

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
 Data File : BF082724.D
 Acq On : 5 Nov 2015 12:41
 Operator : UM/IZ
 Sample : G4241-18
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-11(18-20)

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-BF103015.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	5.058	256	260	262	rBV	1568935	2617822	45.34%	4.839%
2	5.470	293	296	299	rBV	4367951	4557730	78.94%	8.425%
3	6.499	382	386	388	rBV	4890678	5625922	97.44%	10.400%
4	6.636	395	398	400	rBV	4226335	5421763	93.91%	10.022%
5	6.864	415	418	420	rBV	1107576	1084709	18.79%	2.005%
6	7.024	429	432	434	rVB	3189800	3826200	66.27%	7.073%
7	7.424	464	467	469	rBV	3323226	3482139	60.31%	6.437%
8	8.145	528	530	533	rBV	1456112	1358275	23.53%	2.511%
9	9.105	611	614	616	rBV	63238	63413	1.10%	0.117%
10	9.230	622	625	627	rBV	5497226	5773603	100.00%	10.673%
11	9.619	656	659	661	rBV	1210444	1056039	18.29%	1.952%
12	9.905	681	684	686	rBV	1583407	1700912	29.46%	3.144%
13	10.350	721	723	724	rVB	66810	82689	1.43%	0.153%
14	10.568	739	742	744	rBV	63005	76869	1.33%	0.142%
15	10.693	749	753	755	rVV	2945506	4093869	70.91%	7.568%
16	10.819	762	764	768	rVB	164967	224340	3.89%	0.415%
17	11.265	801	803	804	rBV	173544	144103	2.50%	0.266%
18	11.299	804	806	808	rVB	64616	64188	1.11%	0.119%
19	11.379	811	813	816	rVV	1756560	1673178	28.98%	3.093%
20	11.688	838	840	843	rVB	102840	103503	1.79%	0.191%
21	11.916	858	860	863	rBV	272951	421648	7.30%	0.779%
22	12.099	873	876	878	rBV	98767	90627	1.57%	0.168%
23	12.488	908	910	912	rVB	76094	61478	1.06%	0.114%
24	12.705	927	929	936	rBV	171565	197676	3.42%	0.365%
25	12.796	936	937	941	rVB	54764	77054	1.33%	0.142%
26	12.876	941	944	946	rVB2	44119	91352	1.58%	0.169%
27	12.968	950	952	955	rVB	3934165	5464950	94.65%	10.102%
28	13.219	970	974	975	rBV2	42437	77356	1.34%	0.143%
29	13.448	989	994	998	rBV	150569	258482	4.48%	0.478%
30	13.505	998	999	1002	rVV2	56424	73352	1.27%	0.136%
31	13.562	1002	1004	1007	rVB	43150	69343	1.20%	0.128%
32	13.871	1029	1031	1039	rBV	475957	568667	9.85%	1.051%
33	14.019	1041	1044	1046	rBV	2010795	1851857	32.07%	3.423%
34	14.202	1058	1060	1063	rBV2	65392	71485	1.24%	0.132%

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SB-11(18-20)

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-BF103015.M
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35	14.522	1086	1088	1090	rBV	64407	88189	1.53%	0.163%
36	14.899	1118	1121	1123	rBV	105616	124478	2.16%	0.230%
37	15.460	1167	1170	1173	rBV	1037252	1359054	23.54%	2.512%
38	15.985	1214	1216	1220	rVB3	33561	59113	1.02%	0.109%
39	17.677	1359	1364	1368	rVB5	20443	58760	1.02%	0.109%

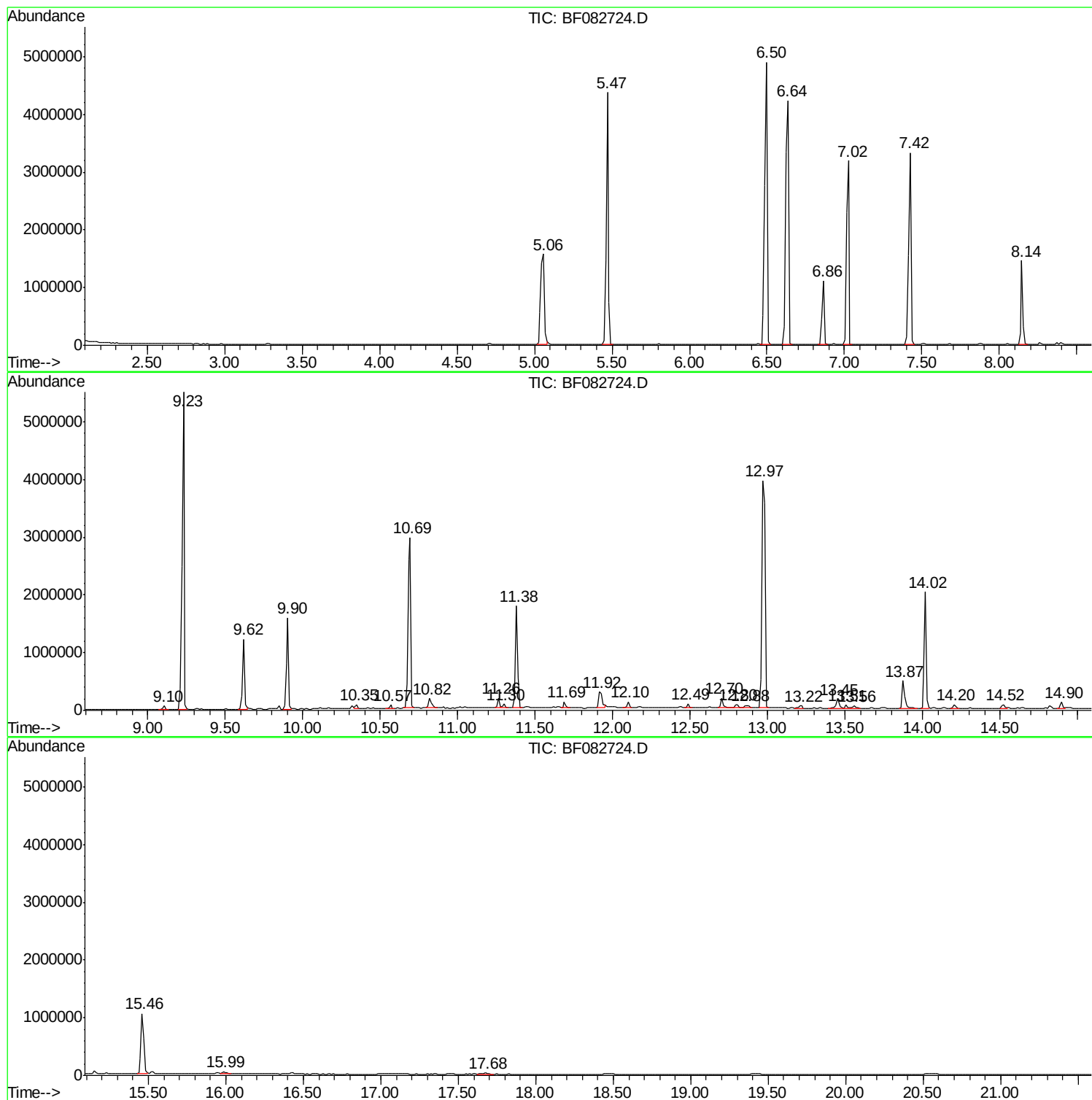
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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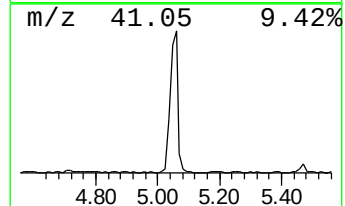
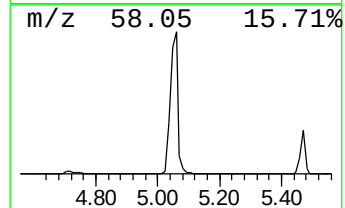
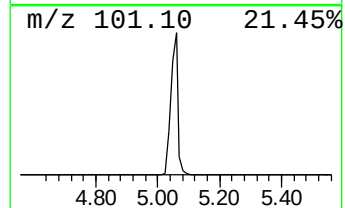
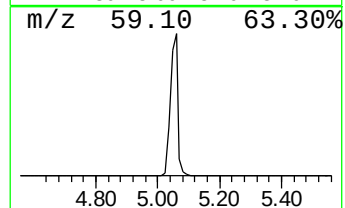
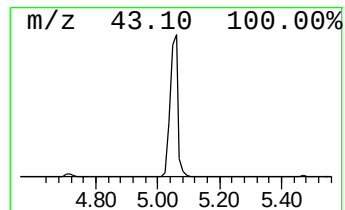
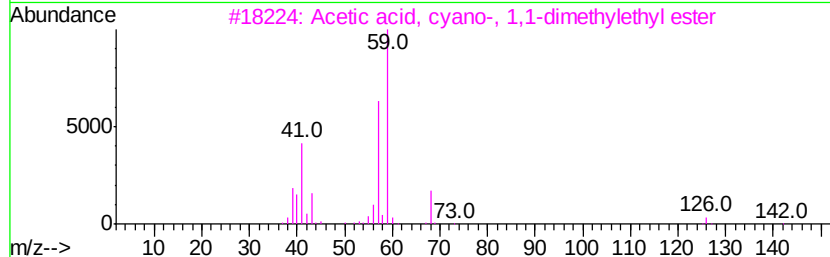
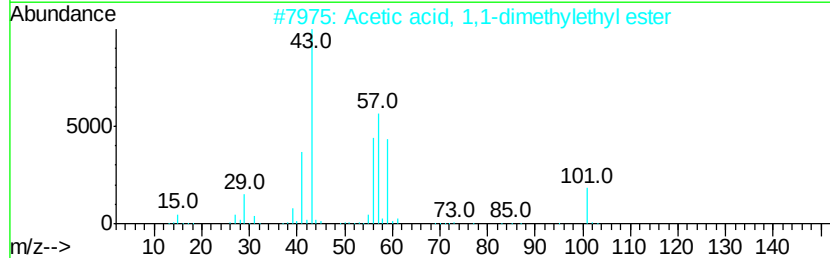
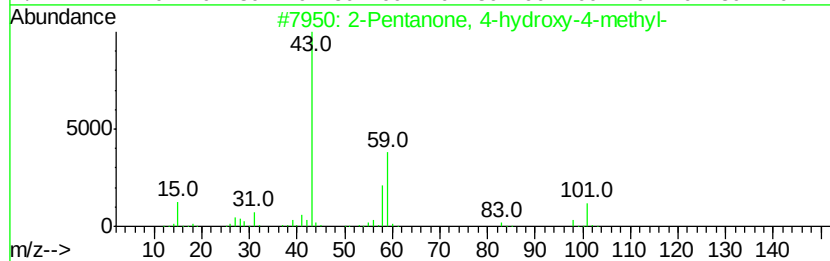
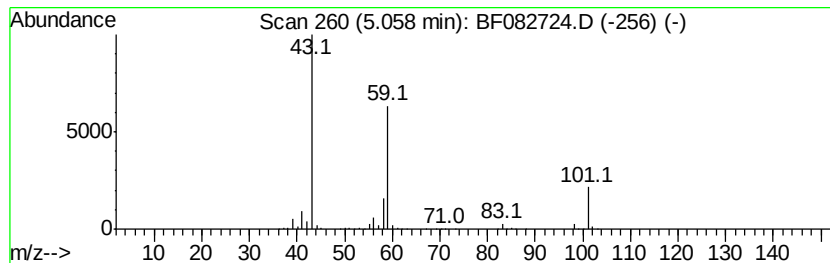
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.06	48.27 ng	2617820	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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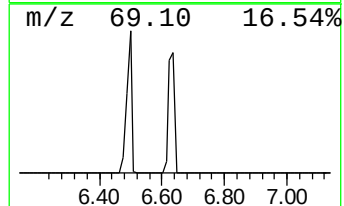
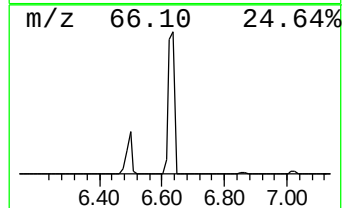
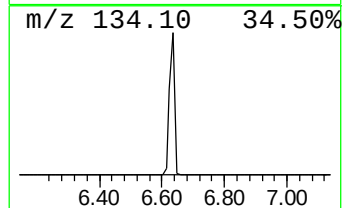
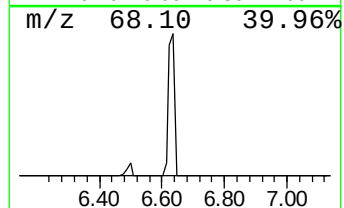
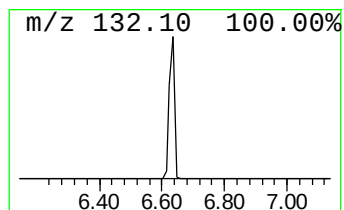
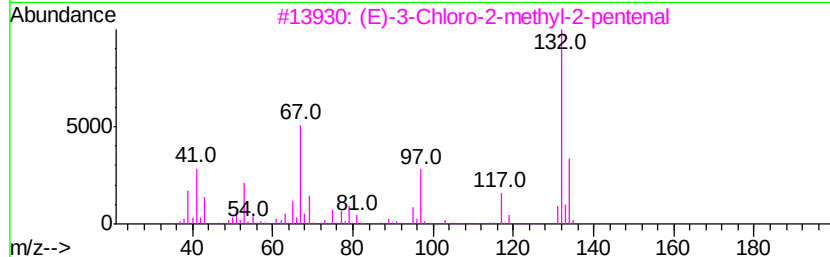
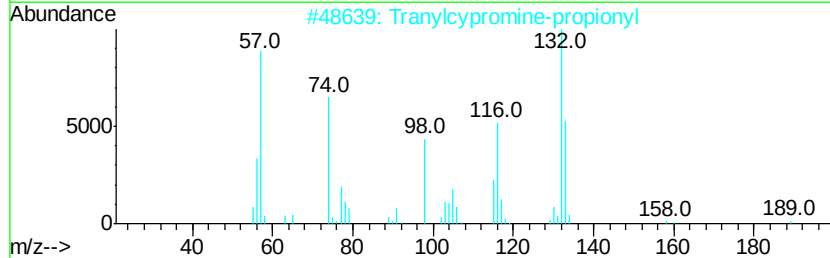
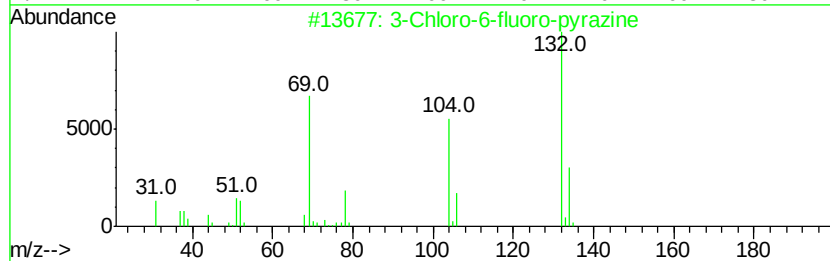
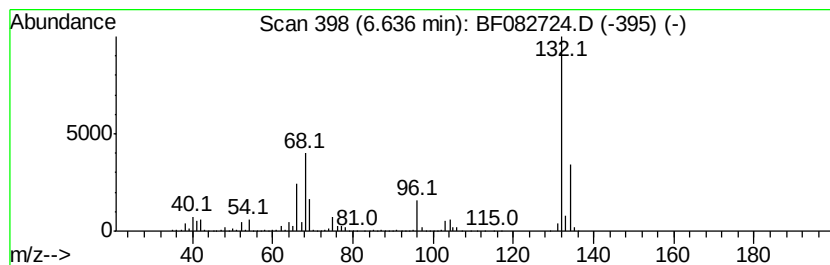
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	99.97 ng	5421760	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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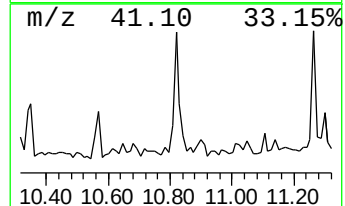
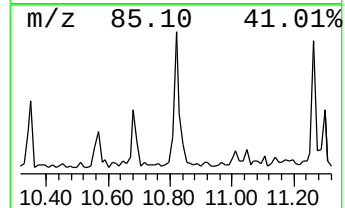
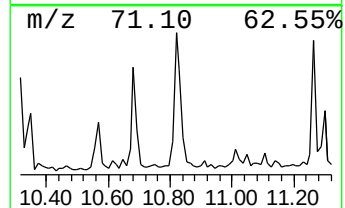
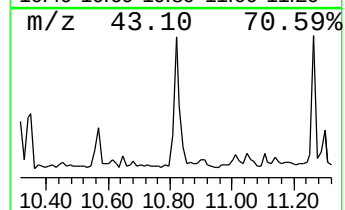
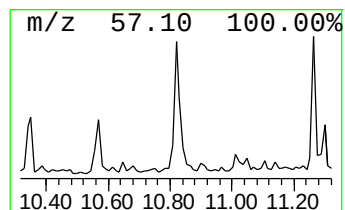
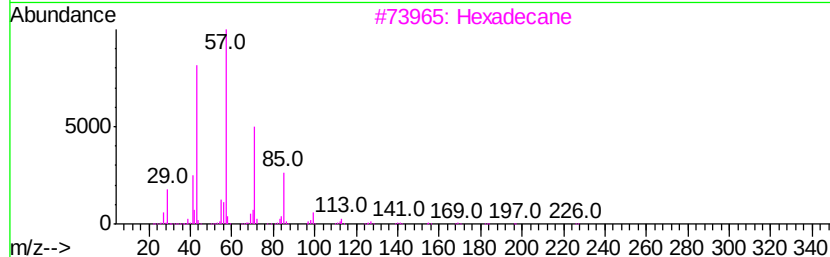
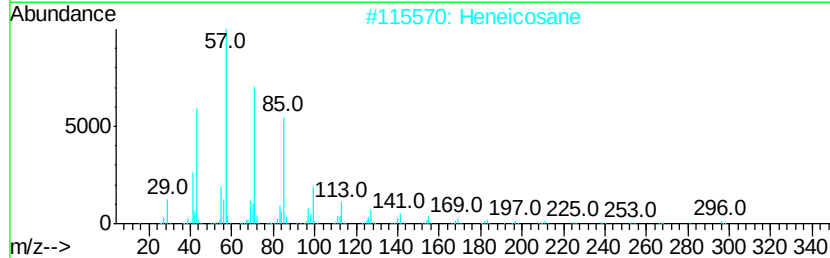
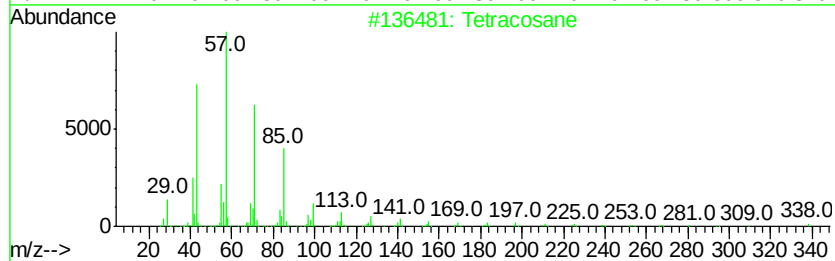
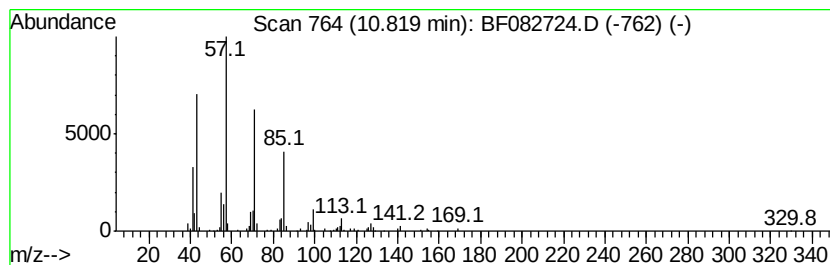
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.68 ng	224340	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexadecane	226	C16H34	000544-76-3	90
4		Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
5		Nonadecane	268	C19H40	000629-92-5	86



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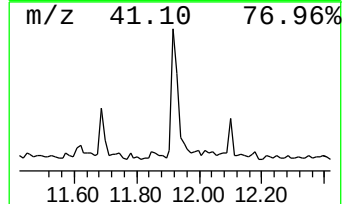
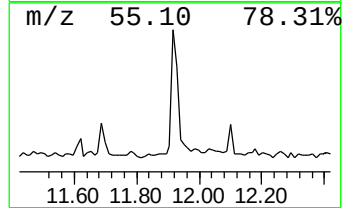
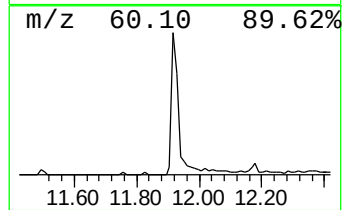
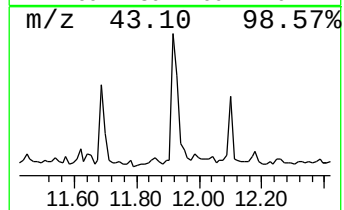
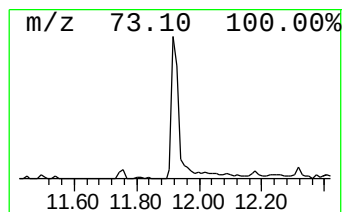
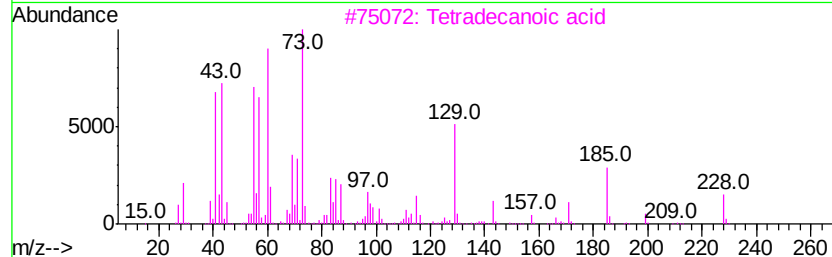
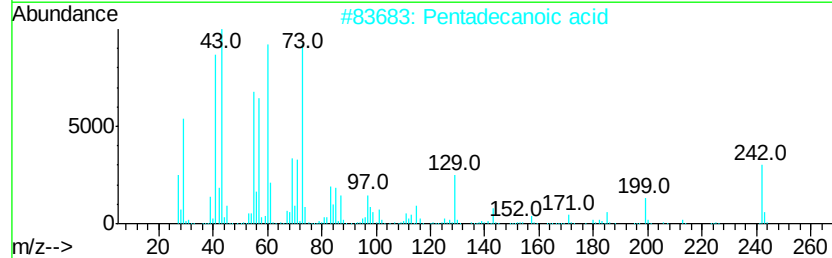
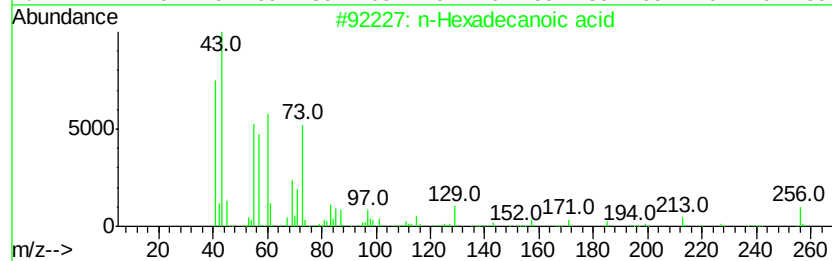
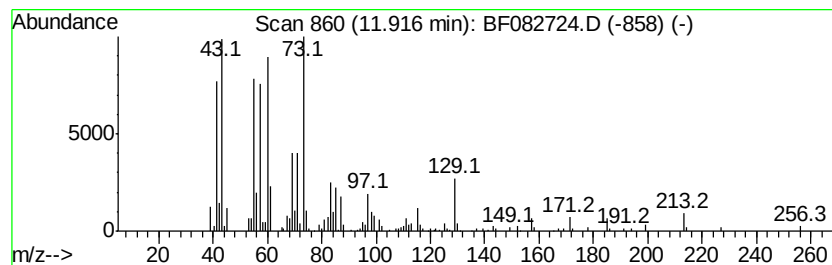
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.92	5.04 ng	421648	Phenanthrene-d10		11.38
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	78



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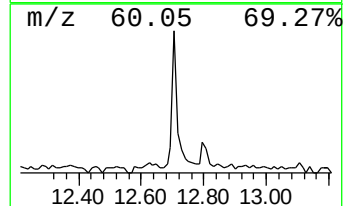
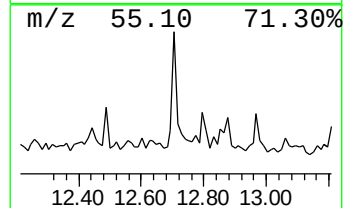
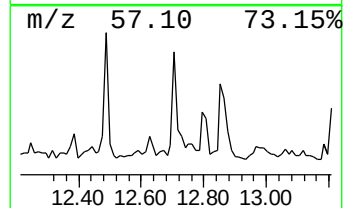
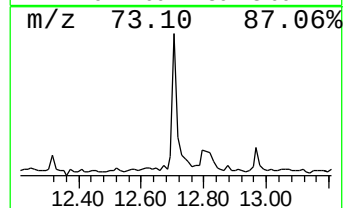
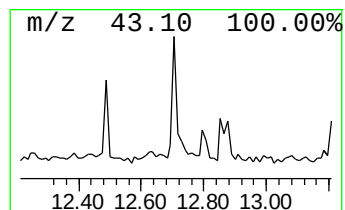
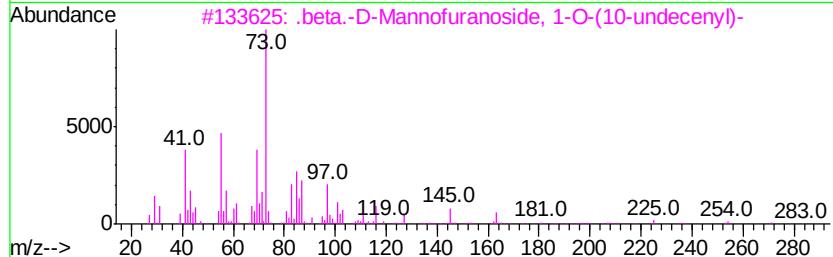
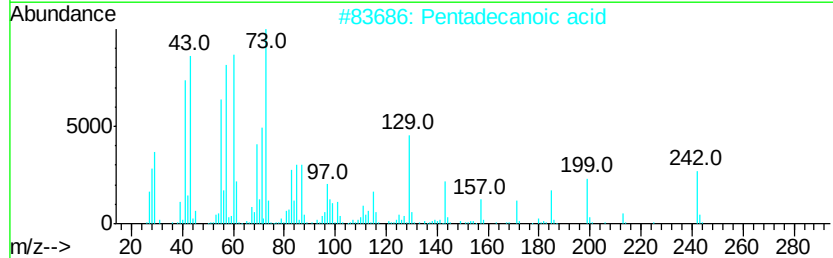
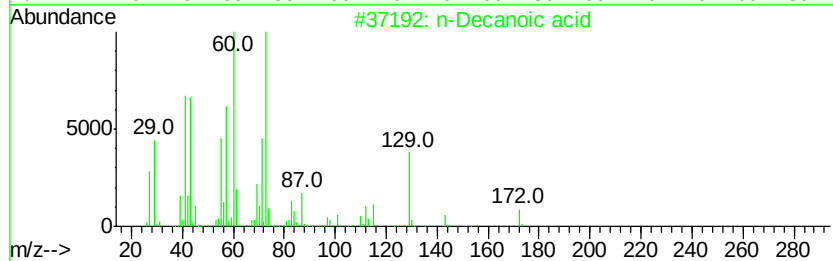
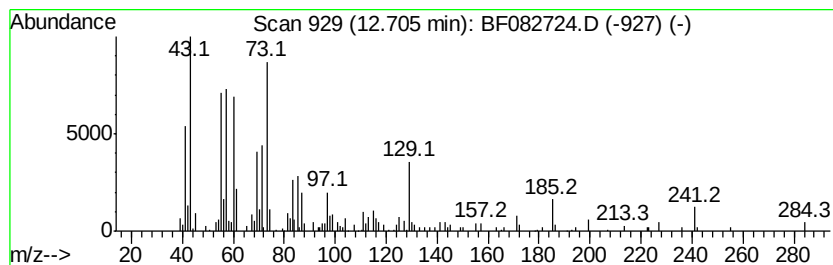
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Decanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.71	2.13 ng	197676	Chrysene-d12	14.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	70	
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52	
3	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	38	
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	25	
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	20	



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Misc :
ALS Vial : 29 Sample Multiplier: 1

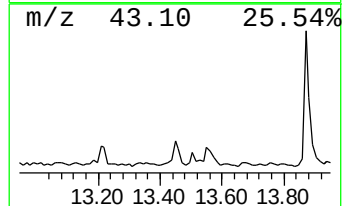
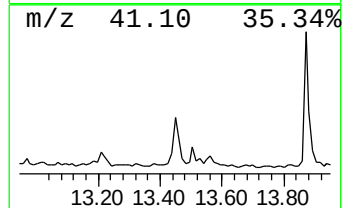
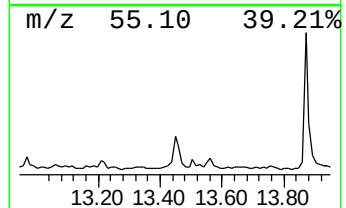
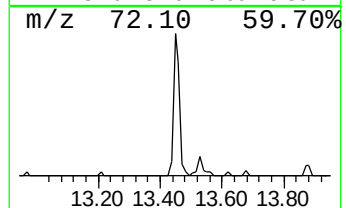
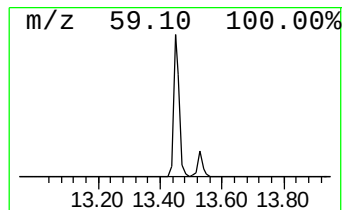
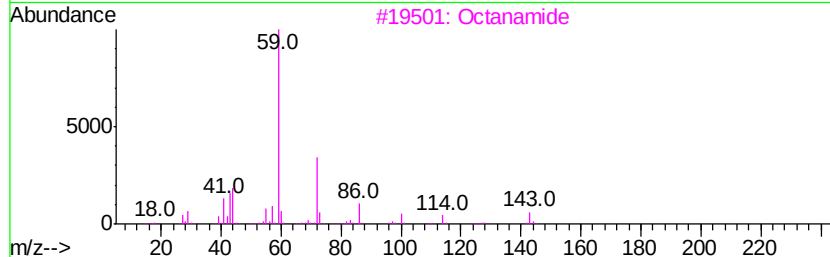
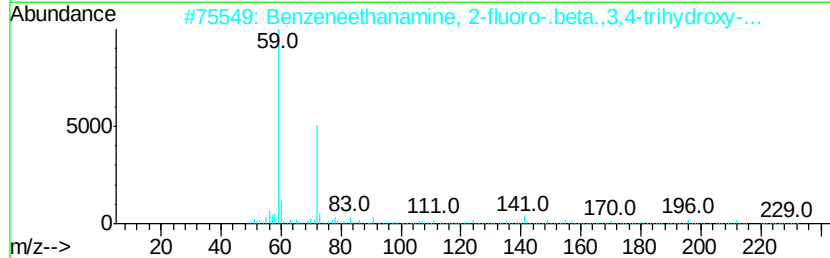
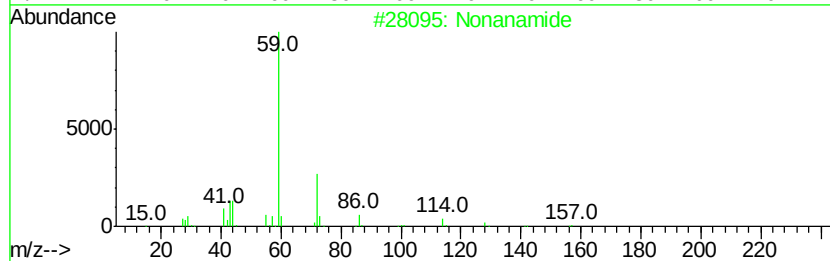
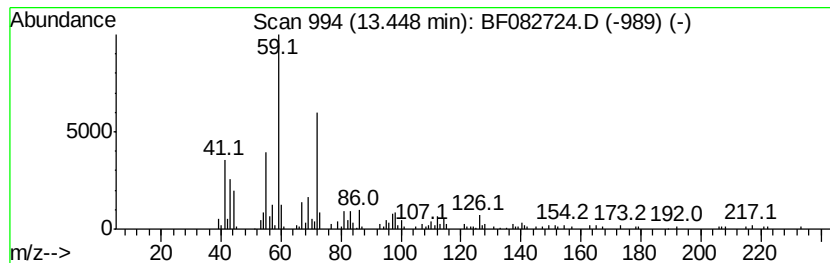
Instrument :
BNA_F
ClientSampleId :
SB-11(18-20)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Nonanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	2.79 ng	258482	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonanamide		157 C9H19NO	001120-07-6 72
2	Benzeneethanamine, 2-fluoro-.bet...		229 C11H16FN03	061338-98-5 64
3	Octanamide		143 C8H17NO	000629-01-6 64
4	Dodecanamide		199 C12H25NO	001120-16-7 64
5	Pentanamide, 4-methyl-		115 C6H13NO	001119-29-5 59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF110615\
Data File : BF082724.D
Acq On : 5 Nov 2015 12:41
Operator : UM/IZ
Sample : G4241-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11(18-20)

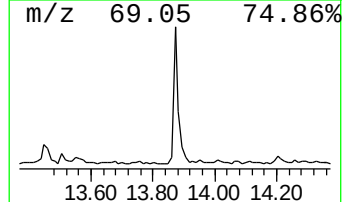
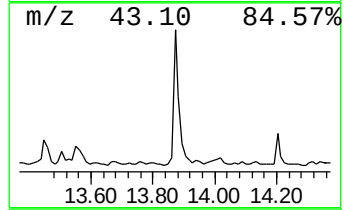
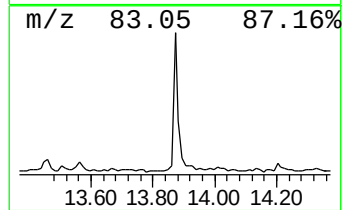
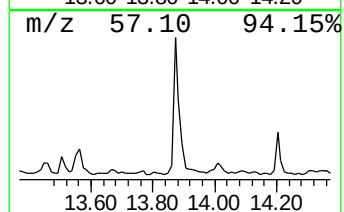
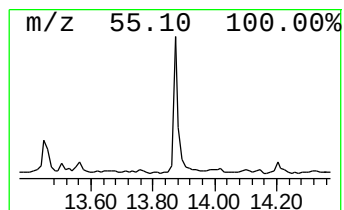
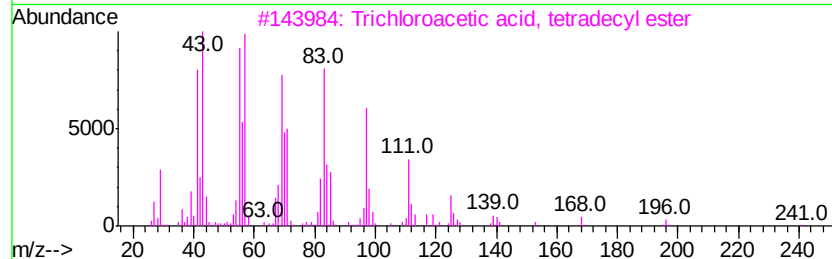
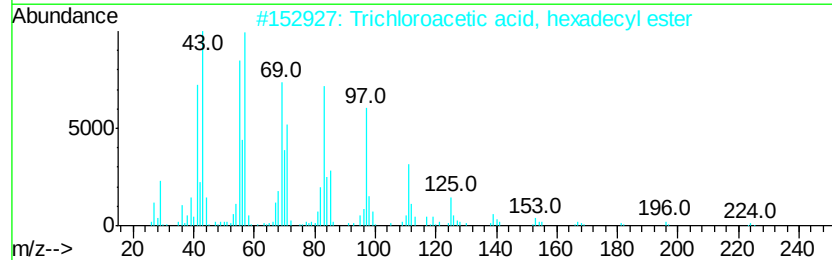
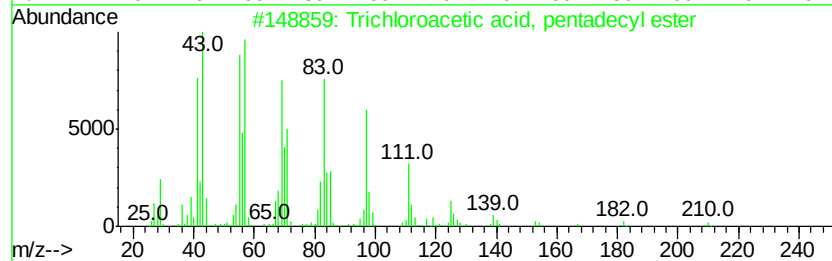
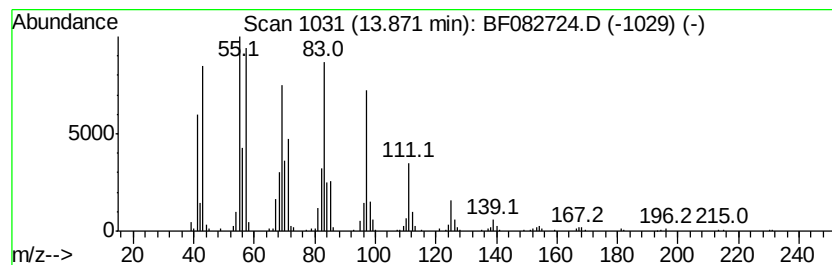
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.14 ng	568667	Chrysene-d12	14.02

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4			1-Heptadecanol	256	C17H36O	001454-85-9	90
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110615\
Data File : BF082724.D
Acq On : 5 Nov 2015 12:41
Operator : UM/IZ
Sample : G4241-18
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11(18-20)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.06	48.3	ng	2617820	1	6.86	1084710	20.0
unknown6.64	6.64	100.0	ng	5421760	1	6.86	1084710	20.0
Tetracosane	10.82	2.7	ng	224340	4	11.38	1673180	20.0
n-Hexadecanoic acid	11.92	5.0	ng	421648	4	11.38	1673180	20.0
n-Decanoic acid	12.71	2.1	ng	197676	5	14.02	1851860	20.0
Nonanamide	13.45	2.8	ng	258482	5	14.02	1851860	20.0
Trichloroacetic a...	13.87	6.1	ng	568667	5	14.02	1851860	20.0