

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
 Data File : BF088667.D
 Acq On : 4 Jul 2016 00:47
 Operator : UM/SJ
 Sample : H3817-09
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-4A-2-9FT

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-BF063016.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	1.850	21	23	35	rVB	125258	177802	5.59%	0.595%
2	2.021	35	38	41	rVB	54068	81806	2.57%	0.274%
3	3.016	123	125	137	rBV	59362	121326	3.81%	0.406%
4	4.959	292	295	302	rVB	192911	276219	8.68%	0.924%
5	5.382	329	332	334	rBV	2833508	2984148	93.75%	9.987%
6	6.056	389	391	393	rBV	270836	225681	7.09%	0.755%
7	6.422	420	423	425	rBV	2783493	3182971	100.00%	10.653%
8	6.547	431	434	437	rBV	2467091	3116294	97.91%	10.429%
9	6.787	452	455	456	rBV	548223	690126	21.68%	2.310%
10	6.822	456	458	460	rVV	72081	65918	2.07%	0.221%
11	6.936	466	468	471	rVB	1957690	2113223	66.39%	7.072%
12	7.027	475	476	478	rBV	35778	48968	1.54%	0.164%
13	7.347	501	504	506	rBV	2025992	2053418	64.51%	6.872%
14	7.987	557	560	565	rBV	45174	64426	2.02%	0.216%
15	8.067	565	567	569	rVB	1195318	1020906	32.07%	3.417%
16	9.142	658	661	664	rVB	2563630	2657314	83.49%	8.893%
17	9.542	693	696	698	rBV	412998	461804	14.51%	1.546%
18	9.816	717	720	722	rBV	1262359	1102861	34.65%	3.691%
19	10.113	742	746	752	rBV2	21734	113365	3.56%	0.379%
20	10.605	786	789	791	rBV	2037879	2244677	70.52%	7.512%
21	10.731	798	800	805	rVB	52733	53206	1.67%	0.178%
22	11.176	837	839	841	rBV	104911	94308	2.96%	0.316%
23	11.291	847	849	852	rVV	1229250	1076344	33.82%	3.602%
24	11.359	852	855	859	rVB2	29194	65365	2.05%	0.219%
25	11.599	875	876	879	rVB	56730	54664	1.72%	0.183%
26	12.879	985	988	990	rBV	2558320	2539331	79.78%	8.499%
27	13.359	1028	1030	1034	rBV	71867	72479	2.28%	0.243%
28	13.794	1066	1068	1076	rVB	132758	196316	6.17%	0.657%
29	13.919	1076	1079	1081	rBV	907964	996073	31.29%	3.334%
30	14.422	1119	1123	1134	rBV	172285	333271	10.47%	1.115%
31	14.685	1143	1146	1150	rBV	292943	298618	9.38%	0.999%
32	15.051	1177	1178	1185	rVB2	32660	65828	2.07%	0.220%
33	15.303	1198	1200	1202	rBV	536734	767026	24.10%	2.567%
34	15.348	1202	1204	1208	rVB	80784	132865	4.17%	0.445%

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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 >
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35	16.148	1271	1274	1277	rBV	33329	56664	1.78%	0.190%
36	17.223	1363	1368	1370	rBV3	24415	68172	2.14%	0.228%
37	17.691	1405	1409	1415	rVB4	26020	69299	2.18%	0.232%
38	17.943	1427	1431	1438	rVB6	13946	50961	1.60%	0.171%
39	19.063	1524	1529	1537	rVB2	27765	85587	2.69%	0.286%

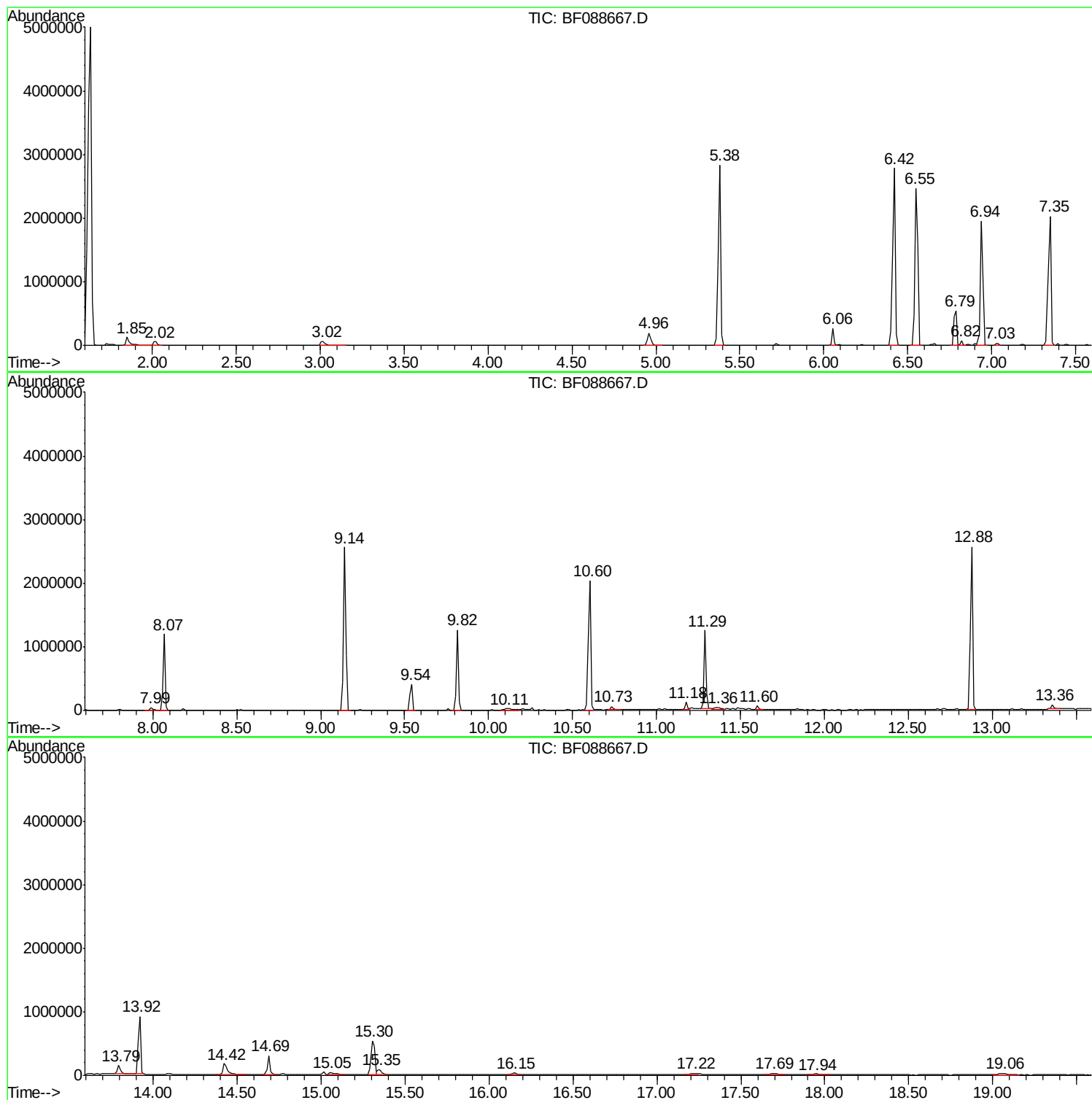
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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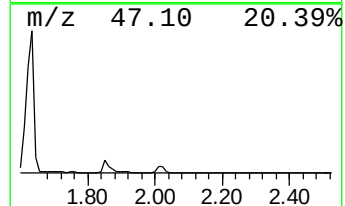
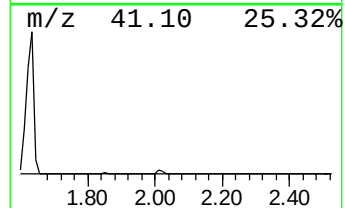
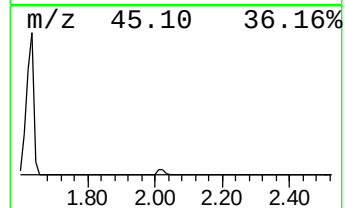
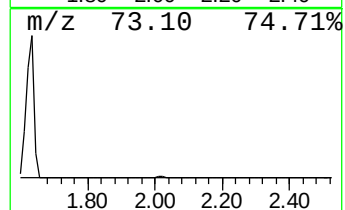
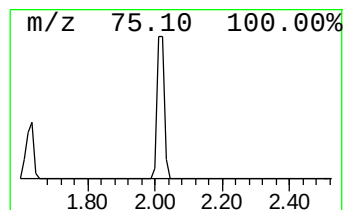
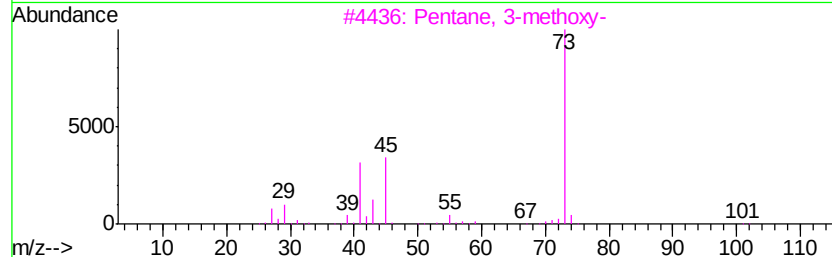
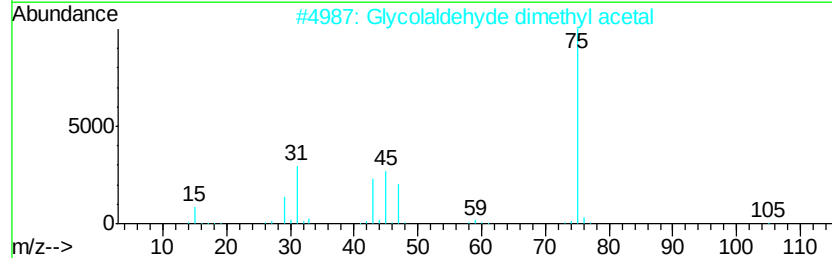
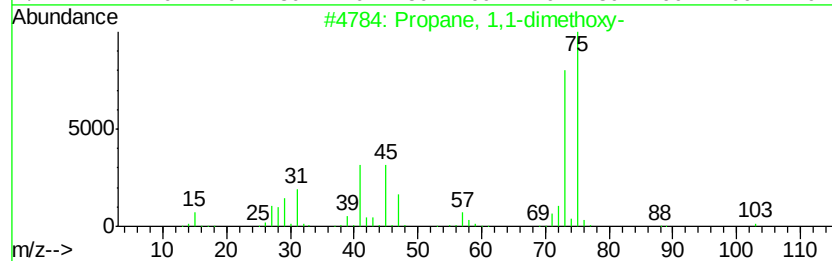
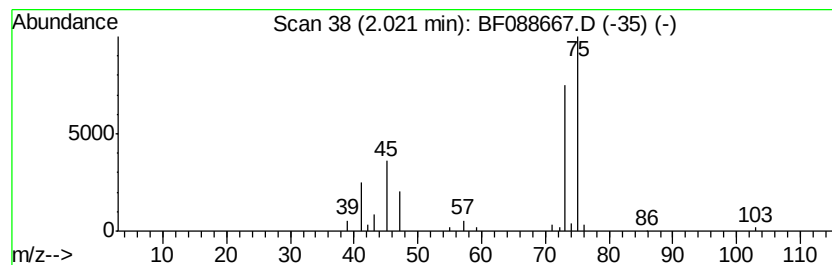
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	2.37 ng	81806	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
4		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9



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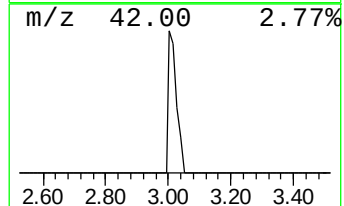
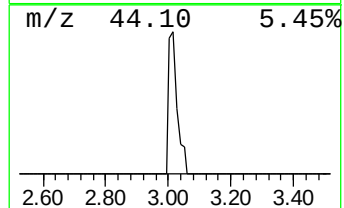
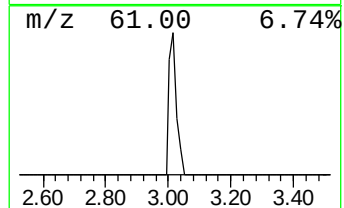
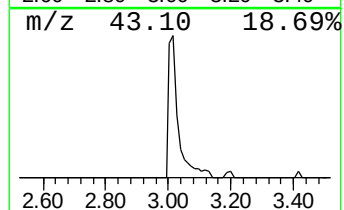
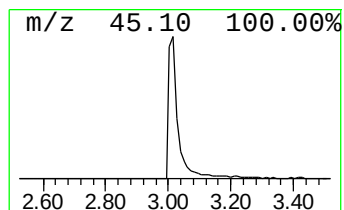
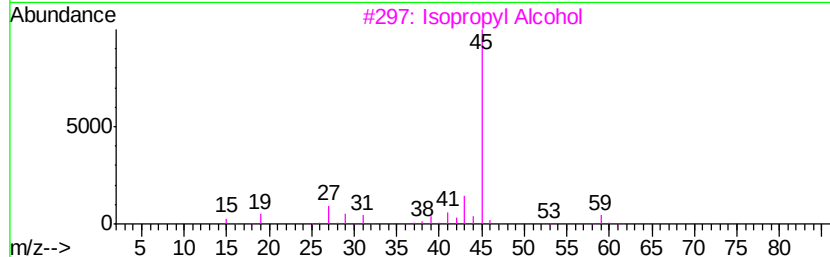
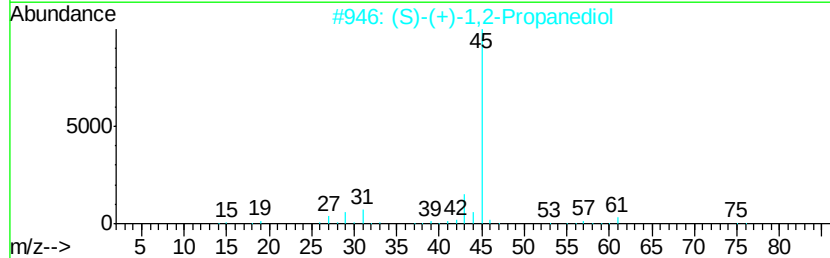
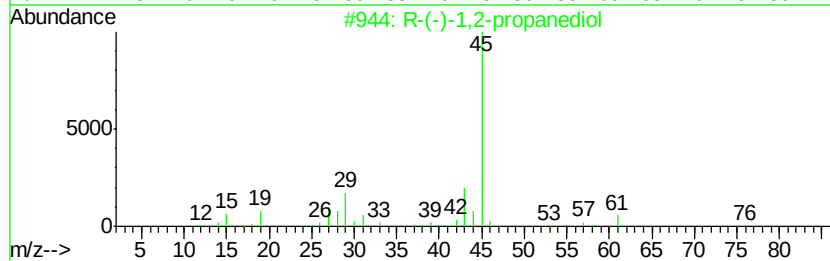
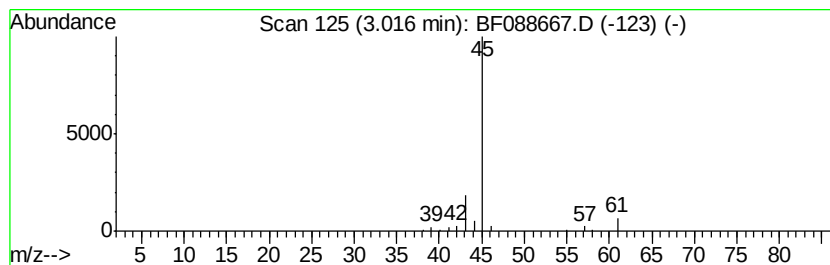
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	3.52 ng	121326	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		Formamide	45	CH3NO	000075-12-7	7



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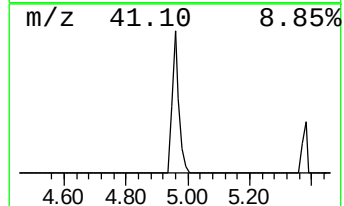
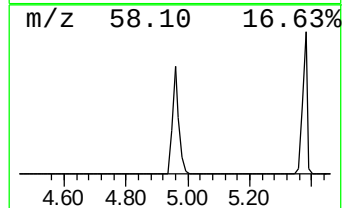
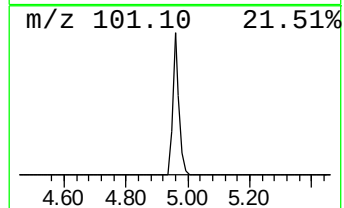
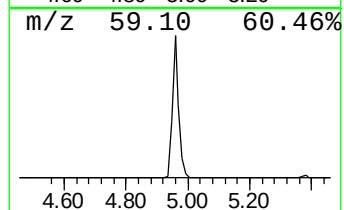
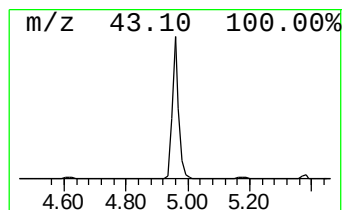
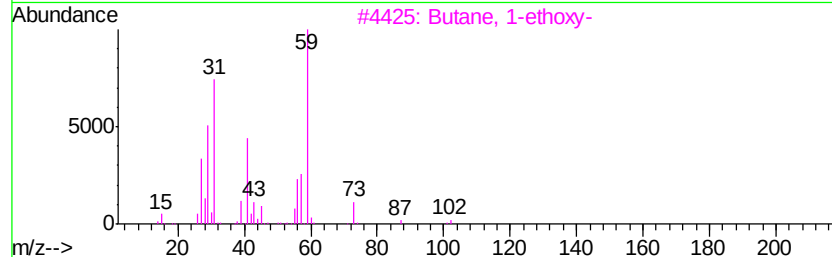
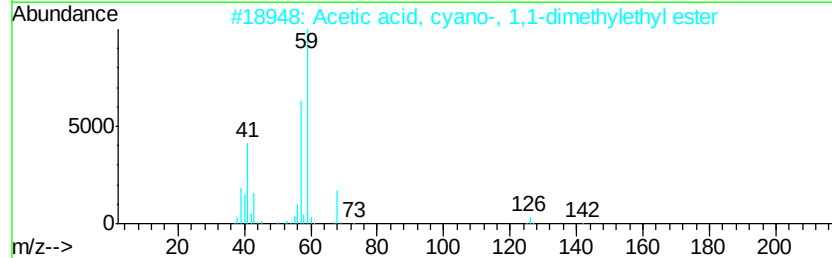
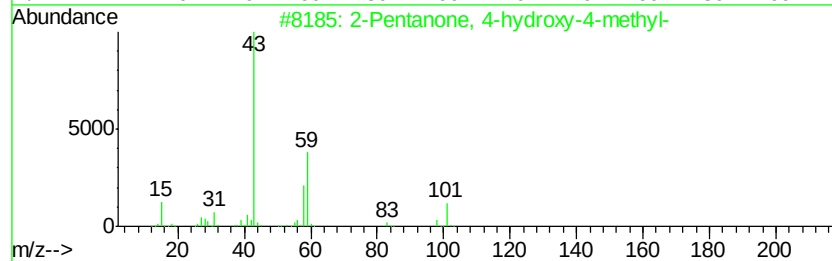
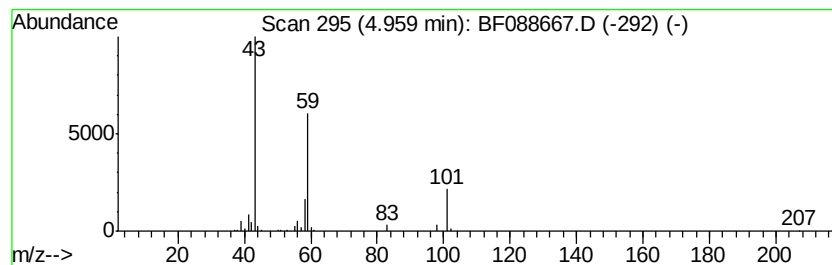
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.00 ng	276219	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	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		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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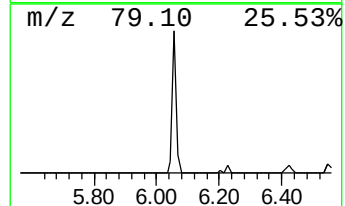
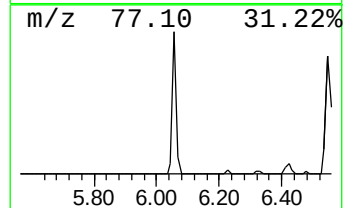
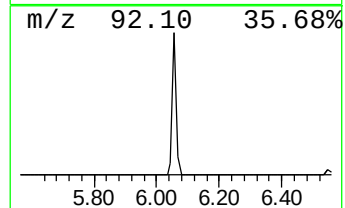
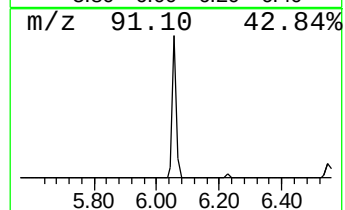
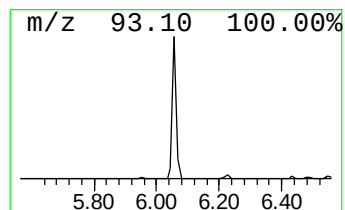
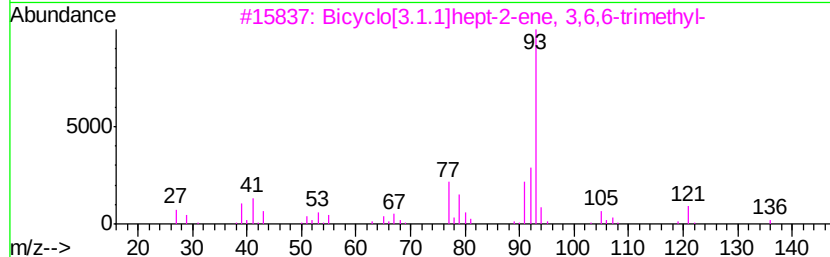
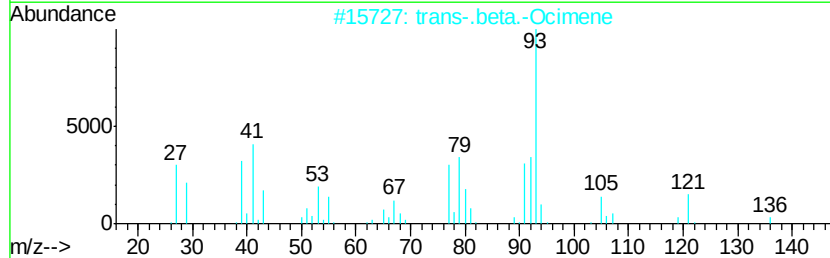
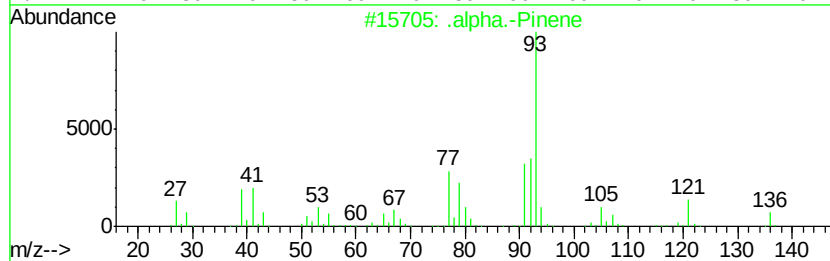
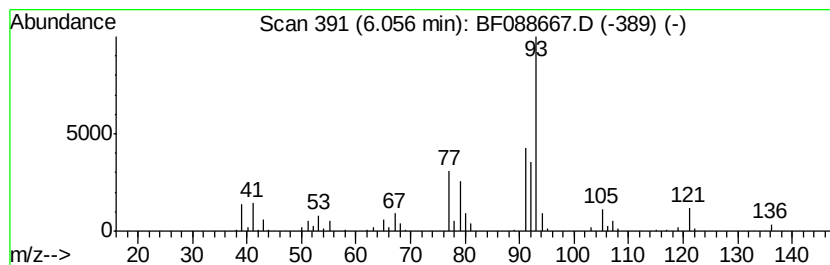
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 .alpha.-Pinene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.06	6.54 ng	225681	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Pinene	136	C10H16	000080-56-8	94
2		trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
3		Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4		Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5		(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	90



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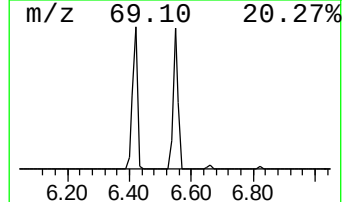
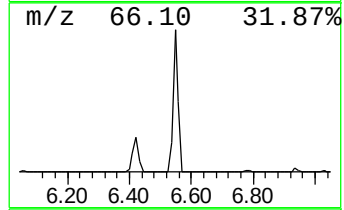
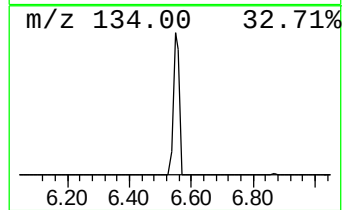
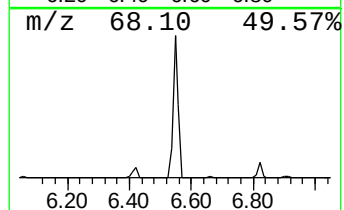
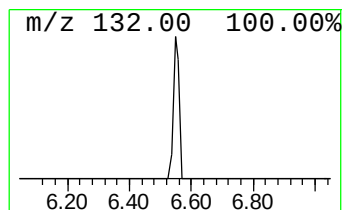
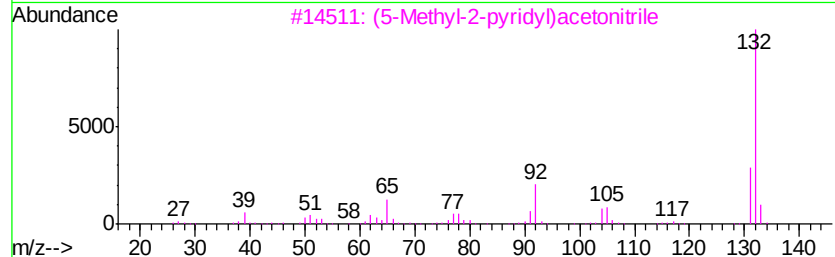
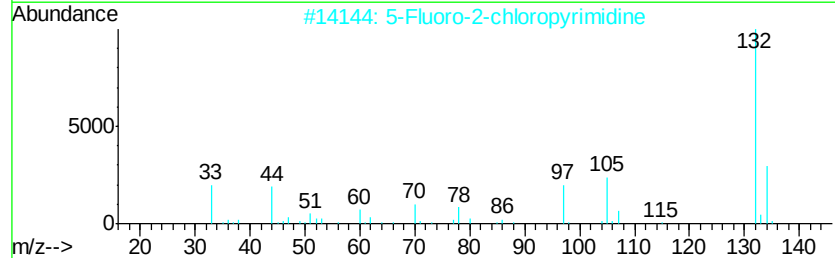
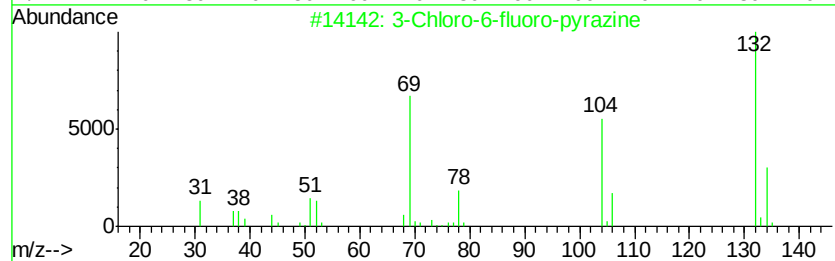
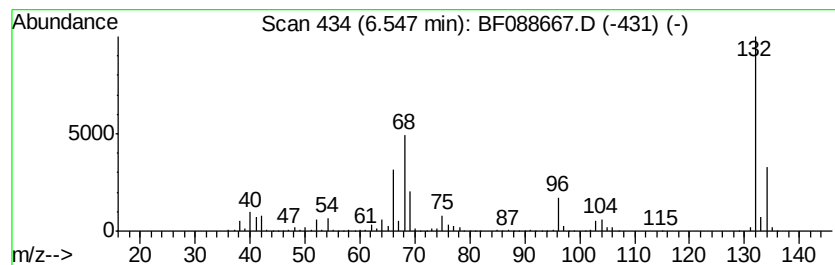
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Peak Number 6 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	90.31 ng	3116290	1,4-Dichlorobenzene-d4	6.79

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		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088667.D
Acq On : 4 Jul 2016 00:47
Operator : UM/SJ
Sample : H3817-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-4A-2-9FT

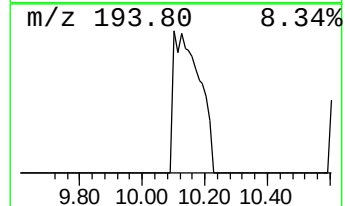
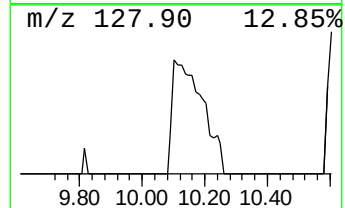
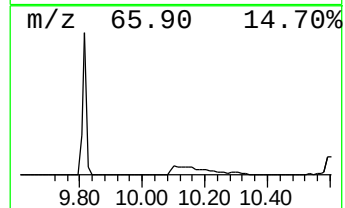
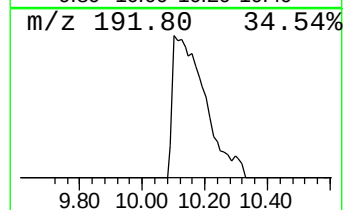
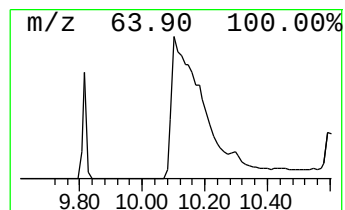
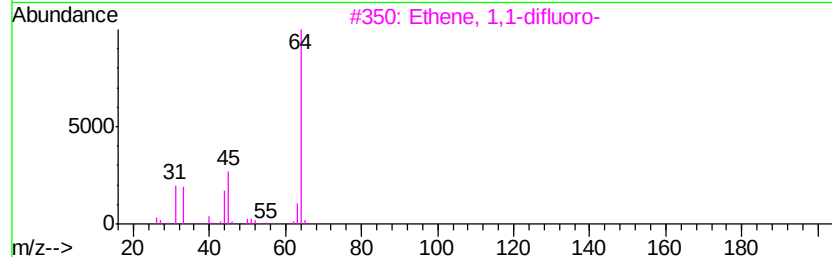
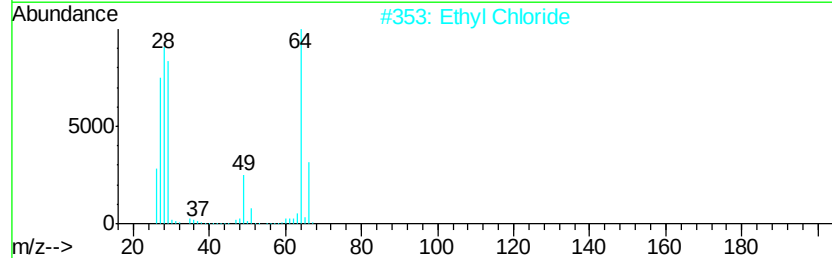
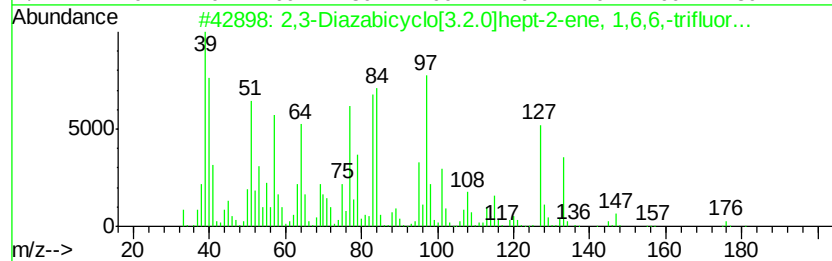
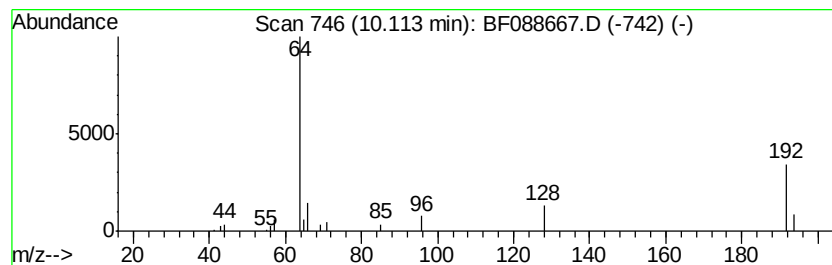
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2,3-Diazabicyclo[3.2.0]hept... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.11	2.06 ng	113365	Acenaphthene-d10	9.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	50
2		Ethyl Chloride	64	C2H5Cl	000075-00-3	4
3		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4		Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	4
5		1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	4



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088667.D
Acq On : 4 Jul 2016 00:47
Operator : UM/SJ
Sample : H3817-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

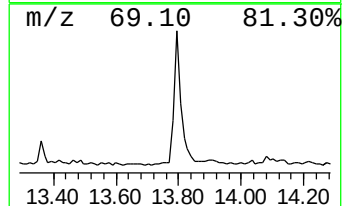
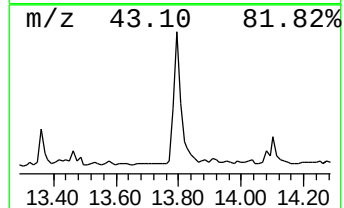
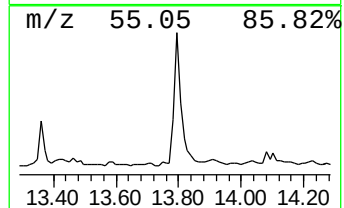
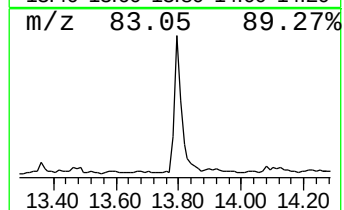
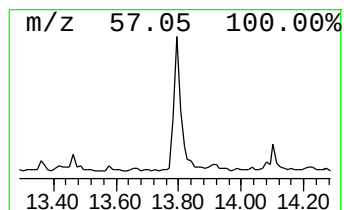
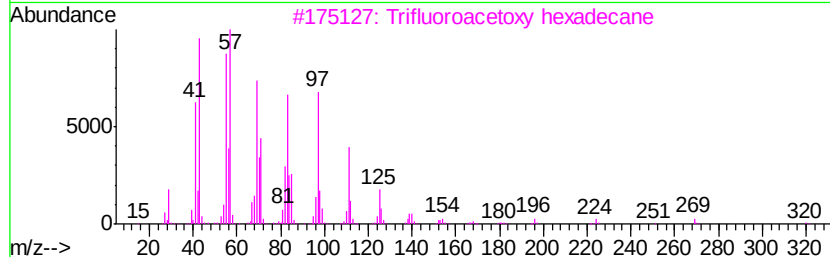
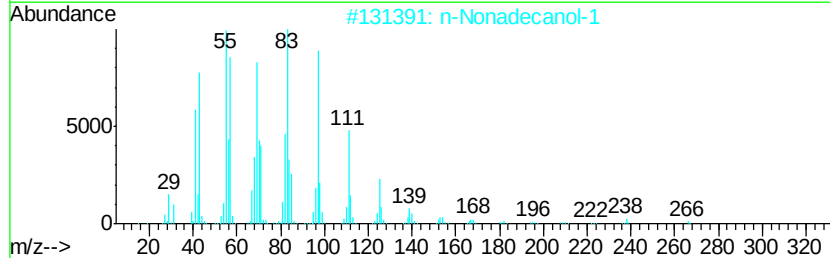
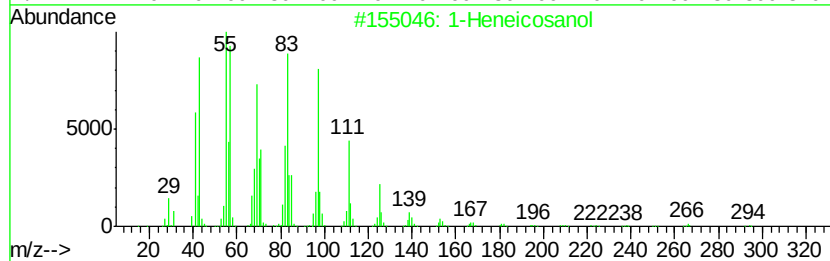
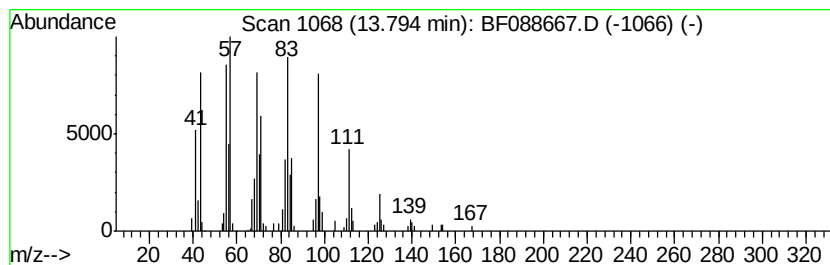
Instrument :
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ClientSampleId :
BS-4A-2-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.79	3.94 ng	196316	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088667.D
Acq On : 4 Jul 2016 00:47
Operator : UM/SJ
Sample : H3817-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

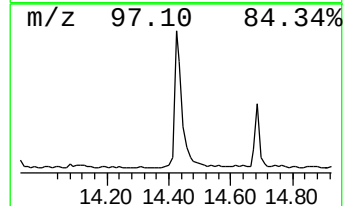
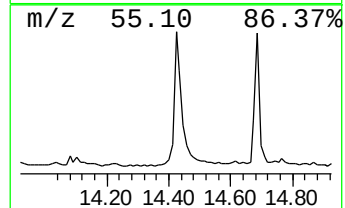
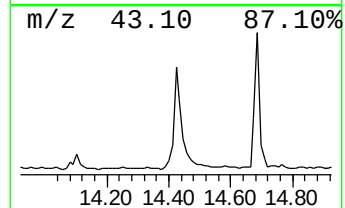
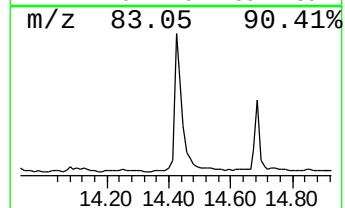
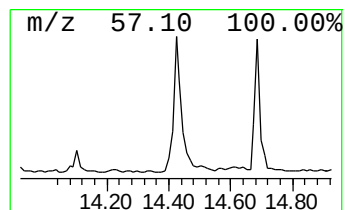
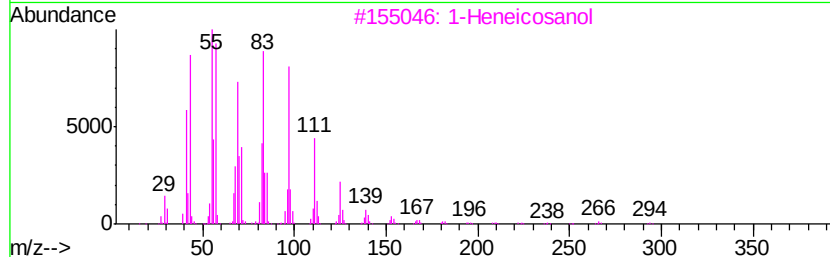
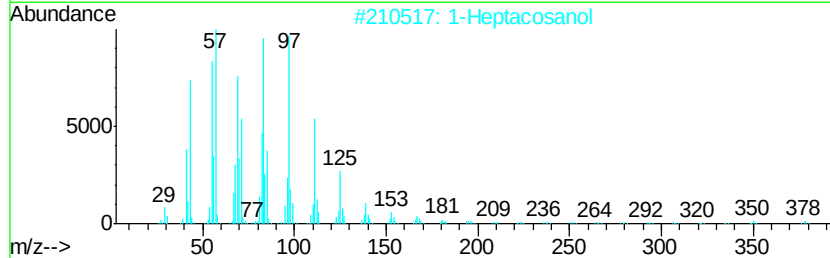
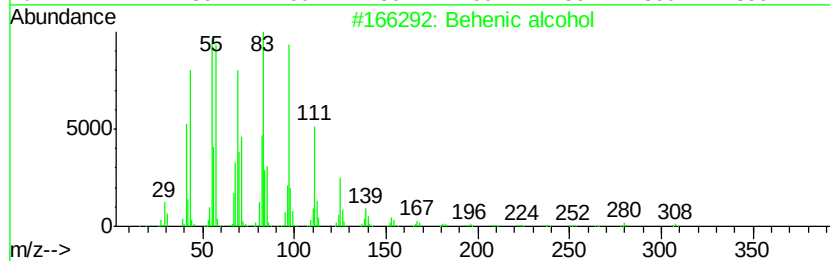
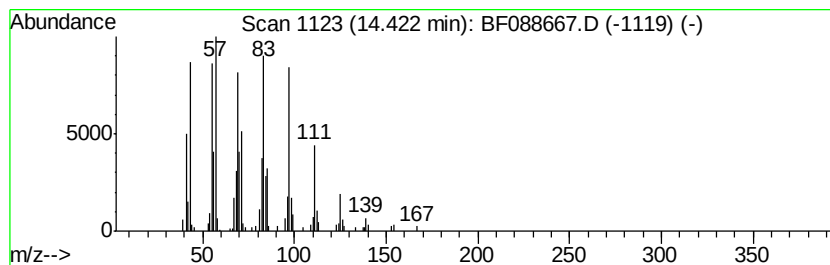
Instrument :
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ClientSampleId :
BS-4A-2-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.42	6.69 ng	333271	Chrysene-d12		13.92
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088667.D
Acq On : 4 Jul 2016 00:47
Operator : UM/SJ
Sample : H3817-09
Misc :
ALS Vial : 29 Sample Multiplier: 1

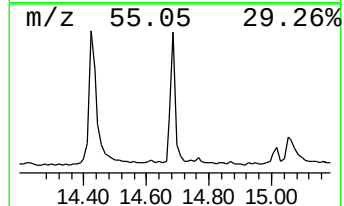
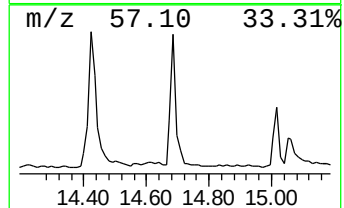
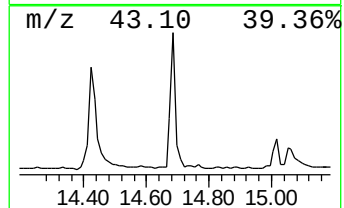
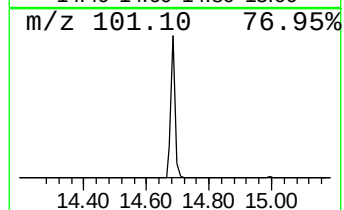
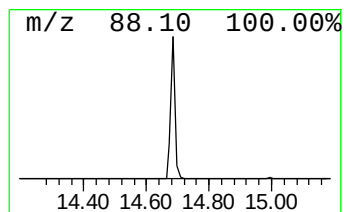
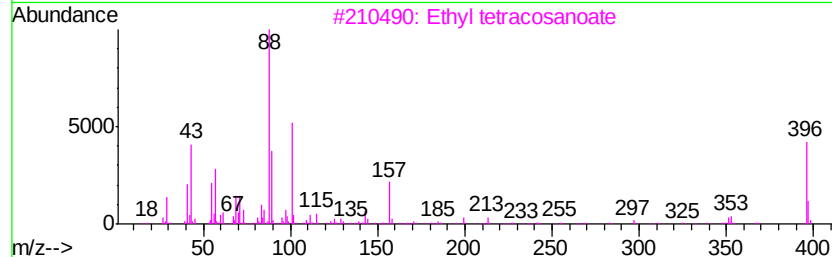
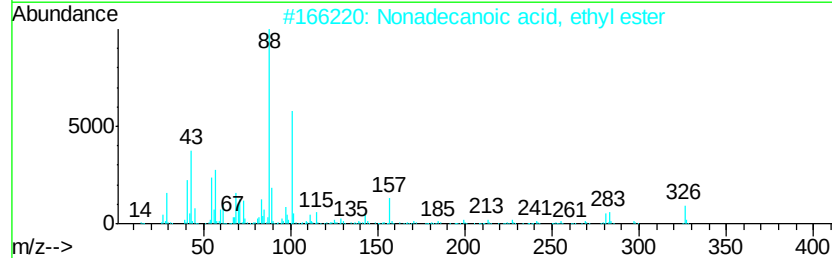
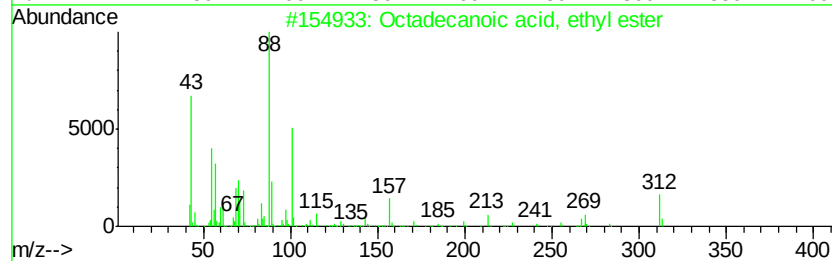
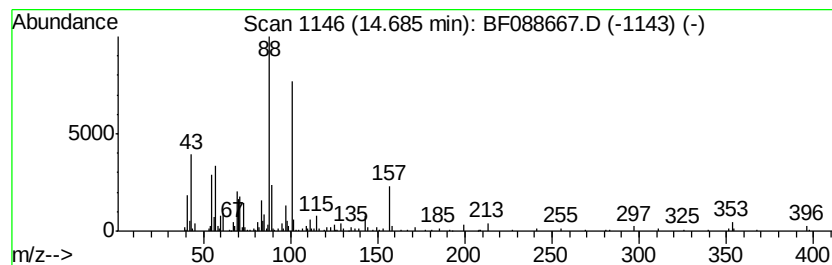
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Octadecanoic acid, ethyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.69	7.79 ng	298618	Perylene-d12		15.31	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, ethyl ester	312	C20H40O2	000111-61-5	90
2		Nonadecanoic acid, ethyl ester	326	C21H42O2	018281-04-4	86
3		Ethyl tetracosanoate	396	C26H52O2	024634-95-5	81
4		Heptadecanoic acid, ethyl ester	298	C19H38O2	014010-23-2	78
5		Pentadecanoic acid, ethyl ester	270	C17H34O2	041114-00-5	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088667.D
Acq On : 4 Jul 2016 00:47
Operator : UM/SJ
Sample : H3817-09
Misc :
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Instrument :
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BS-4A-2-9FT

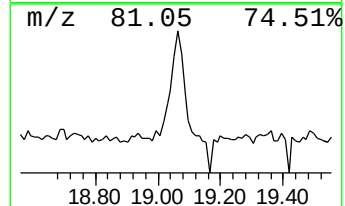
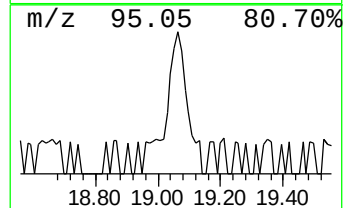
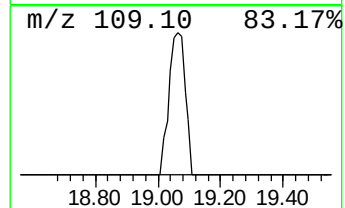
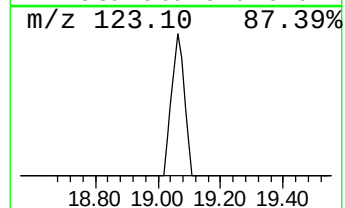
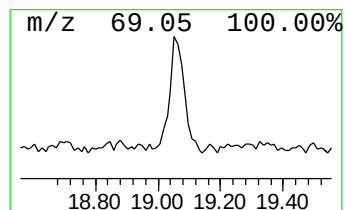
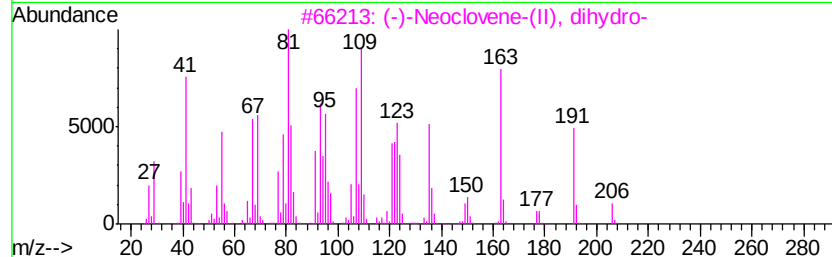
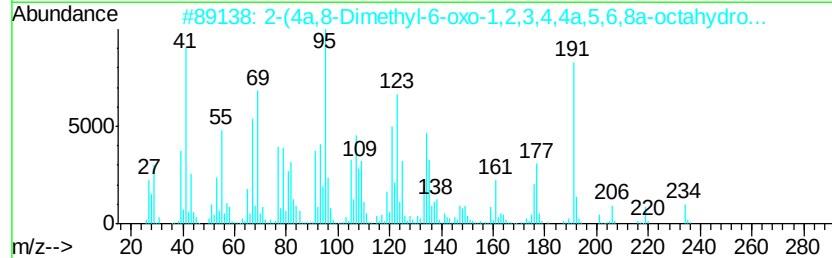
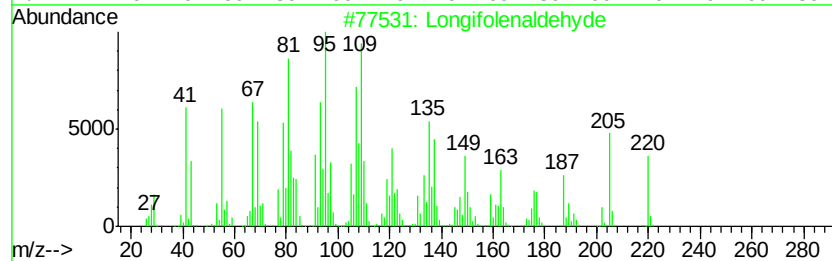
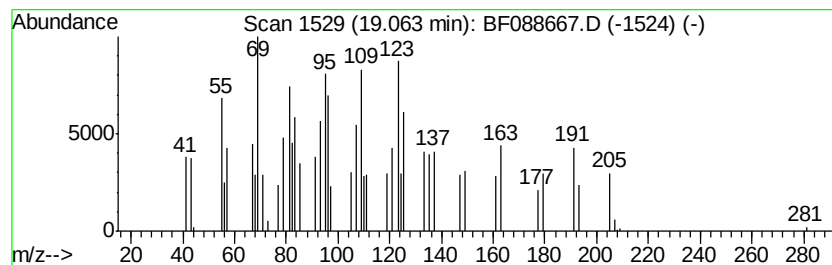
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown19.06 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	2.23 ng	85587	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Longifolenaldehyde	220	C15H24O	019890-84-7	49
2		2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	47
3		(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	38
4		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	38
5		2-Methyl-3-(3-methyl-but-2-enyl)...	222	C15H26O	1000144-10-2	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
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ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BS-4A-2-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.02	2.4	ng	81806	1	6.79	690126	20.0
R-(-)-1,2-propane...	3.02	3.5	ng	121326	1	6.79	690126	20.0
2-Pentanone, 4-hy...	4.96	8.0	ng	276219	1	6.79	690126	20.0
.alpha.-Pinene	6.06	6.5	ng	225681	1	6.79	690126	20.0
unknown6.55	6.55	90.3	ng	3116290	1	6.79	690126	20.0
2,3-Diazabicyclo[...	10.11	2.1	ng	113365	3	9.82	1102860	20.0
1-Heneicosanol	13.79	3.9	ng	196316	5	13.92	996073	20.0
Behenic alcohol	14.42	6.7	ng	333271	5	13.92	996073	20.0
Octadecanoic acid...	14.69	7.8	ng	298618	6	15.31	767026	20.0
unknown19.06	19.06	2.2	ng	85587	6	15.31	767026	20.0