

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF032218\
 Data File : BF103845.D
 Acq On : 22 Mar 2018 11:55
 Operator : JU/SJ
 Sample : J1946-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-104(14-15)

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-BF031518.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	2.322	33	40	46	rVB	134711	184990	4.52%	0.499%
2	5.222	526	533	544	rVB	91601	120078	2.93%	0.324%
3	5.598	591	597	600	rBV	3552132	3734318	91.15%	10.068%
4	5.916	648	651	660	rVB	123342	110723	2.70%	0.299%
5	6.592	760	766	770	rBV	3099551	3780016	92.26%	10.191%
6	6.739	786	791	795	rBV	3475331	3797103	92.68%	10.237%
7	6.969	827	830	834	rBV	1047415	844664	20.62%	2.277%
8	7.128	853	857	860	rBV	3312193	2989242	72.96%	8.059%
9	7.533	920	926	929	rBV	2417779	2434940	59.43%	6.565%
10	8.251	1044	1048	1052	rBV	1392979	1157772	28.26%	3.121%
11	9.327	1226	1231	1234	rBV	4303829	4097072	100.00%	11.046%
12	9.716	1293	1297	1300	rBV	419887	332285	8.11%	0.896%
13	9.927	1327	1333	1336	rVB	100520	84730	2.07%	0.228%
14	10.010	1343	1347	1351	rBV2	1465179	1308564	31.94%	3.528%
15	10.427	1415	1418	1421	rVB	137602	99652	2.43%	0.269%
16	10.645	1451	1455	1458	rBV	35125	44266	1.08%	0.119%
17	10.804	1478	1482	1486	rBV	2615458	2624955	64.07%	7.077%
18	10.898	1496	1498	1503	rVB	101827	102145	2.49%	0.275%
19	11.351	1571	1575	1578	rBV	56608	46477	1.13%	0.125%
20	11.504	1597	1601	1604	rBV	1517338	1317451	32.16%	3.552%
21	11.527	1604	1605	1610	rVB2	66198	43923	1.07%	0.118%
22	12.016	1684	1688	1697	rBV3	111062	146195	3.57%	0.394%
23	12.721	1804	1808	1812	rBV	65974	59480	1.45%	0.160%
24	12.951	1845	1847	1849	rBV	58593	47778	1.17%	0.129%
25	13.098	1866	1872	1875	rBV	3691335	3884255	94.81%	10.472%
26	13.557	1938	1950	1954	rBV9	119647	346044	8.45%	0.933%
27	13.674	1967	1970	1977	rVB3	32335	48021	1.17%	0.129%
28	13.933	2006	2014	2015	rBV4	31309	60041	1.47%	0.162%
29	13.968	2017	2020	2030	rVB	640378	680516	16.61%	1.835%
30	14.157	2047	2052	2055	rBV	1275013	1129781	27.58%	3.046%
31	14.615	2127	2130	2137	rVB3	51593	56921	1.39%	0.153%
32	15.086	2207	2210	2213	rBV4	29919	44815	1.09%	0.121%
33	15.151	2214	2221	2223	rBV4	61537	125575	3.06%	0.339%
34	15.692	2308	2313	2320	rBV	685693	911691	22.25%	2.458%

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Instrument :
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MW-104(14-15)

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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.215	2397	2402	2412	rBV	68348	133885	3.27%	0.361%
36	17.439	2605	2610	2619	rVB9	21308	47089	1.15%	0.127%
37	17.874	2678	2684	2694	rVB9	46254	113229	2.76%	0.305%

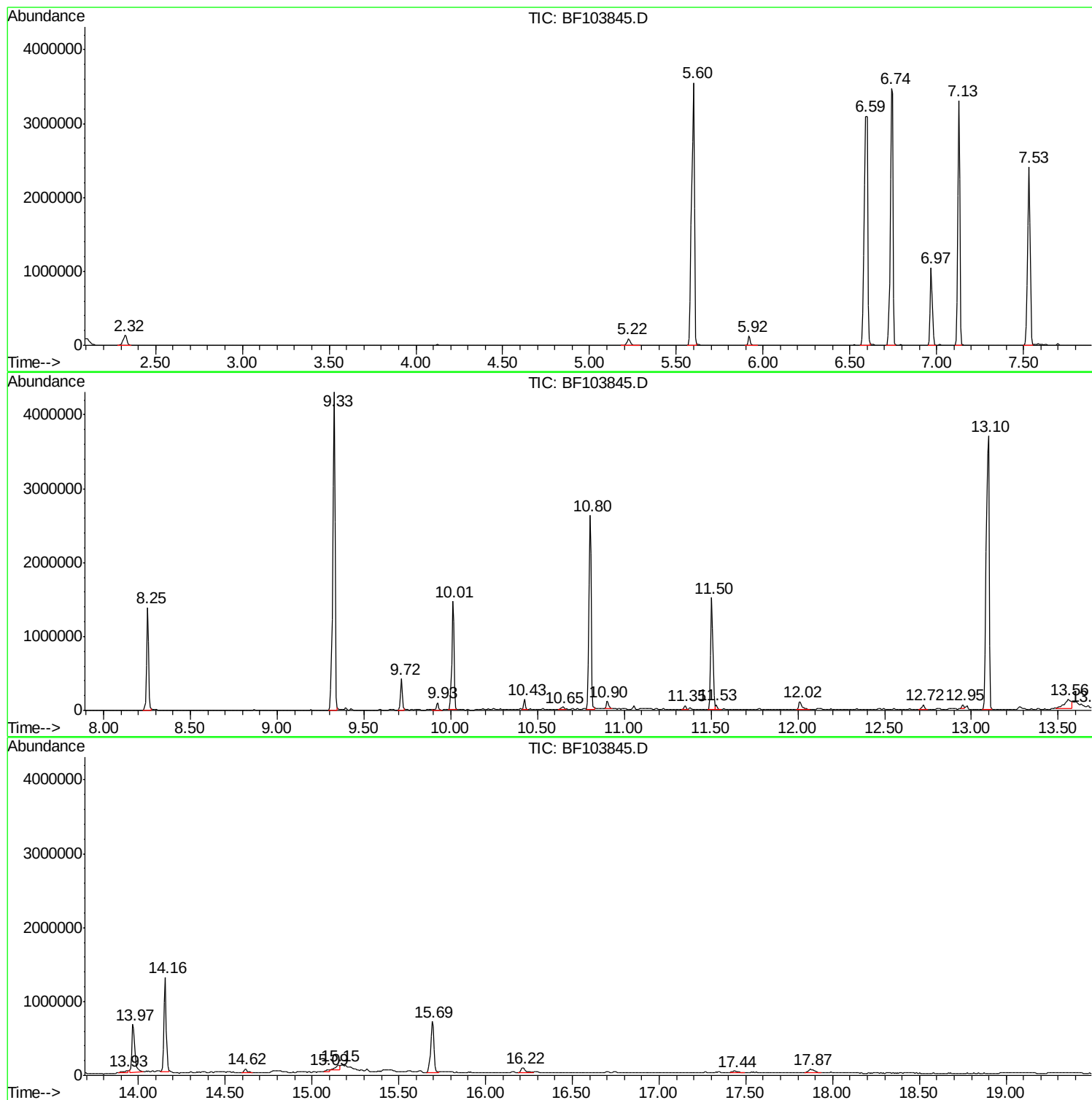
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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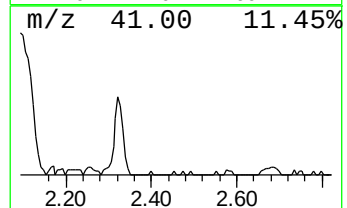
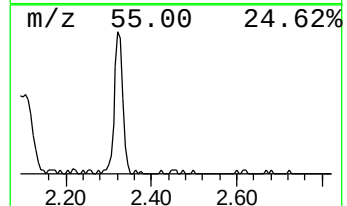
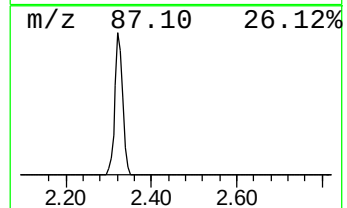
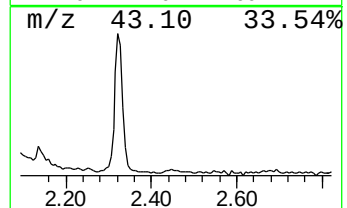
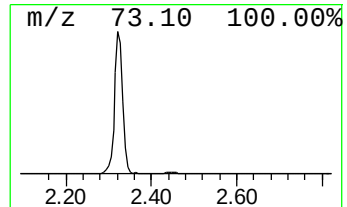
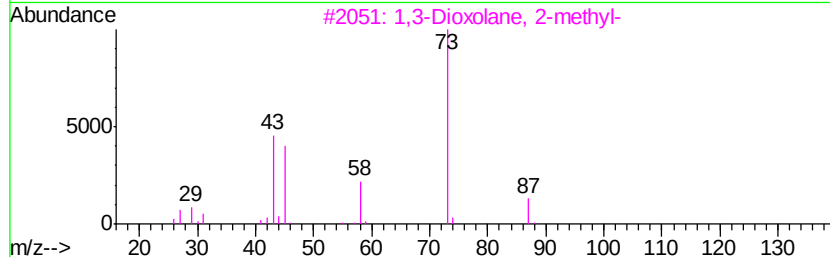
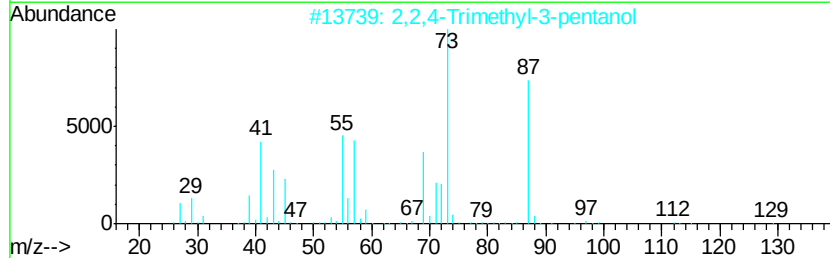
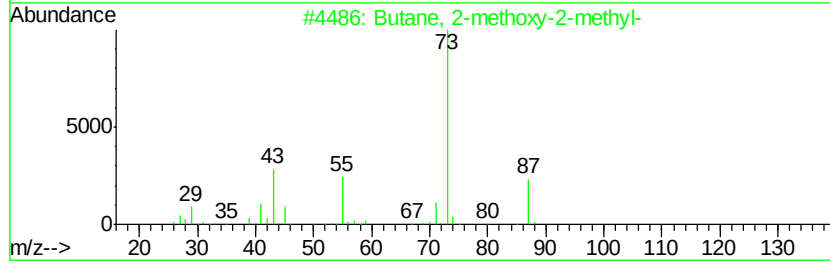
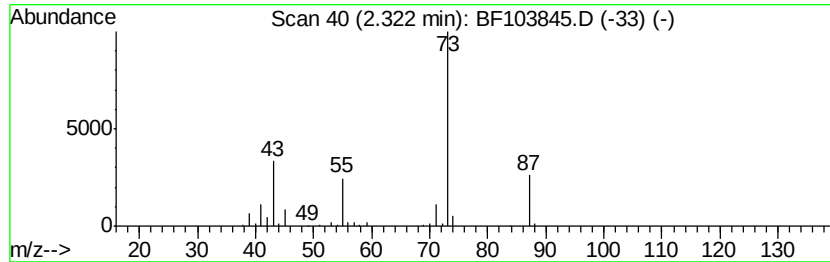
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	4.38 ng	184990	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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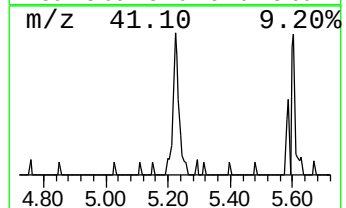
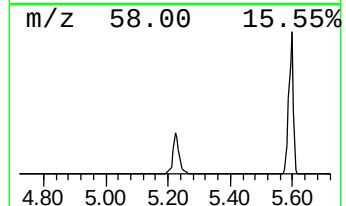
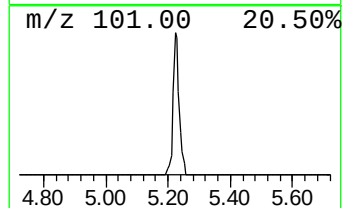
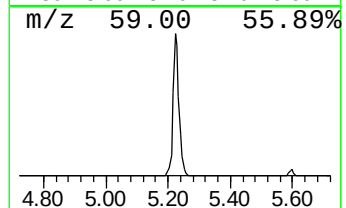
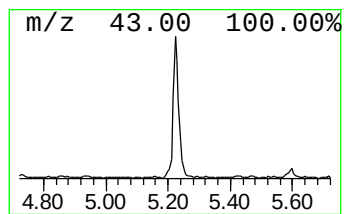
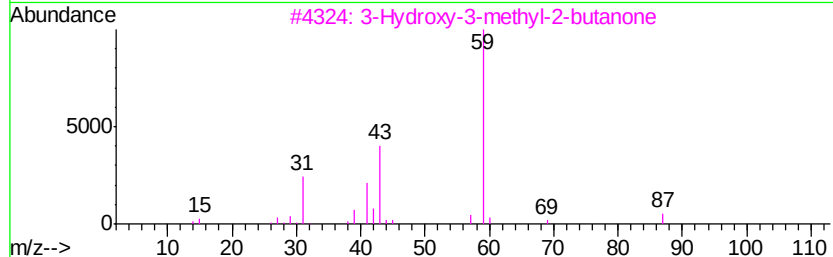
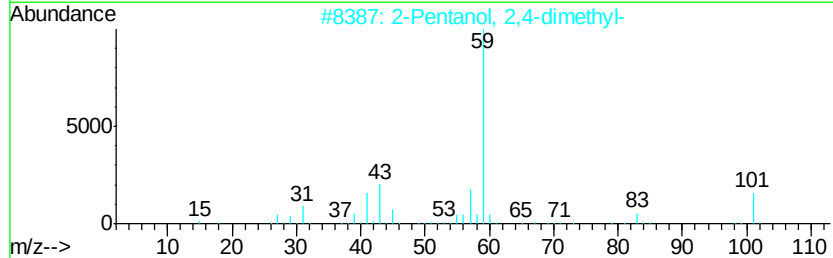
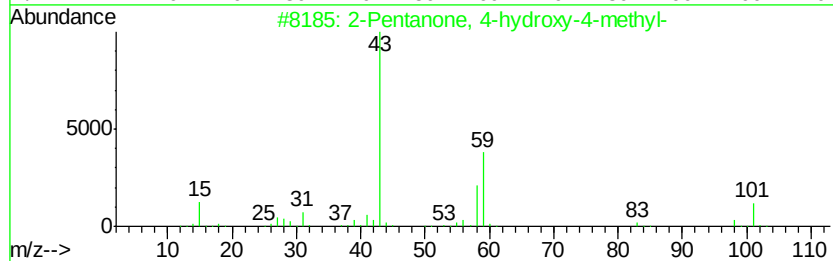
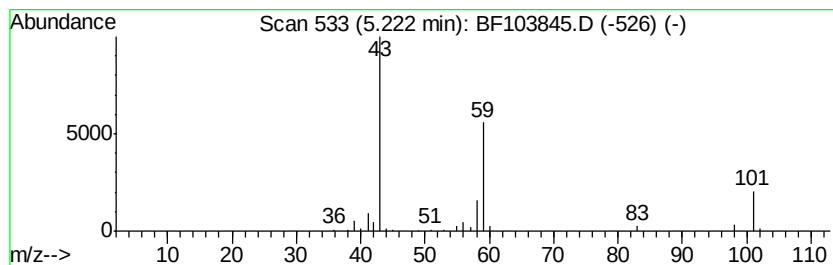
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.22 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.84 ng	120078	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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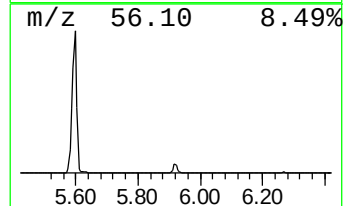
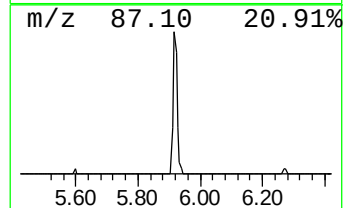
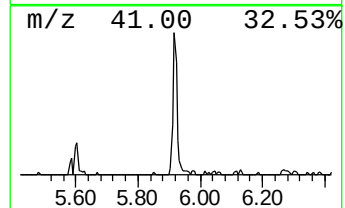
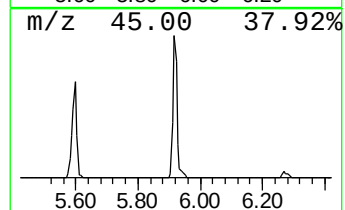
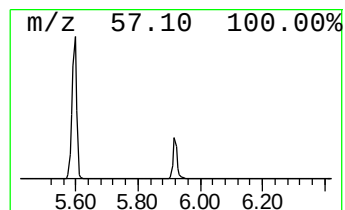
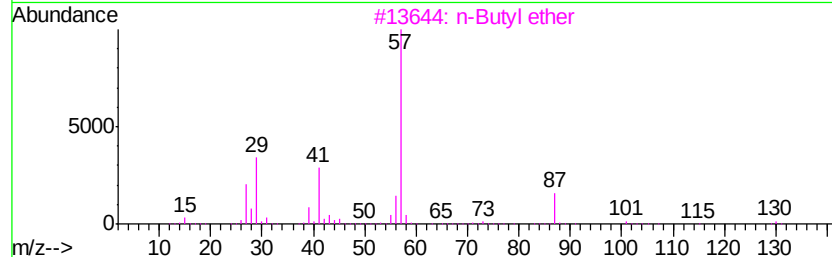
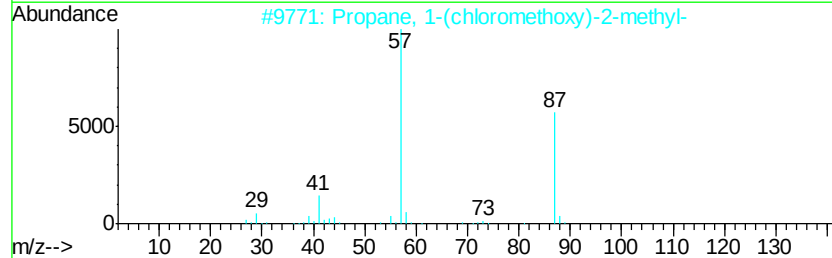
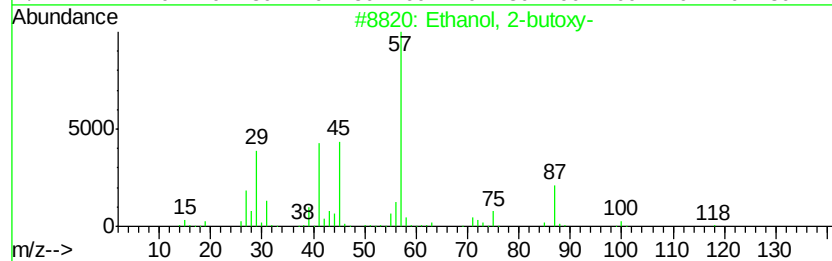
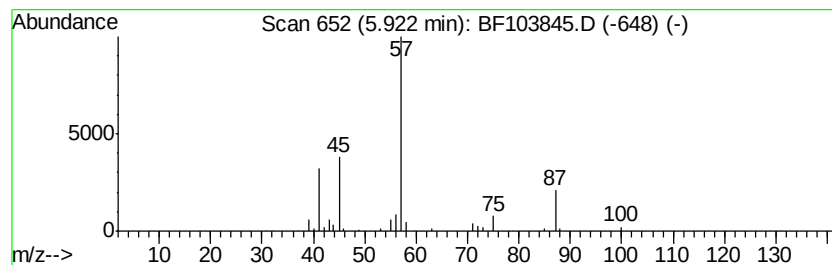
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	2.62 ng	110723	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	72
2		Propane, 1-(chloromethoxy)-2-met...	122	C5H11ClO	034180-11-5	43
3		n-Butyl ether	130	C8H18O	000142-96-1	37
4		Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	36
5		Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	28



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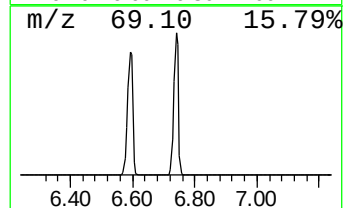
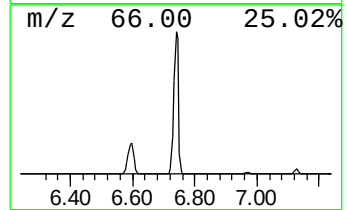
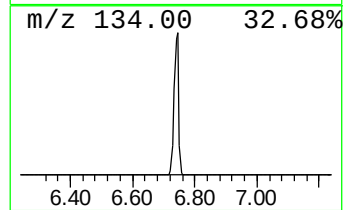
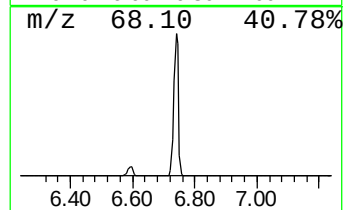
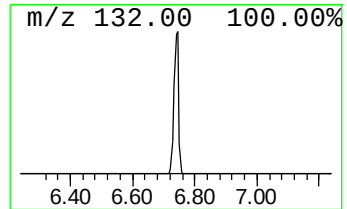
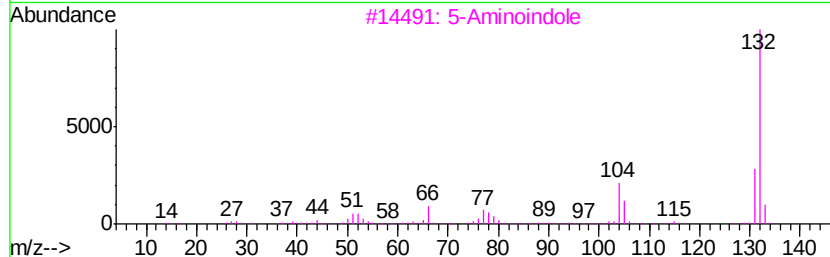
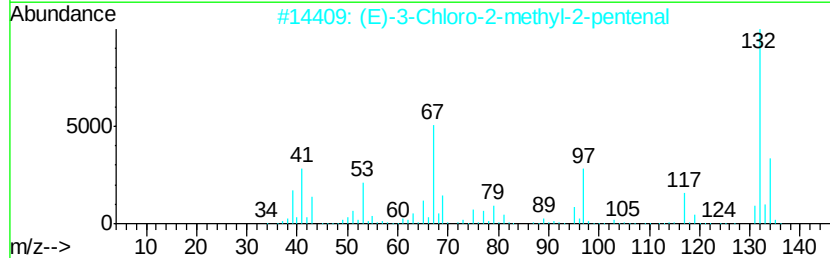
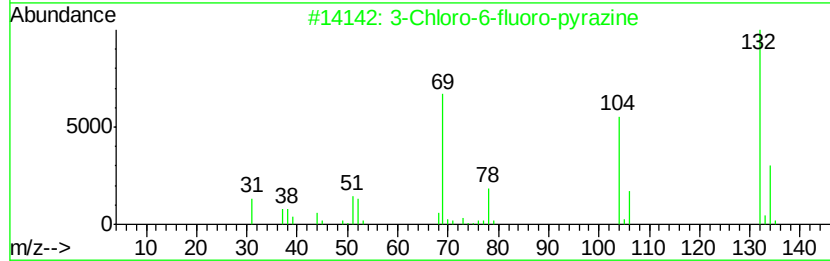
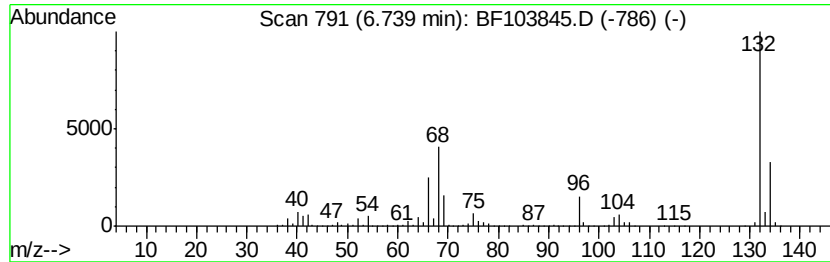
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	89.91 ng	3797100	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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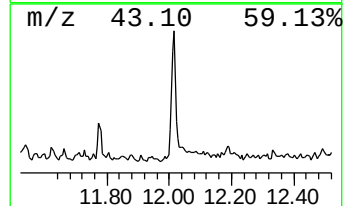
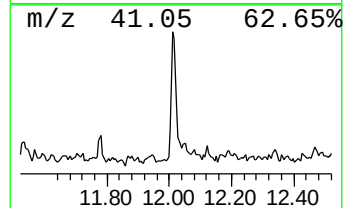
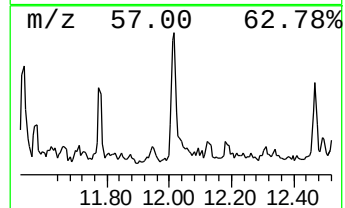
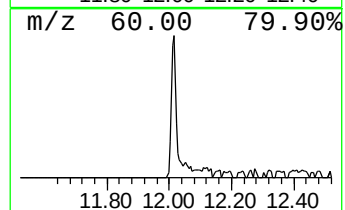
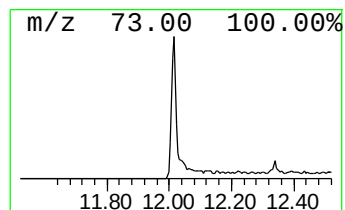
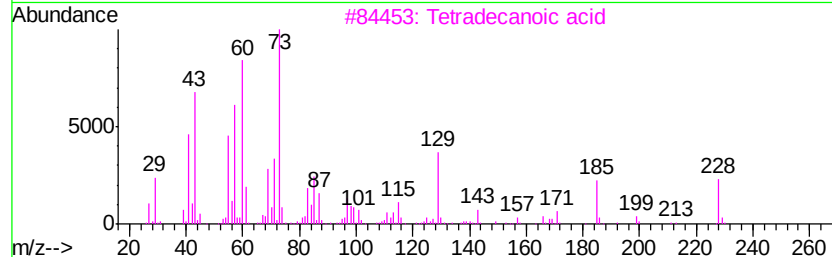
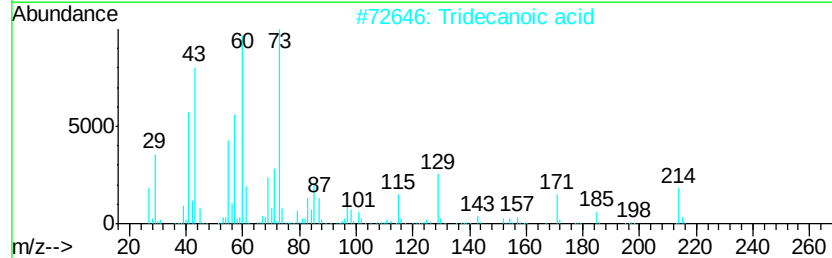
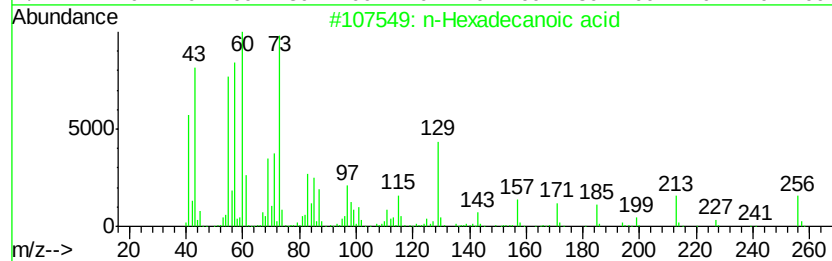
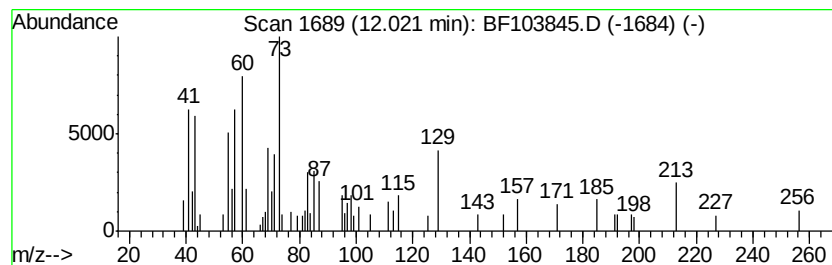
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.22 ng	146195	Phenanthrene-d10	11.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5		Tetradecane	198	C14H30	000629-59-4	53



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Acq On : 22 Mar 2018 11:55
Operator : JU/SJ
Sample : J1946-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

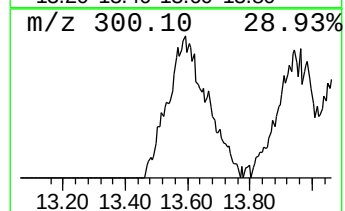
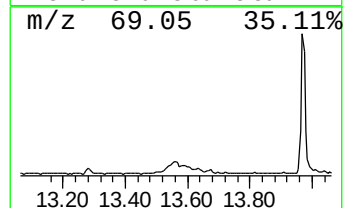
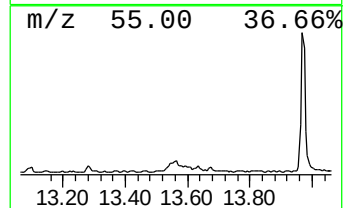
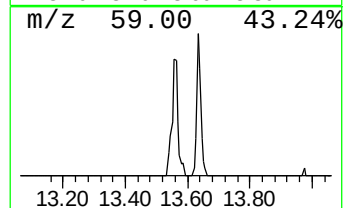
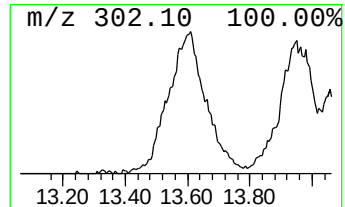
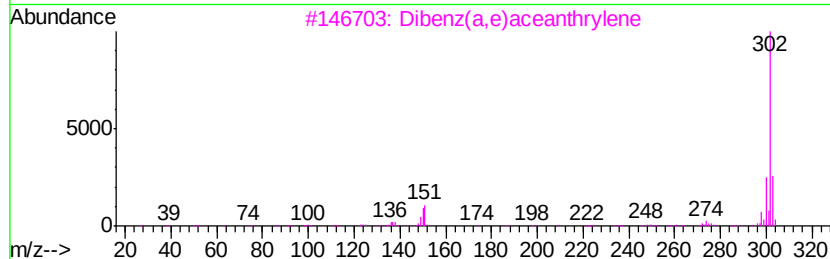
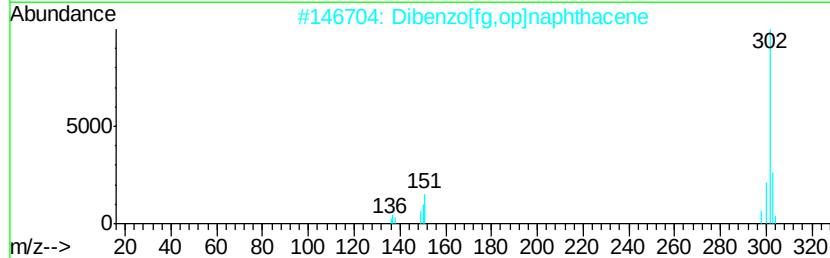
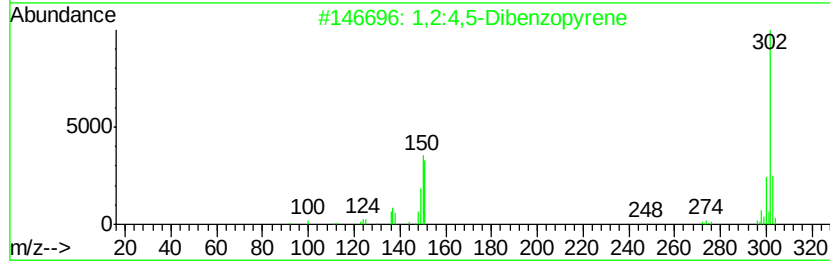
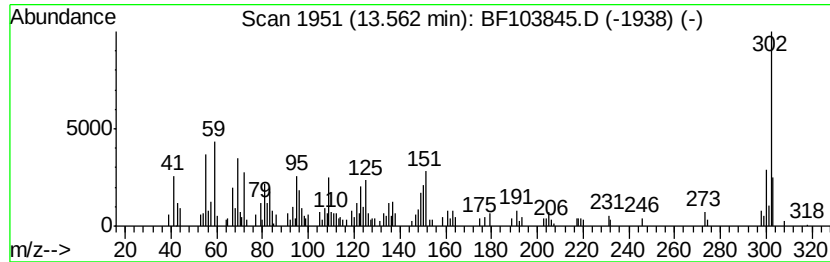
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ClientSampleId :
MW-104(14-15)

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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 1,2:4,5-Dibenzopyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.56	6.13 ng	346044	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	60
2	Dibenzo[fg,op]naphthacene	302	C24H14	000192-51-8	58
3	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	58
4	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	52
5	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	49



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103845.D
Acq On : 22 Mar 2018 11:55
Operator : JU/SJ
Sample : J1946-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-104(14-15)

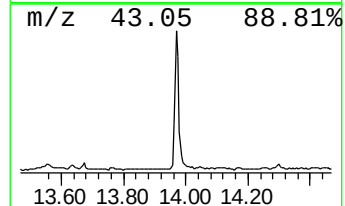
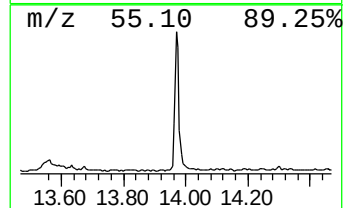
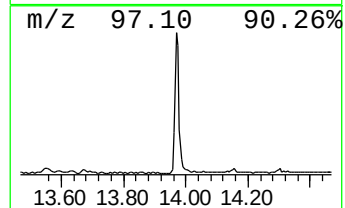
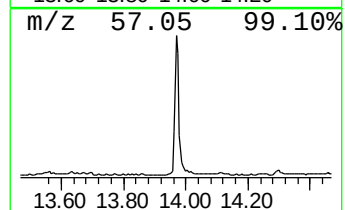
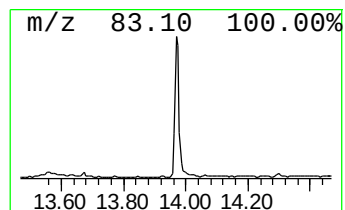
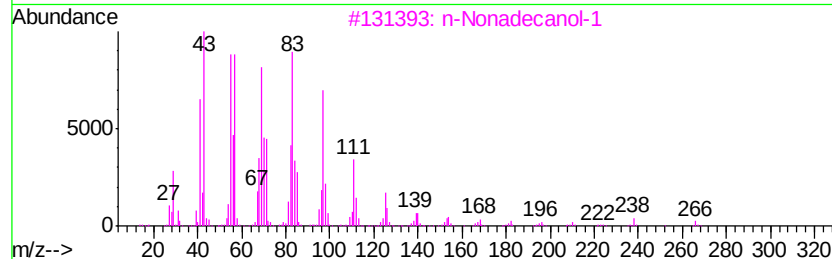
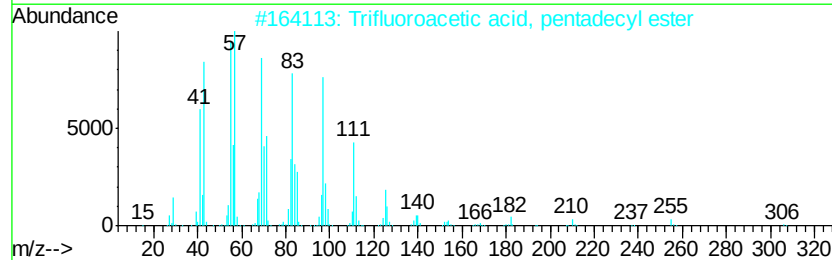
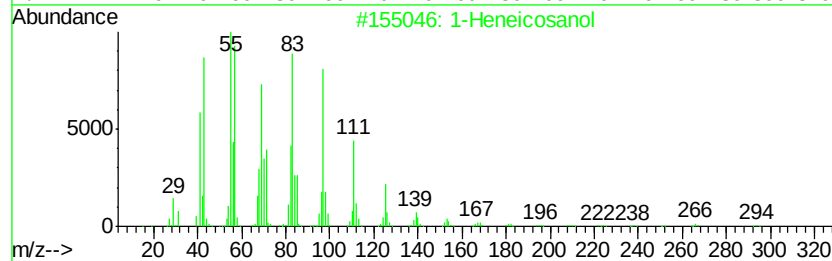
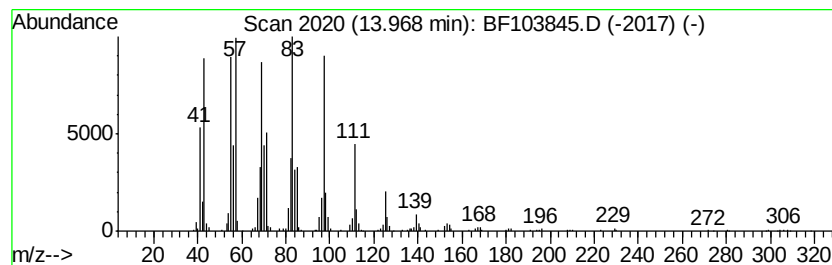
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	12.05 ng	680516	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103845.D
Acq On : 22 Mar 2018 11:55
Operator : JU/SJ
Sample : J1946-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-104(14-15)

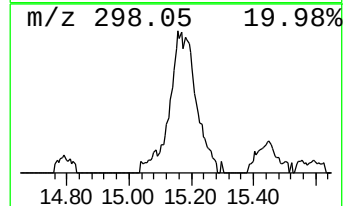
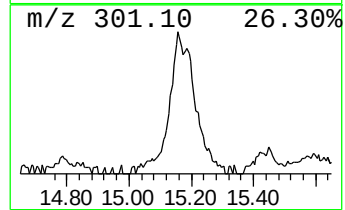
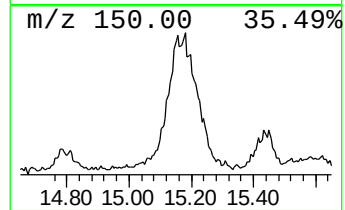
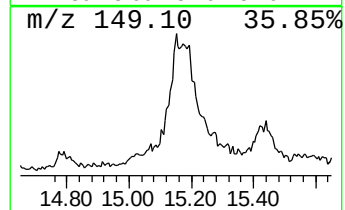
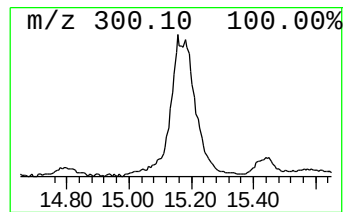
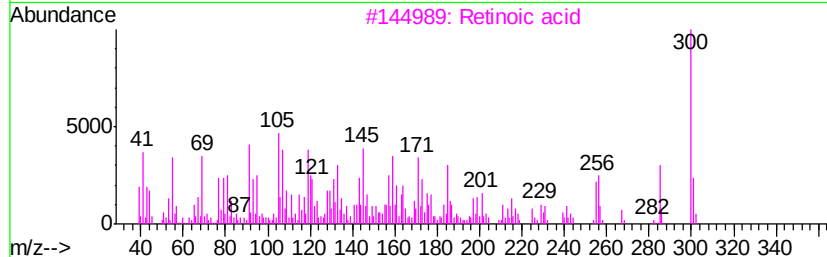
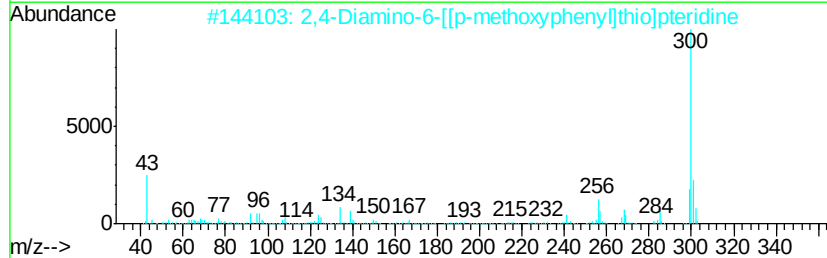
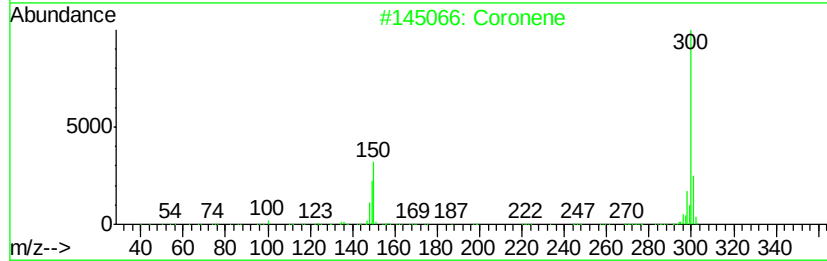
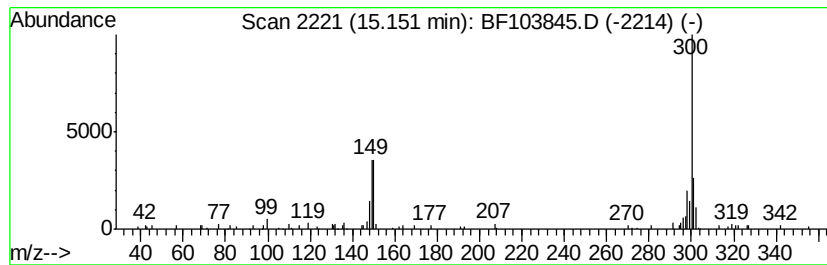
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Coronene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	2.75 ng	125575	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Coronene	300	C24H12	000191-07-1	95
2		2,4-Diamino-6-[[p-methoxyphenyl]...	300	C13H12N6OS	077900-97-1	47
3		Retinoic acid	300	C20H28O2	000302-79-4	38
4		But-2-enoic acid, 3-(1,2,3,6-tet...	300	C18H24N2O2	1000302-46-1	32
5		Silane, dimethyldi(2,3-dimethylp...	300	C18H24O2Si	1000347-44-7	28



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF032218\
Data File : BF103845.D
Acq On : 22 Mar 2018 11:55
Operator : JU/SJ
Sample : J1946-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-104(14-15)

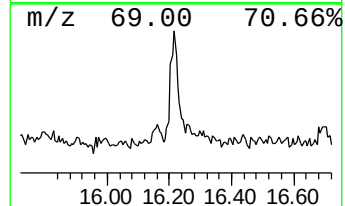
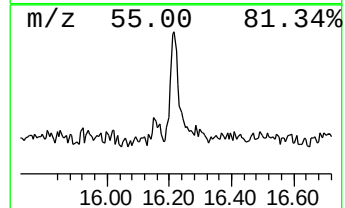
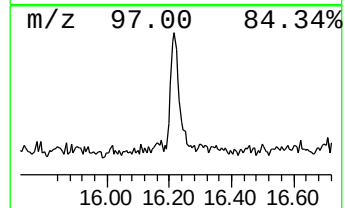
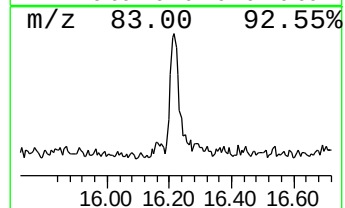
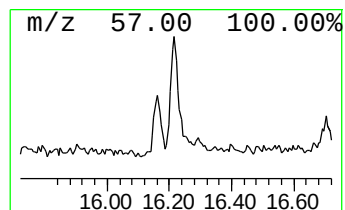
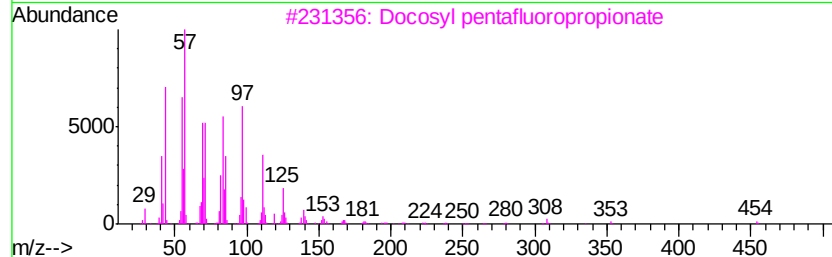
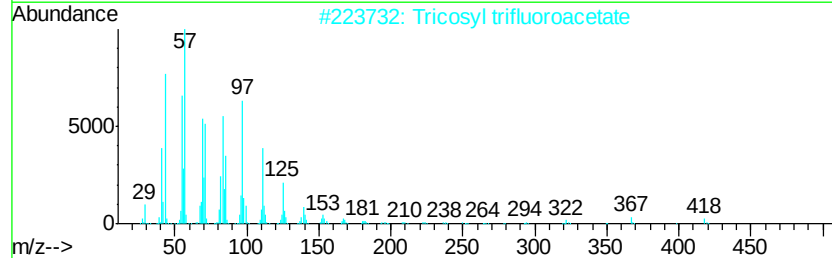
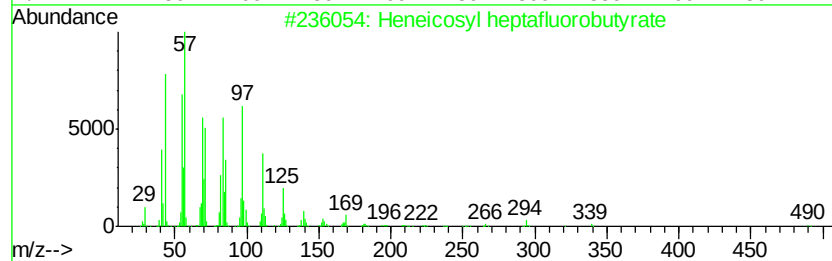
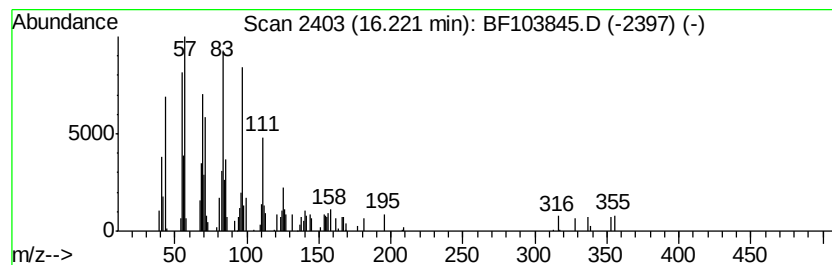
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	2.94 ng	133885	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	95
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	94
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
4		Octacosanol	410	C28H58O	000557-61-9	94
5		Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	93



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ALS Vial : 7 Sample Multiplier: 1

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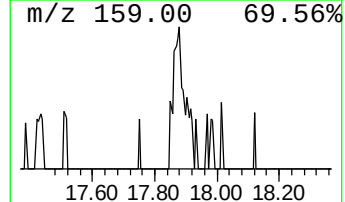
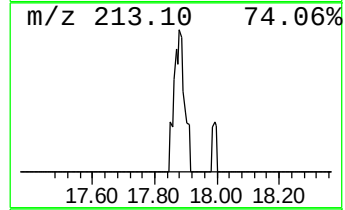
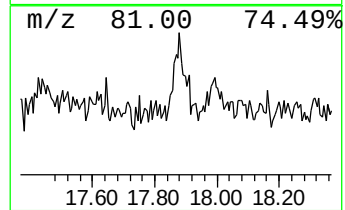
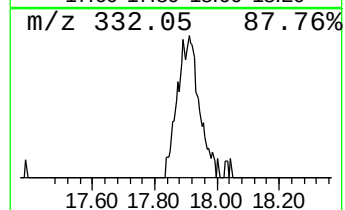
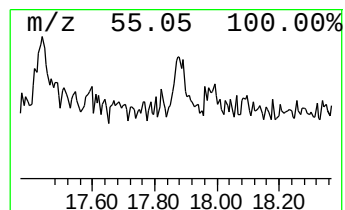
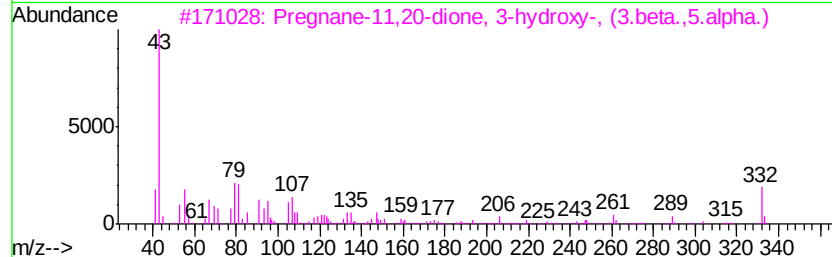
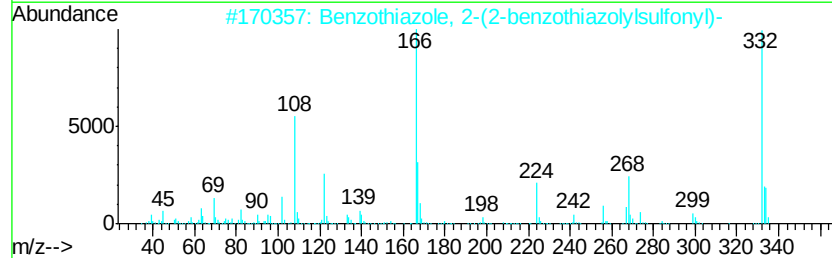
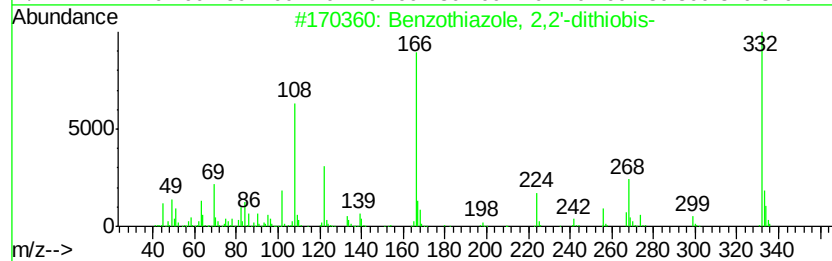
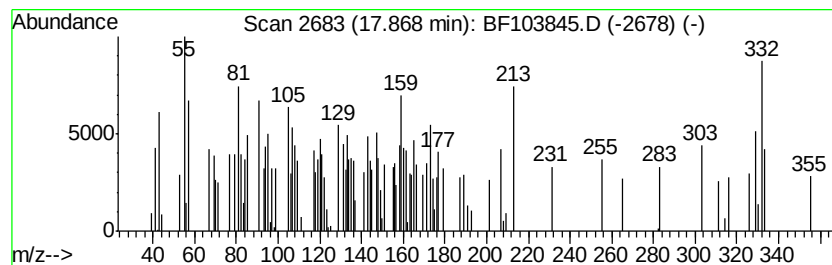
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown17.87 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.48 ng	113229	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzothiazole, 2,2'-dithiobis-	332	C14H8N2S4	000120-78-5	27
2		Benzothiazole, 2-(2-benzothiazol...	332	C14H8N2O2S3	119993-83-8	27
3		Pregnane-11,20-dione, 3-hydroxy-...	332	C21H32O3	000600-59-9	27
4		Bicyclo[2.2.1]heptan-2-one, 1,7,...	332	C16H20N4O4	002628-66-2	11
5		1-(2,5-Dimethoxybenzenesulfonyl)...	332	C16H16N2O4S	332021-84-8	10



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF032218\
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 Sample : J1946-05
 Misc :
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Instrument :
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 ClientSampleId :
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 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
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unknown5.22	5.22	2.8	ng	120078	1	6.97	844664	20.0
Ethanol, 2-butoxy-	5.92	2.6	ng	110723	1	6.97	844664	20.0
unknown6.74	6.74	89.9	ng	3797100	1	6.97	844664	20.0
n-Hexadecanoic acid	12.02	2.2	ng	146195	4	11.50	1317450	20.0
1,2:4,5-Dibenzopy...	13.56	6.1	ng	346044	5	14.16	1129780	20.0
1-Heneicosanol	13.97	12.1	ng	680516	5	14.16	1129780	20.0
Coronene	15.15	2.8	ng	125575	6	15.69	911691	20.0
Heneicosyl heptaf...	16.22	2.9	ng	133885	6	15.69	911691	20.0
unknown17.87	17.87	2.5	ng	113229	6	15.69	911691	20.0