

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
 Data File : BF086872.D
 Acq On : 10 May 2016 21:08
 Operator : UM/SJ
 Sample : H2916-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-CSPH3-3K

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	4.841	239	241	250	rBV	384709	655775	16.65%	1.903%
2	5.287	277	280	282	rBV	3169671	3854878	97.85%	11.189%
3	5.687	313	315	325	rVB	50973	85550	2.17%	0.248%
4	6.350	370	373	375	rBV	2988493	3939517	100.00%	11.435%
5	6.453	380	382	385	rBV	3147453	3622619	91.96%	10.515%
6	6.682	400	402	409	rVB	1116434	1014957	25.76%	2.946%
7	6.842	413	416	418	rBV	3301360	3227919	81.94%	9.369%
8	7.253	450	452	455	rBV	2245579	2341631	59.44%	6.797%
9	7.973	512	515	517	rBV	1157959	1145379	29.07%	3.325%
10	9.048	607	609	612	rBV	4003953	3556086	90.27%	10.322%
11	9.448	642	644	648	rBV	439765	405047	10.28%	1.176%
12	9.665	661	663	665	rBV	118018	124482	3.16%	0.361%
13	9.722	665	668	670	rBV	1048500	1085235	27.55%	3.150%
14	9.893	679	683	684	rBV	25860	40390	1.03%	0.117%
15	10.156	704	706	708	rVB	246763	197240	5.01%	0.572%
16	10.373	722	725	728	rBV	73816	120432	3.06%	0.350%
17	10.511	734	737	739	rBV	1556225	1939302	49.23%	5.629%
18	10.625	746	747	752	rBV	212536	282332	7.17%	0.819%
19	10.819	762	764	766	rBV	33630	44725	1.14%	0.130%
20	11.071	785	786	788	rBV	104846	111245	2.82%	0.323%
21	11.196	795	797	801	rBV	1015922	901262	22.88%	2.616%
22	11.745	842	845	848	rBV	30253	59069	1.50%	0.171%
23	12.774	933	935	938	rBV	1997426	2799438	71.06%	8.126%
24	13.014	954	956	964	rBV	26209	70925	1.80%	0.206%
25	13.688	1013	1015	1024	rBV	374601	803241	20.39%	2.331%
26	13.825	1024	1027	1029	rBV	714973	792863	20.13%	2.301%
27	14.271	1063	1066	1068	rBV	144015	210917	5.35%	0.612%
28	14.339	1070	1072	1076	rVB2	43046	91065	2.31%	0.264%
29	14.660	1098	1100	1103	rBV	44458	44395	1.13%	0.129%
30	15.197	1144	1147	1154	rBV	553423	676322	17.17%	1.963%
31	15.608	1180	1183	1186	rBV	32886	52579	1.33%	0.153%
32	15.700	1187	1191	1197	rVB4	41398	155598	3.95%	0.452%

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ALS Vial : 21 Sample Multiplier: 1

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ClientSampleId :
VITALE-FILL-CSPH3-3K

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

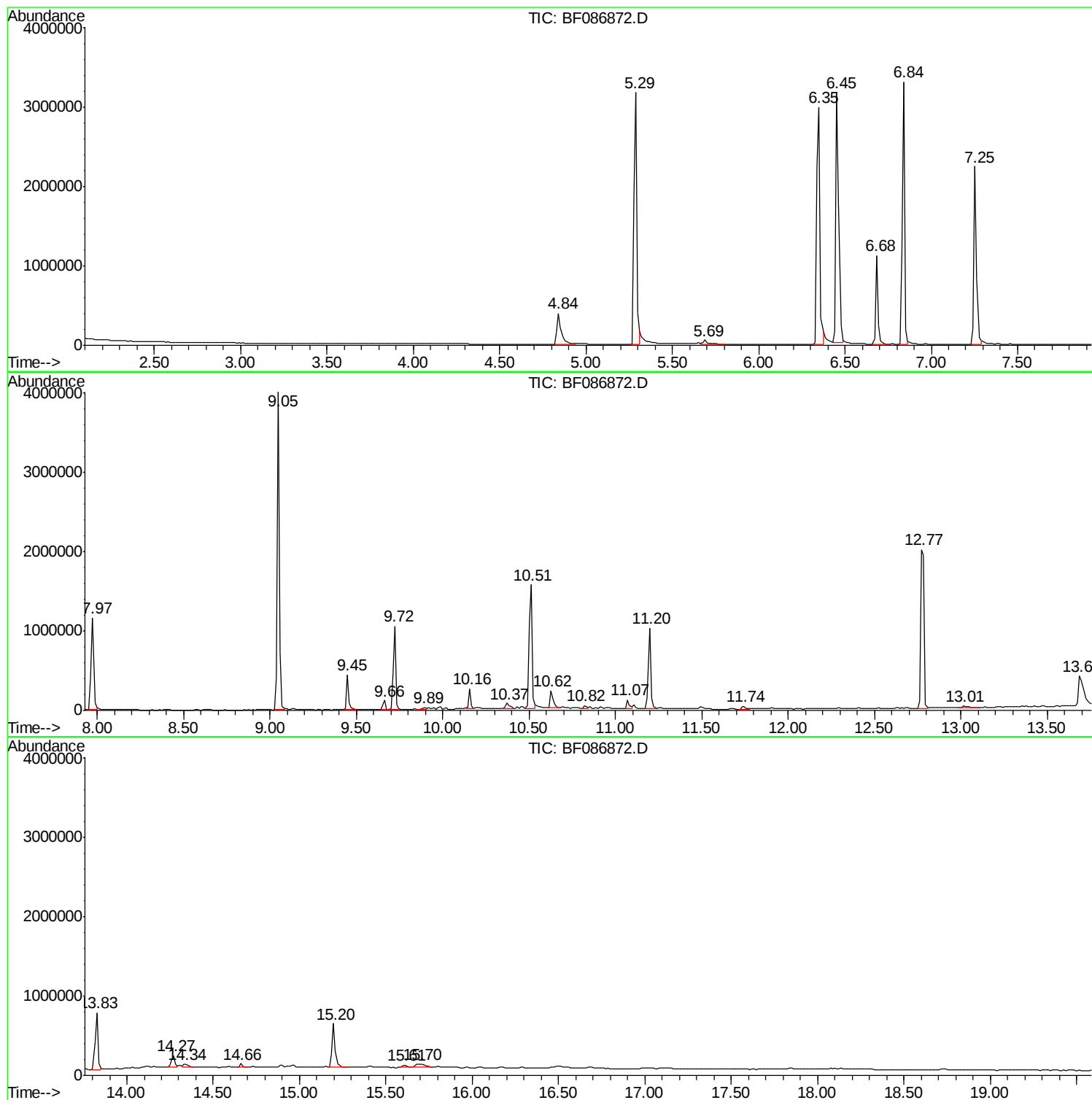
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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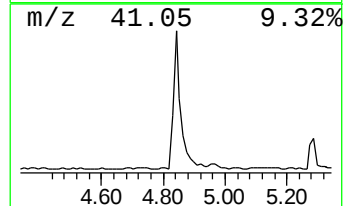
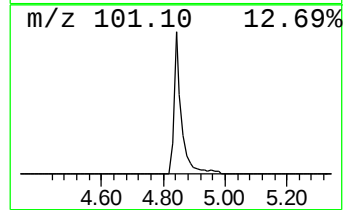
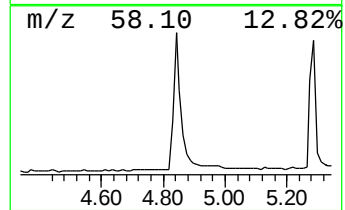
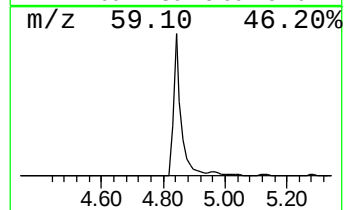
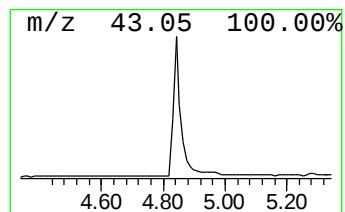
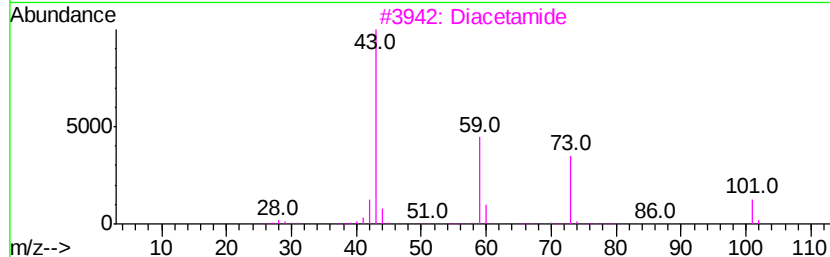
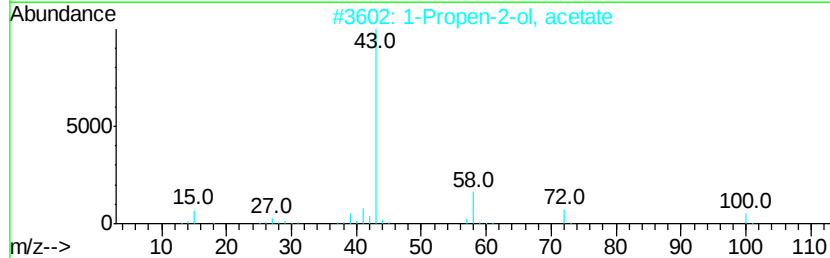
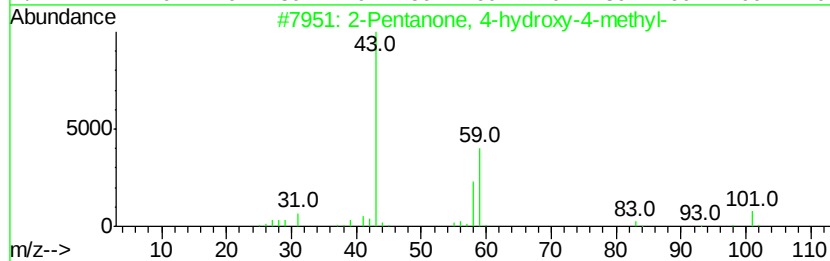
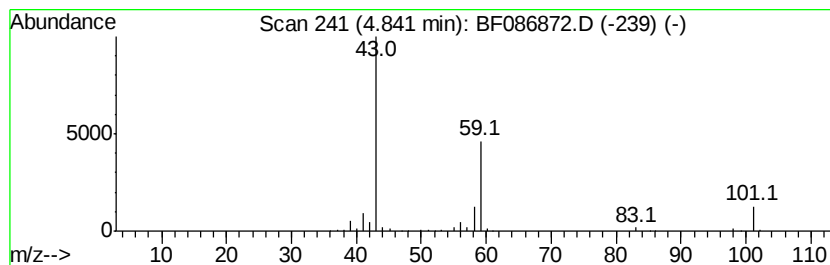
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	12.92 ng	655775	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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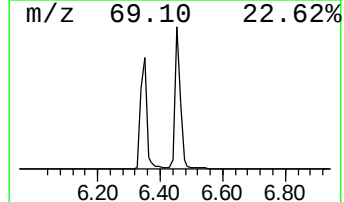
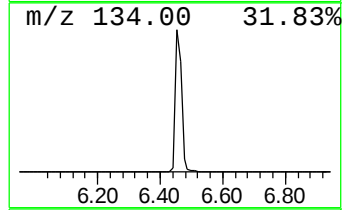
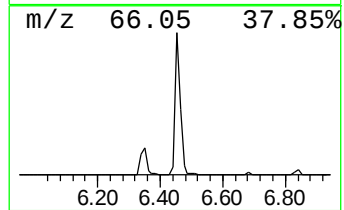
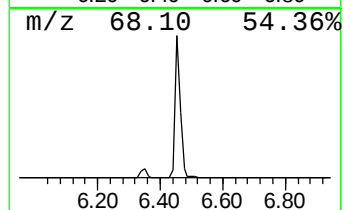
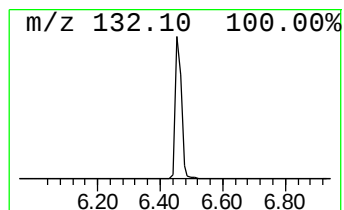
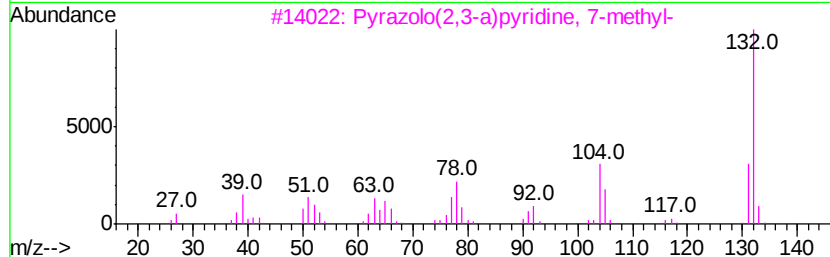
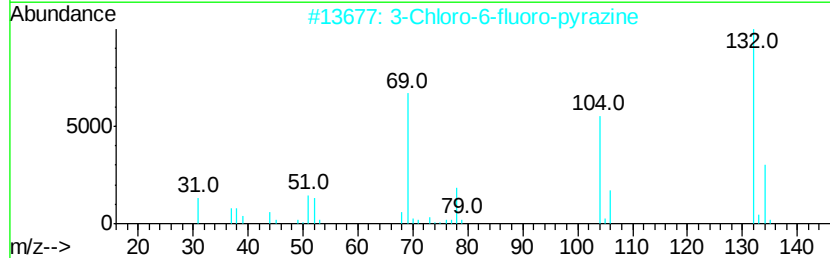
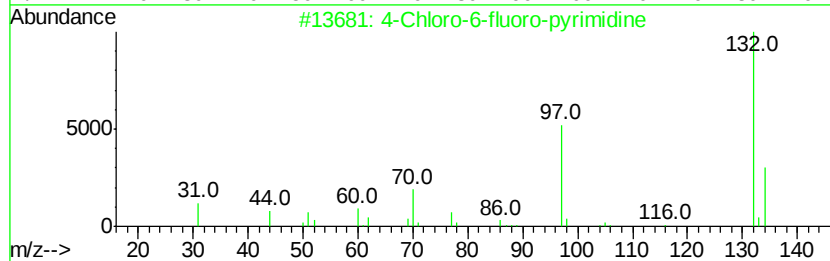
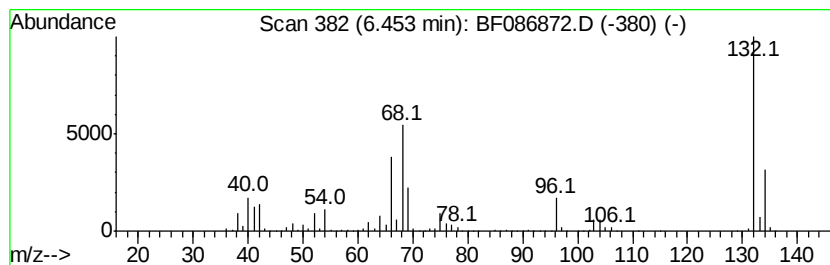
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Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	71.38 ng	3622620	1,4-Dichlorobenzene-d4	6.68

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



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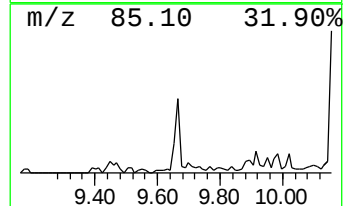
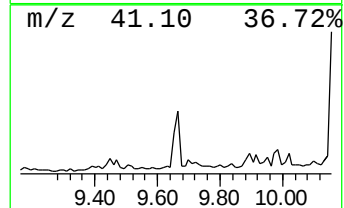
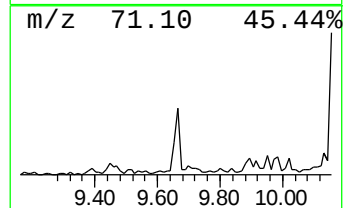
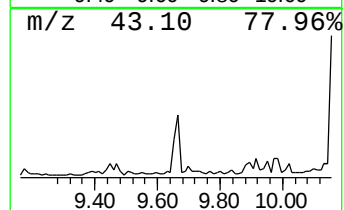
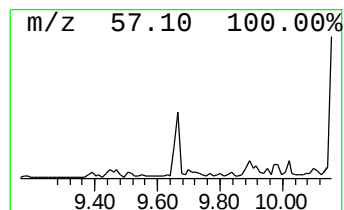
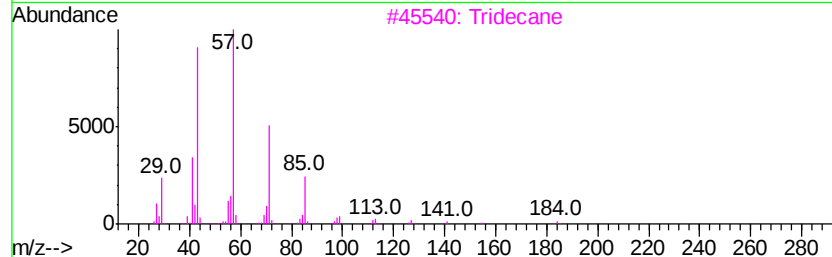
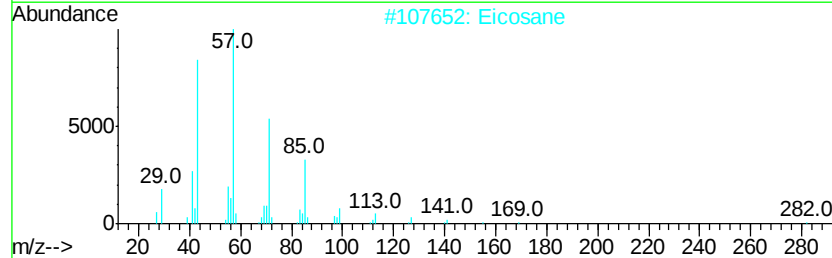
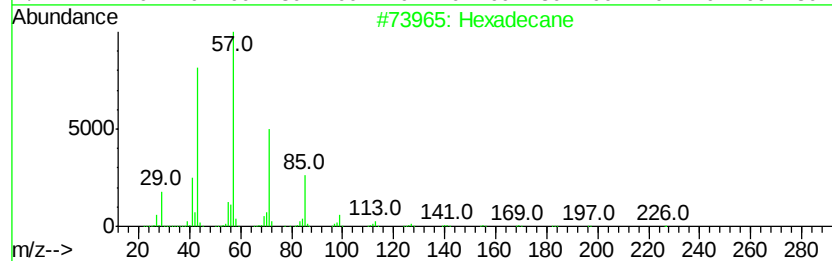
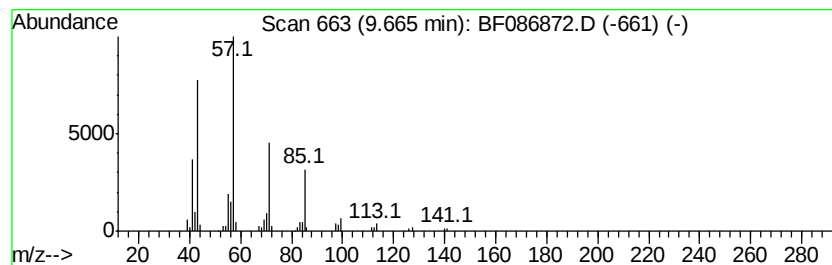
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	2.29 ng	124482	Acenaphthene-d10	9.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	91
2		Eicosane	282	C20H42	000112-95-8	86
3		Tridecane	184	C13H28	000629-50-5	80
4		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5		Pentadecane	212	C15H32	000629-62-9	72



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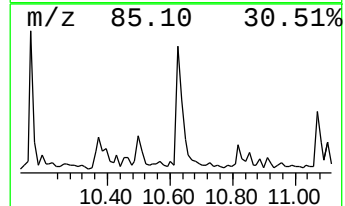
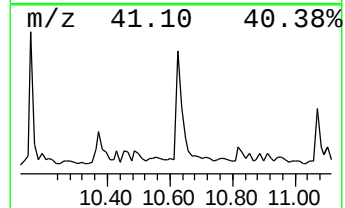
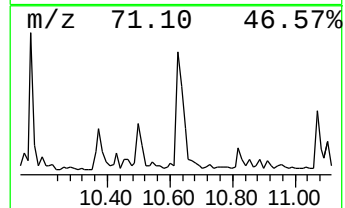
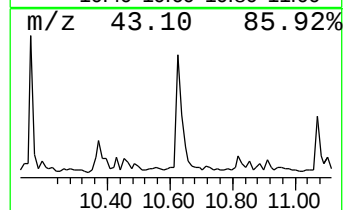
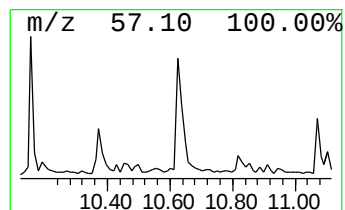
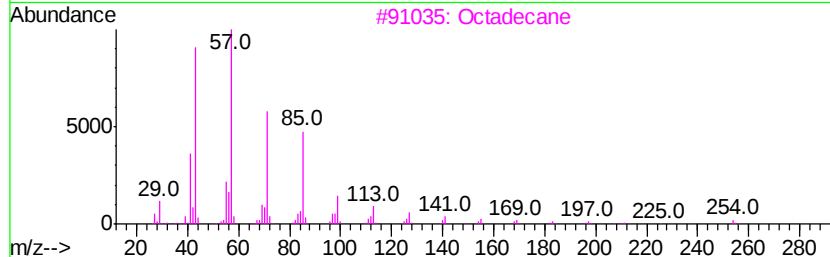
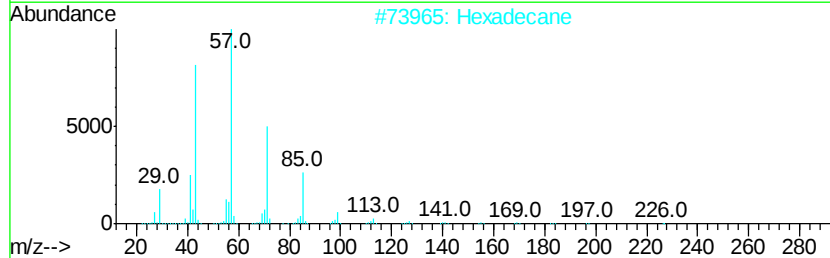
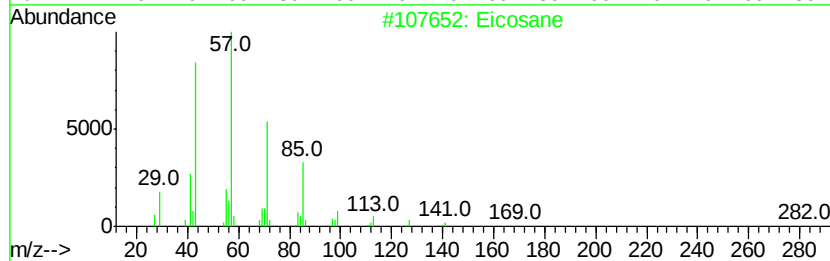
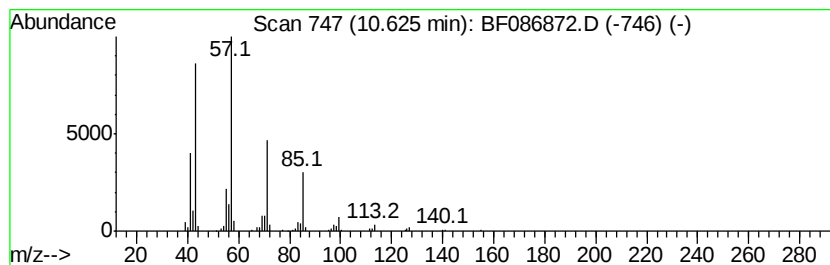
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	6.27 ng	282332	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Hexadecane		226	C16H34	000544-76-3	91
3	Octadecane		254	C18H38	000593-45-3	86
4	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	86
5	Tridecane		184	C13H28	000629-50-5	83



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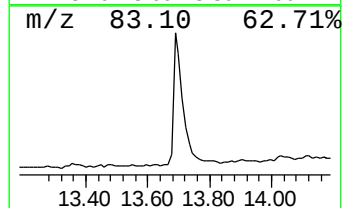
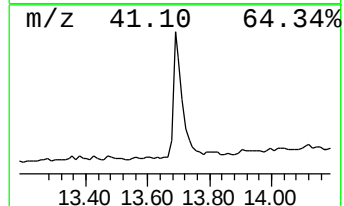
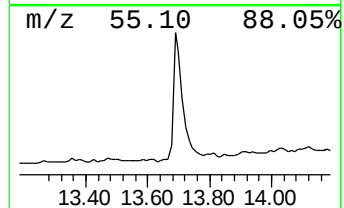
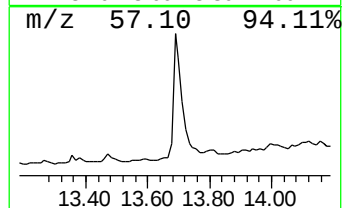
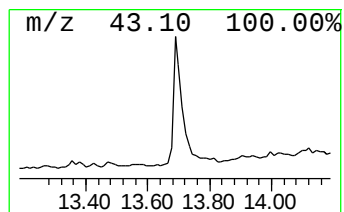
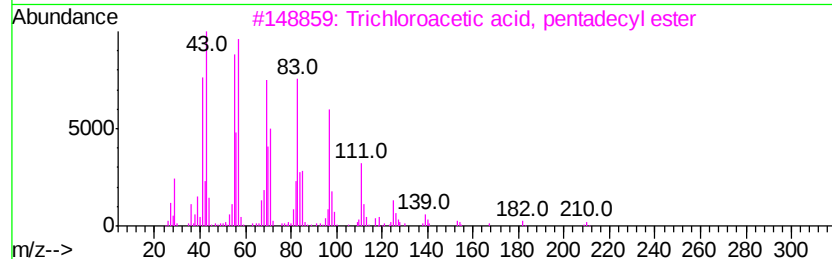
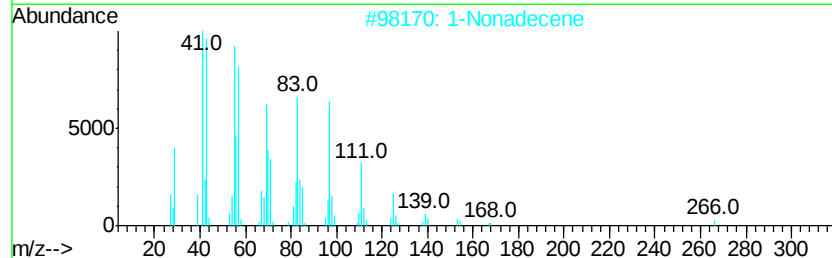
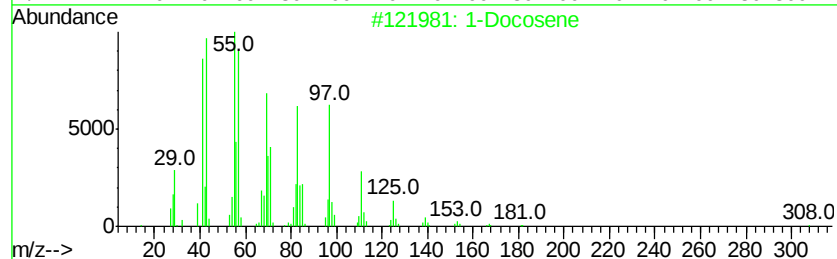
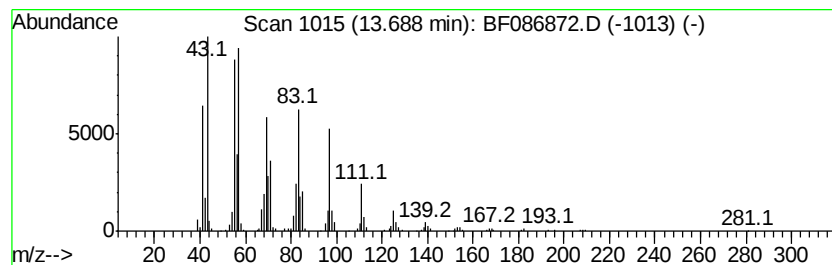
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	20.26 ng	803241	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	95
2	1-Nonadecene		266	C19H38	018435-45-5	91
3	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	90
4	3-Eicosene, (E)-		280	C20H40	074685-33-9	87
5	Heptafluorobutyric acid, n-tetra...		410	C18H29F7O2	007365-36-8	83



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ClientSampleId :
VITALE-FILL-CSPH3-3K

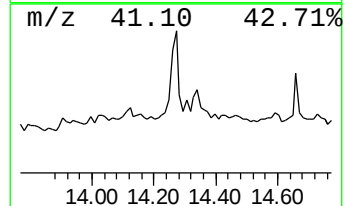
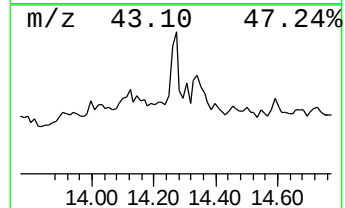
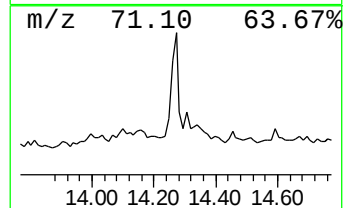
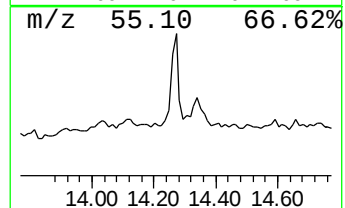
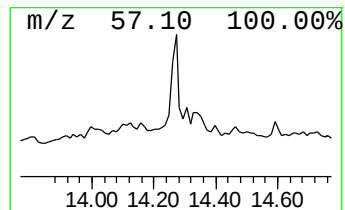
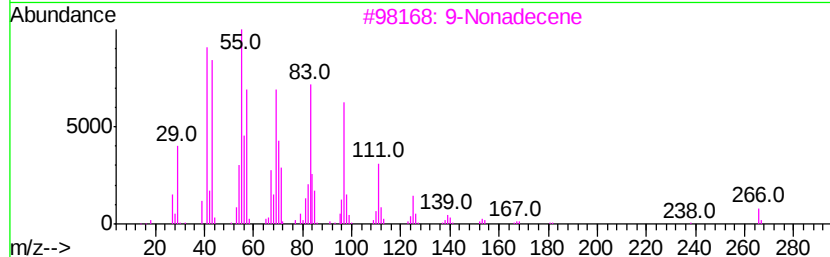
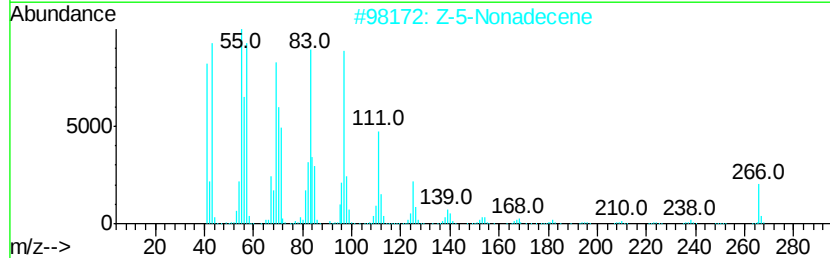
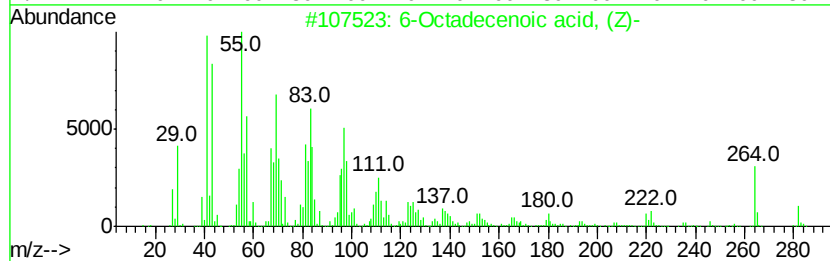
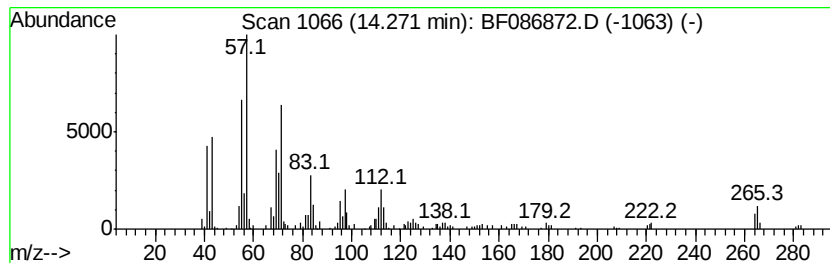
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.27 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	5.32 ng	210917	Chrysene-d12	13.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	38
2			Z-5-Nonadecene	266	C19H38	1000131-11-8	38
3			9-Nonadecene	266	C19H38	031035-07-1	35
4			Dodecyl acrylate	240	C15H28O2	002156-97-0	27
5			1-Heptadecene	238	C17H34	006765-39-5	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086872.D
Acq On : 10 May 2016 21:08
Operator : UM/SJ
Sample : H2916-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-3K

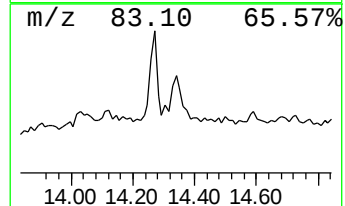
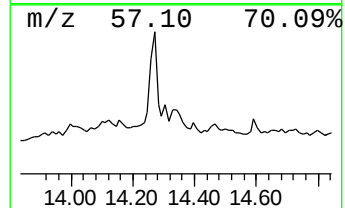
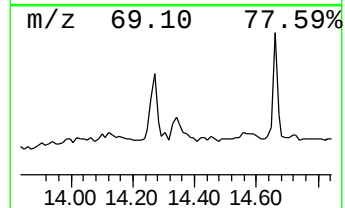
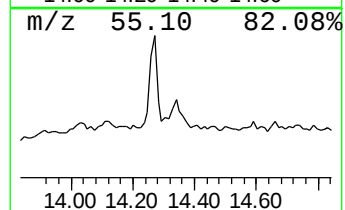
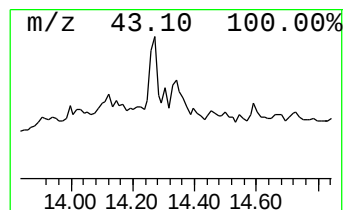
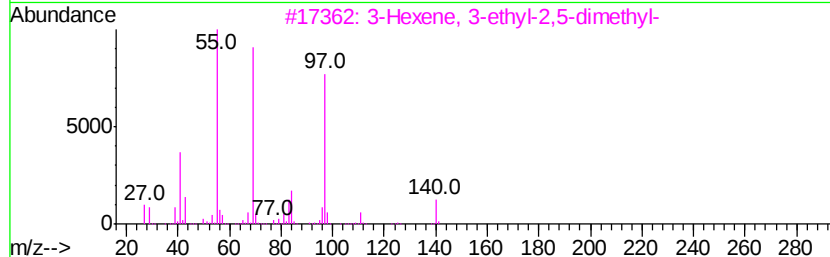
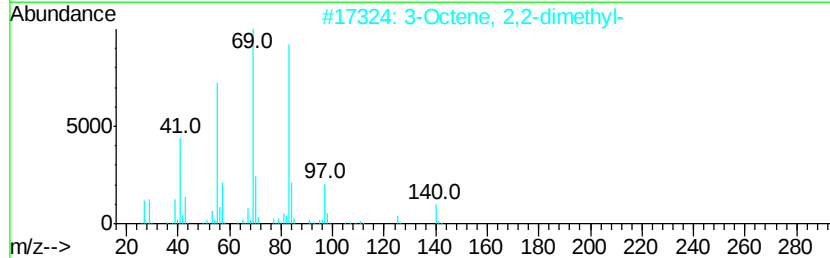
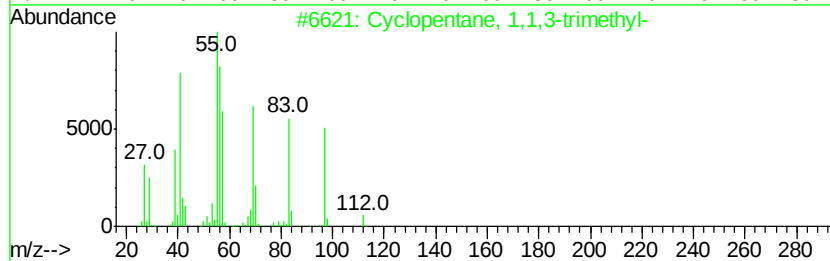
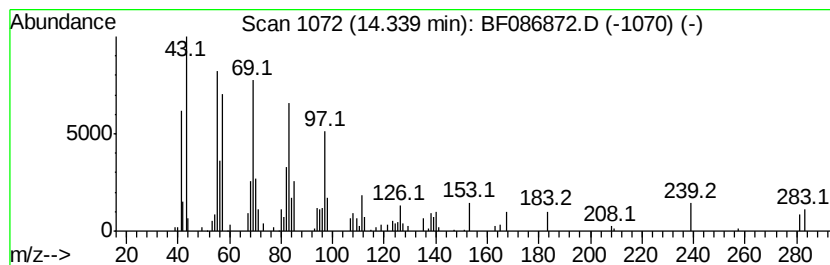
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.30 ng	91065	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52
2		3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	46
3		3-Hexene, 3-ethyl-2,5-dimethyl-	140	C10H20	062338-08-3	43
4		17-Pentatriacontene	491	C35H70	006971-40-0	38
5		Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086872.D
Acq On : 10 May 2016 21:08
Operator : UM/SJ
Sample : H2916-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

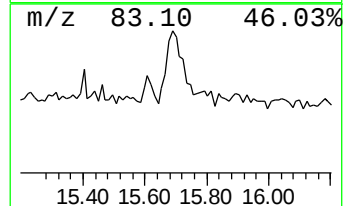
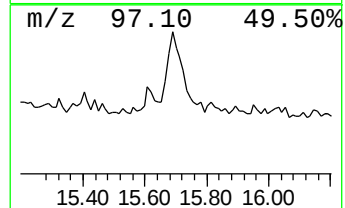
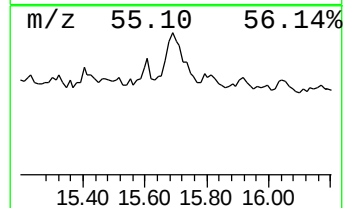
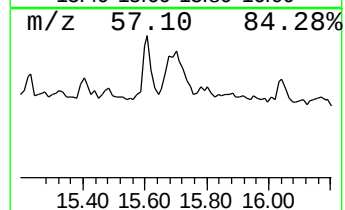
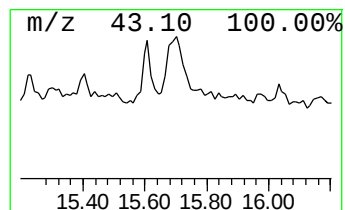
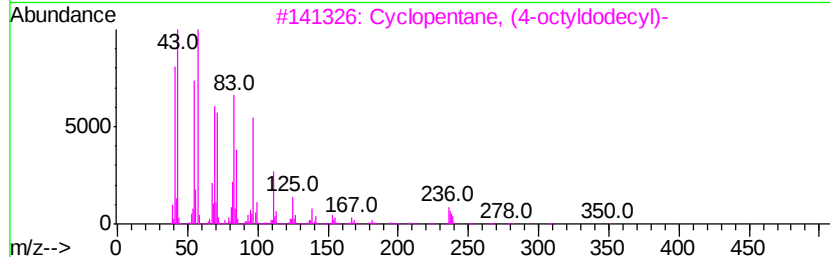
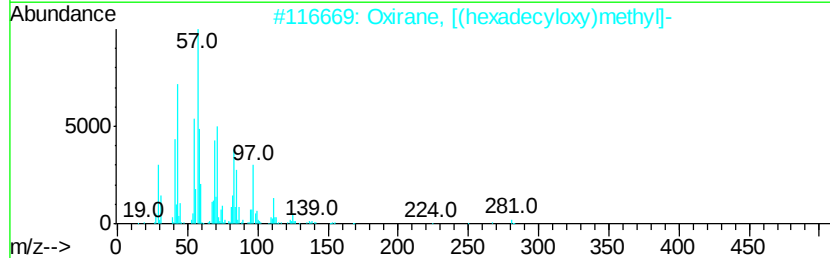
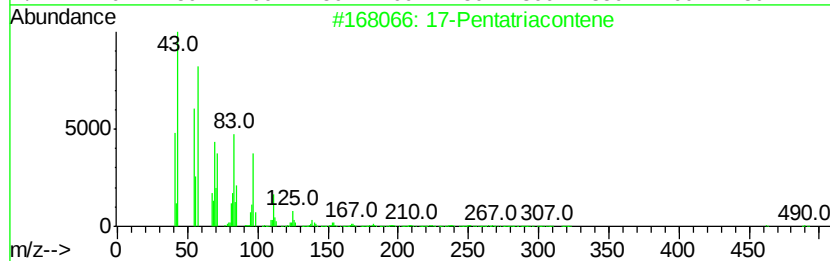
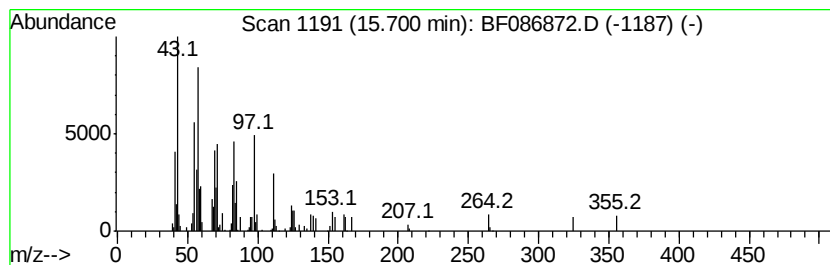
Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-3K

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 12 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.70	4.60 ng	155598	Perylene-d12	15.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	70
2	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	58
3	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	52
4	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	52
5	1-Hexacosanol	382	C26H54O	000506-52-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086872.D
Acq On : 10 May 2016 21:08
Operator : UM/SJ
Sample : H2916-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-3K

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...	4.84	12.9	ng	655775	1	6.68	1014960	20.0
unknown6.45	6.45	71.4	ng	3622620	1	6.68	1014960	20.0
Hexadecane	9.66	2.3	ng	124482	3	9.72	1085240	20.0
Eicosane	10.62	6.3	ng	282332	4	11.20	901262	20.0
1-Docosene	13.69	20.3	ng	803241	5	13.83	792863	20.0
unknown14.27	14.27	5.3	ng	210917	5	13.83	792863	20.0
Cyclopentane, 1,1...	14.34	2.3	ng	91065	5	13.83	792863	20.0
17-Pentatriacontene	15.70	4.6	ng	155598	6	15.20	676322	20.0