

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
 Data File : BF092901.D
 Acq On : 10 Feb 2017 23:34
 Operator : SJ/MA
 Sample : I1777-08
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 38-SB-01-0-2

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-BF013017.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	5.081	258	262	272	rBV	1084318	1765847	41.34%	4.132%
2	5.504	296	299	301	rBV	3128972	4150487	97.17%	9.712%
3	6.533	386	389	392	rBV	3498160	3962095	92.76%	9.271%
4	6.659	398	400	403	rBV	3259333	3931632	92.04%	9.200%
5	6.887	418	420	423	rBV	987253	978320	22.90%	2.289%
6	7.047	432	434	437	rBV	3192878	2952383	69.12%	6.909%
7	7.459	467	470	472	rBV	2508222	2531511	59.26%	5.924%
8	8.179	530	533	535	rBV	1552145	1411257	33.04%	3.302%
9	9.253	624	627	630	rBV	3722889	4271553	100.00%	9.996%
10	9.653	659	662	664	rBV	263535	280531	6.57%	0.656%
11	9.859	676	680	684	rBV	82995	119429	2.80%	0.279%
12	9.928	684	686	689	rBV	1248064	1644247	38.49%	3.848%
13	10.362	715	724	726	rBV	158836	176988	4.14%	0.414%
14	10.579	740	743	746	rBV	49996	69787	1.63%	0.163%
15	10.728	752	756	758	rBV	2356979	2829235	66.23%	6.620%
16	10.831	763	765	770	rVB	173782	241282	5.65%	0.565%
17	11.276	802	804	806	rBV	88765	128458	3.01%	0.301%
18	11.414	814	816	819	rBV	1265610	1821298	42.64%	4.262%
19	11.974	864	865	868	rVB2	33296	49487	1.16%	0.116%
20	12.031	868	870	874	rVB2	53109	83336	1.95%	0.195%
21	12.625	920	922	925	rVB	385043	371362	8.69%	0.869%
22	12.854	937	942	945	rBV2	323443	418803	9.80%	0.980%
23	13.002	952	955	958	rBV	3061720	4105314	96.11%	9.607%
24	13.082	958	962	966	rVB3	25237	43841	1.03%	0.103%
25	13.185	968	971	973	rBV	51146	72628	1.70%	0.170%
26	13.802	1022	1025	1026	rBV2	33665	47734	1.12%	0.112%
27	13.894	1032	1033	1039	rVB2	182934	252618	5.91%	0.591%
28	14.054	1044	1047	1053	rVB2	1415922	1752844	41.04%	4.102%
29	14.214	1058	1061	1063	rBV3	23533	46887	1.10%	0.110%
30	14.442	1076	1081	1082	rBV	36109	46855	1.10%	0.110%
31	14.534	1086	1089	1091	rBV3	47765	100791	2.36%	0.236%
32	14.820	1112	1114	1119	rVB	27254	44334	1.04%	0.104%
33	15.082	1135	1137	1141	rBV	140788	273890	6.41%	0.641%
34	15.151	1141	1143	1145	rVV2	42289	49921	1.17%	0.117%

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Integration Parameters: rteint.p
Integrator: RTE
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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 >
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35	15.380	1160	1163	1166	rVB	79706	99618	2.33%	0.233%
36	15.437	1166	1168	1171	rBV	98849	129912	3.04%	0.304%
37	15.505	1171	1174	1181	rVB	863651	1153631	27.01%	2.700%
38	15.940	1209	1212	1216	rBV	49672	95101	2.23%	0.223%
39	16.923	1295	1298	1302	rVB2	38585	81518	1.91%	0.191%
40	17.014	1302	1306	1310	rBV2	23789	49958	1.17%	0.117%
41	17.357	1332	1336	1342	rBV	35731	97740	2.29%	0.229%

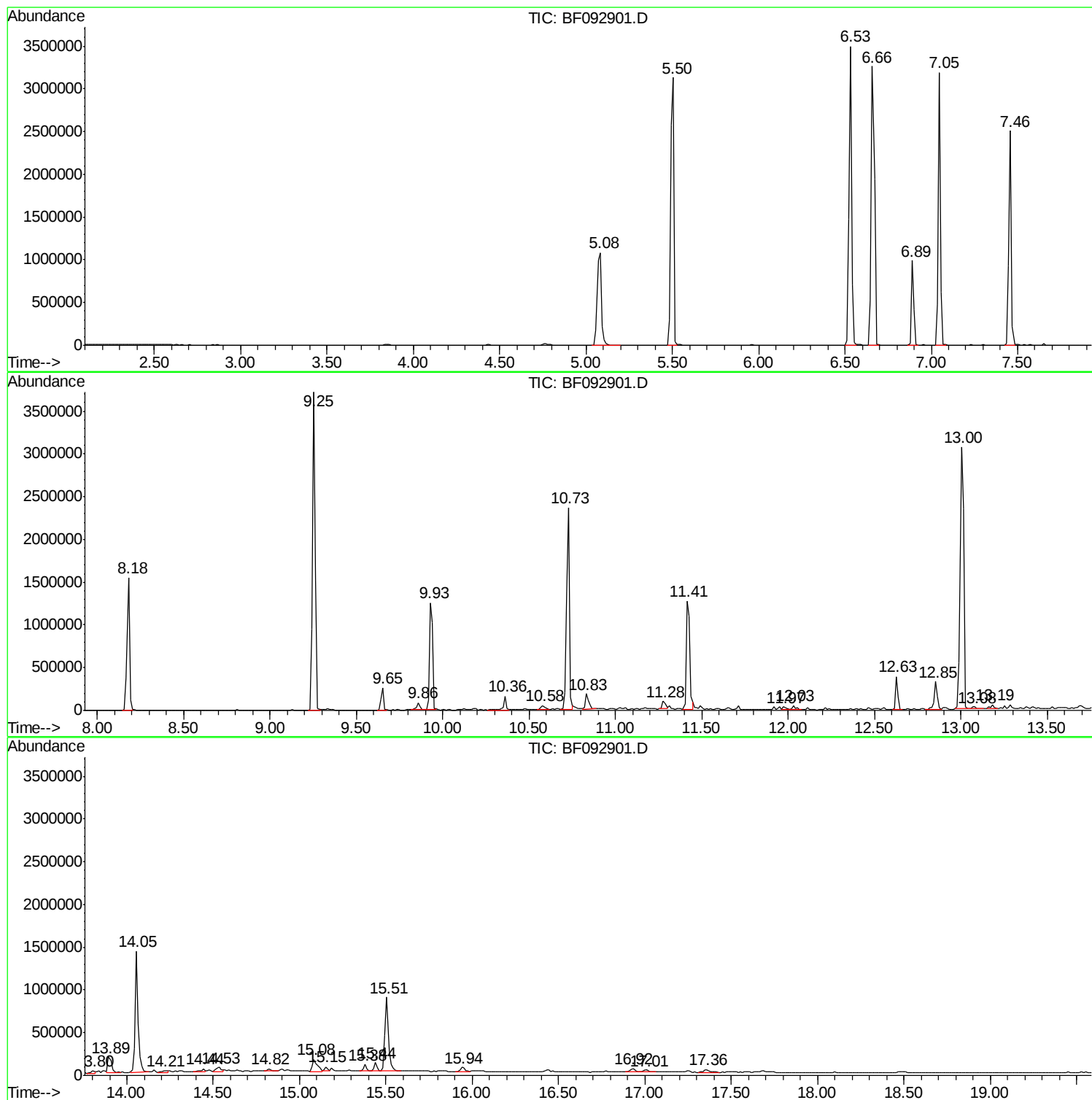
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ClientSampled :
38-SB-01-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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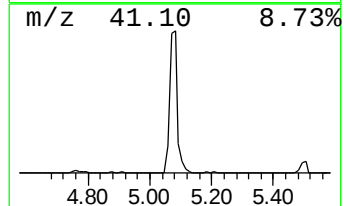
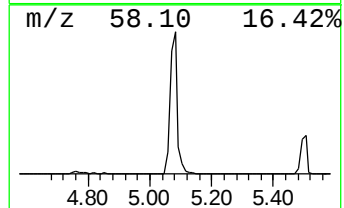
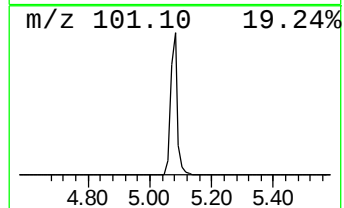
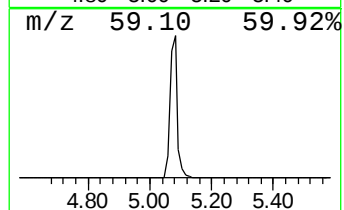
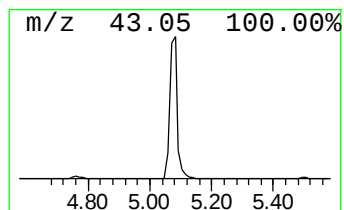
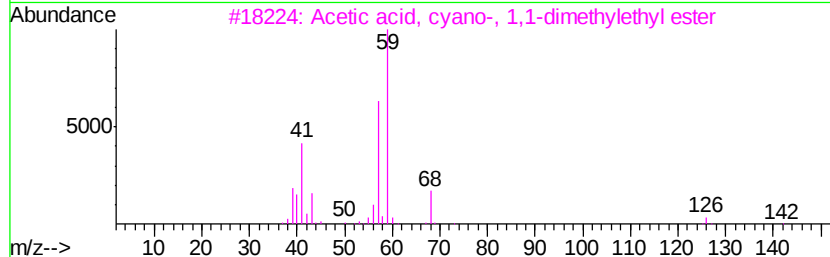
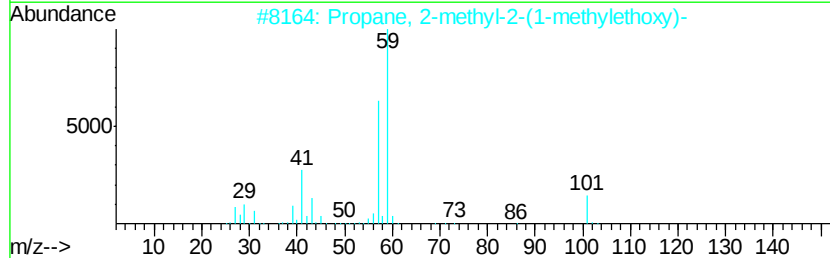
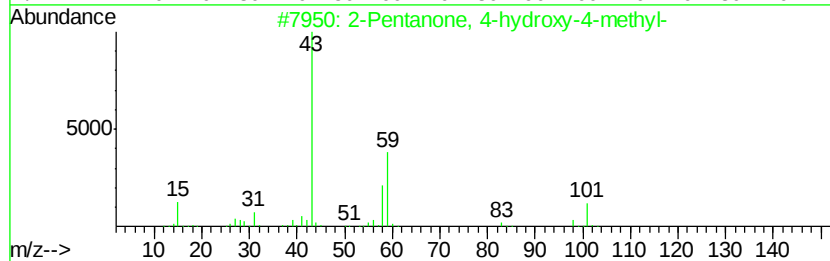
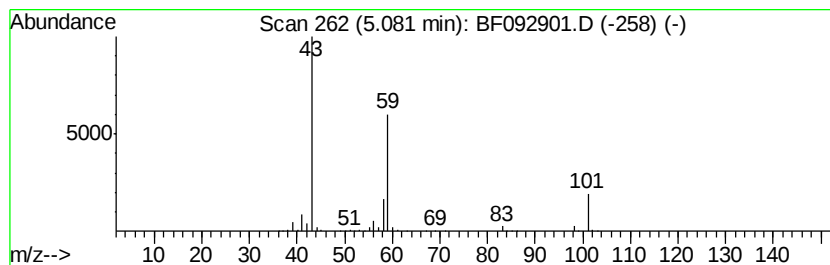
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.08	36.10 ng	1765850	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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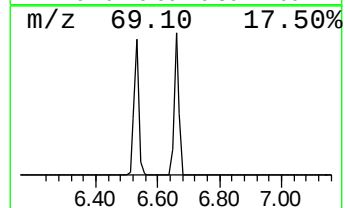
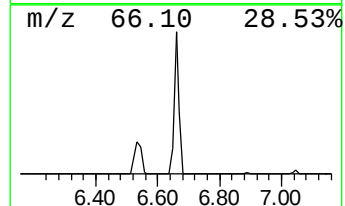
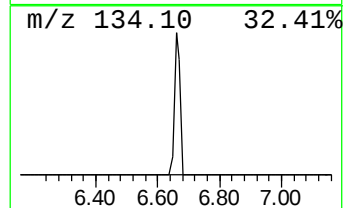
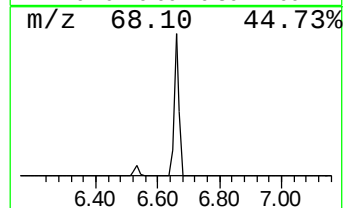
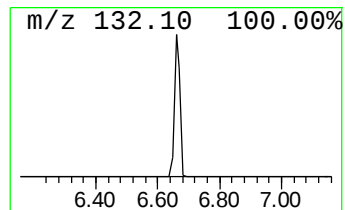
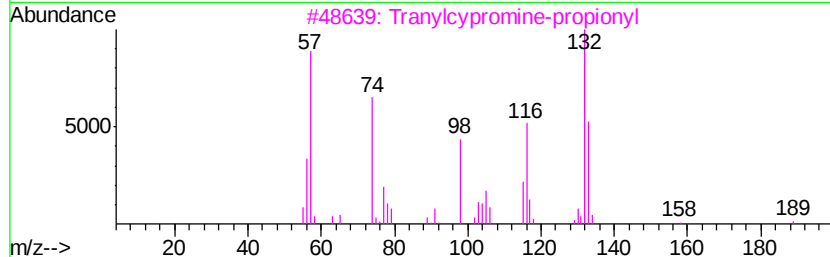
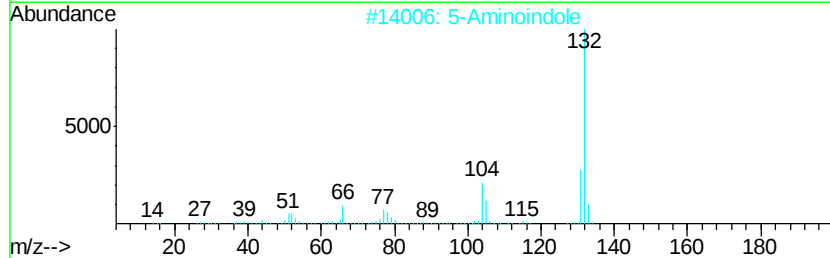
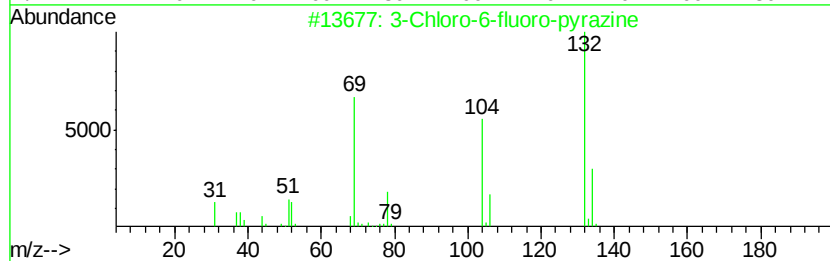
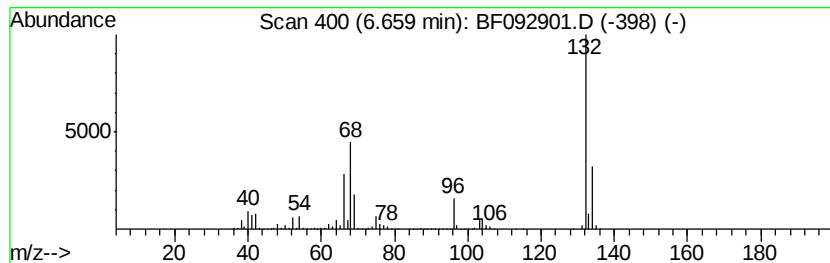
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	80.38 ng	3931630	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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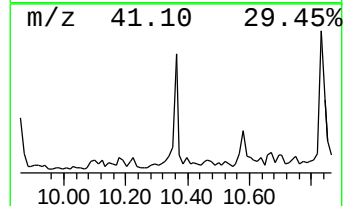
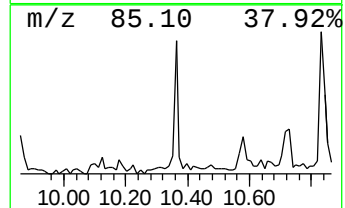
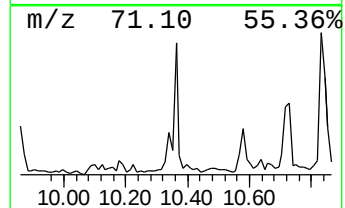
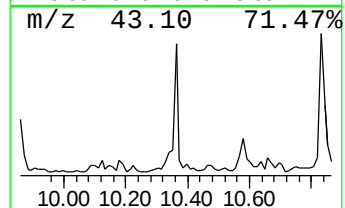
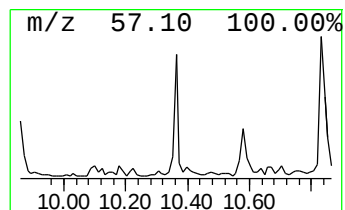
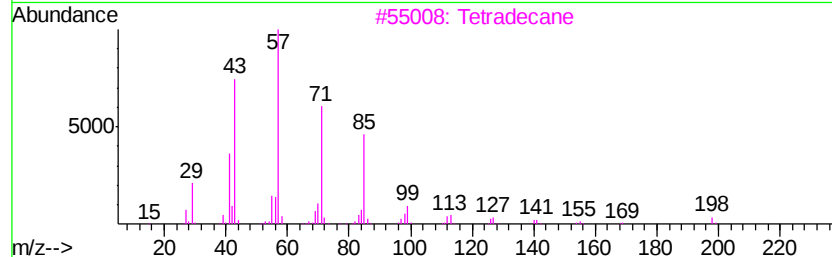
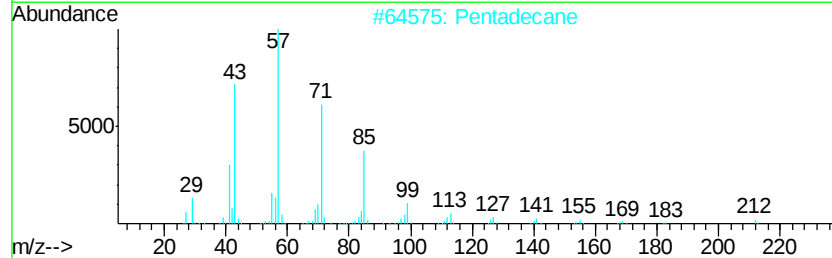
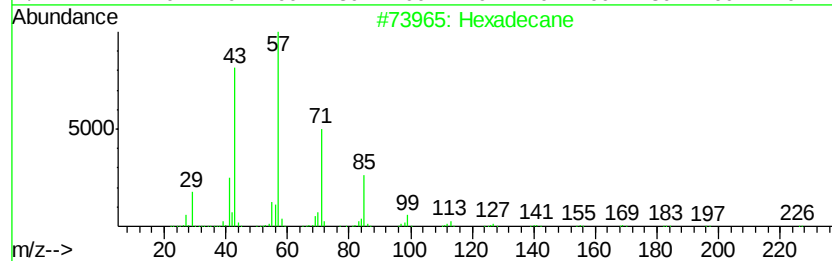
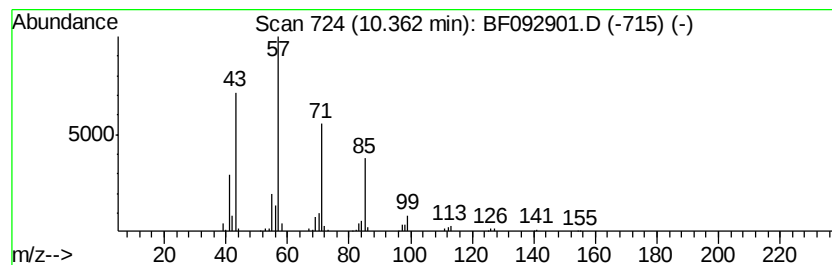
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.36	2.15 ng	176988	Acenaphthene-d10		9.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Pentadecane		212	C15H32	000629-62-9	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	83
5	Tridecane		184	C13H28	000629-50-5	78



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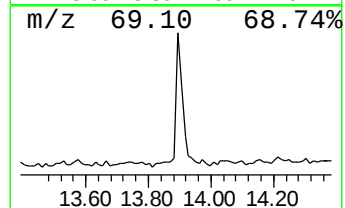
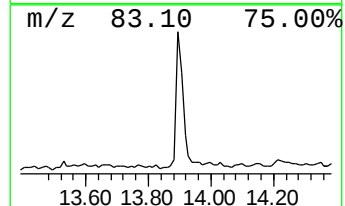
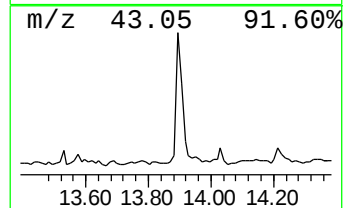
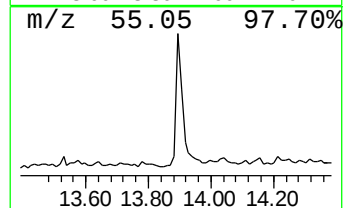
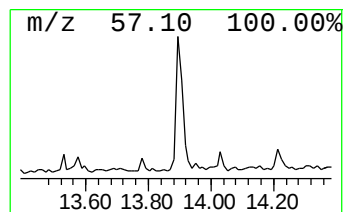
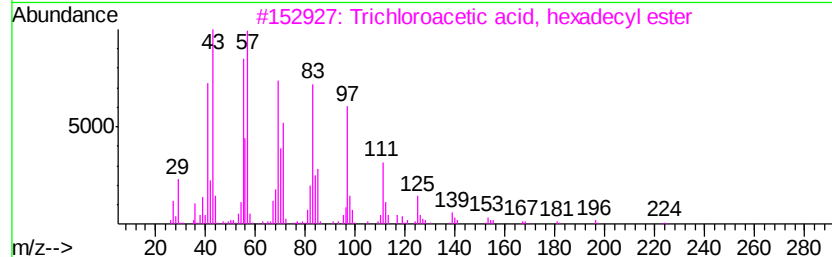
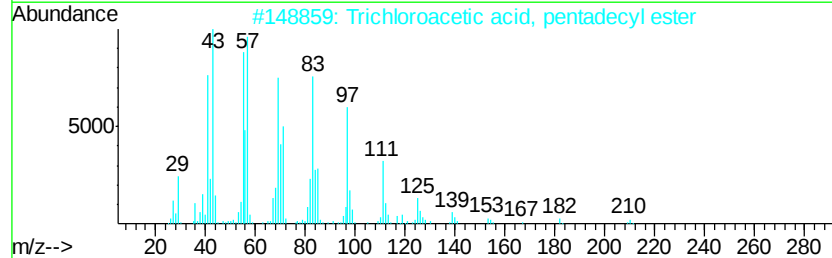
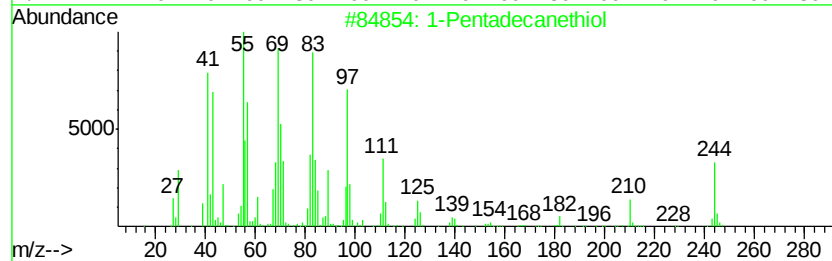
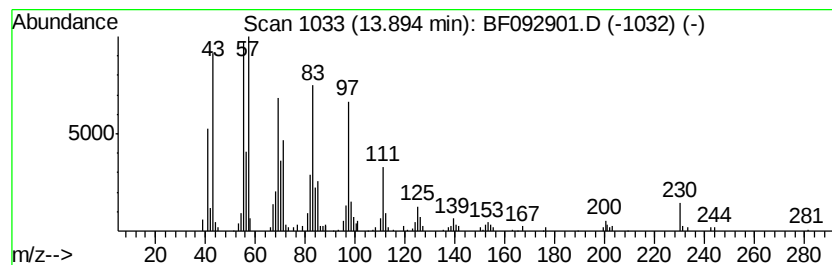
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Peak Number 6 1-Pentadecanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.89	2.88 ng	252618	Chrysene-d12	14.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentadecanethiol	244	C15H32S	025276-70-4	95
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		1-Docosene	308	C22H44	001599-67-3	94
5		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	36.1	ng	1765850	1	6.89	978320	20.0
unknown6.66	6.66	80.4	ng	3931630	1	6.89	978320	20.0
Hexadecane	10.36	2.1	ng	176988	3	9.93	1644250	20.0
1-Pentadecanethiol	13.89	2.9	ng	252618	5	14.05	1752840	20.0