

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
 Data File : BF092937.D
 Acq On : 14 Feb 2017 12:10
 Operator : SJ/MA
 Sample : I1789-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EFF-WW

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-BF013017.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	5.047	256	259	263	rVB	623147	693331	1.66%	0.192%
2	5.424	289	292	296	rBV	611990	978621	2.35%	0.271%
3	5.607	305	308	311	rBV	389783	935680	2.24%	0.259%
4	5.916	324	335	337	rBV	6589127	32838019	78.71%	9.102%
5	6.453	376	382	383	rVV2	234757	714162	1.71%	0.198%
6	6.499	385	386	393	rVV2	309921	721903	1.73%	0.200%
7	6.659	393	400	403	rVV3	2142071	4060741	9.73%	1.126%
8	6.750	403	408	412	rVB	587212	1754504	4.21%	0.486%
9	6.876	417	419	422	rBV	938980	920753	2.21%	0.255%
10	7.024	423	432	436	rBV3	8180724	41722843	100.00%	11.565%
11	7.299	452	456	458	rBV	267687	487551	1.17%	0.135%
12	7.459	465	470	471	rBV	2236186	3352667	8.04%	0.929%
13	7.779	477	498	502	rBV3	2799150	20632133	49.45%	5.719%
14	7.836	502	503	505	rVV2	506153	648188	1.55%	0.180%
15	7.882	505	507	509	rVB	1230833	1172080	2.81%	0.325%
16	8.019	514	519	521	rVV	773164	1388525	3.33%	0.385%
17	8.167	528	532	534	rVB	1211672	1385468	3.32%	0.384%
18	8.830	585	590	591	rVV	840629	1516147	3.63%	0.420%
19	8.887	591	595	597	rVV3	902015	1827015	4.38%	0.506%
20	9.242	622	626	628	rBV	4823311	5129439	12.29%	1.422%
21	9.322	630	633	634	rBV	424515	562855	1.35%	0.156%
22	9.916	683	685	687	rVB	2028288	2013624	4.83%	0.558%
23	10.133	702	704	709	rBV2	304522	458081	1.10%	0.127%
24	10.328	719	721	724	rBV2	590165	863633	2.07%	0.239%
25	10.705	751	754	756	rBV	1698531	1894871	4.54%	0.525%
26	10.819	762	764	767	rBV2	394056	742278	1.78%	0.206%
27	10.933	772	774	775	rVV	1371654	1328489	3.18%	0.368%
28	10.956	775	776	778	rVV	2802515	3266364	7.83%	0.905%
29	10.990	778	779	784	rVB	1554047	1677057	4.02%	0.465%
30	11.265	801	803	806	rVB	380836	555429	1.33%	0.154%
31	11.356	809	811	812	rBV	473963	449788	1.08%	0.125%
32	11.390	812	814	817	rBV	945976	1240362	2.97%	0.344%
33	11.619	833	834	836	rBV	467038	587796	1.41%	0.163%
34	11.688	839	840	843	rBV	530955	502788	1.21%	0.139%

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35	11.756	843	846	847	rBV	248749	546184	1.31%	0.151%
36	11.848	852	854	859	rBV	2068237	2394538	5.74%	0.664%
37	11.962	859	864	867	rBV2	1458497	5340867	12.80%	1.480%
38	12.065	872	873	874	rVV	1427330	1710948	4.10%	0.474%
39	12.122	877	878	881	rVV	1616328	3451513	8.27%	0.957%
40	12.191	881	884	885	rVV	4966784	8855543	21.22%	2.455%
41	12.225	885	887	891	rVV	5128295	15022357	36.01%	4.164%
42	12.282	891	892	894	rVV	2460249	4543829	10.89%	1.259%
43	12.316	894	895	897	rVV2	2155081	4341048	10.40%	1.203%
44	12.351	897	898	899	rVV	2497835	2937040	7.04%	0.814%
45	12.408	899	903	905	rVV2	4095277	13548921	32.47%	3.755%
46	12.442	905	906	910	rVV3	4632195	14540892	34.85%	4.030%
47	12.499	910	911	916	rVV4	5120108	14972374	35.89%	4.150%
48	12.579	916	918	919	rVV	3385356	6573350	15.75%	1.822%
49	12.613	919	921	926	rVV3	5138015	16500154	39.55%	4.573%
50	12.728	926	931	936	rVV5	6569763	34052203	81.62%	9.438%
51	12.842	940	941	943	rVV	4272778	5165941	12.38%	1.432%
52	12.876	943	944	948	rVV	5440352	8675496	20.79%	2.405%
53	12.945	948	950	952	rVV2	5421587	8594037	20.60%	2.382%
54	13.002	952	955	958	rVV	3951674	10732969	25.72%	2.975%
55	13.059	958	960	963	rVV3	1719289	5001488	11.99%	1.386%
56	13.128	963	966	973	rVV5	2112317	9724833	23.31%	2.695%
57	13.219	973	974	977	rVV2	1125100	1713212	4.11%	0.475%
58	13.299	978	981	982	rVV	2505498	2998898	7.19%	0.831%
59	13.334	982	984	987	rVV2	805560	1411729	3.38%	0.391%
60	13.402	987	990	991	rVV2	1426524	2922280	7.00%	0.810%
61	13.436	991	993	998	rVB2	1728126	4371130	10.48%	1.212%
62	13.551	1001	1003	1006	rVB	989102	1048767	2.51%	0.291%
63	13.619	1006	1009	1010	rBV	845011	890535	2.13%	0.247%
64	13.654	1010	1012	1014	rVB	1138078	1572529	3.77%	0.436%
65	13.745	1014	1020	1021	rBV2	463403	696524	1.67%	0.193%
66	13.882	1030	1032	1035	rVB	467600	548521	1.31%	0.152%
67	13.985	1039	1041	1043	rVB	1363182	1148278	2.75%	0.318%
68	14.031	1043	1045	1048	rBV	767689	993340	2.38%	0.275%
69	14.248	1062	1064	1066	rBV2	498727	525890	1.26%	0.146%
70	14.499	1083	1086	1089	rVB	395703	422330	1.01%	0.117%
71	15.151	1142	1143	1153	rVB	226798	433324	1.04%	0.120%

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72	15.459	1168	1170	1176	rBV	520960	817170	1.96%	0.227%
73	18.134	1397	1404	1414	rVB2	180915	949323	2.28%	0.263%
74	18.946	1470	1475	1493	rVB	257010	1067736	2.56%	0.296%

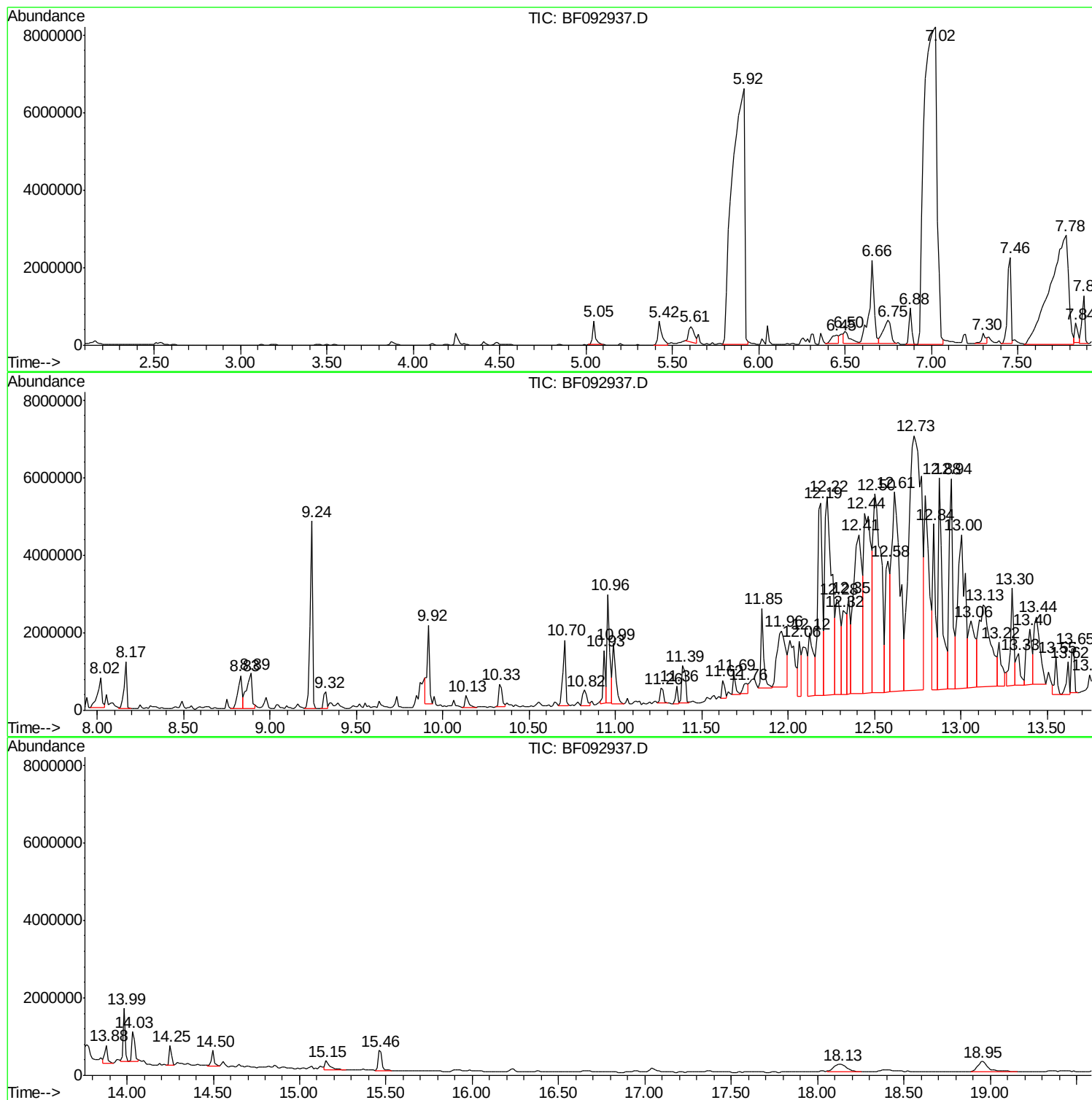
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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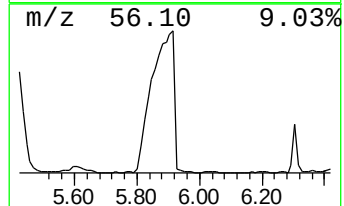
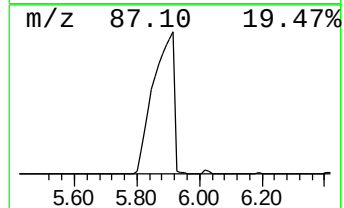
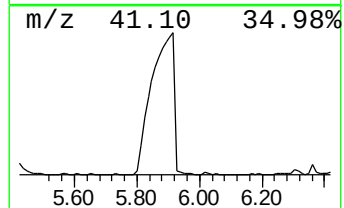
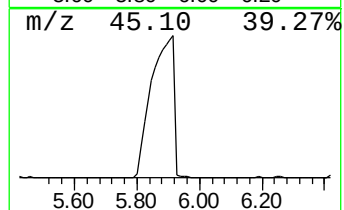
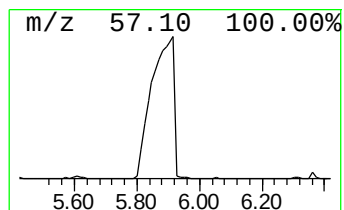
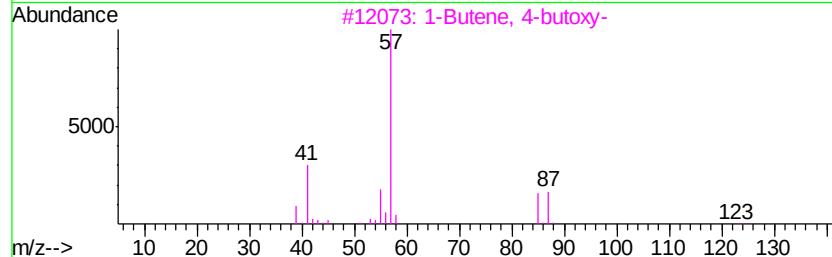
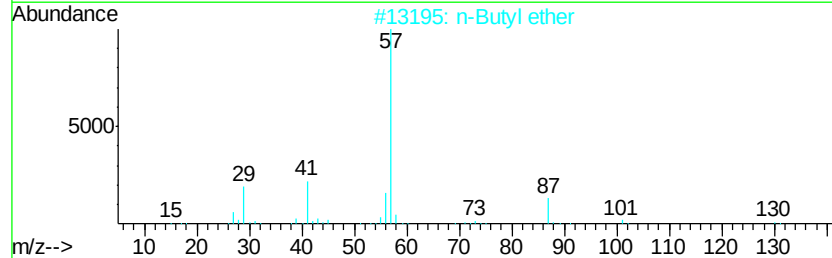
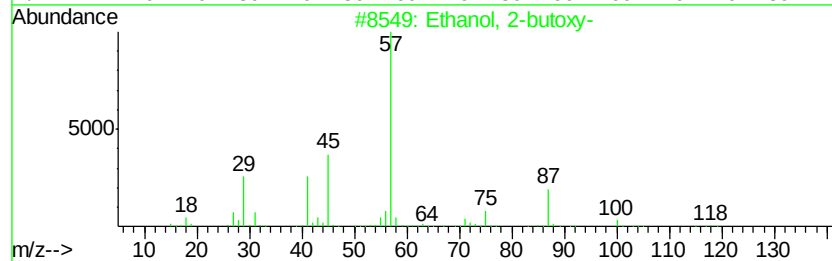
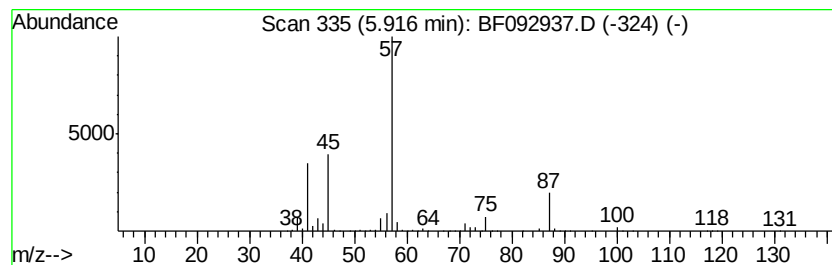
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.92	713.29 ng	32838000	1,4-Dichlorobenzene-d4	6.88	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	91
2	n-Butyl ether	130	C8H18O	000142-96-1	25
3	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	23
4	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	14
5	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	12



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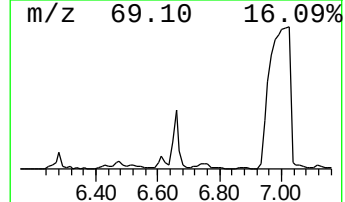
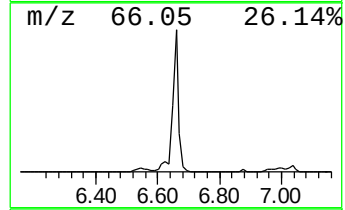
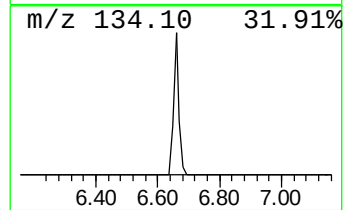
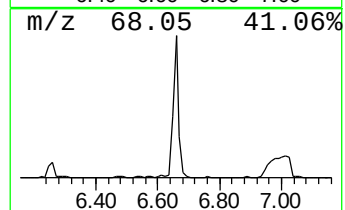
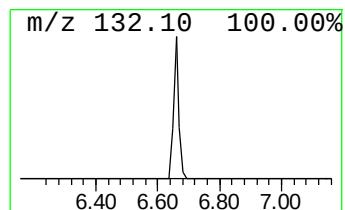
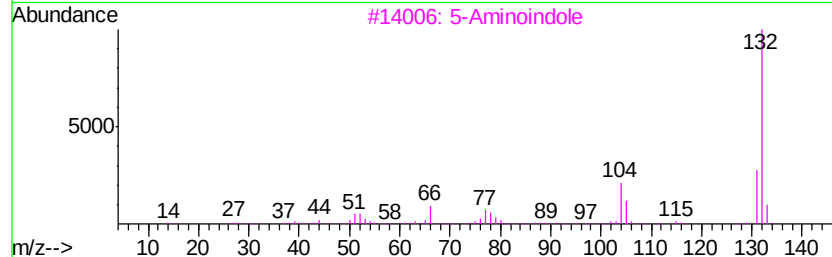
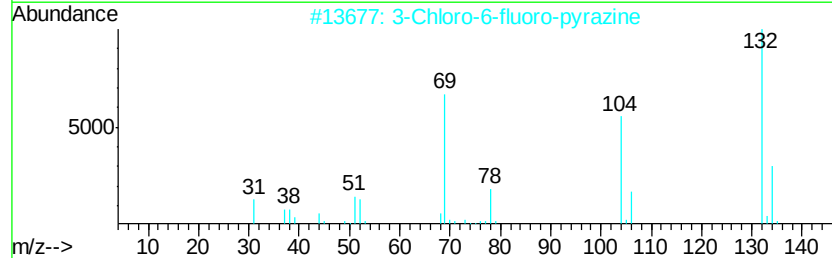
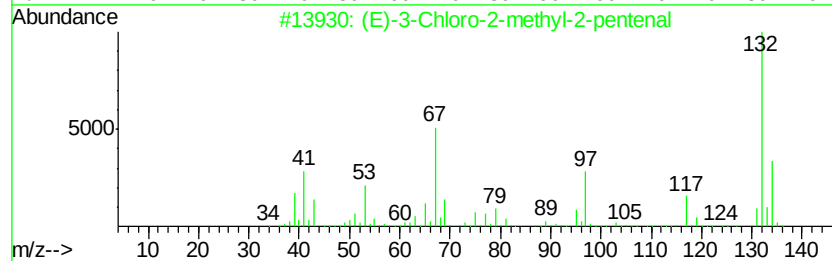
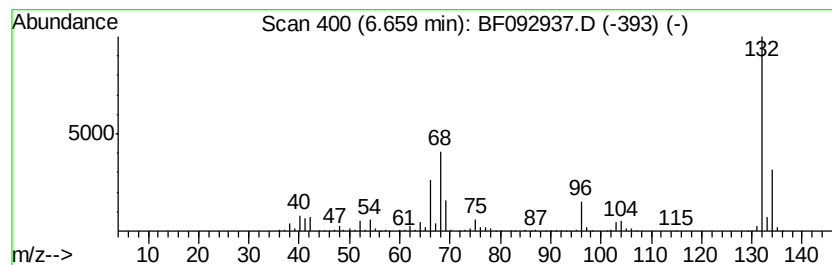
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.66 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	88.20 ng	4060740	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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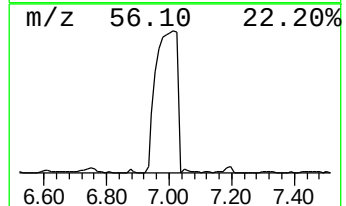
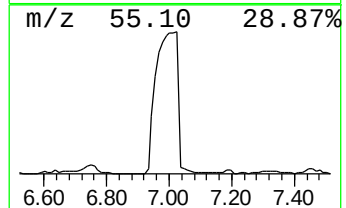
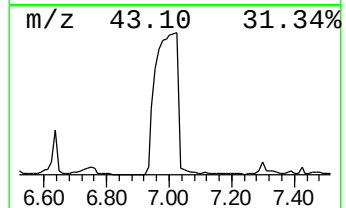
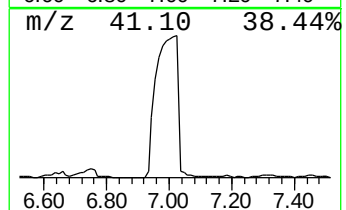
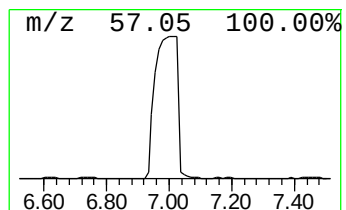
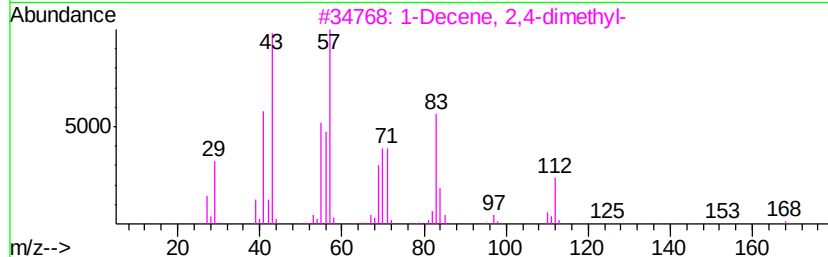
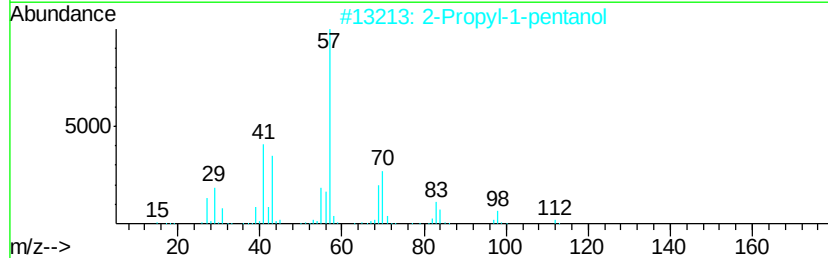
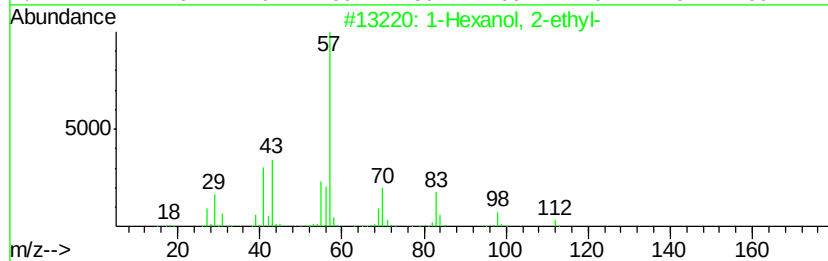
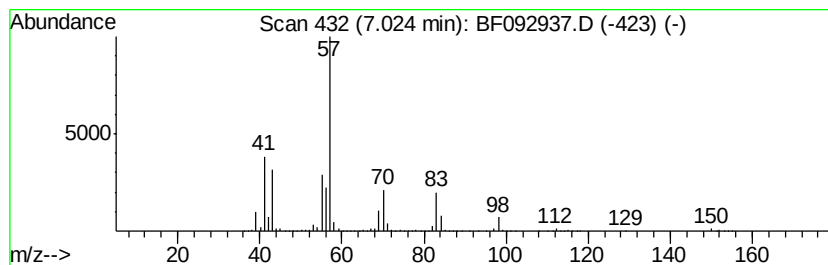
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	906.28 ng	41722800	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
3		1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	42
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42
5		dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	42



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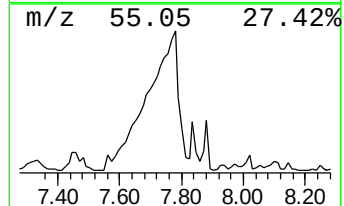
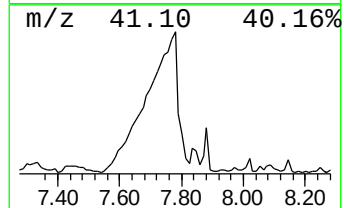
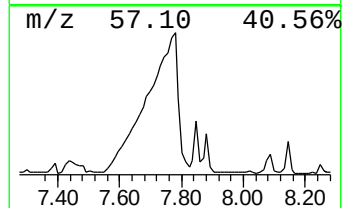
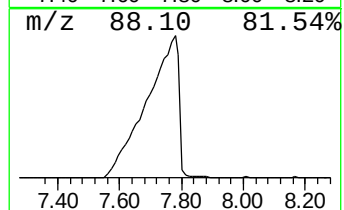
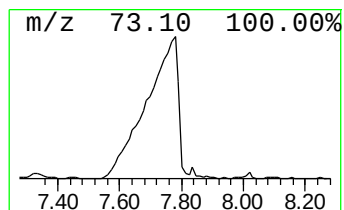
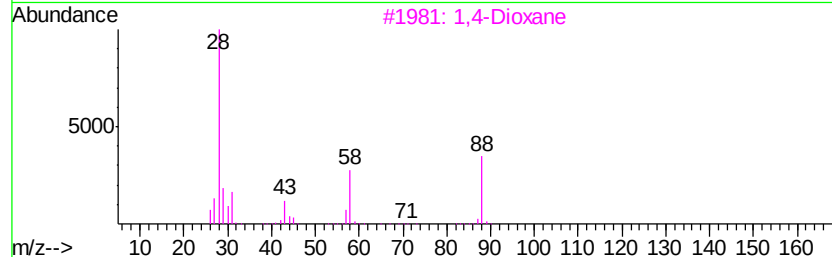
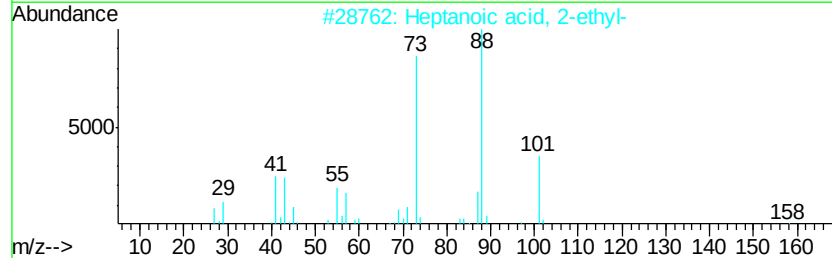
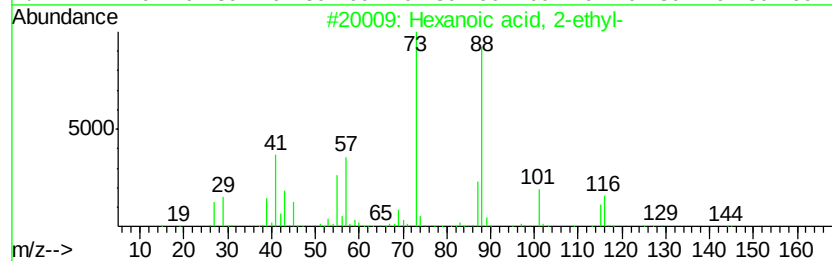
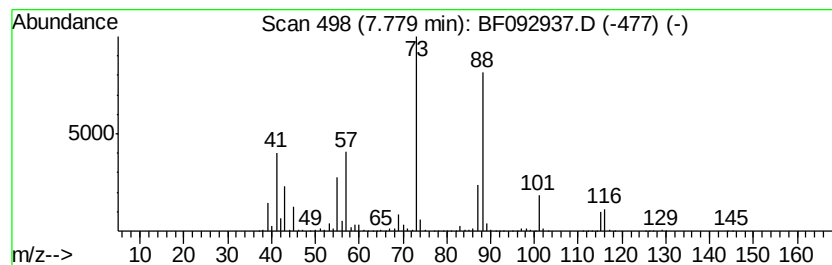
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	297.84 ng	20632100	Naphthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3		1,4-Dioxane	88	C4H8O2	000123-91-1	47
4		Heptanoic acid, 2-methyl-, methy...	158	C9H18O2	051209-78-0	43
5		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
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Operator : SJ/MA
Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

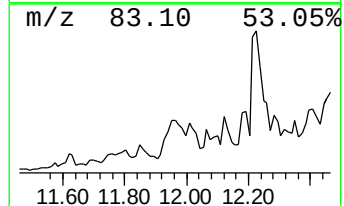
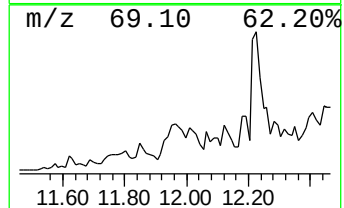
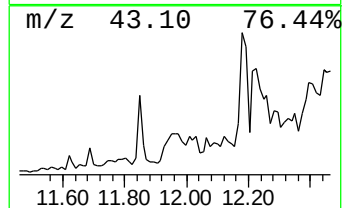
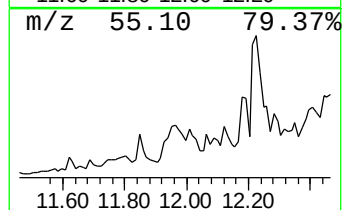
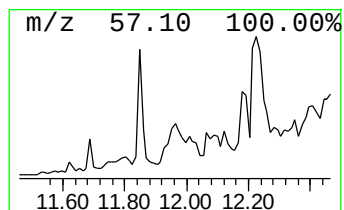
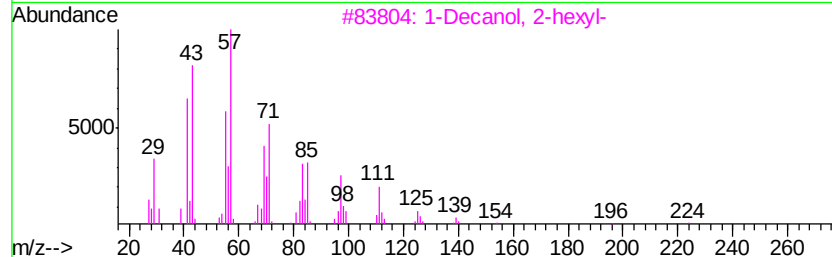
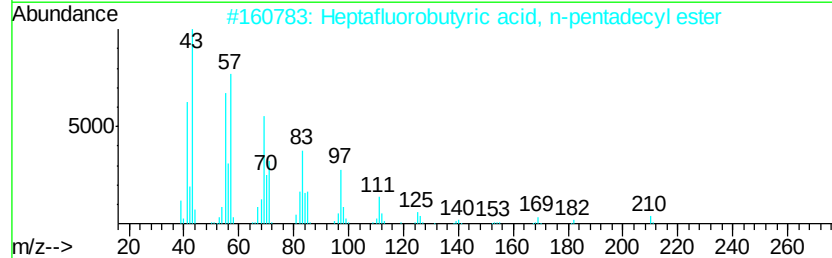
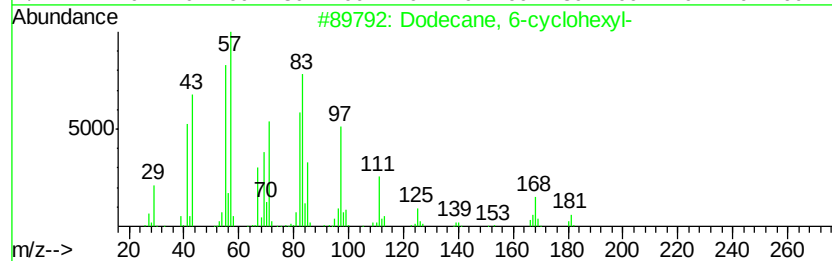
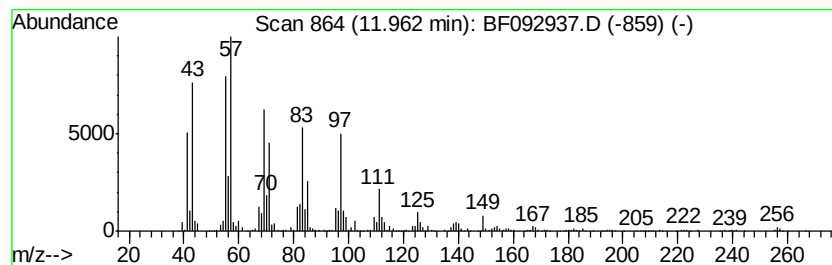
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dodecane, 6-cyclohexyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.96	86.12 ng	5340870	Phenanthrene-d10	11.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	91	
2	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	72	
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70	
4	9-Nonadecene	266	C19H38	031035-07-1	70	
5	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	49	



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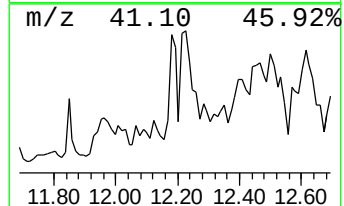
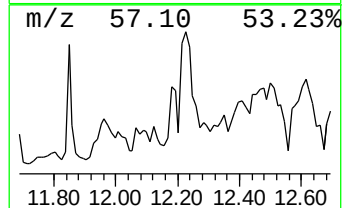
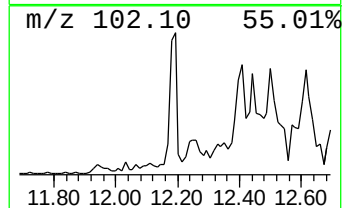
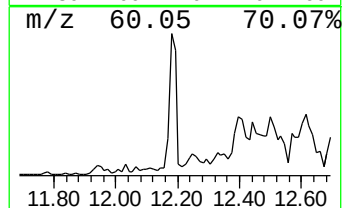
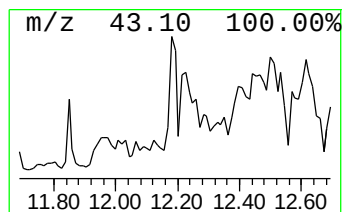
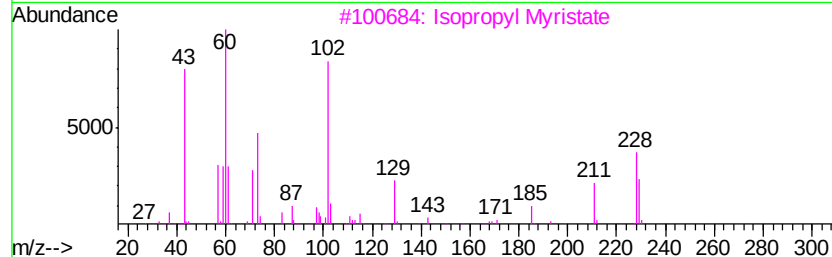
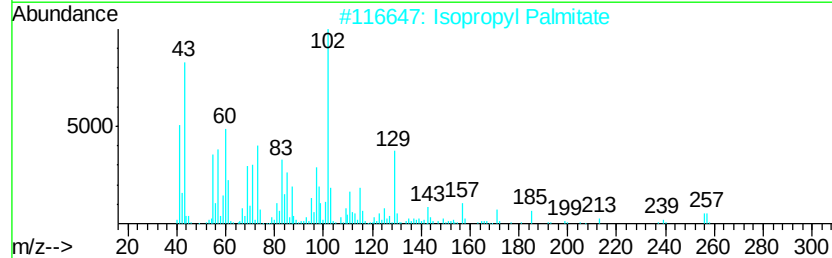
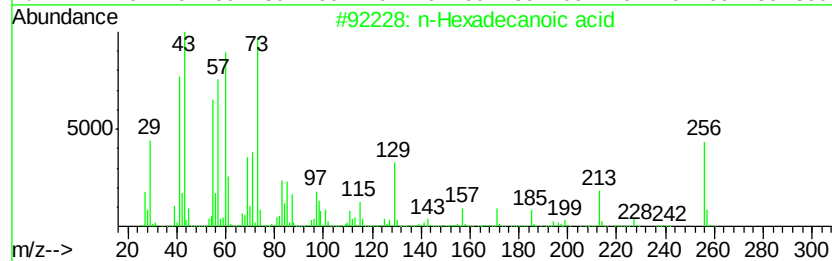
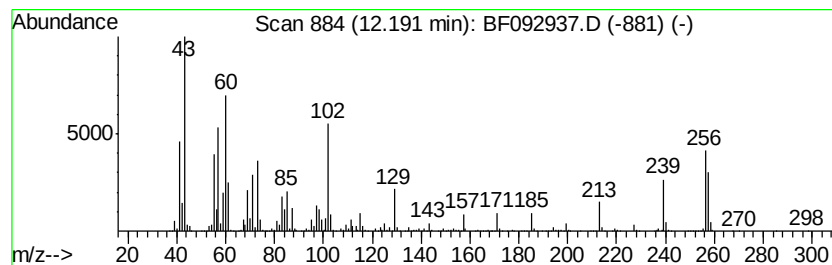
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	142.79 ng	8855540	Phenanthrene-d10	11.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 90
2		Isopropyl Palmitate	298 C19H38O2	000142-91-6 74
3		Isopropyl Myristate	270 C17H34O2	000110-27-0 53
4		Dodecanoic acid, 1-methylethyl e...	242 C15H30O2	010233-13-3 43
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129 C5H7NOS	029926-41-8 18



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Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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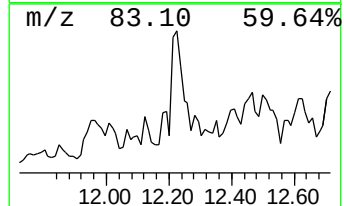
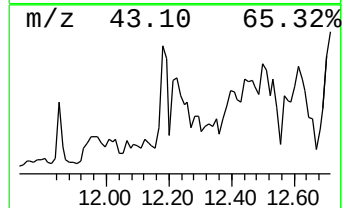
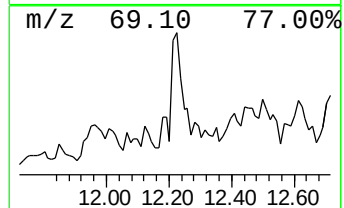
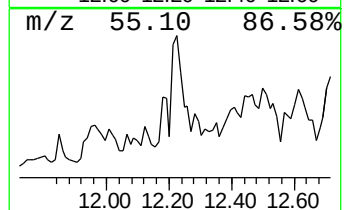
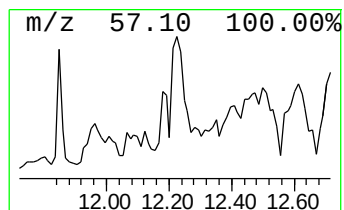
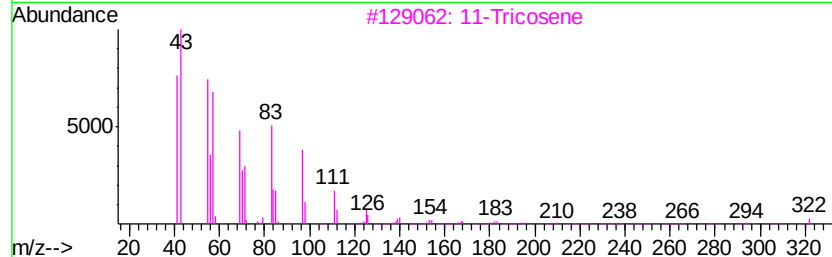
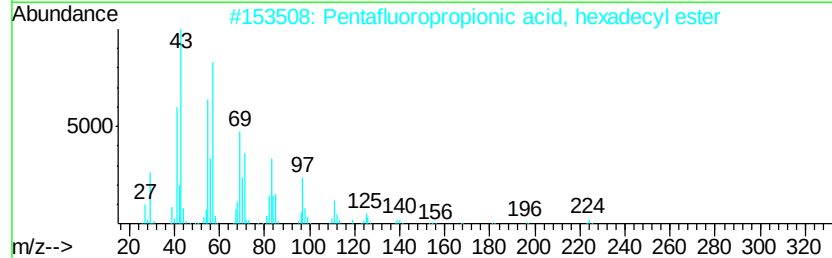
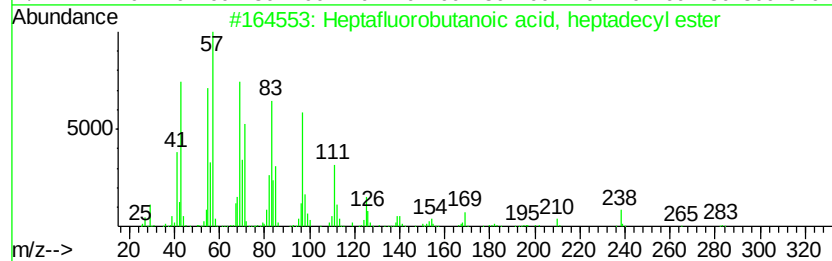
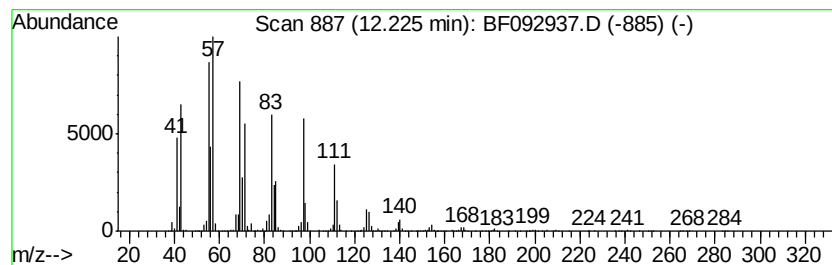
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	242.23 ng	15022400	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
3		11-Tricosene	322	C23H46	052078-56-5	86
4		17-Pentatriacontene	491	C35H70	006971-40-0	86
5		1-Undecene, 7-methyl-	168	C12H24	074630-42-5	58



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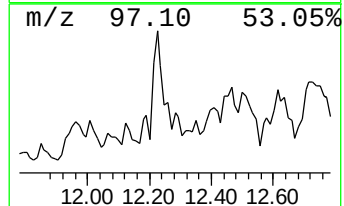
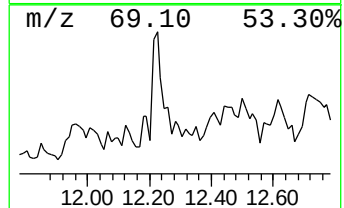
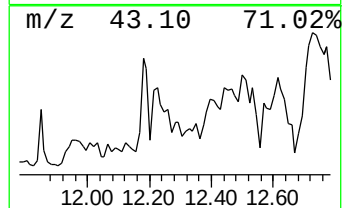
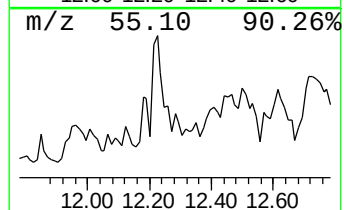
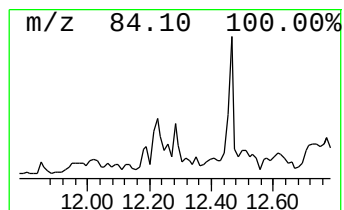
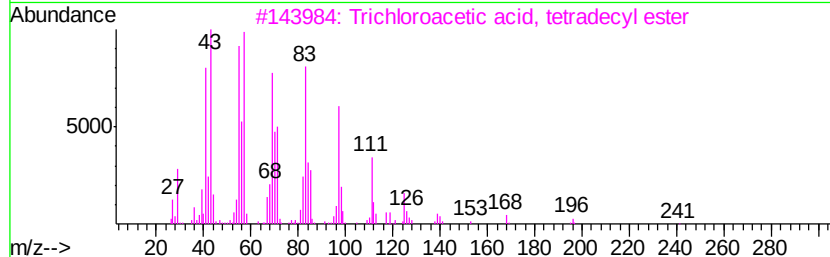
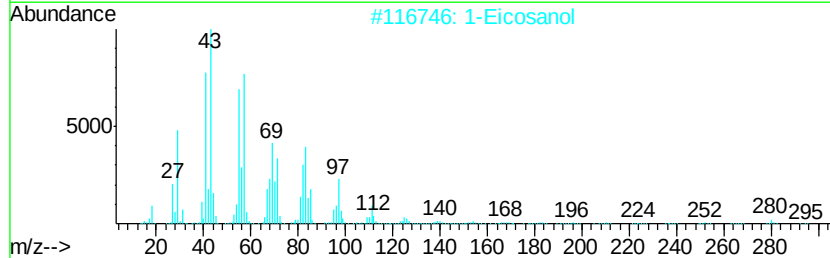
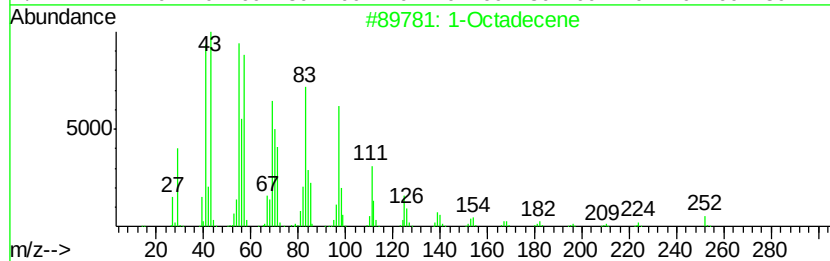
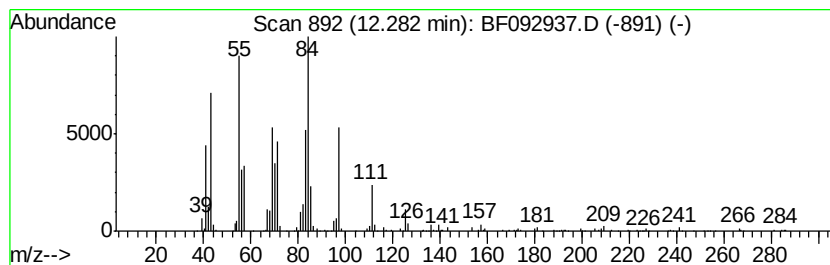
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Octadecene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	73.27 ng	4543830	Phenanthrene-d10	11.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecene	252 C18H36	000112-88-9	52
2	1-Eicosanol	298 C20H42O	000629-96-9	50
3	Trichloroacetic acid, tetradecyl...	358 C16H29Cl3O2	074339-52-9	46
4	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	43
5	4-Heptafluorobutyroxytridecane	396 C17H27F7O2	1000245-49-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
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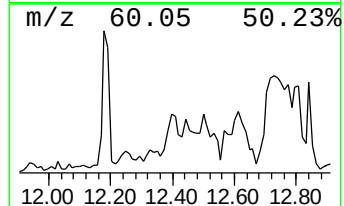
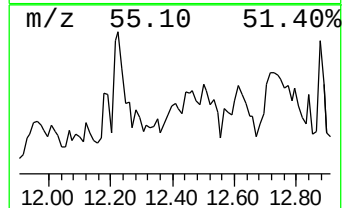
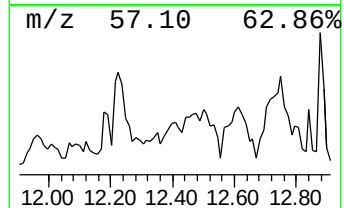
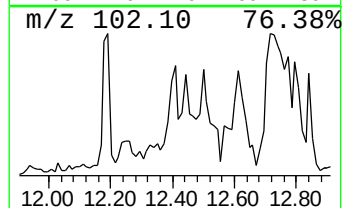
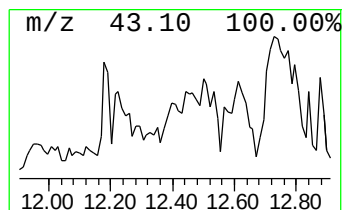
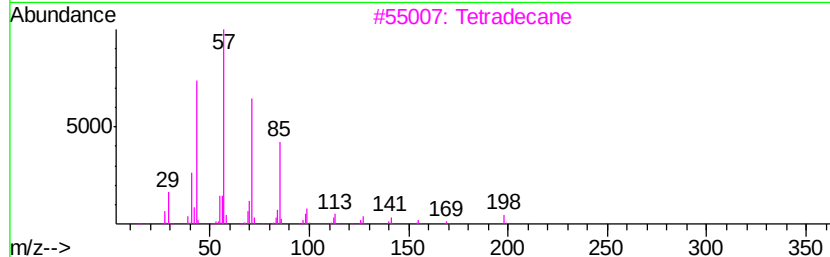
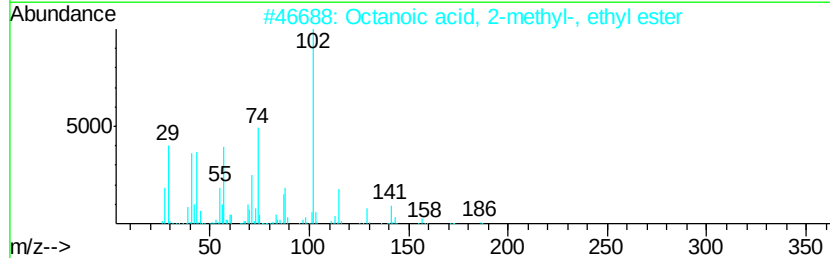
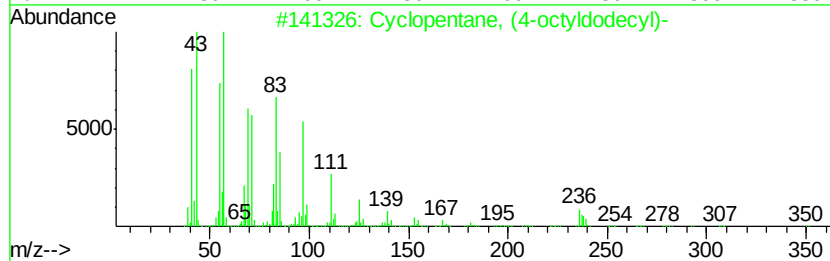
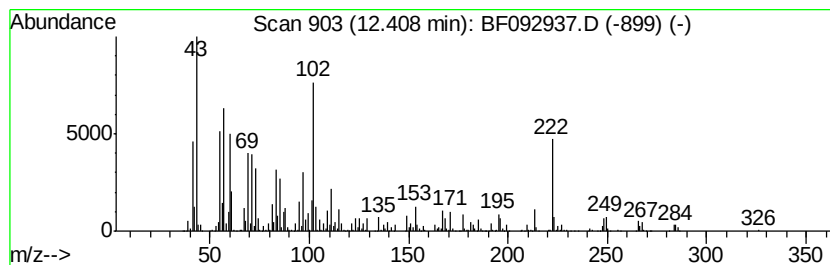
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown12.41 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	218.47 ng	13548900	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	18
2		Octanoic acid, 2-methyl-, ethyl ...	186	C11H22O2	030982-02-6	18
3		Tetradecane	198	C14H30	000629-59-4	11
4		Heptadecane	240	C17H36	000629-78-7	11
5		Tridecane	184	C13H28	000629-50-5	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
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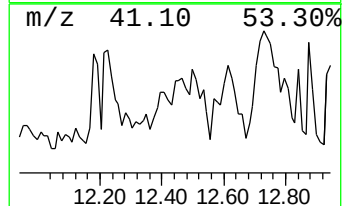
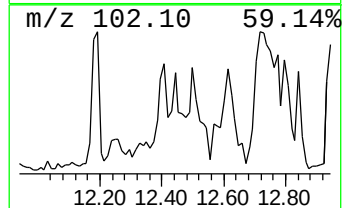
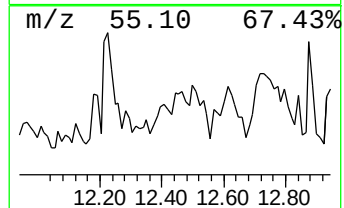
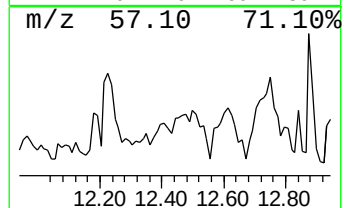
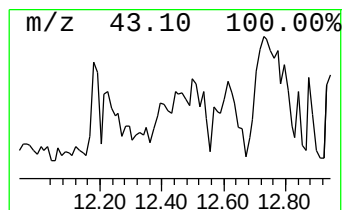
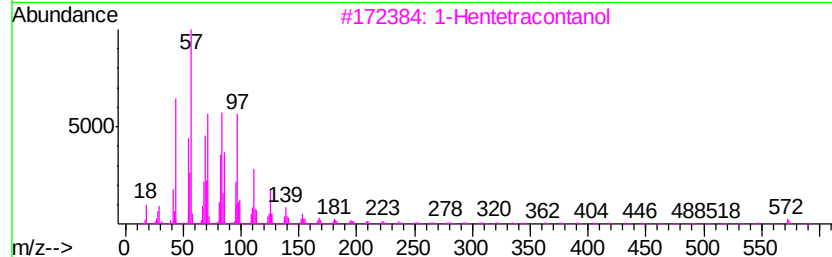
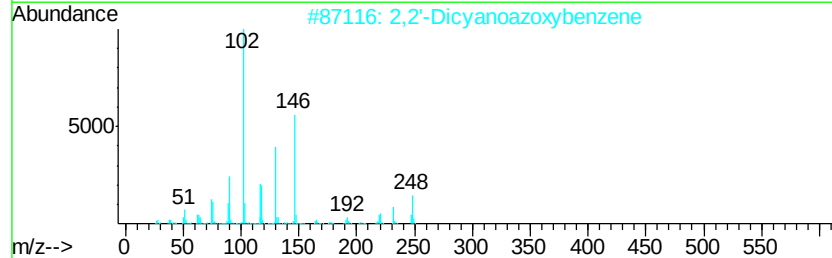
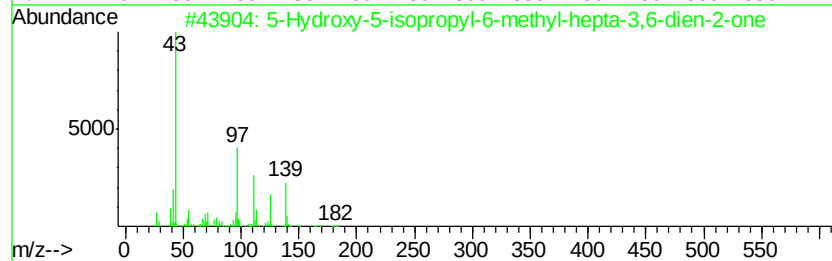
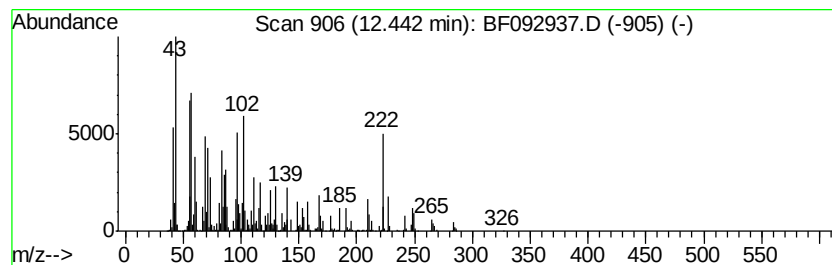
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown12.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.44	234.46 ng	14540900	Phenanthrene-d10	11.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxy-5-isopropyl-6-methyl-h...	182	C11H18O2	1000187-15-9	38	
2	2,2'-Dicyanoazoxybenzene	248	C14H8N4O	001885-69-4	30	
3	1-Hentetracontanol	593	C41H84O	040710-42-7	18	
4	Pentadec-7-ene, 7-bromomethyl-	302	C16H31Br	1000259-58-5	14	
5	Cyclohexanecarboxylic acid, 4-he...	320	C20H29FO2	133856-78-7	12	



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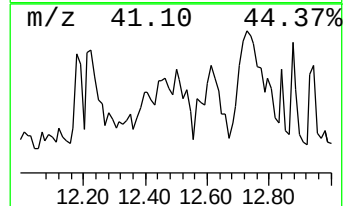
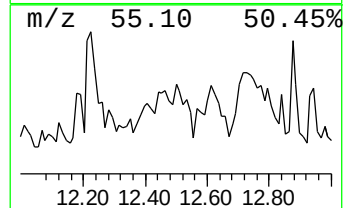
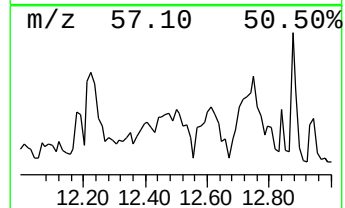
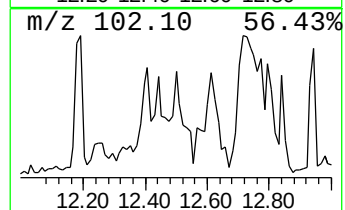
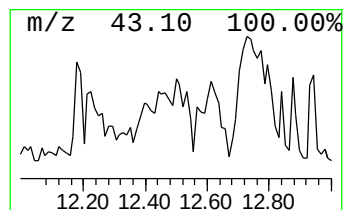
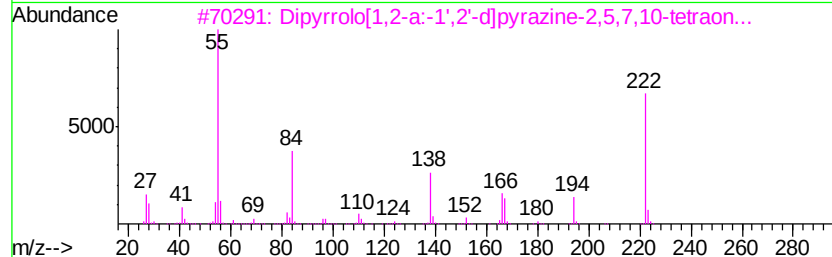
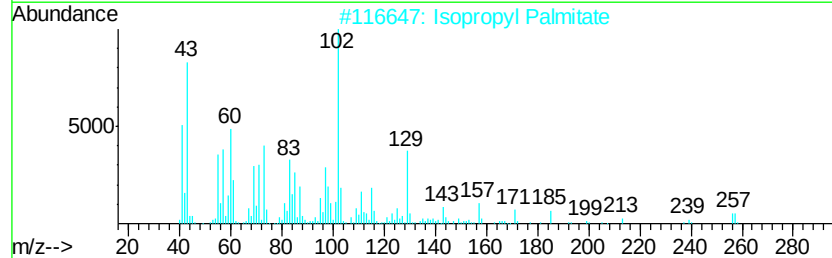
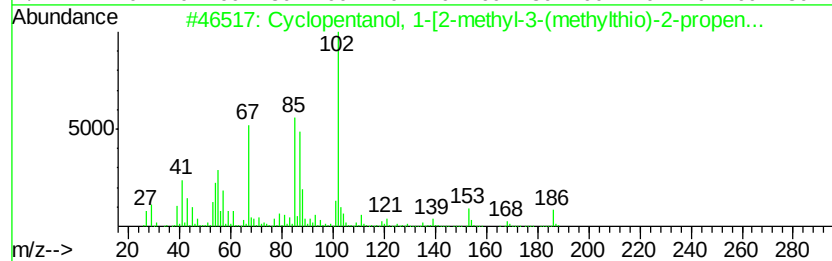
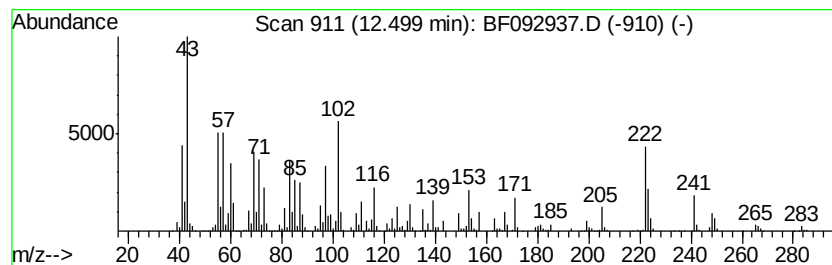
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown12.50 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.50	241.42 ng	14972400	Phenanthrene-d10	11.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentanol, 1-[2-methyl-3-(me...	186	C10H18OS	063297-93-8	12
2		Isopropyl Palmitate	298	C19H38O2	000142-91-6	12
3		Dipyrrolo[1,2-a:-1',2'-d]pyrazin...	222	C10H10N2O4	063667-06-1	10
4		Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	10
5		Heptanoic acid, 2,2-dimethyl-6-o...	186	C10H18O3	000926-27-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
Operator : SJ/MA
Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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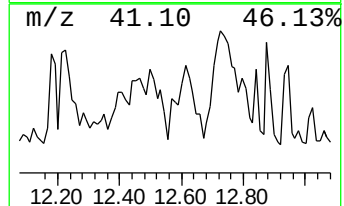
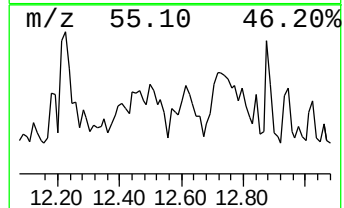
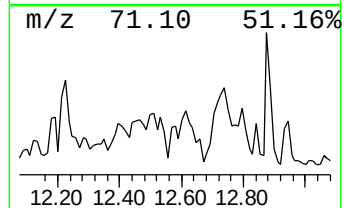
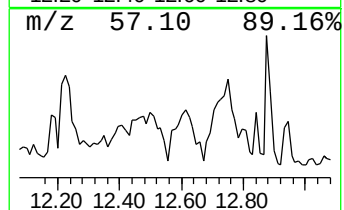
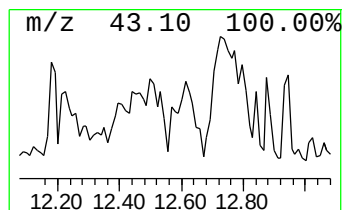
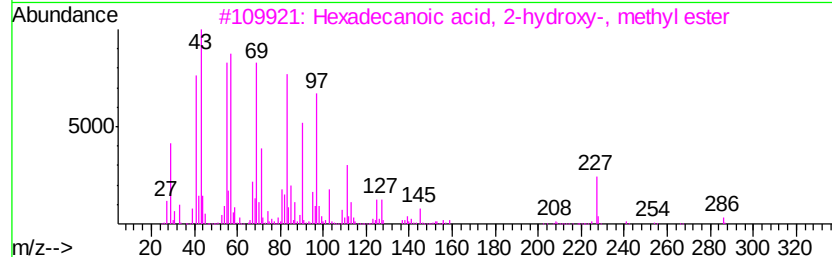
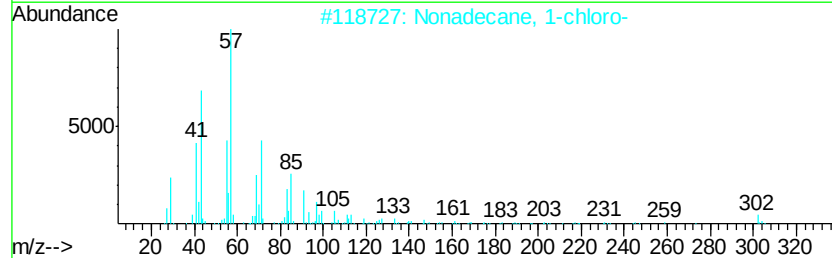
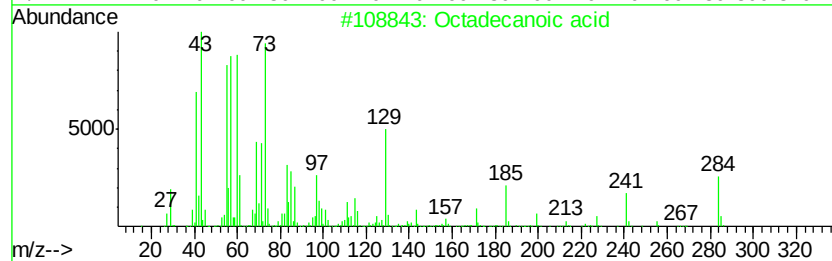
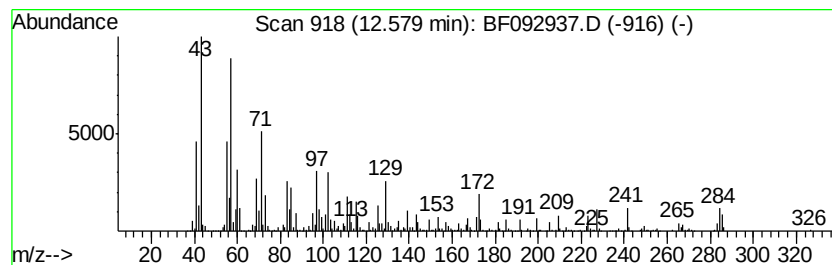
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown12.58 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	105.99 ng	6573350	Phenanthrene-d10	11.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	38
2		Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	30
3		Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	25
4		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	25
5		Undecane	156	C11H24	001120-21-4	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
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Misc :
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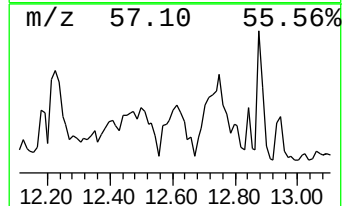
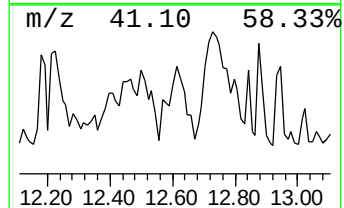
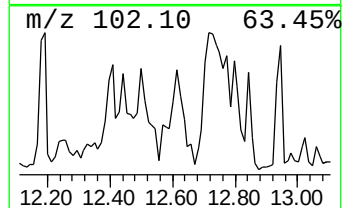
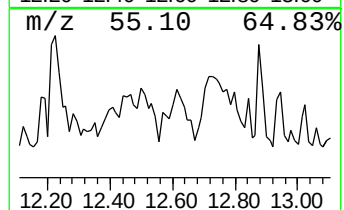
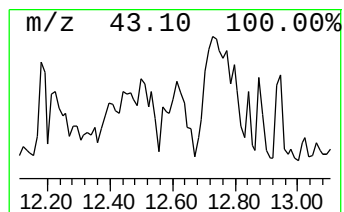
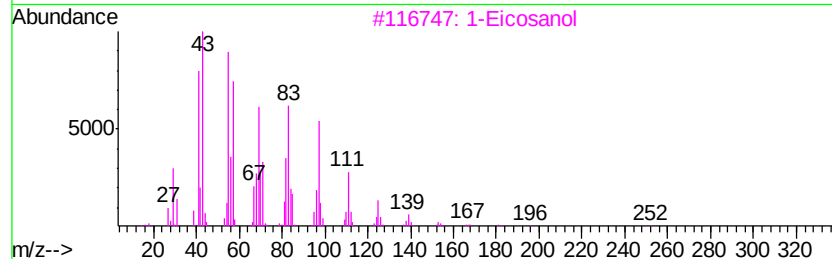
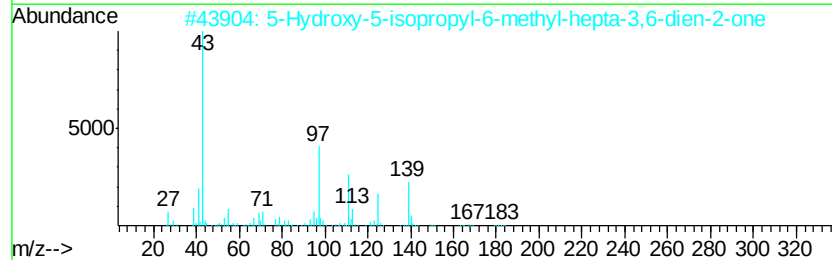
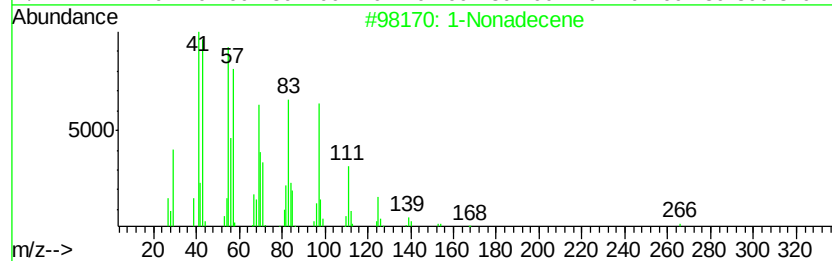
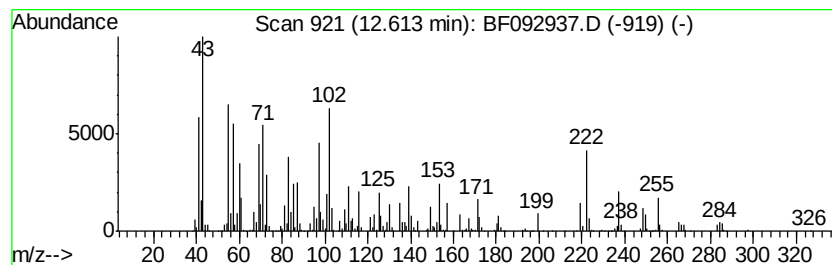
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown12.61 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.61	266.05 ng	16500200	Phenanthrene-d10	11.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene		266 C19H38	018435-45-5 42
2	5-Hydroxy-5-isopropyl-6-methyl-h...		182 C11H18O2	1000187-15-9 27
3	1-Eicosanol		298 C20H42O	000629-96-9 22
4	Cyclohexane, 1,2,3,4,5,6-hexaethyl-		252 C18H36	001795-14-8 22
5	E-14-Hexadecenal		238 C16H30O	330207-53-9 15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
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Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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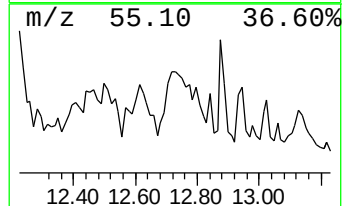
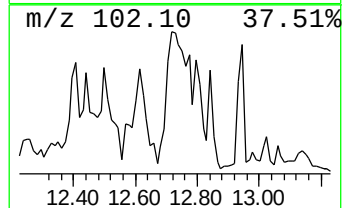
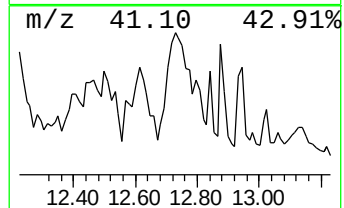
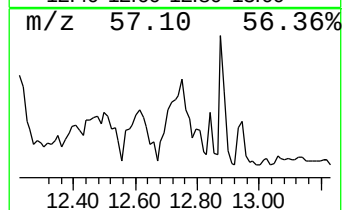
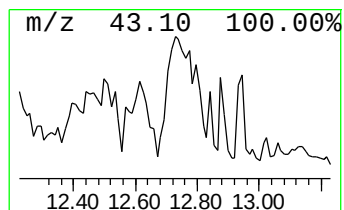
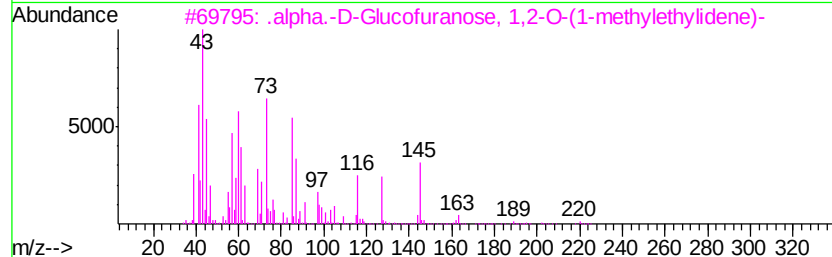
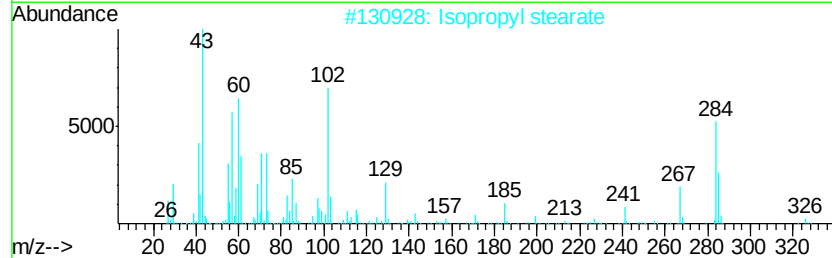
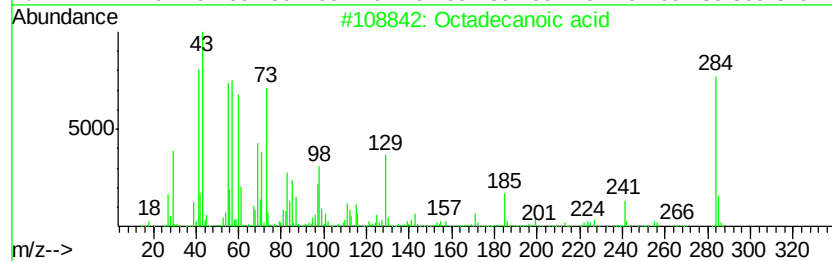
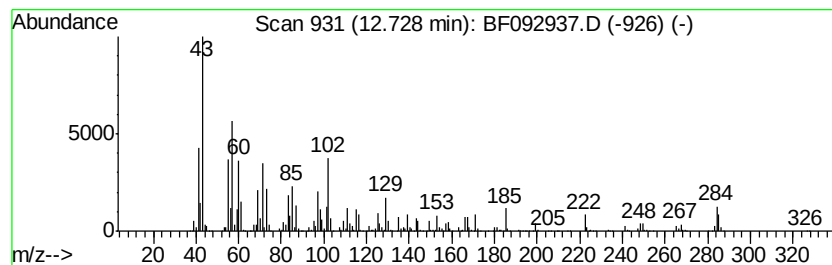
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown12.73 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	685.61 ng	34052200	Chrysene-d12	14.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	46
2		Isopropyl stearate	326	C21H42O2	000112-10-7	38
3		.alpha.-D-Glucofuranose, 1,2-O-(...	220	C9H16O6	018549-40-1	35
4		n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	25
5		N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
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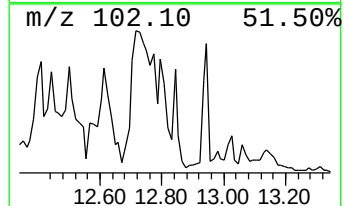
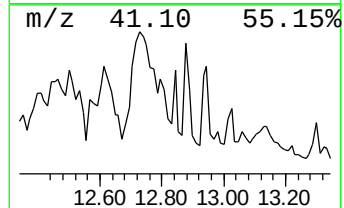
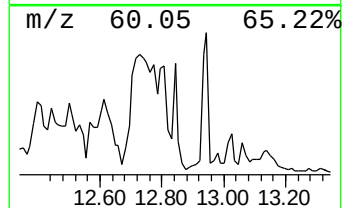
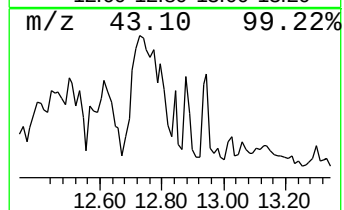
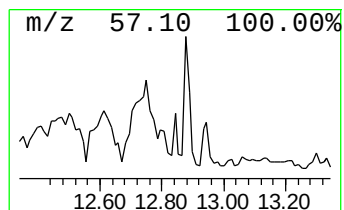
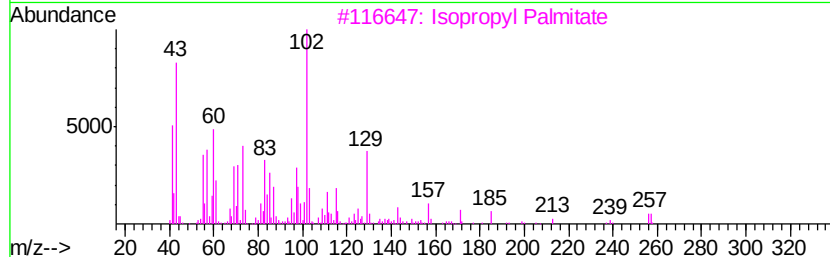
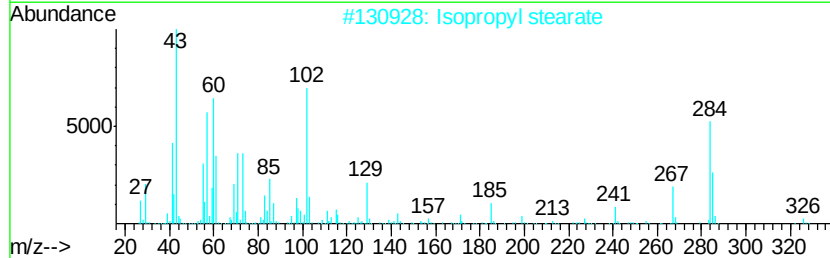
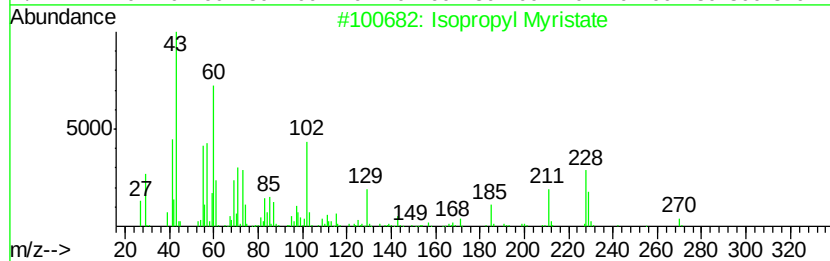
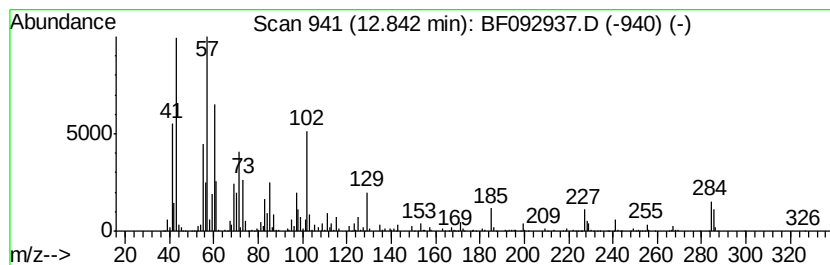
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Isopropyl Myristate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	104.01 ng	5165940	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Isopropyl Myristate	270 C17H34O2	000110-27-0	72
2	Isopropyl stearate	326 C21H42O2	000112-10-7	64
3	Isopropyl Palmitate	298 C19H38O2	000142-91-6	49
4	Octadecanoic acid	284 C18H36O2	000057-11-4	46
5	n-Decanoic acid	172 C10H20O2	000334-48-5	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
Operator : SJ/MA
Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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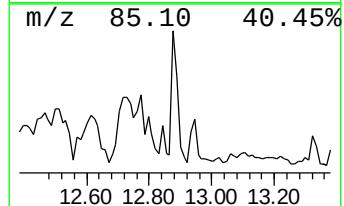
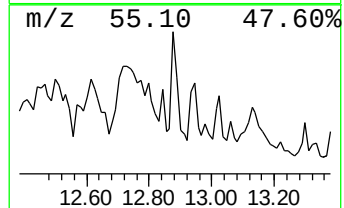
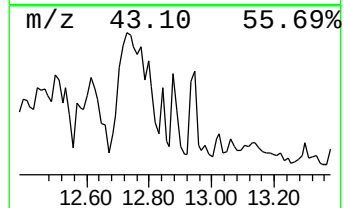
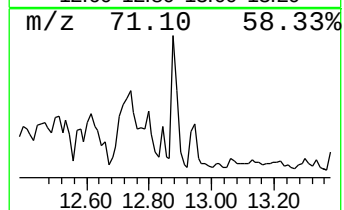
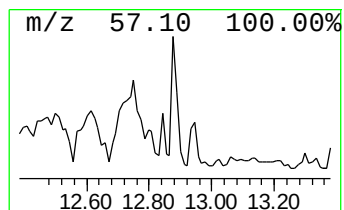
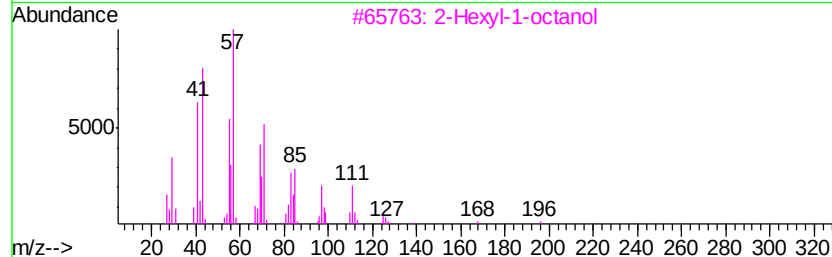
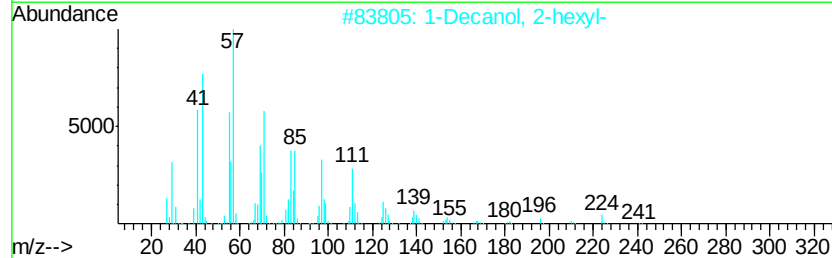
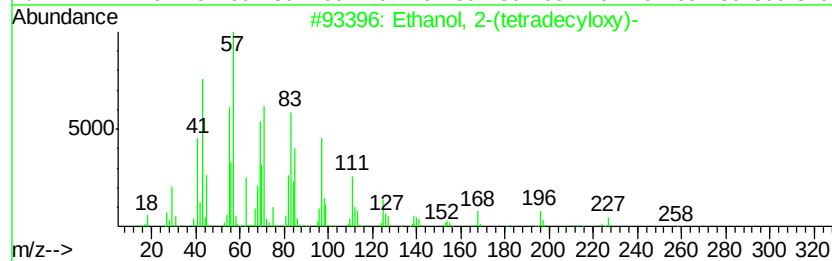
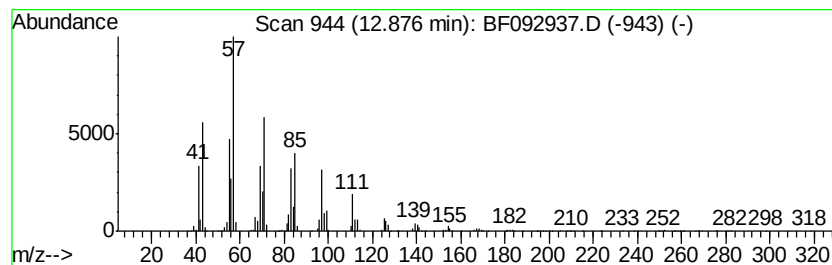
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Ethanol, 2-(tetradecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	174.67 ng	8675500	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
3		2-Hexyl-1-octanol	214	C14H30O	019780-79-1	80
4		Nonane	128	C9H20	000111-84-2	60
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
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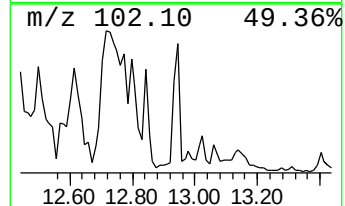
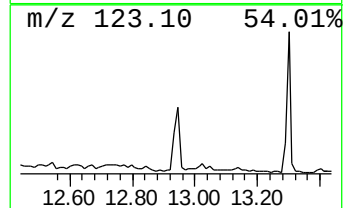
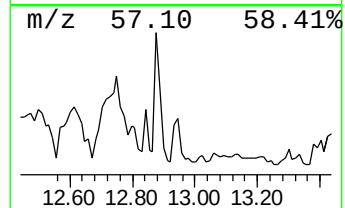
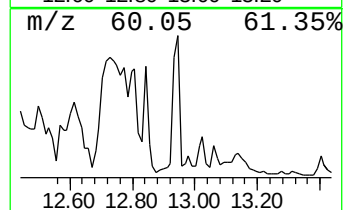
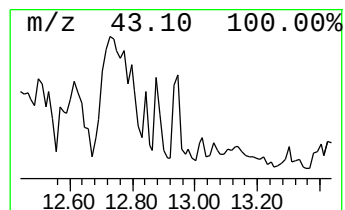
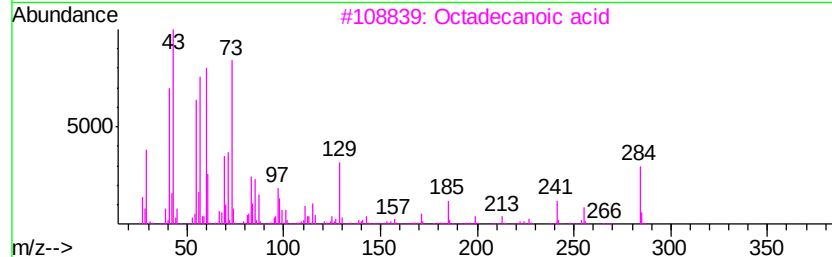
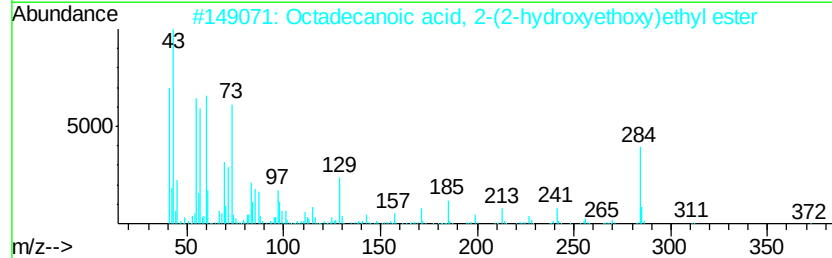
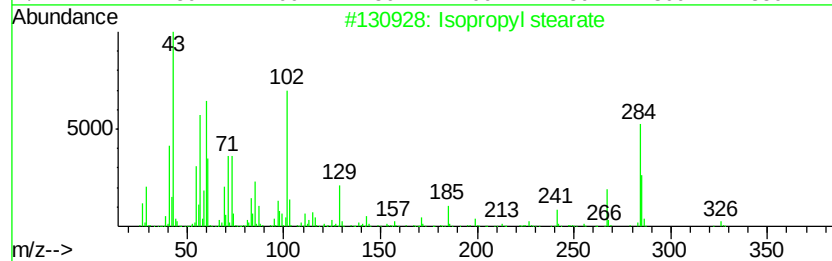
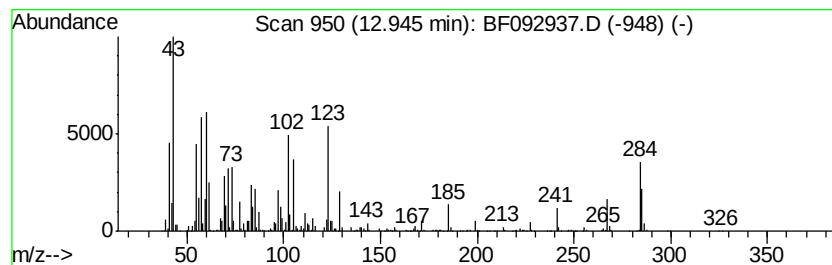
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Isopropyl stearate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.94	173.03 ng	8594040	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Isopropyl stearate	326 C21H42O2	000112-10-7	76
2	Octadecanoic acid, 2-(2-hydroxye...	372 C22H44O4	000106-11-6	45
3	Octadecanoic acid	284 C18H36O2	000057-11-4	41
4	Isopropyl Myristate	270 C17H34O2	000110-27-0	35
5	Methyl isopropylidene-.beta.-d-a...	204 C9H16O5	1000129-88-1	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
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Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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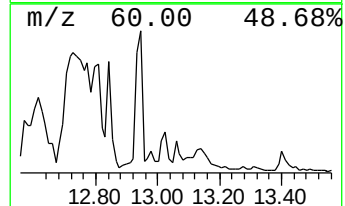
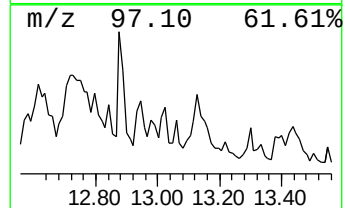
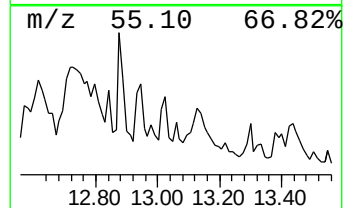
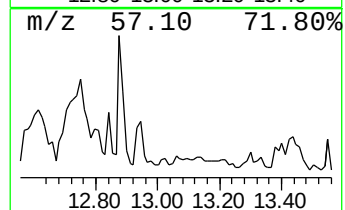
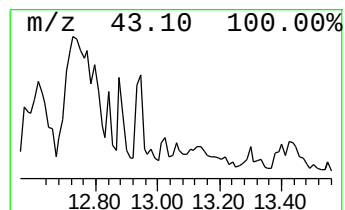
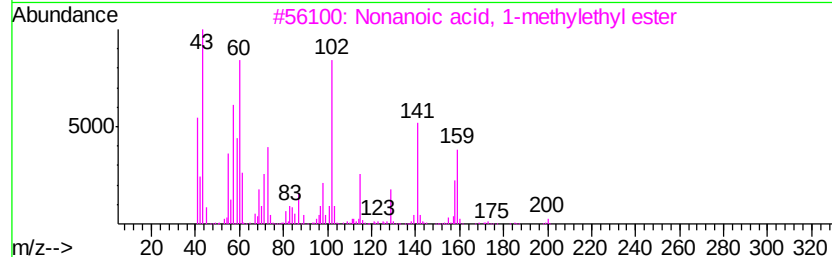
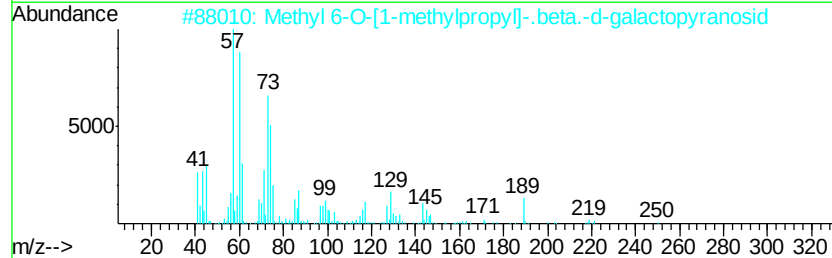
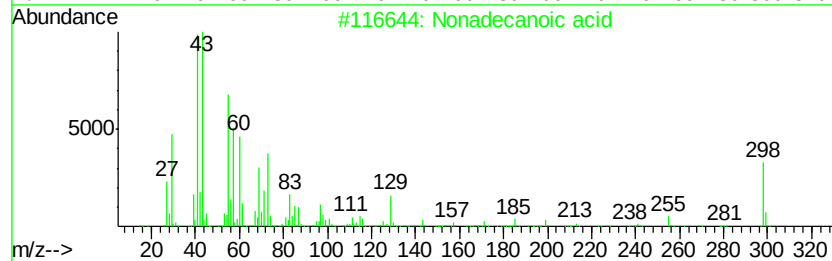
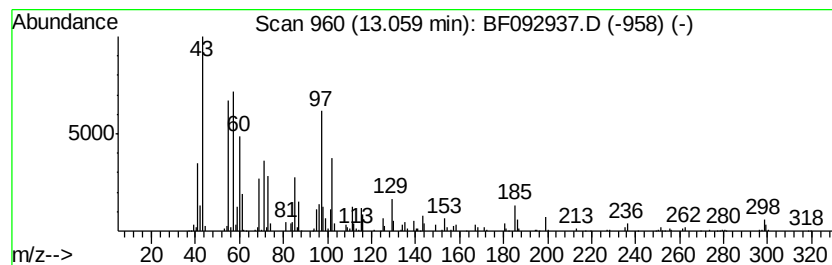
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown13.06 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	100.70 ng	5001490	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecanoic acid	298	C19H38O2	000646-30-0	41
2		Methyl 6-O-[1-methylpropyl]-.bet...	250	C11H22O6	1000126-15-7	38
3		Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	37
4		.alpha.-D-Glucofuranose, 1,2-O-(...	220	C9H16O6	018549-40-1	35
5		D-Erythro-Pentose, 2-deoxy-	134	C5H10O4	000533-67-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
Operator : SJ/MA
Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

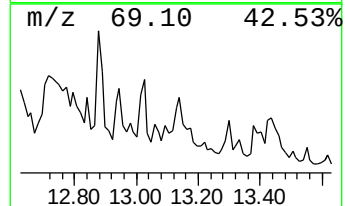
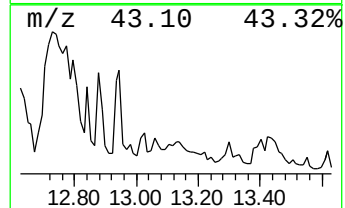
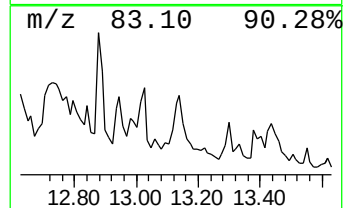
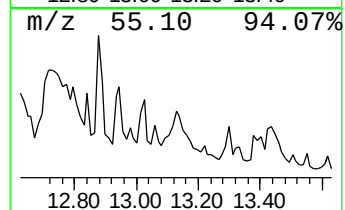
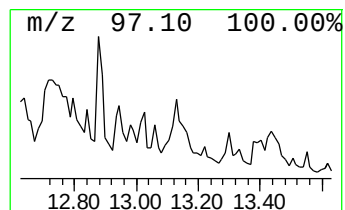
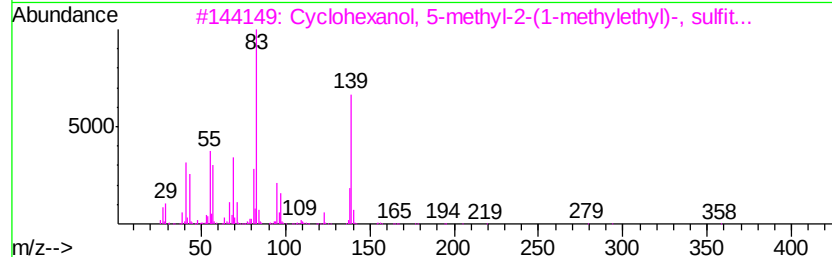
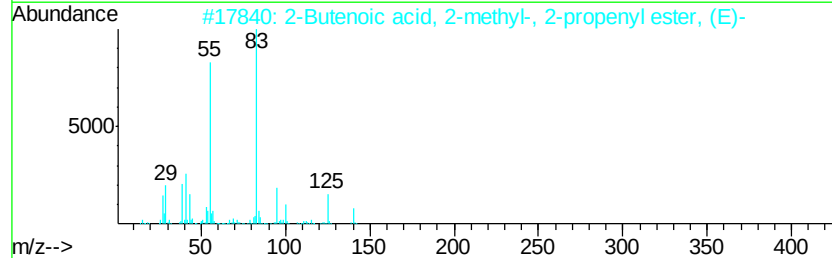
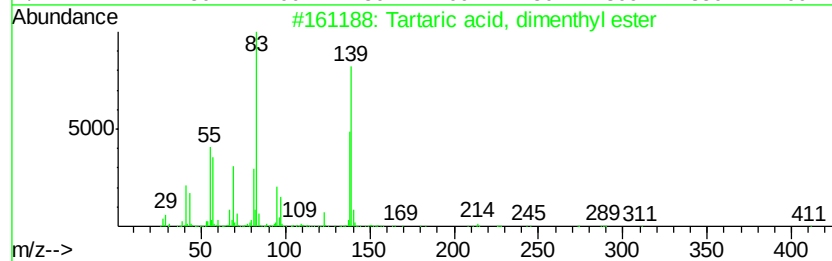
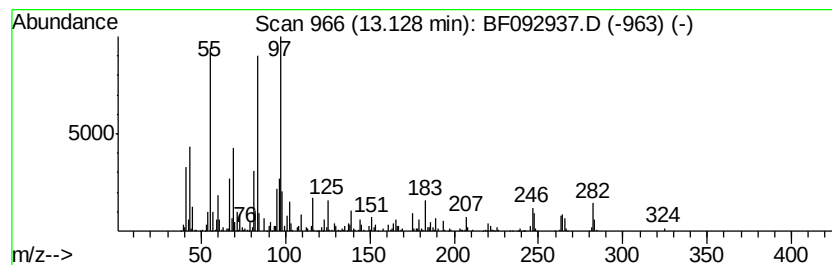
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown13.13 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	195.80 ng	9724830	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tartaric acid, dimethyl ester	426	C24H42O6	1000149-89-9	35
2		2-Butenoic acid, 2-methyl-, 2-propenyl ester, (E)-	140	C8H12O2	007493-71-2	27
3		Cyclohexanol, 5-methyl-2-(1-methylethyl)-, sulfite	358	C20H38O3S	026510-92-9	27
4		5-Amino-3-methylpyrazole	97	C4H7N3	031230-17-8	27
5		2,2,3,3-Tetramethylcyclopropanecarboxylic acid	238	C15H26O2	1000221-97-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092937.D
Acq On : 14 Feb 2017 12:10
Operator : SJ/MA
Sample : I1789-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EFF-WW

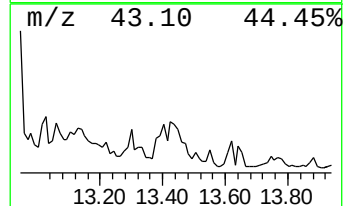
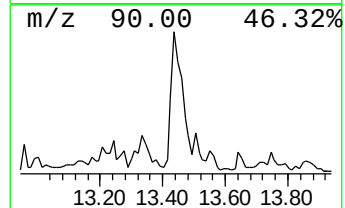
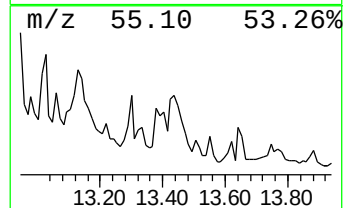
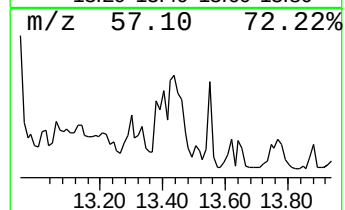
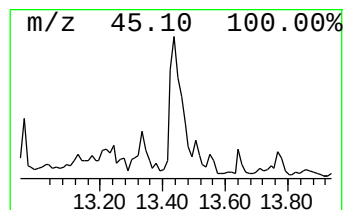
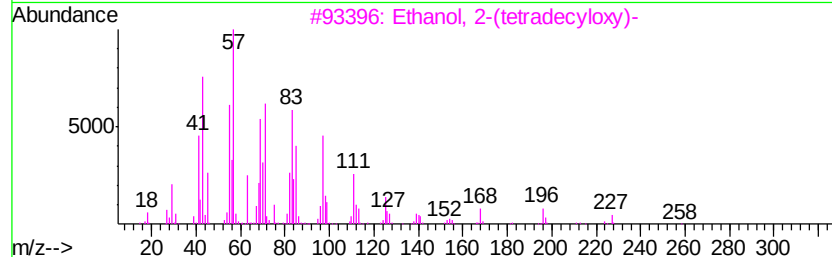
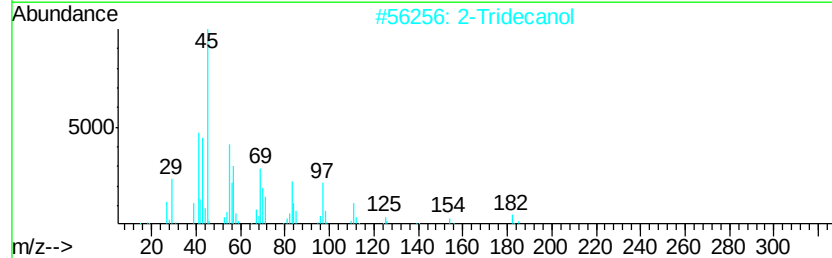
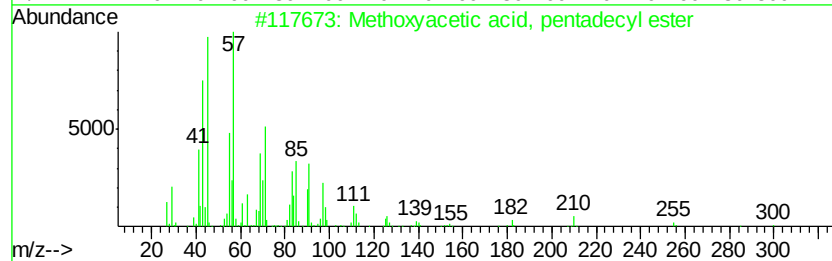
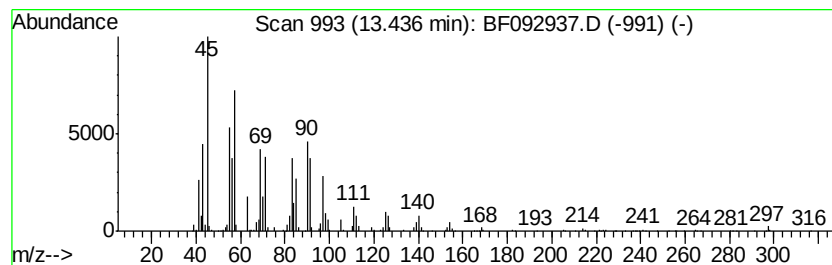
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Methoxyacetic acid, pentade... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	88.01 ng	4371130	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methoxyacetic acid, pentadecyl e...	300	C18H36O3	1000281-82-2	64
2		2-Tridecanol	200	C13H28O	001653-31-2	53
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	43
4		2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	43
5		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
 Data File : BF092937.D
 Acq On : 14 Feb 2017 12:10
 Operator : SJ/MA
 Sample : I1789-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EFF-WW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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
Ethanol, 2-butoxy-	5.92	713.3	ng	32838000	1	6.88	920753	20.0
unknown6.66	6.66	88.2	ng	4060740	1	6.88	920753	20.0
1-Hexanol, 2-ethyl-	7.02	906.3	ng	41722800	1	6.88	920753	20.0
Hexanoic acid, 2-...	7.78	297.8	ng	20632100	2	8.17	1385470	20.0
Dodecane, 6-cyclo...	11.96	86.1	ng	5340870	4	11.39	1240360	20.0
n-Hexadecanoic acid	12.19	142.8	ng	8855540	4	11.39	1240360	20.0
Heptafluorobutano...	12.22	242.2	ng	15022400	4	11.39	1240360	20.0
1-Octadecene	12.28	73.3	ng	4543830	4	11.39	1240360	20.0
unknown12.41	12.41	218.5	ng	13548900	4	11.39	1240360	20.0
unknown12.44	12.44	234.5	ng	14540900	4	11.39	1240360	20.0
unknown12.50	12.50	241.4	ng	14972400	4	11.39	1240360	20.0
unknown12.58	12.58	106.0	ng	6573350	4	11.39	1240360	20.0
unknown12.61	12.61	266.1	ng	16500200	4	11.39	1240360	20.0
unknown12.73	12.73	685.6	ng	34052200	5	14.03	993340	20.0
Isopropyl Myristate	12.84	104.0	ng	5165940	5	14.03	993340	20.0
Ethanol, 2-(tetra...	12.88	174.7	ng	8675500	5	14.03	993340	20.0
Isopropyl stearate	12.94	173.0	ng	8594040	5	14.03	993340	20.0
unknown13.06	13.06	100.7	ng	5001490	5	14.03	993340	20.0
unknown13.13	13.13	195.8	ng	9724830	5	14.03	993340	20.0
Methoxyacetic aci...	13.44	88.0	ng	4371130	5	14.03	993340	20.0