

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062615\
 Data File : BF080199.D
 Acq On : 26 Jun 2015 19:56
 Operator : TP/IZ
 Sample : G2785-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF061715.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	5.510	210	212	216	rVB	47426	48104	3.04%	0.545%
2	5.898	244	246	249	rBV	353879	387288	24.51%	4.391%
3	6.893	331	333	336	rBV	248439	248513	15.73%	2.817%
4	7.064	345	348	350	rBV	747276	748854	47.39%	8.489%
5	7.293	366	368	370	rVB	223332	198911	12.59%	2.255%
6	7.453	380	382	385	rVB	905874	742664	47.00%	8.419%
7	7.853	415	417	419	rBV	722675	597177	37.79%	6.770%
8	8.584	479	481	484	rBV	305341	258596	16.36%	2.932%
9	9.659	573	575	578	rVB	1297452	1147218	72.60%	13.006%
10	9.807	586	588	591	rBV	44314	41129	2.60%	0.466%
11	10.047	608	609	612	rBV2	20555	16902	1.07%	0.192%
12	10.356	634	636	639	rVB	358732	303300	19.19%	3.438%
13	10.882	681	682	686	rVB	11020	15822	1.00%	0.179%
14	11.145	703	705	708	rBV2	554322	694114	43.92%	7.869%
15	11.202	708	710	713	rVV	262026	273319	17.30%	3.099%
16	11.865	766	768	770	rBV	256599	313294	19.83%	3.552%
17	12.413	814	816	822	rBV	235455	275183	17.41%	3.120%
18	13.522	910	913	915	rBV	1426027	1580283	100.00%	17.915%
19	14.551	1000	1003	1007	rBV2	28990	57769	3.66%	0.655%
20	14.631	1007	1010	1016	rVV	58706	90539	5.73%	1.026%
21	14.756	1019	1021	1024	rVV	381272	377176	23.87%	4.276%
22	15.705	1102	1104	1109	rBV	20592	39784	2.52%	0.451%
23	16.597	1178	1182	1185	rBV	244061	365016	23.10%	4.138%

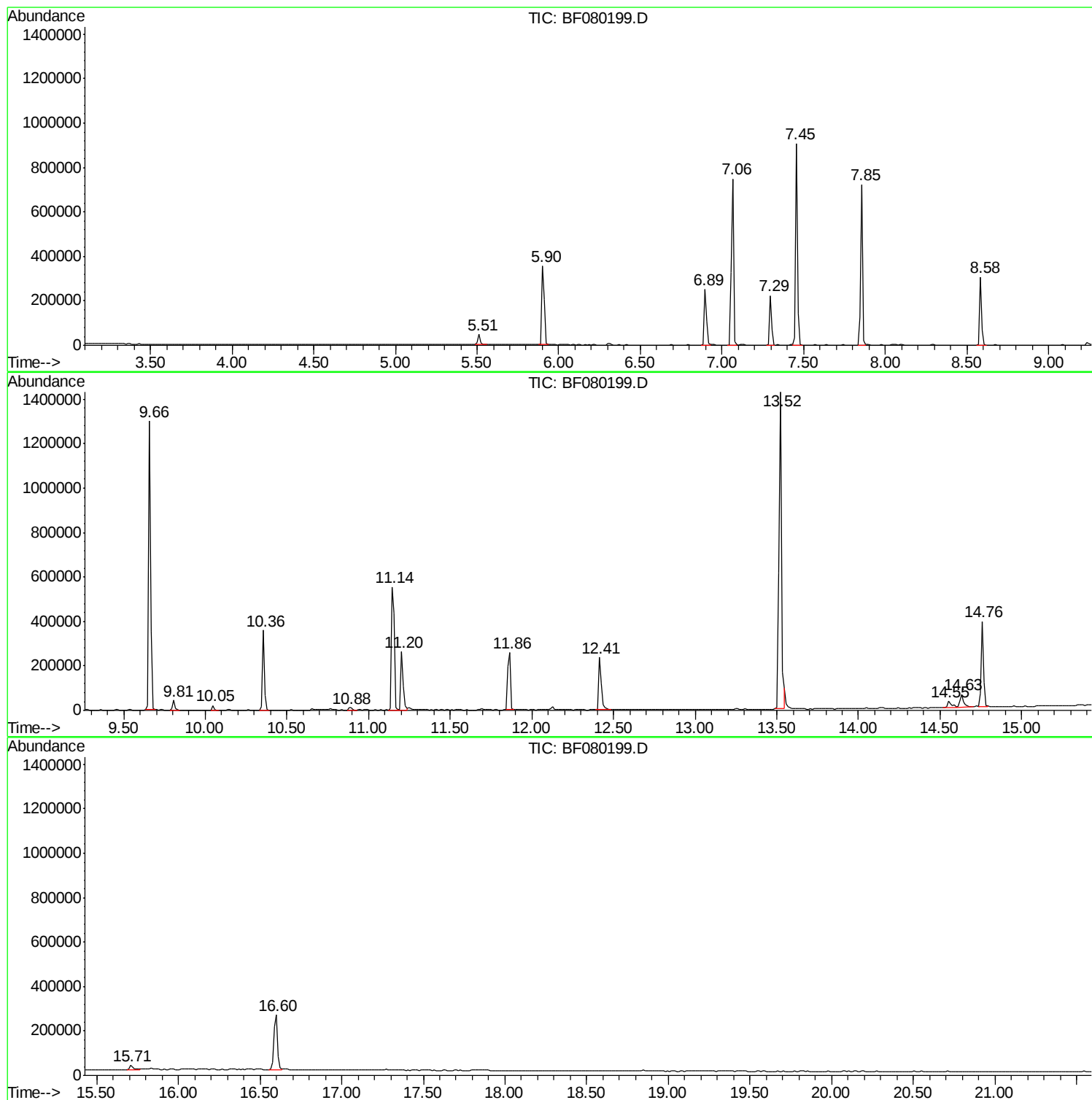
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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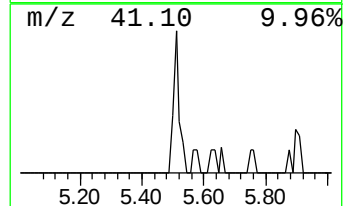
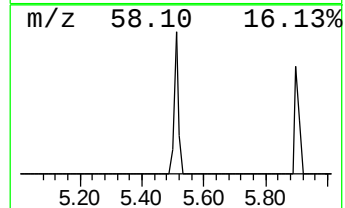
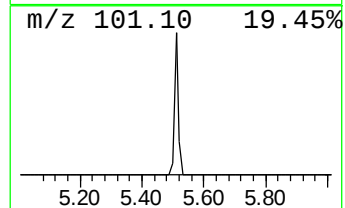
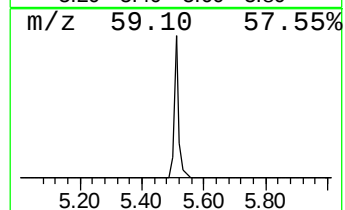
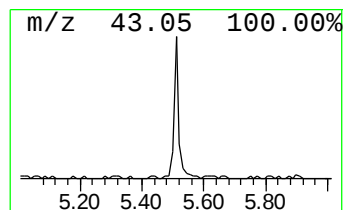
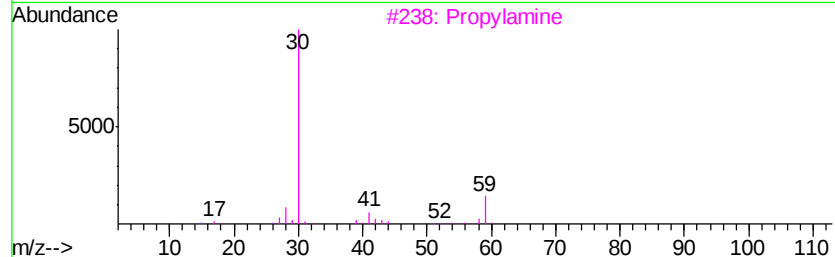
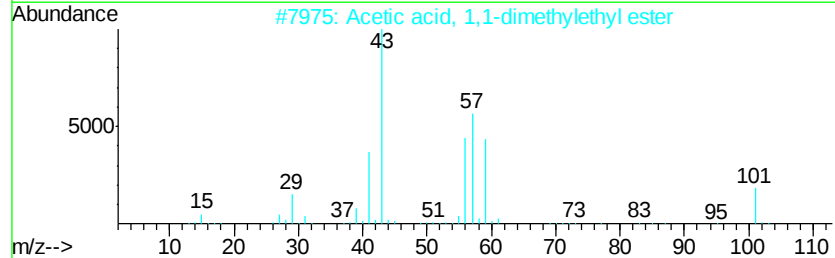
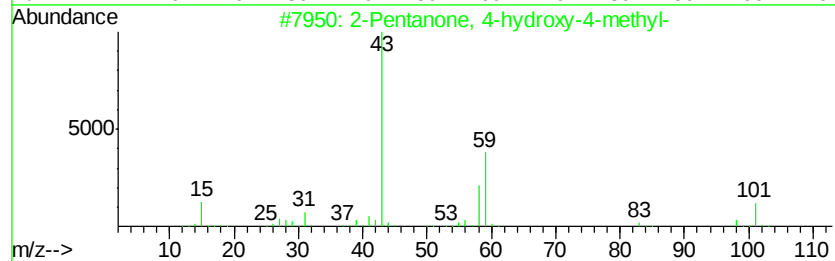
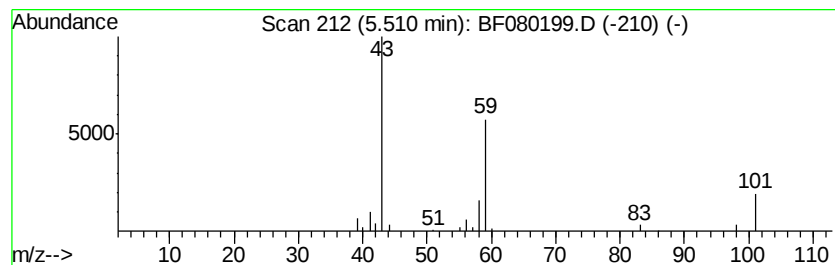
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	4.84 ng	48104	1,4-Dichlorobenzene-d4	7.29

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			Propylamine	59	C3H9N	000107-10-8	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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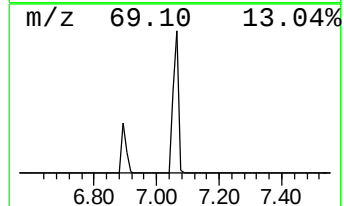
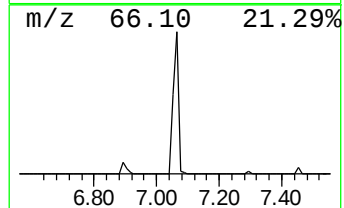
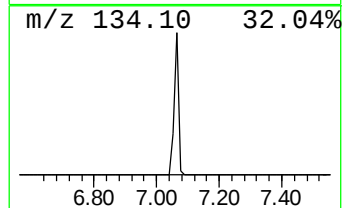
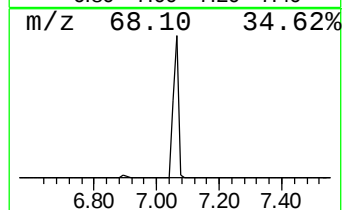
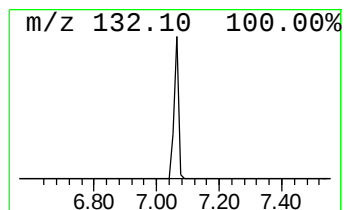
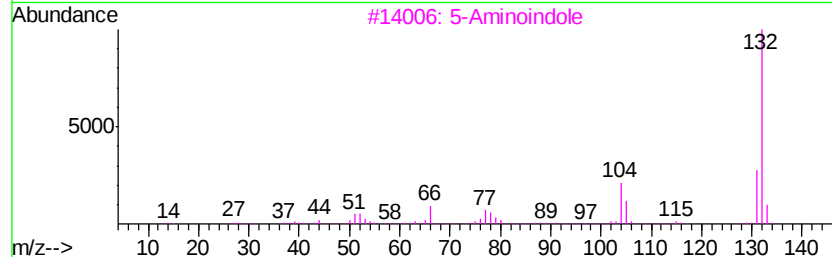
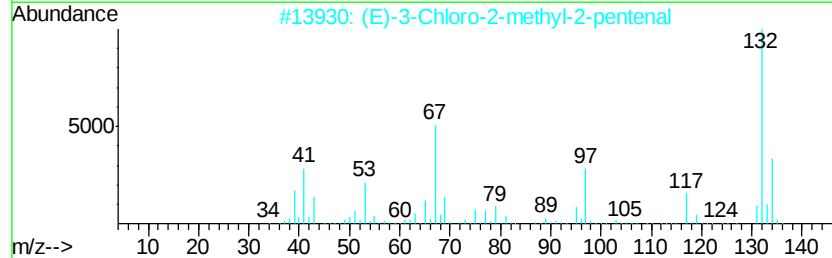
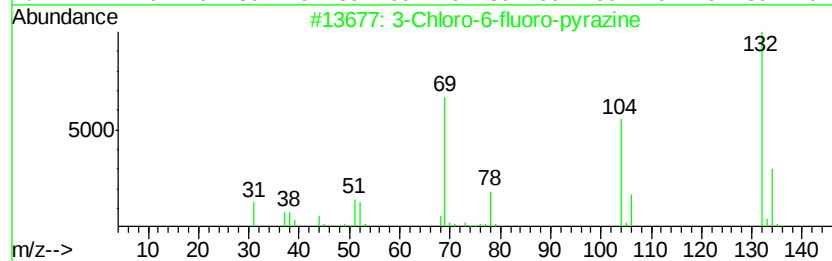
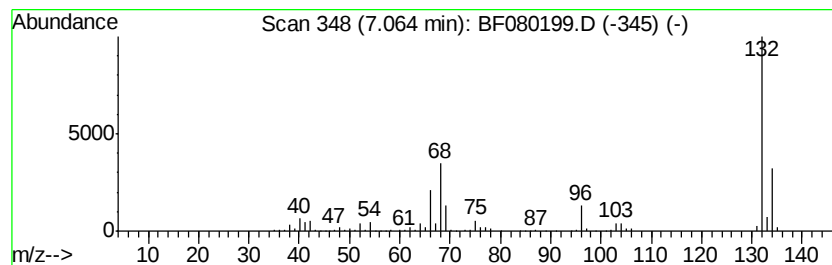
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.06 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	75.30 ng	748854	1,4-Dichlorobenzene-d4	7.29

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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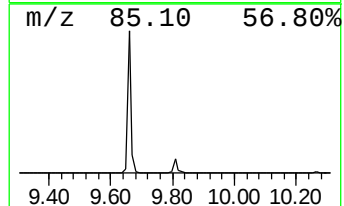
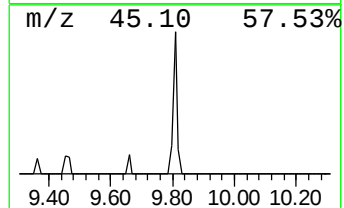
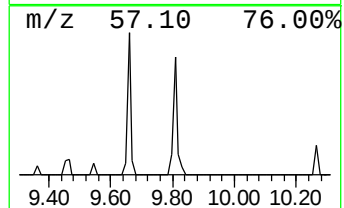
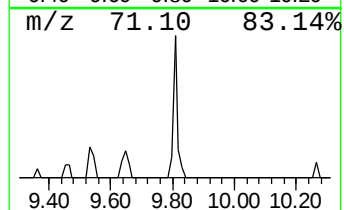
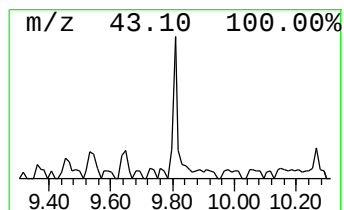
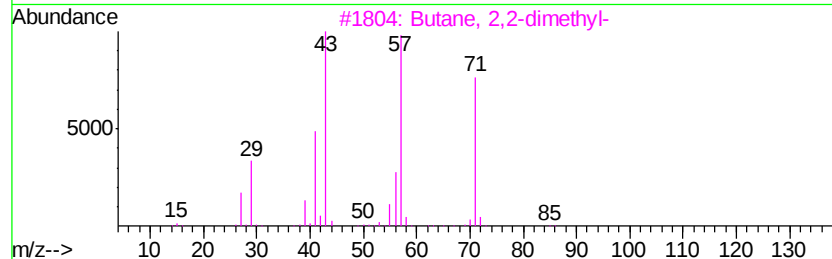
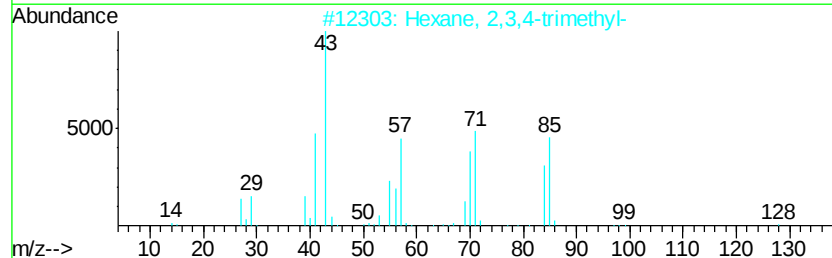
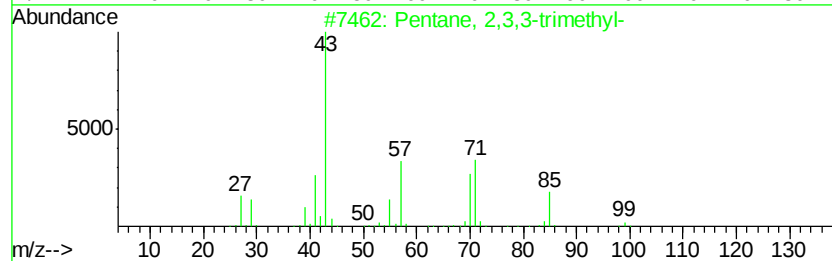
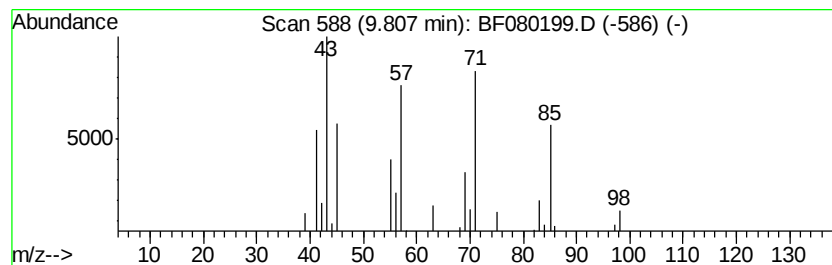
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Peak Number 4 unknown9.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.81	2.71 ng	41129	Acenaphthene-d10	10.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	47
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	40
3		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	25
4		Ether, heptyl hexyl	200	C13H28O	007289-40-9	16
5		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	16



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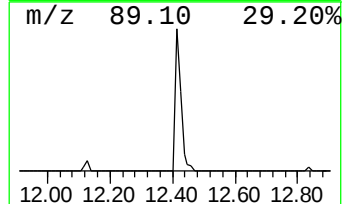
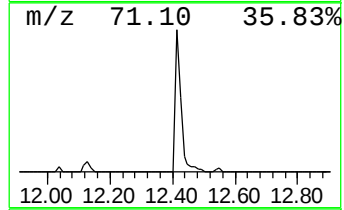
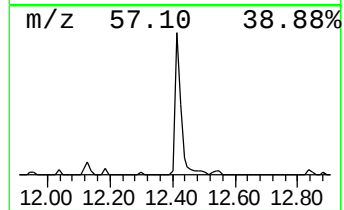
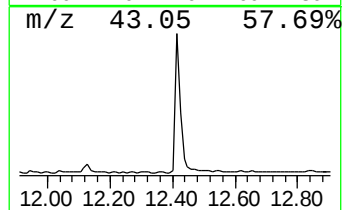
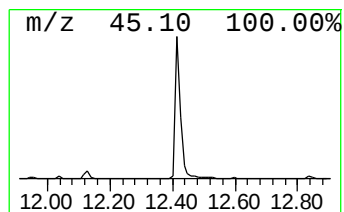
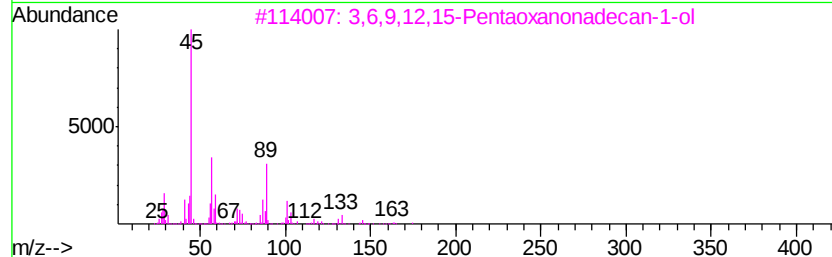
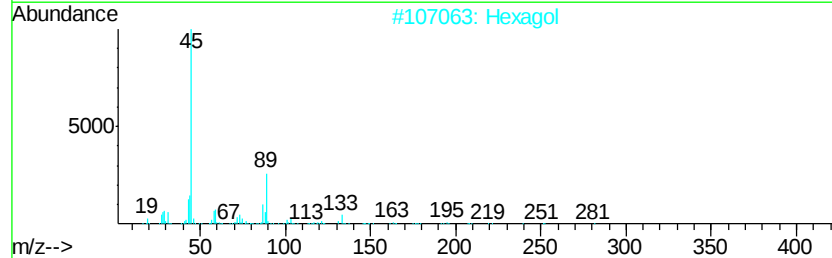
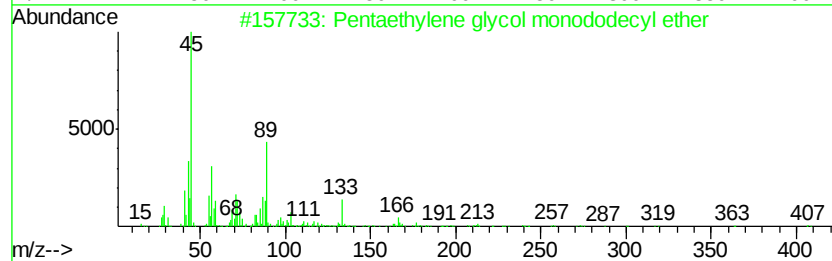
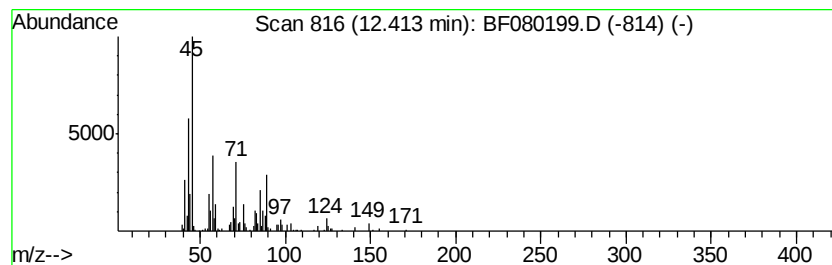
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Pentaethylene glycol monodo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	17.57 ng	275183	Phenanthrene-d10	11.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	64
2		Hexagol	282	C12H26O7	002615-15-8	58
3		3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	53
4		Octaethylene glycol	370	C16H34O9	1000289-34-2	53
5		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	52



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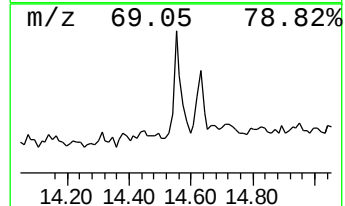
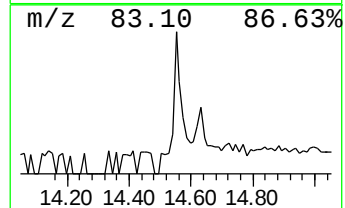
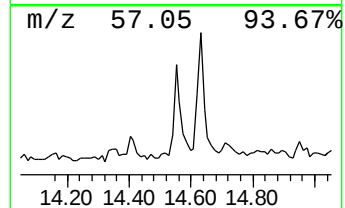
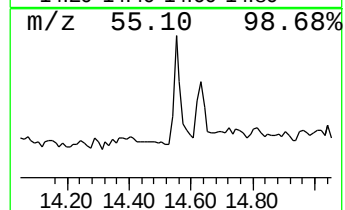
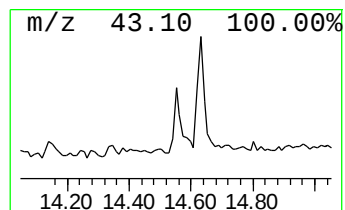
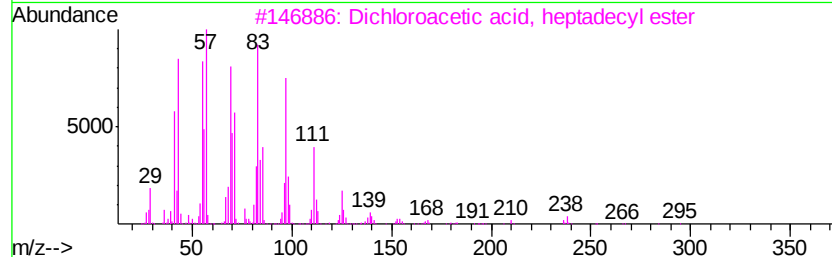
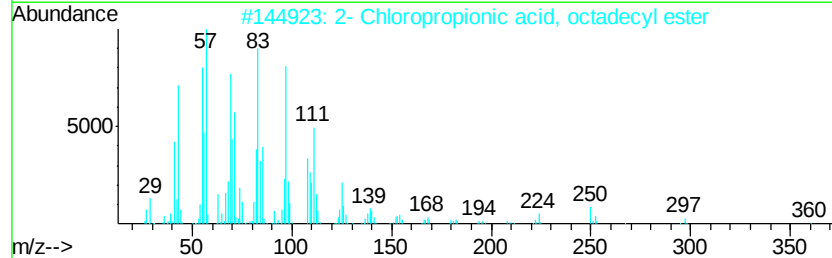
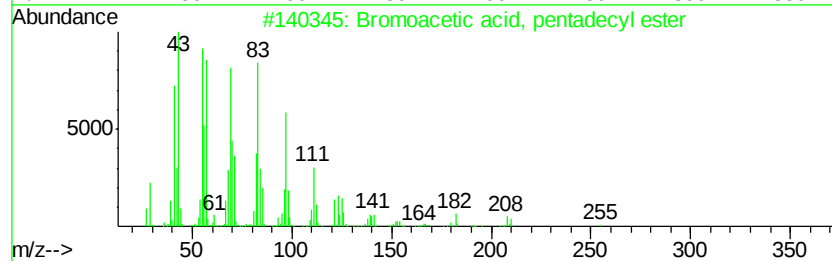
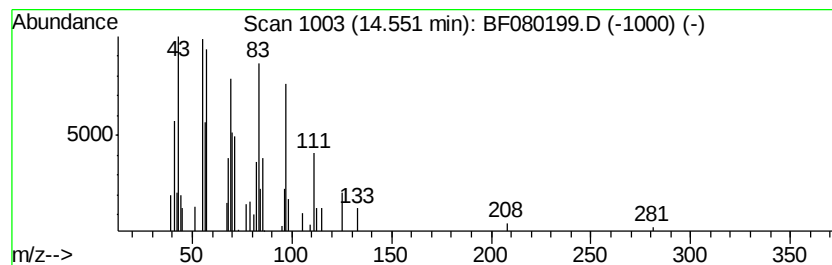
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Bromoacetic acid, pentadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	3.06 ng	57769	Chrysene-d12	14.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	93
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	87



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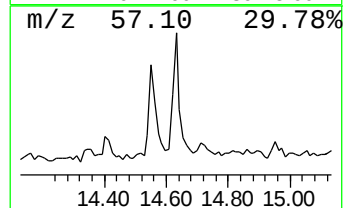
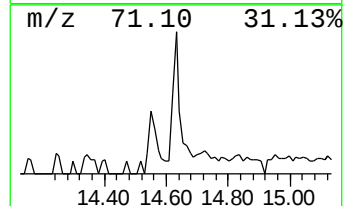
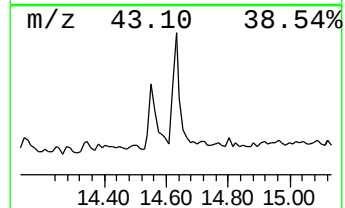
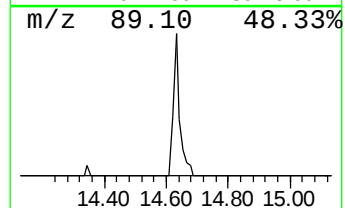
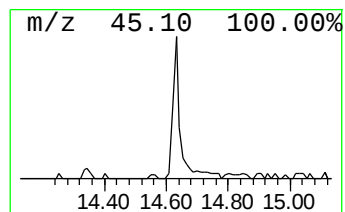
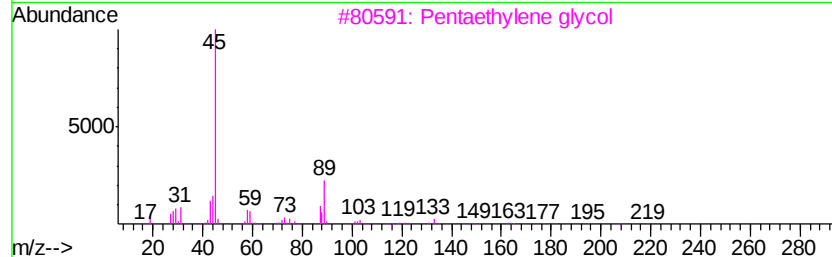
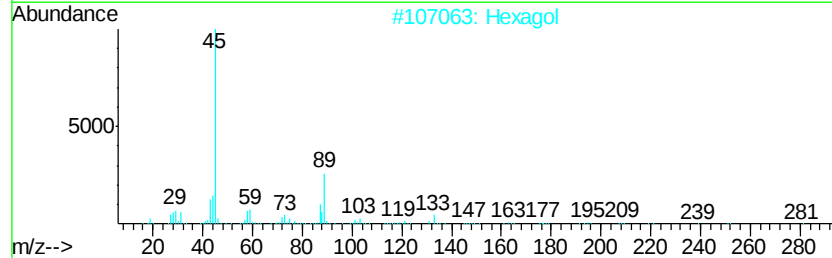
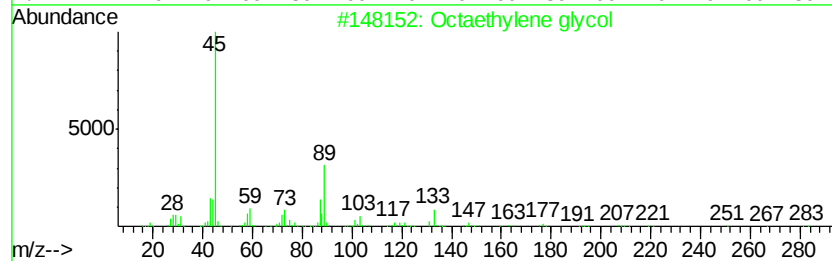
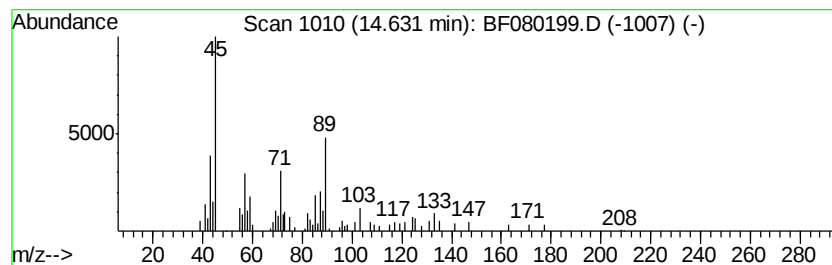
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.80 ng	90539	Chrysene-d12	14.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octaethylene glycol	370	C16H34O9	1000289-34-2	80
2		Hexagol	282	C12H26O7	002615-15-8	72
3		Pentaethylene glycol	238	C10H22O6	004792-15-8	64
4		Ethanol, 1-[2-[2-(1-methylethoxy...	192	C9H20O4	029681-21-8	64
5		1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062615\
Data File : BF080199.D
Acq On : 26 Jun 2015 19:56
Operator : TP/IZ
Sample : G2785-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

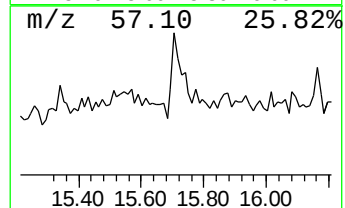
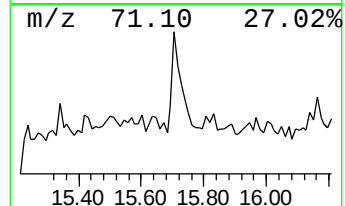
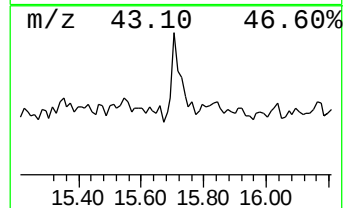
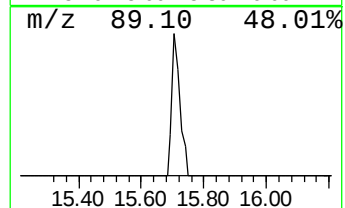
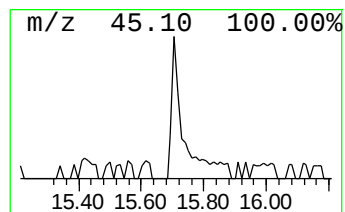
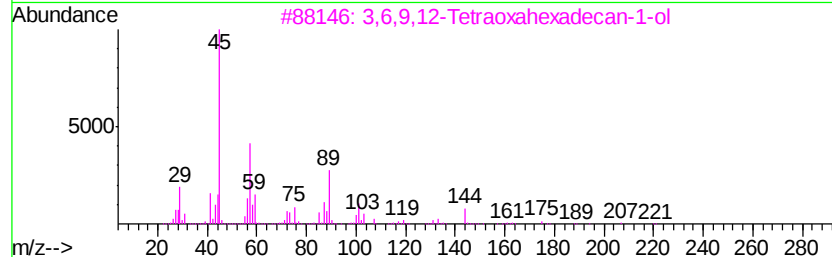
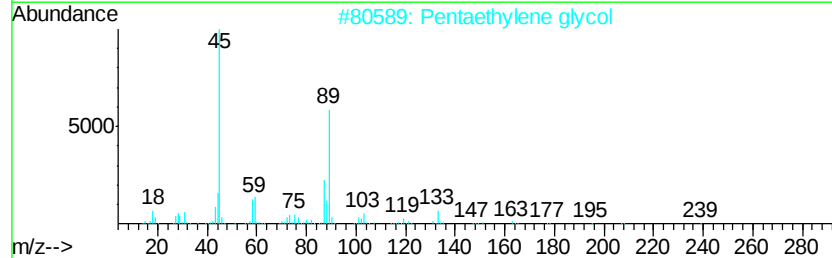
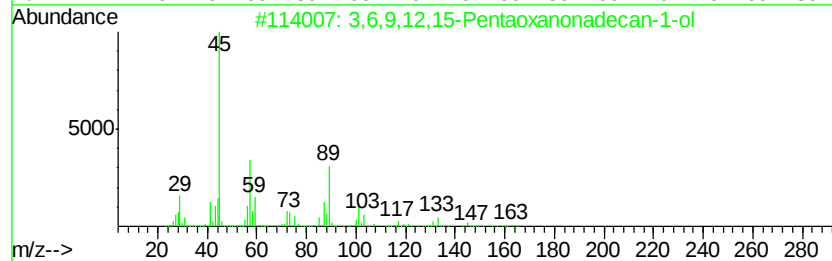
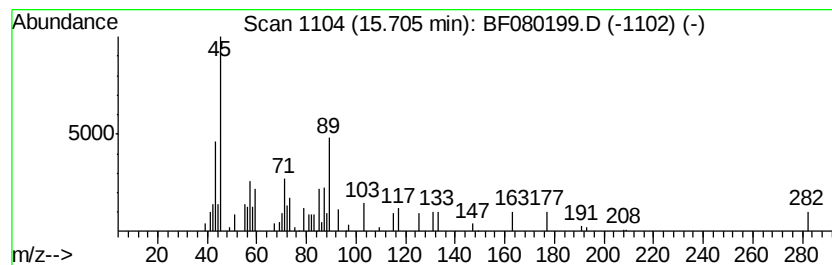
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.18 ng	39784	Perylene-d12	16.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	59
2		Pentaethylene glycol	238	C10H22O6	004792-15-8	53
3		3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	53
4		Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	53
5		15-Crown-5	220	C10H20O5	033100-27-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062615\
Data File : BF080199.D
Acq On : 26 Jun 2015 19:56
Operator : TP/IZ
Sample : G2785-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061715.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...	5.51	4.8	ng	48104	1	7.29	198911	20.0
unknown7.06	7.06	75.3	ng	748854	1	7.29	198911	20.0
unknown9.81	9.81	2.7	ng	41129	3	10.36	303300	20.0
Pentaethylene gly...	12.41	17.6	ng	275183	4	11.86	313294	20.0
Bromoacetic acid,...	14.55	3.1	ng	57769	5	14.76	377176	20.0
Octaethylene glycol	14.63	4.8	ng	90539	5	14.76	377176	20.0
3,6,9,12,15-Penta...	15.71	2.2	ng	39784	6	16.60	365016	20.0