LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012216\
Data File : BF084585.D
Acq On : 22 Jan 2016 13:18
Operator : SJ/IZ
Sample : PB87895BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB87895BL

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-BF123115.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	4.236	185	188	195	rVB	211838	281899	4.53%	0.579%
2	4.921	244	248	251	rBV	2875536	4940771	79.35%	10.142%
3	5.344	283	285	288	rBV	3218096	3452029	55.44%	7.086%
4	5.744	318	320	323	rBV	249297	249478	4.01%	0.512%
5	6.384	373	376	379	rBV	3149976	3260989	52.37%	6.694%
6	6.510	385	387	390	rBV	3805985	3464352	55.64%	7.111%
7	6.739	405	407	410	rBV	1186440	1210019	19.43%	2.484%
8	6.899	418	421	423	rBV	4410284	3887660	62.44%	7.980%
9	7.310	454	457	459	rBV	3304577	3242715	52.08%	6.656%
10	8.030	517	520	522	rBV	1938647	1794743	28.83%	3.684%
11	9.105	611	614	617	rBV	4195602	6188667	99.40%	12.704%
12	9.779	670	673	676	rBV	1700518	1987018	31.91%	4.079%
13	10.568	739	742	745	rBV	2569193	2740767	44.02%	5.626%
14	11.265	800	803	805	rBV	2436765	2116411	33.99%	4.344%
15	12.682	925	927	930	rBV	87431	102018	1.64%	0.209%
16	12.854	939	942	945	rBV	5110361	6226233	100.00%	12.781%
17	13.391	988	989	991	rVB	93365	70172	1.13%	0.144%
18	13.894	1031	1033	1036	rBV	1444736	1895968	30.45%	3.892%
19	15.288	1152	1155	1158	rBV	1038932	1323795	21.26%	2.717%
20	15.540	1171	1177	1188	rVB	71836	279580	4.49%	0.574%

Sum of corrected areas: 48715284

LSC Report - Integrated Chromatogram

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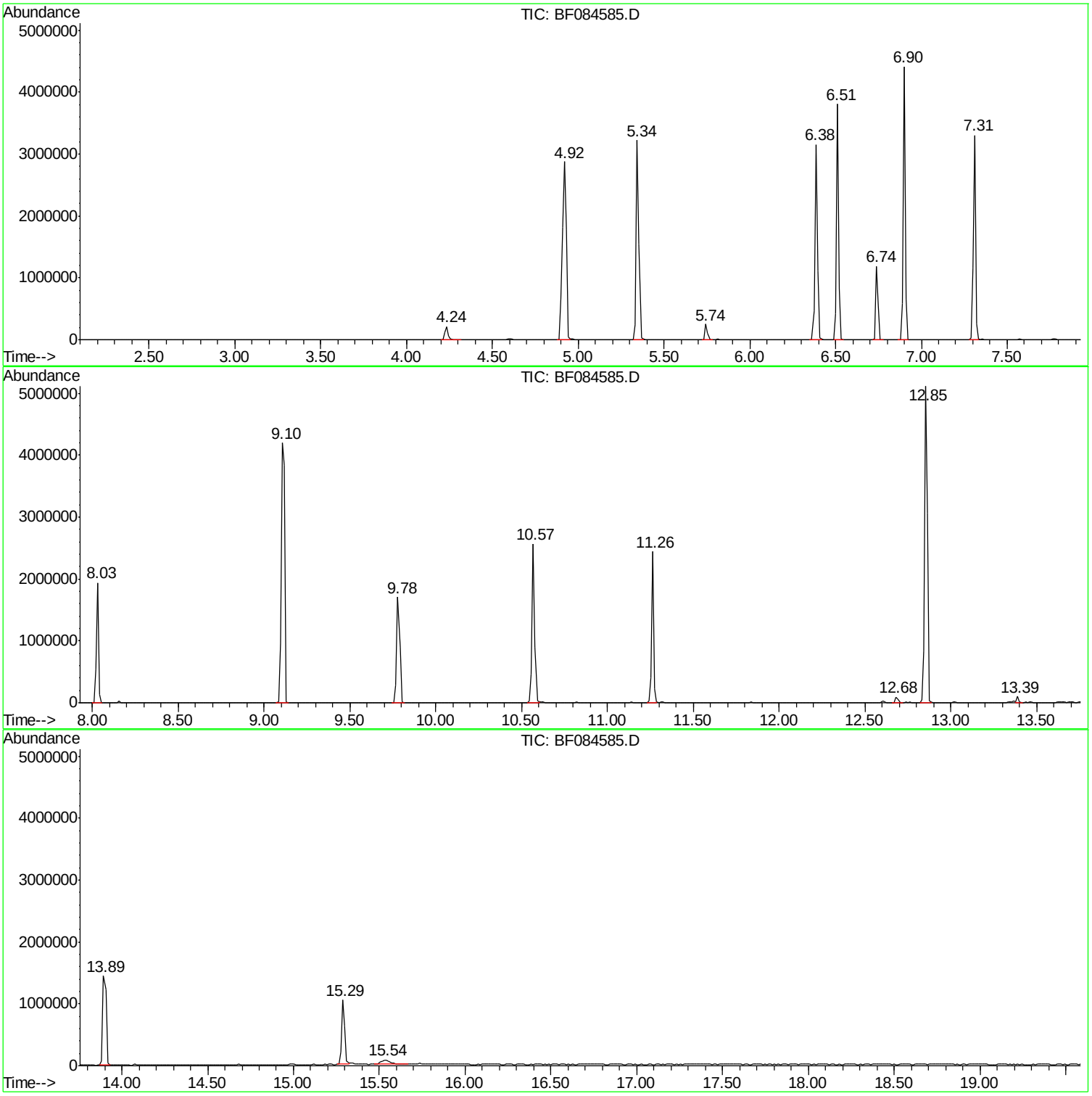
Instrument :
BNA_F
ClientSampleId :
PB87895BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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Sample : PB87895BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB87895BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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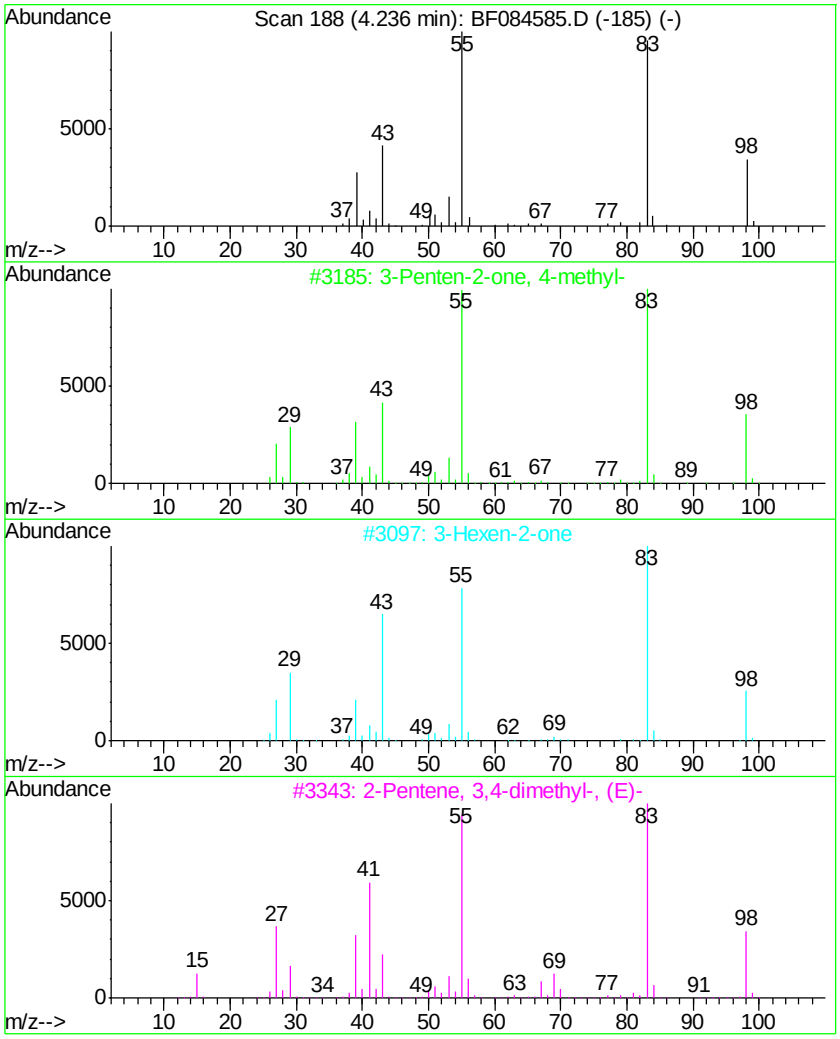
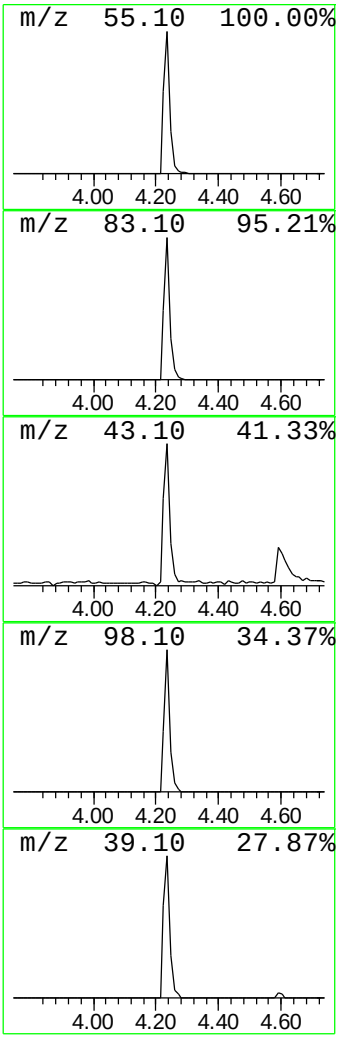
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	4.66 ng	281899	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB87895BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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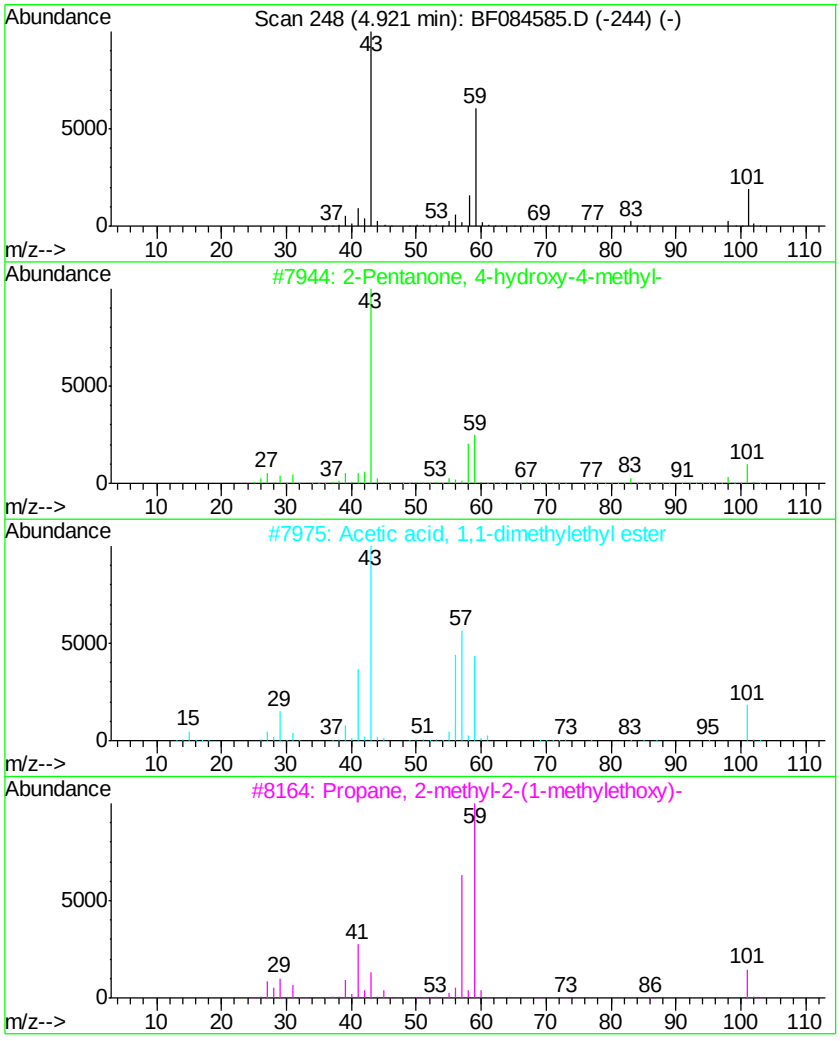
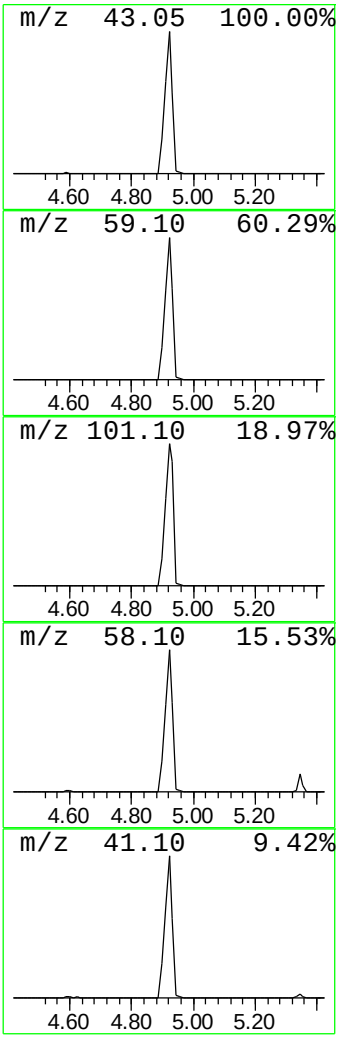
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	81.66 ng	4940770	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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ClientSampleId : PB87895BL

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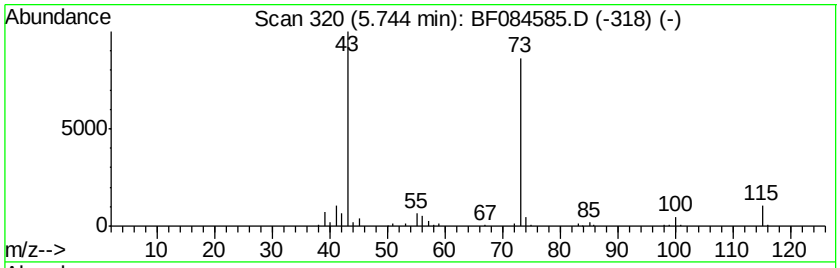
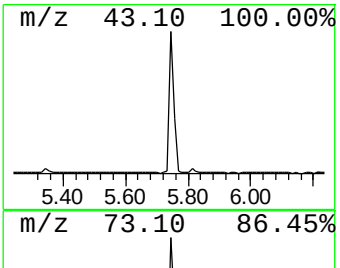
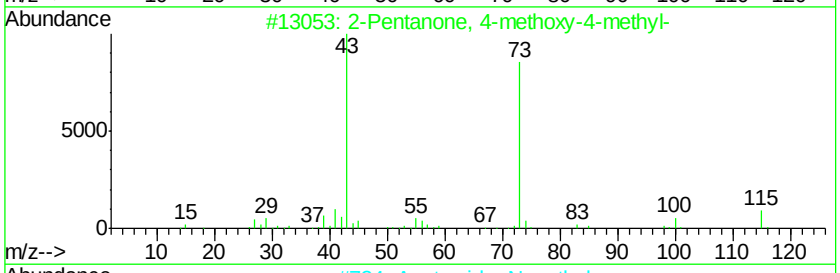
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

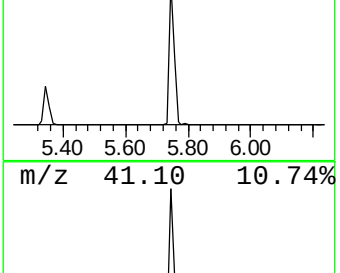
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	4.12 ng	249478	1,4-Dichlorobenzene-d4	6.74

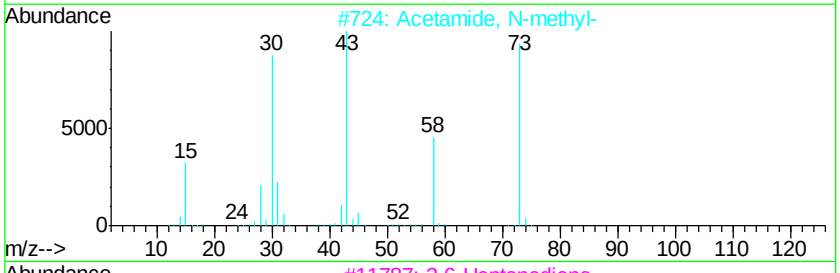
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	3,6-Heptanedione	128	C7H12O2	001703-51-1	23
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
5	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10

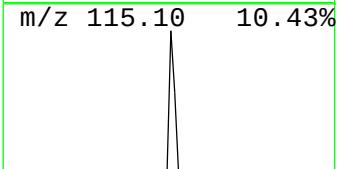


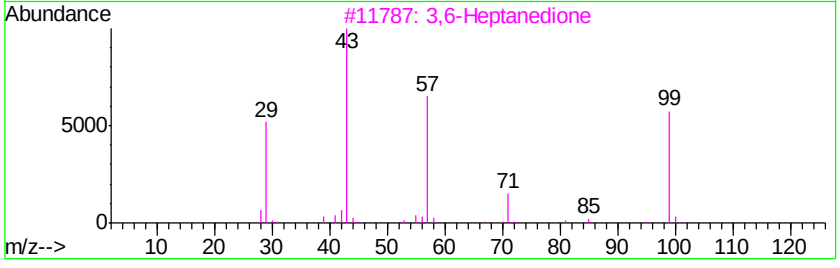


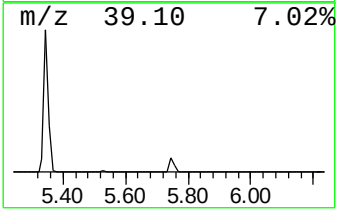












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

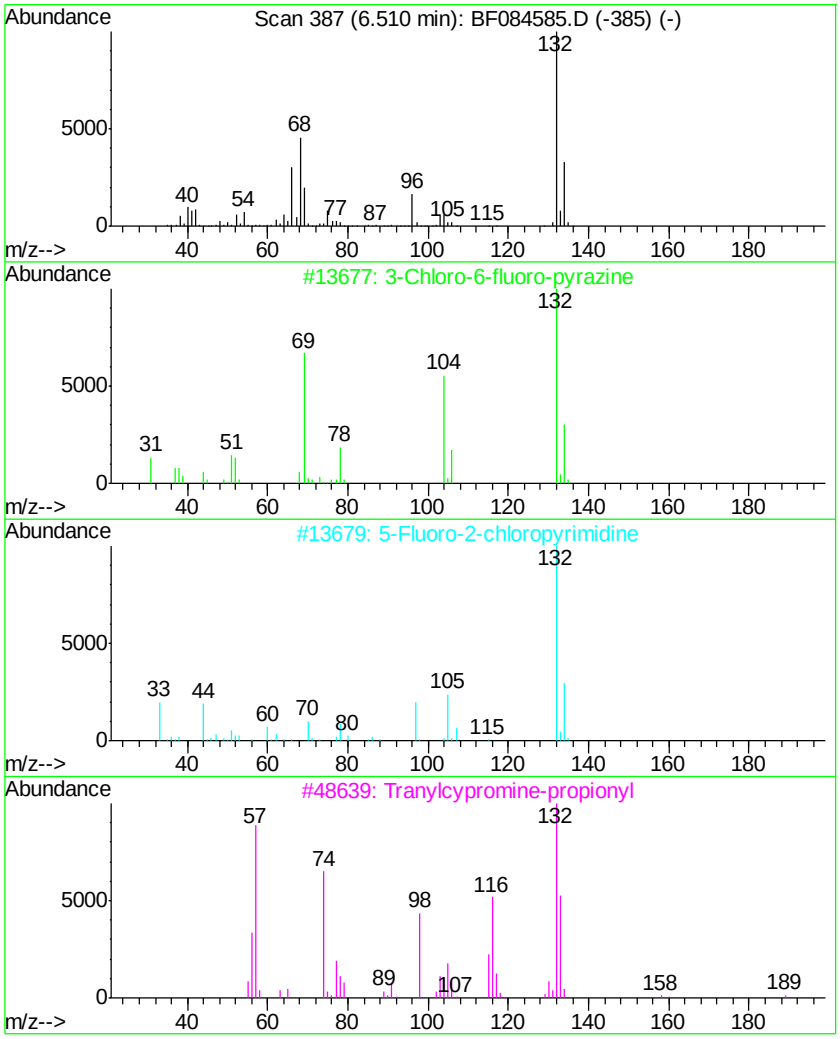
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

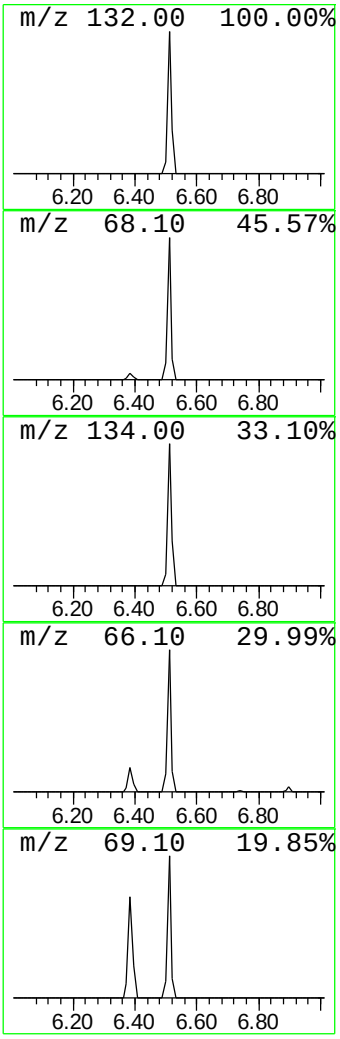
****

Peak Number 4 unknown6.51 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	57.26 ng	3464350	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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

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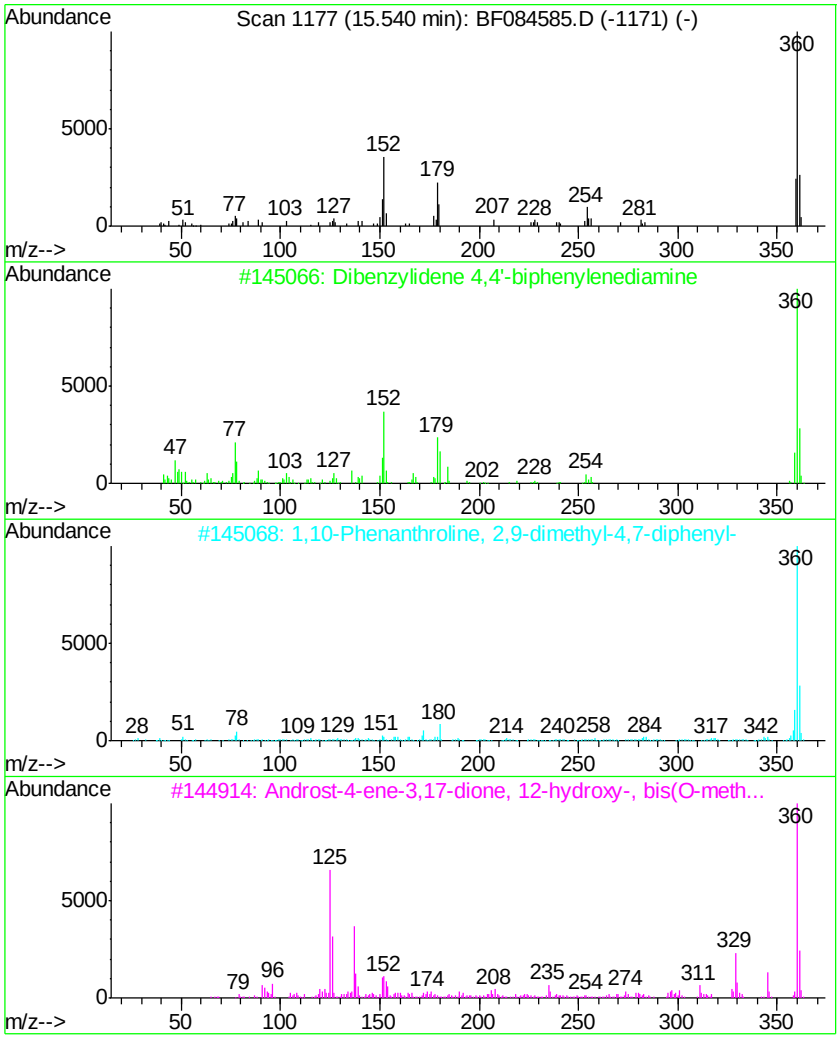
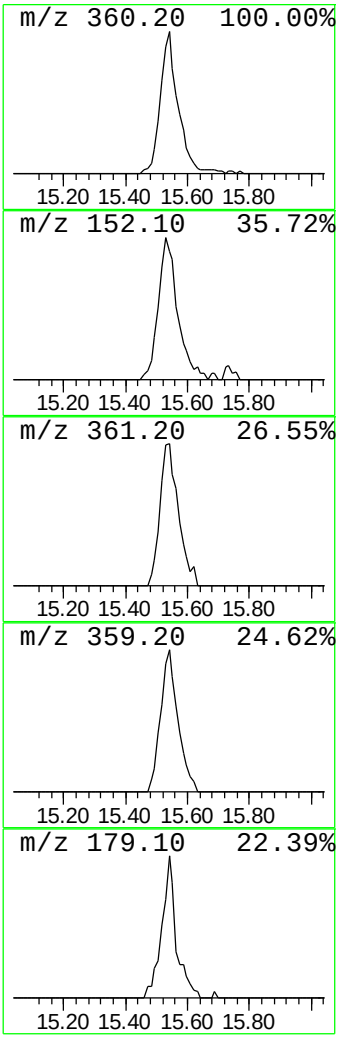
Peak Number 6 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	4.22 ng	279580	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	90
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	52
3	Androst-4-ene-3,17-dione, 12-hyd...	360	C21H32N2O3	069688-31-9	50
4	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	50
5	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	49





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.24	4.7	ng	281899	1	6.74	1210020	20.0
2-Pentanone, 4-hy...	4.92	81.7	ng	4940770	1	6.74	1210020	20.0
2-Pentanone, 4-me...	5.74	4.1	ng	249478	1	6.74	1210020	20.0
unknown6.51	6.51	57.3	ng	3464350	1	6.74	1210020	20.0
Dibenzylidene 4,4...	15.54	4.2	ng	279580	6	15.29	1323800	20.0