

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
 Data File : BF085323.D
 Acq On : 10 Mar 2016 2:49
 Operator : UM/SJ
 Sample : H1722-06
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-29(0.5-3.0)

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-BF030316.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	3.978	145	148	152	rBV	484352	770478	12.45%	1.426%
2	5.076	239	244	249	rVV3	32520	78593	1.27%	0.145%
3	5.167	249	252	258	rVB	264480	434757	7.02%	0.805%
4	5.441	273	276	277	rBV2	39833	76565	1.24%	0.142%
5	5.556	283	286	288	rVB	3853187	4905480	79.25%	9.079%
6	5.853	310	312	314	rBV	107309	95272	1.54%	0.176%
7	6.573	372	375	378	rVB	3371790	5624367	90.86%	10.409%
8	6.721	384	388	390	rBV	3858256	5644414	91.18%	10.446%
9	6.767	390	392	395	rVB	67795	80008	1.29%	0.148%
10	6.939	405	407	410	rBV	872767	1137261	18.37%	2.105%
11	7.099	419	421	424	rVB	3245425	4266636	68.93%	7.896%
12	7.510	453	457	459	rBV	3134821	3475527	56.15%	6.432%
13	7.590	461	464	467	rVB	97076	136284	2.20%	0.252%
14	8.230	517	520	522	rBV	1845278	1613647	26.07%	2.986%
15	9.305	611	614	617	rBV	4208648	6190142	100.00%	11.456%
16	9.705	646	649	650	rBV	812124	1080597	17.46%	2.000%
17	9.910	665	667	669	rVB	101734	125402	2.03%	0.232%
18	9.990	671	674	676	rVB	1617171	1700925	27.48%	3.148%
19	10.413	708	711	713	rBV	228853	253773	4.10%	0.470%
20	10.630	728	730	734	rBV	62869	121622	1.96%	0.225%
21	10.779	740	743	745	rBV	3552762	3719095	60.08%	6.883%
22	10.893	751	753	757	rBV	176612	261222	4.22%	0.483%
23	11.088	767	770	774	rBV4	30595	84679	1.37%	0.157%
24	11.339	789	792	793	rBV	144601	136863	2.21%	0.253%
25	11.476	801	804	806	rBV	1623767	1748202	28.24%	3.235%
26	11.533	807	809	812	rVB3	39310	78043	1.26%	0.144%
27	11.693	821	823	827	rBV	129235	145284	2.35%	0.269%
28	11.762	827	829	831	rVV	82576	68375	1.10%	0.127%
29	12.002	848	850	852	rBV	427471	469363	7.58%	0.869%
30	12.253	869	872	874	rBV	52650	69437	1.12%	0.129%
31	12.688	908	910	912	rBV	65518	94836	1.53%	0.176%
32	12.779	916	918	922	rBV	125505	151020	2.44%	0.279%
33	12.905	928	929	936	rVB2	43490	99070	1.60%	0.183%
34	13.065	940	943	945	rVV	4718381	4919085	79.47%	9.104%

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Instrument :
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ClientSampleId :
W170TH-SB-29(0.5-3.0)

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.248	957	959	963	rVV	41124	70619	1.14%	0.131%
36	13.945	1018	1020	1026	rBV	214486	361337	5.84%	0.669%
37	14.094	1030	1033	1037	rBV2	1690617	2572596	41.56%	4.761%
38	14.494	1063	1068	1070	rBV4	24845	65495	1.06%	0.121%
39	14.859	1098	1100	1104	rBV	171622	244643	3.95%	0.453%
40	14.962	1107	1109	1113	rVB	61482	78684	1.27%	0.146%
41	15.568	1159	1162	1165	rBV	522520	782578	12.64%	1.448%

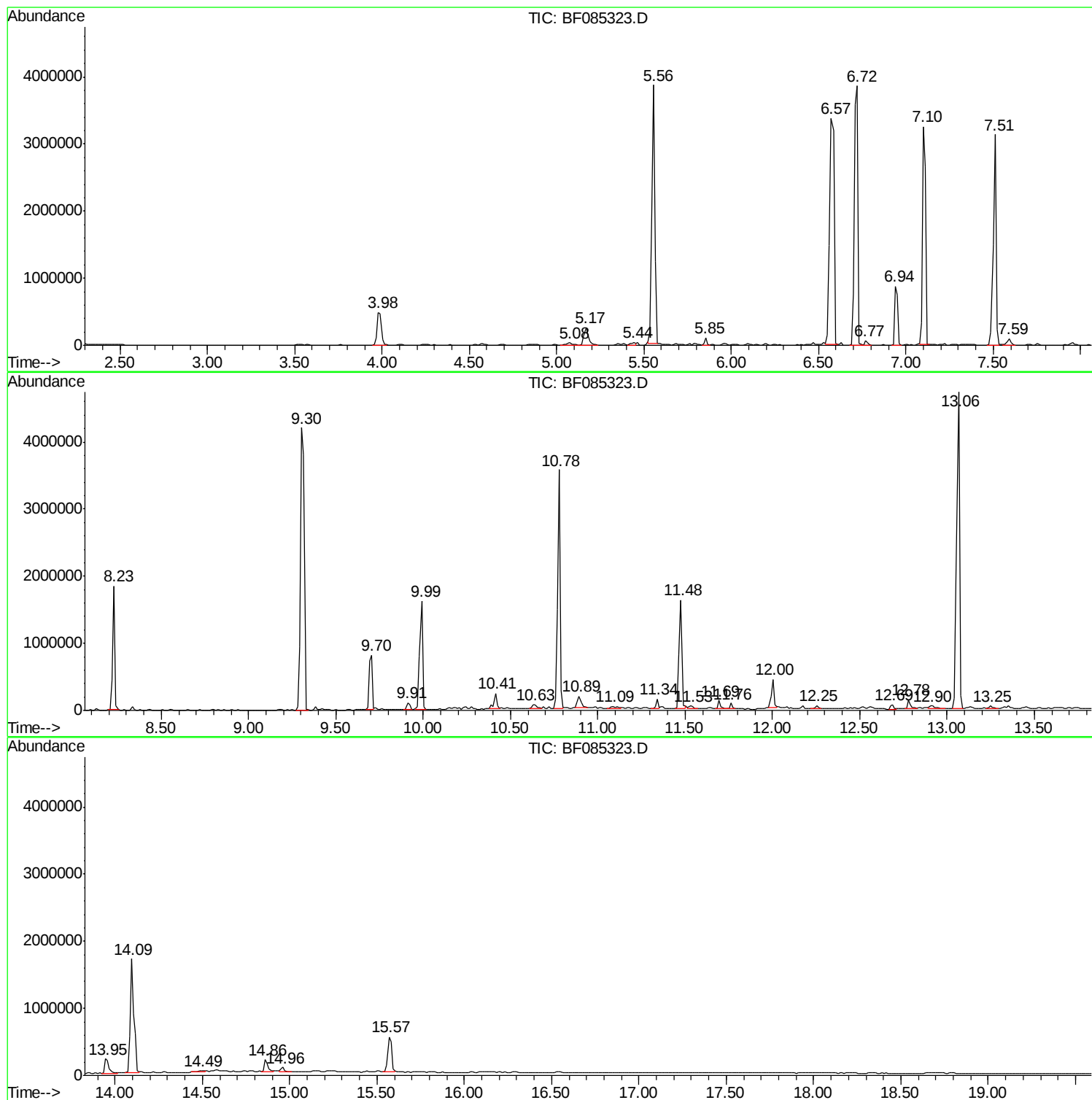
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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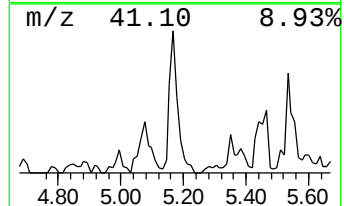
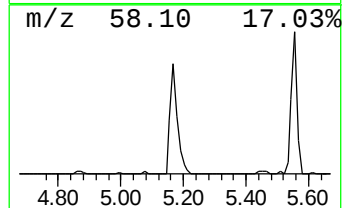
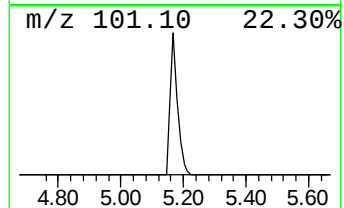
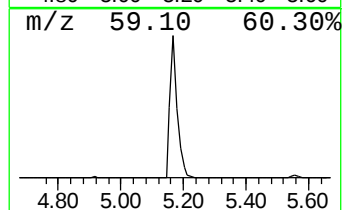
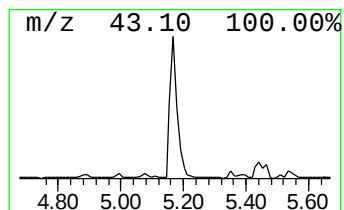
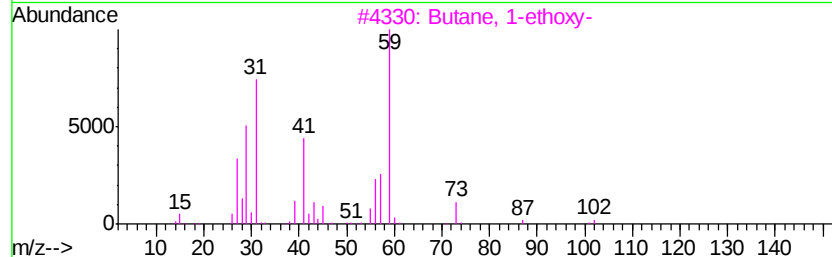
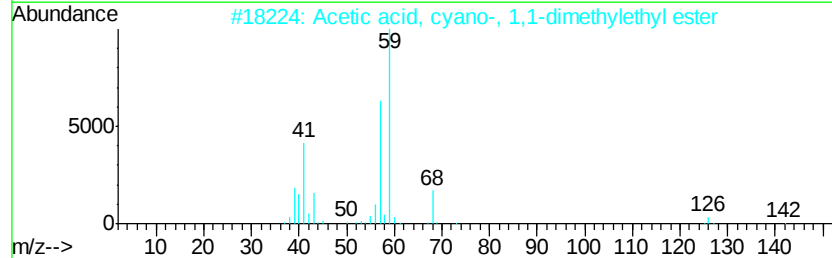
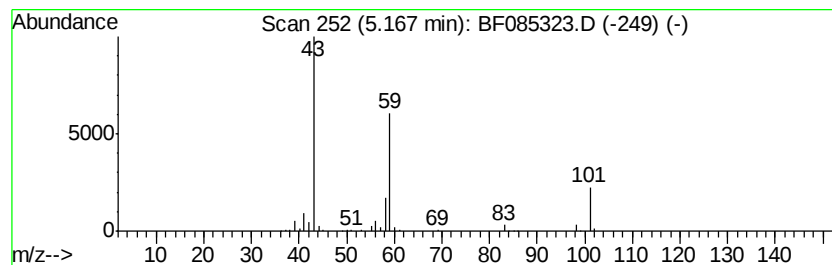
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	7.65 ng	434757	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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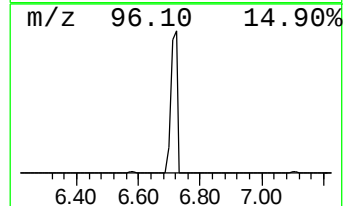
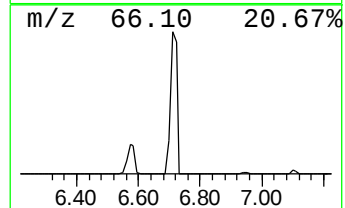
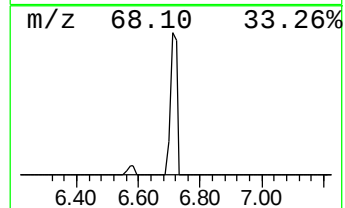
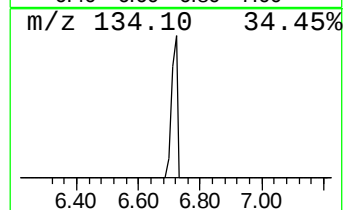
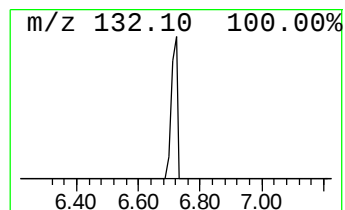
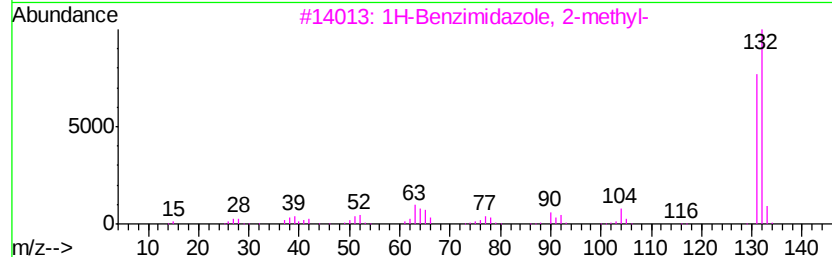
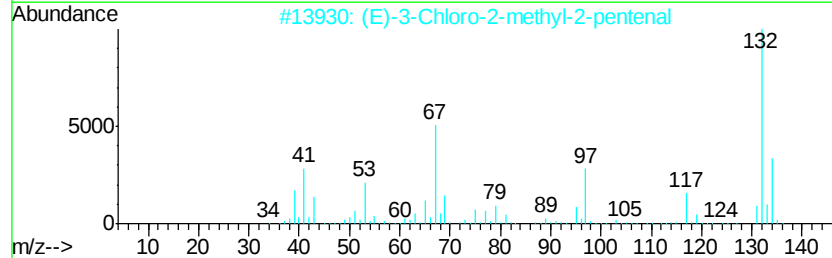
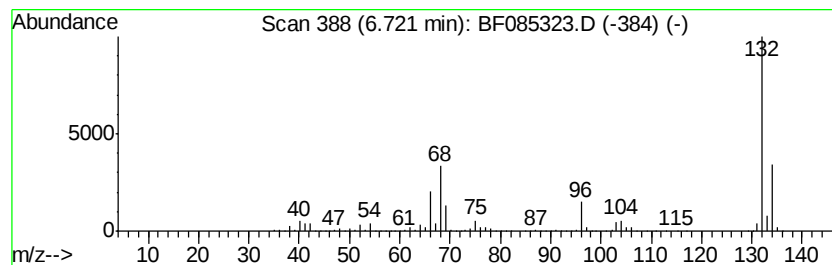
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	99.26 ng	5644410	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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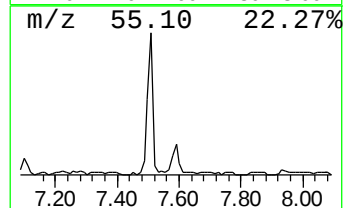
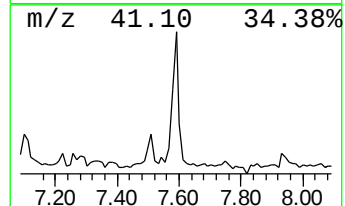
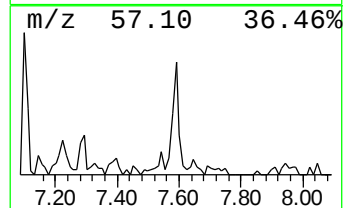
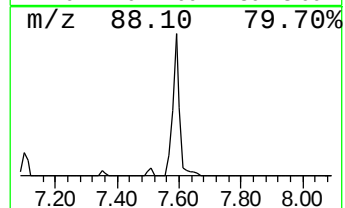
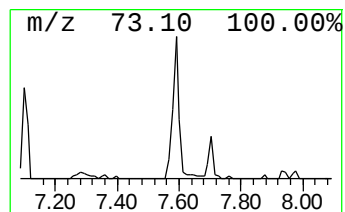
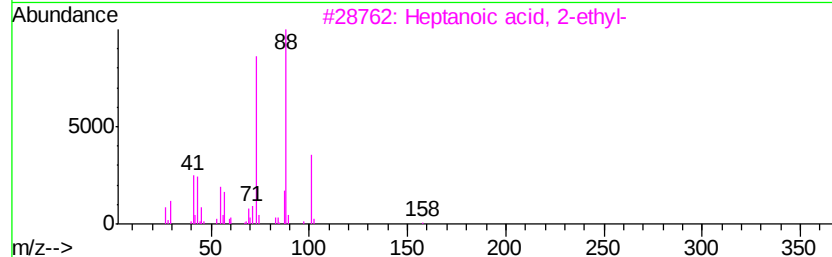
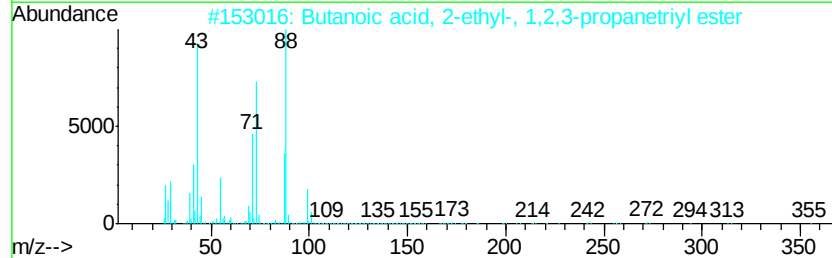
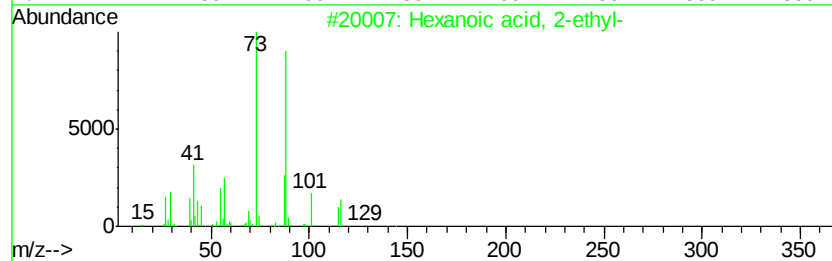
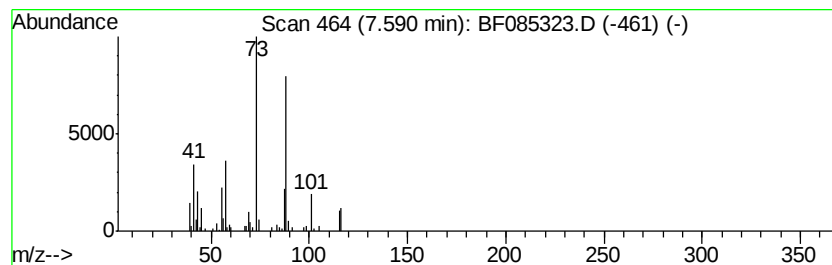
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	2.40 ng	136284	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4		1,4-Dioxane	88	C4H8O2	000123-91-1	43
5		Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	33



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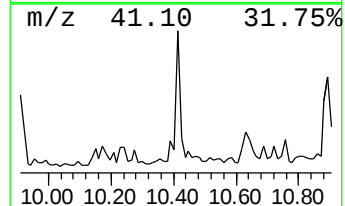
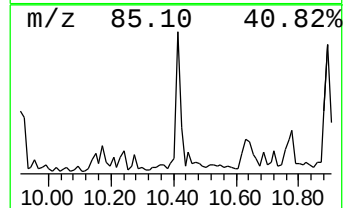
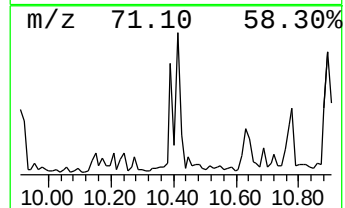
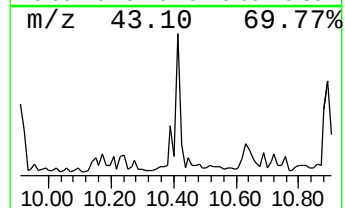
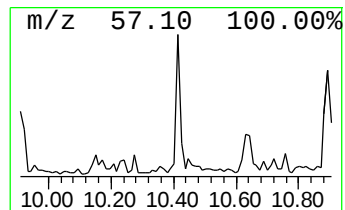
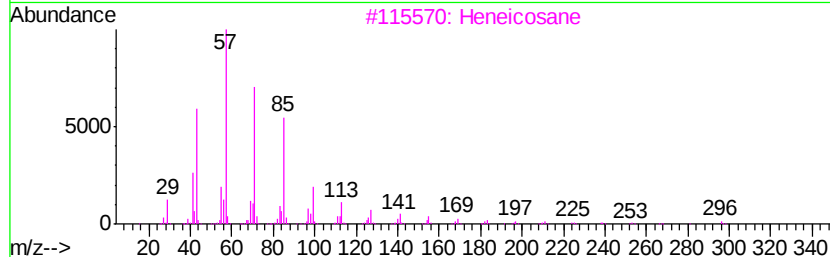
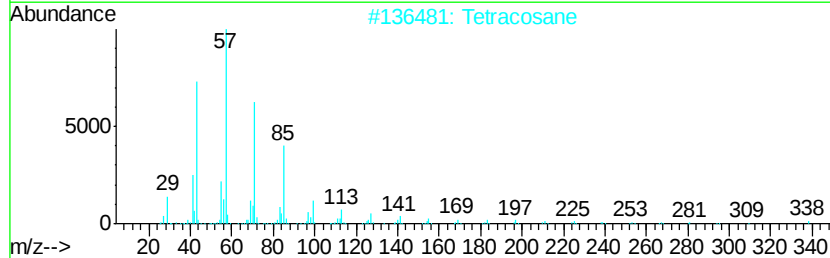
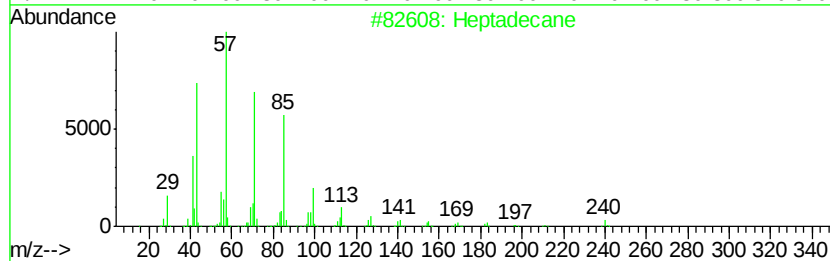
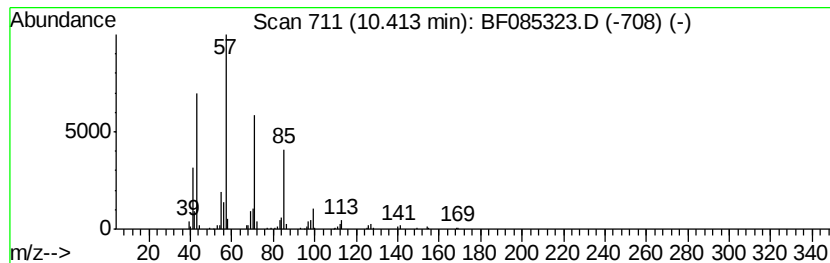
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	2.98 ng	253773	Acenaphthene-d10	9.99
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	Tetracosane	338 C24H50	000646-31-1	90
3	Heneicosane	296 C21H44	000629-94-7	83
4	Eicosane	282 C20H42	000112-95-8	80
5	Hexadecane	226 C16H34	000544-76-3	74



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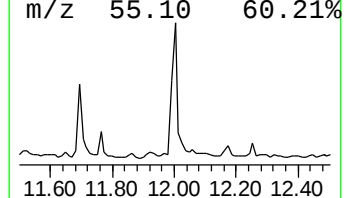
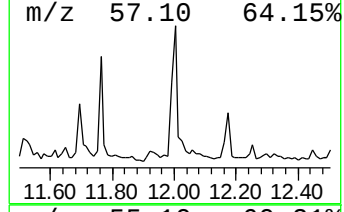
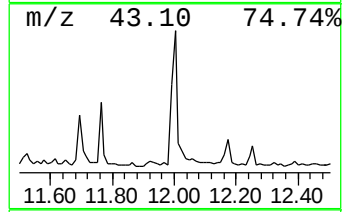
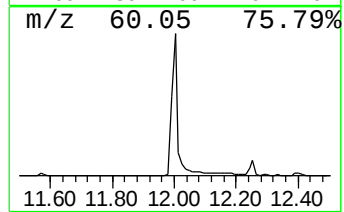
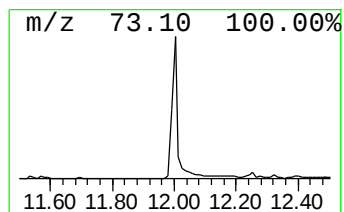
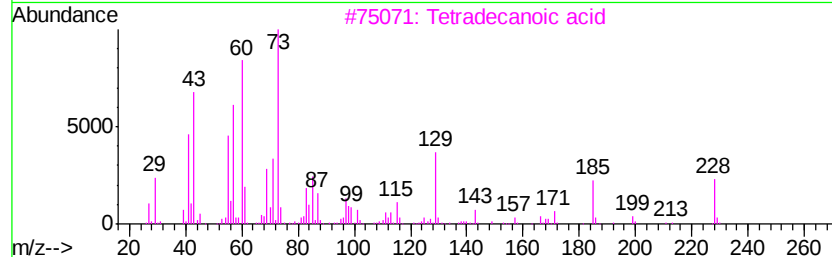
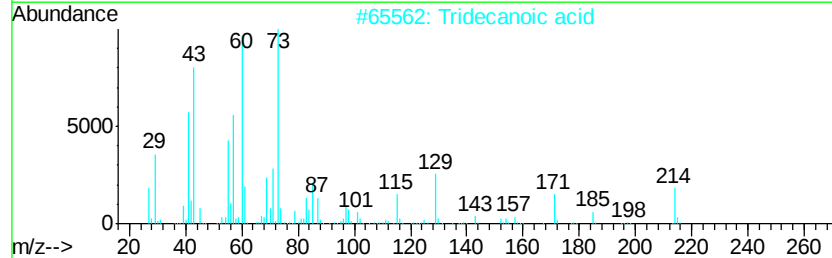
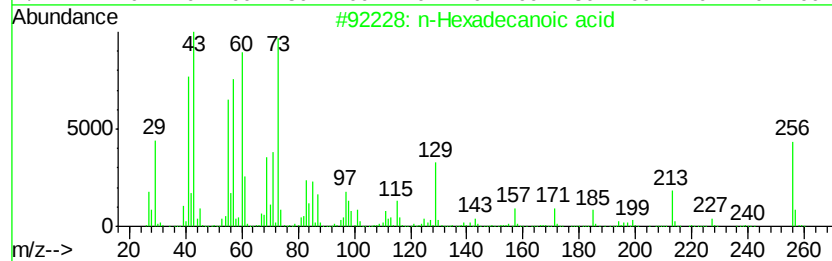
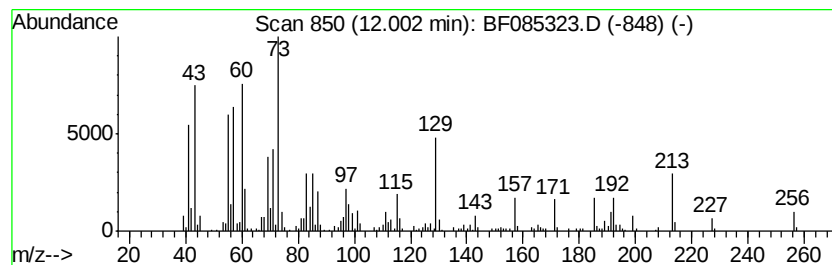
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Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.00	5.37 ng	469363	Phenanthrene-d10		11.48	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Tridecanoic acid		214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
5	n-Decanoic acid		172	C10H20O2	000334-48-5	76



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-29(0.5-3.0)

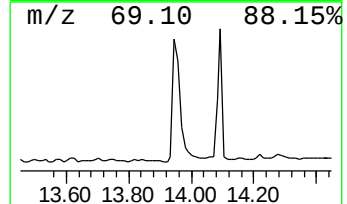
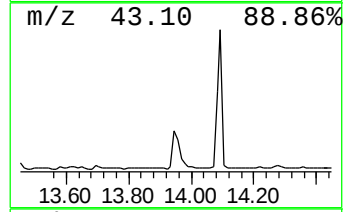
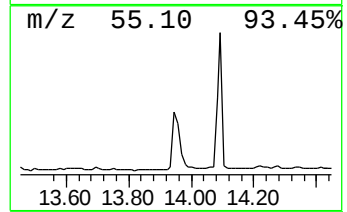
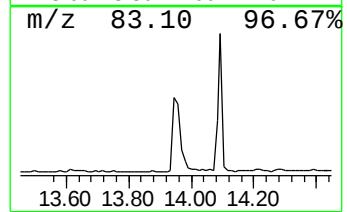
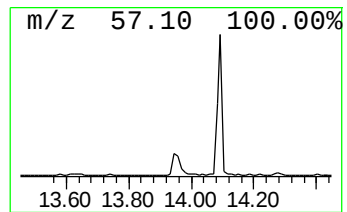
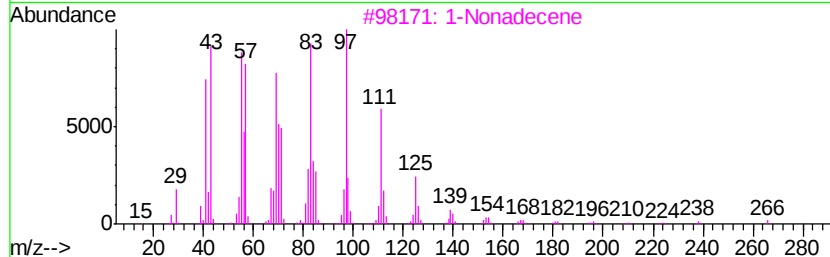
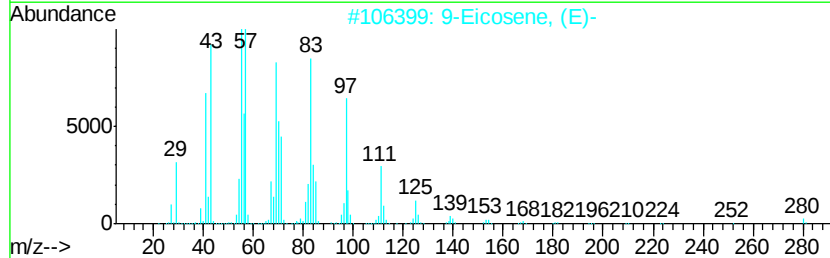
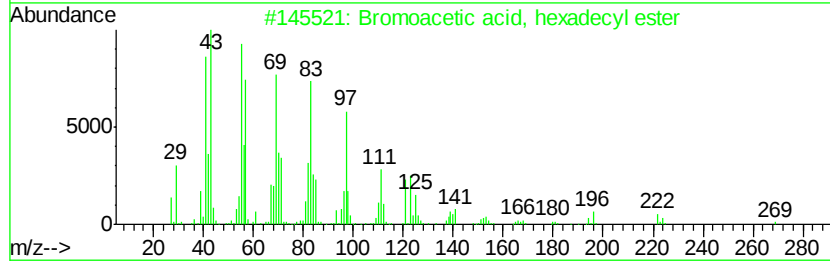
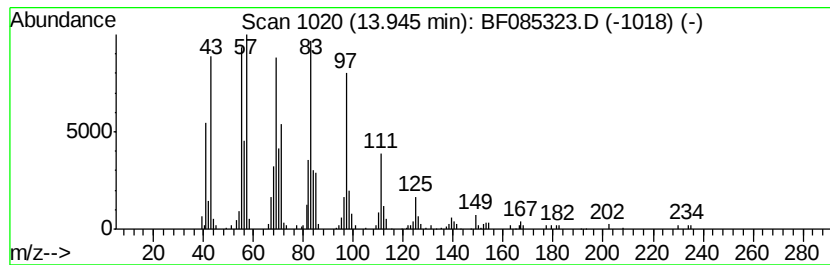
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromoacetic acid, hexadecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.81 ng	361337	Chrysene-d12	14.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
3			1-Nonadecene	266	C19H38	018435-45-5	91
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085323.D
Acq On : 10 Mar 2016 2:49
Operator : UM/SJ
Sample : H1722-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-29(0.5-3.0)

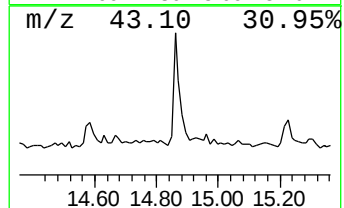
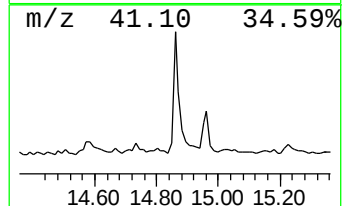
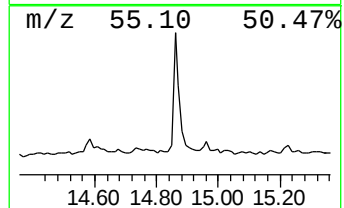
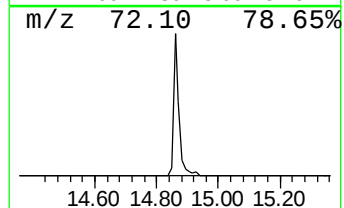
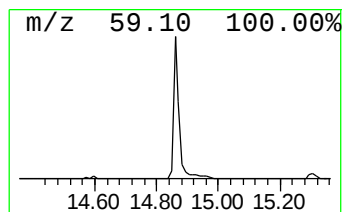
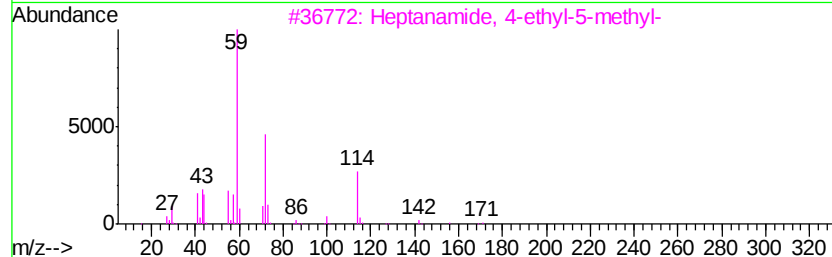
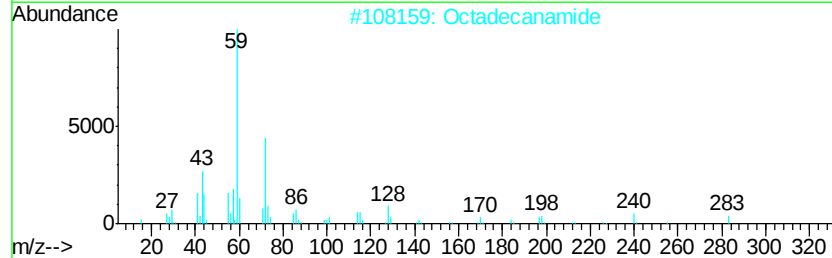
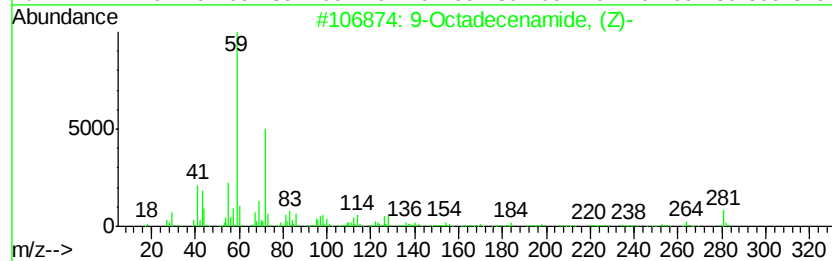
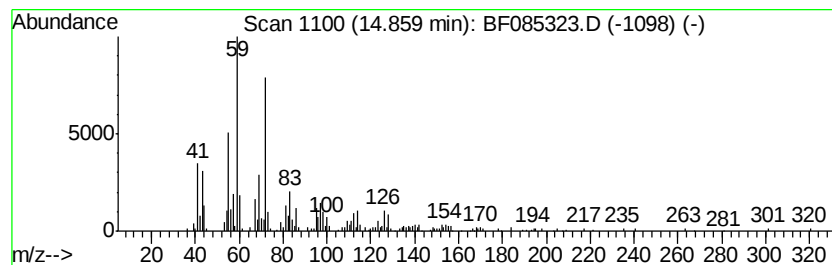
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	6.25 ng	244643	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2		Octadecanamide	283	C18H37NO	000124-26-5	47
3		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	38
4		Dodecanamide	199	C12H25NO	001120-16-7	38
5		2-Methyl-2-decanol	172	C11H24O	003396-02-9	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085323.D
Acq On : 10 Mar 2016 2:49
Operator : UM/SJ
Sample : H1722-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

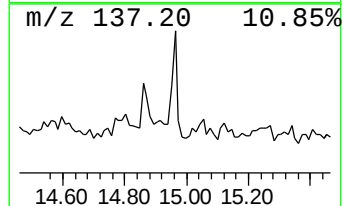
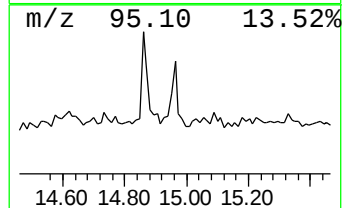
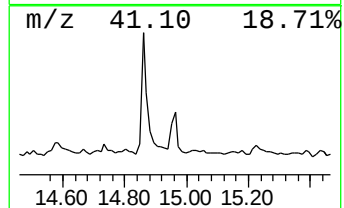
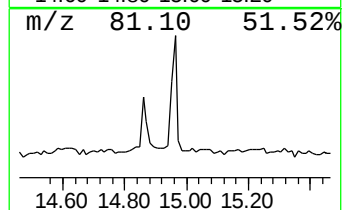
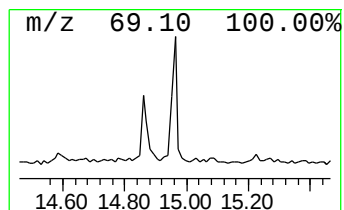
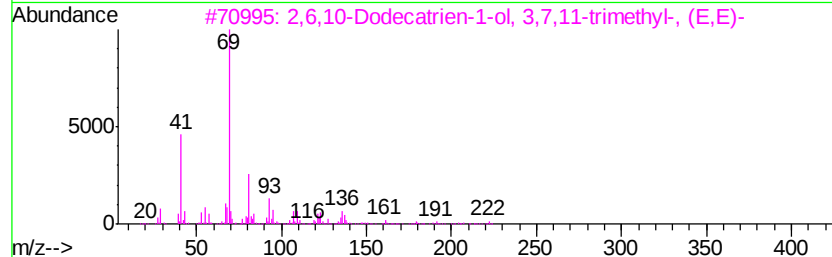
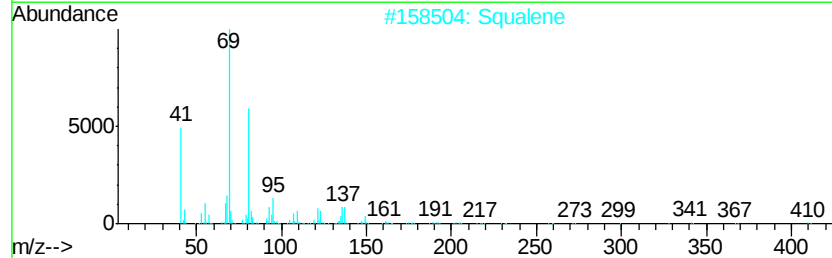
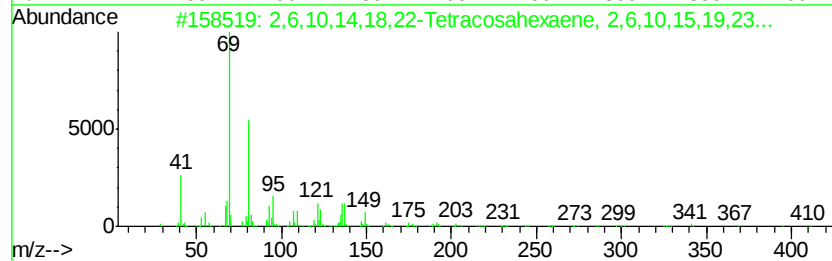
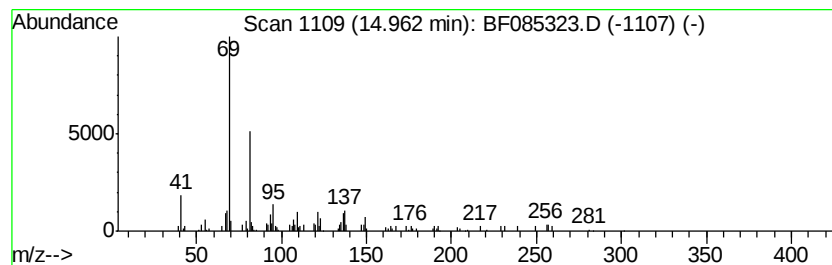
Instrument :
BNA_F
ClientSampleId :
W170TH-SB-29(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.01 ng	78684	Perylene-d12	15.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
2	Squalene	410 C30H50	007683-64-9	91
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	86
4	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	83
5	.psi.,.psi.-Carotene, 7,7',8,8',...	547 C40H66	000502-62-5	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085323.D
Acq On : 10 Mar 2016 2:49
Operator : UM/SJ
Sample : H1722-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-29(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.17	7.7	ng	434757	1	6.95	1137260	20.0
unknown6.72	6.72	99.3	ng	5644410	1	6.95	1137260	20.0
Hexanoic acid, 2-...	7.59	2.4	ng	136284	1	6.95	1137260	20.0
Heptadecane	10.41	3.0	ng	253773	3	9.99	1700930	20.0
n-Hexadecanoic acid	12.00	5.4	ng	469363	4	11.48	1748200	20.0
Bromoacetic acid,...	13.95	2.8	ng	361337	5	14.11	2572600	20.0
9-Octadecenamide,...	14.86	6.3	ng	244643	6	15.57	782578	20.0
2,6,10,14,18,22-T...	14.96	2.0	ng	78684	6	15.57	782578	20.0