

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102747.D
 Acq On : 5 Feb 2018 19:27
 Operator : SJ/JU
 Sample : J1456-06
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-ST-LATERAL-LINE-2-NW@4

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	10	16	21	rVB	524152	679476	13.05%	1.456%
2	5.122	512	516	527	rVB	132727	178970	3.44%	0.384%
3	5.498	575	580	583	rBV	4652708	5205295	100.00%	11.157%
4	6.504	745	751	755	rBV	4205096	5199596	99.89%	11.145%
5	6.651	771	776	779	rBV	5047197	5047559	96.97%	10.819%
6	6.881	811	815	818	rBV	1577419	1290486	24.79%	2.766%
7	7.040	837	842	845	rBV	3848148	3592508	69.02%	7.700%
8	7.445	900	911	914	rBV	3273461	3386942	65.07%	7.260%
9	8.163	1029	1033	1036	rBV	2074216	1712968	32.91%	3.672%
10	9.239	1211	1216	1219	rBV	4848039	4344290	83.46%	9.312%
11	9.316	1225	1229	1231	rBV	110791	102944	1.98%	0.221%
12	9.628	1278	1282	1285	rBV	638194	495117	9.51%	1.061%
13	9.822	1310	1315	1316	rBV2	49592	71771	1.38%	0.154%
14	9.845	1316	1319	1322	rVB	250876	212988	4.09%	0.457%
15	9.916	1327	1331	1335	rVB	1864074	1762613	33.86%	3.778%
16	10.163	1370	1373	1377	rBV3	56107	60768	1.17%	0.130%
17	10.345	1401	1404	1407	rVB	271823	228136	4.38%	0.489%
18	10.563	1436	1441	1444	rBV	75650	98099	1.88%	0.210%
19	10.704	1459	1465	1469	rBV	2738241	2794489	53.69%	5.990%
20	10.816	1481	1484	1494	rVB	249762	254172	4.88%	0.545%
21	11.263	1557	1560	1562	rBV	112791	85608	1.64%	0.183%
22	11.404	1580	1584	1587	rBV	1764171	1479813	28.43%	3.172%
23	11.927	1666	1673	1685	rBV	790934	871718	16.75%	1.868%
24	12.616	1787	1790	1798	rBV	113581	151788	2.92%	0.325%
25	12.710	1802	1806	1814	rBV	183315	241619	4.64%	0.518%
26	12.845	1826	1829	1833	rVB	79403	85969	1.65%	0.184%
27	12.986	1849	1853	1857	rBV	2966974	2974750	57.15%	6.376%
28	13.874	2001	2004	2015	rVB	1074576	939626	18.05%	2.014%
29	14.039	2027	2032	2035	rBV	1220789	1118336	21.48%	2.397%
30	14.510	2109	2112	2115	rBV	88521	86298	1.66%	0.185%
31	14.798	2157	2161	2169	rBV	375981	526700	10.12%	1.129%
32	15.080	2206	2209	2216	rVB	45719	91572	1.76%	0.196%
33	15.521	2279	2284	2293	rVB	732419	976273	18.76%	2.093%
34	16.039	2368	2372	2380	rBV	139029	222290	4.27%	0.476%

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ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.192	2565	2568	2579	rVB	37304	82548	1.59%	0.177%
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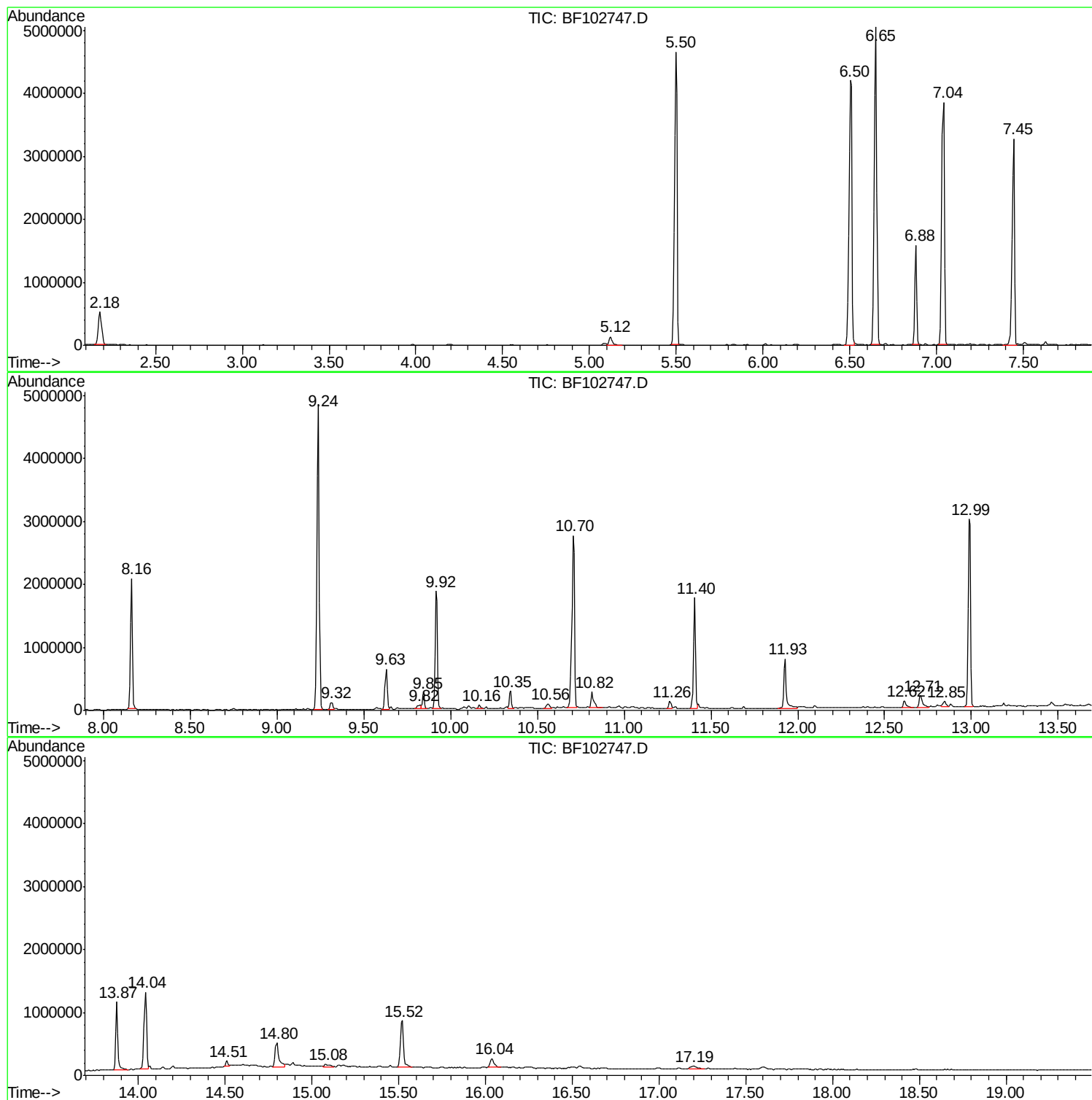
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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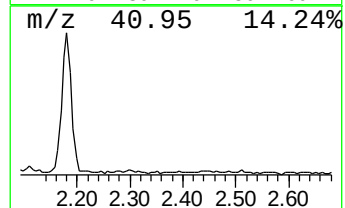
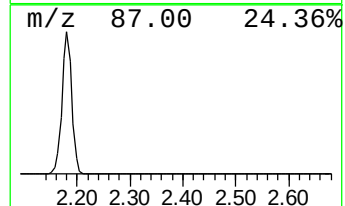
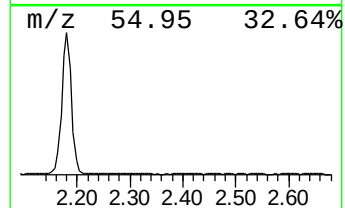
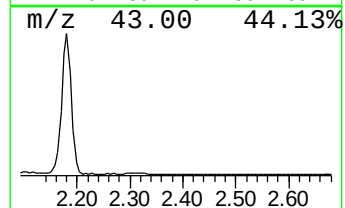
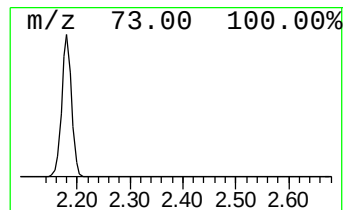
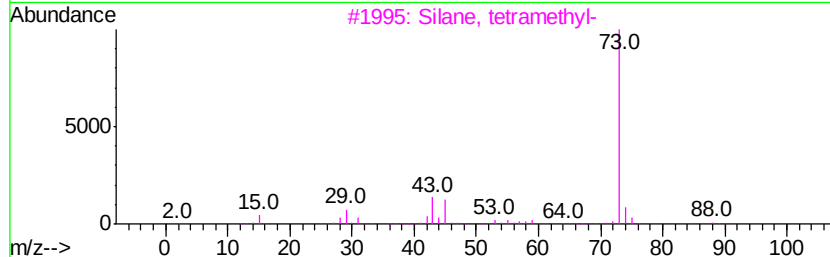
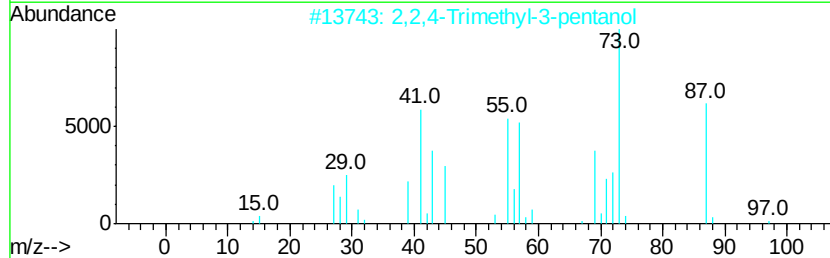
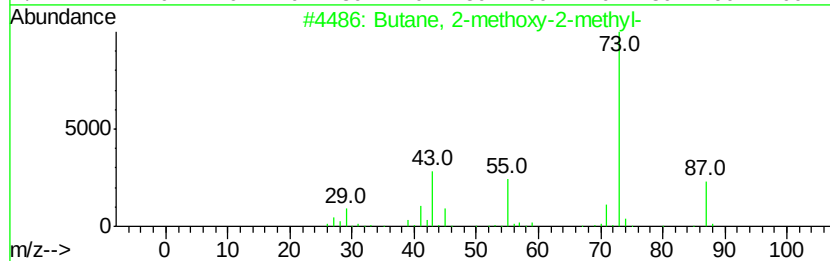
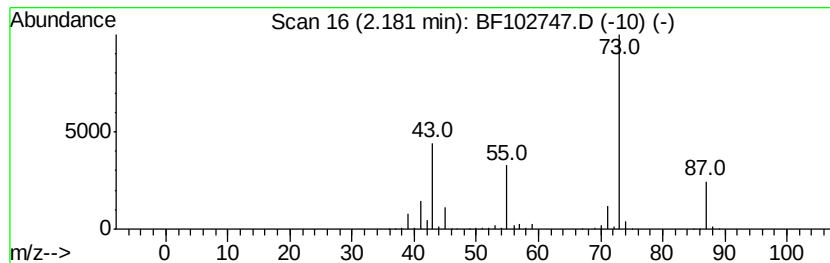
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	10.53 ng	679476	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	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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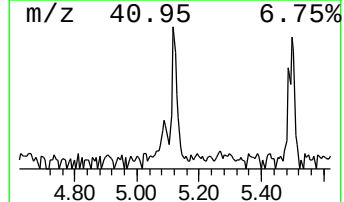
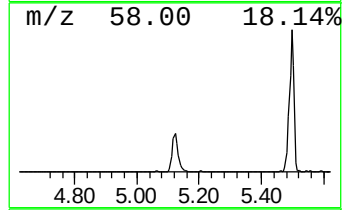
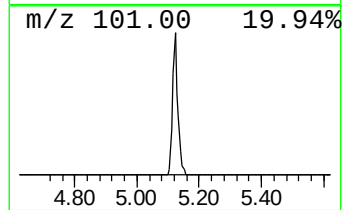
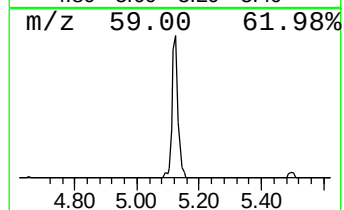
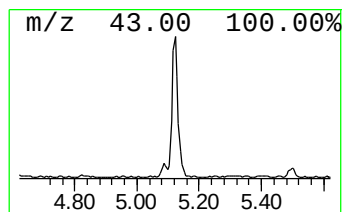
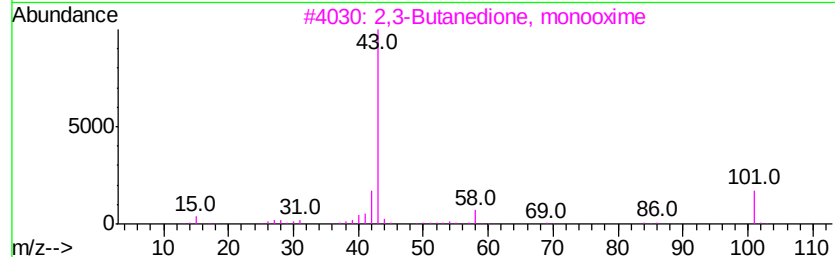
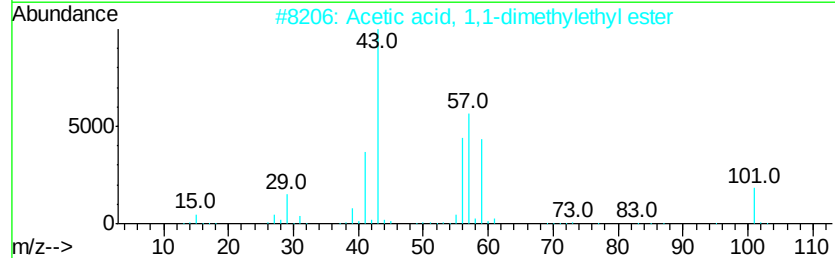
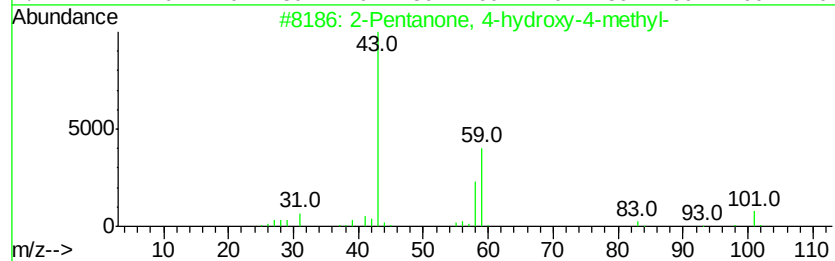
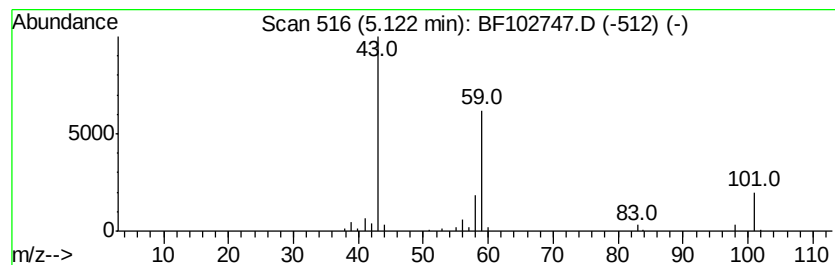
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.77 ng	178970	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	25
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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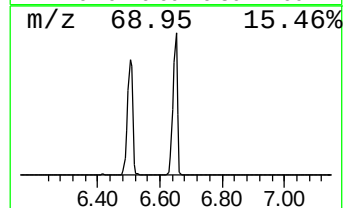
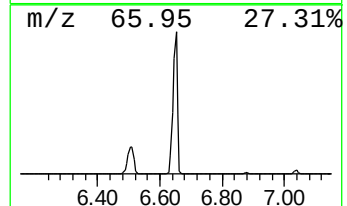
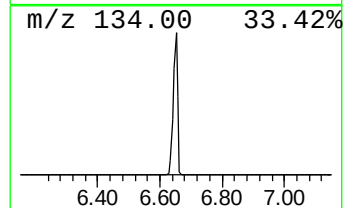
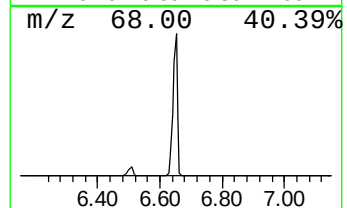
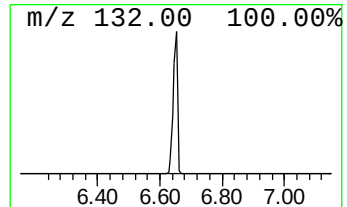
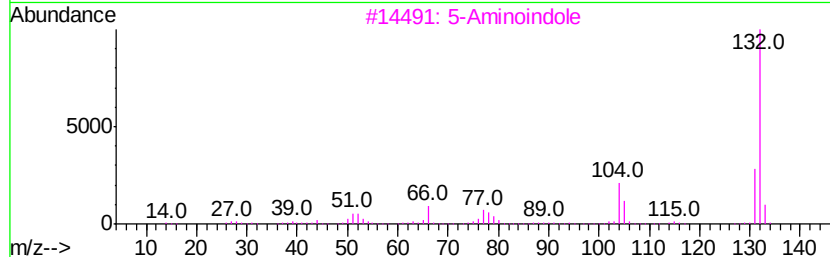
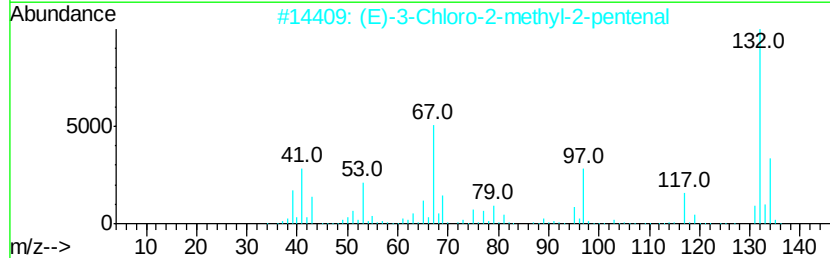
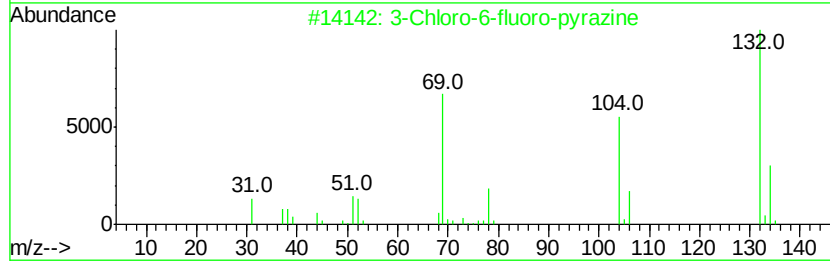
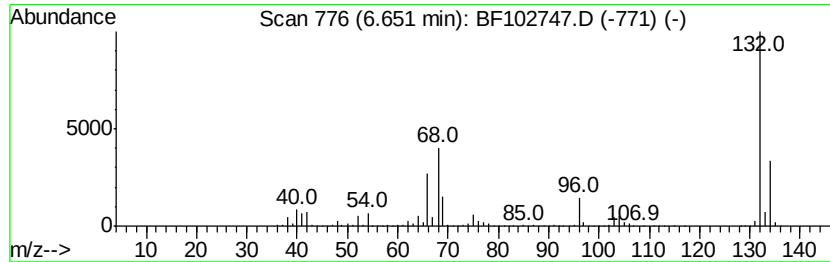
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	78.23 ng	5047560	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	16
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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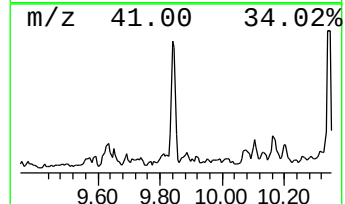
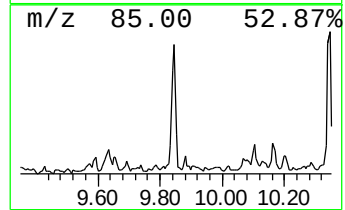
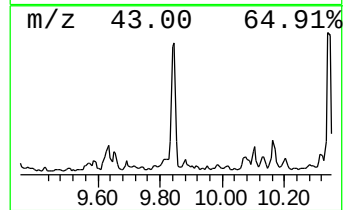
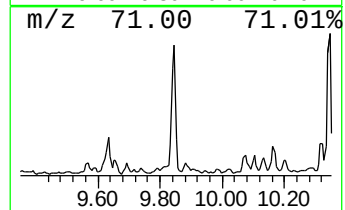
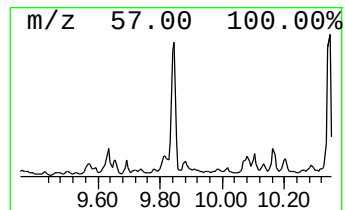
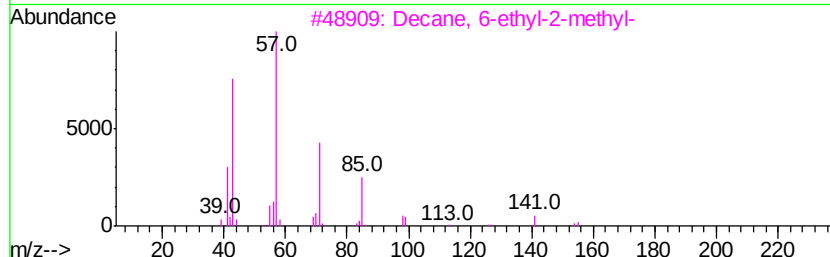
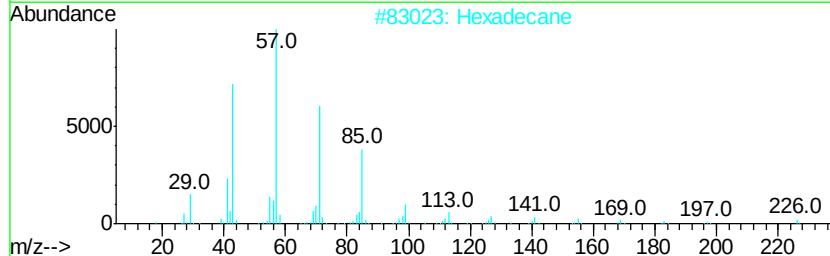
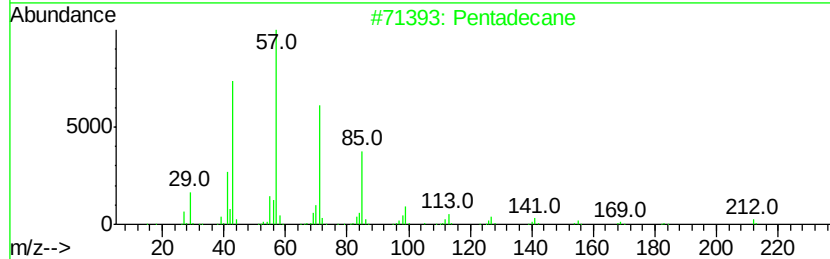
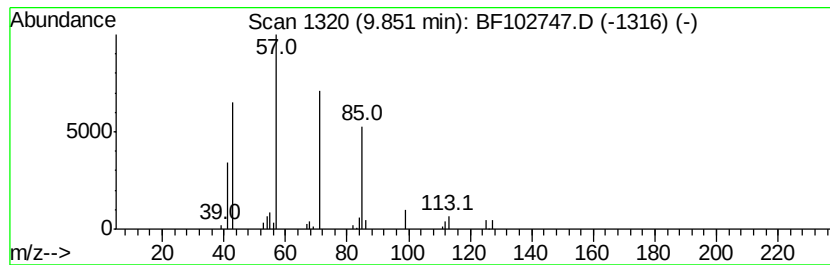
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.42 ng	212988	Acenaphthene-d10	9.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	80
2	Hexadecane		226	C16H34	000544-76-3	80
3	Decane, 6-ethyl-2-methyl-		184	C13H28	062108-21-8	72
4	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	64
5	Dodecane, 3-methyl-		184	C13H28	017312-57-1	64



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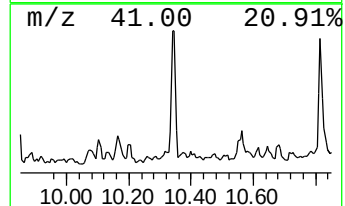
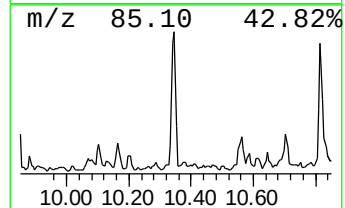
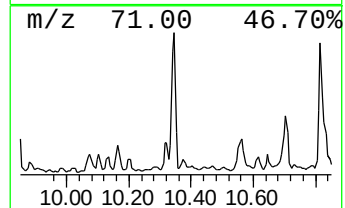
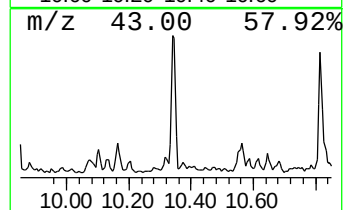
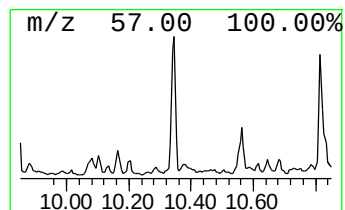
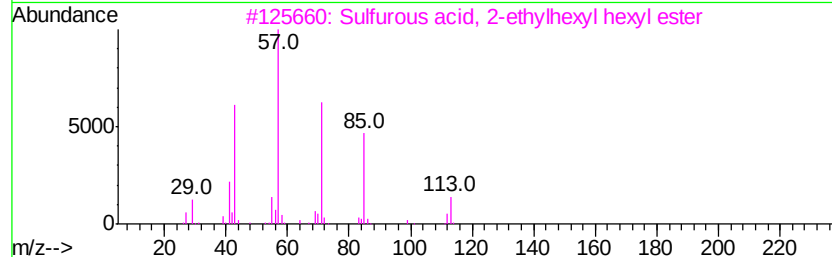
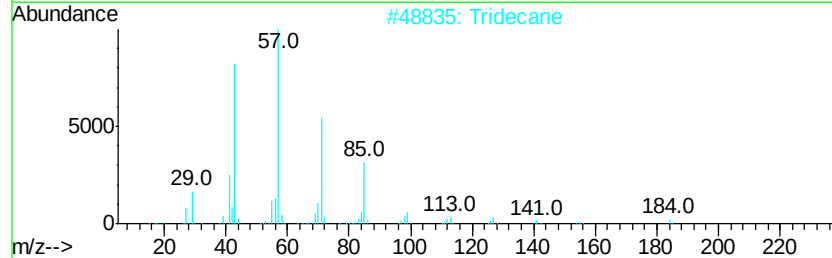
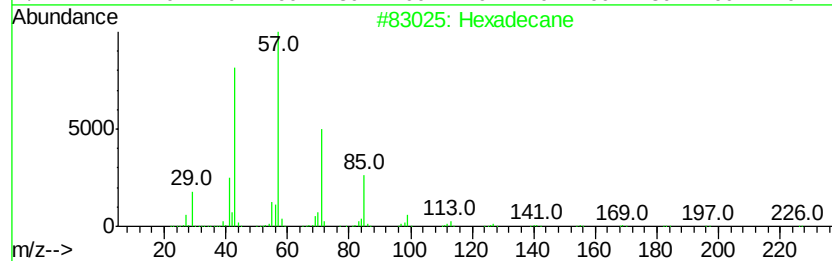
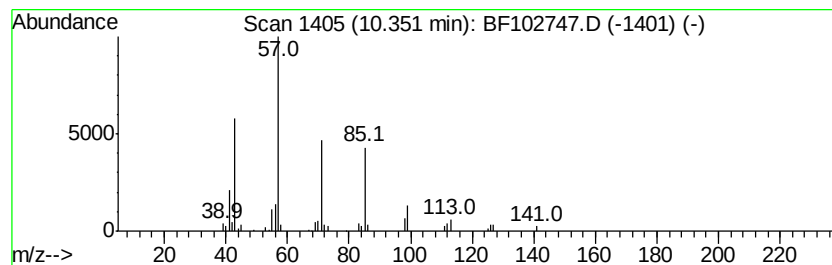
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Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.59 ng	228136	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	86
2	Tridecane	184 C13H28	000629-50-5	83
3	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	80
4	Tetradecane	198 C14H30	000629-59-4	78
5	Tridecane, 2-methyl-	198 C14H30	001560-96-9	72



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BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

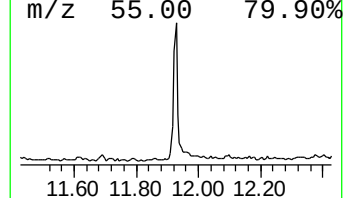
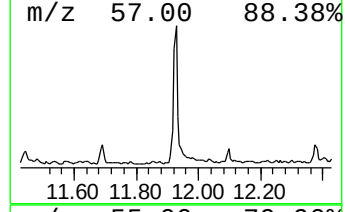
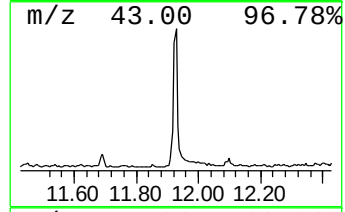
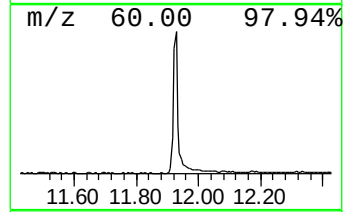
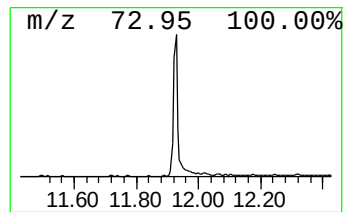
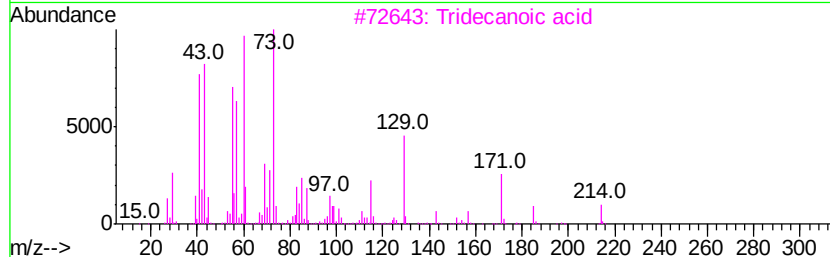
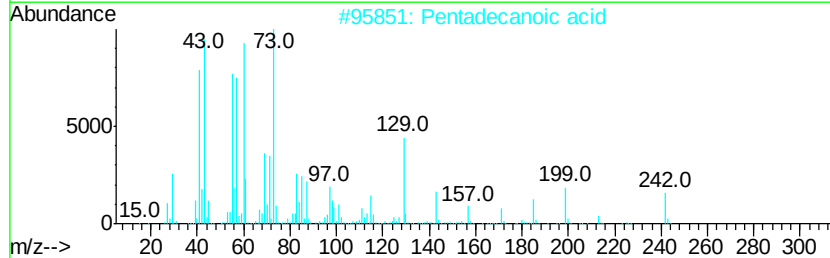
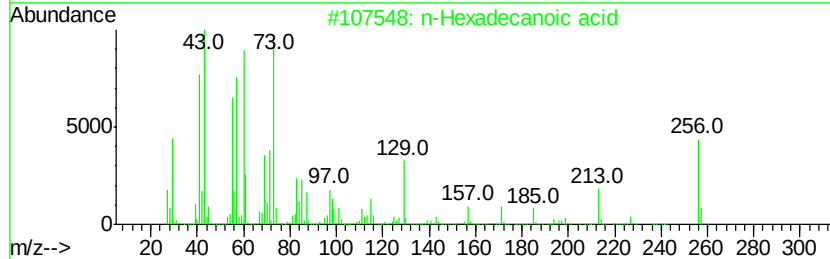
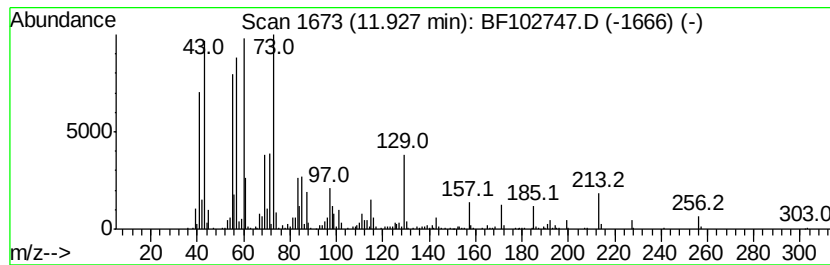
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	11.78 ng	871718	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102747.D
Acq On : 5 Feb 2018 19:27
Operator : SJ/JU
Sample : J1456-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

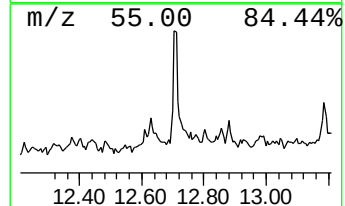
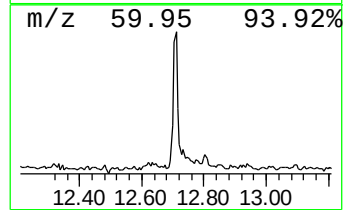
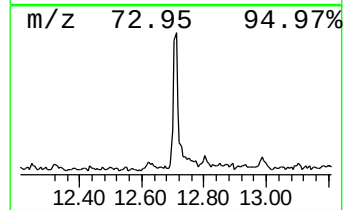
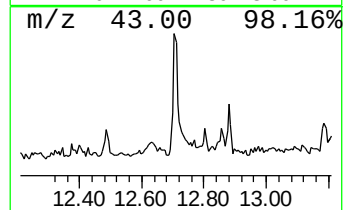
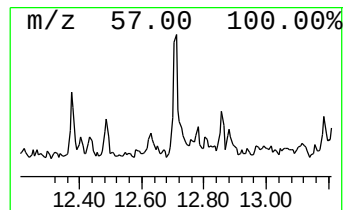
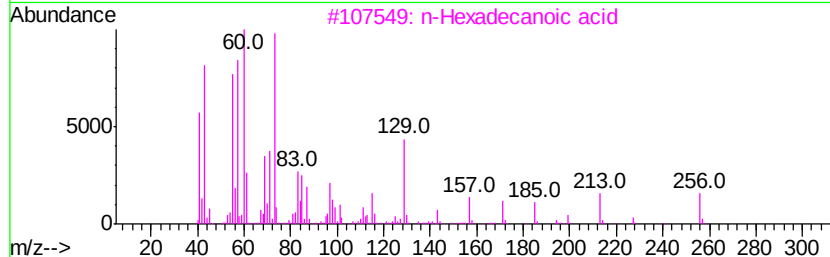
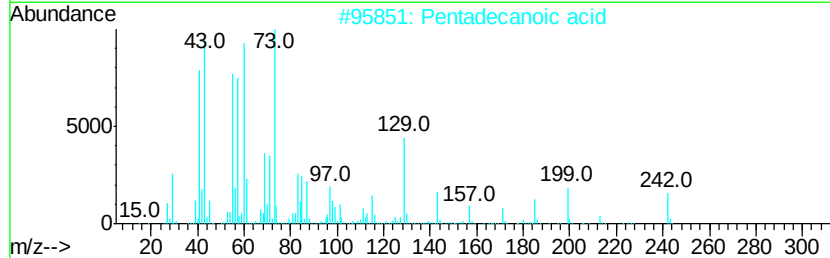
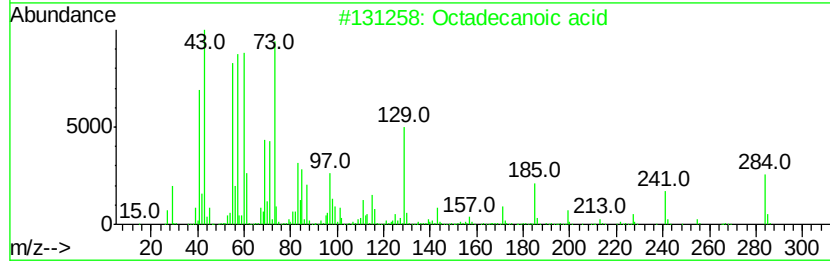
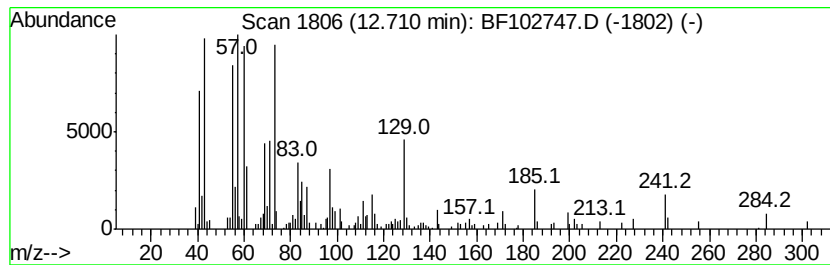
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.27 ng	241619	Phenanthrene-d10	11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	89
5			Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	86



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
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Acq On : 5 Feb 2018 19:27
Operator : SJ/JU
Sample : J1456-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

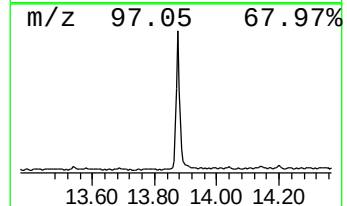
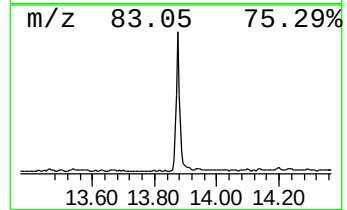
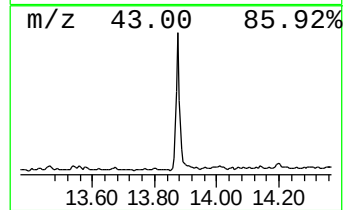
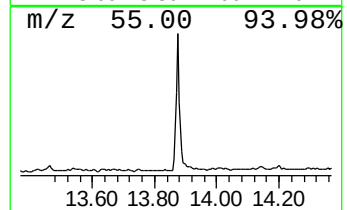
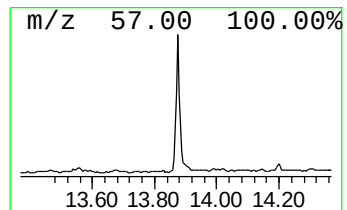
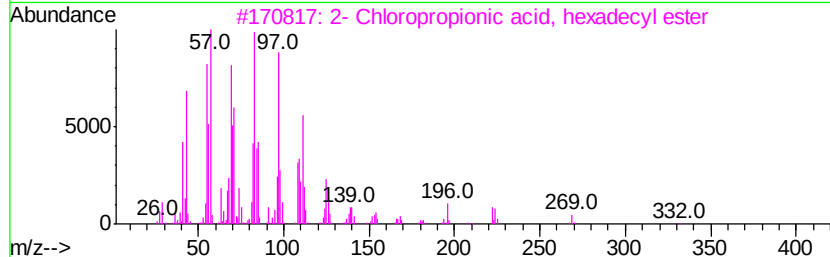
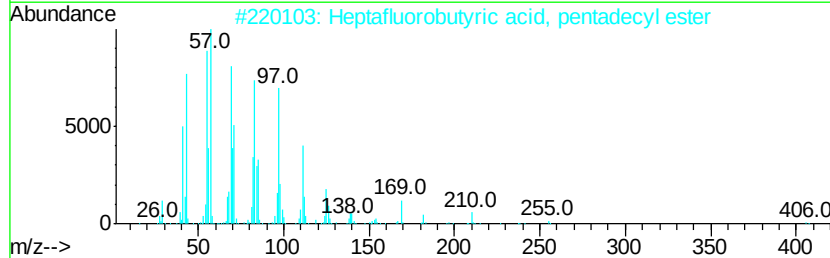
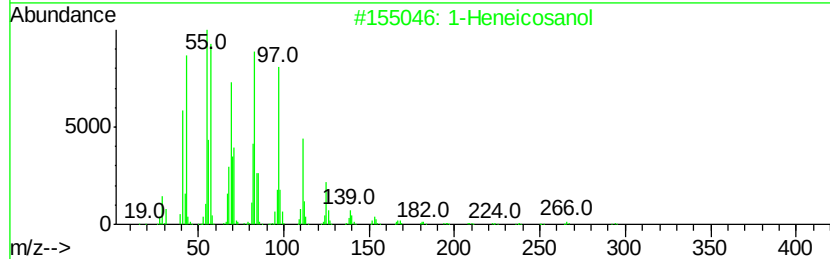
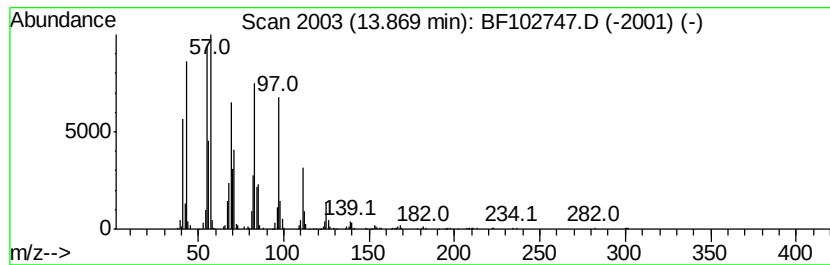
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ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

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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 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.87	16.80 ng	939626	Chrysene-d12	14.04		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102747.D
Acq On : 5 Feb 2018 19:27
Operator : SJ/JU
Sample : J1456-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

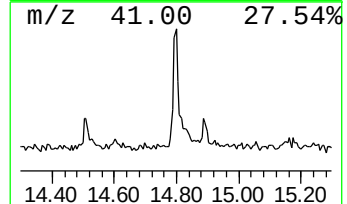
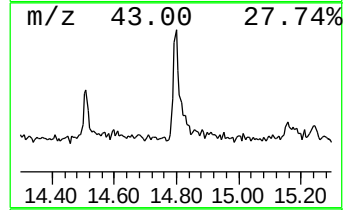
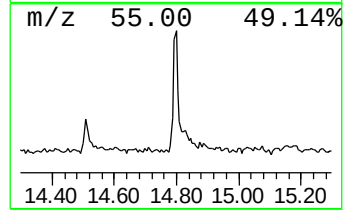
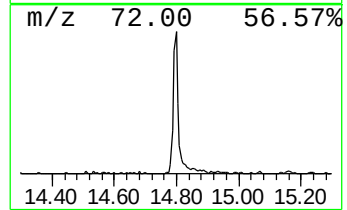
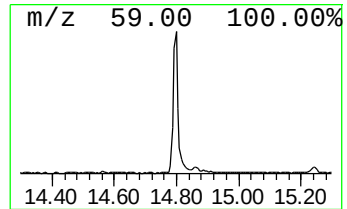
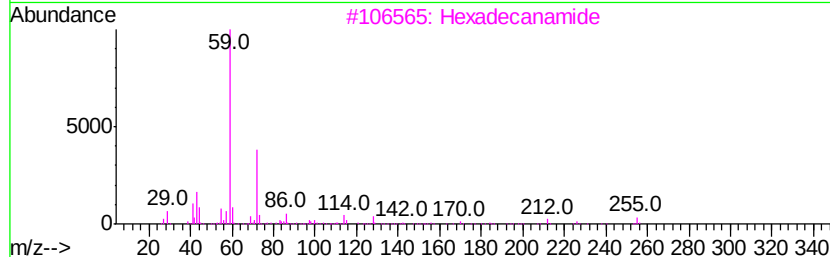
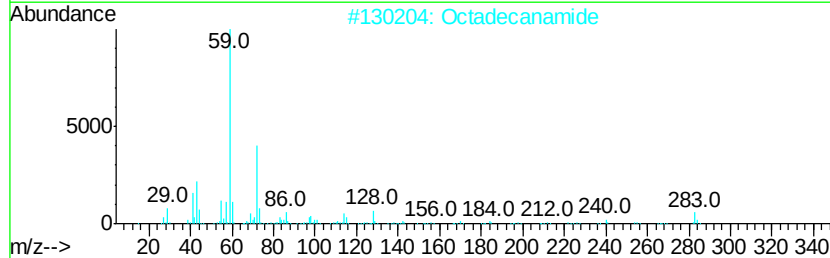
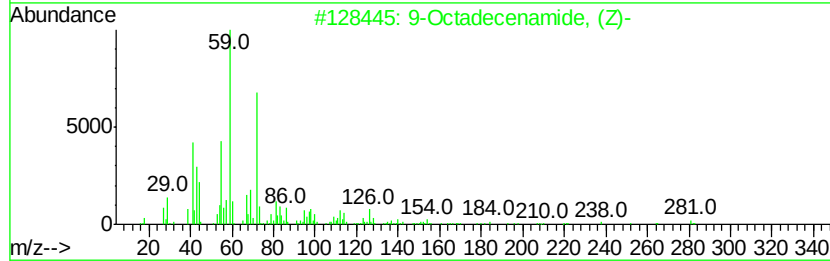
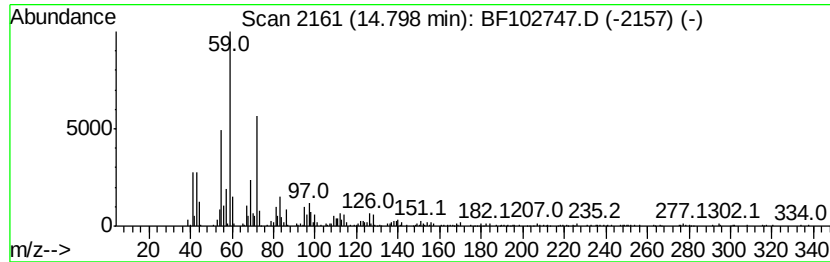
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	10.79 ng	526700	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Octadecanamide	283	C18H37NO	000124-26-5	72
3		Hexadecanamide	255	C16H33NO	000629-54-9	72
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
5		Tetradecanamide	227	C14H29NO	000638-58-4	64



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102747.D
Acq On : 5 Feb 2018 19:27
Operator : SJ/JU
Sample : J1456-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SA-ST-LATERAL-LINE-2-NW@4

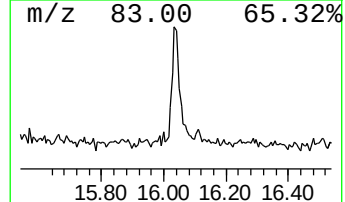
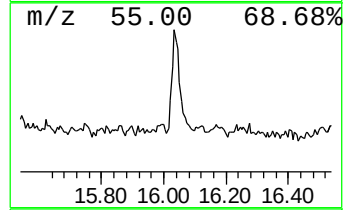
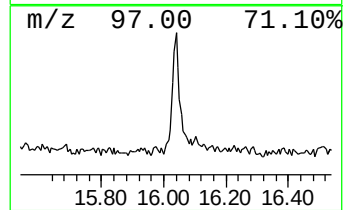
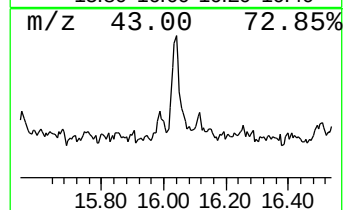
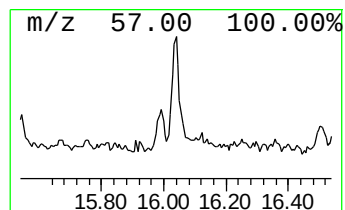
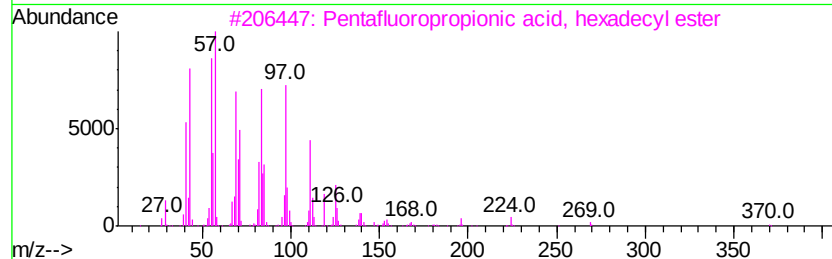
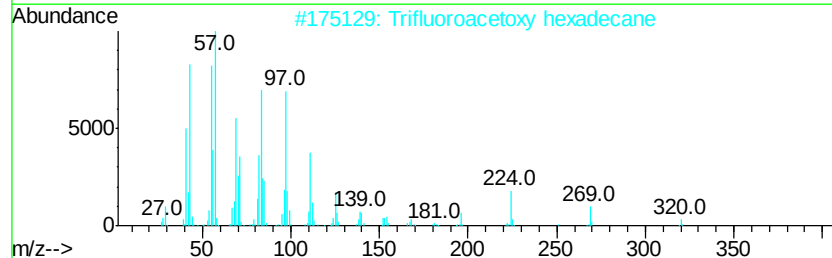
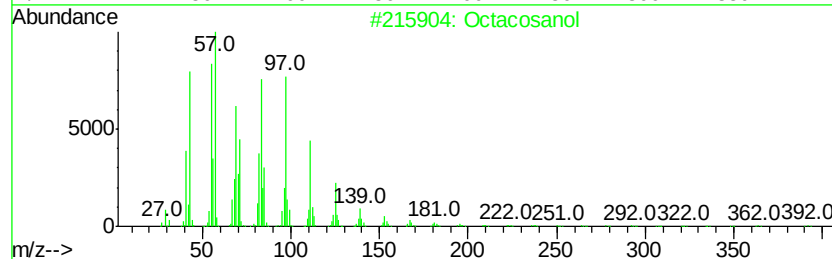
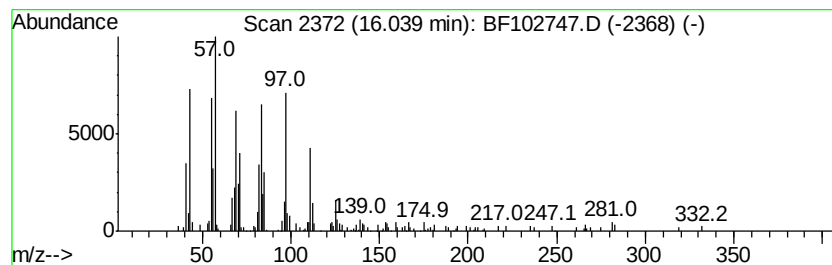
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	4.55 ng	222290	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	86
4		Triacetyl acetate	480	C32H64O2	041755-58-2	74
5		Z-5-Nonadecene	266	C19H38	1000131-11-8	74



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102747.D
Acq On : 5 Feb 2018 19:27
Operator : SJ/JU
Sample : J1456-06
Misc :
ALS Vial : 22 Sample Multiplier: 1

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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2-Pentanone, 4-hy...	5.12	2.8	ng	178970	1	6.88	1290490	20.0
unknown6.65	6.65	78.2	ng	5047560	1	6.88	1290490	20.0
Pentadecane	9.85	2.4	ng	212988	3	9.92	1762610	20.0
Hexadecane	10.35	2.6	ng	228136	3	9.92	1762610	20.0
n-Hexadecanoic acid	11.93	11.8	ng	871718	4	11.40	1479810	20.0
Octadecanoic acid	12.71	3.3	ng	241619	4	11.40	1479810	20.0
1-Heneicosanol	13.87	16.8	ng	939626	5	14.04	1118340	20.0
9-Octadecenamide, ...	14.80	10.8	ng	526700	6	15.52	976273	20.0
Octacosanol	16.04	4.5	ng	222290	6	15.52	976273	20.0