

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
 Data File : BF092514.D
 Acq On : 26 Jan 2017 9:57
 Operator : SJ/MA
 Sample : I1312-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CAS-SB-03-5-7

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-BF012417.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	2.281	16	17	26	rVB3	15673	44074	1.03%	0.100%
2	3.390	112	114	126	rBV	16707	56149	1.31%	0.128%
3	5.161	265	269	275	rBV	1273538	1809019	42.08%	4.109%
4	5.561	301	304	307	rBV	3019393	3918201	91.13%	8.900%
5	6.590	391	394	397	rBV	3718992	4299495	100.00%	9.767%
6	6.727	403	406	409	rBV	3111906	3911743	90.98%	8.886%
7	6.967	424	427	429	rVB	1190901	1039565	24.18%	2.361%
8	7.127	438	441	443	rBV	2731928	3021537	70.28%	6.864%
9	7.527	473	476	479	rBV	2079237	2452079	57.03%	5.570%
10	8.259	537	540	542	rBV	1605071	1446629	33.65%	3.286%
11	9.345	632	635	637	rBV	4014569	4154886	96.64%	9.438%
12	9.733	667	669	672	rBV	807110	686232	15.96%	1.559%
13	9.950	686	688	692	rBV	49255	44345	1.03%	0.101%
14	10.019	692	694	696	rVV	1635083	1475046	34.31%	3.351%
15	10.316	718	720	722	rBV	66484	67679	1.57%	0.154%
16	10.431	728	730	731	rBV	48957	50933	1.18%	0.116%
17	10.453	731	732	734	rVB	131450	98041	2.28%	0.223%
18	10.671	749	751	755	rBV	33148	60180	1.40%	0.137%
19	10.808	760	763	766	rBV2	1963843	2318939	53.94%	5.268%
20	10.933	772	774	778	rVB	106106	173916	4.05%	0.395%
21	11.116	788	790	795	rBV4	24327	56076	1.30%	0.127%
22	11.379	809	813	814	rBV	129909	132362	3.08%	0.301%
23	11.402	814	815	819	rVB	43558	58008	1.35%	0.132%
24	11.505	822	824	828	rBV2	1285625	1736083	40.38%	3.944%
25	11.585	828	831	832	rVB	88275	98813	2.30%	0.224%
26	11.733	841	844	845	rBV2	35070	43947	1.02%	0.100%
27	11.802	848	850	852	rVV	109974	98858	2.30%	0.225%
28	12.008	866	868	869	rBV	65097	55826	1.30%	0.127%
29	12.042	869	871	872	rVV	86832	103149	2.40%	0.234%
30	12.122	876	878	882	rVB2	131088	178708	4.16%	0.406%
31	12.214	882	886	887	rBV	56531	55865	1.30%	0.127%
32	12.305	892	894	898	rVB2	55806	85805	2.00%	0.195%
33	12.556	914	916	918	rBV	62124	74405	1.73%	0.169%
34	12.602	918	920	922	rVV2	46891	57421	1.34%	0.130%

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35	12.648	922	924	927	rVB3	32447	45323	1.05%	0.103%
36	12.728	928	931	933	rVB	531657	647767	15.07%	1.471%
37	12.785	933	936	937	rBV3	20433	45683	1.06%	0.104%
38	12.819	937	939	941	rBV	42580	44711	1.04%	0.102%
39	12.945	947	950	953	rBV2	424737	657554	15.29%	1.494%
40	13.105	961	964	966	rVV	2851092	3415576	79.44%	7.759%
41	13.174	966	970	974	rVV3	47303	83124	1.93%	0.189%
42	13.276	975	979	981	rVV2	107311	164545	3.83%	0.374%
43	13.345	983	985	986	rVV	98172	88916	2.07%	0.202%
44	13.379	986	988	992	rVB2	78248	113877	2.65%	0.259%
45	13.677	1010	1014	1018	rBV4	32355	108036	2.51%	0.245%
46	13.791	1021	1024	1026	rVB3	34709	72964	1.70%	0.166%
47	13.894	1031	1033	1035	rBV2	35170	56630	1.32%	0.129%
48	13.997	1040	1042	1047	rVB	342662	412110	9.59%	0.936%
49	14.145	1052	1055	1061	rVB2	1123218	1627373	37.85%	3.697%
50	14.248	1062	1064	1066	rBV3	32120	45958	1.07%	0.104%
51	14.534	1087	1089	1090	rBV	48694	43597	1.01%	0.099%
52	14.625	1095	1097	1099	rBV2	87266	101752	2.37%	0.231%
53	15.185	1144	1146	1152	rBV	173876	450007	10.47%	1.022%
54	15.300	1154	1156	1159	rVB	64446	84136	1.96%	0.191%
55	15.494	1171	1173	1176	rVB	120870	174254	4.05%	0.396%
56	15.562	1176	1179	1181	rBV	157975	221992	5.16%	0.504%
57	15.620	1181	1184	1187	rBV	579191	965128	22.45%	2.192%
58	16.168	1229	1232	1238	rVB6	44539	100384	2.33%	0.228%
59	17.094	1310	1313	1318	rBV2	78835	175792	4.09%	0.399%
60	17.540	1349	1352	1356	rBV	55661	111431	2.59%	0.253%

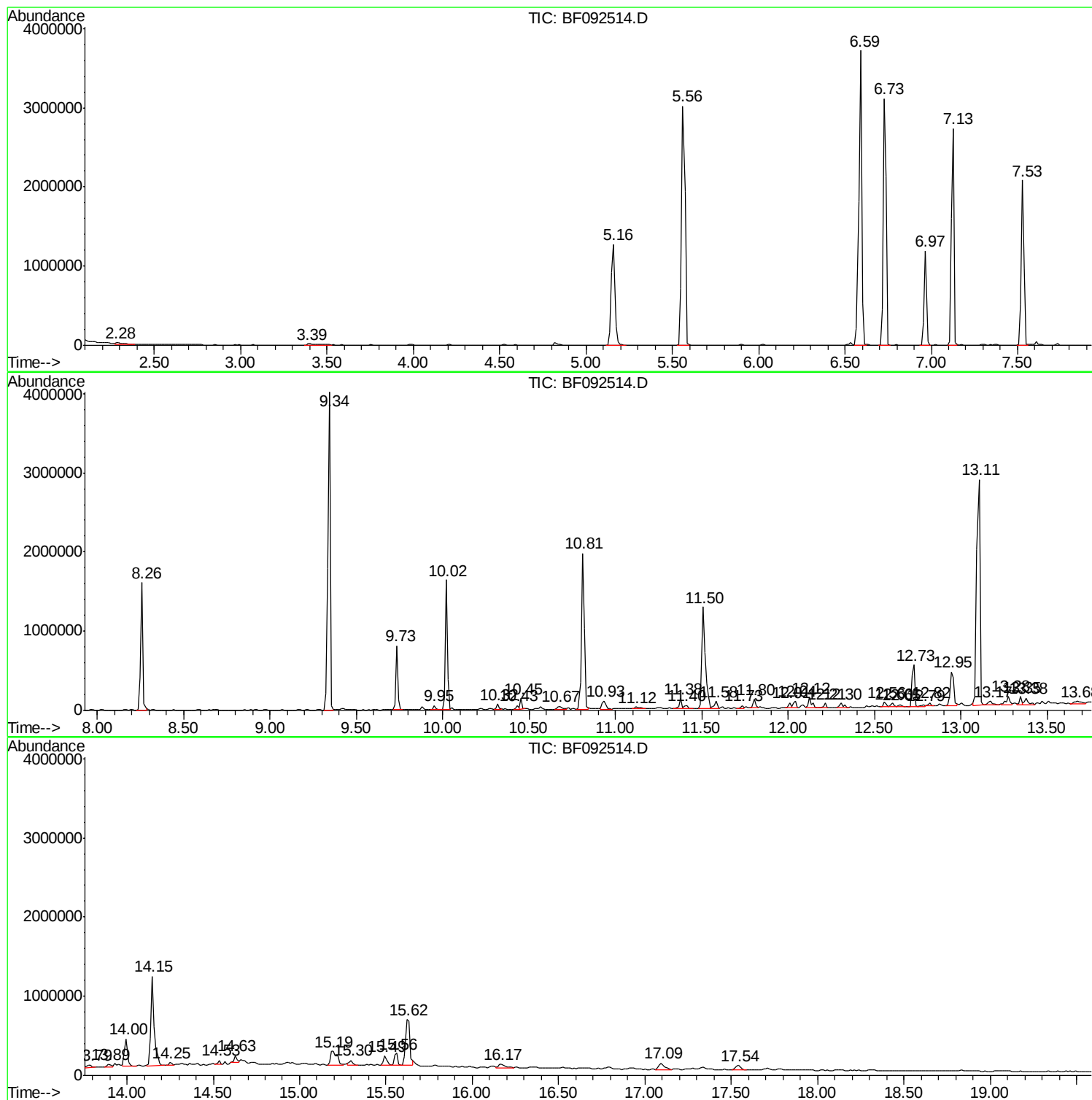
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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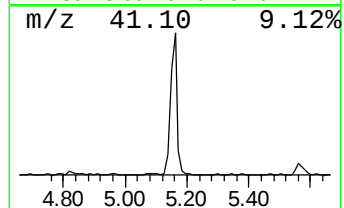
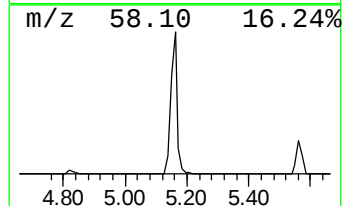
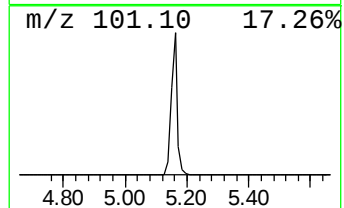
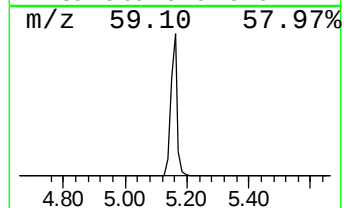
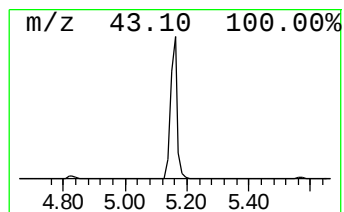
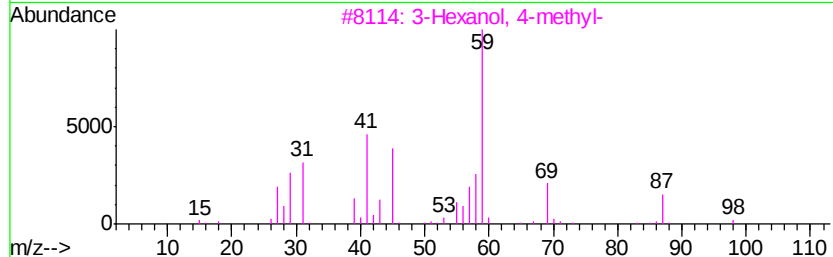
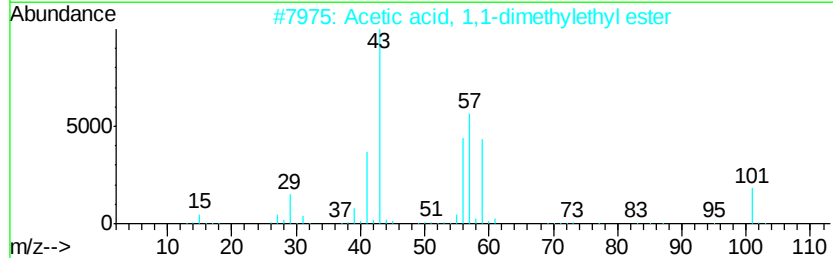
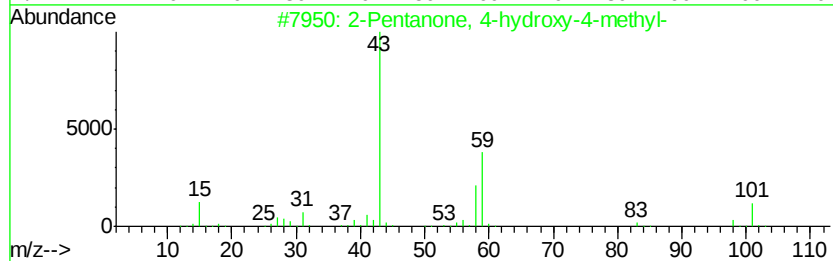
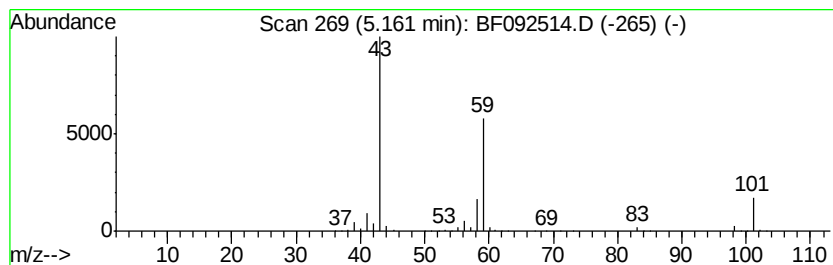
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.16	34.80 ng	1809020	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	9



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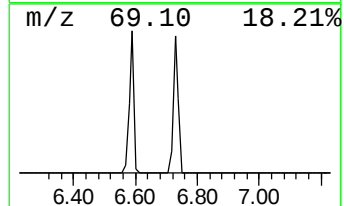
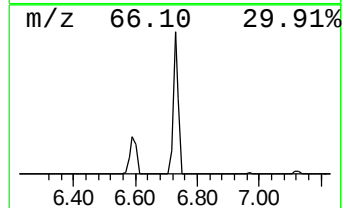
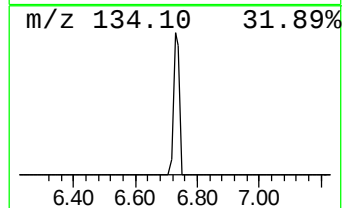
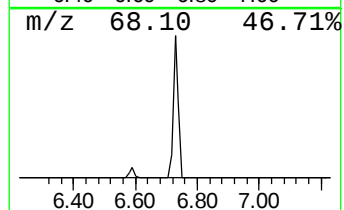
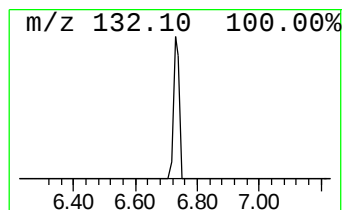
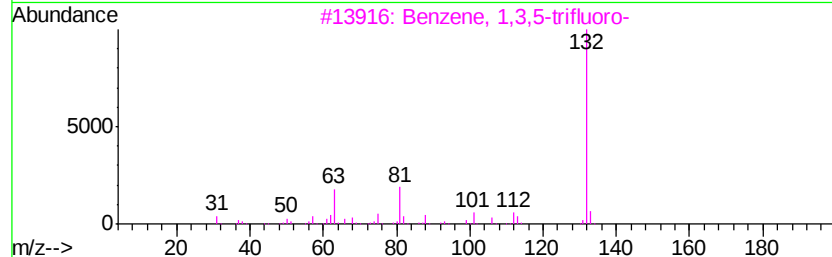
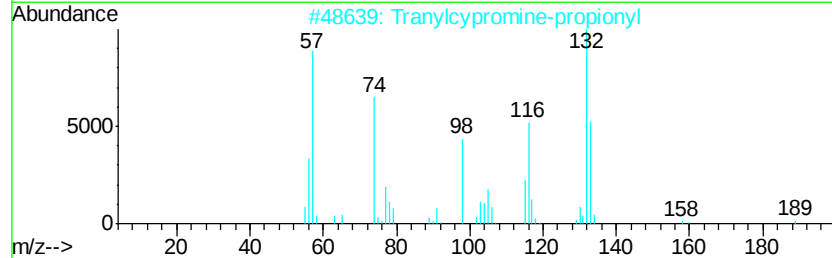
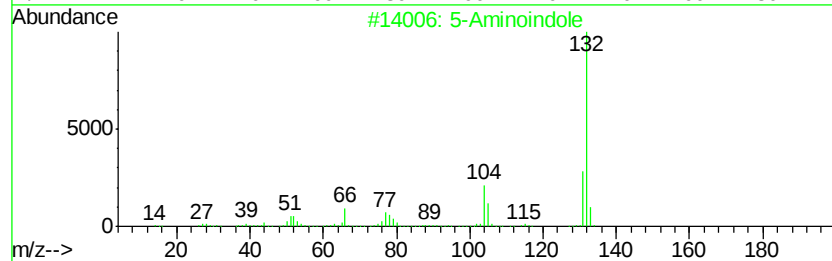
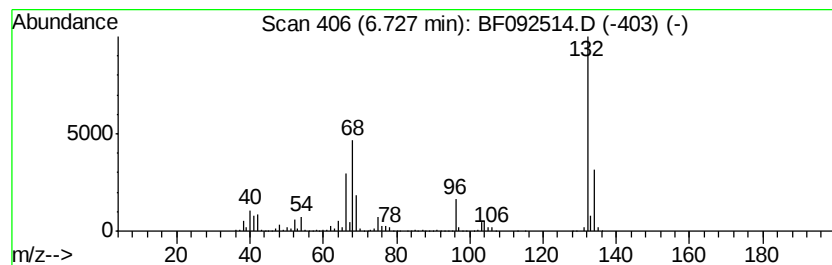
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	75.26 ng	3911740	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranvlcypropamine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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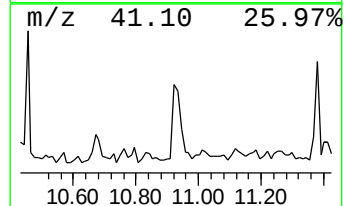
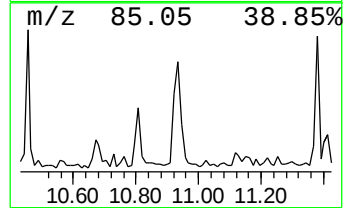
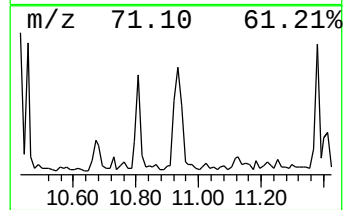
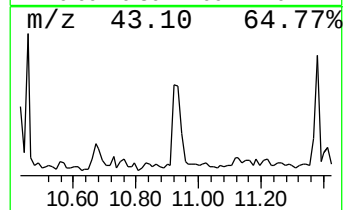
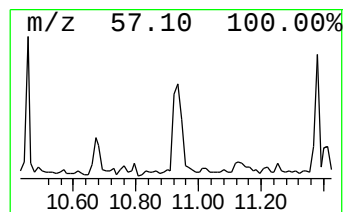
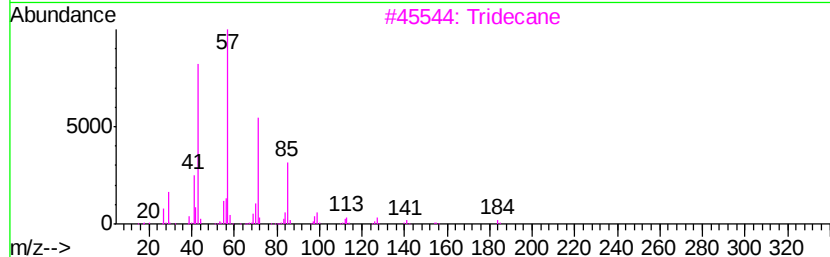
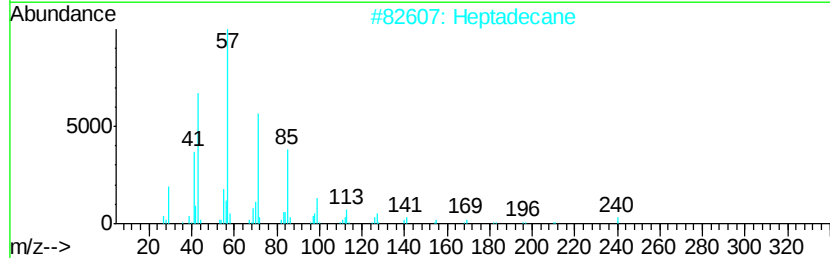
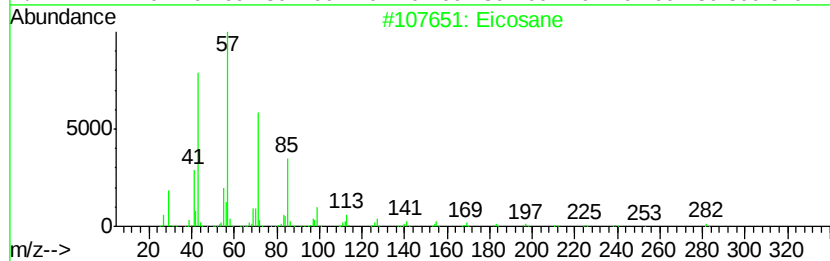
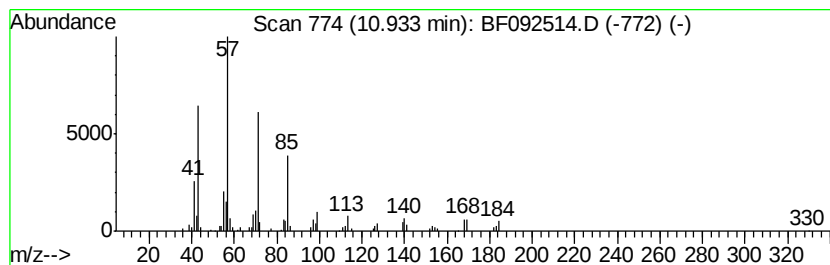
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2.00 ng	173916	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	83
2	Heptadecane		240	C17H36	000629-78-7	80
3	Tridecane		184	C13H28	000629-50-5	76
4	Heptacosane		380	C27H56	000593-49-7	74
5	Tetracosane		338	C24H50	000646-31-1	74



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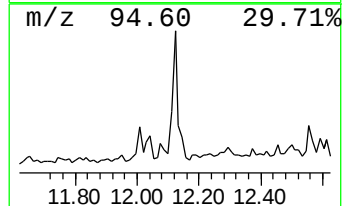
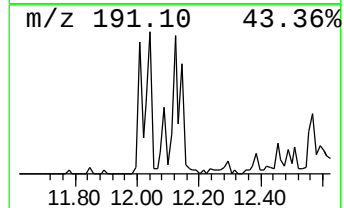
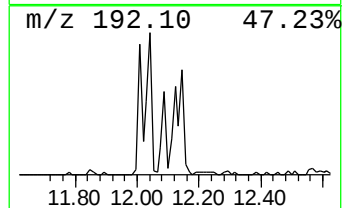
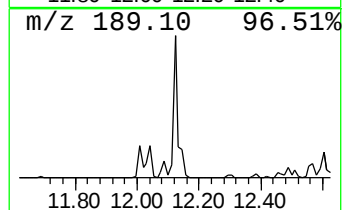
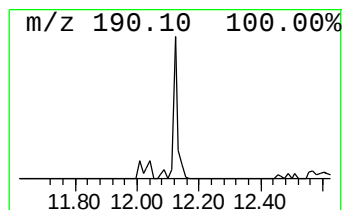
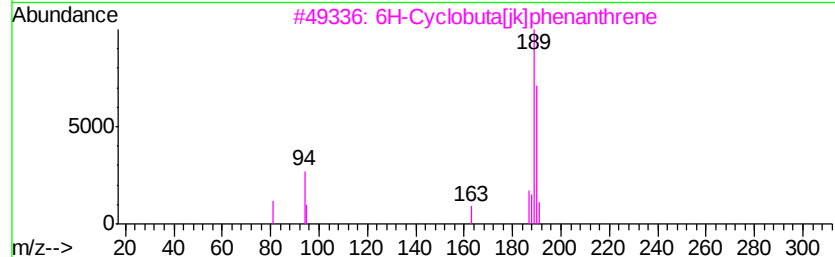
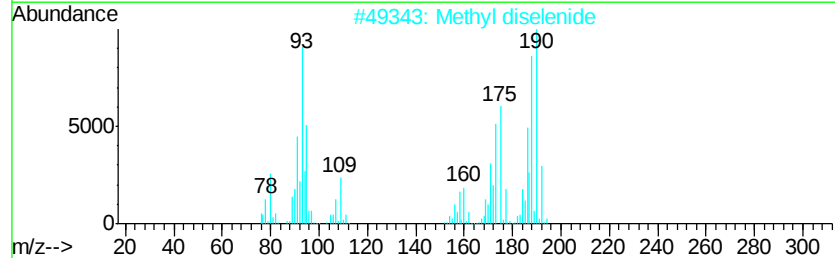
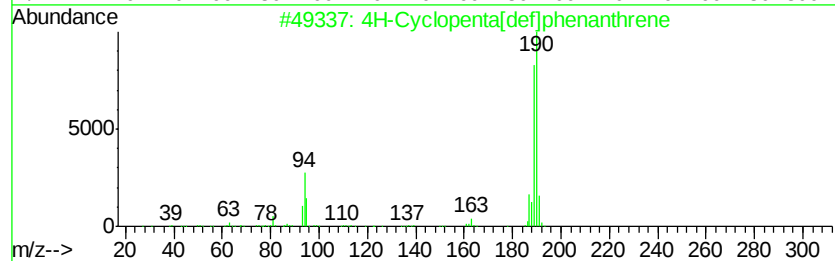
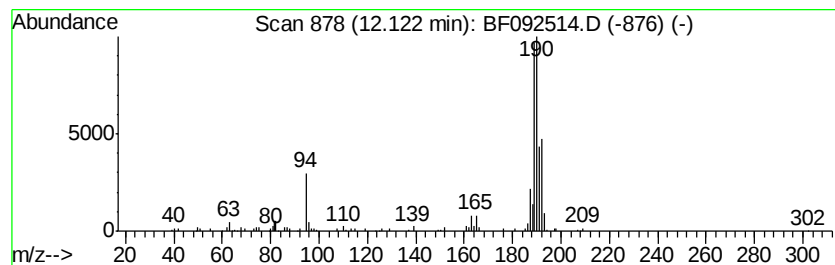
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	2.06 ng	178708	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2		Methyl diselenide	190	C2H6Se2	007101-31-7	45
3		6H-Cyclobuta[f]phenanthrene	190	C15H10	083469-43-6	42
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5		Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	33



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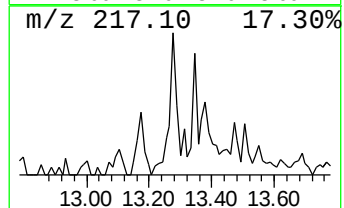
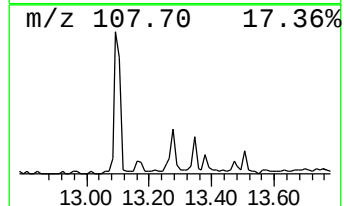
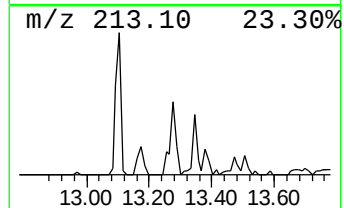
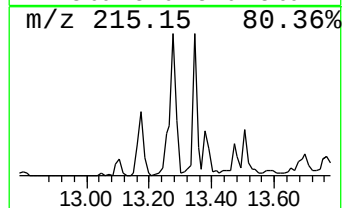
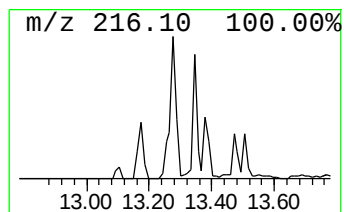
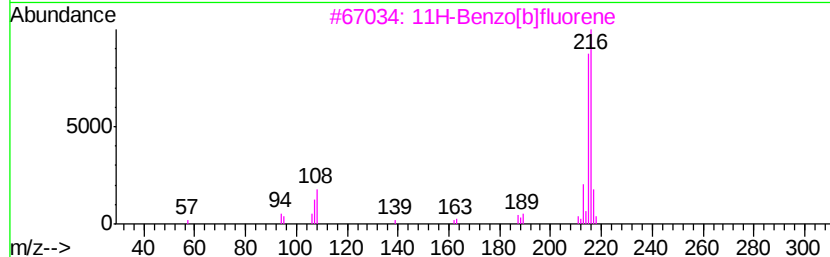
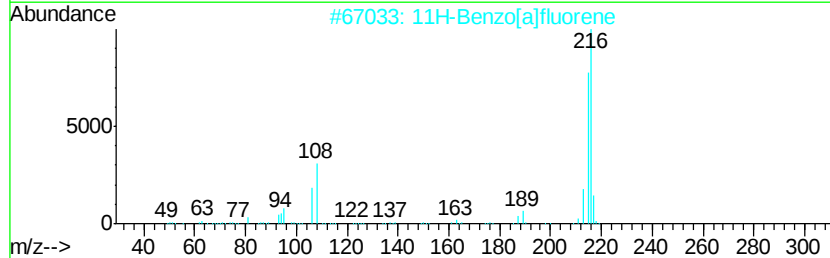
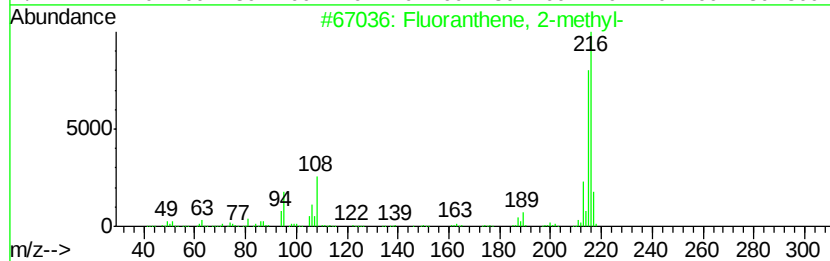
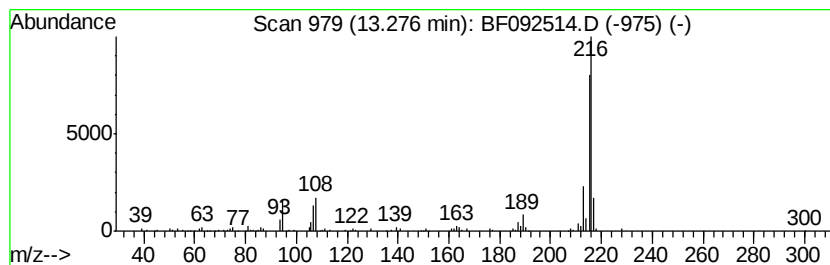
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Fluoranthene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	2.02 ng	164545	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
2		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
3		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
4		Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092514.D
Acq On : 26 Jan 2017 9:57
Operator : SJ/MA
Sample : I1312-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS-SB-03-5-7

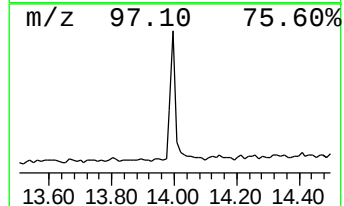
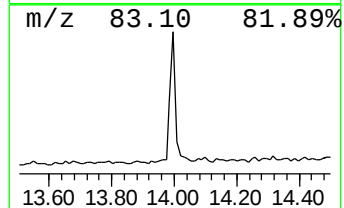
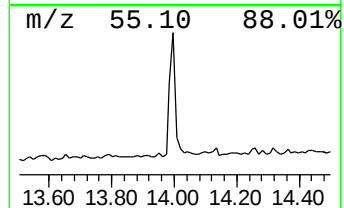
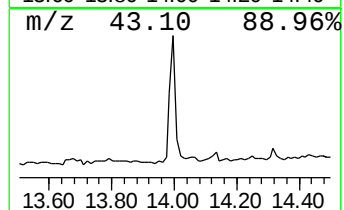
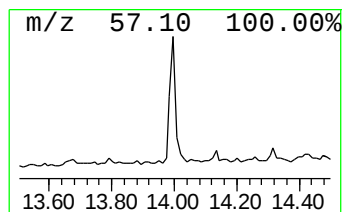
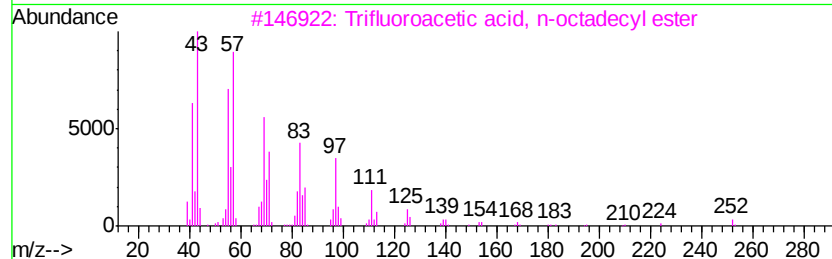
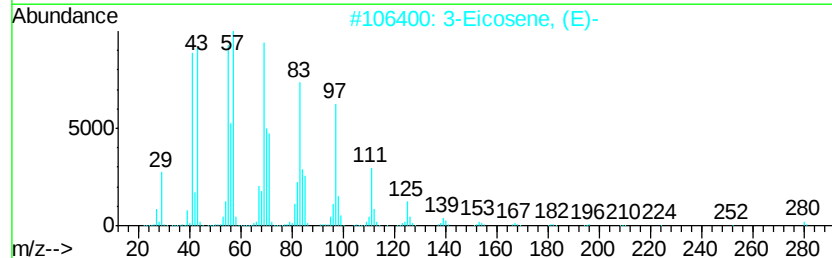
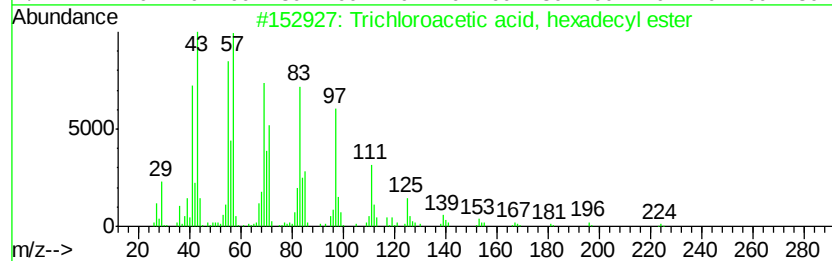
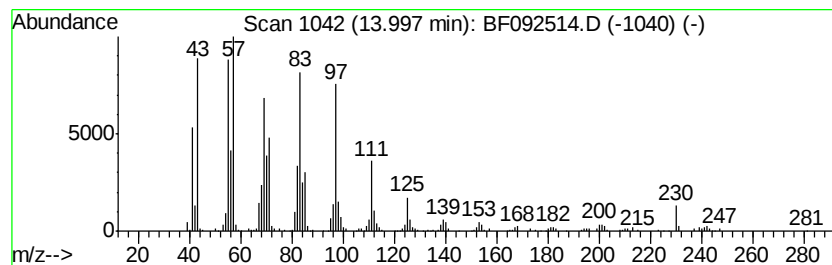
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	5.06 ng	412110	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
4		1-Docosene	308	C22H44	001599-67-3	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092514.D
Acq On : 26 Jan 2017 9:57
Operator : SJ/MA
Sample : I1312-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS-SB-03-5-7

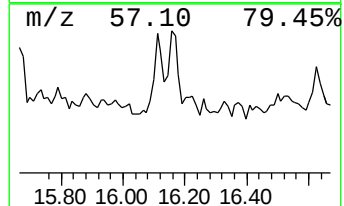
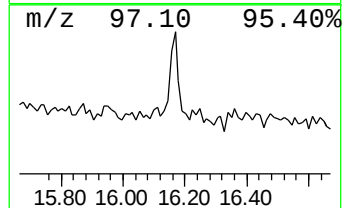
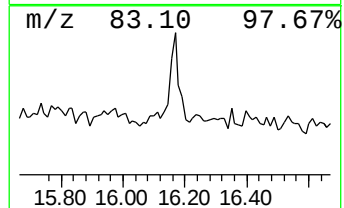
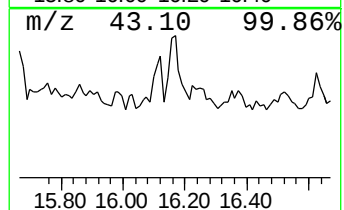
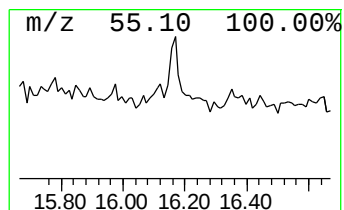
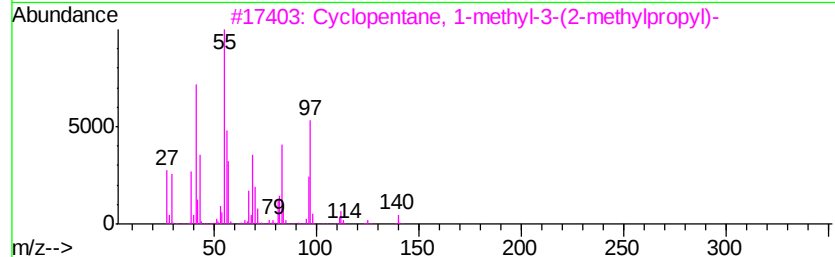
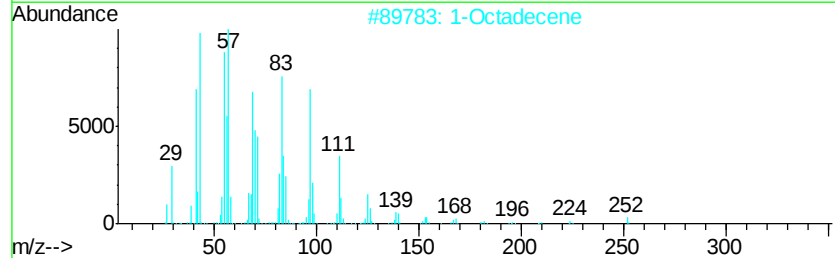
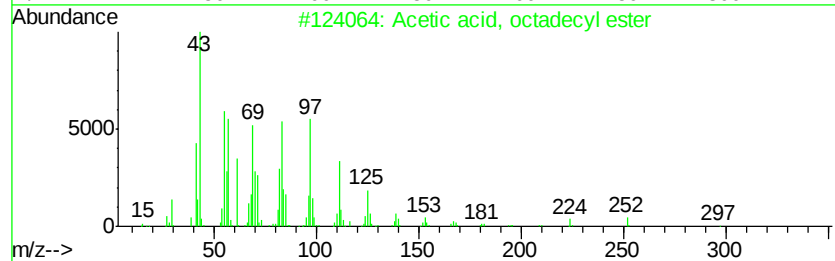
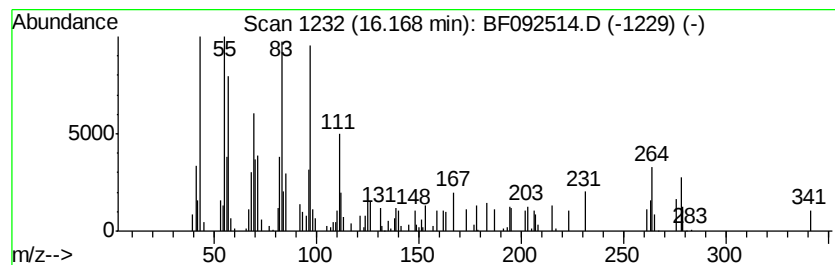
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Acetic acid, octadecyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.08 ng	100384	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	52
2		1-Octadecene	252	C18H36	000112-88-9	52
3		Cyclopentane, 1-methyl-3-(2-methylpropyl)-	140	C10H20	029053-04-1	46
4		Cyclohexane, 1-(cyclohexylmethyl)-	194	C14H26	054823-97-1	38
5		Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092514.D
Acq On : 26 Jan 2017 9:57
Operator : SJ/MA
Sample : I1312-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CAS-SB-03-5-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.16	34.8	ng	1809020	1	6.97	1039570	20.0
unknown6.73	6.73	75.3	ng	3911740	1	6.97	1039570	20.0
Eicosane	10.93	2.0	ng	173916	4	11.50	1736080	20.0
4H-Cyclopenta[def...	12.12	2.1	ng	178708	4	11.50	1736080	20.0
Fluoranthene, 2-m...	13.28	2.0	ng	164545	5	14.15	1627370	20.0
Trichloroacetic a...	14.00	5.1	ng	412110	5	14.15	1627370	20.0
Acetic acid, octa...	16.17	2.1	ng	100384	6	15.63	965128	20.0