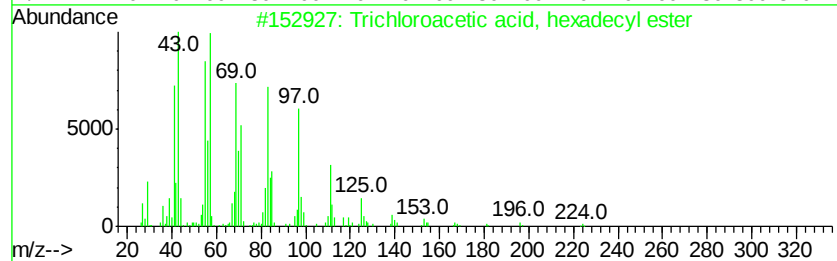
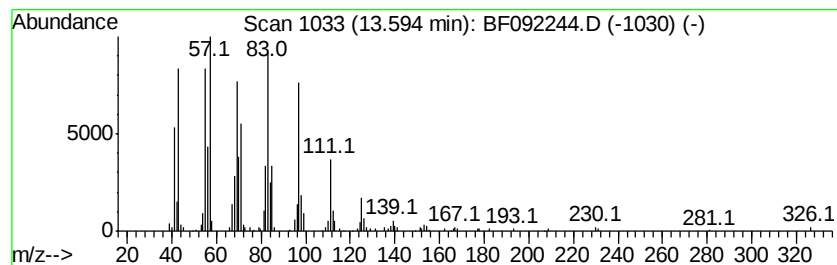
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	6.07 ng	488182	Chrysene-d12	13.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
3		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



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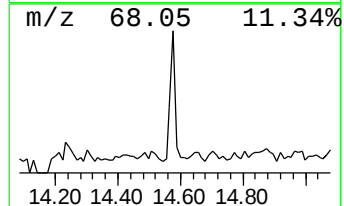
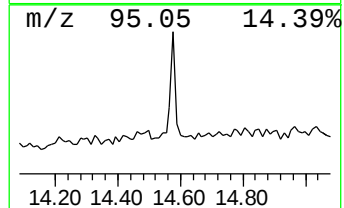
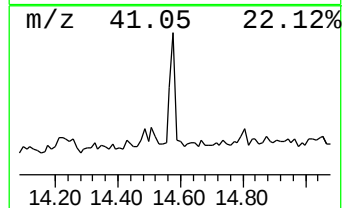
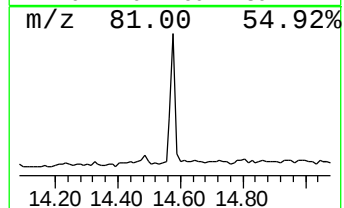
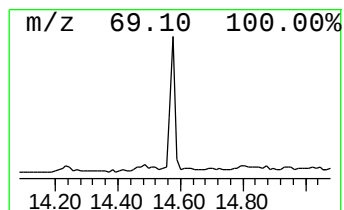
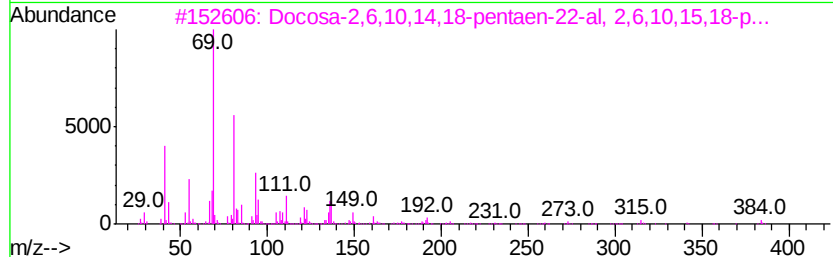
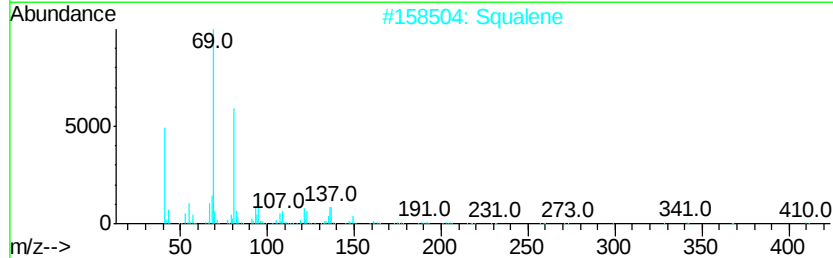
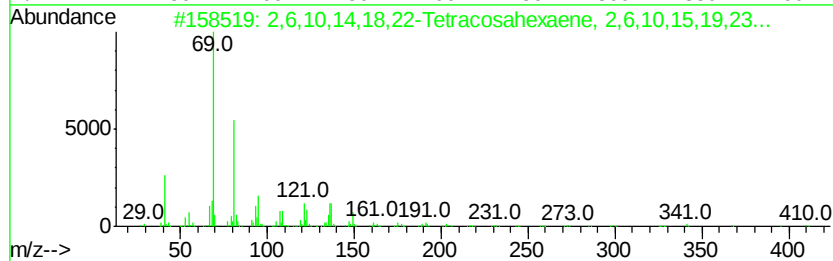
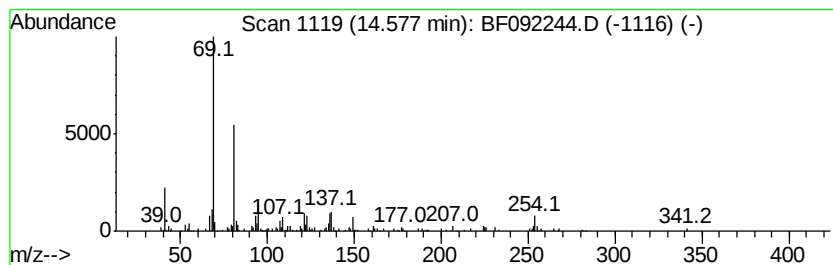
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Peak Number 5 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.42 ng	154774	Perylene-d12	15.08

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87		
2	Squalene	410	C30H50	007683-64-9	87		
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83		
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64		
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011317\
Data File : BF092244.D
Acq On : 13 Jan 2017 12:49
Operator : UM/SJ
Sample : I1131-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-002

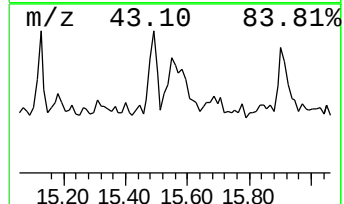
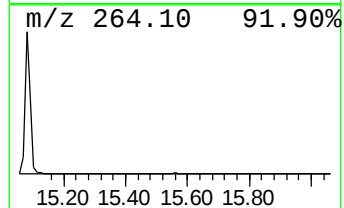
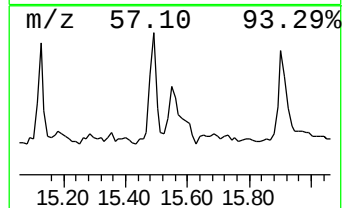
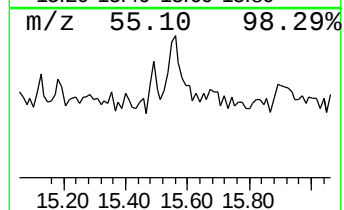
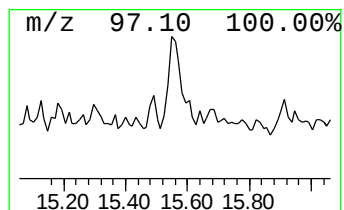
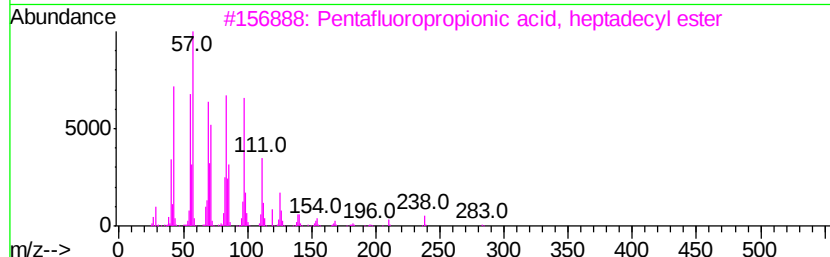
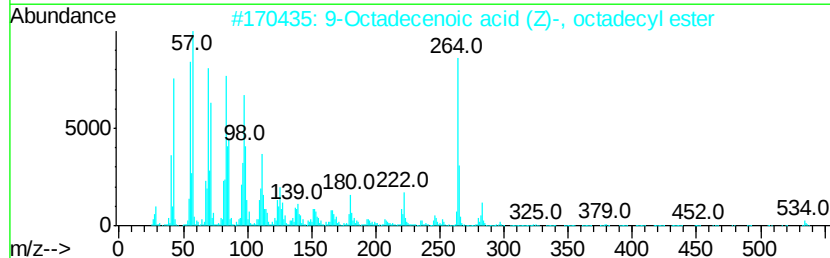
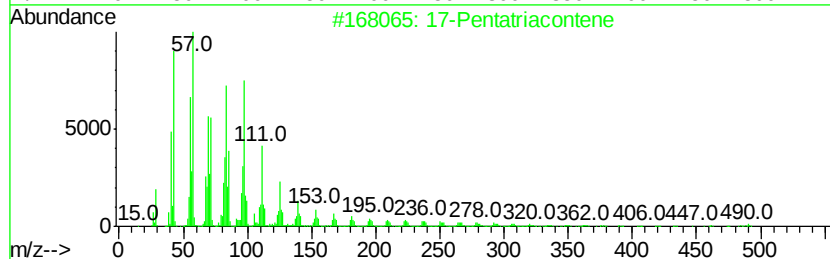
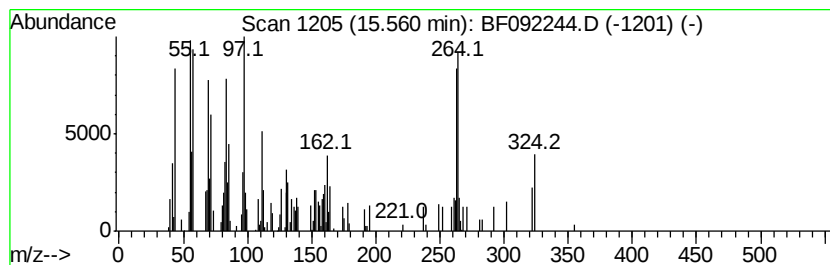
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	2.32 ng	148097	Perylene-d12	15.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	38
2		9-Octadecenoic acid (Z)-, octade...	535	C36H70O2	017673-49-3	38
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	35
4		2-Methyl-2-docosene	322	C23H46	1000131-16-9	27
5		Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011317\
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Sample : I1131-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-002

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.71	50.5	ng	3159830	1	6.59	1251900	20.0
unknown6.36	6.36	95.5	ng	5978850	1	6.59	1251900	20.0
Tridecanoic acid	11.65	3.3	ng	324595	4	11.09	1956790	20.0
Trichloroacetic a...	13.59	6.1	ng	488182	5	13.72	1609830	20.0
2,6,10,14,18,22-T...	14.58	2.4	ng	154774	6	15.08	1277790	20.0
unknown15.56	15.56	2.3	ng	148097	6	15.08	1277790	20.0