

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111116\
 Data File : BF091139.D
 Acq On : 11 Nov 2016 14:49
 Operator : UM/SJ
 Sample : PB94644BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB94644BL

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-BF110316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF091138.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.744	3	5	15	rBV	1916277	3807263	75.92%	9.953%
2	1.870	15	16	53	rVB	222263	1227209	24.47%	3.208%
3	4.784	268	271	282	rBV	672389	1008881	20.12%	2.637%
4	5.241	309	311	313	rBV	1682688	2225815	44.39%	5.819%
5	6.293	400	403	405	rBV	2435074	2392184	47.70%	6.253%
6	6.407	411	413	416	rBV	2693678	2498378	49.82%	6.531%
7	6.636	432	433	444	rVB	561653	906995	18.09%	2.371%
8	6.796	444	447	450	rBV	3609125	3355389	66.91%	8.771%
9	7.207	481	483	486	rBV	1906391	2527533	50.40%	6.607%
10	7.927	544	546	558	rBV	1194979	1274968	25.42%	3.333%
11	9.013	637	641	643	rBV	3628588	5014756	100.00%	13.109%
12	9.676	696	699	701	rBV	1448632	1307234	26.07%	3.417%
13	10.465	765	768	784	rBV	1553936	1596371	31.83%	4.173%
14	11.151	826	828	831	rBV	1185322	1326893	26.46%	3.469%
15	12.739	964	967	970	rBV	4388718	4989785	99.50%	13.044%
16	13.779	1056	1058	1061	rBV	1284350	1381577	27.55%	3.612%
17	15.025	1161	1167	1175	rBV2	14386	64065	1.28%	0.167%
18	15.151	1175	1178	1187	rVV	1168583	1348331	26.89%	3.525%

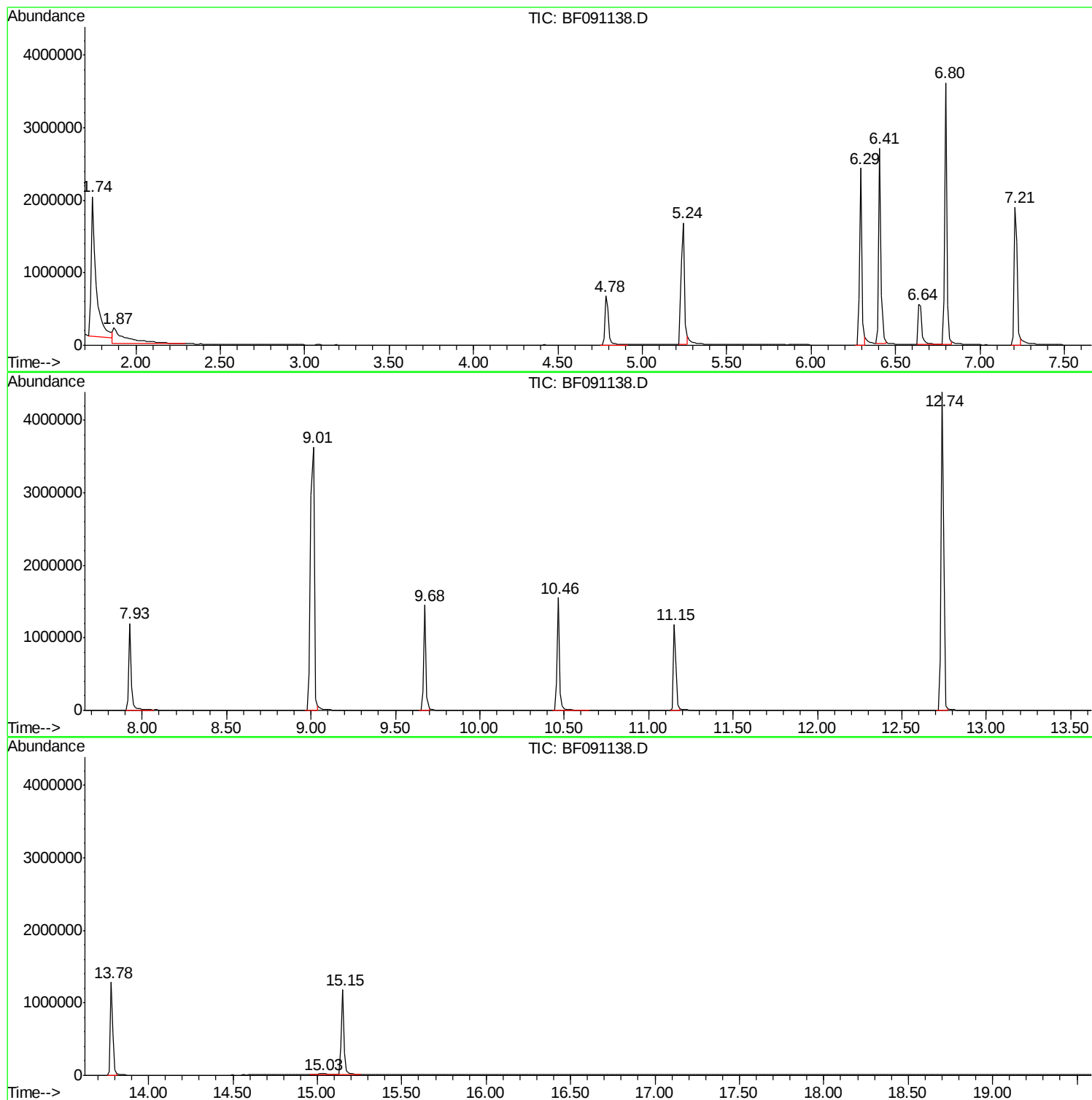
Sum of corrected areas: 38253627

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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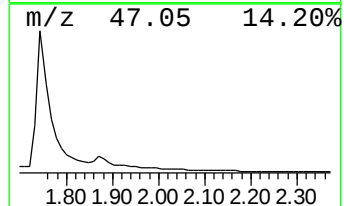
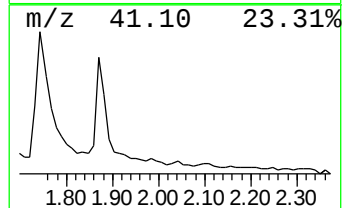
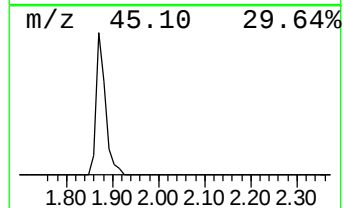
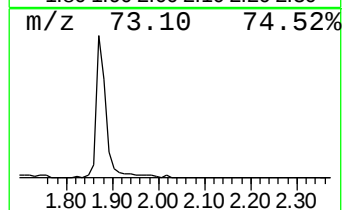
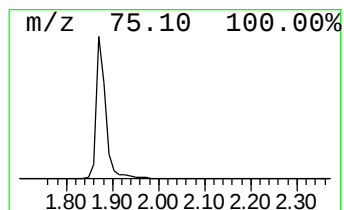
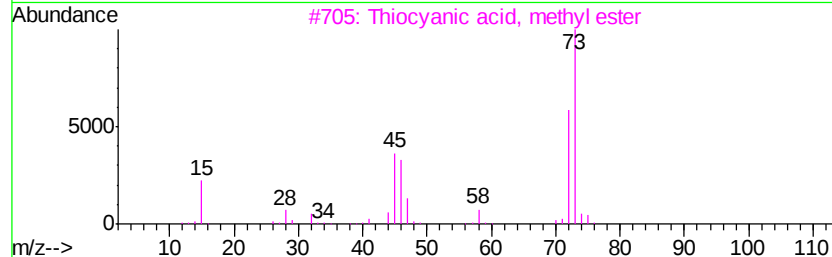
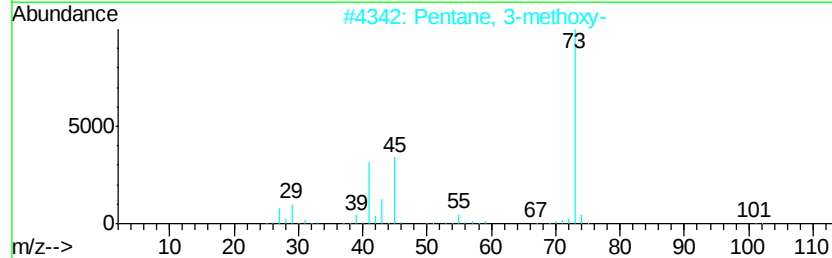
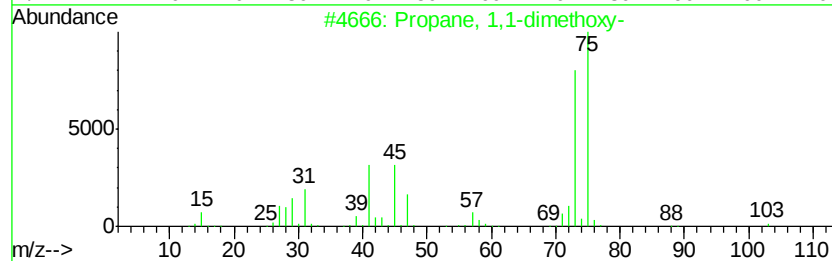
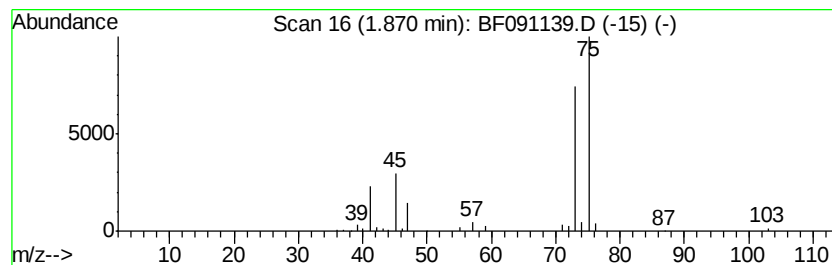
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	27.06 ng	1227210	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	14
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	12
4		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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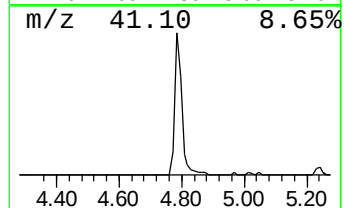
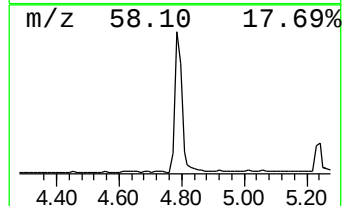
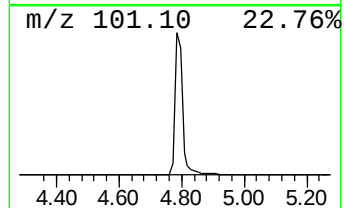
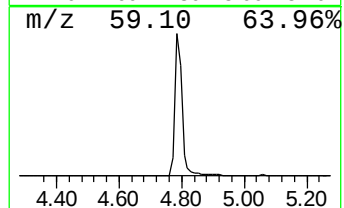
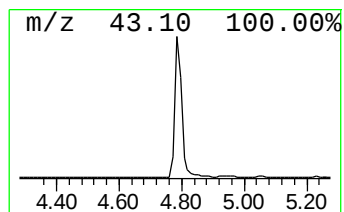
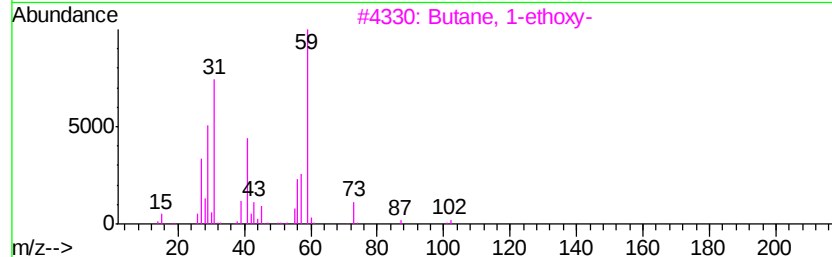
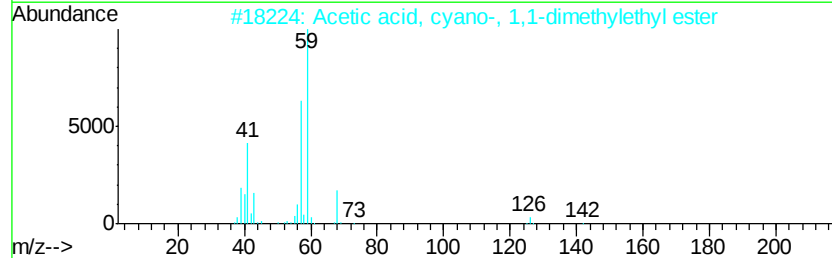
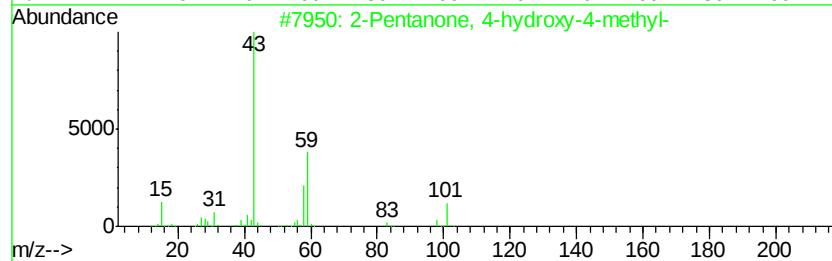
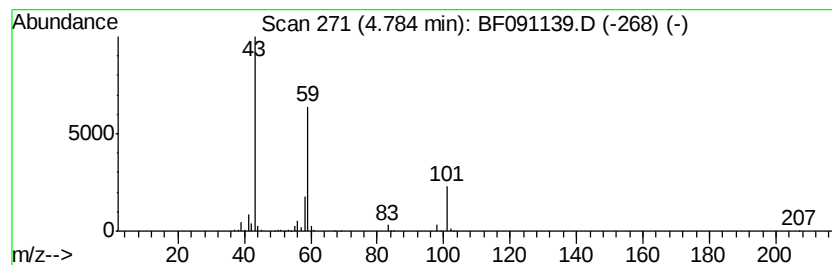
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	22.25 ng	1008880	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	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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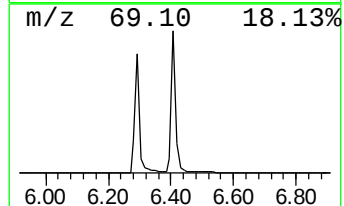
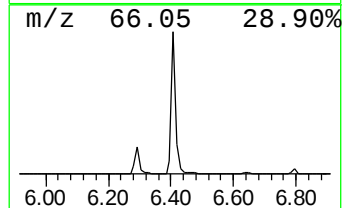
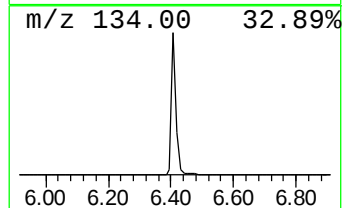
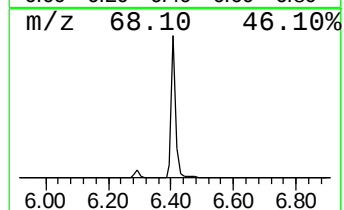
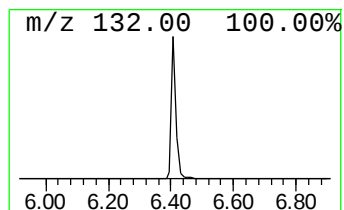
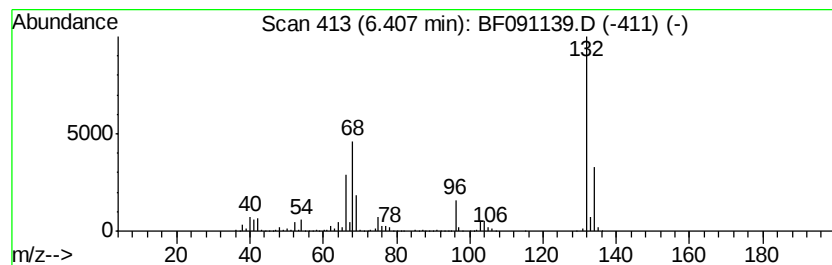
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Peak Number 4 unknown6.41 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	55.09 ng	2498380	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.87	27.1	ng	1227210	1	6.65	906995	20.0
2-Pentanone, 4-hy...	4.78	22.3	ng	1008880	1	6.65	906995	20.0
unknown6.41	6.41	55.1	ng	2498380	1	6.65	906995	20.0