

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101416\
 Data File : BF090597.D
 Acq On : 15 Oct 2016 9:50
 Operator : UM/SJ
 Sample : H5228-01
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5

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-BF101316.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	5.103	240	242	251	rBV	705070	992105	25.41%	2.715%
2	5.526	276	279	299	rBV	3692385	3904799	100.00%	10.687%
3	6.554	366	369	371	rBV	3158412	3841387	98.38%	10.514%
4	6.680	378	380	383	rBV	2763204	3861644	98.89%	10.569%
5	6.920	398	401	412	rBV	1130663	1305785	33.44%	3.574%
6	7.069	412	414	417	rBV	2068180	2581829	66.12%	7.066%
7	7.480	447	450	465	rBV	2064048	2477712	63.45%	6.781%
8	8.200	511	513	516	rBV	1399877	1658048	42.46%	4.538%
9	9.286	605	608	610	rBV	2820274	3259475	83.47%	8.921%
10	9.675	640	642	644	rBV	728409	595415	15.25%	1.630%
11	9.960	665	667	670	rBV	2178892	1880362	48.16%	5.146%
12	10.395	703	705	706	rVB	76180	60079	1.54%	0.164%
13	10.612	721	724	727	rBV	26186	42009	1.08%	0.115%
14	10.749	733	736	745	rBV	1873566	1950832	49.96%	5.339%
15	10.863	745	746	753	rVB	89300	127136	3.26%	0.348%
16	11.320	784	786	787	rBV	34599	49496	1.27%	0.135%
17	11.446	795	797	811	rBV	1343638	1544338	39.55%	4.227%
18	11.675	815	817	821	rBV	92963	106253	2.72%	0.291%
19	12.658	901	903	906	rBV	49958	57729	1.48%	0.158%
20	12.852	918	920	922	rBV	121273	139451	3.57%	0.382%
21	12.886	922	923	926	rVB2	43643	50318	1.29%	0.138%
22	13.035	933	936	945	rBV	2366062	2481177	63.54%	6.791%
23	13.561	980	982	984	rBV	100045	96541	2.47%	0.264%
24	13.926	1012	1014	1020	rBV	184258	245970	6.30%	0.673%
25	14.086	1026	1028	1036	rBV	871500	1164495	29.82%	3.187%
26	14.567	1068	1070	1073	rBV2	56317	101534	2.60%	0.278%
27	14.864	1094	1096	1101	rVV	30966	46247	1.18%	0.127%
28	14.955	1101	1104	1107	rVB2	46282	92162	2.36%	0.252%
29	15.207	1124	1126	1132	rVB	34247	65147	1.67%	0.178%
30	15.389	1139	1142	1145	rBV	74038	106558	2.73%	0.292%
31	15.549	1153	1156	1167	rVB	682420	1121724	28.73%	3.070%
32	15.881	1182	1185	1192	rVB	90928	215673	5.52%	0.590%
33	16.018	1194	1197	1199	rBV	31329	47559	1.22%	0.130%
34	16.475	1233	1237	1240	rBV	65757	176455	4.52%	0.483%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.184	1296	1299	1304	rBV2	37203	89443	2.29%	0.245%
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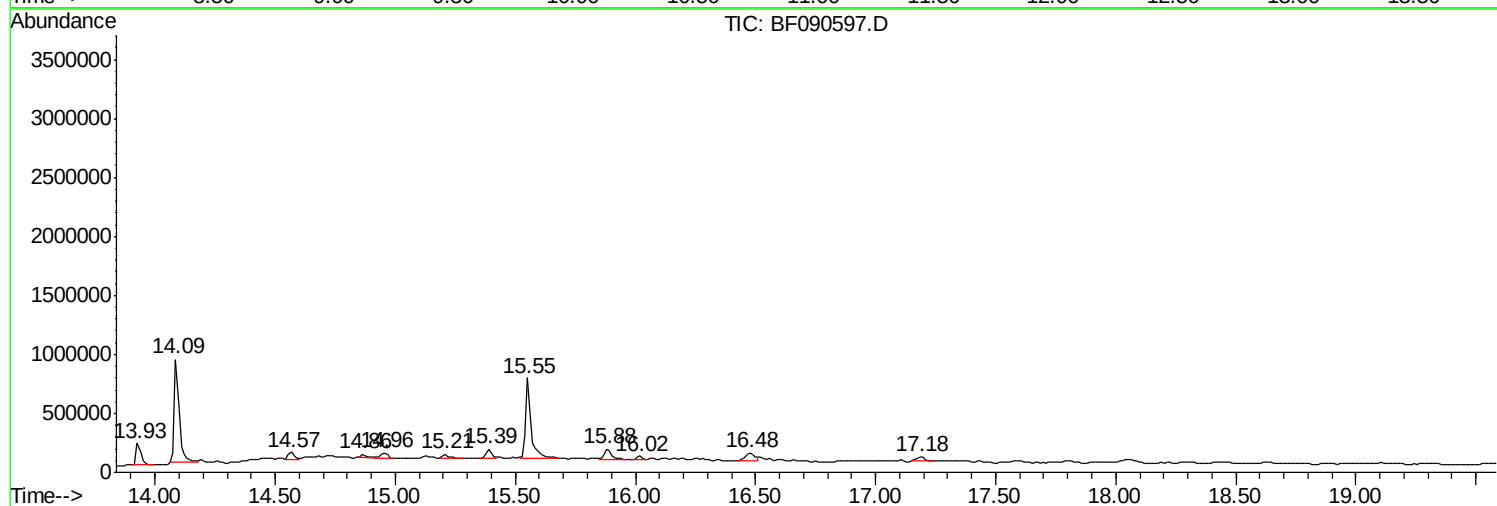
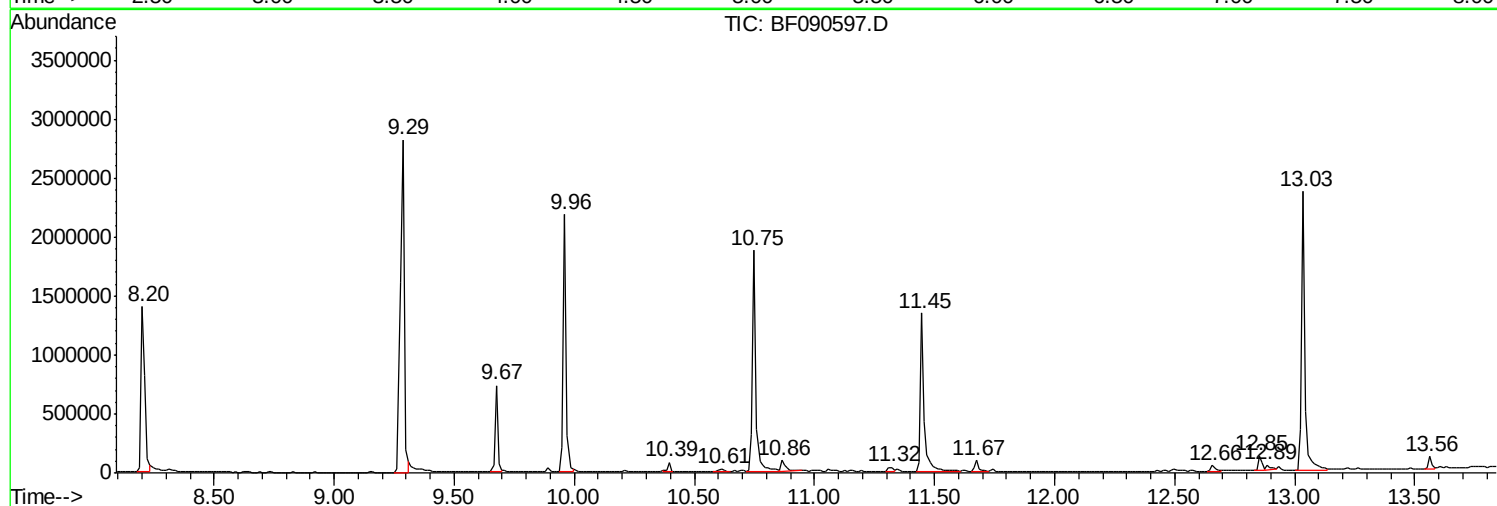
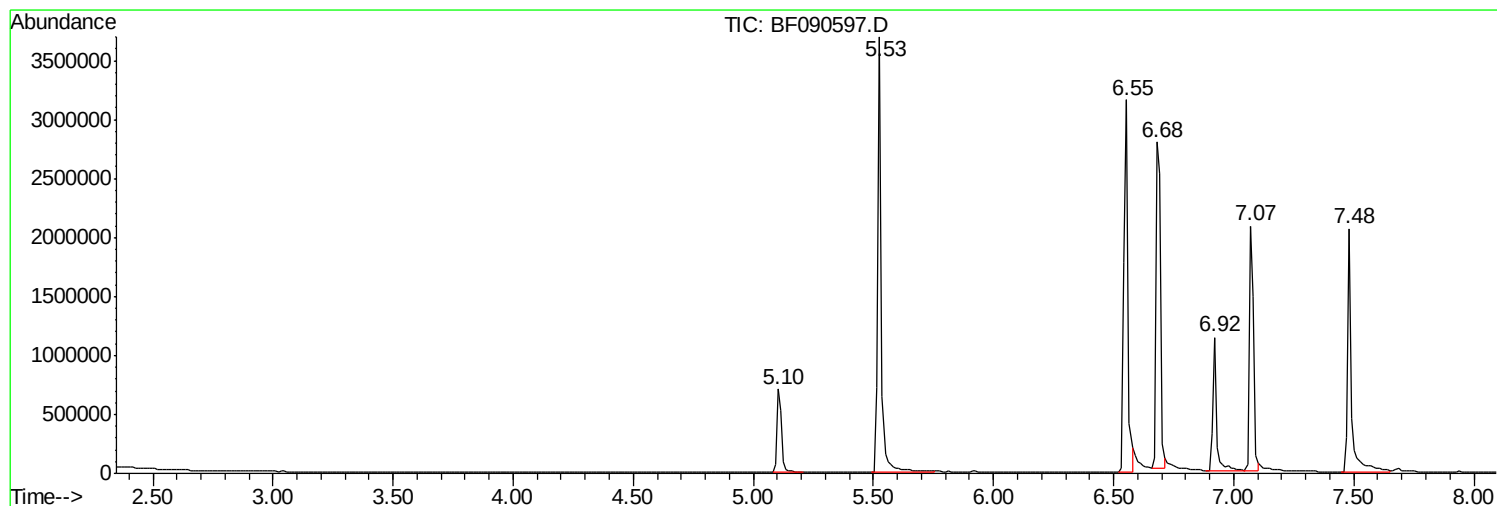
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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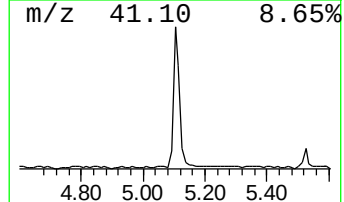
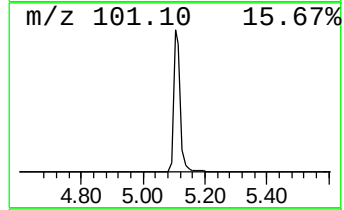
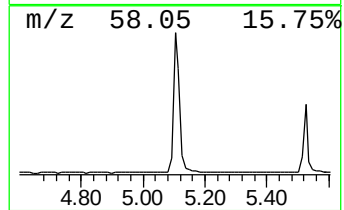
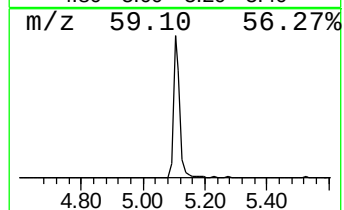
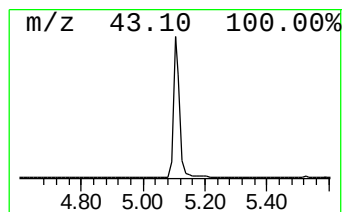
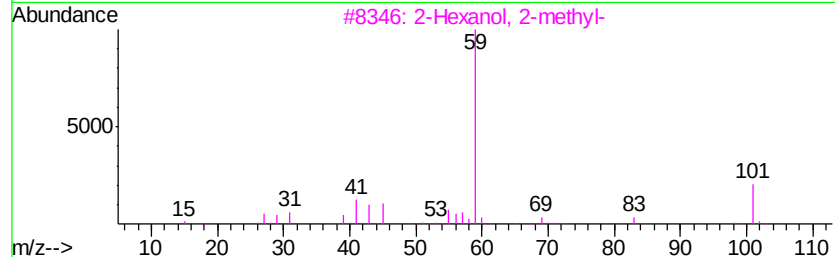
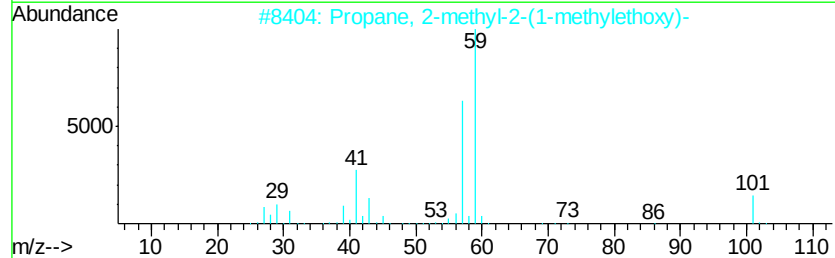
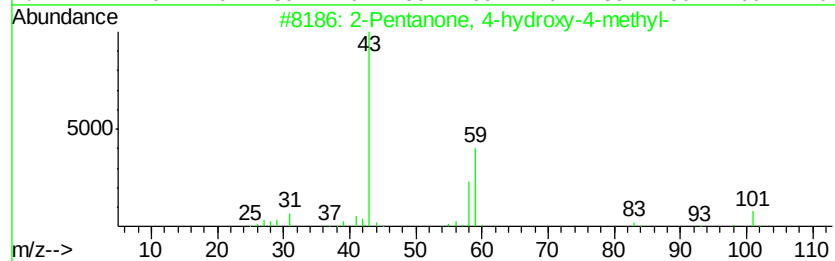
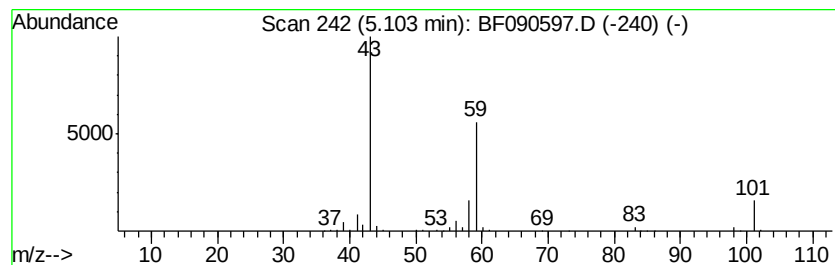
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.10	15.20 ng	992105	1,4-Dichlorobenzene-d4	6.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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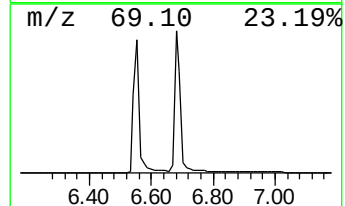
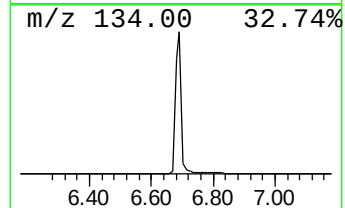
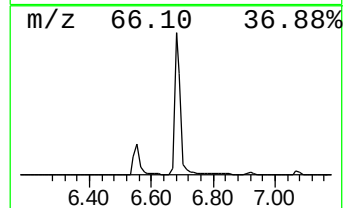
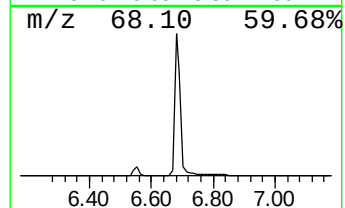
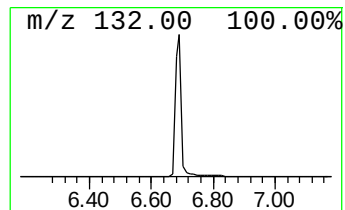
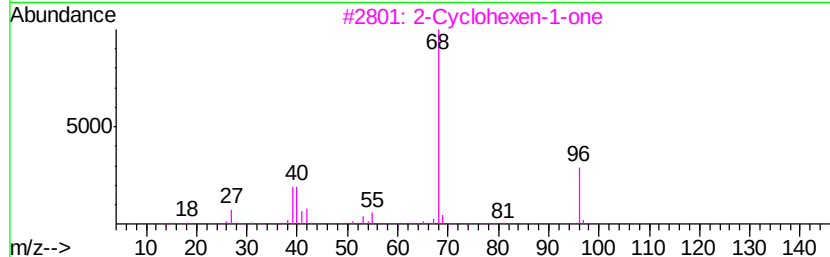
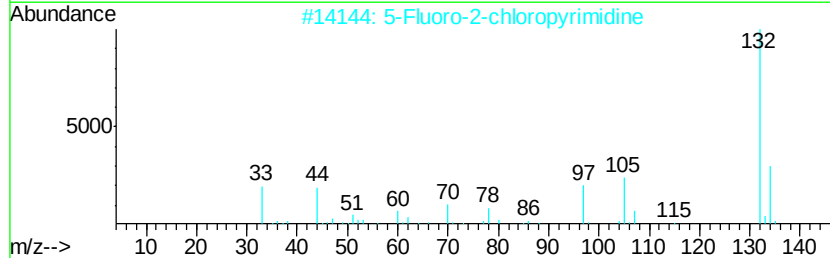
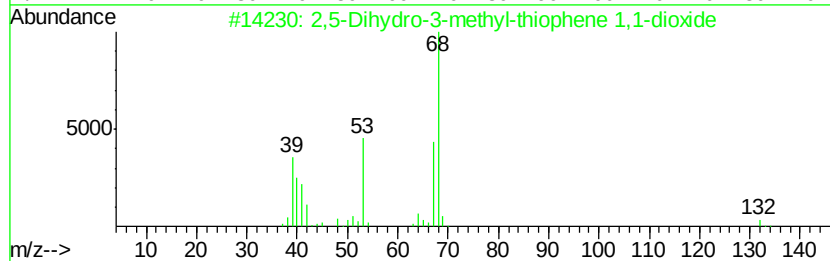
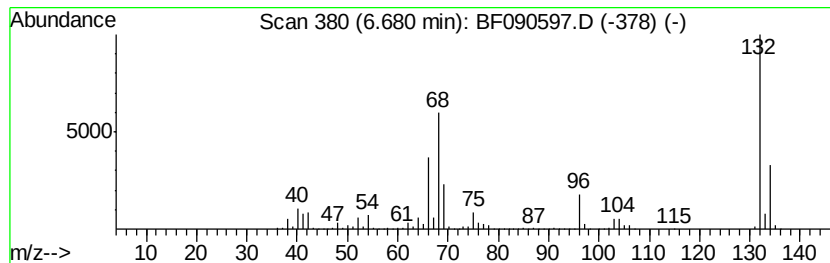
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	59.15 ng	3861640	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	17
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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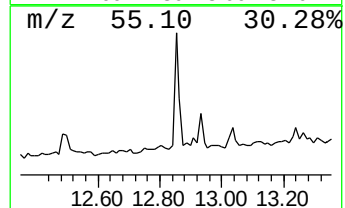
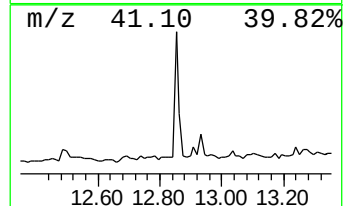
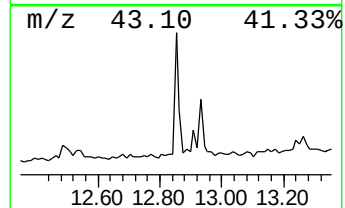
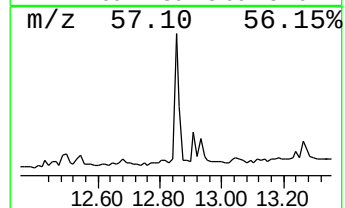
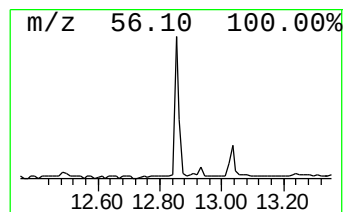
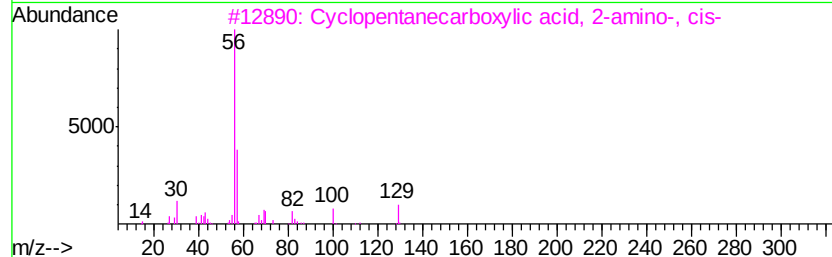
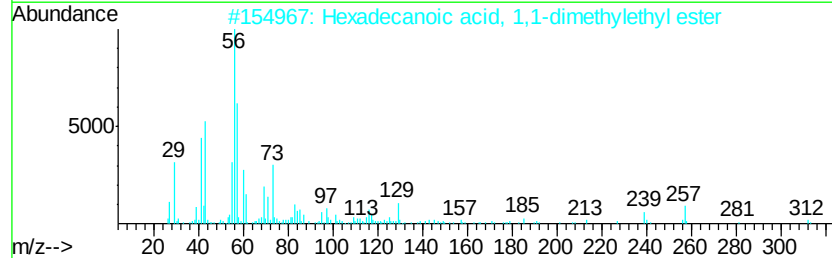
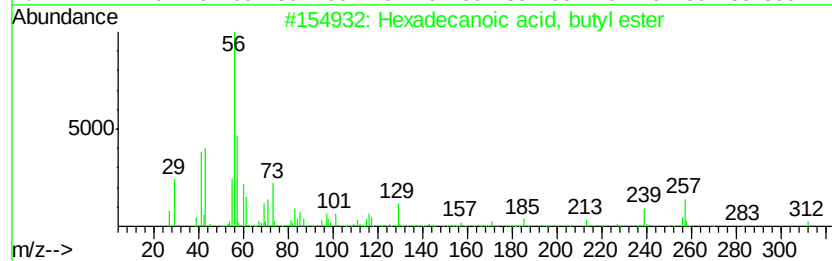
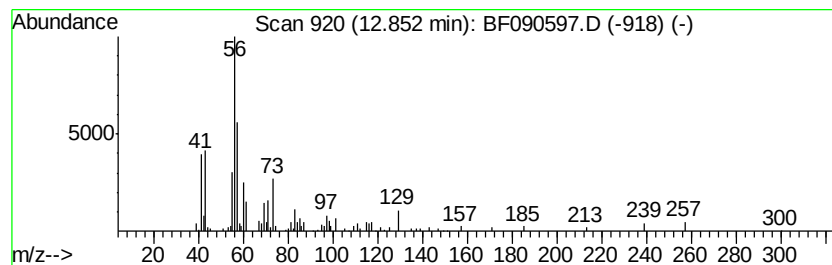
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.40 ng	139451	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	80
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38



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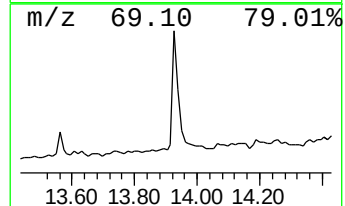
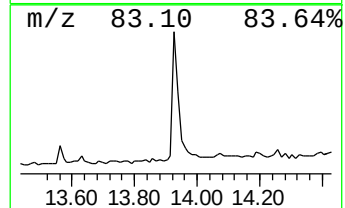
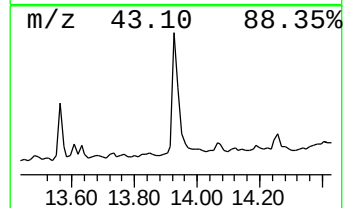
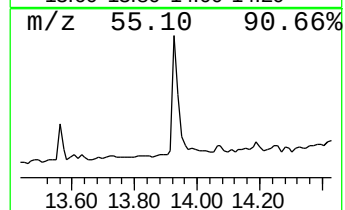
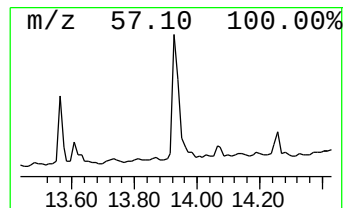
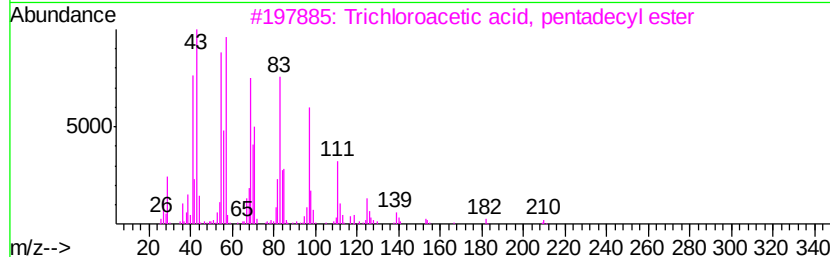
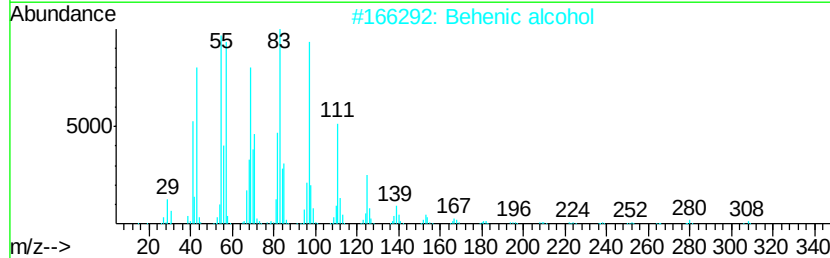
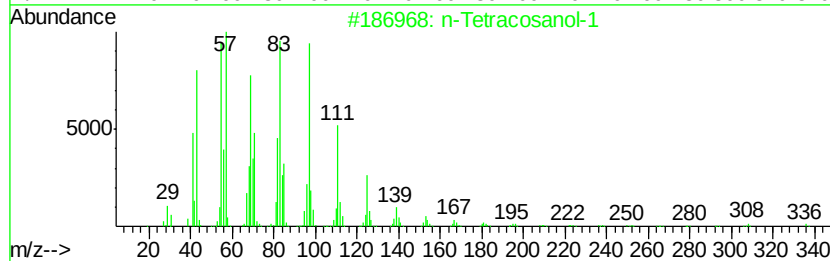
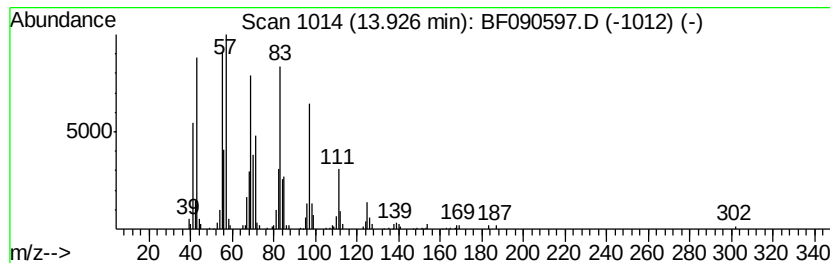
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	4.22 ng	245970	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		Behenic alcohol	326	C22H46O	000661-19-8	94
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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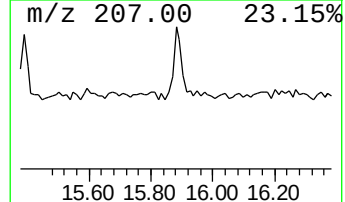
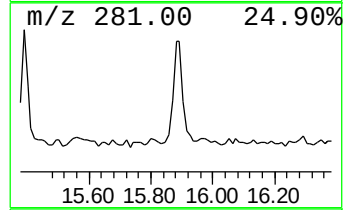
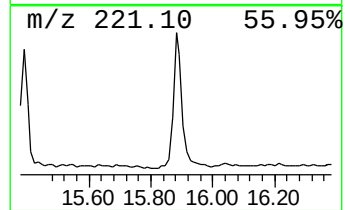
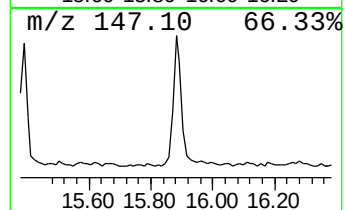
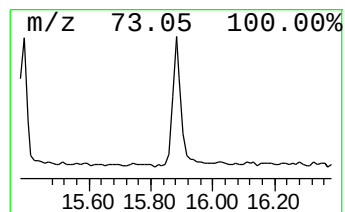
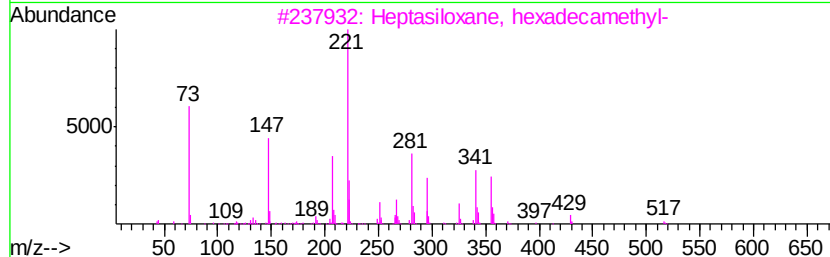
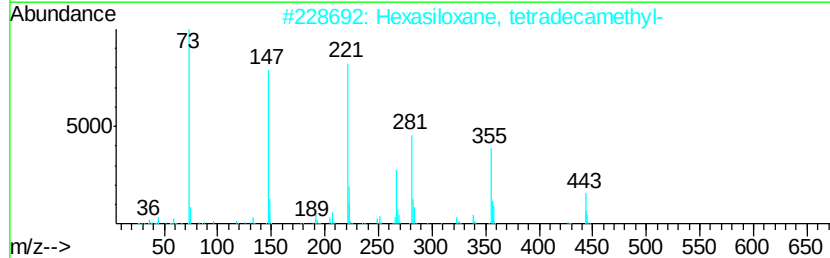
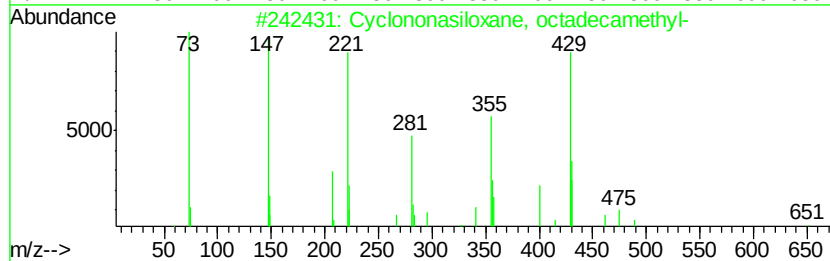
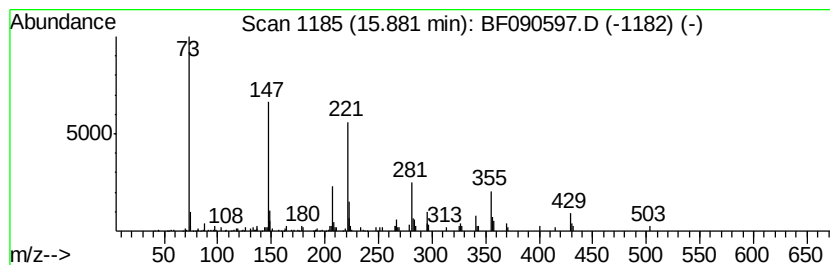
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.85 ng	215673	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H5409Si9	000556-71-8	64
2		Hexasiloxane, tetradecamethyl-	458	C14H4205Si6	000107-52-8	59
3		Heptasiloxane, hexadecamethyl-	532	C16H4806Si7	000541-01-5	42
4		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H3002Si4	004342-25-0	32
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H5207Si7	071579-69-6	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101416\
Data File : BF090597.D
Acq On : 15 Oct 2016 9:50
Operator : UM/SJ
Sample : H5228-01
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
5

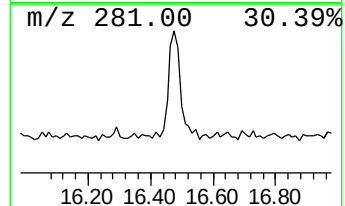
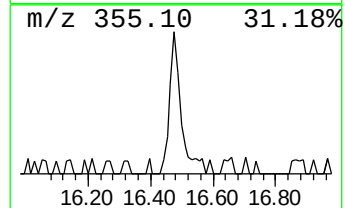
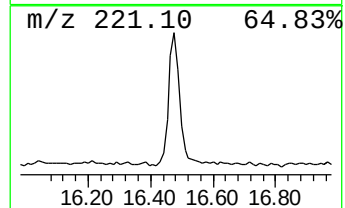
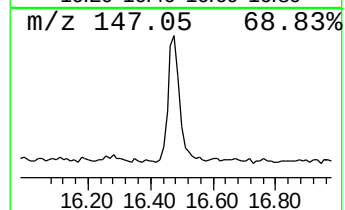
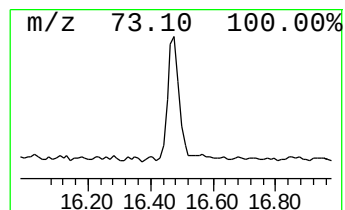
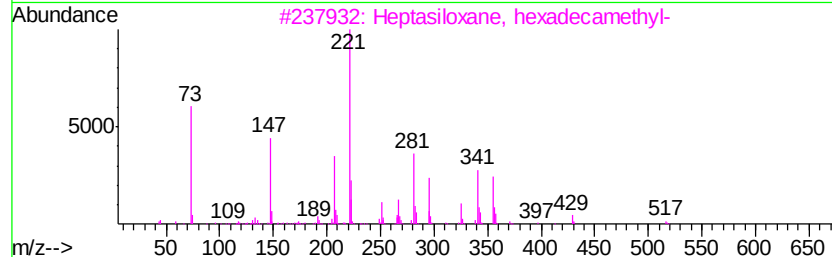
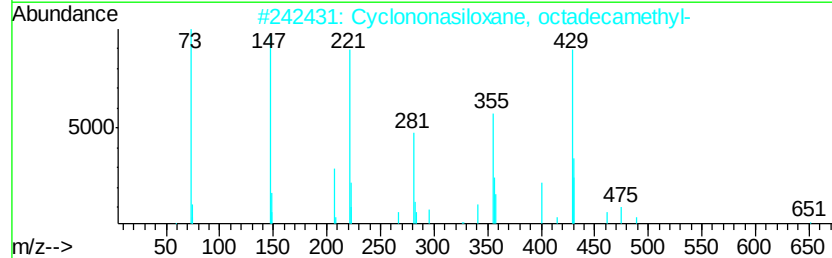
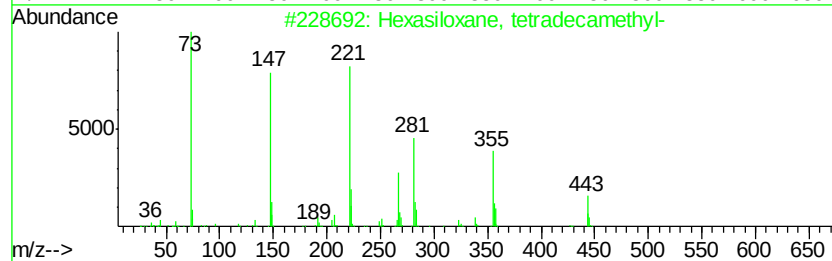
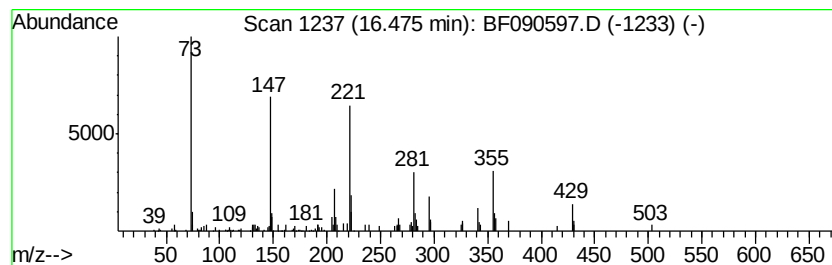
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexasiloxane, tetradecamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	3.15 ng	176455	Perylene-d12	15.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	46
4			3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	43
5			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101416\
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Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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...	5.10	15.2	ng	992105	1	6.92	1305790	20.0
unknown6.68	6.68	59.1	ng	3861640	1	6.92	1305790	20.0
Hexadecanoic acid...	12.85	2.4	ng	139451	5	14.09	1164500	20.0
n-Tetracosanol-1	13.93	4.2	ng	245970	5	14.09	1164500	20.0
Cyclononasiloxane...	15.88	3.9	ng	215673	6	15.55	1121720	20.0
Hexasiloxane, tet...	16.48	3.1	ng	176455	6	15.55	1121720	20.0