

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102770.D
 Acq On : 6 Feb 2018 6:38
 Operator : SJ/JU
 Sample : J1454-04
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 8-SAN-5-EW(4-8)

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	2.175	9	15	22	rVB	436336	582388	12.73%	1.386%
2	5.116	512	515	523	rVB	117284	144551	3.16%	0.344%
3	5.498	575	580	583	rBV	4434421	4574366	100.00%	10.887%
4	6.504	744	751	754	rBV	3862956	4565524	99.81%	10.866%
5	6.651	771	776	779	rBV	4582322	4464399	97.60%	10.626%
6	6.881	811	815	818	rBV	1624939	1297458	28.36%	3.088%
7	7.039	837	842	845	rBV	3373208	3205083	70.07%	7.628%
8	7.445	902	911	914	rBV	2822235	2978685	65.12%	7.090%
9	8.163	1027	1033	1036	rBV	2119816	1788246	39.09%	4.256%
10	9.239	1211	1216	1219	rBV	4440736	4012248	87.71%	9.550%
11	9.316	1225	1229	1231	rBV	52699	46372	1.01%	0.110%
12	9.627	1279	1282	1285	rBV	383305	296819	6.49%	0.706%
13	9.845	1315	1319	1321	rVB	135063	108239	2.37%	0.258%
14	9.874	1321	1324	1327	rBV	58472	58969	1.29%	0.140%
15	9.916	1327	1331	1335	rVV	1856212	1767612	38.64%	4.207%
16	10.345	1401	1404	1406	rVB	179616	143471	3.14%	0.341%
17	10.563	1436	1441	1443	rBV	55540	66690	1.46%	0.159%
18	10.710	1459	1466	1469	rBV	2315196	2430261	53.13%	5.784%
19	10.816	1481	1484	1494	rVB	182934	202580	4.43%	0.482%
20	11.263	1557	1560	1562	rBV	84111	66279	1.45%	0.158%
21	11.292	1562	1565	1572	rVB3	35376	49552	1.08%	0.118%
22	11.404	1580	1584	1587	rBV	1735167	1478575	32.32%	3.519%
23	11.927	1669	1673	1680	rBV2	466388	471216	10.30%	1.122%
24	12.616	1784	1790	1796	rBV	93782	95871	2.10%	0.228%
25	12.710	1802	1806	1815	rBV	102048	137534	3.01%	0.327%
26	12.804	1819	1822	1825	rBV	157043	130333	2.85%	0.310%
27	12.845	1826	1829	1833	rVB2	72446	77827	1.70%	0.185%
28	12.986	1849	1853	1857	rBV	2822940	2826117	61.78%	6.726%
29	13.463	1930	1934	1939	rBV2	58823	66331	1.45%	0.158%
30	13.510	1939	1942	1945	rVV	91173	72561	1.59%	0.173%
31	13.874	2001	2004	2014	rVB	688286	620340	13.56%	1.476%
32	14.039	2028	2032	2035	rBV	1129523	1091700	23.87%	2.598%
33	14.062	2035	2036	2045	rVB	49867	47975	1.05%	0.114%
34	14.145	2047	2050	2054	rVB2	59033	54722	1.20%	0.130%

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8-SAN-5-EW(4-8)

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
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.198	2056	2059	2066	rBV3	44477	72402	1.58%	0.172%
36	14.509	2108	2112	2116	rBV	97121	118306	2.59%	0.282%
37	14.798	2157	2161	2169	rBV2	300523	433300	9.47%	1.031%
38	15.080	2206	2209	2212	rBV2	34884	49453	1.08%	0.118%
39	15.156	2219	2222	2225	rBV	59252	66465	1.45%	0.158%
40	15.521	2278	2284	2296	rBV	701905	1032622	22.57%	2.458%
41	15.986	2359	2363	2367	rVB2	49758	71829	1.57%	0.171%
42	16.033	2367	2371	2378	rBV2	83539	149664	3.27%	0.356%

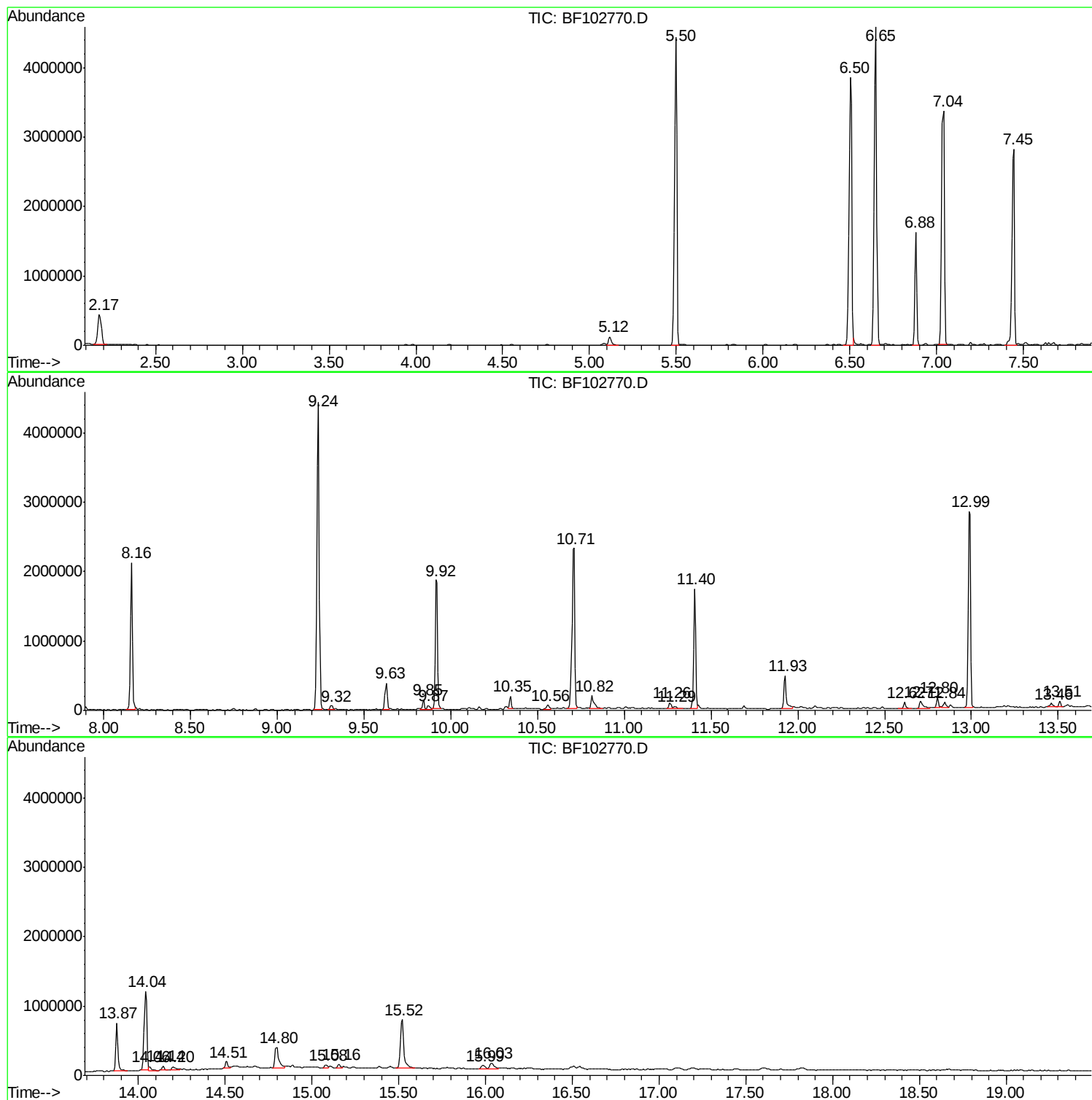
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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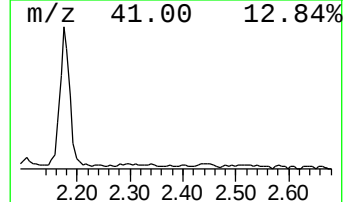
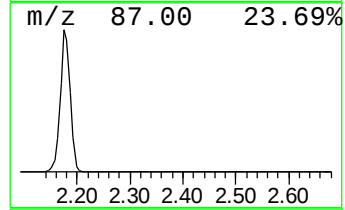
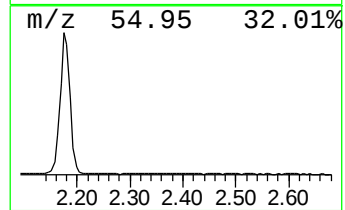
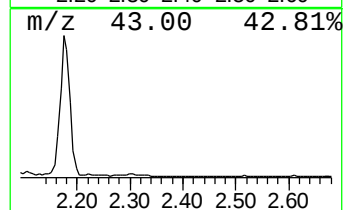
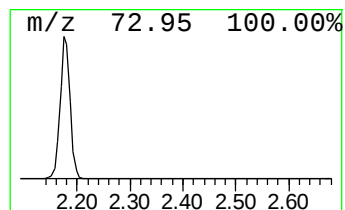
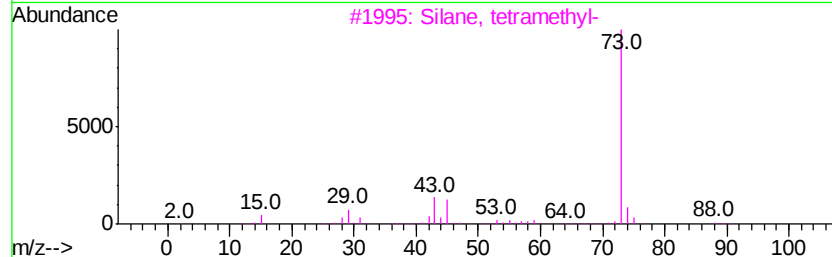
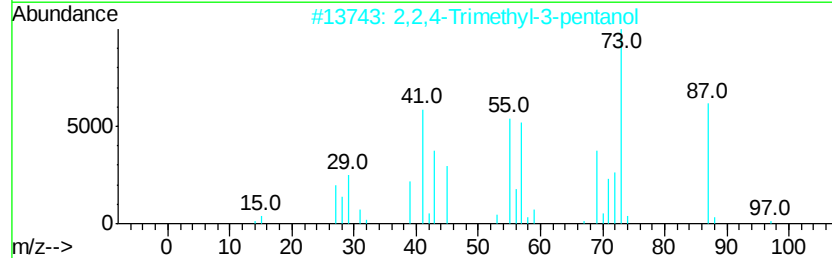
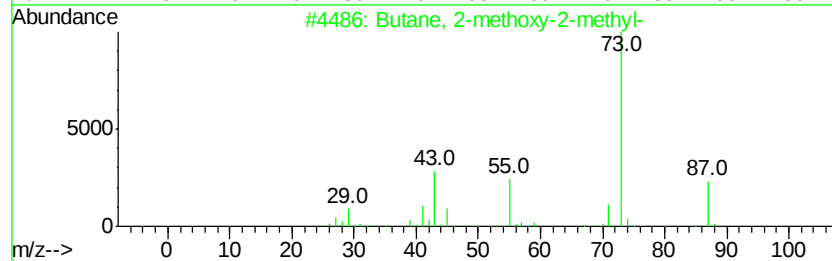
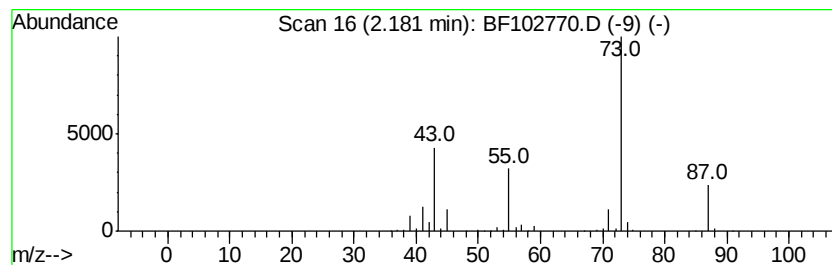
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	8.98 ng	582388	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		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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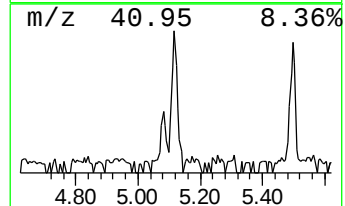
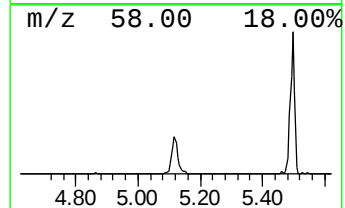
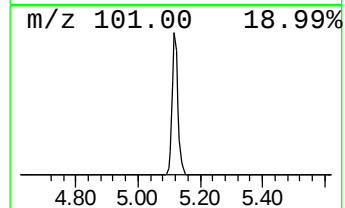
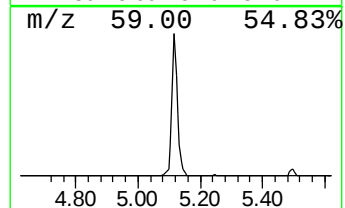
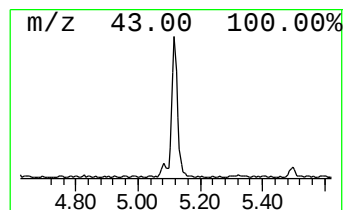
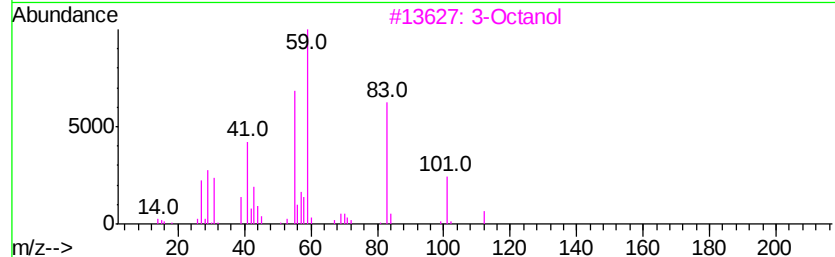
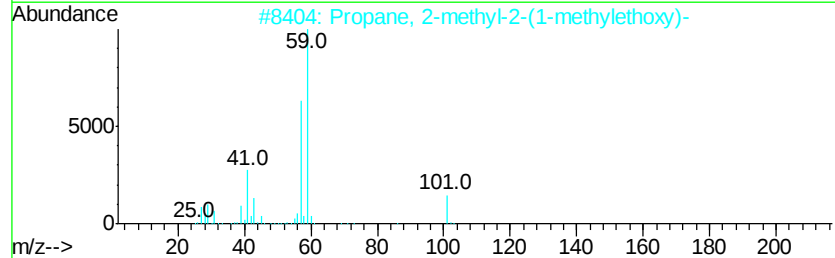
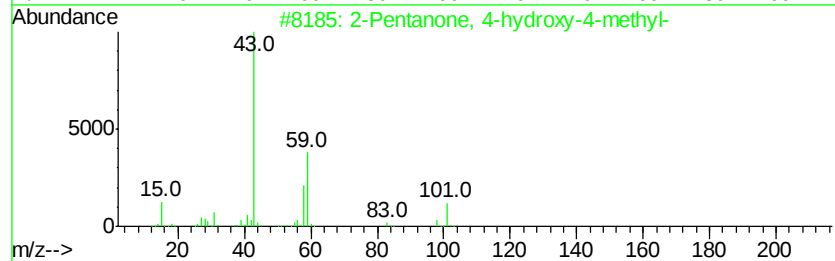
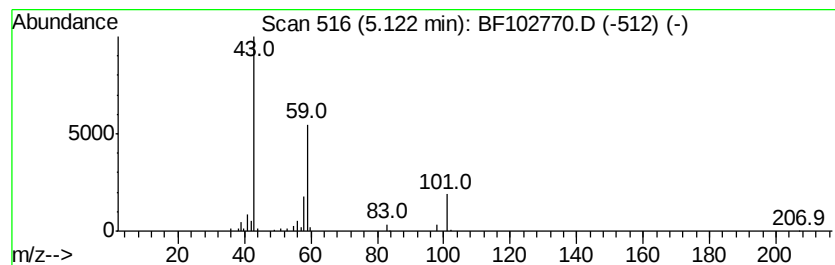
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.23 ng	144551	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	59
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
3		3-Octanol	130	C8H18O	000589-98-0	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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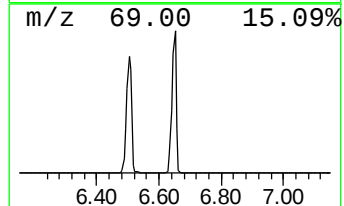
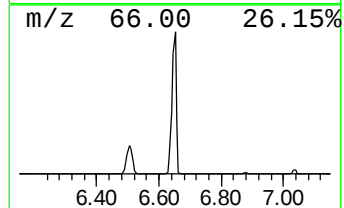
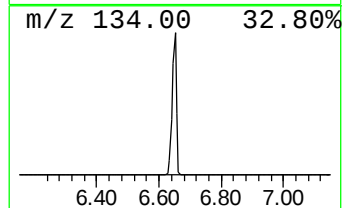
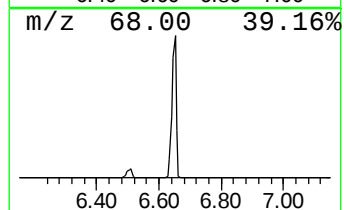
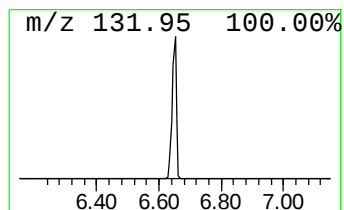
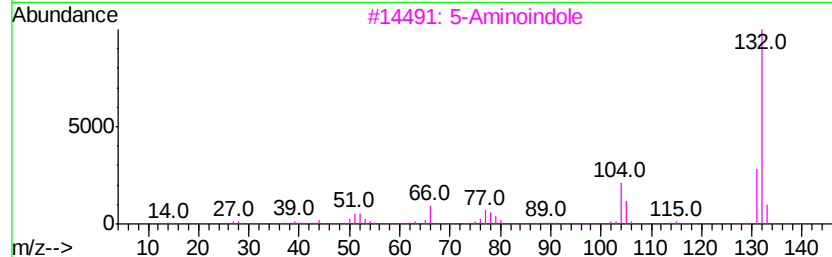
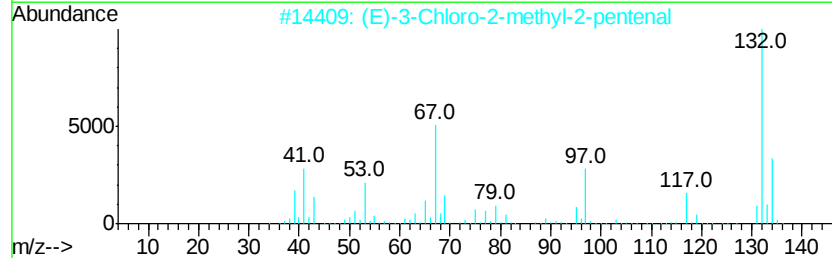
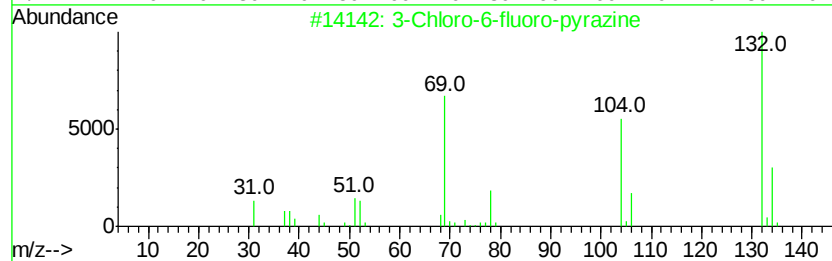
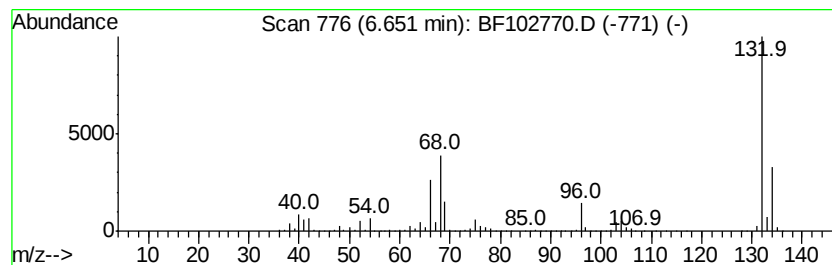
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	68.82 ng	4464400	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	17
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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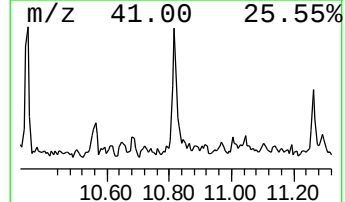
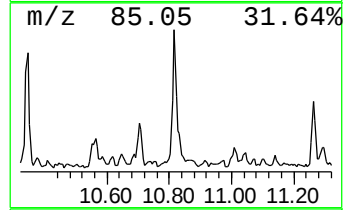
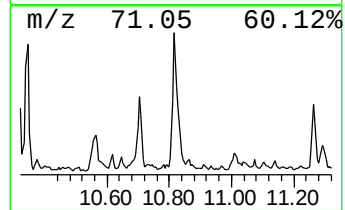
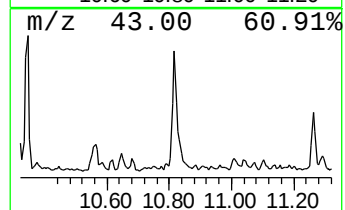
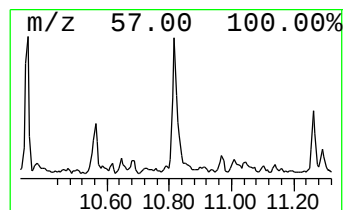
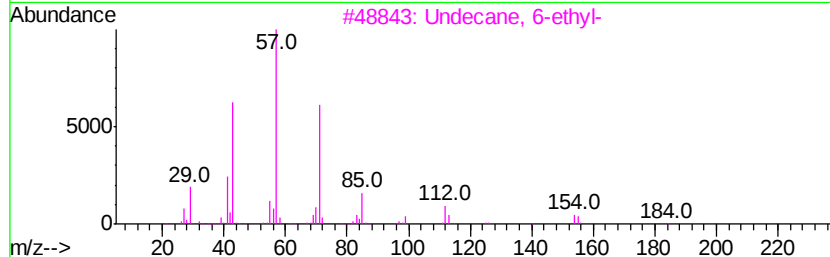
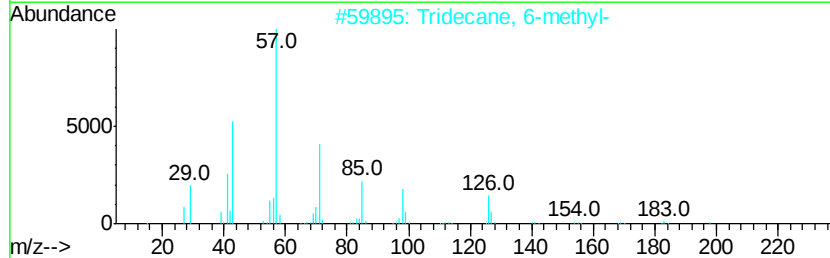
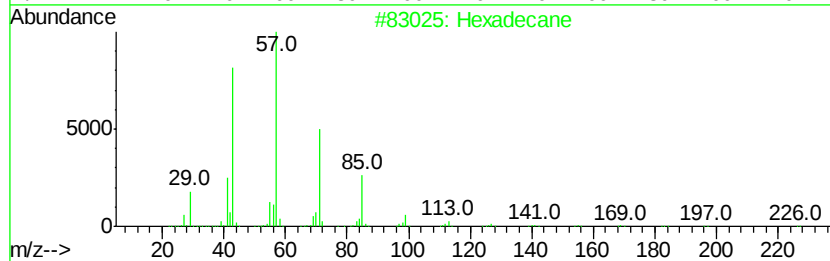
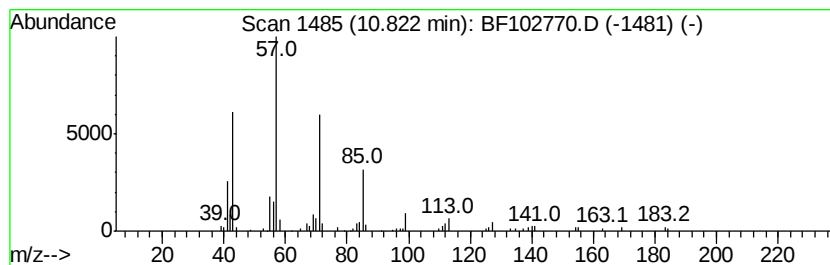
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.74 ng	202580	Phenanthrene-d10	11.40
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	86
2	Tridecane, 6-methyl-	198 C14H30	013287-21-3	78
3	Undecane, 6-ethyl-	184 C13H28	017312-60-6	72
4	2-Bromotetradecane	276 C14H29Br	074036-95-6	72
5	Sulfurous acid, 2-ethylhexyl hex...	278 C14H30O3S	1000309-20-2	72



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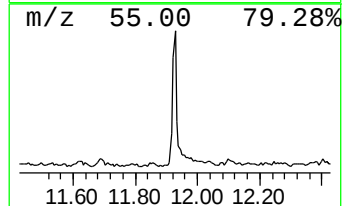
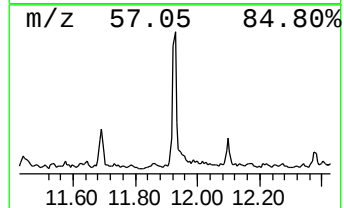
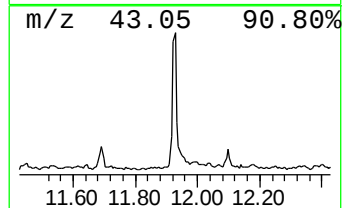
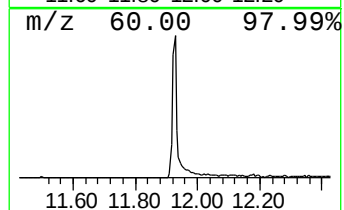
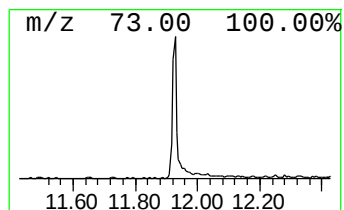
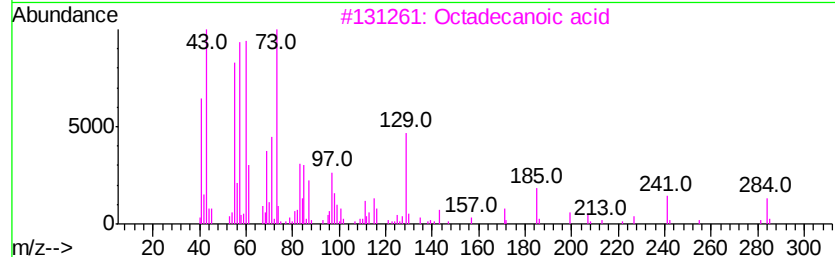
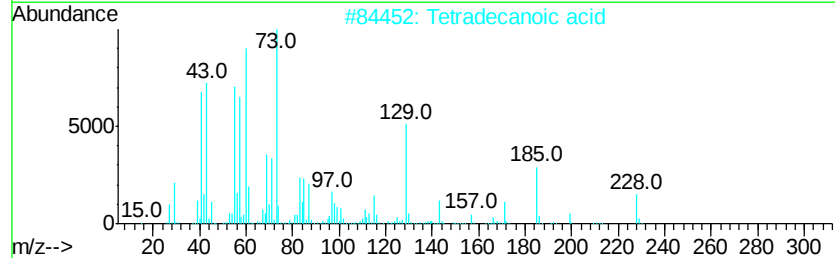
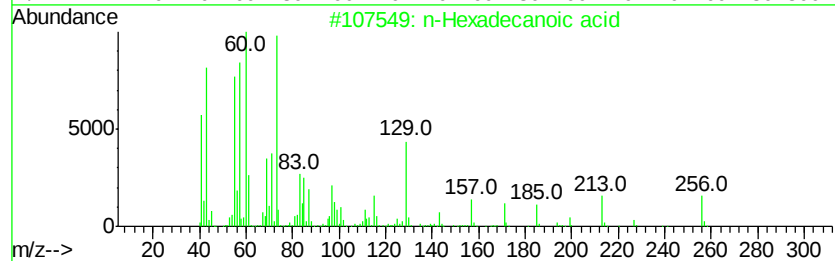
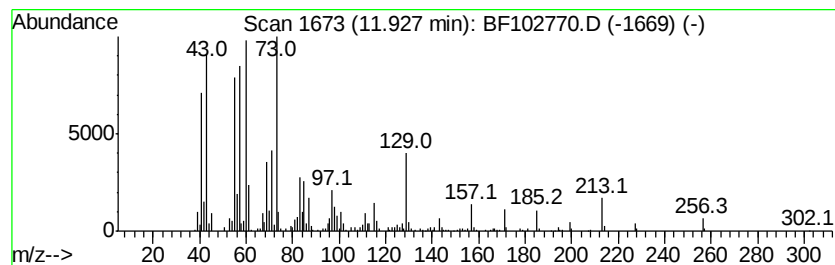
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.93	6.37 ng	471216	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102770.D
Acq On : 6 Feb 2018 6:38
Operator : SJ/JU
Sample : J1454-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
8-SAN-5-EW(4-8)

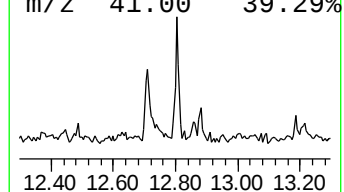
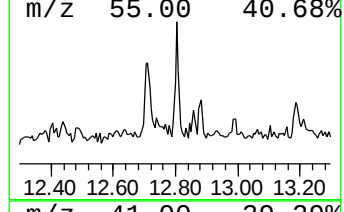
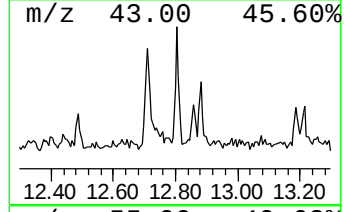
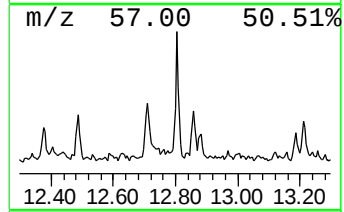
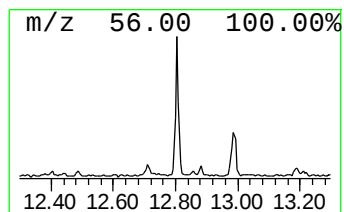
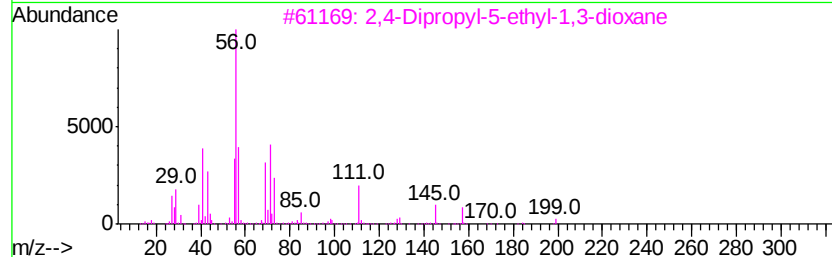
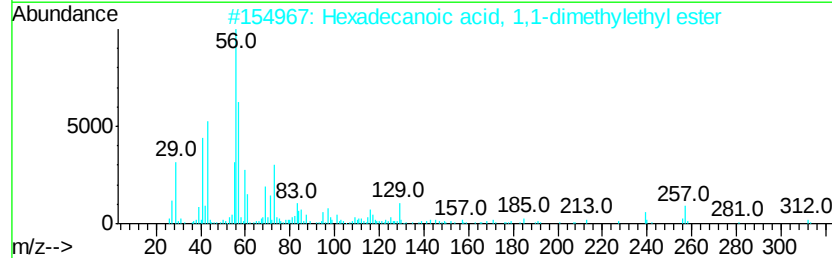
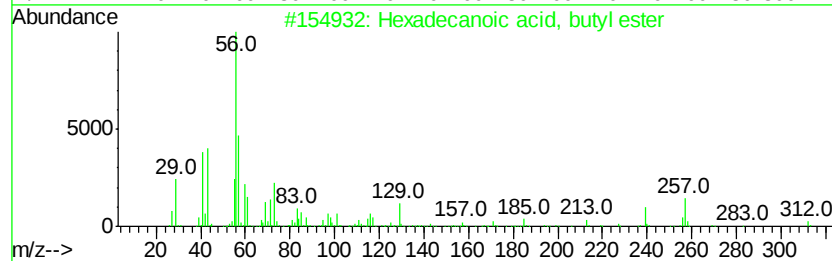
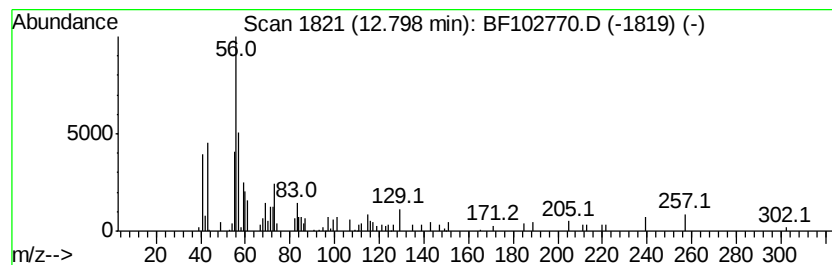
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.39 ng	130333	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	81
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38
5		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102770.D
Acq On : 6 Feb 2018 6:38
Operator : SJ/JU
Sample : J1454-04
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Instrument :
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ClientSampleId :
8-SAN-5-EW(4-8)

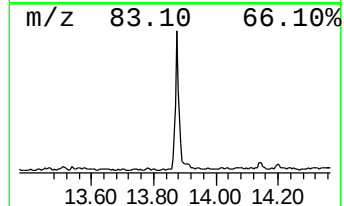
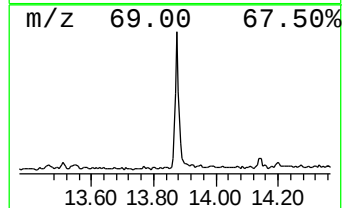
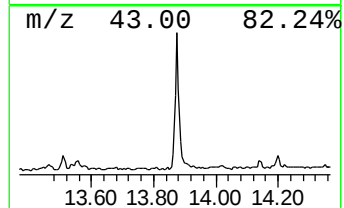
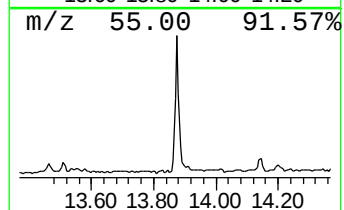
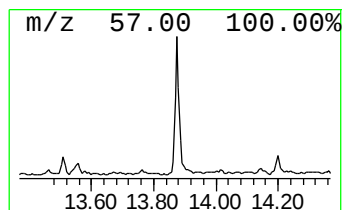
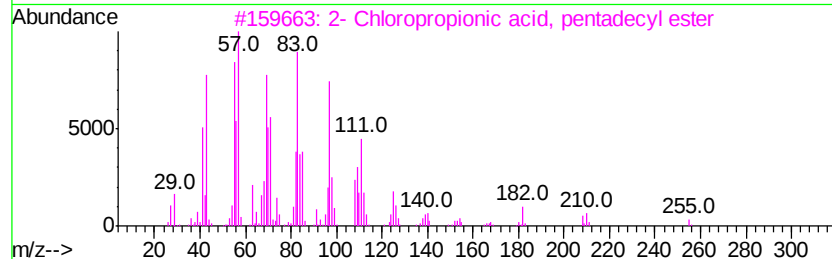
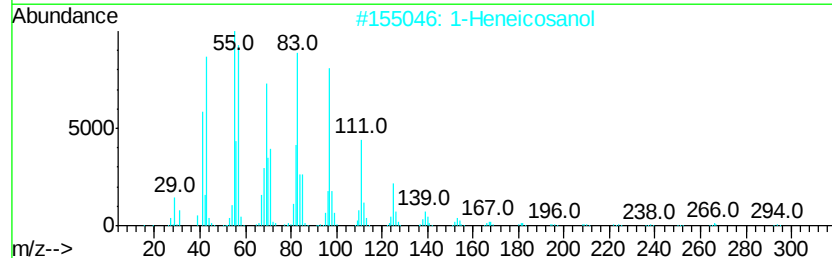
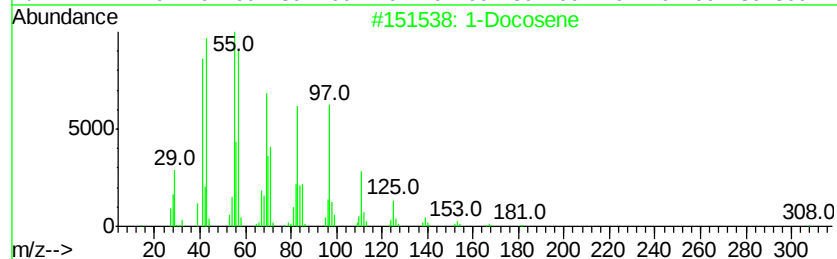
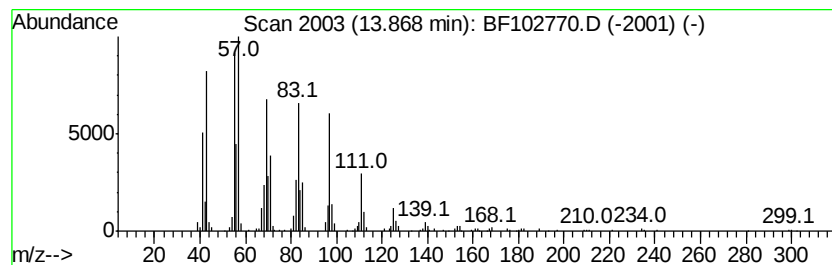
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	11.36 ng	620340	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
4		10-Heneicosene (c,t)	294	C21H42	095008-11-0	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102770.D
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Operator : SJ/JU
Sample : J1454-04
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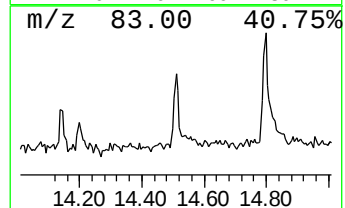
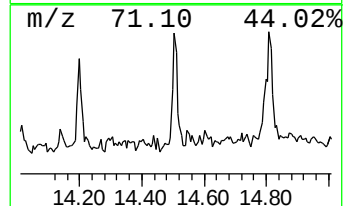
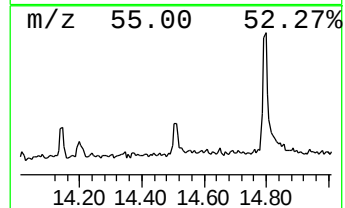
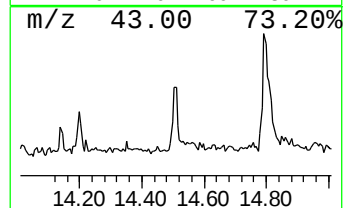
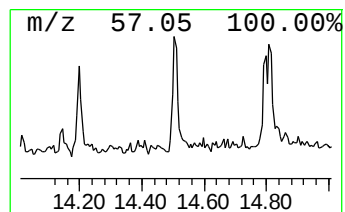
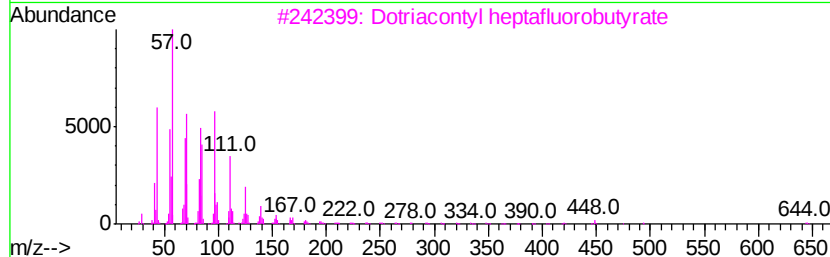
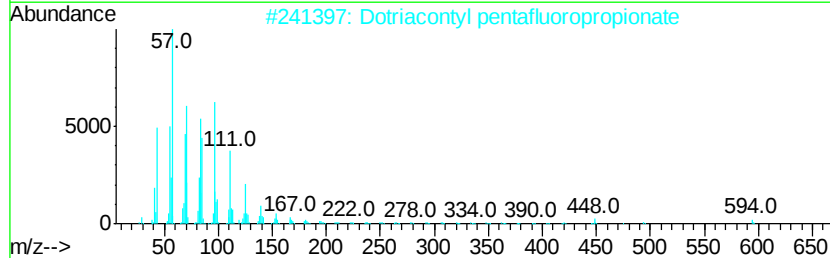
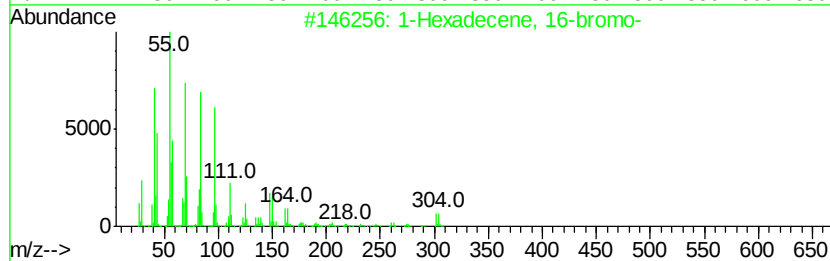
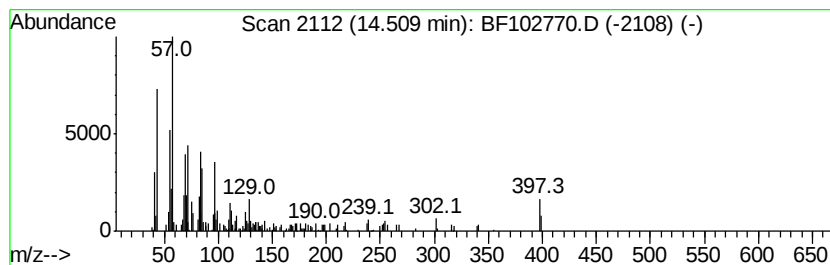
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8-SAN-5-EW(4-8)

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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-Hexadecene, 16-bromo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.17 ng	118306	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Hexadecene, 16-bromo-	302 C16H31Br	118625-56-2 93
2		Dotriacontyl pentafluoropropionate	612 C35H65F5O2	1000351-81-4 68
3		Dotriacontyl heptafluorobutvrate	662 C36H65F7O2	1000351-84-2 68
4		Triacontyl pentafluoropropionate	584 C33H61F5O2	1000351-80-0 68
5		Oxalic acid, cyclobutyl heptadec...	382 C23H42O4	1000309-70-7 64



Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
Data File : BF102770.D
Acq On : 6 Feb 2018 6:38
Operator : SJ/JU
Sample : J1454-04
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
8-SAN-5-EW(4-8)

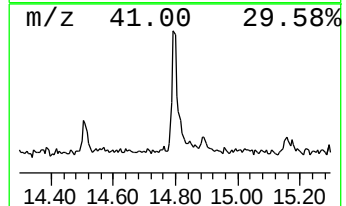
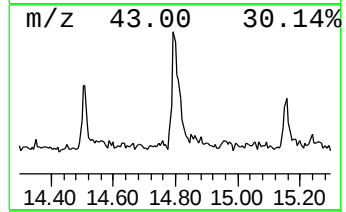
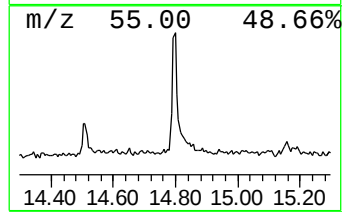
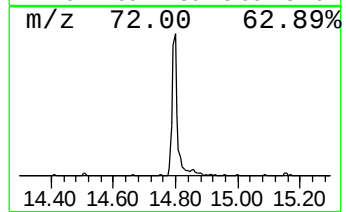
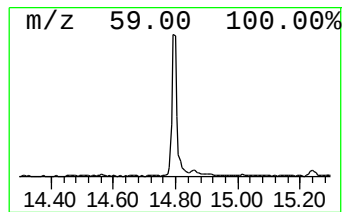
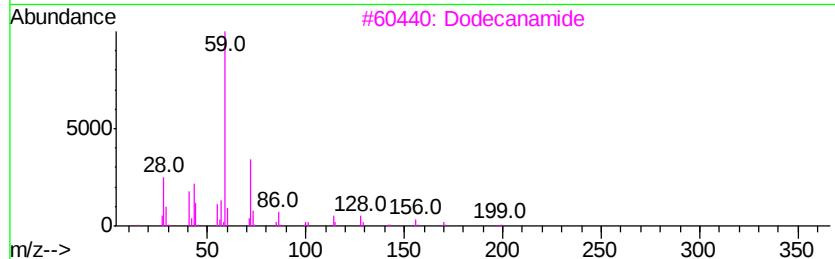
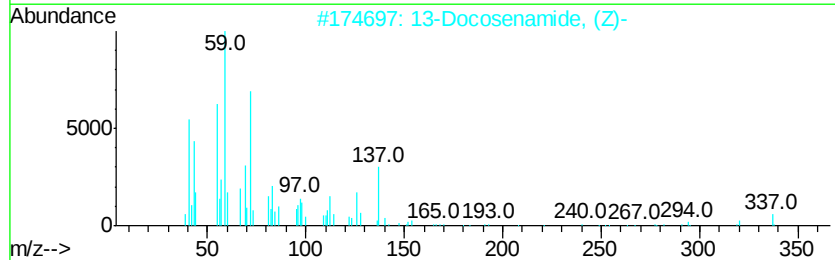
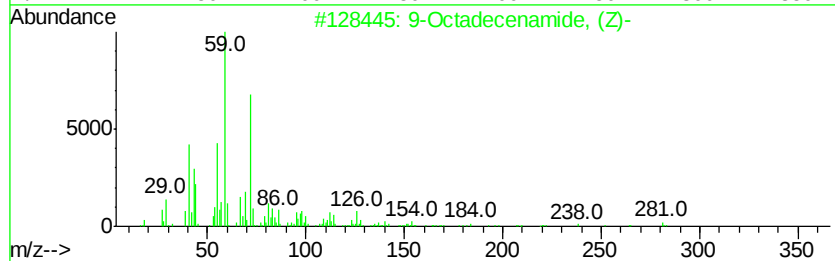
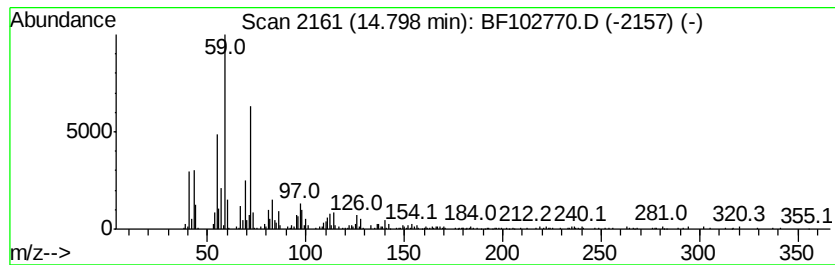
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	8.39 ng	433300	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	94
3		Dodecanamide	199	C12H25NO	001120-16-7	62
4		Hexadecanamide	255	C16H33NO	000629-54-9	59
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102770.D
Acq On : 6 Feb 2018 6:38
Operator : SJ/JU
Sample : J1454-04
Misc :
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Instrument :
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ClientSampleId :
8-SAN-5-EW(4-8)

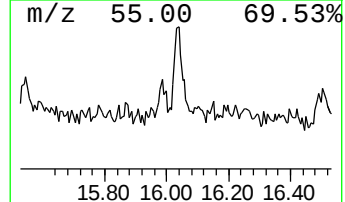
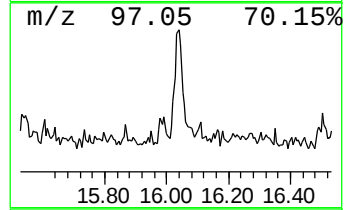
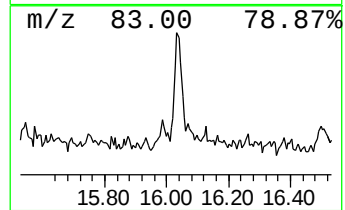
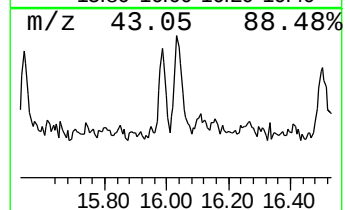
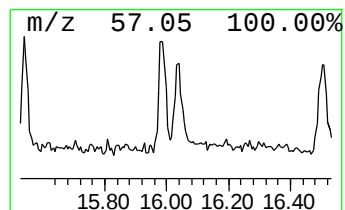
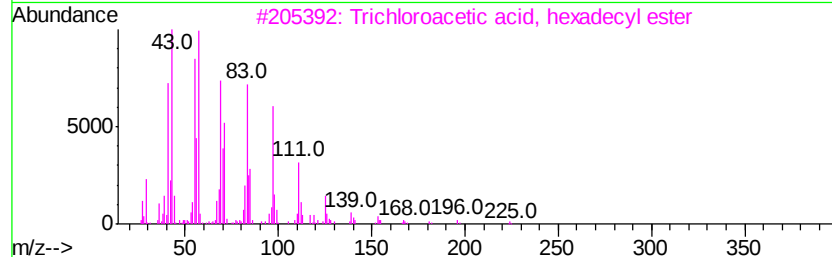
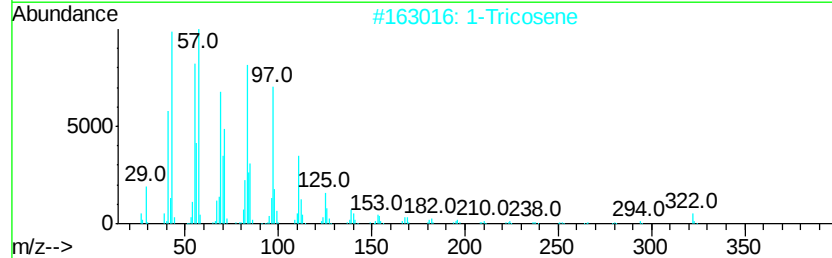
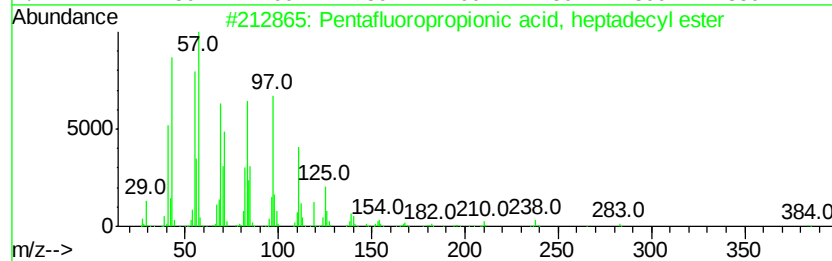
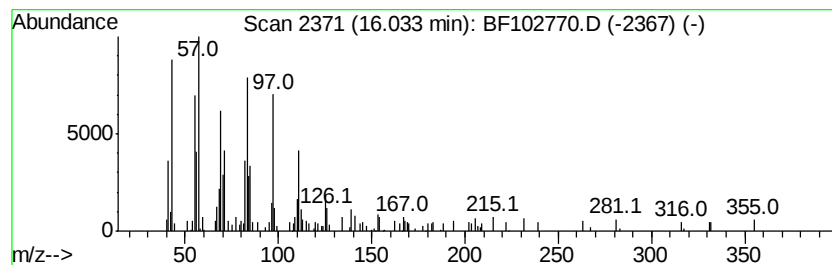
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.90 ng	149664	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2		1-Tricosene	322	C23H46	018835-32-0	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



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8-SAN-5-EW(4-8)

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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	9.0 ng		582388	1	6.88	1297460	20.0
2-Pentanone, 4-hy...	5.12	2.2 ng		144551	1	6.88	1297460	20.0
unknown6.65	6.65	68.8 ng		4464400	1	6.88	1297460	20.0
Hexadecane	10.82	2.7 ng		202580	4	11.40	1478580	20.0
n-Hexadecanoic acid	11.93	6.4 ng		471216	4	11.40	1478580	20.0
Hexadecanoic acid...	12.80	2.4 ng		130333	5	14.04	1091700	20.0
1-Docosene	13.87	11.4 ng		620340	5	14.04	1091700	20.0
1-Hexadecene, 16-...	14.51	2.2 ng		118306	5	14.04	1091700	20.0
9-Octadecenamide, ...	14.80	8.4 ng		433300	6	15.52	1032620	20.0
Pentafluoropropio...	16.03	2.9 ng		149664	6	15.52	1032620	20.0