

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031815\
 Data File : BF077826.D
 Acq On : 19 Mar 2015 7:35
 Operator : TP/IZ
 Sample : G1535-03 2X
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP3B-6B-7B-10(6-15)

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-BF031115.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	1.310	34	37	39	rBV	2525490	2772934	100.00%	28.534%
2	1.435	45	48	50	rBV	56517	72591	2.62%	0.747%
3	1.595	60	62	65	rVB	30168	40005	1.44%	0.412%
4	1.790	77	79	86	rVB	91489	126323	4.56%	1.300%
5	4.922	352	353	363	rVB	54524	75103	2.71%	0.773%
6	5.413	391	396	398	rVB2	31796	65197	2.35%	0.671%
7	5.459	398	400	403	rBV	438955	470328	16.96%	4.840%
8	6.579	493	498	499	rBV4	24257	39652	1.43%	0.408%
9	6.670	504	506	510	rBV	36574	34106	1.23%	0.351%
10	6.739	510	512	514	rBV	490030	474267	17.10%	4.880%
11	6.876	522	524	527	rBV	573874	522610	18.85%	5.378%
12	6.945	528	530	532	rBV	87251	77999	2.81%	0.803%
13	7.162	546	549	551	rBV	257167	231243	8.34%	2.379%
14	7.345	563	565	567	rBV	415271	398345	14.37%	4.099%
15	7.562	582	584	586	rBV	36942	39645	1.43%	0.408%
16	7.859	605	610	612	rBV	309884	345924	12.48%	3.560%
17	8.739	685	687	689	rBV	310460	286509	10.33%	2.948%
18	10.088	803	805	807	rBV	474122	476022	17.17%	4.898%
19	10.911	875	877	879	rBV	314535	303258	10.94%	3.121%
20	11.894	960	963	965	rBV	218690	297193	10.72%	3.058%
21	12.751	1035	1038	1040	rBV	342511	344166	12.41%	3.541%
22	14.122	1154	1158	1160	rBV	22209	31447	1.13%	0.324%
23	14.248	1167	1169	1172	rBV	49997	54876	1.98%	0.565%
24	14.534	1192	1194	1196	rBV	51883	60546	2.18%	0.623%
25	14.740	1210	1212	1215	rBV	482291	538984	19.44%	5.546%
26	15.345	1262	1265	1270	rBV6	9770	34973	1.26%	0.360%
27	15.677	1289	1294	1295	rBV5	11700	33133	1.19%	0.341%
28	15.780	1299	1303	1304	rBV3	14498	30261	1.09%	0.311%
29	15.928	1314	1316	1322	rBV	66166	89307	3.22%	0.919%
30	16.031	1322	1325	1327	rBV	407460	559954	20.19%	5.762%
31	16.694	1381	1383	1385	rBV2	22822	28986	1.05%	0.298%
32	16.763	1385	1389	1394	rVV3	54642	140741	5.08%	1.448%
33	17.220	1427	1429	1430	rBV	34765	51558	1.86%	0.531%
34	17.334	1437	1439	1441	rBV	37525	54536	1.97%	0.561%

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ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
COMP3B-6B-7B-10(6-15)

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-BF031115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.780	1476	1478	1483	rBV	330920	515436	18.59%	5.304%
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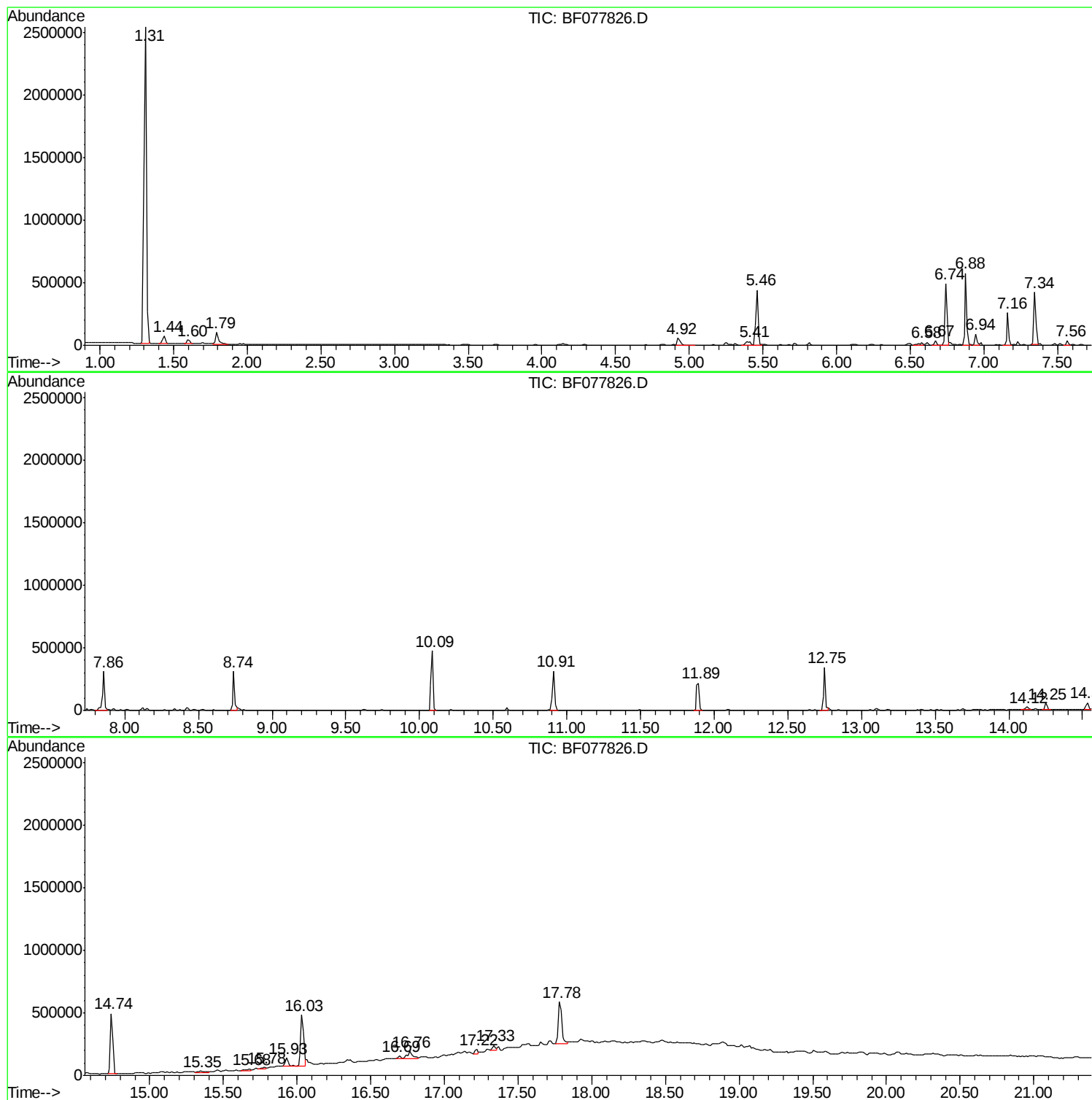
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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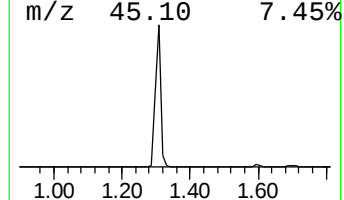
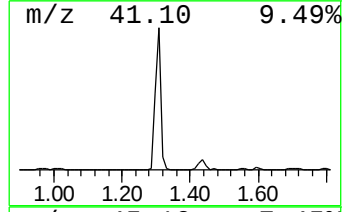
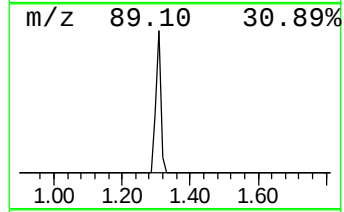
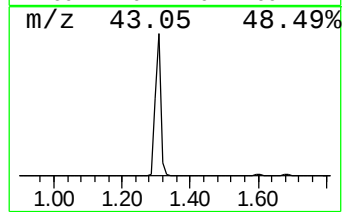
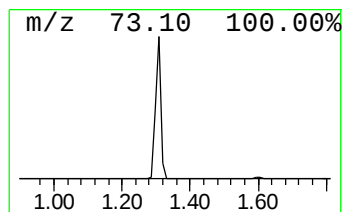
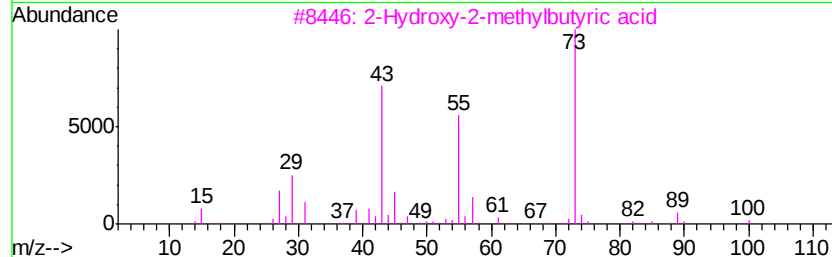
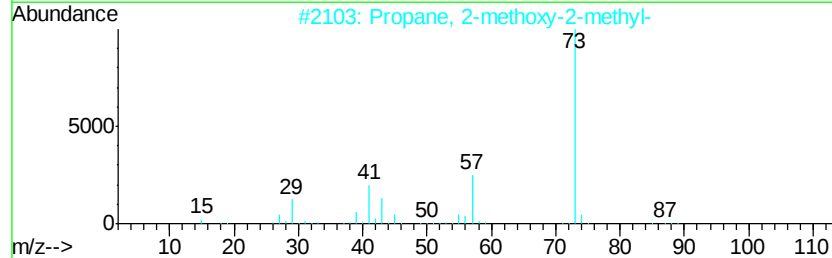
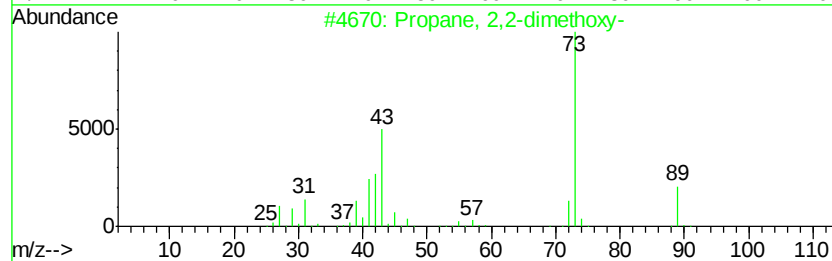
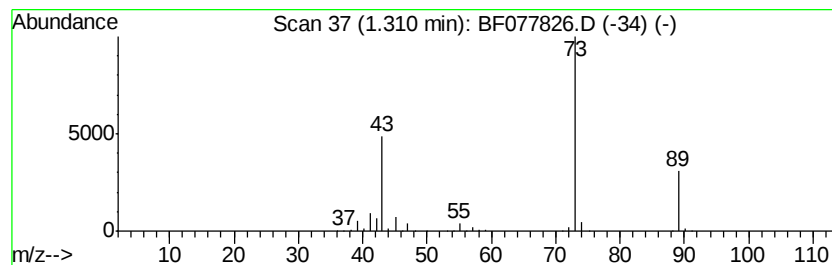
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown1.31 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.31	239.83 ng	2772930	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	5
5		1,3,5-Trioxane	90	C3H6O3	000110-88-3	4



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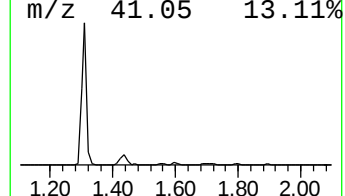
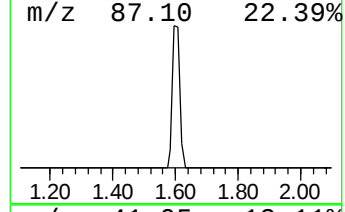
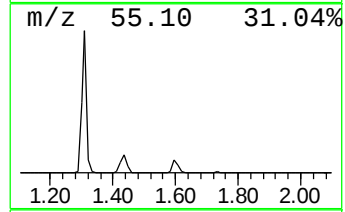
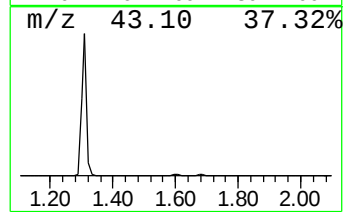
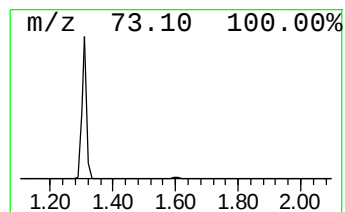
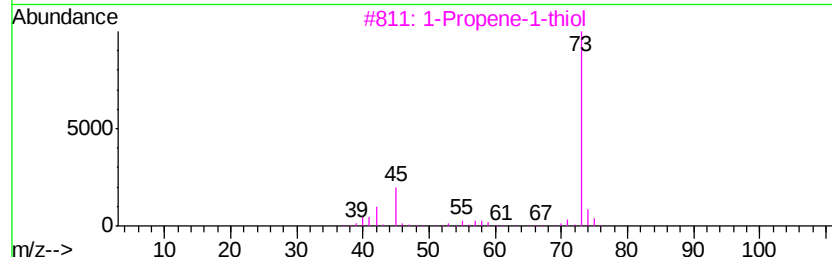
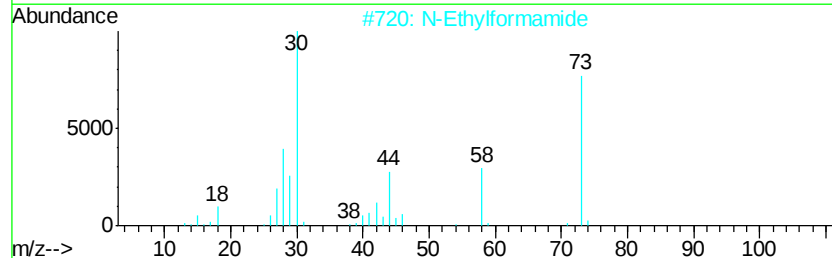
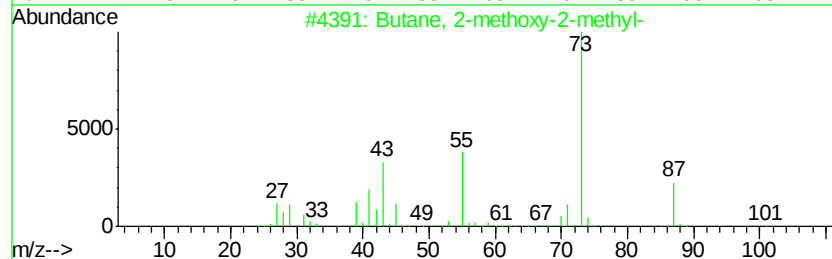
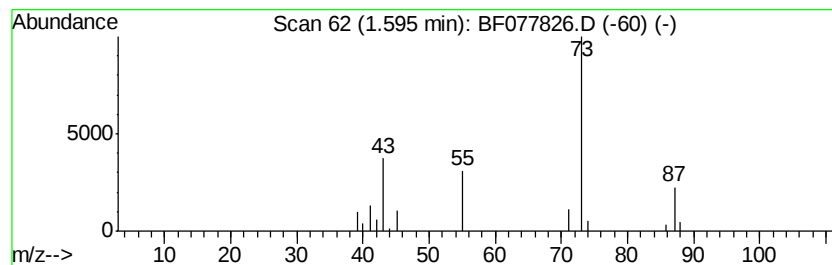
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.60	3.46 ng	40005	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		N-Ethylformamide	73	C3H7NO	000627-45-2	5
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	5
4		1,4-Butanediamine	88	C4H12N2	000110-60-1	5
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



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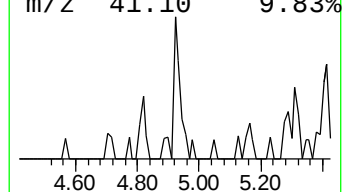
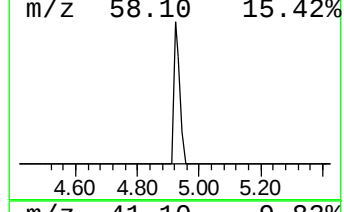
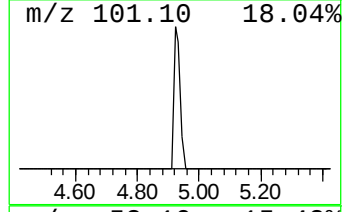
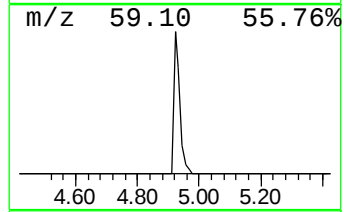
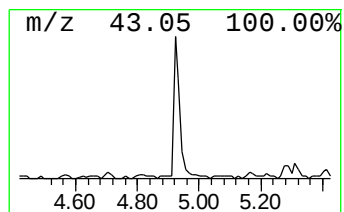
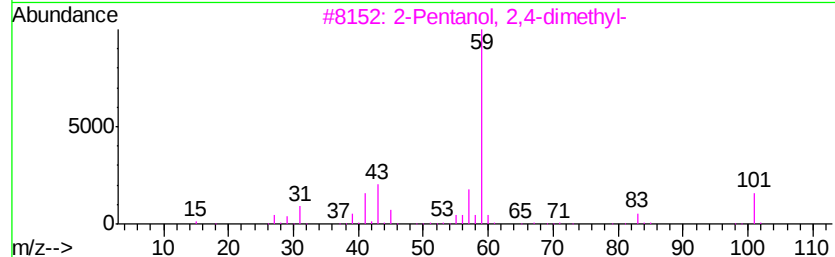
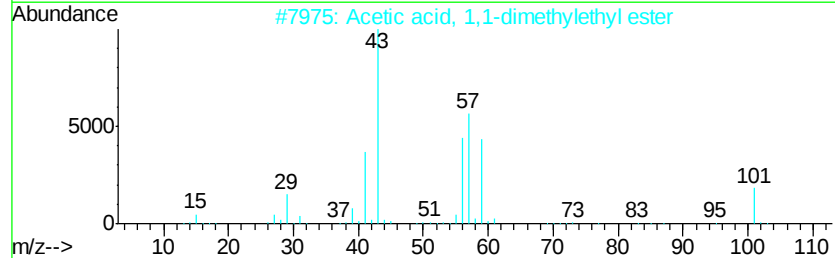
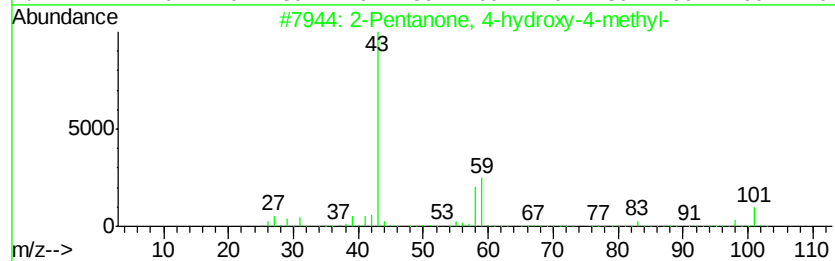
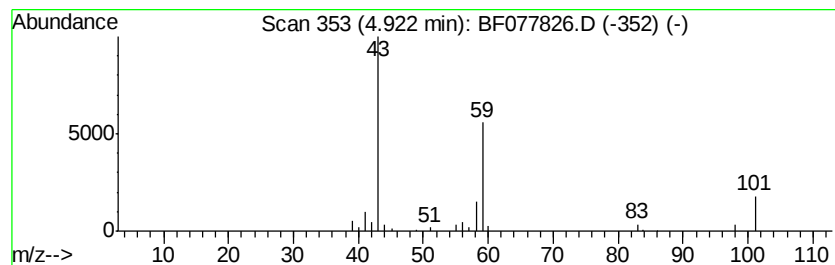
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.50 ng	75103	1,4-Dichlorobenzene-d4	7.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38	
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38	
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	12	



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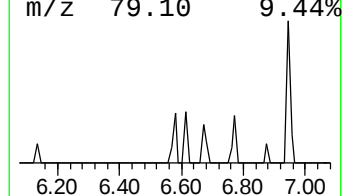
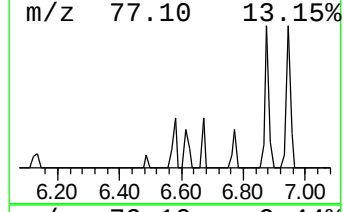
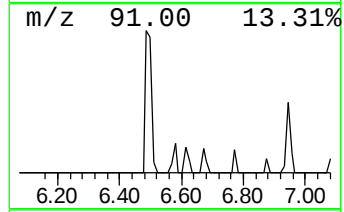
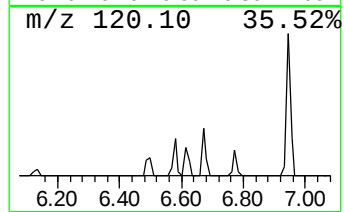
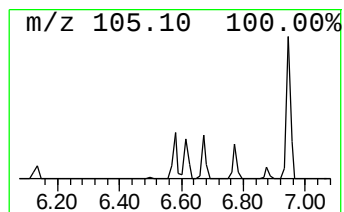
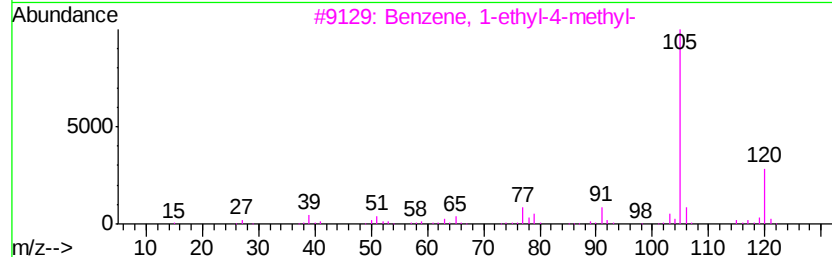
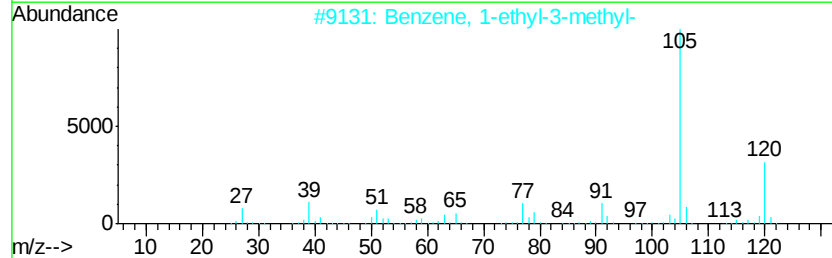
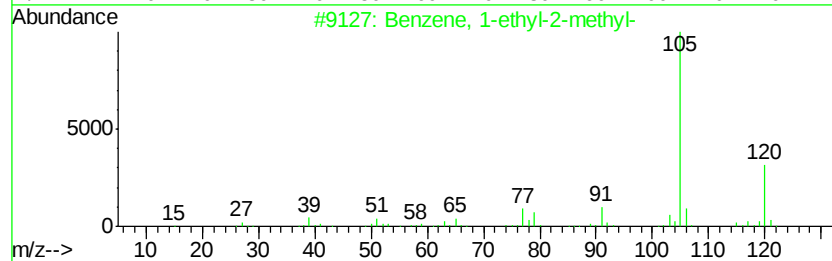
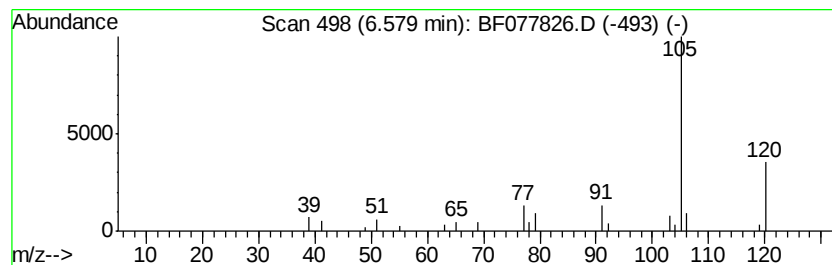
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	3.43 ng	39652	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
4		Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	72
5		1-Hexene, 6-phenyl-4-(1-phenylet...	280	C20H24O	1000190-48-6	53



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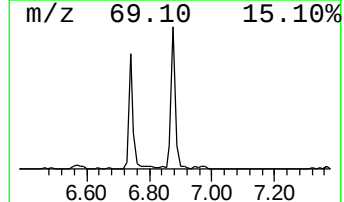
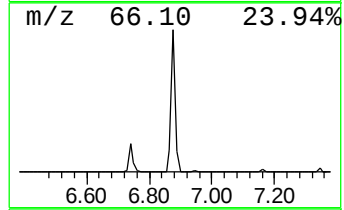
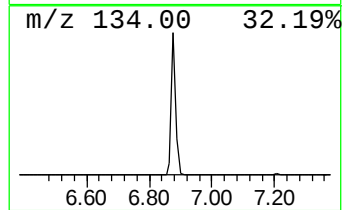
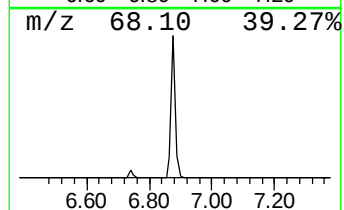
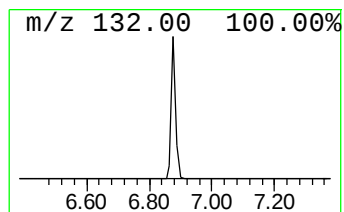
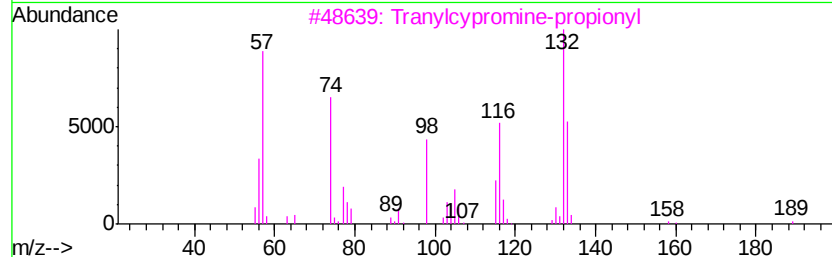
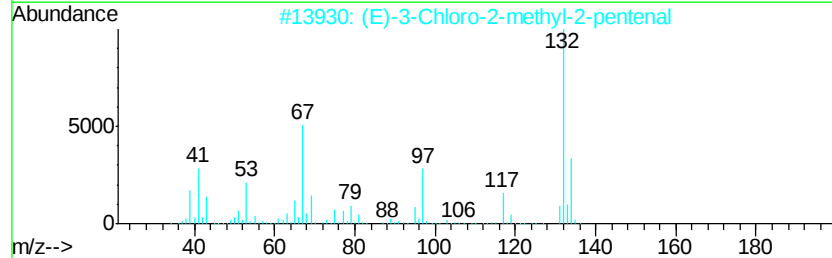
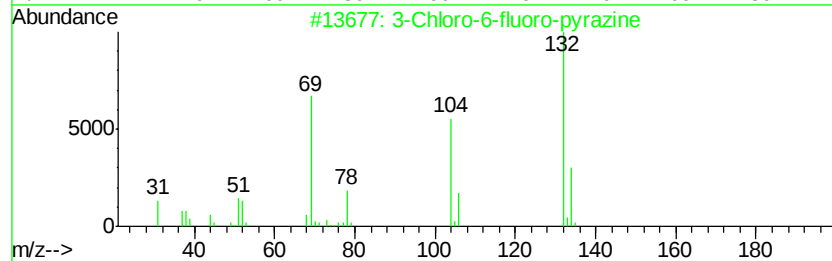
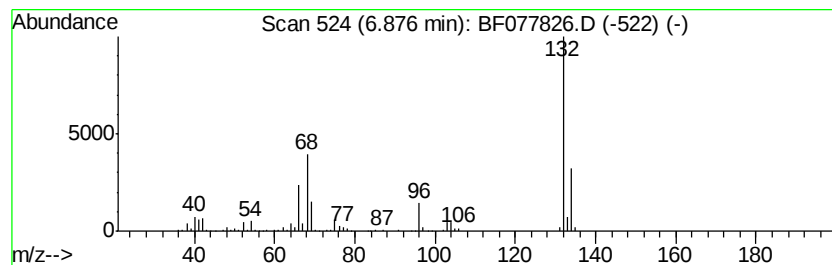
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Peak Number 8 unknown6.88 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	45.20 ng	522610	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031815\
Data File : BF077826.D
Acq On : 19 Mar 2015 7:35
Operator : TP/IZ
Sample : G1535-03 2X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP3B-6B-7B-10(6-15)

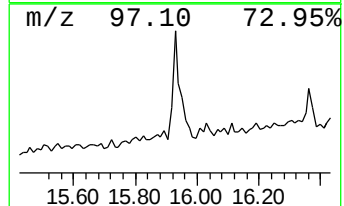
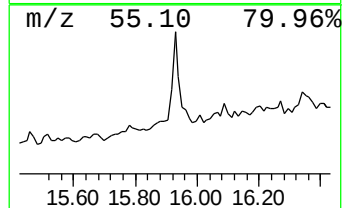
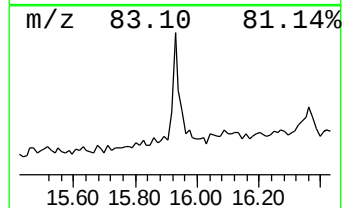
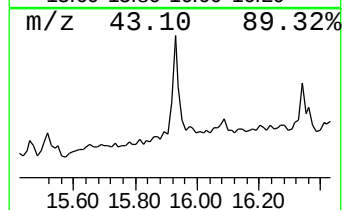
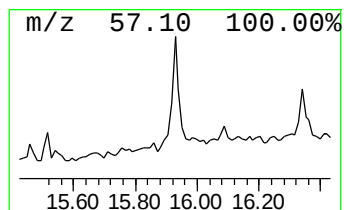
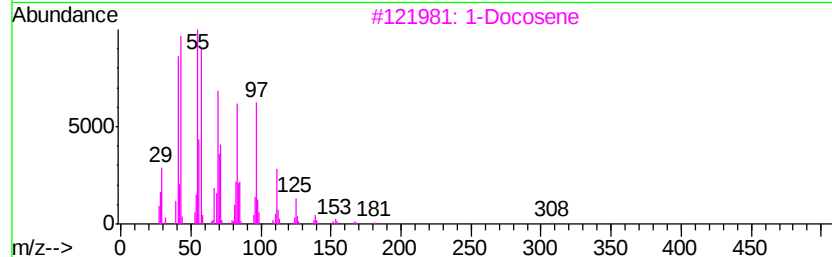
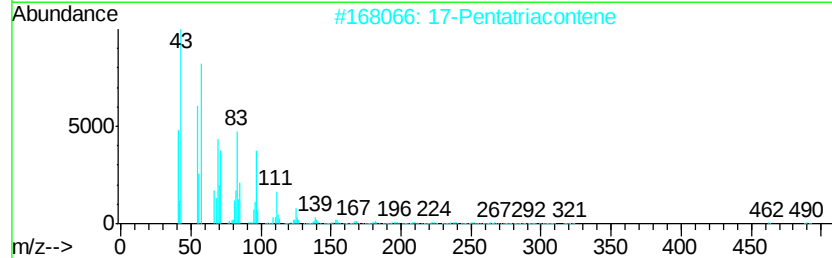
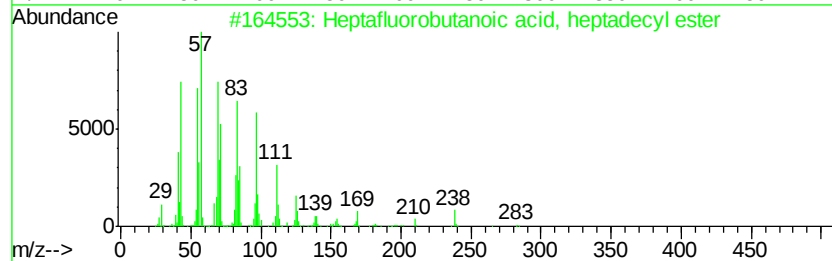
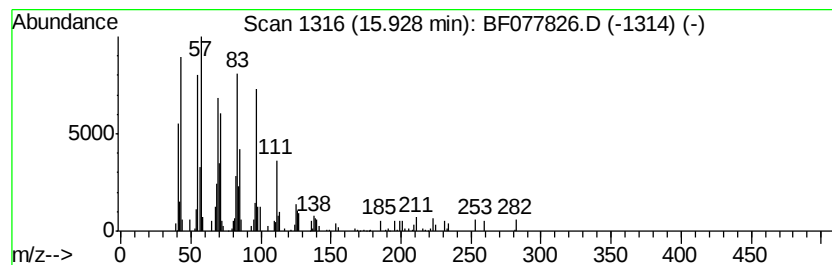
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptafluorobutanoic acid, h... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.19 ng	89307	Chrysene-d12	16.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
2			17-Pentatriacontene	491	C35H70	006971-40-0	74
3			1-Docosene	308	C22H44	001599-67-3	68
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	64
5			1-Nonadecene	266	C19H38	018435-45-5	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031815\
Data File : BF077826.D
Acq On : 19 Mar 2015 7:35
Operator : TP/IZ
Sample : G1535-03 2X
Misc :
ALS Vial : 35 Sample Multiplier: 1

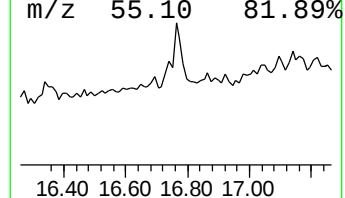
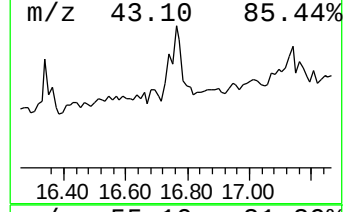
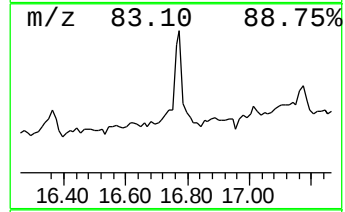
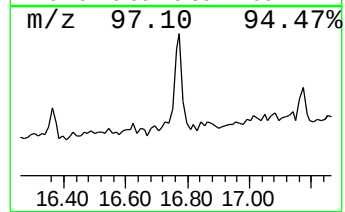
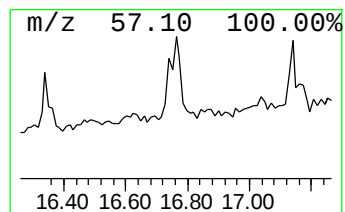
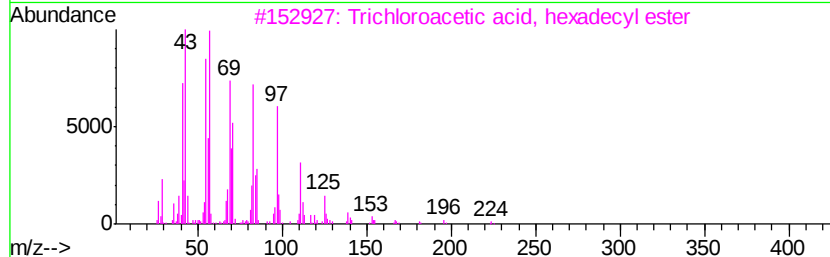
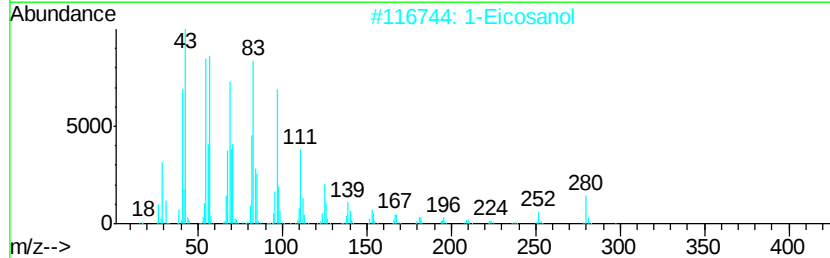
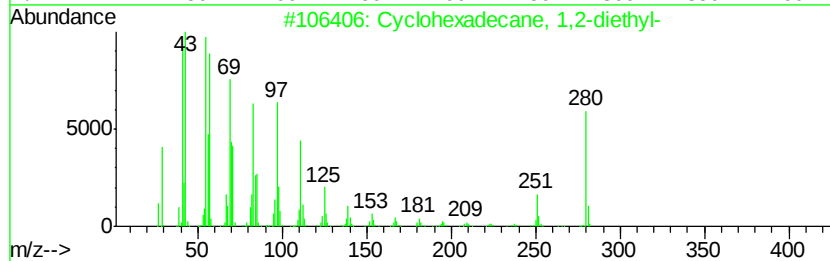
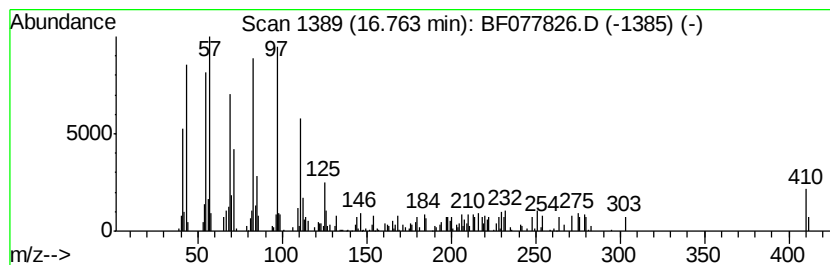
Instrument :
BNA_F
ClientSampleId :
COMP3B-6B-7B-10(6-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Cyclohexadecane, 1,2-diethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.76	5.03 ng	140741	Chrysene-d12	16.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	74
2	1-Eicosanol	298	C20H42O	000629-96-9	59
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	59
4	Cycloeicosane	280	C20H40	000296-56-0	58
5	1-Eicosene	280	C20H40	003452-07-1	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031815\
Data File : BF077826.D
Acq On : 19 Mar 2015 7:35
Operator : TP/IZ
Sample : G1535-03 2X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP3B-6B-7B-10(6-15)

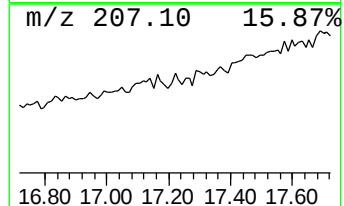
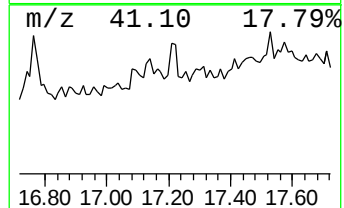
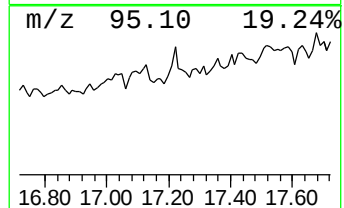
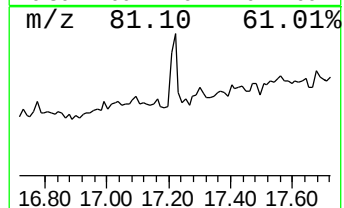
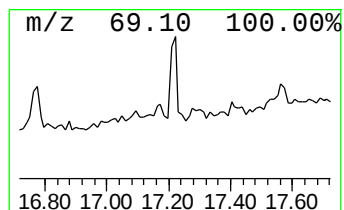
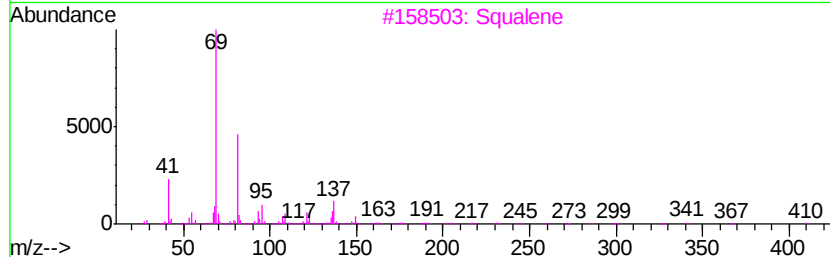
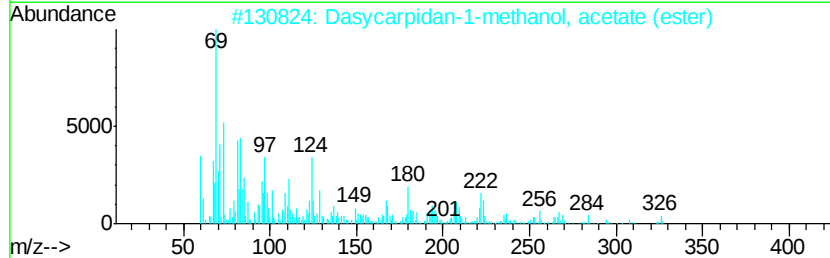
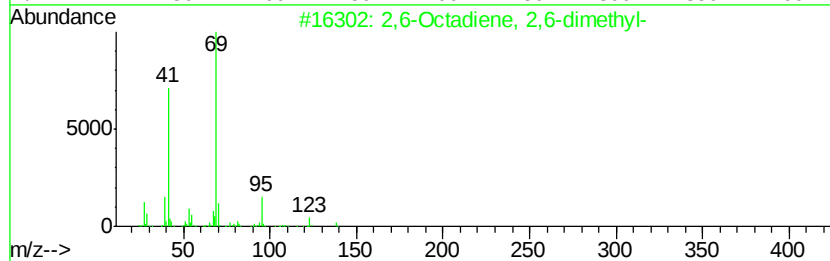
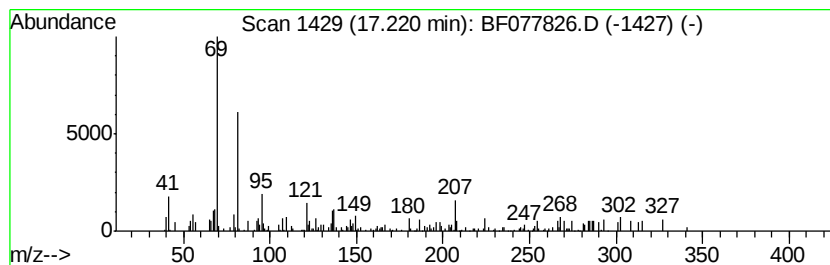
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,6-Octadiene, 2,6-dimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.22	2.00 ng	51558	Perylene-d12	17.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	58
2		Dasycarpidan-1-methanol, acetate...	326	C20H26N2O2	055724-48-6	53
3		Squalene	410	C30H50	007683-64-9	52
4		3,7,11,15-Tetramethylhexadeca-1,...	290	C20H34O	068931-30-6	50
5		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031815\
Data File : BF077826.D
Acq On : 19 Mar 2015 7:35
Operator : TP/IZ
Sample : G1535-03 2X
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP3B-6B-7B-10(6-15)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
unknown1.31	1.31	239.8	ng	2772930	1	7.16	231243	20.0
Butane, 2-methoxy...	1.60	3.5	ng	40005	1	7.16	231243	20.0
2-Pentanone, 4-hy...	4.92	6.5	ng	75103	1	7.16	231243	20.0
Benzene, 1-ethyl-...	6.58	3.4	ng	39652	1	7.16	231243	20.0
unknown6.88	6.88	45.2	ng	522610	1	7.16	231243	20.0
Heptafluorobutano...	15.93	3.2	ng	89307	5	16.03	559954	20.0
Cyclohexadecane, ...	16.76	5.0	ng	140741	5	16.03	559954	20.0
2,6-Octadiene, 2,...	17.22	2.0	ng	51558	6	17.78	515436	20.0