

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
 Data File : BF088658.D
 Acq On : 3 Jul 2016 20:24
 Operator : UM/SJ
 Sample : H3817-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-3B-10-10.5FT

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	32	rVB2	40441	58918	2.11%	0.214%
2	2.021	36	38	41	rBV	47529	60461	2.17%	0.220%
3	3.050	123	128	131	rBV	142569	407157	14.60%	1.481%
4	4.959	292	295	299	rBB	144680	208139	7.46%	0.757%
5	5.382	329	332	334	rBV	2393326	2475186	88.73%	9.001%
6	6.422	420	423	425	rVB	2437550	2789520	100.00%	10.144%
7	6.547	431	434	437	rBV	2254933	2389356	85.65%	8.689%
8	6.787	452	455	457	rBV	546306	667171	23.92%	2.426%
9	6.936	466	468	471	rVB	1741873	1914505	68.63%	6.962%
10	7.347	501	504	506	rBV	1733995	1755663	62.94%	6.384%
11	7.439	510	512	515	rBV	26256	44744	1.60%	0.163%
12	7.987	557	560	565	rBV	28801	54398	1.95%	0.198%
13	8.068	565	567	569	rVB	1086077	943175	33.81%	3.430%
14	9.142	658	661	664	rBV	2426155	2548273	91.35%	9.267%
15	9.542	693	696	698	rVB	486580	534399	19.16%	1.943%
16	9.816	717	720	722	rBV	1207160	1043301	37.40%	3.794%
17	10.193	751	753	755	rBV	443284	507380	18.19%	1.845%
18	10.605	786	789	791	rBV	1666897	1847171	66.22%	6.717%
19	10.731	798	800	804	rVB	60358	61547	2.21%	0.224%
20	11.176	837	839	841	rBV	126190	115002	4.12%	0.418%
21	11.291	847	849	851	rVB	1154290	1011339	36.25%	3.678%
22	11.359	851	855	859	rVB3	39623	89792	3.22%	0.327%
23	11.565	871	873	875	rBV2	38035	84197	3.02%	0.306%
24	11.599	875	876	883	rVB	120404	143695	5.15%	0.523%
25	12.399	941	946	953	rBV	83069	206406	7.40%	0.751%
26	12.879	985	988	990	rBV	2582235	2449776	87.82%	8.909%
27	13.325	1025	1027	1029	rBV	30992	42959	1.54%	0.156%
28	13.759	1063	1065	1066	rBV	42341	49458	1.77%	0.180%
29	13.817	1066	1070	1076	rVV	131204	353575	12.68%	1.286%
30	13.920	1076	1079	1081	rVB	1006239	1016915	36.45%	3.698%
31	14.457	1124	1126	1135	rBV	49804	129888	4.66%	0.472%
32	15.017	1172	1175	1177	rBV	36829	38204	1.37%	0.139%
33	15.108	1179	1183	1190	rBV3	11563	40108	1.44%	0.146%
34	15.314	1197	1201	1203	rBV	485242	742609	26.62%	2.700%

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Stop Thrs : 0 Peak Location: TOP

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35	15.897	1247	1252	1268	rBV6	11426	62073	2.23%	0.226%
36	17.691	1405	1409	1416	rVB2	56374	135913	4.87%	0.494%
37	17.988	1429	1435	1449	rBV2	74051	356265	12.77%	1.296%
38	19.063	1522	1529	1538	rVB2	37728	120481	4.32%	0.438%

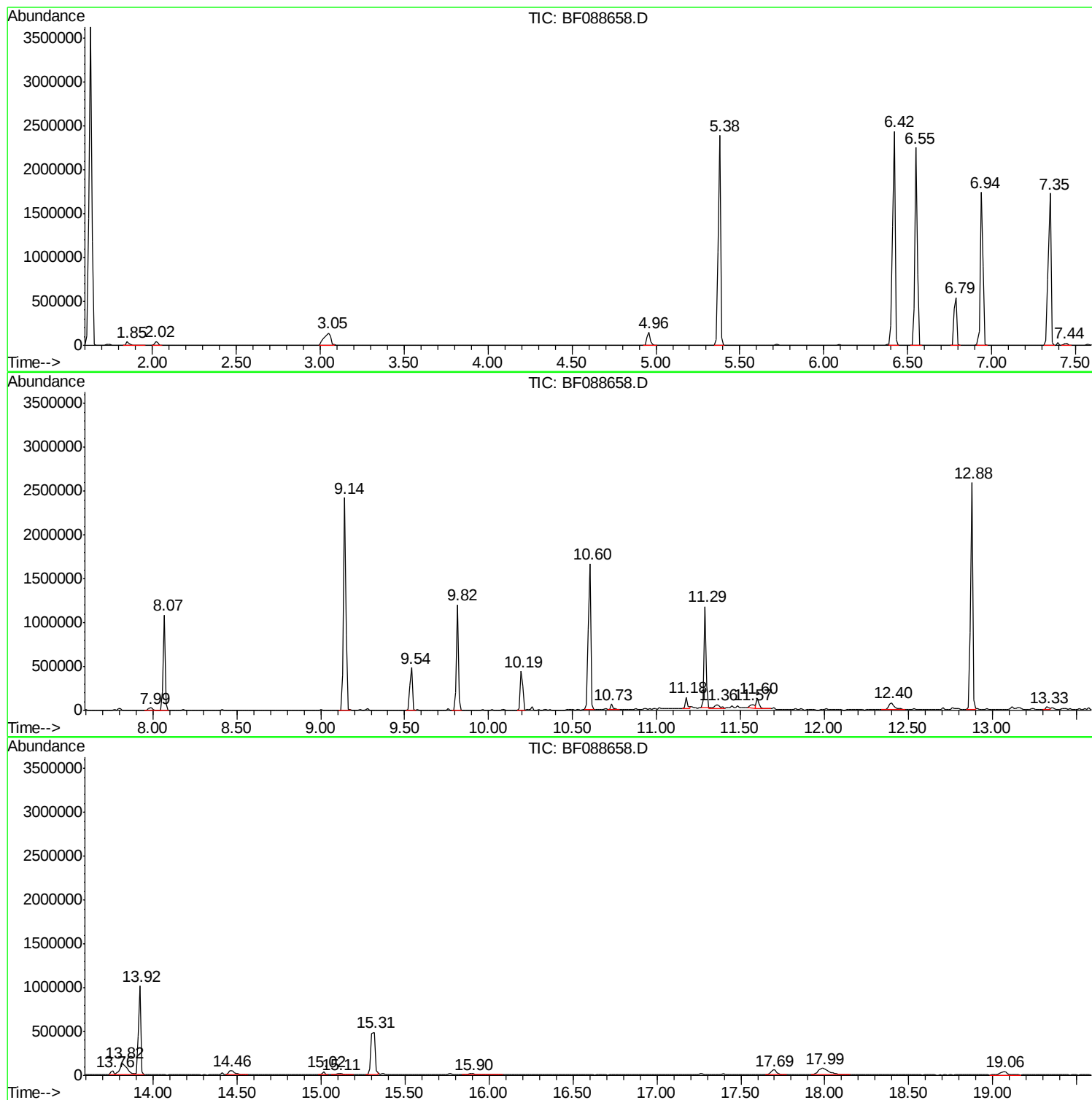
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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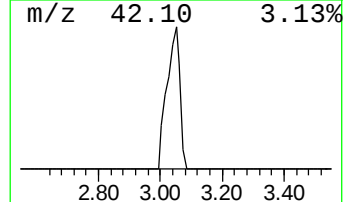
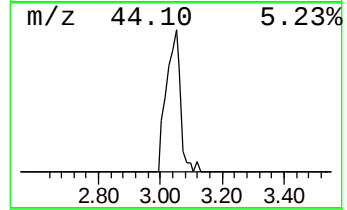
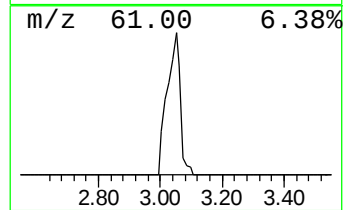
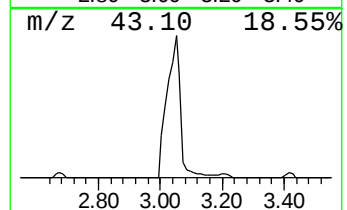
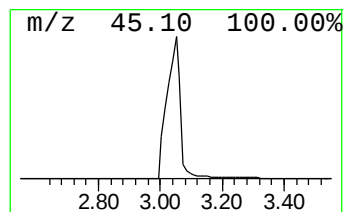
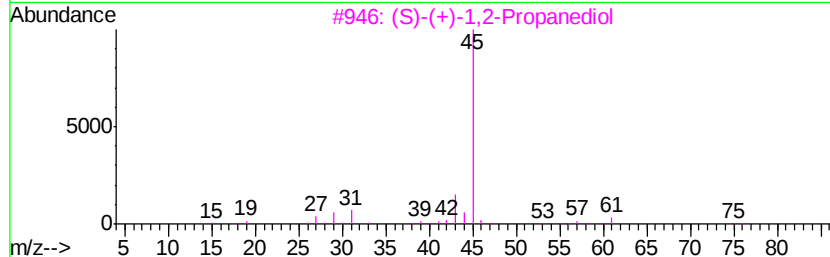
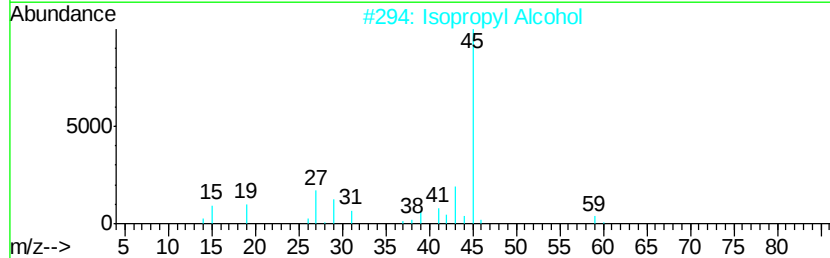
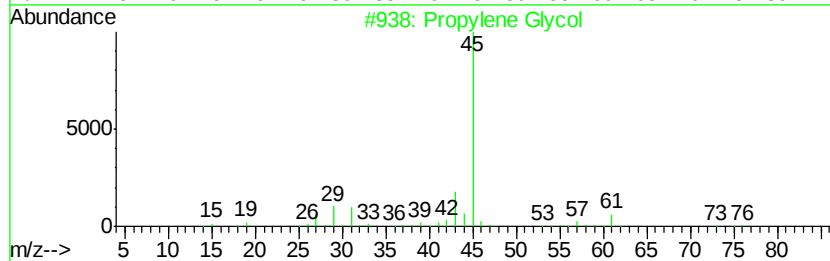
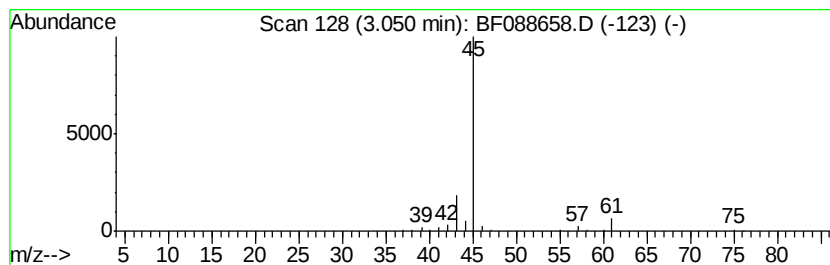
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	12.21 ng	407157	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	83
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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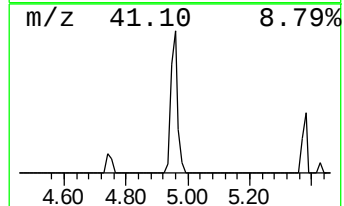
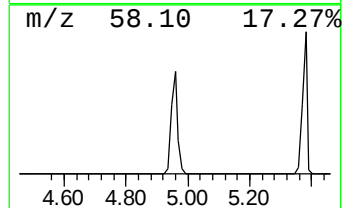
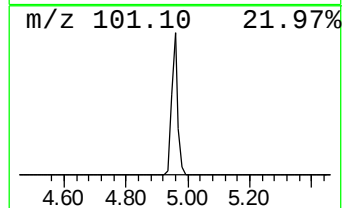
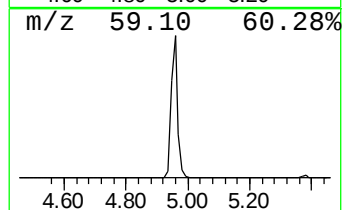
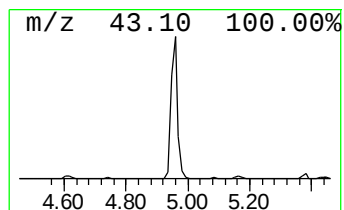
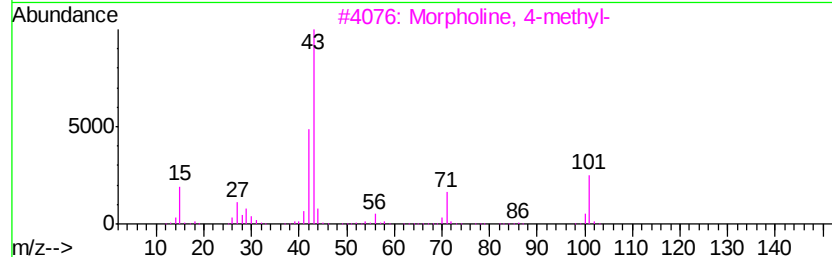
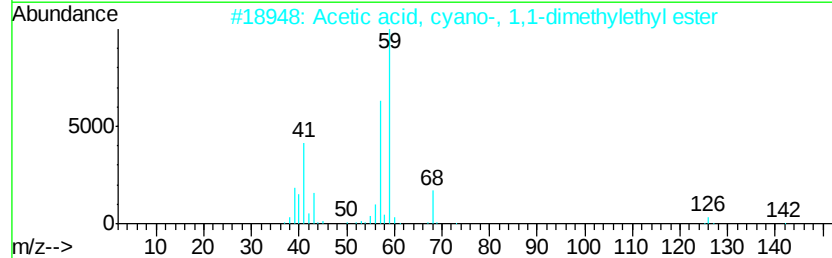
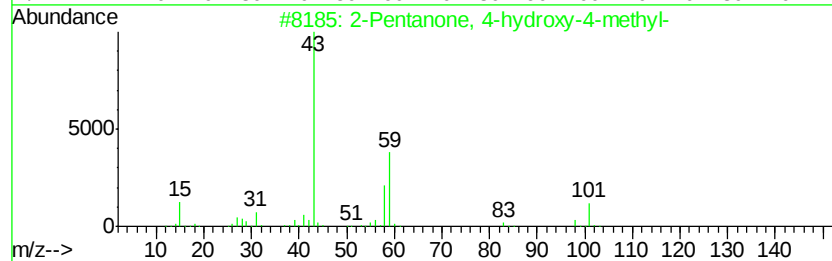
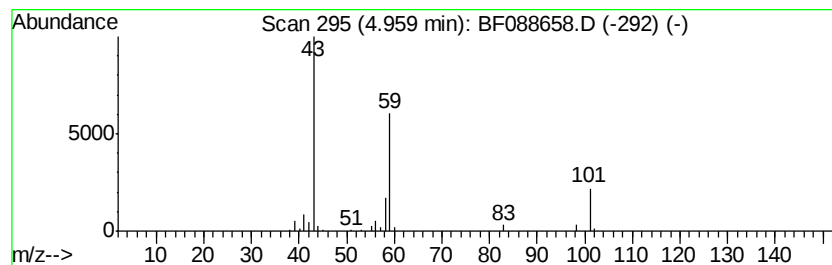
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	6.24 ng	208139	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		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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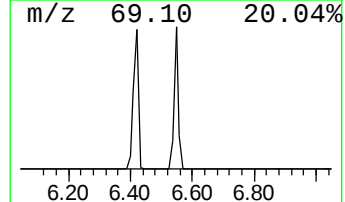
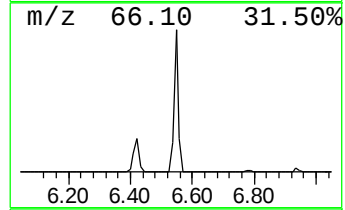
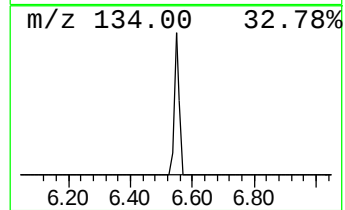
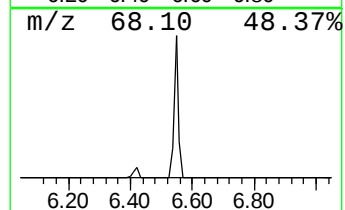
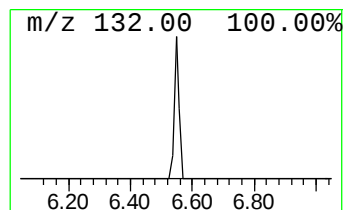
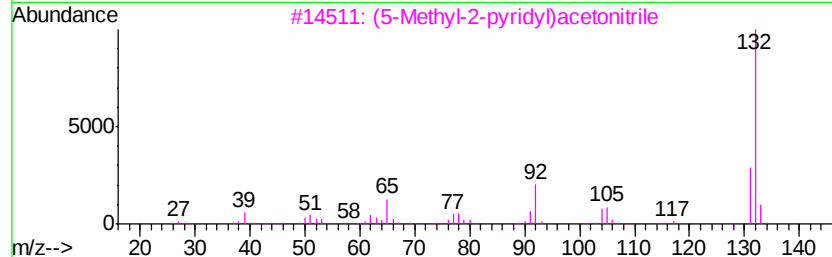
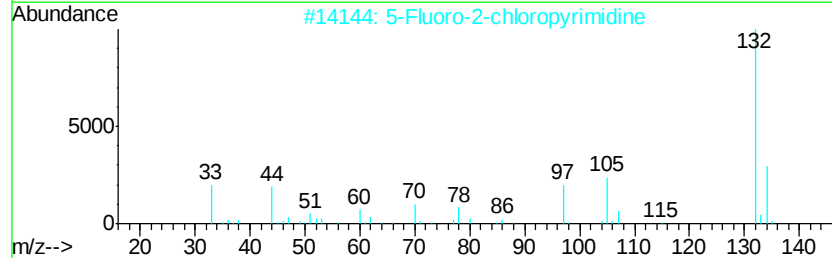
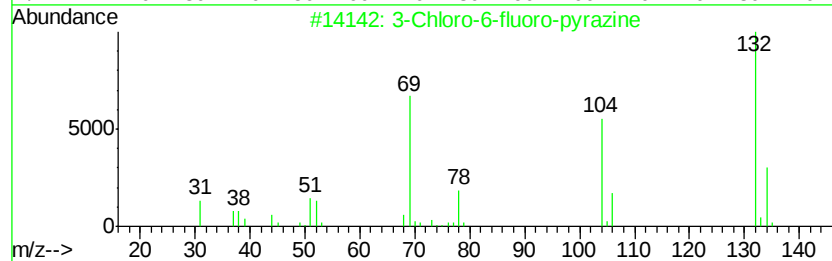
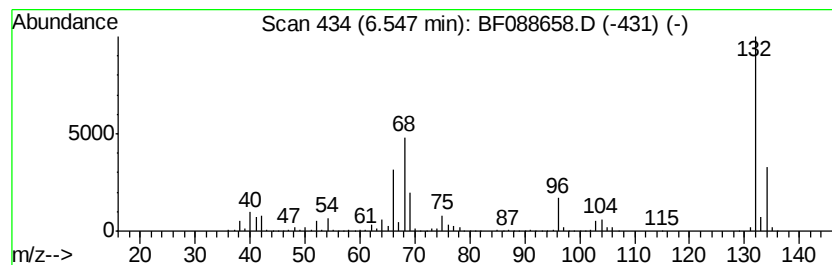
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Peak Number 3 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	71.63 ng	2389360	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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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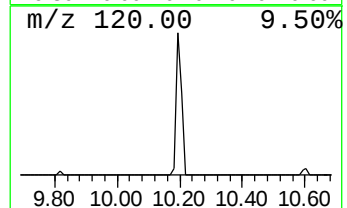
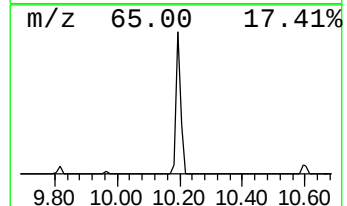
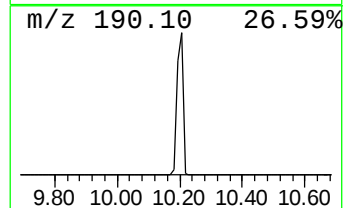
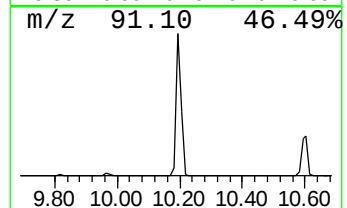
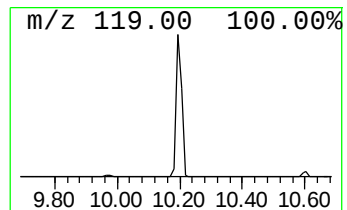
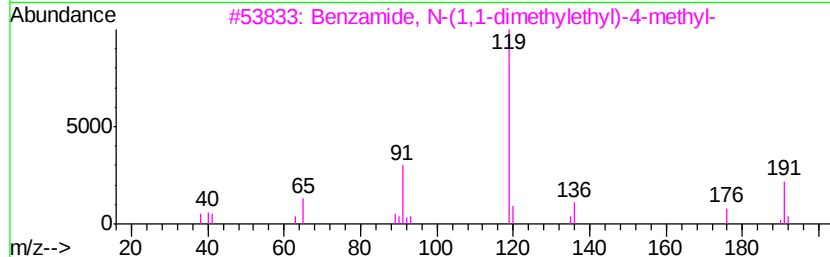
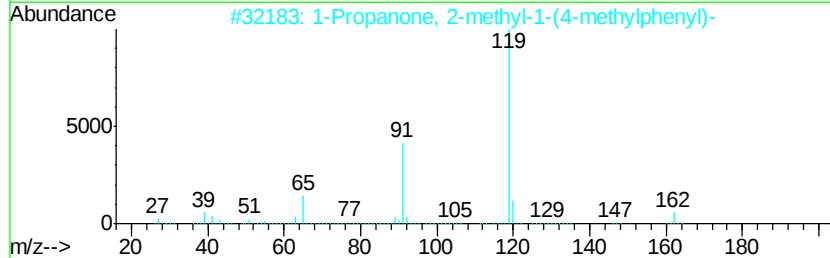
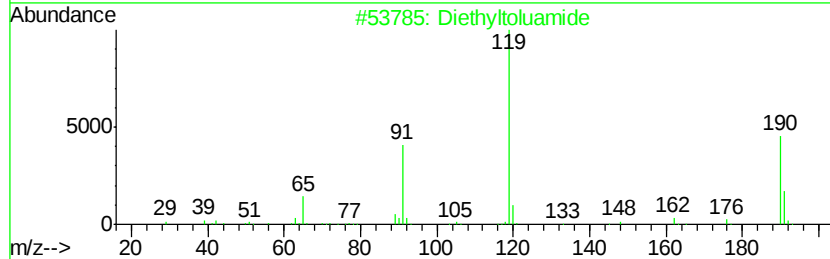
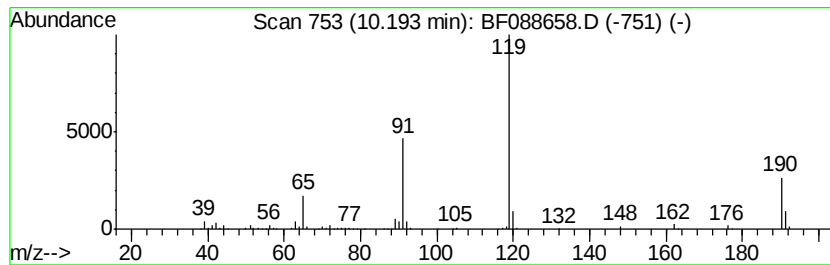
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Peak Number 5 Diethyltoluamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	9.73 ng	507380	Acenaphthene-d10	9.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Diethyltoluamide	191 C12H17NO	000134-62-3 97
2		1-Propanone, 2-methyl-1-(4-methylphenyl)-	162 C11H14O	050390-51-7 74
3		Benzamide, N-(1,1-dimethylethyl)-	191 C12H17NO	042498-32-8 72
4		L-Valine, N-(4-methylbenzoyl)-, ...	277 C16H23NO3	1000346-63-8 72
5		p-Toluic acid, 5-fluoro-2-nitrophenyl-	275 C14H10FN04	1000292-64-6 64



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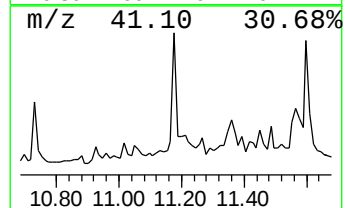
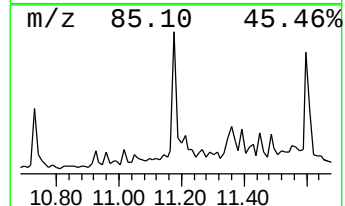
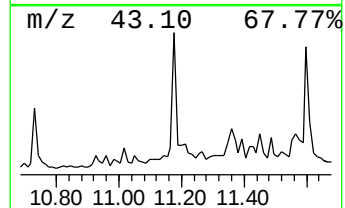
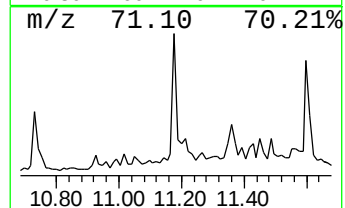
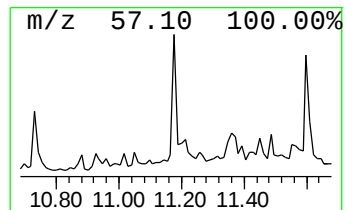
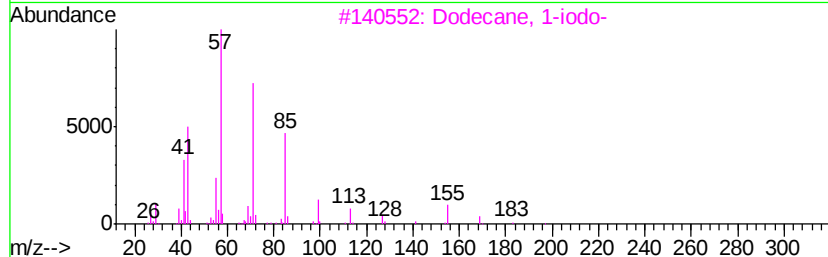
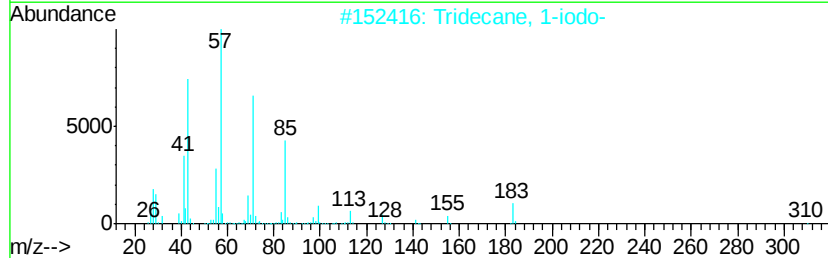
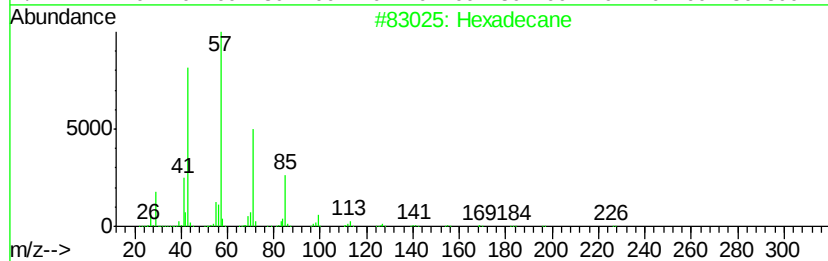
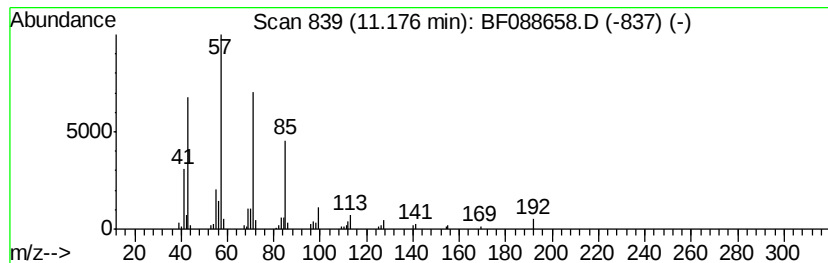
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Peak Number 6 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.27 ng	115002	Phenanthrene-d10	11.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	90
2	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	86
3	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	86
5	Sulfurous acid, pentadecyl 2-pro...	334 C18H38O3S	1000309-12-6	80



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
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Acq On : 3 Jul 2016 20:24
Operator : UM/SJ
Sample : H3817-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BS-3B-10-10.5FT

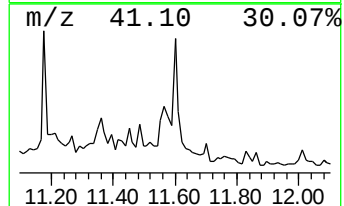
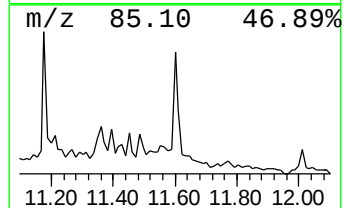
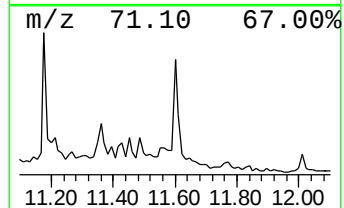
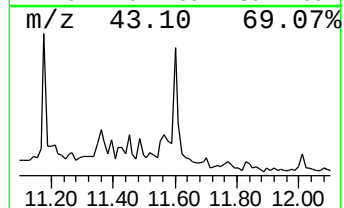
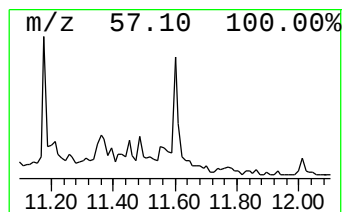
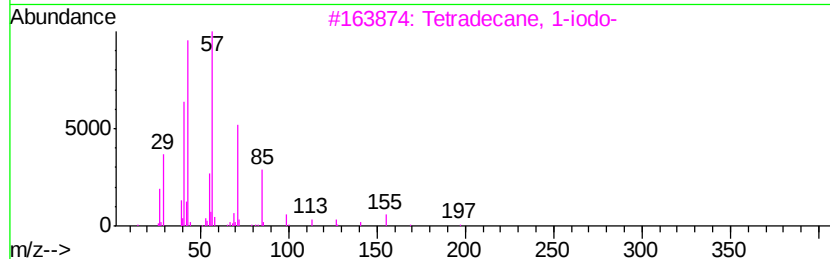
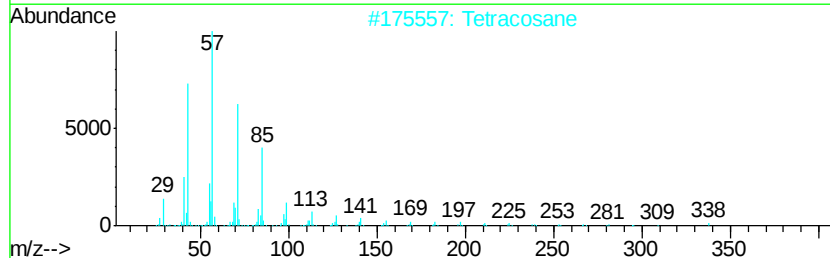
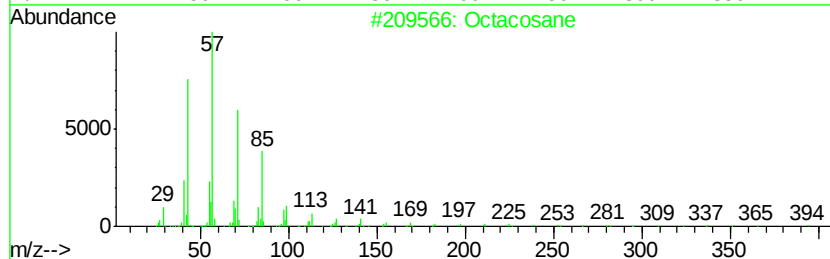
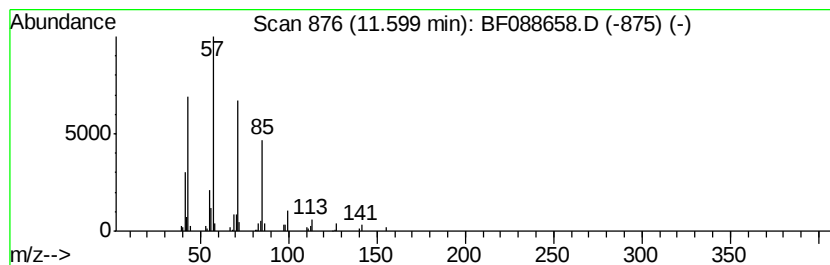
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.60	2.84 ng	143695	Phenanthrene-d10	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Tetracosane	338	C24H50	000646-31-1	90
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	83
4		Pentadecane	212	C15H32	000629-62-9	72
5		Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088658.D
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Sample : H3817-02
Misc :
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Instrument :
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ClientSampleId :
BS-3B-10-10.5FT

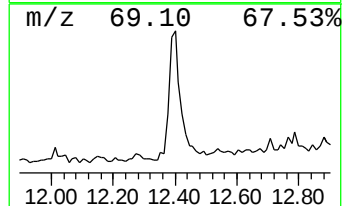
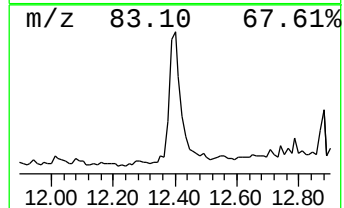
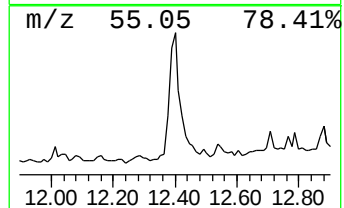
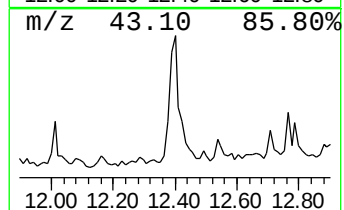
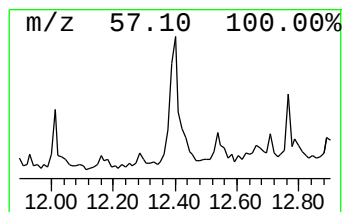
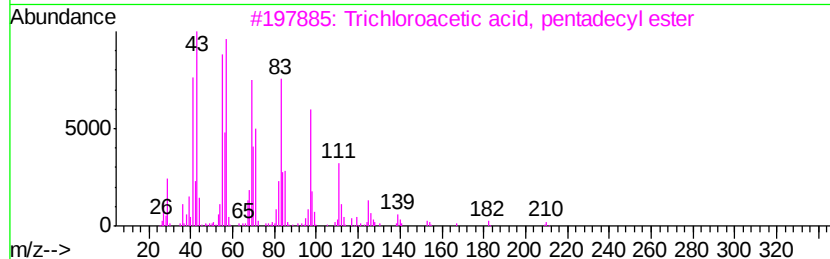
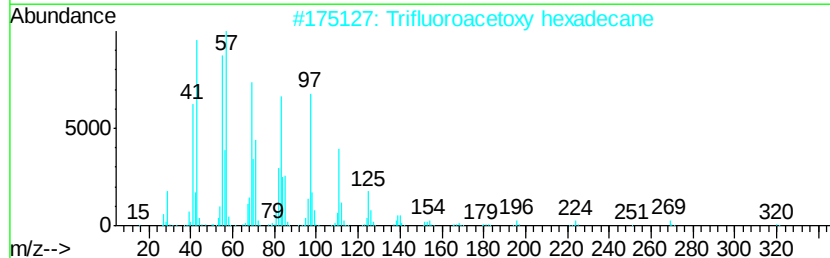
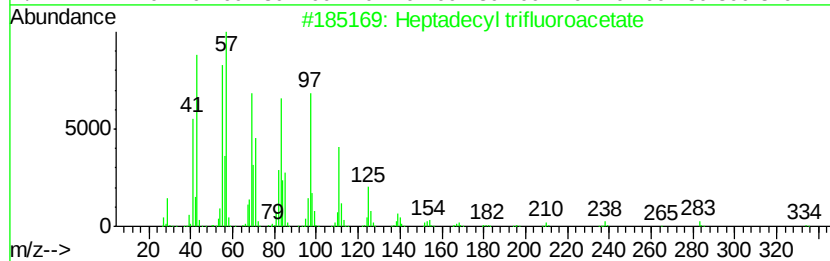
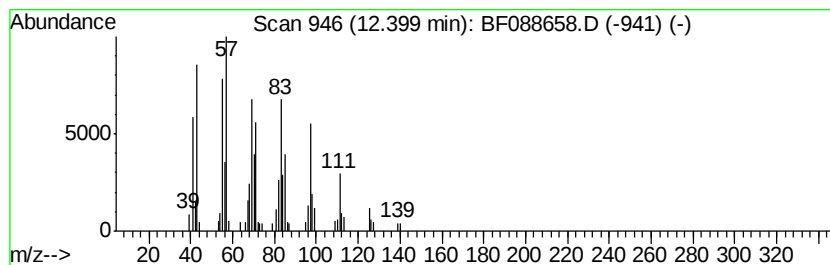
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	4.08 ng	206406	Phenanthrene-d10	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
4		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	83
5		Dodecyl isobutyl carbonate	286	C17H34O3	959067-22-2	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088658.D
Acq On : 3 Jul 2016 20:24
Operator : UM/SJ
Sample : H3817-02
Misc :
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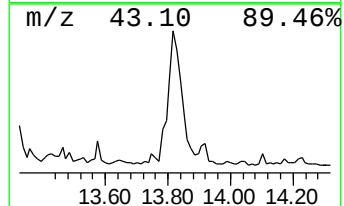
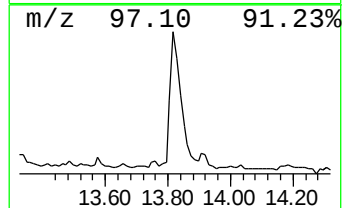
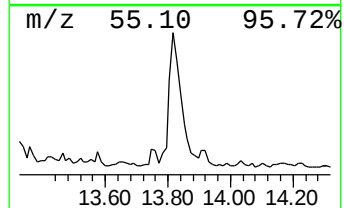
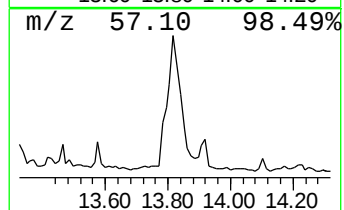
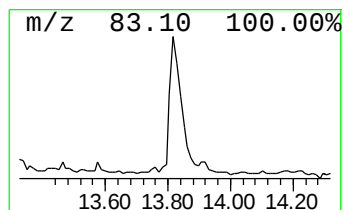
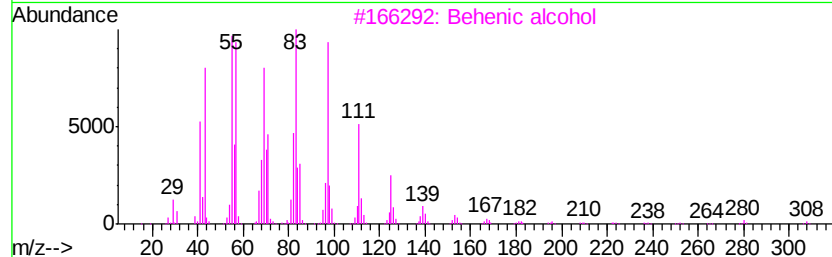
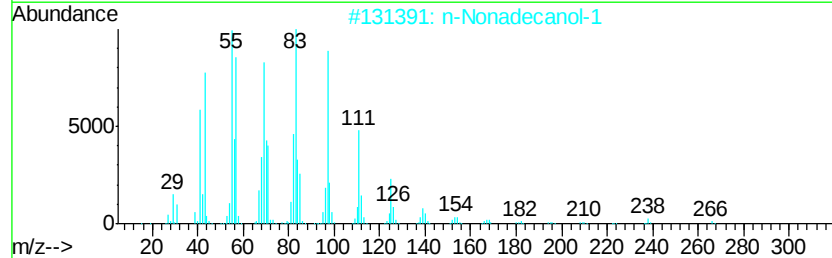
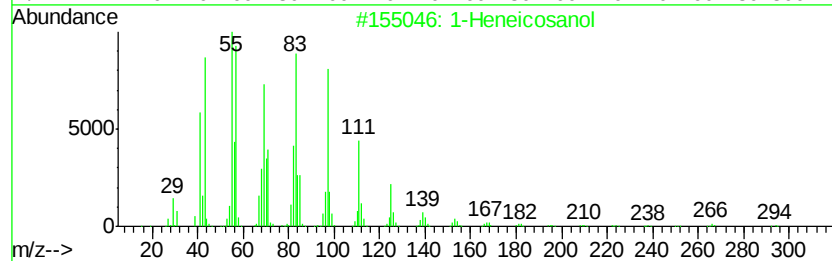
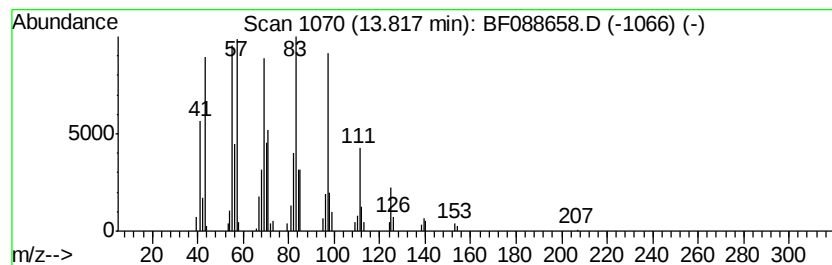
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.82	6.95 ng	353575	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	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Hexadecanol	242	C16H34O	036653-82-4	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
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Acq On : 3 Jul 2016 20:24
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Sample : H3817-02
Misc :
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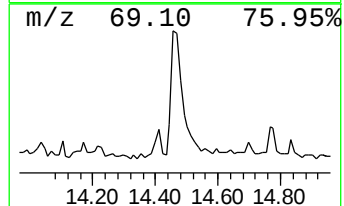
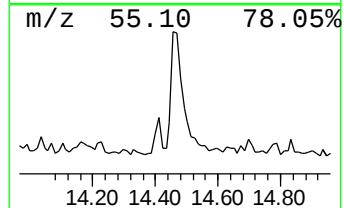
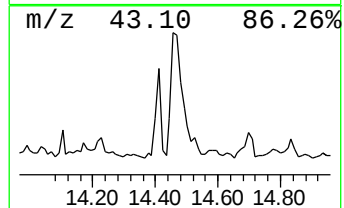
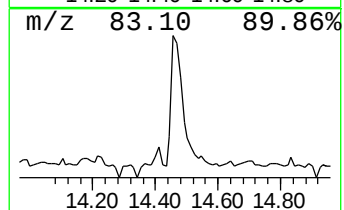
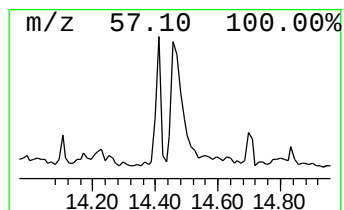
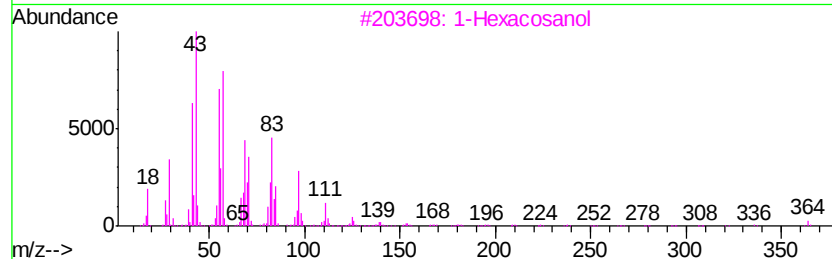
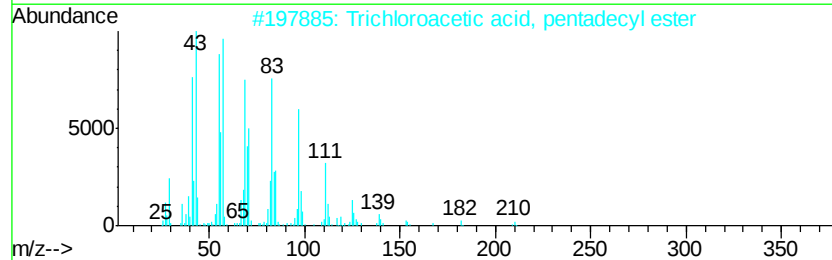
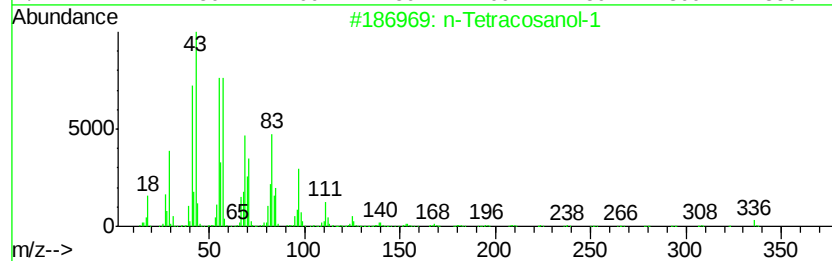
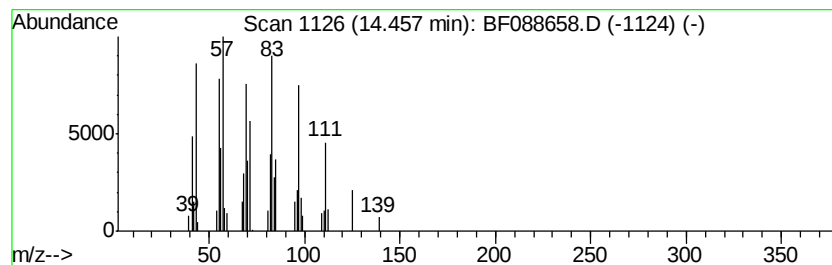
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.46	2.55 ng	129888	Chrysene-d12	13.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	1-Docosene	308	C22H44	001599-67-3	76



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088658.D
Acq On : 3 Jul 2016 20:24
Operator : UM/SJ
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Misc :
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ClientSampleId :
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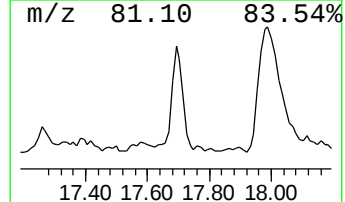
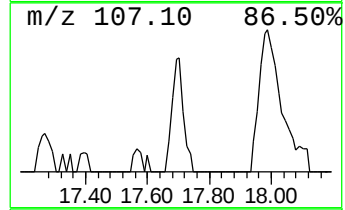
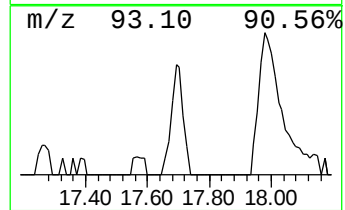
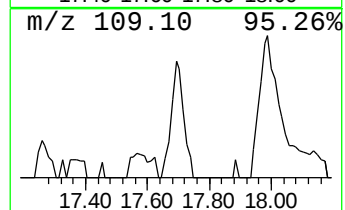
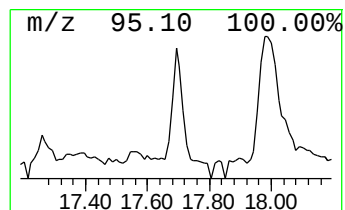
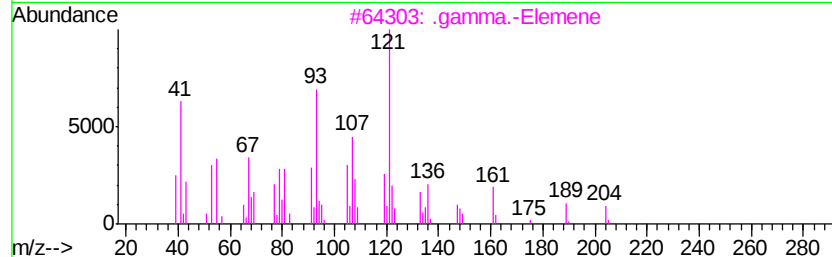
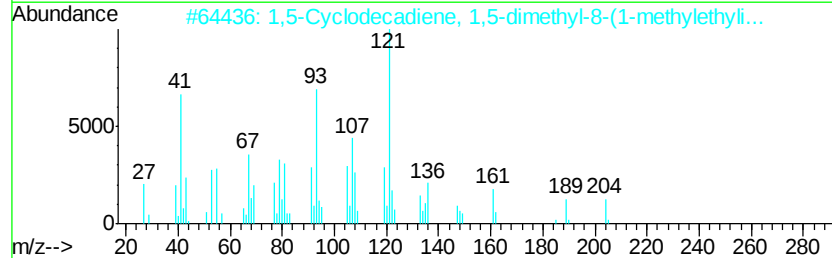
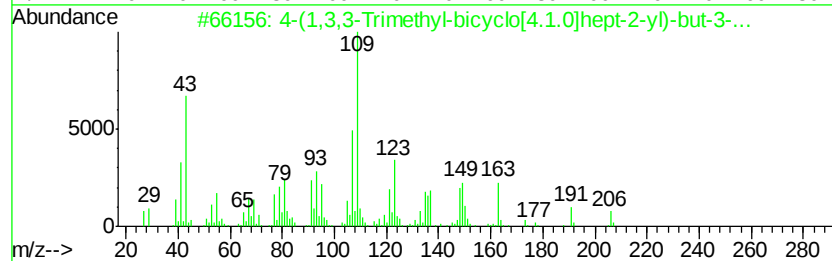
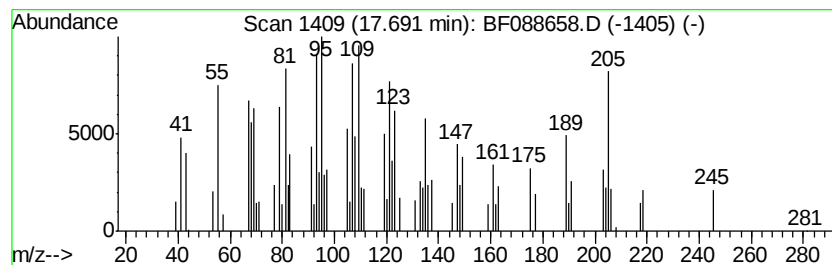
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.69 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	3.66 ng	135913	Perylene-d12	15.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(1,3,3-Trimethyl-bicyclo[4.1.0]hept-2-yl)-but-3-en-2-ol	206	C14H22O	077143-31-8	48
2			1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethyl)-	204	C15H24	015423-57-1	46
3			.gamma.-Elemene	204	C15H24	029873-99-2	46
4			Carvophyllene-(I1)	204	C15H24	1000158-18-5	44
5			2-Butenal, 2-methyl-4-(2,6,6-trimethyl-3-oxy-1,2,3,4-tetrahydronaphthalen-1-yl)-	206	C14H22O	003155-71-3	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
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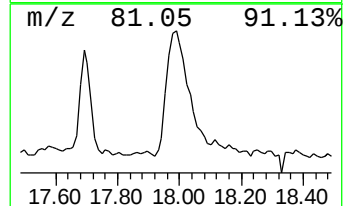
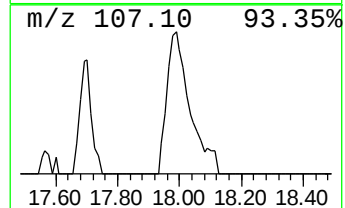
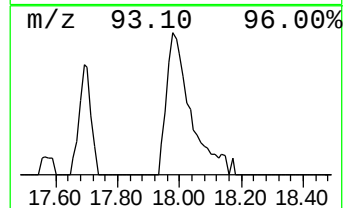
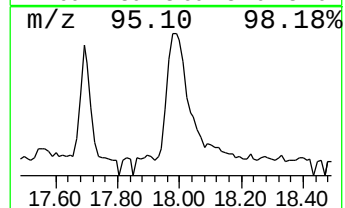
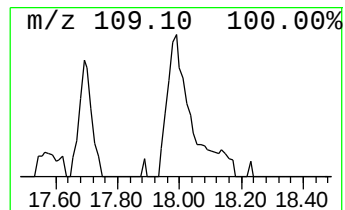
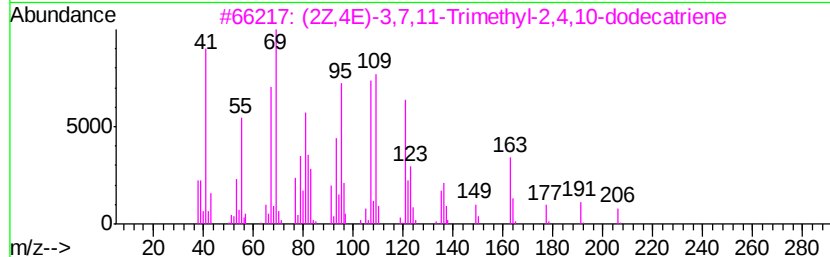
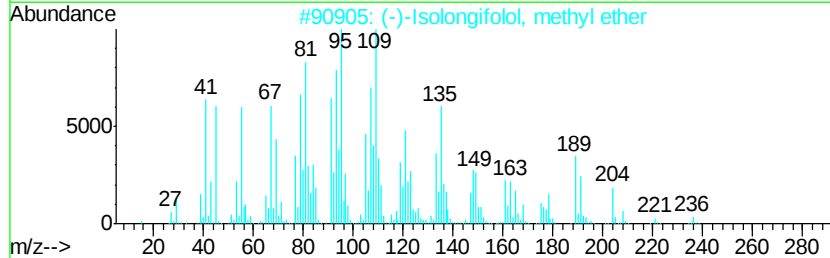
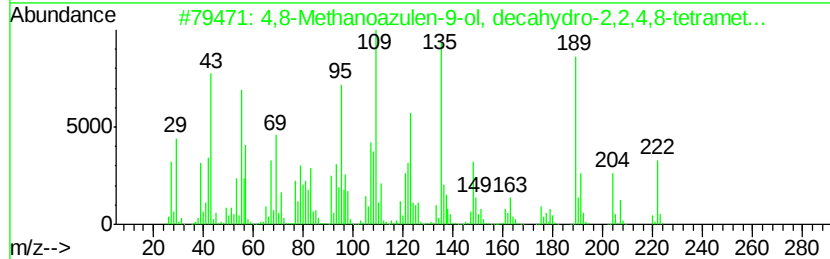
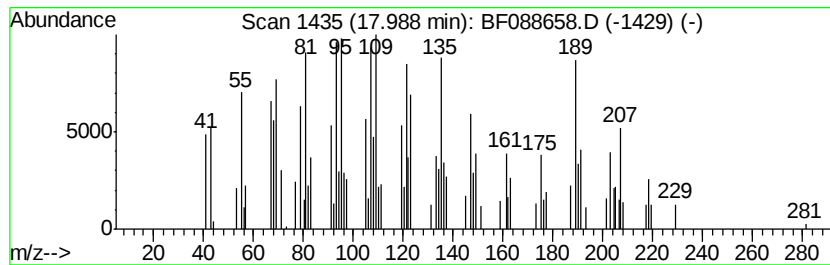
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 4,8-Methanoazulen-9-ol, dec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.99	9.59 ng	356265	Perylene-d12	15.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,8-Methanoazulen-9-ol, decahydr...	222	C15H26O	004586-22-5	53
2			(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	49
3			(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	42
4			6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	42
5			4-Hydroxy-.beta.-ionone	208	C13H20O2	116296-75-4	25



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088658.D
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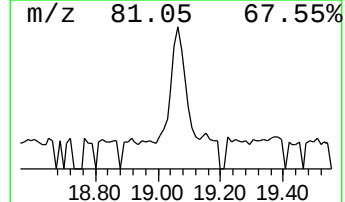
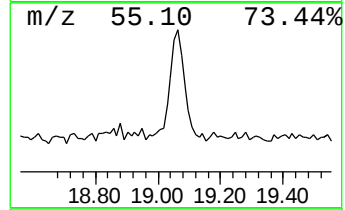
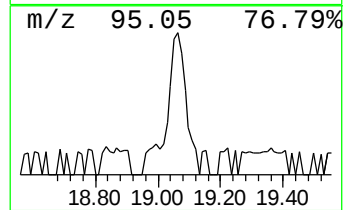
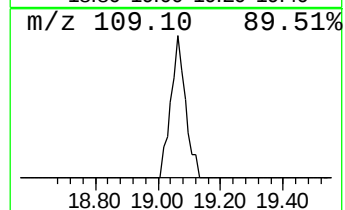
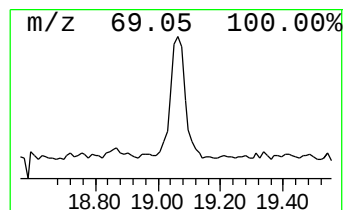
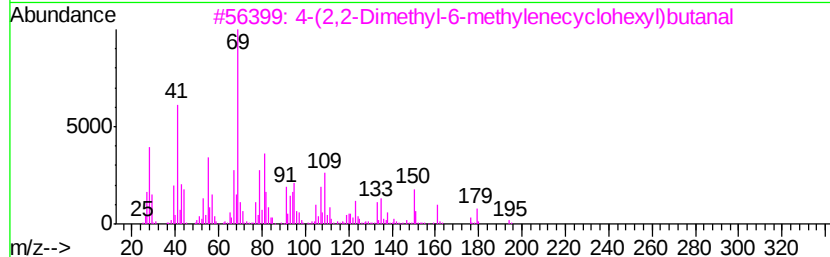
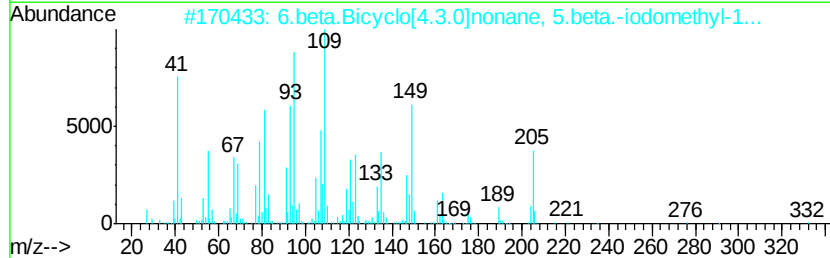
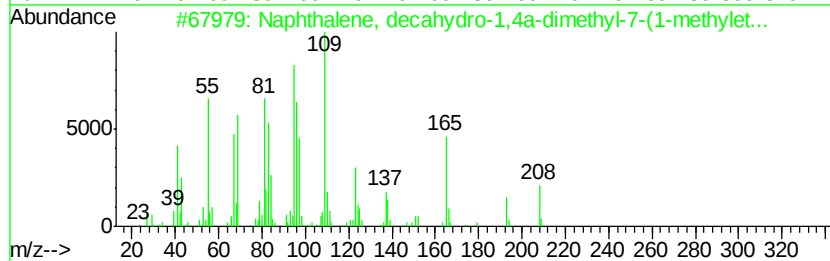
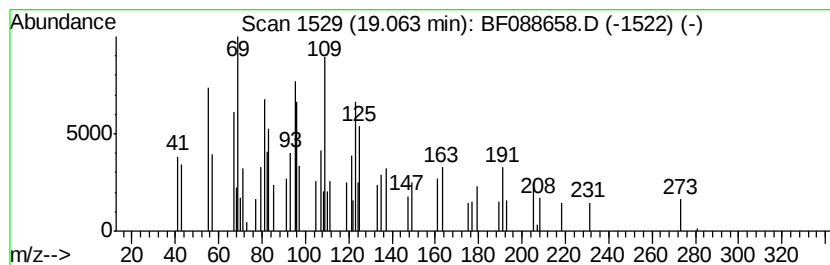
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Naphthalene, decahydro-1,4a... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	3.24 ng	120481	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	50
2		6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	46
3		4-(2,2-Dimethyl-6-methylenecyclo...	194	C13H22O	095452-13-4	35
4		2,4,5,5,8a-Pentamethyl-4a,5,6,7,...	208	C14H24O	1000195-30-1	30
5		Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
 Data File : BF088658.D
 Acq On : 3 Jul 2016 20:24
 Operator : UM/SJ
 Sample : H3817-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BS-3B-10-10.5FT

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
Propylene Glycol	3.05	12.2	ng	407157	1	6.79	667171	20.0
2-Pentanone, 4-hy...	4.96	6.2	ng	208139	1	6.79	667171	20.0
unknown6.55	6.55	71.6	ng	2389360	1	6.79	667171	20.0
Diethyltoluamide	10.19	9.7	ng	507380	3	9.82	1043300	20.0
Hexadecane	11.18	2.3	ng	115002	4	11.29	1011340	20.0
Octacosane	11.60	2.8	ng	143695	4	11.29	1011340	20.0
Heptadecyl triflu...	12.40	4.1	ng	206406	4	11.29	1011340	20.0
1-Heneicosanol	13.82	7.0	ng	353575	5	13.92	1016920	20.0
n-Tetracosanol-1	14.46	2.5	ng	129888	5	13.92	1016920	20.0
unknown17.69	17.69	3.7	ng	135913	6	15.31	742609	20.0
4,8-Methanoazulen...	17.99	9.6	ng	356265	6	15.31	742609	20.0
Naphthalene, deca...	19.06	3.2	ng	120481	6	15.31	742609	20.0