

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
 Data File : BF104479.D
 Acq On : 13 Apr 2018 15:34
 Operator : JU/SJ
 Sample : J2364-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-A

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-BF040618.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	5.040	498	502	514	rVB	143791	224559	5.72%	0.607%
2	5.434	562	569	572	rBV	3301012	3816112	97.21%	10.321%
3	6.081	675	679	694	rVB	131835	228454	5.82%	0.618%
4	6.451	735	742	745	rBV	3195281	3925819	100.00%	10.618%
5	6.581	759	764	768	rBV	3391662	3923886	99.95%	10.613%
6	6.810	799	803	806	rBV	1091084	832038	21.19%	2.250%
7	6.969	825	830	833	rBV	3301664	2988443	76.12%	8.083%
8	7.381	893	900	903	rBV	2354500	2596200	66.13%	7.022%
9	8.092	1015	1021	1024	rBV	1412200	1150284	29.30%	3.111%
10	9.169	1199	1204	1207	rBV	3663914	3859689	98.32%	10.439%
11	9.245	1213	1217	1219	rBV	63949	55849	1.42%	0.151%
12	9.504	1257	1261	1263	rBV	149455	130402	3.32%	0.353%
13	9.563	1267	1271	1274	rBV	823188	669124	17.04%	1.810%
14	9.775	1305	1307	1310	rVB	136945	92711	2.36%	0.251%
15	9.851	1316	1320	1323	rVV	1359592	1222252	31.13%	3.306%
16	10.251	1385	1388	1390	rBV3	39833	43496	1.11%	0.118%
17	10.275	1390	1392	1395	rVB	160860	130144	3.32%	0.352%
18	10.498	1425	1430	1433	rBV	66508	88830	2.26%	0.240%
19	10.645	1448	1455	1458	rBV	2516167	2628457	66.95%	7.109%
20	10.751	1470	1473	1474	rBV	143158	135202	3.44%	0.366%
21	10.763	1474	1475	1482	rVB2	159838	143026	3.64%	0.387%
22	11.339	1569	1573	1575	rBV	1413072	1164785	29.67%	3.150%
23	11.357	1575	1576	1580	rVV	114029	103590	2.64%	0.280%
24	11.863	1660	1662	1666	rBV4	38102	40723	1.04%	0.110%
25	12.551	1776	1779	1783	rVB	276825	225758	5.75%	0.611%
26	12.780	1813	1818	1823	rVB	214174	208219	5.30%	0.563%
27	12.933	1839	1844	1847	rVB	2905116	2971467	75.69%	8.037%
28	13.204	1887	1890	1895	rBV5	30594	45124	1.15%	0.122%
29	13.816	1991	1994	2002	rVB2	288752	317772	8.09%	0.859%
30	13.980	2018	2022	2025	rBV	861025	926682	23.60%	2.506%
31	14.010	2025	2027	2035	rVB	118938	132119	3.37%	0.357%
32	14.204	2058	2060	2064	rVB3	49296	47521	1.21%	0.129%
33	14.463	2101	2104	2109	rBV	67469	81653	2.08%	0.221%
34	14.633	2131	2133	2138	rVB4	90564	94519	2.41%	0.256%

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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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.839	2165	2168	2170	rVB	45925	46863	1.19%	0.127%
36	15.021	2196	2199	2203	rBV	86903	133423	3.40%	0.361%
37	15.098	2209	2212	2216	rBV	214933	217068	5.53%	0.587%
38	15.386	2258	2261	2267	rVB	58989	82627	2.10%	0.223%
39	15.457	2268	2273	2280	rVB	603378	808777	20.60%	2.187%
40	15.910	2346	2350	2355	rBV	139452	211649	5.39%	0.572%
41	16.704	2482	2485	2490	rVB4	62765	93657	2.39%	0.253%
42	18.045	2709	2713	2721	rVB10	59863	135217	3.44%	0.366%

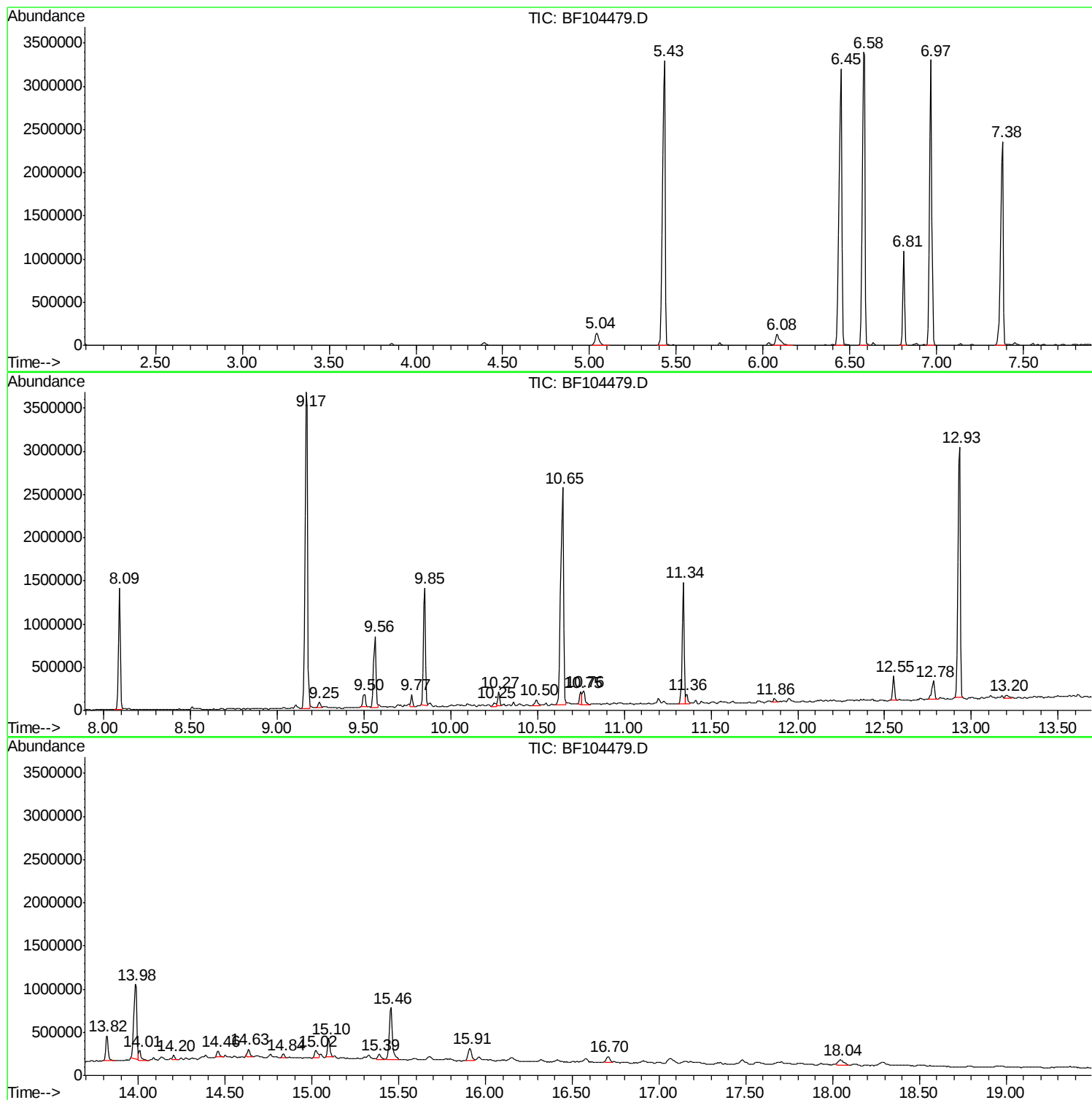
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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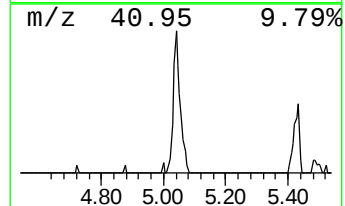
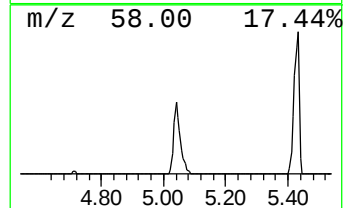
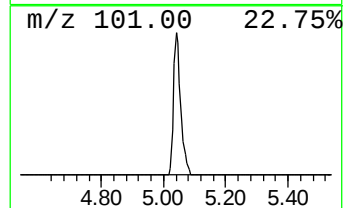
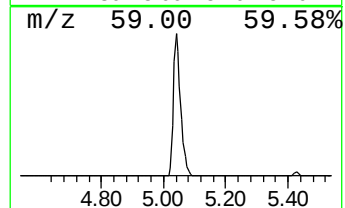
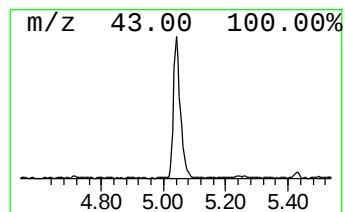
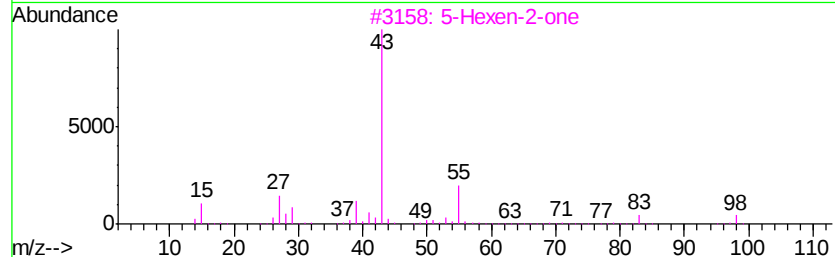
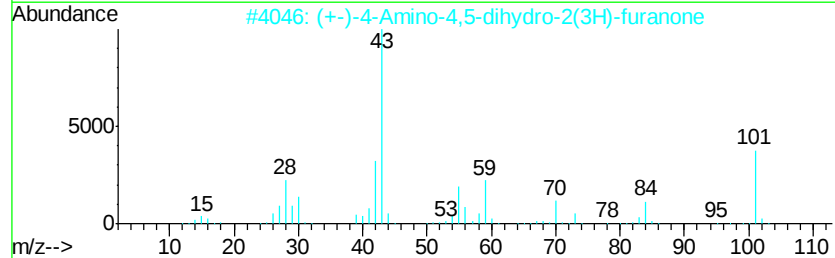
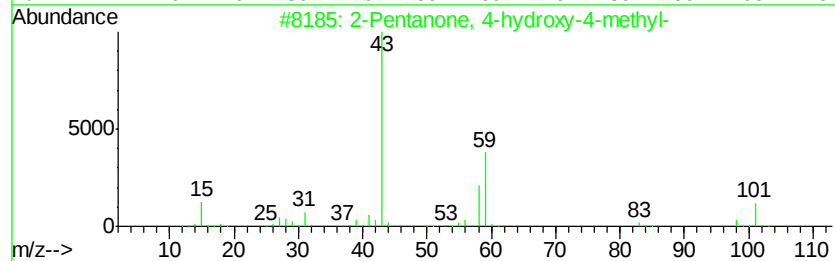
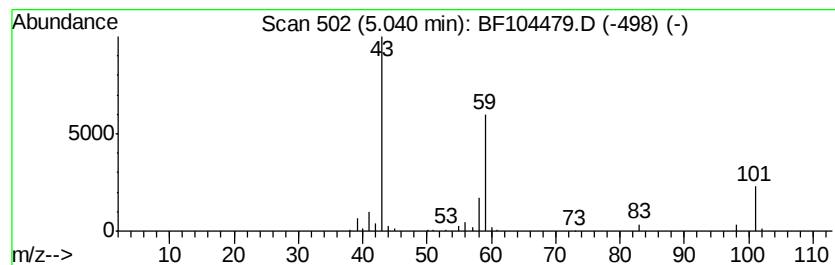
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	5.40 ng	224559	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	9
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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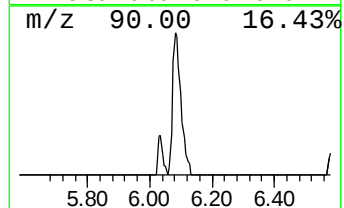
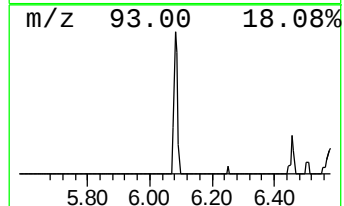
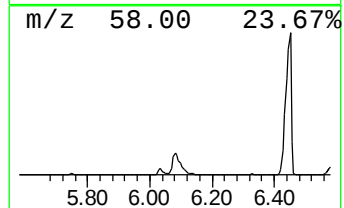
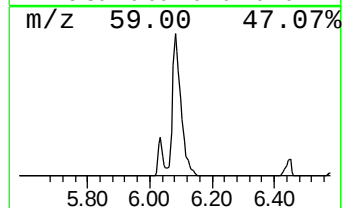
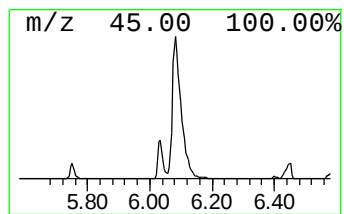
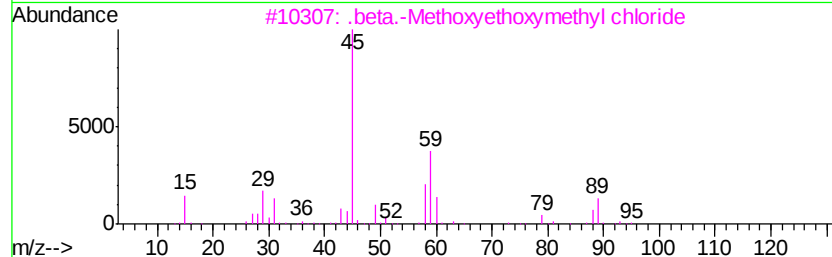
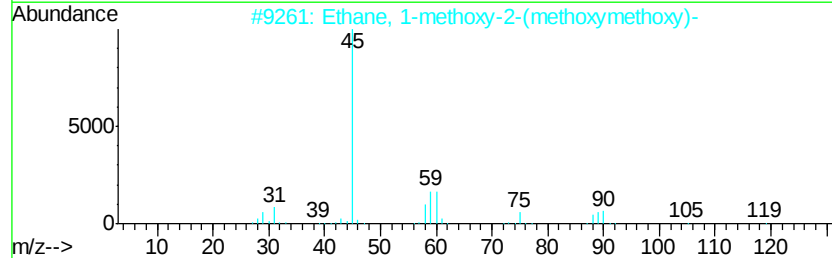
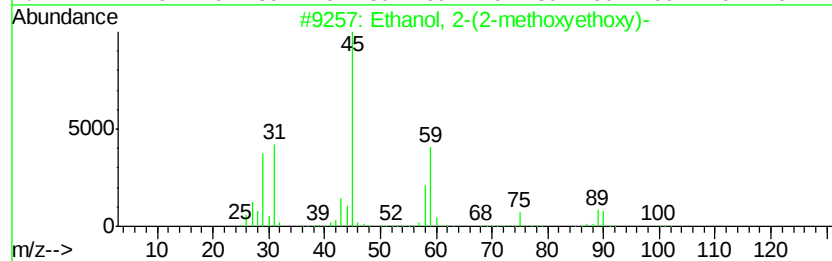
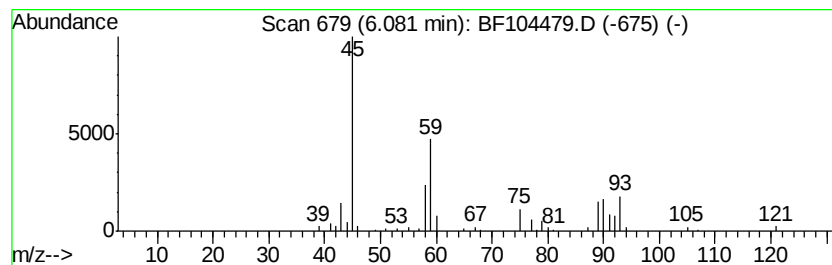
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.08	5.49 ng	228454	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	78
2		Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	64
3		.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	50
4		Methyl 2-(2-methoxyethoxy)acetate	148	C6H12O4	1000366-88-1	36
5		Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	33



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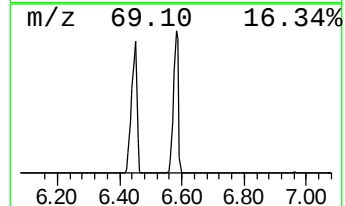
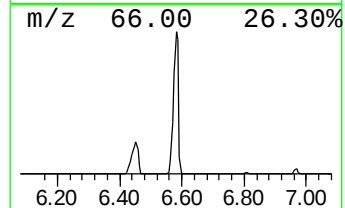
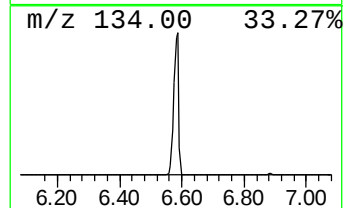
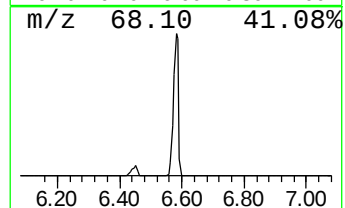
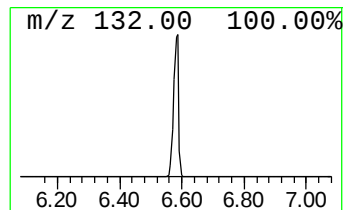
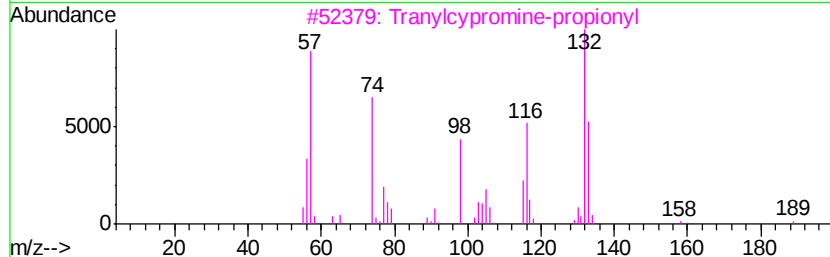
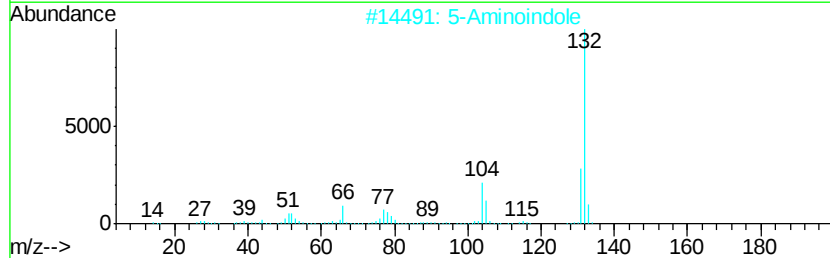
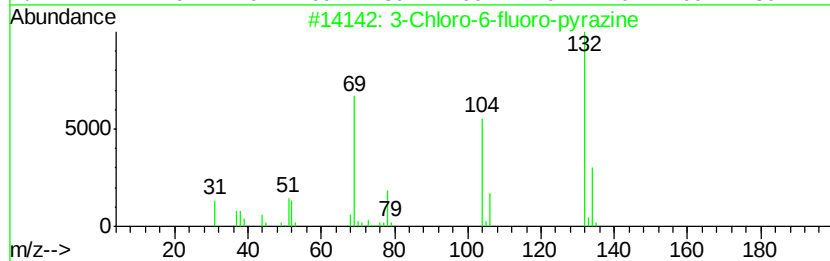
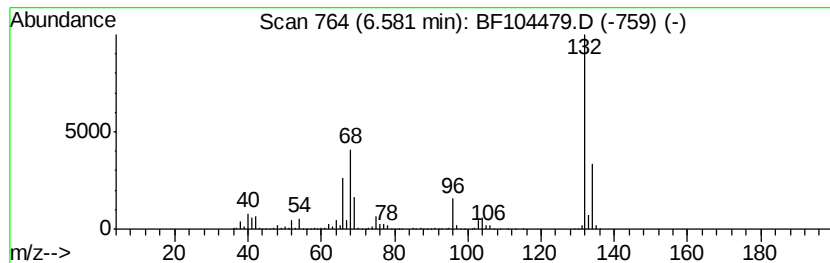
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	94.32 ng	3923890	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10	
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9	
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9	



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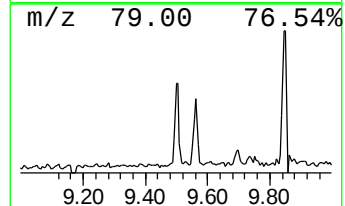
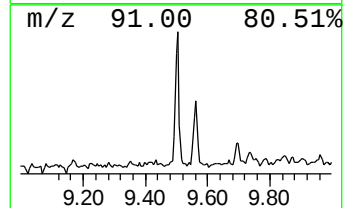
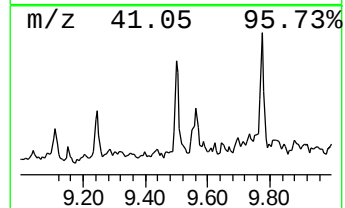
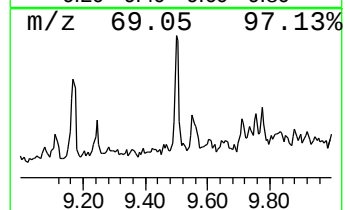
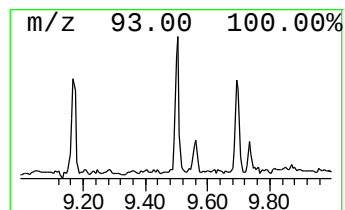
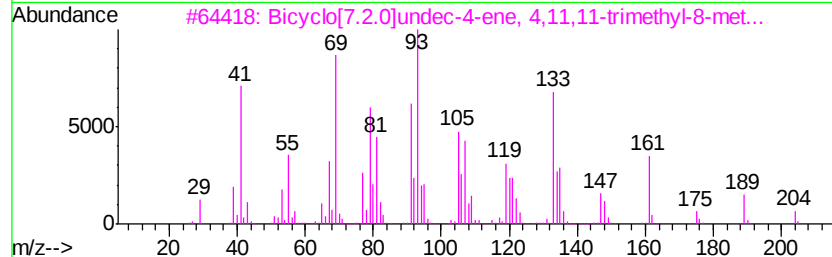
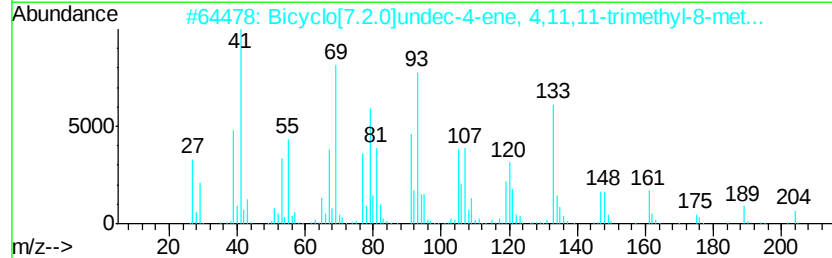
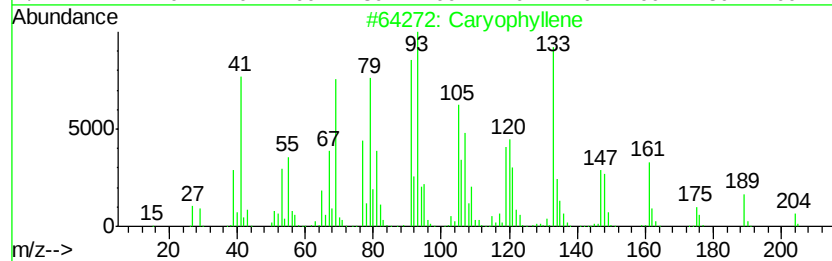
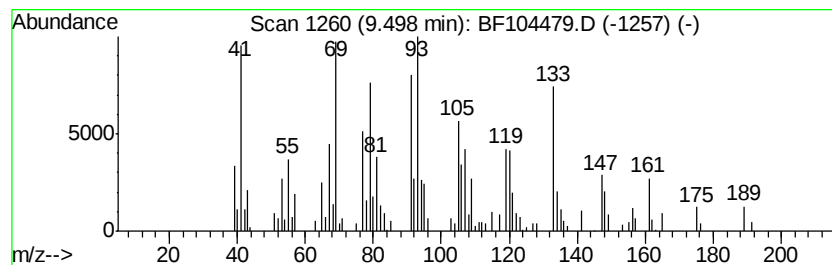
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Caryophyllene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	2.13 ng	130402	Acenaphthene-d10	9.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Caryophyllene	204	C15H24	000087-44-5	99
2		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	95
3		Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
4		Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	93
5		Alloaromadendrene	204	C15H24	025246-27-9	48



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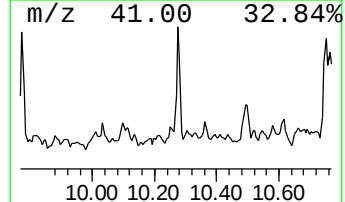
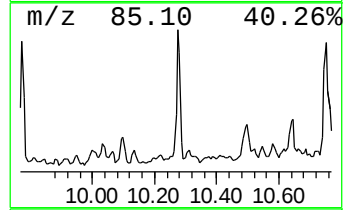
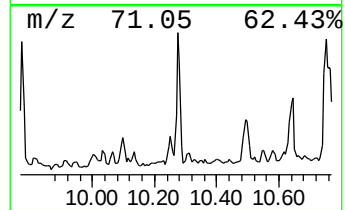
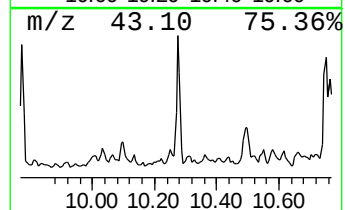
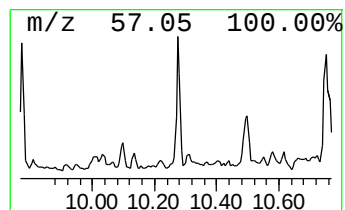
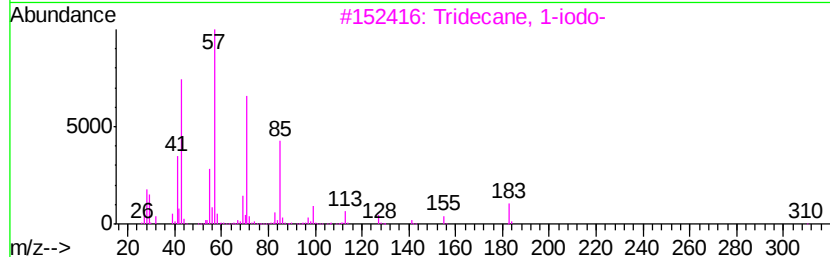
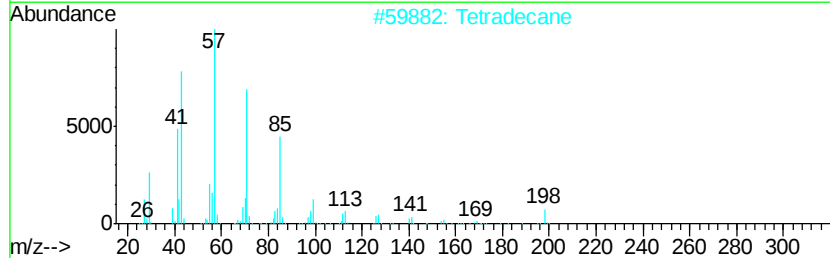
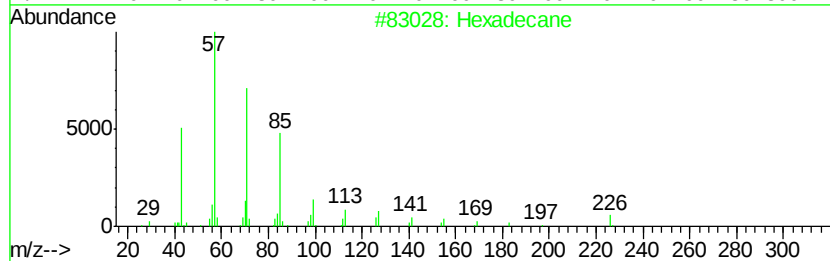
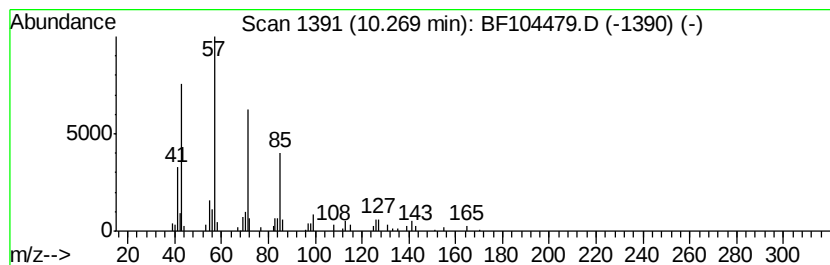
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.13 ng	130144	Acenaphthene-d10	9.85
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	97
2	Tetradecane	198 C14H30	000629-59-4	91
3	Tridecane, 1-iodo-	310 C13H27I	035599-77-0	90
4	Dodecane, 1-iodo-	296 C12H25I	004292-19-7	86
5	Pentadecane	212 C15H32	000629-62-9	86



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Data File : BF104479.D
Acq On : 13 Apr 2018 15:34
Operator : JU/SJ
Sample : J2364-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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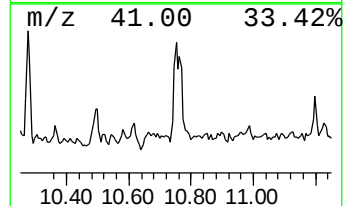
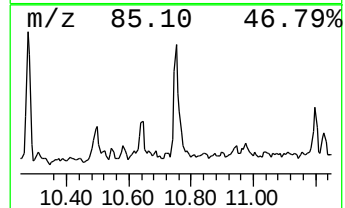
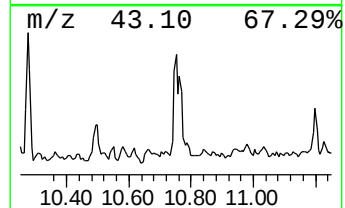
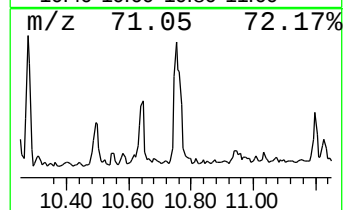
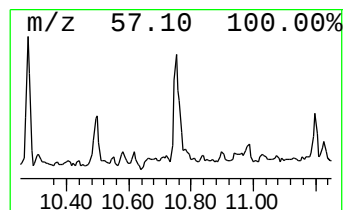
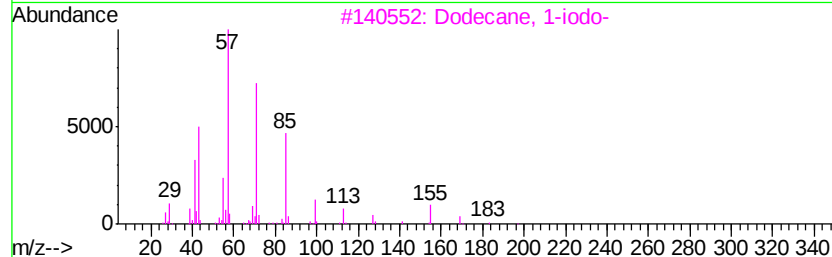
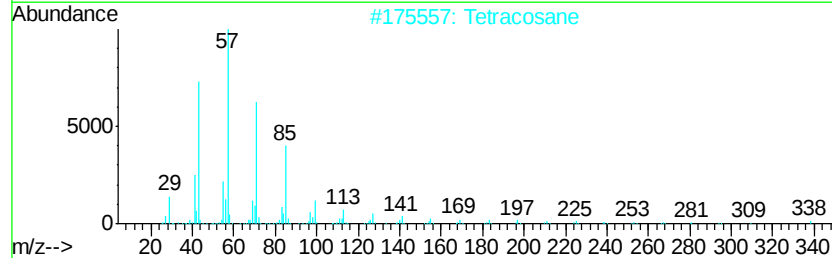
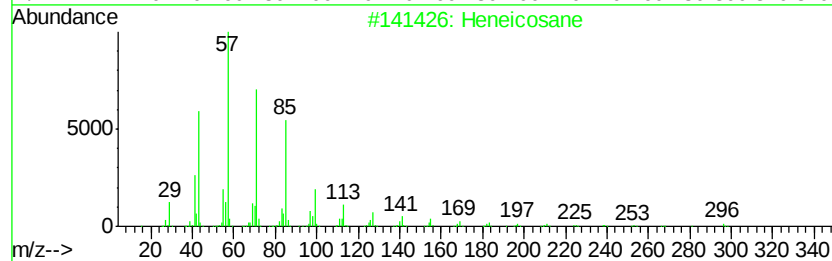
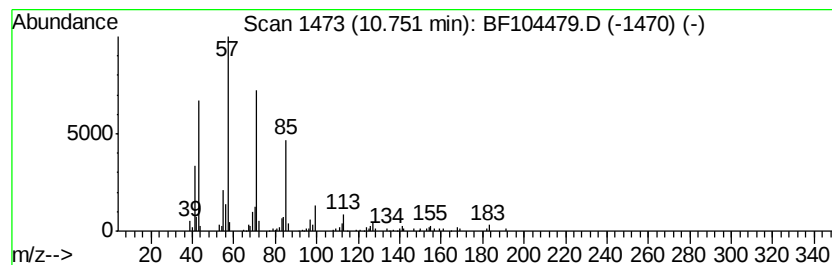
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.32 ng	135202	Phenanthrene-d10	11.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Tetracosane		338	C24H50	000646-31-1	87
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
4	Sulfurous acid, 2-propyl tetra...		320	C17H36O3S	1000309-12-5	86
5	Heptacosane		380	C27H56	000593-49-7	72



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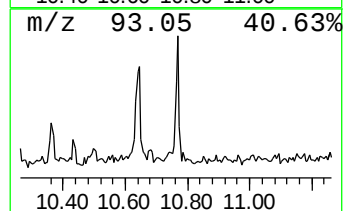
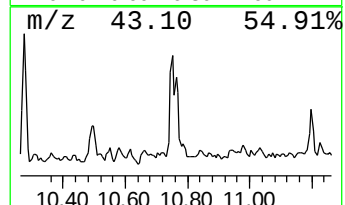
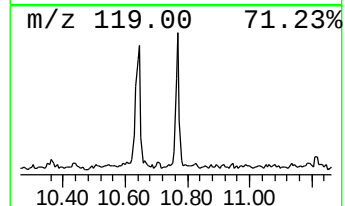
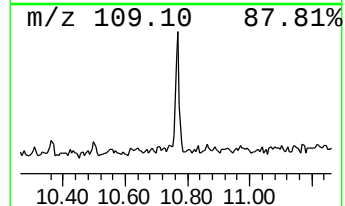
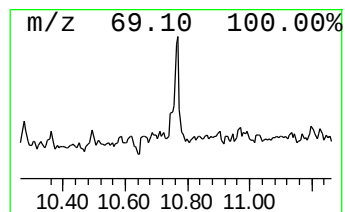
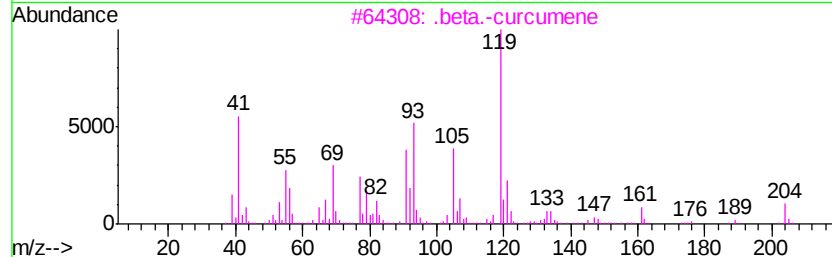
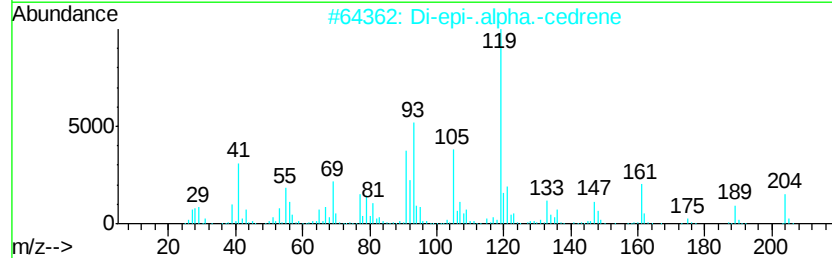
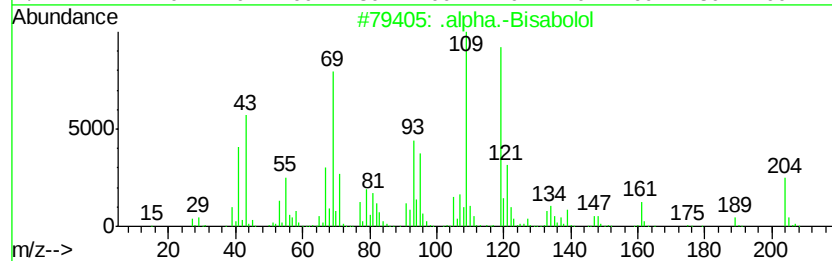
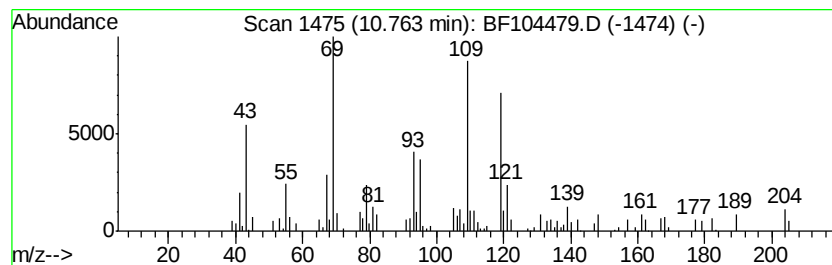
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .alpha.-Bisabolol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.76	2.46 ng	143026	Phenanthrene-d10	11.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Bisabolol	222	C15H26O	000515-69-5	78
2	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	45
3	.beta.-curcumene	204	C15H24	1000374-17-4	44
4	Cyclohexene, 3-(1,5-dimethyl-4-h...	204	C15H24	020307-83-9	38
5	trans-1,2-Bis(bromomethyl)cycloh...	268	C8H14Br2	1000216-87-8	22



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Operator : JU/SJ
Sample : J2364-01
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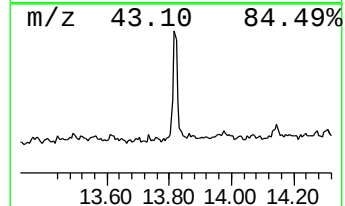
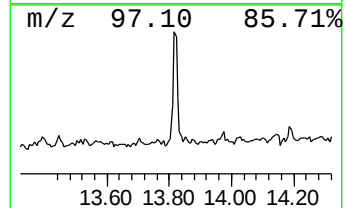
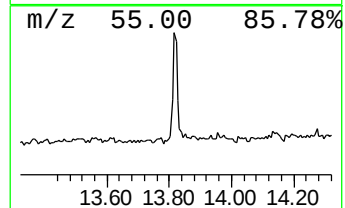
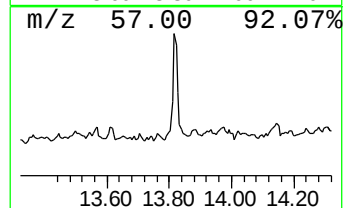
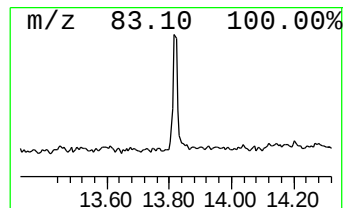
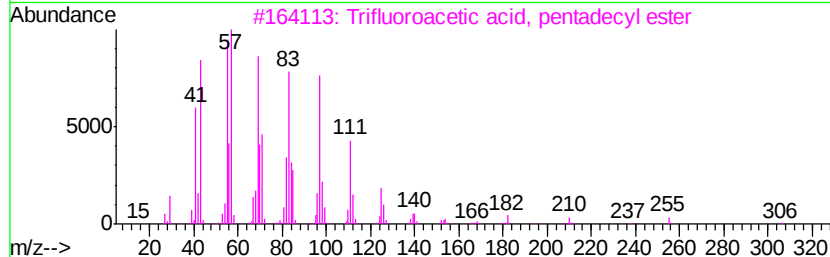
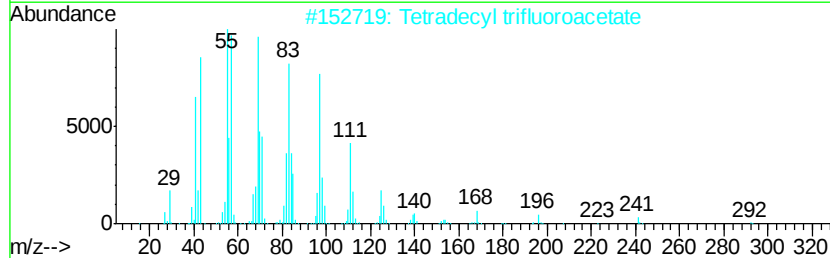
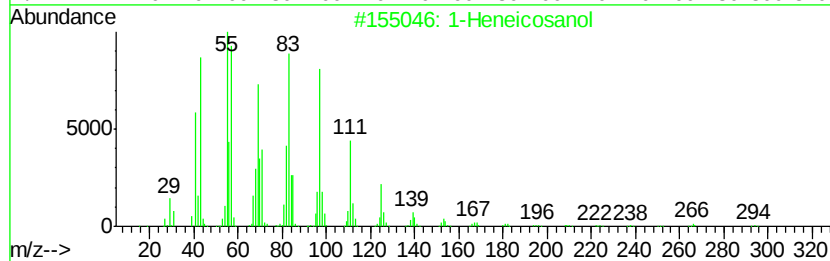
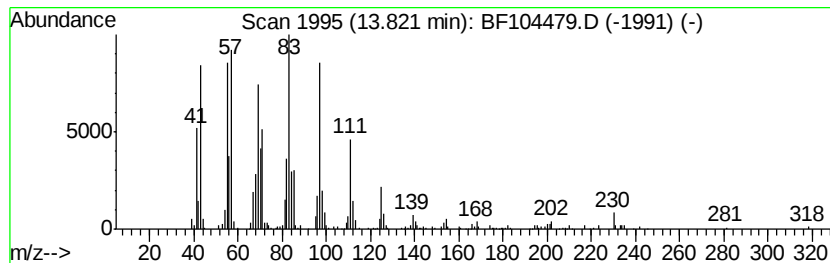
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	6.86 ng	317772	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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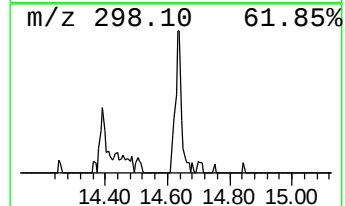
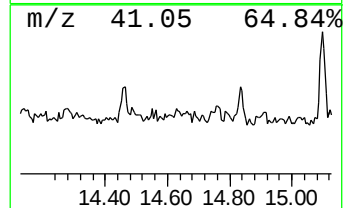
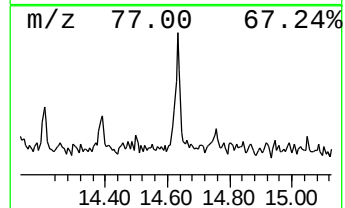
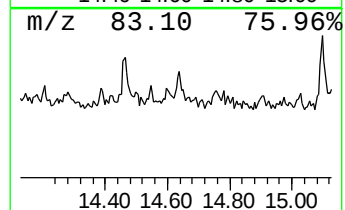
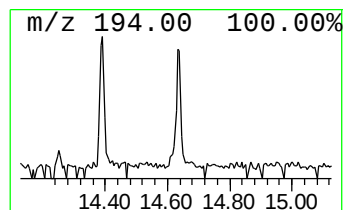
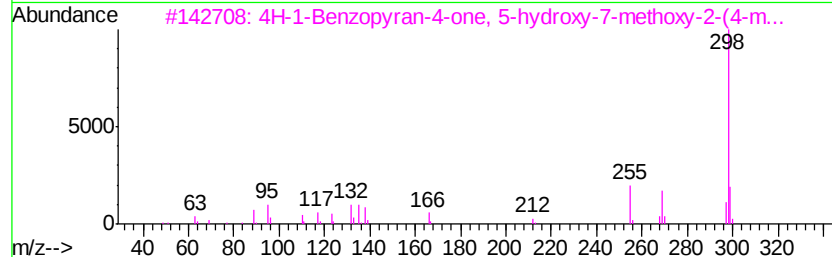
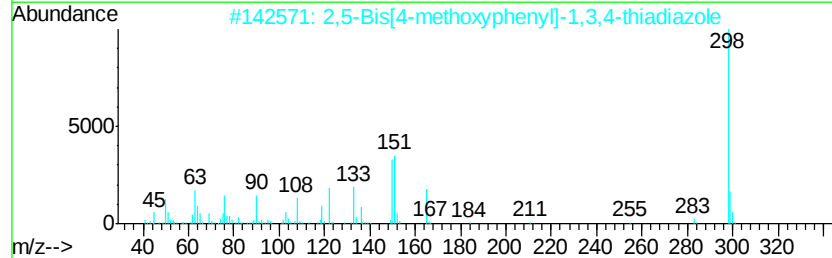
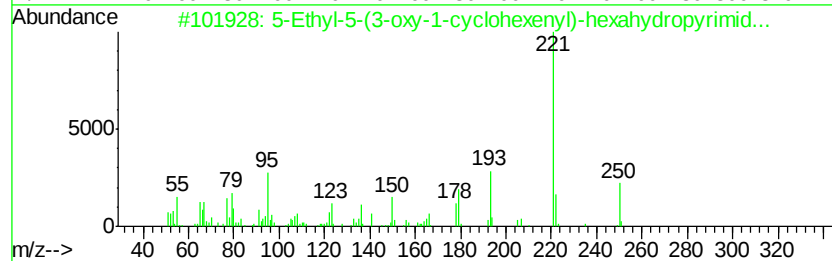
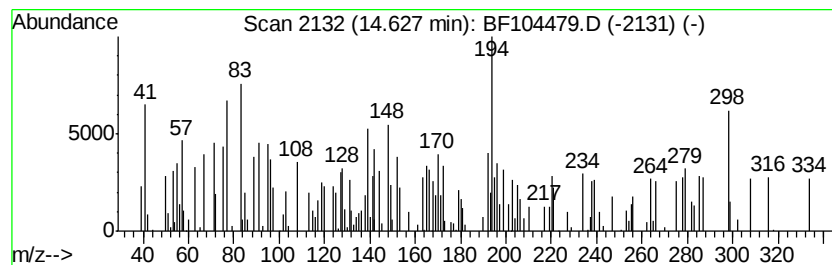
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown14.63 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.04 ng	94519	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Ethyl-5-(3-oxv-1-cvclohexenvl)...	250	C12H14N2O4	035305-10-3	25
2		2,5-Bis[4-methoxyphenyl]-1,3,4-t...	298	C16H14N2O2S	017453-03-1	25
3		4H-1-Benzopvran-4-one, 5-hydroxv...	298	C17H14O5	005128-44-9	15
4		Vanillin, pentafluoropropionate	298	C11H7F5O4	1000375-93-7	15
5		1,1'-Biphenyl, 4-(1-azido-1-meth...	237	C15H15N3	051677-40-8	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
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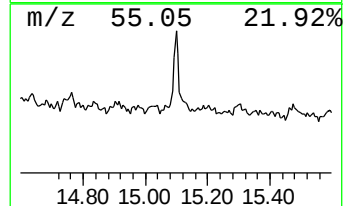
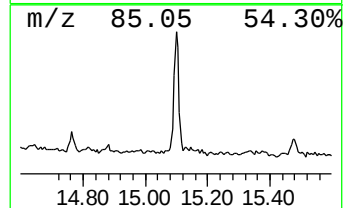
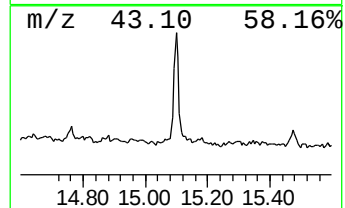
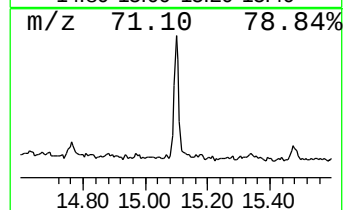
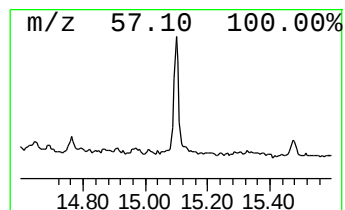
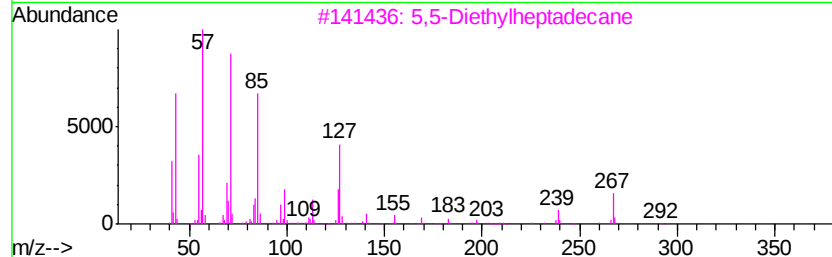
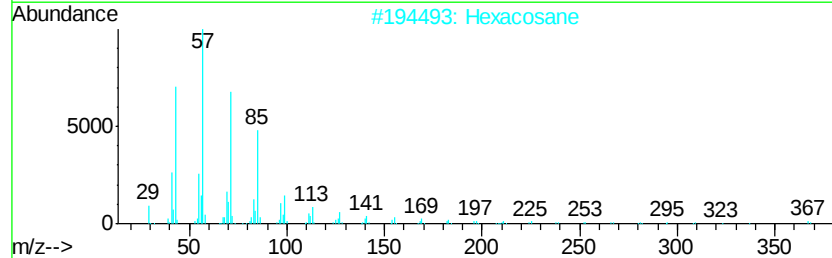
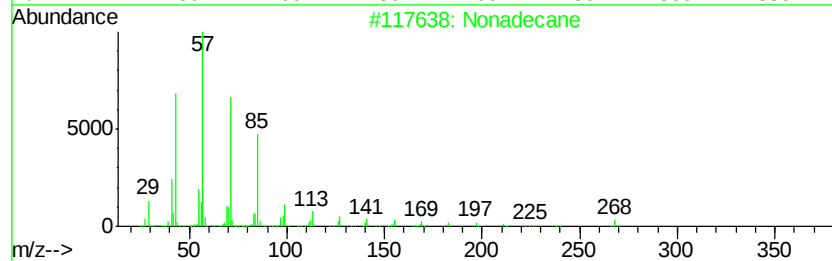
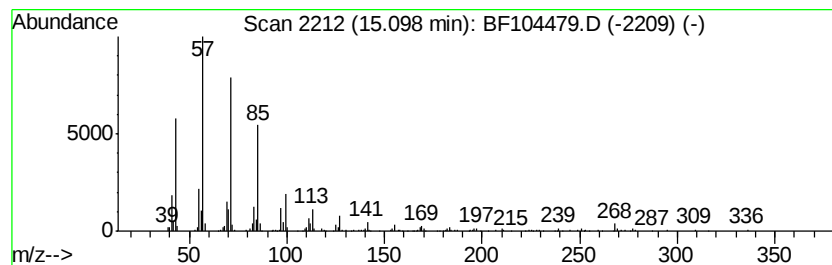
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	5.37 ng	217068	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	96
2		Hexacosane	366	C26H54	000630-01-3	90
3		5,5-Diethylheptadecane	296	C21H44	1000360-41-7	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



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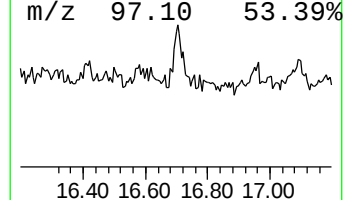
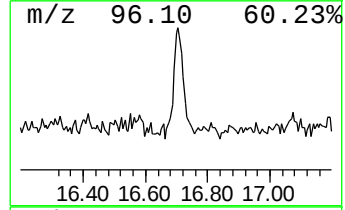
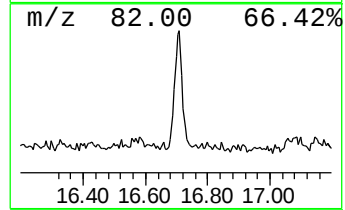
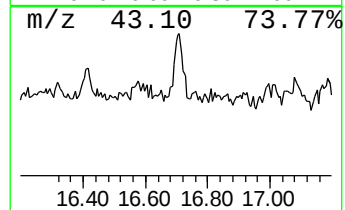
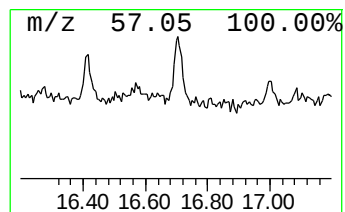
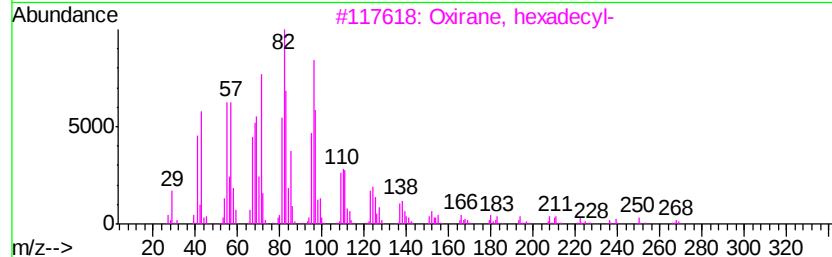
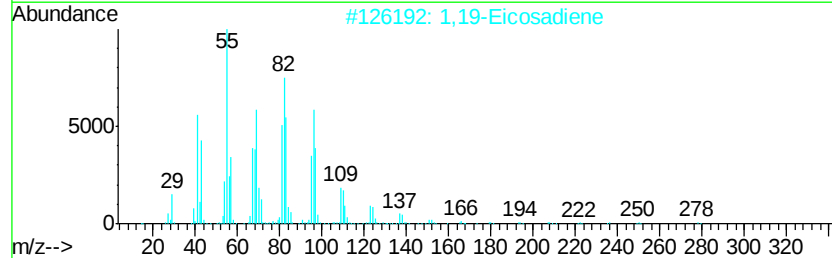
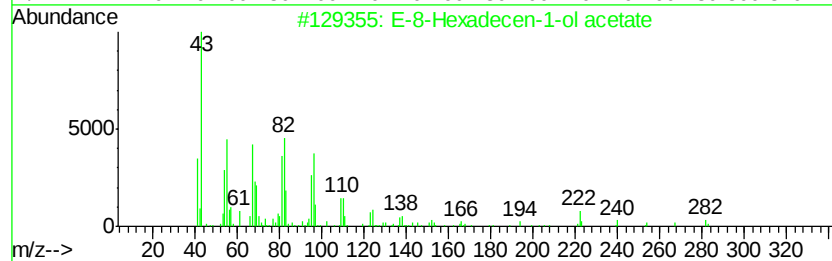
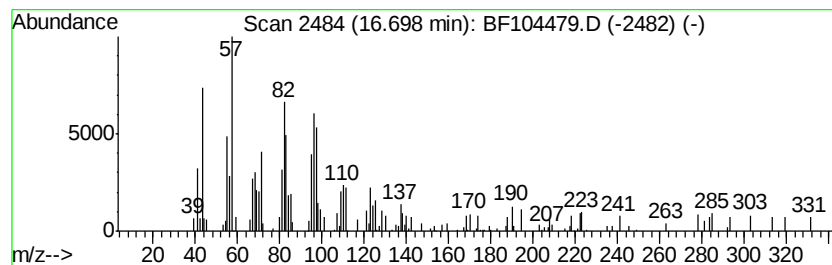
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 E-8-Hexadecen-1-ol acetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	2.32 ng	93657	Perylene-d12	15.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	86
2		1,19-Eicosadiene	278	C20H38	014811-95-1	83
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
4		Octadecanal	268	C18H36O	000638-66-4	64
5		Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	60



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
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ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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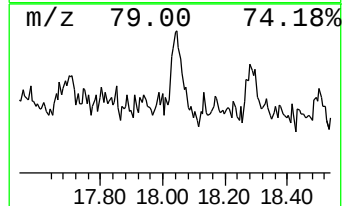
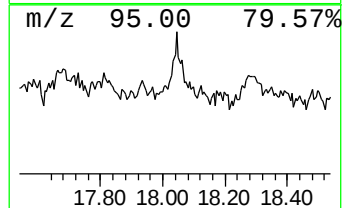
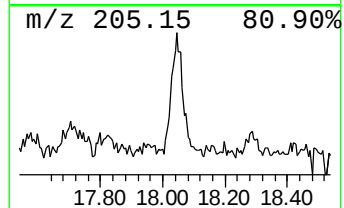
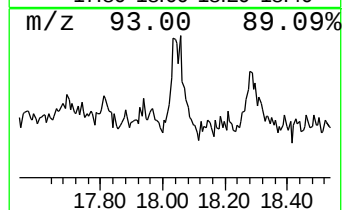
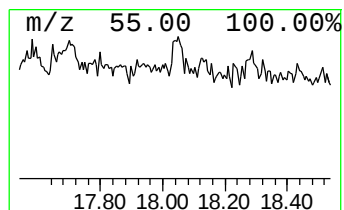
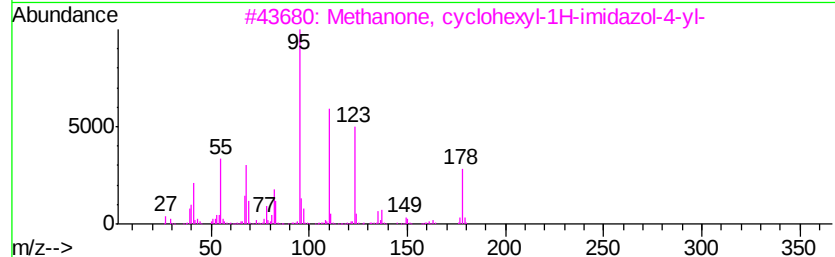
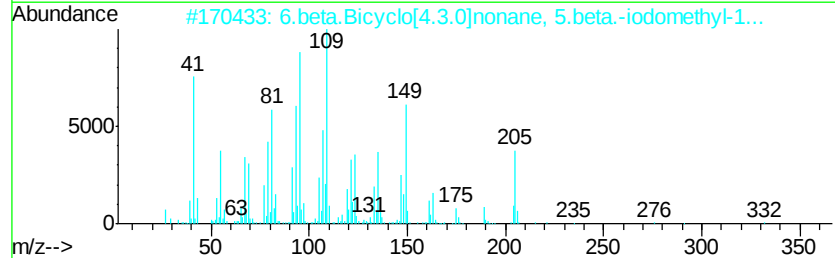
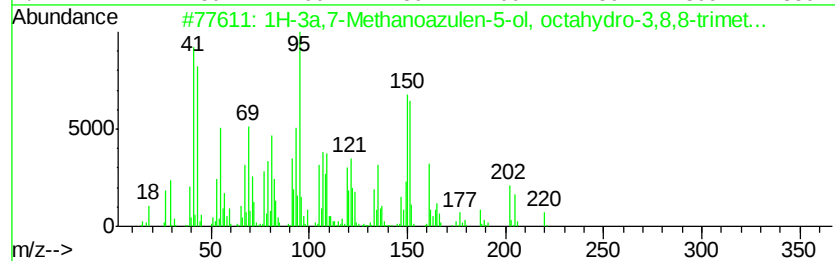
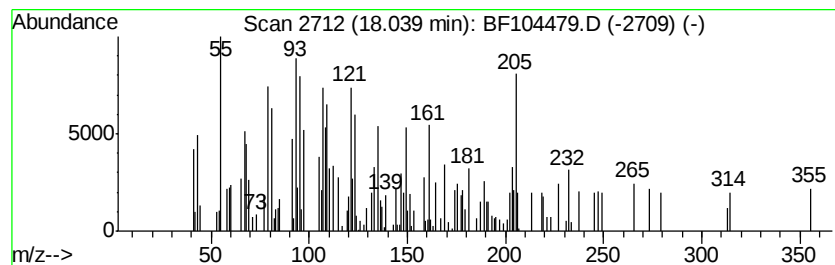
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1H-3a,7-Methanoazulen-5-ol,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	3.34 ng	135217	Perylene-d12	15.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-3a,7-Methanoazulen-5-ol, octa...	220	C15H24O	028231-03-0	50
2			6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	47
3			Methanone, cvclohexvl-1H-imidazo...	178	C10H14N2O	061985-29-3	30
4			9-Cedranone	220	C15H24O	1000156-23-2	27
5			1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
 Data File : BF104479.D
 Acq On : 13 Apr 2018 15:34
 Operator : JU/SJ
 Sample : J2364-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.04	5.4	ng	224559	1	6.81	832038	20.0
Ethanol, 2-(2-met...	6.08	5.5	ng	228454	1	6.81	832038	20.0
unknown6.58	6.58	94.3	ng	3923890	1	6.81	832038	20.0
Caryophyllene	9.50	2.1	ng	130402	3	9.85	1222250	20.0
Hexadecane	10.27	2.1	ng	130144	3	9.85	1222250	20.0
Heneicosane	10.75	2.3	ng	135202	4	11.34	1164790	20.0
.alpha.-Bisabolol	10.76	2.5	ng	143026	4	11.34	1164790	20.0
1-Heneicosanol	13.82	6.9	ng	317772	5	13.99	926682	20.0
unknown14.63	14.63	2.0	ng	94519	5	13.99	926682	20.0
Nonadecane	15.10	5.4	ng	217068	6	15.46	808777	20.0
E-8-Hexadecen-1-o...	16.70	2.3	ng	93657	6	15.46	808777	20.0
1H-3a,7-Methanoaz...	18.04	3.3	ng	135217	6	15.46	808777	20.0