

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091417\
 Data File : BF098550.D
 Acq On : 15 Sep 2017 1:39
 Operator : SJ/JU
 Sample : I5219-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-PS-01-015

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-BF091117.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	4.828	462	466	480	rBV	308051	494351	12.60%	1.414%
2	5.257	534	539	556	rBV	3703683	3733132	95.17%	10.680%
3	6.304	712	717	733	rBV	3598725	3852260	98.21%	11.020%
4	6.422	733	737	740	rBV	4224918	3711163	94.61%	10.617%
5	6.645	772	775	781	rBV	1042939	866560	22.09%	2.479%
6	6.804	798	802	805	rBV	3212993	2780365	70.88%	7.954%
7	7.222	868	873	875	rBV	2258015	2308689	58.86%	6.605%
8	7.928	990	993	1008	rBV	1242783	1170847	29.85%	3.350%
9	9.010	1172	1177	1180	rBV	4455041	3922532	100.00%	11.221%
10	9.404	1240	1244	1252	rVB	583481	452803	11.54%	1.295%
11	9.681	1287	1291	1295	rBV	1445431	1194676	30.46%	3.418%
12	10.469	1421	1425	1440	rVB	1954694	1930196	49.21%	5.522%
13	10.586	1442	1445	1450	rBV	78680	73857	1.88%	0.211%
14	11.163	1539	1543	1546	rBV	1122507	995228	25.37%	2.847%
15	12.745	1807	1812	1815	rBV	2884317	2593861	66.13%	7.420%
16	13.639	1960	1964	1972	rBV	181088	221054	5.64%	0.632%
17	13.792	1986	1990	1994	rBV	916478	813405	20.74%	2.327%
18	14.268	2066	2071	2077	rBV3	93643	144497	3.68%	0.413%
19	14.621	2129	2131	2137	rVB	51942	54157	1.38%	0.155%
20	14.757	2151	2154	2158	rBV5	28473	45277	1.15%	0.130%
21	14.863	2169	2172	2177	rBV	406490	448174	11.43%	1.282%
22	15.192	2223	2228	2234	rBV	753914	877600	22.37%	2.511%
23	15.504	2278	2281	2285	rBV2	36947	46713	1.19%	0.134%
24	15.598	2292	2297	2302	rBV	361719	482458	12.30%	1.380%
25	16.568	2459	2462	2469	rVB3	76033	144480	3.68%	0.413%
26	16.956	2523	2528	2532	rBV3	88277	171065	4.36%	0.489%
27	17.039	2533	2542	2551	rVB8	218180	694511	17.71%	1.987%
28	17.292	2580	2585	2591	rVB3	84784	175427	4.47%	0.502%
29	17.415	2602	2606	2615	rBV3	75785	200302	5.11%	0.573%
30	17.727	2652	2659	2663	rBV6	135880	355874	9.07%	1.018%

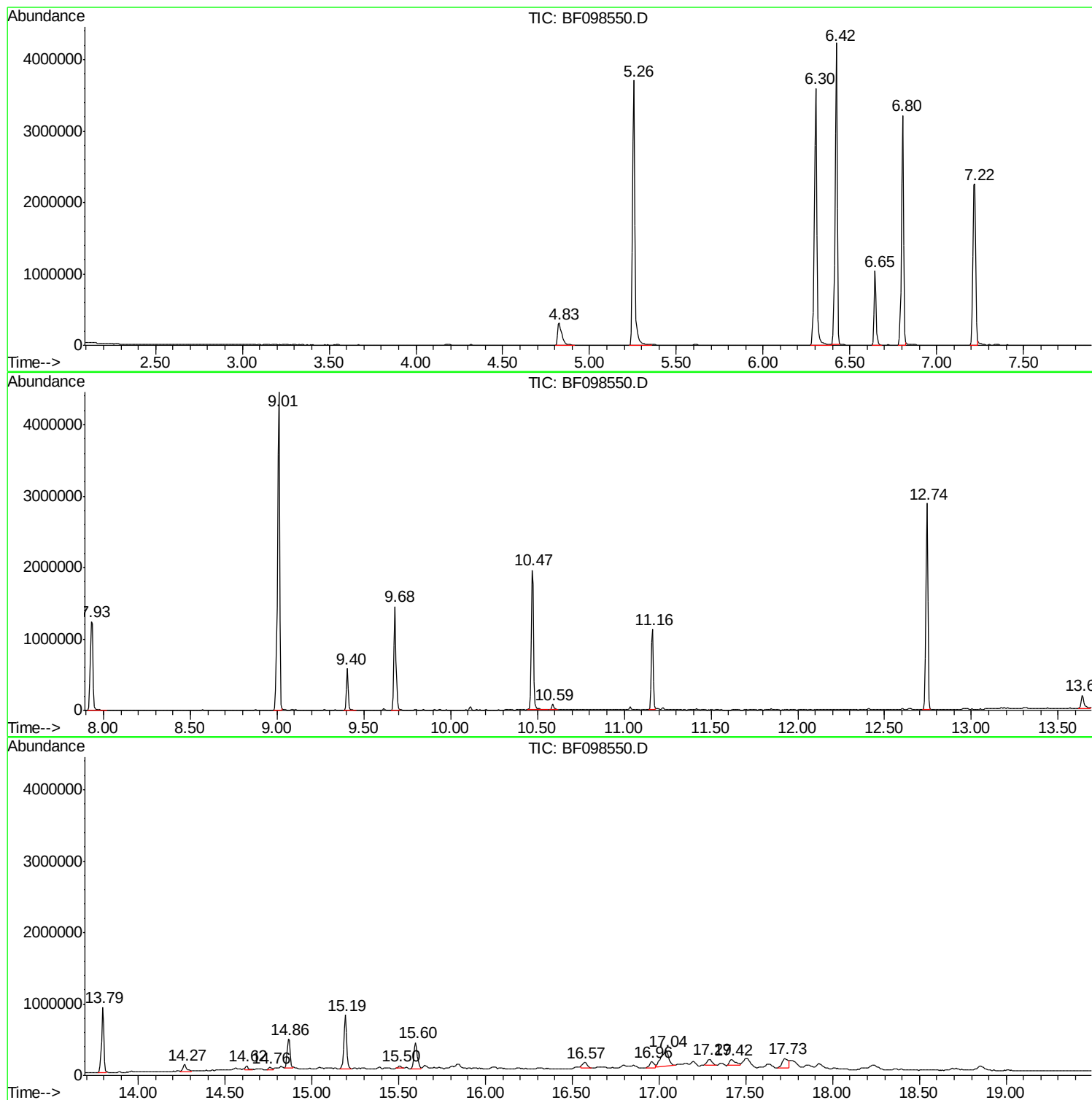
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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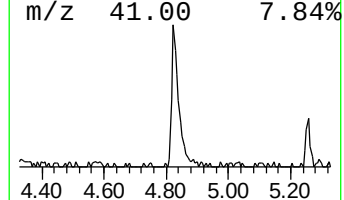
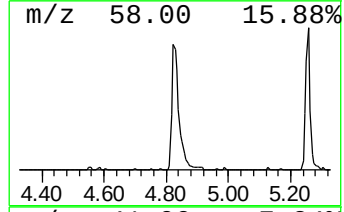
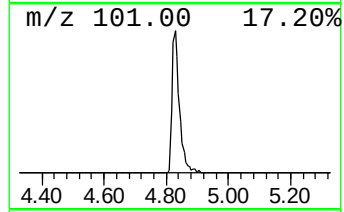
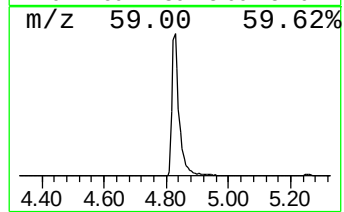
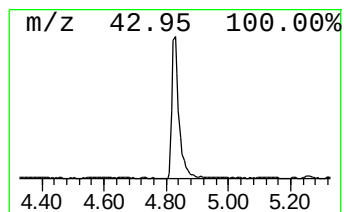
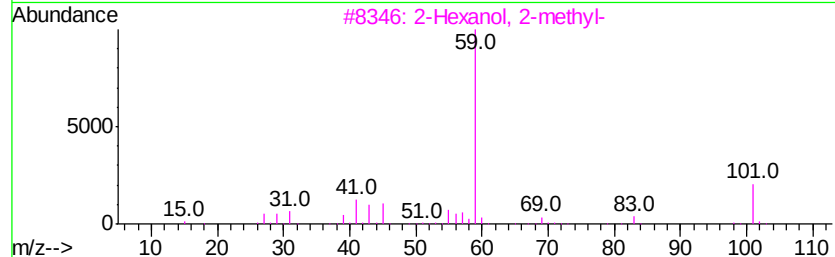
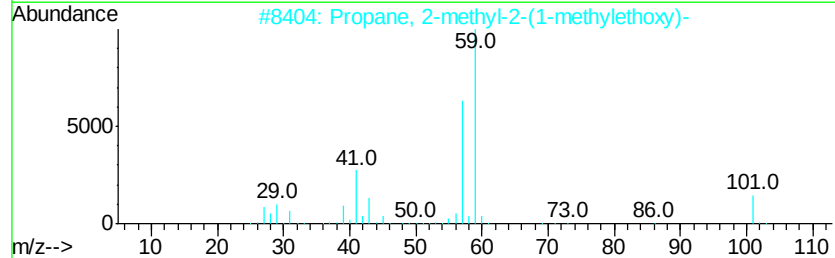
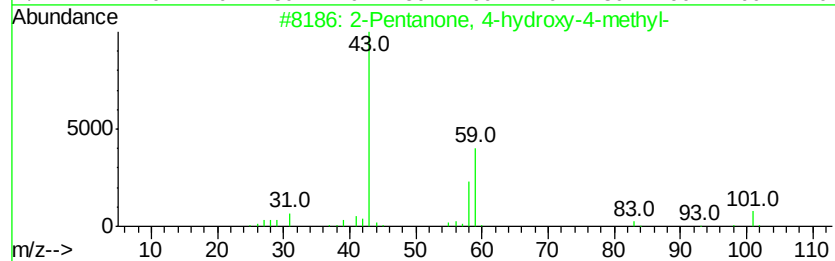
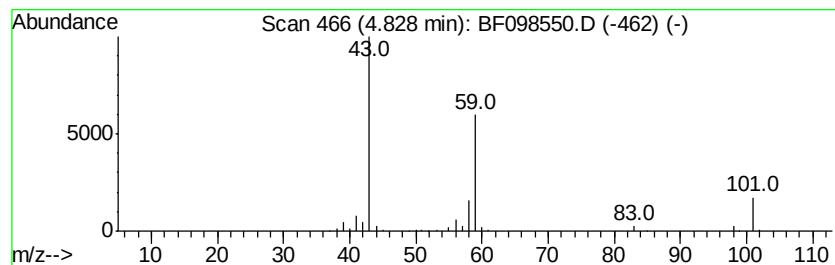
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	11.41 ng	494351	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
5		3-Octanol	130	C8H18O	000589-98-0	33



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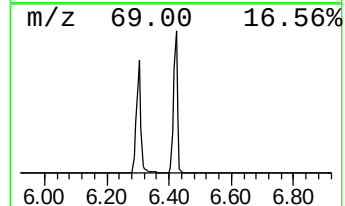
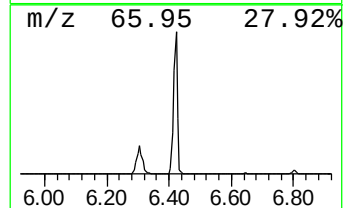
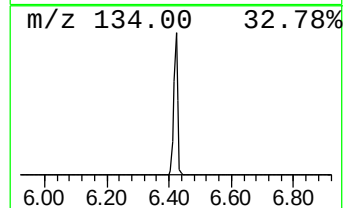
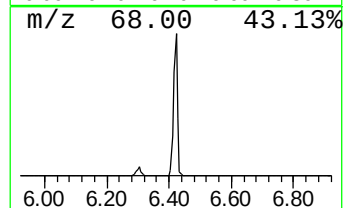
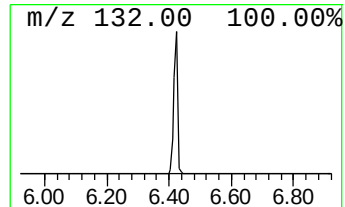
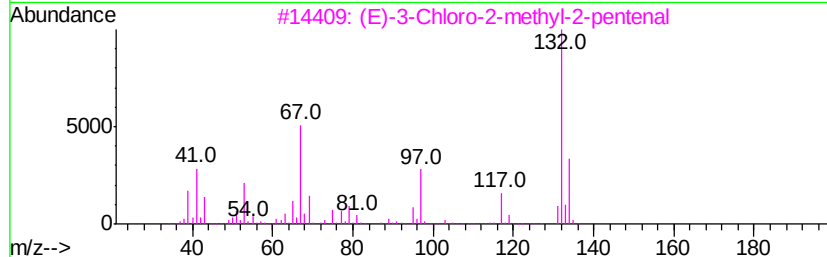
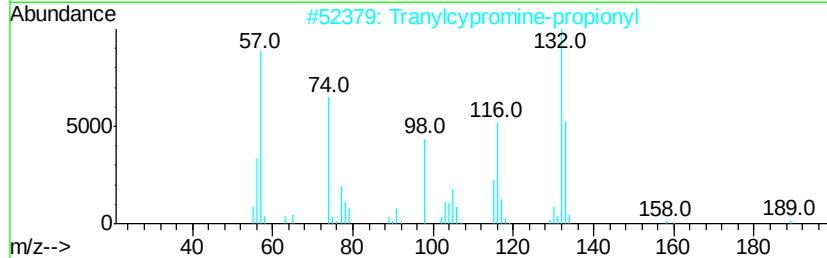
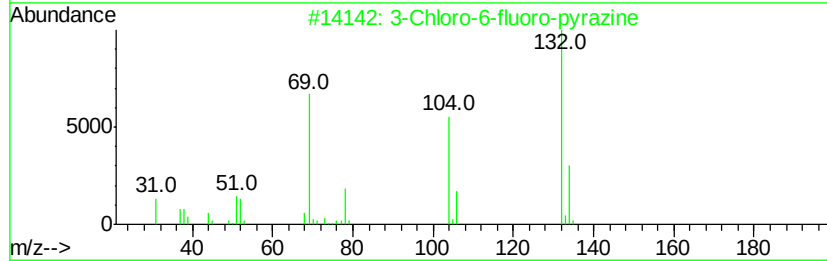
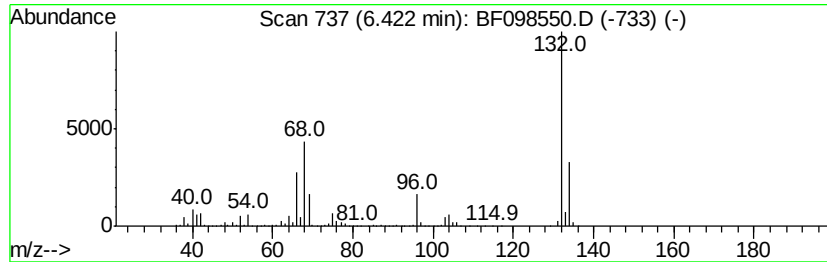
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Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	85.65 ng	3711160	1,4-Dichlorobenzene-d4	6.65

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	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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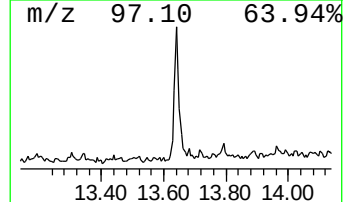
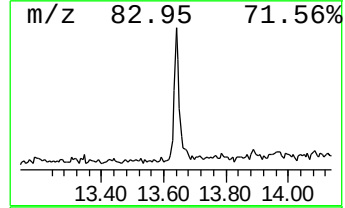
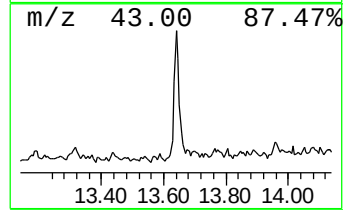
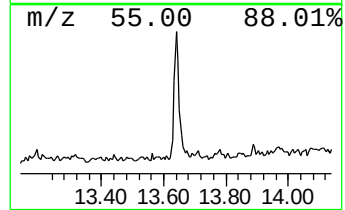
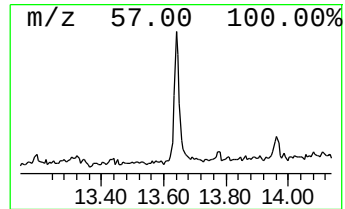
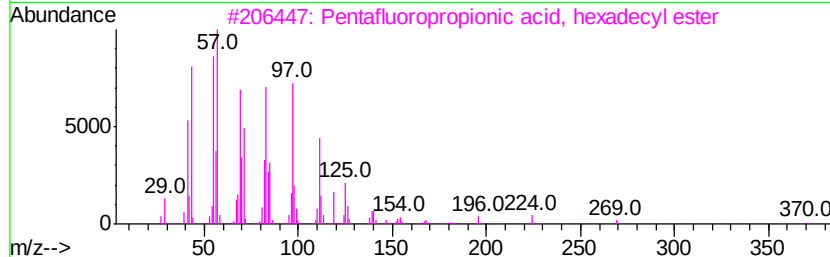
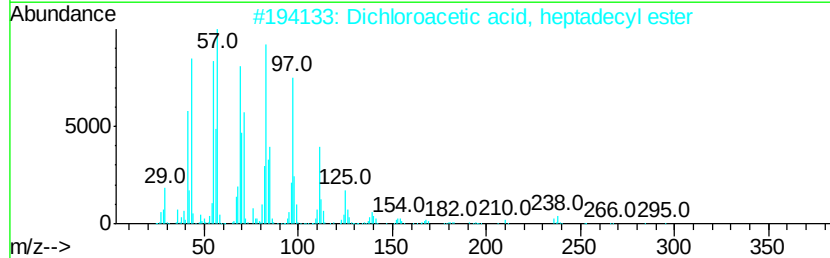
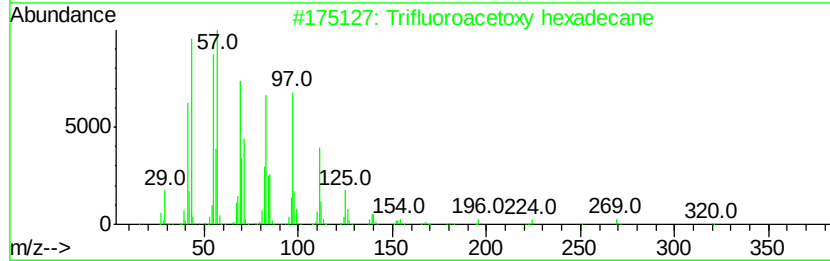
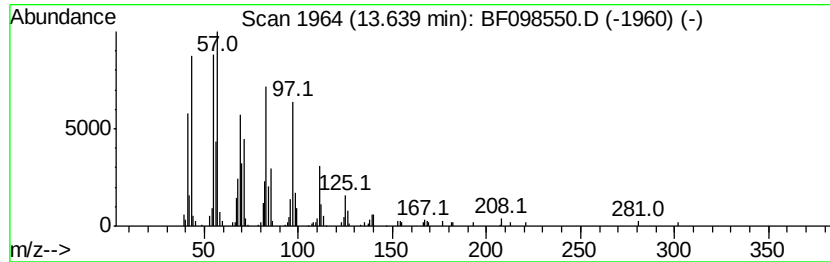
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.64	5.44 ng	221054	Chrysene-d12		13.79
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



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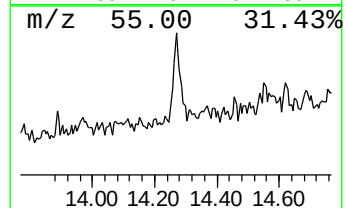
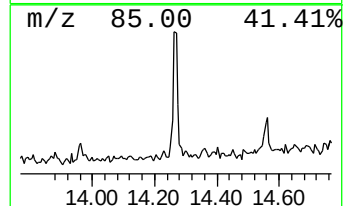
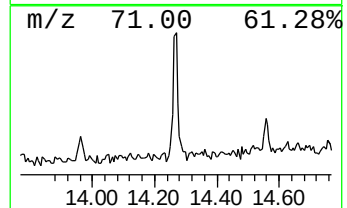
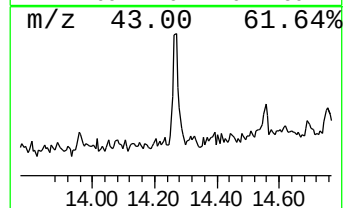
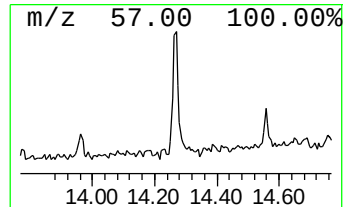
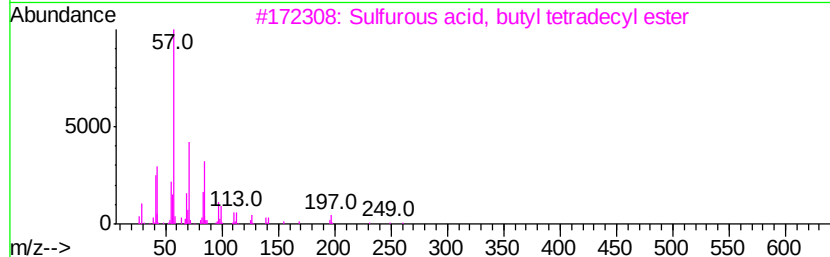
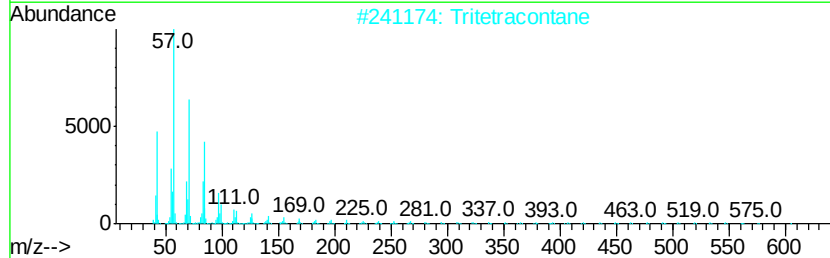
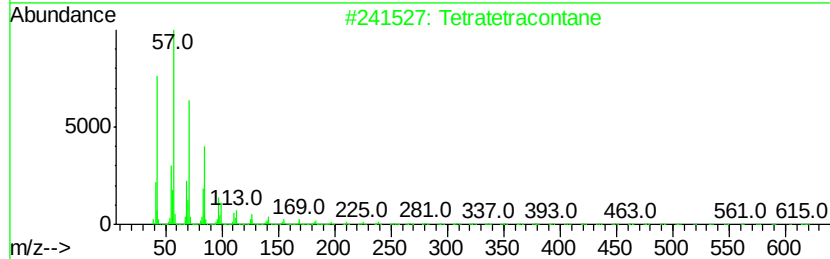
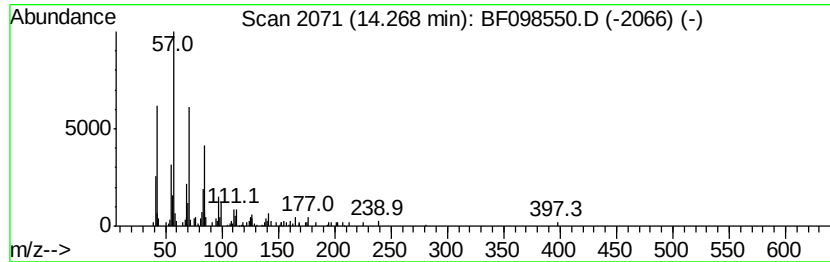
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Peak Number 5 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	3.55 ng	144497	Chrysene-d12	13.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Tritetracontane	605	C43H88	007098-21-7	90
3		Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	87



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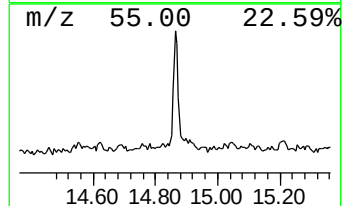
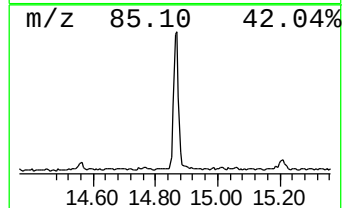
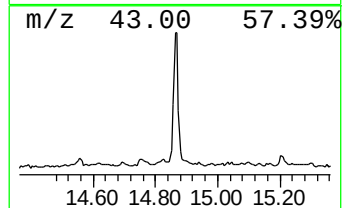
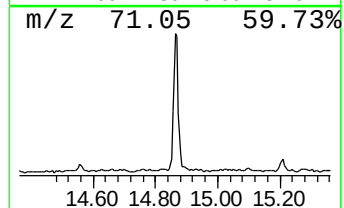
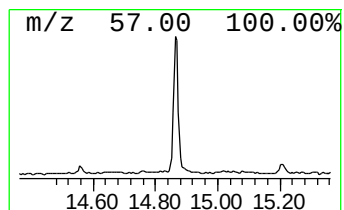
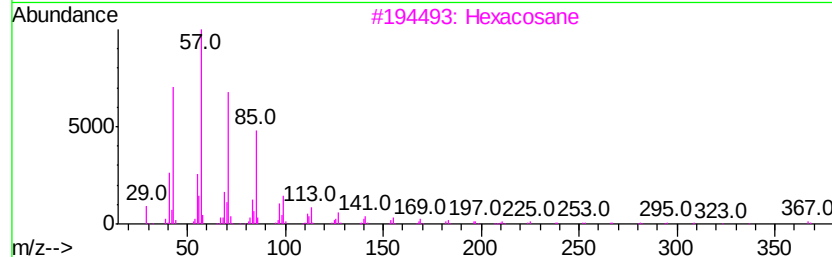
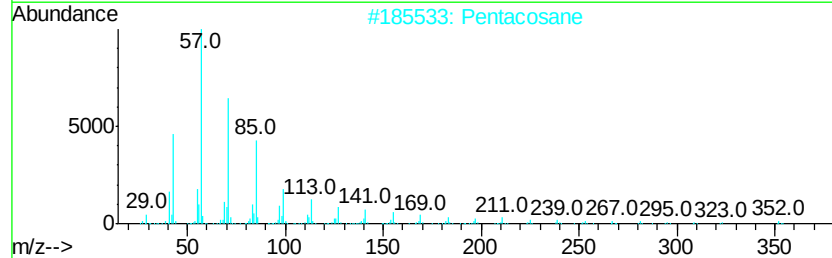
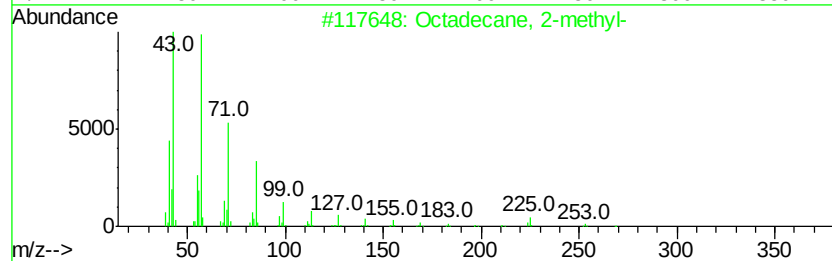
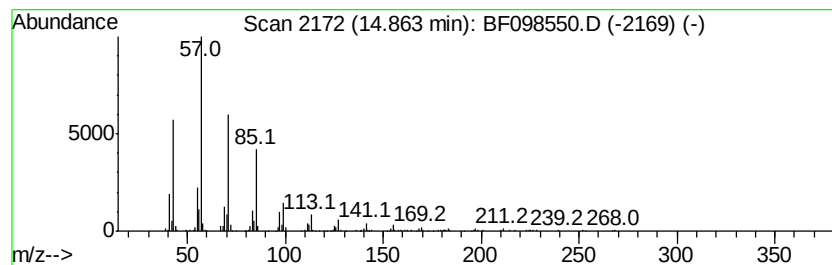
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 Peak Number 6 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	10.21 ng	448174	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2		Pentacosane	352	C25H52	000629-99-2	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptacosane	380	C27H56	000593-49-7	91



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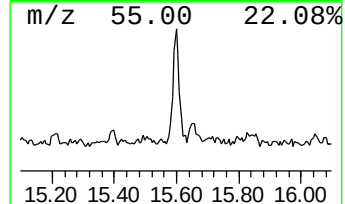
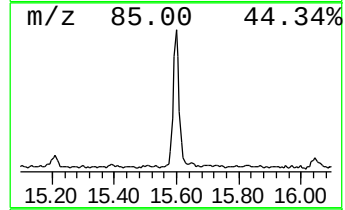
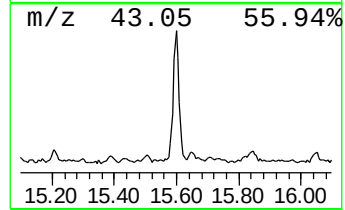
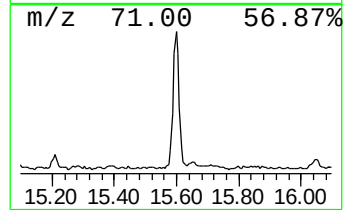
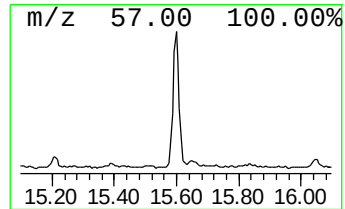
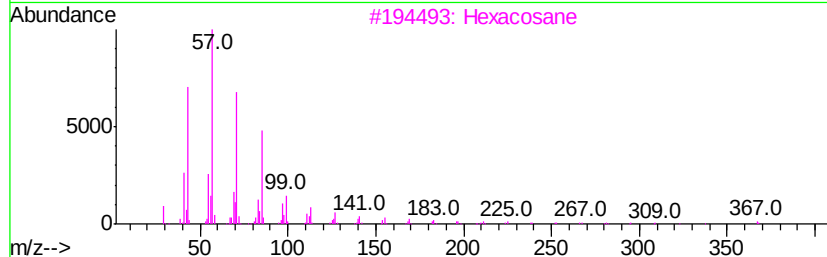
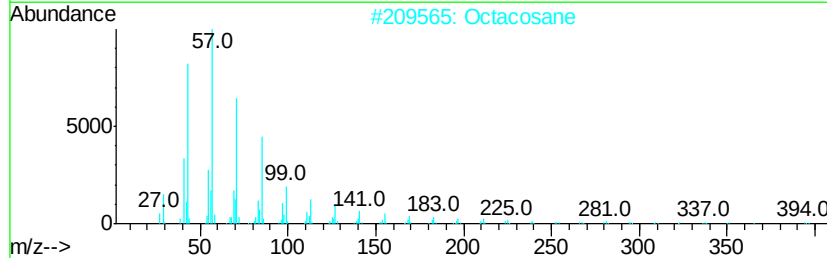
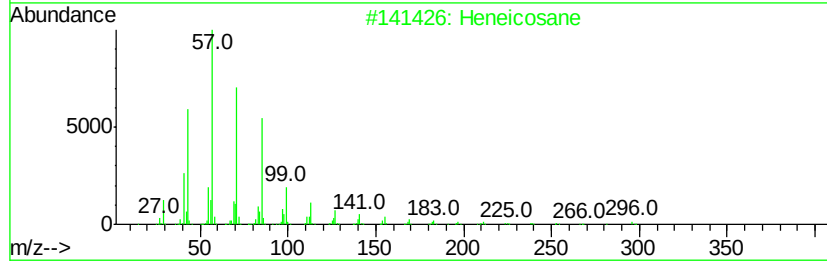
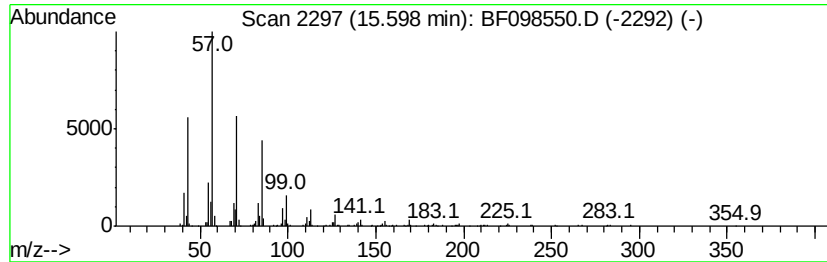
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	10.99 ng	482458	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90
5	Pentacosane	352	C25H52	000629-99-2	90



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Sample : I5219-01
Misc :
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ClientSampleId :
FK-PS-01-015

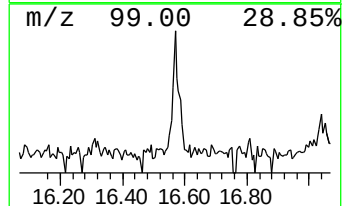
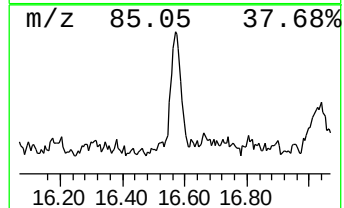
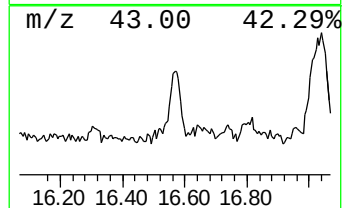
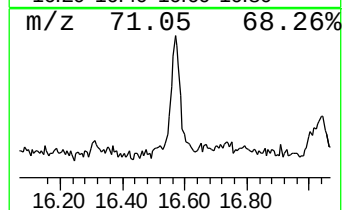
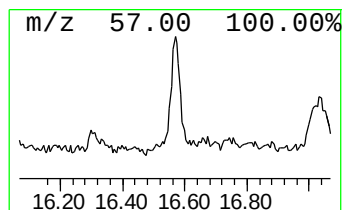
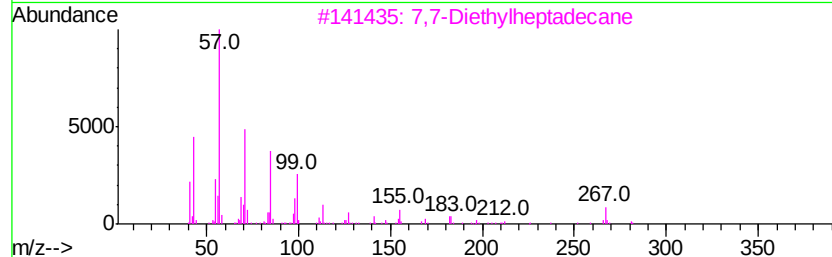
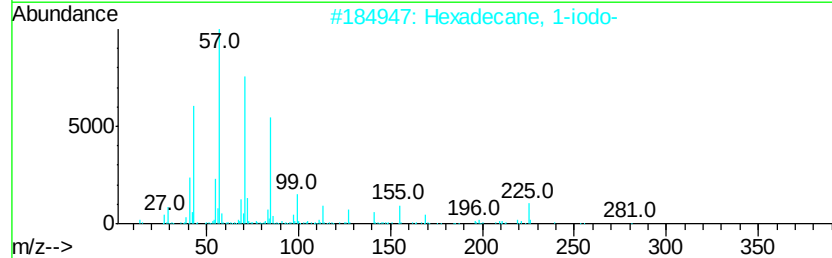
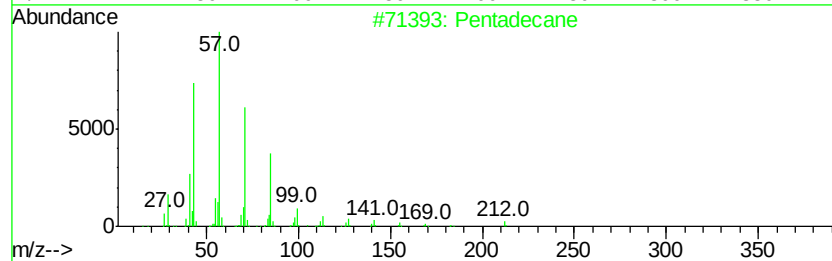
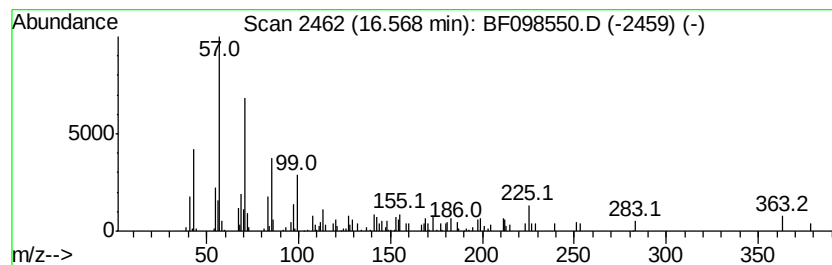
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Pentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.57	3.29 ng	144480	Perylene-d12	15.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	53
2	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	52
3	7,7-Diethylheptadecane		296	C21H44	1000360-41-5	50
4	Hentriacontane		437	C31H64	000630-04-6	49
5	Tetratetracontane		619	C44H90	007098-22-8	49



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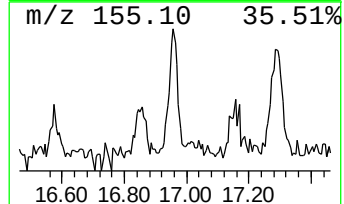
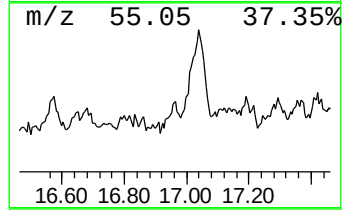
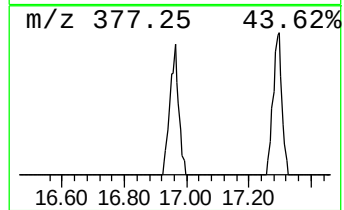
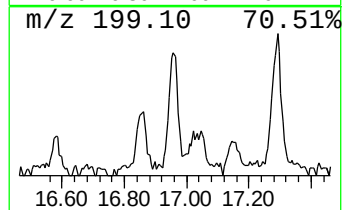
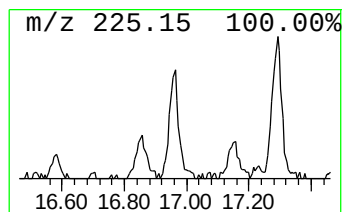
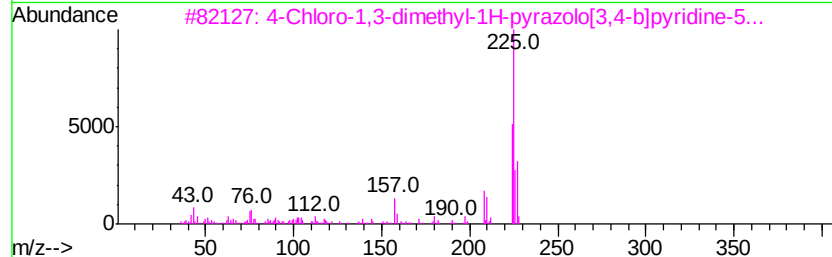
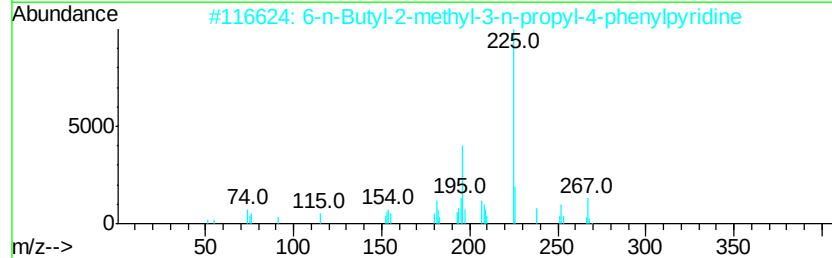
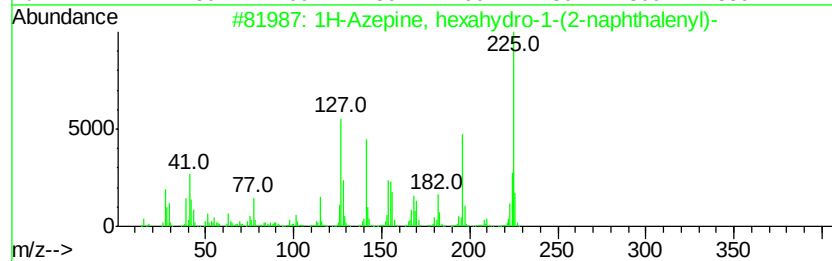
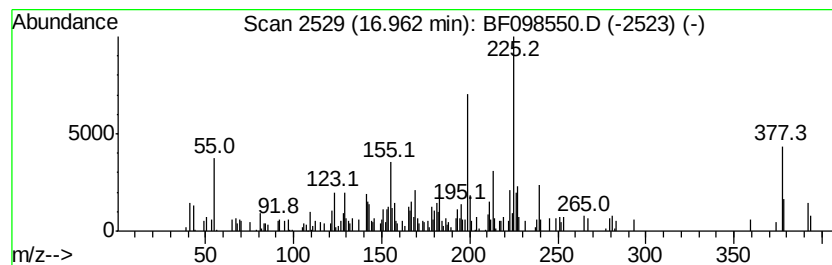
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown16.96 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	3.90 ng	171065	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Azepine, hexahydro-1-(2-napht...	225	C16H19N	055045-05-1	35
2		6-n-Butyl-2-methyl-3-n-propyl-4-...	267	C19H25N	073669-41-7	25
3		4-Chloro-1,3-dimethyl-1H-pyrazol...	225	C9H8ClN3O2	1000293-90-4	22
4		2-Methylidene-hydrazono-3-methyl...	225	C9H8ClN3S	1000147-91-3	18
5		6,7-Dihydro-2-isopropylamino-8-m...	225	C9H15N5O2	1000101-98-2	15



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091417\
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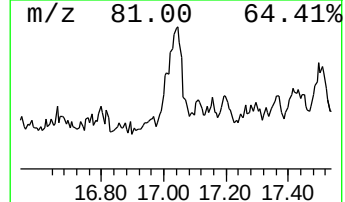
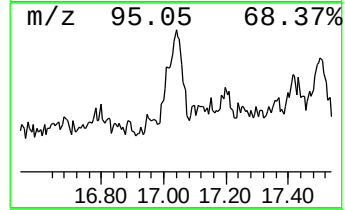
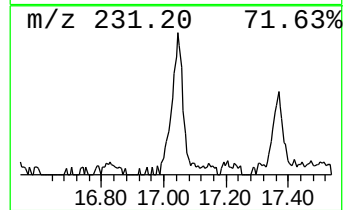
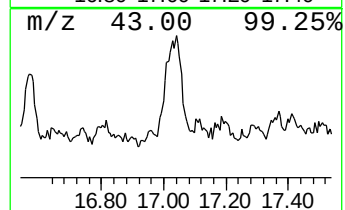
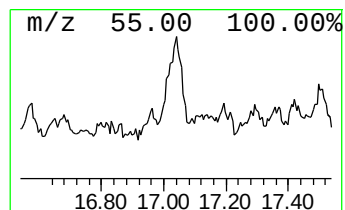
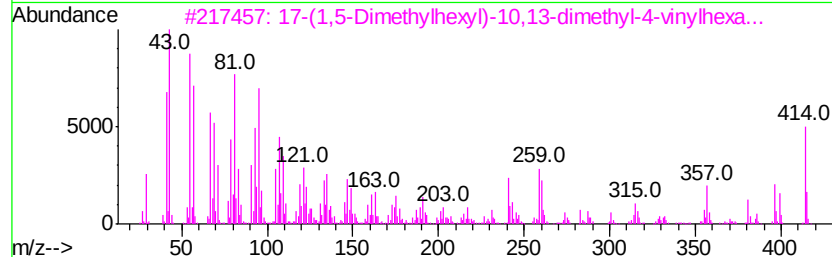
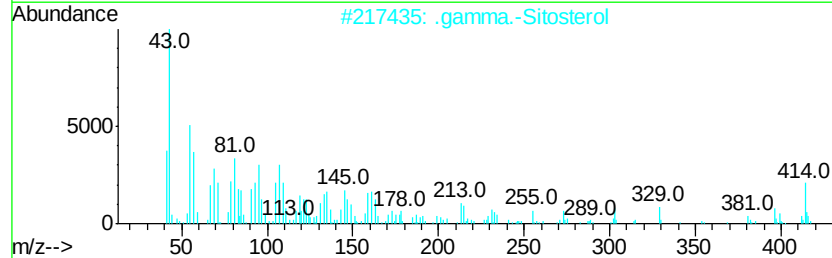
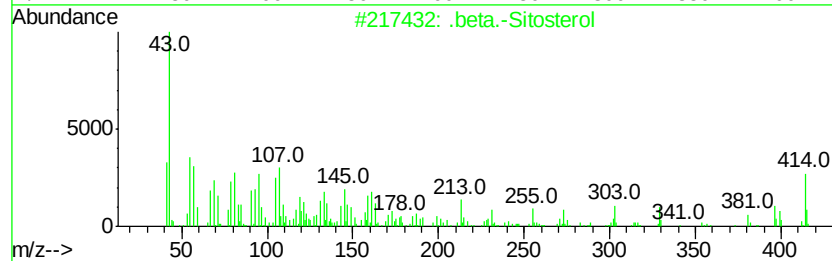
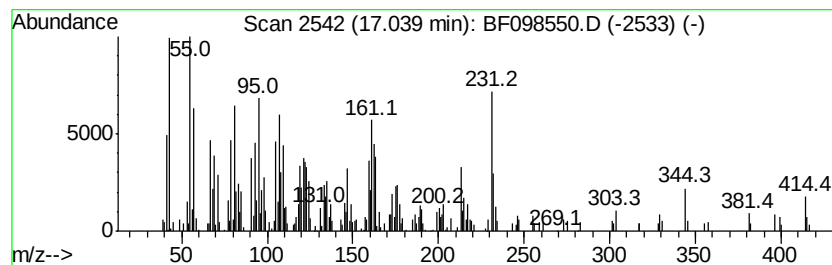
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.04	15.83 ng	694511	Perylene-d12	15.19
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 64
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 56
3		17-(1,5-Dimethylhexyl)-10,13-dim...	414 C29H50O	1000210-86-9 44
4		Cholestan-3-one, 4,4-dimethyl-, ...	414 C29H50O	002097-85-0 38
5		Stigmastan-7-one	414 C29H50O	055331-88-9 20



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091417\
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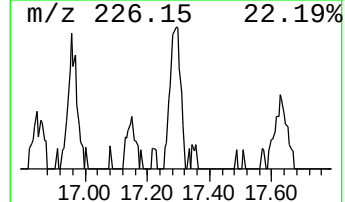
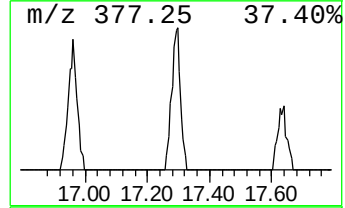
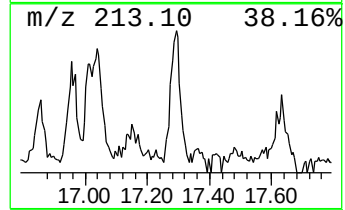
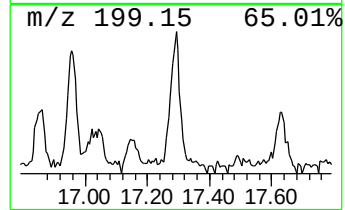
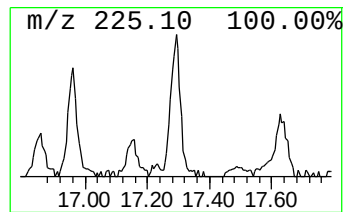
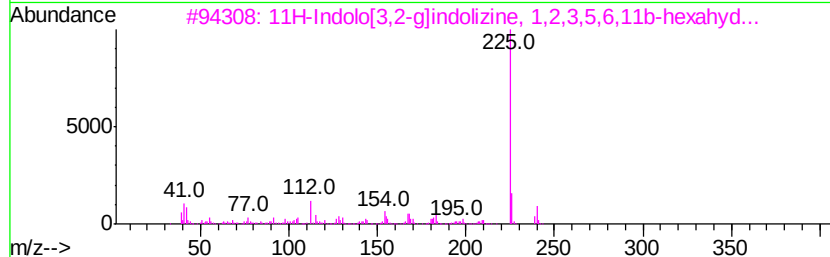
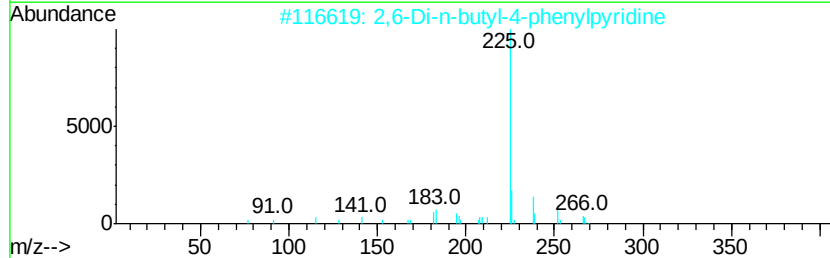
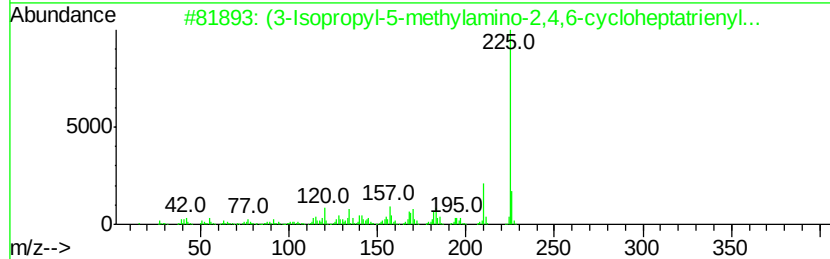
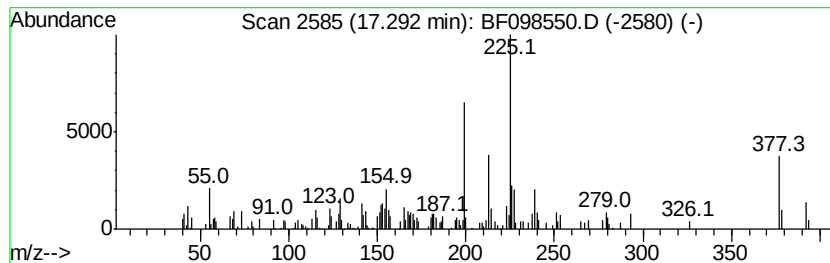
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown17.29 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.29	4.00 ng	175427	Perylene-d12	15.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		(3-Isopropyl-5-methylamino-2,4,6...	225	C14H15N3	014204-00-3	35
2		2,6-Di-n-butyl-4-phenylpyridine	267	C19H25N	073669-42-8	25
3		11H-Indolo[3,2-a]indolizine, 1,2...	240	C16H20N2	1000264-72-5	25
4		(E)-4-Nitrostilbene	225	C14H11NO2	001694-20-8	25
5		Propionitrile, 3-(5-methyl-3-phe...	225	C13H11N3O	1000263-77-0	25



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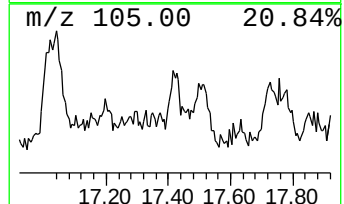
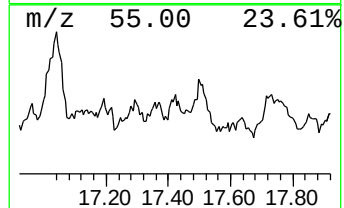
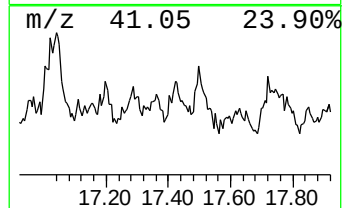
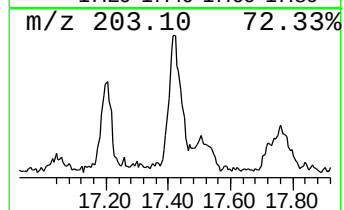
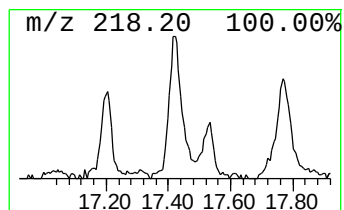
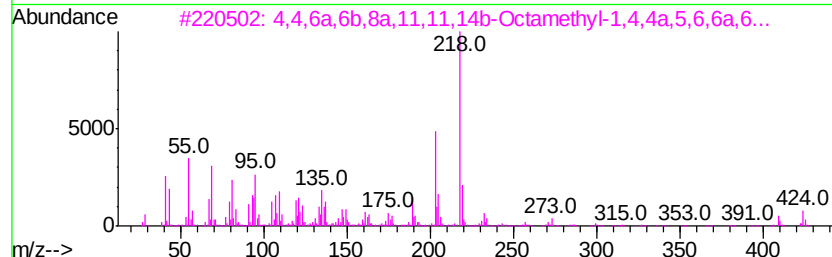
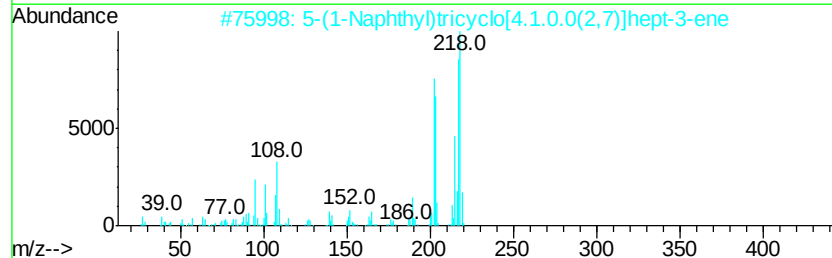
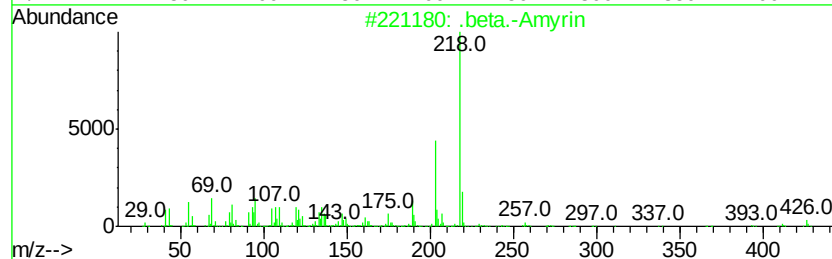
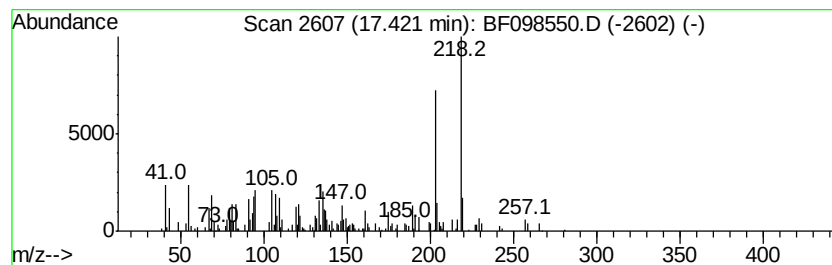
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 .beta.-Amyrin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	4.56 ng	200302	Perylene-d12	15.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Amyrin	426	C30H50O	000559-70-6	89
2		5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	81
3		4,4,6a,6b,8a,11,11,14b-Octamethv...	424	C30H48O	1000194-62-4	64
4		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	49
5		.alpha.-Amyrin	426	C30H50O	000638-95-9	49



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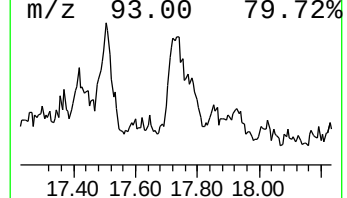
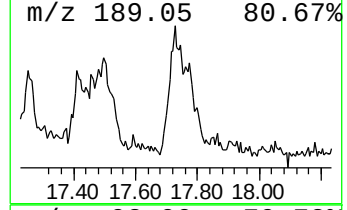
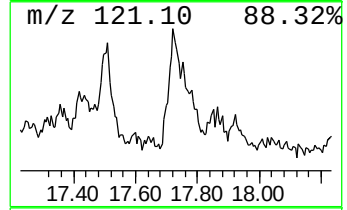
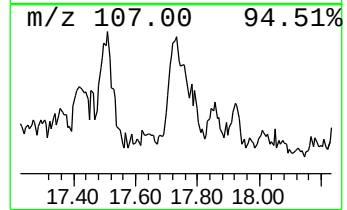
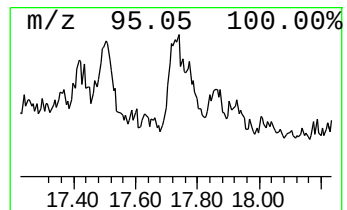
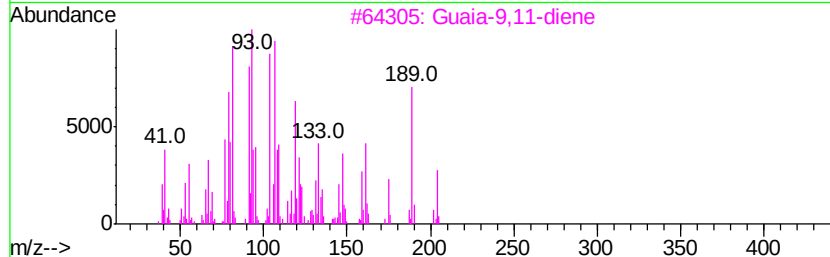
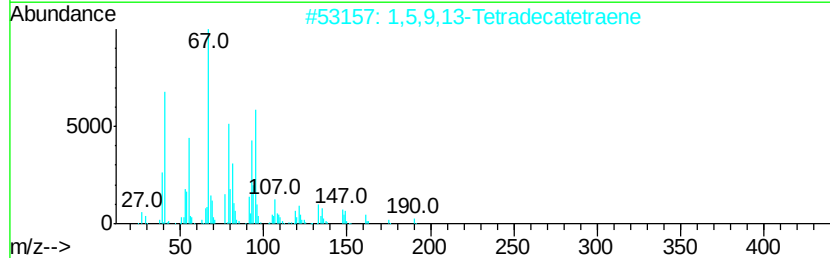
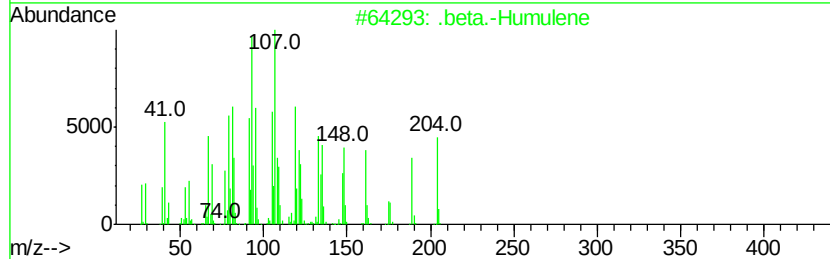
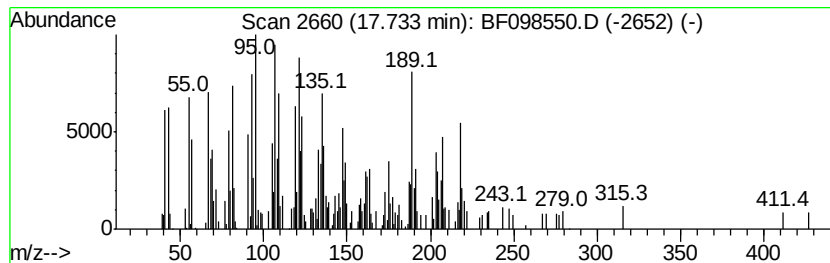
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 .beta.-Humulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.73	8.11 ng	355874	Perylene-d12		15.19	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	.beta.-Humulene		204	C15H24	000116-04-1	92
2	1,5,9,13-Tetradecatetraene		190	C14H22	051487-38-8	68
3	Guaia-9,11-diene		204	C15H24	1000374-19-8	59
4	1-Isopropenyl-3-propenylcyclopent...		150	C11H18	1000192-81-2	53
5	Longifolene		204	C15H24	000475-20-7	50



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Data File : BF098550.D
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Sample : I5219-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	11.4	ng	494351	1	6.65	866560	20.0
unknown6.42	6.42	85.7	ng	3711160	1	6.65	866560	20.0
Trifluoroacetoxy ...	13.64	5.4	ng	221054	5	13.79	813405	20.0
Tetratetracontane	14.27	3.5	ng	144497	5	13.79	813405	20.0
Octadecane, 2-met...	14.86	10.2	ng	448174	6	15.19	877600	20.0
Heneicosane	15.60	11.0	ng	482458	6	15.19	877600	20.0
Pentadecane	16.57	3.3	ng	144480	6	15.19	877600	20.0
unknown16.96	16.96	3.9	ng	171065	6	15.19	877600	20.0
.beta.-Sitosterol	17.04	15.8	ng	694511	6	15.19	877600	20.0
unknown17.29	17.29	4.0	ng	175427	6	15.19	877600	20.0
.beta.-Amyrin	17.42	4.6	ng	200302	6	15.19	877600	20.0
.beta.-Humulene	17.73	8.1	ng	355874	6	15.19	877600	20.0