

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
 Data File : BF102858.D
 Acq On : 8 Feb 2018 16:12
 Operator : SJ/JU
 Sample : J1469-19
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-4

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-BF020318.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	2.169	8	14	22	rVB	466422	630048	12.97%	1.579%
2	3.981	316	322	330	rVB	417124	544022	11.20%	1.363%
3	5.122	512	516	525	rVB	125356	171555	3.53%	0.430%
4	5.504	576	581	585	rBV	4427152	4732524	97.41%	11.861%
5	6.516	747	753	766	rBV	4155476	4858237	100.00%	12.176%
6	6.657	772	777	780	rBV	4635333	4533681	93.32%	11.363%
7	6.886	812	816	819	rBV	1630503	1313810	27.04%	3.293%
8	7.045	838	843	846	rBV	3549624	3306912	68.07%	8.288%
9	7.451	906	912	915	rBV	2909651	3027348	62.31%	7.587%
10	7.522	921	924	931	rBV	46959	49775	1.02%	0.125%
11	7.628	937	942	945	rVB	56465	50739	1.04%	0.127%
12	8.169	1030	1034	1037	rBV	2031411	1669710	34.37%	4.185%
13	9.245	1212	1217	1220	rBV	3977062	3805698	78.33%	9.538%
14	9.316	1226	1229	1232	rVB	107520	80445	1.66%	0.202%
15	9.633	1279	1283	1286	rBV	435807	371895	7.65%	0.932%
16	9.845	1311	1319	1323	rBV	253521	233075	4.80%	0.584%
17	9.927	1329	1333	1341	rVB	1666965	1591657	32.76%	3.989%
18	10.169	1371	1374	1378	rBV2	51031	51145	1.05%	0.128%
19	10.345	1402	1404	1407	rVB	269042	203718	4.19%	0.511%
20	10.569	1437	1442	1444	rBV	65109	79741	1.64%	0.200%
21	10.716	1463	1467	1477	rVB	1869112	1928069	39.69%	4.832%
22	10.821	1481	1485	1493	rVB	285622	336267	6.92%	0.843%
23	11.269	1558	1561	1563	rBV	106132	81908	1.69%	0.205%
24	11.416	1582	1586	1589	rBV	1292254	1235583	25.43%	3.097%
25	11.927	1670	1673	1677	rBV3	56951	62169	1.28%	0.156%
26	12.886	1833	1836	1839	rVB2	69204	56483	1.16%	0.142%
27	12.998	1851	1855	1858	rBV	2318134	2180504	44.88%	5.465%
28	13.468	1931	1935	1941	rBV	121494	129808	2.67%	0.325%
29	13.880	2002	2005	2012	rBV	248014	267336	5.50%	0.670%
30	14.051	2030	2034	2038	rBV	1070508	1078605	22.20%	2.703%
31	15.162	2220	2223	2227	rVB2	80376	92437	1.90%	0.232%
32	15.539	2282	2287	2296	rVB2	708573	1003976	20.67%	2.516%
33	15.998	2362	2365	2370	rVB	98660	141355	2.91%	0.354%

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ClientSampleId :
3N-4

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

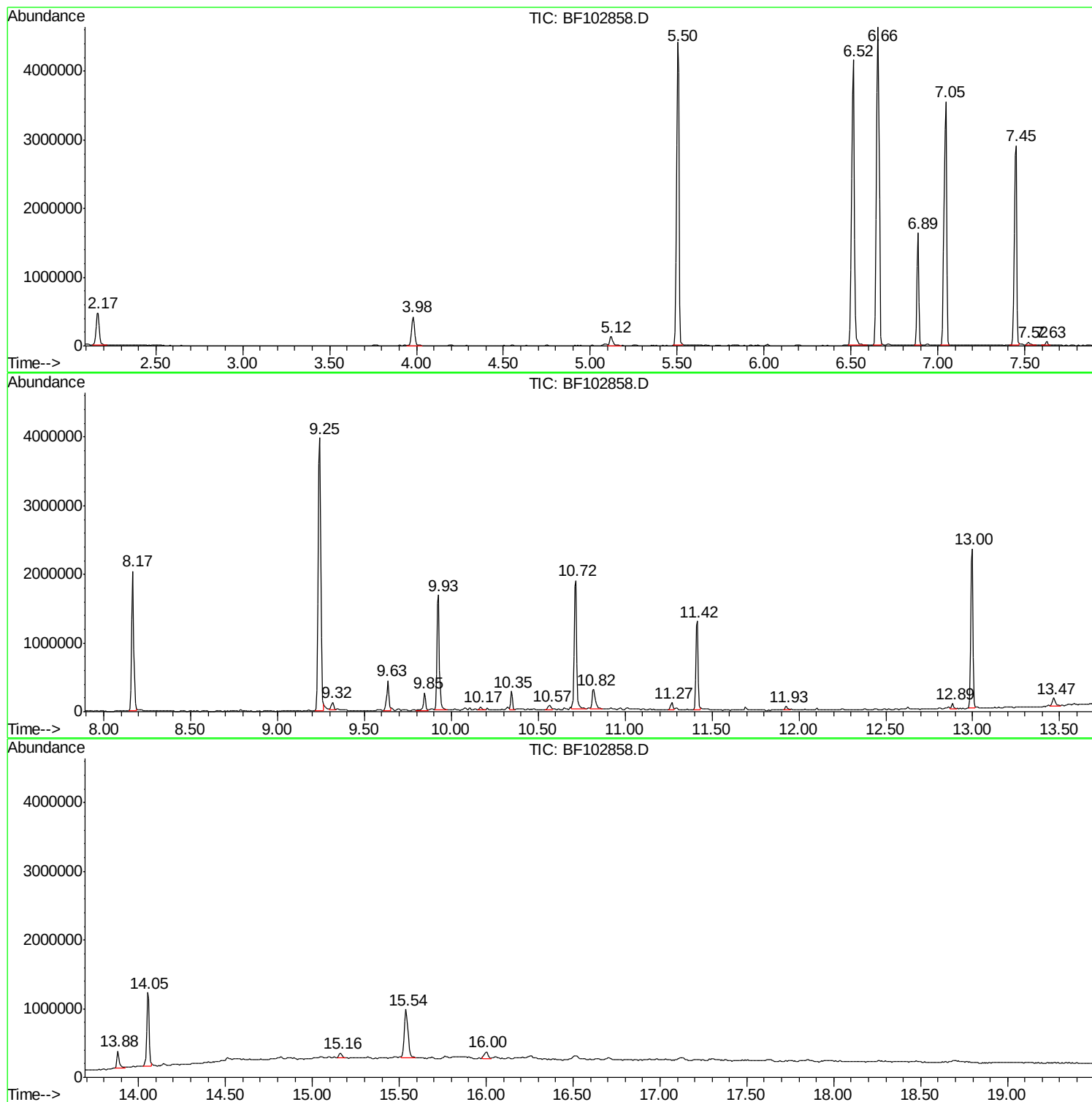
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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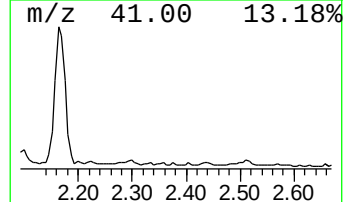
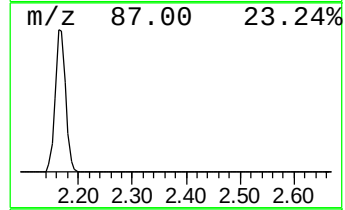
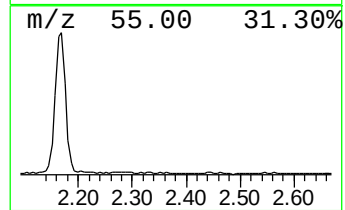
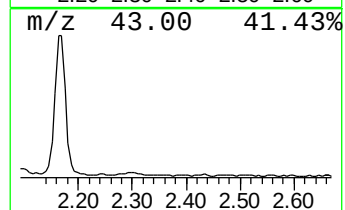
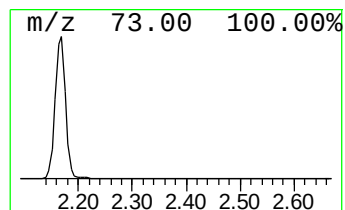
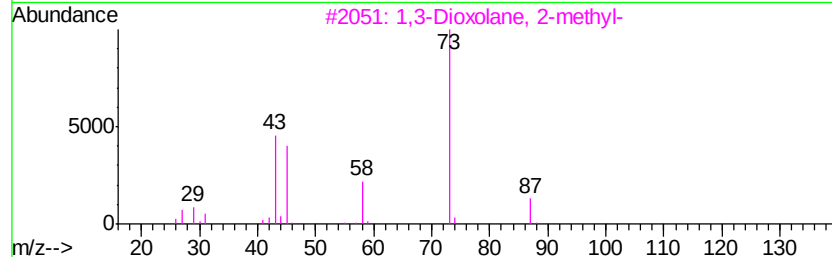
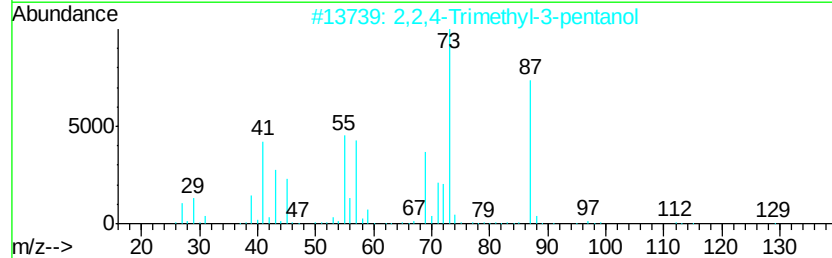
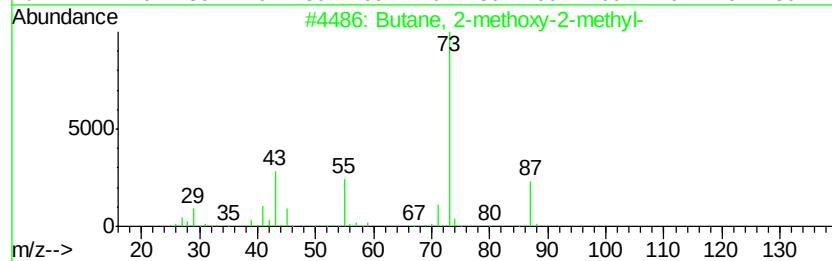
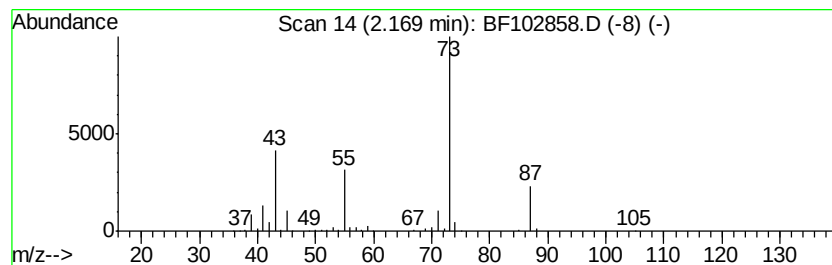
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	9.59 ng	630048	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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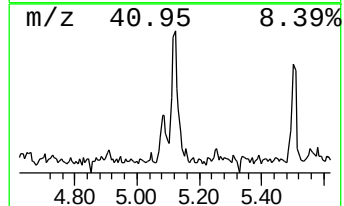
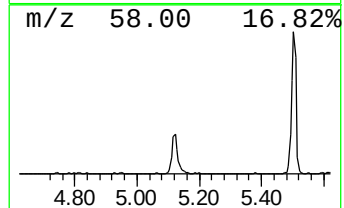
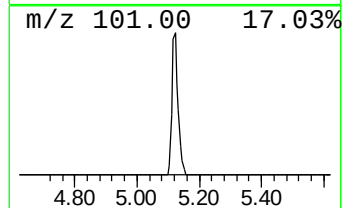
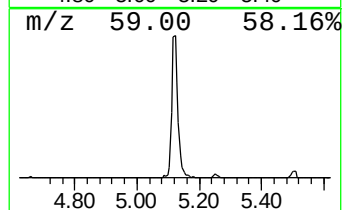
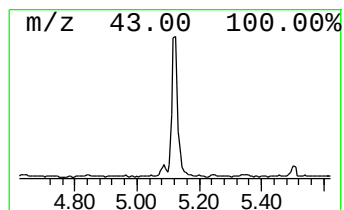
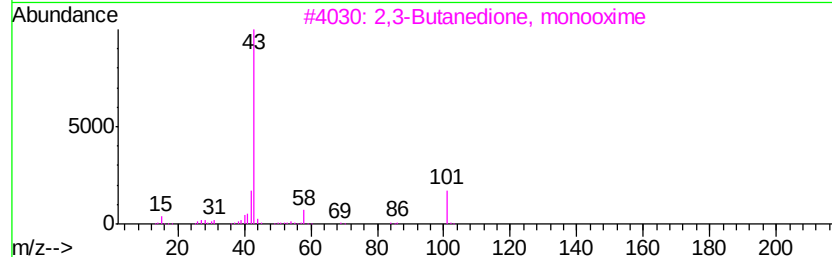
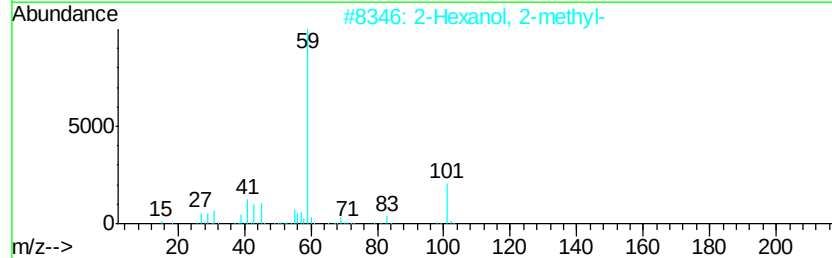
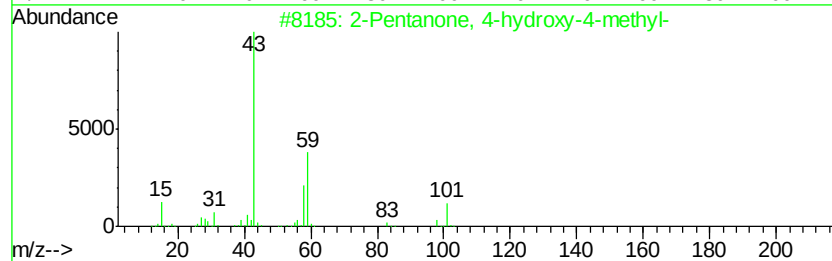
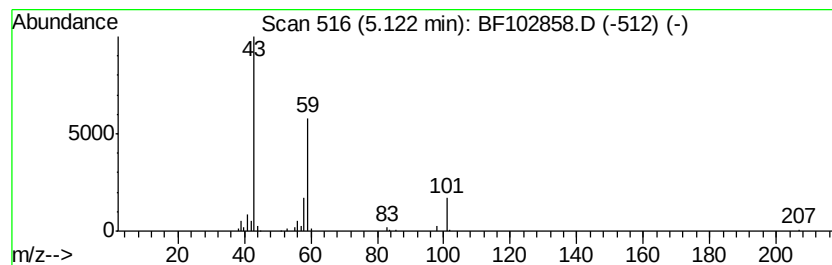
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.61 ng	171555	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4		Acetone	58	C3H6O	000067-64-1	9
5		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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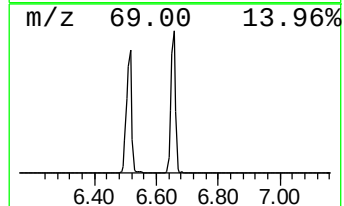
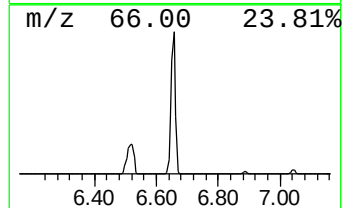
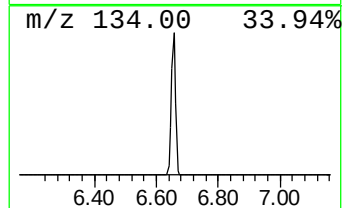
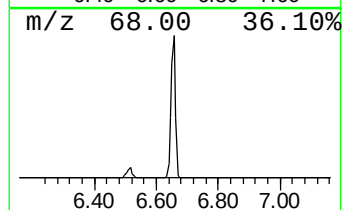
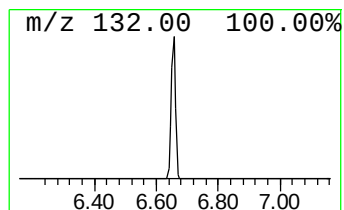
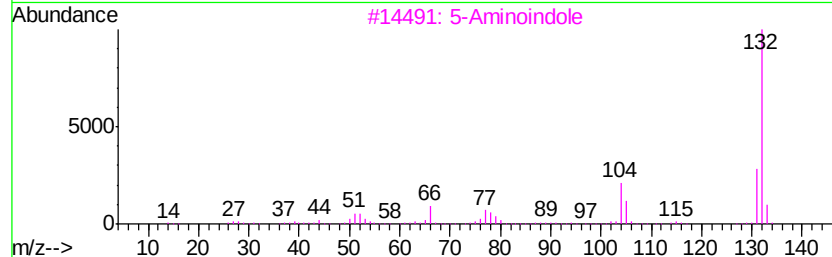
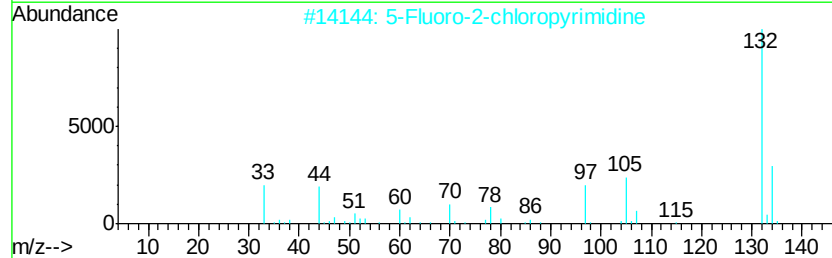
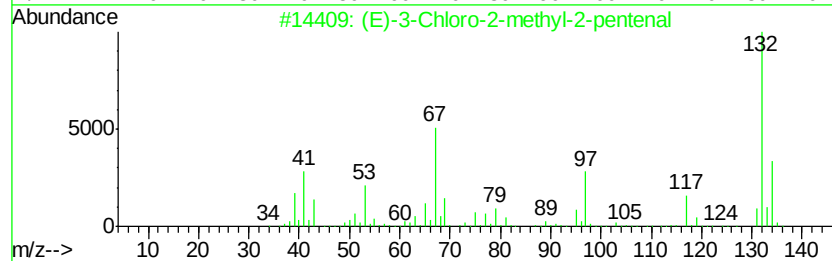
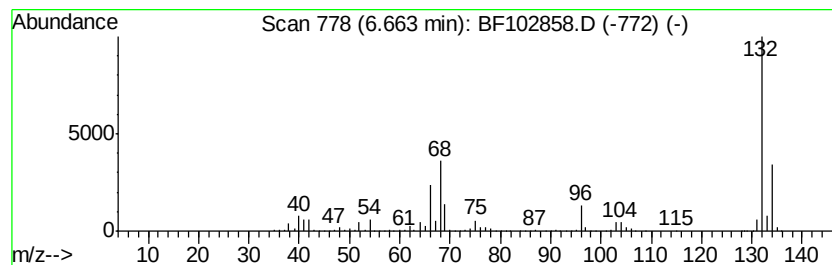
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.02 ng	4533680	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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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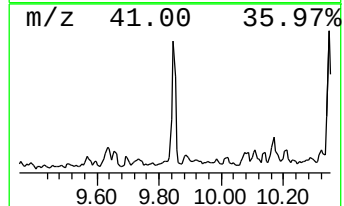
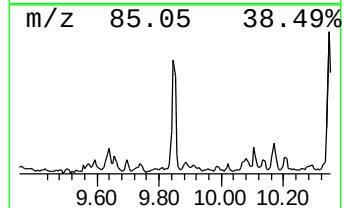
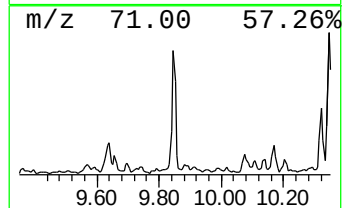
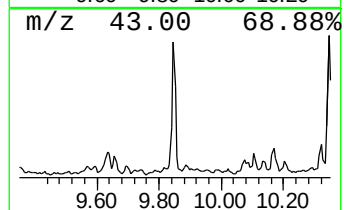
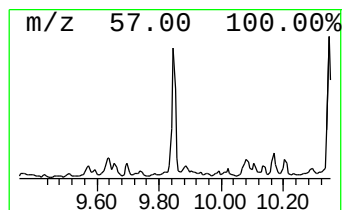
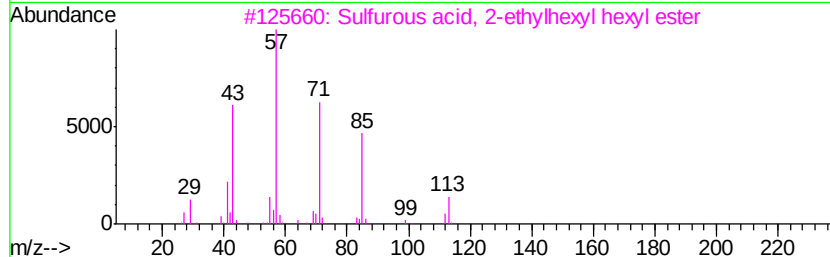
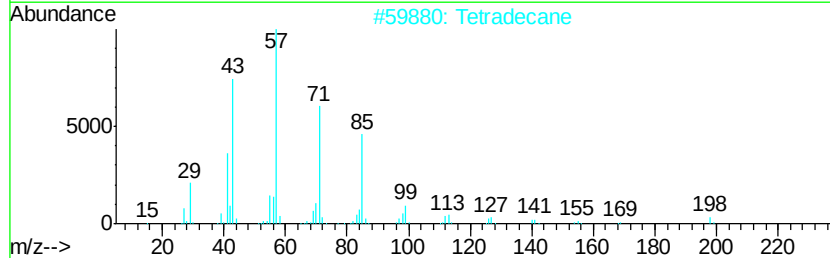
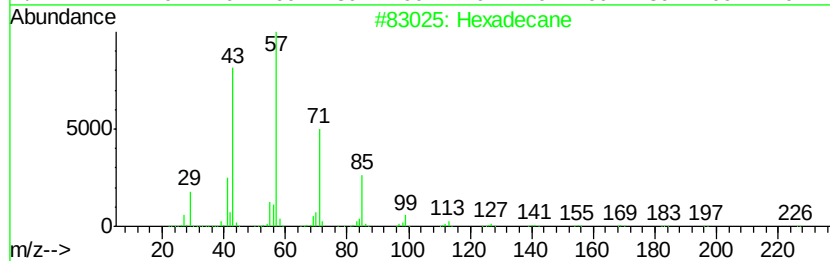
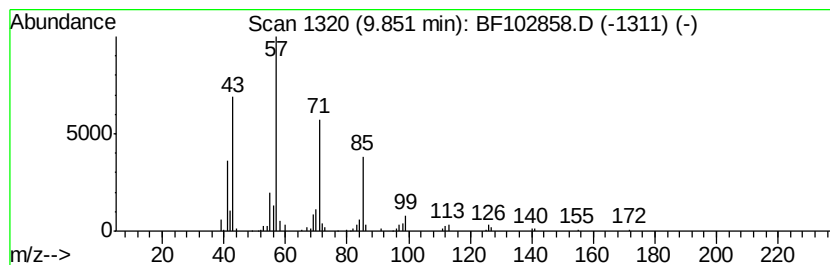
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.93 ng	233075	Acenaphthene-d10	9.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tetradecane		198	C14H30	000629-59-4	86
3	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	86
4	Nonane, 5-butyl-		184	C13H28	017312-63-9	80
5	Pentadecane		212	C15H32	000629-62-9	80



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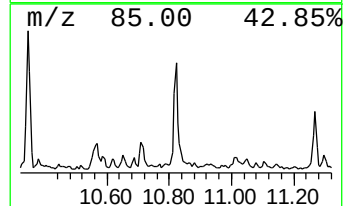
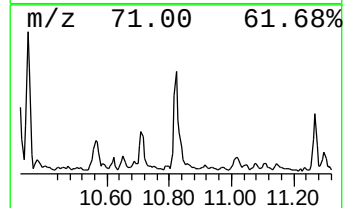
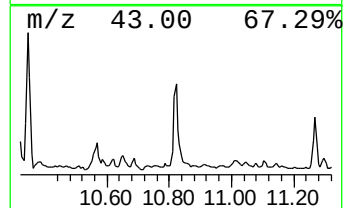
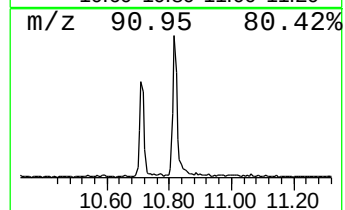
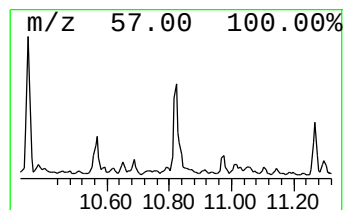
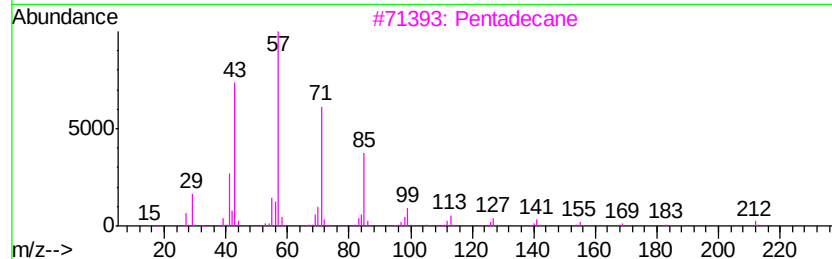
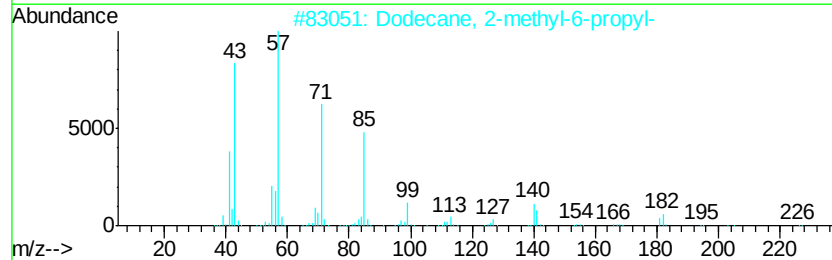
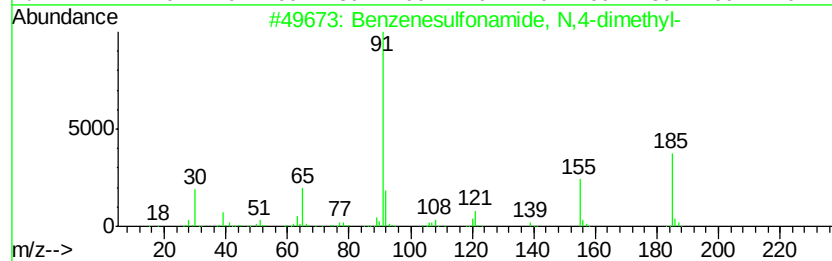
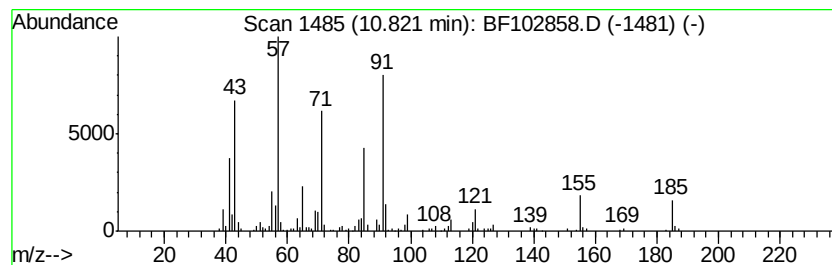
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown10.82 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	5.44 ng	336267	Phenanthrene-d10	11.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	49
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	46
3	Pentadecane	212	C15H32	000629-62-9	46
4	Heptacosane	380	C27H56	000593-49-7	46
5	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	46



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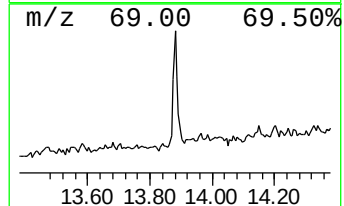
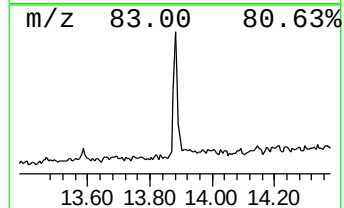
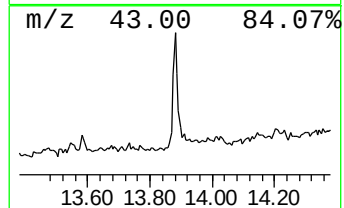
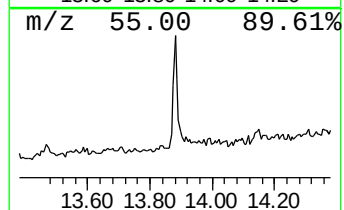
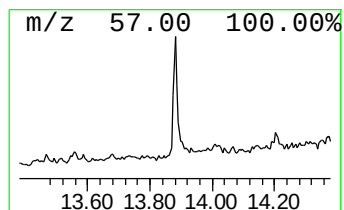
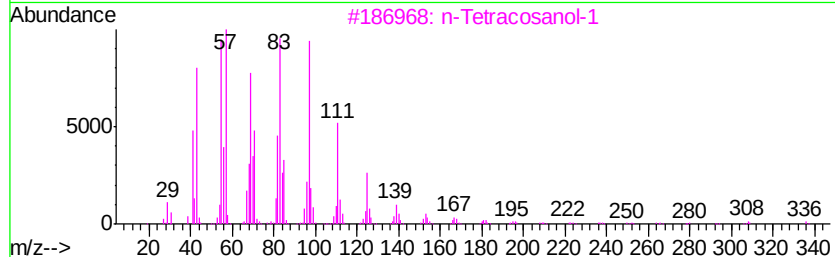
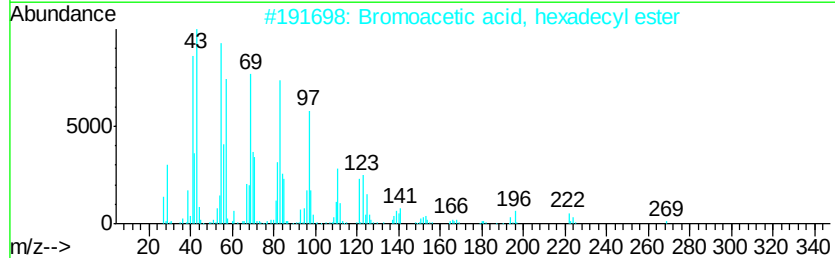
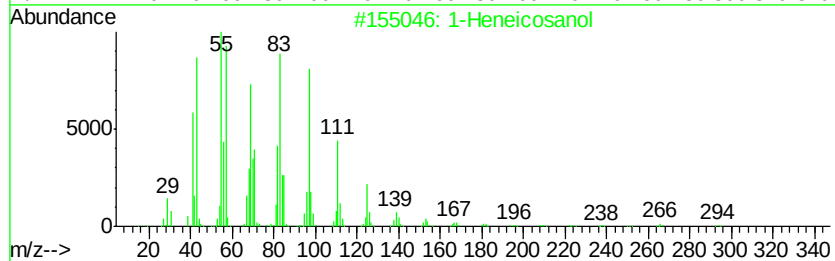
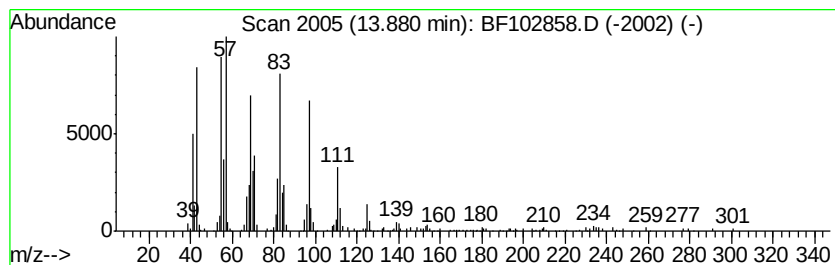
Instrument :
BNA_F
ClientSampleId :
3N-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.88	4.96 ng	267336	Chrysene-d12	14.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102858.D
Acq On : 8 Feb 2018 16:12
Operator : SJ/JU
Sample : J1469-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-4

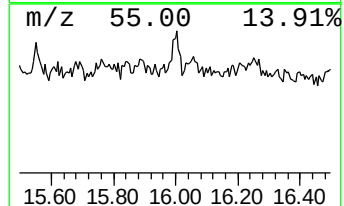
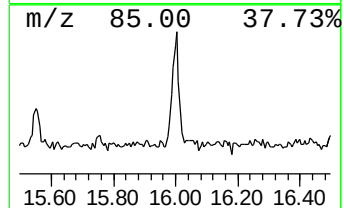
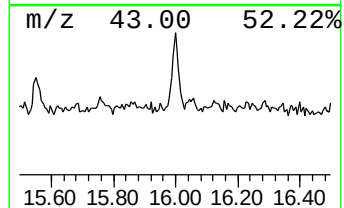
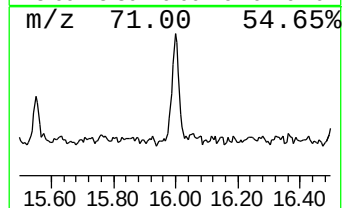
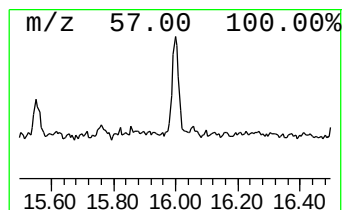
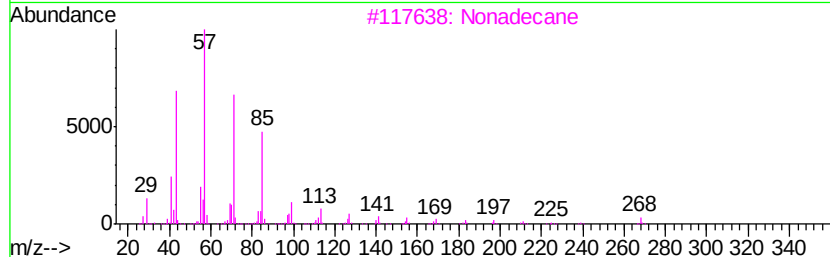
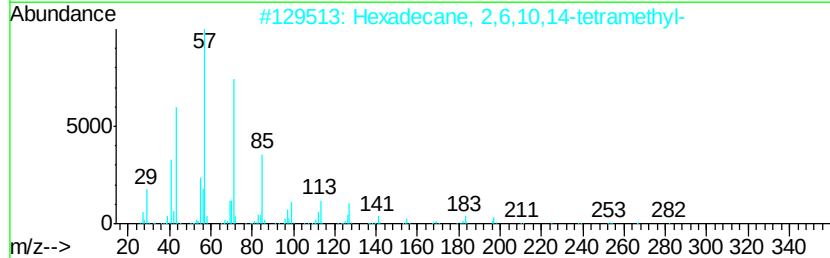
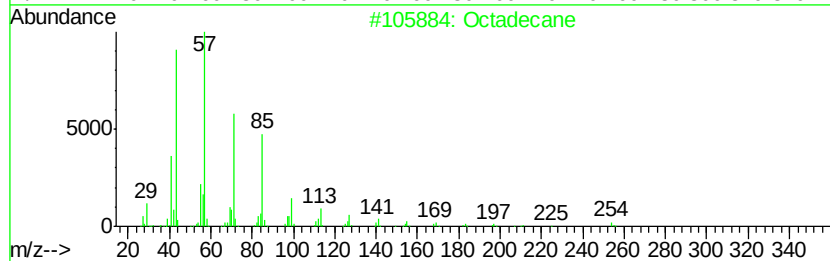
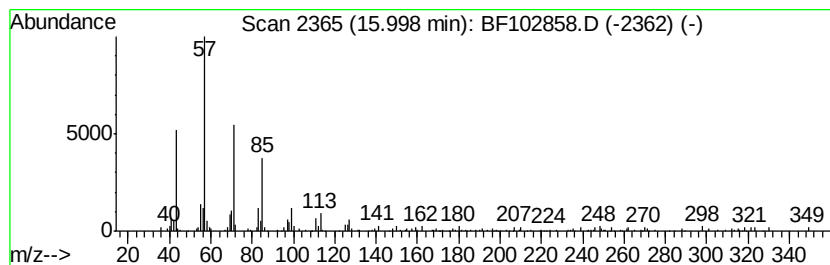
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.82 ng	141355	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	91
3		Nonadecane	268	C19H40	000629-92-5	83
4		Heptadecane	240	C17H36	000629-78-7	83
5		Docosane	310	C22H46	000629-97-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102858.D
Acq On : 8 Feb 2018 16:12
Operator : SJ/JU
Sample : J1469-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.17	9.6	ng	630048	1	6.89	1313810	20.0
2-Pentanone, 4-hy...	5.12	2.6	ng	171555	1	6.89	1313810	20.0
unknown6.66	6.66	69.0	ng	4533680	1	6.89	1313810	20.0
Hexadecane	9.85	2.9	ng	233075	3	9.93	1591660	20.0
unknown10.82	10.82	5.4	ng	336267	4	11.42	1235580	20.0
1-Heneicosanol	13.88	5.0	ng	267336	5	14.05	1078610	20.0
Octadecane	16.00	2.8	ng	141355	6	15.54	1003980	20.0