

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110715\
 Data File : BF082785.D
 Acq On : 7 Nov 2015 2:45
 Operator : UM/IZ
 Sample : G4257-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WABUT-1(0-2)

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-BF110715.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	2.304	17	19	33	rVB4	26614	102096	1.79%	0.193%
2	2.841	62	66	70	rBV	40092	71982	1.26%	0.136%
3	4.384	199	201	205	rBV	97293	145989	2.57%	0.277%
4	5.036	255	258	261	rBV	1914980	2486083	43.69%	4.711%
5	5.459	292	295	297	rBV	4826911	5014444	88.12%	9.502%
6	6.476	381	384	387	rBV	4610848	4725155	83.03%	8.954%
7	6.613	393	396	399	rBV	4867018	4552596	80.00%	8.627%
8	6.842	414	416	419	rBV	1231612	1337113	23.50%	2.534%
9	7.002	428	430	433	rBV	3699035	3427346	60.23%	6.494%
10	7.402	462	465	468	rBV	2237200	3055736	53.70%	5.790%
11	8.133	526	529	531	rBV	2100690	2041711	35.88%	3.869%
12	9.208	620	623	626	rBV	4313065	5022818	88.26%	9.518%
13	9.608	655	658	660	rBV	975550	1060335	18.63%	2.009%
14	9.882	679	682	685	rBV	1693574	1970909	34.63%	3.735%
15	10.305	712	719	720	rBV	73300	72275	1.27%	0.137%
16	10.671	748	751	754	rBV	3339628	3349195	58.85%	6.346%
17	10.808	761	763	767	rVB	86596	134227	2.36%	0.254%
18	11.254	799	802	803	rBV2	155663	140650	2.47%	0.267%
19	11.368	809	812	814	rVV	2760224	2416676	42.47%	4.579%
20	11.425	814	817	822	rVB2	25908	61464	1.08%	0.116%
21	11.676	837	839	842	rBV	84322	71593	1.26%	0.136%
22	11.905	857	859	864	rBV2	136894	183669	3.23%	0.348%
23	12.785	934	936	939	rBV	476140	467086	8.21%	0.885%
24	12.865	939	943	945	rVB2	68998	79092	1.39%	0.150%
25	12.957	948	951	954	rBV	6091962	5690656	100.00%	10.783%
26	13.494	996	998	1001	rBV	381963	321083	5.64%	0.608%
27	13.539	1001	1002	1006	rVB2	38172	62391	1.10%	0.118%
28	13.894	1029	1033	1040	rBV3	185139	679260	11.94%	1.287%
29	13.997	1040	1042	1045	rVB	1662963	1995631	35.07%	3.781%
30	14.191	1056	1059	1061	rBV	57876	67839	1.19%	0.129%
31	14.865	1115	1118	1120	rBV	96898	98002	1.72%	0.186%
32	15.117	1138	1140	1145	rVB	54097	64276	1.13%	0.122%
33	15.425	1164	1167	1170	rBV	1322458	1668954	29.33%	3.162%
34	16.031	1214	1220	1221	rBV2	18872	59467	1.04%	0.113%

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ClientSampleId :
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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-BF110715.M
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35	20.466	1599	1608	1614	rBV5	16205	76375	1.34%	0.145%
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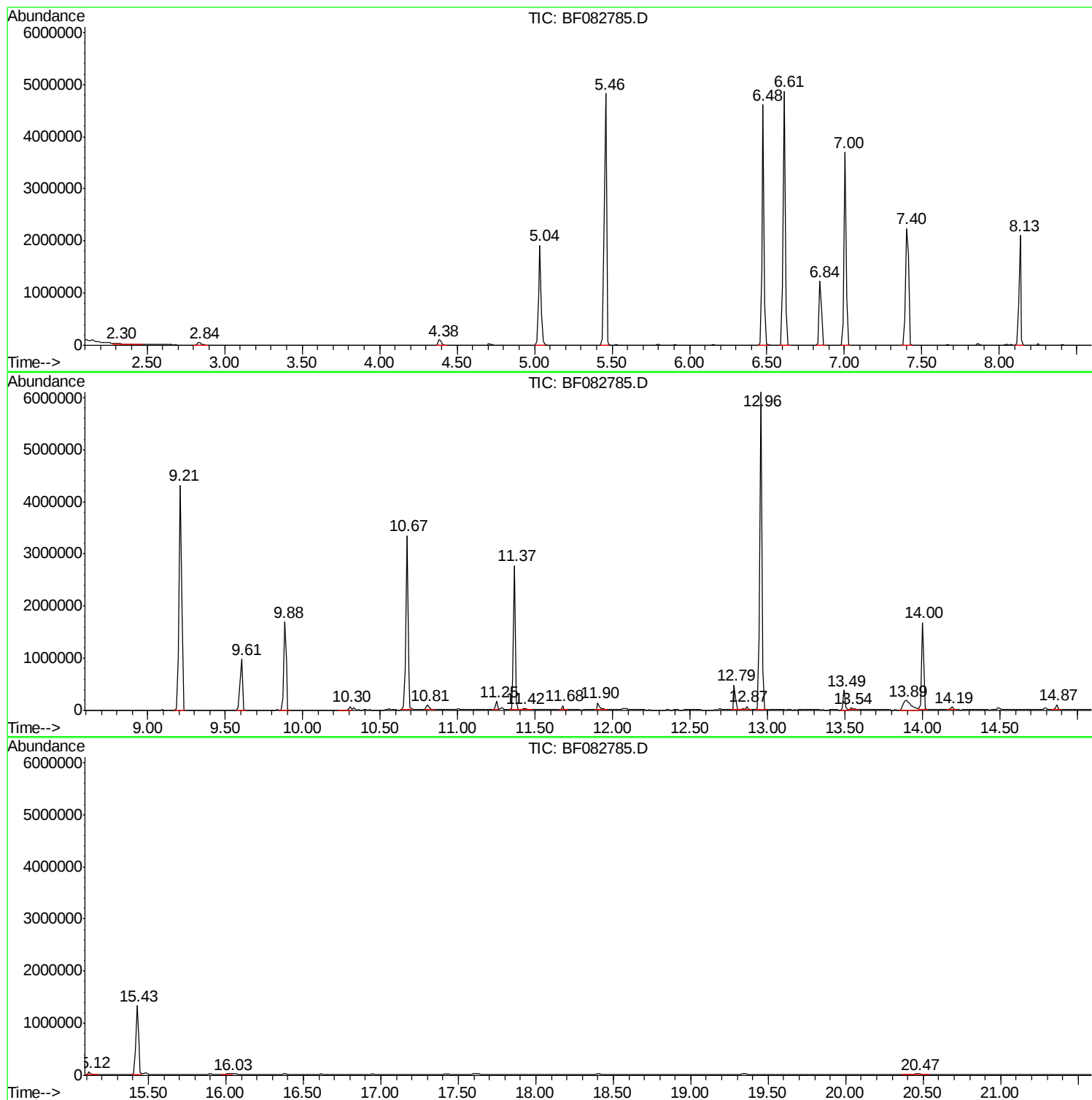
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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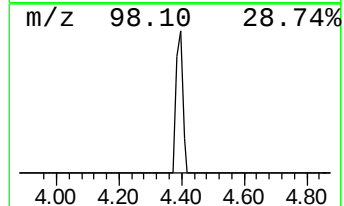
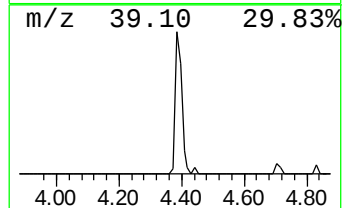
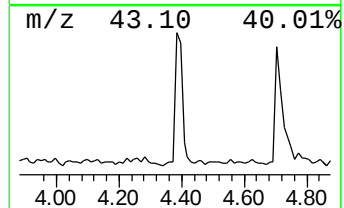
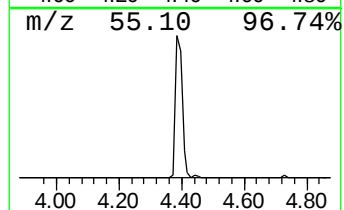
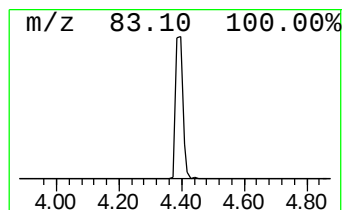
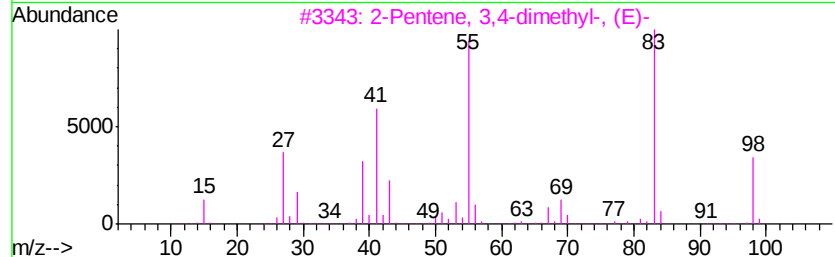
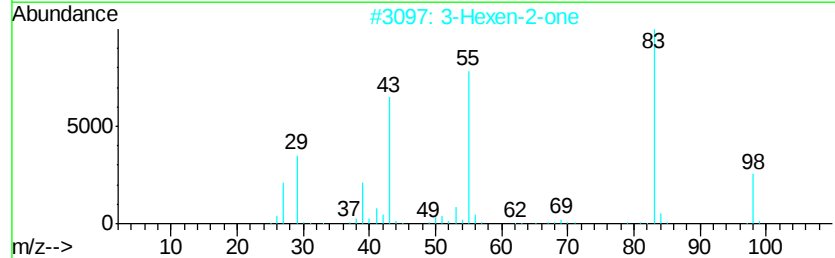
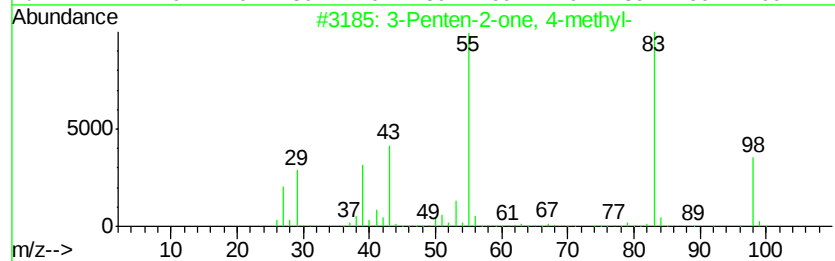
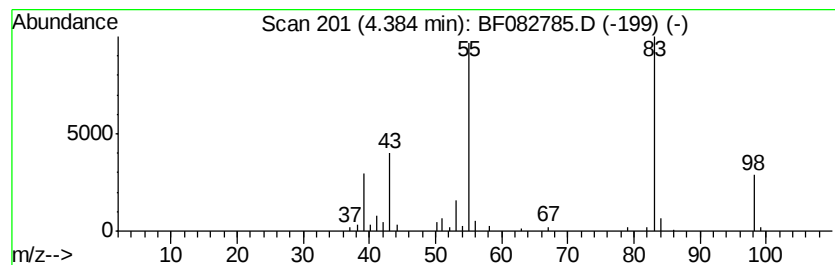
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	2.18 ng	145989	1,4-Dichlorobenzene-d4	6.84

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	87
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	83
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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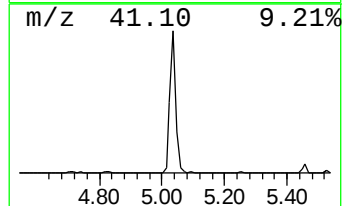
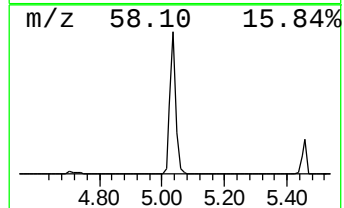
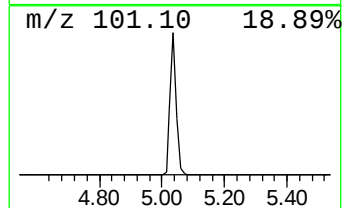
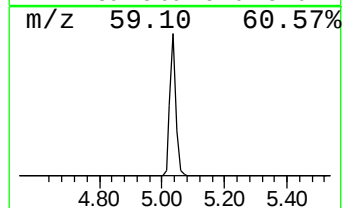
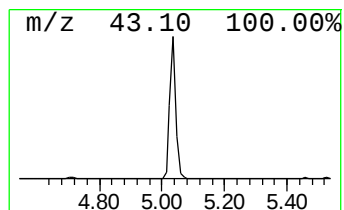
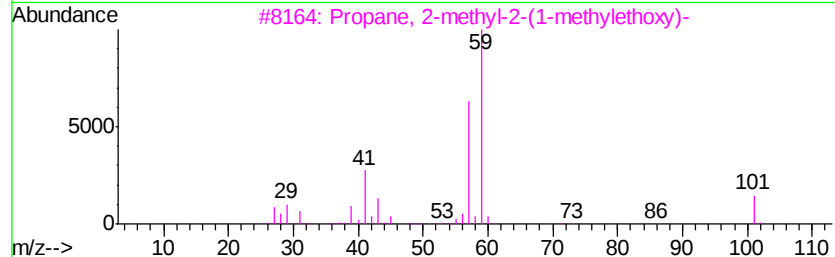
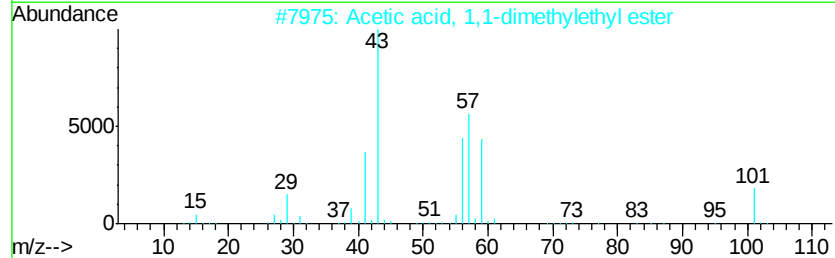
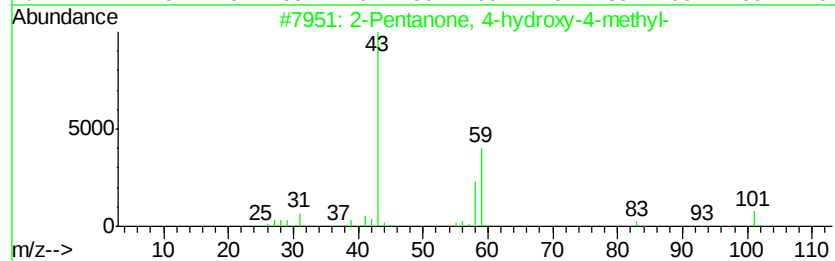
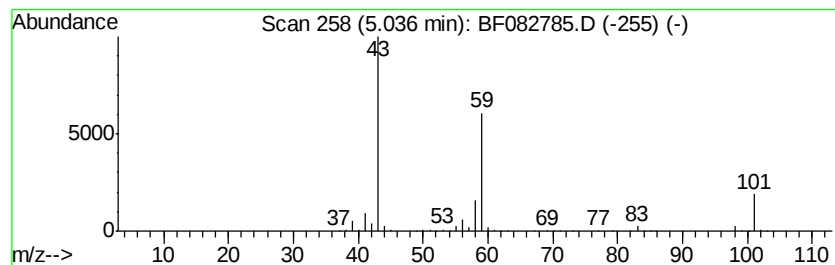
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	37.19 ng	2486080	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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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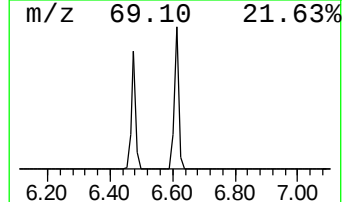
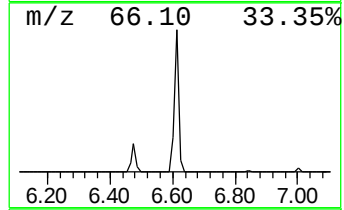
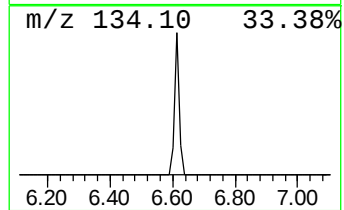
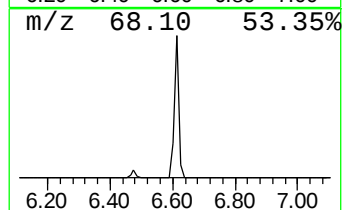
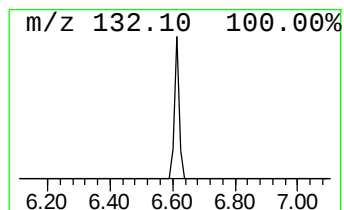
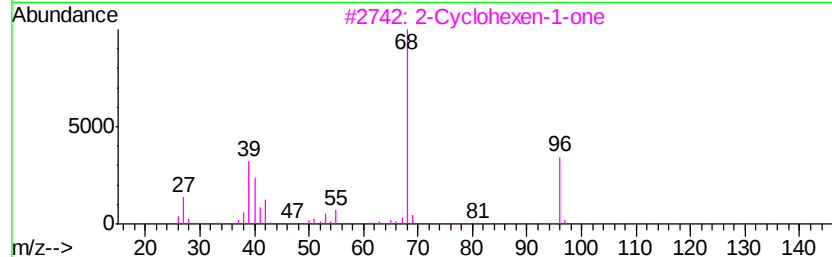
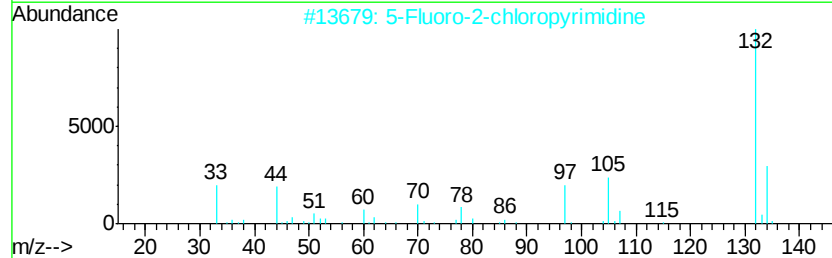
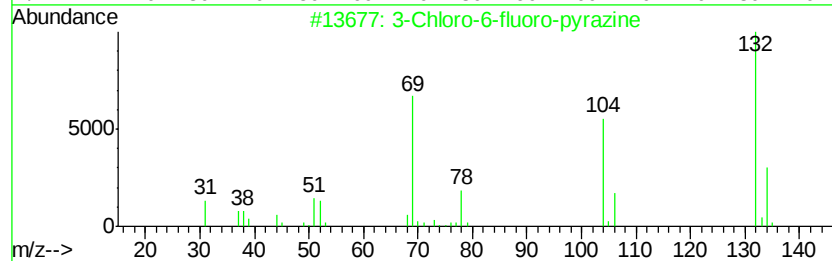
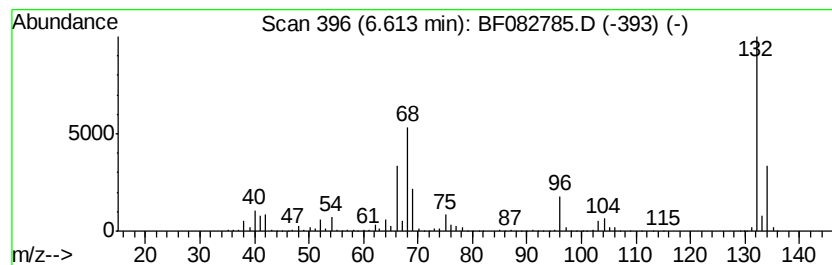
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	68.10 ng	4552600	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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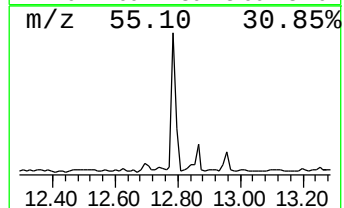
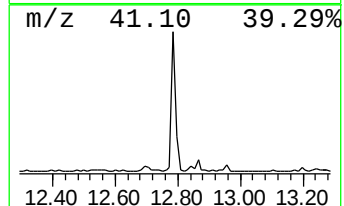
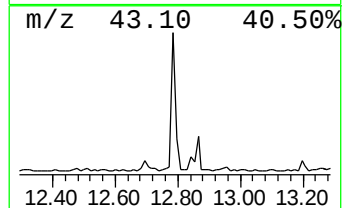
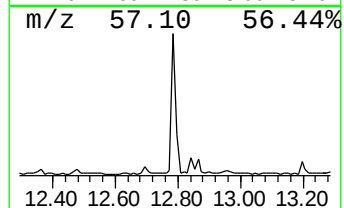
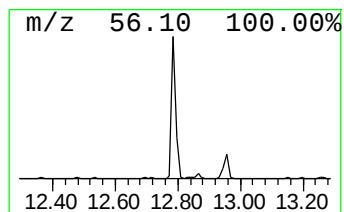
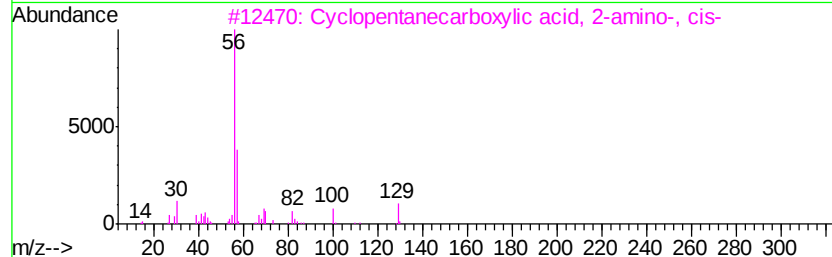
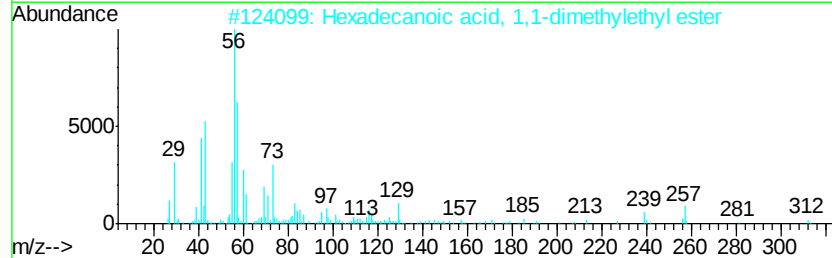
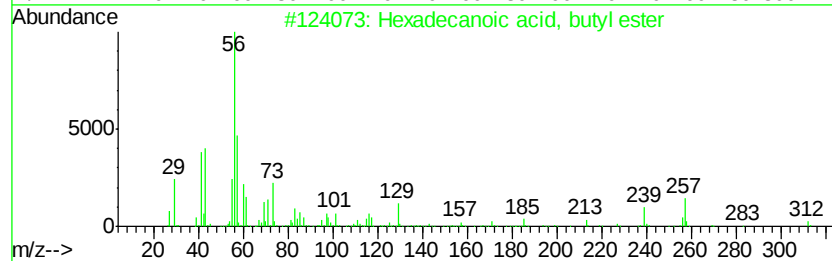
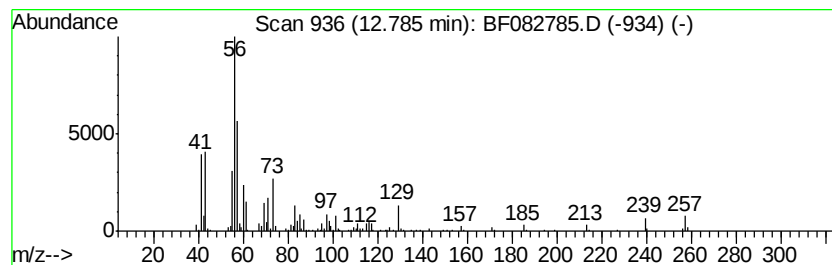
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.68 ng	467086	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecanoic acid, butyl ester	312 C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312 C20H40O2	031158-91-5	76
3	Cyclopentanecarboxylic acid, 2-a...	129 C6H11NO2	037910-65-9	43
4	1-Pentene, 2,4-dimethyl-	98 C7H14	002213-32-3	43
5	Cyclopentanecarboxylic acid, 2-a...	129 C6H11NO2	040482-05-1	43



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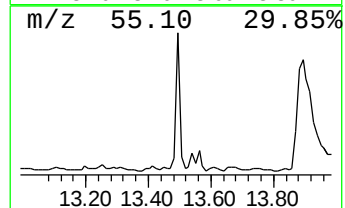
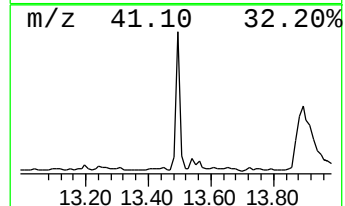
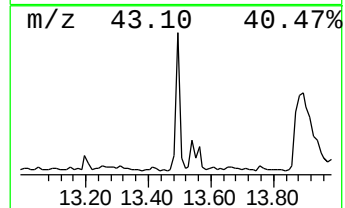
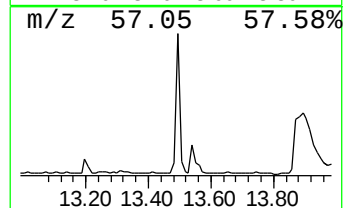
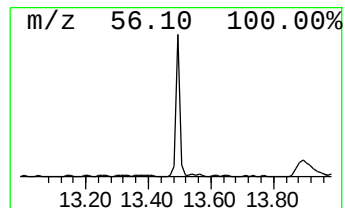
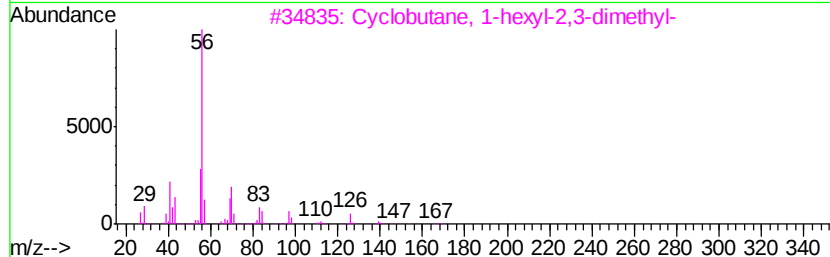
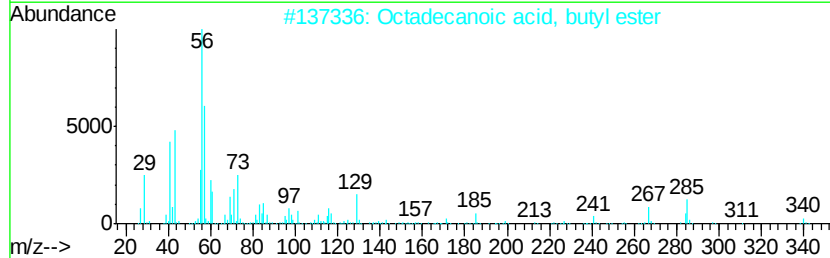
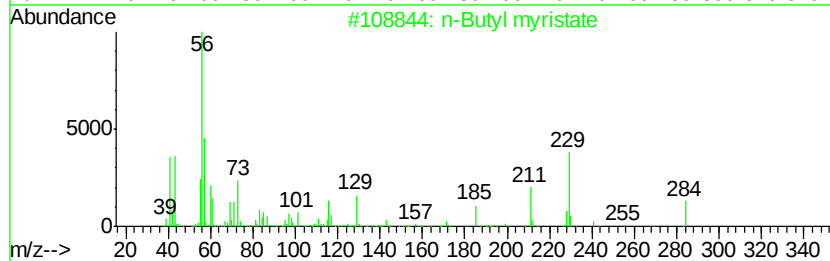
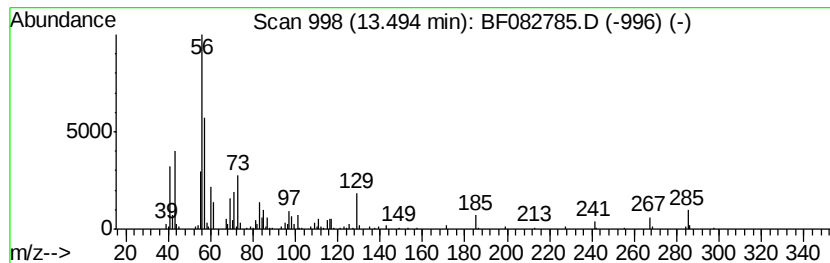
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Peak Number 6 n-Butyl myristate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.22 ng	321083	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Butyl myristate	284 C18H36O2	000110-36-1	64
2	Octadecanoic acid, butyl ester	340 C22H44O2	000123-95-5	53
3	Cyclobutane, 1-hexyl-2,3-dimethyl-	168 C12H24	055170-84-8	38
4	Pentadecane, 8-methylene-	224 C16H32	055668-09-2	37
5	Cyclohexanol, 4-amino-, trans-	115 C6H13NO	027489-62-9	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110715\
Data File : BF082785.D
Acq On : 7 Nov 2015 2:45
Operator : UM/IZ
Sample : G4257-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-1(0-2)

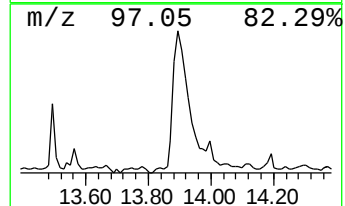
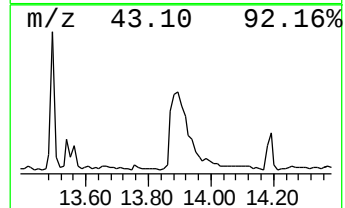
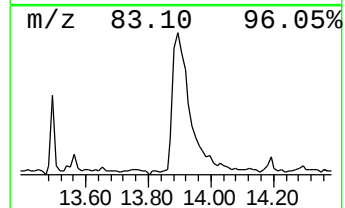
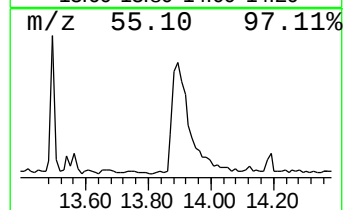
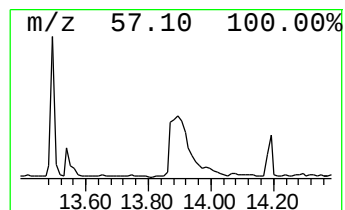
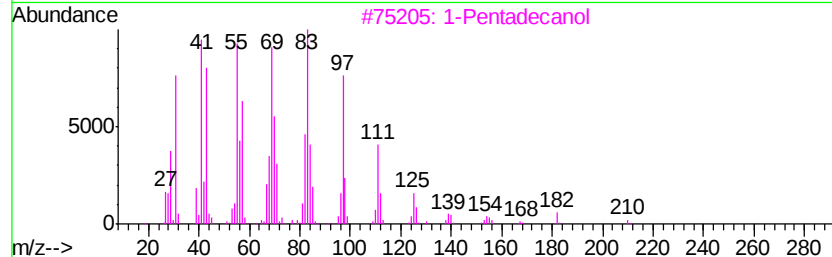
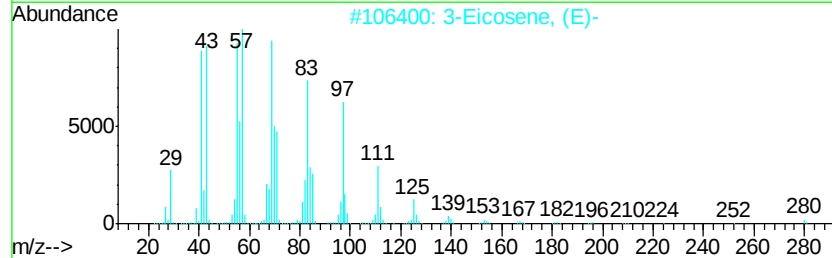
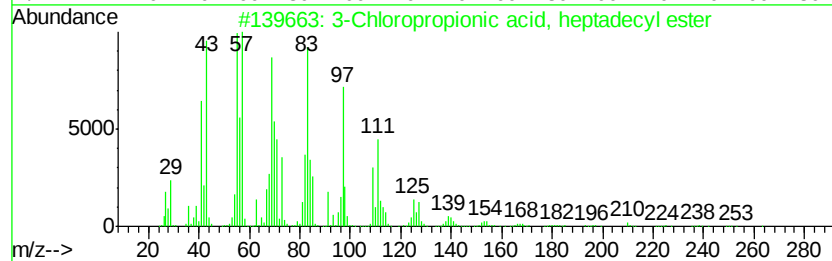
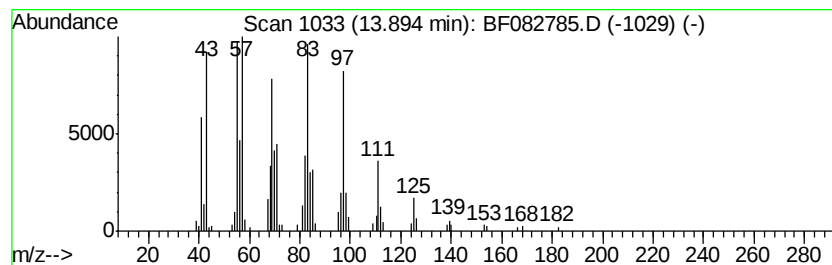
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.81 ng	679260	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3		1-Pentadecanol	228	C15H32O	000629-76-5	90
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		9-Eicosene, (E)-	280	C20H40	074685-29-3	87



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WABUT-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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-Penten-2-one, 4...	4.38	2.2	ng	145989	1	6.84	1337110	20.0
2-Pentanone, 4-hy...	5.04	37.2	ng	2486080	1	6.84	1337110	20.0
unknown6.61	6.61	68.1	ng	4552600	1	6.84	1337110	20.0
Hexadecanoic acid...	12.79	4.7	ng	467086	5	14.00	1995630	20.0
n-Butyl myristate	13.49	3.2	ng	321083	5	14.00	1995630	20.0
3-Chloropropionic...	13.89	6.8	ng	679260	5	14.00	1995630	20.0