

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123605.D
 Acq On : 16 Apr 2021 22:22
 Operator : JU/CG
 Sample : M2040-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FILL-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	4	12	17	rVB	3448512	4438755	54.45%	7.510%
2	5.104	510	513	518	rVB	99172	113013	1.39%	0.191%
3	5.504	576	581	584	rBV	8314288	7863100	96.45%	13.303%
4	6.510	747	752	755	rBV	7750632	8152629	100.00%	13.793%
5	6.698	781	784	788	rVB2	97484	124419	1.53%	0.211%
6	6.869	809	813	816	rBV	2206163	1645292	20.18%	2.784%
7	7.434	901	909	912	rBV	5690067	5468233	67.07%	9.252%
8	8.151	1026	1031	1034	rBV	2355428	2144884	26.31%	3.629%
9	8.810	1136	1143	1146	rBV6	81126	148960	1.83%	0.252%
10	9.181	1204	1206	1209	rBV	159048	121972	1.50%	0.206%
11	9.233	1211	1215	1218	rBV	8297179	7386699	90.61%	12.497%
12	9.304	1224	1227	1232	rBV3	429328	574508	7.05%	0.972%
13	9.351	1232	1235	1239	rVV3	172298	183351	2.25%	0.310%
14	9.481	1254	1257	1260	rBV4	187836	159815	1.96%	0.270%
15	9.575	1270	1273	1275	rVB2	255244	220899	2.71%	0.374%
16	9.628	1279	1282	1288	rVV2	510743	641706	7.87%	1.086%
17	9.681	1288	1291	1295	rBV6	137859	201631	2.47%	0.341%
18	9.769	1303	1306	1307	rBV	299327	283672	3.48%	0.480%
19	9.786	1307	1309	1314	rVV2	321345	426418	5.23%	0.721%
20	9.828	1314	1316	1319	rVV	700564	560759	6.88%	0.949%
21	9.916	1325	1331	1334	rBV	2589205	2498972	30.65%	4.228%
22	9.945	1334	1336	1343	rVB4	571235	836459	10.26%	1.415%
23	10.033	1348	1351	1354	rBV3	269591	286502	3.51%	0.485%
24	10.075	1356	1358	1360	rBV	140992	138131	1.69%	0.234%
25	10.186	1374	1377	1378	rBV2	183156	166990	2.05%	0.283%
26	10.257	1387	1389	1392	rVB3	272554	207761	2.55%	0.352%
27	10.292	1392	1395	1398	rBV3	300592	338987	4.16%	0.574%
28	10.328	1398	1401	1404	rBV	530009	512117	6.28%	0.866%
29	10.380	1407	1410	1412	rBV3	282075	300127	3.68%	0.508%
30	10.575	1440	1443	1446	rVB	522106	452647	5.55%	0.766%
31	10.710	1461	1466	1469	rBV	4305987	4383434	53.77%	7.416%
32	10.839	1485	1488	1495	rVB	1611937	1650468	20.24%	2.792%
33	11.310	1565	1568	1573	rVB	1001615	944899	11.59%	1.599%
34	11.410	1582	1585	1587	rBV	1672032	1566005	19.21%	2.649%
35	13.010	1854	1857	1861	rBV	4369598	3961711	48.59%	6.703%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

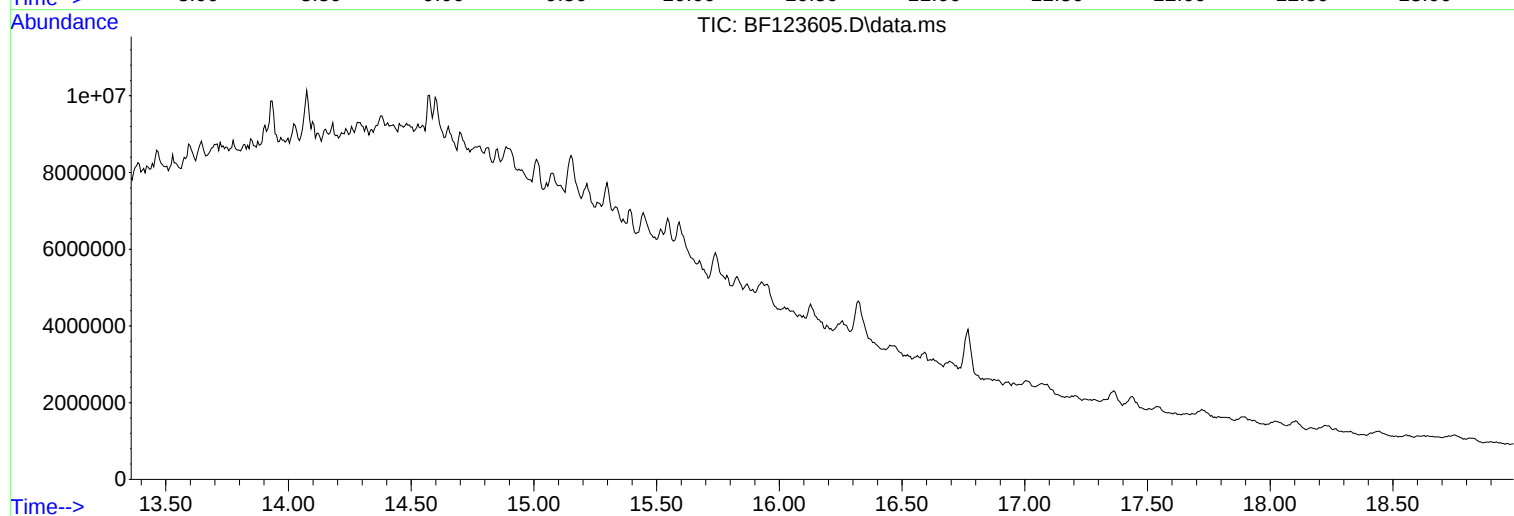
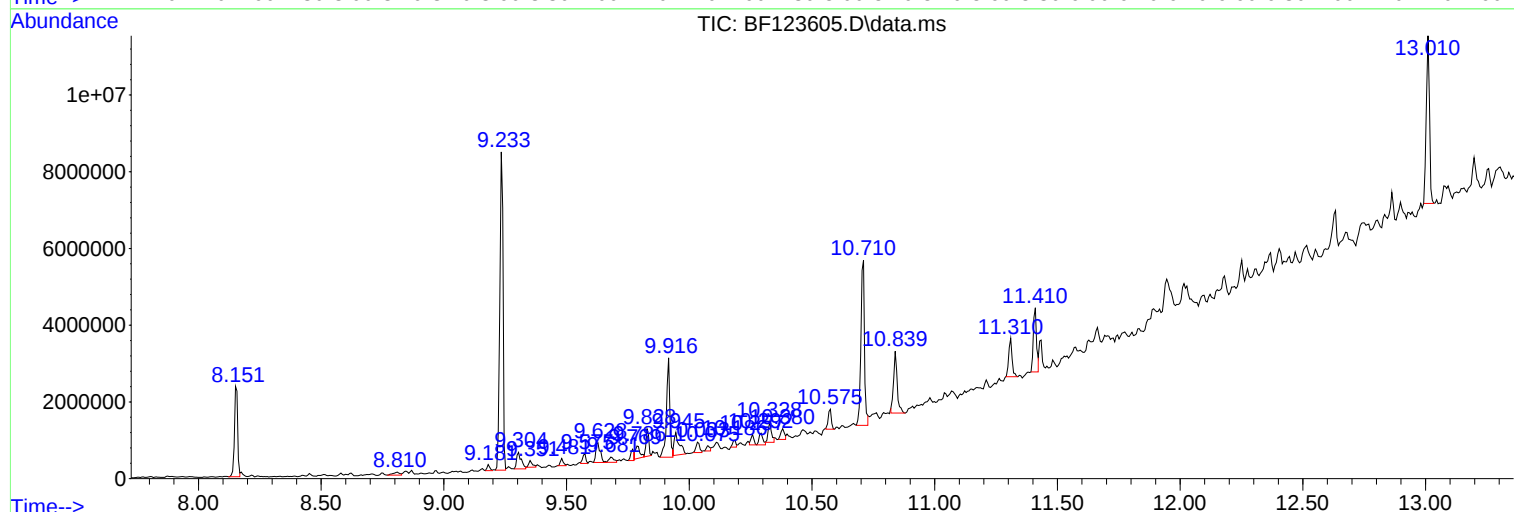
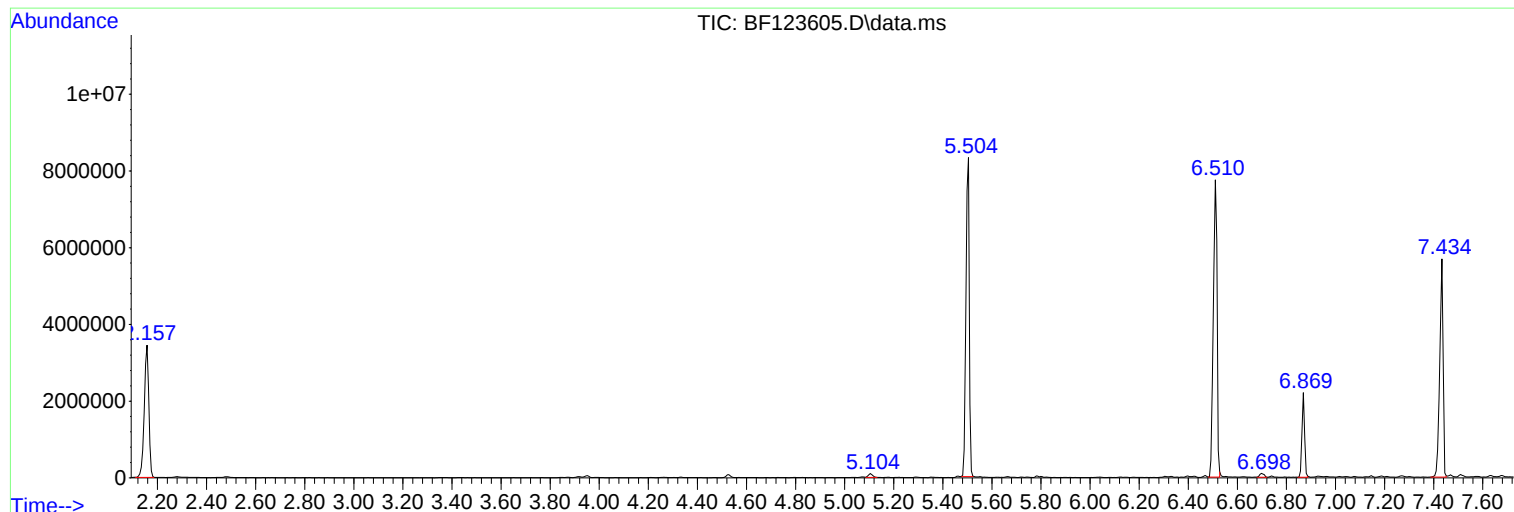
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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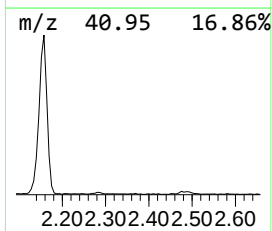
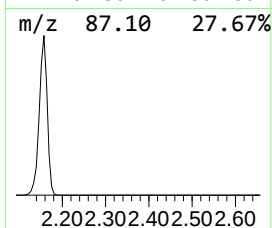
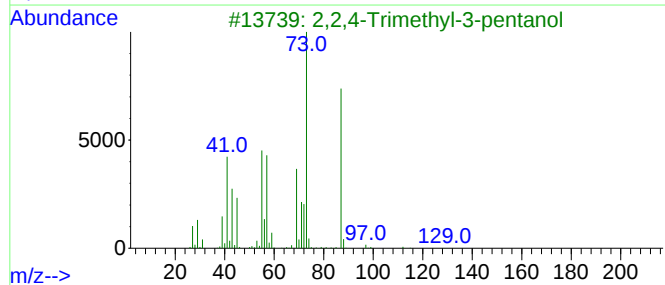
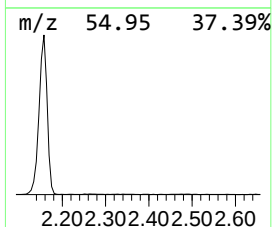
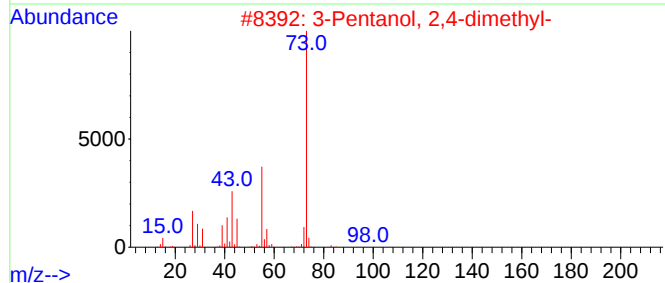
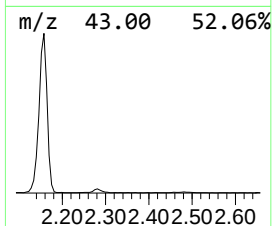
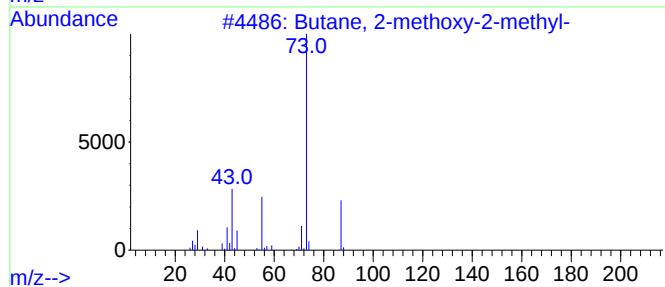
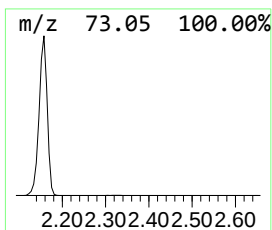
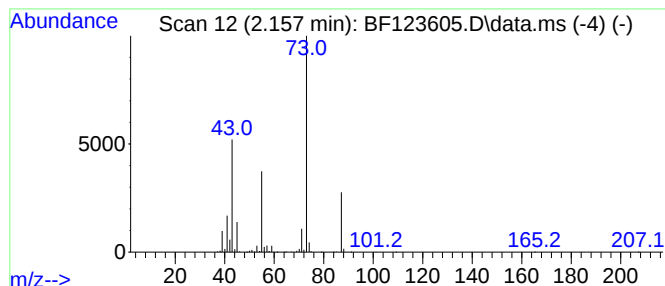
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	53.96 ng	4438760	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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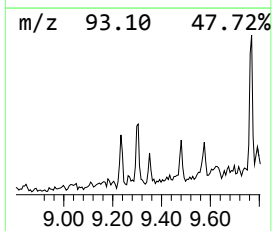
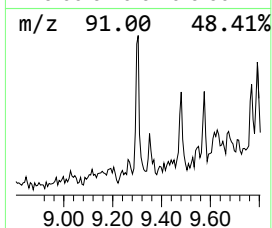
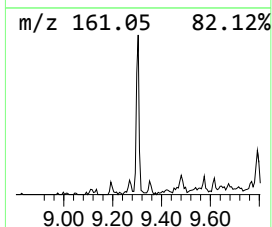
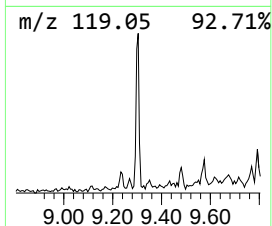
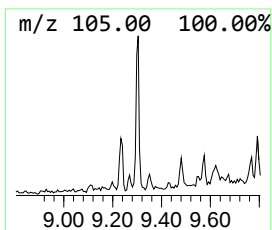
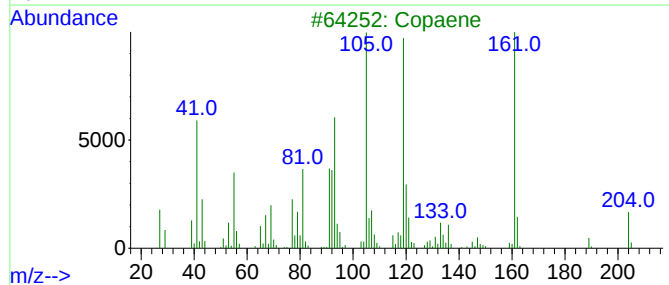
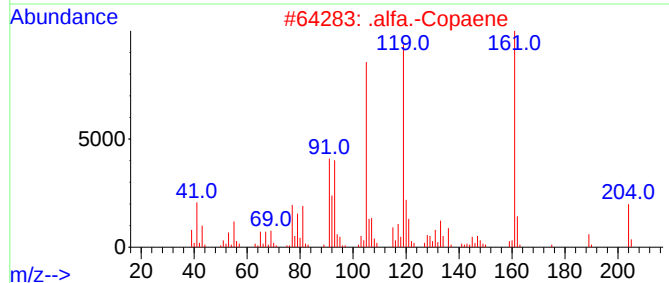
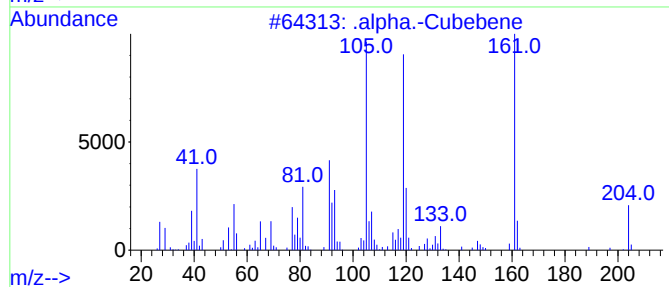
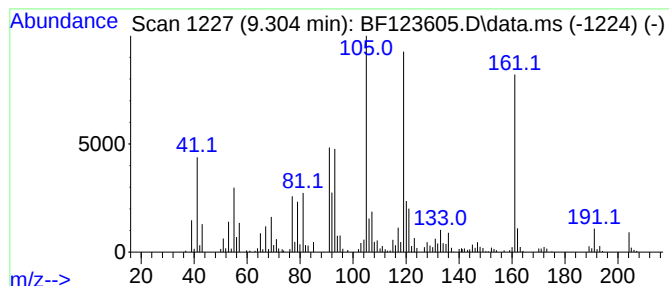
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Peak Number 2 .alpha.-Cubebene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	4.60 ng	574508	Acenaphthene-d10	9.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.alpha.-Cubebene	204	C15H24	017699-14-8	97
2		.alfa.-Copaene	204	C15H24	1000360-33-0	96
3		Copaene	204	C15H24	003856-25-5	96
4		1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	91
5		cis-muurola-3,5-diene	204	C15H24	1000365-95-4	89



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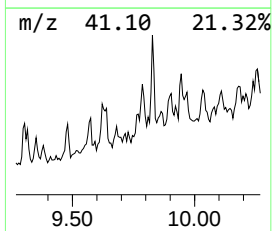
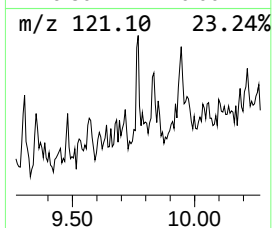
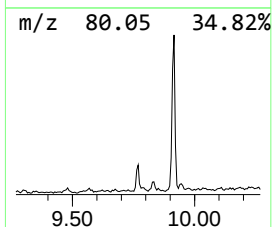
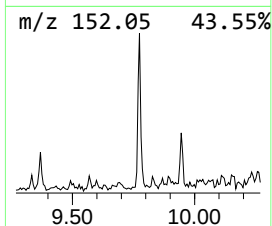
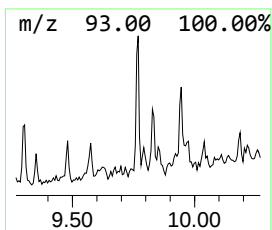
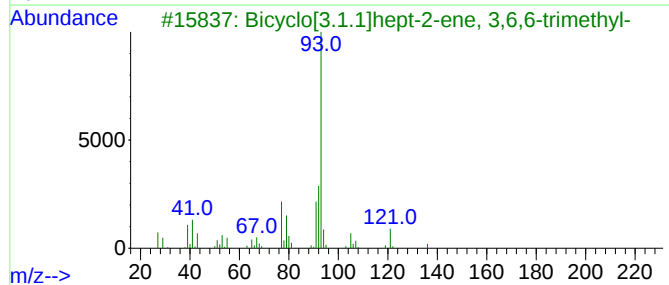
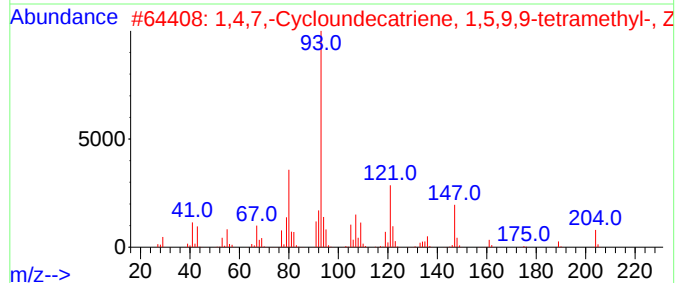
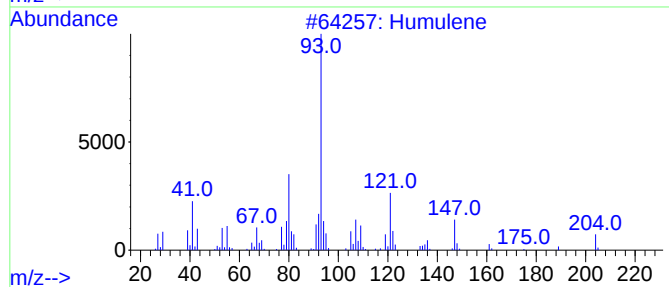
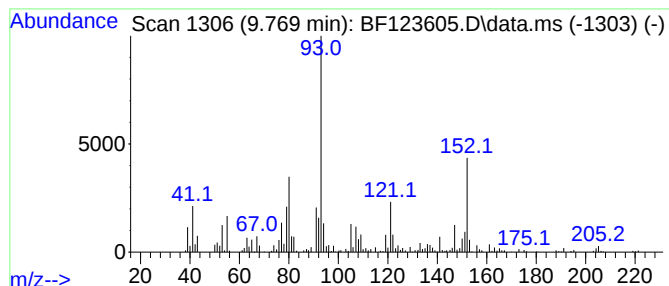
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Humulene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.769	2.27 ng	283672	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Humulene	204	C15H24	006753-98-6	86
2			1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	83
3			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	43
4			Ethanone, 1-cyclopropyl-2-(4-pyr...	161	C10H11NO	006580-95-6	38
5			Acrylanilide	147	C9H9NO	002210-24-4	35



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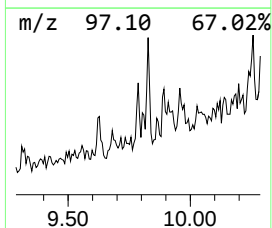
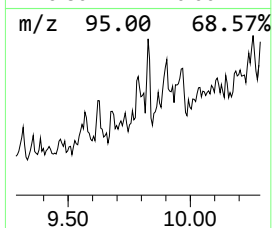
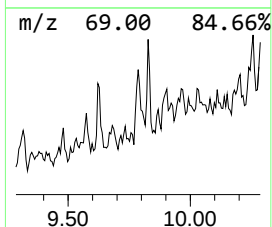
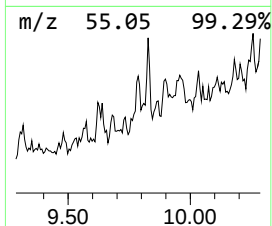
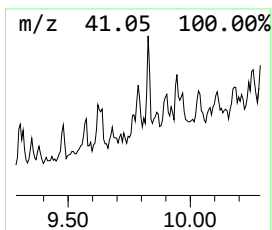
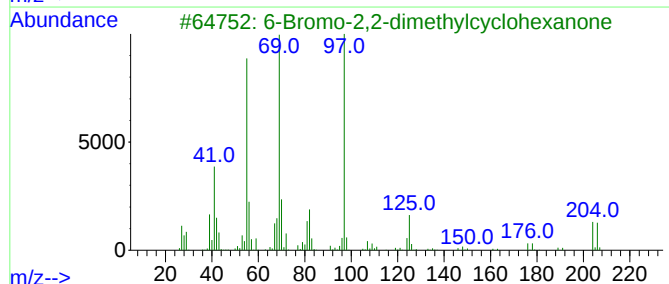
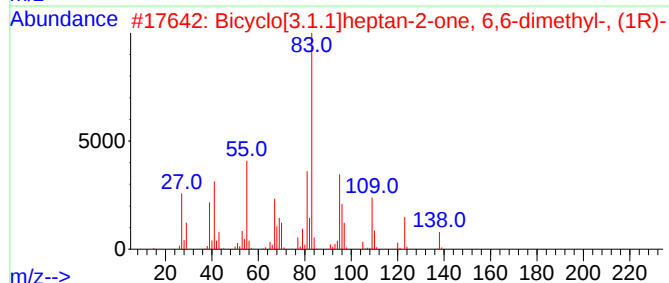
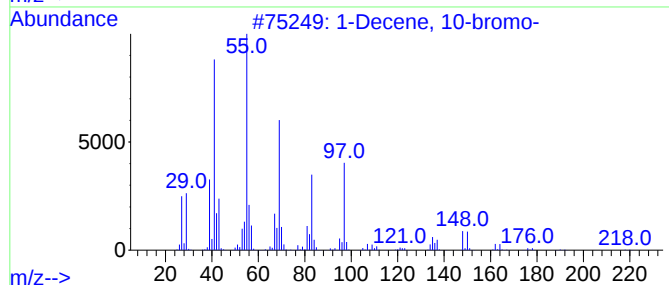
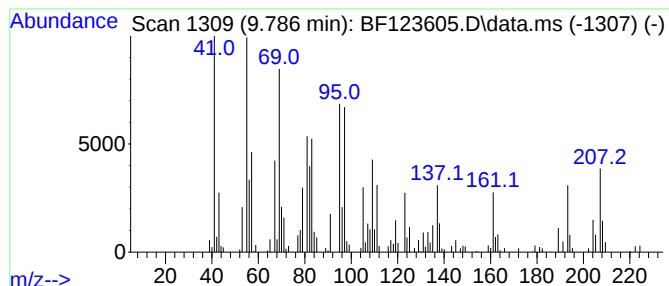
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Peak Number 4 unknown9.786 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.786	3.41 ng	426418	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 10-bromo-		218	C10H19Br	062871-09-4	27	
2	Bicyclo[3.1.1]heptan-2-one, 6,6-...		138	C9H14O	038651-65-9	25	
3	6-Bromo-2,2-dimethylcyclohexanone		204	C8H13BrO	021690-26-6	25	
4	2(1H)-Naphthalenone, octahydro-1...		194	C13H22O	000775-54-2	25	
5	Diethylmalonic acid, monochlorid...		282	C14H15ClO4	1000369-96-3	22	



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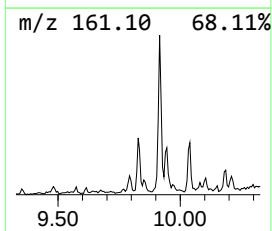
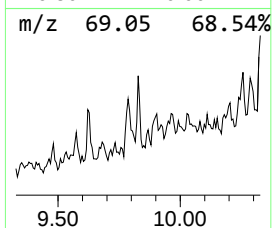
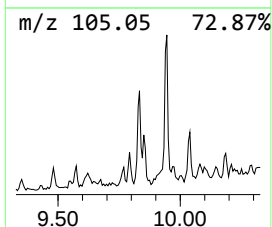
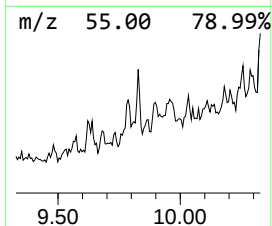
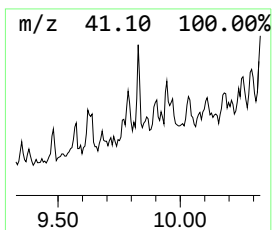
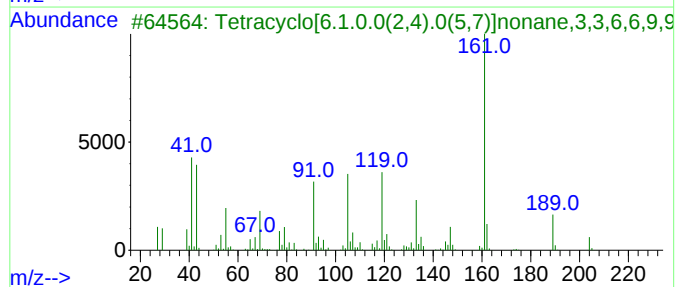
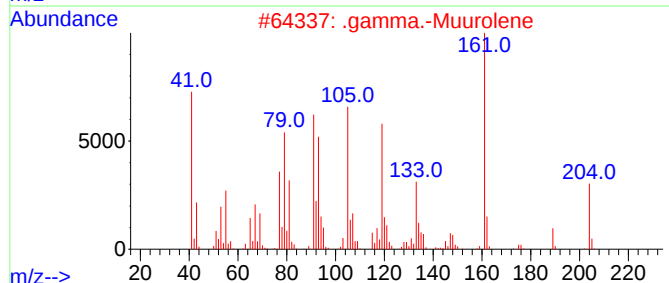
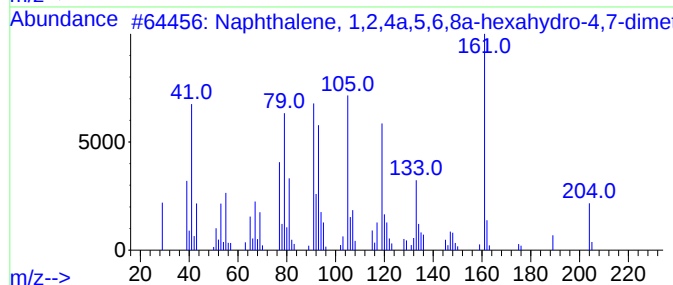
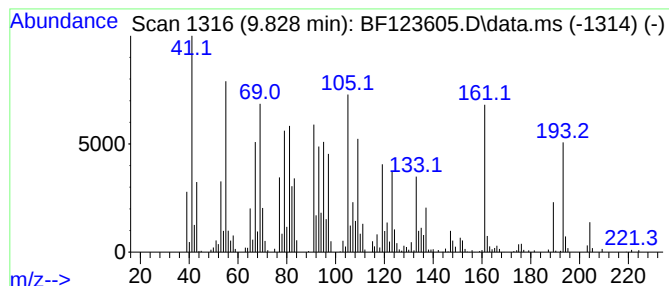
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.828	4.49 ng	560759	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	91
2	.gamma.-Murolene	204	C15H24	030021-74-0	66
3	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	55
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	49
5	Tricyclo[4.1.0.0(2,4)]heptane, 3...	204	C15H24	056348-21-1	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123605.D
Acq On : 16 Apr 2021 22:22
Operator : JU/CG
Sample : M2040-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

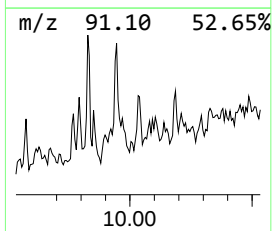
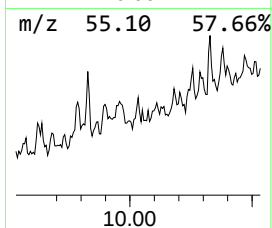
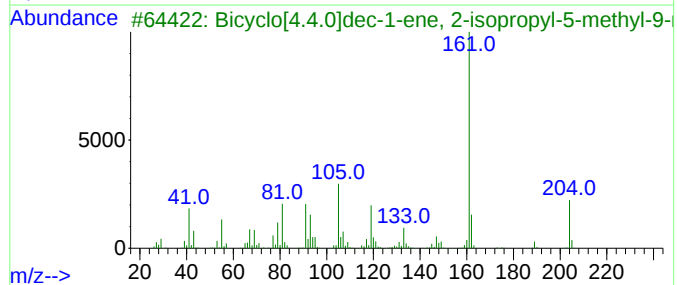
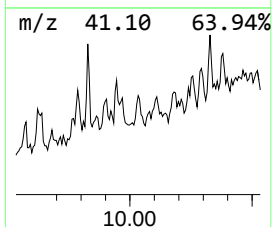
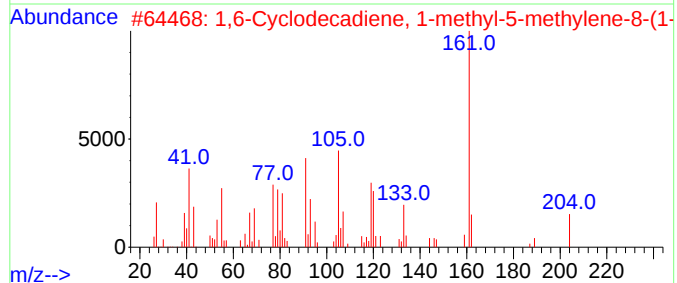
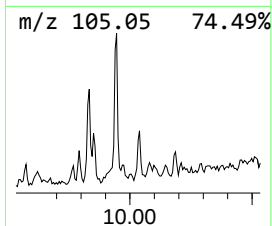
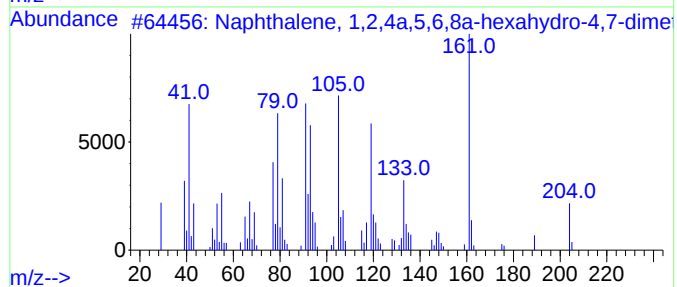
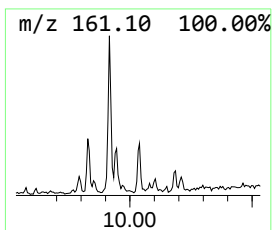
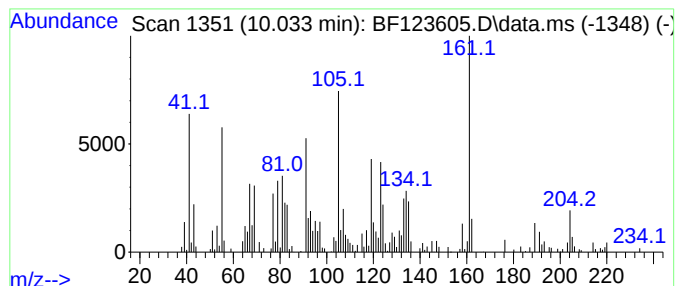
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,6-Cyclodecadiene, 1-methy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.033	2.29 ng	286502	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	78
2	1,6-Cyclodecadiene, 1-methyl-5-m...	204	C15H24	023986-74-5	70
3	Bicyclo[4.4.0]dec-1-ene, 2-isopr...	204	C15H24	150320-52-8	70
4	.gamma.-Muurolene	204	C15H24	030021-74-0	60
5	Isolodene	204	C15H24	1000156-10-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
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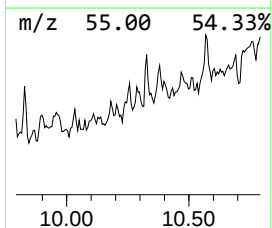
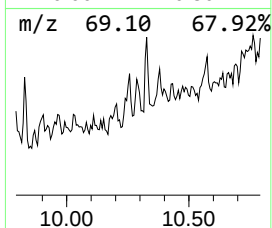
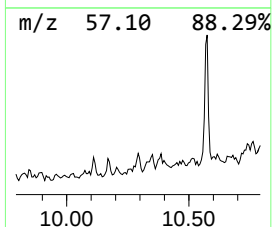
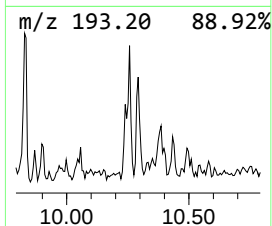
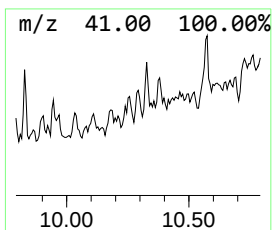
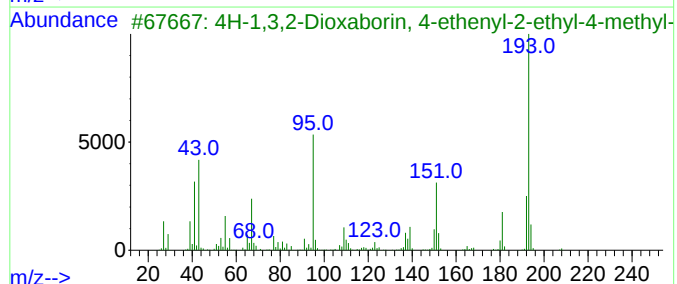
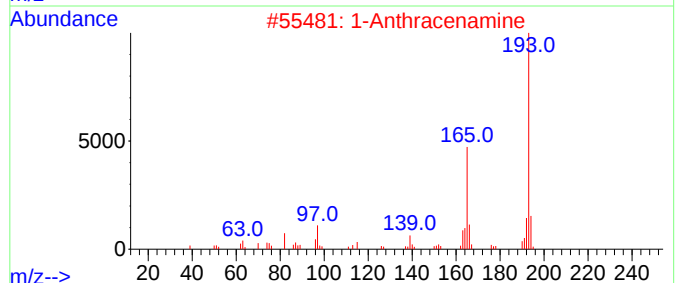
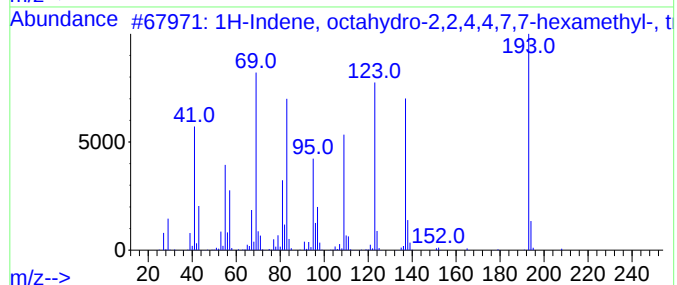
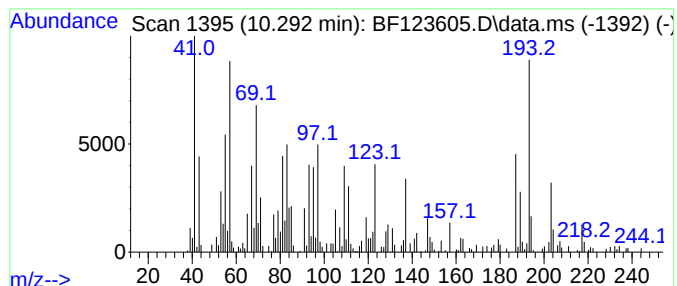
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown10.292 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.292	2.71 ng	338987	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37		
2	1-Anthracenamine	193	C14H11N	000610-49-1	22		
3	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21B02	074630-04-9	16		
4	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25B0	057387-76-5	16		
5	4-t-Butyl-2-(1-methyl-2-nitroeth...	241	C13H23N03	1000192-74-8	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123605.D
Acq On : 16 Apr 2021 22:22
Operator : JU/CG
Sample : M2040-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

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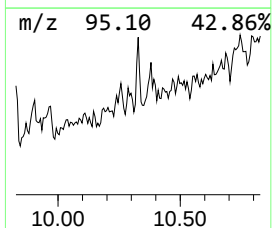
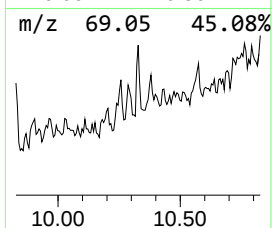
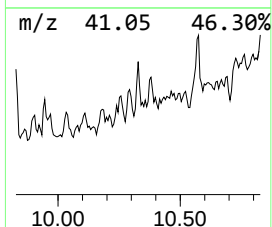
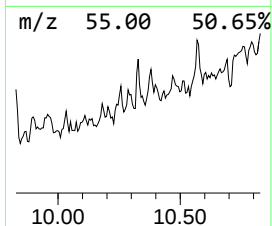
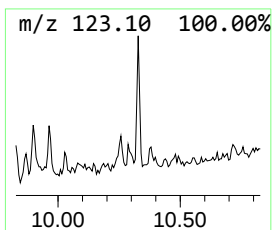
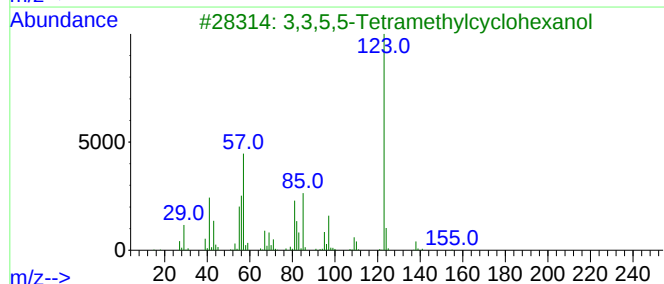
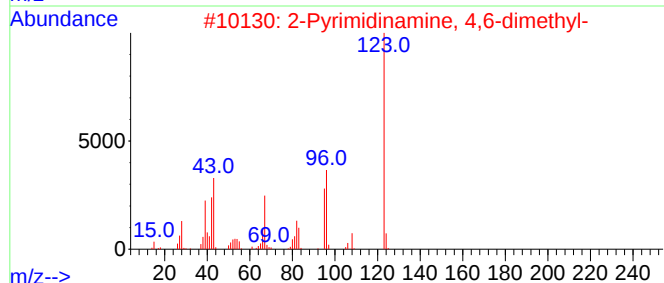
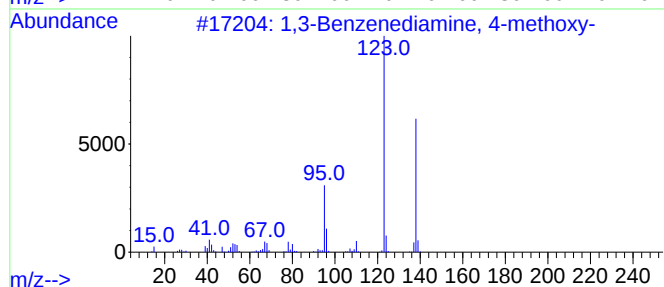
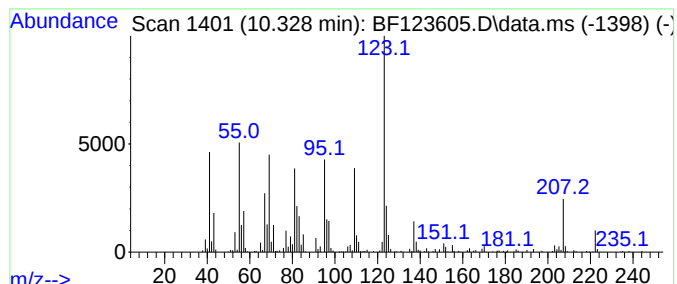
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown10.328 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	4.10 ng	512117	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	43
2			2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	35
3			3,3,5,5-Tetramethylcyclohexanol	156	C10H20O	002650-40-0	35
4			4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	27
5			(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1000299-95-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123605.D
Acq On : 16 Apr 2021 22:22
Operator : JU/CG
Sample : M2040-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

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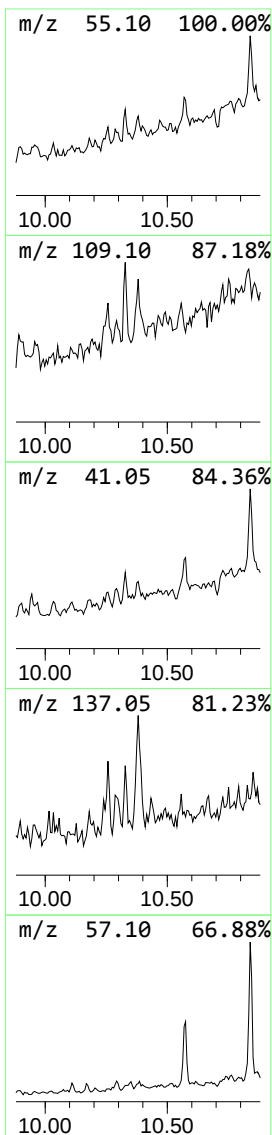
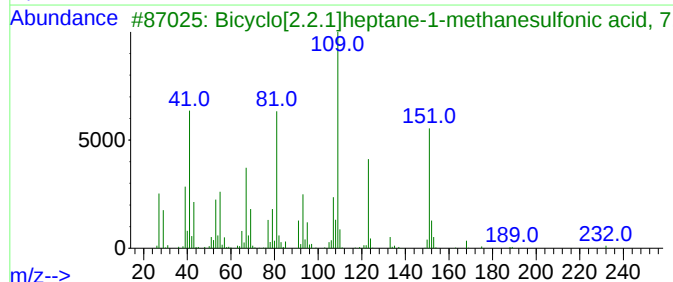
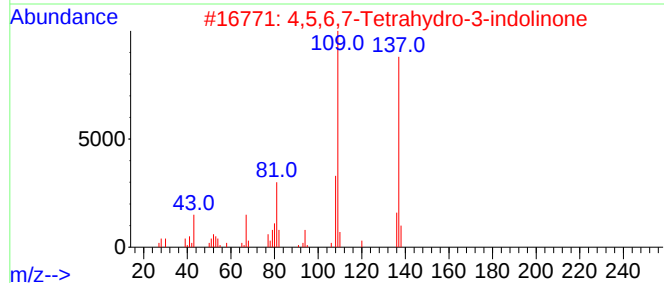
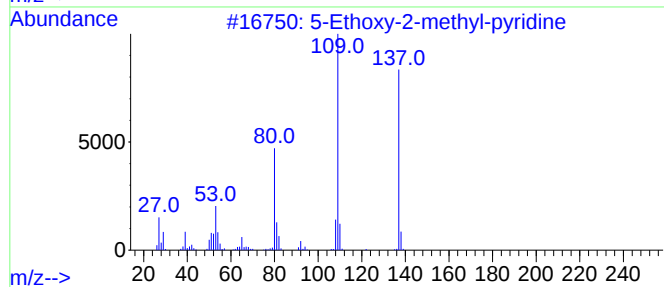
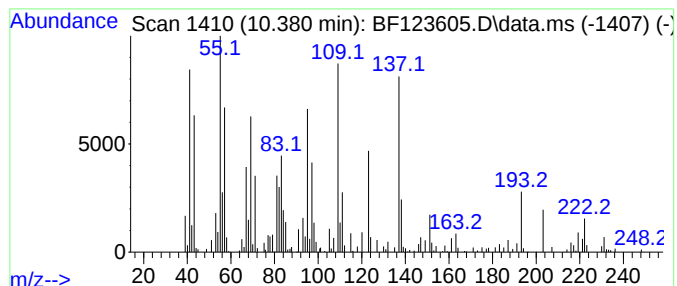
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown10.381 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.381	2.40 ng	300127	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethoxy-2-methyl-pyridine	137	C8H11NO	055270-48-9	38
2			4,5,6,7-Tetrahydro-3-indolinone	137	C8H11NO	058074-25-2	35
3			Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	25
4			Benzene, 1,2-dichloro-4-nitro-	191	C6H3Cl2NO2	000099-54-7	25
5			4-Acetyl-1-methylcyclohexene	138	C9H14O	006090-09-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123605.D
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Operator : JU/CG
Sample : M2040-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

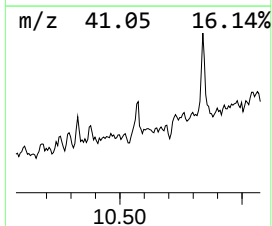
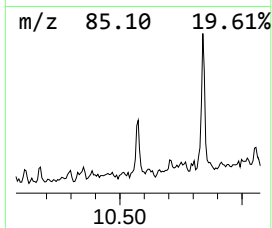
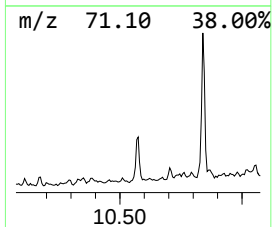
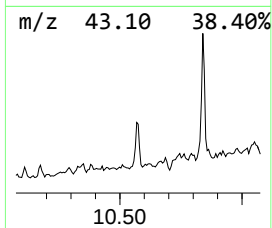
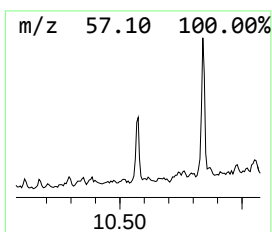
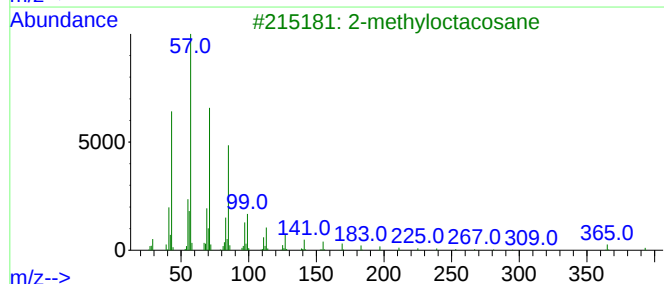
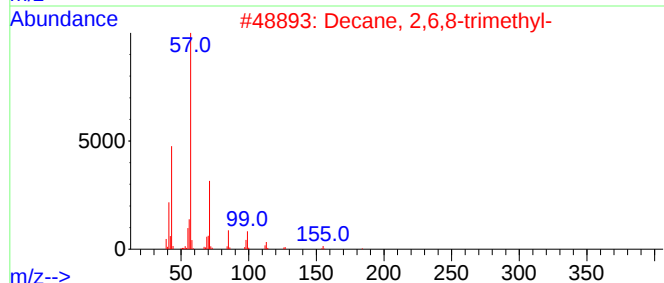
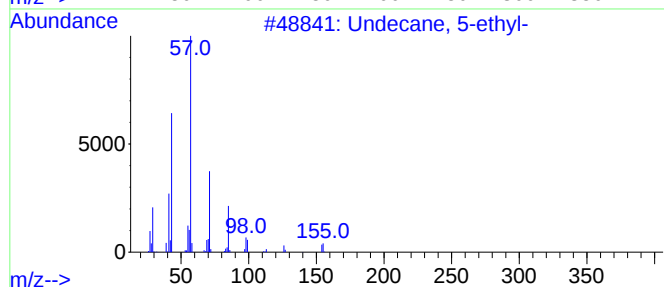
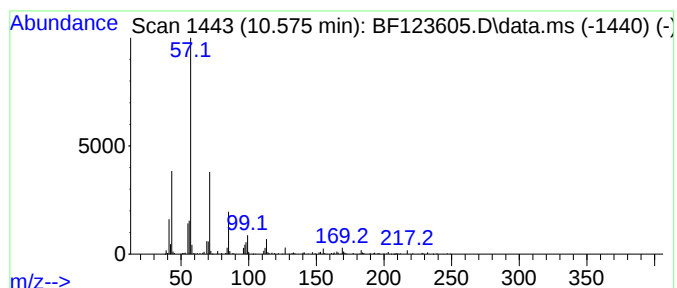
Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Undecane, 5-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.575	3.62 ng	452647	Acenaphthene-d10	9.916	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 5-ethyl-	184	C13H28	017453-94-0	72
2	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	70
3	2-methyloctacosane	408	C29H60	1000376-72-8	64
4	Tridecane, 6-methyl-	198	C14H30	013287-21-3	64
5	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
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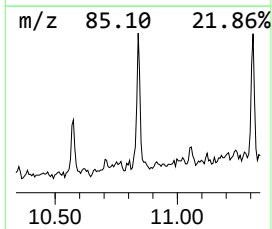
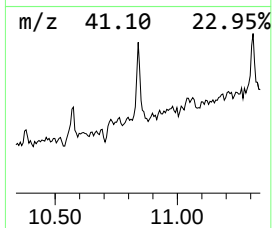
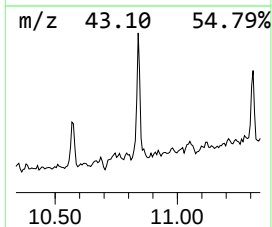
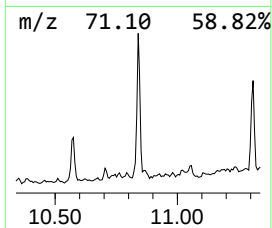
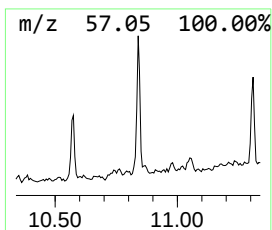
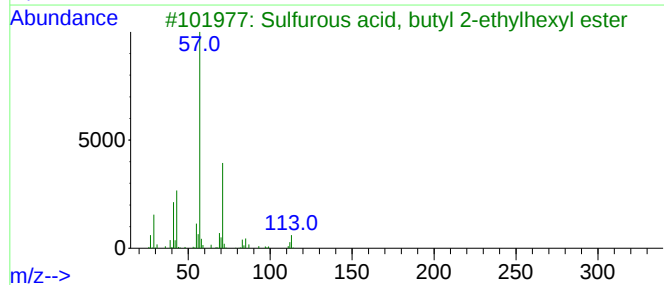
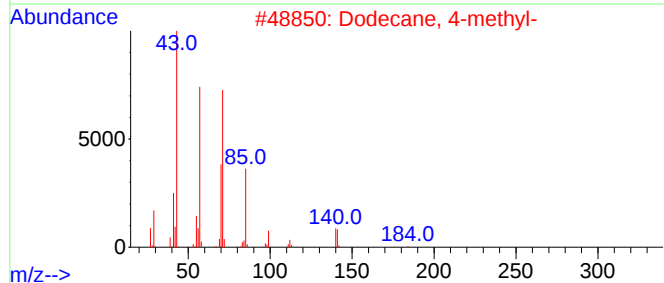
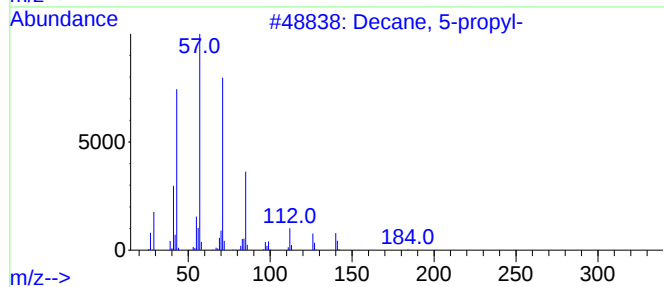
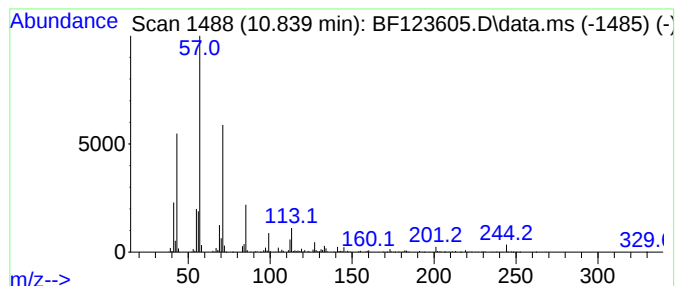
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Decane, 5-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.839	21.08 ng	1650470	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 5-propyl-	184	C13H28	017312-62-8	70
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	60
3	Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	53
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	53
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123605.D
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Instrument :
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ClientSampleId :
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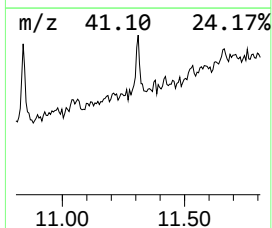
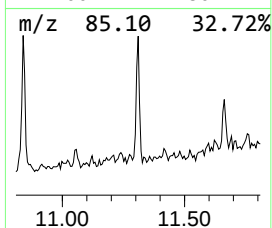
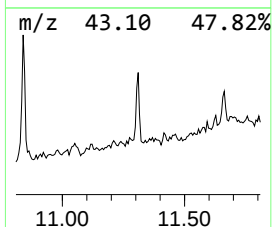
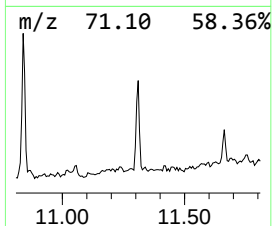
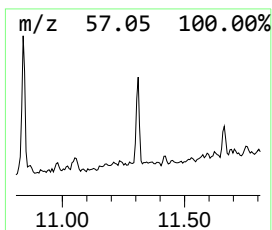
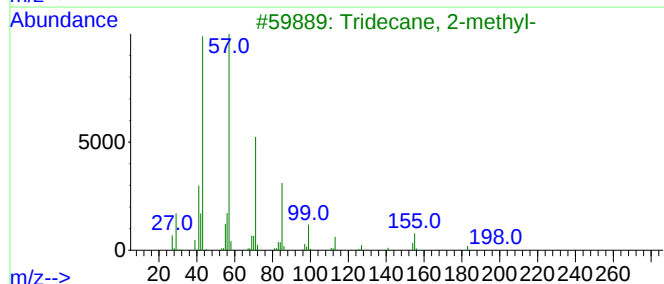
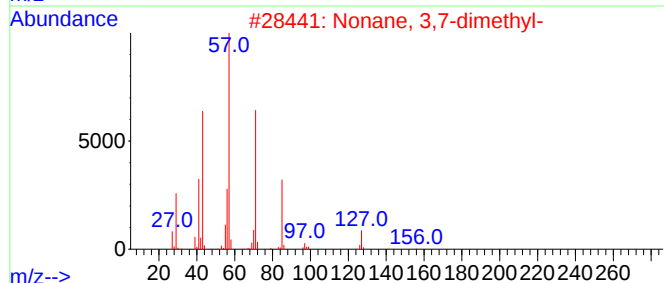
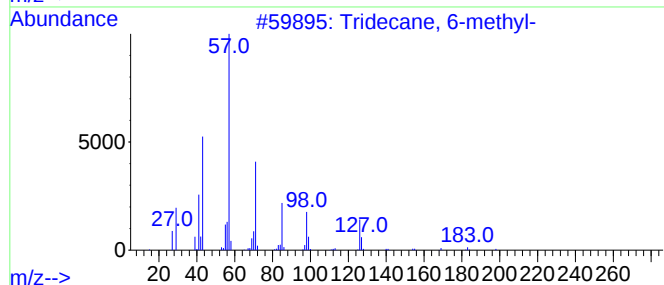
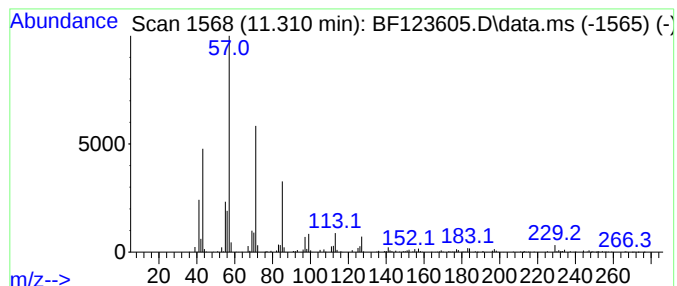
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tridecane, 6-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.310	12.07 ng	944899	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 6-methyl-	198	C14H30	013287-21-3	90
2		Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	87
3		Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
4		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
5		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123605.D
 Acq On : 16 Apr 2021 22:22
 Operator : JU/CG
 Sample : M2040-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FILL-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	54.0	ng	4438760	1	6.869	1645290	20.0
.alpha.-Cubebene	9.304	4.6	ng	574508	3	9.916	2498970	20.0
Humulene	9.769	2.3	ng	283672	3	9.916	2498970	20.0
unknown9.786	9.786	3.4	ng	426418	3	9.916	2498970	20.0
Naphthalene, 1,...	9.828	4.5	ng	560759	3	9.916	2498970	20.0
1,6-Cyclodecadi...	10.033	2.3	ng	286502	3	9.916	2498970	20.0
unknown10.292	10.292	2.7	ng	338987	3	9.916	2498970	20.0
unknown10.328	10.328	4.1	ng	512117	3	9.916	2498970	20.0
unknown10.381	10.381	2.4	ng	300127	3	9.916	2498970	20.0
Undecane, 5-ethyl-	10.575	3.6	ng	452647	3	9.916	2498970	20.0
Decane, 5-propyl-	10.839	21.1	ng	1650470	4	11.410	1566010	20.0
Tridecane, 6-me...	11.310	12.1	ng	944899	4	11.410	1566010	20.0