

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050916\
 Data File : BF086847.D
 Acq On : 10 May 2016 3:48
 Operator : UM/SJ
 Sample : H2895-13
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP11-8-9FT

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-BF050916.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	4.864	241	243	250	rBV	292923	511048	9.22%	1.092%
2	5.298	278	281	283	rBV	4713987	5544233	100.00%	11.845%
3	5.699	314	316	327	rVB	29633	58526	1.06%	0.125%
4	6.350	370	373	376	rBV	4187982	5355396	96.59%	11.442%
5	6.464	381	383	385	rBV	5279739	5190695	93.62%	11.090%
6	6.693	400	403	405	rBV	836479	1090414	19.67%	2.330%
7	6.841	414	416	419	rBV	3227546	3313557	59.77%	7.079%
8	7.264	450	453	455	rBV	3473257	3749942	67.64%	8.012%
9	7.973	513	515	518	rBV	1556746	1445286	26.07%	3.088%
10	9.059	607	610	612	rBV	3405548	4220620	76.13%	9.017%
11	9.447	642	644	647	rBV	265315	379630	6.85%	0.811%
12	9.665	661	663	666	rBV	168014	148298	2.67%	0.317%
13	9.722	666	668	671	rVB	1669639	1564321	28.22%	3.342%
14	10.168	704	707	708	rVB	174587	183104	3.30%	0.391%
15	10.385	723	726	729	rBV	67993	113134	2.04%	0.242%
16	10.510	734	737	740	rBV2	2738965	3417196	61.64%	7.301%
17	10.636	746	748	755	rVB	205122	262798	4.74%	0.561%
18	11.082	783	787	788	rBV	71987	77988	1.41%	0.167%
19	11.208	795	798	800	rBV	1020118	1501329	27.08%	3.208%
20	11.745	843	845	849	rBV2	297577	334213	6.03%	0.714%
21	11.813	849	851	856	rVB2	41637	83117	1.50%	0.178%
22	12.408	901	903	905	rBV	192491	183765	3.31%	0.393%
23	12.636	919	923	924	rBV	129279	178825	3.23%	0.382%
24	12.785	933	936	939	rVB	3419702	3206574	57.84%	6.851%
25	12.968	948	952	954	rVB	29372	57351	1.03%	0.123%
26	13.025	954	957	959	rBV	52910	69022	1.24%	0.147%
27	13.276	975	979	983	rVB2	26260	77564	1.40%	0.166%
28	13.699	1013	1016	1021	rBV2	130805	282914	5.10%	0.604%
29	13.825	1024	1027	1033	rVB	1086643	1224650	22.09%	2.616%
30	14.305	1065	1069	1070	rBV3	86799	168461	3.04%	0.360%
31	14.351	1072	1073	1077	rVB4	52981	83532	1.51%	0.178%
32	14.591	1092	1094	1099	rVB5	23385	56026	1.01%	0.120%
33	14.671	1099	1101	1105	rBV2	34504	67339	1.21%	0.144%
34	14.831	1112	1115	1120	rBV	86124	263992	4.76%	0.564%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.899	1120	1121	1126	rVB2	58665	117653	2.12%	0.251%
36	15.094	1135	1138	1140	rVB	41359	56313	1.02%	0.120%
37	15.151	1140	1143	1145	rVB	81981	129175	2.33%	0.276%
38	15.208	1145	1148	1150	rBV	660713	1002150	18.08%	2.141%
39	15.402	1163	1165	1170	rVB6	27141	64492	1.16%	0.138%
40	15.665	1185	1188	1190	rBV3	153885	253454	4.57%	0.541%
41	15.722	1190	1193	1195	rVB4	90953	198204	3.57%	0.423%
42	16.488	1257	1260	1264	rBV	30806	70395	1.27%	0.150%
43	16.694	1275	1278	1287	rVB10	27722	109713	1.98%	0.234%
44	16.877	1291	1294	1296	rBV	26392	60451	1.09%	0.129%
45	18.488	1433	1435	1438	rVB4	91412	159197	2.87%	0.340%
46	18.751	1455	1458	1464	rVB7	19808	63063	1.14%	0.135%
47	19.026	1478	1482	1485	rVB6	20677	57470	1.04%	0.123%

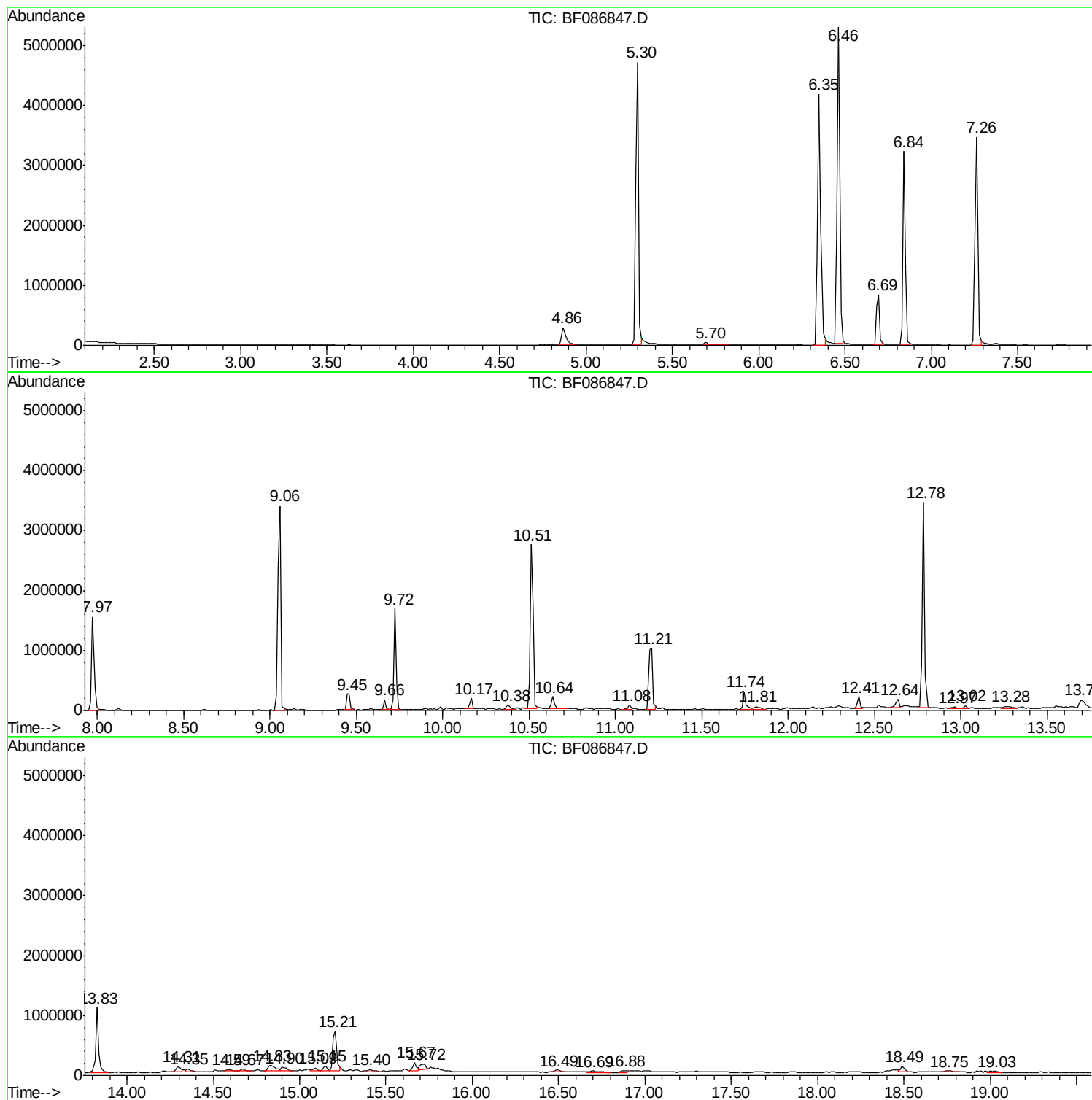
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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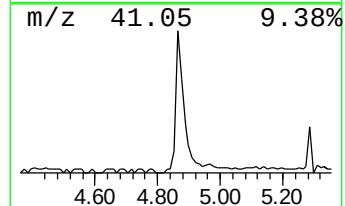
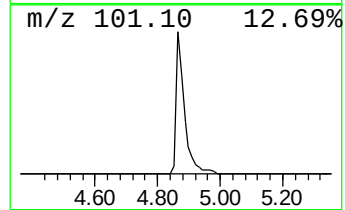
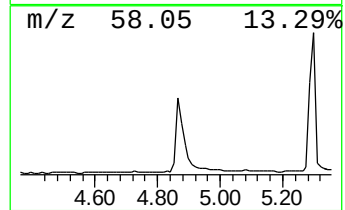
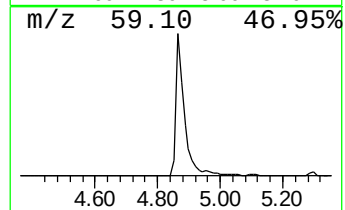
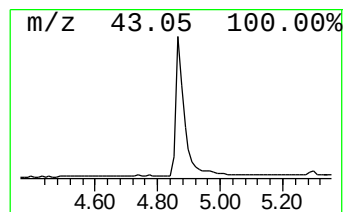
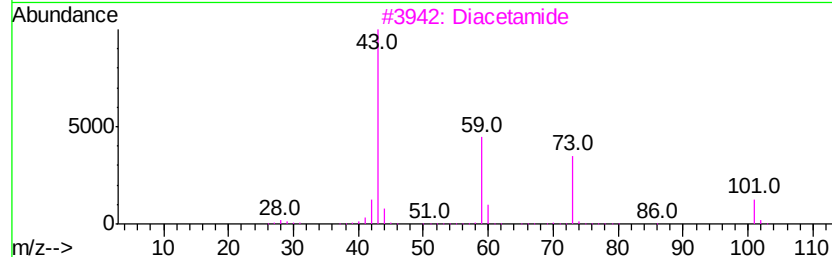
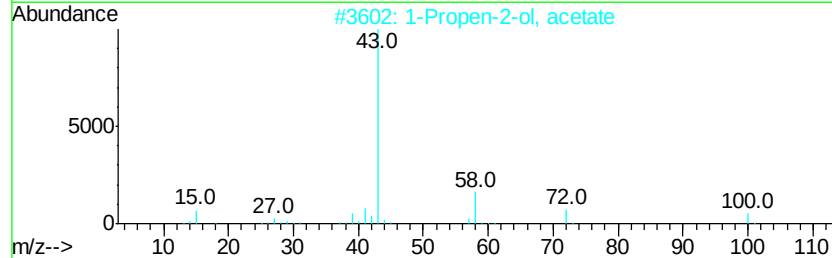
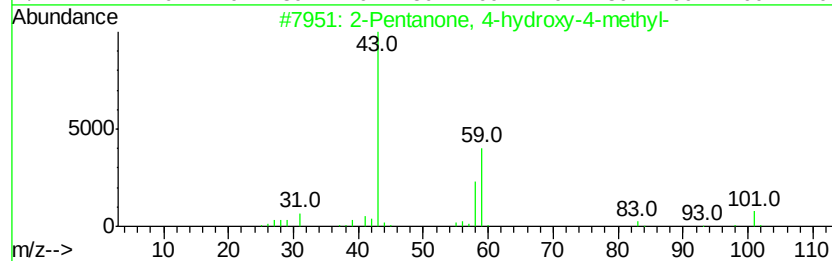
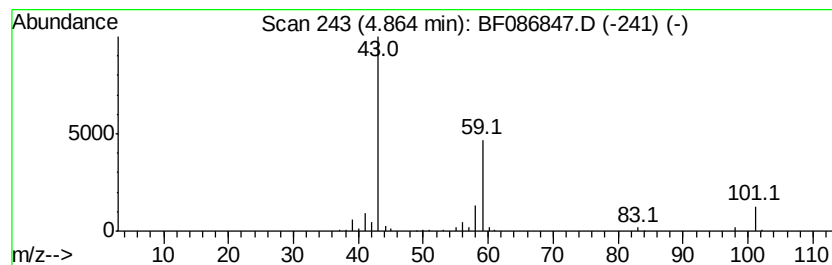
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.86	9.37 ng	511048	1,4-Dichlorobenzene-d4	6.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Diacetamide	101	C4H7NO2	000625-77-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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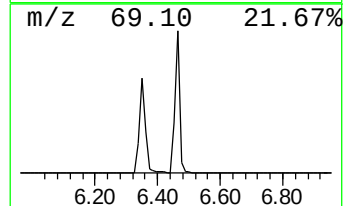
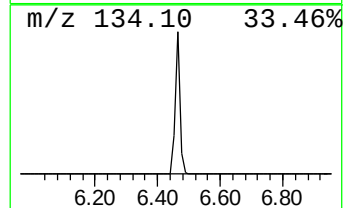
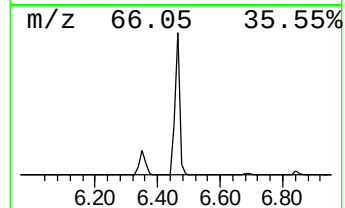
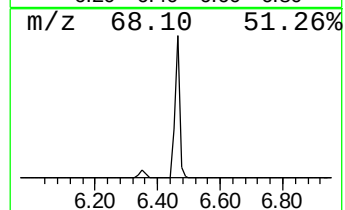
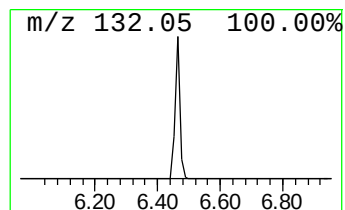
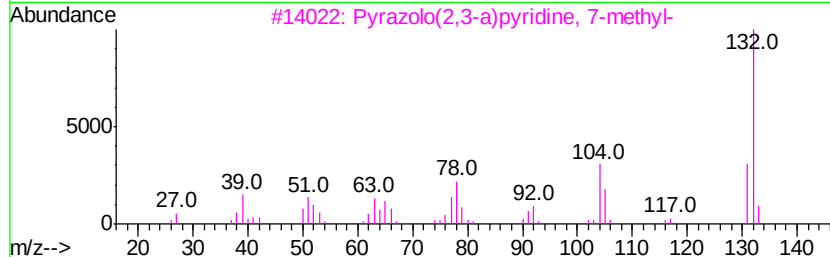
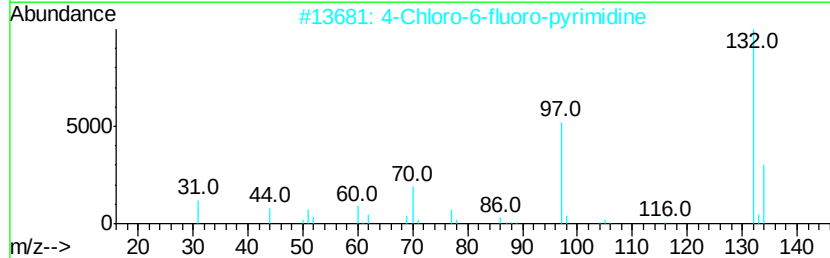
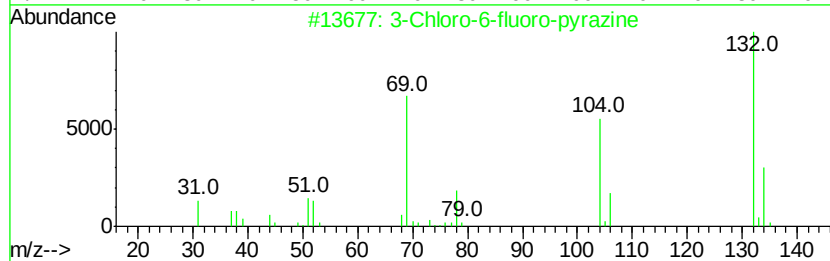
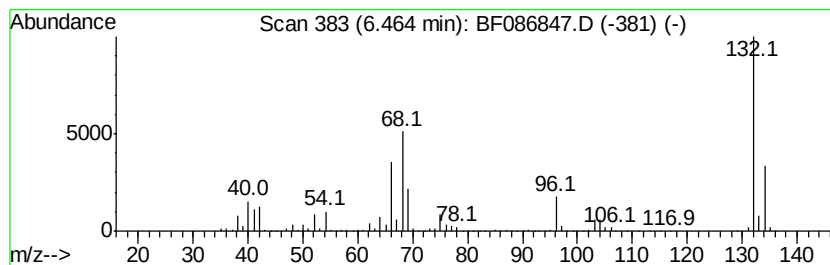
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	95.21 ng	5190700	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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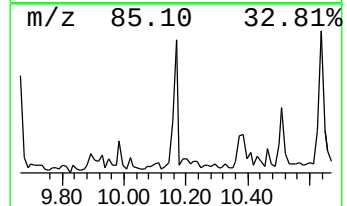
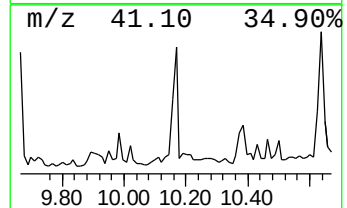
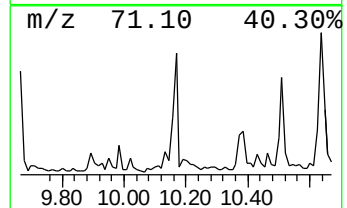
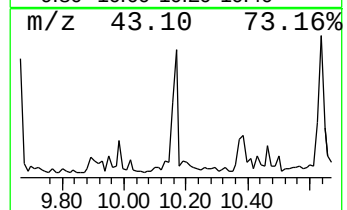
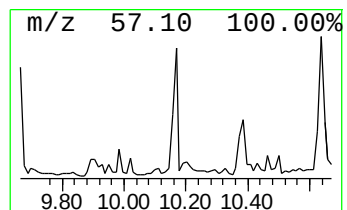
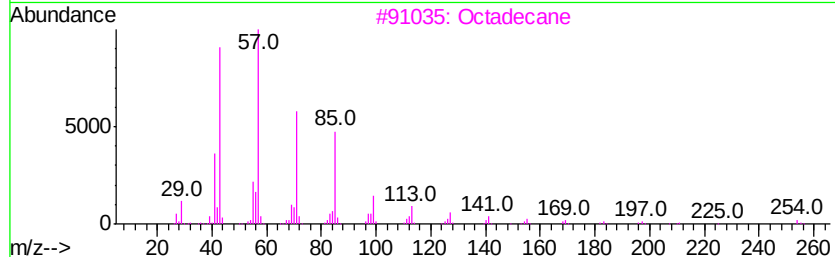
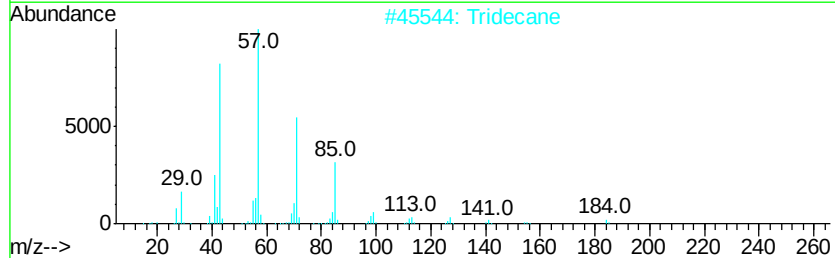
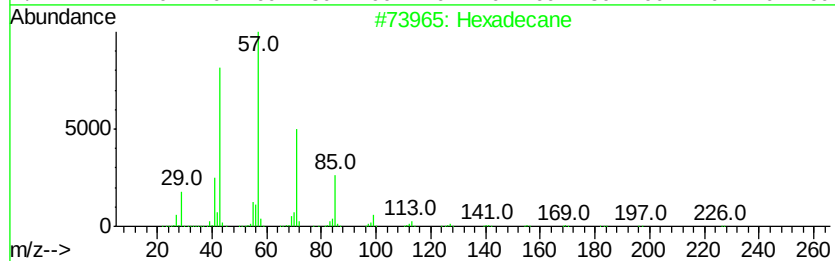
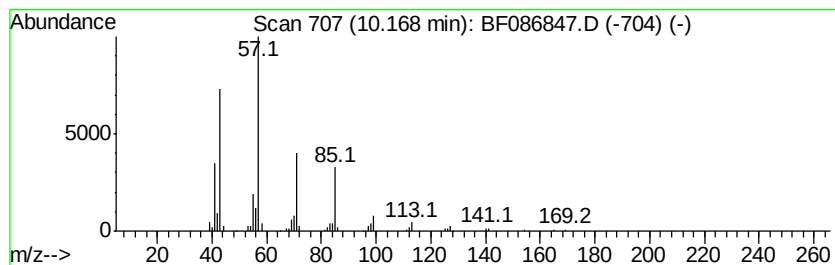
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	2.34 ng	183104	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Tridecane	184	C13H28	000629-50-5	86
3		Octadecane	254	C18H38	000593-45-3	80
4		Tetradecane	198	C14H30	000629-59-4	80
5		Dodecane, 3-methyl-	184	C13H28	017312-57-1	64



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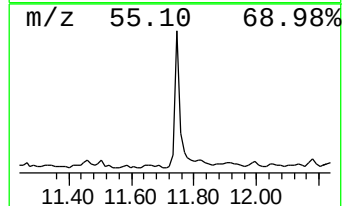
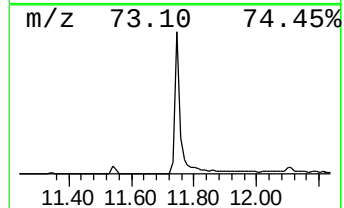
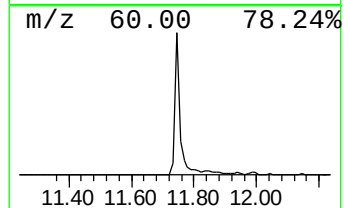
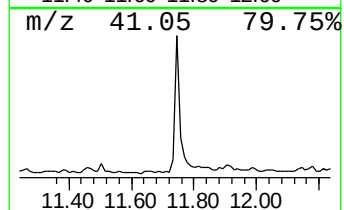
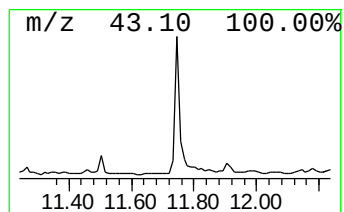
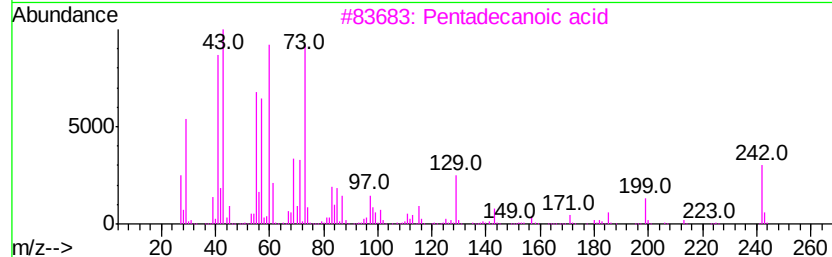
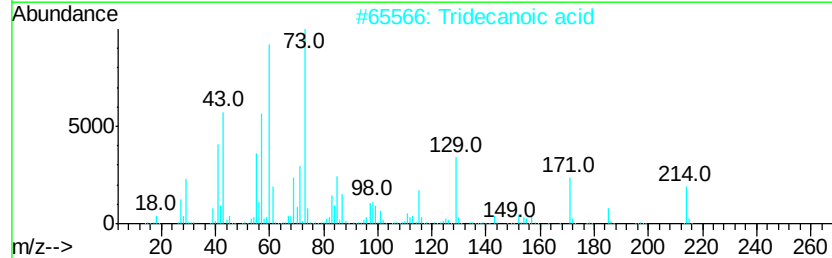
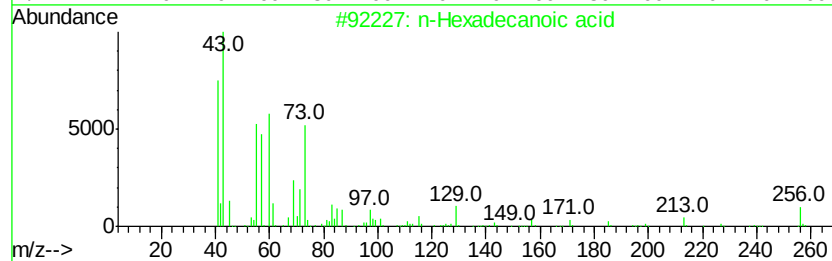
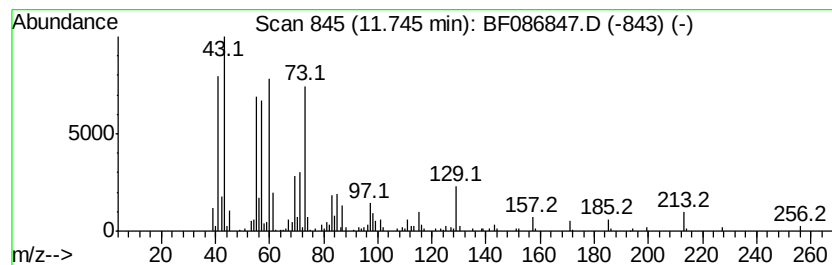
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	4.45 ng	334213	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	78



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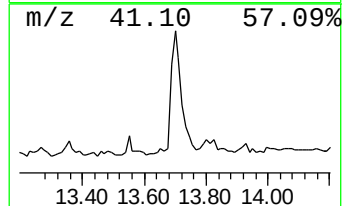
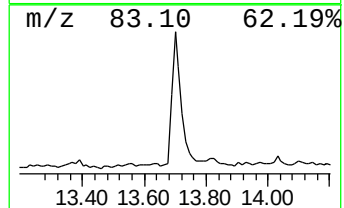
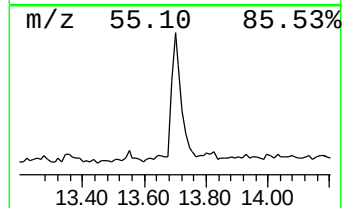
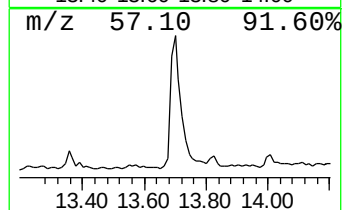
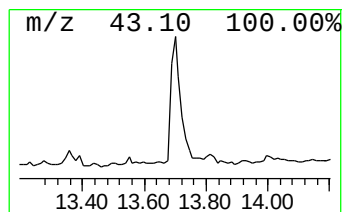
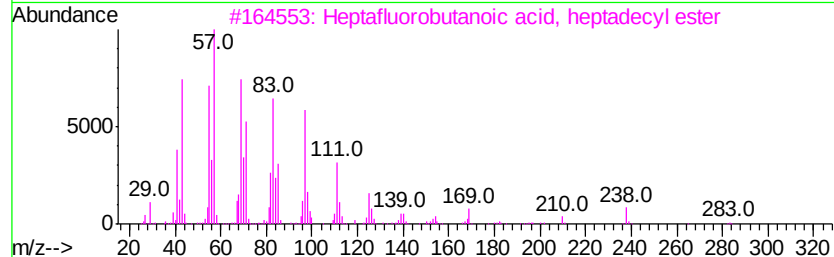
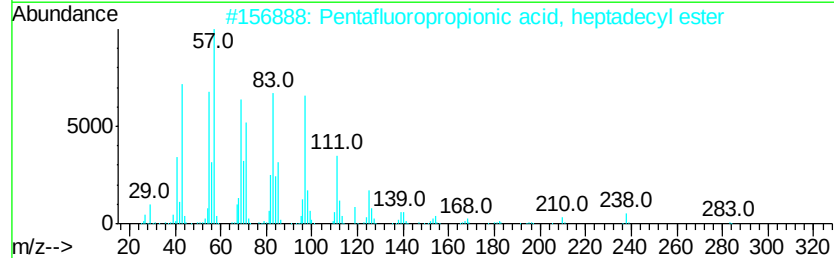
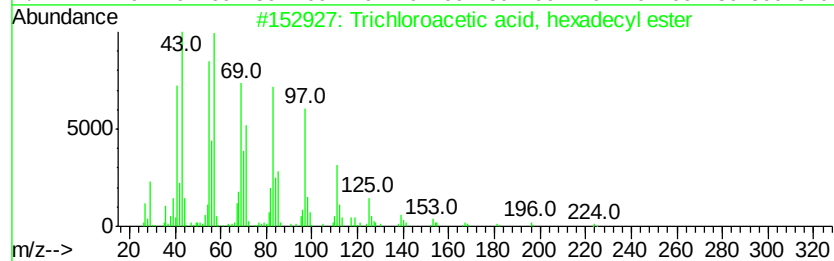
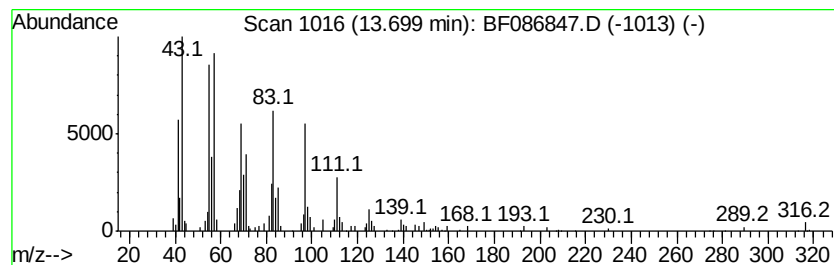
Instrument :
BNA_F
ClientSampleId :
TP11-8-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.70	4.62 ng	282914	Chrysene-d12	13.82		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	81
5		1-Octadecanol	270	C18H38O	000112-92-5	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
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Acq On : 10 May 2016 3:48
Operator : UM/SJ
Sample : H2895-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

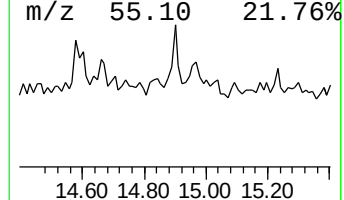
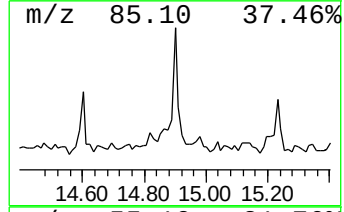
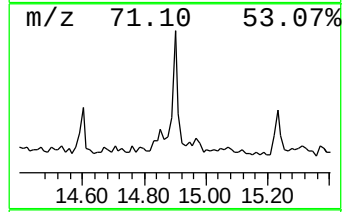
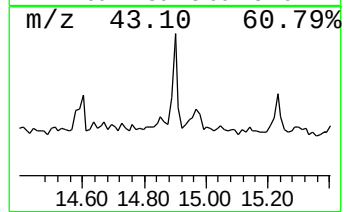
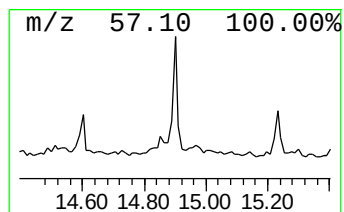
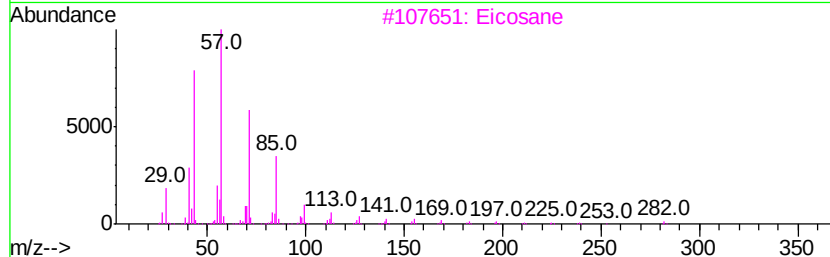
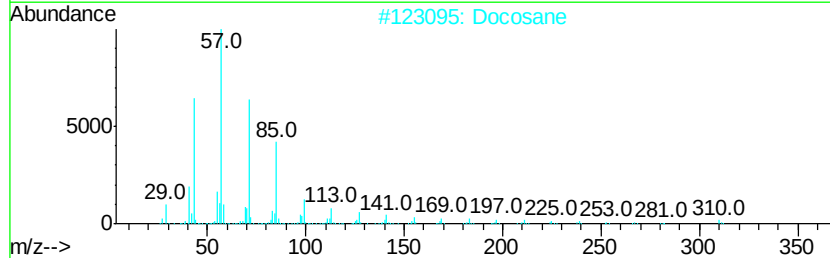
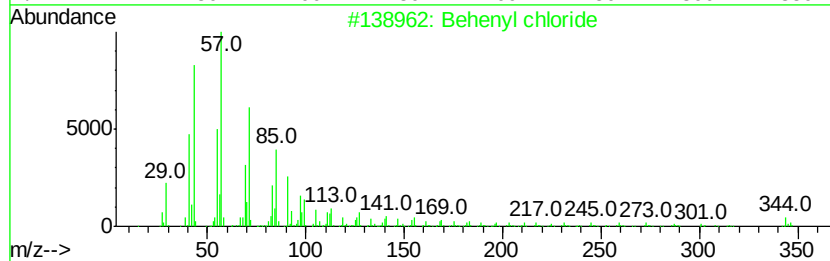
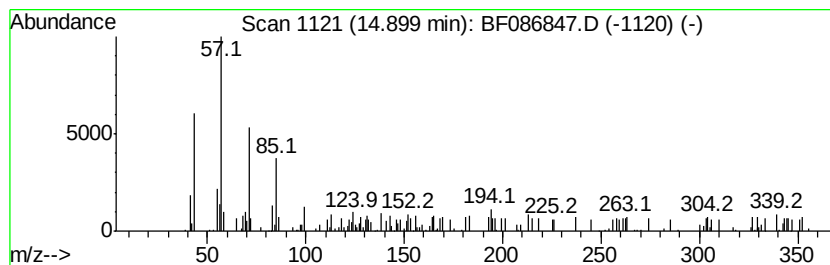
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Behenyl chloride Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.90	2.35 ng	117653	Perylene-d12	15.21	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenyl chloride	344	C22H45Cl	042217-03-8	58
2	Docosane	310	C22H46	000629-97-0	55
3	Eicosane	282	C20H42	000112-95-8	55
4	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	55
5	Pentacosane	352	C25H52	000629-99-2	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050916\
Data File : BF086847.D
Acq On : 10 May 2016 3:48
Operator : UM/SJ
Sample : H2895-13
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP11-8-9FT

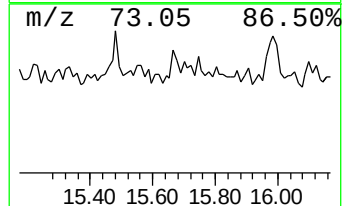
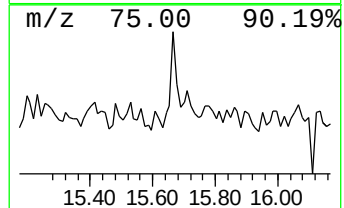
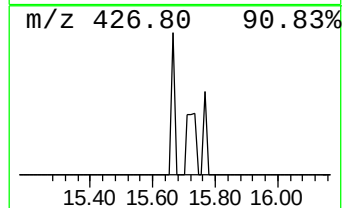
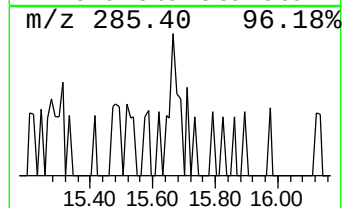
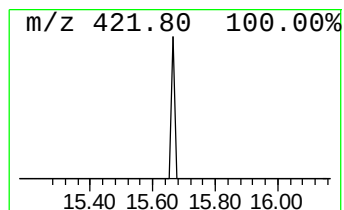
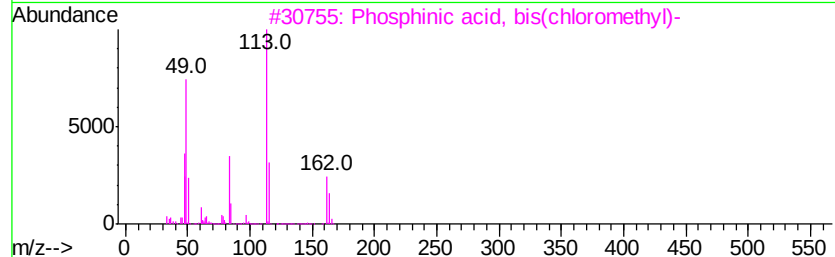
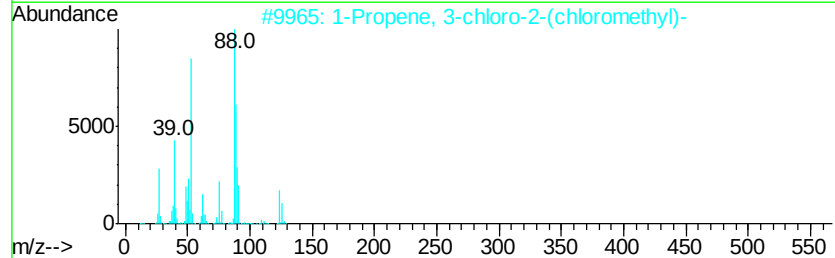
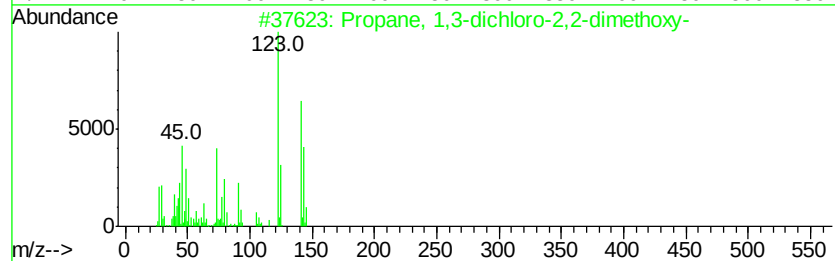
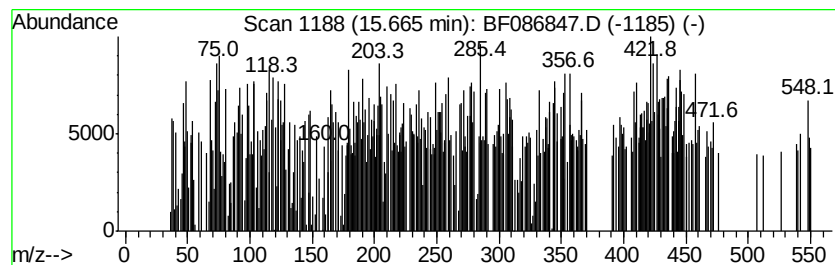
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.67 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	5.06 ng	253454	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,3-dichloro-2,2-dimeth...	172	C5H10Cl2O2	006626-57-9	27
2		1-Propene, 3-chloro-2-(chloromet...	124	C4H6Cl2	001871-57-4	27
3		Phosphinic acid, bis(chloromethyl)-	162	C2H5Cl2O2P	013274-83-4	27
4		Pseudo-solasodine 3-O-acetate-N-[...	526	C32H50N2O4	034638-85-2	25
5		1-Propene, 1,3-dichloro-, (Z)-	110	C3H4Cl2	010061-01-5	16



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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP11-8-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.86	9.4	ng	511048	1	6.69	1090410	20.0
unknown6.46	6.46	95.2	ng	5190700	1	6.69	1090410	20.0
Hexadecane	10.17	2.3	ng	183104	3	9.72	1564320	20.0
n-Hexadecanoic acid	11.74	4.5	ng	334213	4	11.21	1501330	20.0
Trichloroacetic a...	13.70	4.6	ng	282914	5	13.82	1224650	20.0
Behenyl chloride	14.90	2.4	ng	117653	6	15.21	1002150	20.0
unknown15.67	15.67	5.1	ng	253454	6	15.21	1002150	20.0