

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
 Data File : BF091977.D
 Acq On : 27 Dec 2016 19:40
 Operator : UM/SJ
 Sample : H6244-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-5

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-BF122116.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	4.258	188	190	196	rVB	43823	65495	1.06%	0.173%
2	4.876	242	244	250	rBV	794276	943399	15.31%	2.493%
3	5.264	276	278	283	rVB	37616	64872	1.05%	0.171%
4	5.344	283	285	293	rBV	612406	926053	15.03%	2.448%
5	6.407	376	378	384	rBV	524297	695349	11.28%	1.838%
6	6.510	384	387	389	rBV	1473619	1613460	26.18%	4.264%
7	6.727	404	406	408	rBV	1564503	1469315	23.84%	3.883%
8	6.887	417	420	422	rBV	3616303	4095174	66.45%	10.823%
9	7.139	439	442	446	rBV2	45554	63772	1.03%	0.169%
10	7.299	453	456	457	rBV	3723106	3709179	60.18%	9.803%
11	7.333	457	459	461	rVB	172513	238046	3.86%	0.629%
12	7.756	494	496	499	rBV	519406	659853	10.71%	1.744%
13	7.836	499	503	507	rVB4	59348	131550	2.13%	0.348%
14	8.019	516	519	521	rBV	1977527	1944889	31.56%	5.140%
15	8.167	529	532	535	rVB	296426	303625	4.93%	0.802%
16	8.270	535	541	542	rBV2	61608	133491	2.17%	0.353%
17	9.093	610	613	616	rBV	4522010	6163122	100.00%	16.289%
18	9.436	640	643	646	rBV4	37077	74919	1.22%	0.198%
19	9.493	646	648	650	rVV	953658	785490	12.75%	2.076%
20	9.539	650	652	658	rVB5	32989	99961	1.62%	0.264%
21	9.665	658	663	665	rBV4	26565	76627	1.24%	0.203%
22	9.768	670	672	674	rBV	2456143	2192315	35.57%	5.794%
23	10.213	707	711	715	rBV4	74930	144658	2.35%	0.382%
24	10.556	739	741	744	rVB	1038051	1104152	17.92%	2.918%
25	10.682	751	752	756	rVB	180343	204170	3.31%	0.540%
26	11.128	790	791	793	rBV	120386	106818	1.73%	0.282%
27	11.253	800	802	804	rBV	2028527	1862295	30.22%	4.922%
28	11.825	848	852	854	rBV	160662	282087	4.58%	0.746%
29	11.859	854	855	859	rVB4	44066	70019	1.14%	0.185%
30	12.271	888	891	894	rBV4	33239	80992	1.31%	0.214%
31	12.614	918	921	923	rBV3	22581	65881	1.07%	0.174%
32	12.842	938	941	943	rBV	4887718	4718480	76.56%	12.471%
33	13.882	1030	1032	1035	rBV	1035563	1484907	24.09%	3.925%
34	14.739	1104	1107	1115	rVB	56956	116027	1.88%	0.307%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.288	1152	1155	1158	rbV	969493	1146041	18.60%	3.029%
----	--------	------	------	------	-----	--------	---------	--------	--------

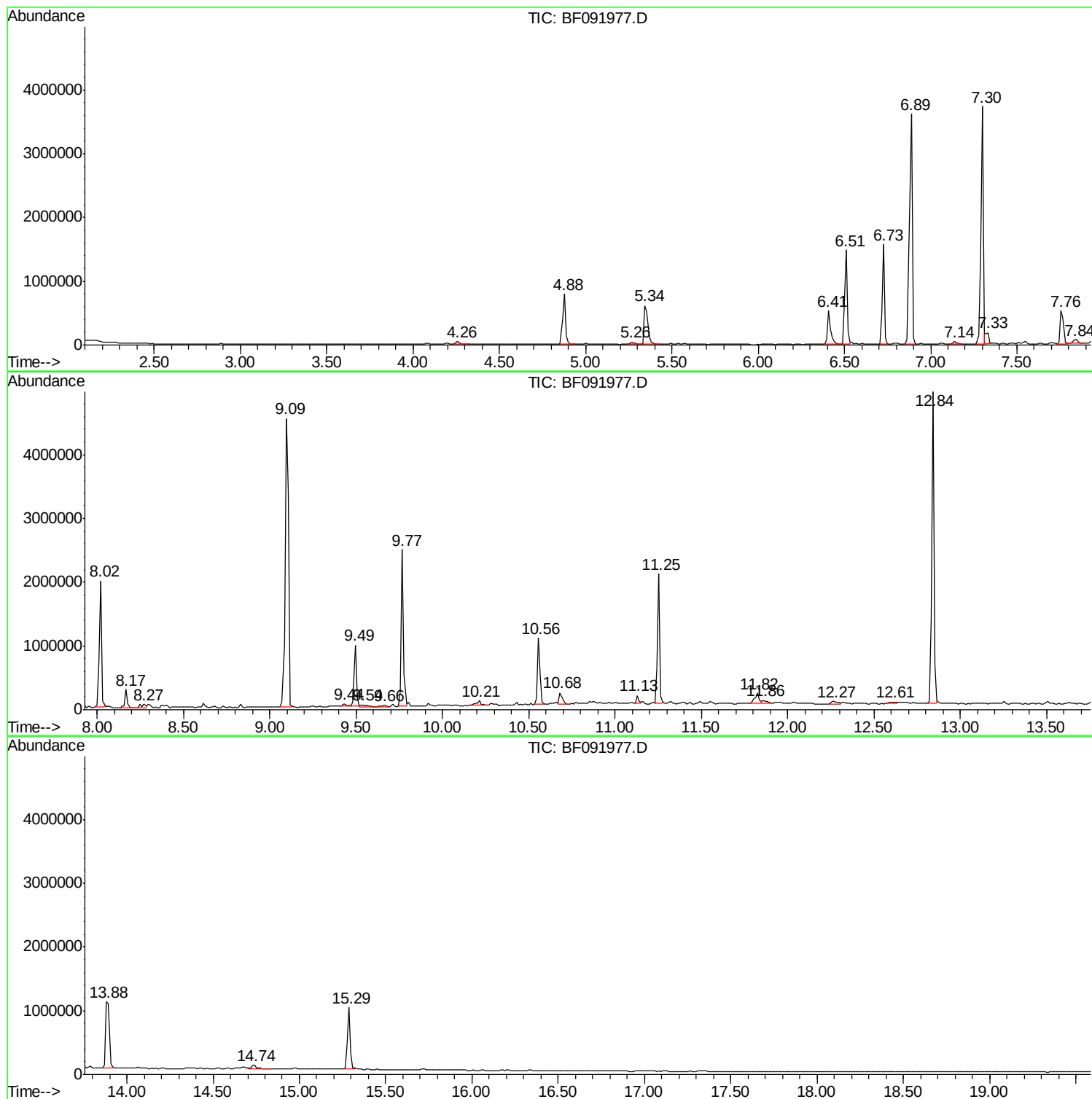
Sum of corrected areas: 37836483

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

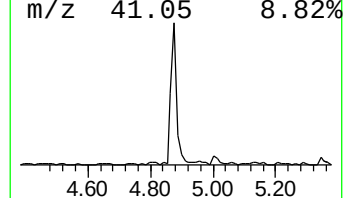
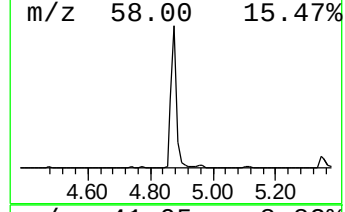
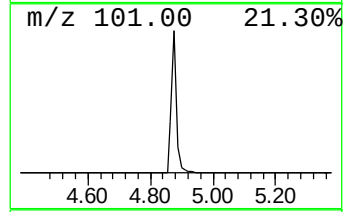
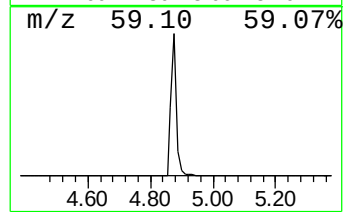
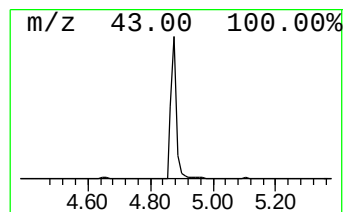
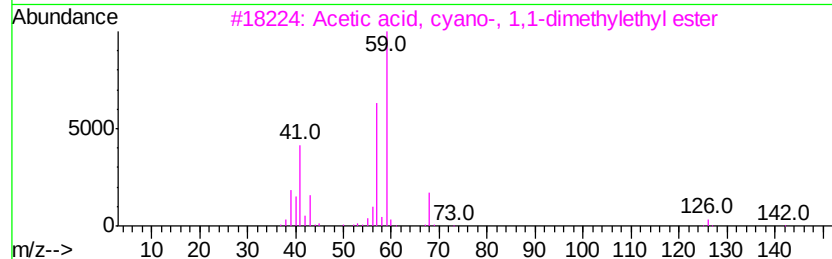
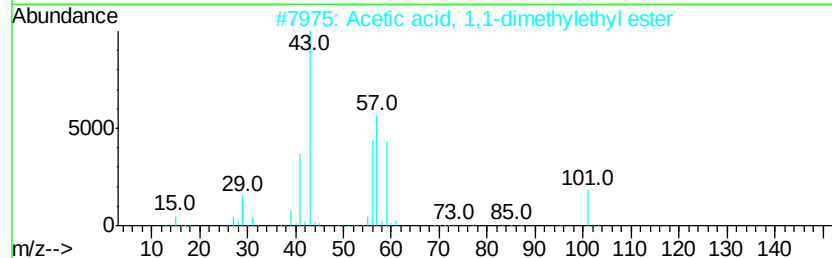
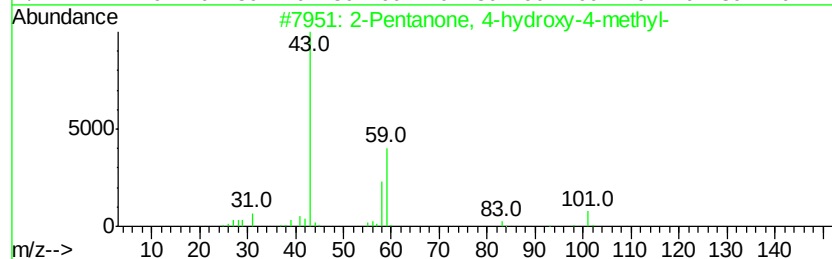
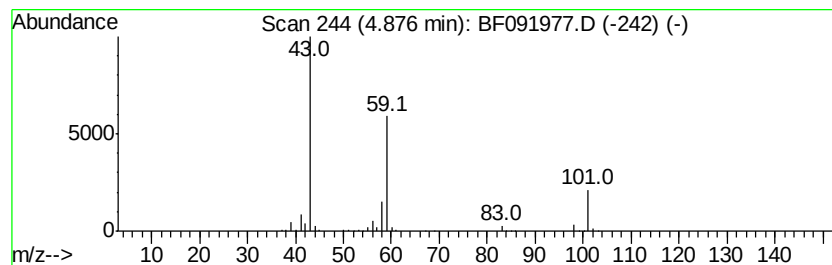
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	12.84 ng	943399	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

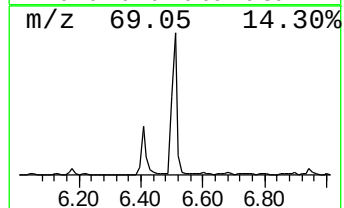
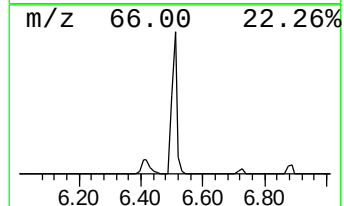
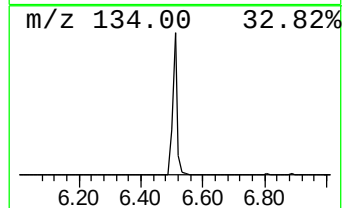
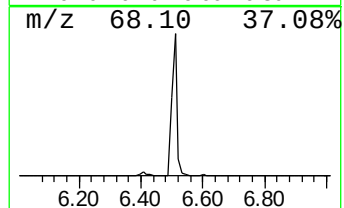
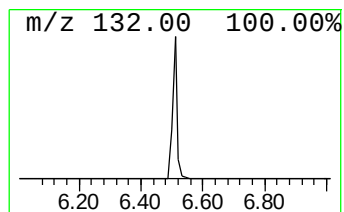
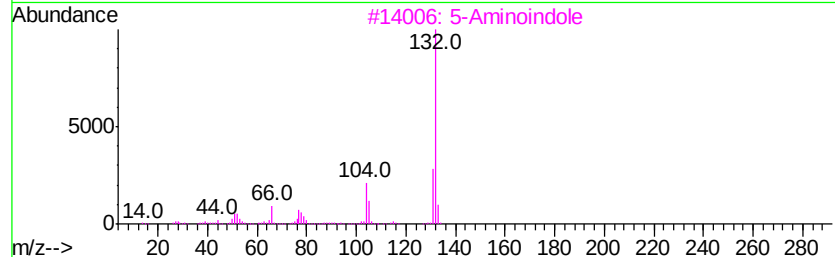
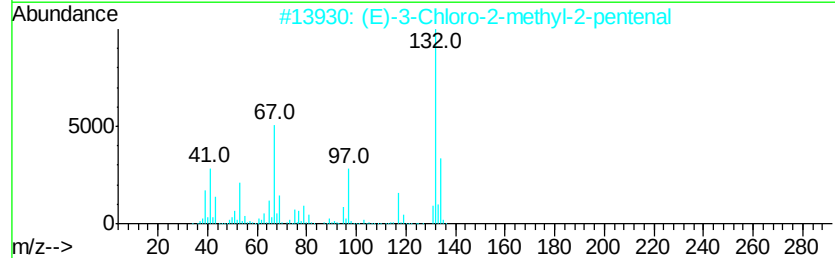
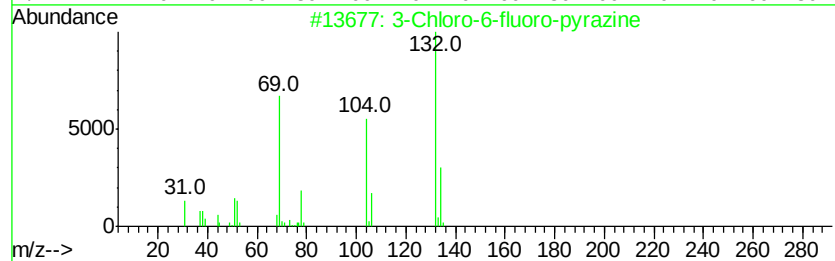
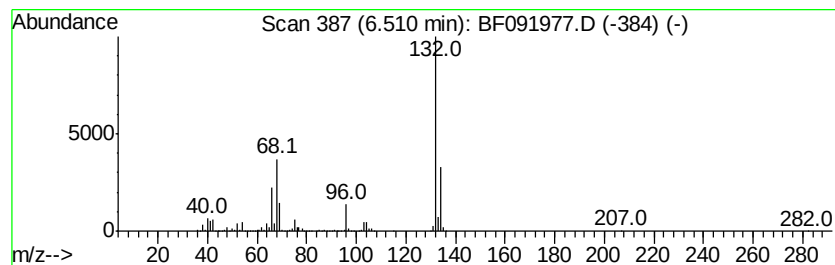
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	21.96 ng	1613460	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

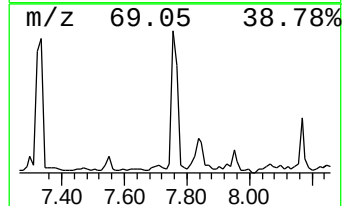
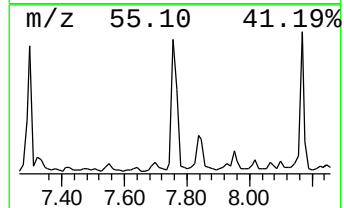
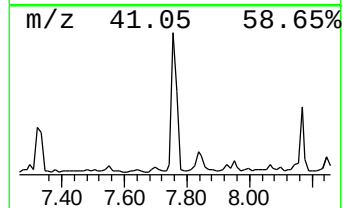
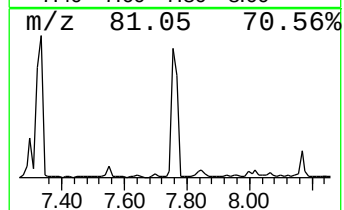
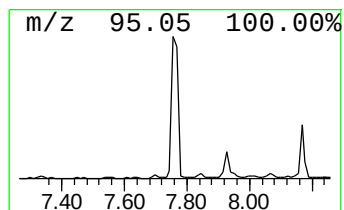
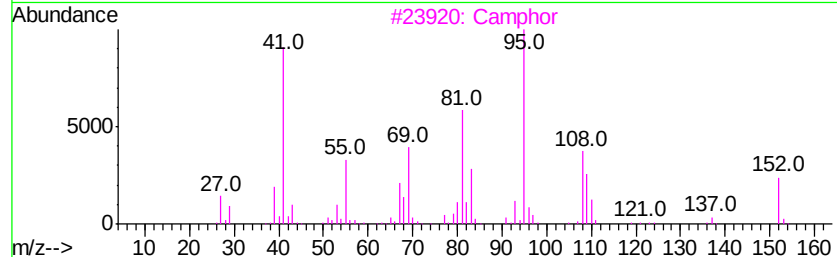
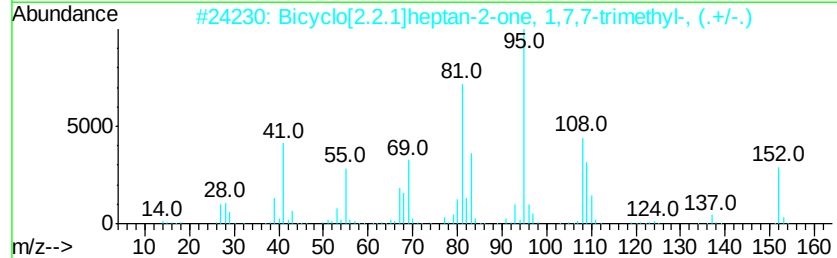
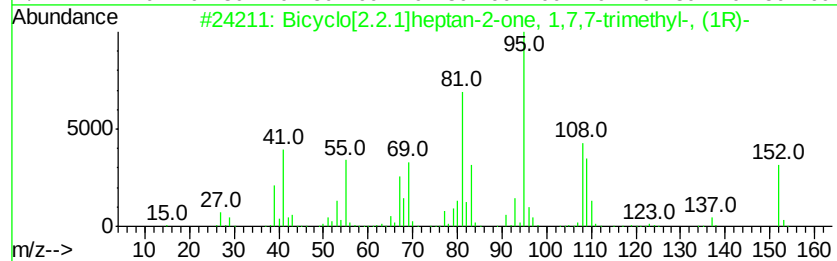
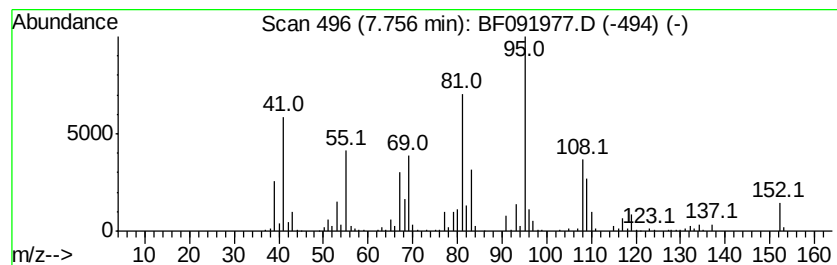
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	6.79 ng	659853	Napthalene-d8	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	97
2		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	97
3		Camphor	152	C10H16O	000076-22-2	97
4		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
5		5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

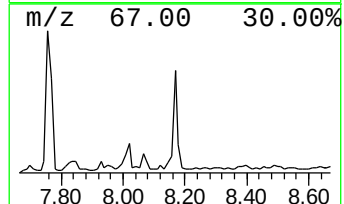
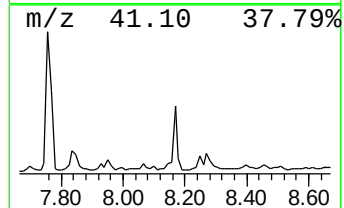
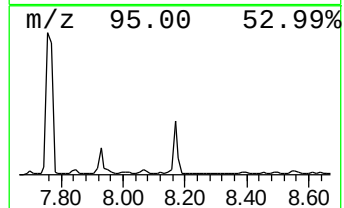
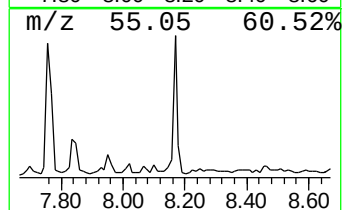
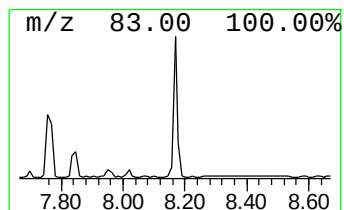
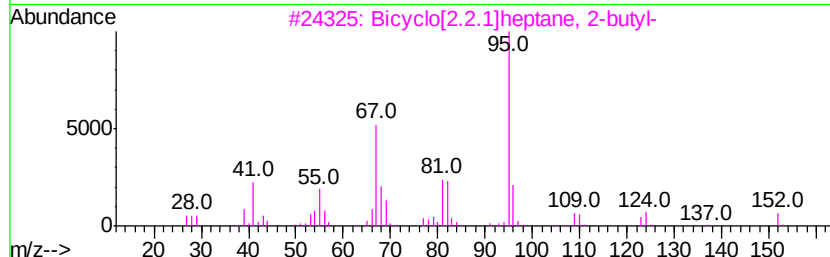
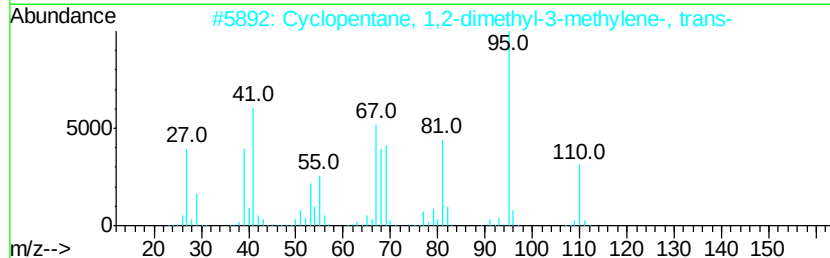
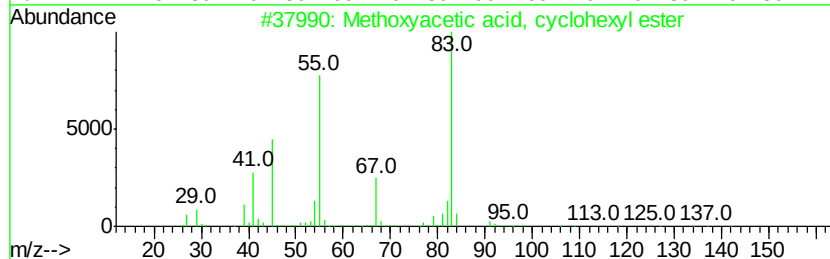
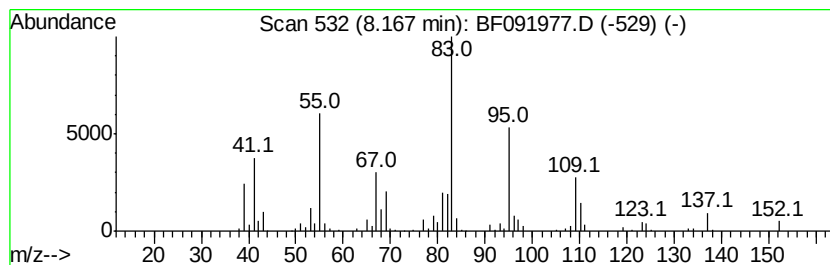
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown8.17 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	3.12 ng	303625	Naphthalene-d8	8.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Methoxyvacetic acid, cvclohexyl e...	172	C9H16O3	1000282-69-4	38
2		Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	30
3		Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	30
4		trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	27
5		Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

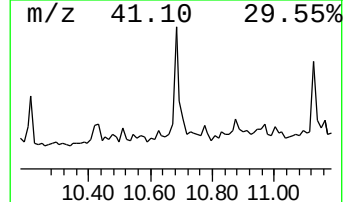
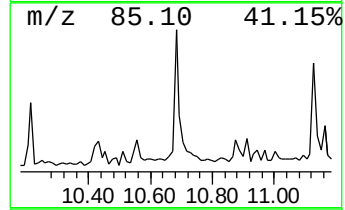
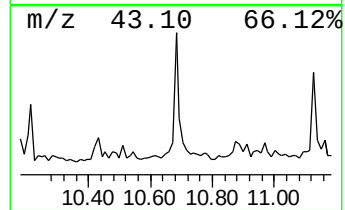
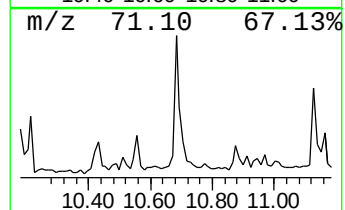
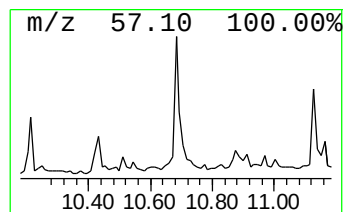
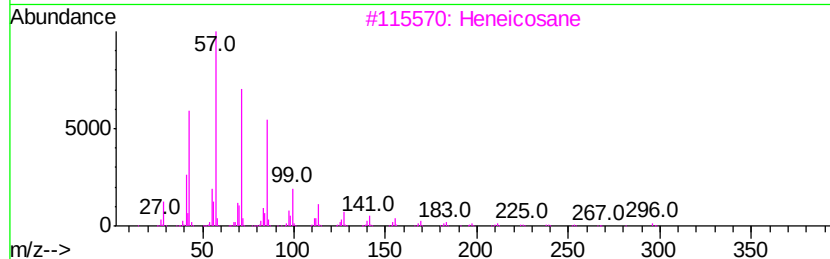
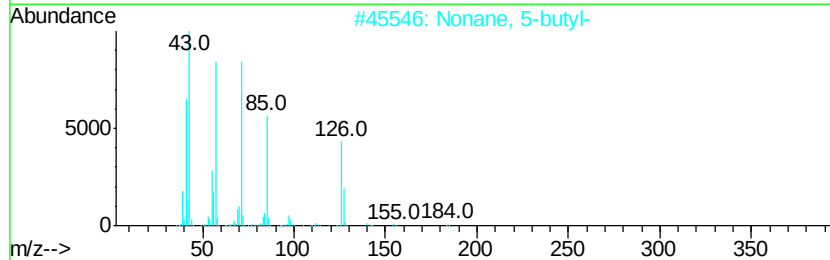
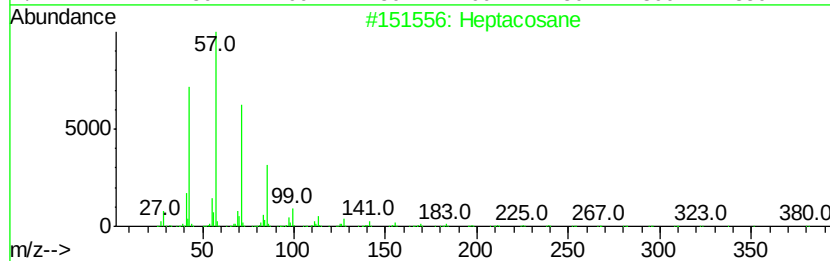
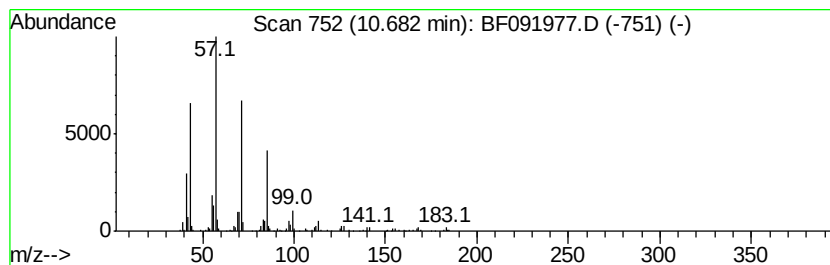
Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.68	2.19 ng	204170	Phenanthrene-d10		11.25
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Nonane, 5-butyl-	184	C13H28	017312-63-9	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
MW-5

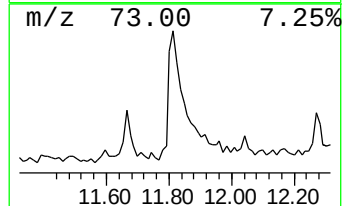
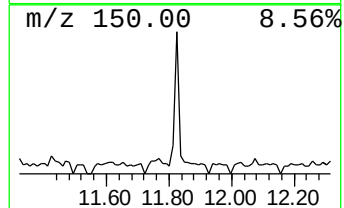
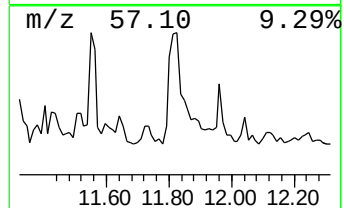
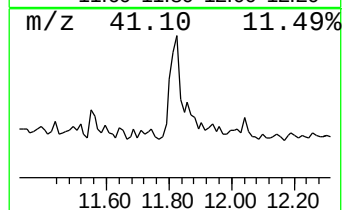
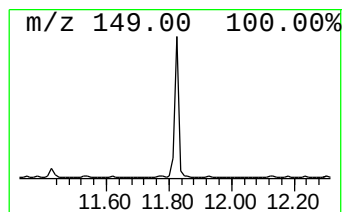
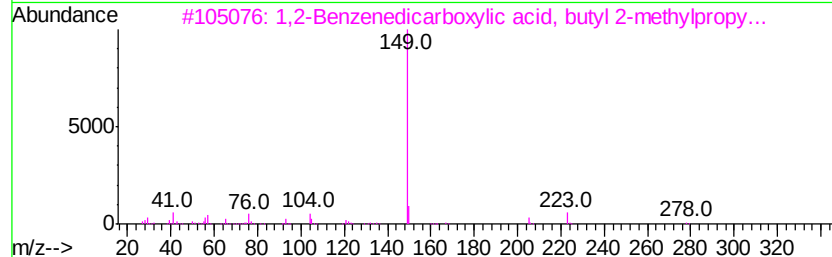
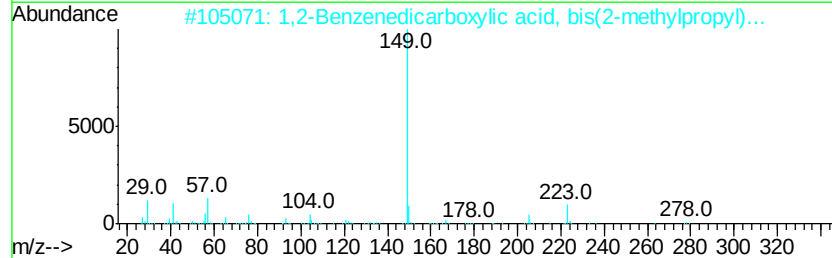
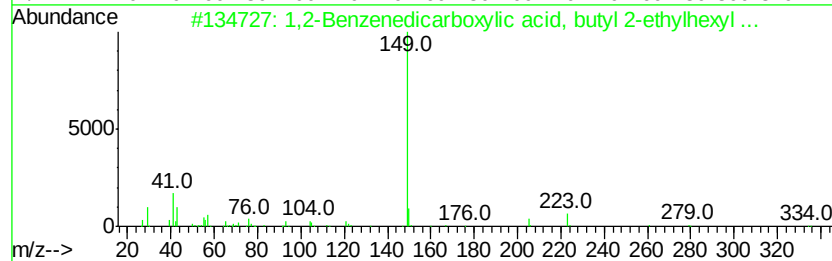
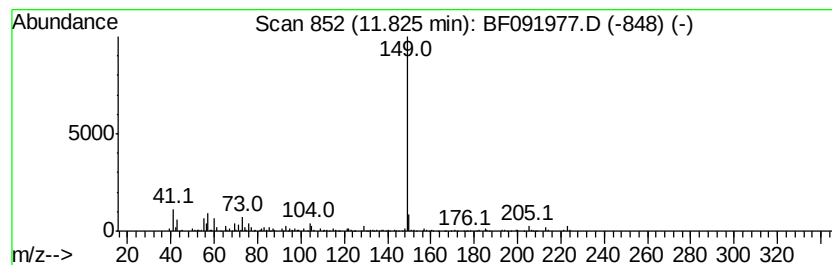
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,2-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	3.03 ng	282087	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	78
2		1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	78
3		1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	64
4		1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-19-0	64
5		1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

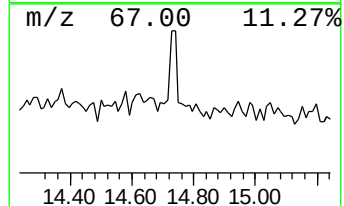
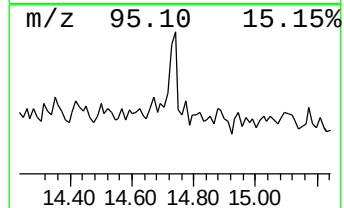
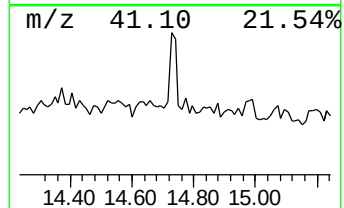
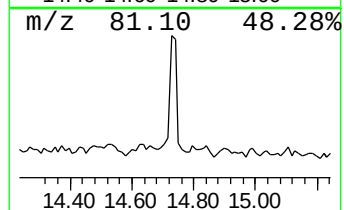
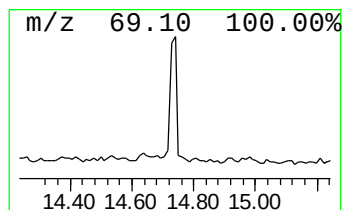
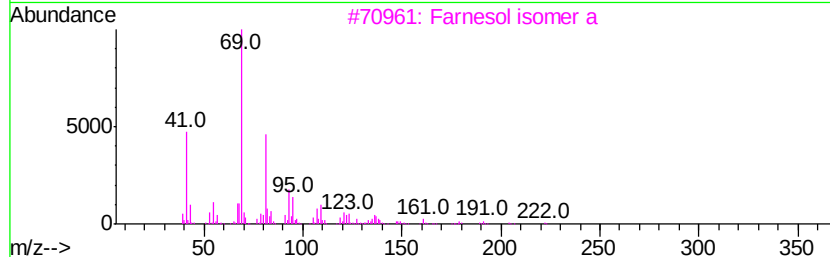
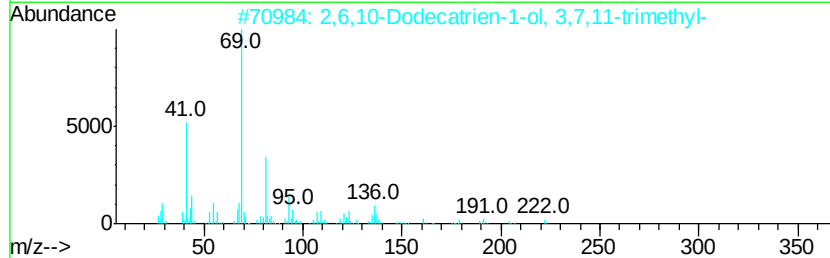
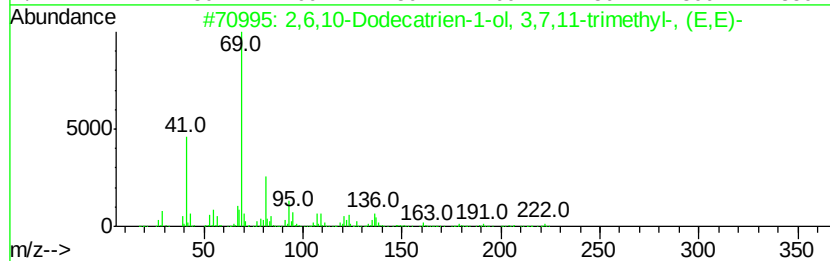
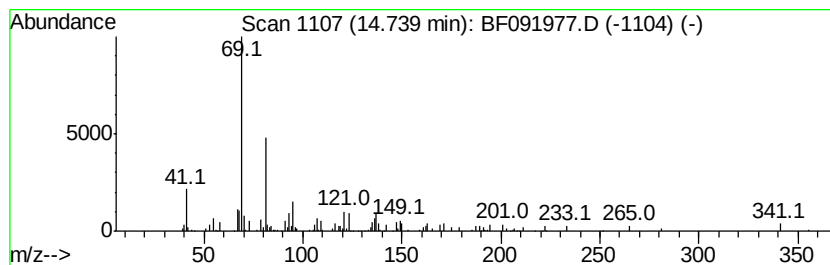
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.02 ng	116027	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	93
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	87
3		Farnesol isomer a	222	C15H26O	1000108-92-4	86
4		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122716\
Data File : BF091977.D
Acq On : 27 Dec 2016 19:40
Operator : UM/SJ
Sample : H6244-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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
2-Pentanone, 4-hy...	4.88	12.8	ng	943399	1	6.73	1469320	20.0
unknown6.51	6.51	22.0	ng	1613460	1	6.73	1469320	20.0
Bicyclo[2.2.1]hep...	7.76	6.8	ng	659853	2	8.02	1944890	20.0
unknown8.17	8.17	3.1	ng	303625	2	8.02	1944890	20.0
Heptacosane	10.68	2.2	ng	204170	4	11.25	1862300	20.0
1,2-Benzenedicarb...	11.82	3.0	ng	282087	4	11.25	1862300	20.0
2,6,10-Dodecatric...	14.74	2.0	ng	116027	6	15.29	1146040	20.0