

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
 Data File : BF081065.D
 Acq On : 19 Aug 2015 4:18
 Operator : UM/IZ
 Sample : G3278-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

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-BF081715.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	3.976	172	174	181	rBV	56221	85808	3.18%	0.475%
2	4.719	236	239	249	rBV	408390	558933	20.68%	3.095%
3	5.176	276	279	281	rBV	680367	926553	34.28%	5.130%
4	5.599	314	316	318	rBV	59835	65274	2.42%	0.361%
5	6.239	370	372	375	rBV	481667	538245	19.92%	2.980%
6	6.364	381	383	386	rBV	1272794	1630160	60.32%	9.026%
7	6.604	402	404	406	rBV	476609	397496	14.71%	2.201%
8	6.765	415	418	420	rBV	1692154	1686149	62.39%	9.336%
9	7.176	451	454	456	rBV	1409947	1416930	52.43%	7.845%
10	7.382	470	472	474	rBV	22726	29893	1.11%	0.166%
11	7.633	492	494	497	rBV	73399	77585	2.87%	0.430%
12	7.885	514	516	518	rBV	409584	515705	19.08%	2.855%
13	7.942	518	521	527	rVB2	36888	68760	2.54%	0.381%
14	8.696	583	587	589	rBV	20210	28635	1.06%	0.159%
15	8.970	608	611	613	rBV	2547239	2368300	87.63%	13.113%
16	9.290	637	639	644	rBV3	14072	34167	1.26%	0.189%
17	9.370	644	646	648	rVB	43201	60401	2.23%	0.334%
18	9.633	667	669	671	rBV	684863	604393	22.36%	3.346%
19	9.839	685	687	692	rVB3	12757	27093	1.00%	0.150%
20	10.422	735	738	740	rBV	1579597	1654838	61.23%	9.162%
21	10.559	748	750	753	rVB	28074	43996	1.63%	0.244%
22	11.108	795	798	800	rBV	712178	665553	24.63%	3.685%
23	11.656	844	846	850	rBV	56633	66053	2.44%	0.366%
24	11.828	857	861	867	rVB3	19250	34079	1.26%	0.189%
25	12.537	920	923	925	rBV	135787	134145	4.96%	0.743%
26	12.605	925	929	932	rVB2	27450	41957	1.55%	0.232%
27	12.697	934	937	939	rBV	2500456	2702512	100.00%	14.963%
28	13.234	982	984	987	rBV2	135536	136681	5.06%	0.757%
29	13.611	1015	1017	1024	rBV2	29472	86667	3.21%	0.480%
30	13.725	1024	1027	1029	rBV	656181	684500	25.33%	3.790%
31	13.919	1042	1044	1046	rVB	42953	37109	1.37%	0.205%
32	14.228	1069	1071	1073	rBV	26425	29945	1.11%	0.166%
33	14.514	1094	1096	1099	rVB	38239	38691	1.43%	0.214%
34	14.582	1099	1102	1103	rBV	26194	30235	1.12%	0.167%

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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

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35	14.811	1119	1122	1125	rVB	20767	32278	1.19%	0.179%
36	15.062	1141	1144	1147	rBV	368631	488168	18.06%	2.703%
37	15.120	1147	1149	1156	rVB	20392	33465	1.24%	0.185%

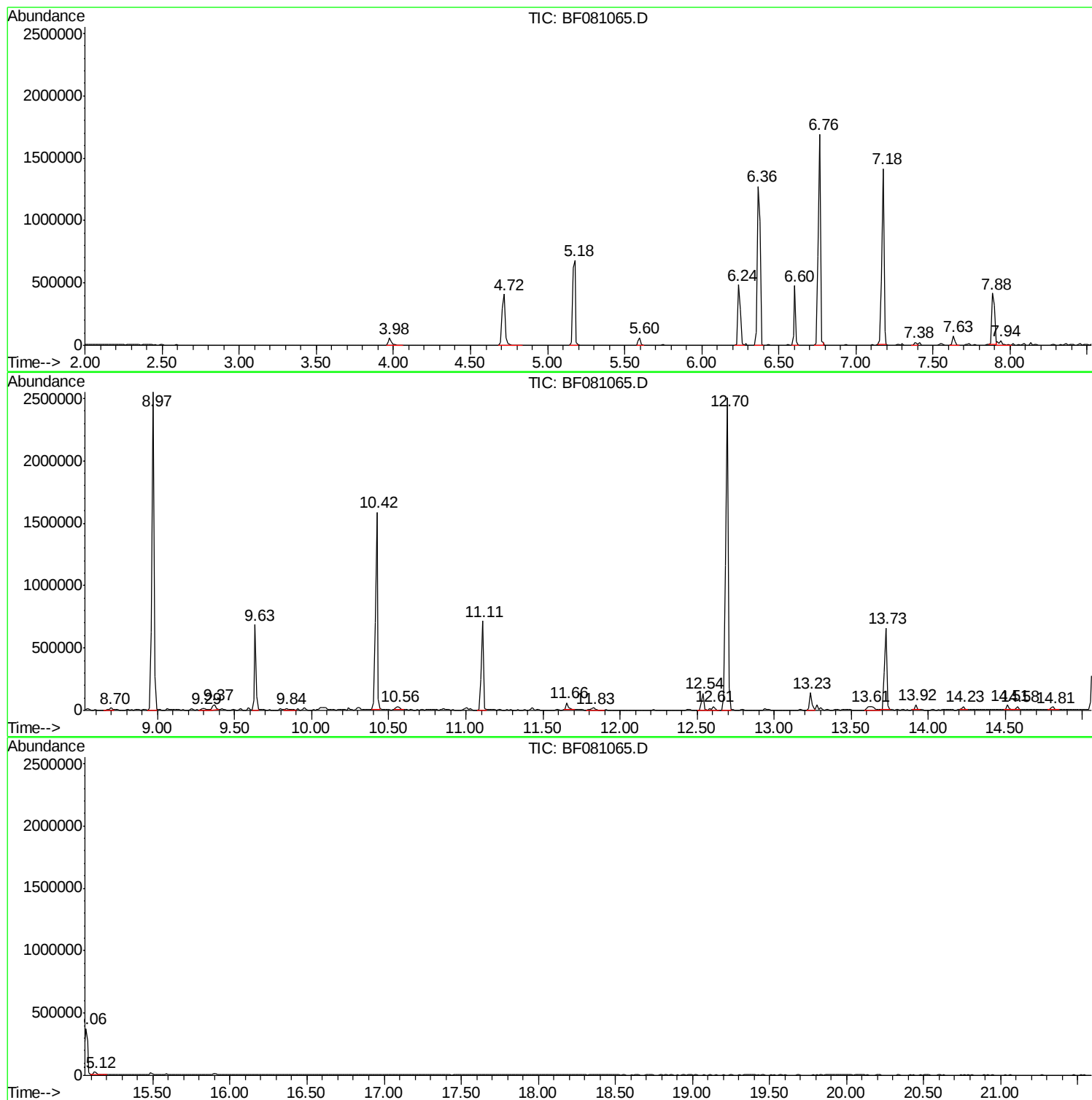
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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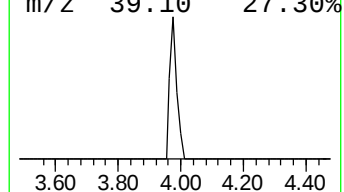
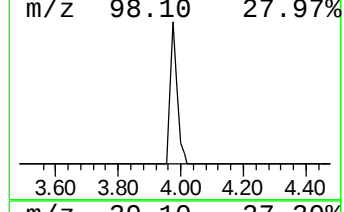
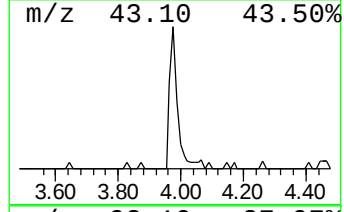
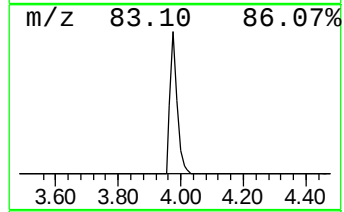
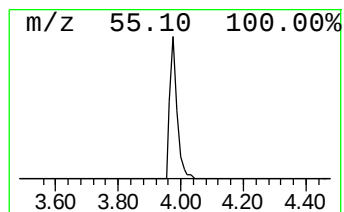
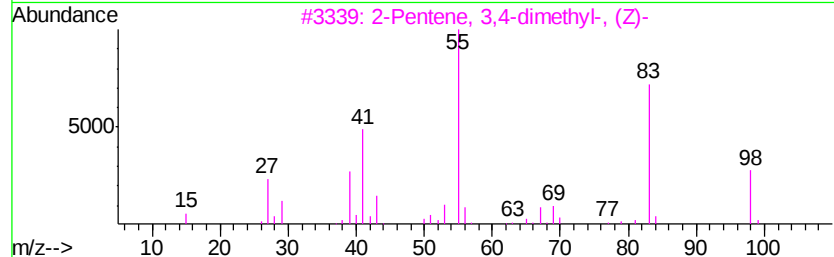
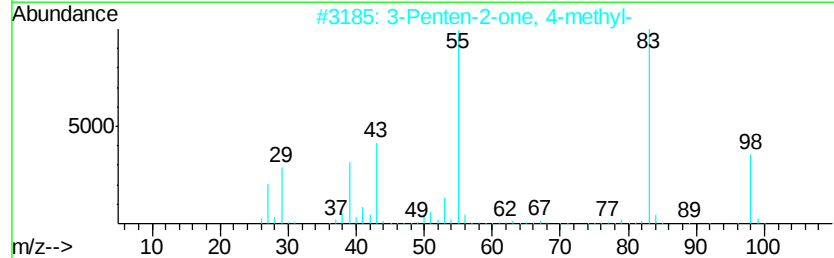
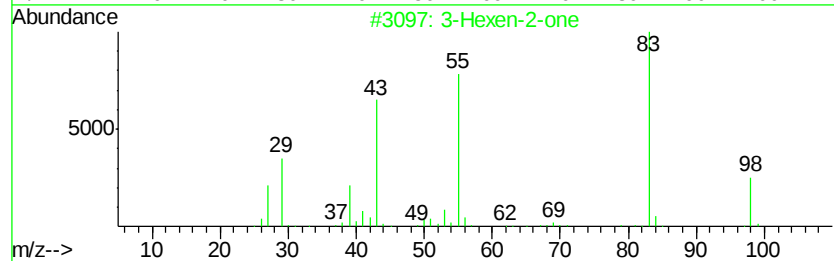
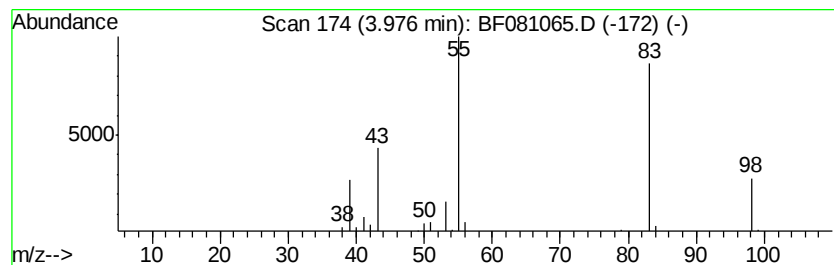
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	4.32 ng	85808	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	90
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80



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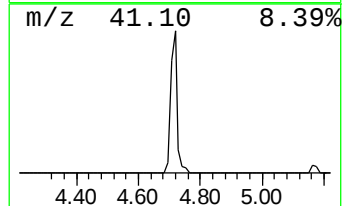
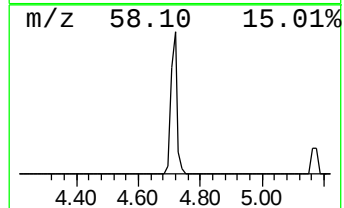
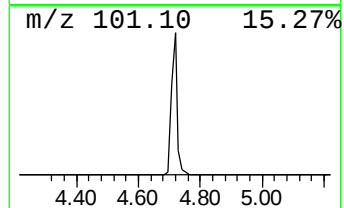
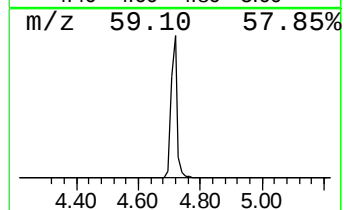
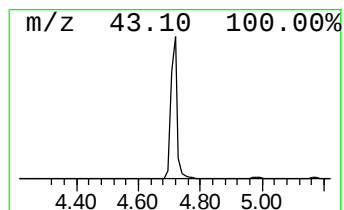
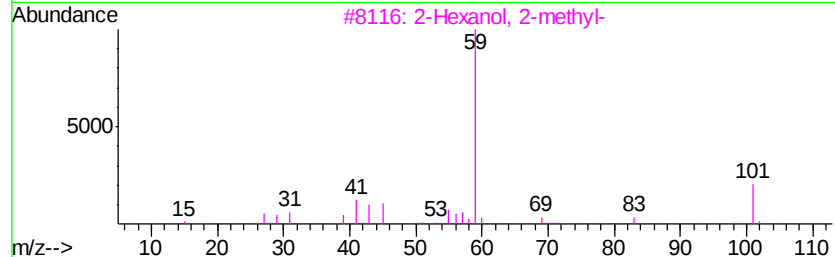
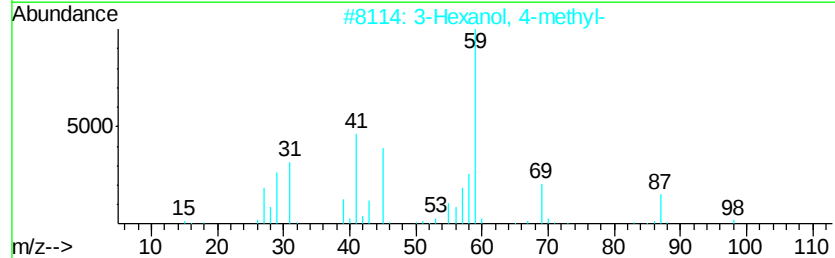
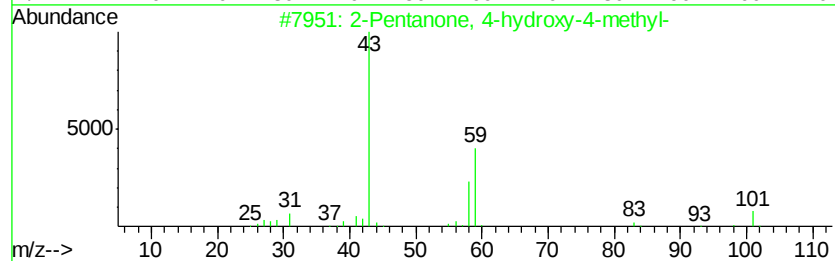
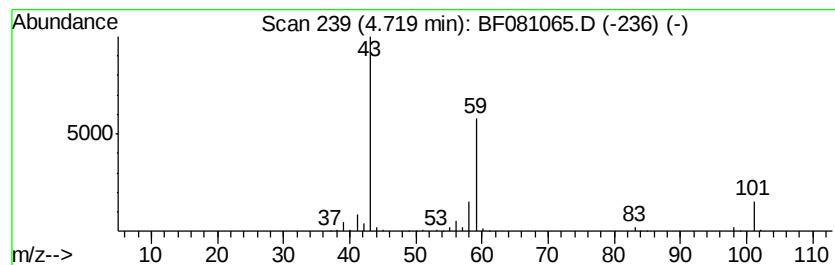
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	28.12 ng	558933	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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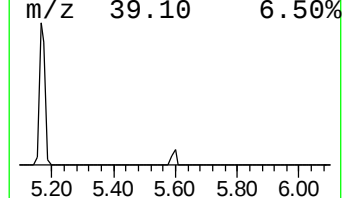
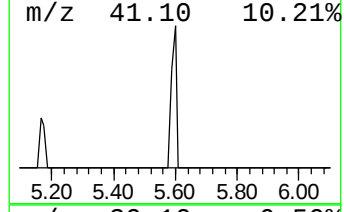
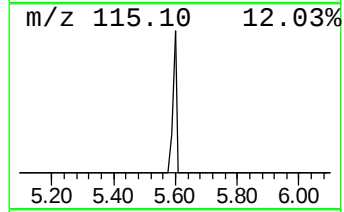
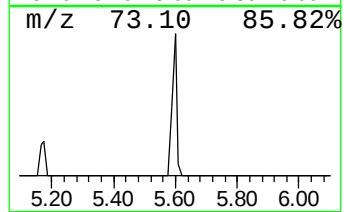
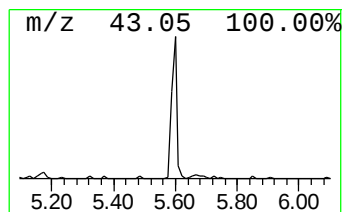
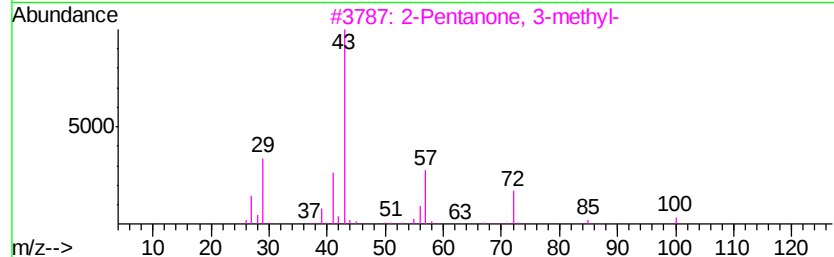
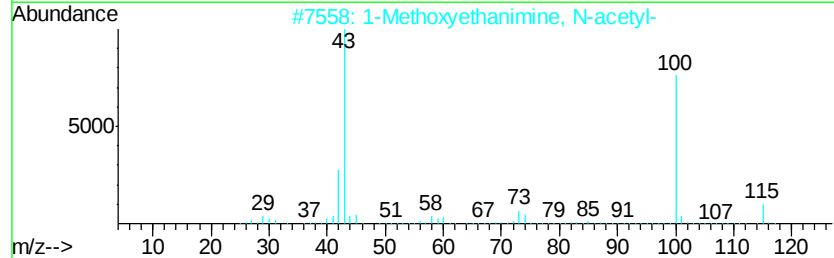
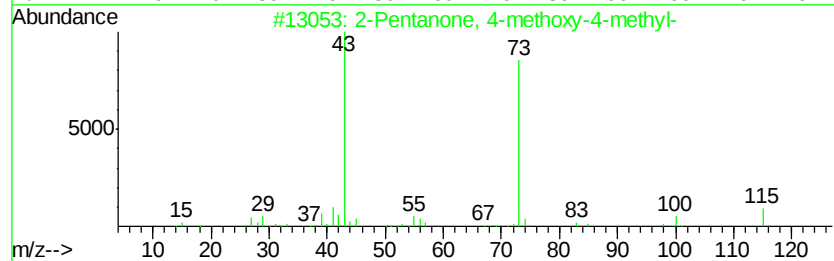
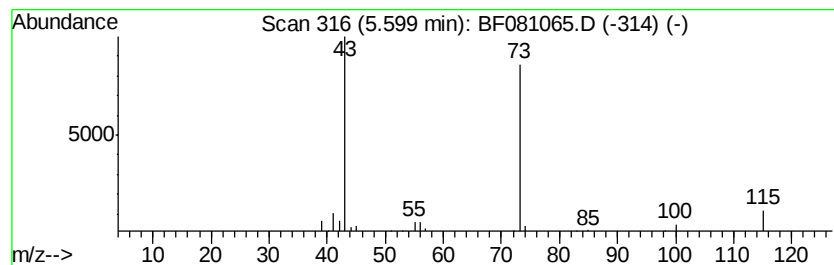
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	3.28 ng	65274	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	43
3		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
4		Hexane, 2-methyl-	100	C7H16	000591-76-4	9
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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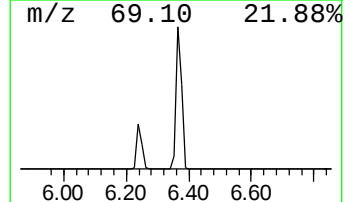
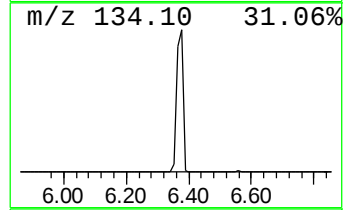
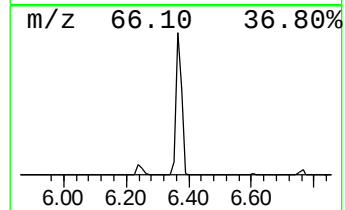
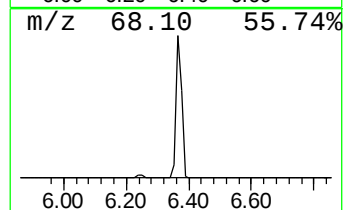
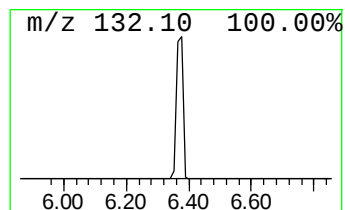
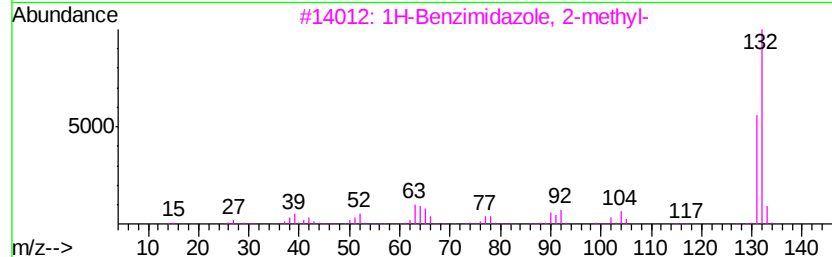
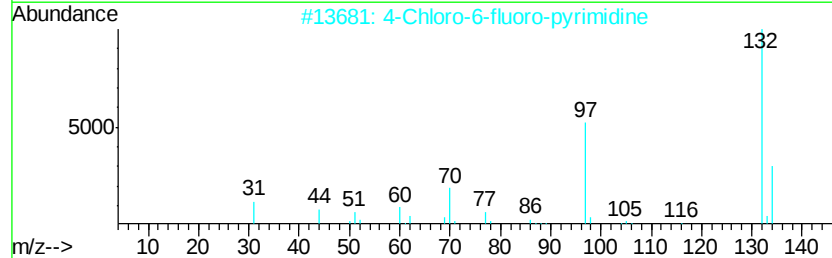
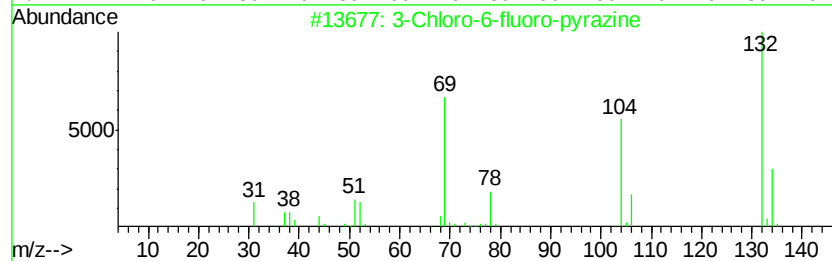
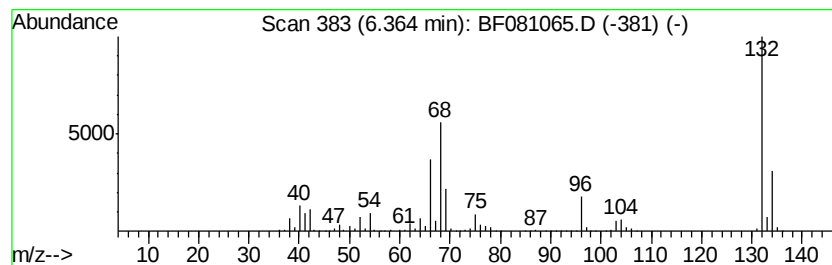
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	82.02 ng	1630160	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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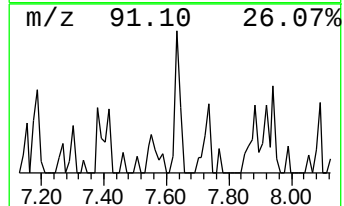
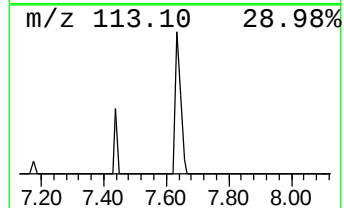
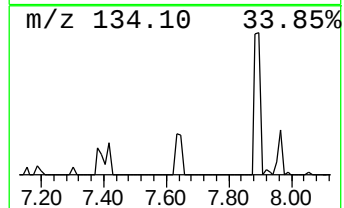
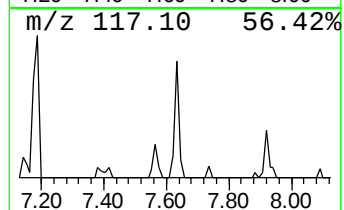
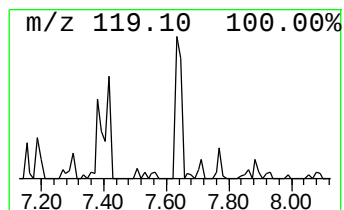
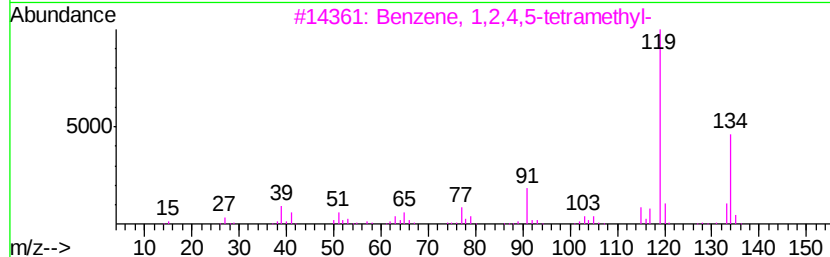
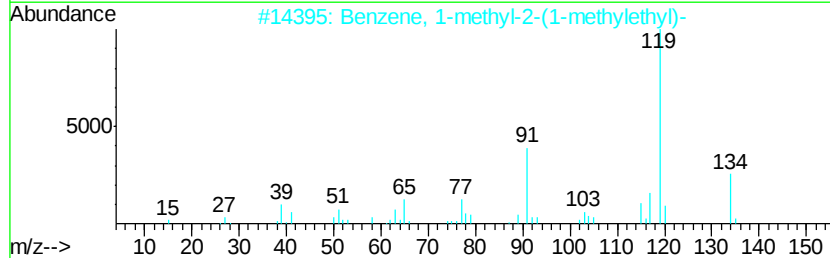
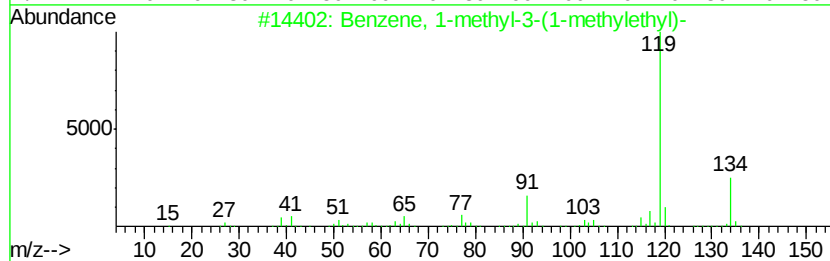
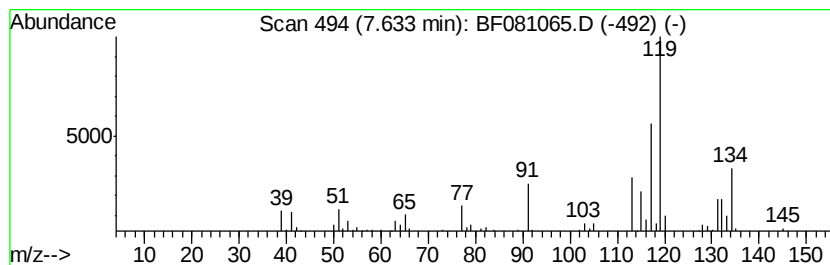
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	3.01 ng	77585	Napthalene-d8	7.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	55
2			Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	55
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	55
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	50
5			Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081065.D
Acq On : 19 Aug 2015 4:18
Operator : UM/IZ
Sample : G3278-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

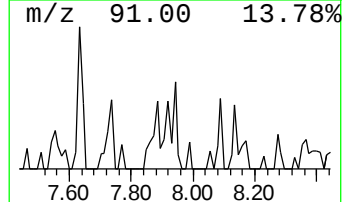
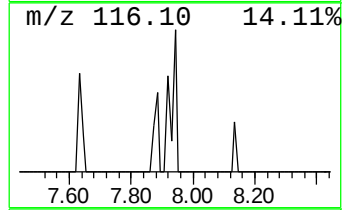
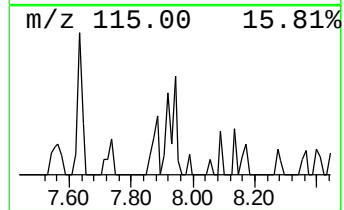
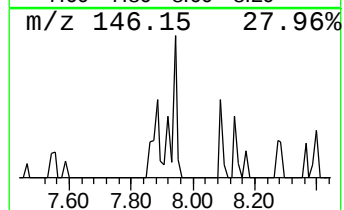
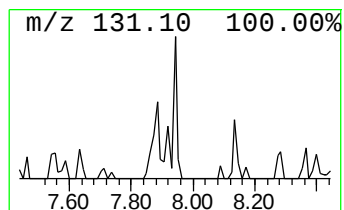
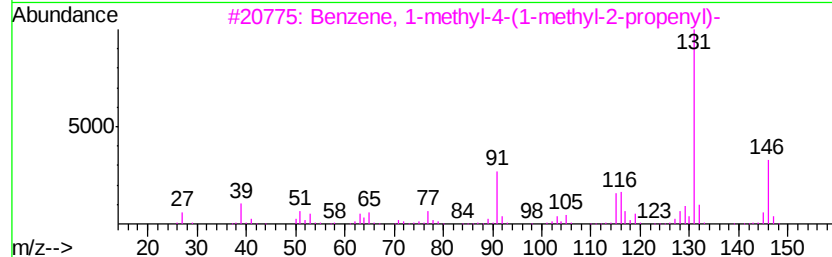
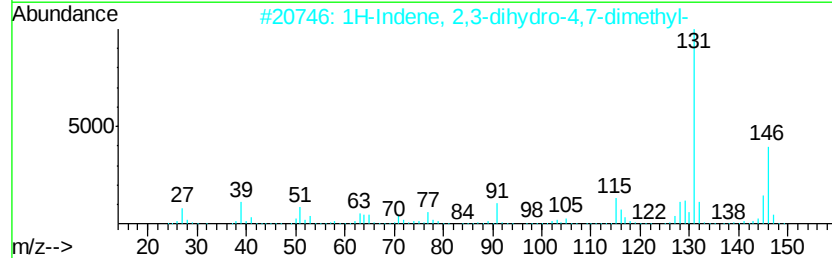
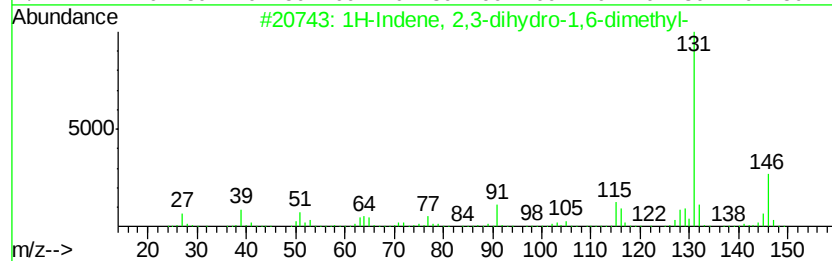
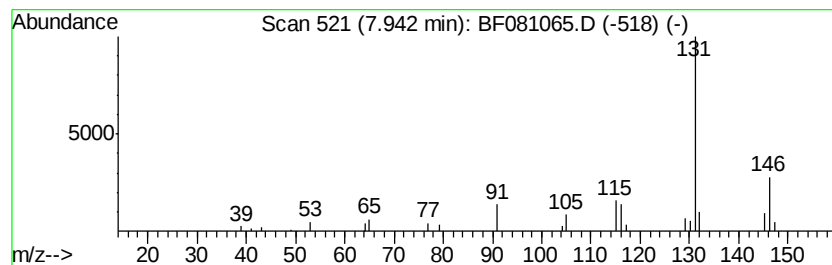
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.94	2.67 ng	68760	Naphthalene-d8	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	91
2		1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	91
3		Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	87
4		1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	87
5		Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
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Acq On : 19 Aug 2015 4:18
Operator : UM/IZ
Sample : G3278-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

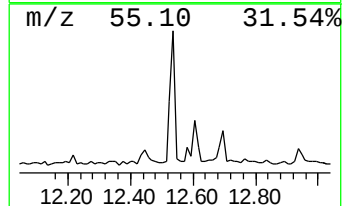
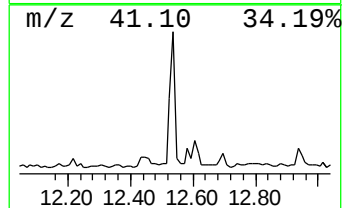
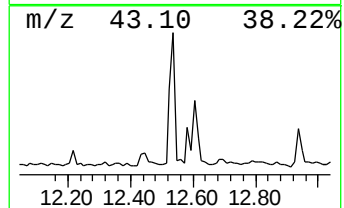
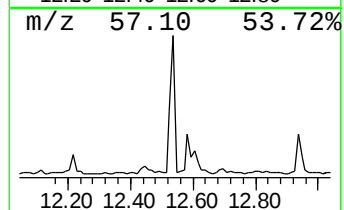
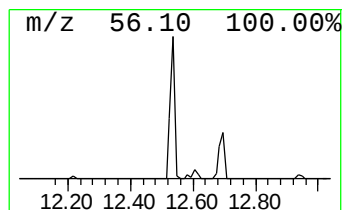
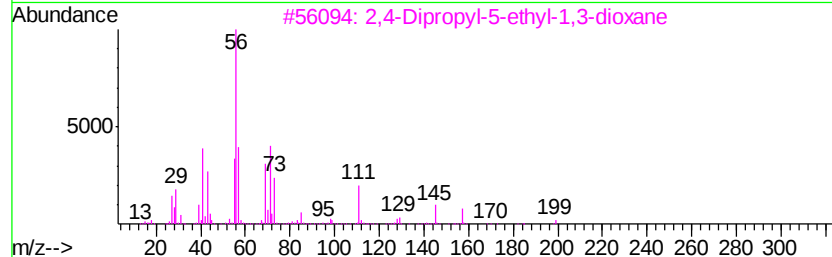
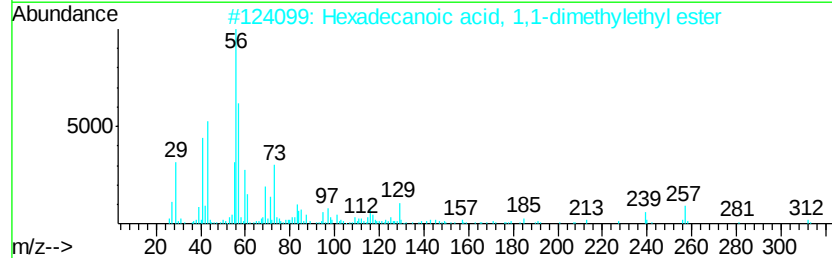
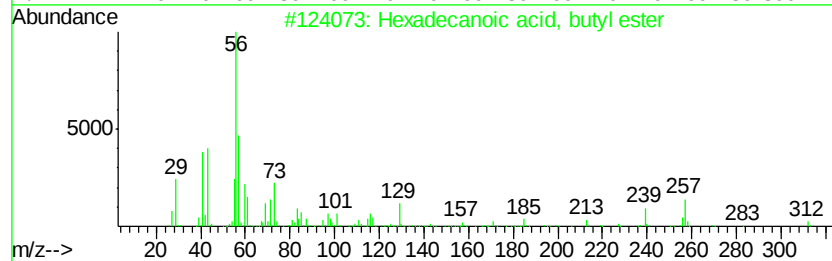
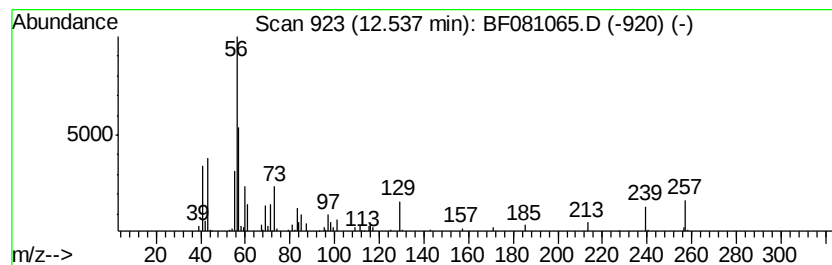
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	3.92 ng	134145	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5		1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081065.D
Acq On : 19 Aug 2015 4:18
Operator : UM/IZ
Sample : G3278-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

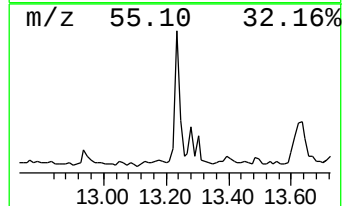
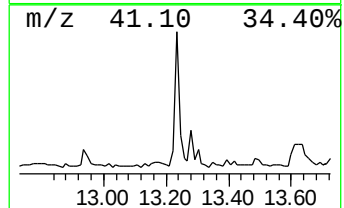
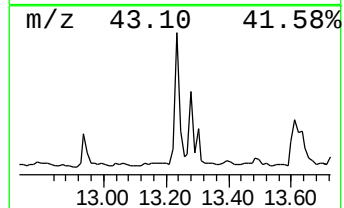
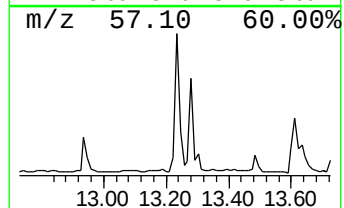
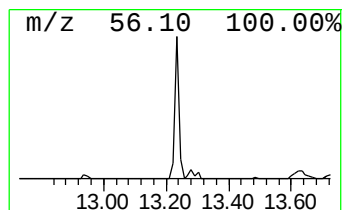
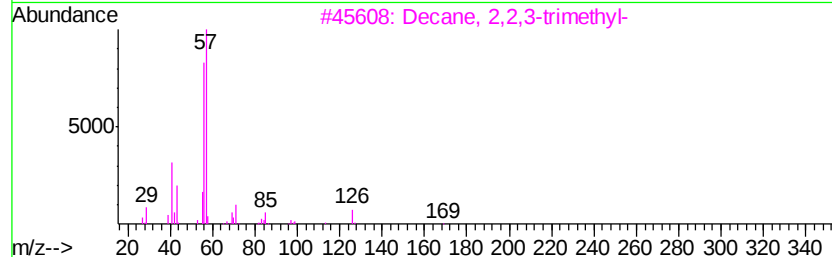
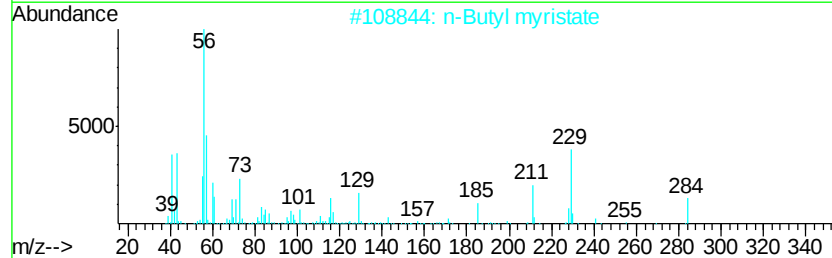
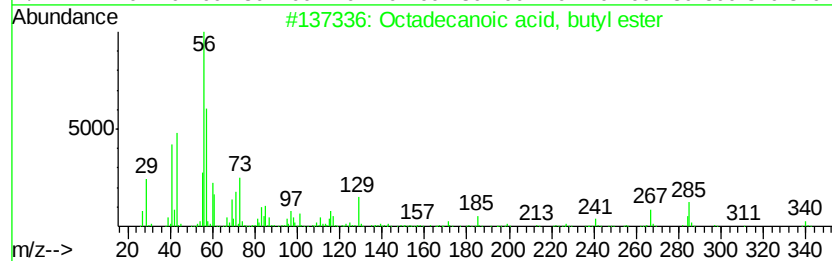
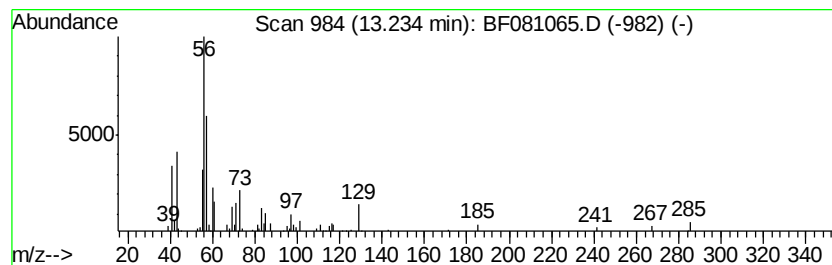
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	3.99 ng	136681	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
Data File : BF081065.D
Acq On : 19 Aug 2015 4:18
Operator : UM/IZ
Sample : G3278-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

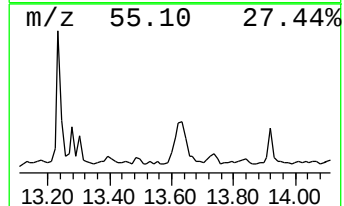
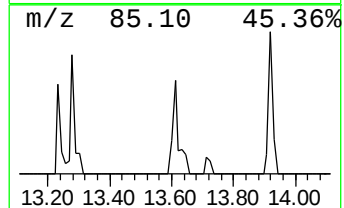
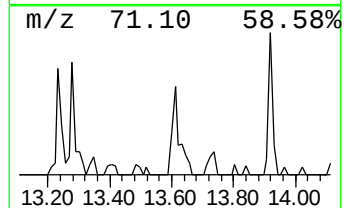
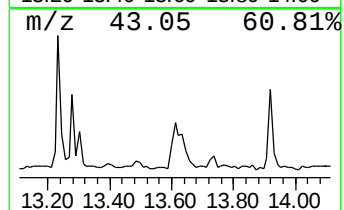
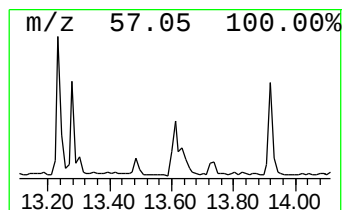
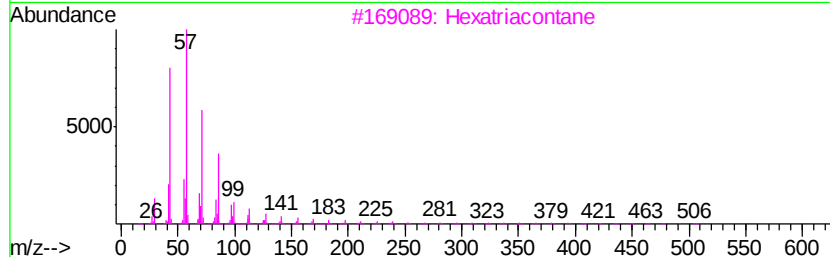
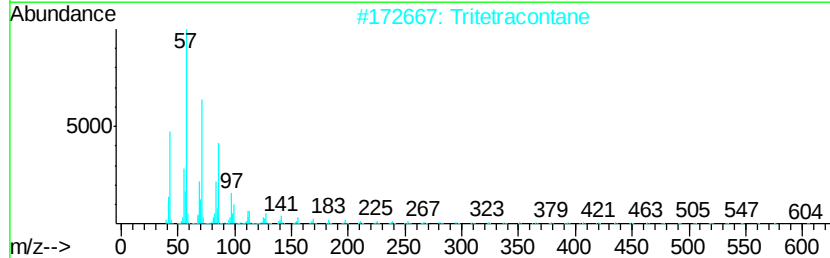
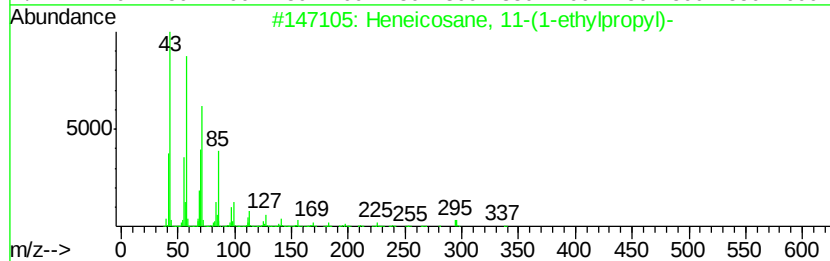
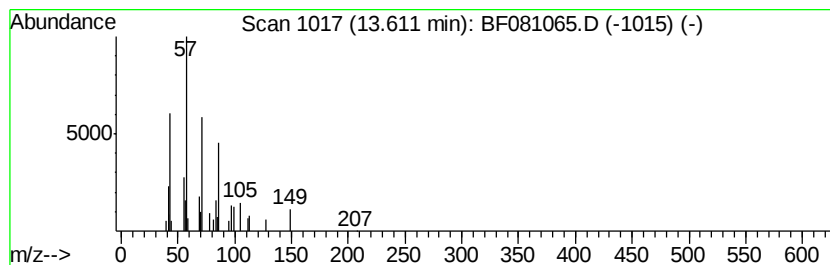
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane, 11-(1-ethylpro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.53 ng	86667	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
2		Tritetracontane	605	C43H88	007098-21-7	80
3		Hexatriacontane	507	C36H74	000630-06-8	80
4		Tetratetracontane	619	C44H90	007098-22-8	80
5		Octacosane	394	C28H58	000630-02-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081815\
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Acq On : 19 Aug 2015 4:18
Operator : UM/IZ
Sample : G3278-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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-Hexen-2-one	3.98	4.3	ng	85808	1	6.60	397496	20.0
2-Pentanone, 4-hy...	4.72	28.1	ng	558933	1	6.60	397496	20.0
2-Pentanone, 4-me...	5.60	3.3	ng	65274	1	6.60	397496	20.0
unknown6.36	6.36	82.0	ng	1630160	1	6.60	397496	20.0
Benzene, 1-methyl...	7.63	3.0	ng	77585	2	7.88	515705	20.0
1H-Indene, 2,3-di...	7.94	2.7	ng	68760	2	7.88	515705	20.0
Hexadecanoic acid...	12.54	3.9	ng	134145	5	13.73	684500	20.0
Octadecanoic acid...	13.23	4.0	ng	136681	5	13.73	684500	20.0
Heneicosane, 11-(...	13.61	2.5	ng	86667	5	13.73	684500	20.0