

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
 Data File : BF103632.D  
 Acq On : 14 Mar 2018 5:55  
 Operator : SJ/JU  
 Sample : J1895-01  
 Misc :  
 ALS Vial : 35 Sample Multiplier: 1

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-BF022218.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

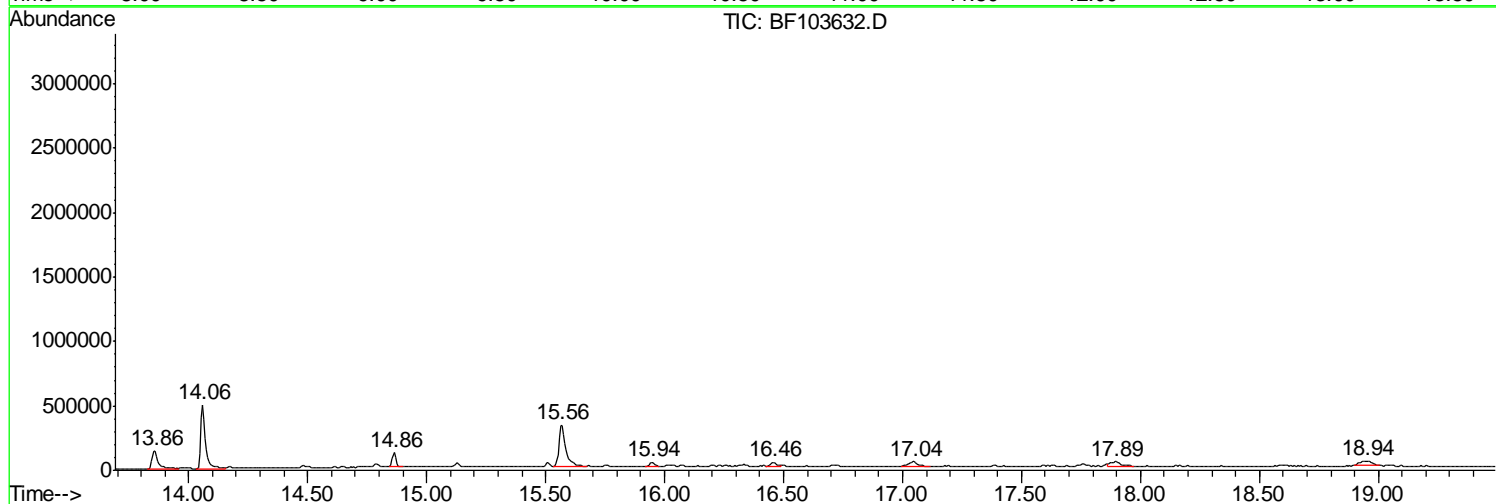
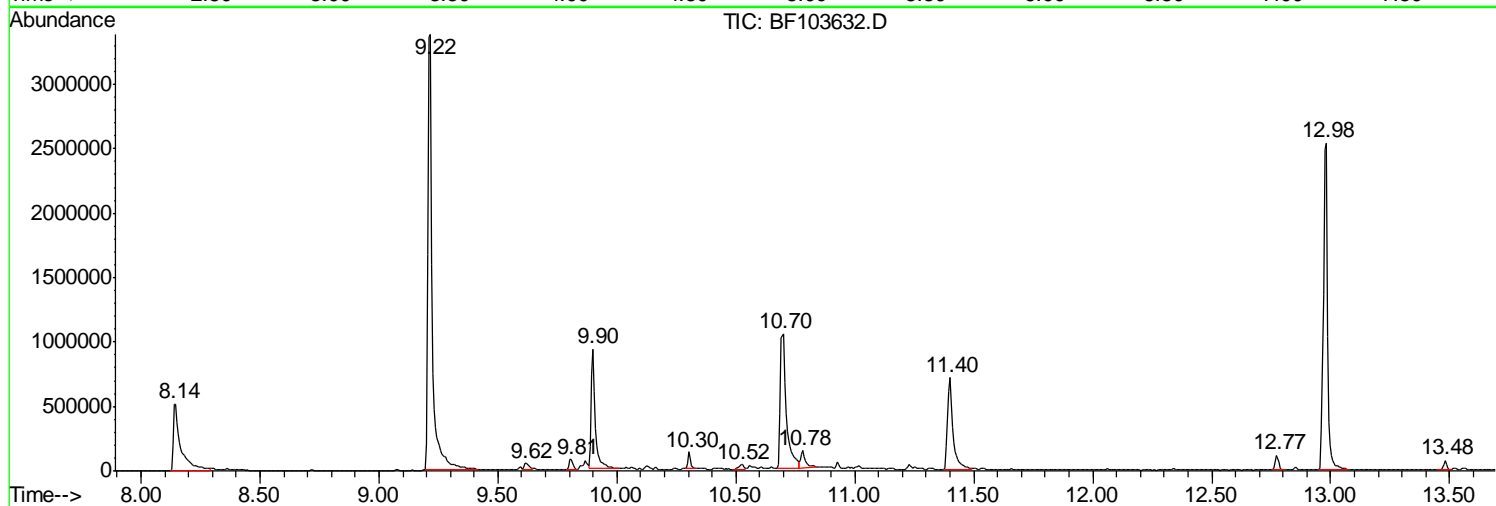
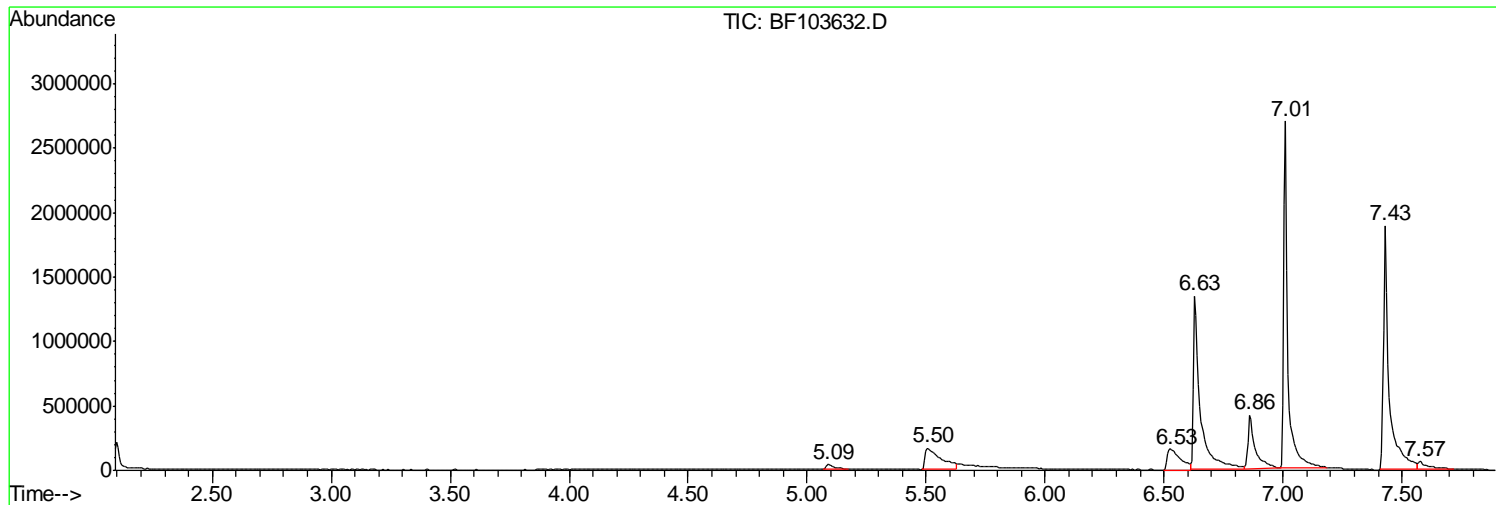
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	507	510	524	rBV	39341	99981	2.12%	0.361%
2	5.504	577	581	602	rBV2	162936	786764	16.70%	2.842%
3	6.528	750	755	769	rBV2	160094	609602	12.94%	2.202%
4	6.628	769	772	808	rVV	1342544	2772238	58.83%	10.015%
5	6.857	808	811	833	rVV	414544	864560	18.35%	3.123%
6	7.010	833	837	866	rVV	2687596	3468196	73.60%	12.530%
7	7.428	905	908	931	rBV	1891671	3143480	66.71%	11.356%
8	7.575	931	933	957	rVB	58555	165202	3.51%	0.597%
9	8.139	1026	1029	1055	rBV	513174	1150728	24.42%	4.157%
10	9.216	1208	1212	1246	rBV	3377202	4712345	100.00%	17.024%
11	9.616	1278	1280	1285	rBV	44072	52142	1.11%	0.188%
12	9.810	1309	1313	1317	rBV	77460	78664	1.67%	0.284%
13	9.898	1325	1328	1346	rVB	931670	1191850	25.29%	4.306%
14	10.304	1394	1397	1401	rBV	130208	101189	2.15%	0.366%
15	10.521	1429	1434	1437	rBV	37484	50328	1.07%	0.182%
16	10.698	1460	1464	1475	rBV	1051239	1717766	36.45%	6.206%
17	10.780	1475	1478	1487	rVB	126370	183971	3.90%	0.665%
18	11.398	1579	1583	1599	rBV	710405	1116193	23.69%	4.032%
19	12.774	1814	1817	1822	rBV	115750	96224	2.04%	0.348%
20	12.980	1847	1852	1868	rBV	2540222	3066561	65.08%	11.079%
21	13.480	1932	1937	1942	rBV	74462	67972	1.44%	0.246%
22	13.857	1996	2001	2018	rBV	143425	247383	5.25%	0.894%
23	14.057	2031	2035	2052	rBV	495164	737081	15.64%	2.663%
24	14.862	2169	2172	2178	rVB	110730	105853	2.25%	0.382%
25	15.562	2286	2291	2310	rBV	320369	655610	13.91%	2.369%
26	15.945	2352	2356	2361	rVB	33429	48704	1.03%	0.176%
27	16.456	2438	2443	2449	rBV3	30230	55457	1.18%	0.200%
28	17.045	2535	2543	2555	rVB5	35461	108330	2.30%	0.391%
29	17.892	2682	2687	2700	rVB5	33104	102270	2.17%	0.369%
30	18.944	2858	2866	2876	rVB5	36467	123505	2.62%	0.446%

Sum of corrected areas: 27680149

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Misc :  
ALS Vial : 35 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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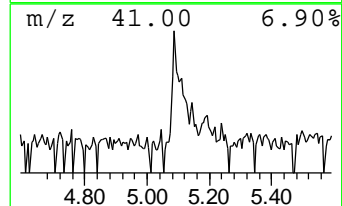
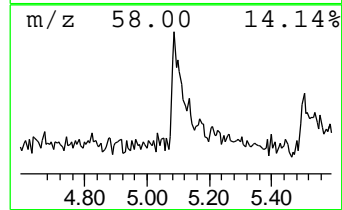
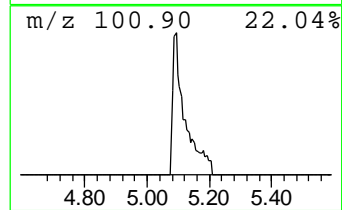
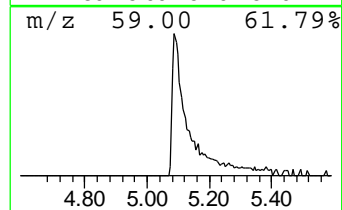
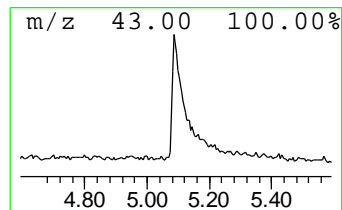
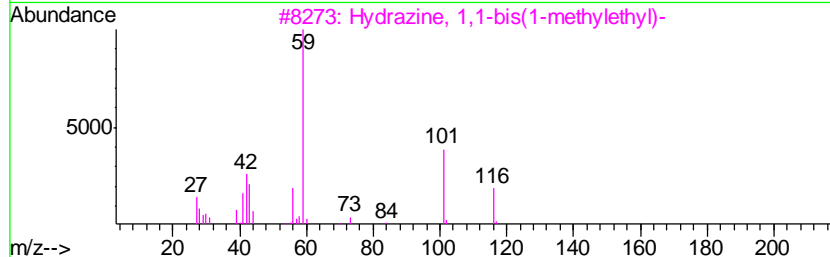
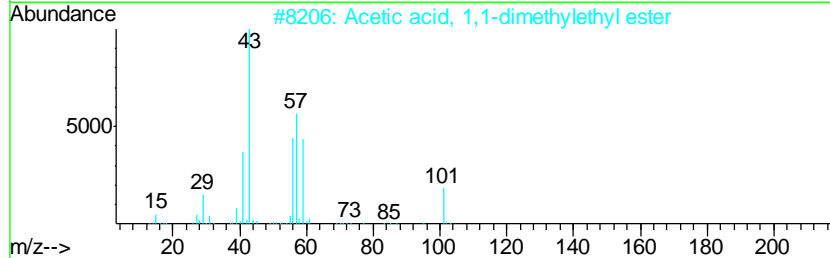
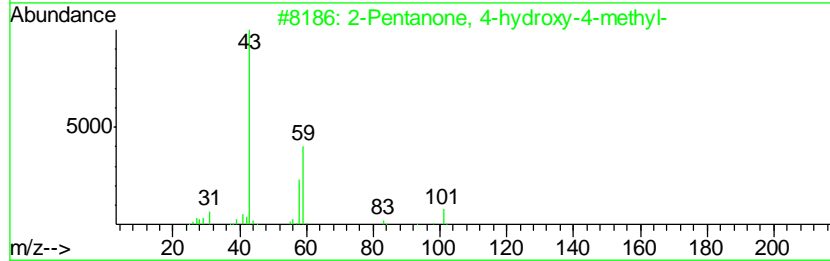
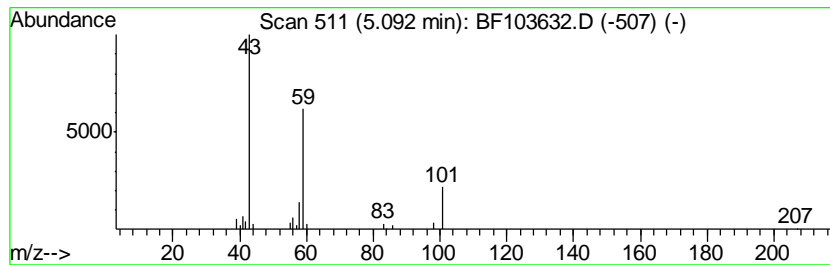
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.31 ng	99981	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	23
4		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5		Acetone	58	C3H6O	000067-64-1	9



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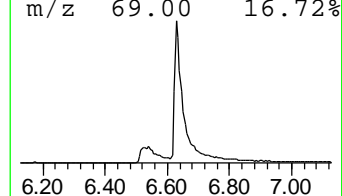
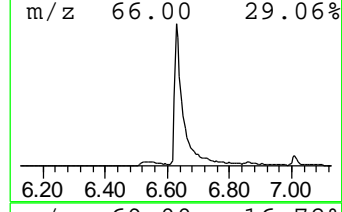
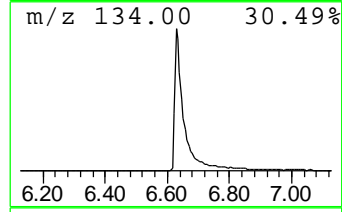
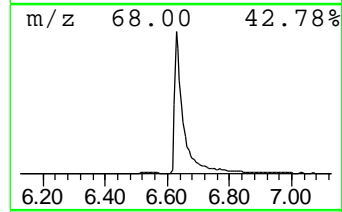
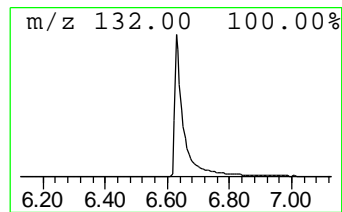
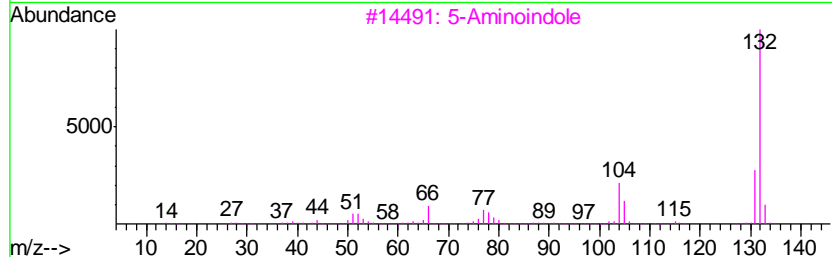
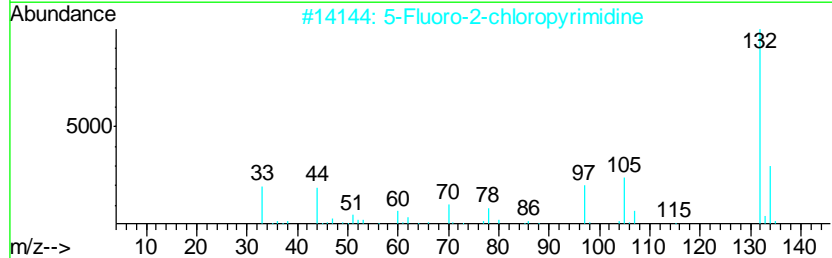
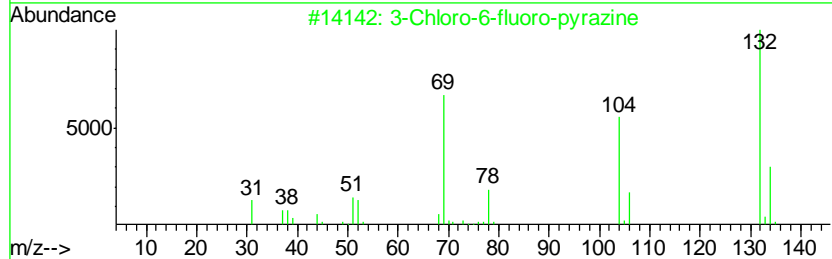
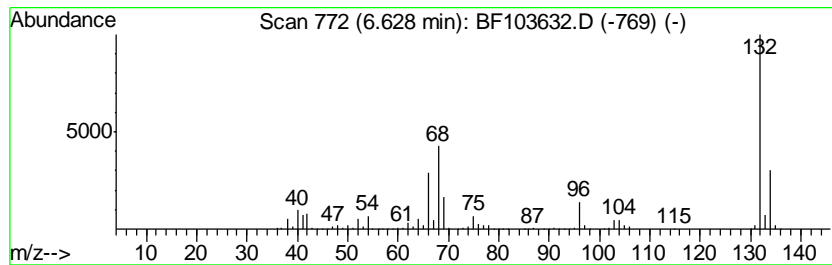
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 Peak Number 2 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	64.13 ng	2772240	1,4-Dichlorobenzene-d4	6.86

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-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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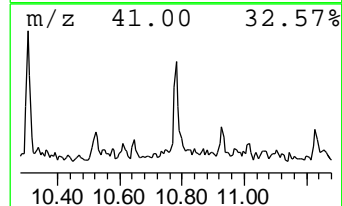
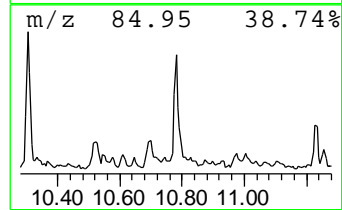
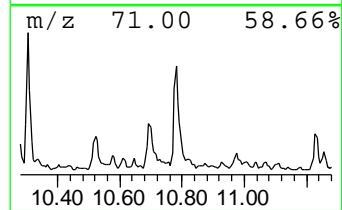
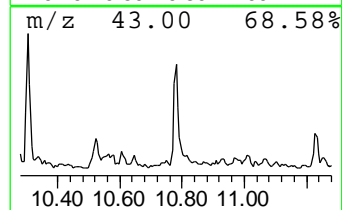
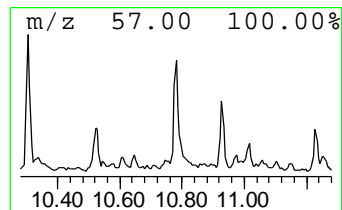
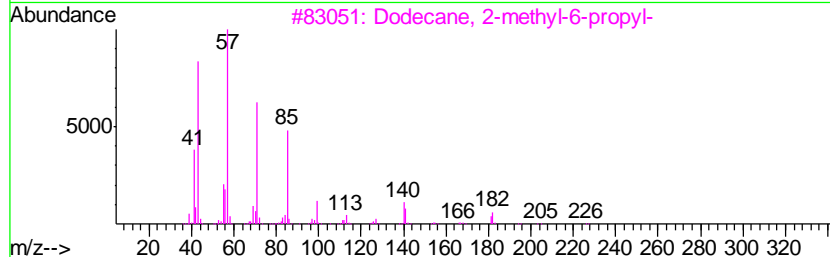
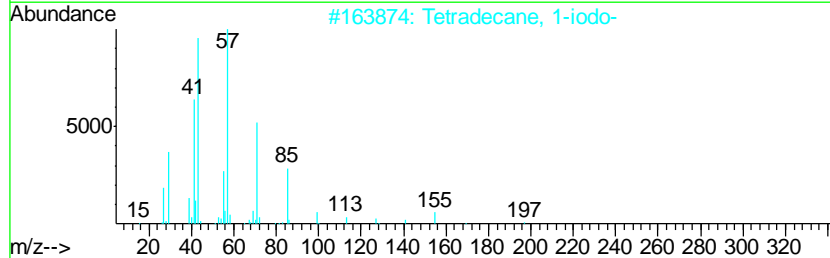
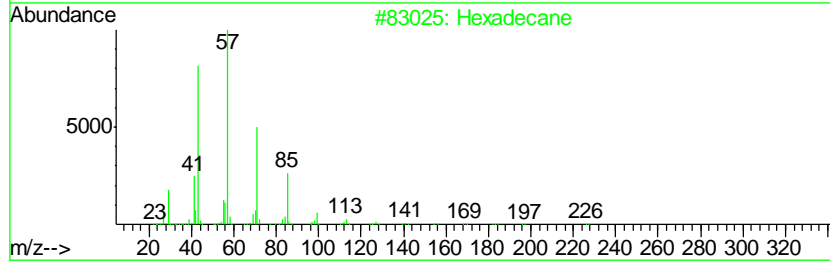
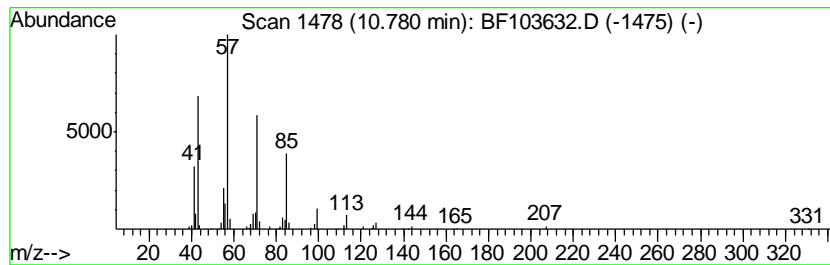
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.78	3.30 ng	183971	Phenanthrene-d10	11.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
3		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83



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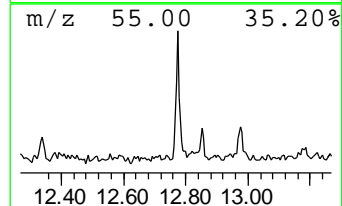
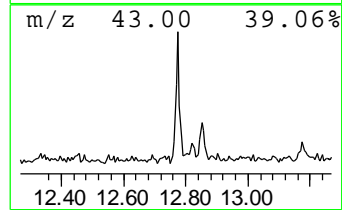
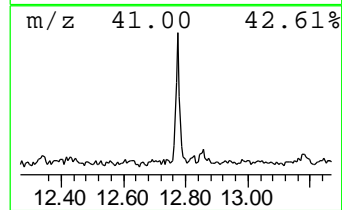
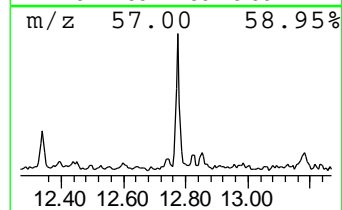
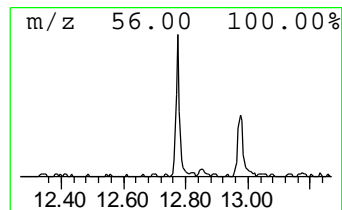
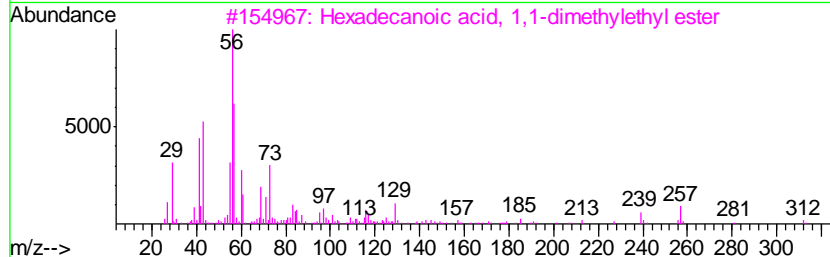
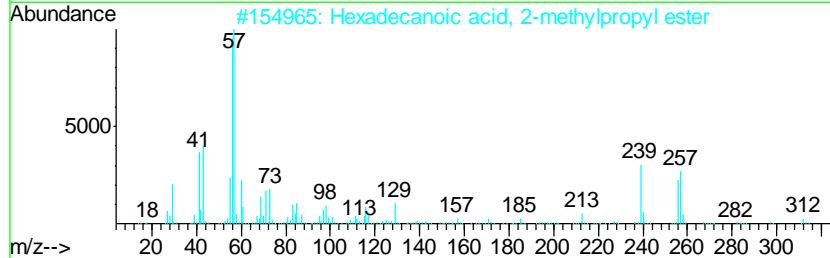
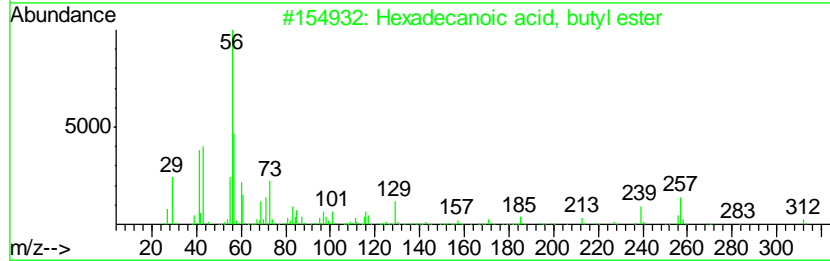
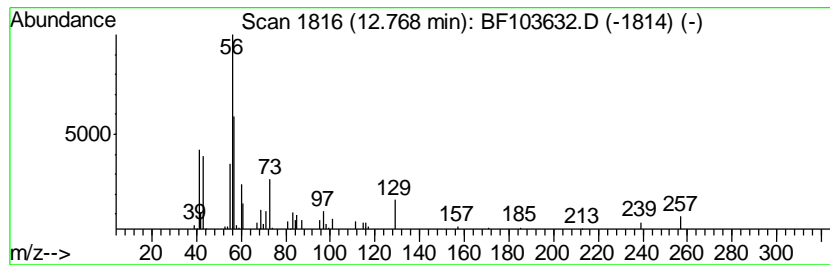
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.61 ng	96224	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
4		4-Ethyl-4-methyl-5-methylene-[1,...	142	C7H10O3	080956-52-1	35
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	32



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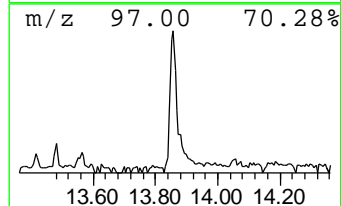
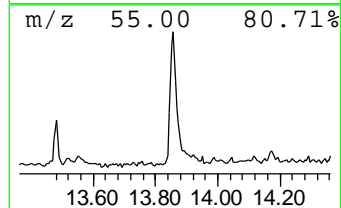
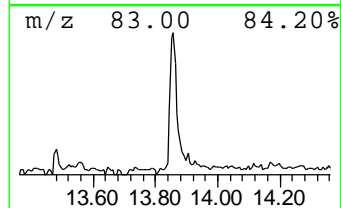
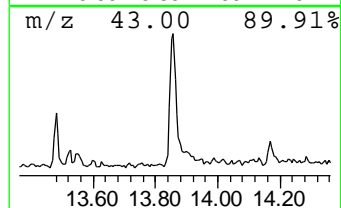
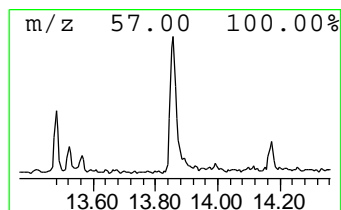
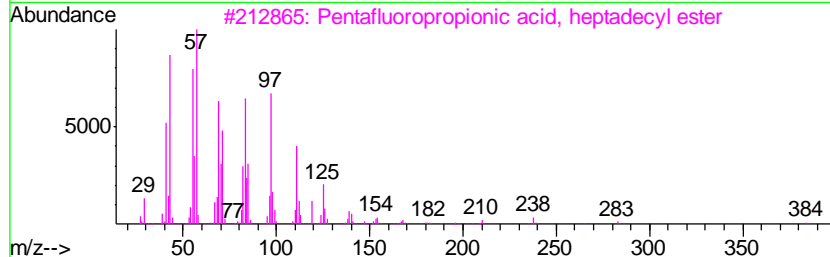
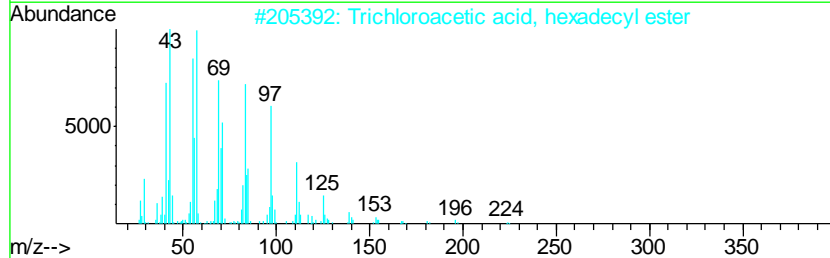
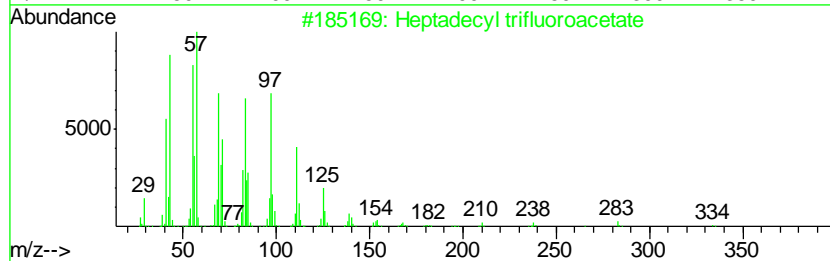
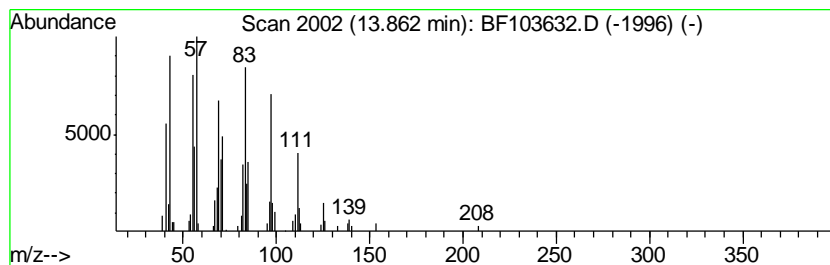
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	6.71 ng	247383	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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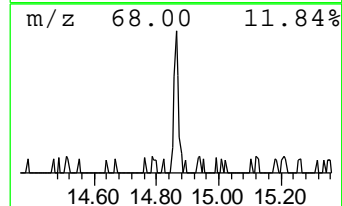
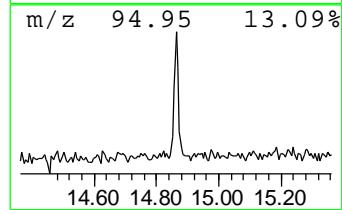
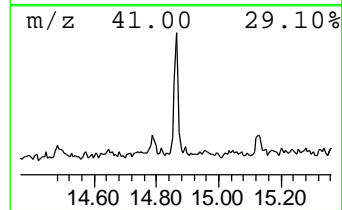
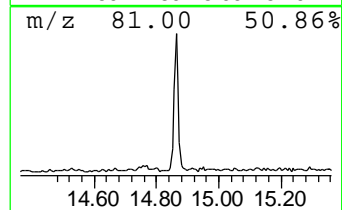
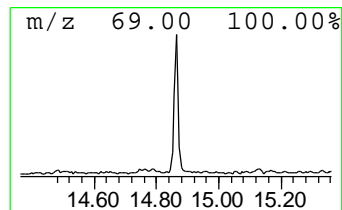
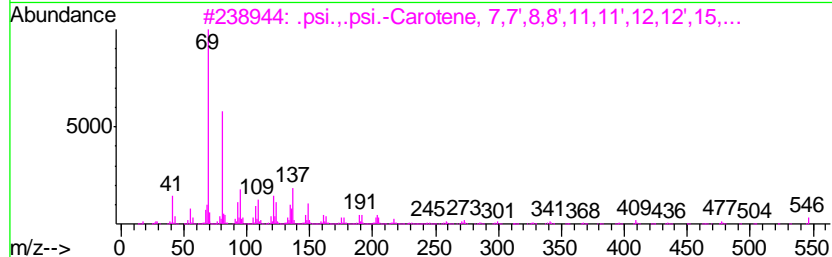
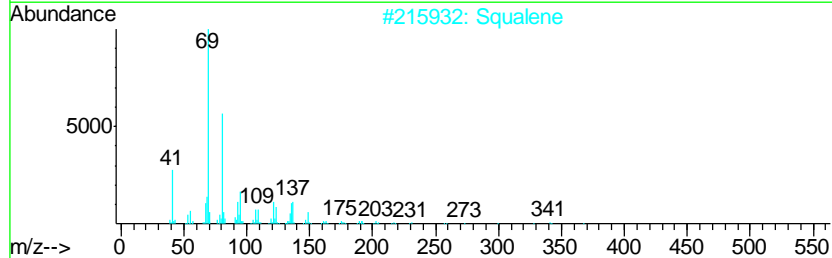
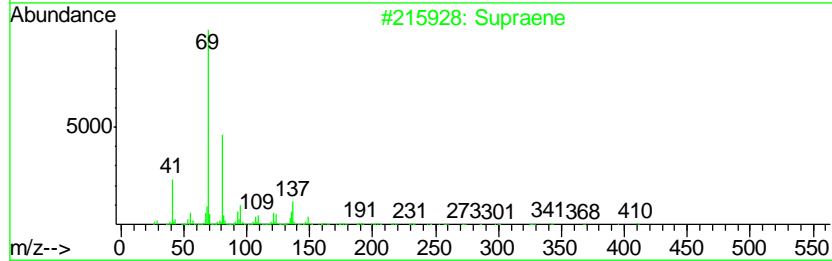
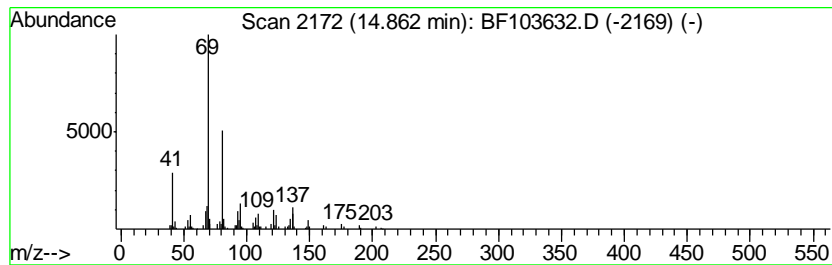
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.23 ng	105853	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		.psi...psi.-Carotene, 7,7',8,8',....	547	C40H66	000502-62-5	83
4		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
5		1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
 Data File : BF103632.D  
 Acq On : 14 Mar 2018 5:55  
 Operator : SJ/JU  
 Sample : J1895-01  
 Misc :  
 ALS Vial : 35 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

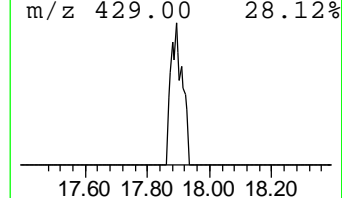
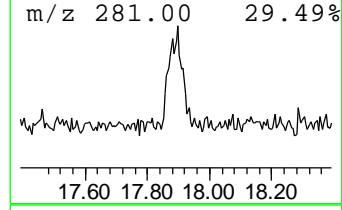
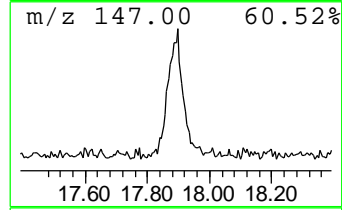
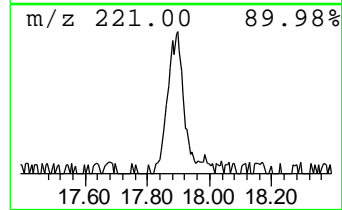
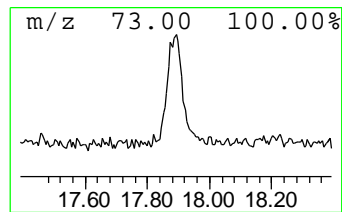
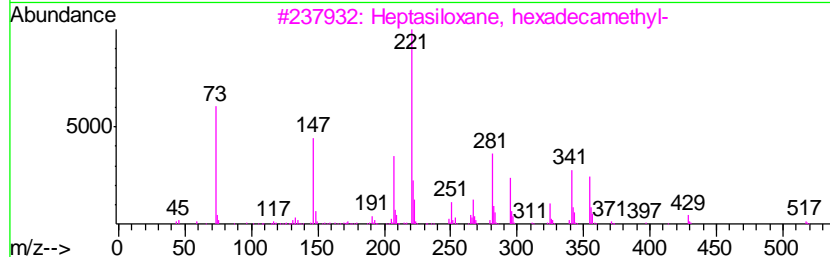
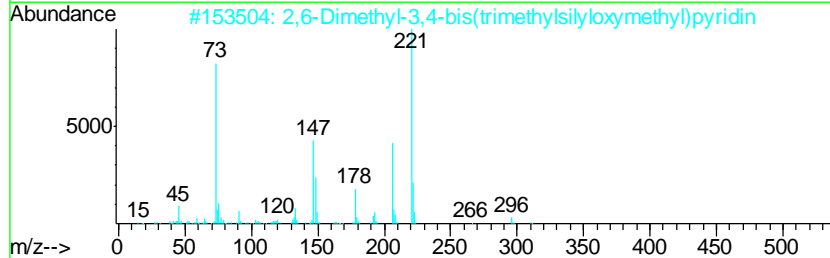
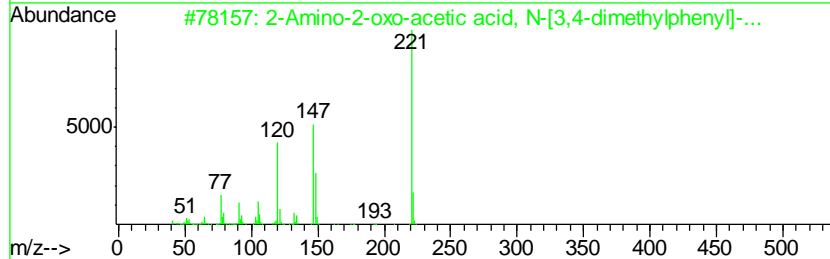
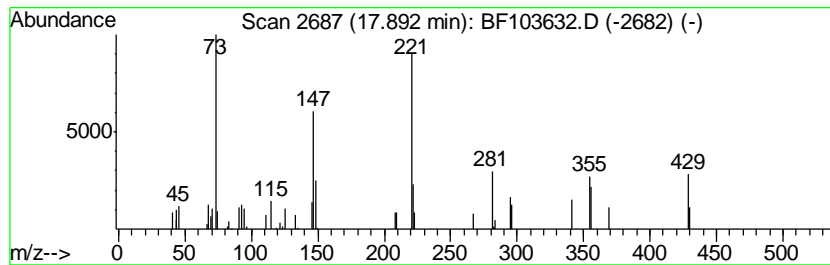
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 10 unknown17.89 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	3.12 ng	102270	Perylene-d12	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	38
2		2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	25
3		Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	17
4		2-tert-Butyl-6-methylphenol, O-t...	278	C17H30OSi	1000374-86-0	16
5		Tris(trimethylsilyl)borate	278	C9H27BO3Si3	004325-85-3	12



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF031318\  
Data File : BF103632.D  
Acq On : 14 Mar 2018 5:55  
Operator : SJ/JU  
Sample : J1895-01  
Misc :  
ALS Vial : 35 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF022218.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...	5.09	2.3	ng	99981	1	6.86	864560	20.0
unknown6.63	6.63	64.1	ng	2772240	1	6.86	864560	20.0
Hexadecane	10.78	3.3	ng	183971	4	11.40	1116190	20.0
Hexadecanoic acid...	12.77	2.6	ng	96224	5	14.06	737081	20.0
Heptadecyl triflu...	13.86	6.7	ng	247383	5	14.06	737081	20.0
Supraene	14.86	3.2	ng	105853	6	15.57	655610	20.0
unknown17.89	17.89	3.1	ng	102270	6	15.57	655610	20.0