

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085525.D
 Acq On : 18 Mar 2016 8:04
 Operator : UM/SJ
 Sample : H1776-10
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-05(0.5-3.0)

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-BF031516.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	243	245	251	rBV	62456	90390	2.30%	0.252%
2	5.487	276	280	282	rBV	2737999	3926832	100.00%	10.927%
3	6.516	366	370	372	rBV	3103474	3900176	99.32%	10.853%
4	6.642	379	381	384	rBV	2977154	3698964	94.20%	10.293%
5	6.870	399	401	404	rBV	705308	783699	19.96%	2.181%
6	7.030	413	415	418	rBV	2807910	2873225	73.17%	7.995%
7	7.442	448	451	453	rBV	2330701	2415161	61.50%	6.721%
8	7.533	456	459	466	rVB	70208	96038	2.45%	0.267%
9	8.162	511	514	516	rBV	1241720	1069126	27.23%	2.975%
10	9.236	605	608	611	rBV	3083230	3752299	95.56%	10.441%
11	9.636	640	643	645	rBV	717384	760199	19.36%	2.115%
12	9.853	659	662	664	rVB	55010	67075	1.71%	0.187%
13	9.922	665	668	670	rVB	734137	1030914	26.25%	2.869%
14	10.345	704	705	707	rVB	109245	100724	2.57%	0.280%
15	10.562	722	724	728	rBV	36978	70571	1.80%	0.196%
16	10.711	734	737	739	rBV2	1854016	2400109	61.12%	6.679%
17	10.825	745	747	751	rBV	92291	152526	3.88%	0.424%
18	11.271	784	786	787	rBV	73639	76729	1.95%	0.214%
19	11.396	795	797	800	rBV	1035075	988334	25.17%	2.750%
20	11.853	834	837	840	rBV	30752	60091	1.53%	0.167%
21	11.933	842	844	846	rBV	405369	488325	12.44%	1.359%
22	12.608	901	903	904	rBV	68120	67953	1.73%	0.189%
23	12.711	910	912	919	rVB	125458	148268	3.78%	0.413%
24	12.836	921	923	924	rVB	53044	43374	1.10%	0.121%
25	12.985	933	936	938	rBV	3056356	2784689	70.91%	7.749%
26	13.877	1012	1014	1020	rBV	284928	322965	8.22%	0.899%
27	14.037	1025	1028	1030	rBV	703097	851504	21.68%	2.369%
28	14.505	1067	1069	1071	rBV	55667	70047	1.78%	0.195%
29	14.688	1082	1085	1087	rBV	1009317	1048313	26.70%	2.917%
30	14.779	1091	1093	1097	rVV2	146899	246864	6.29%	0.687%
31	15.054	1115	1117	1121	rVB	32471	57613	1.47%	0.160%
32	15.134	1121	1124	1125	rBV	45143	60458	1.54%	0.168%
33	15.477	1151	1154	1156	rBV	458960	765200	19.49%	2.129%
34	15.922	1190	1193	1195	rBV	61791	103336	2.63%	0.288%

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W170TH-SB-05(0.5-3.0)

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-BF031516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.968	1195	1197	1205	rVB8	40093	94949	2.42%	0.264%
36	16.403	1232	1235	1237	rBV	62859	116783	2.97%	0.325%
37	16.974	1282	1285	1290	rVB2	50099	110025	2.80%	0.306%
38	17.648	1341	1344	1349	rVB	52678	131908	3.36%	0.367%
39	18.437	1409	1413	1418	rBV2	35540	111444	2.84%	0.310%

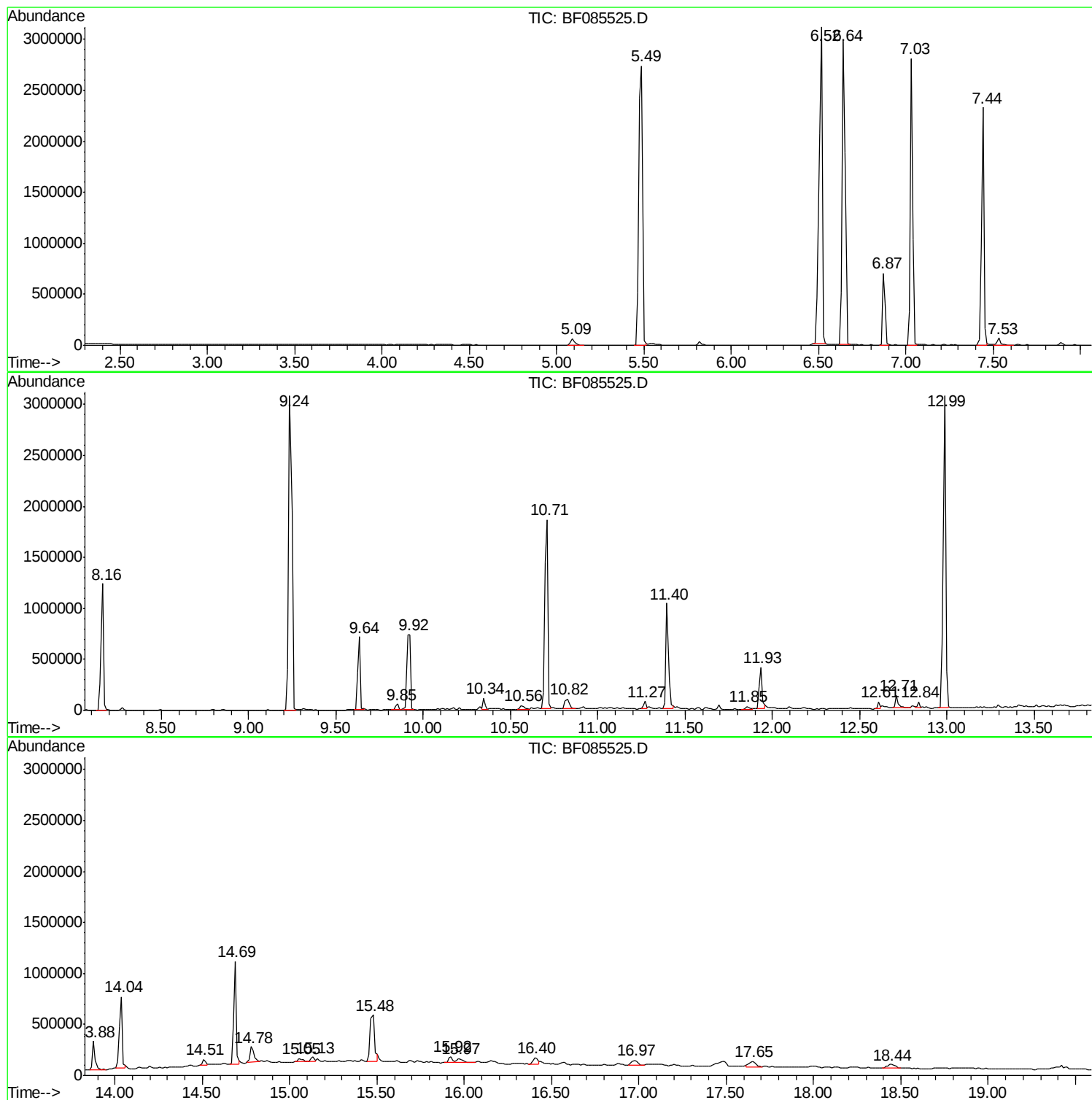
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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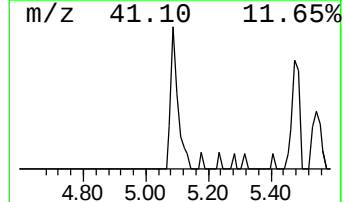
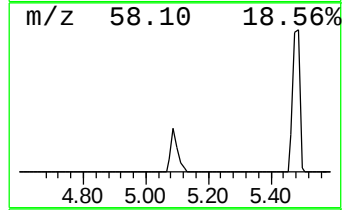
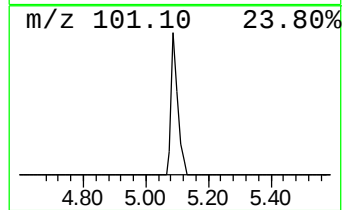
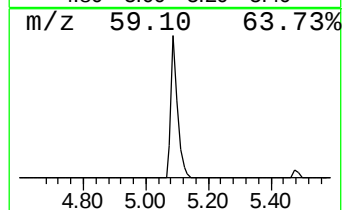
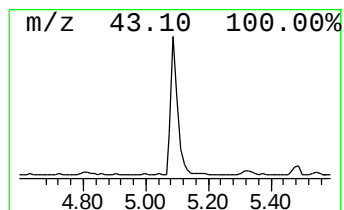
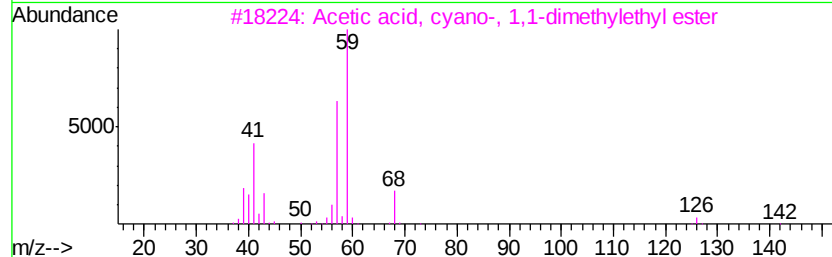
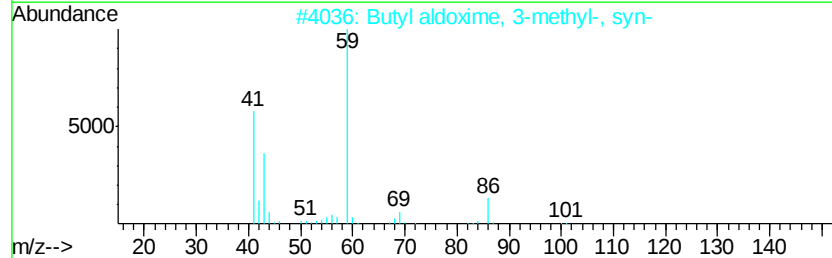
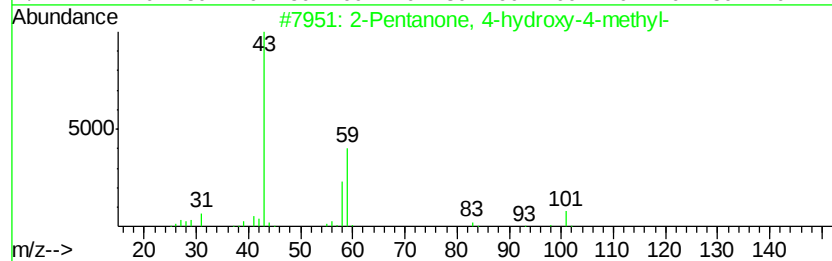
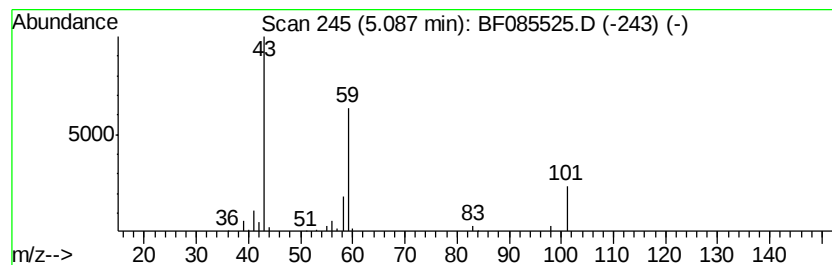
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.31 ng	90390	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Acetone	58	C3H6O	000067-64-1	9



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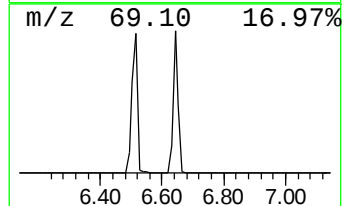
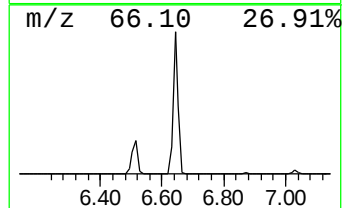
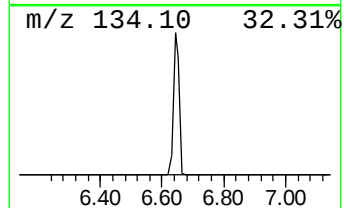
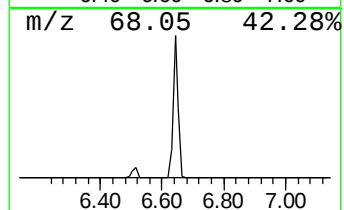
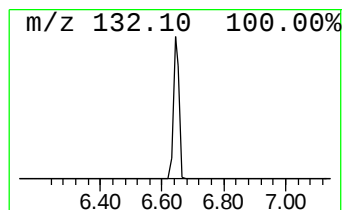
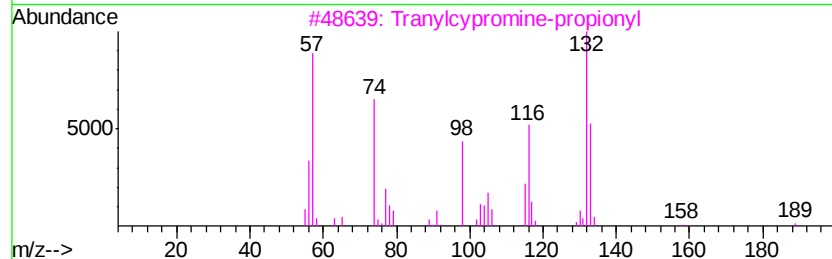
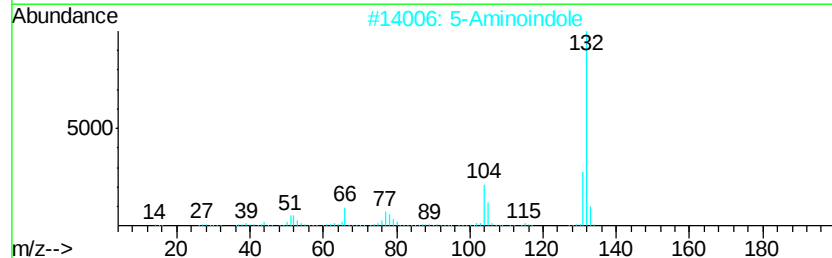
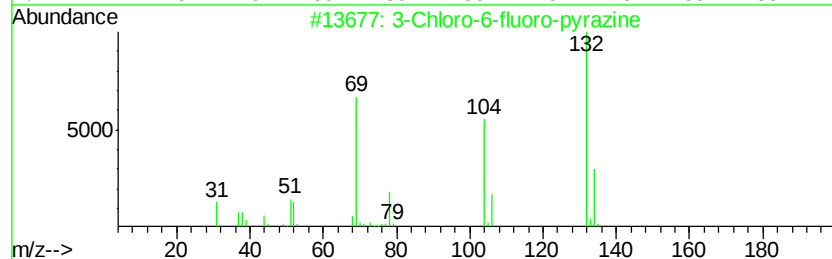
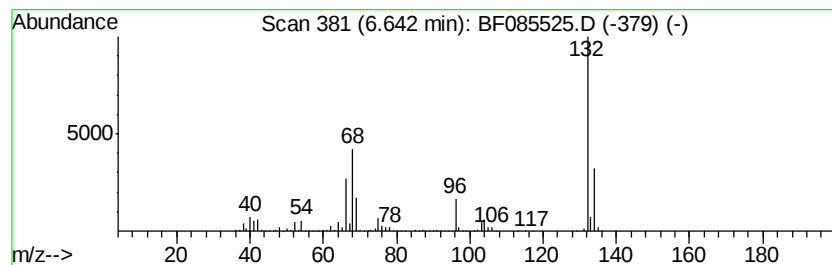
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	94.40 ng	3698960	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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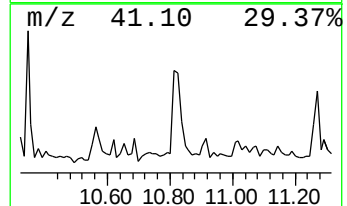
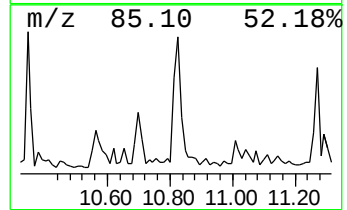
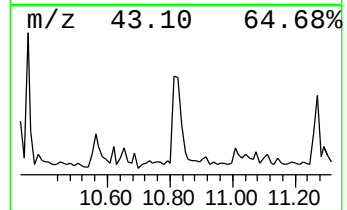
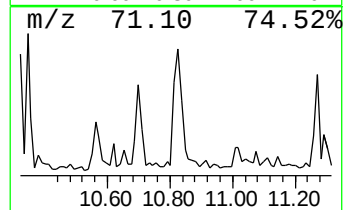
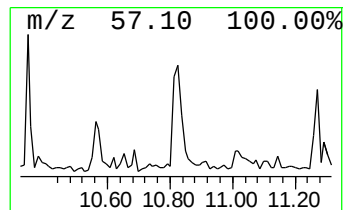
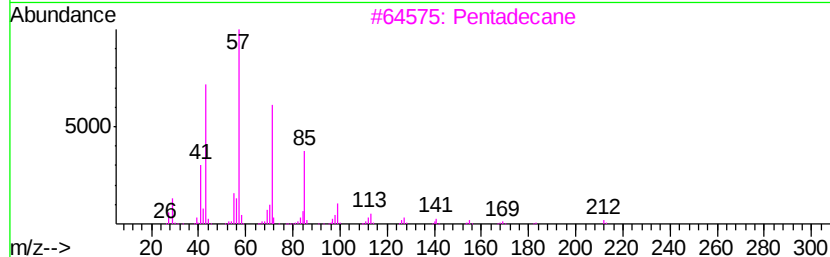
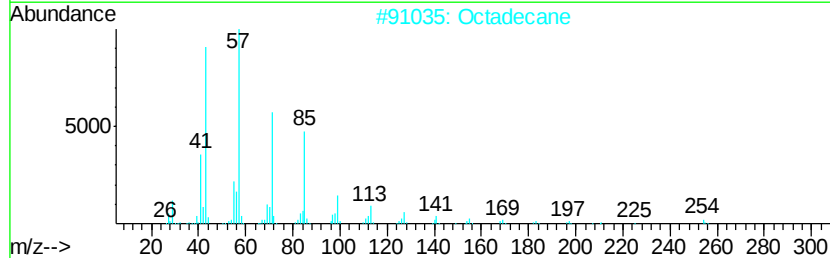
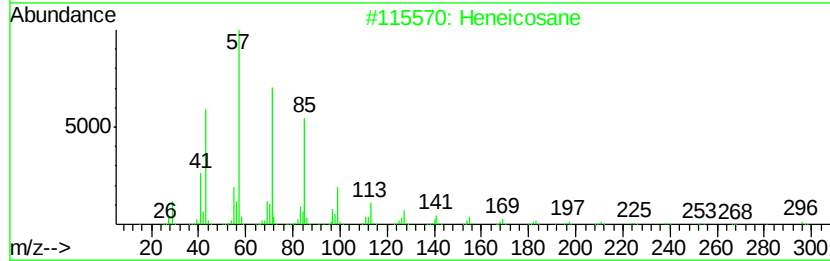
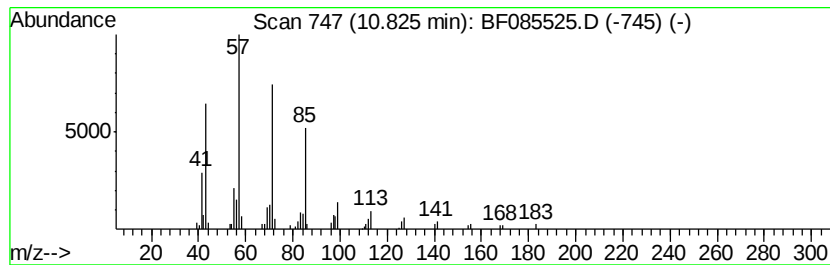
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	3.09 ng	152526	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Hexadecane	226	C16H34	000544-76-3	91



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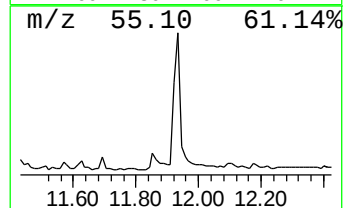
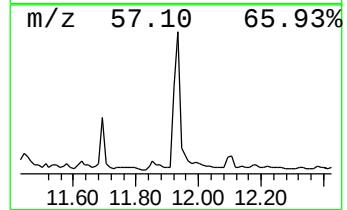
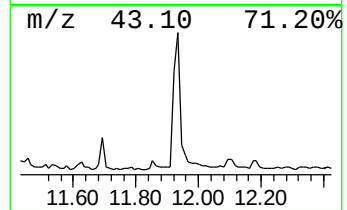
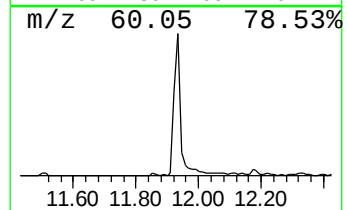
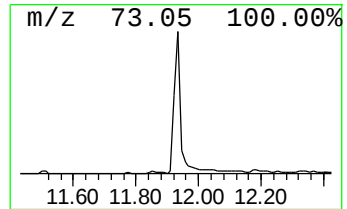
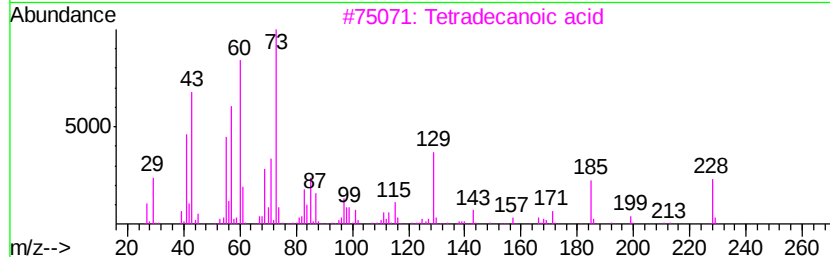
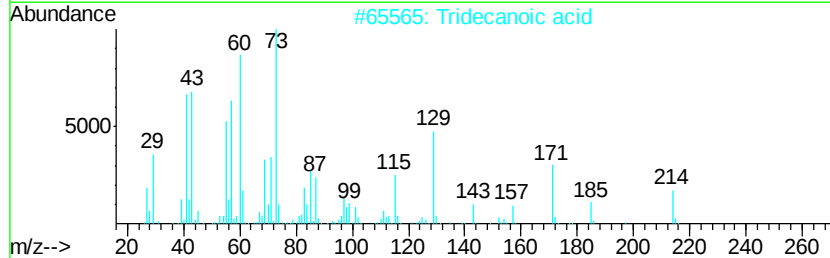
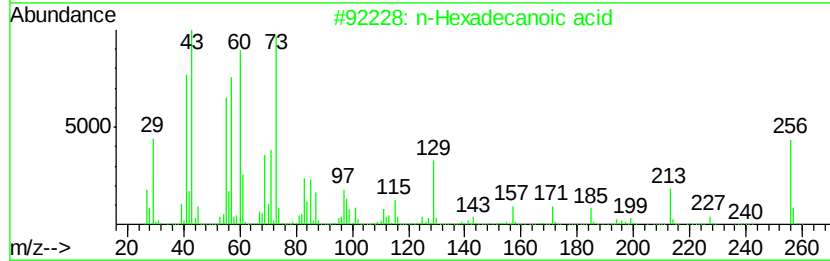
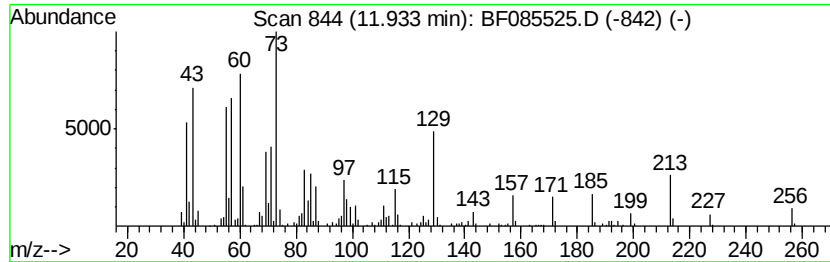
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	9.88 ng	488325	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76



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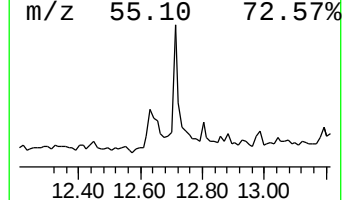
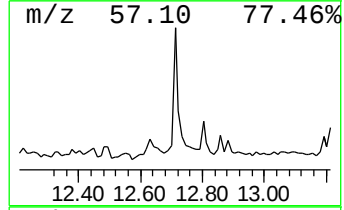
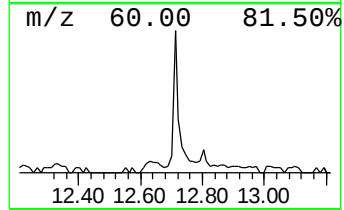
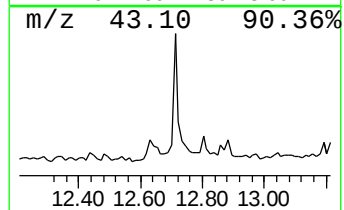
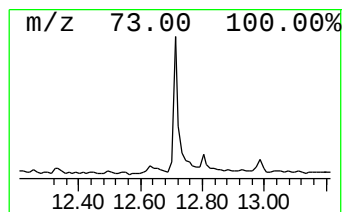
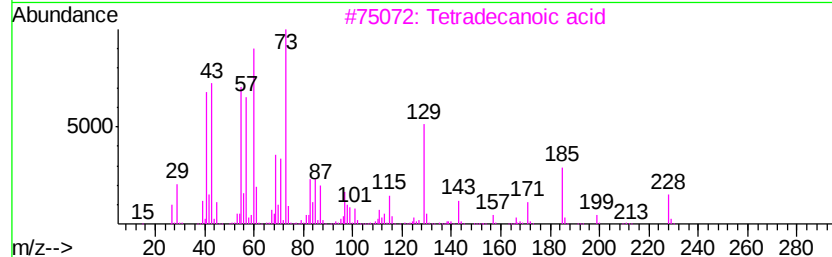
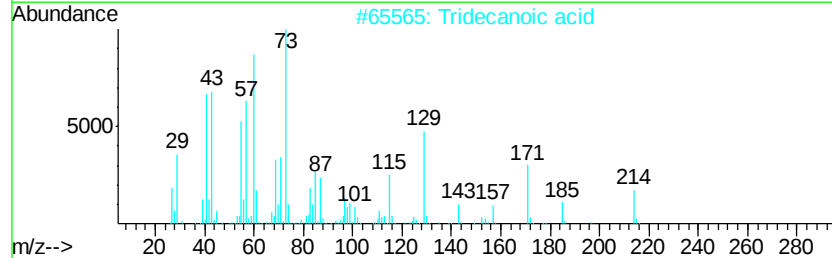
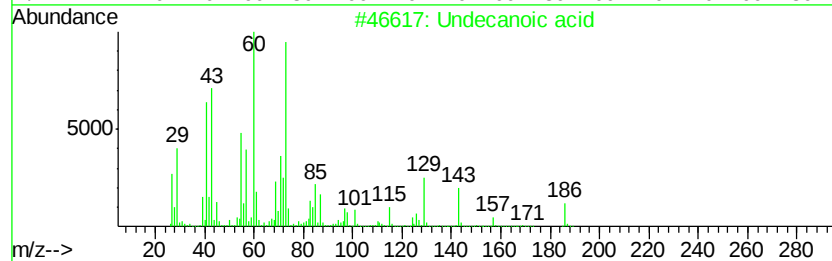
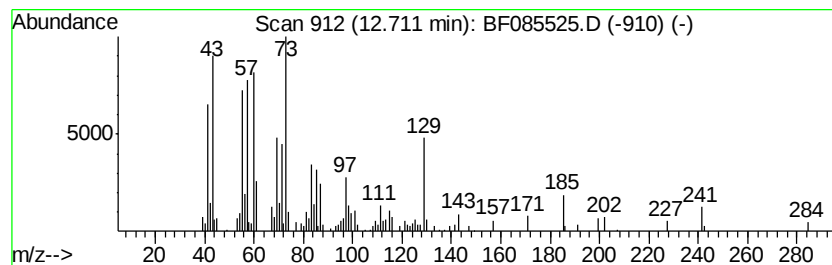
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.00 ng	148268	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid		186	C11H22O2	000112-37-8	83
2	Tridecanoic acid		214	C13H26O2	000638-53-9	80
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	58
4	Acetamide, N-(4-hydroxycyclohexy...		157	C8H15NO2	027489-61-8	18
5	Ethanol, 2-(hexadecyloxy)-		286	C18H38O2	002136-71-2	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
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ClientSampleId :
W170TH-SB-05(0.5-3.0)

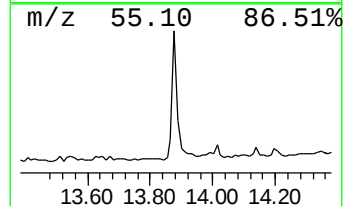
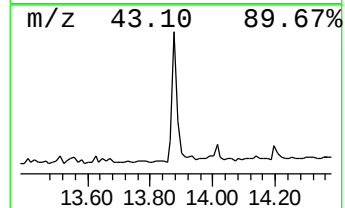
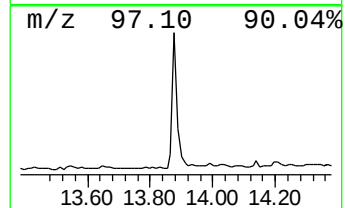
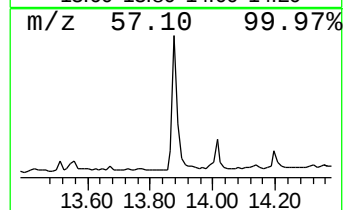
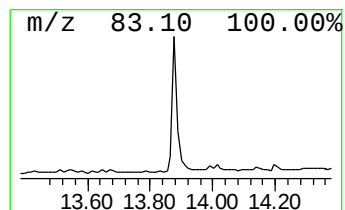
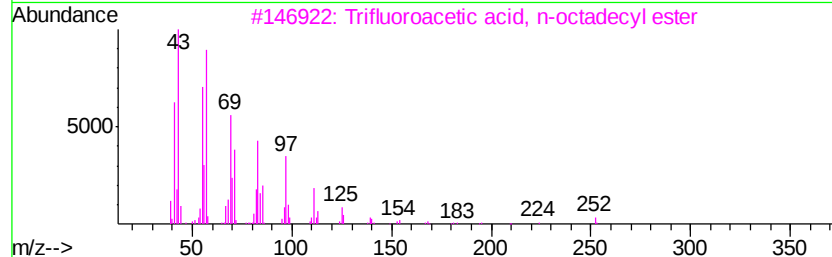
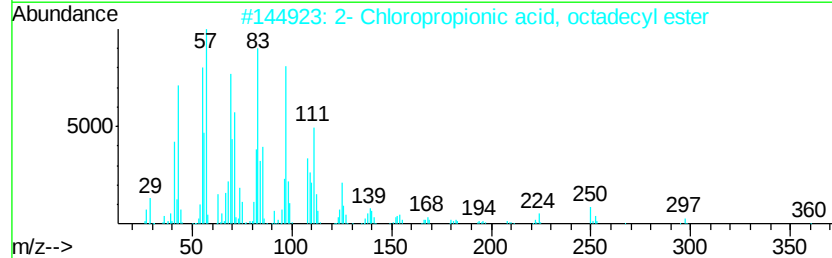
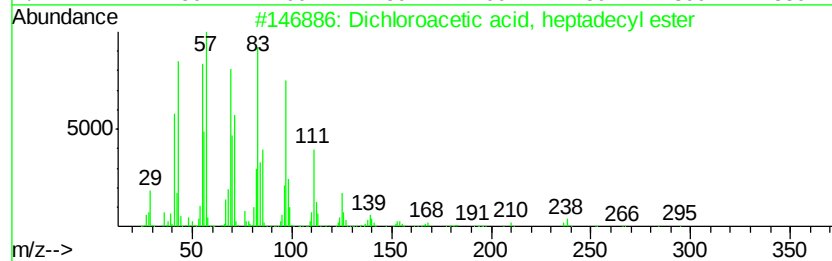
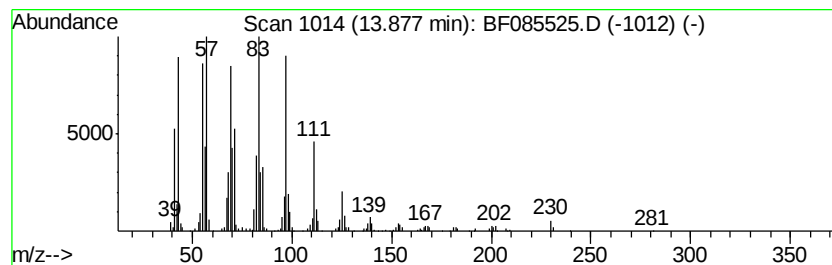
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.59 ng	322965	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
3		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

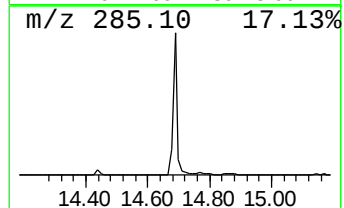
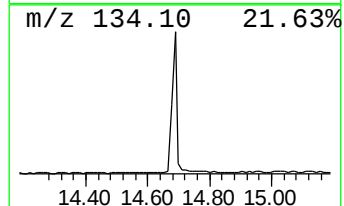
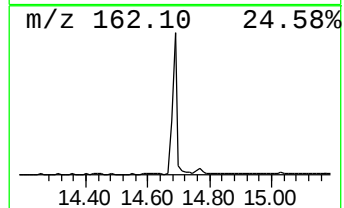
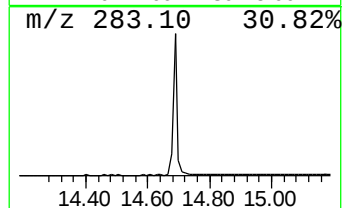
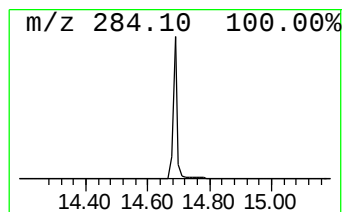
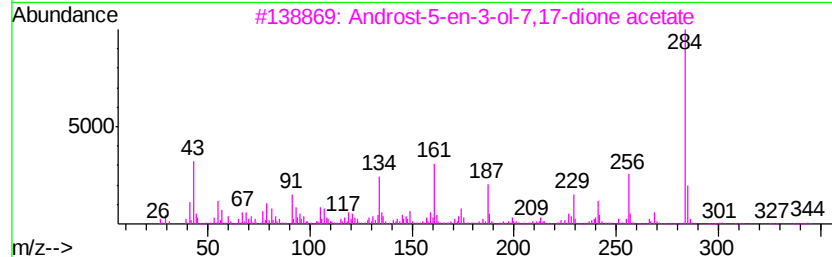
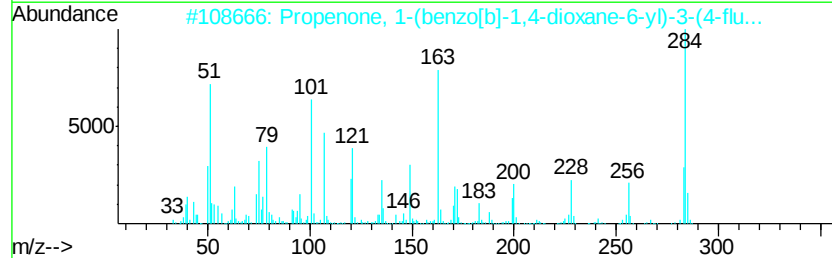
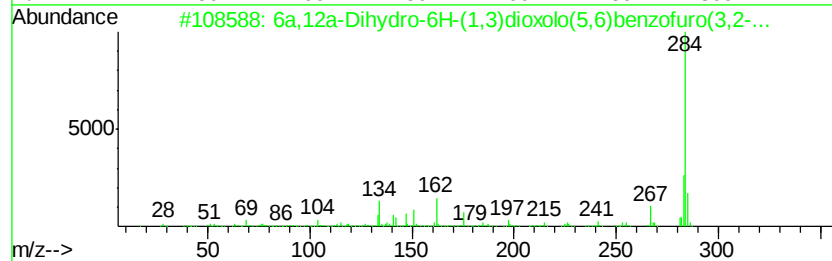
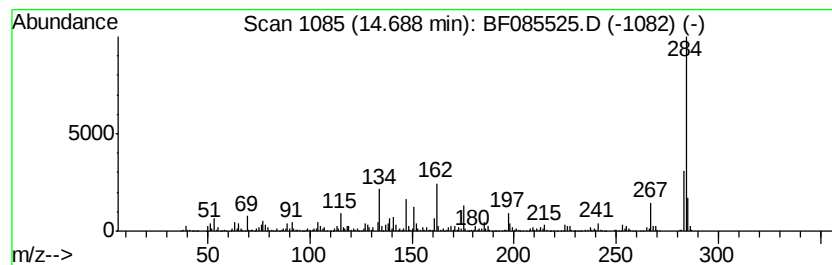
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ClientSampleId :
W170TH-SB-05(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.69	24.62 ng	1048310	Chrysene-d12	14.04		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	95	
2	Propenone, 1-(benzo[b]-1,4-dioxa...	284	C17H13F03	133188-35-9	55	
3	Androst-5-en-3-ol-7,17-dione ace...	344	C21H28O4	001449-61-2	43	
4	4-Amino-5-(4-nitrophenylazo)benz...	284	C12H8N6O3	166766-07-0	43	
5	Thiazole, 2-(4-fluorophenylamino...	284	C16H13FN2S	340801-58-3	38	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
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ClientSampleId :
W170TH-SB-05(0.5-3.0)

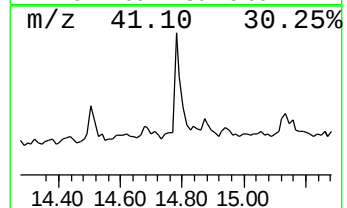
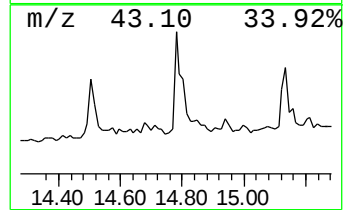
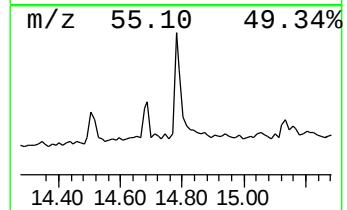
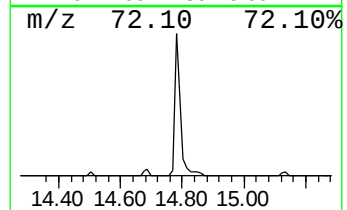
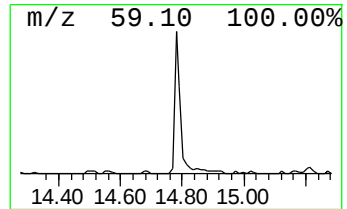
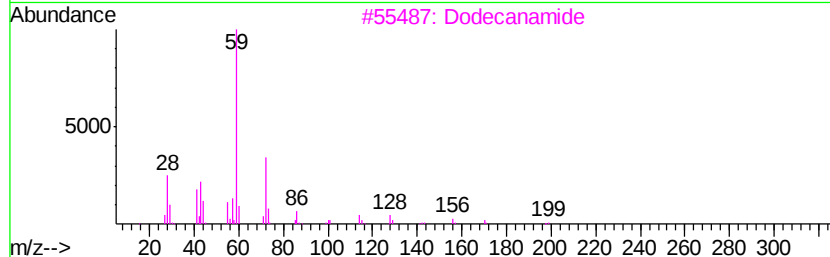
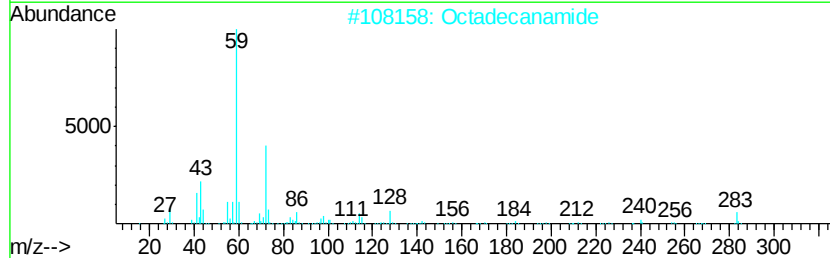
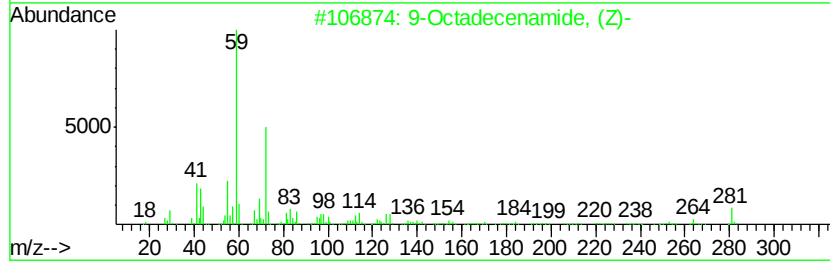
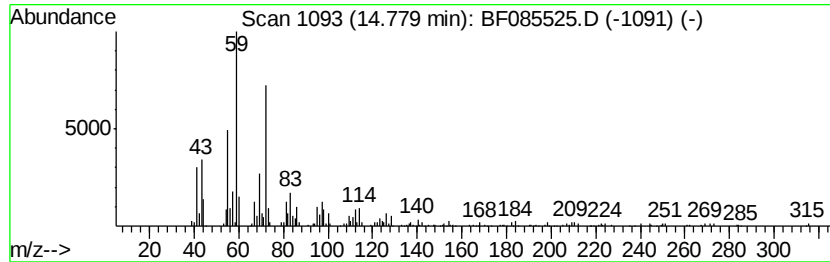
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	6.45 ng	246864	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Octadecanamide	283	C18H37NO	000124-26-5	56
3		Dodecanamide	199	C12H25NO	001120-16-7	53
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5		Tetradecanamide	227	C14H29NO	000638-58-4	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

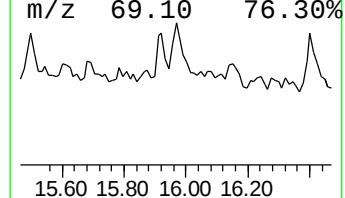
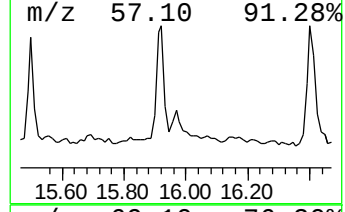
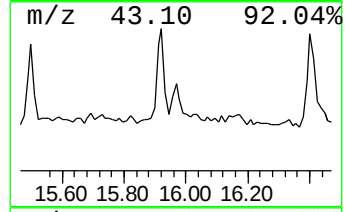
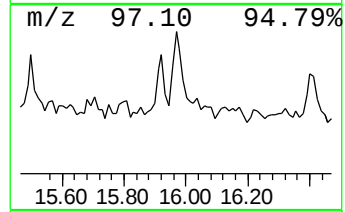
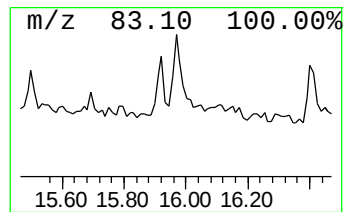
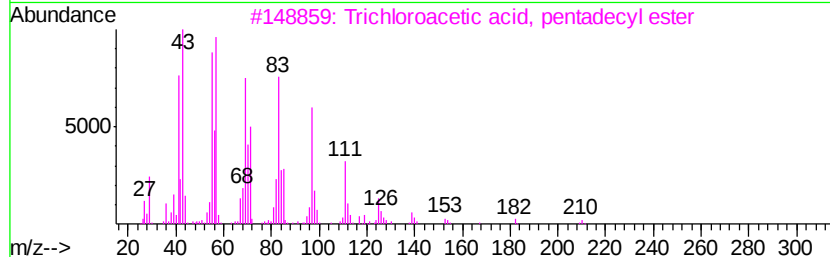
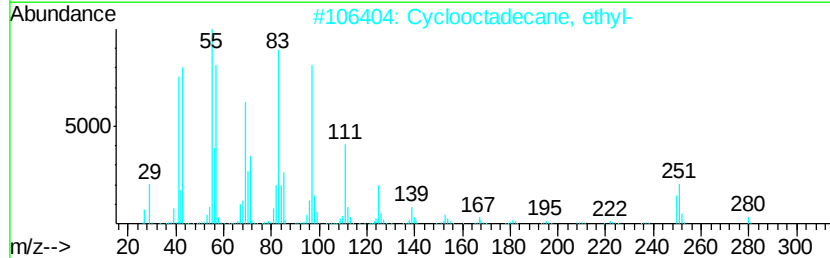
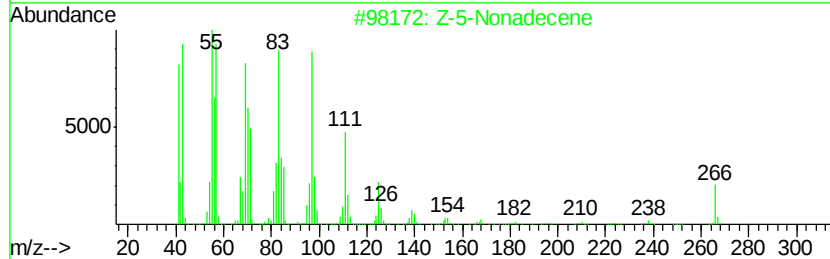
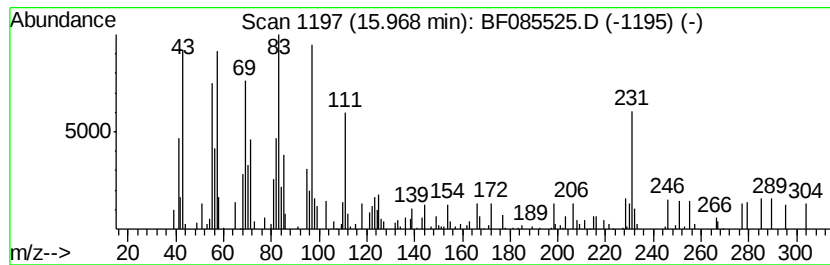
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ClientSampleId :
W170TH-SB-05(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Z-5-Nonadecene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.48 ng	94949	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Z-5-Nonadecene	266 C19H38	1000131-11-8 74
2		Cyclooctadecane, ethyl-	280 C20H40	1000151-22-5 49
3		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0 45
4		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 45
5		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W170TH-SB-05(0.5-3.0)

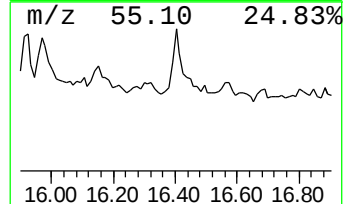
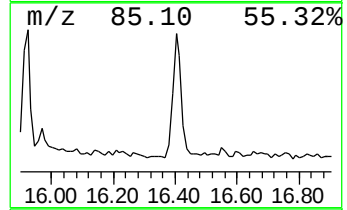
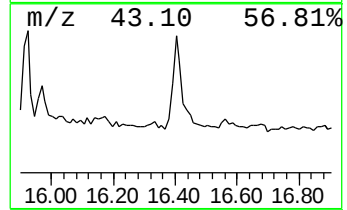
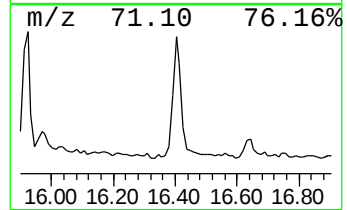
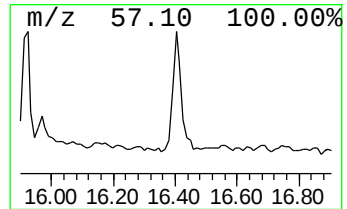
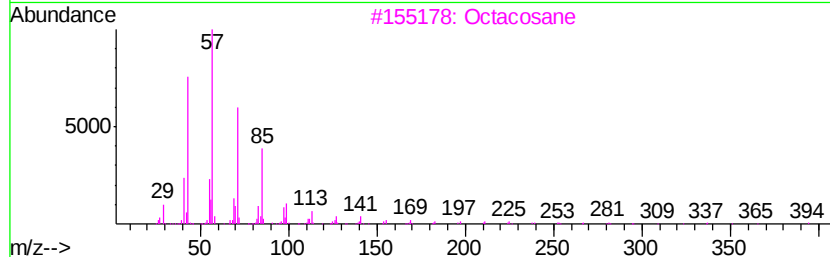
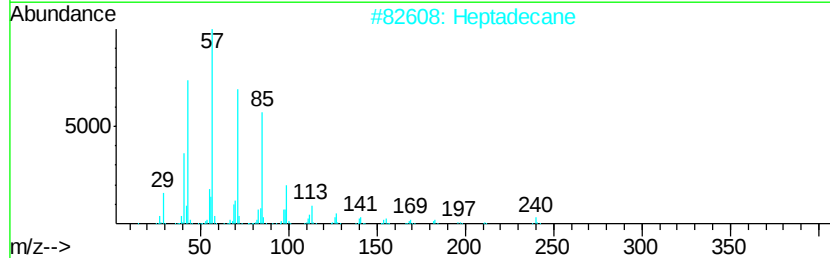
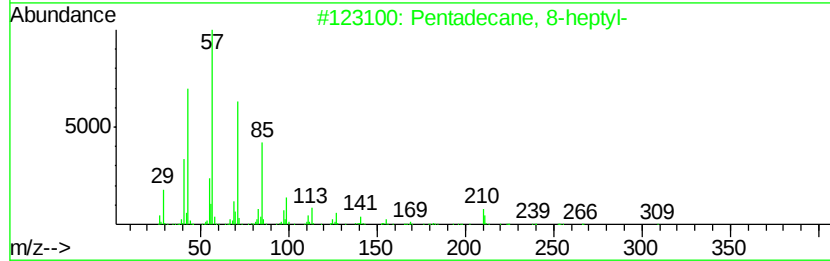
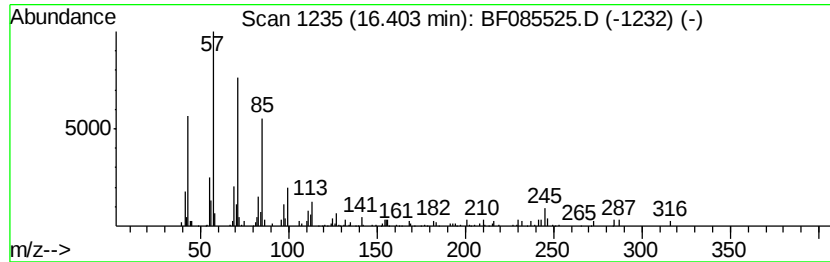
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecane, 8-heptyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	3.05 ng	116783	Perylene-d12	15.48

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
2			Heptadecane	240	C17H36	000629-78-7	86
3			Octacosane	394	C28H58	000630-02-4	86
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
Sample : H1776-10
Misc :
ALS Vial : 45 Sample Multiplier: 1

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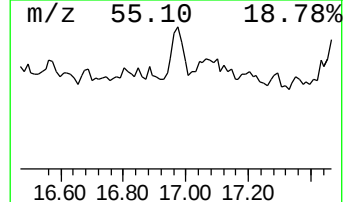
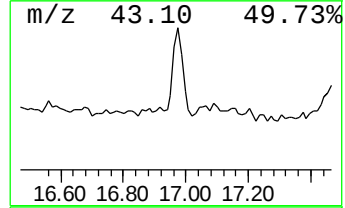
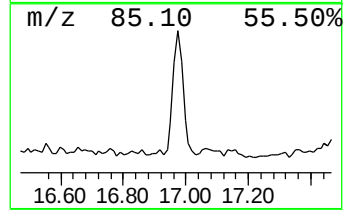
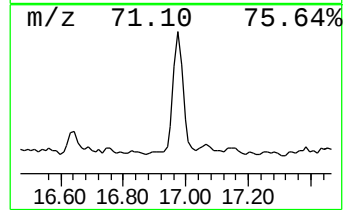
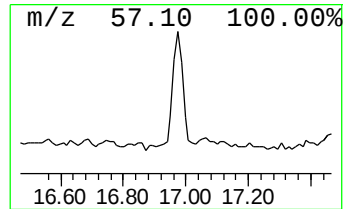
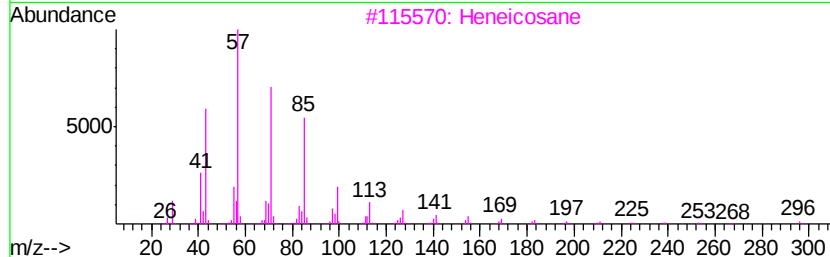
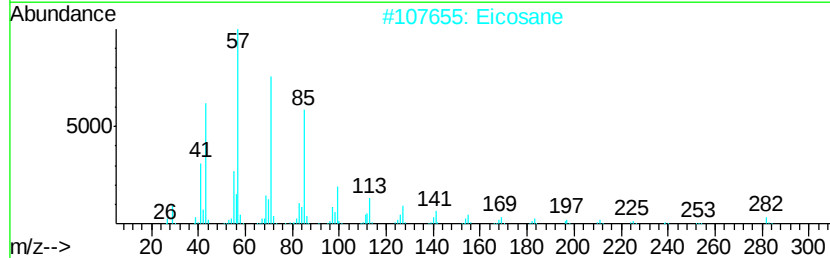
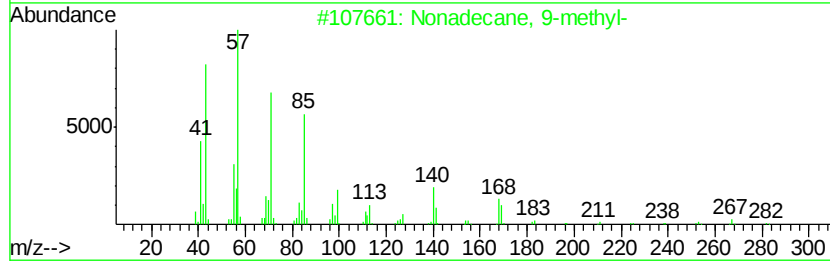
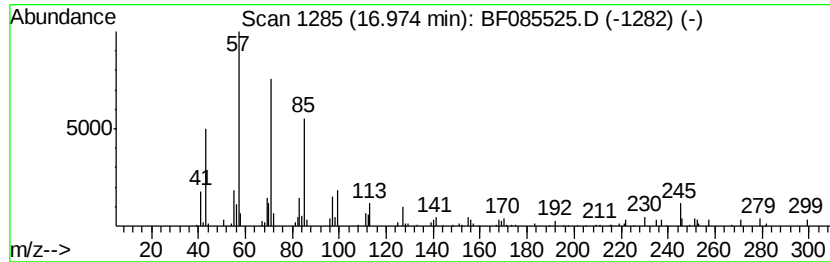
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonadecane, 9-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	2.88 ng	110025	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2		Eicosane	282	C20H42	000112-95-8	86
3		Heneicosane	296	C21H44	000629-94-7	62
4		Nonadecane	268	C19H40	000629-92-5	58
5		Heptadecane	240	C17H36	000629-78-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085525.D
Acq On : 18 Mar 2016 8:04
Operator : UM/SJ
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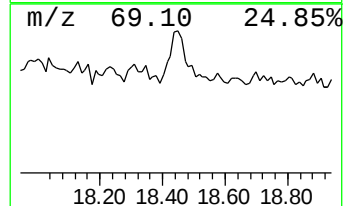
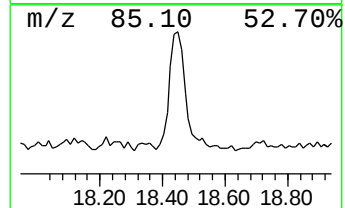
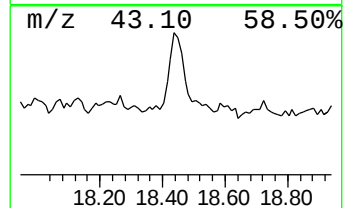
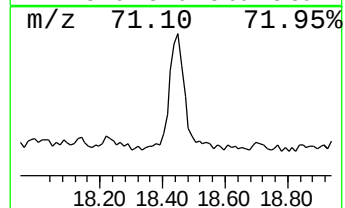
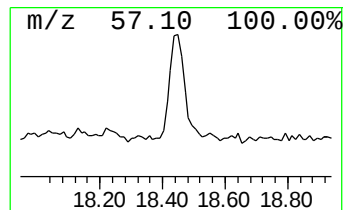
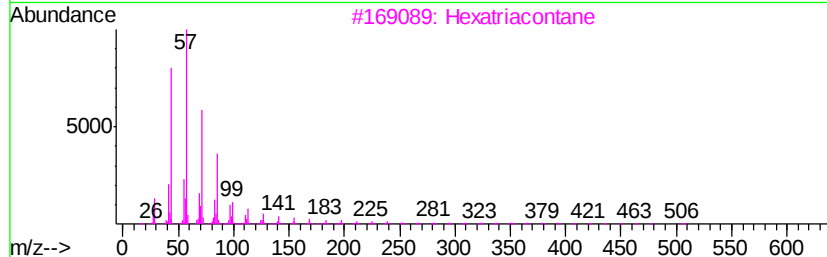
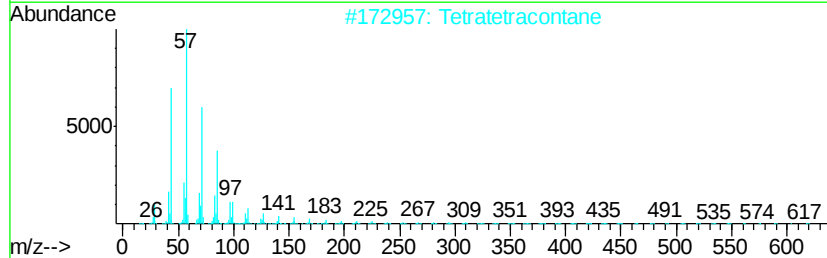
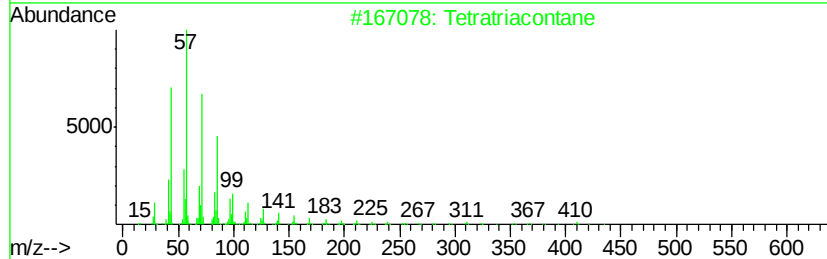
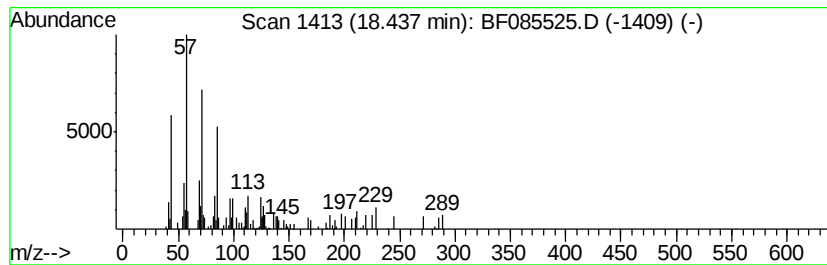
Instrument :
BNA_F
ClientSampleId :
W170TH-SB-05(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Tetratriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.44	2.91 ng	111444	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tetratriacontane	479 C34H70	014167-59-0 64
2		Tetratetracontane	619 C44H90	007098-22-8 64
3		Hexatriacontane	507 C36H74	000630-06-8 59
4		Nonacosane	408 C29H60	000630-03-5 58
5		Docosane	310 C22H46	000629-97-0 52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085525.D
 Acq On : 18 Mar 2016 8:04
 Operator : UM/SJ
 Sample : H1776-10
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-05(0.5-3.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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...	5.09	2.3	ng	90390	1	6.87	783699	20.0
unknown6.64	6.64	94.4	ng	3698960	1	6.87	783699	20.0
Heneicosane	10.82	3.1	ng	152526	4	11.40	988334	20.0
n-Hexadecanoic acid	11.93	9.9	ng	488325	4	11.40	988334	20.0
Undecanoic acid	12.71	3.0	ng	148268	4	11.40	988334	20.0
Dichloroacetic ac...	13.88	7.6	ng	322965	5	14.04	851504	20.0
6a,12a-Dihydro-6H...	14.69	24.6	ng	1048310	5	14.04	851504	20.0
9-Octadecenamide, ...	14.78	6.5	ng	246864	6	15.48	765200	20.0
Z-5-Nonadecene	15.97	2.5	ng	94949	6	15.48	765200	20.0
Pentadecane, 8-he...	16.40	3.0	ng	116783	6	15.48	765200	20.0
Nonadecane, 9-met...	16.97	2.9	ng	110025	6	15.48	765200	20.0
Tetratriacontane	18.44	2.9	ng	111444	6	15.48	765200	20.0