

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102732.D
 Acq On : 5 Feb 2018 12:25
 Operator : SJ/JU
 Sample : J1436-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B13

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-BF020318.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	2.181	9	16	21	rVB	445605	598286	11.44%	1.251%
2	5.116	512	515	522	rVB	148486	192199	3.68%	0.402%
3	5.498	574	580	583	rBV	4814216	5229091	100.00%	10.931%
4	6.510	745	752	756	rBV	4118227	5171149	98.89%	10.810%
5	6.651	771	776	779	rBV	5064630	5022982	96.06%	10.501%
6	6.881	811	815	819	rVB	1734909	1380091	26.39%	2.885%
7	7.039	837	842	845	rVB	4259146	3875022	74.11%	8.101%
8	7.445	905	911	914	rBV	3380500	3265387	62.45%	6.826%
9	8.163	1029	1033	1036	rBV	2285277	1810294	34.62%	3.784%
10	9.239	1211	1216	1219	rBV	5516919	5025879	96.11%	10.507%
11	9.628	1279	1282	1285	rBV	622725	461690	8.83%	0.965%
12	9.745	1299	1302	1310	rBV4	36132	76250	1.46%	0.159%
13	9.822	1311	1315	1317	rVV	55675	90752	1.74%	0.190%
14	9.845	1317	1319	1322	rVB	76001	59061	1.13%	0.123%
15	9.916	1327	1331	1335	rVB	1926789	1854896	35.47%	3.878%
16	10.222	1377	1383	1393	rBV	107156	221558	4.24%	0.463%
17	10.345	1402	1404	1406	rVB	76602	56049	1.07%	0.117%
18	10.627	1448	1452	1455	rBV	85013	84847	1.62%	0.177%
19	10.704	1460	1465	1469	rBV	2797555	2837950	54.27%	5.933%
20	10.816	1481	1484	1489	rVB	57127	58298	1.11%	0.122%
21	11.263	1558	1560	1570	rVB3	41546	78327	1.50%	0.164%
22	11.404	1580	1584	1587	rBV	1829881	1571933	30.06%	3.286%
23	11.927	1667	1673	1685	rBV	770349	773158	14.79%	1.616%
24	12.621	1787	1791	1794	rBV2	71515	115809	2.21%	0.242%
25	12.710	1802	1806	1814	rBV	284103	283562	5.42%	0.593%
26	12.804	1819	1822	1825	rBV	161214	137839	2.64%	0.288%
27	12.927	1840	1843	1846	rVB	79425	61579	1.18%	0.129%
28	12.992	1849	1854	1857	rBV	3681127	3414785	65.30%	7.139%
29	13.263	1897	1900	1908	rVB	91261	84522	1.62%	0.177%
30	13.510	1939	1942	1945	rBV	109486	96113	1.84%	0.201%
31	13.874	2001	2004	2010	rBV	687907	610090	11.67%	1.275%
32	14.039	2029	2032	2036	rBV	1162838	1076385	20.58%	2.250%
33	14.204	2057	2060	2063	rBV2	57190	60319	1.15%	0.126%
34	14.515	2109	2113	2119	rBV	356157	358080	6.85%	0.749%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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35	15.162	2220	2223	2225	rBV	95610	110469	2.11%	0.231%
36	15.521	2279	2284	2293	rVB2	802249	1067301	20.41%	2.231%
37	15.998	2361	2365	2369	rVB	106876	146025	2.79%	0.305%
38	16.045	2369	2373	2379	rBV	85121	125828	2.41%	0.263%
39	17.374	2595	2599	2607	rVB5	146117	291668	5.58%	0.610%

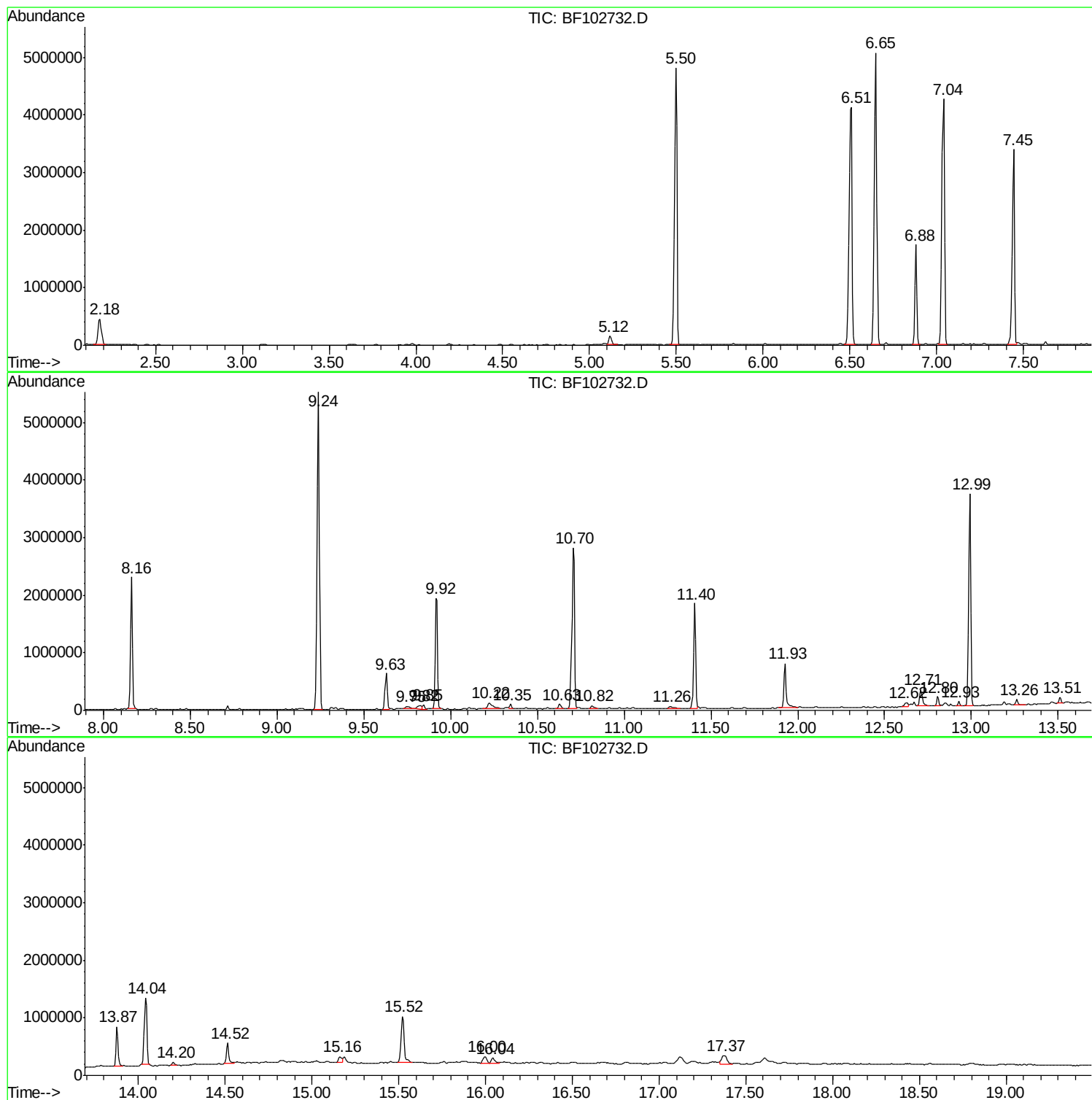
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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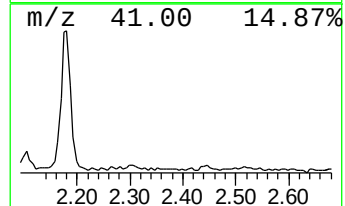
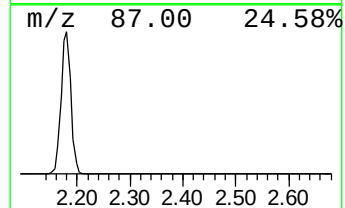
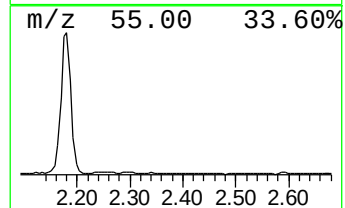
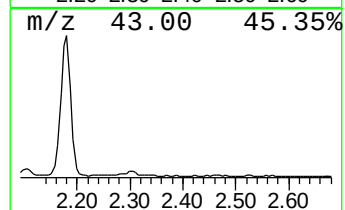
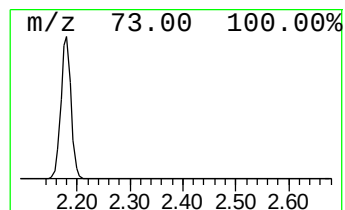
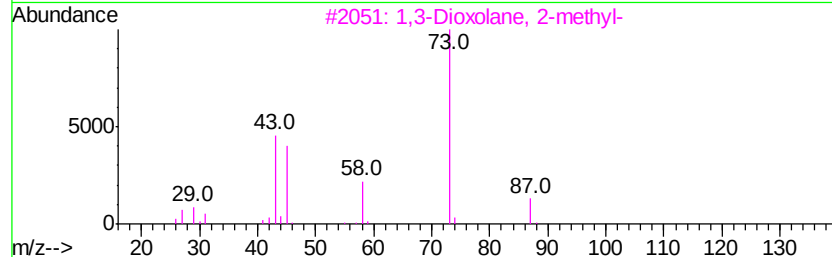
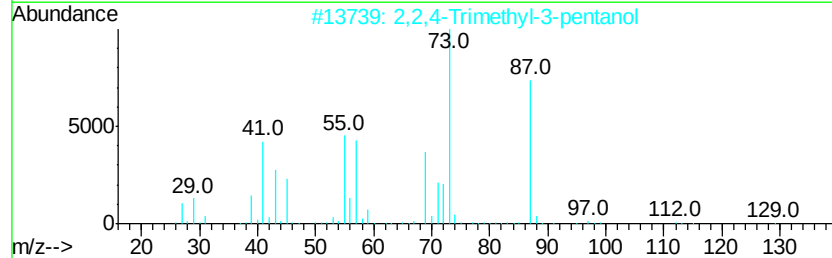
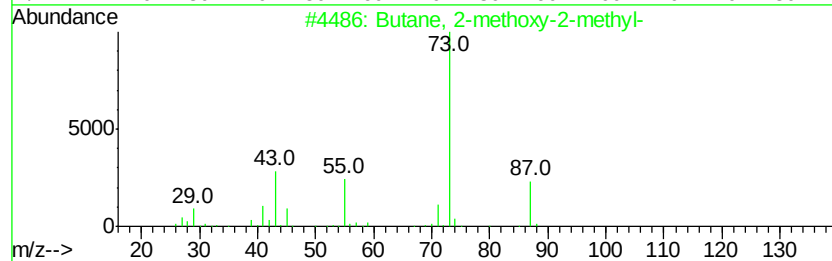
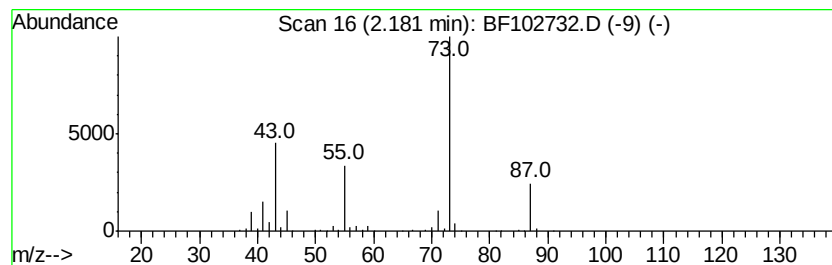
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	8.67 ng	598286	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23



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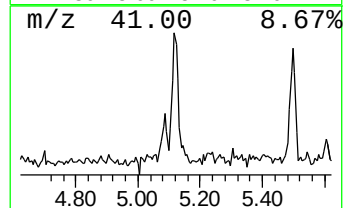
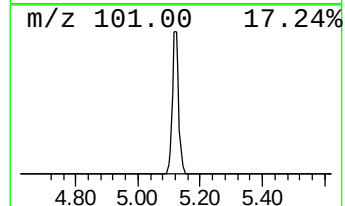
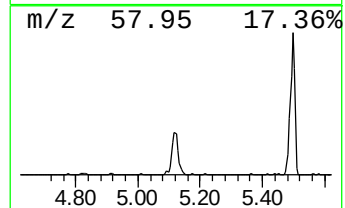
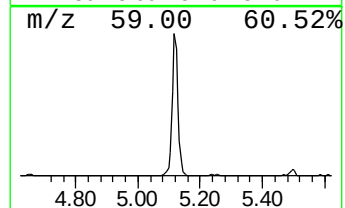
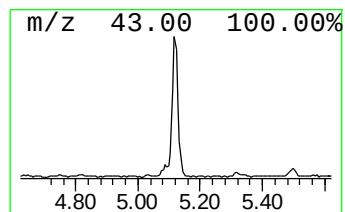
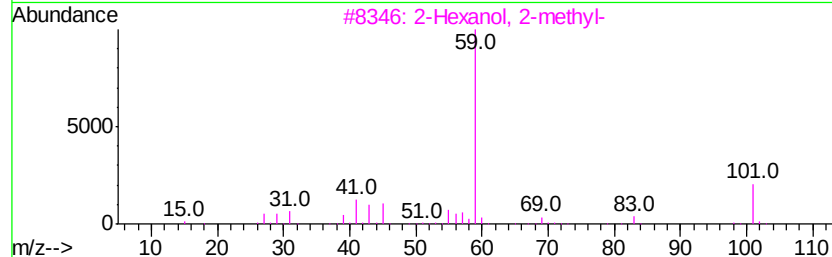
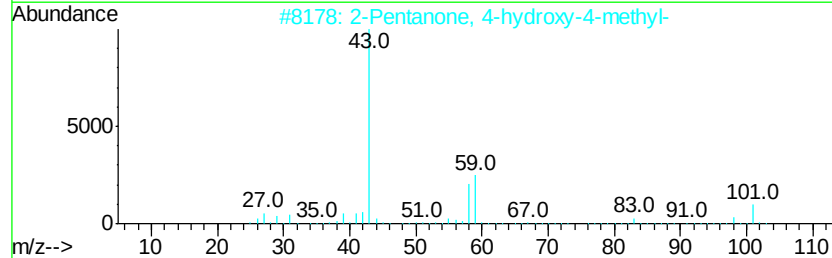
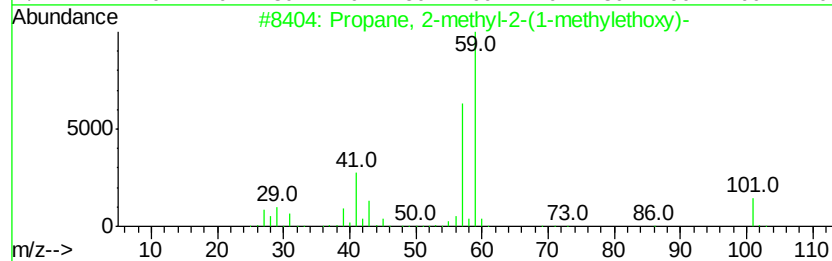
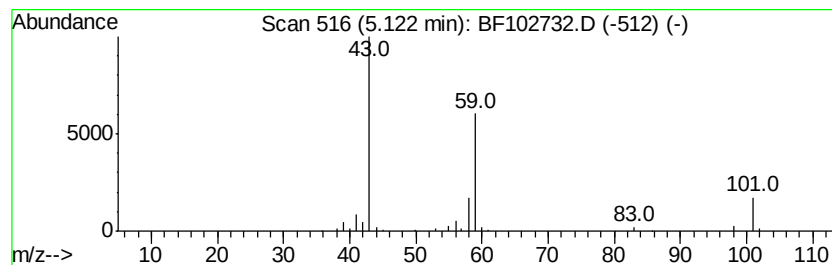
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.79 ng	192199	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		3-Octanol	130	C8H18O	000589-98-0	33



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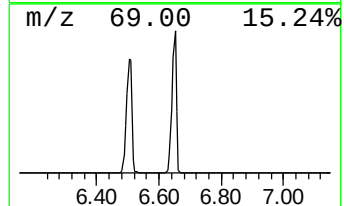
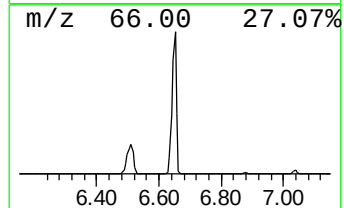
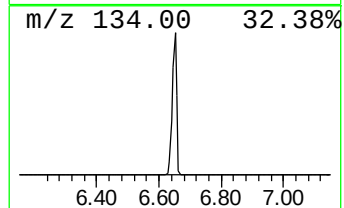
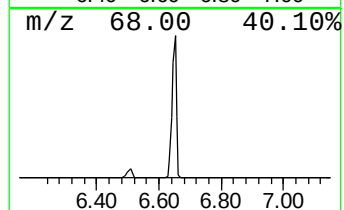
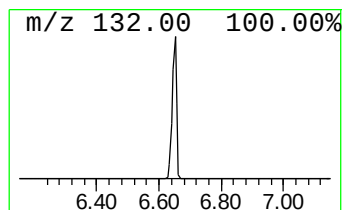
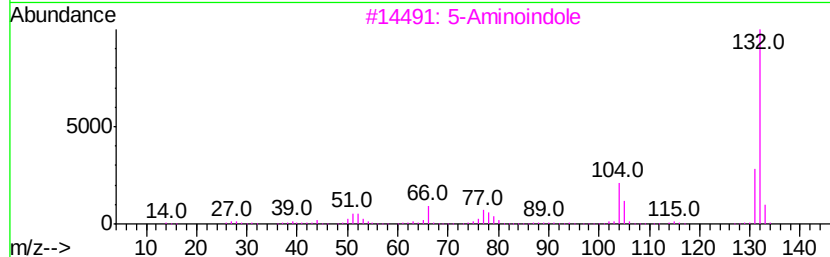
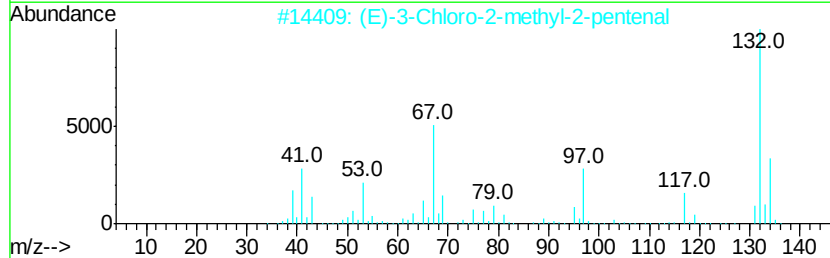
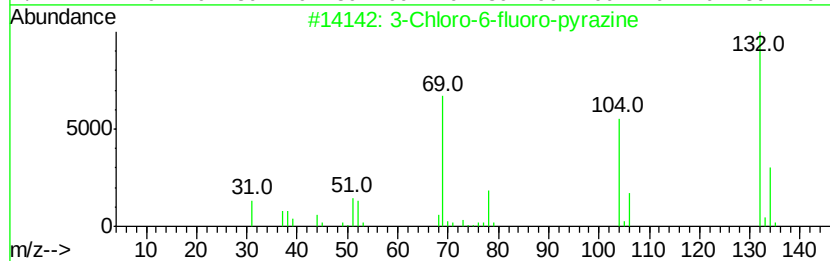
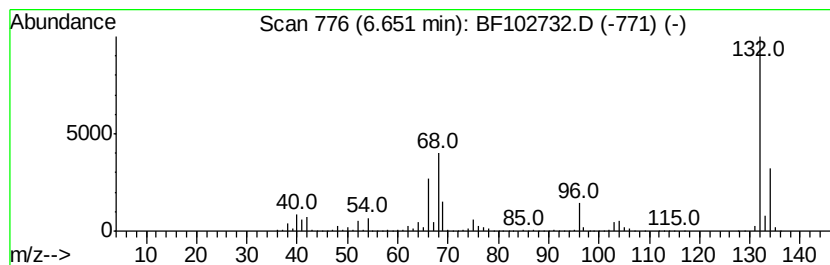
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	72.79 ng	5022980	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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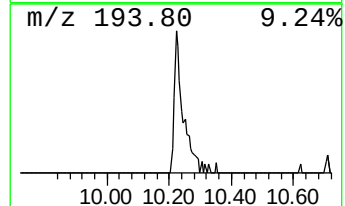
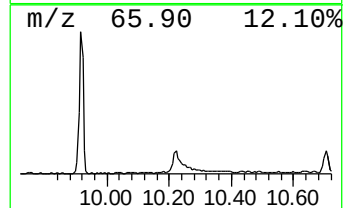
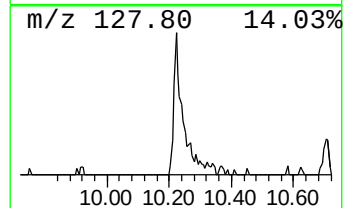
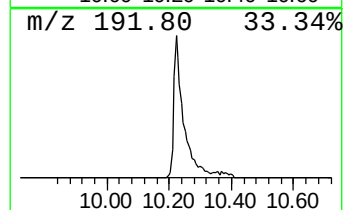
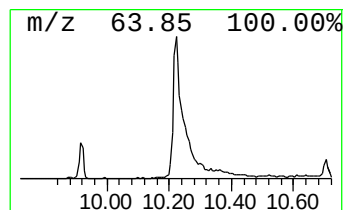
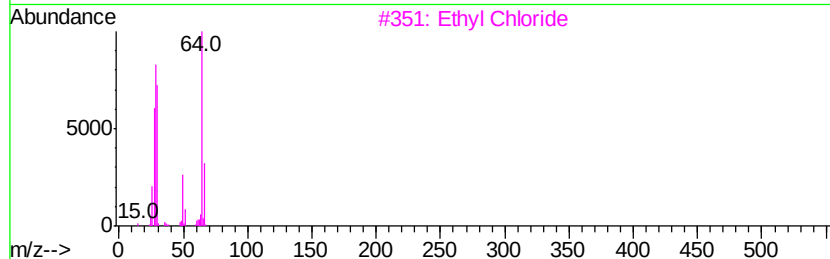
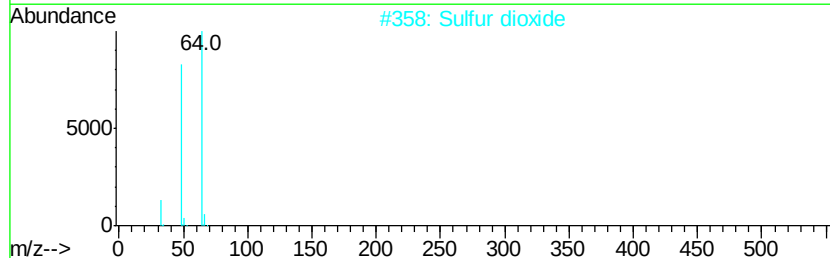
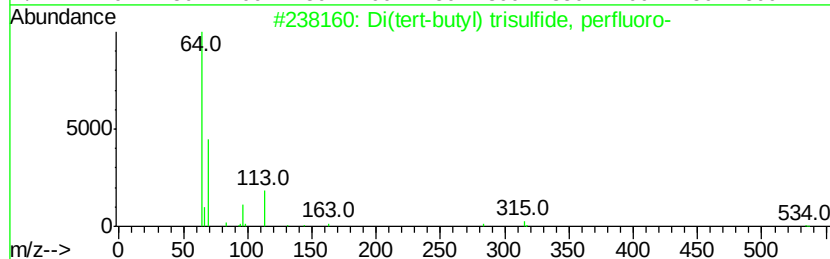
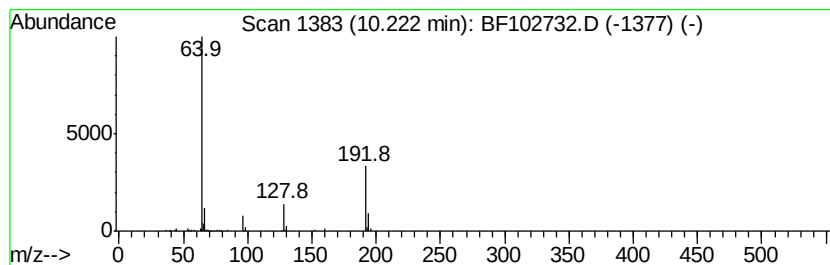
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown10.22 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	2.39 ng	221558	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
2		Sulfur dioxide	64	O2S	007446-09-5	4
3		Ethyl Chloride	64	C2H5Cl	000075-00-3	4
4		Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5		Pentafluorochlorodimethyl trisul...	250	C2ClF5S3	1000226-65-9	4



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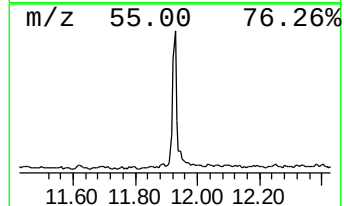
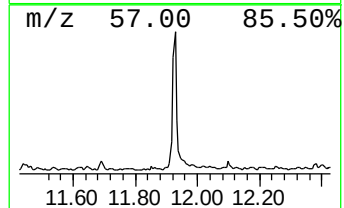
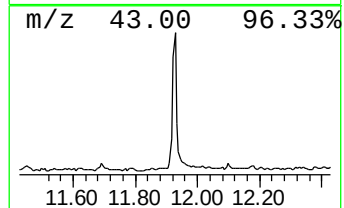
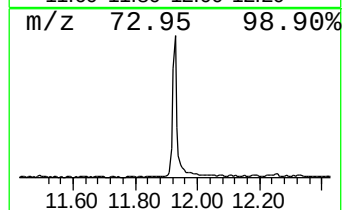
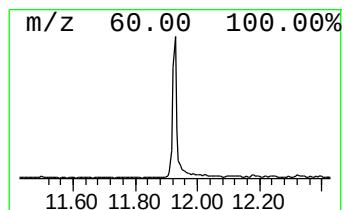
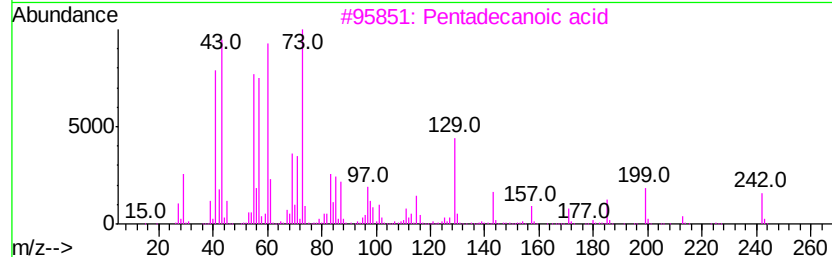
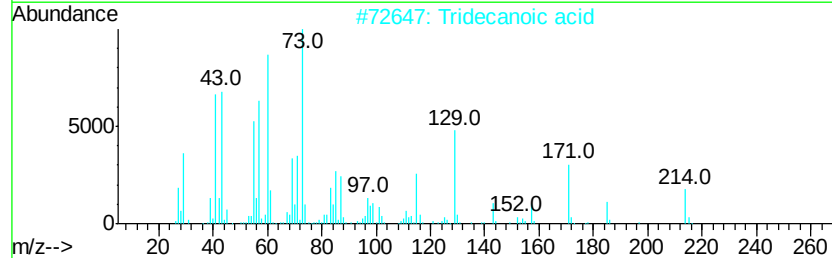
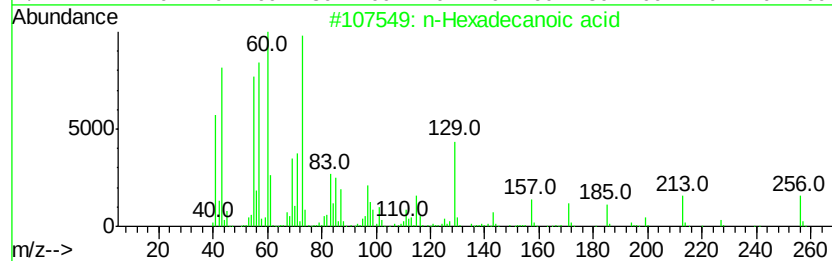
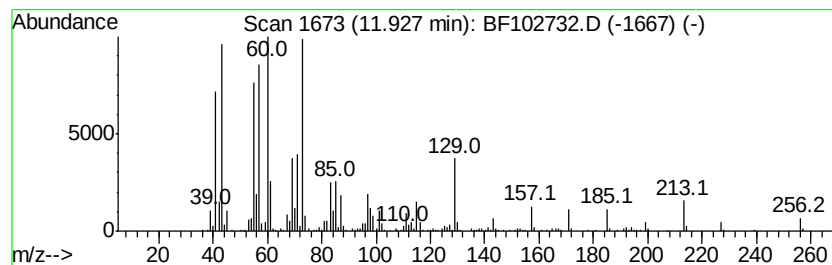
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	9.84 ng	773158	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	96
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Decane	142	C10H22	000124-18-5	25



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Misc :
ALS Vial : 7 Sample Multiplier: 1

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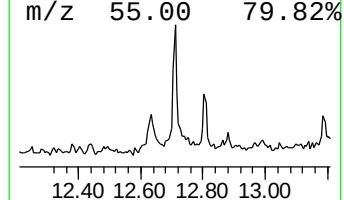
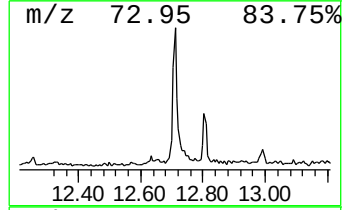
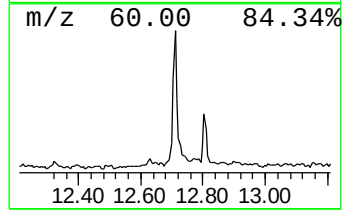
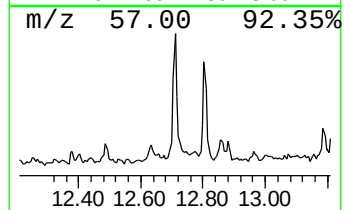
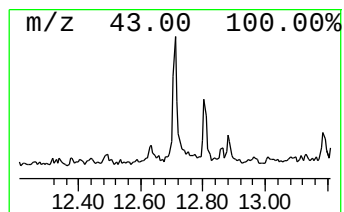
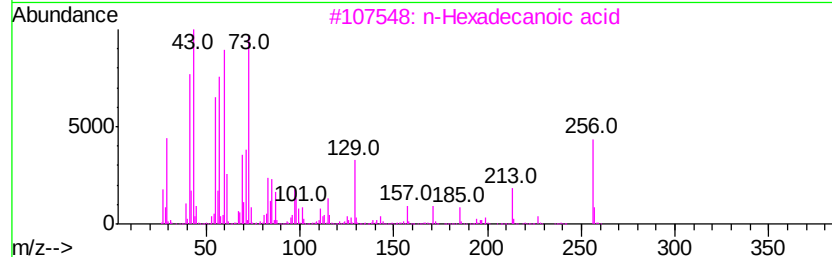
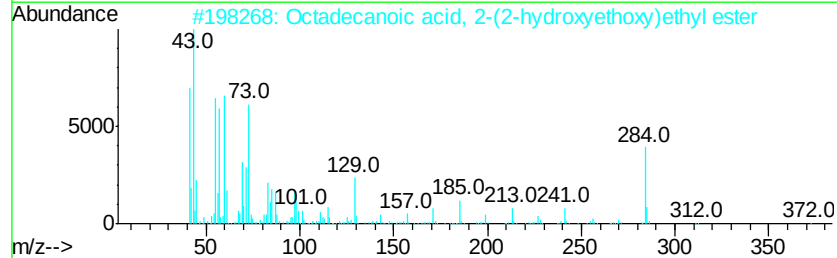
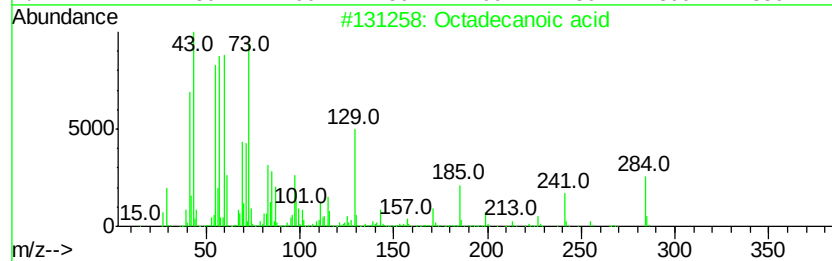
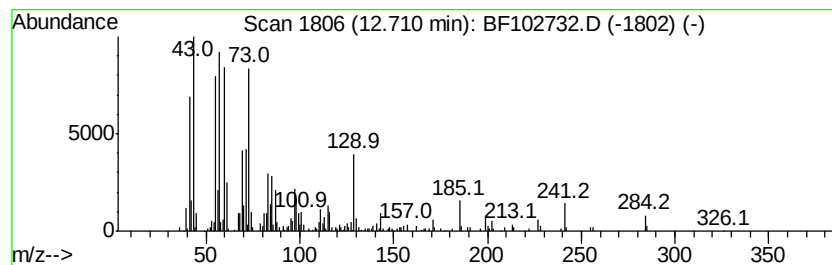
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.71	3.61 ng	283562	Phenanthrene-d10		11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	89



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102732.D
Acq On : 5 Feb 2018 12:25
Operator : SJ/JU
Sample : J1436-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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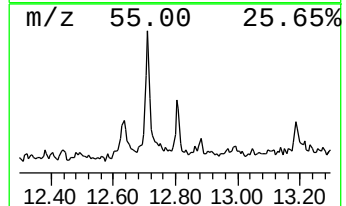
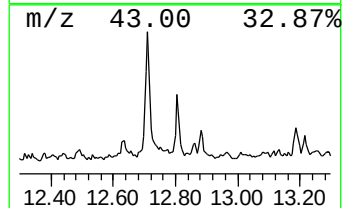
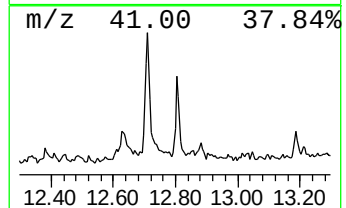
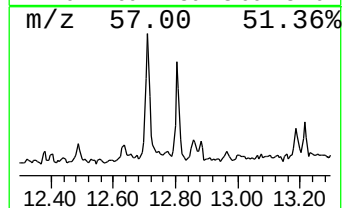
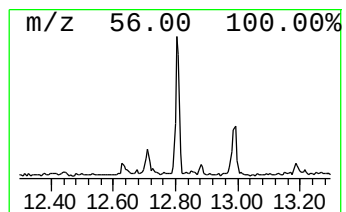
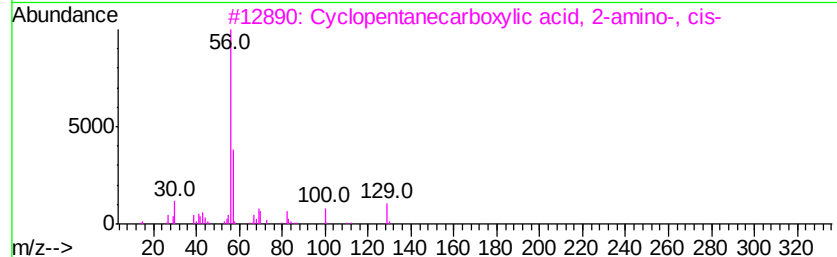
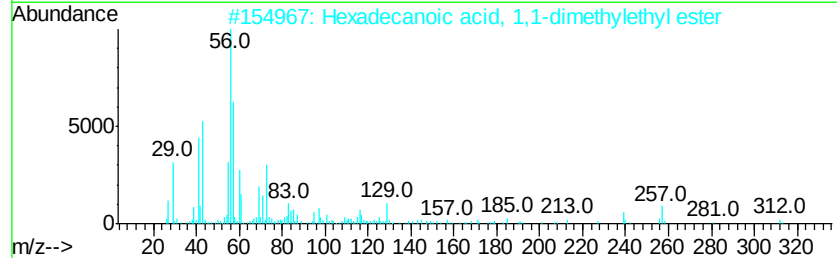
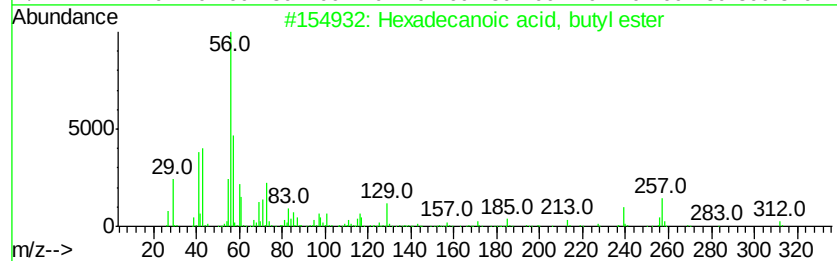
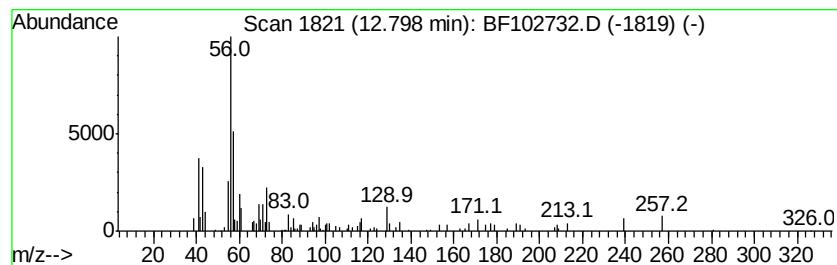
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.56 ng	137839	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102732.D
Acq On : 5 Feb 2018 12:25
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Misc :
ALS Vial : 7 Sample Multiplier: 1

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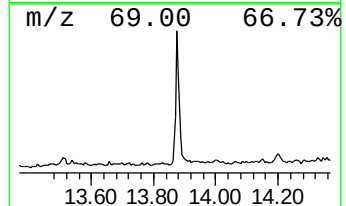
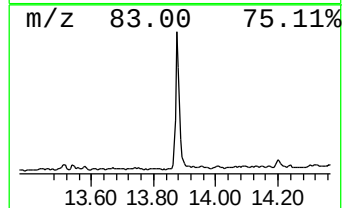
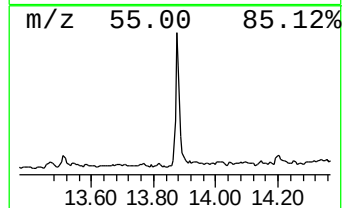
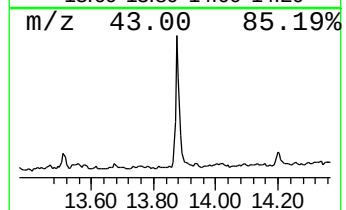
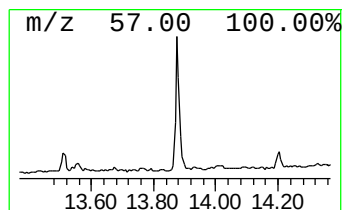
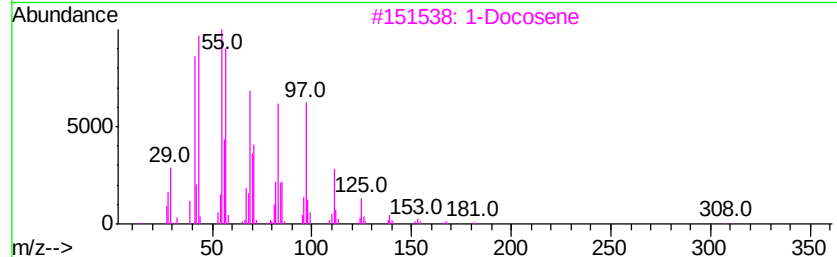
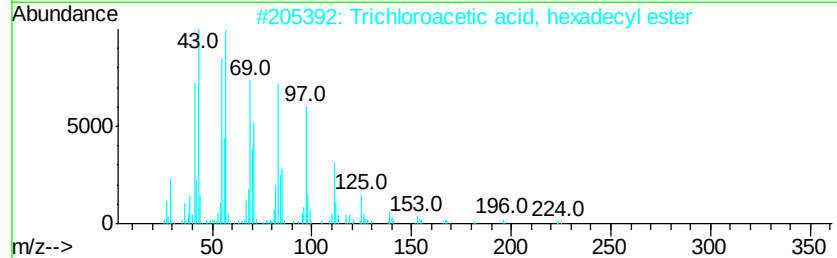
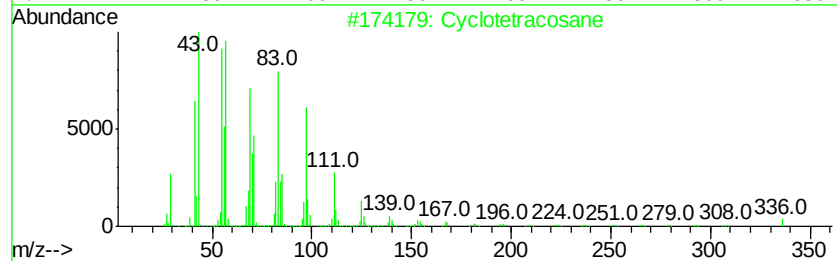
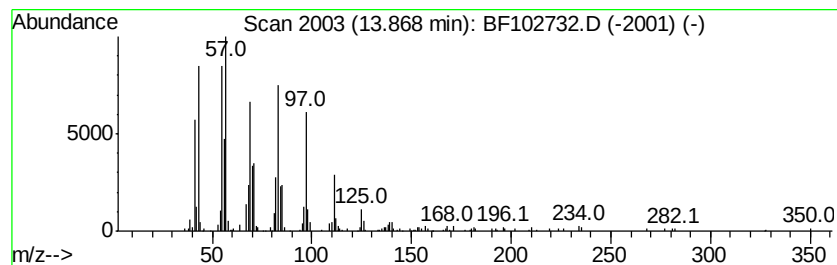
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.34 ng	610090	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		1-Docosene	308	C22H44	001599-67-3	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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Acq On : 5 Feb 2018 12:25
Operator : SJ/JU
Sample : J1436-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

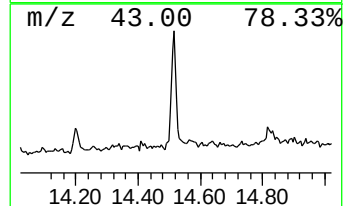
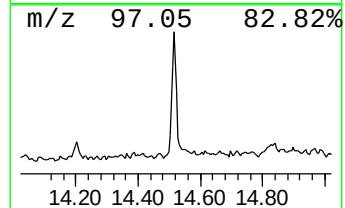
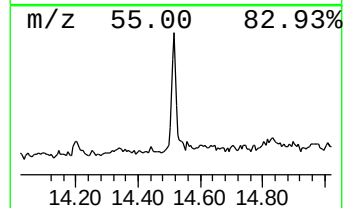
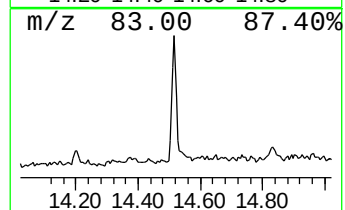
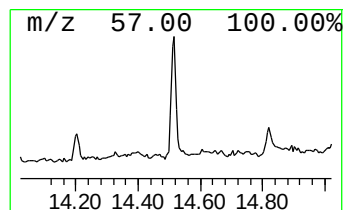
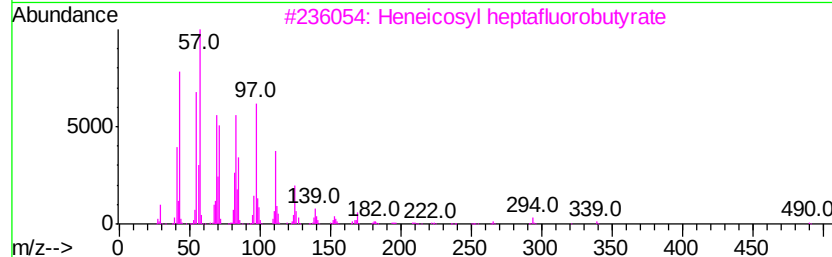
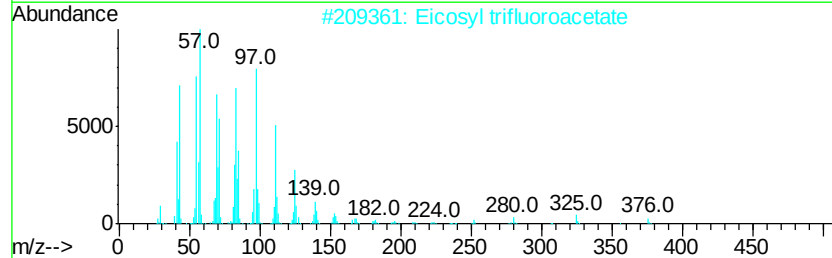
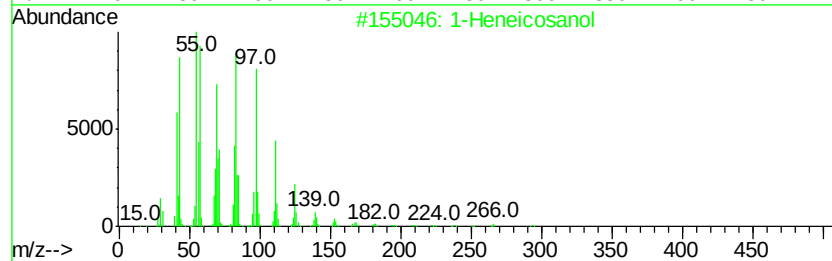
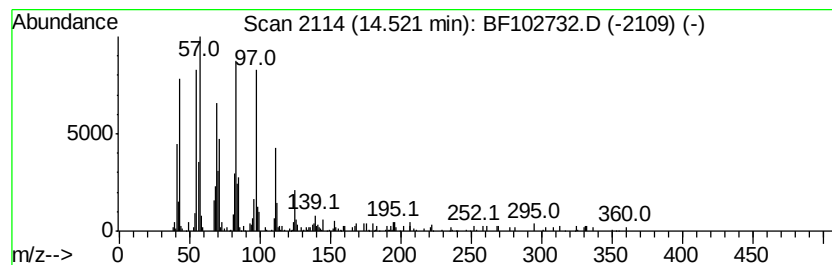
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.52	6.65 ng	358080	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3	Heneicosyl heptafluorobutrate	508	C25H43F7O2	1000351-83-8	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
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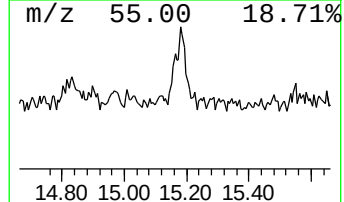
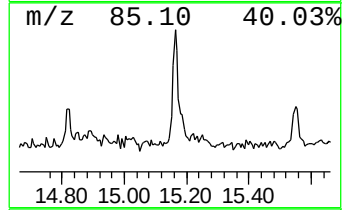
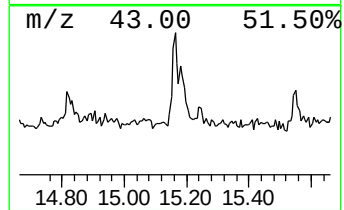
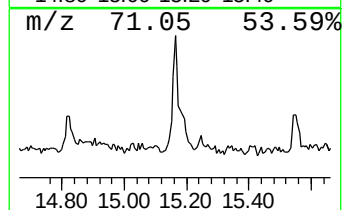
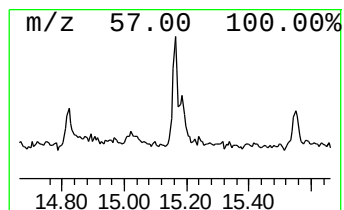
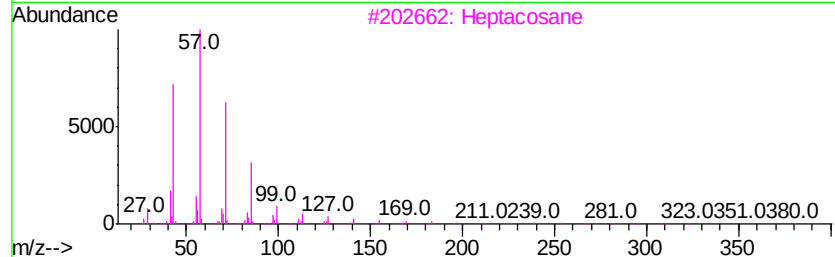
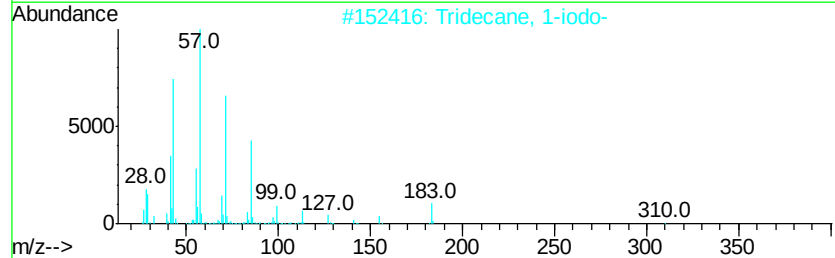
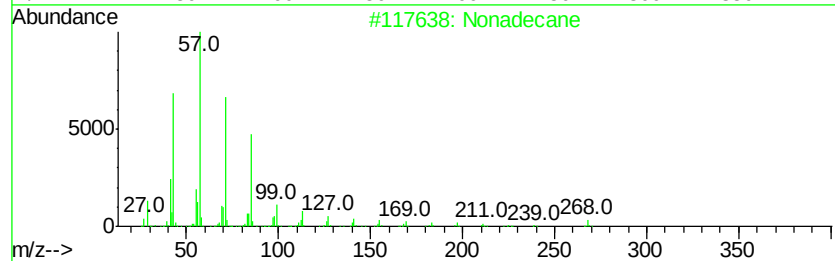
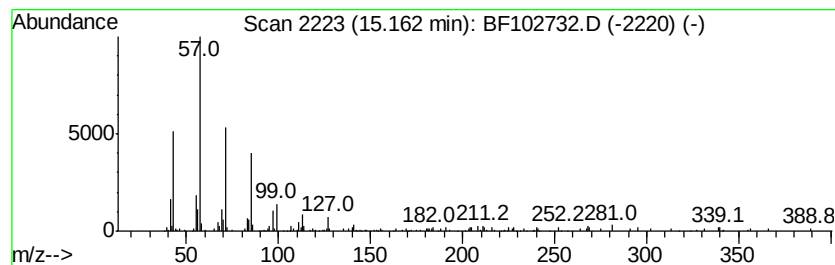
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	2.07 ng	110469	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	91
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
3		Heptacosane	380	C27H56	000593-49-7	80
4		Hentriacontane	437	C31H64	000630-04-6	78
5		Hexatriacontane	507	C36H74	000630-06-8	78



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
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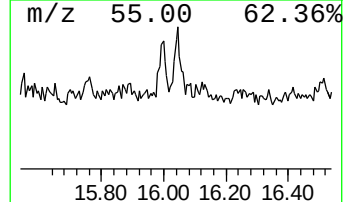
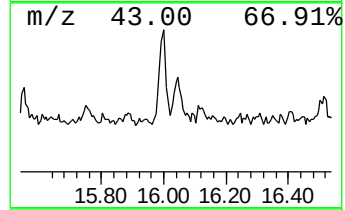
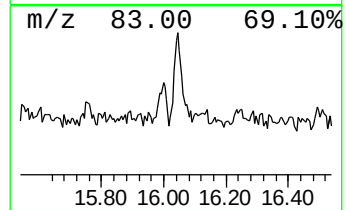
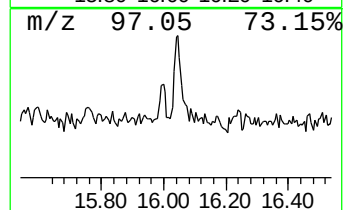
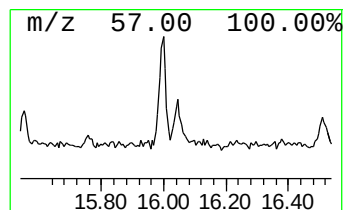
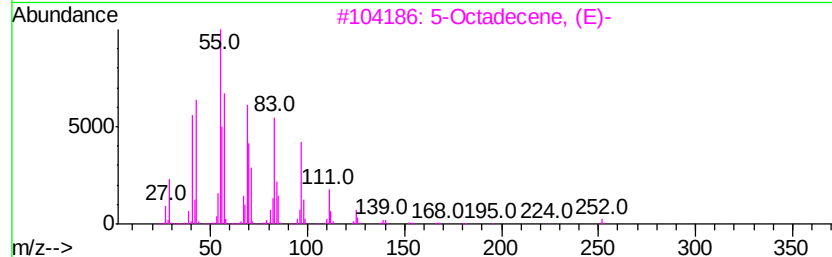
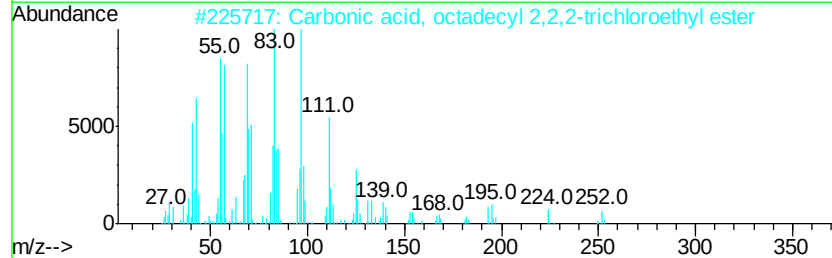
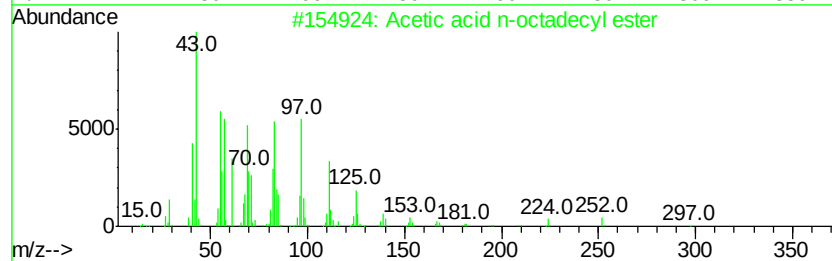
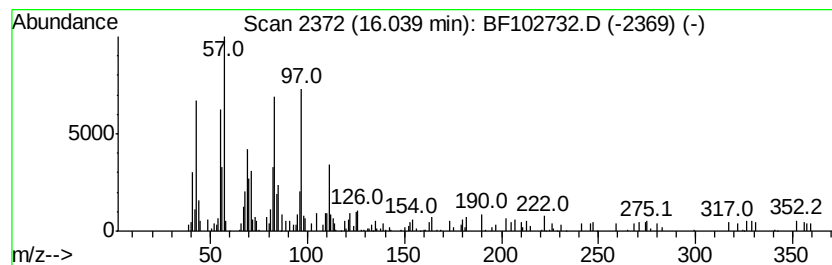
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Acetic acid n-octadecyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.36 ng	125828	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	80
2			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	72
3			5-Octadecene, (E)-	252	C18H36	007206-21-5	68
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	64
5			Disparlure	282	C19H38O	029804-22-6	64



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102732.D
Acq On : 5 Feb 2018 12:25
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Sample : J1436-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

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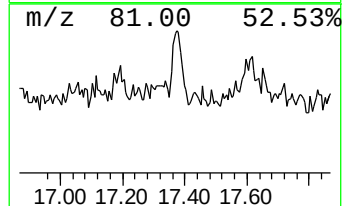
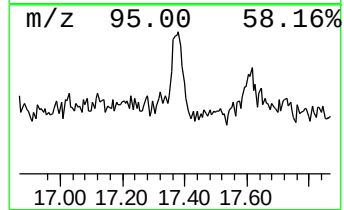
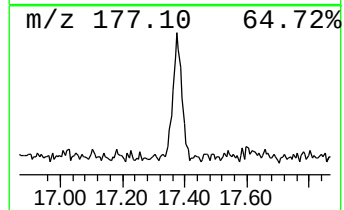
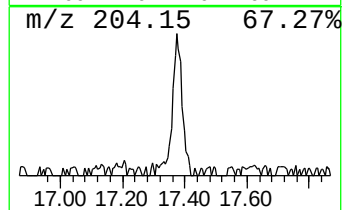
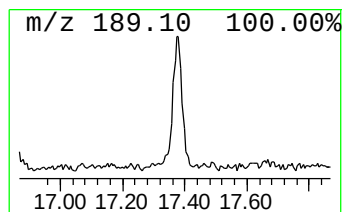
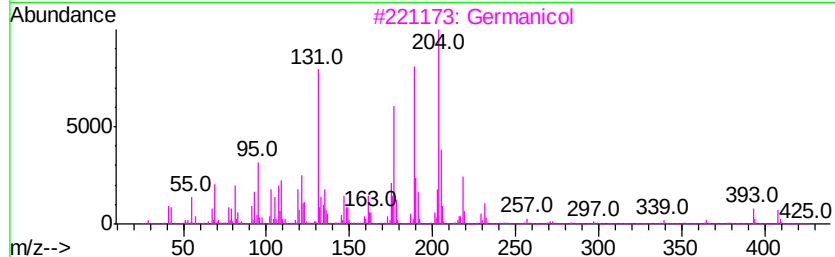
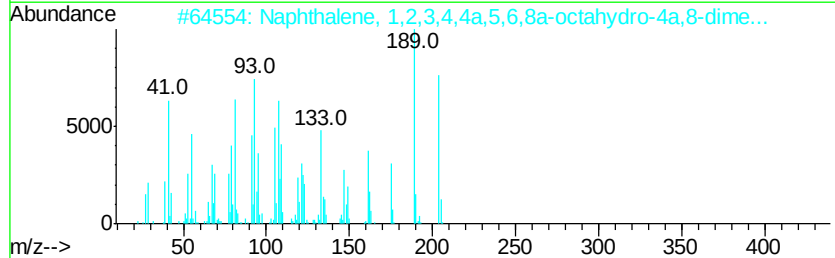
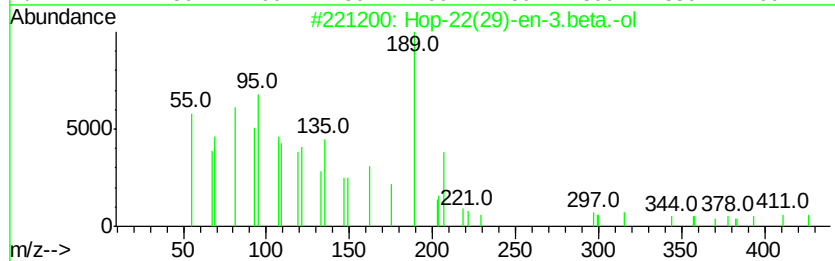
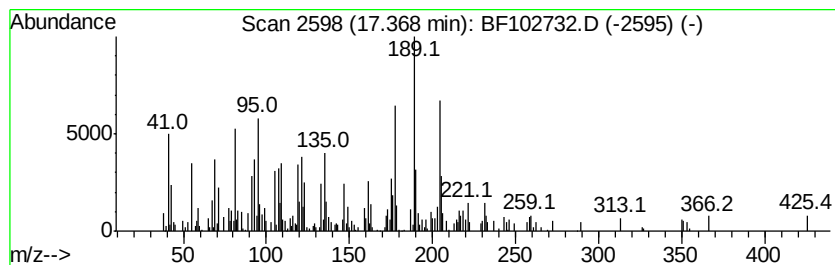
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Hop-22(29)-en-3.beta.-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.37	5.47 ng	291668	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	70
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	50
3		Germanicol	426	C30H50O	000465-02-1	50
4		2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	43
5		1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	38



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
 Data File : BF102732.D
 Acq On : 5 Feb 2018 12:25
 Operator : SJ/JU
 Sample : J1436-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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-methoxy...	2.18	8.7	ng	598286	1	6.88	1380090	20.0
Propane, 2-methyl...	5.12	2.8	ng	192199	1	6.88	1380090	20.0
unknown6.65	6.65	72.8	ng	5022980	1	6.88	1380090	20.0
unknown10.22	10.22	2.4	ng	221558	3	9.92	1854900	20.0
n-Hexadecanoic acid	11.93	9.8	ng	773158	4	11.40	1571930	20.0
Octadecanoic acid	12.71	3.6	ng	283562	4	11.40	1571930	20.0
Hexadecanoic acid...	12.80	2.6	ng	137839	5	14.04	1076390	20.0
Cyclotetracosane	13.87	11.3	ng	610090	5	14.04	1076390	20.0
1-Heneicosanol	14.52	6.7	ng	358080	5	14.04	1076390	20.0
Nonadecane	15.16	2.1	ng	110469	6	15.52	1067300	20.0
Acetic acid n-oct...	16.04	2.4	ng	125828	6	15.52	1067300	20.0
Hop-22(29)-en-3.b...	17.37	5.5	ng	291668	6	15.52	1067300	20.0