

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031115\
 Data File : BF078122.D
 Acq On : 31 Mar 2015 19:05
 Operator : TP/IZ
 Sample : G1700-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S8-0425

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-BF031115.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	1.321	35	38	41	rVB	266842	450249	24.86%	3.417%
2	1.481	49	52	55	rVB	402814	438614	24.22%	3.329%
3	1.618	62	64	71	rVV	50330	115373	6.37%	0.876%
4	1.721	71	73	98	rVB	617473	1035710	57.18%	7.860%
5	4.784	339	341	347	rBV	20428	40225	2.22%	0.305%
6	5.333	386	389	395	rBV	357816	439086	24.24%	3.332%
7	6.636	501	503	505	rBV	234005	249803	13.79%	1.896%
8	6.762	511	514	516	rBV	905290	923494	50.99%	7.009%
9	7.047	537	539	541	rBV	236910	254094	14.03%	1.928%
10	7.230	553	555	557	rBV	1062105	961915	53.11%	7.300%
11	7.744	597	600	602	rBV	764147	758867	41.90%	5.759%
12	8.625	674	677	679	rBV	299716	356215	19.67%	2.703%
13	9.585	757	761	763	rBV	311072	447110	24.69%	3.393%
14	9.973	792	795	797	rBV	1561405	1609674	88.87%	12.216%
15	10.785	864	866	869	rVB	422161	424670	23.45%	3.223%
16	11.768	949	952	954	rBV	925019	880700	48.62%	6.684%
17	12.385	1004	1006	1008	rBV	31637	35125	1.94%	0.267%
18	12.625	1024	1027	1029	rBV	420491	457797	25.28%	3.474%
19	14.625	1199	1202	1204	rBV	1440022	1811214	100.00%	13.746%
20	15.814	1303	1306	1311	rBV	24433	47653	2.63%	0.362%
21	15.905	1311	1314	1317	rBV	466819	490562	27.08%	3.723%
22	17.677	1466	1469	1475	rBV	328560	471205	26.02%	3.576%
23	19.231	1602	1605	1614	rVB8	18819	56614	3.13%	0.430%
24	19.540	1628	1632	1633	rBV3	20450	50542	2.79%	0.384%
25	19.586	1633	1636	1638	rVV2	31228	70180	3.87%	0.533%
26	19.643	1638	1641	1652	rVB	74680	191943	10.60%	1.457%
27	20.854	1743	1747	1750	rBV4	8017	24308	1.34%	0.184%
28	21.003	1756	1760	1764	rBV4	18502	50722	2.80%	0.385%
29	21.152	1769	1773	1777	rVB5	11047	33032	1.82%	0.251%

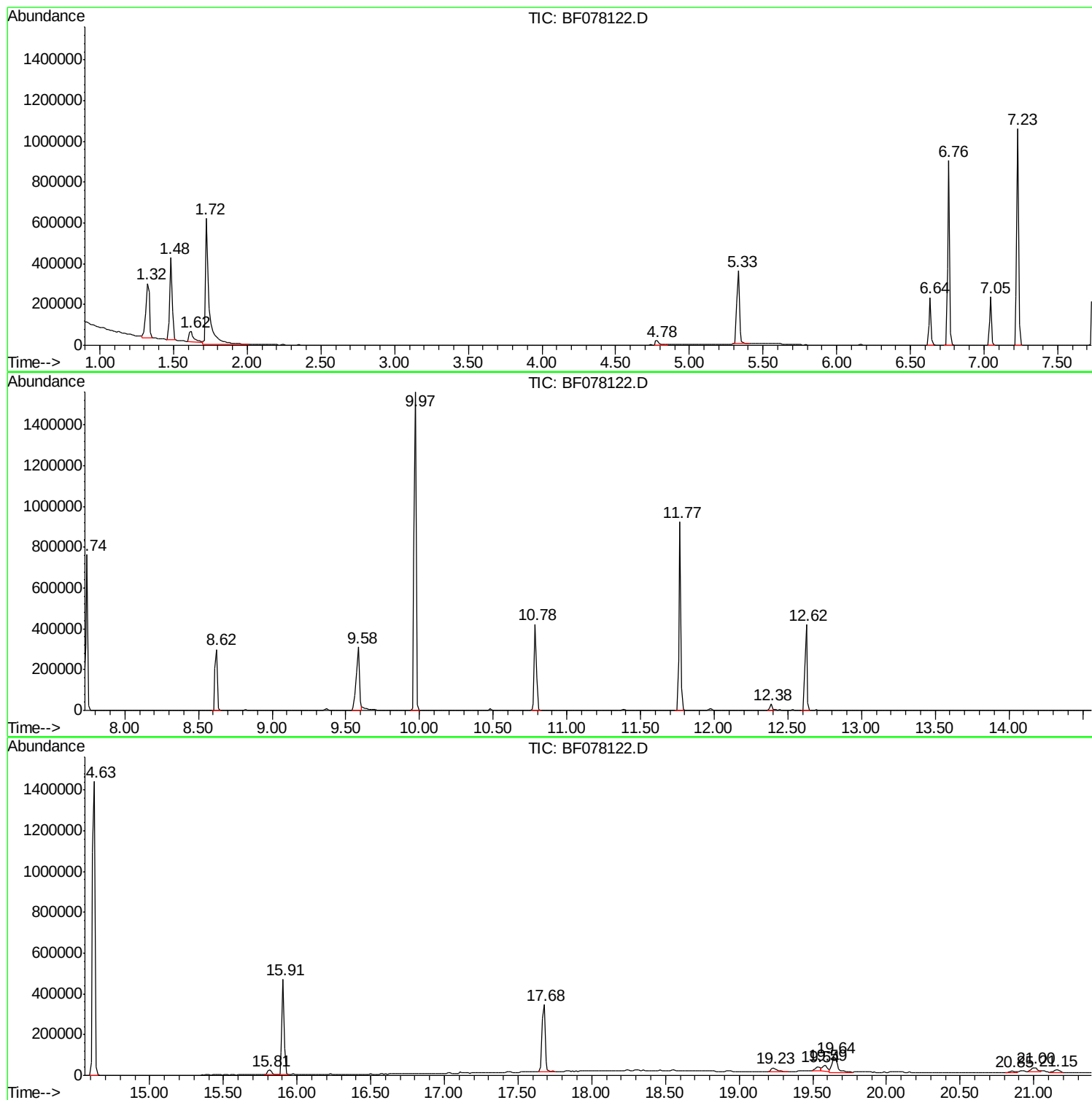
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Data Path : Z:\HPCHEM1\BNA F\DATA\BF033115\
Data File : BF078122.D
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Sample : G1700-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0425

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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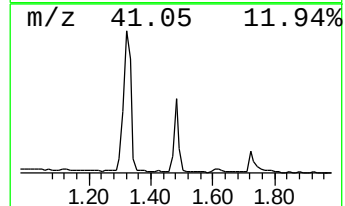
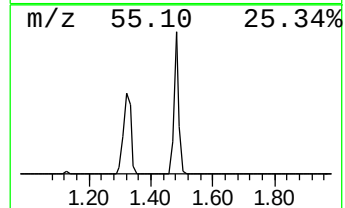
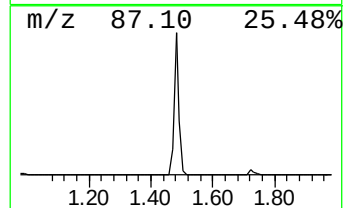
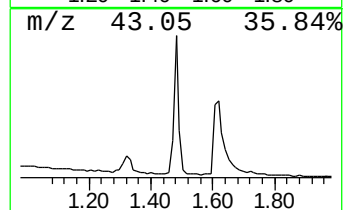
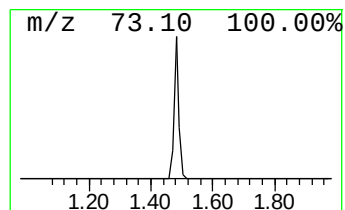
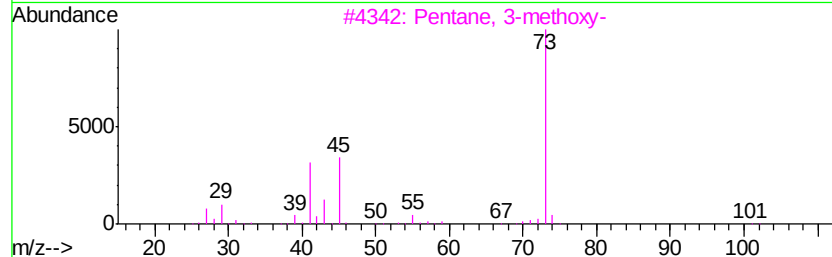
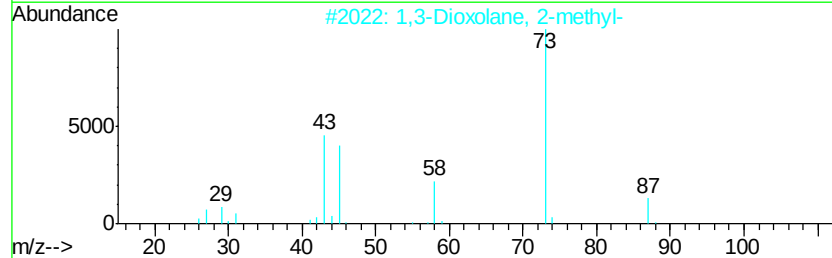
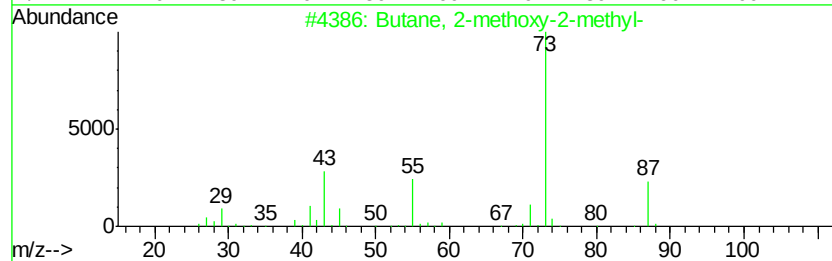
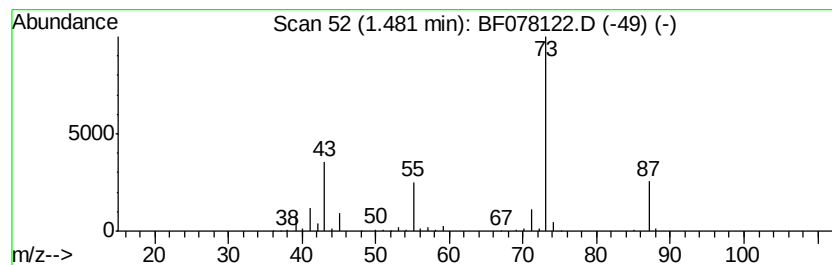
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	34.52 ng	438614	1,4-Dichlorobenzene-d4	7.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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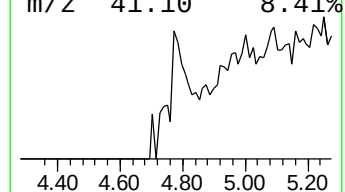
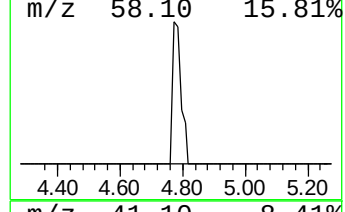
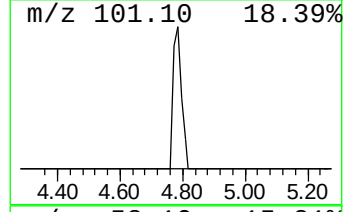
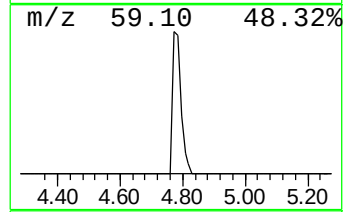
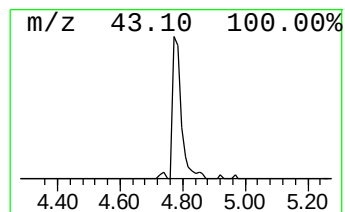
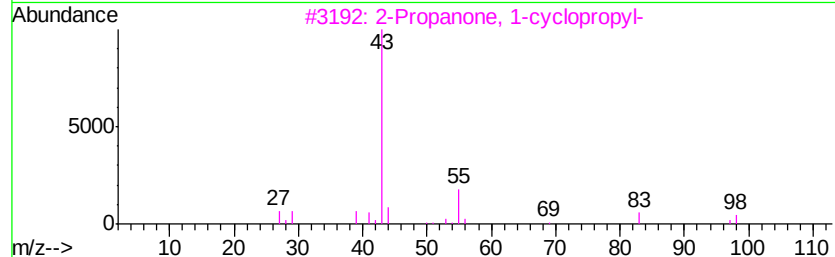
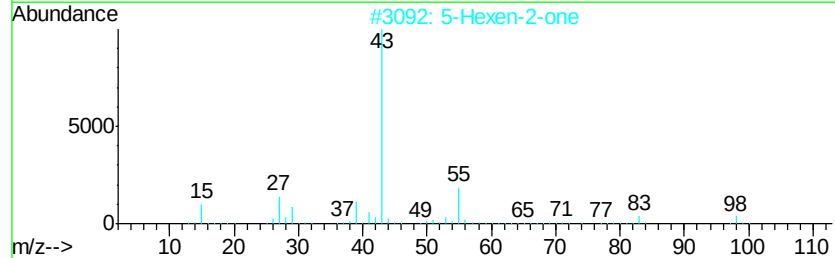
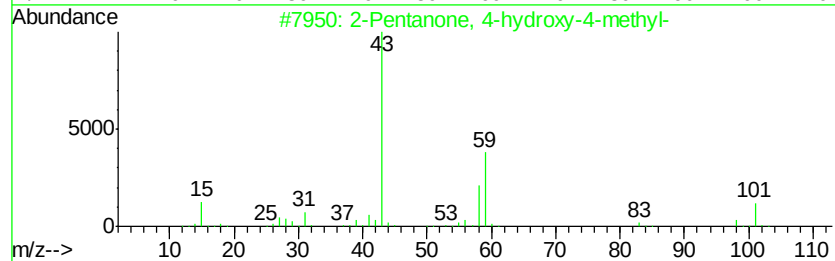
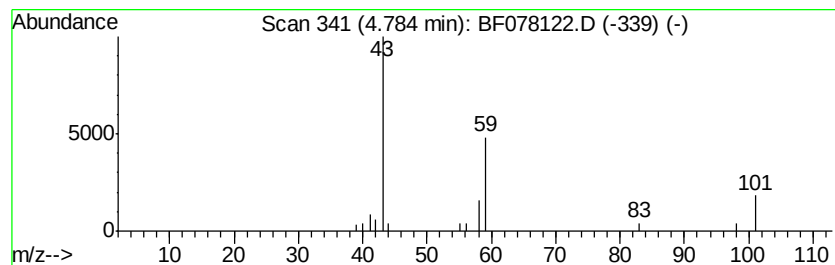
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TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.17 ng	40225	1,4-Dichlorobenzene-d4	7.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		5-Hexen-2-one	98	C6H10O	000109-49-9	12
3		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		Diacetamide	101	C4H7NO2	000625-77-4	7



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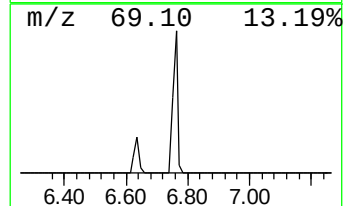
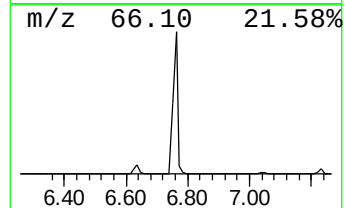
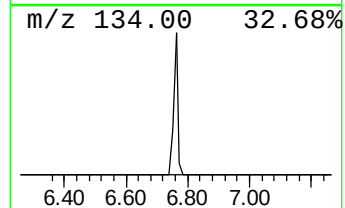
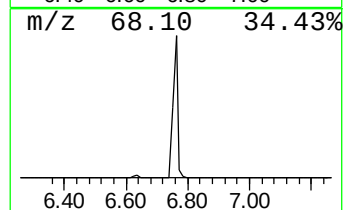
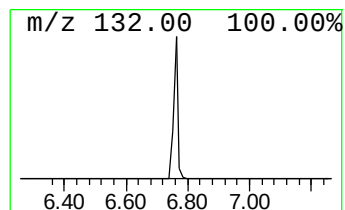
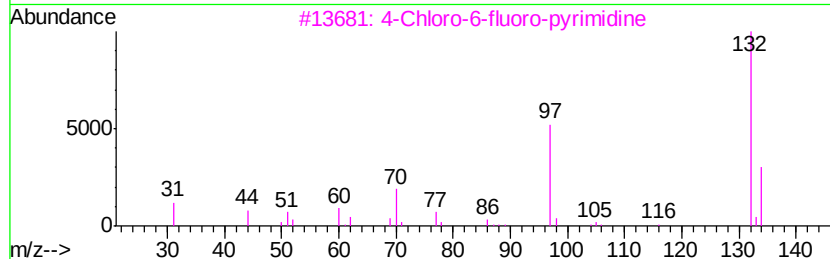
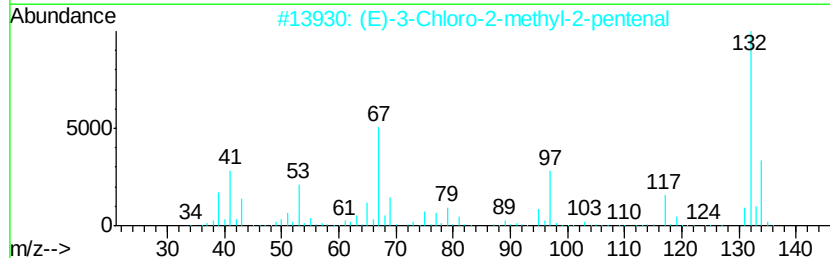
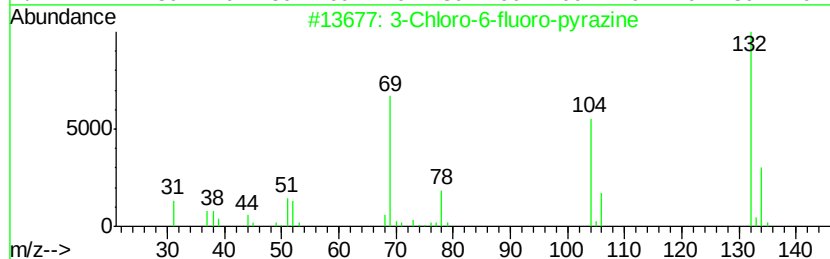
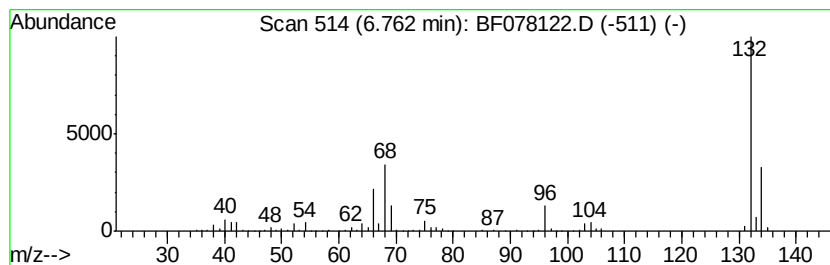
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.76 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	72.69 ng	923494	1,4-Dichlorobenzene-d4	7.05

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	17
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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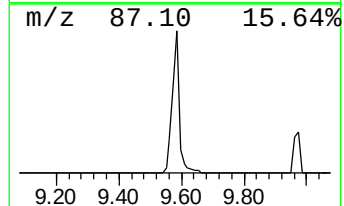
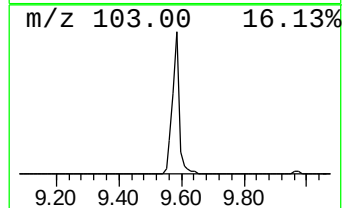
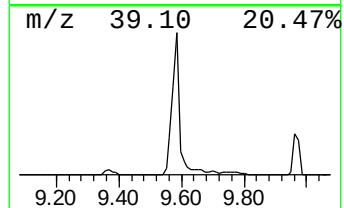
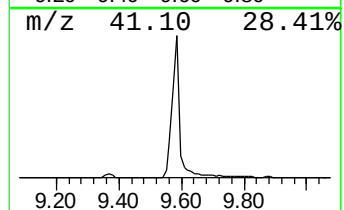
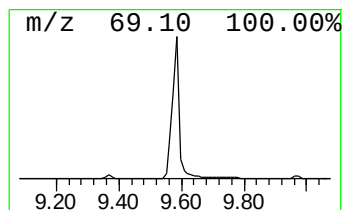
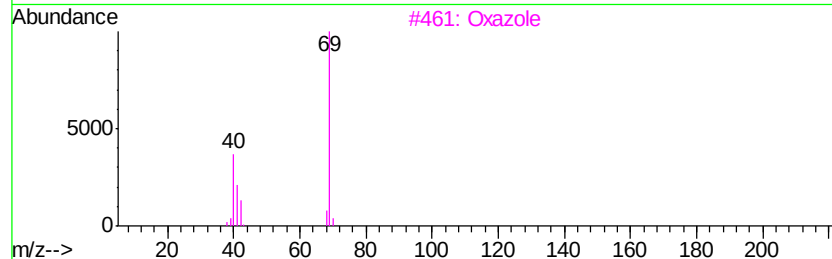
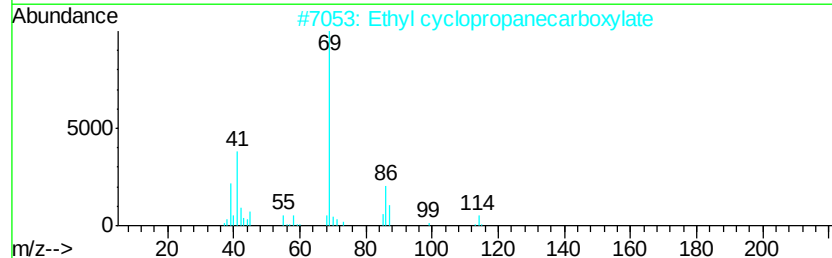
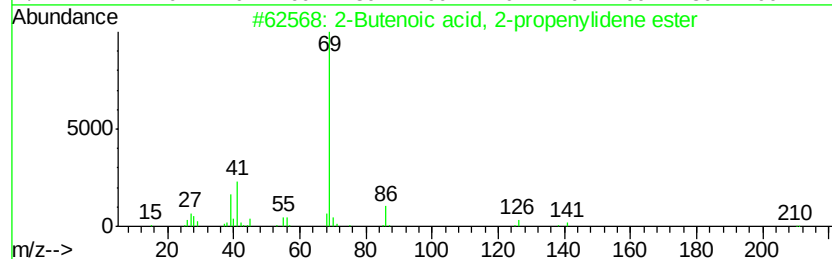
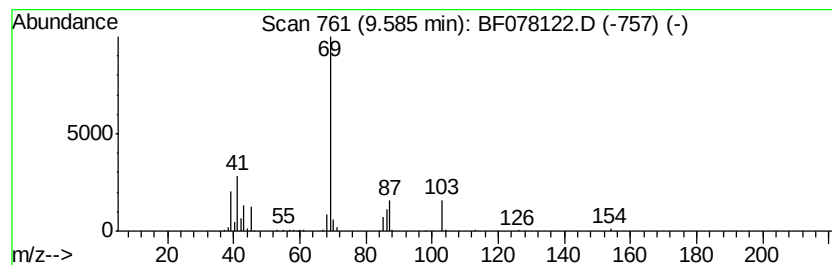
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 unknown9.58 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	25.10 ng	447110	Napthalene-d8	8.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
2		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
3		Oxazole	69	C3H3NO	000288-42-6	9
4		Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	9
5		Vinyl crotonate	112	C6H8O2	014861-06-4	9



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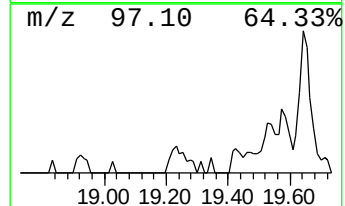
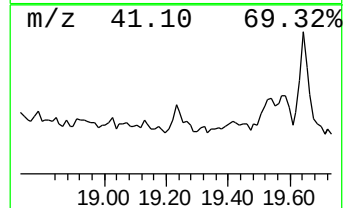
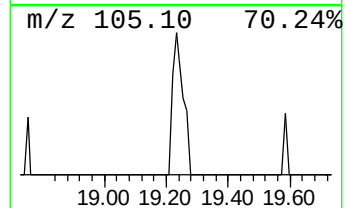
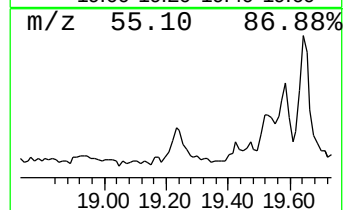
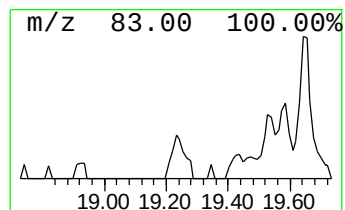
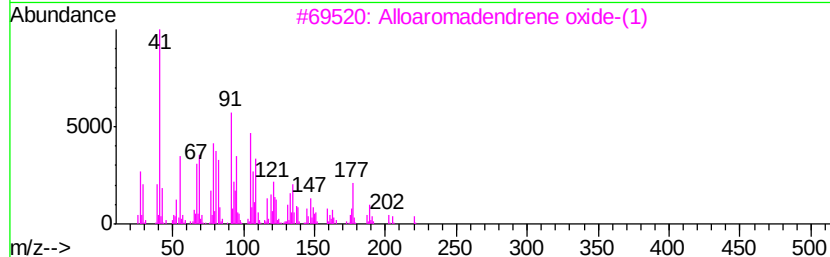
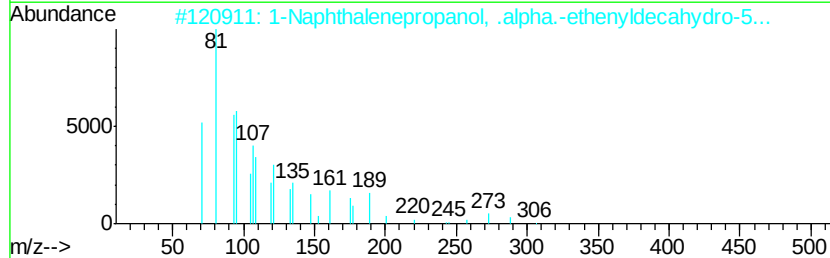
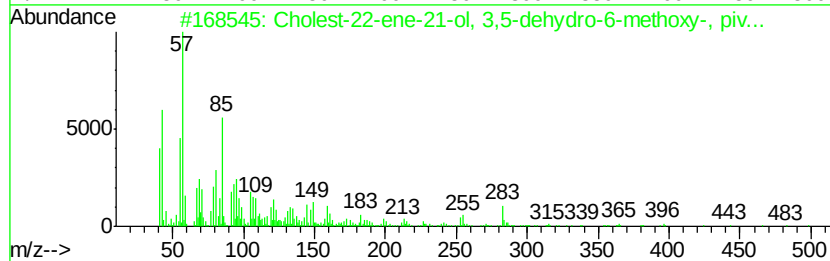
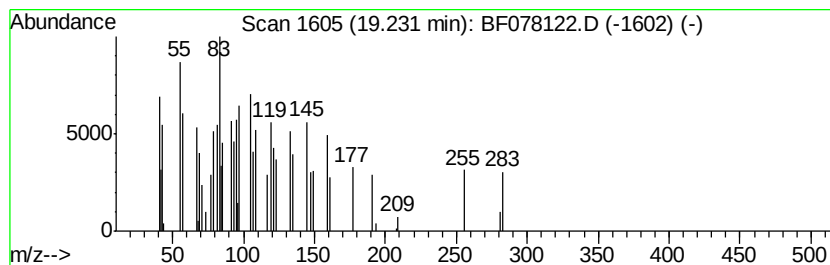
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown19.23 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	2.40 ng	56614	Perylene-d12	17.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholest-22-ene-21-ol, 3,5-dehydr...	498	C33H54O3	1000124-60-2	43
2		1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	004549-12-6	38
3		Alloaromadendrene oxide-(1)	220	C15H24O	1000156-12-8	38
4		2H-Pyran, 2-(7-heptadecynvloxy)t...	336	C22H40O2	056599-50-9	35
5		1,4-Methanoazulen-7-ol, decahydr...	222	C15H26O	018319-27-2	27



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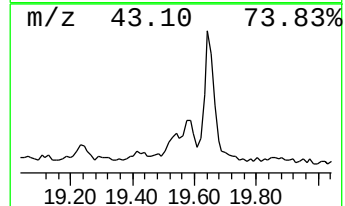
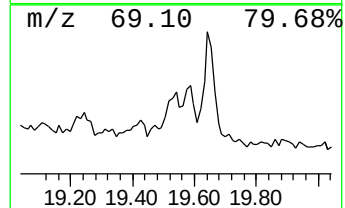
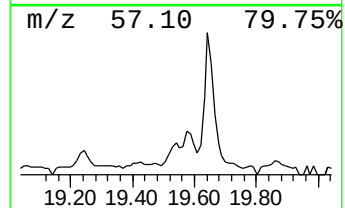
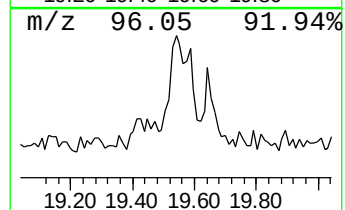
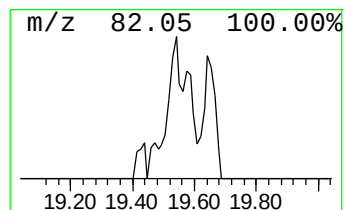
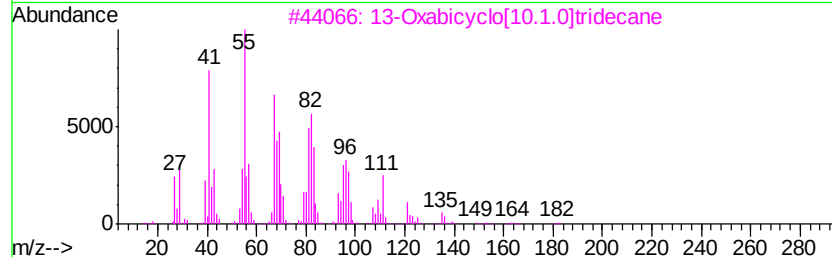
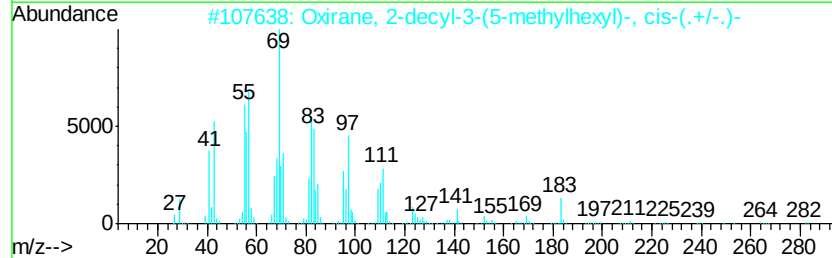
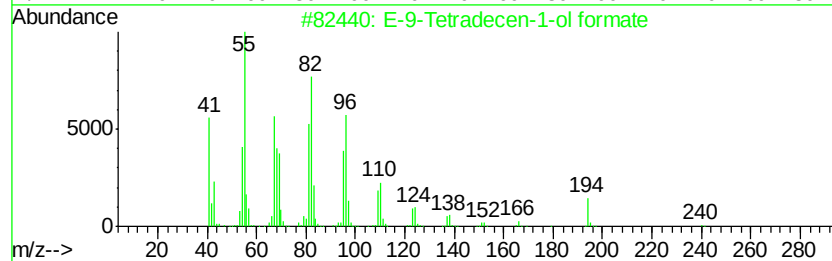
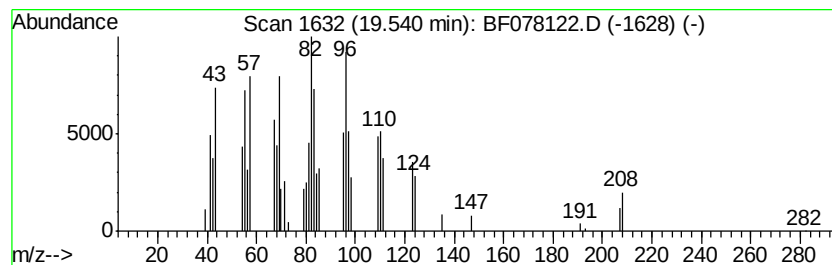
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown19.54 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	2.15 ng	50542	Perylene-d12	17.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-9-Tetradecen-1-ol formate	240	C15H28O2	1000130-78-2	43
2			Oxirane, 2-decyl-3-(5-methylhexy...	282	C19H38O	057457-72-4	38
3			13-Oxabicyclo[10.1.0]tridecane	182	C12H22O	000286-99-7	38
4			1-Cyclohexylheptene	180	C13H24	114614-83-4	38
5			Pentafluoropropionic acid, 10-un...	316	C14H21F5O2	1000280-07-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033115\
Data File : BF078122.D
Acq On : 31 Mar 2015 19:05
Operator : TP/IZ
Sample : G1700-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0425

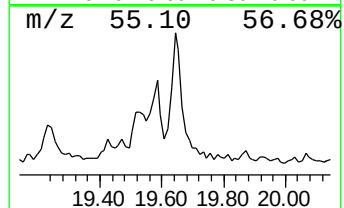
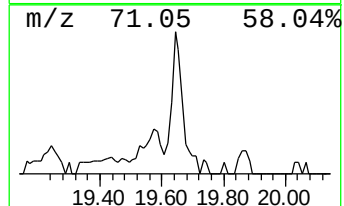
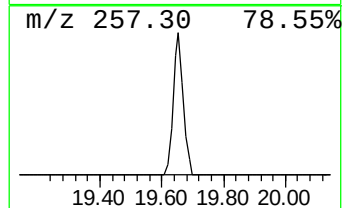
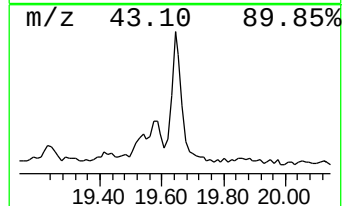
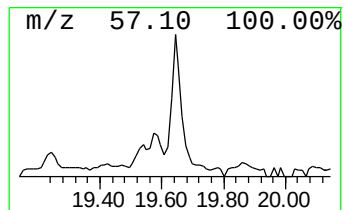
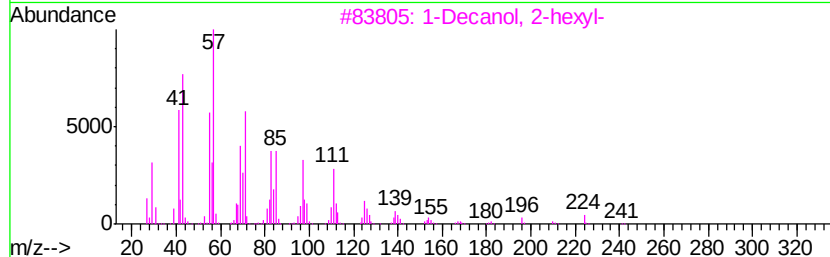
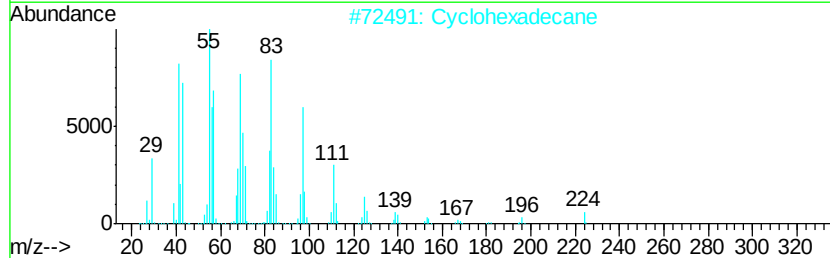
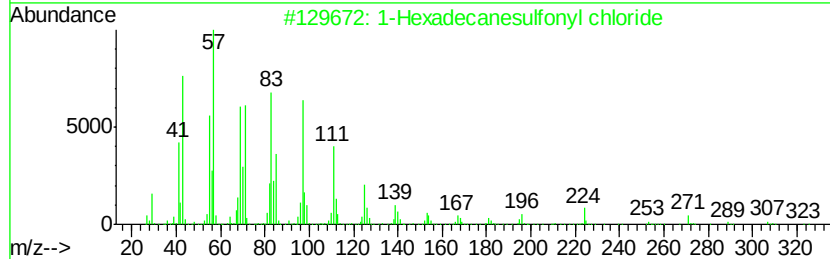
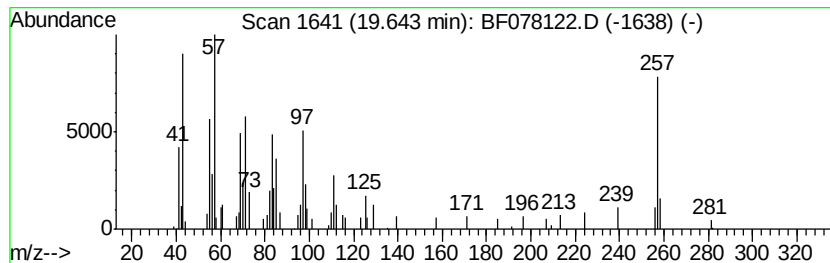
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Hexadecanesulfonyl chloride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	8.15 ng	191943	Perylene-d12	17.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	64
2			Cyclohexadecane	224	C16H32	000295-65-8	64
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	49
4			2-Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	49
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF033115\
Data File : BF078122.D
Acq On : 31 Mar 2015 19:05
Operator : TP/IZ
Sample : G1700-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

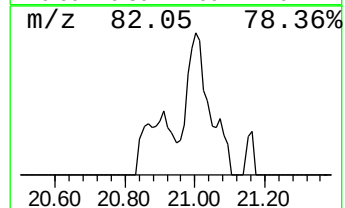
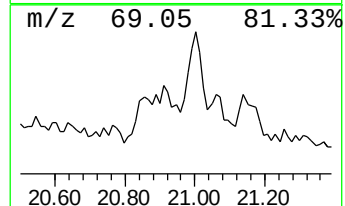
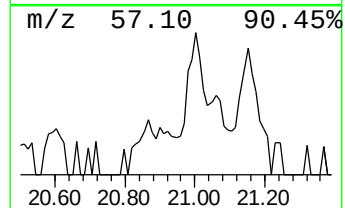
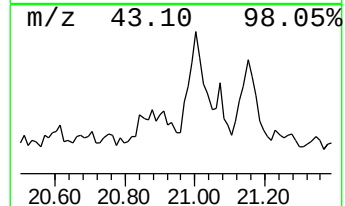
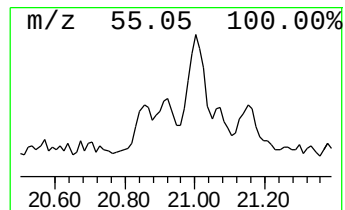
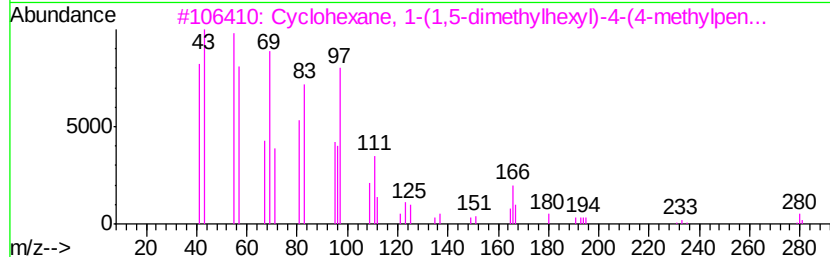
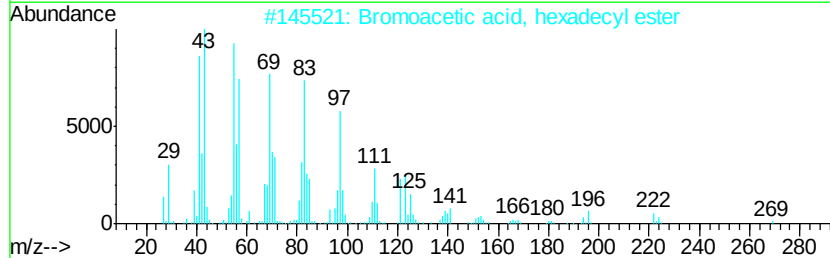
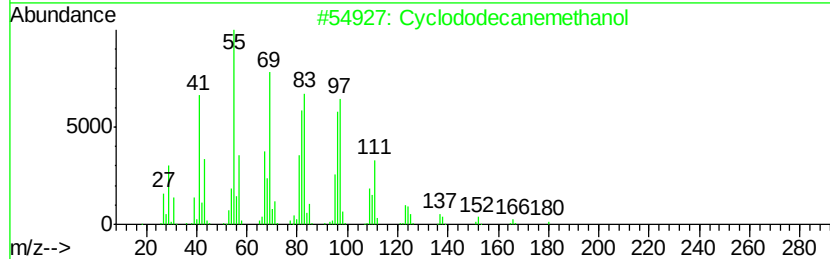
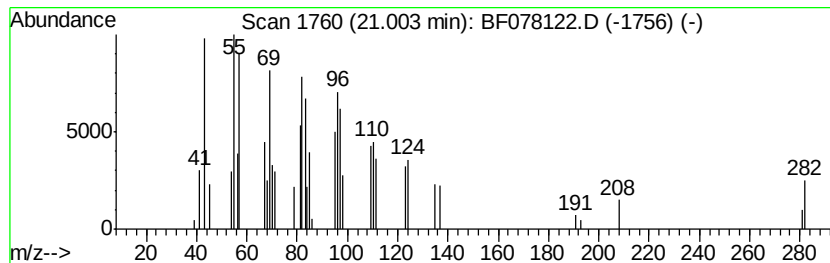
Instrument :
BNA_F
ClientSampled :
S8-0425

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cyclododecanemethanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.00	2.15 ng	50722	Perylene-d12	17.68		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclododecanemethanol	198	C13H26O	001892-12-2	52
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	30
3		Cyclohexane, 1-(1,5-dimethylhexyl)-4-(4-methylphenyl)-	280	C20H40	056009-20-2	30
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	30
5		Cyclohexane, 1-(cyclohexylmethyl)-4-(4-methylphenyl)-	208	C15H28	054934-94-0	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033115\
Data File : BF078122.D
Acq On : 31 Mar 2015 19:05
Operator : TP/IZ
Sample : G1700-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S8-0425

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
Butane, 2-methoxy...	1.48	34.5	ng	438614	1	7.05	254094	20.0
2-Pentanone, 4-hy...	4.78	3.2	ng	40225	1	7.05	254094	20.0
unknown6.76	6.76	72.7	ng	923494	1	7.05	254094	20.0
unknown9.58	9.58	25.1	ng	447110	2	8.62	356215	20.0
unknown19.23	19.23	2.4	ng	56614	6	17.68	471205	20.0
unknown19.54	19.54	2.1	ng	50542	6	17.68	471205	20.0
1-Hexadecanesulfo...	19.64	8.2	ng	191943	6	17.68	471205	20.0
Cyclododecanemeth...	21.00	2.1	ng	50722	6	17.68	471205	20.0