

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
 Data File : BF077464.D
 Acq On : 26 Feb 2015 14:46
 Operator : TP/IZ
 Sample : G1384-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 41A-SW-022515

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	0.944	3	5	7	rVB	274485	384267	17.74%	2.236%
2	1.195	23	27	29	rVB	21775	41694	1.92%	0.243%
3	1.424	45	47	50	rVB	835835	836197	38.60%	4.867%
4	1.561	56	59	62	rVB	137856	207657	9.58%	1.209%
5	1.733	72	74	77	rBV	54135	65283	3.01%	0.380%
6	1.847	81	84	91	rBV2	85741	187709	8.66%	1.092%
7	5.047	362	364	369	rVB	225549	255736	11.80%	1.488%
8	5.562	406	409	411	rBV	1087590	1257302	58.03%	7.318%
9	6.819	517	519	522	rBV	1034271	1283489	59.24%	7.470%
10	6.979	530	533	535	rBV	1477572	1405718	64.88%	8.181%
11	7.265	556	558	560	rBV	351547	332585	15.35%	1.936%
12	7.459	572	575	577	rVB	816409	1044309	48.20%	6.078%
13	7.962	616	619	621	rVB	648017	816356	37.68%	4.751%
14	8.842	694	696	699	rBV	538075	463152	21.38%	2.696%
15	9.550	755	758	760	rBV	33116	29571	1.36%	0.172%
16	10.191	811	814	816	rBV	2012977	1762486	81.35%	10.258%
17	10.693	856	858	860	rVB	55975	44987	2.08%	0.262%
18	11.014	884	886	889	rVB	456261	536807	24.78%	3.124%
19	11.916	963	965	968	rBV	75745	78413	3.62%	0.456%
20	11.996	969	972	975	rBV	1151432	1112693	51.36%	6.476%
21	12.865	1045	1048	1050	rBV	534713	571614	26.38%	3.327%
22	14.865	1220	1223	1225	rBV	1671218	2166521	100.00%	12.609%
23	15.494	1275	1278	1283	rBV	152344	249564	11.52%	1.452%
24	16.043	1323	1326	1334	rBV	238262	327043	15.10%	1.903%
25	16.168	1334	1337	1339	rBV	607318	701626	32.38%	4.084%
26	16.888	1397	1400	1406	rBV4	23993	42775	1.97%	0.249%
27	17.300	1433	1436	1438	rBV3	16006	28567	1.32%	0.166%
28	17.380	1440	1443	1446	rVV	68655	93783	4.33%	0.546%
29	17.700	1469	1471	1475	rBV4	10746	28817	1.33%	0.168%
30	17.963	1491	1494	1497	rBV	586367	714779	32.99%	4.160%
31	18.111	1505	1507	1510	rBV4	13021	33931	1.57%	0.197%
32	18.603	1548	1550	1554	rBV3	38438	76345	3.52%	0.444%

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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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

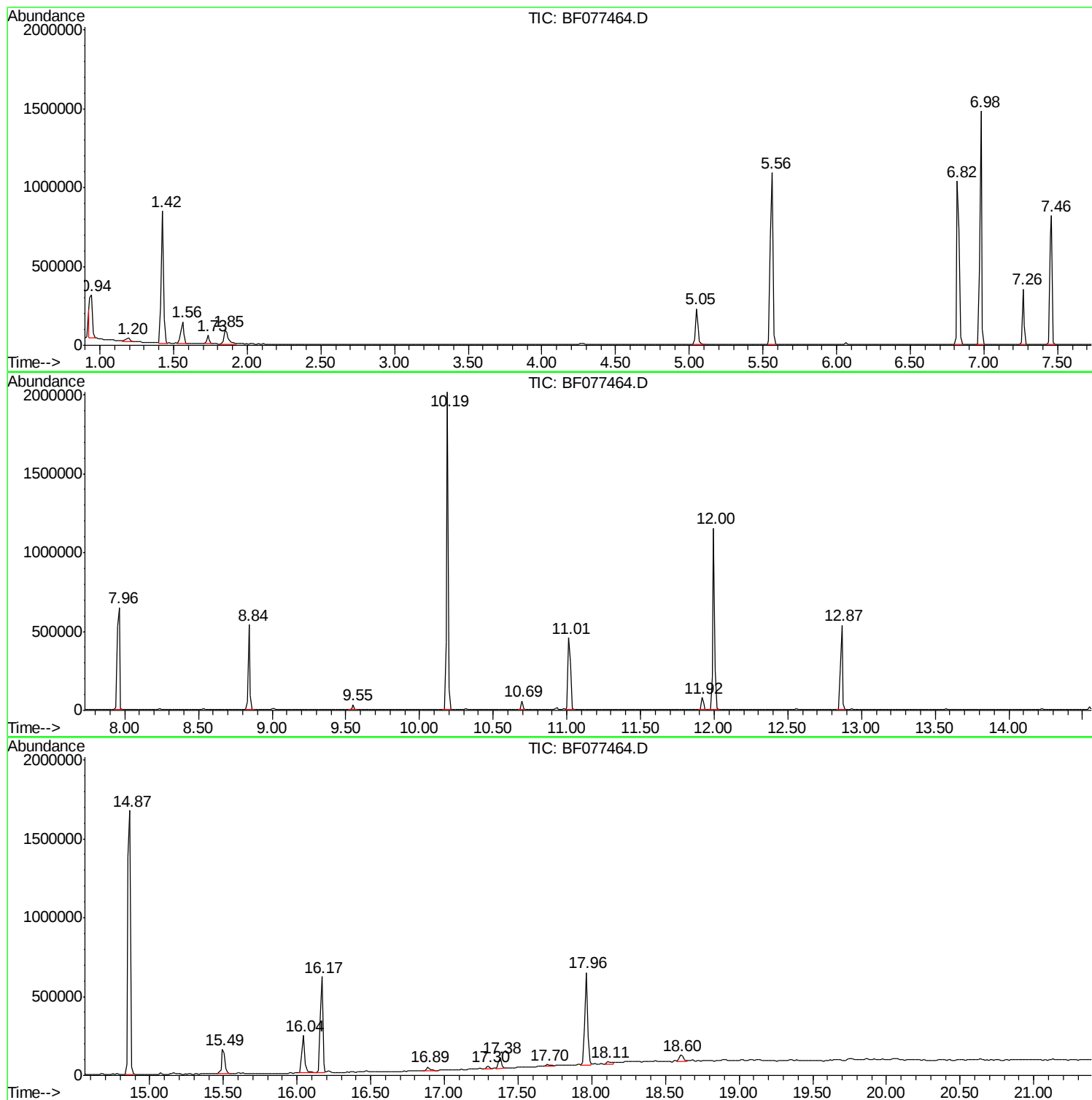
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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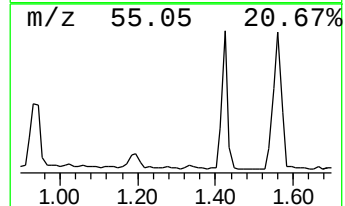
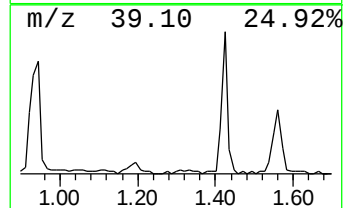
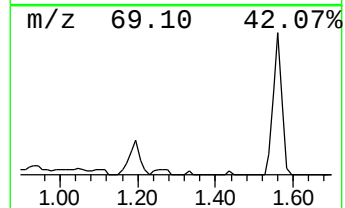
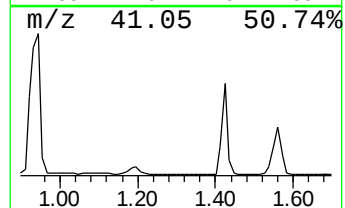
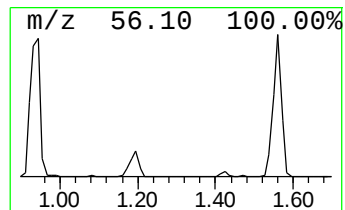
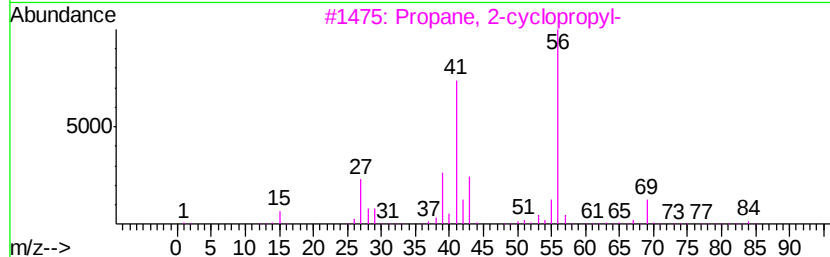
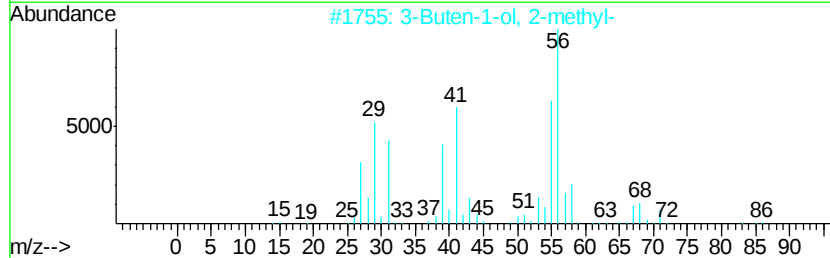
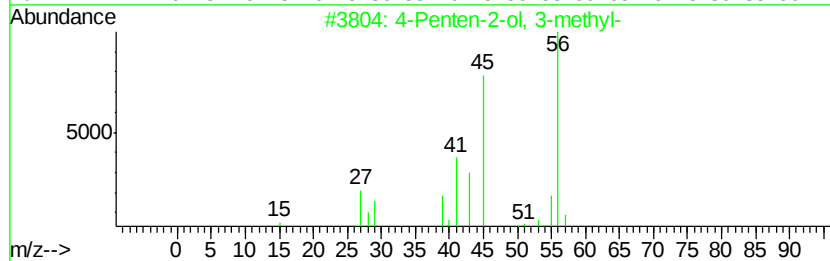
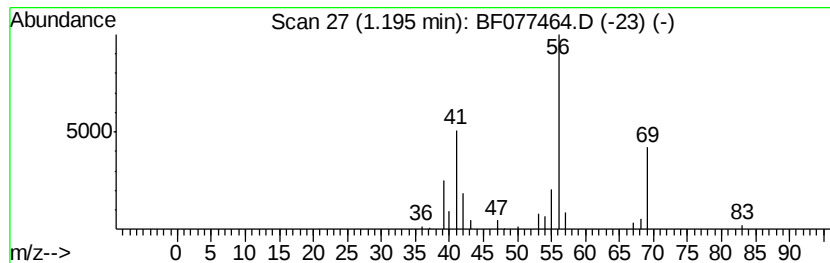
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown1.20 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.20	2.51 ng	41694	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-ol, 3-methyl-	100	C6H12O	001569-59-1	38
2		3-Buten-1-ol, 2-methyl-	86	C5H10O	004516-90-9	9
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9
4		1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	9
5		3-Hexen-1-ol	100	C6H12O	000544-12-7	9



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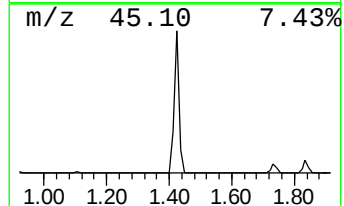
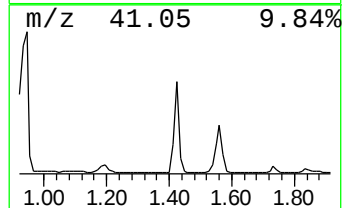
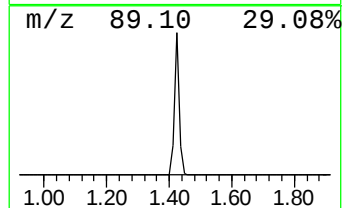
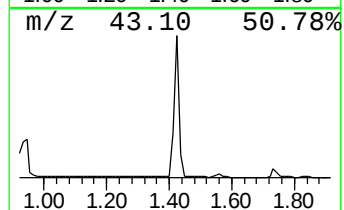
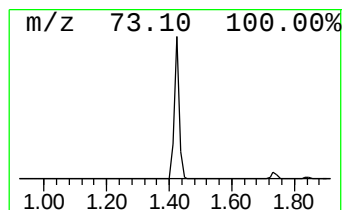
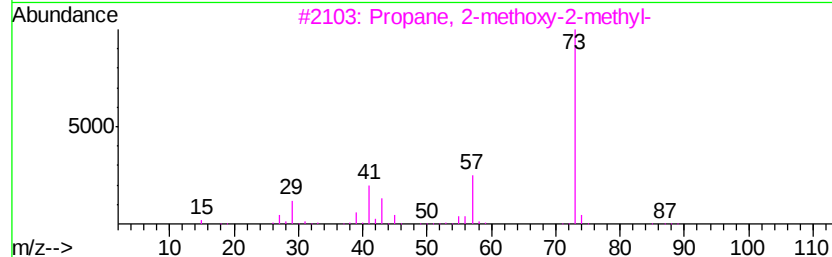
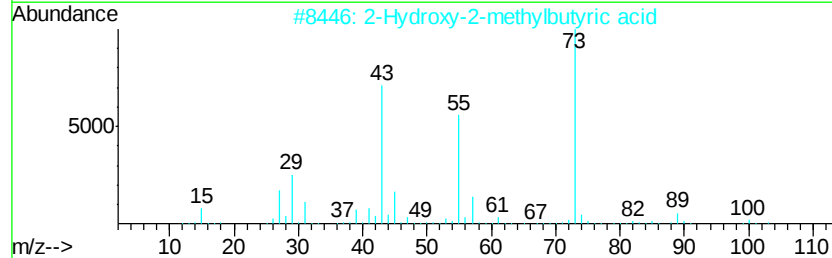
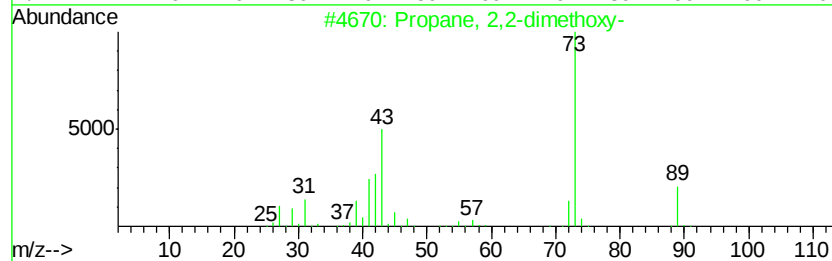
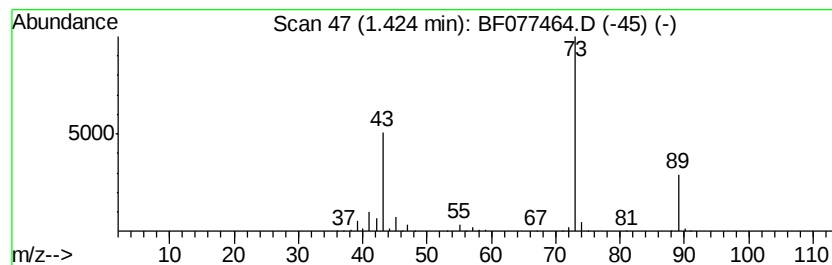
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.42	50.28 ng	836197	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	7
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	7



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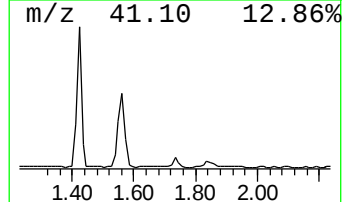
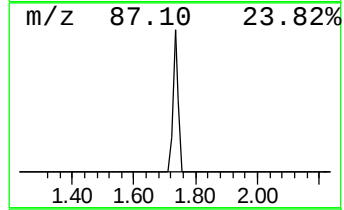
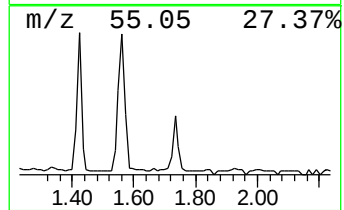
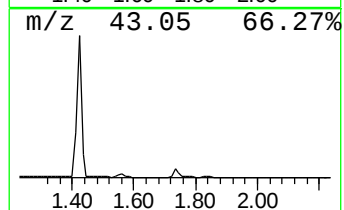
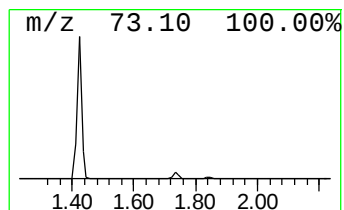
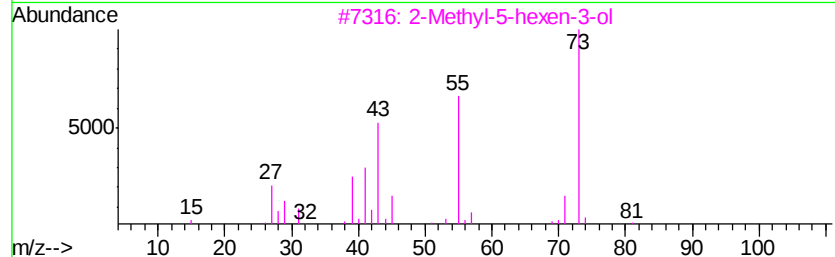
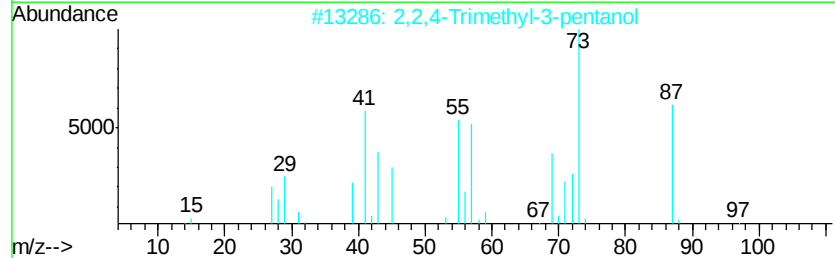
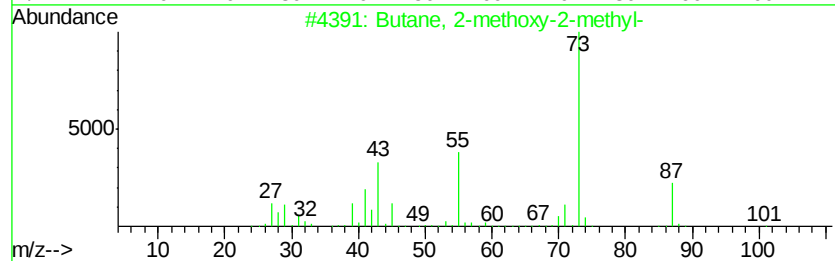
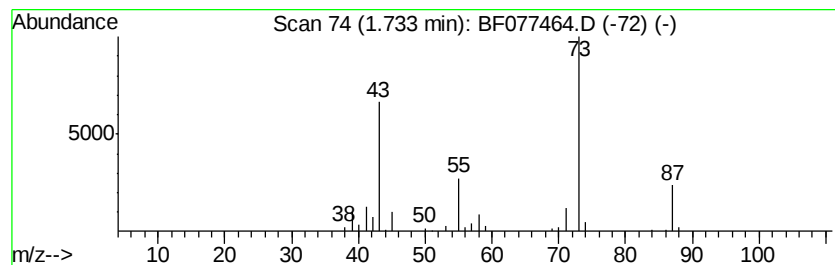
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.73	3.93 ng	65283	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4		3,4-Hexanediol, 2,5-dimethyl-	146	C8H18O2	022607-11-0	12
5		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12



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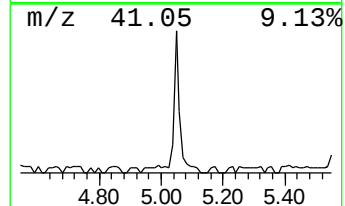
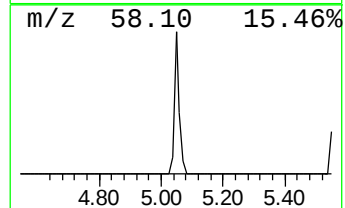
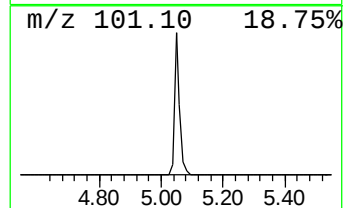
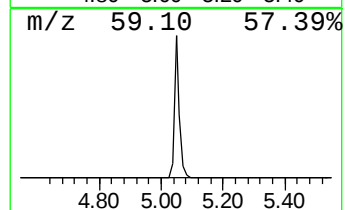
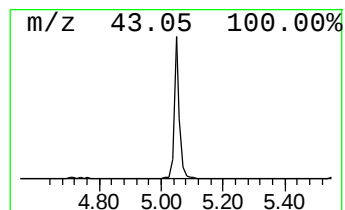
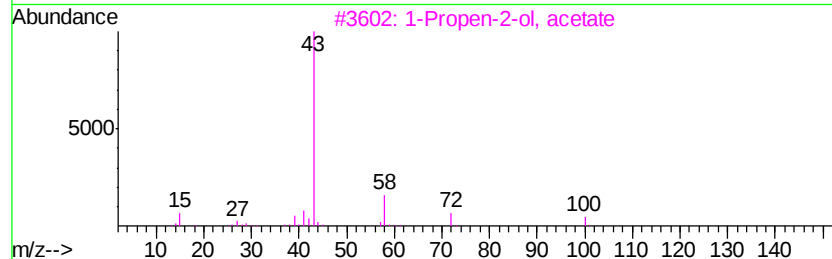
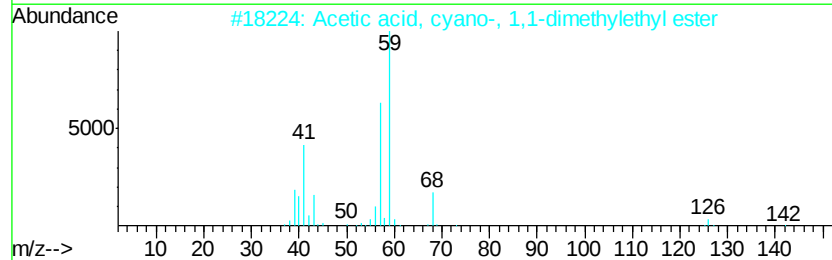
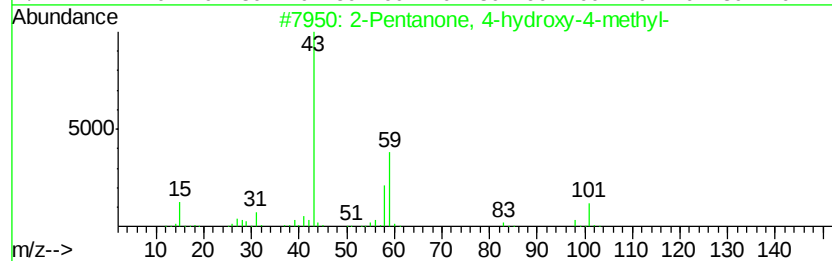
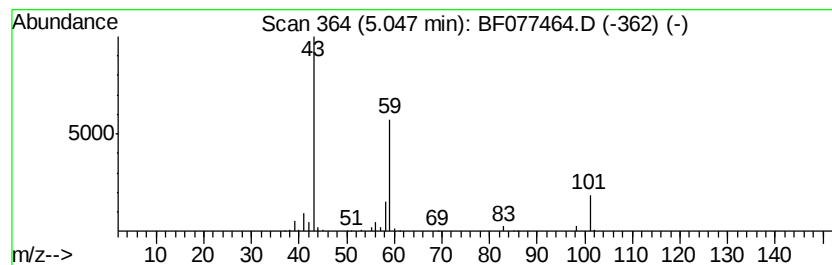
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.38 ng	255736	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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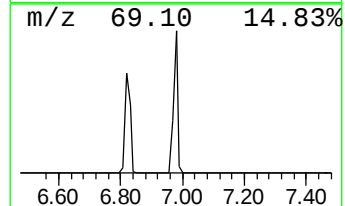
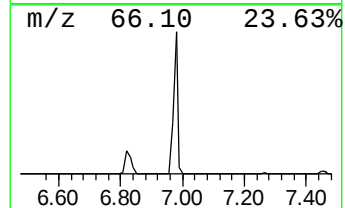
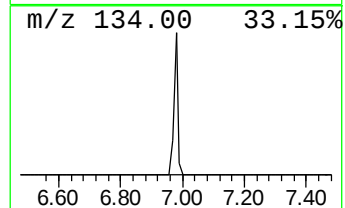
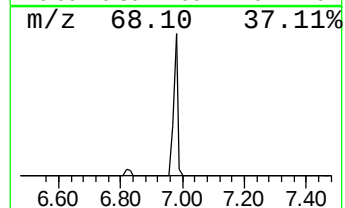
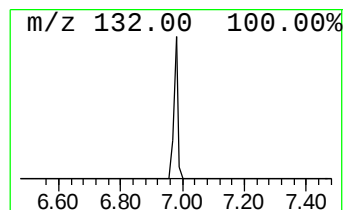
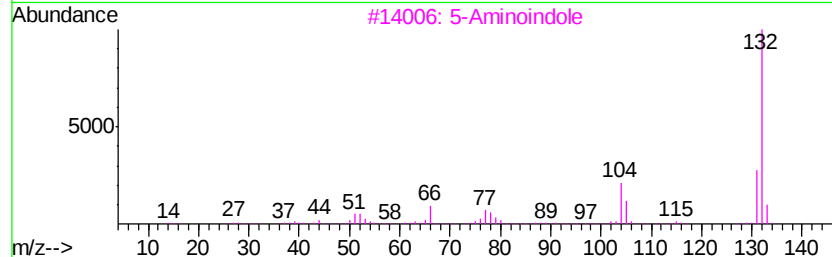
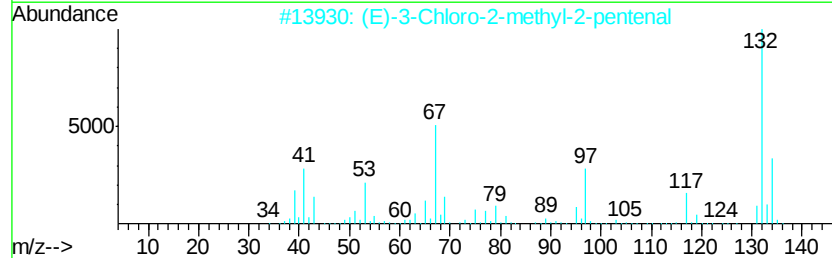
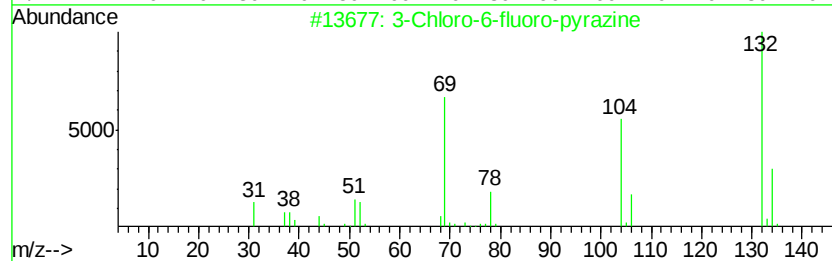
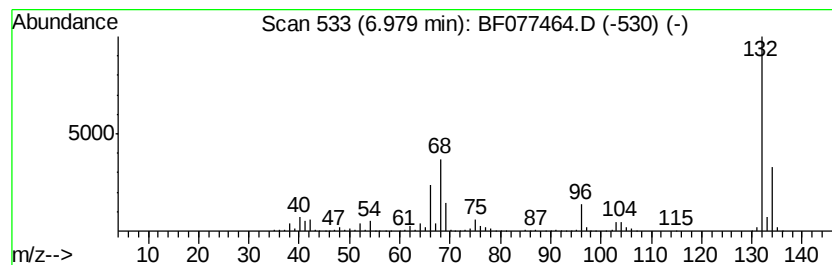
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 unknown6.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	84.53 ng	1405720	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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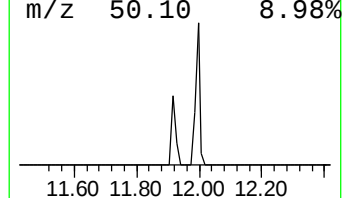
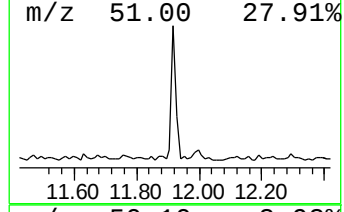
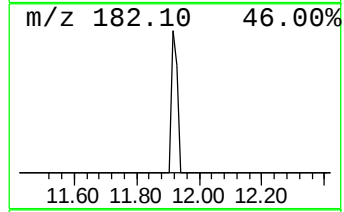
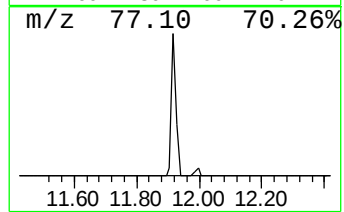
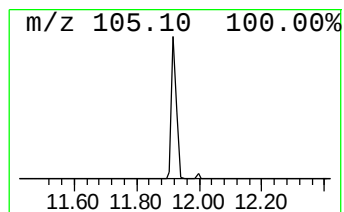
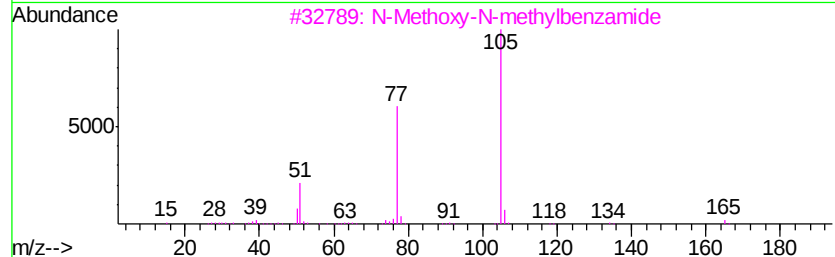
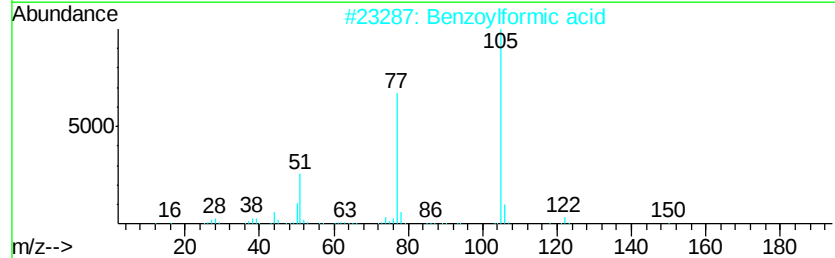
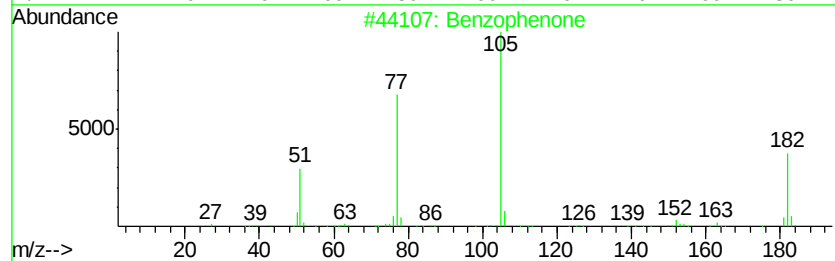
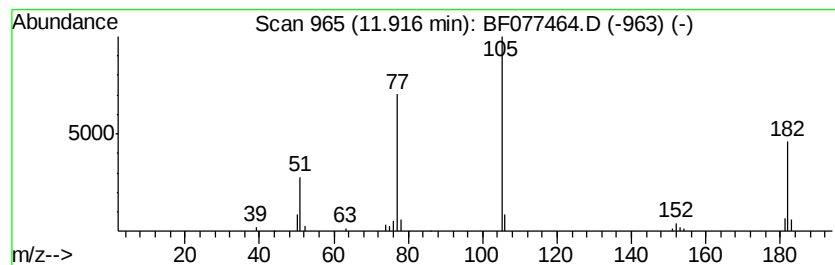
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.92 ng	78413	Acenaphthene-d10	11.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	97
2		Benzoylformic acid	150	C8H6O3	000611-73-4	47
3		N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5		Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
Data File : BF077464.D
Acq On : 26 Feb 2015 14:46
Operator : TP/IZ
Sample : G1384-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
41A-SW-022515

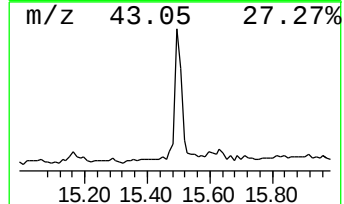
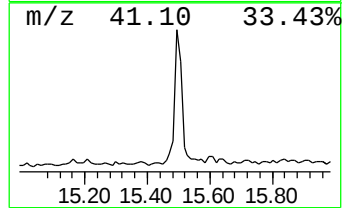
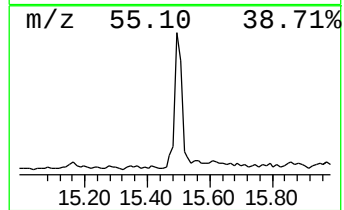
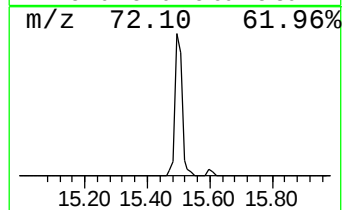
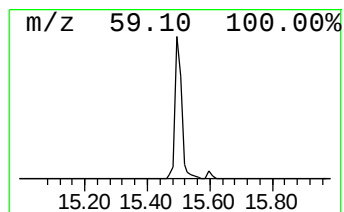
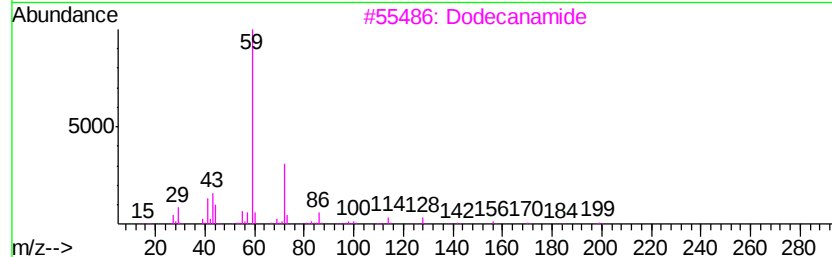
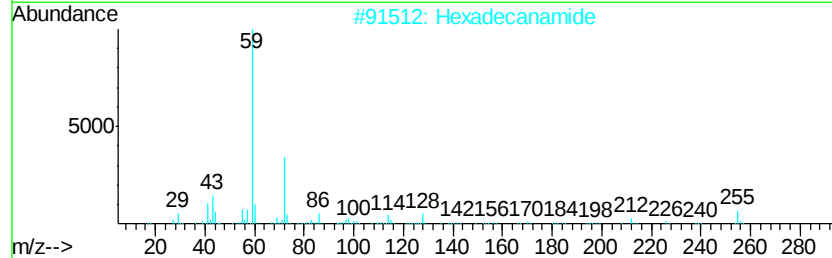
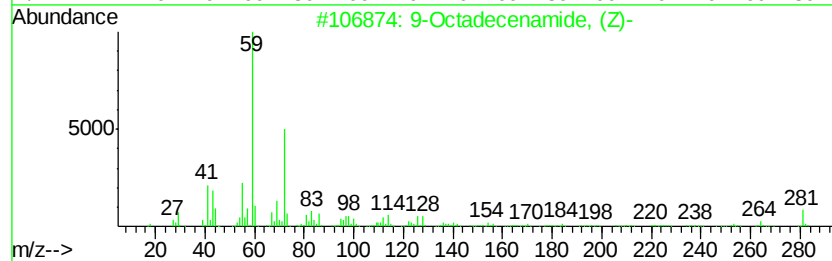
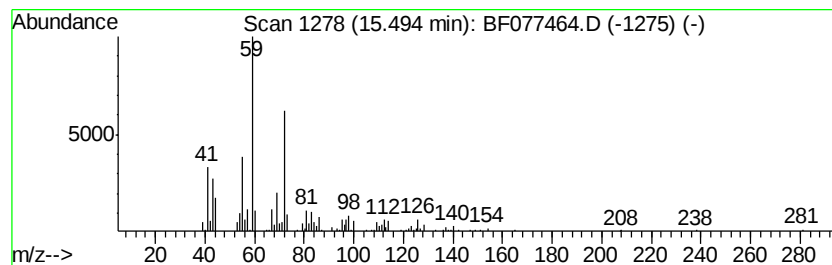
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.49	7.11 ng	249564	Chrysene-d12	16.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Dodecanamide	199	C12H25NO	001120-16-7	64
4		Nonanamide	157	C9H19NO	001120-07-6	59
5		Silane, octyl-	144	C8H20Si	000871-92-1	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
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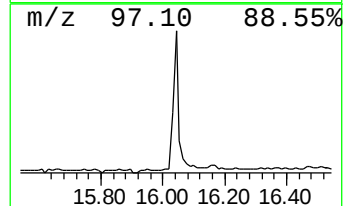
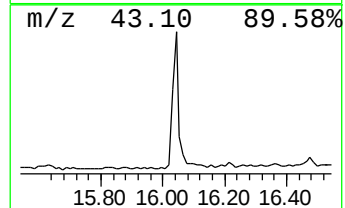
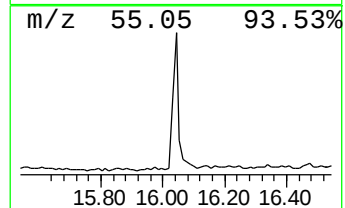
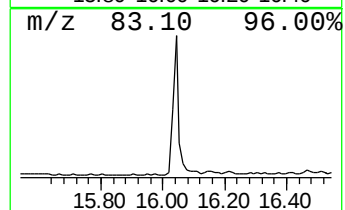
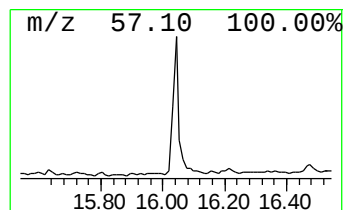
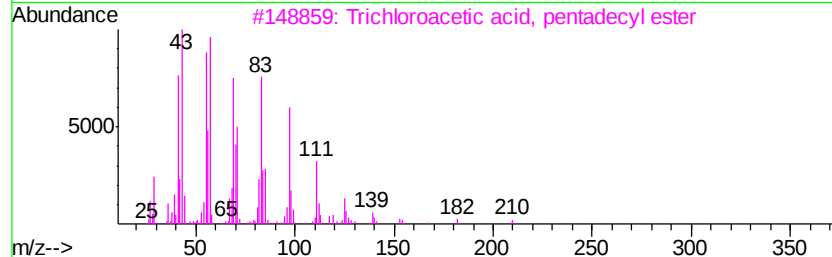
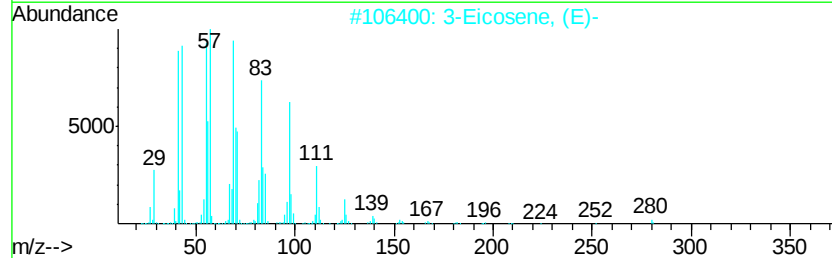
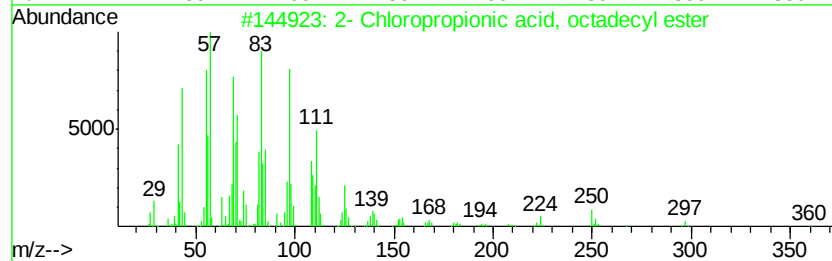
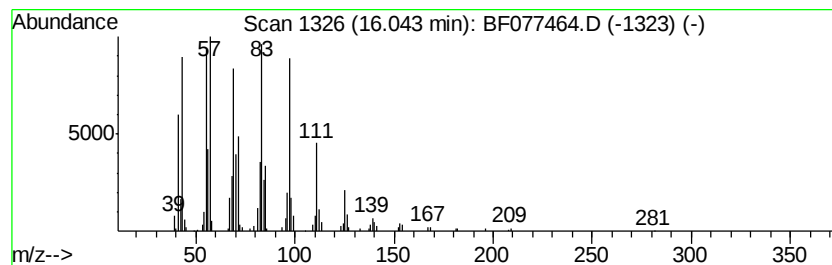
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2- Chloropropionic acid, oc... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	9.32 ng	327043	Chrysene-d12	16.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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Data File : BF077464.D
Acq On : 26 Feb 2015 14:46
Operator : TP/IZ
Sample : G1384-03
Misc :
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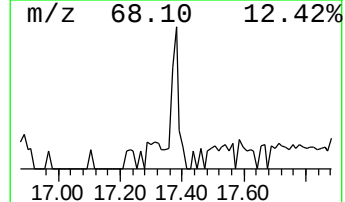
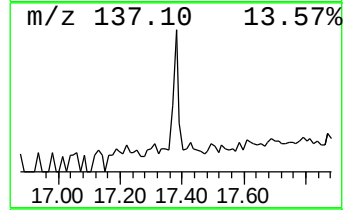
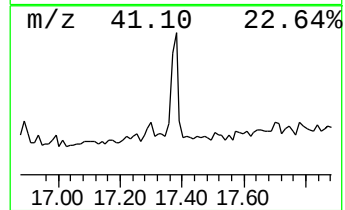
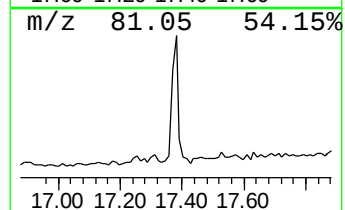
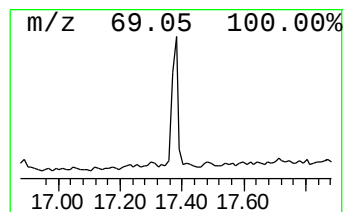
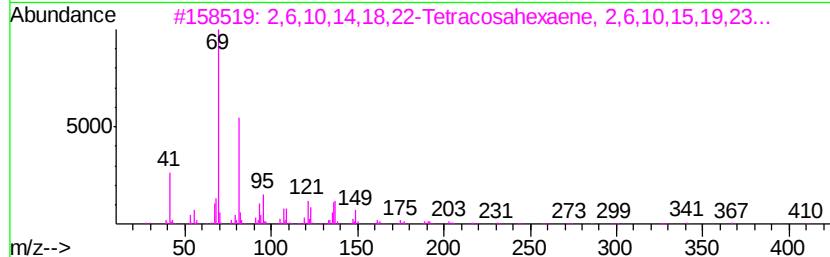
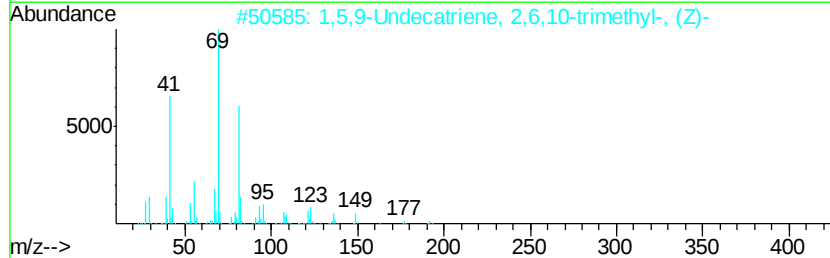
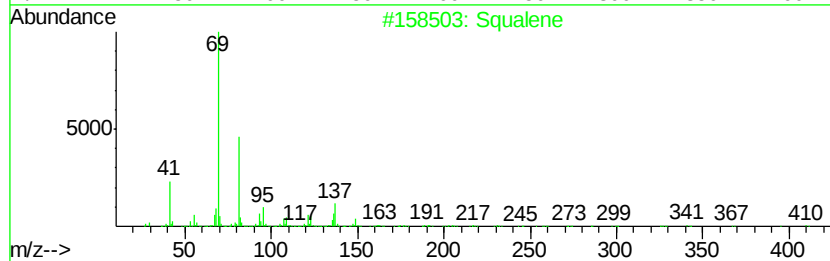
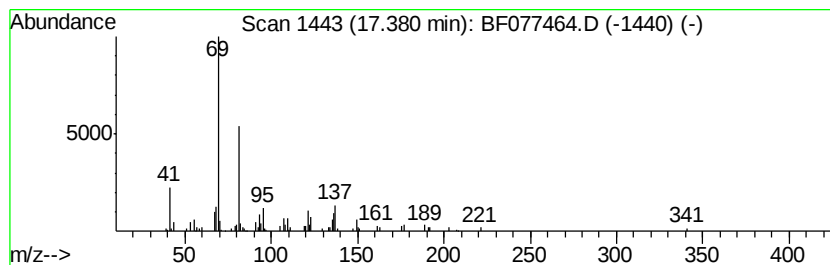
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.38	2.62 ng	93783	Perylene-d12	17.96
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	91
3	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
4	Docosa-2,6,10,14,18-pentaen-22-a...	384 C27H44O	1000163-04-7	91
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	000106-28-5	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022615\
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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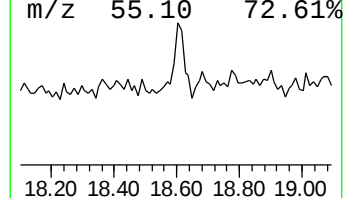
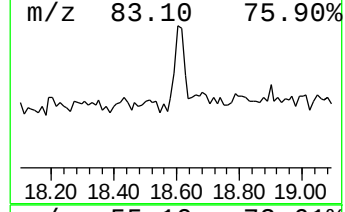
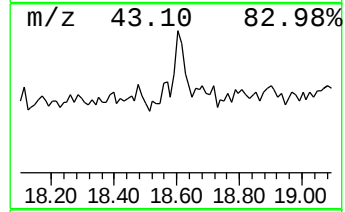
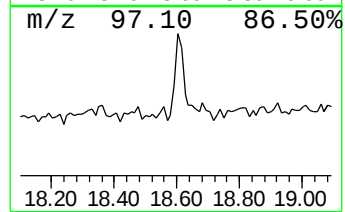
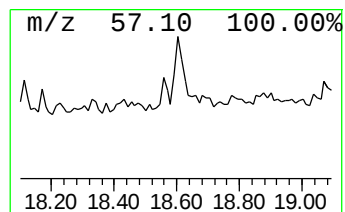
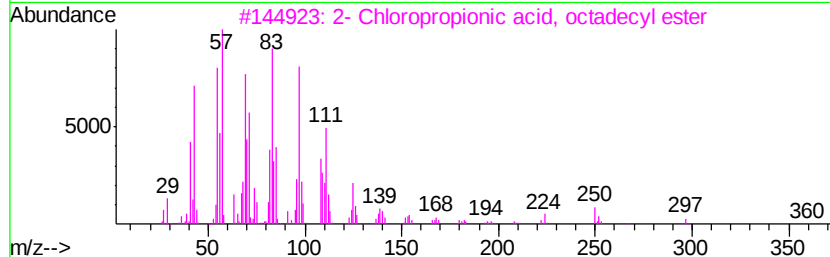
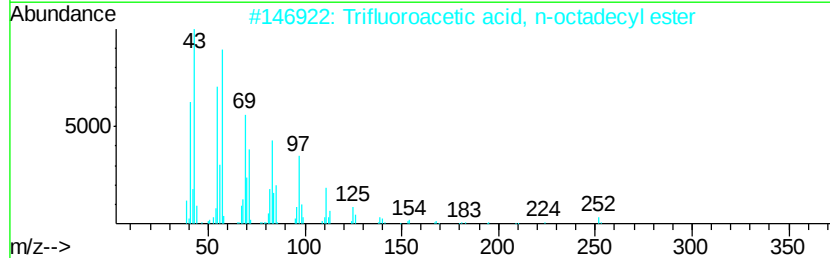
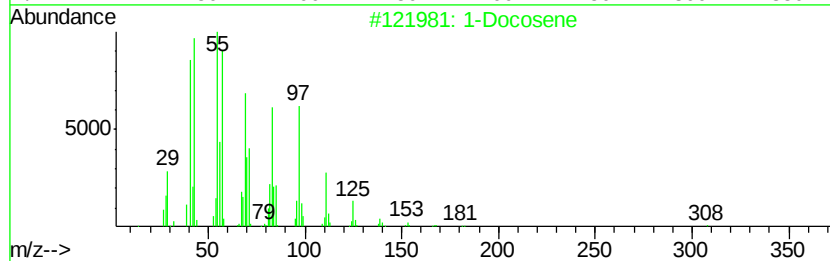
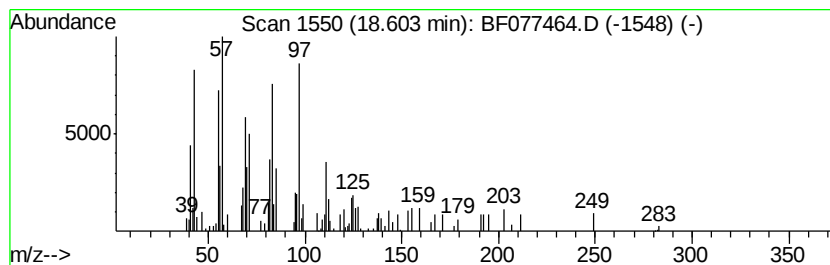
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Docosene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.60	2.14 ng	76345	Perylene-d12	17.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	80
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	74
3		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	74
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	72
5		11-Tricosene	322	C23H46	052078-56-5	64



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Sample : G1384-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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Propane, 2,2-dime...	1.42	50.3	ng	836197	1	7.26	332585	20.0
Butane, 2-methoxy...	1.73	3.9	ng	65283	1	7.26	332585	20.0
2-Pentanone, 4-hy...	5.05	15.4	ng	255736	1	7.26	332585	20.0
unknown6.98	6.98	84.5	ng	1405720	1	7.26	332585	20.0
Benzophenone	11.92	2.9	ng	78413	3	11.01	536807	20.0
9-Octadecenamide, ...	15.49	7.1	ng	249564	5	16.17	701626	20.0
2-Chloropropioni...	16.04	9.3	ng	327043	5	16.17	701626	20.0
Squalene	17.38	2.6	ng	93783	6	17.96	714779	20.0
1-Docosene	18.60	2.1	ng	76345	6	17.96	714779	20.0