

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091917\
 Data File : BF098639.D
 Acq On : 19 Sep 2017 14:11
 Operator : SJ/JU
 Sample : PB102369BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB102369BL

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-BF091117.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	3.181	180	186	198	rBV2	17891	40825	1.10%	0.133%
2	4.157	350	352	364	rBV	124247	191553	5.18%	0.623%
3	4.822	461	465	482	rVB	450829	700315	18.95%	2.277%
4	5.245	533	537	560	rBV	3155636	3372540	91.26%	10.963%
5	6.281	709	713	716	rBV	2955848	3238082	87.62%	10.526%
6	6.398	729	733	736	rBV	3653081	3412613	92.35%	11.093%
7	6.622	768	771	785	rVB	883706	821059	22.22%	2.669%
8	6.781	794	798	818	rVB	2937002	2613773	70.73%	8.497%
9	7.198	864	869	872	rBV	2146326	2127011	57.56%	6.914%
10	7.910	985	990	1000	rBV	1159052	1081190	29.26%	3.515%
11	8.986	1167	1173	1176	rBV	3854891	3695418	100.00%	12.013%
12	9.657	1282	1287	1296	rVB	1317150	1188315	32.16%	3.863%
13	10.451	1417	1422	1425	rBV	2143048	1925916	52.12%	6.261%
14	11.139	1535	1539	1547	rBV	1302684	1061897	28.74%	3.452%
15	12.727	1804	1809	1812	rBV	3623650	3479995	94.17%	11.312%
16	13.774	1983	1987	1996	rVB	1127398	992637	26.86%	3.227%
17	15.168	2219	2224	2234	rVB	703629	819289	22.17%	2.663%

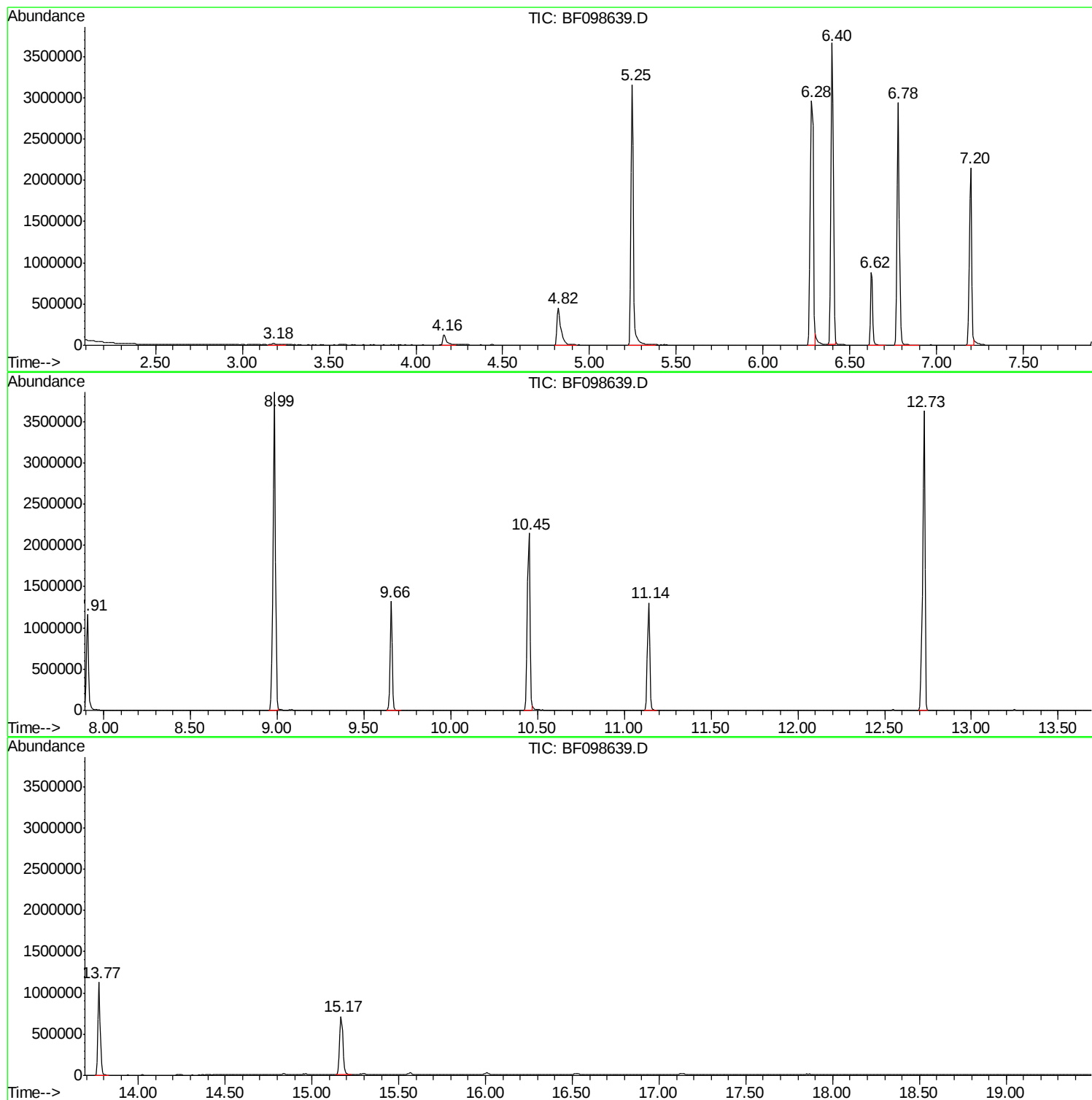
Sum of corrected areas: 30762428

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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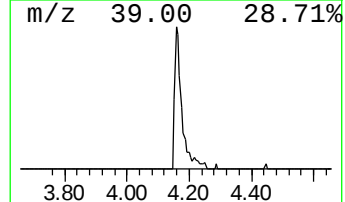
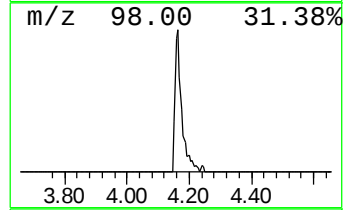
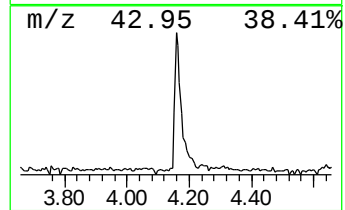
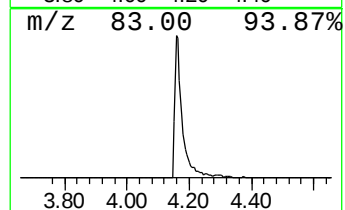
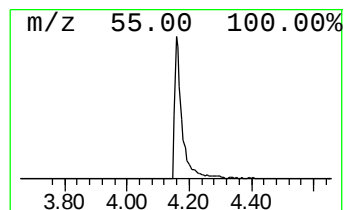
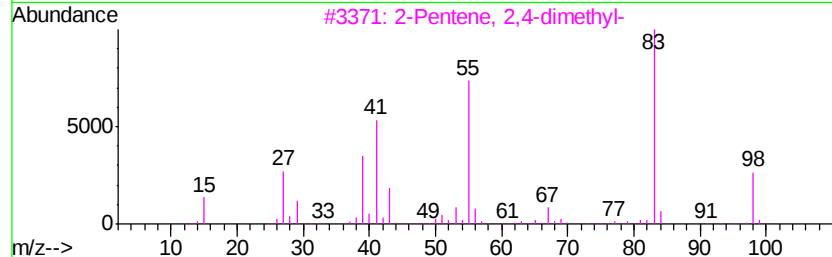
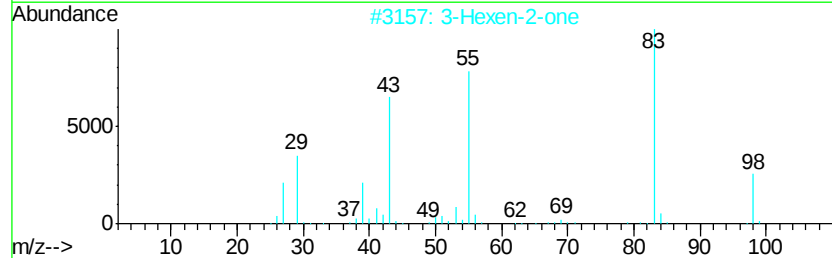
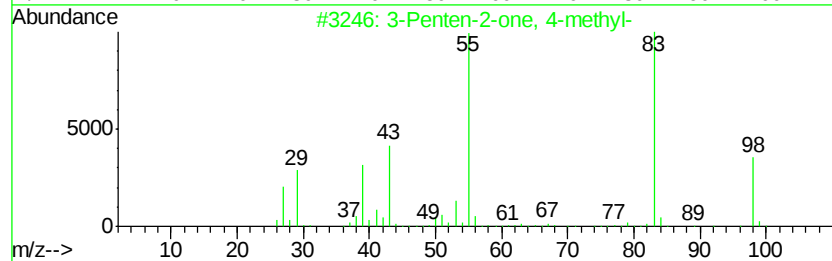
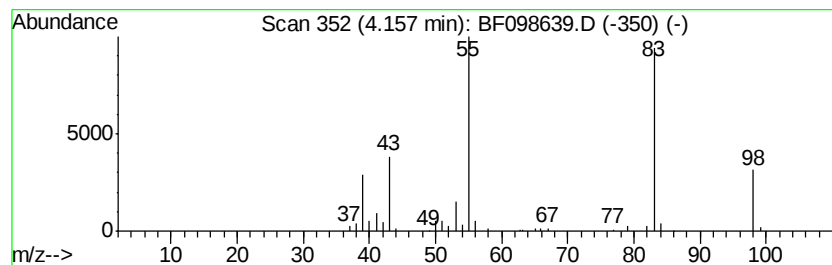
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	4.67 ng	191553	1,4-Dichlorobenzene-d4	6.62

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	80
5			2,4-Azetidinedione, 3,3-diethyl-	141	C7H11N2O2	042282-85-9	78



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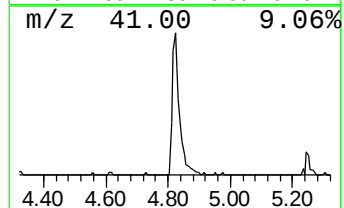
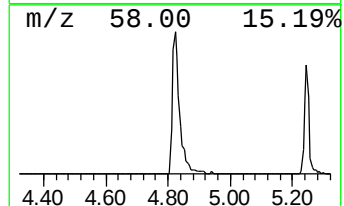
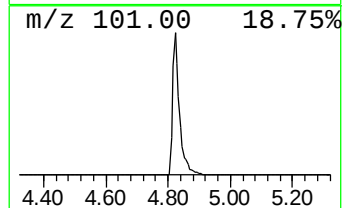
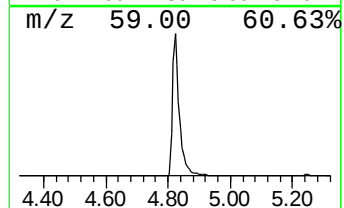
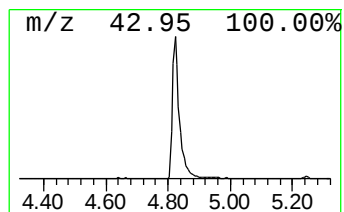
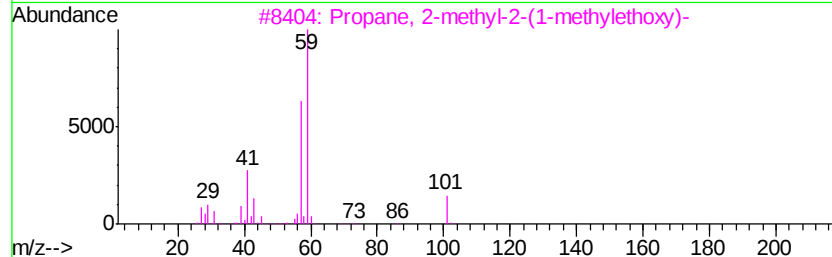
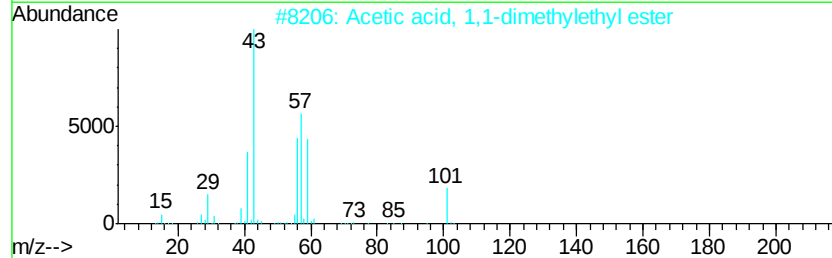
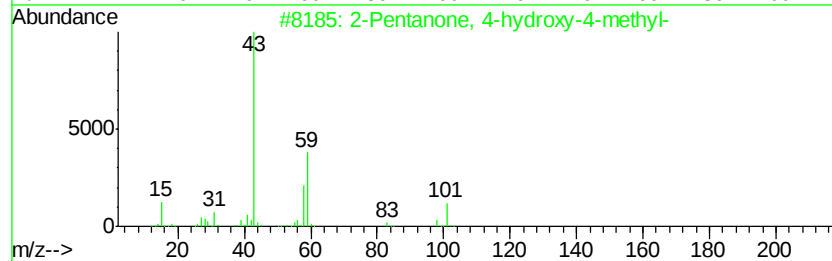
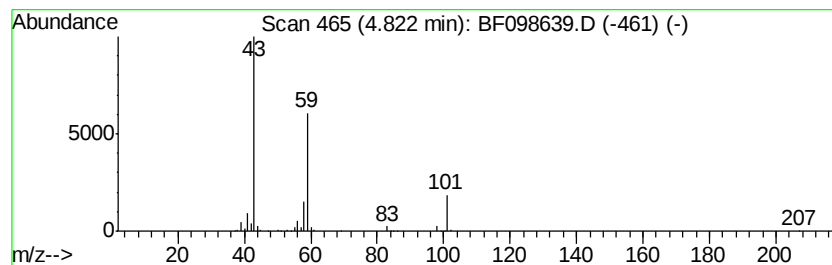
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	17.06 ng	700315	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	33
4		4-Methoxy-1-pentene	100	C6H12O	098386-09-5	32
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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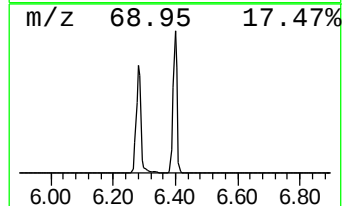
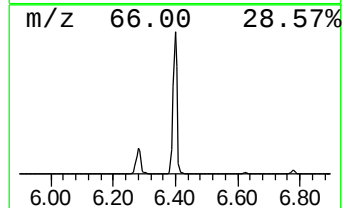
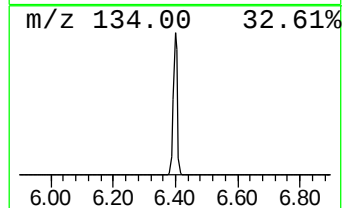
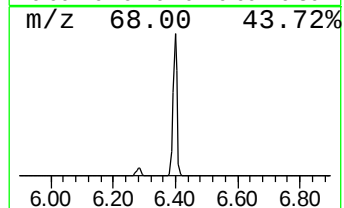
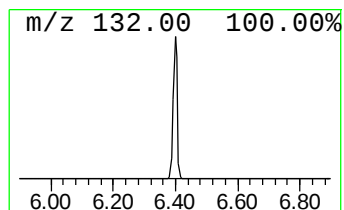
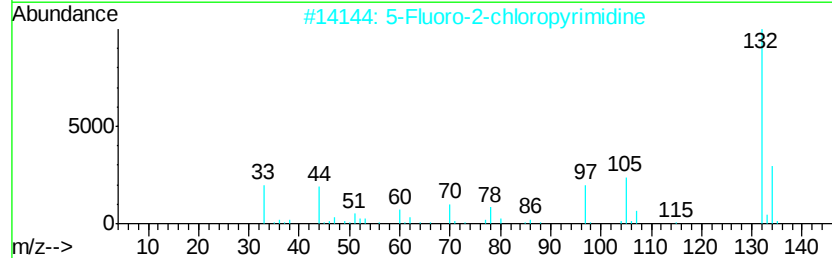
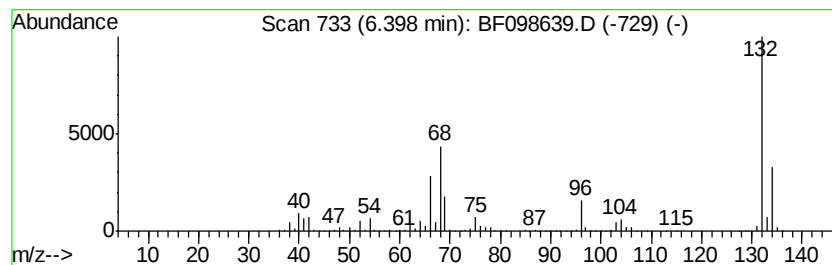
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Peak Number 3 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	83.13 ng	3412610	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.16	4.7	ng	191553	1	6.62	821059	20.0
2-Pentanone, 4-hy...	4.82	17.1	ng	700315	1	6.62	821059	20.0
unknown6.40	6.40	83.1	ng	3412610	1	6.62	821059	20.0