

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
 Data File : BF101964.D
 Acq On : 9 Jan 2018 20:37
 Operator : SJ/JU
 Sample : J1044-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-COMP-A

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-BF010918.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	4.287	370	374	378	rVB	55872	71400	1.02%	0.123%
2	4.945	481	486	497	rVB	393197	606063	8.66%	1.048%
3	5.339	547	553	556	rBV	5721902	6947339	99.30%	12.013%
4	6.363	720	727	731	rBV	5165145	6996549	100.00%	12.098%
5	6.498	744	750	753	rBV	5828417	6510948	93.06%	11.258%
6	6.728	785	789	792	rBV	1854378	1490596	21.30%	2.577%
7	6.886	811	816	819	rBV	5082772	4748987	67.88%	8.212%
8	7.298	879	886	888	rBV	3671023	4146500	59.26%	7.170%
9	8.010	1002	1007	1010	rBV	2194031	1783376	25.49%	3.084%
10	8.569	1097	1102	1105	rBV	241234	203037	2.90%	0.351%
11	9.086	1185	1190	1194	rBV	4996098	4980083	71.18%	8.611%
12	9.480	1253	1257	1261	rBV	588357	439904	6.29%	0.761%
13	9.763	1298	1305	1308	rBV	1735006	1458463	20.85%	2.522%
14	9.792	1308	1310	1314	rVB	171508	130418	1.86%	0.226%
15	9.963	1336	1339	1342	rBV	179006	144163	2.06%	0.249%
16	10.304	1394	1397	1401	rBV	606643	544848	7.79%	0.942%
17	10.474	1422	1426	1429	rVB	477588	432512	6.18%	0.748%
18	10.551	1434	1439	1442	rBV	2697002	2543506	36.35%	4.398%
19	10.680	1457	1461	1467	rVB4	40023	73771	1.05%	0.128%
20	11.139	1537	1539	1545	rVB	114664	115685	1.65%	0.200%
21	11.245	1553	1557	1559	rBV	1422559	1250929	17.88%	2.163%
22	11.269	1559	1561	1564	rVV	1552230	1137982	16.26%	1.968%
23	11.316	1564	1569	1573	rVB	832380	755545	10.80%	1.306%
24	11.780	1644	1648	1652	rBV2	492521	514539	7.35%	0.890%
25	11.857	1657	1661	1663	rBV	184191	164510	2.35%	0.284%
26	12.451	1759	1762	1766	rBV	854306	754630	10.79%	1.305%
27	12.563	1776	1781	1786	rBV2	155643	191216	2.73%	0.331%
28	12.680	1795	1801	1804	rBV	607972	634393	9.07%	1.097%
29	12.833	1823	1827	1830	rBV	3702911	3578584	51.15%	6.188%
30	13.010	1854	1857	1860	rVB2	119548	101061	1.44%	0.175%
31	13.074	1865	1868	1871	rVB	129267	119436	1.71%	0.207%
32	13.727	1976	1979	1989	rBV	918069	869236	12.42%	1.503%
33	13.880	1999	2005	2007	rBV	1496816	1536897	21.97%	2.658%
34	13.904	2007	2009	2012	rVB	256335	194954	2.79%	0.337%

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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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.362	2084	2087	2093	rBV2	183646	216844	3.10%	0.375%
36	14.886	2174	2176	2179	rBV	79583	87760	1.25%	0.152%
37	14.986	2190	2193	2201	rBV4	81808	182419	2.61%	0.315%
38	15.298	2241	2246	2250	rBV	822536	910685	13.02%	1.575%
39	15.756	2321	2324	2328	rBV3	60463	80732	1.15%	0.140%
40	15.804	2328	2332	2339	rVB3	112784	180919	2.59%	0.313%

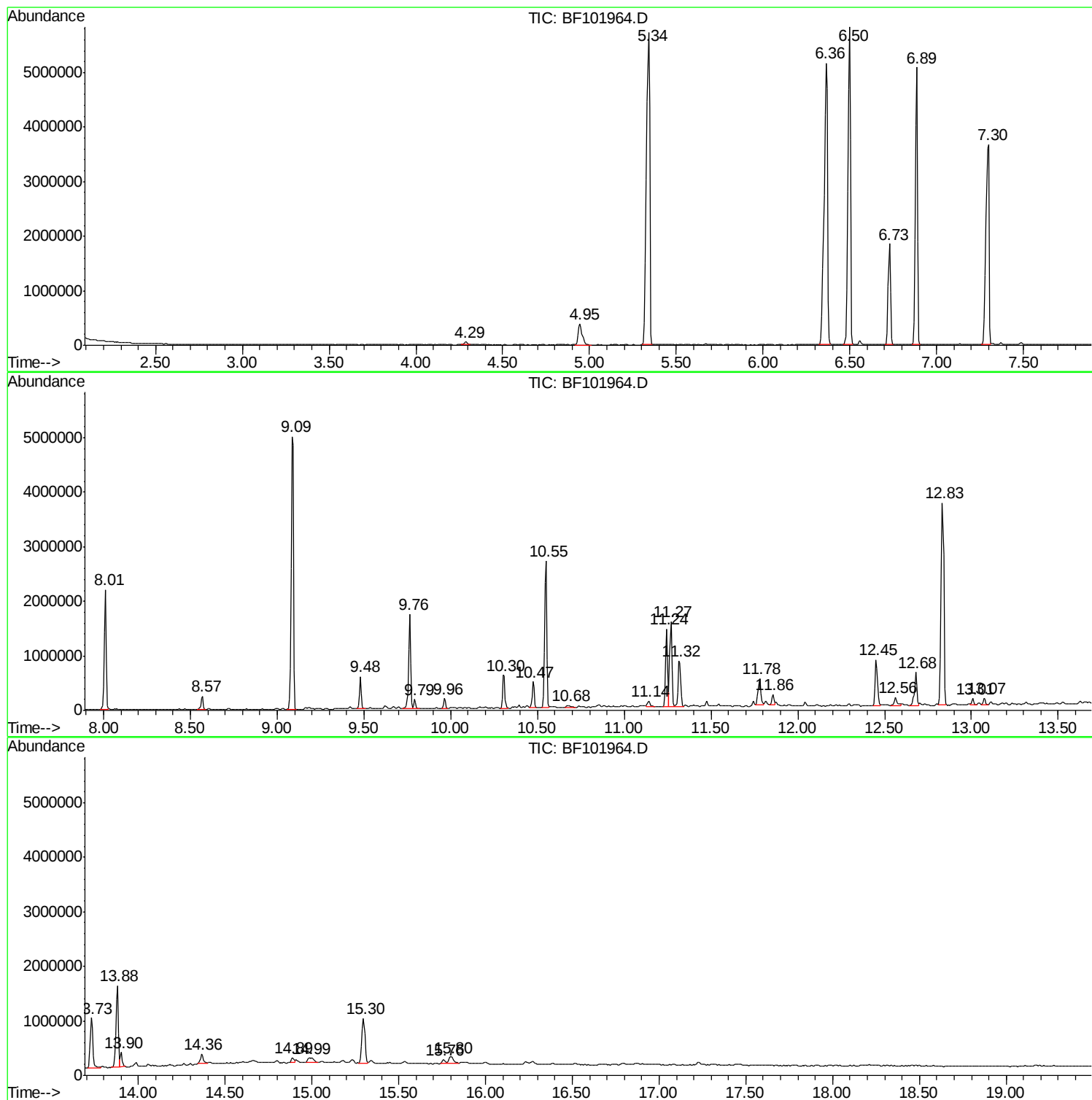
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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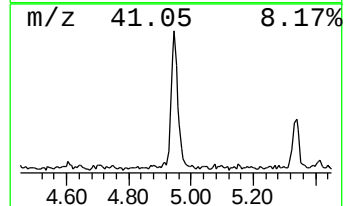
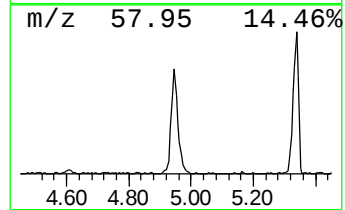
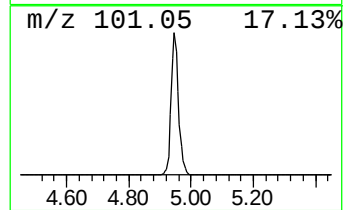
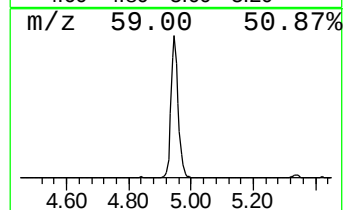
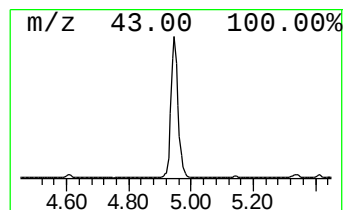
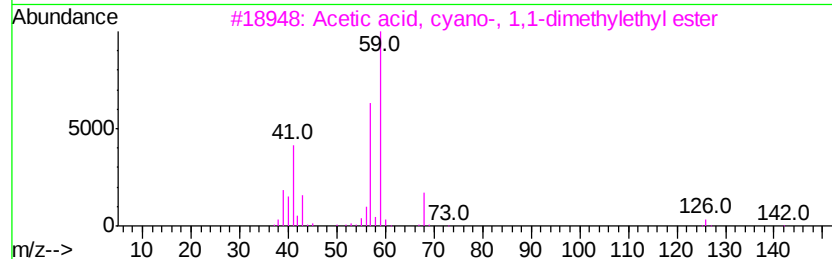
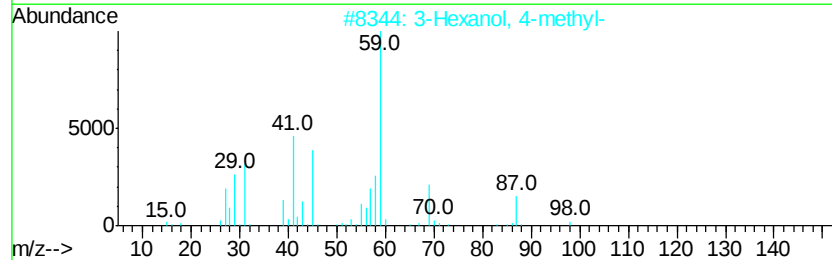
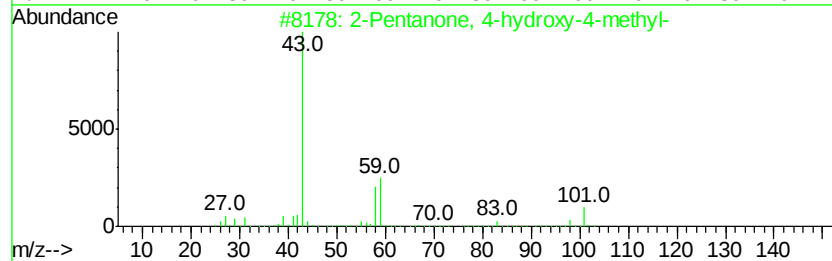
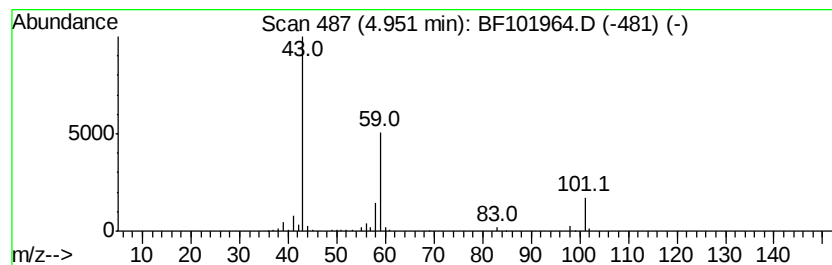
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	8.13 ng	606063	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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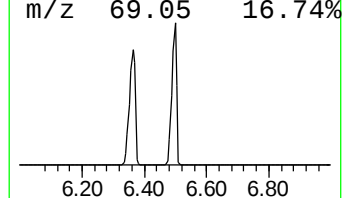
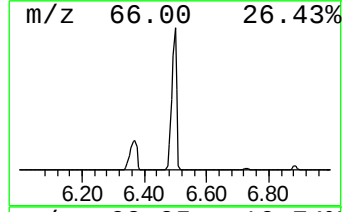
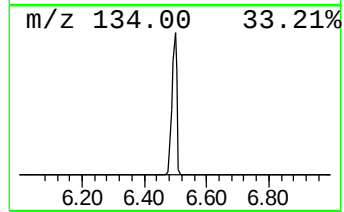
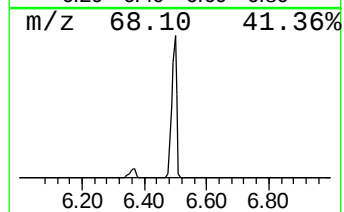
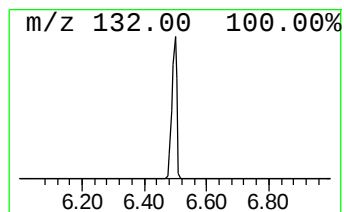
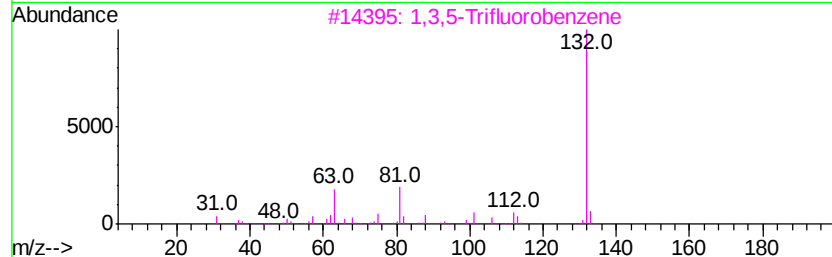
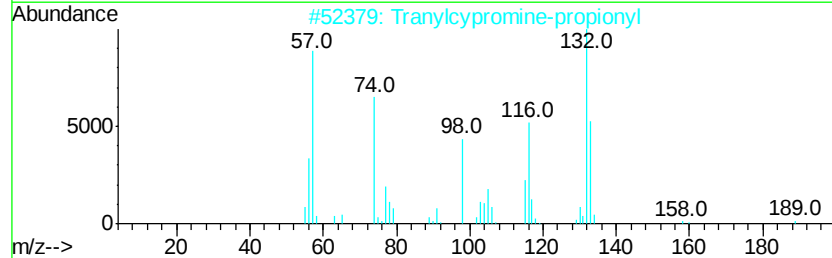
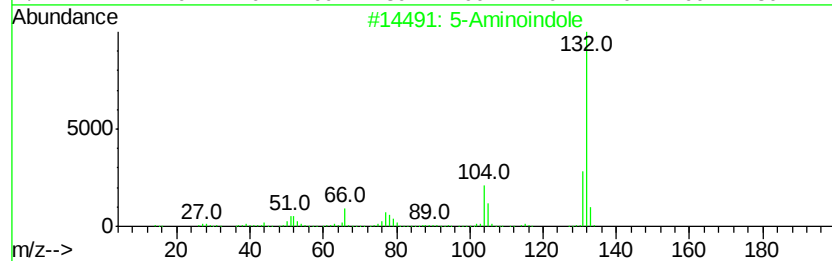
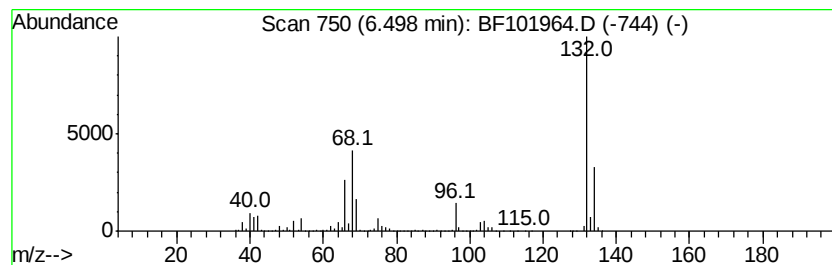
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	87.36 ng	6510950	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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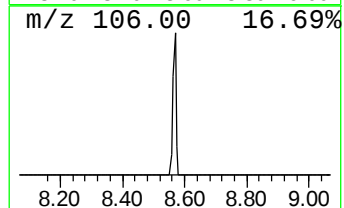
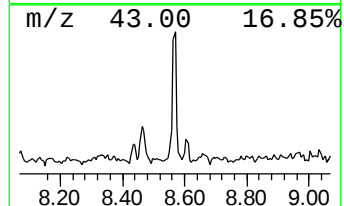
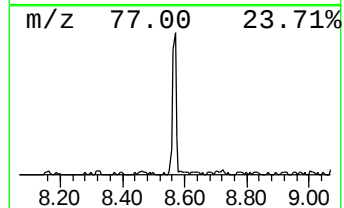
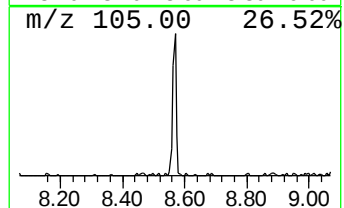
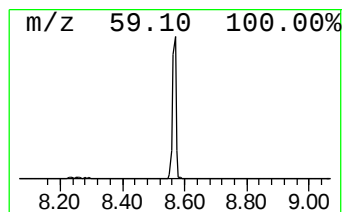
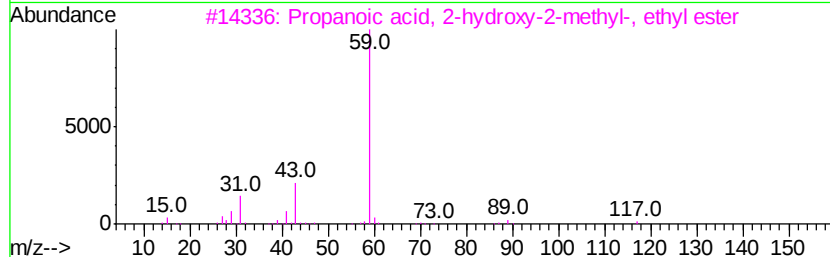
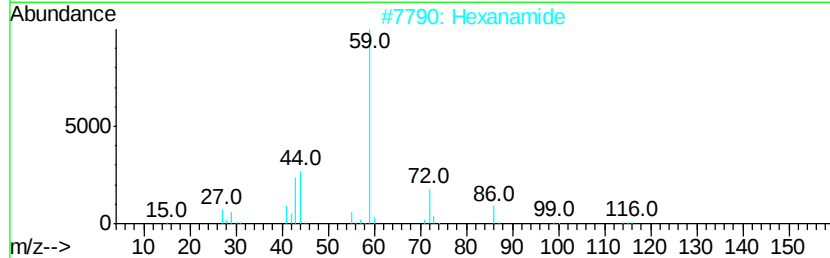
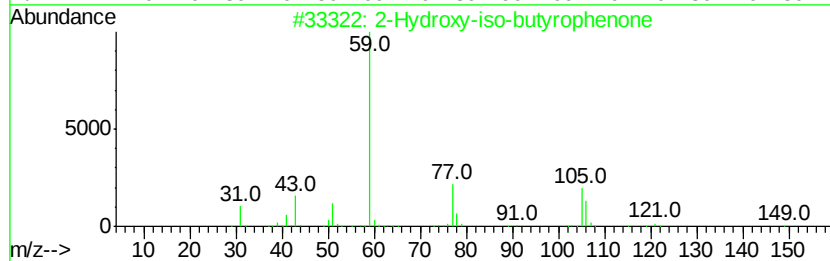
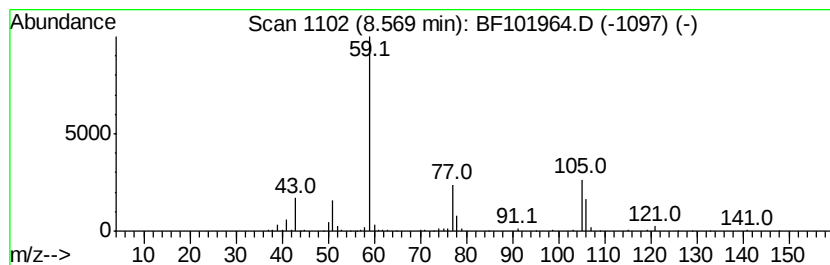
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	2.28 ng	203037	Napthalene-d8	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Hexanamide	115	C6H13NO	000628-02-4	9
3		Propanoic acid, 2-hydroxy-2-methyl-, ethyl ester	132	C6H12O3	000080-55-7	9
4		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	9
5		Guanidine	59	CH5N3	000113-00-8	7



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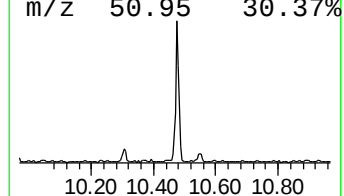
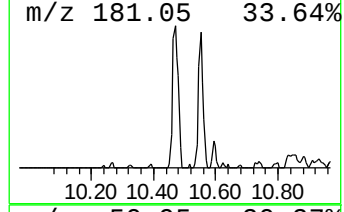
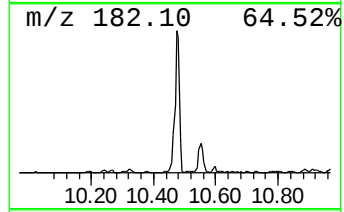
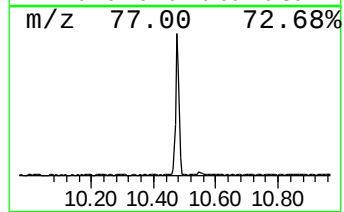
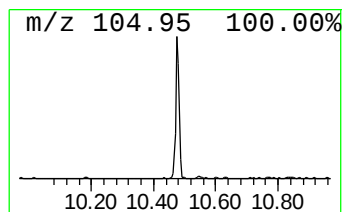
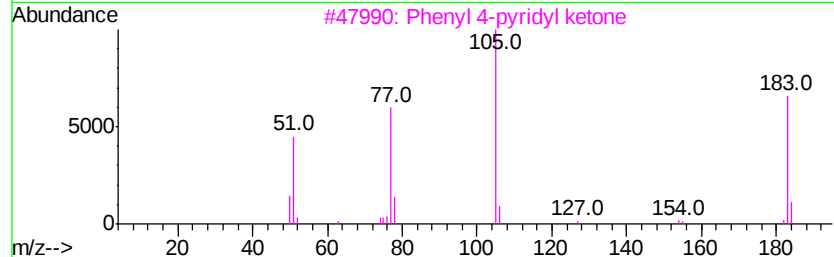
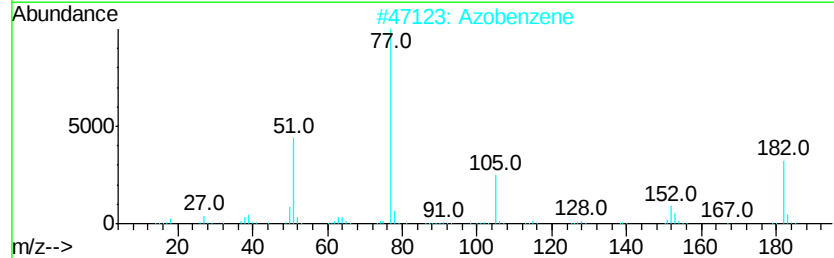
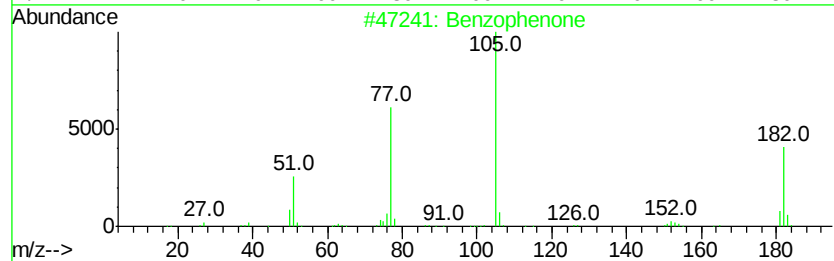
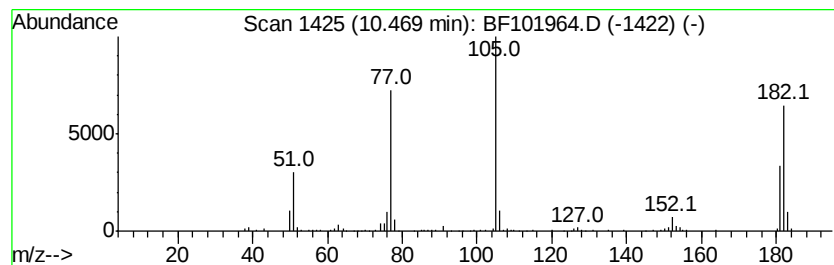
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.47	5.93 ng	432512	Acenaphthene-d10		9.76
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Phenvl 4-pvridvl ketone	183	C12H9NO	014548-46-0	58
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47



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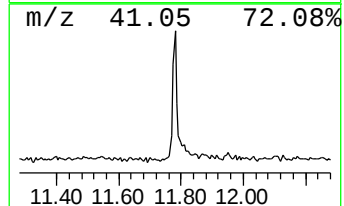
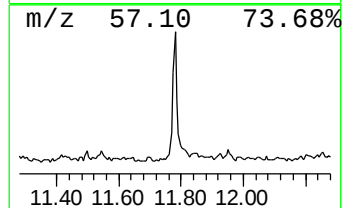
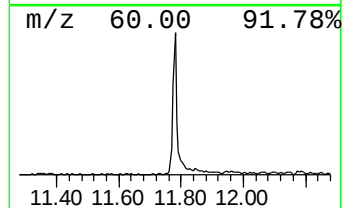
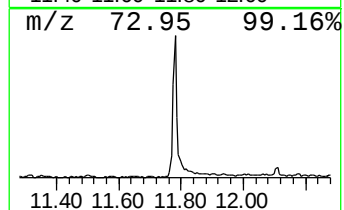
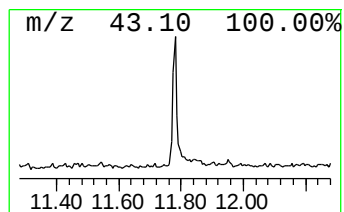
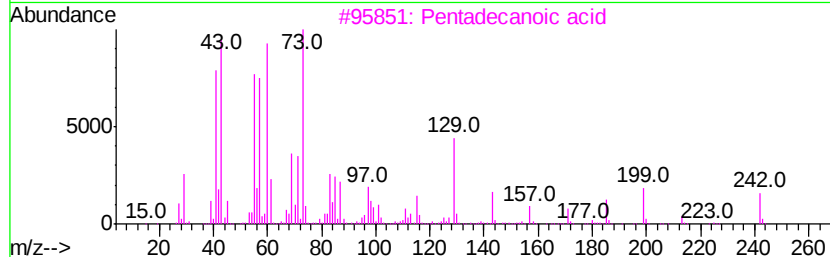
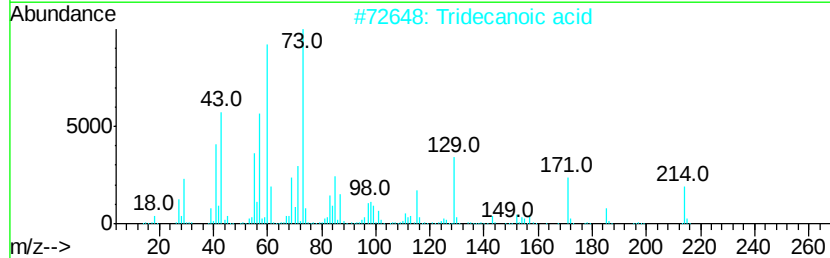
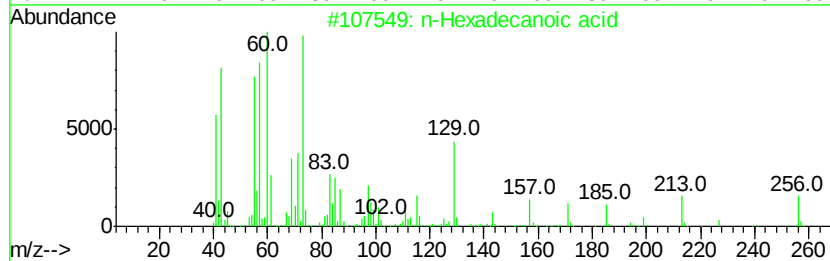
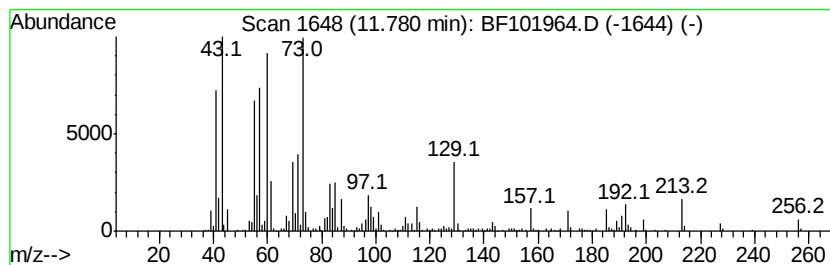
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	8.23 ng	514539	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101964.D
Acq On : 9 Jan 2018 20:37
Operator : SJ/JU
Sample : J1044-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

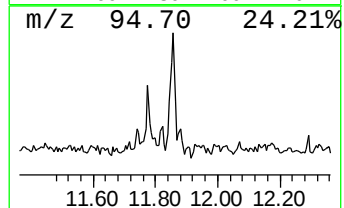
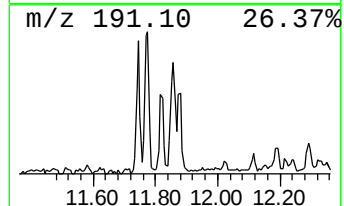
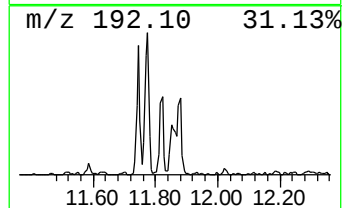
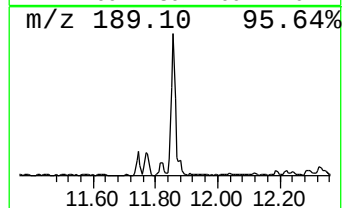
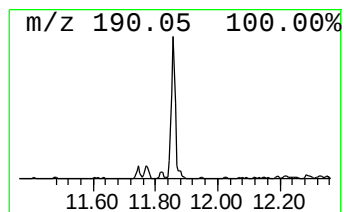
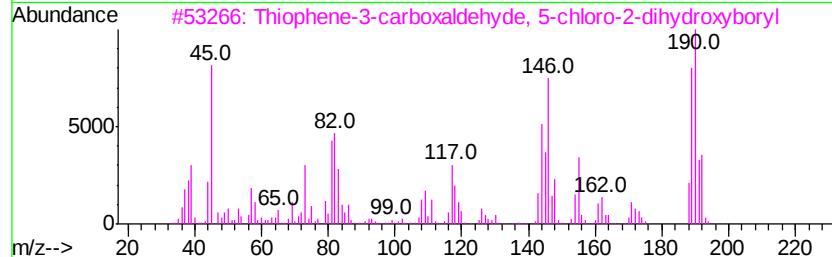
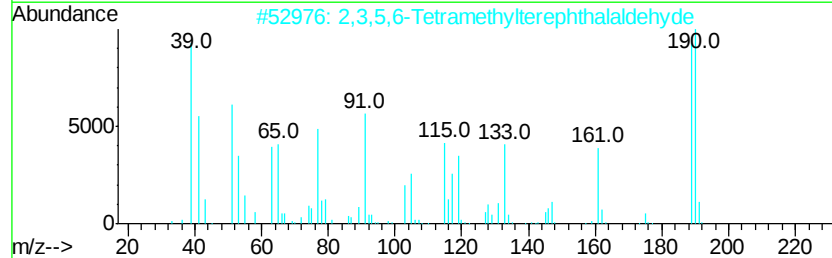
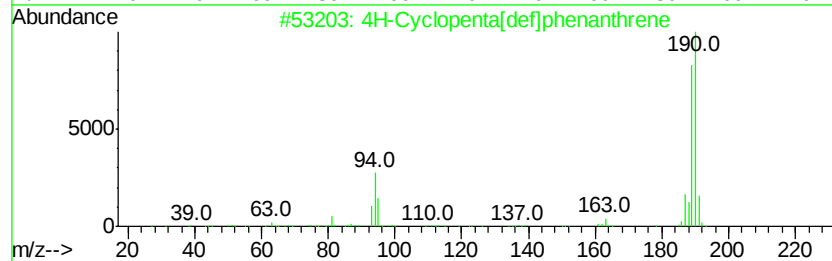
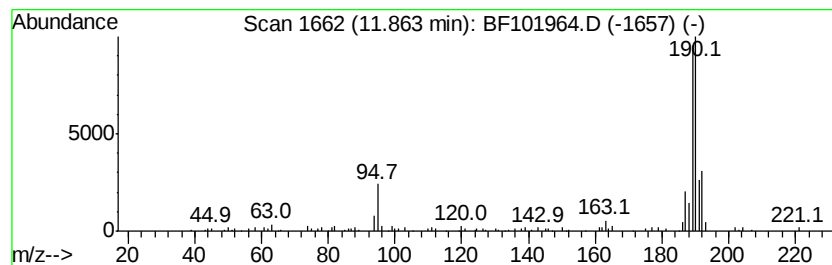
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.86	2.63 ng	164510	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2		2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	33
5		1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	23



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF01964.D
Acq On : 9 Jan 2018 20:37
Operator : SJ/JU
Sample : J1044-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

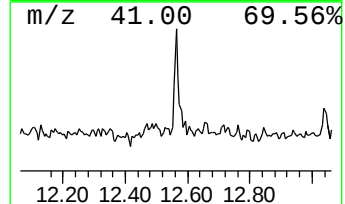
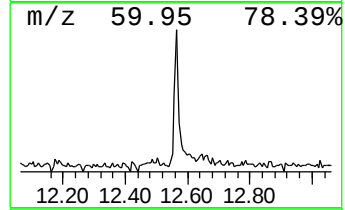
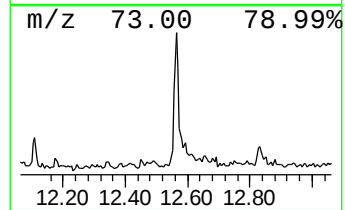
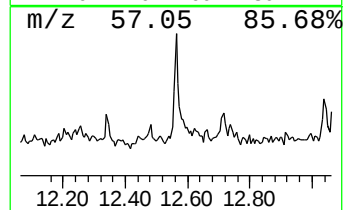
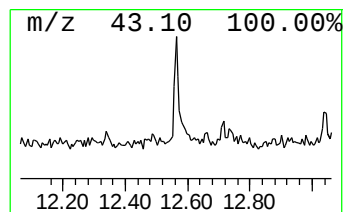
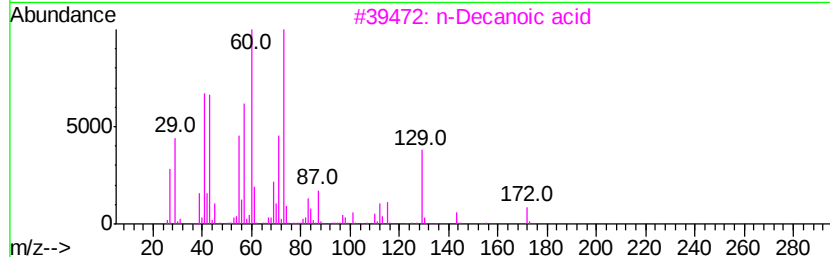
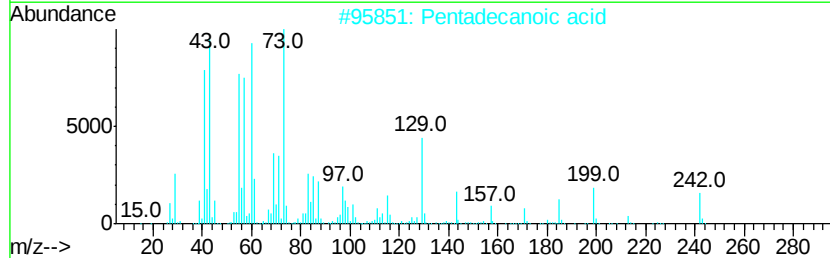
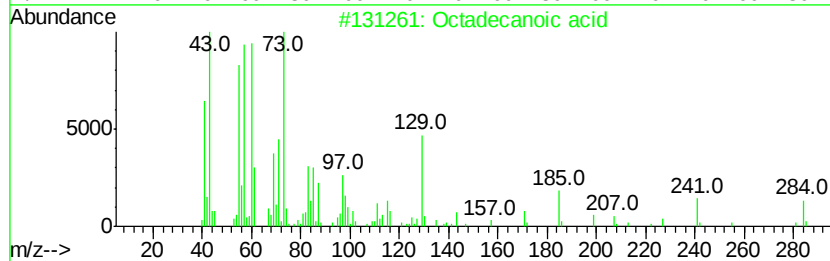
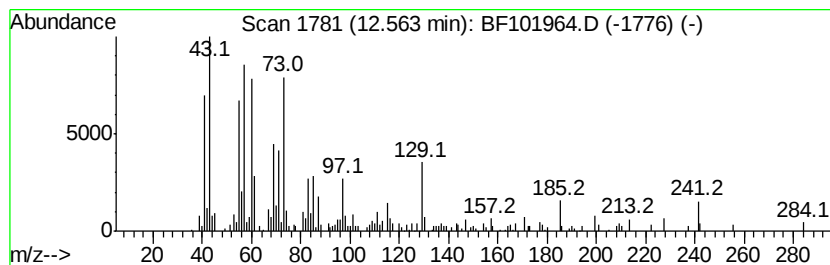
Instrument :
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ClientSampleId :
SP-COMP-A

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	2.49 ng	191216	Chrysene-d12	13.88	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Nonanoic acid	158	C9H18O2	000112-05-0	30
5	Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF01964.D
Acq On : 9 Jan 2018 20:37
Operator : SJ/JU
Sample : J1044-04
Misc :
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Instrument :
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ClientSampleId :
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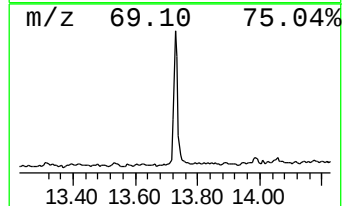
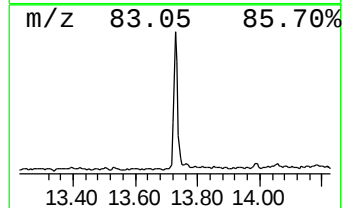
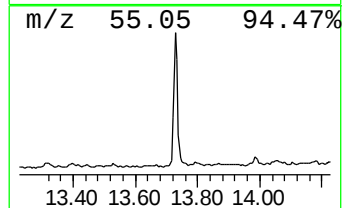
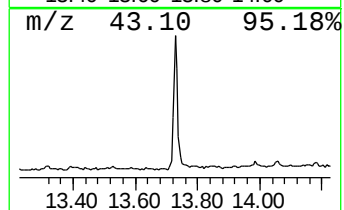
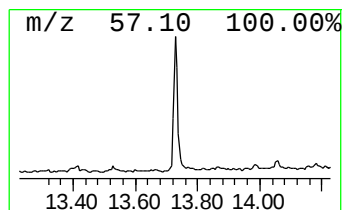
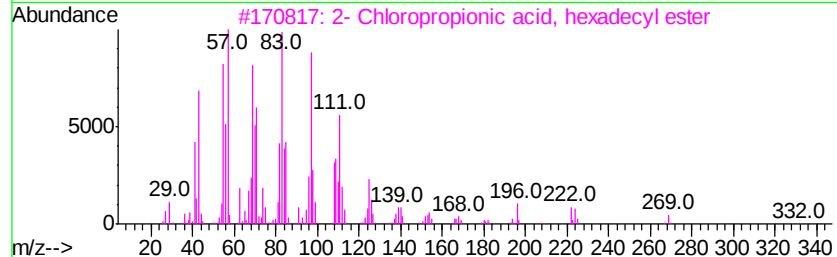
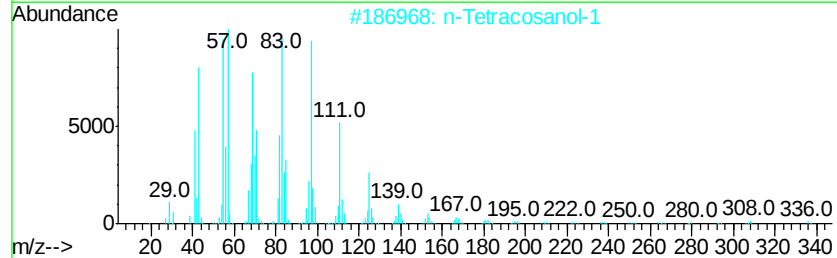
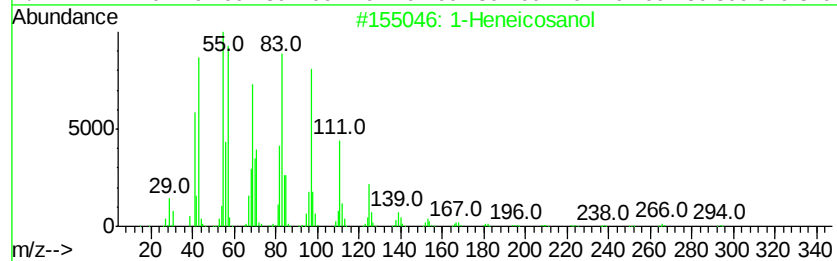
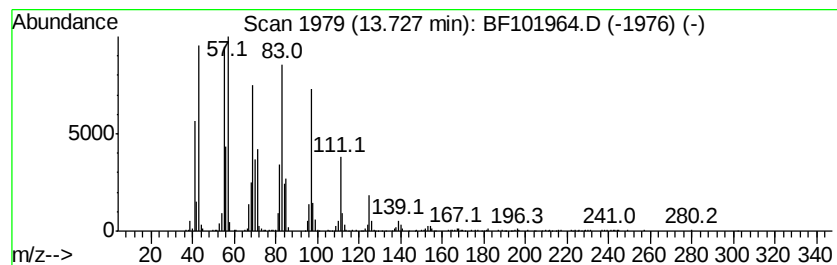
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	11.31 ng	869236	Chrysene-d12	13.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5			3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF01964.D
Acq On : 9 Jan 2018 20:37
Operator : SJ/JU
Sample : J1044-04
Misc :
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Instrument :
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ClientSampleId :
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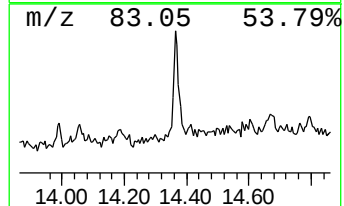
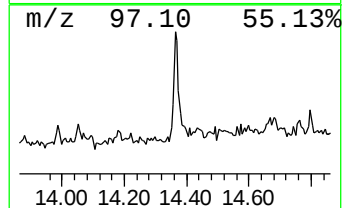
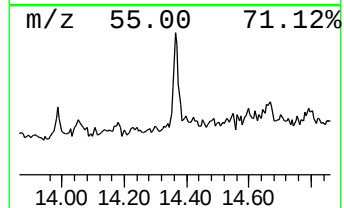
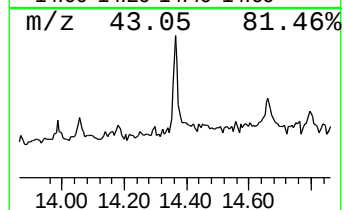
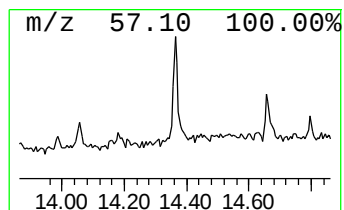
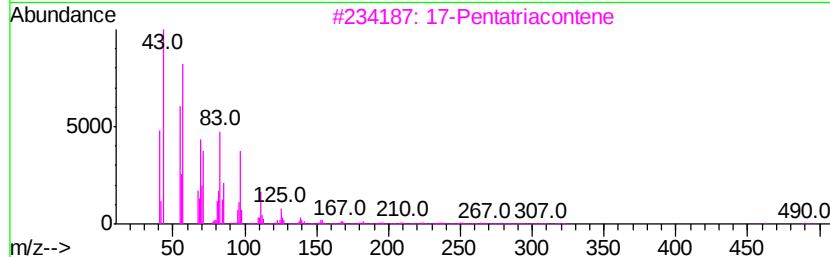
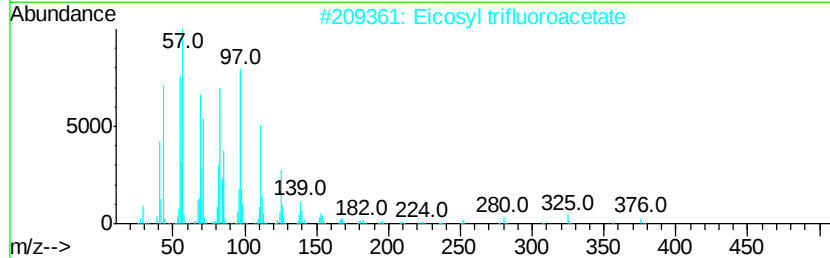
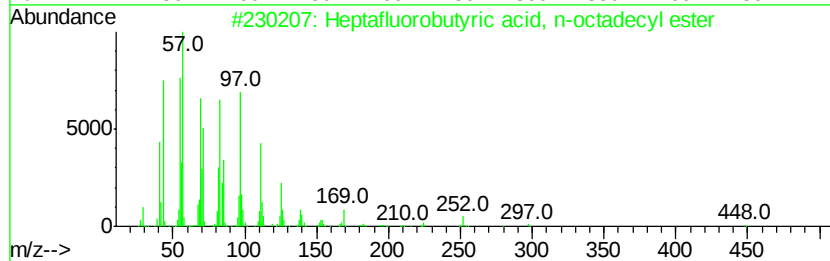
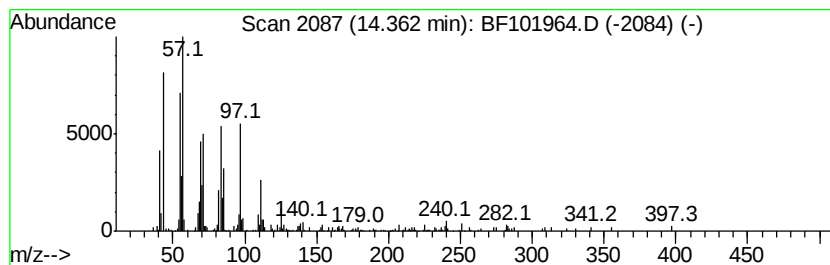
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptafluorobutyric acid, n-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.82 ng	216844	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	90
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	90
3		17-Pentatriacontene	491	C35H70	006971-40-0	86
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101964.D
Acq On : 9 Jan 2018 20:37
Operator : SJ/JU
Sample : J1044-04
Misc :
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Instrument :
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ClientSampleId :
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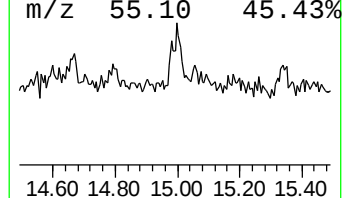
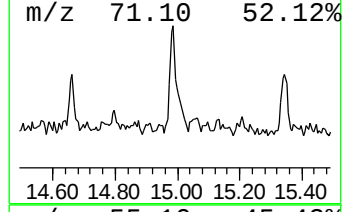
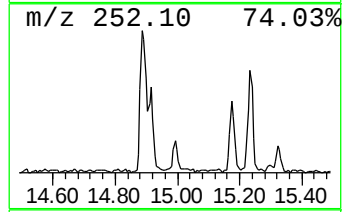
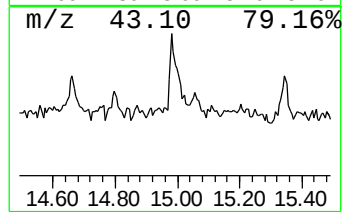
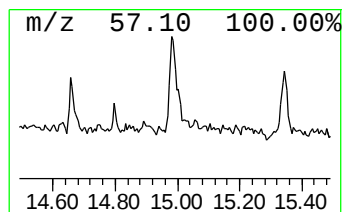
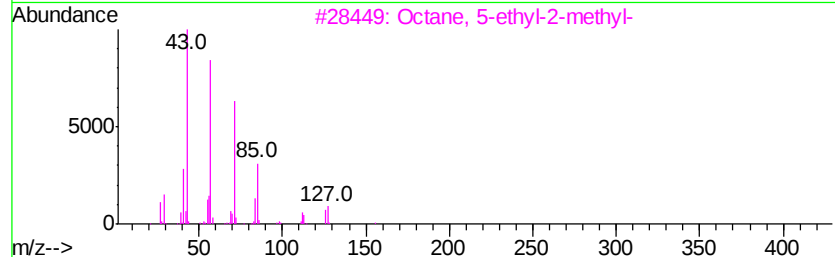
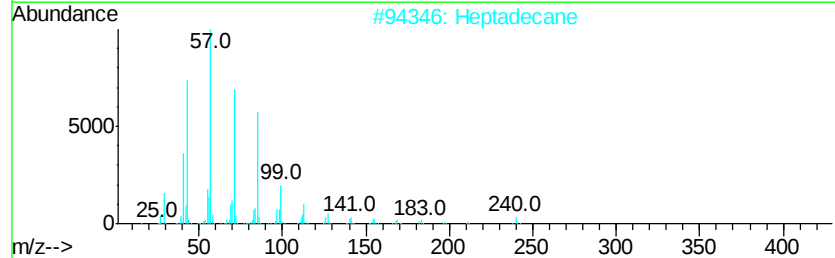
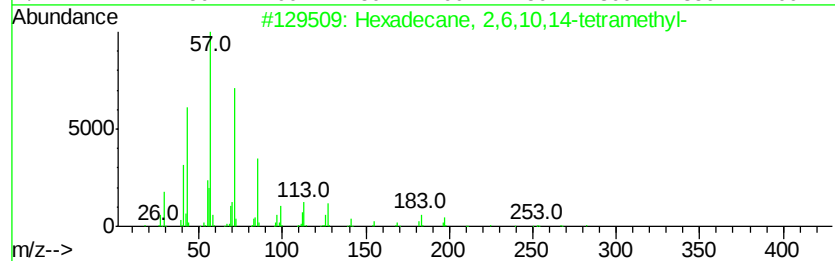
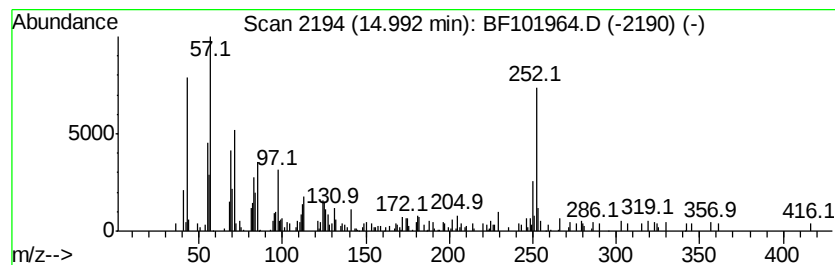
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexadecane, 2,6,10,14-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	4.01 ng	182419	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
2		Heptadecane	240	C17H36	000629-78-7	70
3		Octane, 5-ethyl-2-methyl-	156	C11H24	062016-18-6	70
4		Eicosane	282	C20H42	000112-95-8	62
5		Hexadecane	226	C16H34	000544-76-3	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
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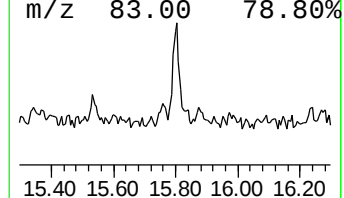
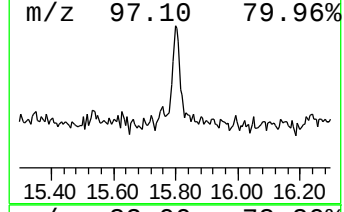
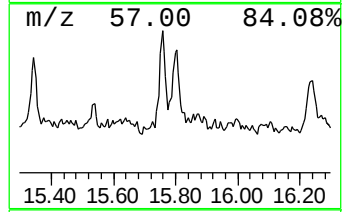
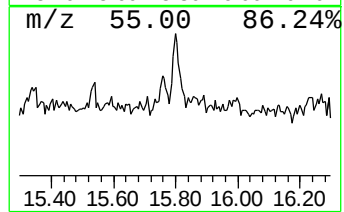
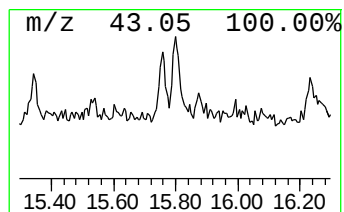
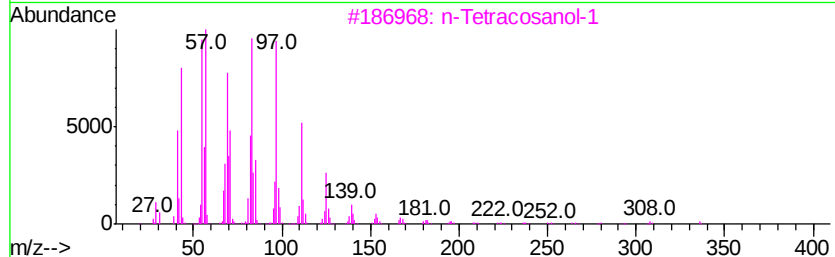
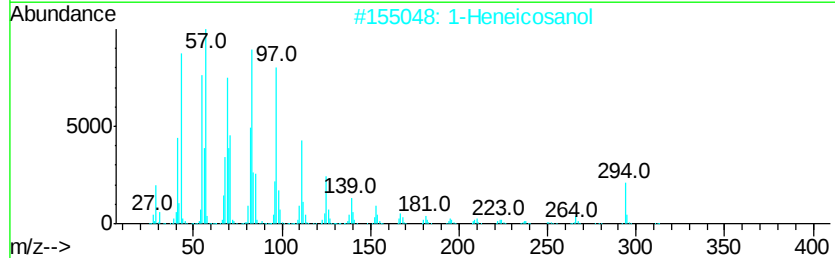
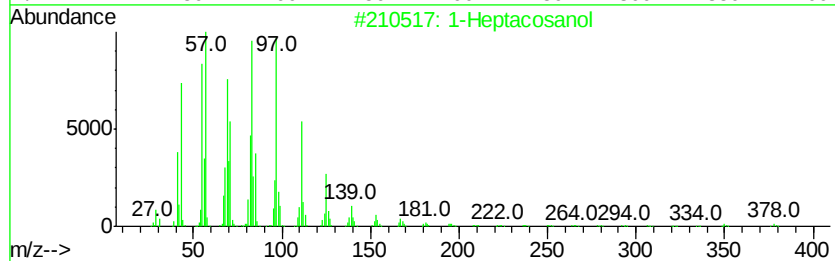
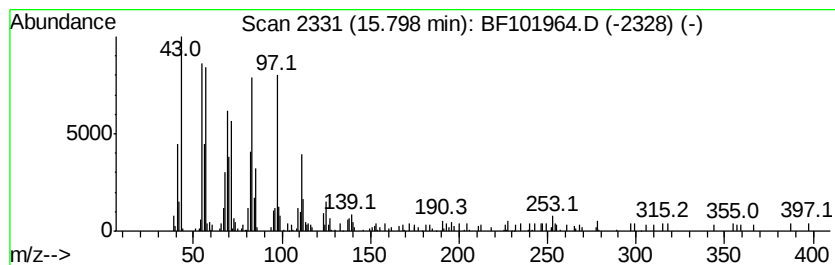
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.97 ng	180919	Perylene-d12	15.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	95
2	1-Heneicosanol	312 C21H44O	015594-90-8	94
3	n-Tetracosanol-1	354 C24H50O	000506-51-4	91
4	Behenic alcohol	326 C22H46O	000661-19-8	90
5	Octacosanol	410 C28H58O	000557-61-9	90



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 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 SP-COMP-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.95	8.1 ng		606063	1	6.73	1490600	20.0
unknown6.50	6.50	87.4 ng		6510950	1	6.73	1490600	20.0
2-Hydroxy-iso-but...	8.57	2.3 ng		203037	2	8.01	1783380	20.0
Benzophenone	10.47	5.9 ng		432512	3	9.76	1458460	20.0
n-Hexadecanoic acid	11.78	8.2 ng		514539	4	11.24	1250930	20.0
4H-Cyclopenta[def...	11.86	2.6 ng		164510	4	11.24	1250930	20.0
Octadecanoic acid	12.56	2.5 ng		191216	5	13.88	1536900	20.0
1-Heneicosanol	13.73	11.3 ng		869236	5	13.88	1536900	20.0
Heptafluorobutyri...	14.36	2.8 ng		216844	5	13.88	1536900	20.0
Hexadecane, 2,6,1...	14.99	4.0 ng		182419	6	15.30	910685	20.0
1-Heptacosanol	15.80	4.0 ng		180919	6	15.30	910685	20.0