

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051716\
 Data File : BF087115.D
 Acq On : 17 May 2016 21:29
 Operator : UM/SJ
 Sample : PB90651BL
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90651BL

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-BF051716.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	1.724	10	12	42	rVB	2340023	4795896	93.35%	10.258%
2	3.999	208	211	222	rBV	110852	255480	4.97%	0.546%
3	4.719	271	274	288	rBV	1030589	2011175	39.14%	4.302%
4	5.187	312	315	337	rBV	3613689	3917201	76.24%	8.379%
5	5.587	348	350	359	rVB	123787	145164	2.83%	0.310%
6	6.262	406	409	411	rBV	3816878	4271465	83.14%	9.136%
7	6.365	416	418	420	rBV	4192743	3945239	76.79%	8.439%
8	6.593	435	438	440	rBV	842850	951524	18.52%	2.035%
9	6.742	449	451	454	rBV	2592030	2863736	55.74%	6.125%
10	7.165	486	488	498	rBV	2488823	2649598	51.57%	5.667%
11	7.873	548	550	553	rBV	921868	1226147	23.87%	2.623%
12	8.959	642	645	648	rBV	4090270	4234489	82.42%	9.057%
13	9.622	701	703	706	rBV	1132684	1392059	27.09%	2.978%
14	10.422	770	773	775	rBV	2487981	3077319	59.90%	6.582%
15	11.108	830	833	835	rBV	1509231	1571458	30.59%	3.361%
16	12.525	955	957	959	rBV	86284	72677	1.41%	0.155%
17	12.697	969	972	974	rBV	4388547	5137785	100.00%	10.989%
18	13.737	1060	1063	1065	rBV	1024476	1406466	27.37%	3.008%
19	14.583	1134	1137	1140	rBV	64918	77349	1.51%	0.165%
20	14.948	1166	1169	1172	rBV	142434	182732	3.56%	0.391%
21	15.085	1178	1181	1184	rBV	865061	1112440	21.65%	2.379%
22	15.360	1201	1205	1209	rBV	177125	283632	5.52%	0.607%
23	15.840	1243	1247	1250	rBV	160063	326990	6.36%	0.699%
24	16.400	1291	1296	1308	rVB	118930	304868	5.93%	0.652%
25	17.097	1352	1357	1368	rVB2	71649	214245	4.17%	0.458%
26	17.954	1425	1432	1439	rBV2	46931	166446	3.24%	0.356%
27	18.994	1517	1523	1533	rVB3	34359	158781	3.09%	0.340%

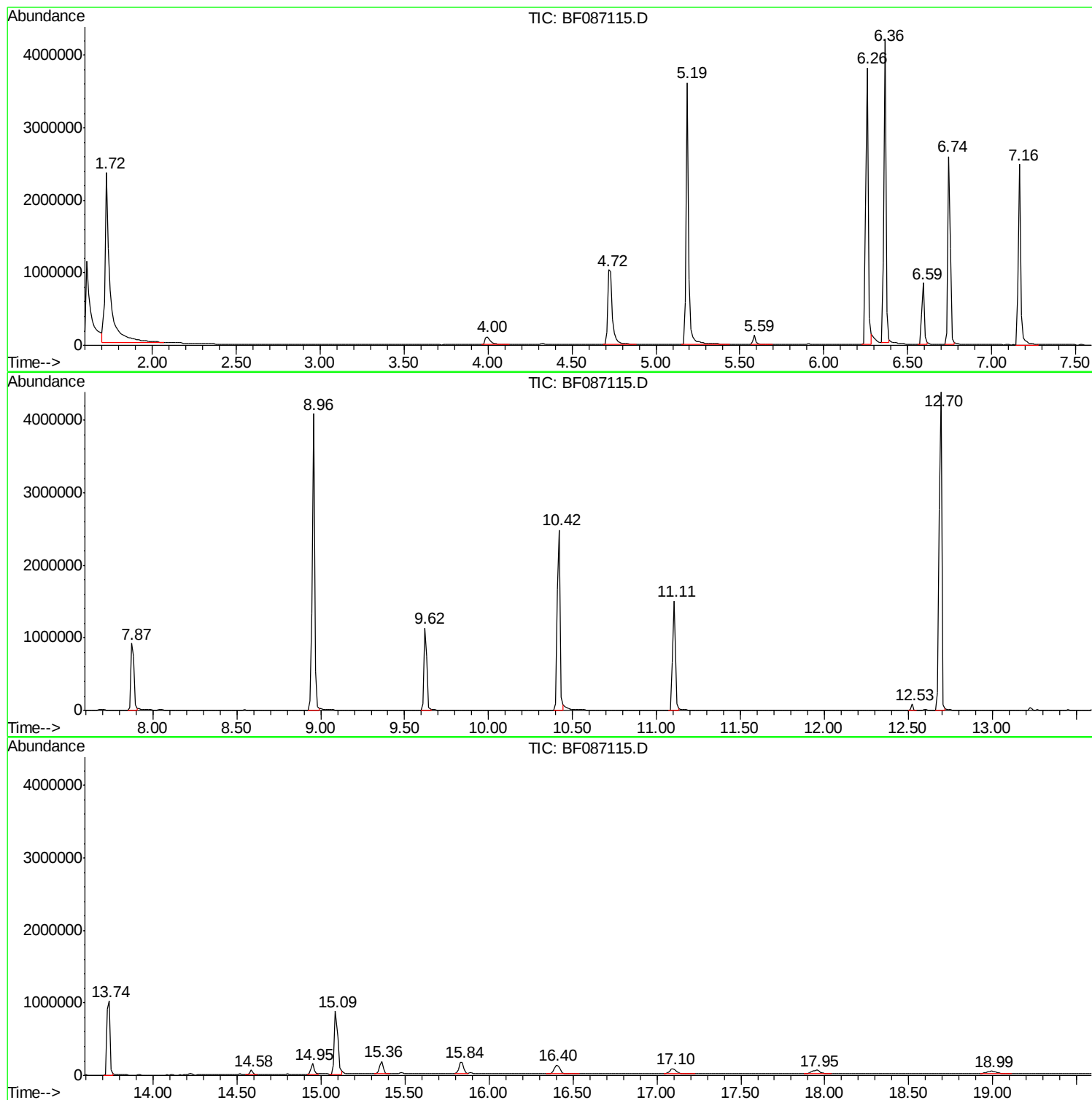
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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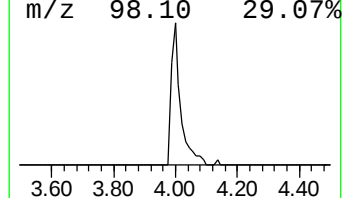
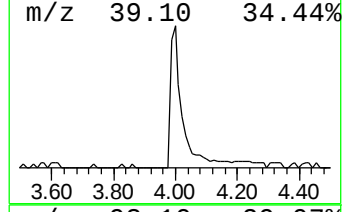
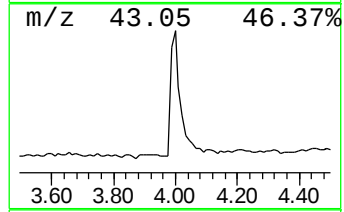
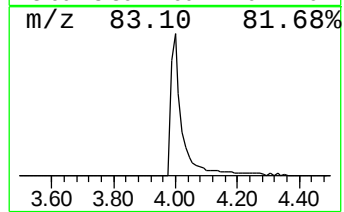
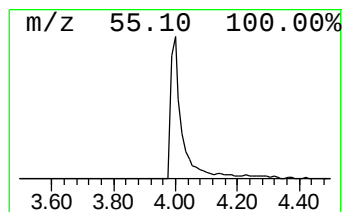
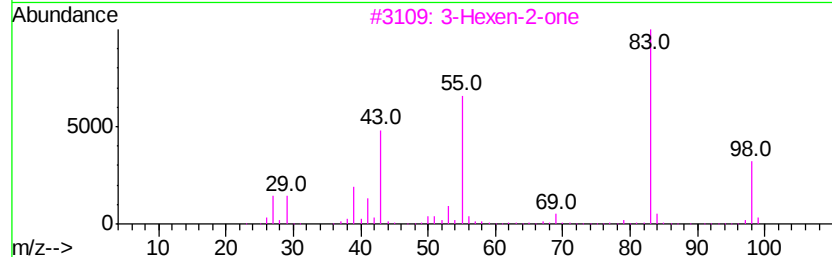
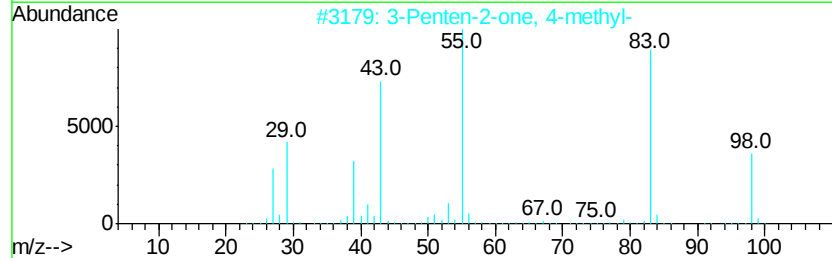
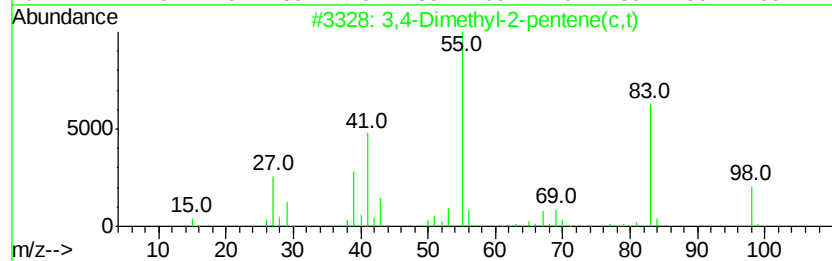
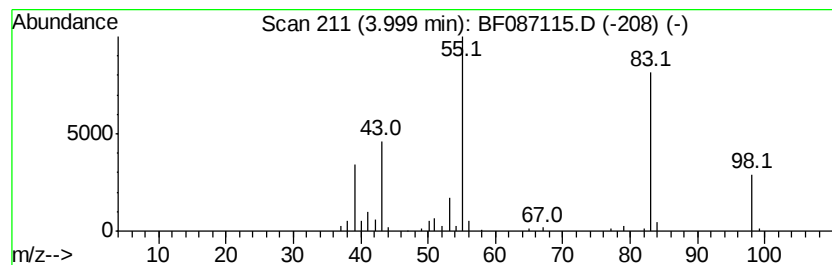
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3,4-Dimethyl-2-pentene(c,t) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	5.37 ng	255480	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	83
3			3-Hexen-2-one	98	C6H10O	000763-93-9	80
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72



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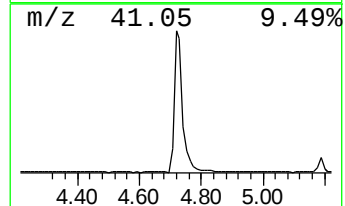
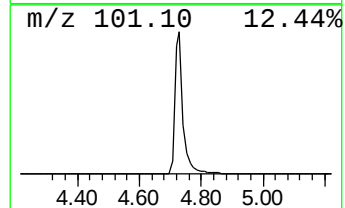
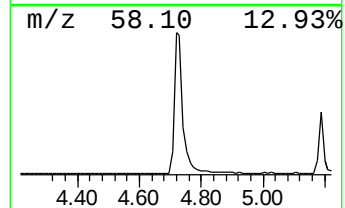
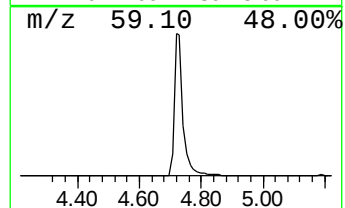
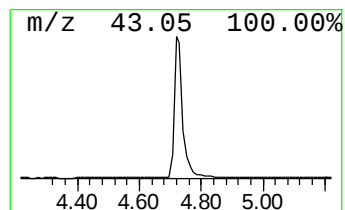
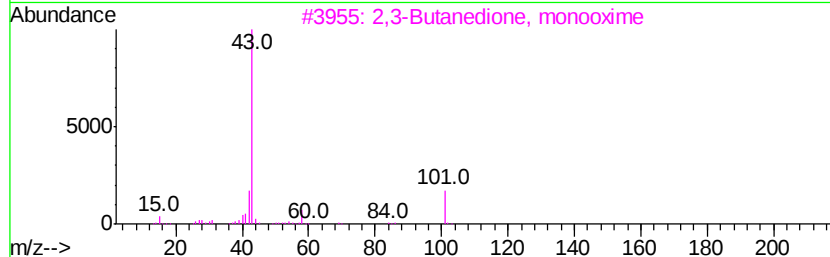
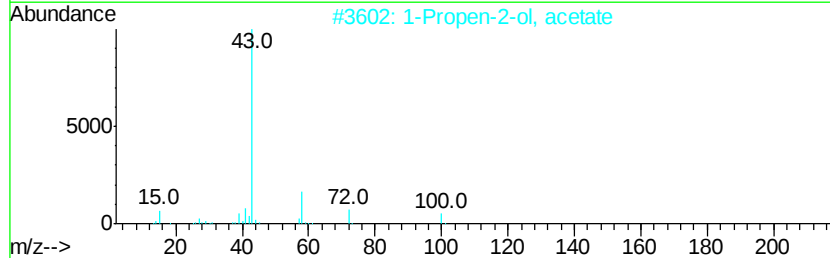
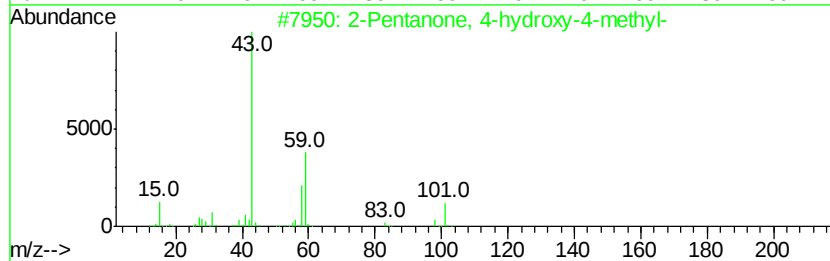
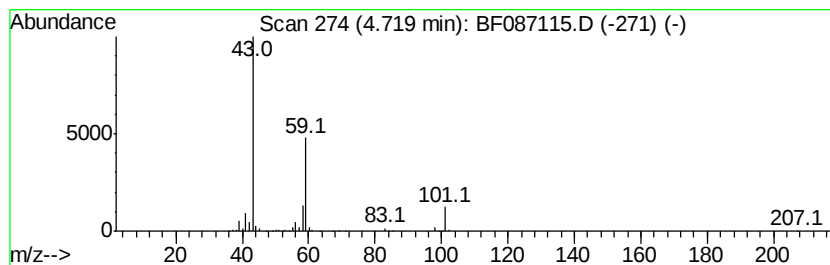
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	42.27 ng	2011180	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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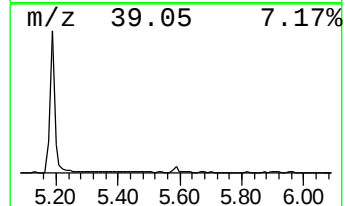
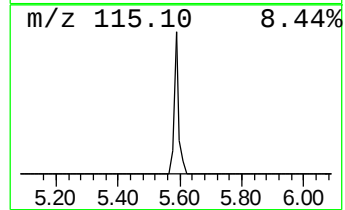
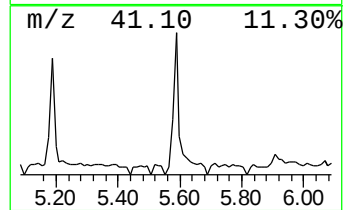
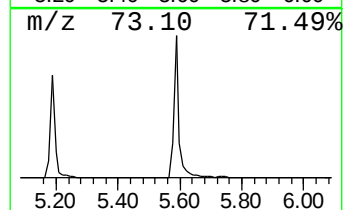
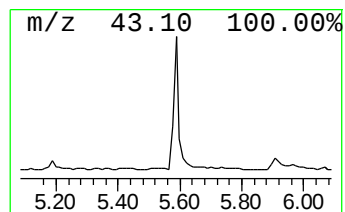
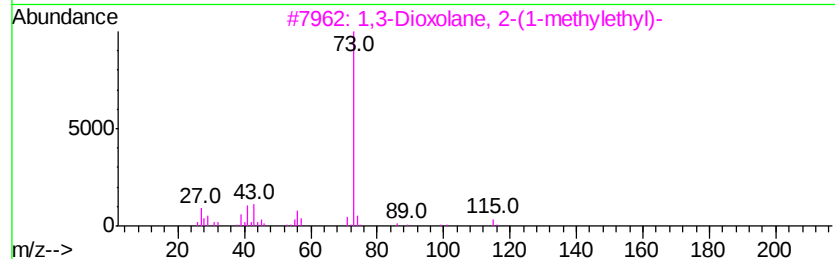
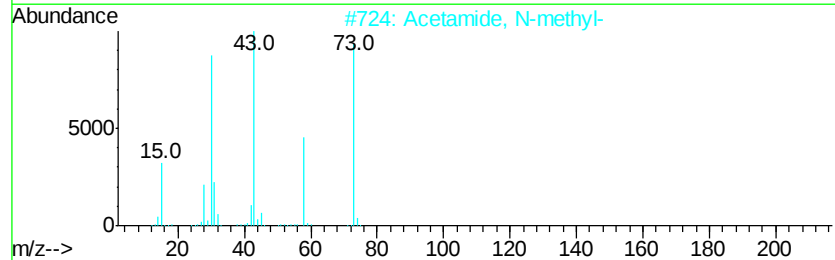
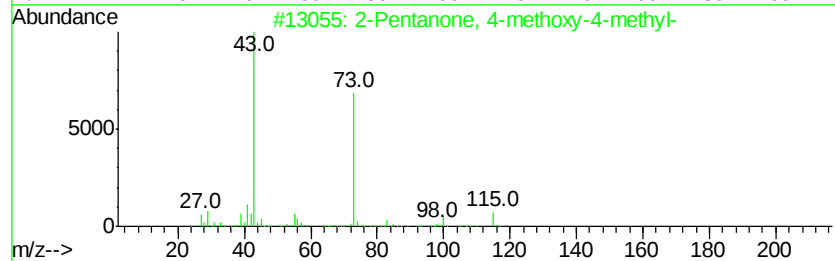
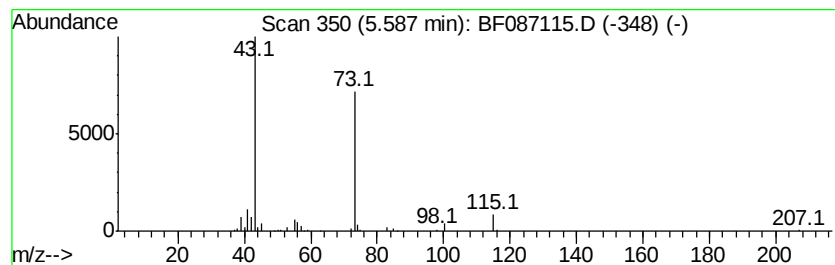
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	3.05 ng	145164	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4			Guanidine, methyl-	73	C2H7N3	000471-29-4	9
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



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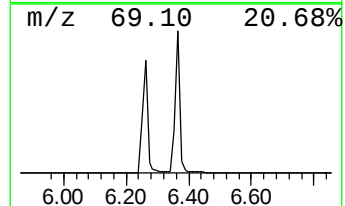
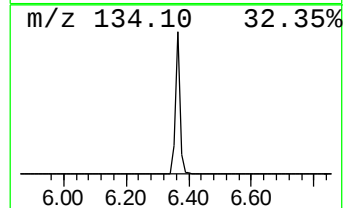
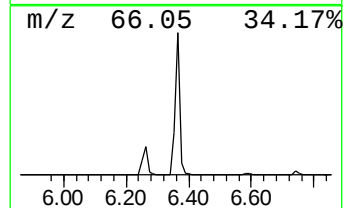
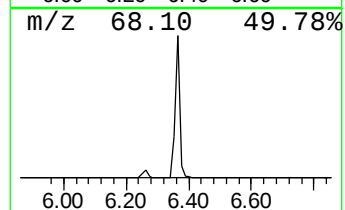
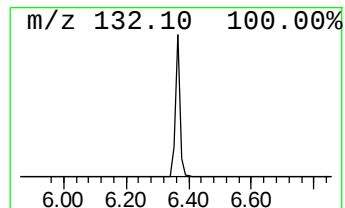
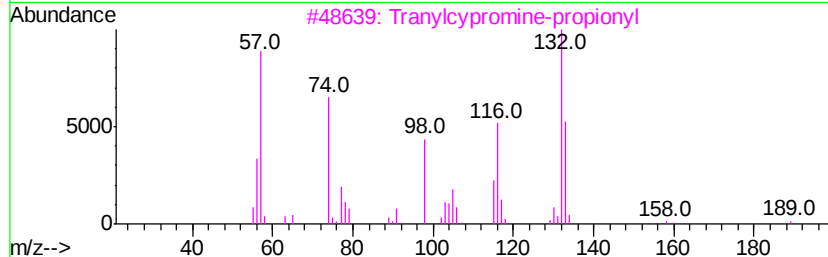
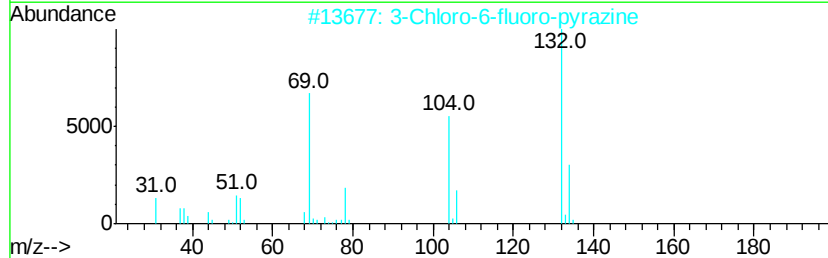
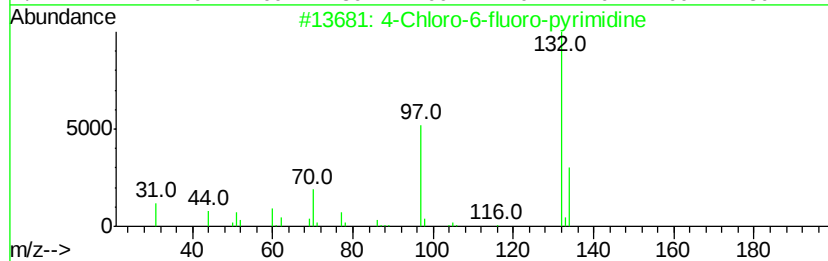
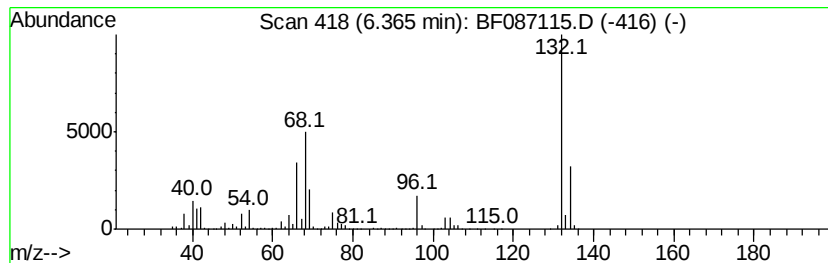
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	82.92 ng	3945240	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27	
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
3	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	22	
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22	
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16	



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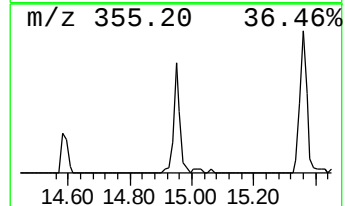
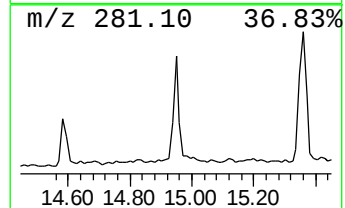
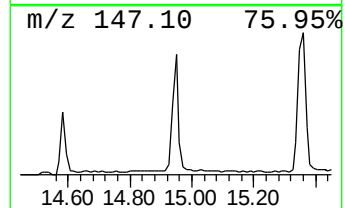
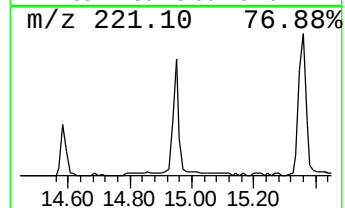
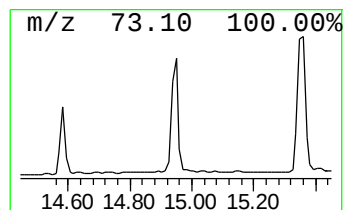
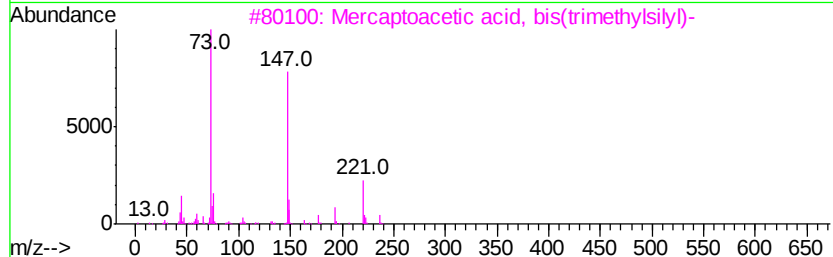
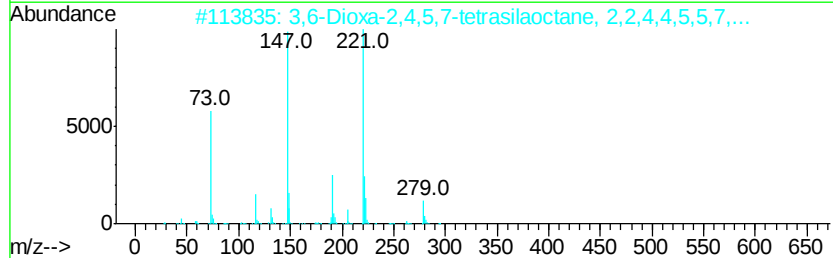
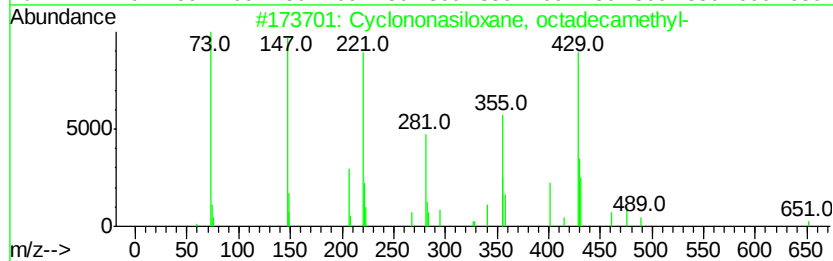
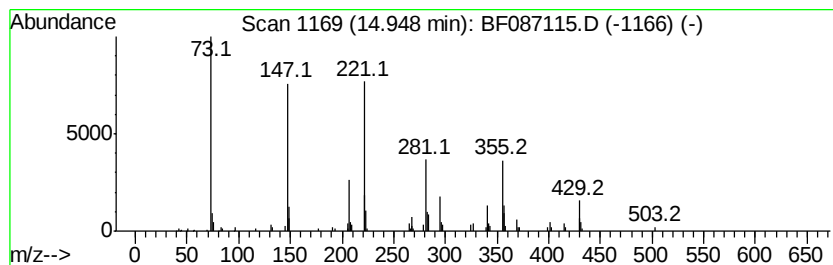
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown14.95 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.29 ng	182732	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	45
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	42
3		Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40
4		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	35
5		N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30



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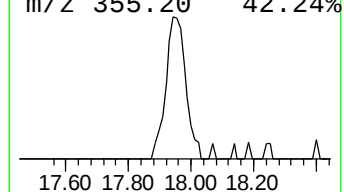
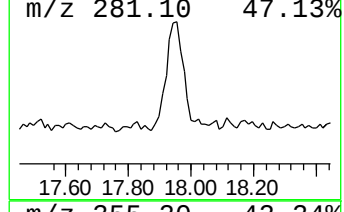
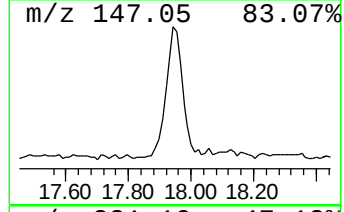
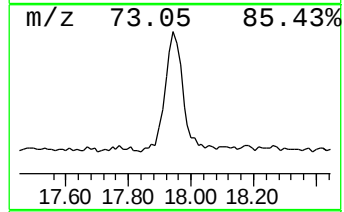
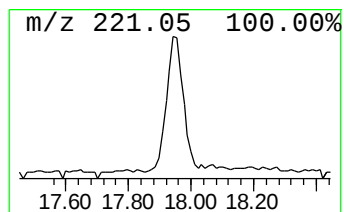
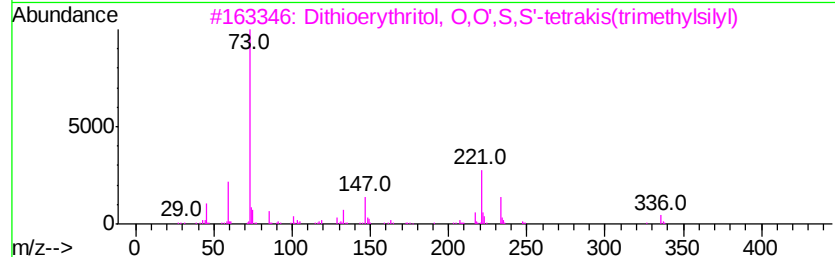
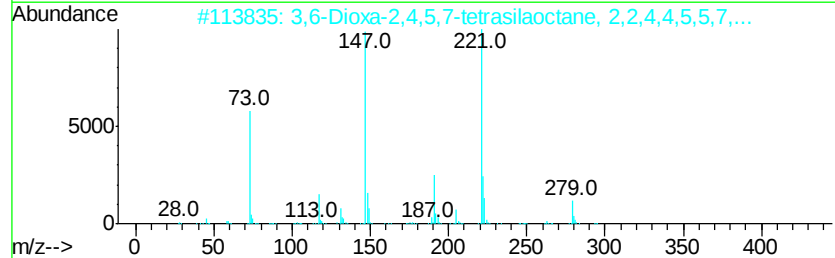
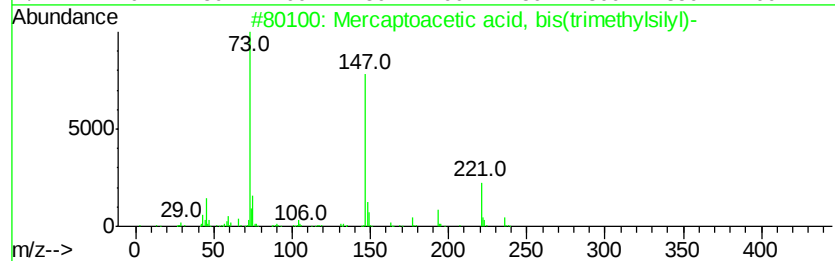
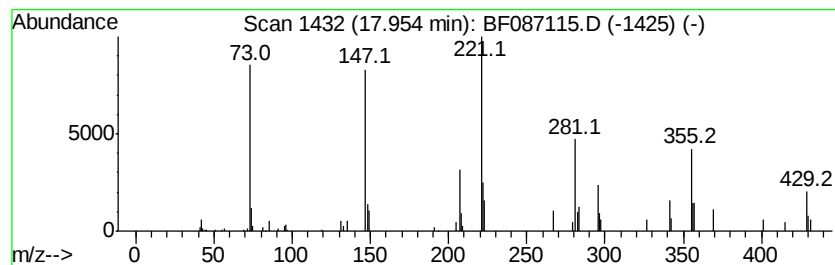
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.95 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	2.99 ng	166446	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	37
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
3		Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	35
4		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	28
5		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087115.D
Acq On : 17 May 2016 21:29
Operator : UM/SJ
Sample : PB90651BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB90651BL

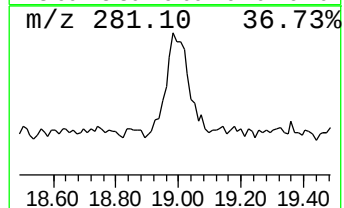
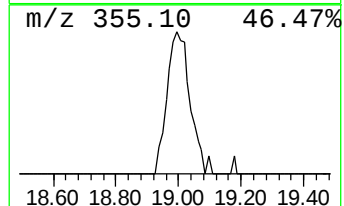
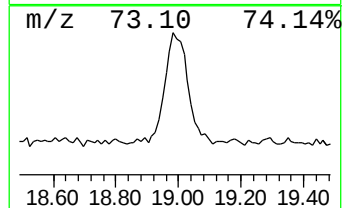
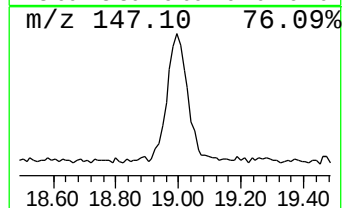
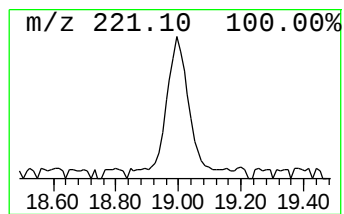
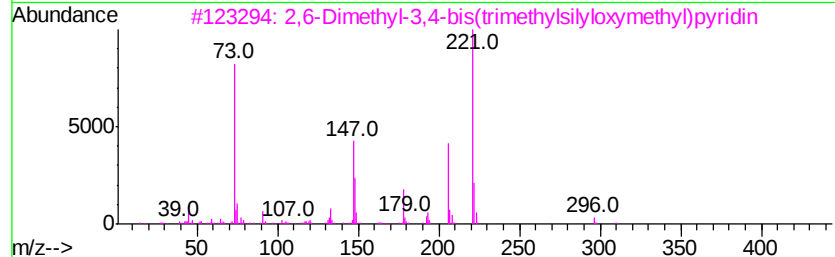
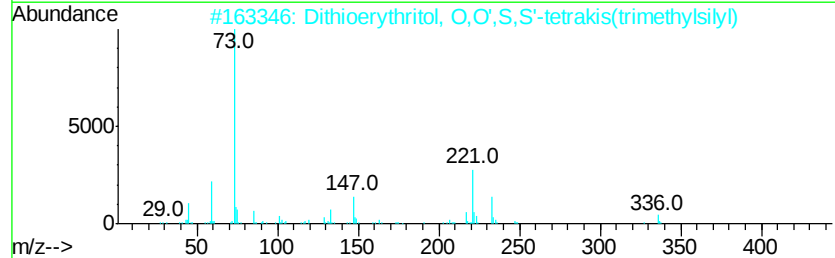
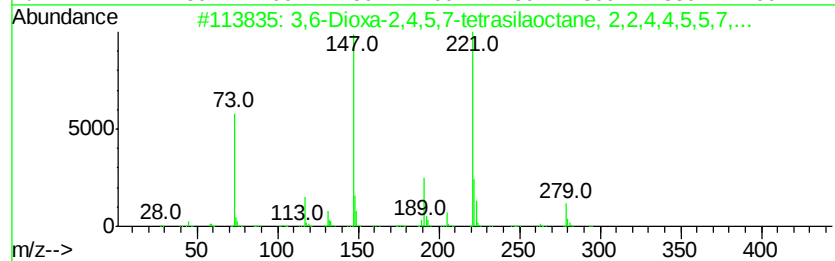
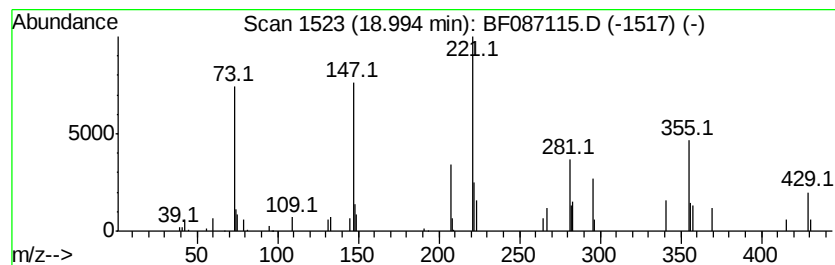
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.99 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.99	2.85 ng	158781	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
2			Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	35
3			2,6-Dimethyl-3,4-bis(trimethylsilyl)...	311	C15H29NO2Si2	1000079-52-1	25
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	22
5			Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
Data File : BF087115.D
Acq On : 17 May 2016 21:29
Operator : UM/SJ
Sample : PB90651BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB90651BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3,4-Dimethyl-2-pe...	4.00	5.4	ng	255480	1	6.59	951524	20.0
2-Pentanone, 4-hy...	4.72	42.3	ng	2011180	1	6.59	951524	20.0
2-Pentanone, 4-me...	5.59	3.0	ng	145164	1	6.59	951524	20.0
unknown6.36	6.36	82.9	ng	3945240	1	6.59	951524	20.0
unknown14.95	14.95	3.3	ng	182732	6	15.09	1112440	20.0
unknown17.95	17.95	3.0	ng	166446	6	15.09	1112440	20.0
unknown18.99	18.99	2.9	ng	158781	6	15.09	1112440	20.0