

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092915\
 Data File : BF081898.D
 Acq On : 30 Sep 2015 5:28
 Operator : UM/IZ
 Sample : G3840-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP219BR-40-42

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-BF092815.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	2.194	3	5	8	rVB	26509	34119	1.11%	0.145%
2	5.120	257	261	273	rBV	774692	1376485	44.68%	5.869%
3	5.520	293	296	298	rBV	2455779	2514362	81.61%	10.720%
4	6.549	383	386	388	rBV	1578260	1748068	56.74%	7.453%
5	6.686	395	398	401	rBV	1844456	1821235	59.11%	7.765%
6	6.926	417	419	430	rBV	229242	384813	12.49%	1.641%
7	7.074	430	432	447	rVB	1394838	1311613	42.57%	5.592%
8	7.486	466	468	482	rBV	982499	1146041	37.20%	4.886%
9	8.206	529	531	540	rBV	515758	525534	17.06%	2.241%
10	9.280	623	625	628	rBV	1485146	1726078	56.02%	7.359%
11	9.680	657	660	662	rBV	450493	419501	13.62%	1.789%
12	9.966	682	685	687	rBV	619343	644873	20.93%	2.749%
13	10.755	751	754	762	rBV	1492817	1624768	52.73%	6.927%
14	10.858	762	763	771	rVB	23757	44975	1.46%	0.192%
15	11.452	813	815	828	rBV	675345	738601	23.97%	3.149%
16	12.583	908	914	915	rBV	139205	465536	15.11%	1.985%
17	12.858	936	938	940	rBV	180840	165571	5.37%	0.706%
18	12.938	943	945	951	rVB	30717	51180	1.66%	0.218%
19	13.041	951	954	957	rBV	2999029	3081012	100.00%	13.136%
20	13.486	991	993	994	rBV	129236	155436	5.04%	0.663%
21	13.521	994	996	998	rVV	649241	719957	23.37%	3.070%
22	13.566	998	1000	1002	rVV2	146421	226673	7.36%	0.966%
23	13.601	1002	1003	1009	rVB2	47200	93378	3.03%	0.398%
24	13.932	1030	1032	1035	rBV	51433	51765	1.68%	0.221%
25	14.092	1044	1046	1053	rVB	872185	1038980	33.72%	4.430%
26	14.252	1058	1060	1076	rVB	72708	146446	4.75%	0.624%
27	14.561	1084	1087	1089	rBV	51072	50503	1.64%	0.215%
28	14.869	1111	1114	1116	rBV	40642	57349	1.86%	0.245%
29	14.938	1118	1120	1123	rVV	50655	56867	1.85%	0.242%
30	15.201	1140	1143	1149	rVB	33131	41469	1.35%	0.177%
31	15.555	1171	1174	1185	rBV	479283	924536	30.01%	3.942%
32	16.012	1211	1214	1221	rVB	21080	36113	1.17%	0.154%
33	16.515	1256	1258	1267	rBV	14945	30977	1.01%	0.132%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

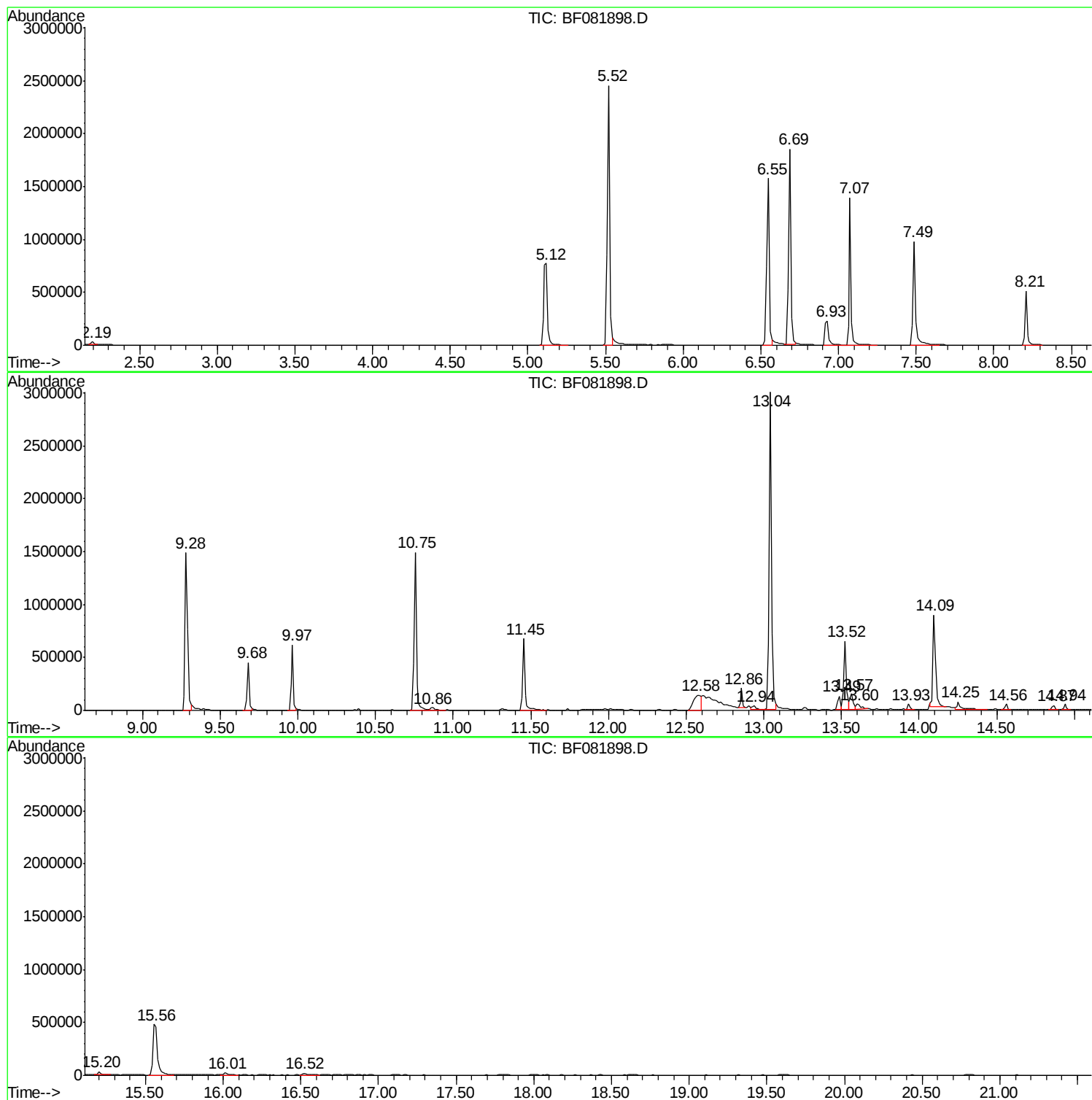
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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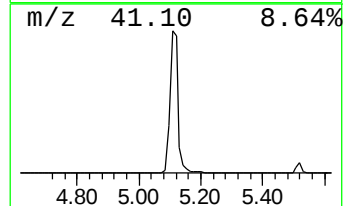
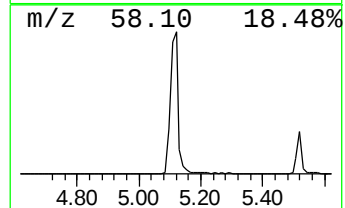
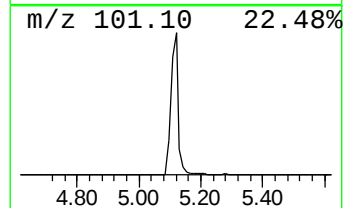
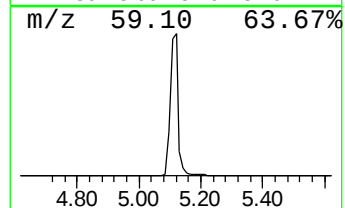
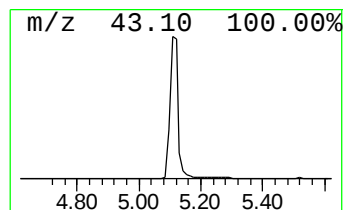
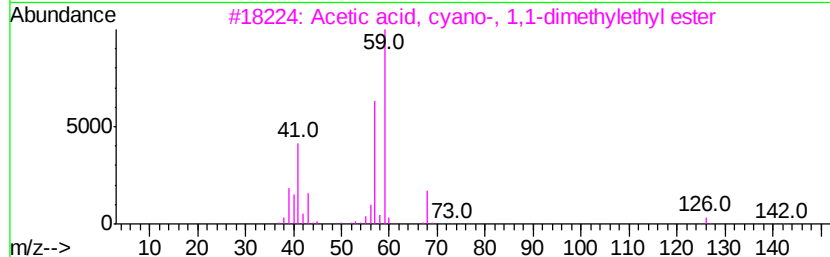
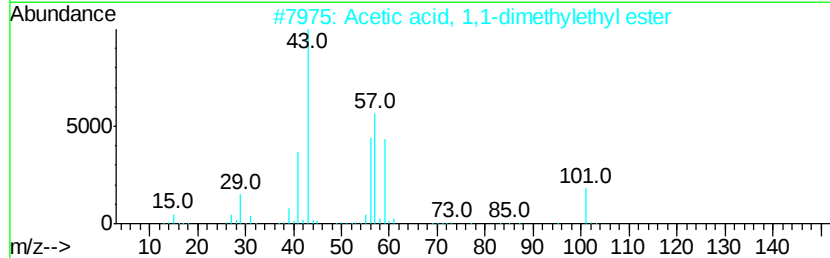
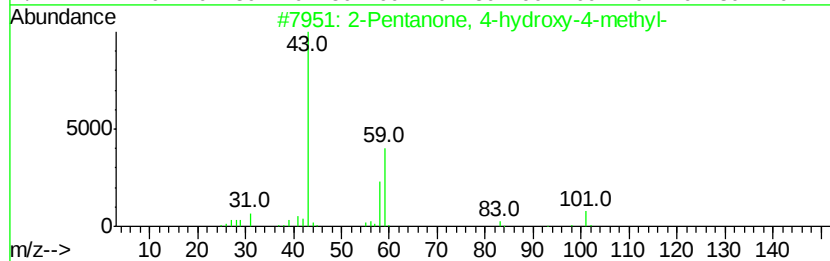
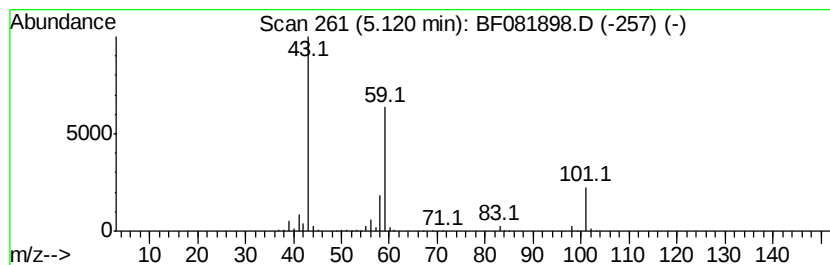
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	71.54 ng	1376490	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Acetone	58	C3H6O	000067-64-1	9



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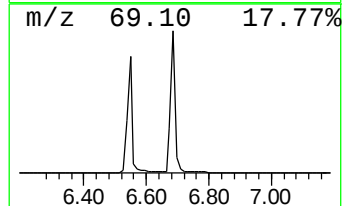
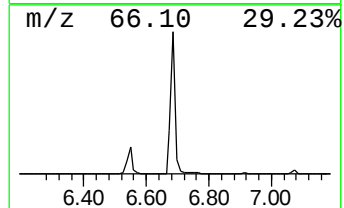
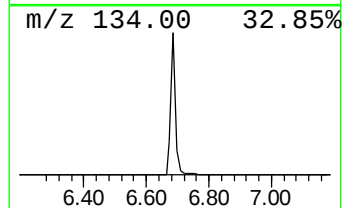
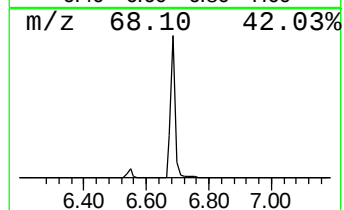
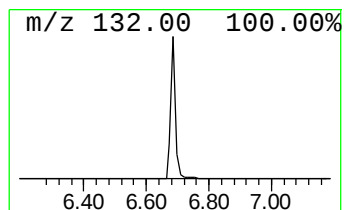
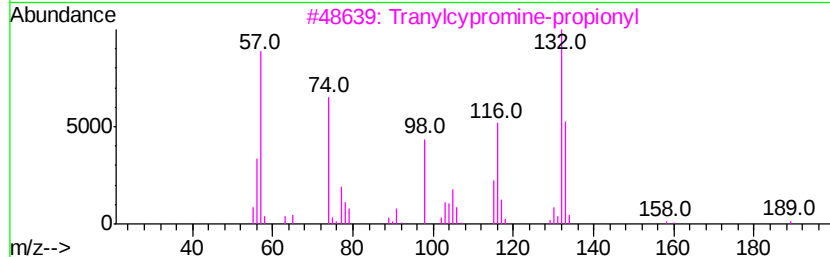
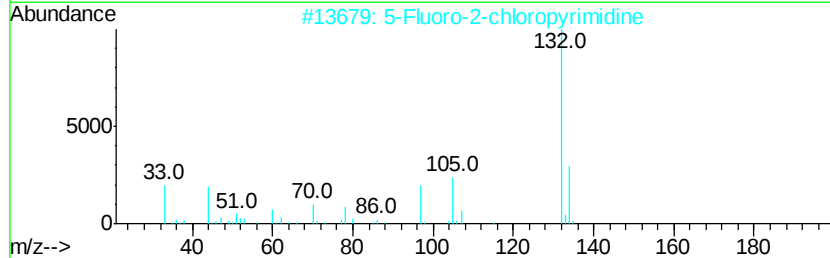
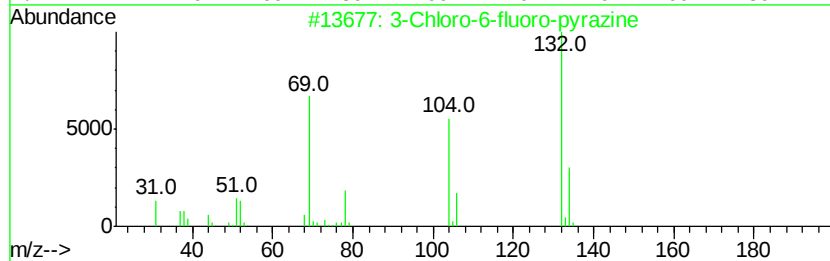
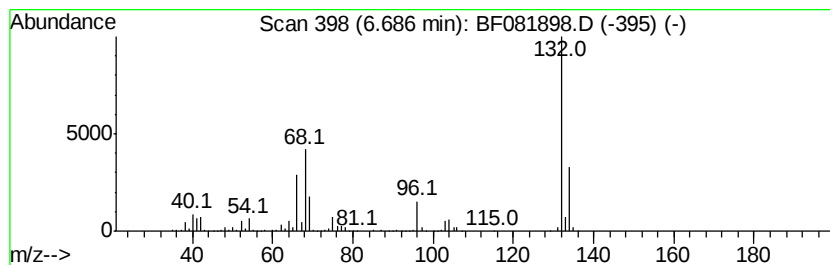
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	94.66 ng	1821240	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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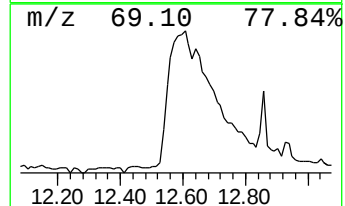
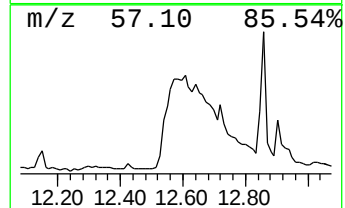
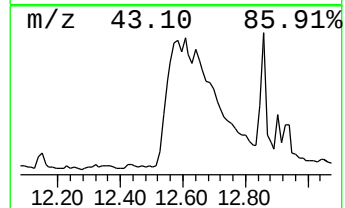
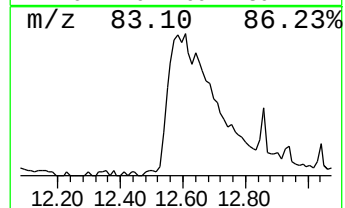
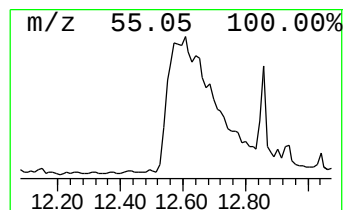
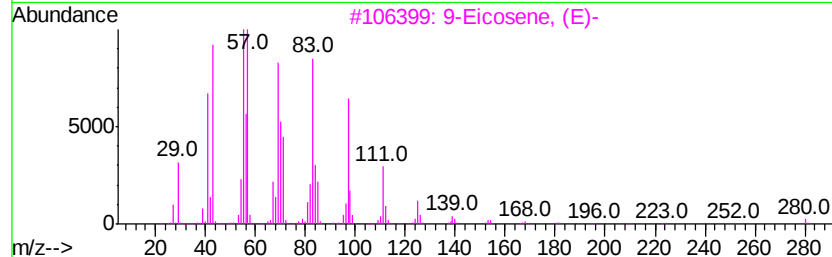
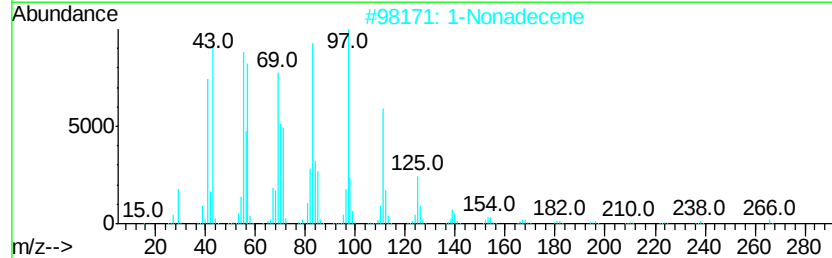
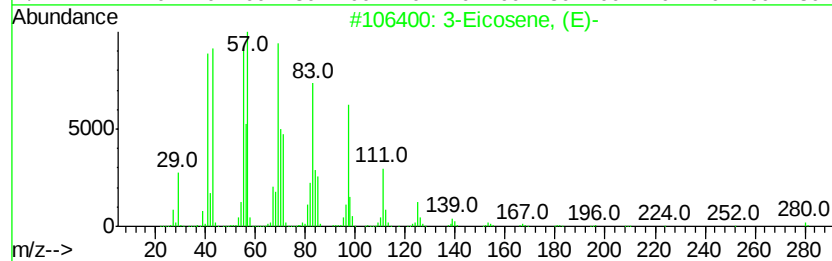
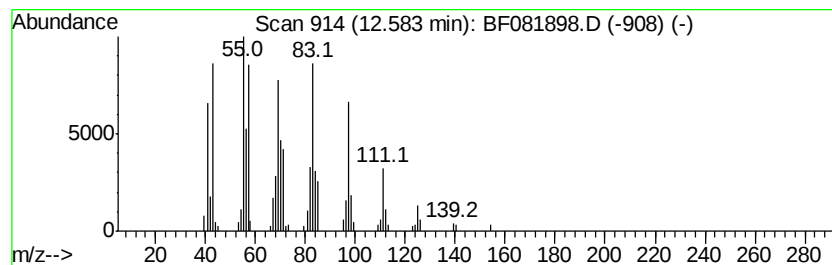
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.58	12.61 ng	465536	Phenanthrene-d10	11.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	1-Nonadecene	266	C19H38	018435-45-5	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91



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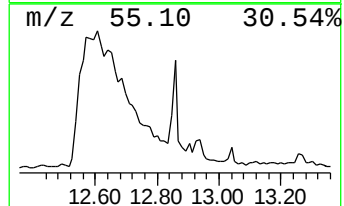
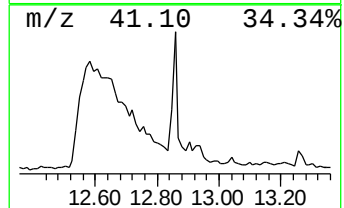
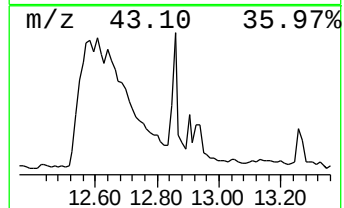
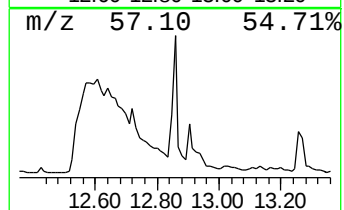
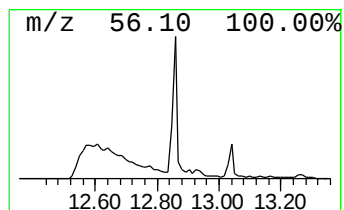
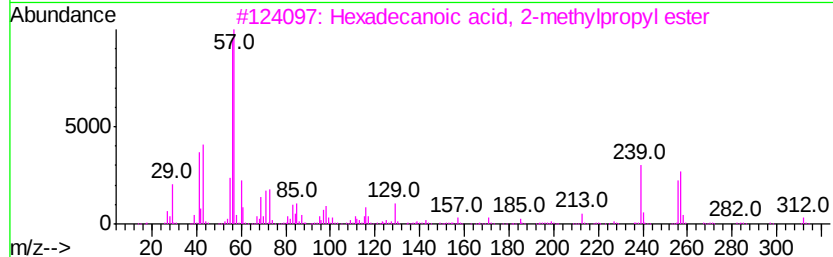
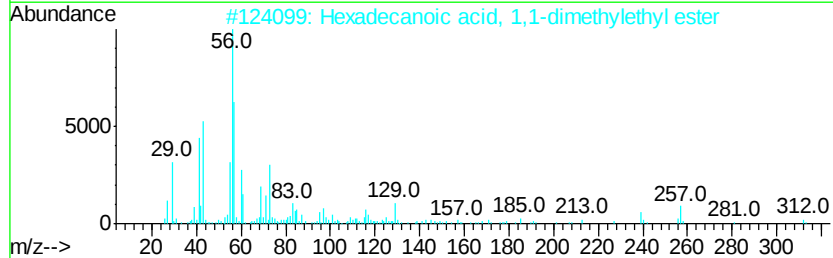
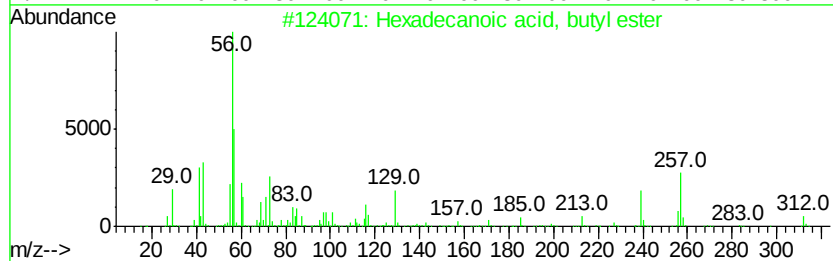
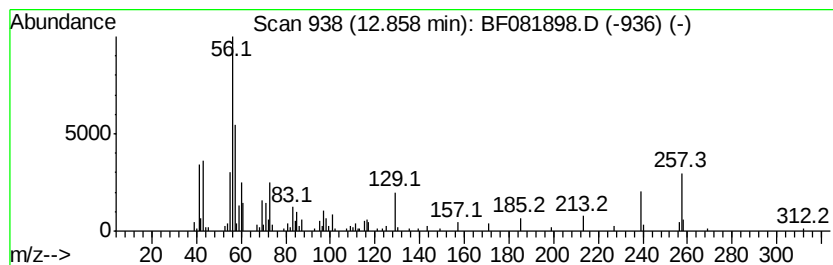
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	3.19 ng	165571	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	43
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35



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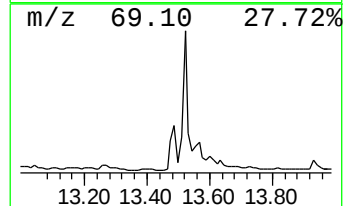
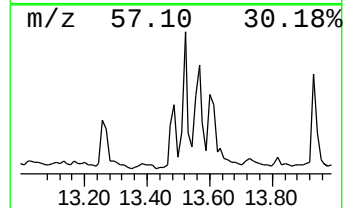
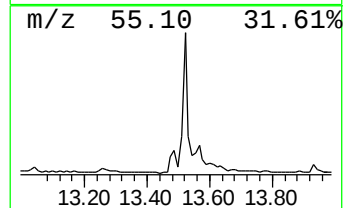
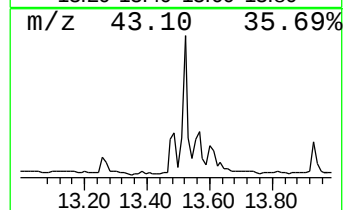
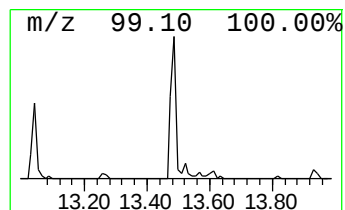
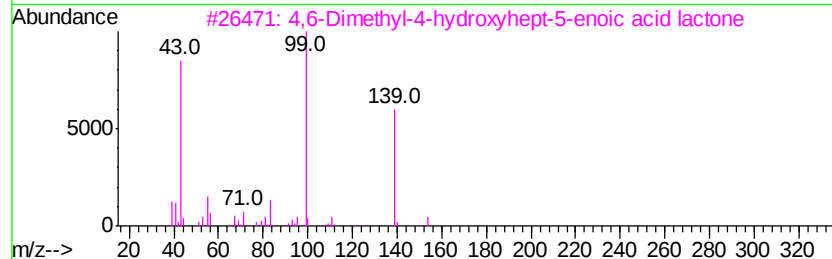
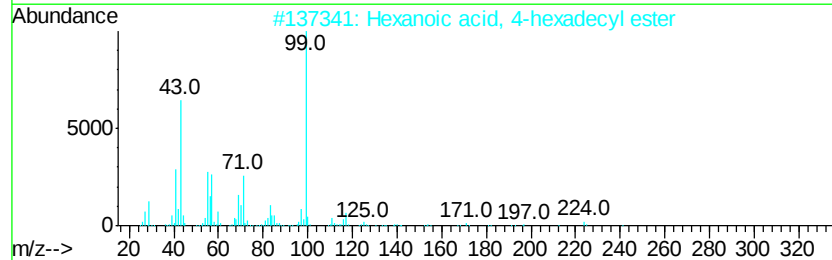
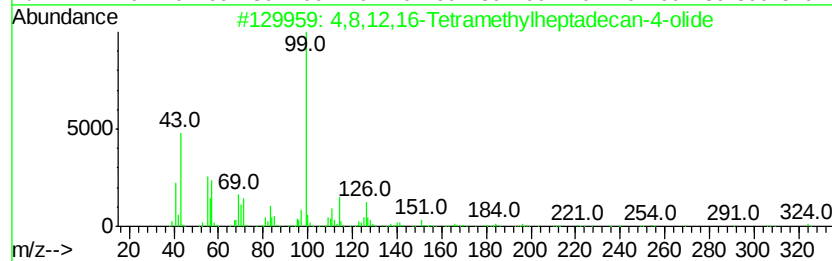
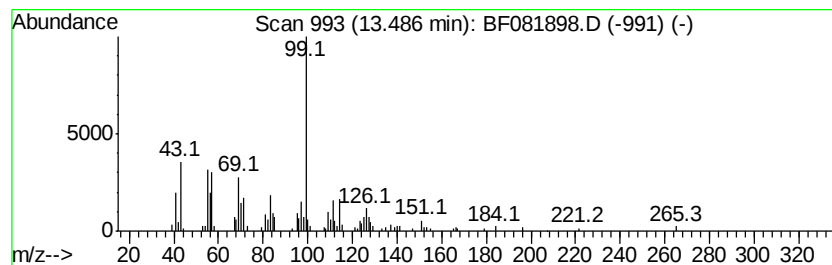
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Peak Number 6 4,8,12,16-Tetramethylheptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.99 ng	155436	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	87
2		Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	53
3		4,6-Dimethyl-4-hydroxyhept-5-eno...	154	C9H14O2	1000122-47-0	47
4		2-Heptyl methylphosphonofluoridate	196	C8H18FO2P	000674-95-3	43
5		Acetaldehyde, diethylhydrazone	114	C6H14N2	007422-91-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092915\
Data File : BF081898.D
Acq On : 30 Sep 2015 5:28
Operator : UM/IZ
Sample : G3840-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP219BR-40-42

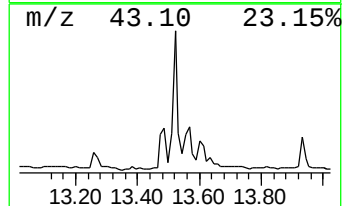
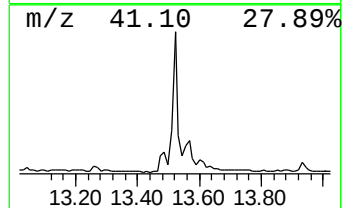
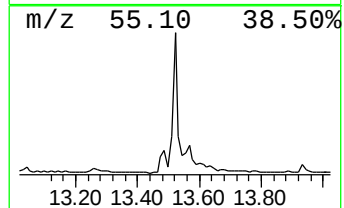
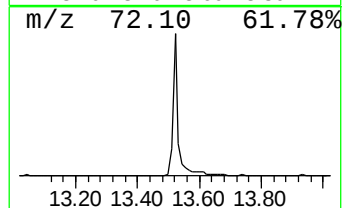
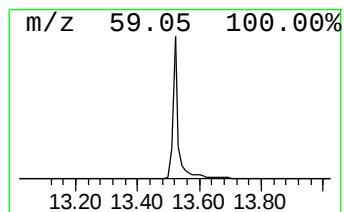
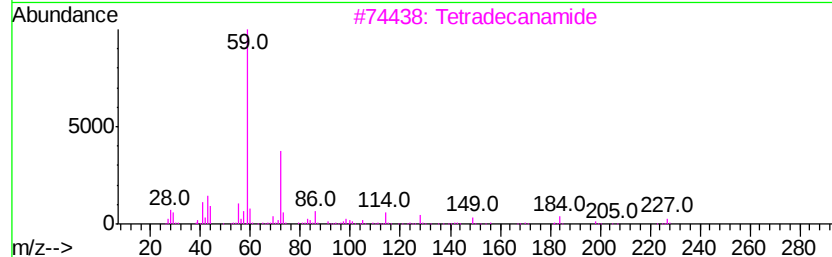
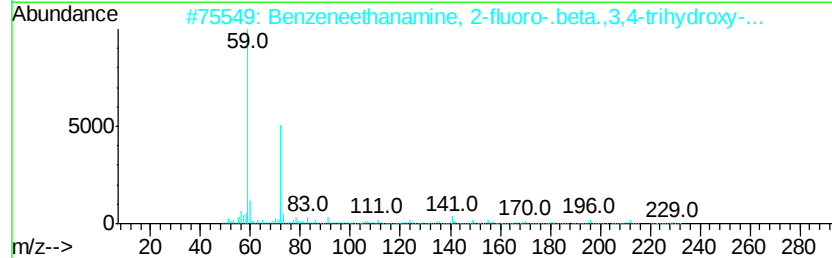
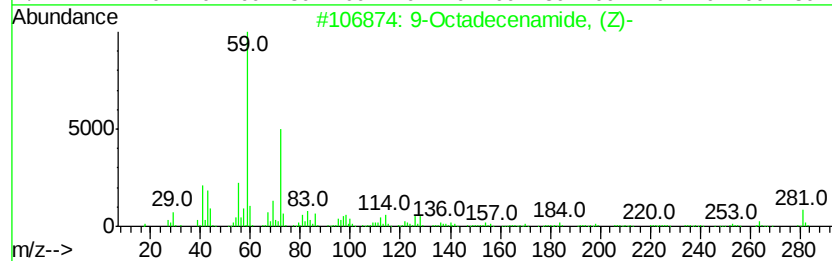
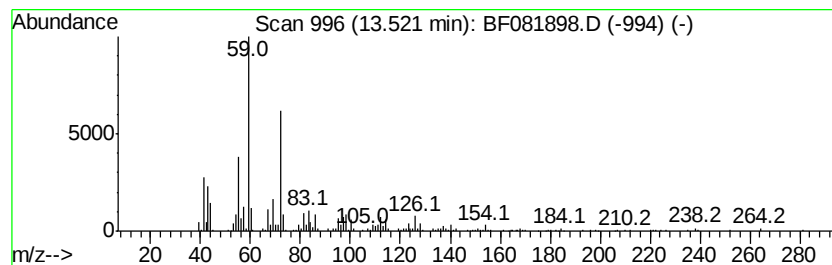
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	13.86 ng	719957	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		Octanamide	143	C8H17NO	000629-01-6	56
5		7-Nonenamide	155	C9H17NO	090949-53-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092915\
Data File : BF081898.D
Acq On : 30 Sep 2015 5:28
Operator : UM/IZ
Sample : G3840-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP219BR-40-42

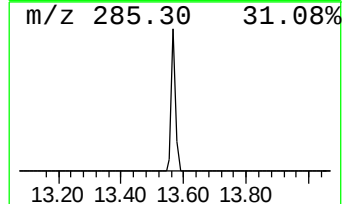
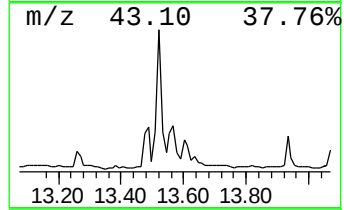
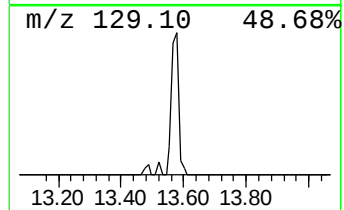
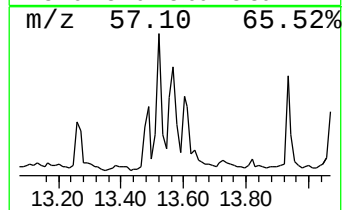
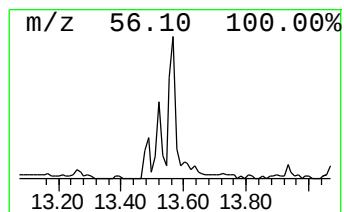
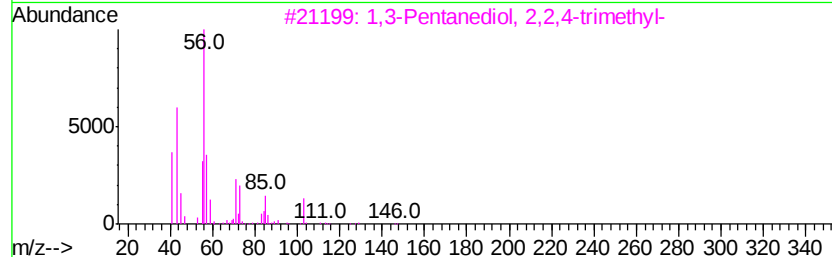
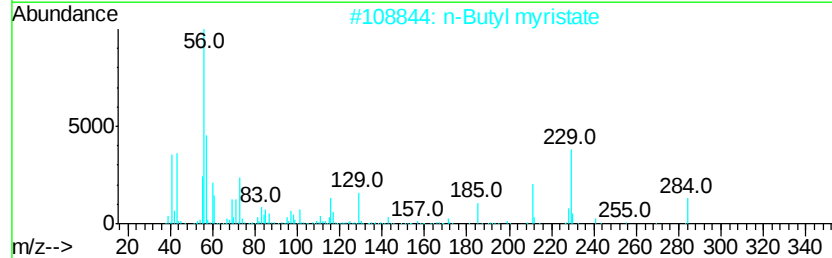
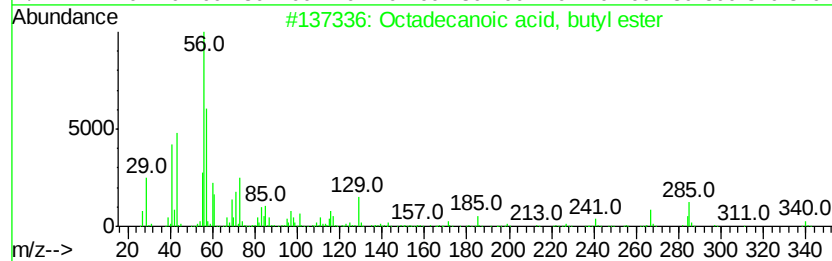
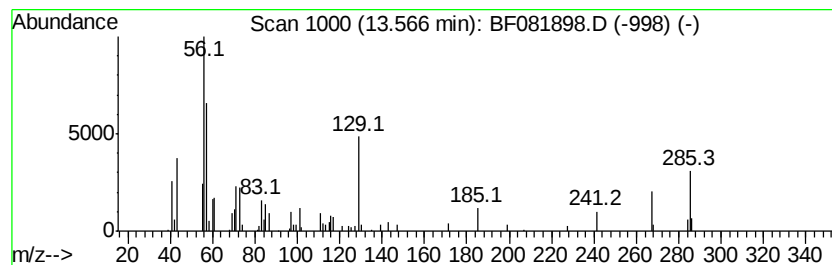
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	4.36 ng	226673	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	50
2		n-Butyl myristate	284	C18H36O2	000110-36-1	43
3		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	25
4		2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	22
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092915\
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Operator : UM/IZ
Sample : G3840-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP219BR-40-42

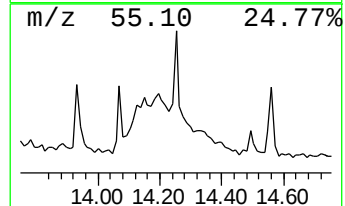
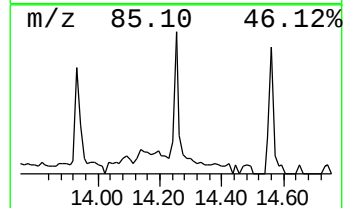
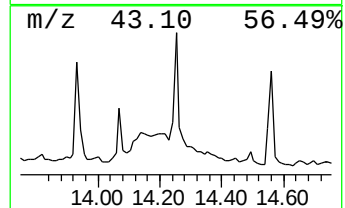
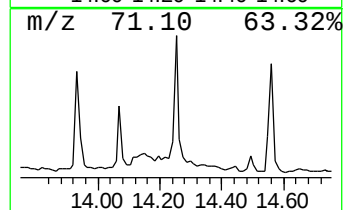
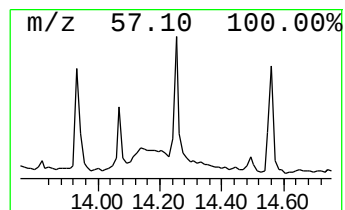
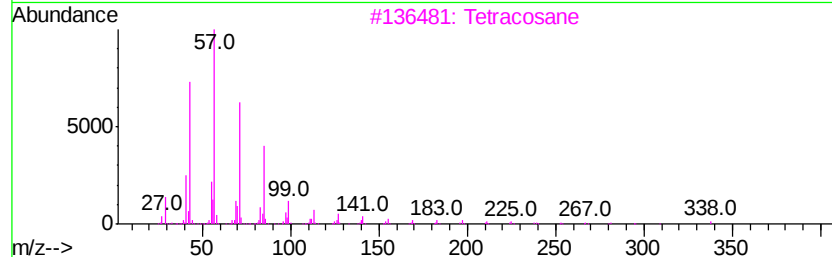
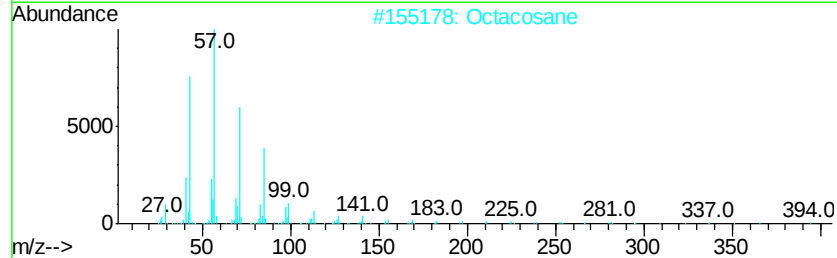
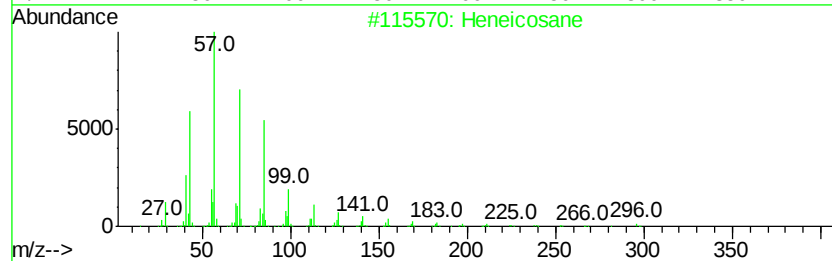
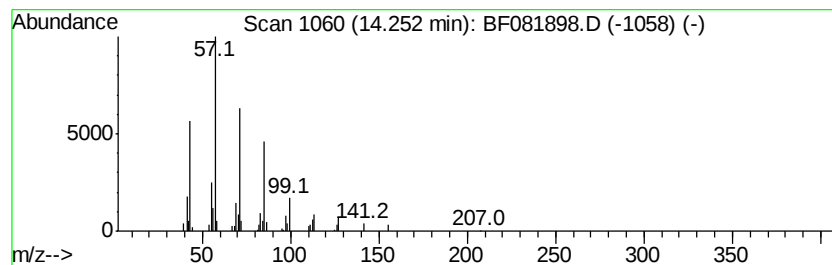
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	2.82 ng	146446	Chrysene-d12	14.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Tetracosane		338	C24H50	000646-31-1	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Heptacosane		380	C27H56	000593-49-7	90



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Operator : UM/IZ
Sample : G3840-02
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP219BR-40-42

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.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...	5.12	71.5	ng	1376490	1	6.93	384813	20.0
unknown6.69	6.69	94.7	ng	1821240	1	6.93	384813	20.0
3-Eicosene, (E)-	12.58	12.6	ng	465536	4	11.45	738601	20.0
Hexadecanoic acid...	12.86	3.2	ng	165571	5	14.09	1038980	20.0
4,8,12,16-Tetrame...	13.49	3.0	ng	155436	5	14.09	1038980	20.0
9-Octadecenamide,...	13.52	13.9	ng	719957	5	14.09	1038980	20.0
Octadecanoic acid...	13.57	4.4	ng	226673	5	14.09	1038980	20.0
Heneicosane	14.25	2.8	ng	146446	5	14.09	1038980	20.0