

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
 Data File : BF100943.D
 Acq On : 28 Nov 2017 19:27
 Operator : SJ/JU
 Sample : I6602-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ETGI-294

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-BF110817.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	5.087	506	510	519	rBB	59499	78245	6.31%	0.697%
2	5.481	573	577	580	rBV	1289519	1155096	93.12%	10.290%
3	6.492	744	749	757	rBV	1129601	1179782	95.11%	10.510%
4	6.628	768	772	775	rBV	1355901	1213082	97.79%	10.807%
5	6.857	808	811	815	rBV	439717	351272	28.32%	3.129%
6	7.016	834	838	841	rBV	1107186	914472	73.72%	8.147%
7	7.422	902	907	910	rBV	814020	691364	55.73%	6.159%
8	8.139	1025	1029	1033	rBV	525206	415192	33.47%	3.699%
9	9.216	1207	1212	1215	rBV	1451840	1240470	100.00%	11.051%
10	9.286	1221	1224	1227	rBV	32906	27683	2.23%	0.247%
11	9.545	1263	1268	1269	rBV5	10236	14384	1.16%	0.128%
12	9.604	1274	1278	1281	rBV2	134948	131279	10.58%	1.169%
13	9.657	1285	1287	1290	rVB3	17617	17636	1.42%	0.157%
14	9.757	1301	1304	1307	rBV2	57339	65871	5.31%	0.587%
15	9.804	1309	1312	1316	rVB2	96984	117639	9.48%	1.048%
16	9.892	1321	1327	1331	rVV	413935	432216	34.84%	3.850%
17	9.927	1331	1333	1336	rBV3	13488	20844	1.68%	0.186%
18	9.992	1342	1344	1347	rBV3	16347	18516	1.49%	0.165%
19	10.139	1367	1369	1373	rBV3	52100	62402	5.03%	0.556%
20	10.210	1379	1381	1382	rBV2	25886	21199	1.71%	0.189%
21	10.227	1382	1384	1386	rVV3	40805	31165	2.51%	0.278%
22	10.263	1388	1390	1393	rVB3	37979	30719	2.48%	0.274%
23	10.298	1393	1396	1398	rBV2	120751	120260	9.69%	1.071%
24	10.351	1402	1405	1407	rBV2	47059	53525	4.31%	0.477%
25	10.686	1458	1462	1466	rBV	575647	547935	44.17%	4.881%
26	10.804	1478	1482	1485	rBV	172592	181610	14.64%	1.618%
27	11.268	1559	1561	1564	rVB	69258	50615	4.08%	0.451%
28	11.380	1577	1580	1585	rBV	374098	370134	29.84%	3.297%
29	12.962	1846	1849	1853	rVB	975484	892663	71.96%	7.952%
30	13.851	1998	2000	2005	rVB3	40178	48443	3.91%	0.432%
31	14.021	2025	2029	2035	rVB	439033	387796	31.26%	3.455%
32	15.492	2274	2279	2288	rBV	274969	341767	27.55%	3.045%

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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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

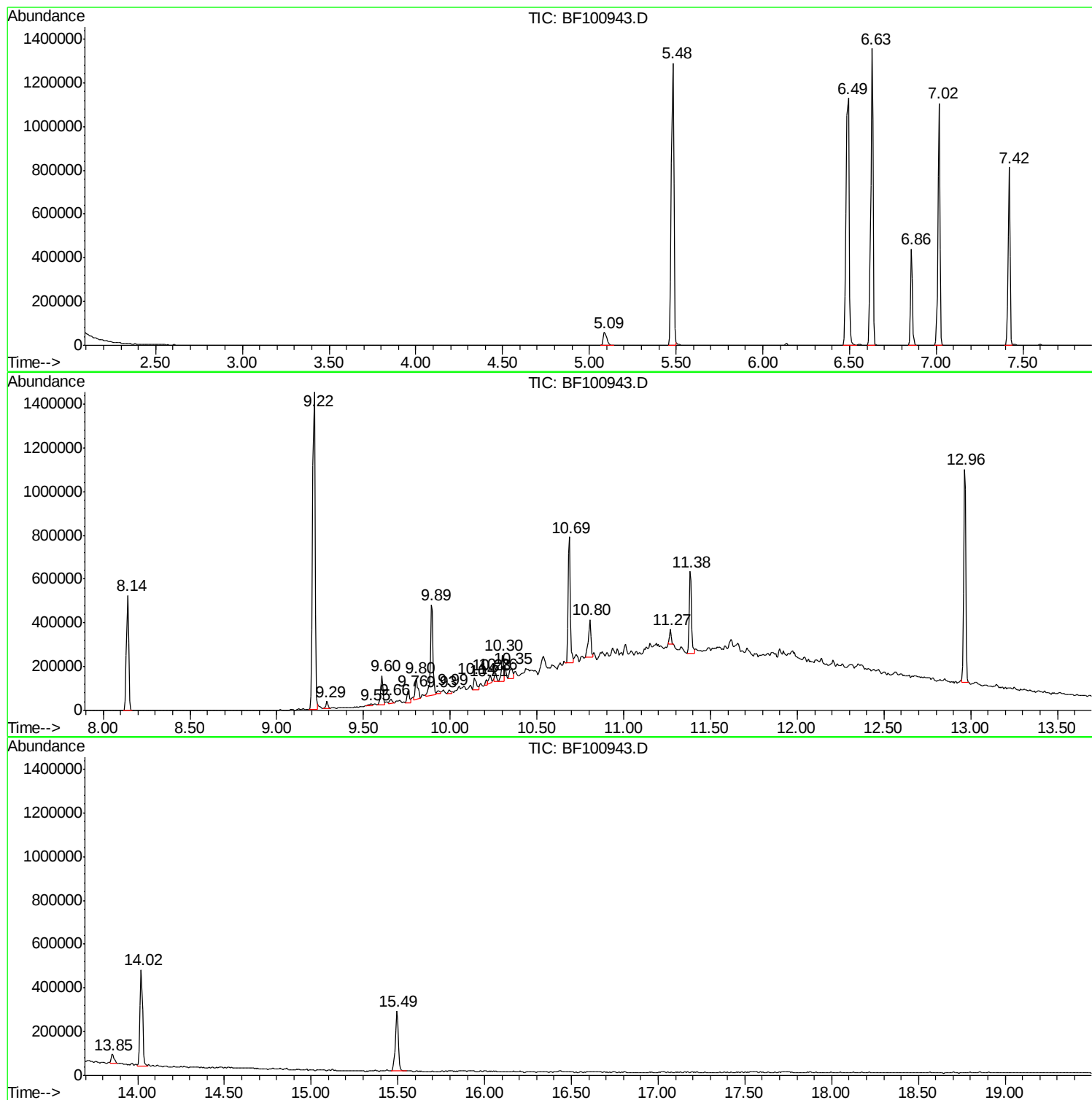
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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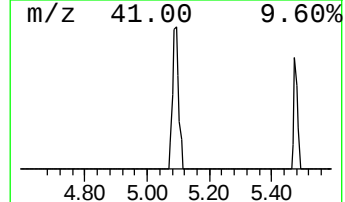
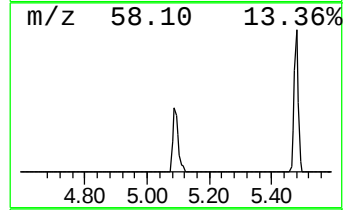
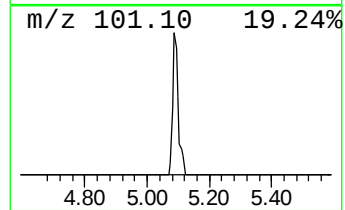
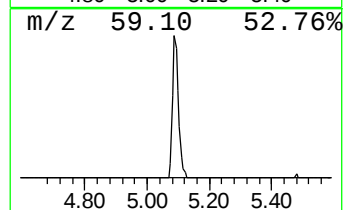
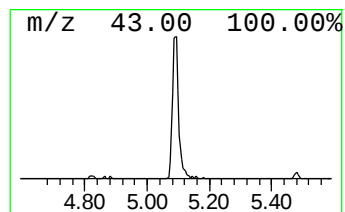
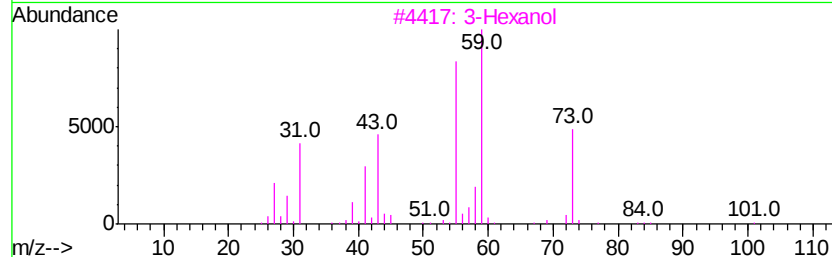
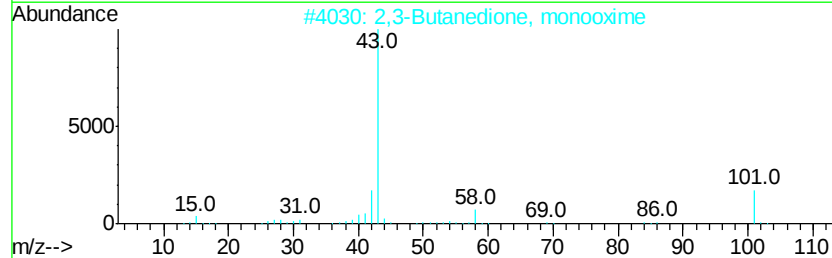
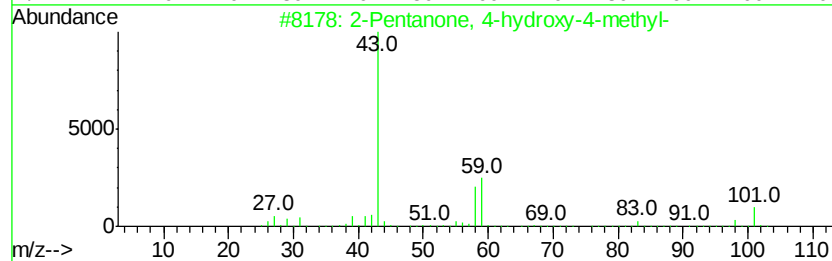
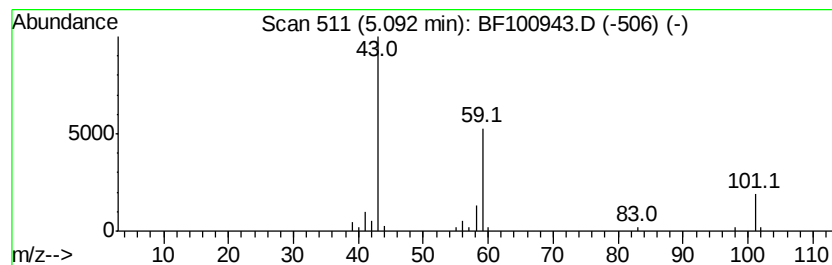
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.45 ng	78245	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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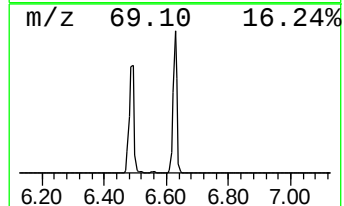
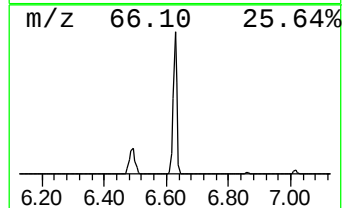
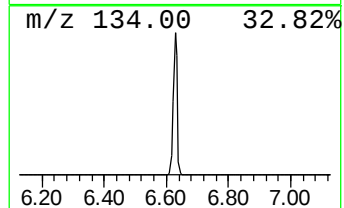
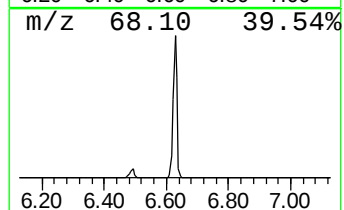
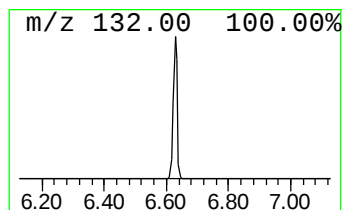
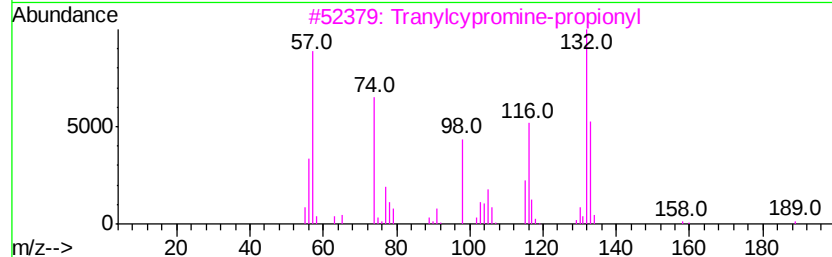
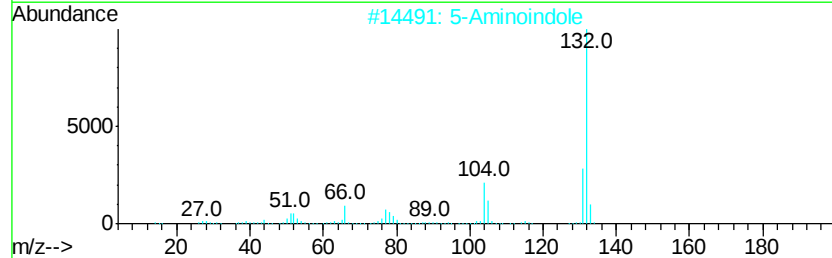
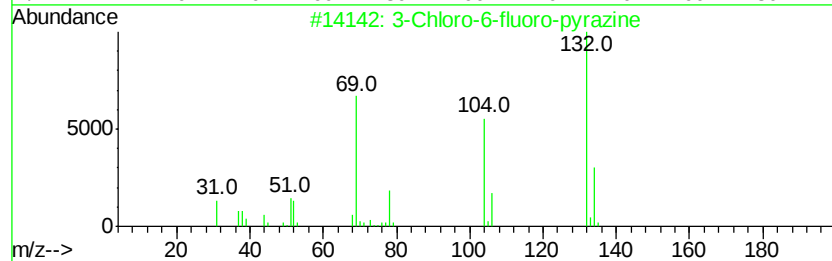
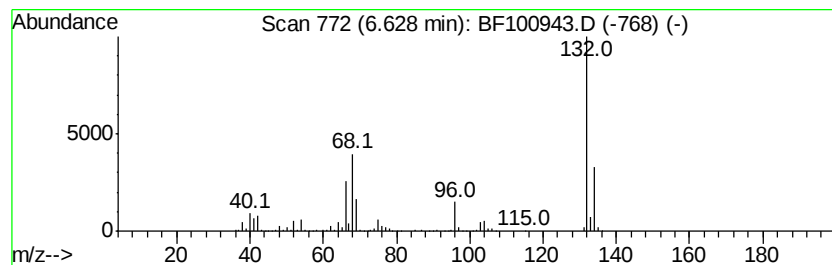
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.07 ng	1213080	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcyproline-propionyl			189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
5	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	9



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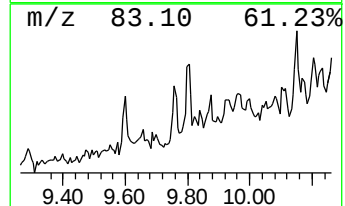
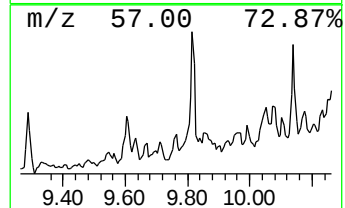
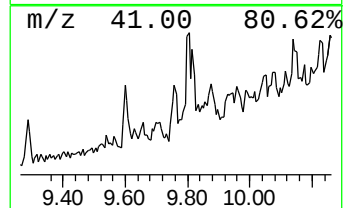
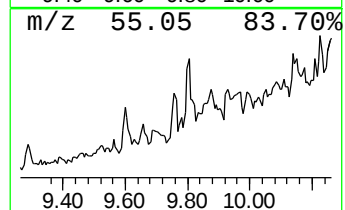
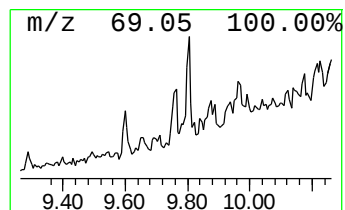
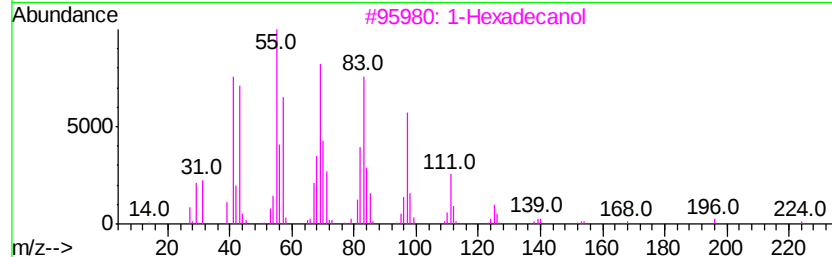
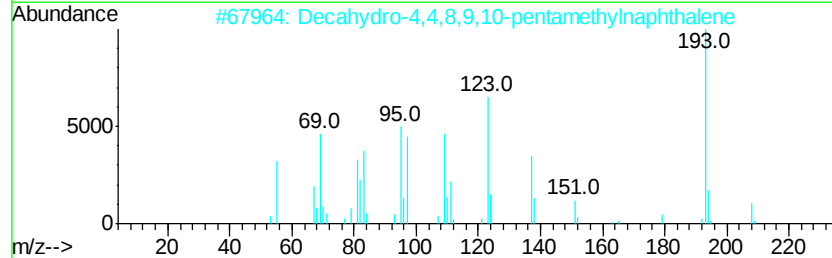
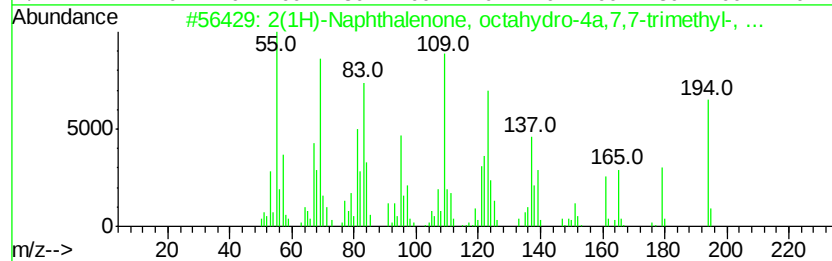
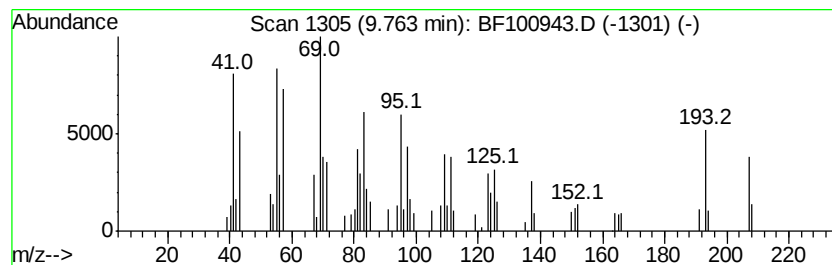
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2(1H)-Naphthalenone, octahydro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	3.05 ng	65871	Acenaphthene-d10	9.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(1H)-Naphthalenone, octahydro-4...	194	C13H22O	054699-31-9	87
2		Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
3		1-Hexadecanol	242	C16H34O	036653-82-4	42
4		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38
5		1,3,7,7-Tetramethyl-9-oxo-2-oxab...	208	C13H20O2	020194-67-6	35



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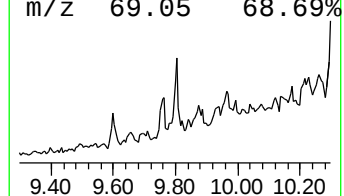
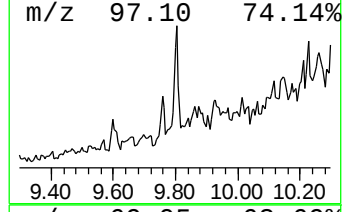
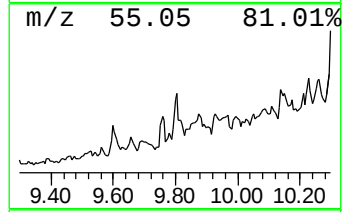
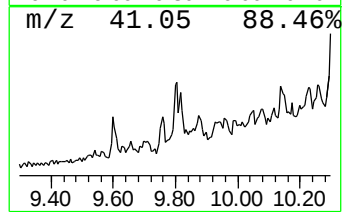
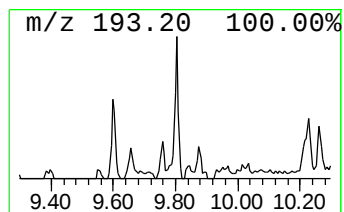
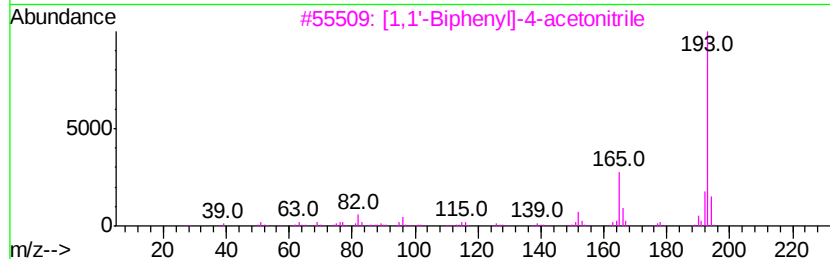
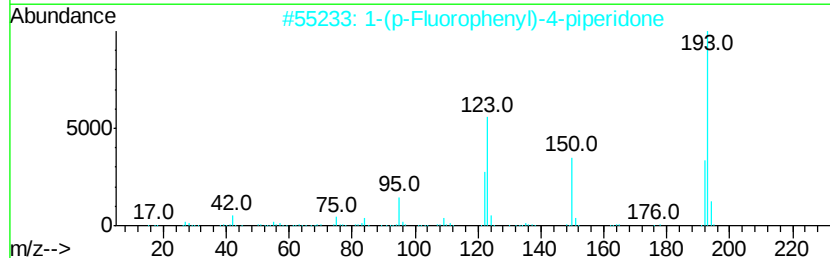
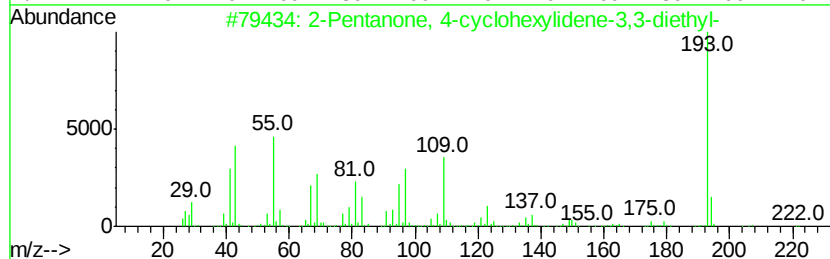
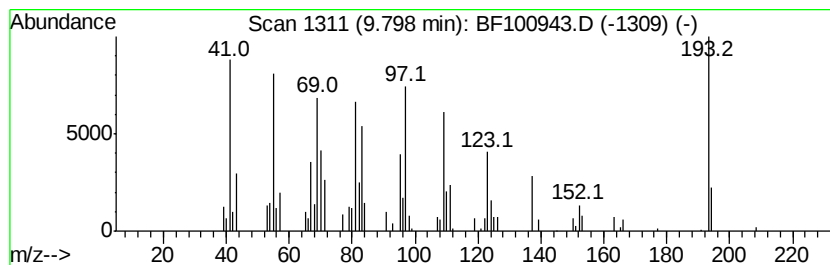
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown9.80 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	5.44 ng	117639	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	37
3		[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	22
4		Cyclododecanemethanol	198	C13H26O	001892-12-2	14
5		Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-95-9	14



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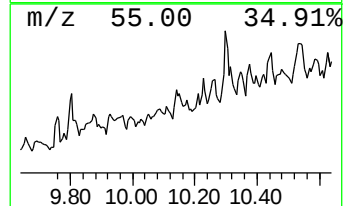
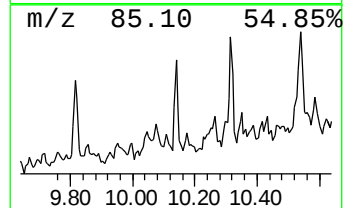
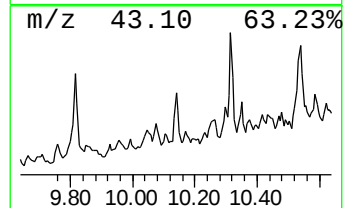
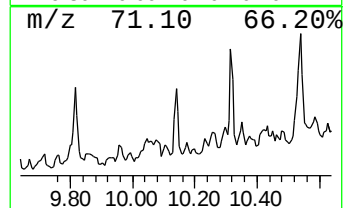
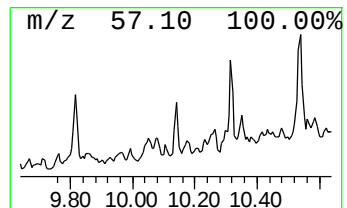
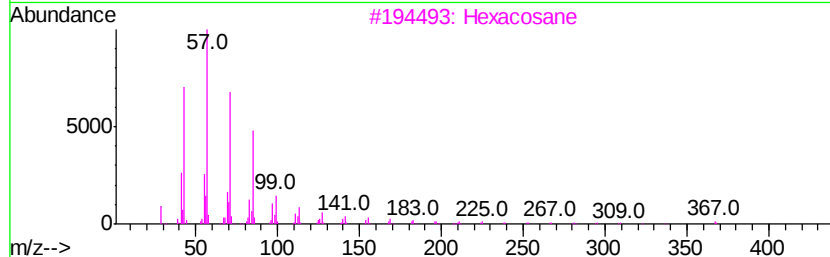
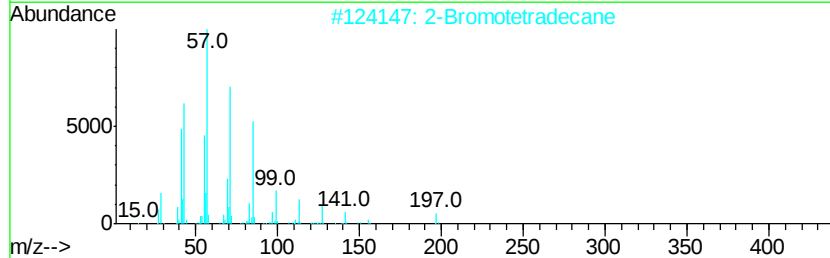
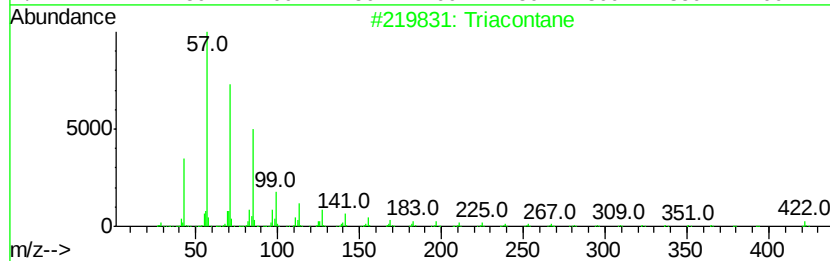
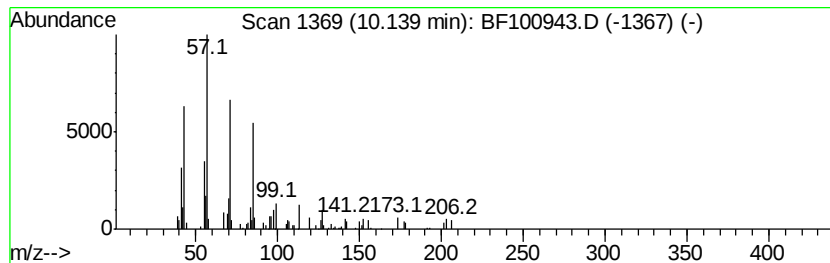
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.14	2.89 ng	62402	Acenaphthene-d10		9.89		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	86
2			2-Bromotetradecane	276	C14H29Br	074036-95-6	80
3			Hexacosane	366	C26H54	000630-01-3	78
4			Octacosane	394	C28H58	000630-02-4	72
5			2-methyloctacosane	408	C29H60	1000376-72-8	64



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Misc :
ALS Vial : 22 Sample Multiplier: 1

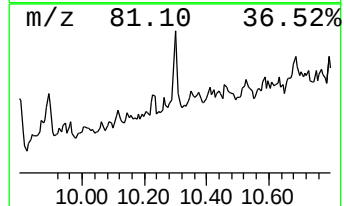
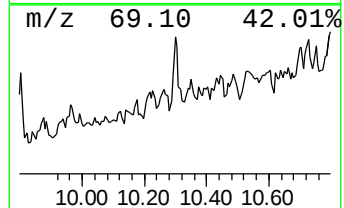
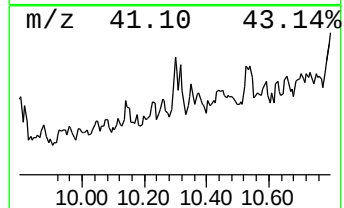
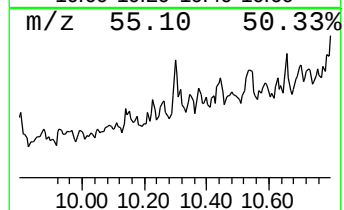
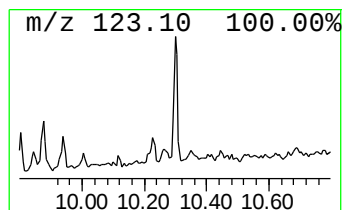
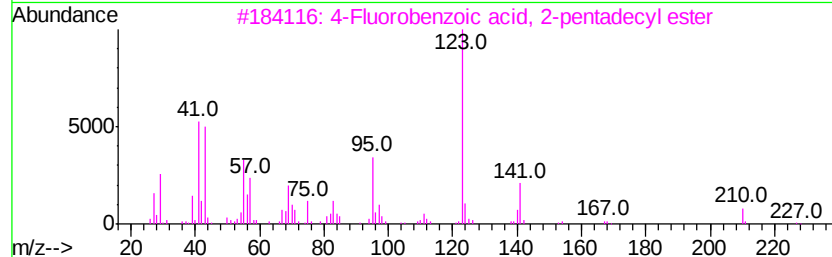
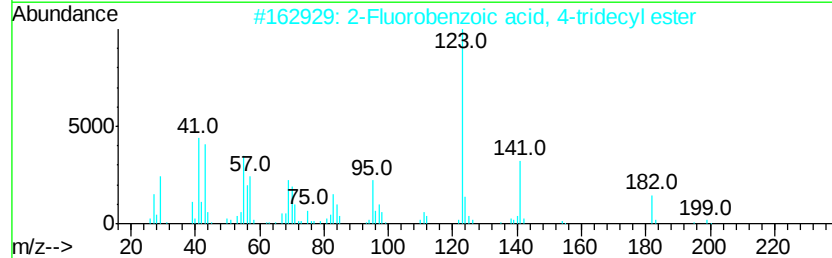
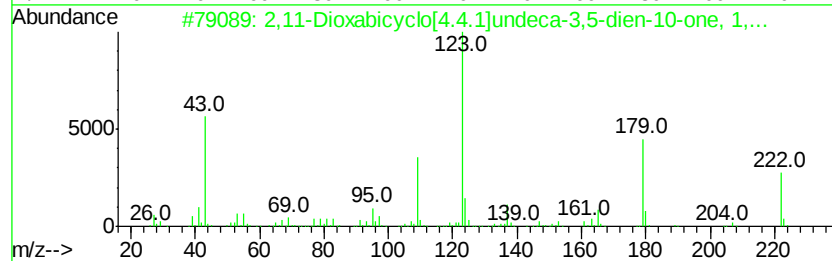
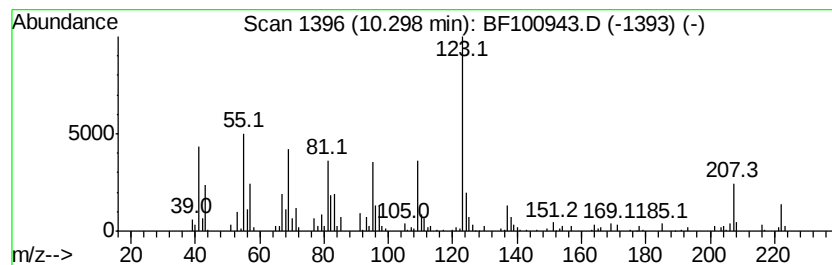
Instrument :
BNA_F
ClientSampleId :
ETGI-294

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.30	5.56 ng	120260	Acenaphthene-d10	9.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	2-Fluorobenzoic acid, 4-tridecyl...	322	C20H31FO2	1000280-61-2	50
3	4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	47
4	4-Fluorobenzoic acid, 3-tetradec...	336	C21H33FO2	1000280-68-1	47
5	4-Fluorobenzoic acid, 5-pentadec...	350	C22H35FO2	1000280-68-6	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100943.D
Acq On : 28 Nov 2017 19:27
Operator : SJ/JU
Sample : I6602-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

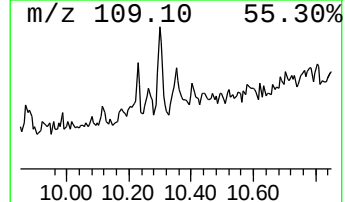
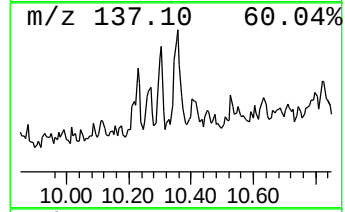
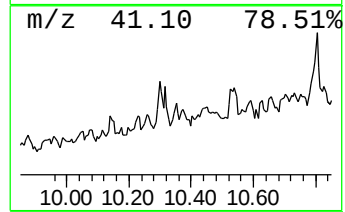
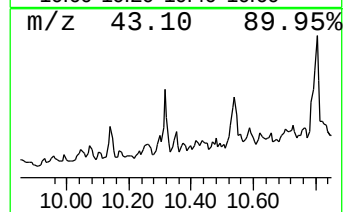
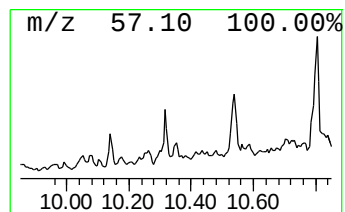
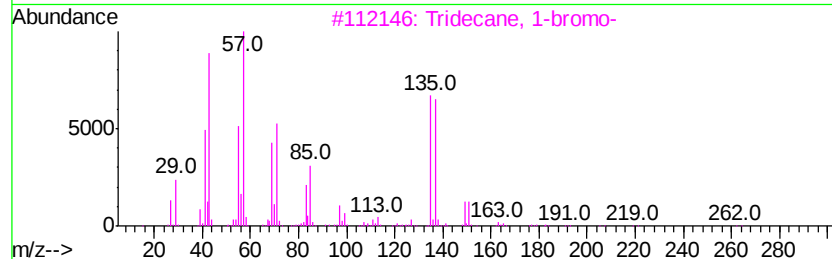
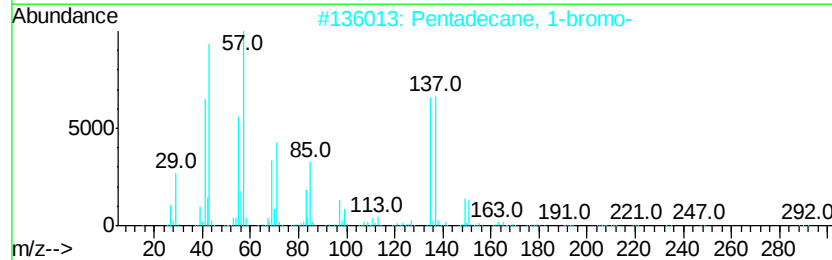
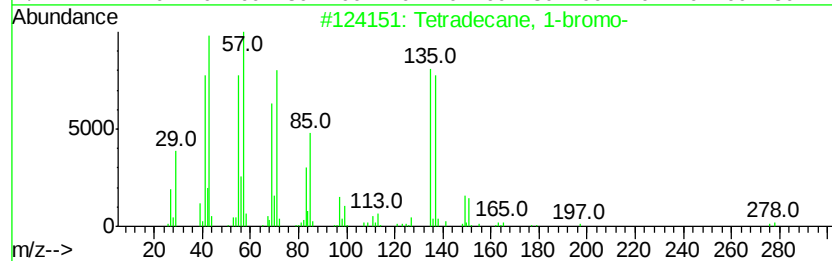
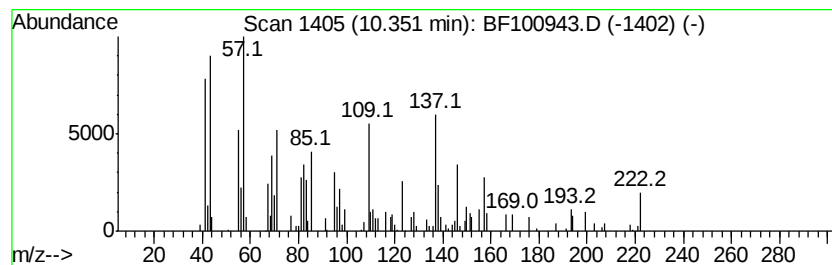
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.35 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.48 ng	53525	Acenaphthene-d10	9.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetradecane, 1-bromo-	276 C14H29Br	000112-71-0 30
2		Pentadecane, 1-bromo-	290 C15H31Br	000629-72-1 25
3		Tridecane, 1-bromo-	262 C13H27Br	000765-09-3 25
4		3,5-Octadiene, 2,2,4,5,7,7-hexam...	194 C14H26	055712-52-2 18
5		1-Octadecanesulphonyl chloride	352 C18H37ClO2S	1000342-70-4 15



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100943.D
Acq On : 28 Nov 2017 19:27
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Sample : I6602-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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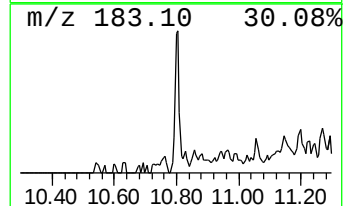
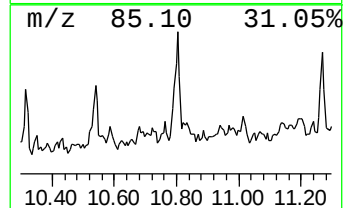
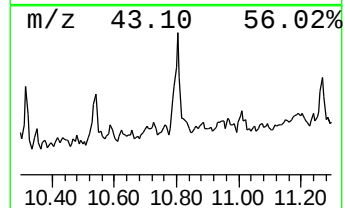
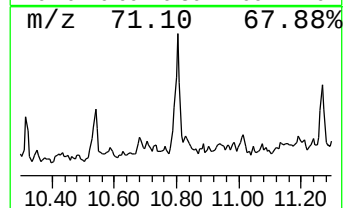
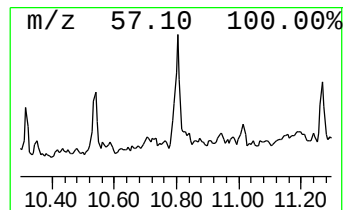
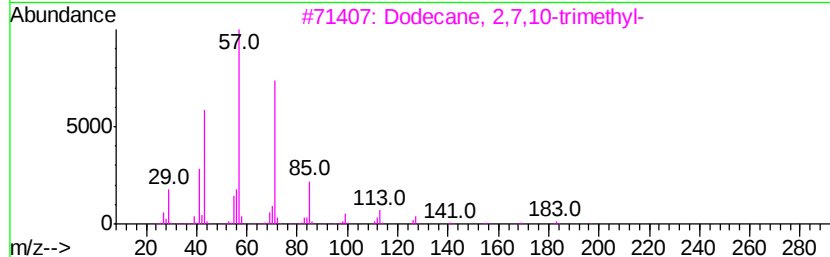
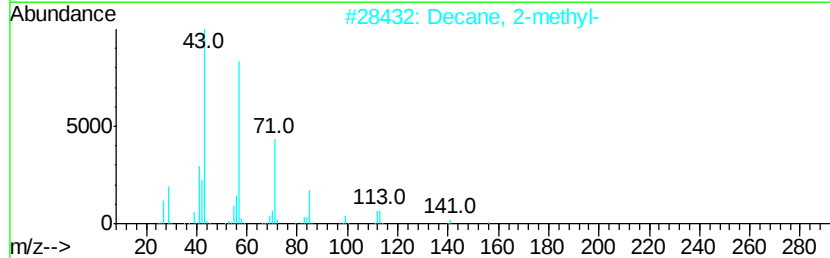
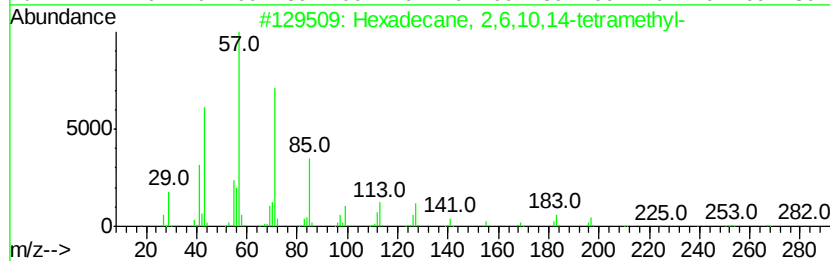
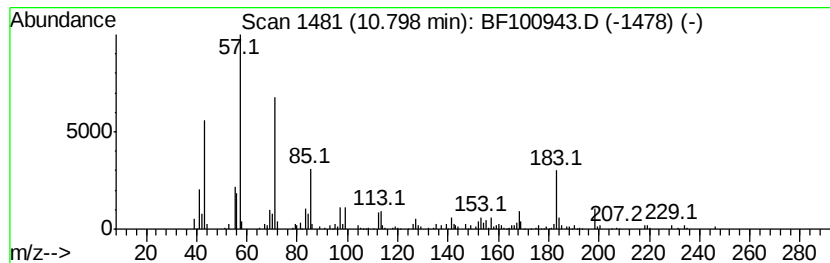
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2,6,10,14-tetra... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	9.81 ng	181610	Phenanthrene-d10	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
2			Decane, 2-methyl-	156	C11H24	006975-98-0	64
3			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112817\
Data File : BF100943.D
Acq On : 28 Nov 2017 19:27
Operator : SJ/JU
Sample : I6602-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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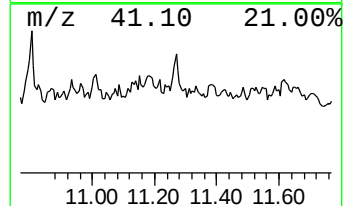
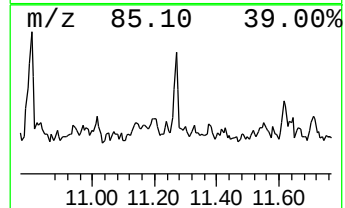
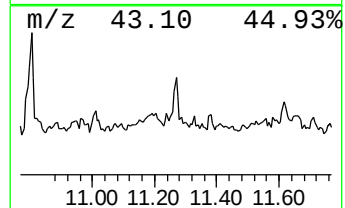
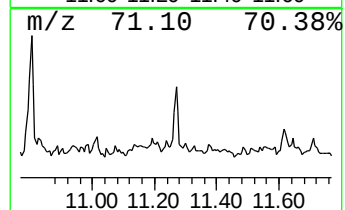
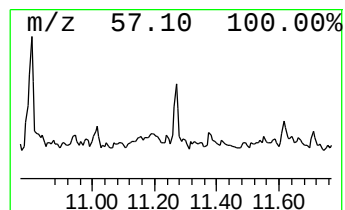
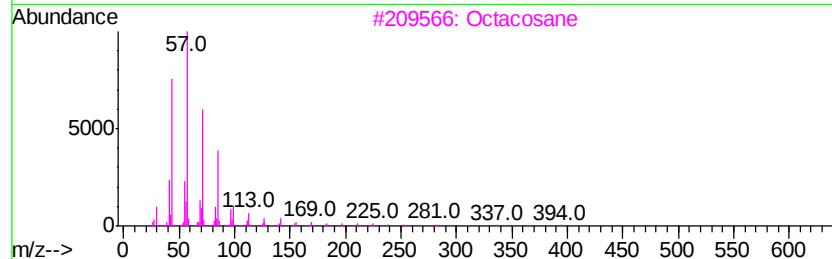
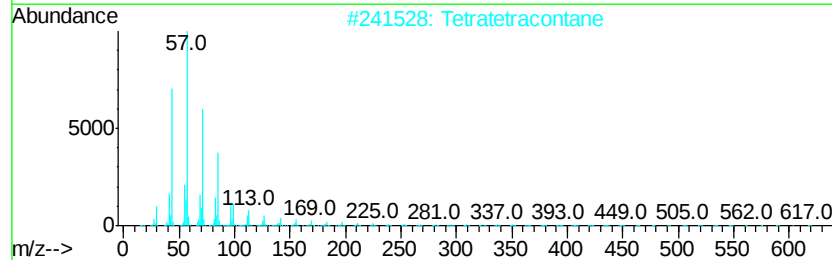
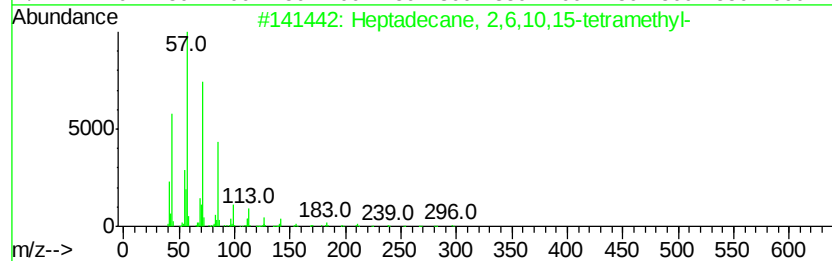
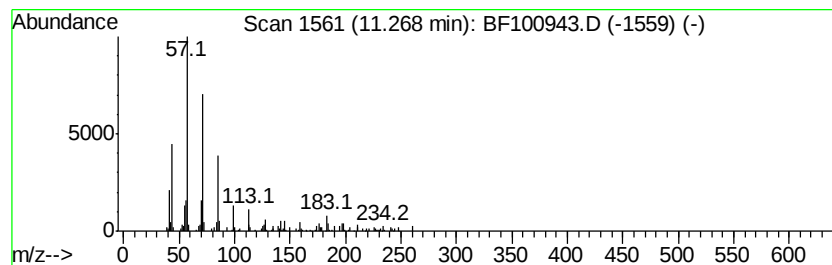
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	2.73 ng	50615	Phenanthrene-d10	11.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
2			Tetratetracontane	619	C44H90	007098-22-8	80
3			Octacosane	394	C28H58	000630-02-4	72
4			2-Bromotetradecane	276	C14H29Br	074036-95-6	72
5			Hentriacontane	437	C31H64	000630-04-6	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
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Sample : I6602-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

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ClientSampleId :
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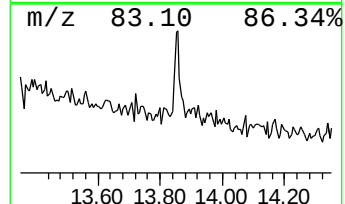
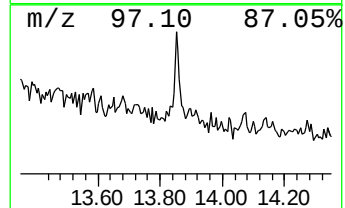
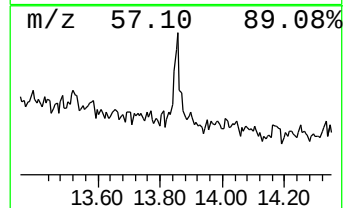
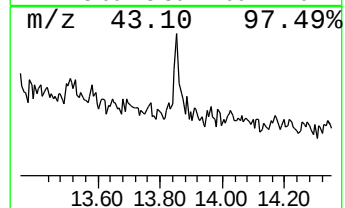
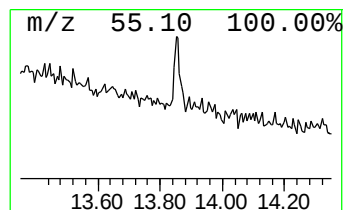
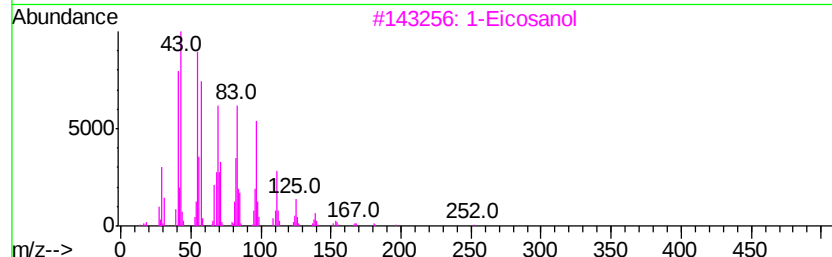
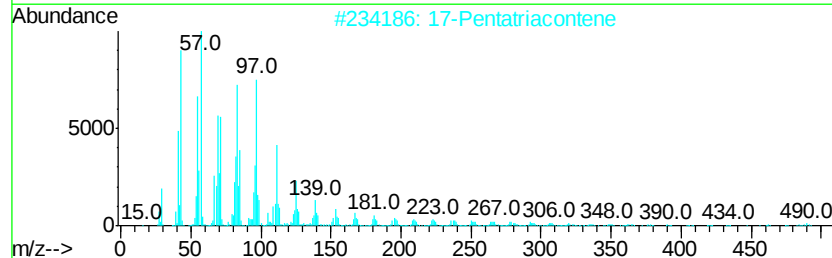
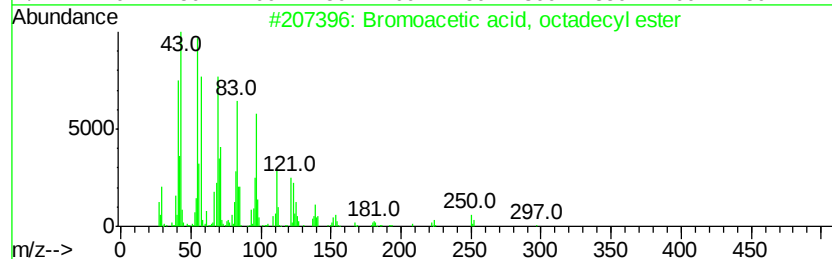
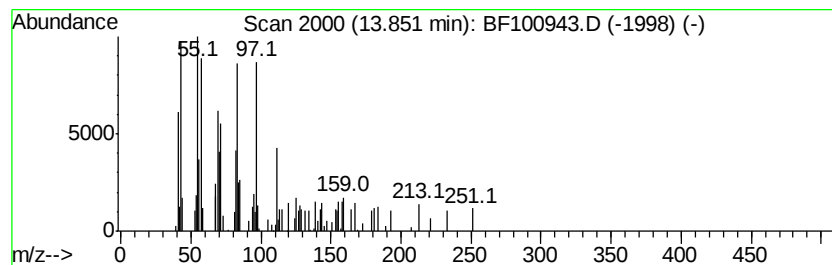
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Bromoacetic acid, octadecyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.50 ng	48443	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	86
2		17-Pentatriacontene	491	C35H70	006971-40-0	80
3		1-Eicosanol	298	C20H42O	000629-96-9	72
4		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	64
5		Triacetyl acetate	480	C32H64O2	041755-58-2	64



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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.09	4.5	ng	78245	1	6.86	351272	20.0
unknown6.63	6.63	69.1	ng	1213080	1	6.86	351272	20.0
2(1H)-Naphthaleno...	9.76	3.0	ng	65871	3	9.89	432216	20.0
unknown9.80	9.80	5.4	ng	117639	3	9.89	432216	20.0
Triacontane	10.14	2.9	ng	62402	3	9.89	432216	20.0
2,11-Dioxabicyclo...	10.30	5.6	ng	120260	3	9.89	432216	20.0
unknown10.35	10.35	2.5	ng	53525	3	9.89	432216	20.0
Hexadecane, 2,6,1...	10.80	9.8	ng	181610	4	11.38	370134	20.0
Heptadecane, 2,6,...	11.27	2.7	ng	50615	4	11.38	370134	20.0
Bromoacetic acid,...	13.85	2.5	ng	48443	5	14.02	387796	20.0