

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
 Data File : BF092373.D
 Acq On : 20 Jan 2017 15:21
 Operator : UM/SJ
 Sample : I1304-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1634-NOTTINGHAM-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-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	4.633	246	249	268	rBV	954454	1878009	29.53%	3.640%
2	5.113	288	291	293	rBV	3786187	4610038	72.49%	8.936%
3	6.187	382	385	388	rBV	3219278	5105445	80.28%	9.896%
4	6.290	392	394	397	rVV	3924029	4510975	70.93%	8.744%
5	6.519	412	414	417	rBV	996409	906643	14.26%	1.757%
6	6.679	425	428	430	rBV	3321082	3571325	56.16%	6.922%
7	7.102	462	465	467	rBV	2724969	3203111	50.37%	6.209%
8	7.810	524	527	529	rBV	1174991	1134699	17.84%	2.199%
9	8.896	618	622	624	rBV	5044988	6359698	100.00%	12.327%
10	9.296	654	657	659	rBV	742153	753675	11.85%	1.461%
11	9.559	677	680	682	rBV	1671792	1799932	28.30%	3.489%
12	10.005	718	719	721	rVB	79183	69756	1.10%	0.135%
13	10.348	746	749	751	rBV	3427026	3546461	55.76%	6.874%
14	10.473	758	760	764	rVB	104200	151911	2.39%	0.294%
15	10.919	798	799	805	rVB	91550	140109	2.20%	0.272%
16	11.033	806	809	810	rVV	1722705	1675947	26.35%	3.249%
17	11.056	810	811	813	rVV	225975	180518	2.84%	0.350%
18	11.353	834	837	839	rVB	57120	82761	1.30%	0.160%
19	11.536	848	853	854	rBV3	55923	70106	1.10%	0.136%
20	11.593	854	858	861	rVV2	316718	440482	6.93%	0.854%
21	11.639	861	862	868	rVB	82557	138946	2.18%	0.269%
22	12.233	912	914	917	rBV	382637	465732	7.32%	0.903%
23	12.371	924	926	931	rBV2	71876	104410	1.64%	0.202%
24	12.462	931	934	937	rBV	465649	476813	7.50%	0.924%
25	12.622	945	948	950	rBV	4270111	4776545	75.11%	9.259%
26	12.794	960	963	966	rVB	40624	95467	1.50%	0.185%
27	12.896	971	972	976	rVB2	50091	71243	1.12%	0.138%
28	13.205	994	999	1004	rBV8	21661	81912	1.29%	0.159%
29	13.319	1004	1009	1012	rBV3	34271	64886	1.02%	0.126%
30	13.422	1015	1018	1021	rBV3	35548	98049	1.54%	0.190%
31	13.548	1025	1029	1036	rBV3	108768	383546	6.03%	0.743%
32	13.662	1036	1039	1044	rVB2	1583326	2003334	31.50%	3.883%
33	14.051	1069	1073	1075	rBV	44243	72146	1.13%	0.140%
34	14.154	1077	1082	1083	rBV4	28553	63678	1.00%	0.123%

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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-BF122116.M
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35	14.508	1111	1113	1117	rBV2	78875	126846	1.99%	0.246%
36	14.657	1124	1126	1131	rBV	195290	338285	5.32%	0.656%
37	14.737	1131	1133	1136	rVB3	36391	69033	1.09%	0.134%
38	14.908	1146	1148	1151	rVB	109497	121367	1.91%	0.235%
39	14.965	1151	1153	1155	rBV	121543	162068	2.55%	0.314%
40	15.011	1155	1157	1164	rVB	727542	1063781	16.73%	2.062%
41	15.400	1188	1191	1195	rBV2	41339	70067	1.10%	0.136%
42	15.800	1223	1226	1231	rVB2	33219	75232	1.18%	0.146%
43	16.234	1261	1264	1273	rVB2	69895	213907	3.36%	0.415%
44	16.588	1292	1295	1302	rBV	53640	105391	1.66%	0.204%
45	16.817	1312	1315	1321	rVB3	28709	72129	1.13%	0.140%
46	17.068	1334	1337	1341	rBV5	36227	83761	1.32%	0.162%

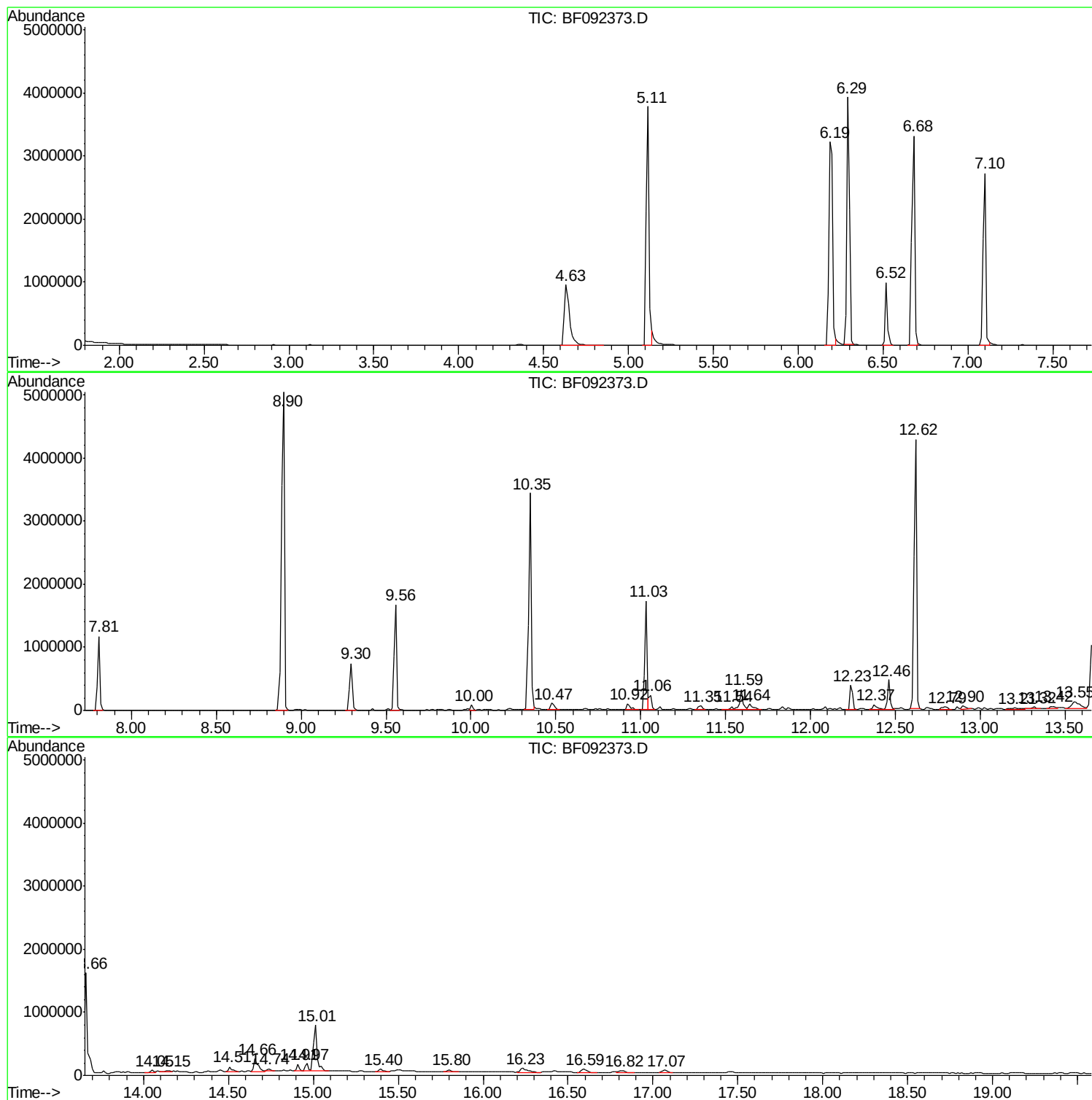
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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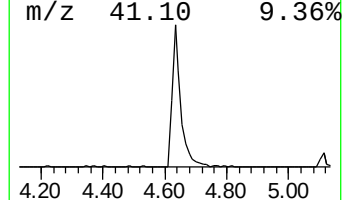
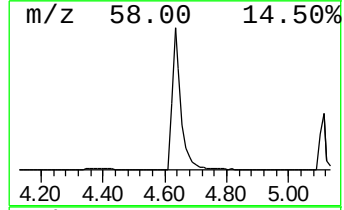
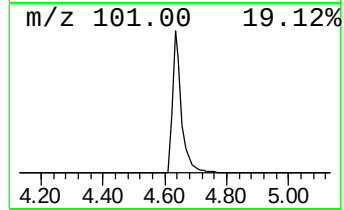
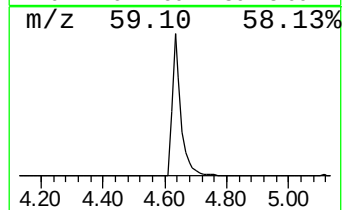
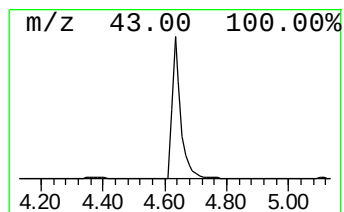
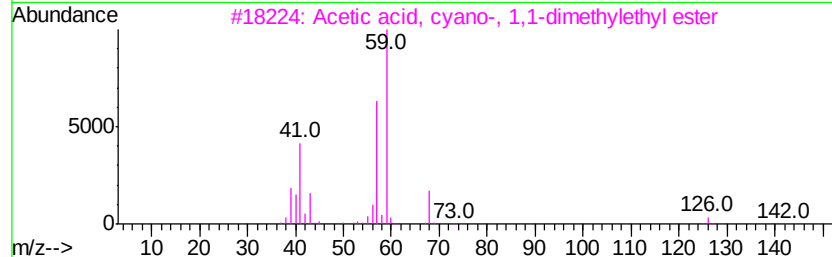
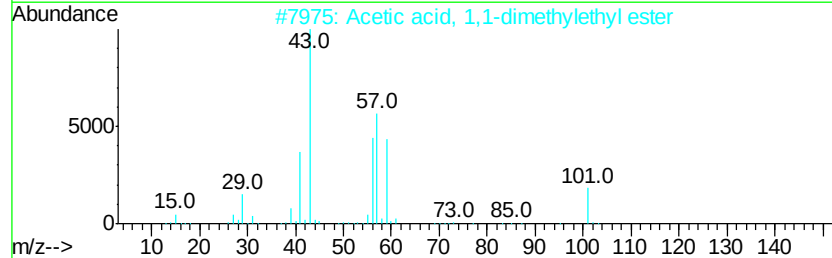
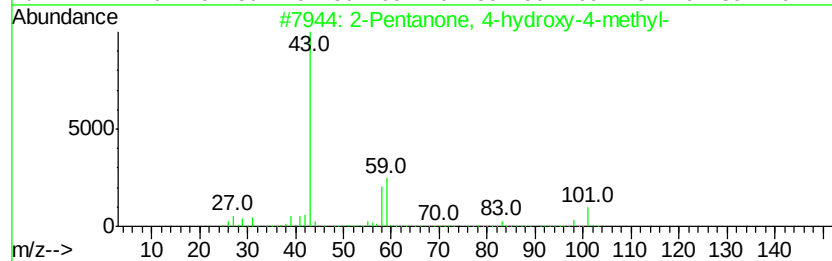
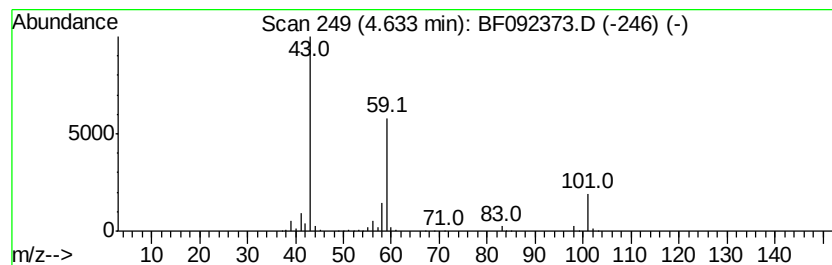
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	41.43 ng	1878010	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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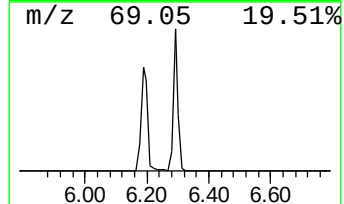
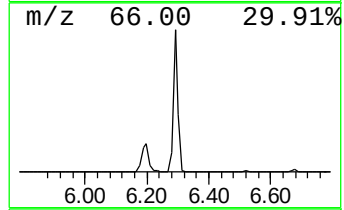
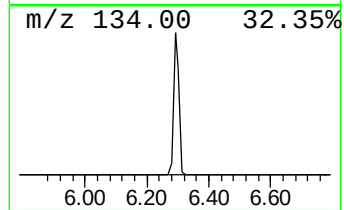
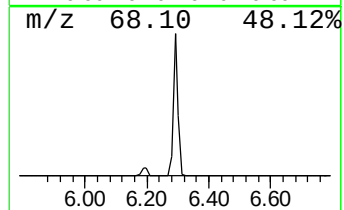
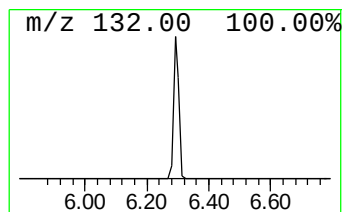
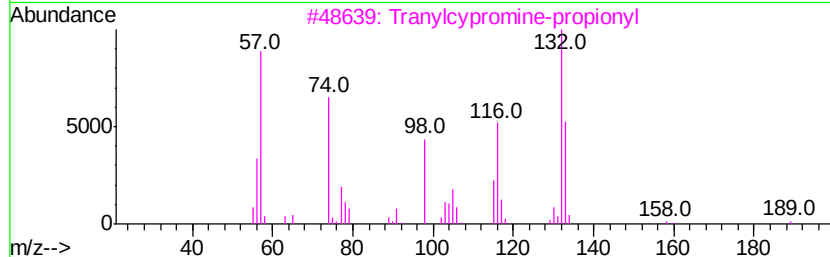
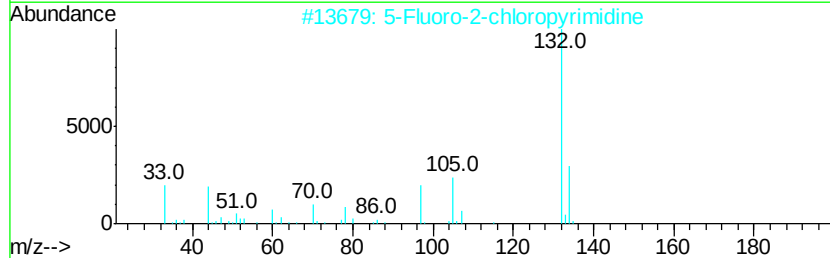
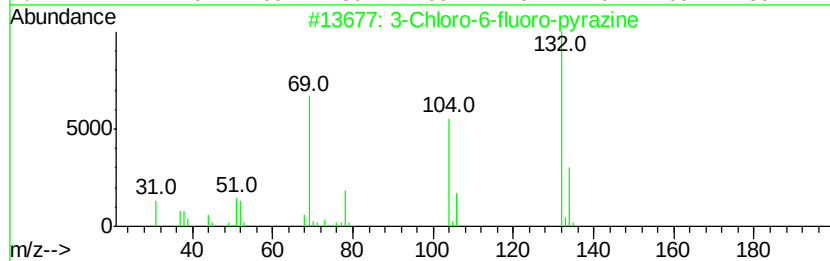
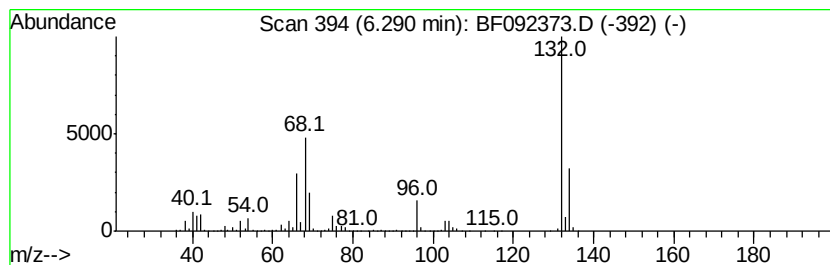
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Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	99.51 ng	4510980	1,4-Dichlorobenzene-d4	6.52

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	12
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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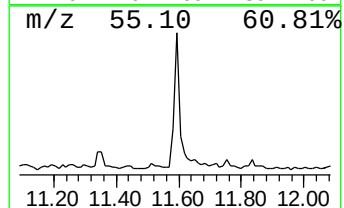
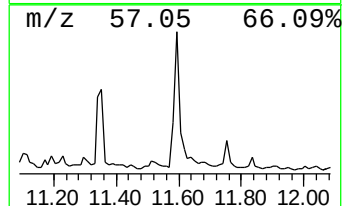
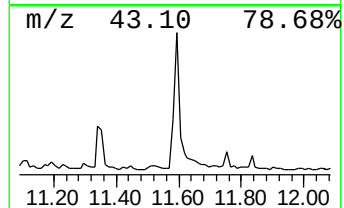
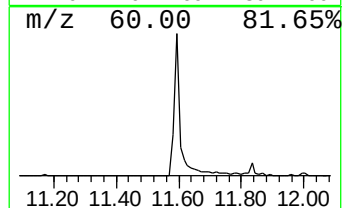
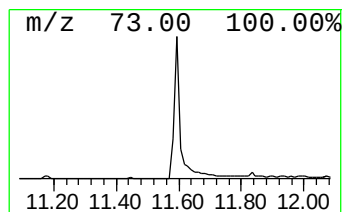
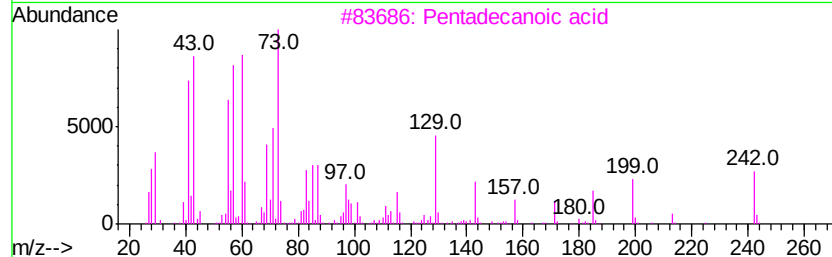
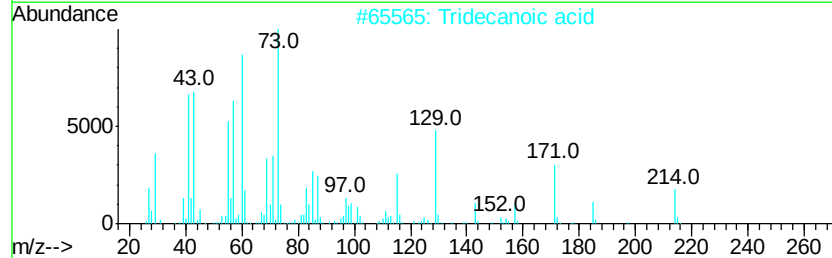
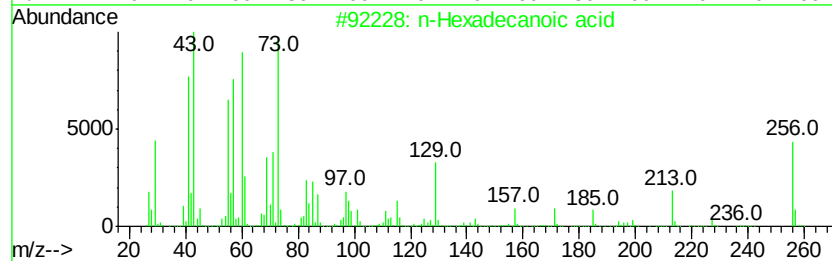
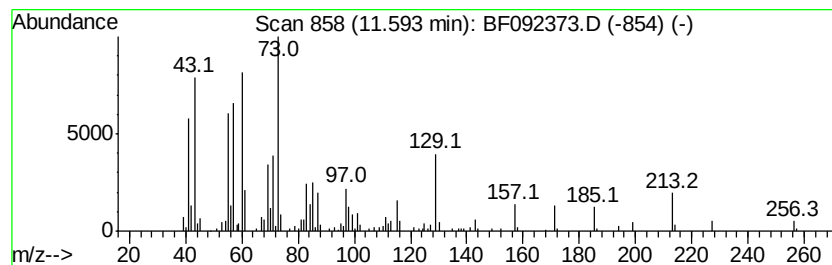
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.59	5.26 ng	440482	Phenanthrene-d10		11.03
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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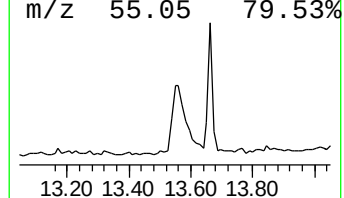
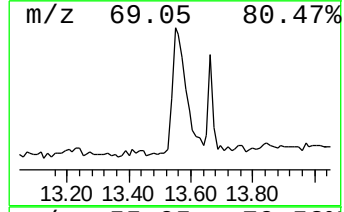
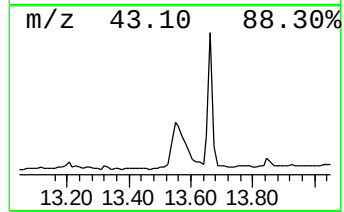
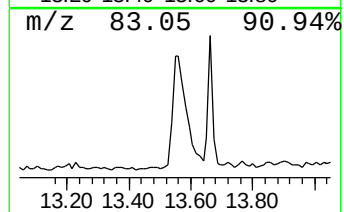
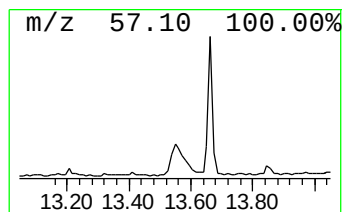
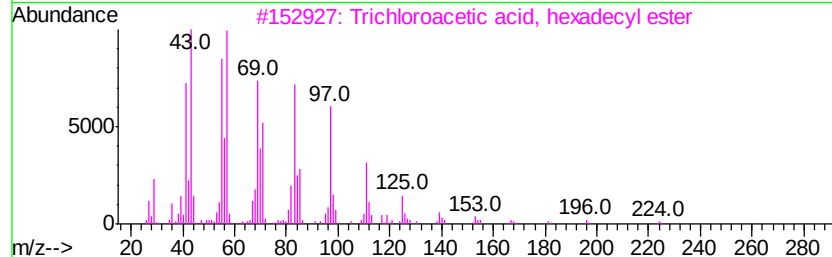
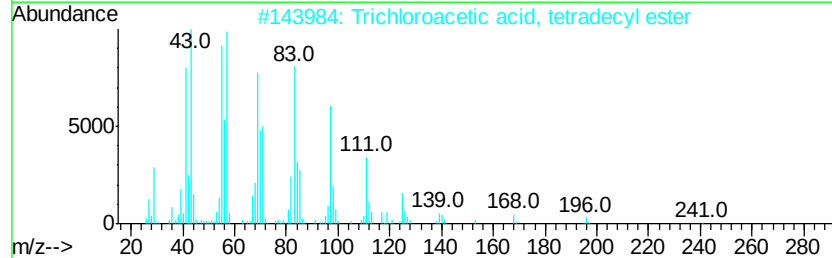
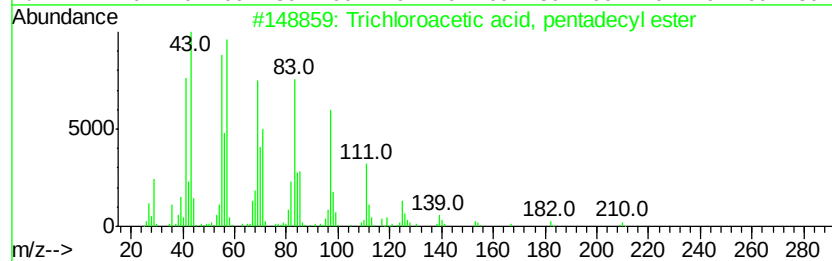
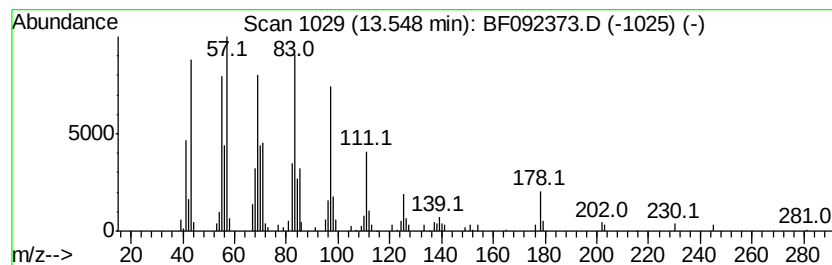
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.83 ng	383546	Chrysene-d12	13.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90
5		1-Nonadecene	266	C19H38	018435-45-5	90



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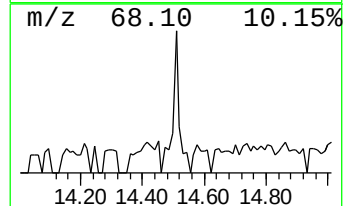
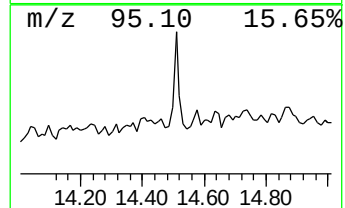
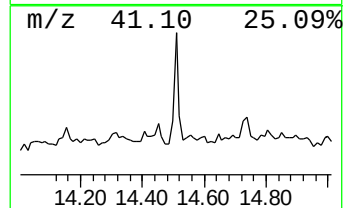
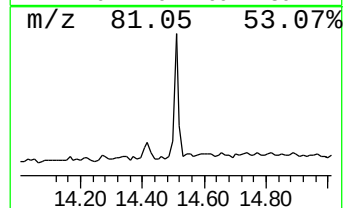
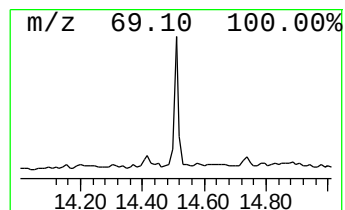
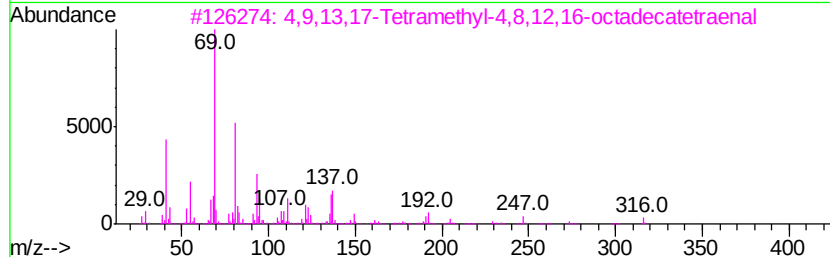
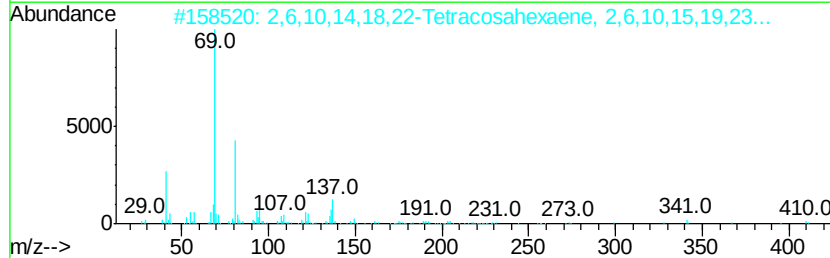
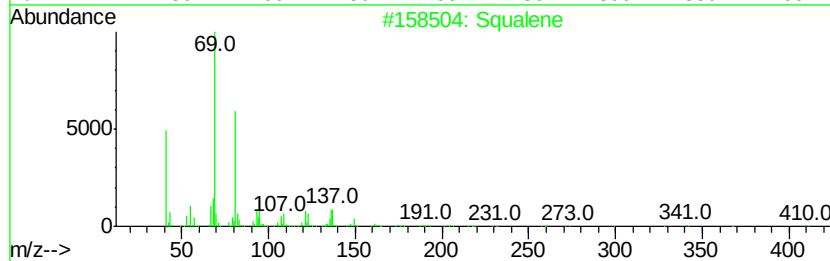
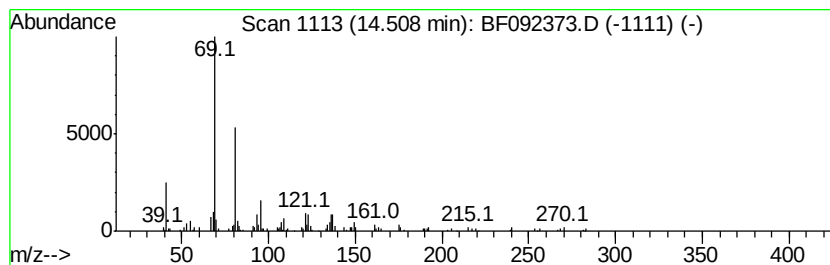
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.38 ng	126846	Perylene-d12	15.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	86
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	83
5	Crotonic acid, o-formylphenyl ester	190 C11H10O3	114636-69-0	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092373.D
Acq On : 20 Jan 2017 15:21
Operator : UM/SJ
Sample : I1304-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1634-NOTTINGHAM-COMP

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...	4.63	41.4	ng	1878010	1	6.52	906643	20.0
unknown6.29	6.29	99.5	ng	4510980	1	6.52	906643	20.0
n-Hexadecanoic acid	11.59	5.3	ng	440482	4	11.03	1675950	20.0
Trichloroacetic a...	13.55	3.8	ng	383546	5	13.66	2003330	20.0
Squalene	14.51	2.4	ng	126846	6	15.01	1063780	20.0