

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071217\
 Data File : BF096711.D
 Acq On : 13 Jul 2017 00:18
 Operator : SJ/JU
 Sample : I4127-03
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-8(6.5-7.0)

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-BF070117.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	4.851	465	470	479	rBV	535029	745171	29.10%	3.559%
2	5.281	538	543	546	rBV	2217916	2240496	87.49%	10.702%
3	6.310	712	718	721	rBV	2318838	2370156	92.55%	11.321%
4	6.439	735	740	743	rBV	2259992	2307639	90.11%	11.023%
5	6.663	775	778	782	rBV	695963	604268	23.60%	2.886%
6	6.822	801	805	809	rBV	2011187	1788537	69.84%	8.543%
7	7.228	869	874	877	rBV	1612555	1516924	59.23%	7.246%
8	7.945	992	996	1000	rBV	1021338	893918	34.91%	4.270%
9	9.027	1174	1180	1183	rBV	2799630	2560990	100.00%	12.233%
10	9.416	1242	1246	1250	rBV	302809	263048	10.27%	1.256%
11	9.698	1290	1294	1298	rBV	951325	802542	31.34%	3.833%
12	10.145	1367	1370	1373	rVB	38447	28271	1.10%	0.135%
13	10.480	1423	1427	1431	rBV	1203768	1129017	44.09%	5.393%
14	10.616	1447	1450	1458	rBV	60385	62246	2.43%	0.297%
15	11.174	1541	1545	1549	rBV	805450	649077	25.34%	3.100%
16	12.598	1783	1787	1790	rBV	42893	36248	1.42%	0.173%
17	12.762	1810	1815	1818	rBV	1767152	1675189	65.41%	8.002%
18	13.662	1963	1968	1977	rBV	109596	134817	5.26%	0.644%
19	13.804	1988	1992	1997	rBV	612631	549875	21.47%	2.626%
20	14.298	2072	2076	2083	rBV3	20617	31467	1.23%	0.150%
21	14.898	2175	2178	2186	rBV5	17194	27690	1.08%	0.132%
22	15.198	2223	2229	2235	rBV	401540	485196	18.95%	2.318%
23	15.245	2235	2237	2243	rVB4	23728	32929	1.29%	0.157%

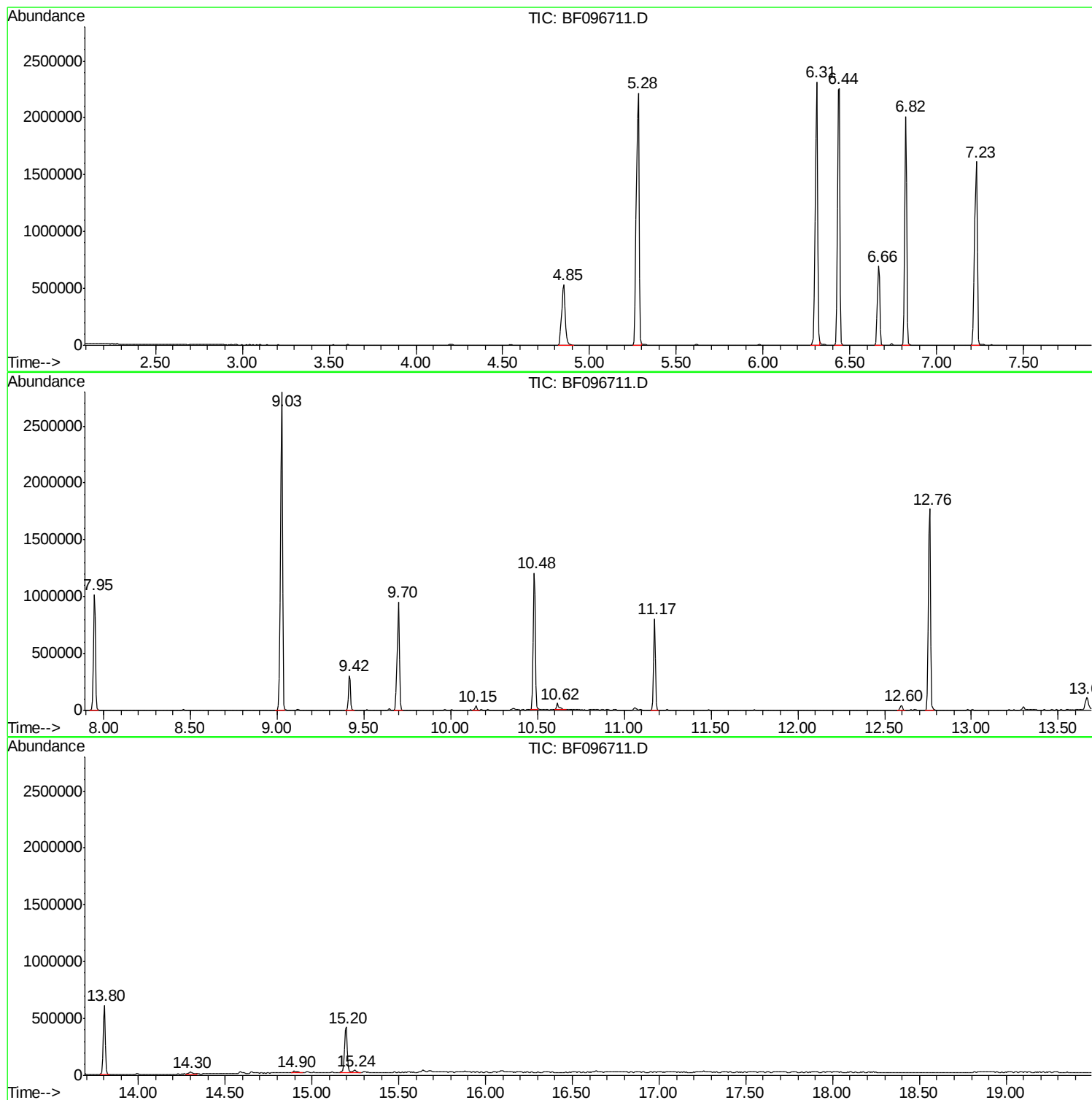
Sum of corrected areas: 20935711

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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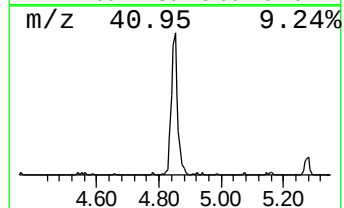
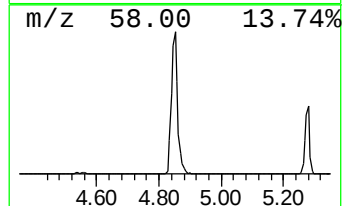
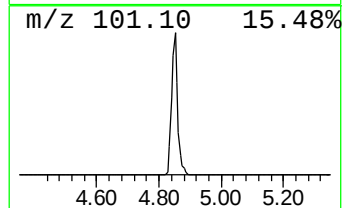
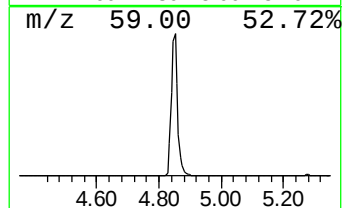
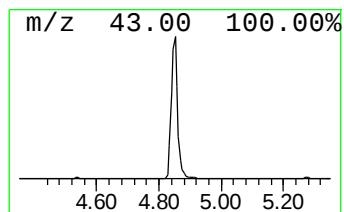
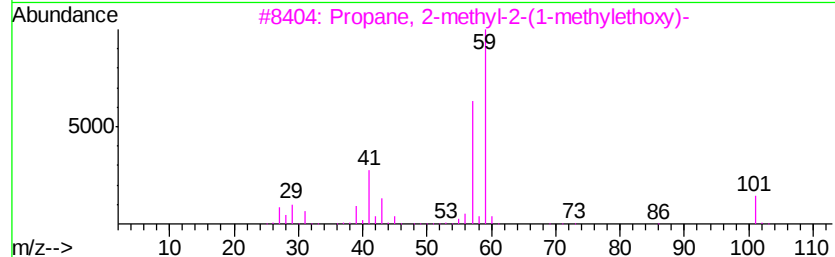
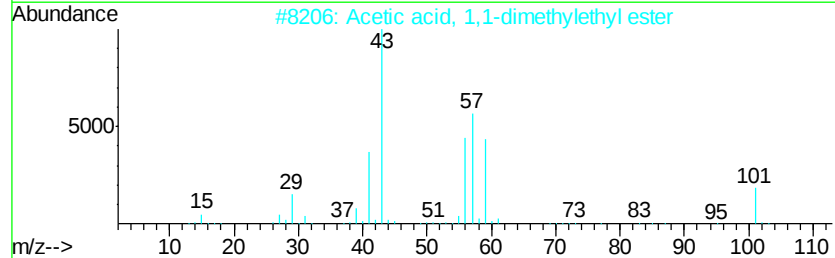
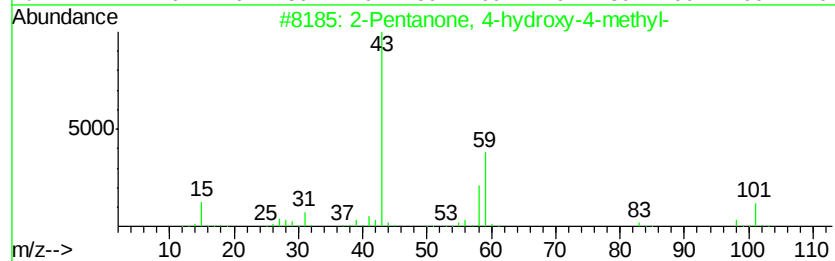
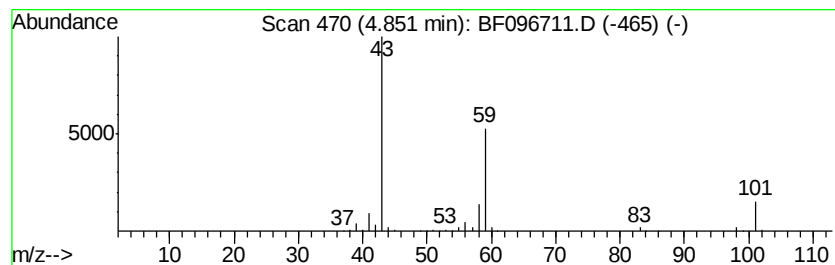
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.85	24.66 ng	745171	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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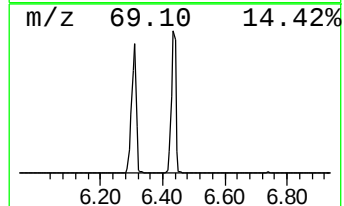
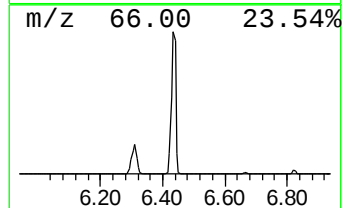
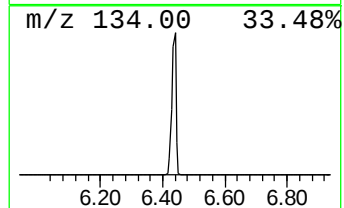
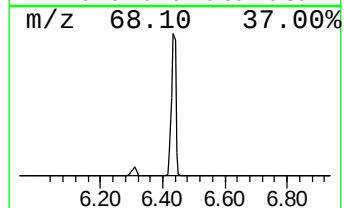
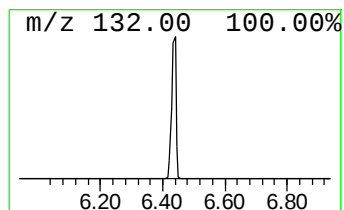
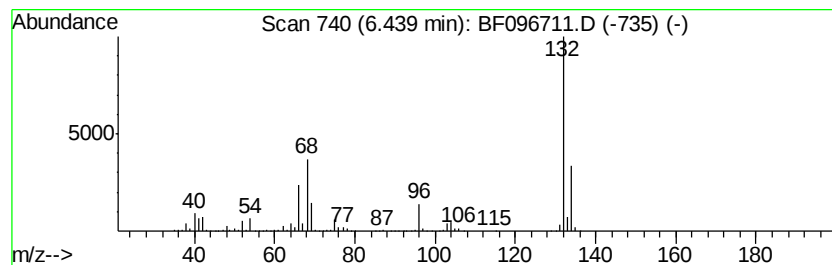
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Peak Number 2 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	76.38 ng	2307640	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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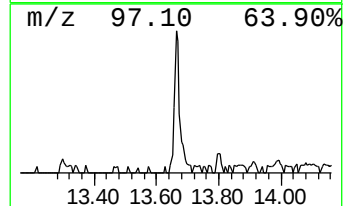
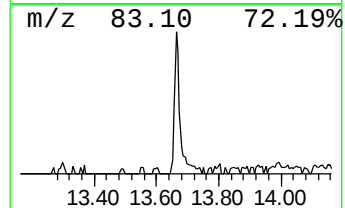
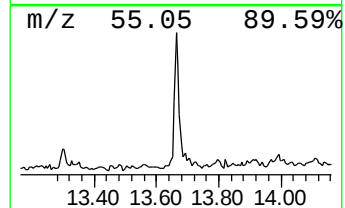
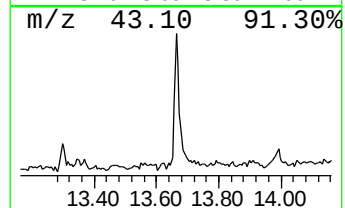
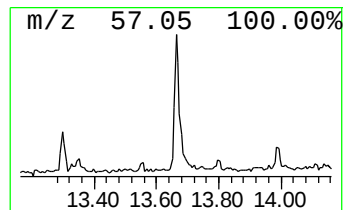
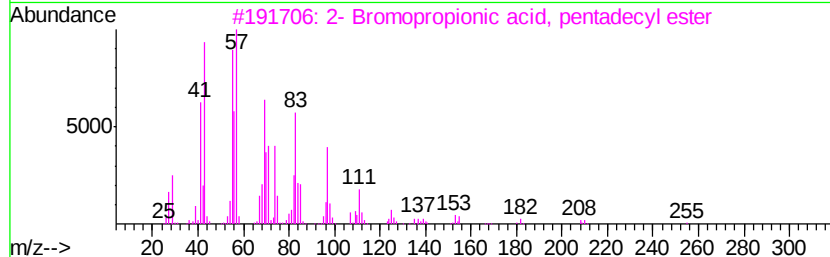
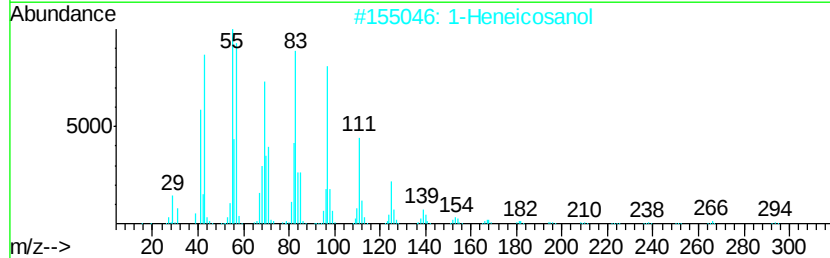
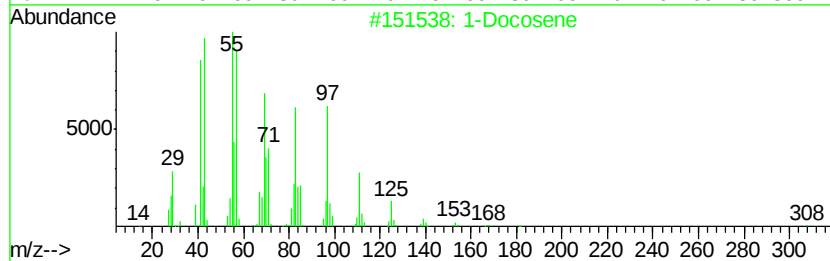
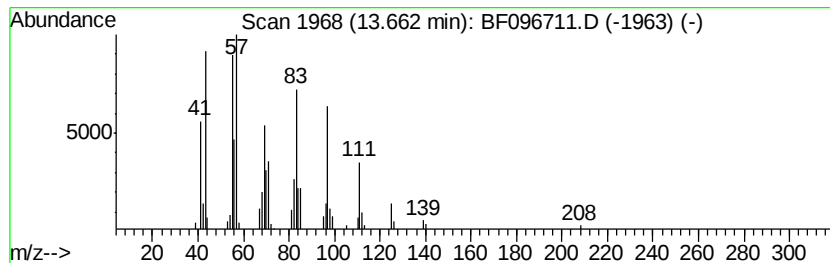
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Peak Number 4 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	4.90 ng	134817	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	24.7	ng	745171	1	6.66	604268	20.0
unknown6.44	6.44	76.4	ng	2307640	1	6.66	604268	20.0
1-Docosene	13.66	4.9	ng	134817	5	13.80	549875	20.0