

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081017\
 Data File : BF097587.D
 Acq On : 11 Aug 2017 5:31
 Operator : SJ/JU
 Sample : I4664-01
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN001

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-BF072517.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	4.510	475	480	495	rBV2	49929	110511	3.90%	0.534%
2	4.981	557	560	593	rBV	890202	1565966	55.30%	7.571%
3	6.069	743	745	758	rBV	605971	941570	33.25%	4.552%
4	6.163	758	761	773	rVB	2269016	2546786	89.93%	12.314%
5	6.387	796	799	811	rVB	591244	643615	22.73%	3.112%
6	6.545	822	826	841	rBV	2212430	2255418	79.65%	10.905%
7	6.969	894	898	915	rBV	1793267	2083503	73.58%	10.074%
8	7.675	1014	1018	1027	rVB	902529	882433	31.16%	4.267%
9	8.134	1093	1096	1104	rBV5	17265	33993	1.20%	0.164%
10	8.628	1177	1180	1187	rBV	25756	34225	1.21%	0.165%
11	8.751	1197	1201	1212	rBV	2764813	2831808	100.00%	13.692%
12	9.157	1266	1270	1281	rVB	156913	153295	5.41%	0.741%
13	9.416	1310	1314	1324	rVB	872629	815274	28.79%	3.942%
14	10.204	1444	1448	1464	rBV	1314490	1485872	52.47%	7.184%
15	10.786	1543	1547	1548	rBV2	31474	37577	1.33%	0.182%
16	10.816	1549	1552	1555	rVV	138132	135275	4.78%	0.654%
17	10.892	1561	1565	1569	rBV	595409	592803	20.93%	2.866%
18	10.951	1572	1575	1576	rBV3	33316	34338	1.21%	0.166%
19	11.163	1605	1611	1614	rBV2	129890	202727	7.16%	0.980%
20	11.451	1658	1660	1663	rBV	102740	106139	3.75%	0.513%
21	11.963	1744	1747	1753	rVB	180611	236987	8.37%	1.146%
22	12.475	1830	1834	1839	rBV	1457084	1493471	52.74%	7.221%
23	13.521	2008	2012	2022	rVB	562396	589812	20.83%	2.852%
24	13.998	2089	2093	2100	rVB5	46606	95657	3.38%	0.463%
25	14.163	2119	2121	2125	rVB2	45516	43352	1.53%	0.210%
26	14.857	2235	2239	2248	rBV	404435	500090	17.66%	2.418%
27	15.233	2298	2303	2306	rVB2	25350	34592	1.22%	0.167%
28	15.386	2323	2329	2331	rBV7	16702	37973	1.34%	0.184%
29	15.539	2349	2355	2357	rBV7	23858	42217	1.49%	0.204%
30	15.615	2364	2368	2373	rVB3	30504	46046	1.63%	0.223%
31	16.068	2440	2445	2450	rVB4	18857	32533	1.15%	0.157%
32	16.139	2452	2457	2461	rBV8	19018	36700	1.30%	0.177%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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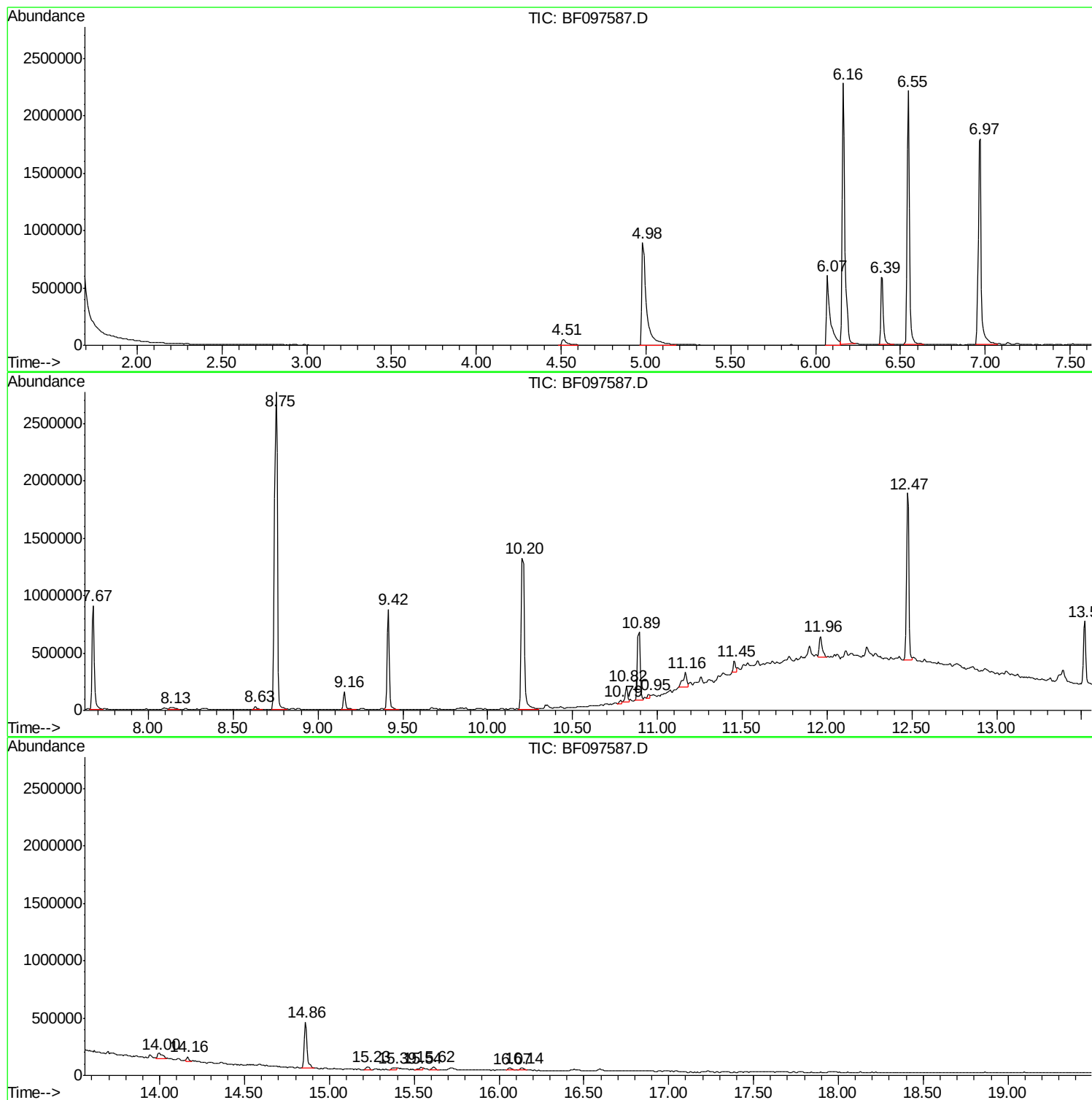
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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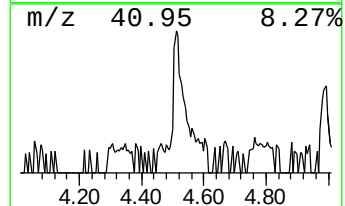
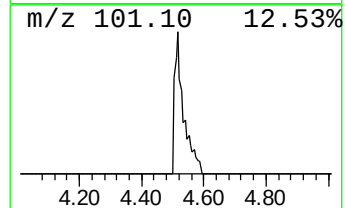
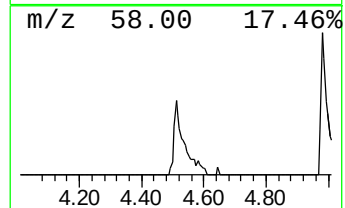
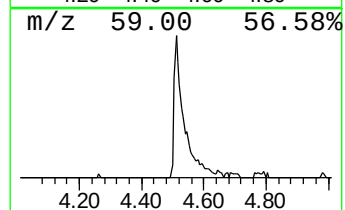
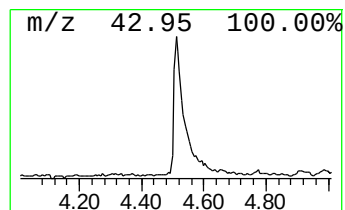
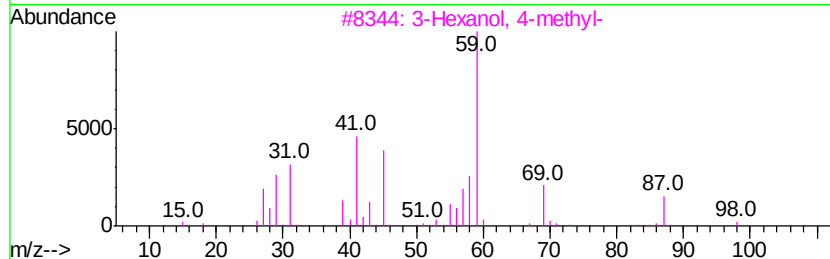
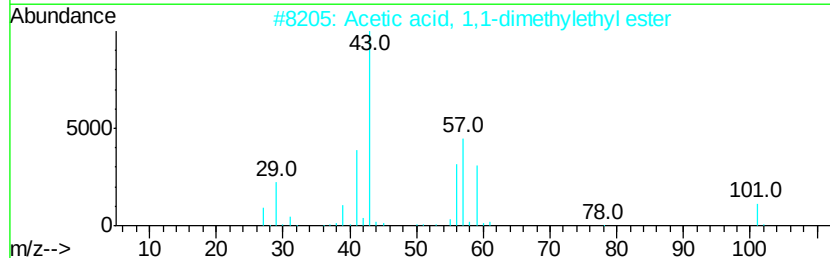
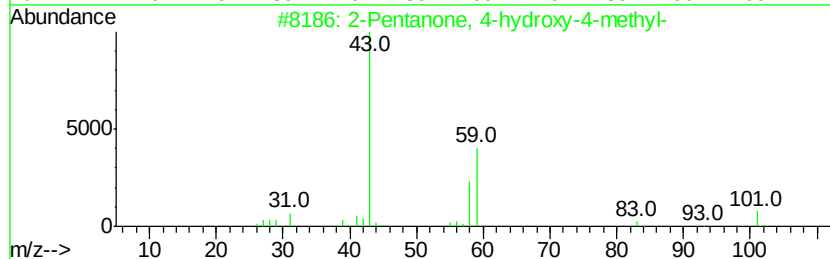
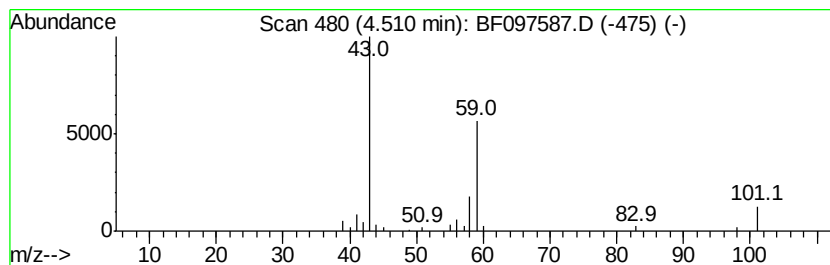
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.51	3.43 ng	110511	1,4-Dichlorobenzene-d4	6.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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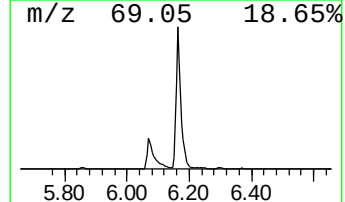
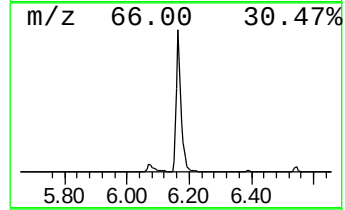
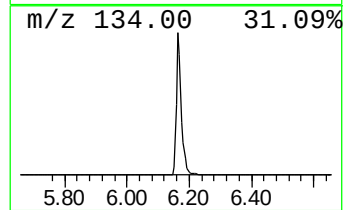
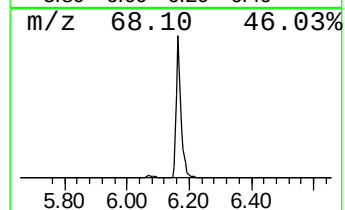
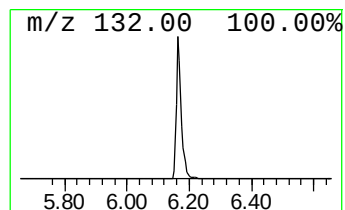
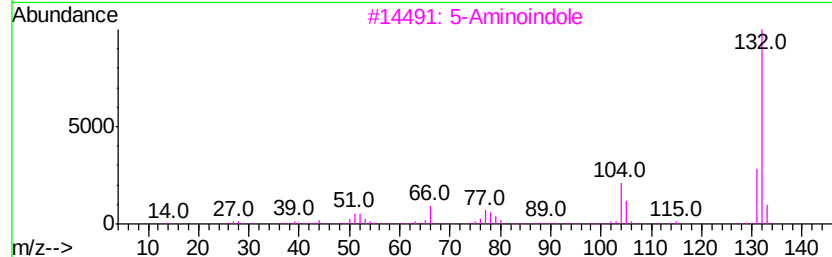
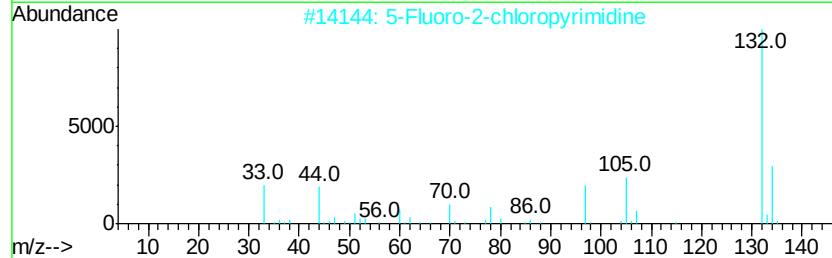
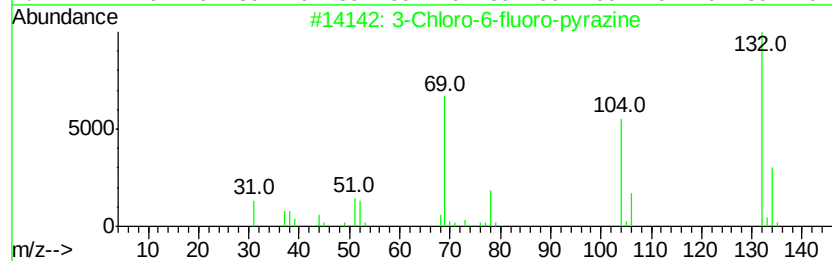
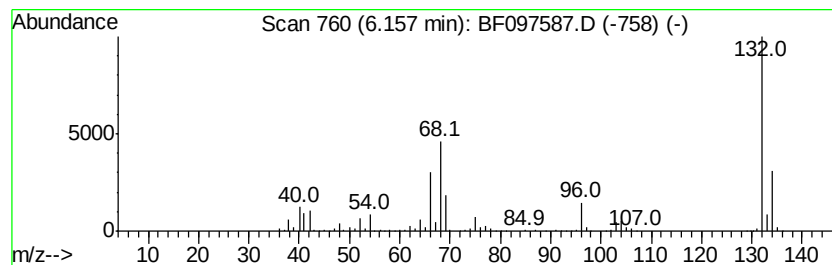
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	79.14 ng	2546790	1,4-Dichlorobenzene-d4	6.39

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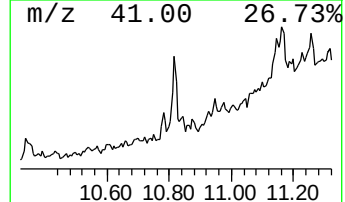
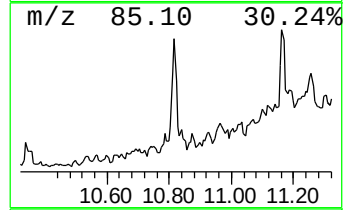
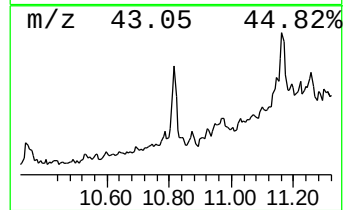
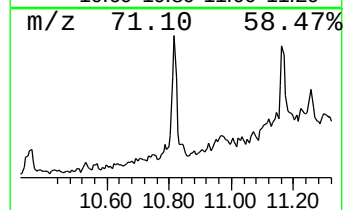
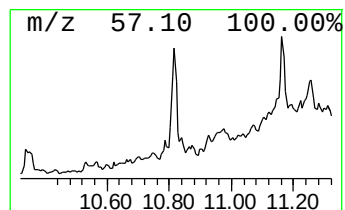
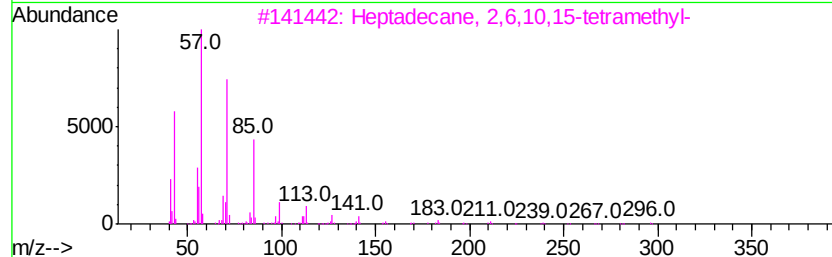
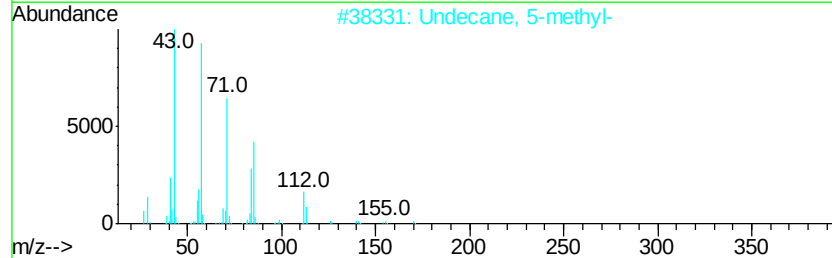
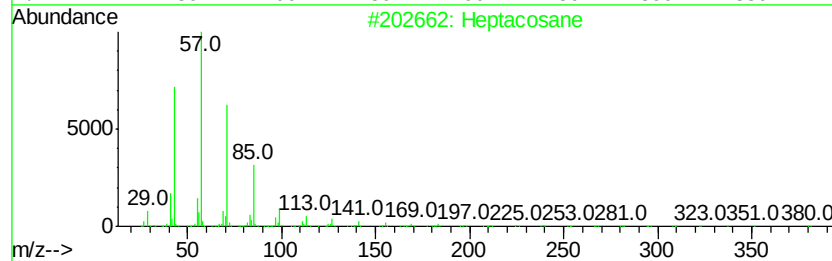
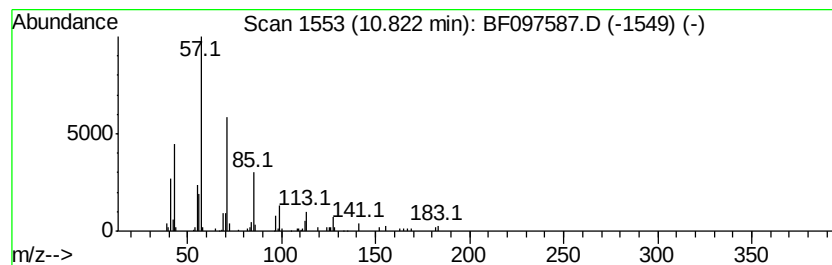
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	4.56 ng	135275	Phenanthrene-d10	10.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Undecane, 5-methyl-	170	C12H26	001632-70-8	81
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	78
5	Octacosane	394	C28H58	000630-02-4	72



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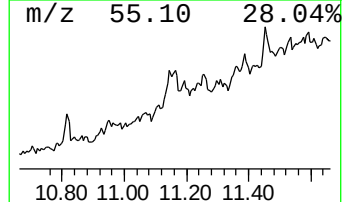
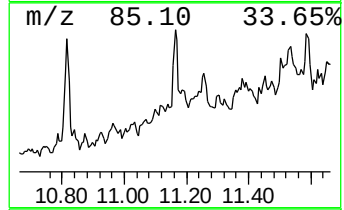
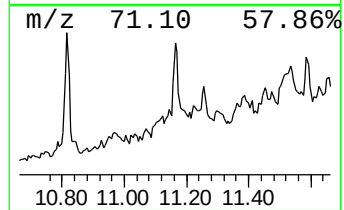
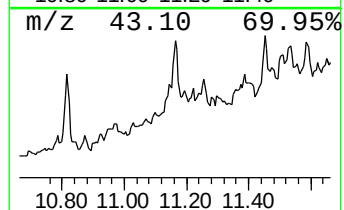
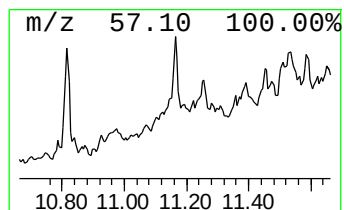
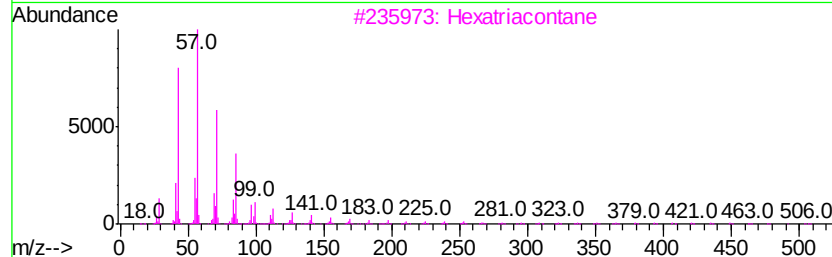
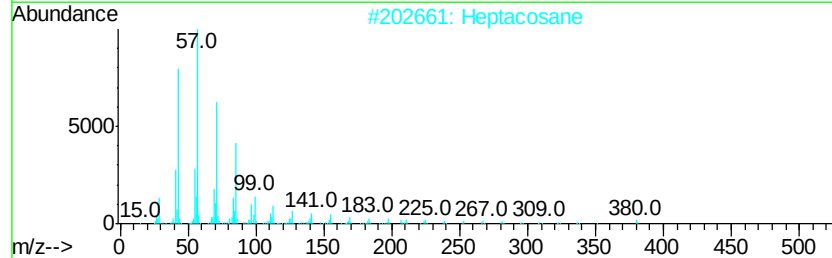
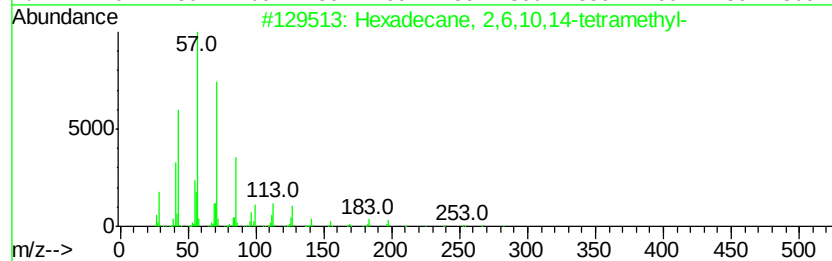
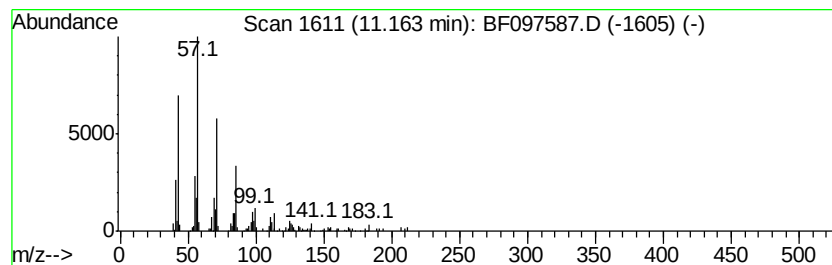
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane, 2,6,10,14-tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	6.84 ng	202727	Phenanthrene-d10	10.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42		000638-36-8	91
2	Heptacosane	380	C27H56		000593-49-7	91
3	Hexatriacontane	507	C36H74		000630-06-8	90
4	Octacosane	394	C28H58		000630-02-4	86
5	Hentriacontane	437	C31H64		000630-04-6	83



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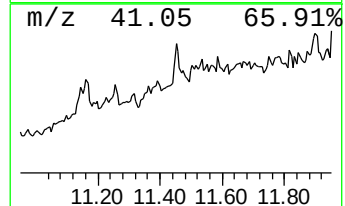
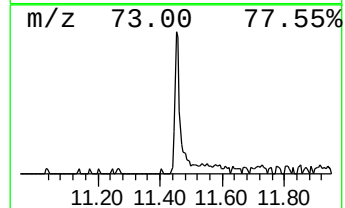
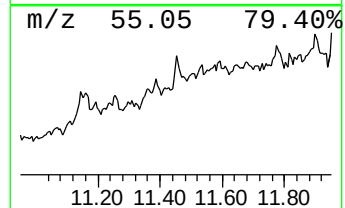
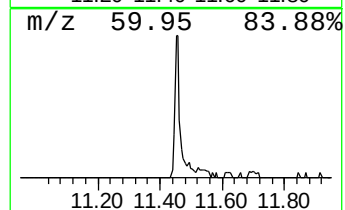
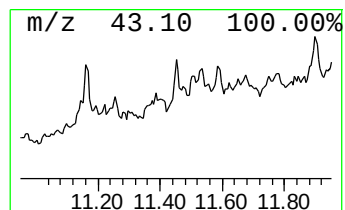
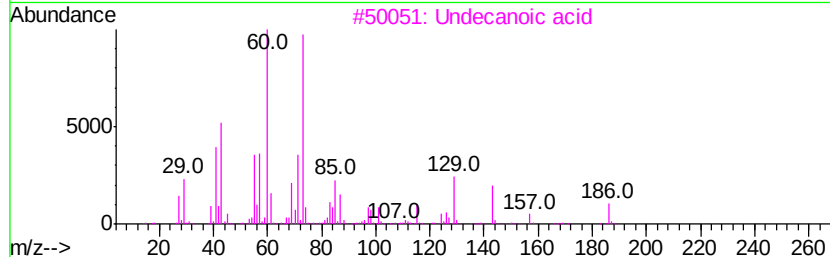
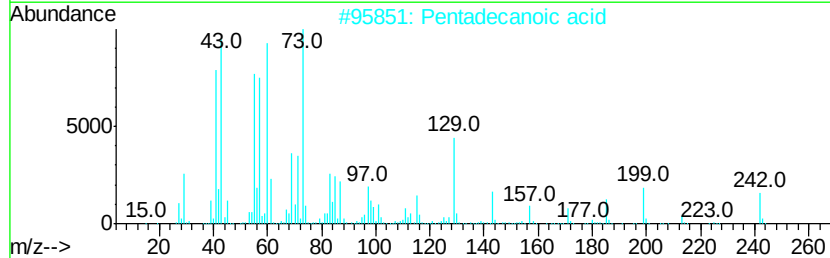
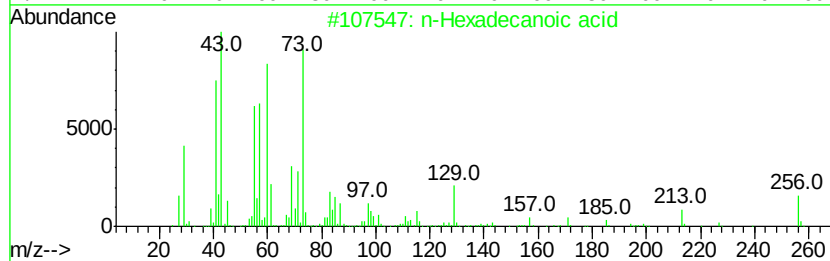
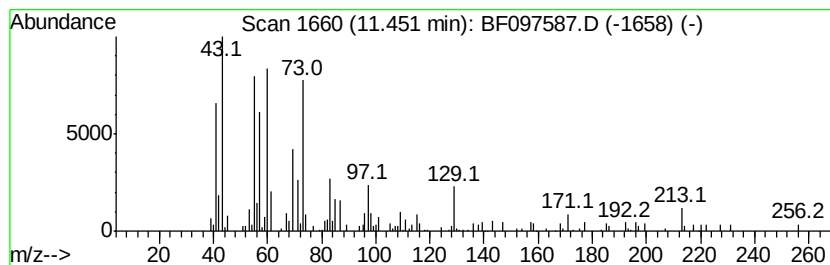
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	3.58 ng	106139	Phenanthrene-d10	10.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Undecanoic acid	186	C11H22O2	000112-37-8	53
4		Nonanoic acid	158	C9H18O2	000112-05-0	52
5		Methyl .beta.-d-galactopyranoside	194	C7H14O6	1000126-04-6	47



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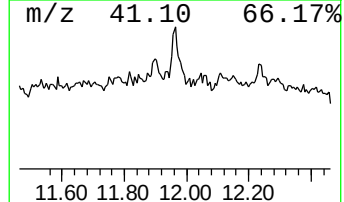
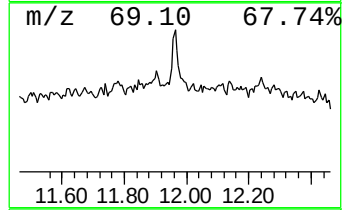
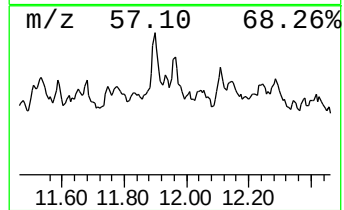
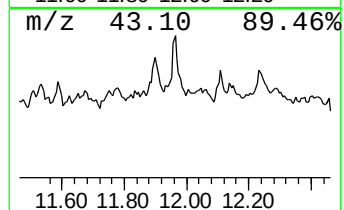
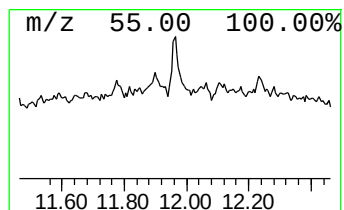
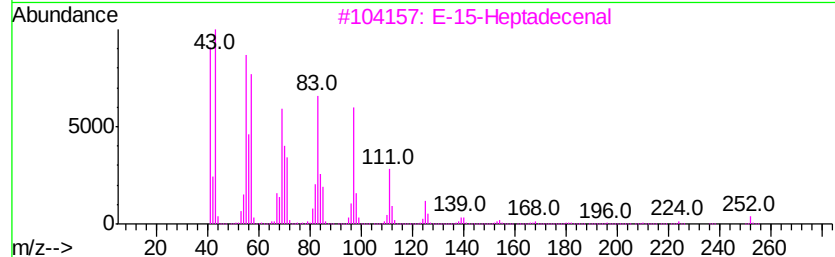
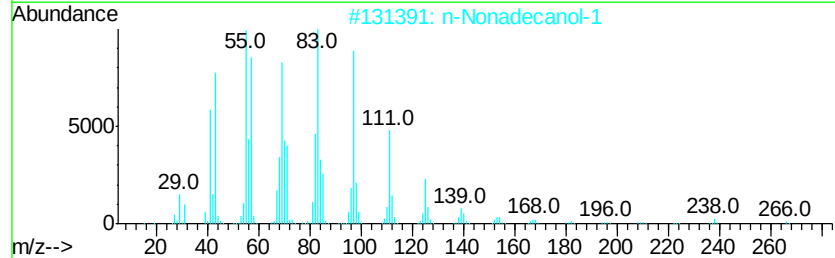
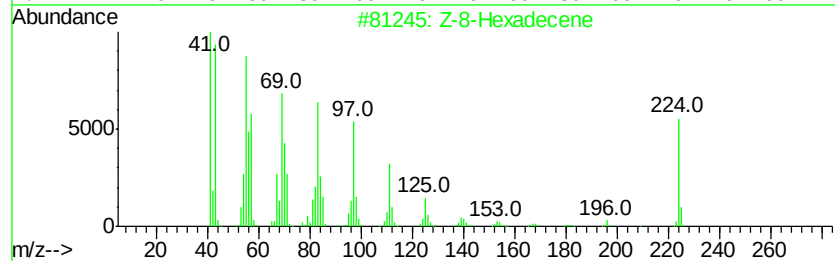
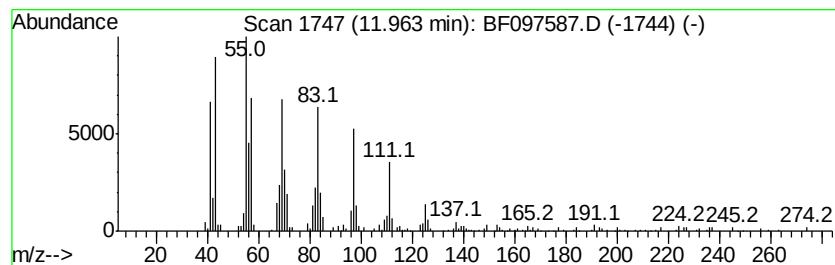
Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Z-8-Hexadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.96	8.00 ng	236987	Phenanthrene-d10	10.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-8-Hexadecene	224	C16H32	1000130-87-5	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	86
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	83
4	1-Hexadecanol	242	C16H34O	036653-82-4	83
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097587.D
Acq On : 11 Aug 2017 5:31
Operator : SJ/JU
Sample : I4664-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

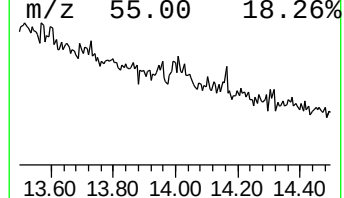
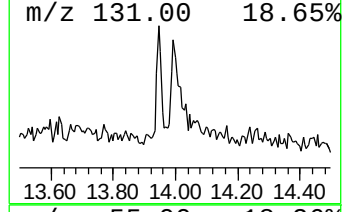
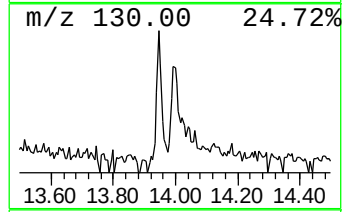
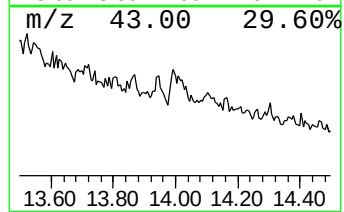
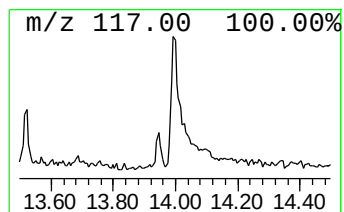
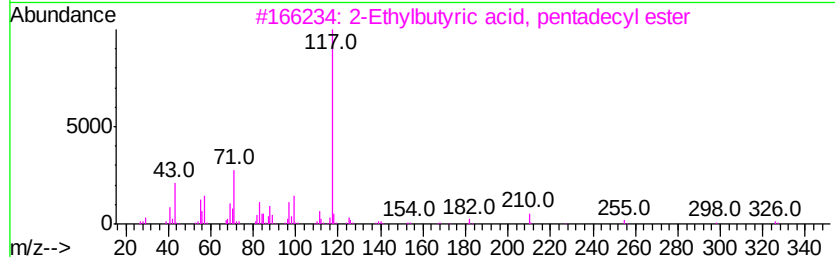
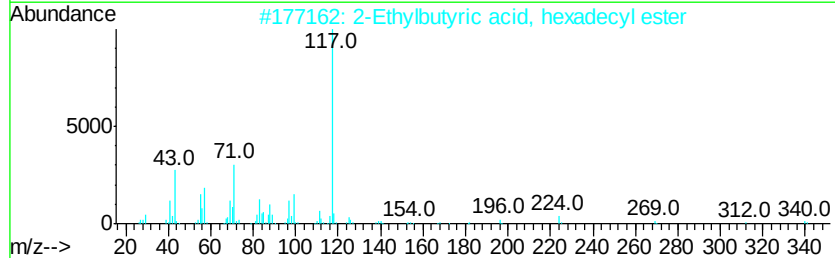
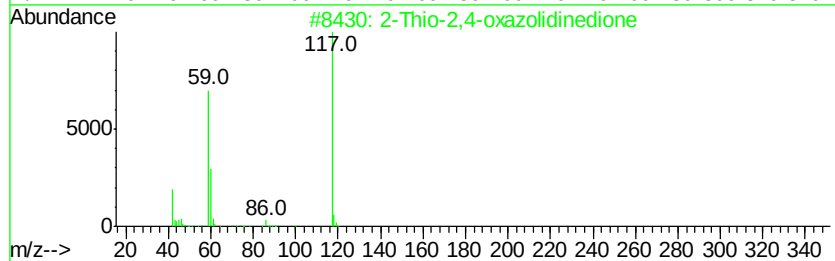
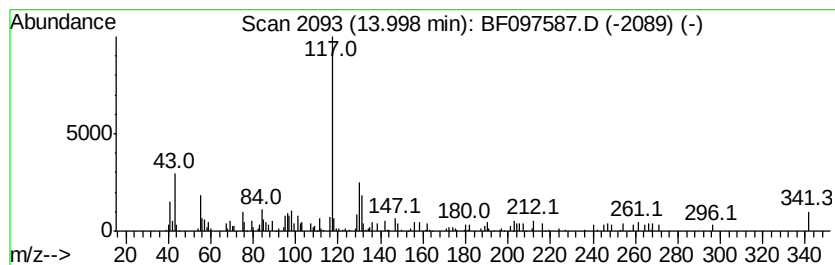
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.00 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	3.24 ng	95657	Chrysene-d12	13.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2	Thio-2,4-oxazolidinedione	117	C3H3N02S	002346-24-9	46
2	2	Ethylbutyric acid, hexadecyl e...	340	C22H44O2	1000369-72-6	43
3	2	Ethylbutyric acid, pentadecyl ...	326	C21H42O2	1000369-75-5	43
4	2	Ethylbutyric acid, tridecyl ester	298	C19H38O2	1000369-71-1	37
5	2	Ethylbutyric acid, octadecyl e...	368	C24H48O2	1000369-75-3	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081017\
Data File : BF097587.D
Acq On : 11 Aug 2017 5:31
Operator : SJ/JU
Sample : I4664-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DSN001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.51	3.4	ng	110511	1	6.39	643615	20.0
unknown6.16	6.16	79.1	ng	2546790	1	6.39	643615	20.0
Heptacosane	10.82	4.6	ng	135275	4	10.89	592803	20.0
Hexadecane, 2,6,1...	11.16	6.8	ng	202727	4	10.89	592803	20.0
n-Hexadecanoic acid	11.45	3.6	ng	106139	4	10.89	592803	20.0
Z-8-Hexadecene	11.96	8.0	ng	236987	4	10.89	592803	20.0
unknown14.00	14.00	3.2	ng	95657	5	13.52	589812	20.0