

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050317\
 Data File : BF094841.D
 Acq On : 3 May 2017 18:58
 Operator : SJ/MA
 Sample : PB98646BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB98646BL

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-BF050217.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	4.137	370	374	386	rBV	46004	91602	3.11%	0.423%
2	5.054	524	530	548	rBV	388027	758193	25.73%	3.503%
3	5.684	633	637	658	rBV	1444858	2084624	70.76%	9.632%
4	6.248	730	733	741	rBV	25834	39844	1.35%	0.184%
5	7.272	901	907	922	rBV	1550867	2023357	68.68%	9.349%
6	7.389	922	927	944	rVB	1772959	2248893	76.33%	10.391%
7	7.725	980	984	992	rBV	434766	516239	17.52%	2.385%
8	7.966	1020	1025	1034	rBV	1560796	1750827	59.43%	8.090%
9	8.625	1131	1137	1156	rBV	1018132	1303128	44.23%	6.021%
10	9.742	1323	1327	1339	rBV	566931	690252	23.43%	3.189%
11	11.519	1623	1629	1633	rBV	2173174	2589781	87.90%	11.966%
12	12.571	1803	1808	1819	rBV2	582665	769335	26.11%	3.555%
13	13.866	2023	2028	2045	rBV	1090152	1453243	49.33%	6.715%
14	14.971	2211	2216	2230	rBV2	661285	834149	28.31%	3.854%
15	17.301	2606	2612	2616	rBV	2297211	2946168	100.00%	13.613%
16	18.636	2835	2839	2849	rBV	751979	846505	28.73%	3.911%
17	20.300	3117	3122	3136	rBV	540662	695828	23.62%	3.215%

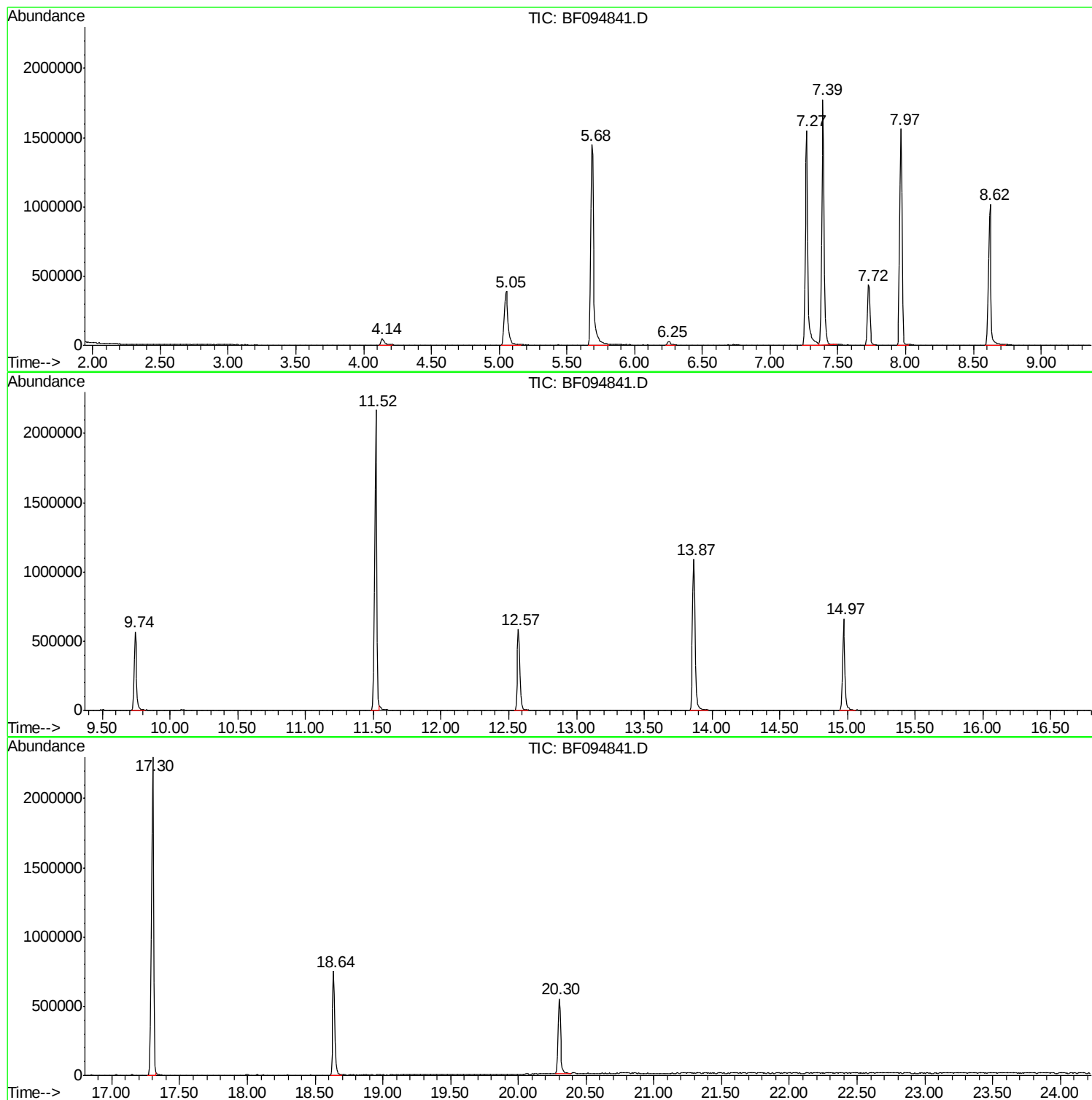
Sum of corrected areas: 21641968

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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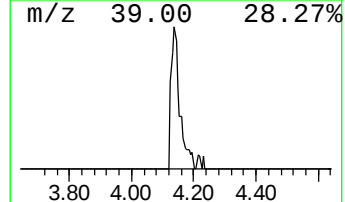
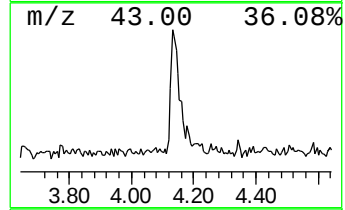
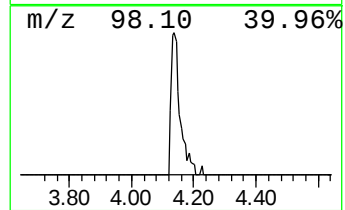
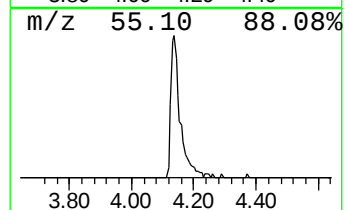
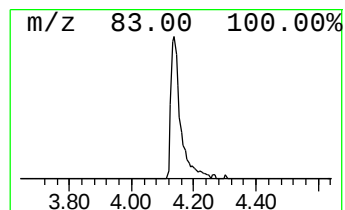
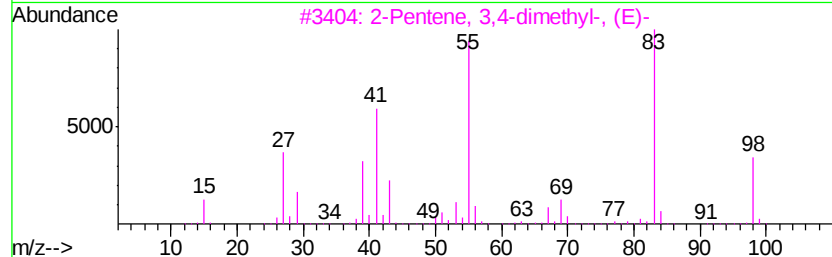
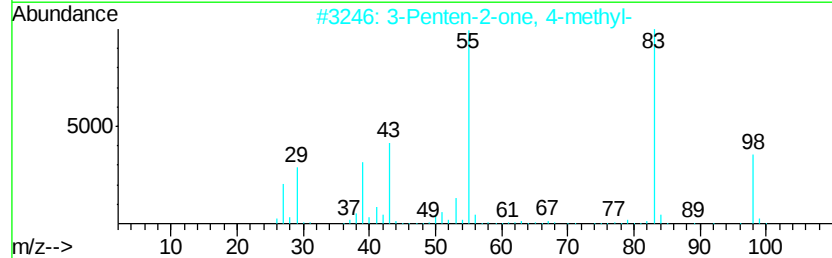
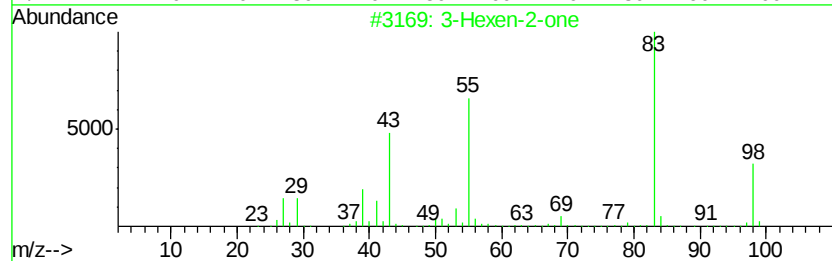
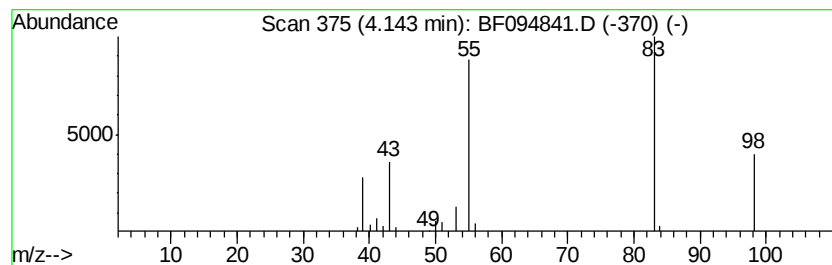
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.14	3.55 ng	91602	1,4-Dichlorobenzene-d4	7.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72



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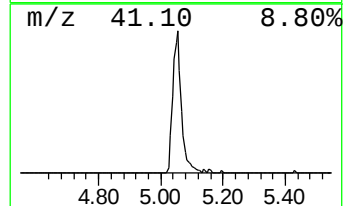
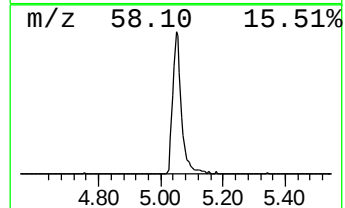
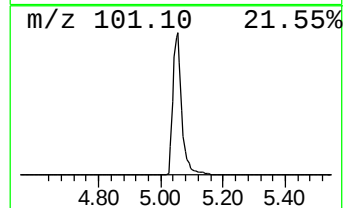
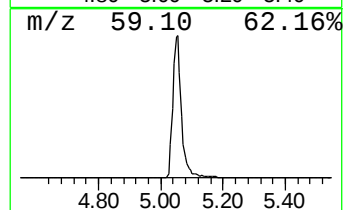
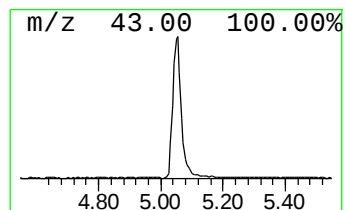
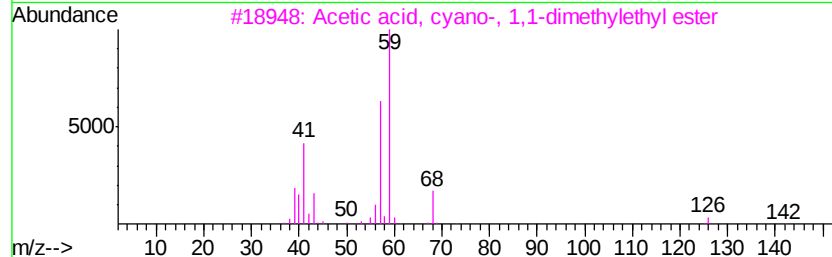
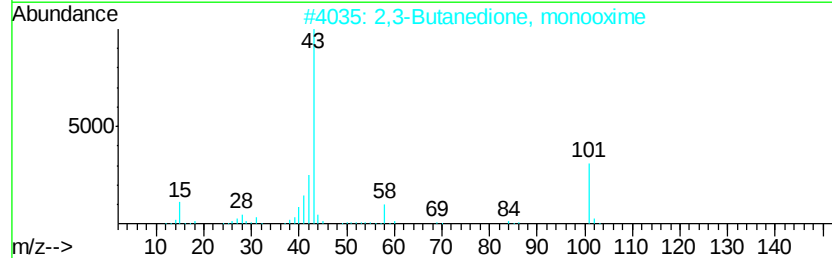
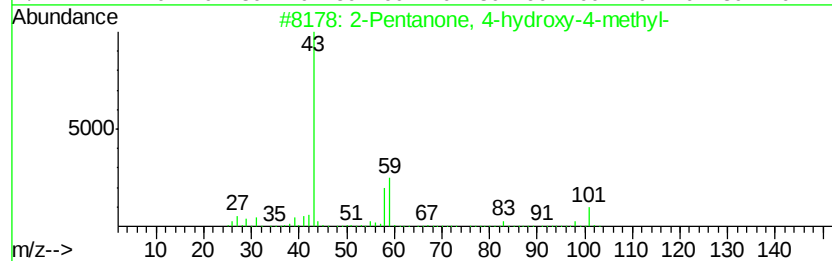
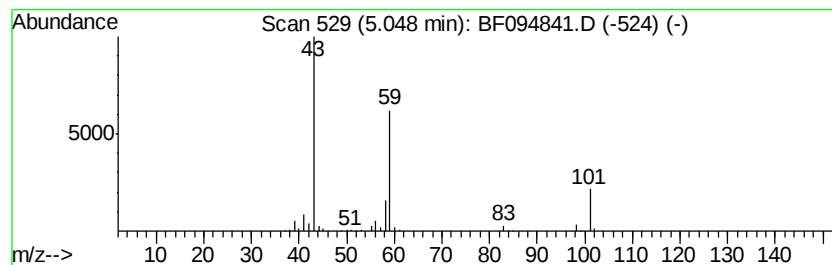
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	29.37 ng	758193	1,4-Dichlorobenzene-d4	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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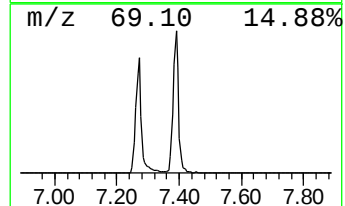
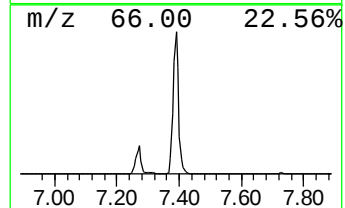
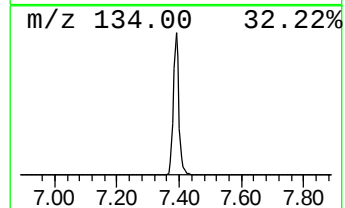
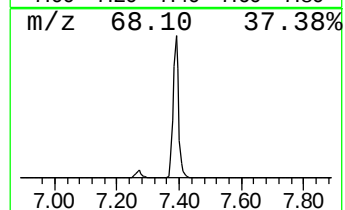
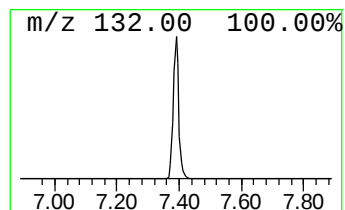
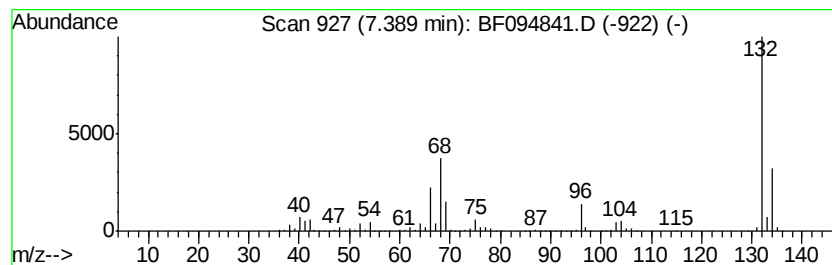
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Peak Number 3 unknown7.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.39	87.13 ng	2248890	1,4-Dichlorobenzene-d4	7.73

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	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.14	3.5	ng	91602	1	7.73	516239	20.0
2-Pentanone, 4-hy...	5.05	29.4	ng	758193	1	7.73	516239	20.0
unknown7.39	7.39	87.1	ng	2248890	1	7.73	516239	20.0