

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100584.D
 Acq On : 15 Nov 2017 13:29
 Operator : SJ/JU
 Sample : I6436-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 153RD-63RD-ST-DRUM

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	2.193	14	18	24	rVB2	20514	33964	1.19%	0.119%
2	5.110	510	514	523	rBV	411082	559347	19.57%	1.961%
3	5.504	574	581	585	rBV	2463703	2741887	95.94%	9.615%
4	5.739	617	621	624	rBV	50623	48096	1.68%	0.169%
5	6.510	745	752	757	rBV	2509167	2858066	100.00%	10.022%
6	6.657	772	777	780	rBV	2560780	2738184	95.81%	9.602%
7	6.881	812	815	819	rBV	941336	800537	28.01%	2.807%
8	7.039	838	842	845	rVB	2270681	2058273	72.02%	7.217%
9	7.445	905	911	914	rBV	1810705	1777099	62.18%	6.231%
10	8.163	1029	1033	1036	rBV	1205332	1053370	36.86%	3.694%
11	8.716	1123	1127	1131	rBV	140606	114266	4.00%	0.401%
12	9.239	1211	1216	1219	rBV	3109424	2797929	97.90%	9.811%
13	9.627	1279	1282	1285	rBV	103292	77245	2.70%	0.271%
14	9.716	1293	1297	1303	rVB	176321	159478	5.58%	0.559%
15	9.922	1327	1332	1335	rBV	1182211	1122388	39.27%	3.936%
16	10.627	1448	1452	1456	rBV	507113	413841	14.48%	1.451%
17	10.710	1461	1466	1474	rVB	1656076	1766881	61.82%	6.196%
18	10.827	1484	1486	1489	rVB	47366	37080	1.30%	0.130%
19	10.880	1492	1495	1497	rBV	78829	62099	2.17%	0.218%
20	10.910	1497	1500	1504	rVV2	72566	88299	3.09%	0.310%
21	10.945	1504	1506	1508	rVV2	79475	64202	2.25%	0.225%
22	10.969	1508	1510	1513	rVV	41708	39222	1.37%	0.138%
23	11.016	1513	1518	1519	rVV	32715	40263	1.41%	0.141%
24	11.057	1522	1525	1529	rVV3	79592	87444	3.06%	0.307%
25	11.098	1529	1532	1534	rVV	88183	74144	2.59%	0.260%
26	11.139	1537	1539	1546	rVB2	47355	39281	1.37%	0.138%
27	11.404	1580	1584	1587	rBV	1237560	1033261	36.15%	3.623%
28	11.427	1587	1588	1591	rVB	81547	40555	1.42%	0.142%
29	11.916	1666	1671	1676	rBV2	236429	260498	9.11%	0.913%
30	12.127	1704	1707	1710	rVB	55505	44613	1.56%	0.156%
31	12.616	1786	1790	1793	rBV	159849	166418	5.82%	0.584%
32	12.704	1802	1805	1811	rBV	134711	136118	4.76%	0.477%
33	12.863	1829	1832	1839	rVB	639051	562210	19.67%	1.971%
34	12.986	1849	1853	1856	rBV	2050241	1843926	64.52%	6.466%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.868	2000	2003	2008	rBV4	73887	86750	3.04%	0.304%
36	14.010	2025	2027	2029	rBV	56904	62008	2.17%	0.217%
37	14.039	2029	2032	2035	rVV	912363	834290	29.19%	2.925%
38	14.062	2035	2036	2042	rVB	63156	50056	1.75%	0.176%
39	14.498	2107	2110	2115	rBV4	35330	46340	1.62%	0.162%
40	14.792	2156	2160	2167	rVB2	94496	140992	4.93%	0.494%
41	15.080	2205	2209	2215	rBV	49238	93039	3.26%	0.326%
42	15.145	2217	2220	2225	rVB3	38719	47550	1.66%	0.167%
43	15.445	2268	2271	2277	rBV	34397	51197	1.79%	0.180%
44	15.515	2278	2283	2291	rVB	750871	992634	34.73%	3.481%
45	15.968	2357	2360	2365	rVB5	22661	34597	1.21%	0.121%
46	16.468	2440	2445	2454	rVB2	91419	185847	6.50%	0.652%
47	17.780	2659	2668	2680	rVB4	54555	152366	5.33%	0.534%

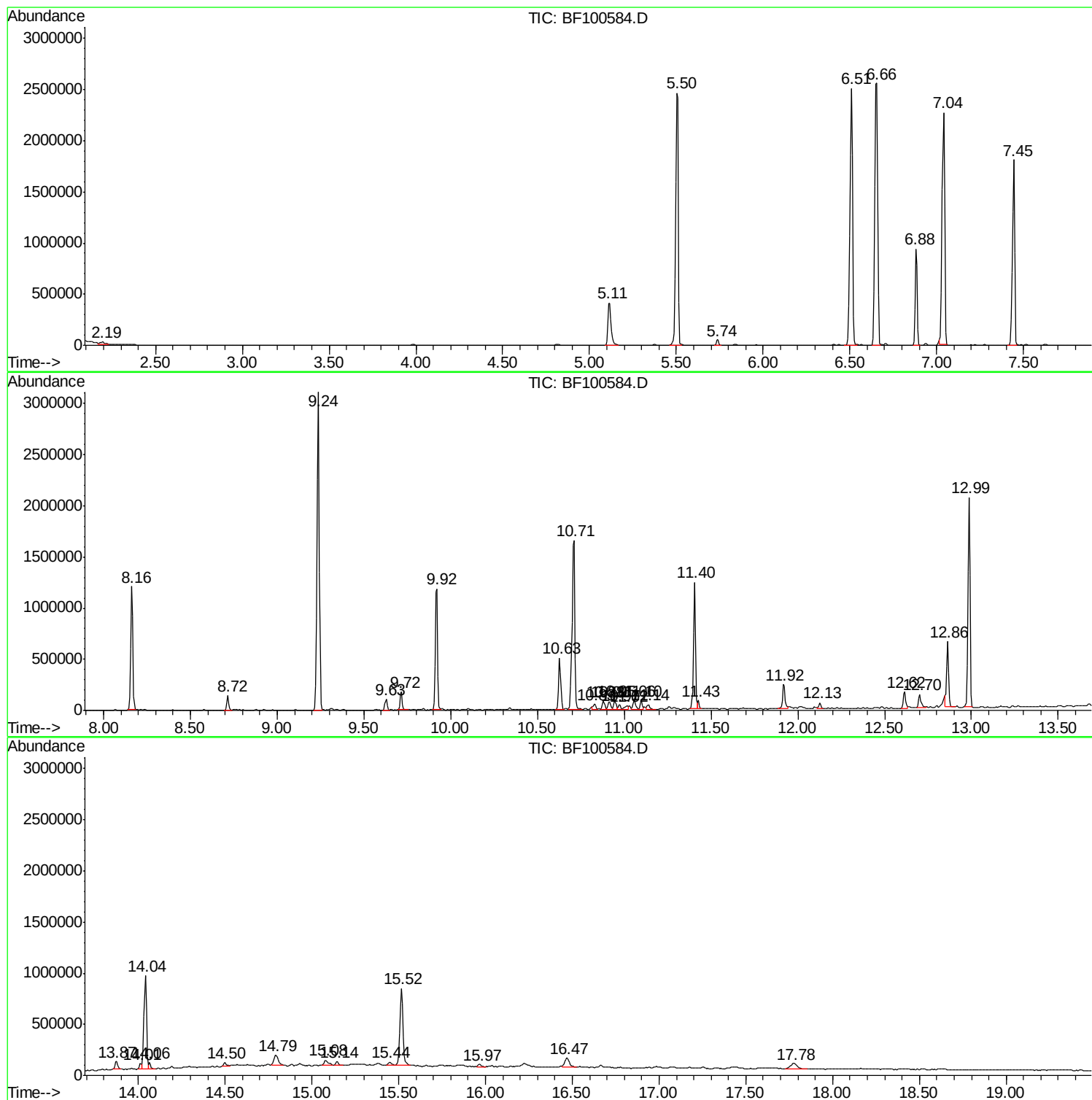
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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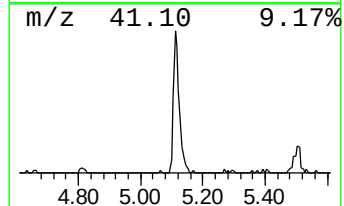
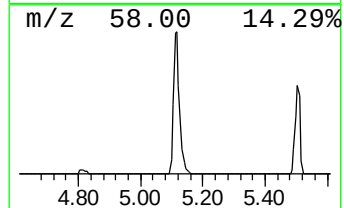
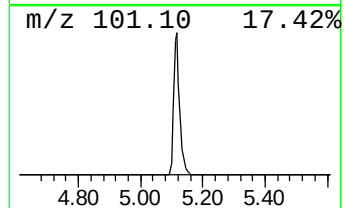
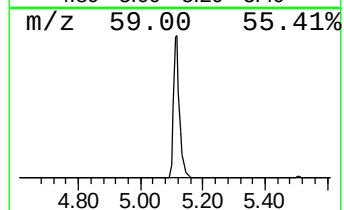
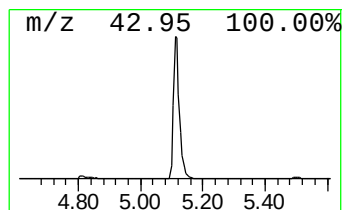
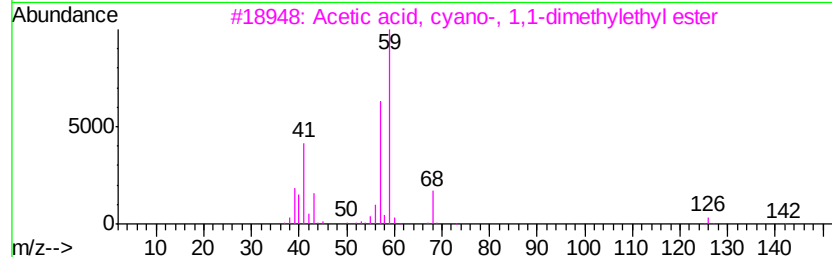
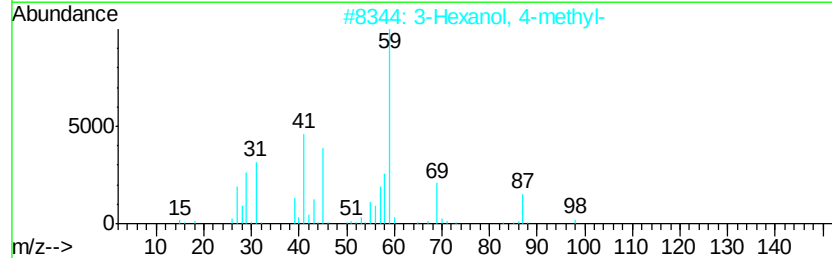
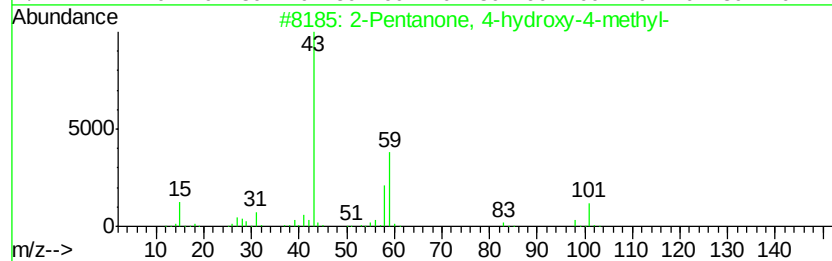
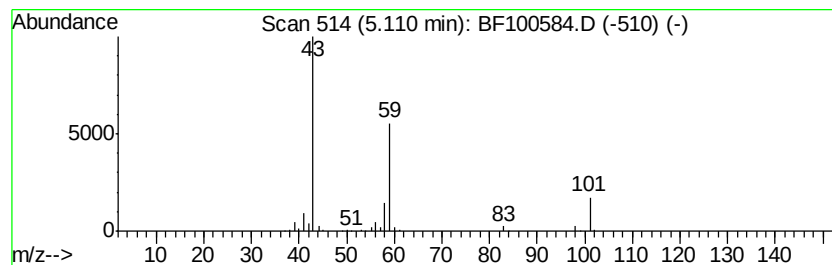
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.97 ng	559347	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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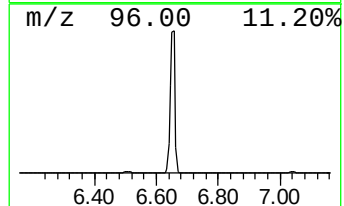
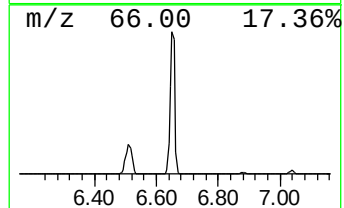
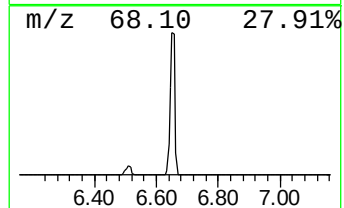
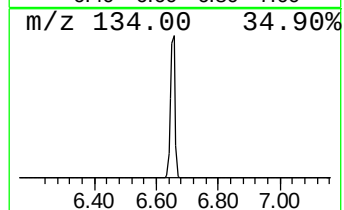
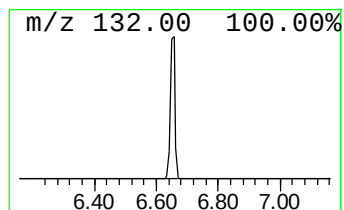
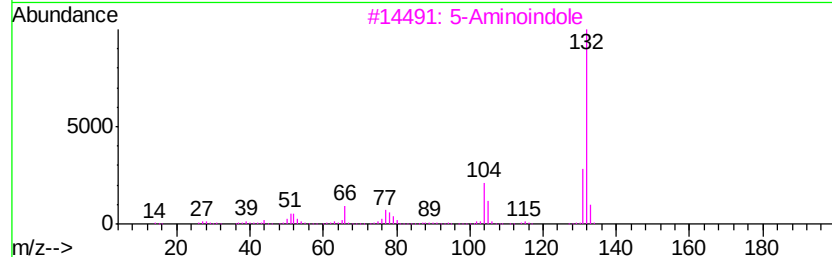
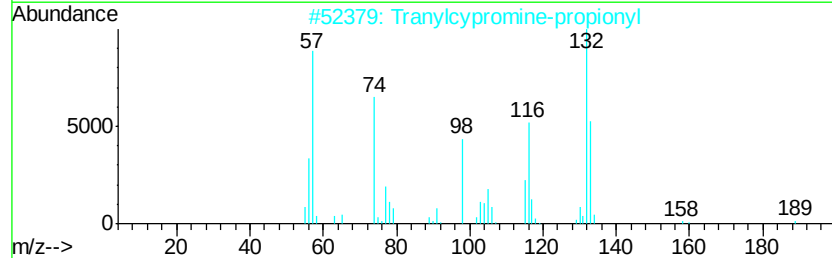
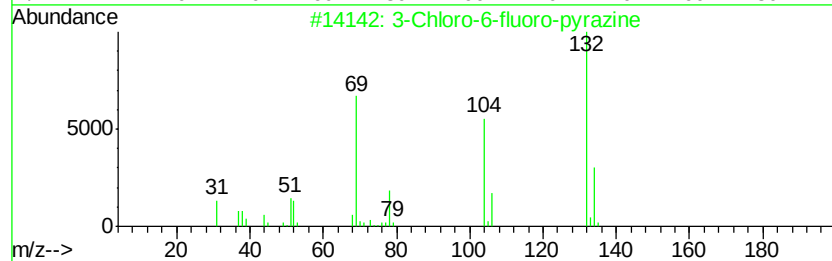
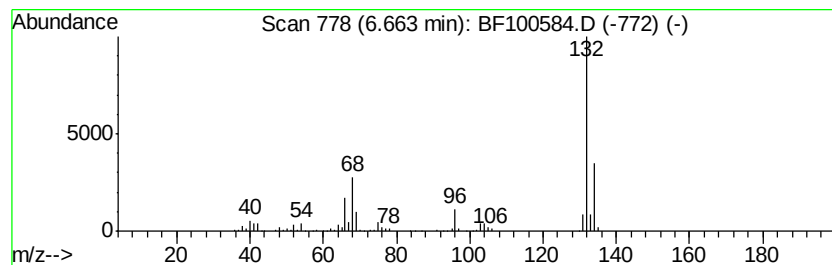
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.41 ng	2738180	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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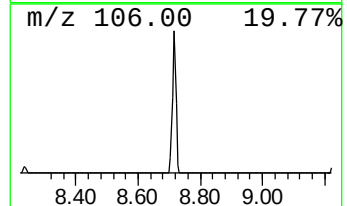
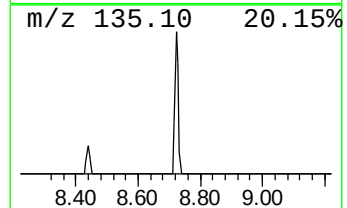
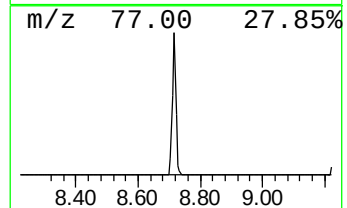
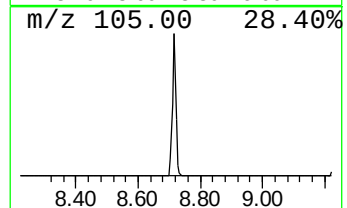
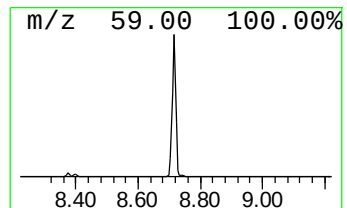
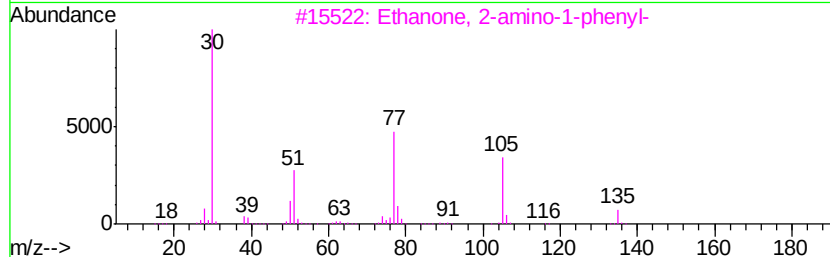
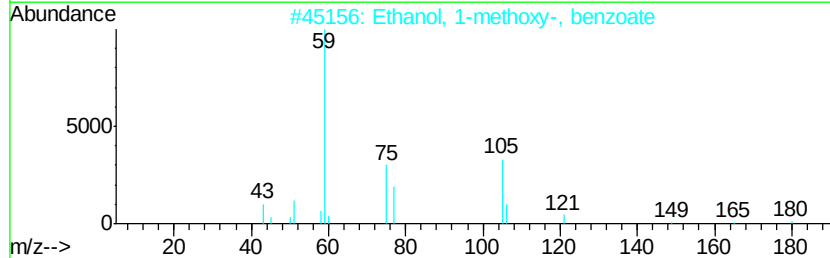
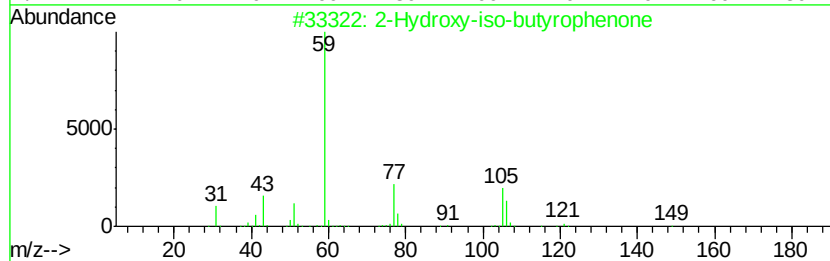
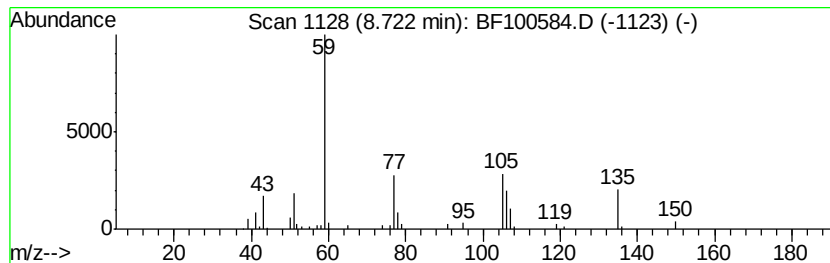
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.17 ng	114266	Napthalene-d8	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	14
4		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5		Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9



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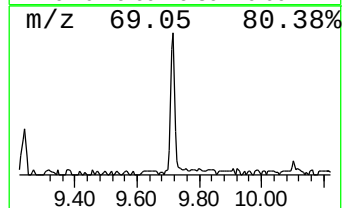
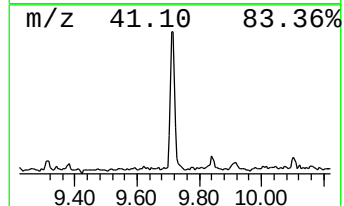
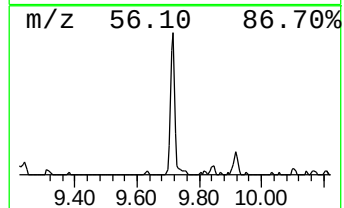
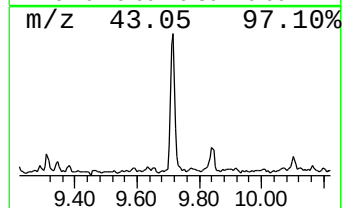
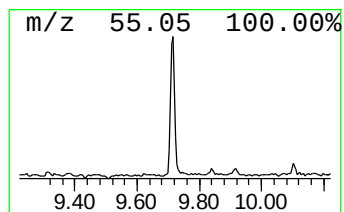
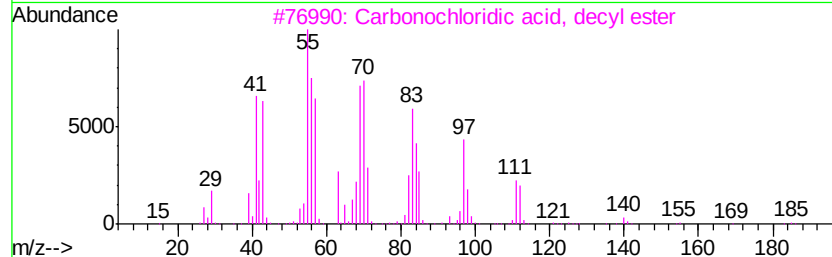
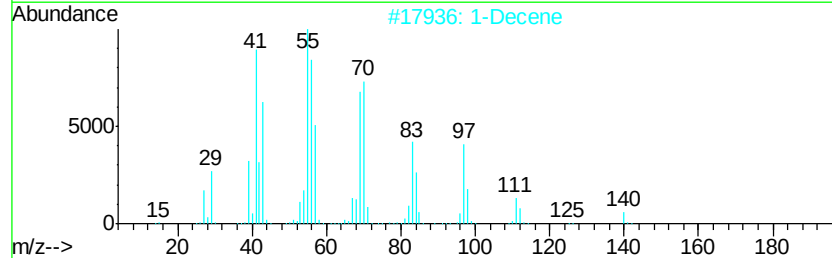
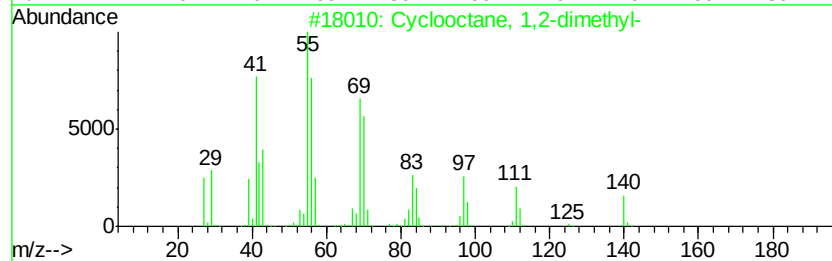
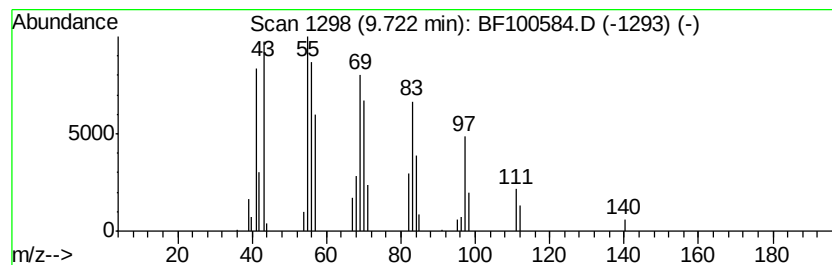
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclooctane, 1,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	2.84 ng	159478	Acenaphthene-d10	9.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclooctane, 1,2-dimethyl-	140	C10H20	013151-94-5	95
2		1-Decene	140	C10H20	000872-05-9	94
3		Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	91
4		Cyclopropane, nonyl-	168	C12H24	074663-85-7	91
5		Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	91



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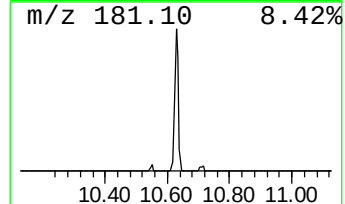
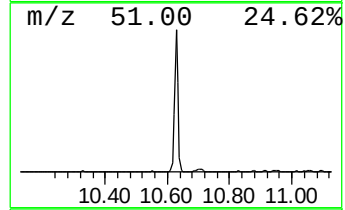
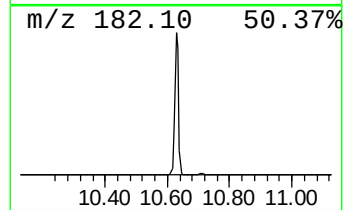
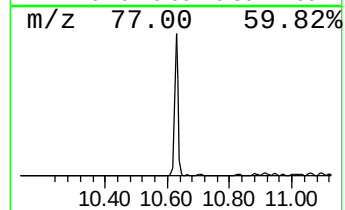
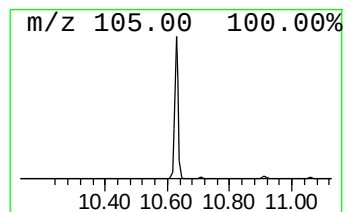
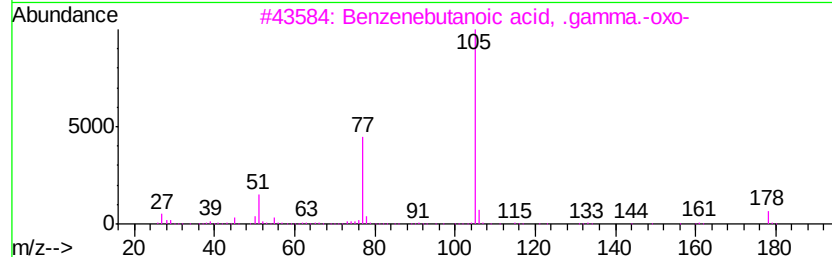
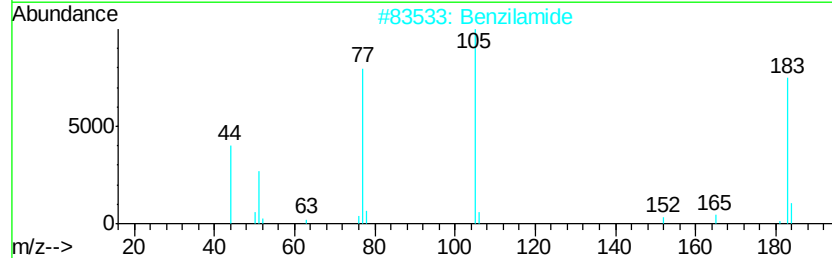
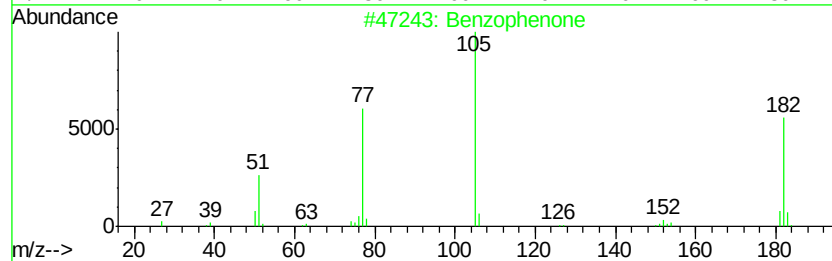
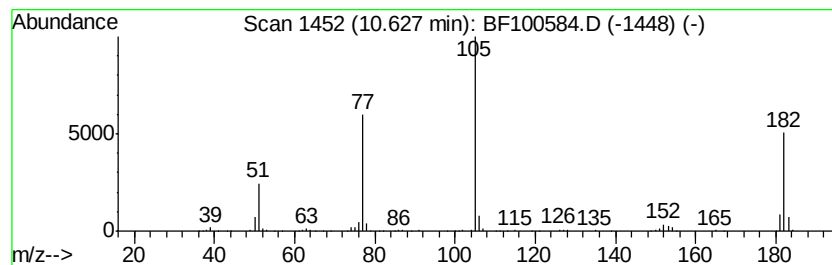
Instrument :
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ClientSampleId :
153RD-63RD-ST-DRUM

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 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.63	7.37 ng	413841	Acenaphthene-d10		9.92		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzilamide	227	C14H13NO2	004746-87-6	47
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzopinacol	366	C26H22O2	000464-72-2	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100584.D
Acq On : 15 Nov 2017 13:29
Operator : SJ/JU
Sample : I6436-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
153RD-63RD-ST-DRUM

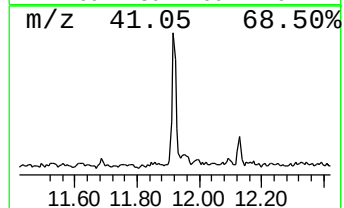
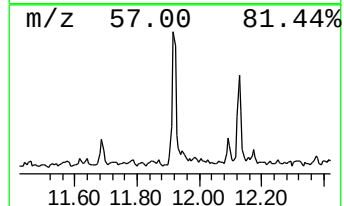
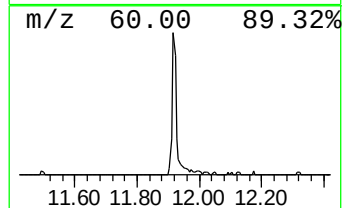
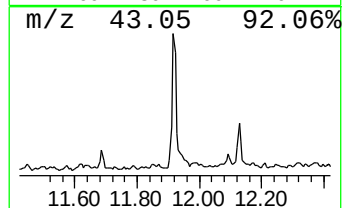
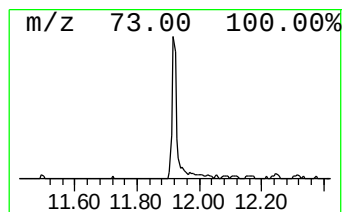
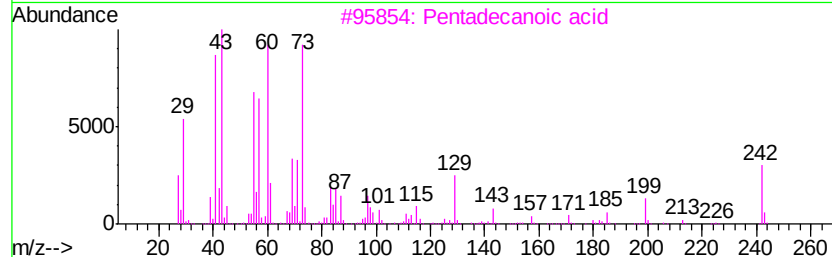
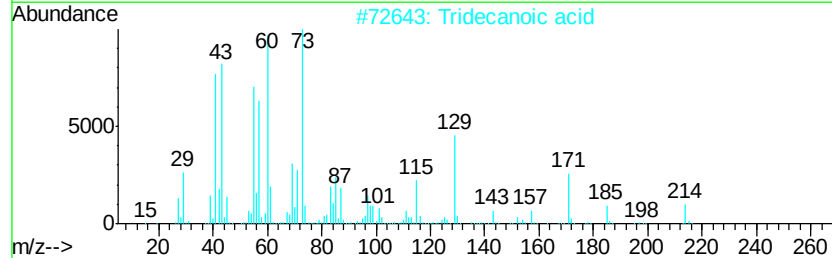
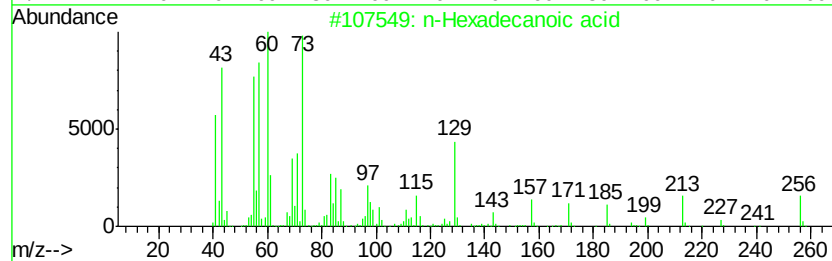
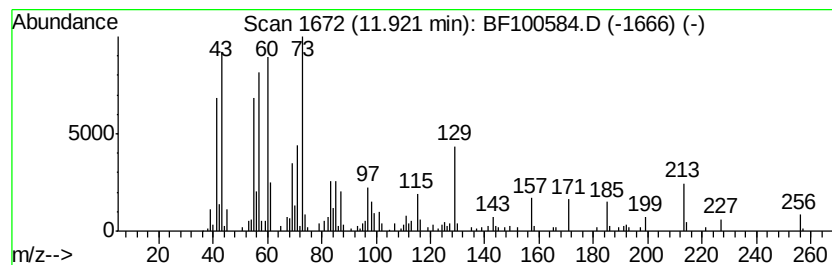
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.04 ng	260498	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
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Acq On : 15 Nov 2017 13:29
Operator : SJ/JU
Sample : I6436-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
153RD-63RD-ST-DRUM

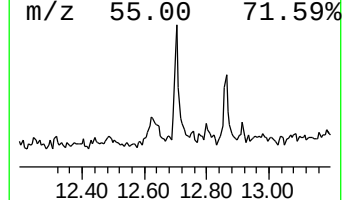
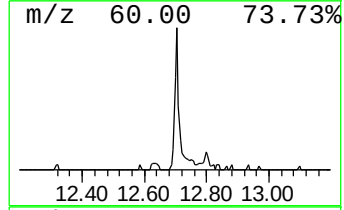
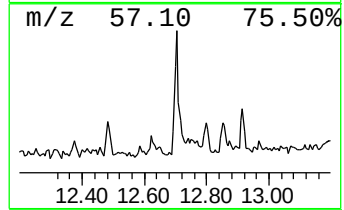
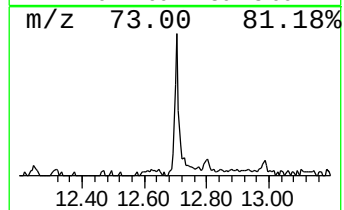
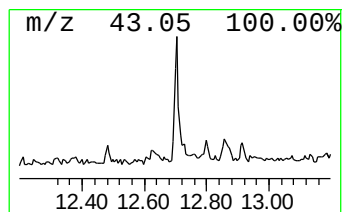
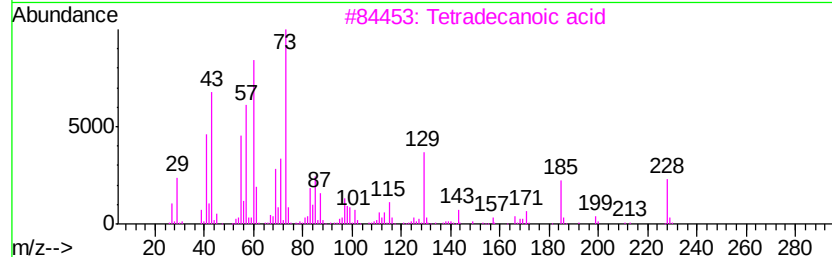
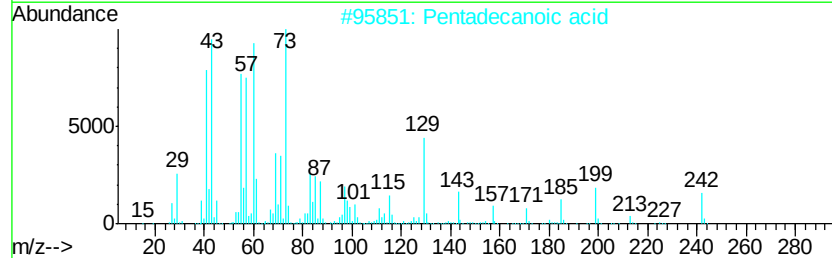
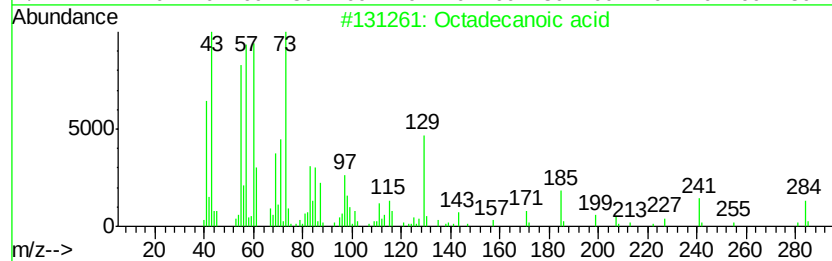
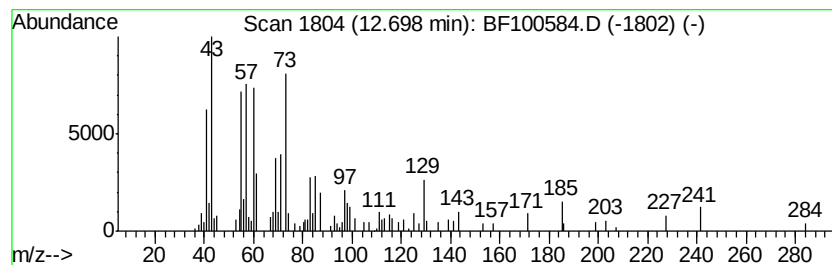
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.63 ng	136118	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5		Tridecanoic acid	214	C13H26O2	000638-53-9	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100584.D
Acq On : 15 Nov 2017 13:29
Operator : SJ/JU
Sample : I6436-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

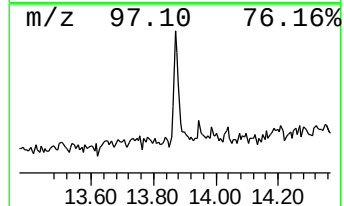
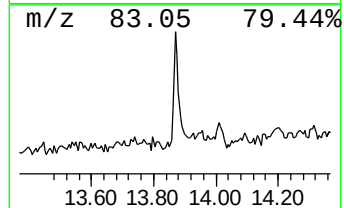
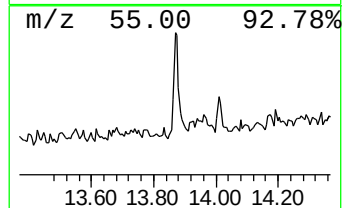
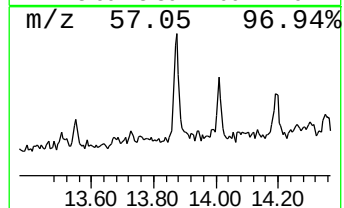
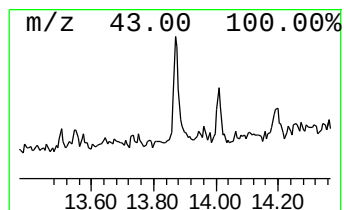
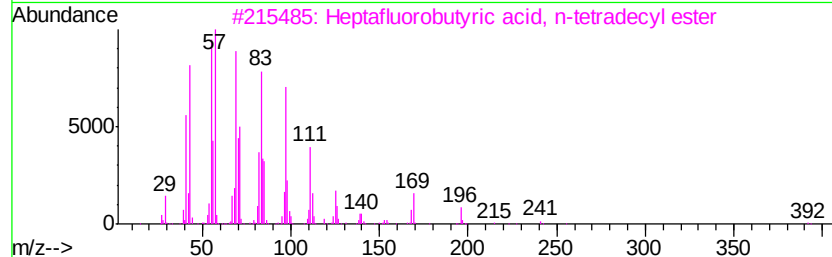
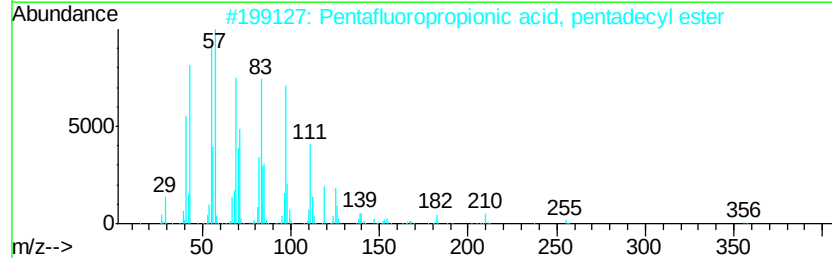
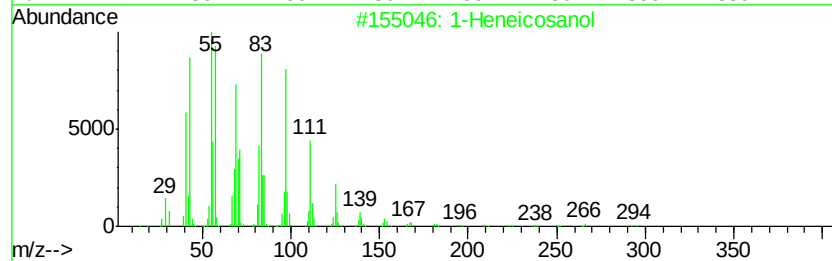
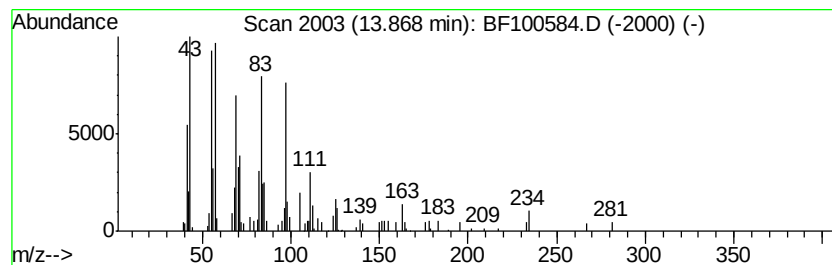
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ClientSampleId :
153RD-63RD-ST-DRUM

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 9 1-Heneicosanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.87	2.08 ng	86750	Chrysene-d12		14.04	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
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Sample : I6436-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
153RD-63RD-ST-DRUM

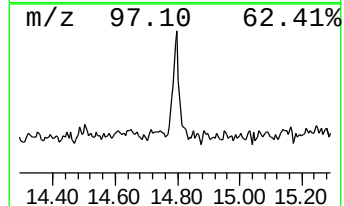
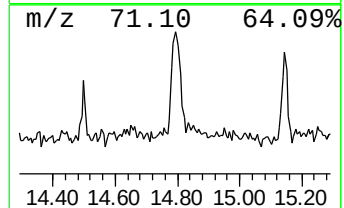
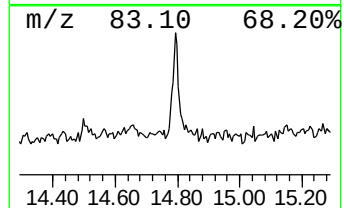
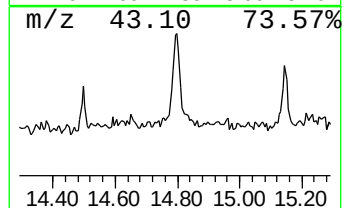
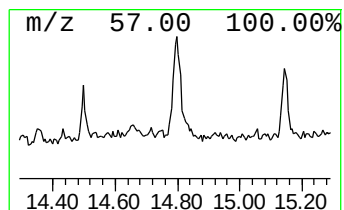
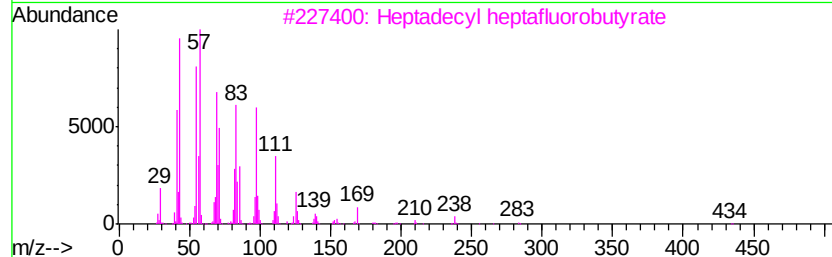
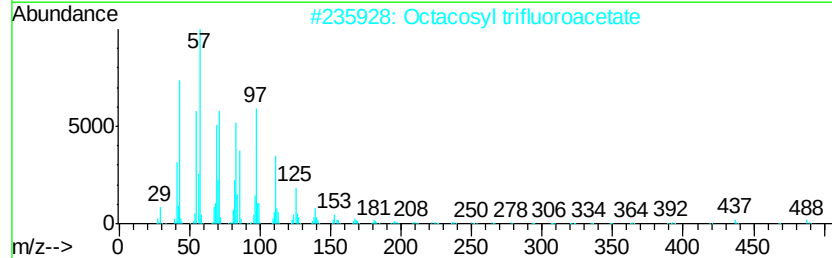
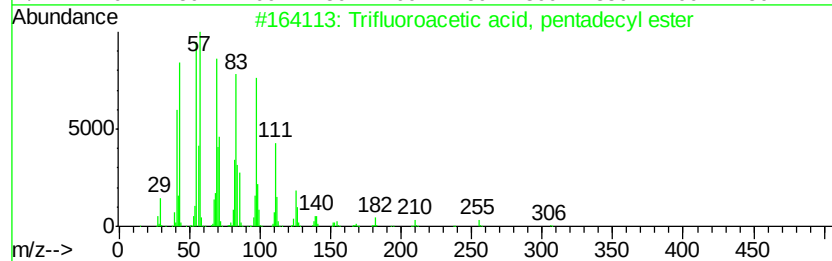
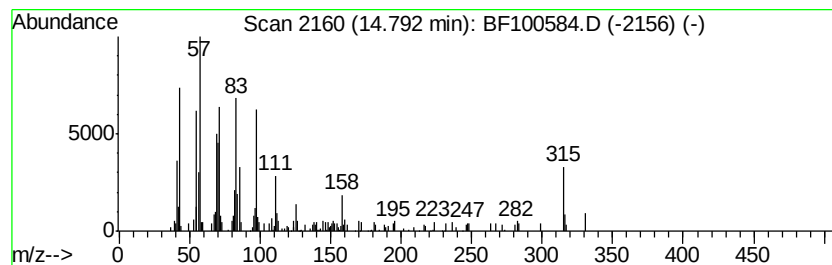
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trifluoroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.84 ng	140992	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	64
3		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62
4		1-Tricosene	322	C23H46	018835-32-0	62
5		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100584.D
Acq On : 15 Nov 2017 13:29
Operator : SJ/JU
Sample : I6436-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
153RD-63RD-ST-DRUM

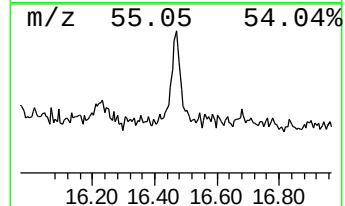
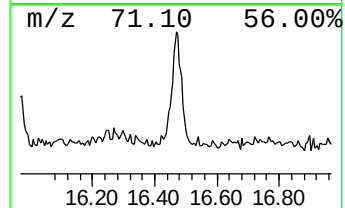
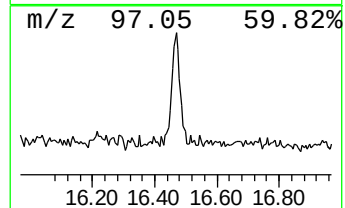
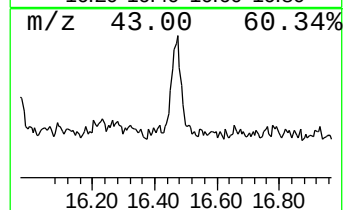
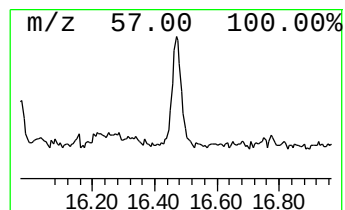
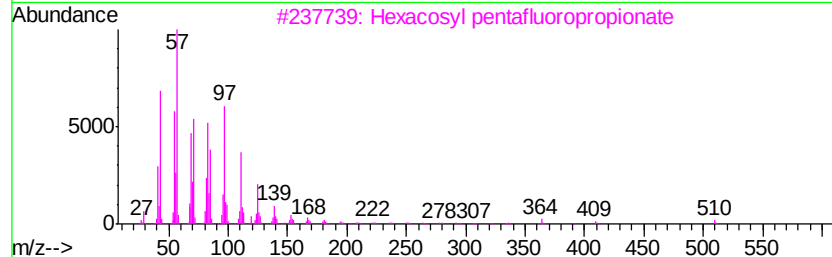
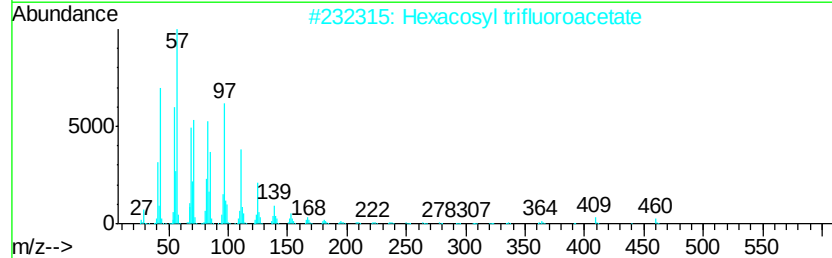
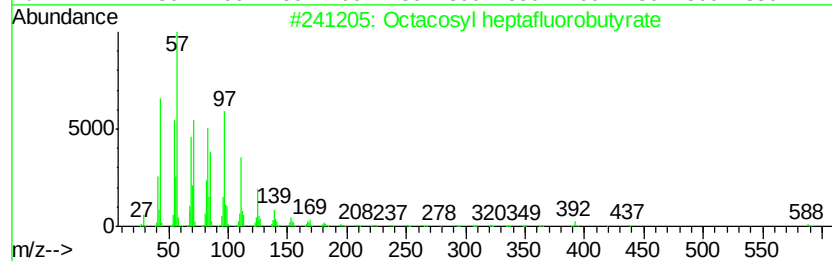
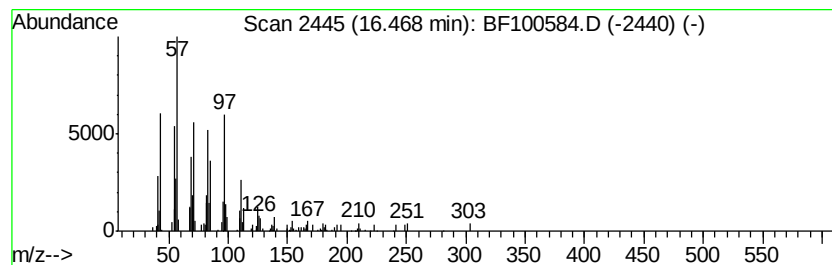
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	3.74 ng	185847	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	90
2		Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
3		Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
4		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5		Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
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Operator : SJ/JU
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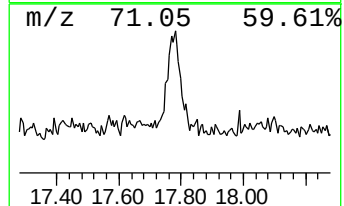
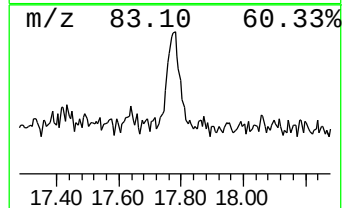
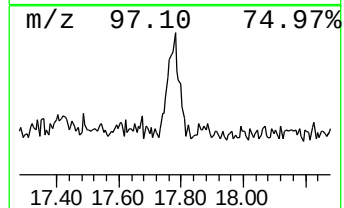
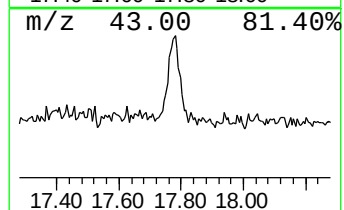
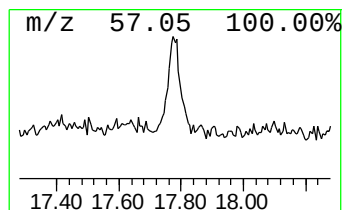
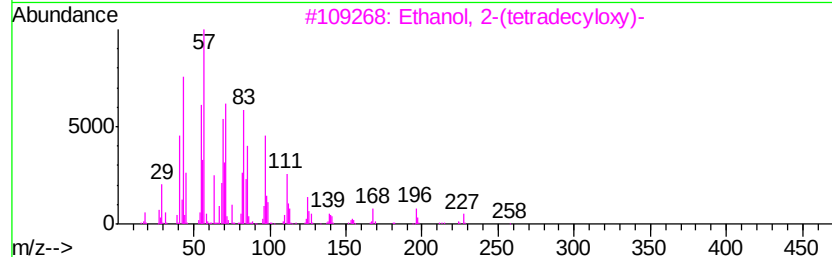
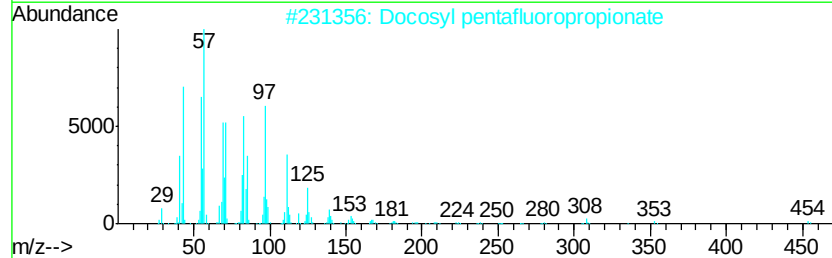
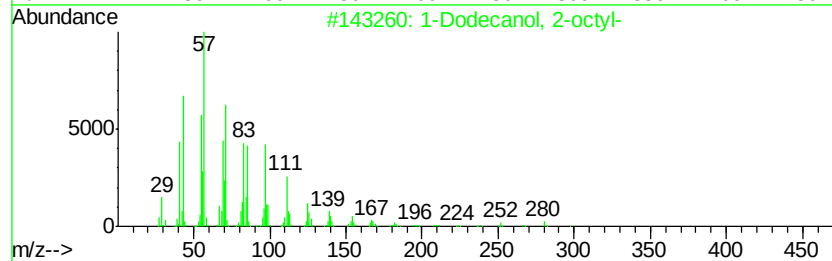
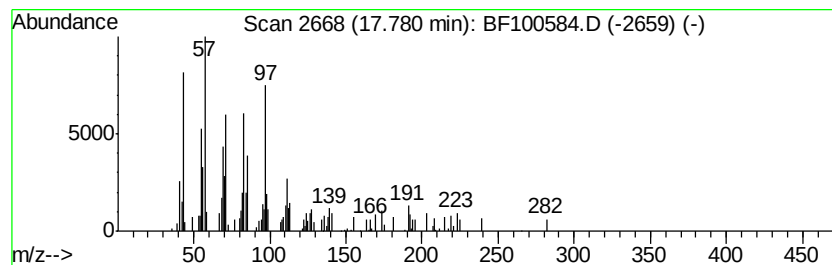
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ClientSampleId :
153RD-63RD-ST-DRUM

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 12 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.78	3.07 ng	152366	Perylene-d12	15.52
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Dodecanol, 2-octyl-	298 C20H42O	005333-42-6	64
2	Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9	64
3	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	58
4	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	53
5	1-Decanol, 2-octyl-	270 C18H38O	045235-48-1	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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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
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unknown6.66	6.66	68.4	ng	2738180	1	6.88	800537	20.0
2-Hydroxy-iso-but...	8.72	2.2	ng	114266	2	8.16	1053370	20.0
Cyclooctane, 1,2-...	9.72	2.8	ng	159478	3	9.92	1122390	20.0
Benzophenone	10.63	7.4	ng	413841	3	9.92	1122390	20.0
n-Hexadecanoic acid	11.92	5.0	ng	260498	4	11.40	1033260	20.0
Octadecanoic acid	12.70	2.6	ng	136118	4	11.40	1033260	20.0
1-Heneicosanol	13.87	2.1	ng	86750	5	14.04	834290	20.0
Trifluoroacetic a...	14.79	2.8	ng	140992	6	15.52	992634	20.0
Octacosyl heptafl...	16.47	3.7	ng	185847	6	15.52	992634	20.0
1-Dodecanol, 2-oc...	17.78	3.1	ng	152366	6	15.52	992634	20.0