

Data Path : U:\HPCHEM1\BNA F\DATA\BF020518\
 Data File : BF102768.D
 Acq On : 6 Feb 2018 5:44
 Operator : SJ/JU
 Sample : J1454-08
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 8-SAN-7-EW(4-7)

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	2.187	11	17	31	rVB	518804	735867	15.40%	1.689%
2	5.116	512	515	524	rVB	189514	236253	4.95%	0.542%
3	5.498	575	580	583	rBV	4340964	4731124	99.04%	10.858%
4	6.504	745	751	760	rBV	3929540	4776820	100.00%	10.963%
5	6.651	771	776	779	rBV	4665050	4636469	97.06%	10.640%
6	6.881	811	815	818	rBV	1654149	1329205	27.83%	3.050%
7	7.040	837	842	845	rBV	3702092	3465003	72.54%	7.952%
8	7.445	903	911	914	rBV	3078307	3110599	65.12%	7.139%
9	7.510	917	922	928	rVB3	42581	52598	1.10%	0.121%
10	8.163	1028	1033	1036	rBV	2200863	1776147	37.18%	4.076%
11	9.239	1210	1216	1219	rBV	4529716	4160677	87.10%	9.549%
12	9.628	1278	1282	1285	rBV	453649	357203	7.48%	0.820%
13	9.845	1315	1319	1322	rVB	145402	128053	2.68%	0.294%
14	9.916	1327	1331	1335	rBV	1874038	1805955	37.81%	4.145%
15	10.345	1401	1404	1407	rVB	214695	172889	3.62%	0.397%
16	10.563	1436	1441	1443	rBV	58460	69389	1.45%	0.159%
17	10.704	1459	1465	1469	rBV	2431615	2483516	51.99%	5.700%
18	10.816	1481	1484	1493	rVB	206700	205314	4.30%	0.471%
19	11.263	1557	1560	1562	rBV	131690	99401	2.08%	0.228%
20	11.292	1562	1565	1571	rVB3	37531	48754	1.02%	0.112%
21	11.404	1580	1584	1587	rBV	1822781	1510339	31.62%	3.466%
22	11.927	1669	1673	1683	rBV	538160	541370	11.33%	1.242%
23	12.710	1802	1806	1816	rBV	127938	158029	3.31%	0.363%
24	12.804	1819	1822	1825	rBV	226903	177147	3.71%	0.407%
25	12.992	1849	1854	1857	rBV	3110596	2942982	61.61%	6.754%
26	13.463	1931	1934	1939	rVB	72868	70515	1.48%	0.162%
27	13.510	1939	1942	1945	rBV	137407	108152	2.26%	0.248%
28	13.874	2001	2004	2012	rBV	962254	846434	17.72%	1.943%
29	14.039	2028	2032	2036	rVB	1068454	1063603	22.27%	2.441%
30	14.145	2047	2050	2052	rVB2	59929	50099	1.05%	0.115%
31	14.198	2056	2059	2062	rBV	52907	55626	1.16%	0.128%
32	14.510	2108	2112	2116	rBV	140773	152113	3.18%	0.349%
33	14.792	2157	2160	2163	rBV	93123	114276	2.39%	0.262%
34	15.157	2219	2222	2224	rBV	41929	49620	1.04%	0.114%

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ClientSampleId :
8-SAN-7-EW(4-7)

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	15.521	2278	2284	2292	rBV	722204	1004237	21.02%	2.305%
36	16.033	2367	2371	2380	rBV	108987	188466	3.95%	0.433%
37	16.539	2454	2457	2462	rVB	48093	76297	1.60%	0.175%
38	17.604	2635	2638	2647	rVB	43329	83545	1.75%	0.192%

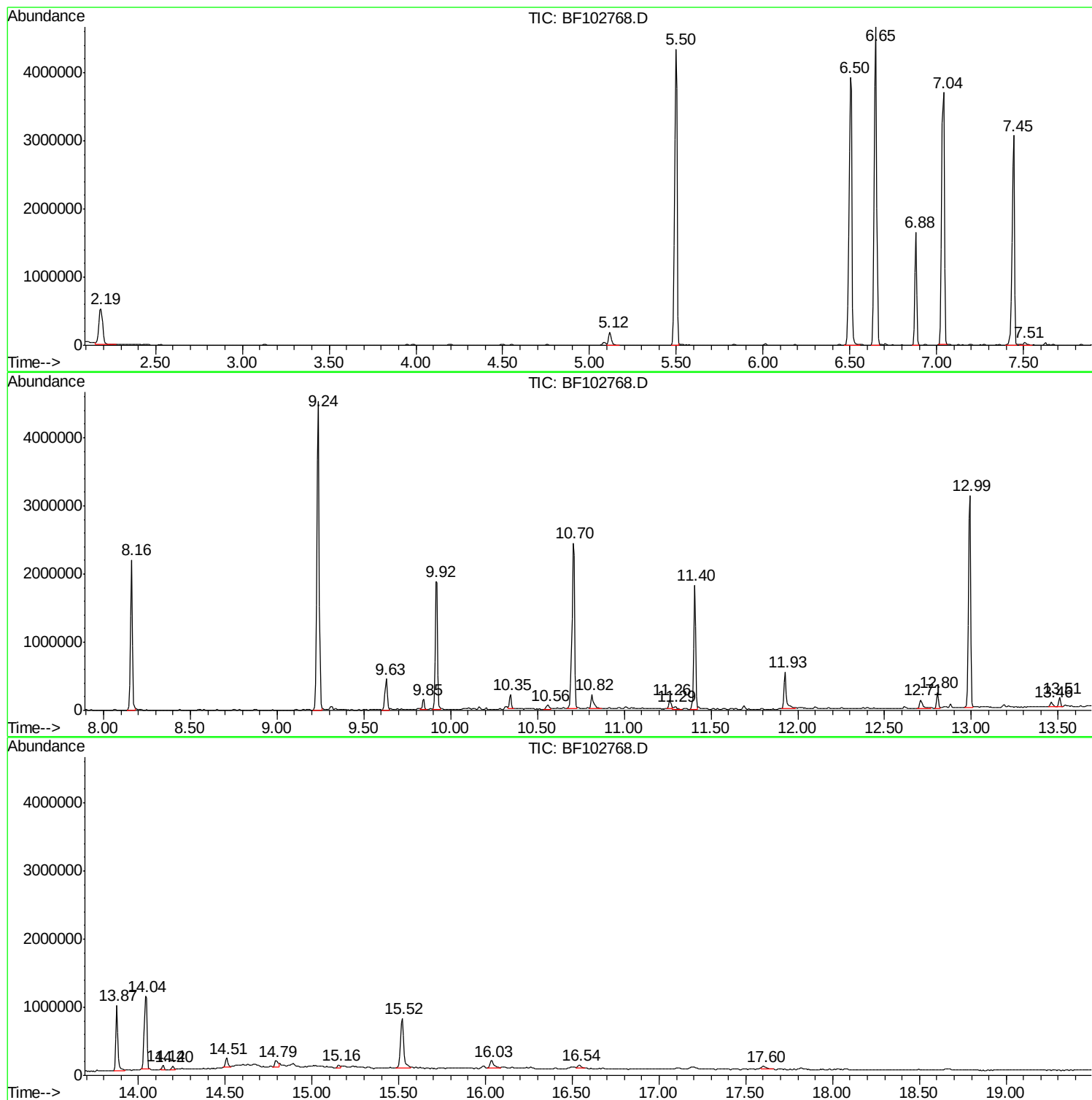
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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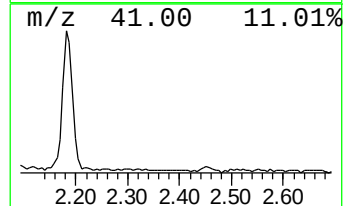
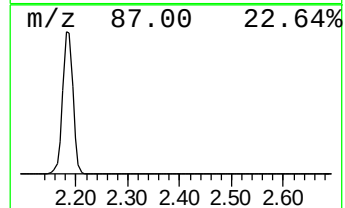
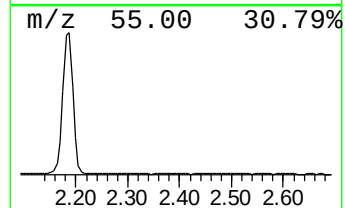
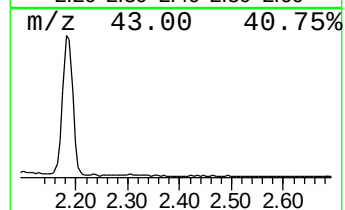
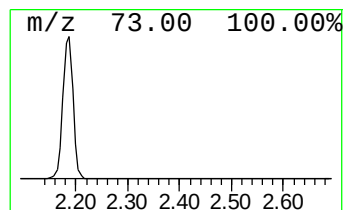
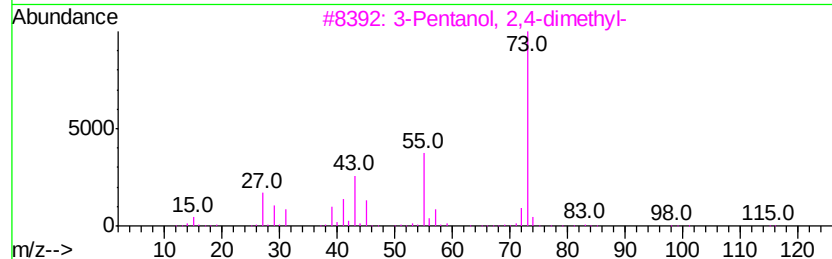
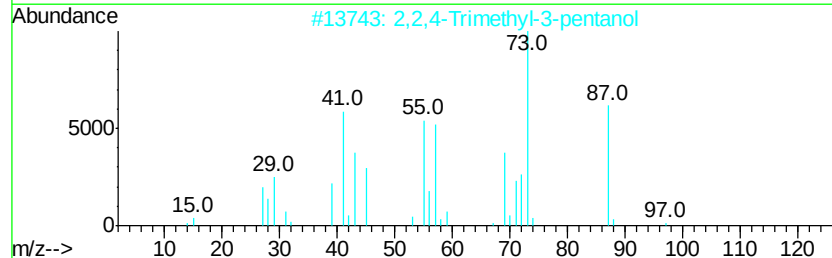
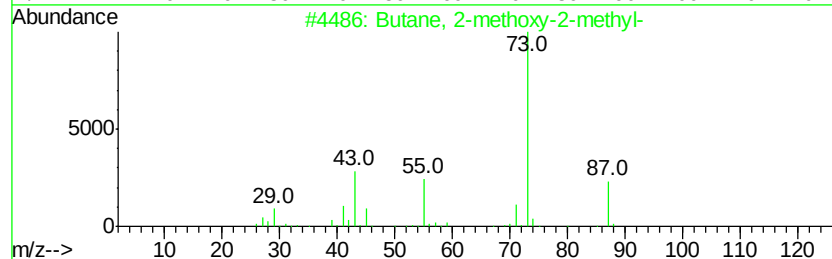
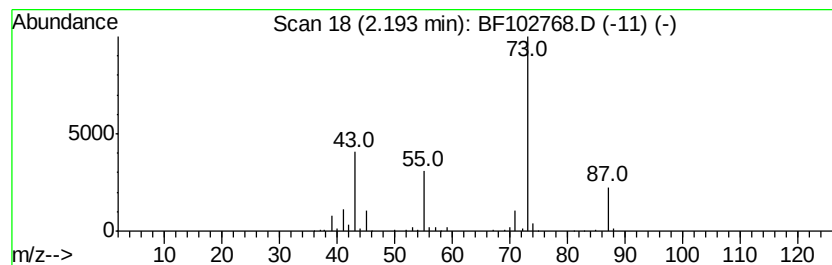
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.19	11.07 ng	735867	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		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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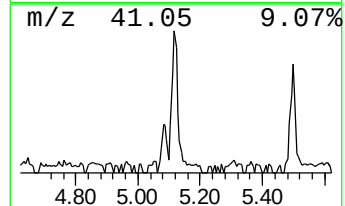
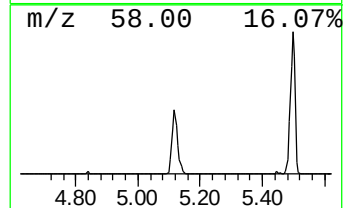
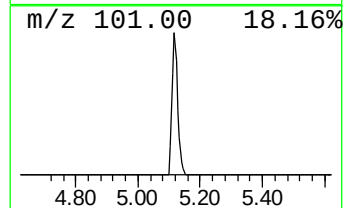
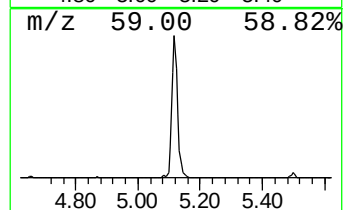
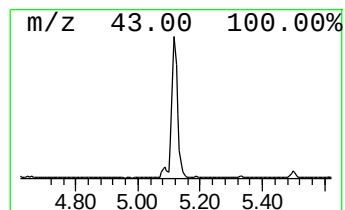
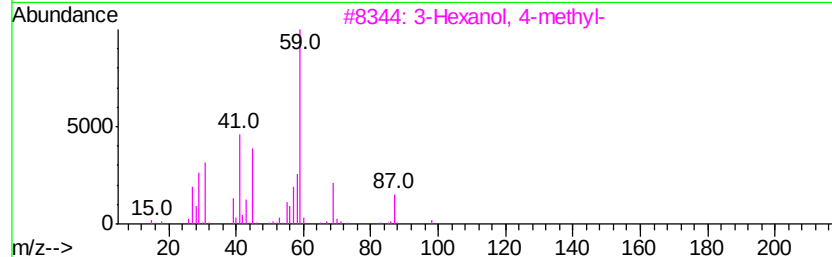
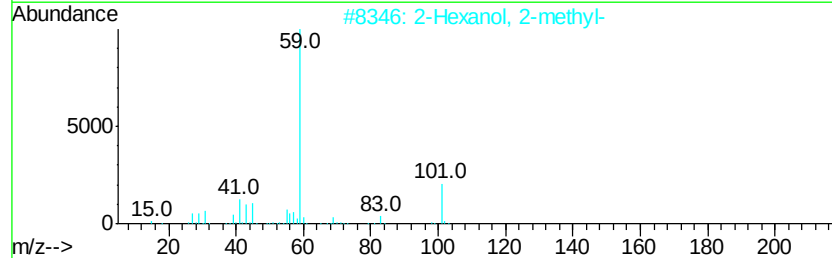
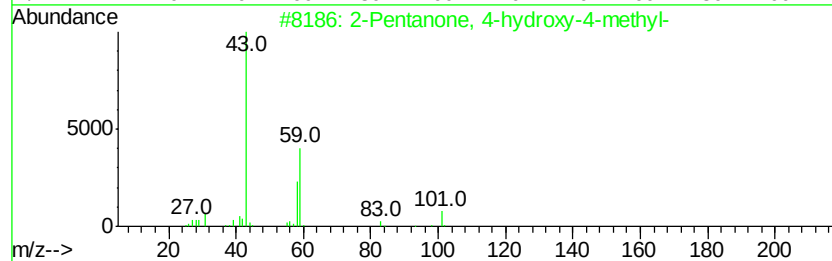
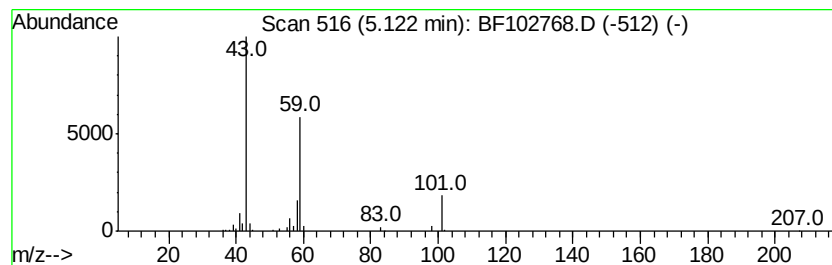
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.55 ng	236253	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	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	23



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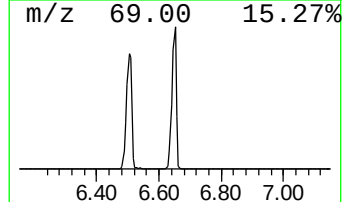
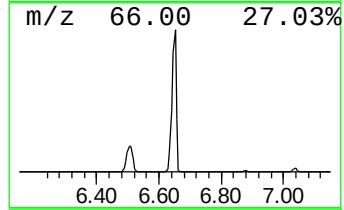
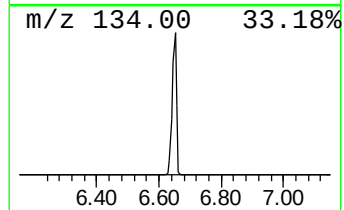
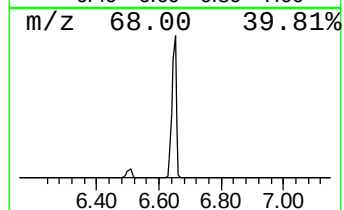
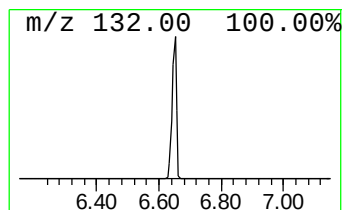
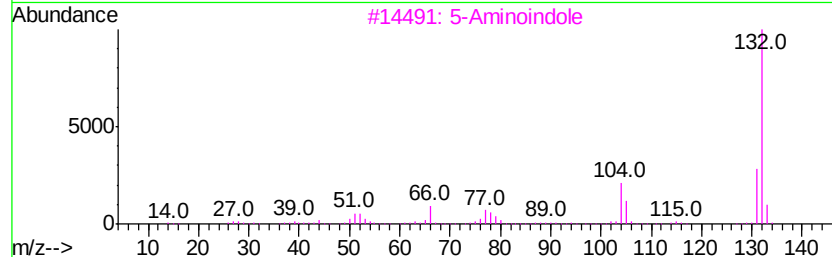
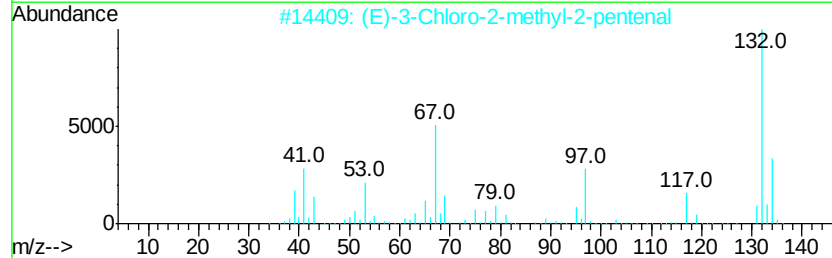
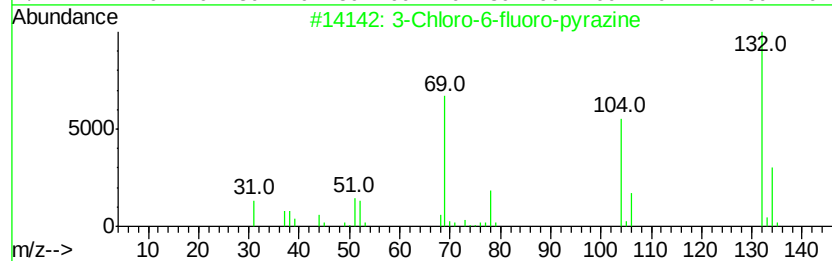
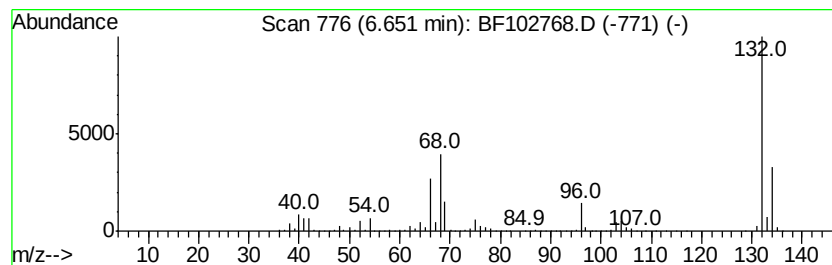
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.76 ng	4636470	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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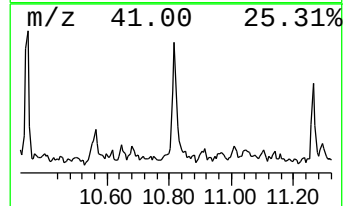
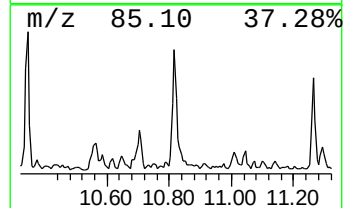
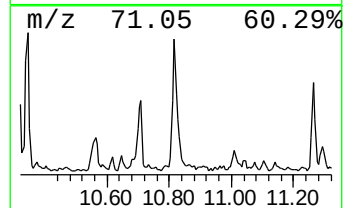
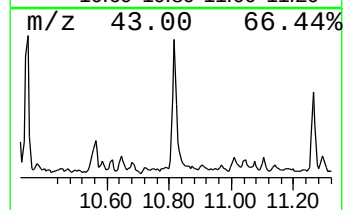
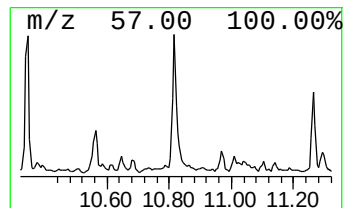
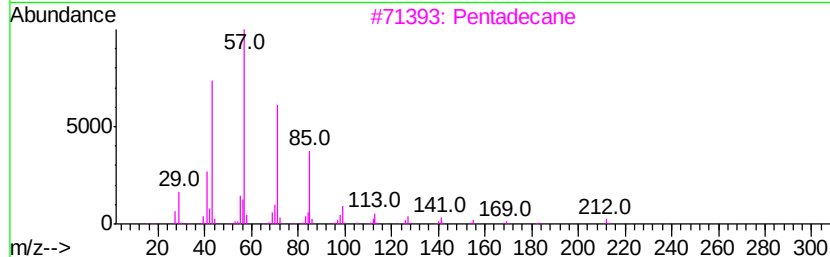
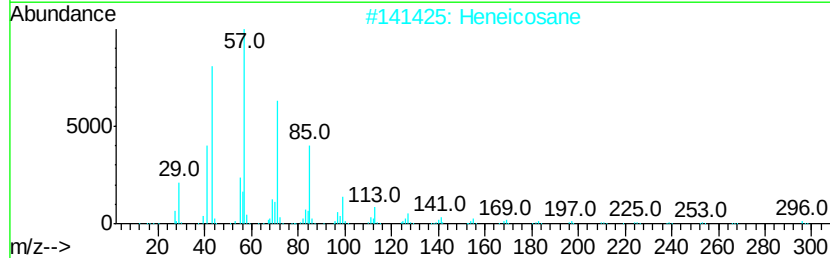
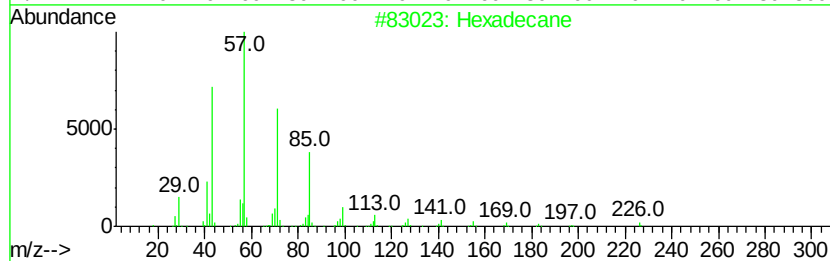
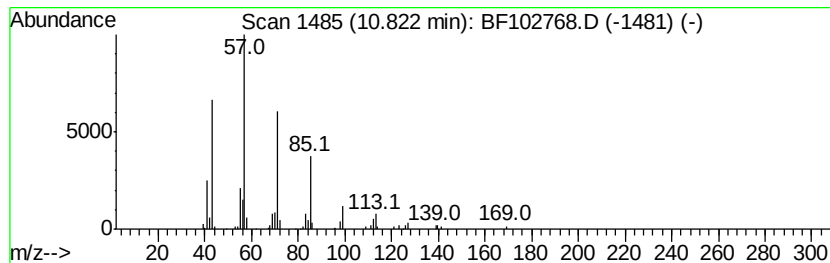
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	2.72 ng	205314	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heneicosane	296	C21H44	000629-94-7	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tetracosane	338	C24H50	000646-31-1	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83



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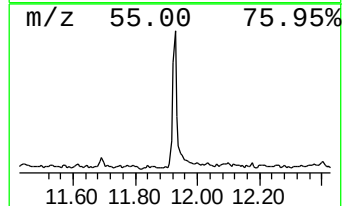
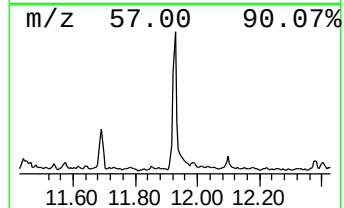
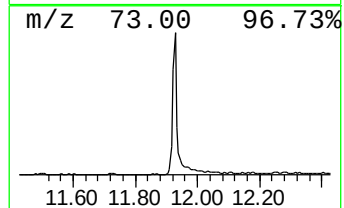
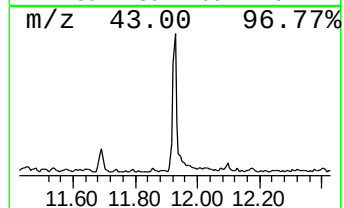
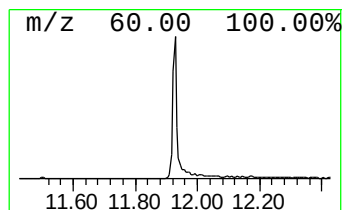
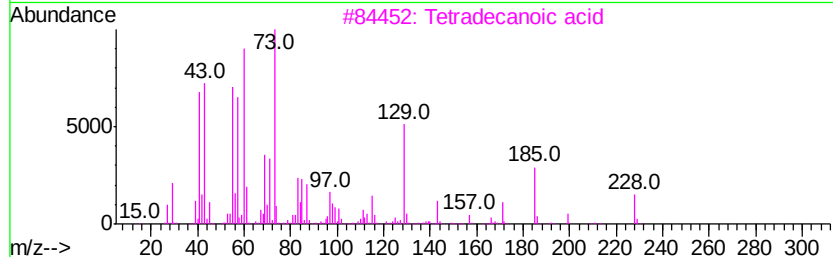
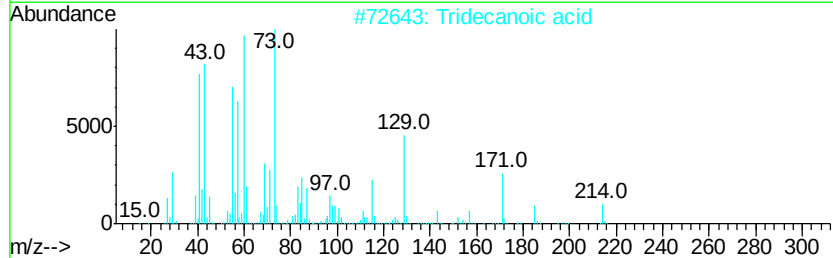
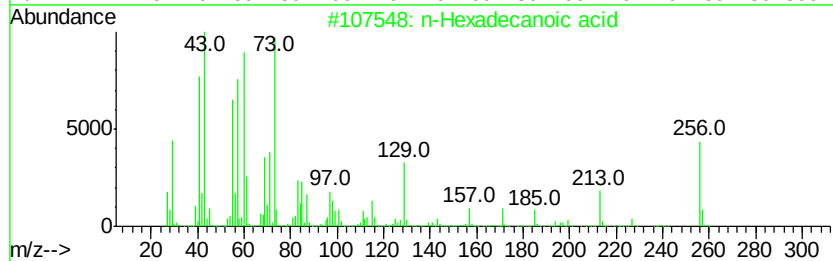
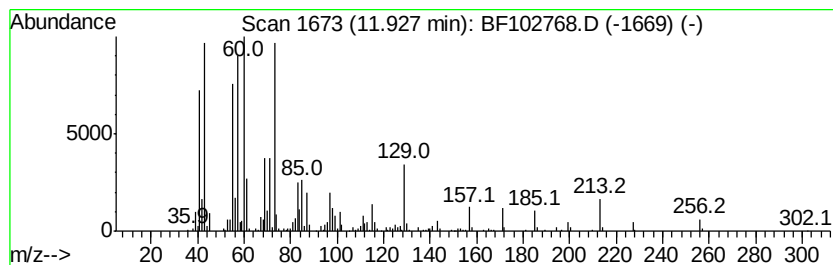
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.93	7.17 ng	541370	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102768.D
Acq On : 6 Feb 2018 5:44
Operator : SJ/JU
Sample : J1454-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
8-SAN-7-EW(4-7)

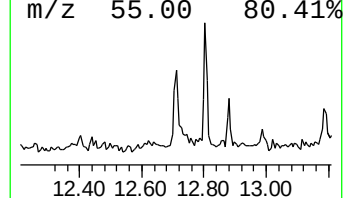
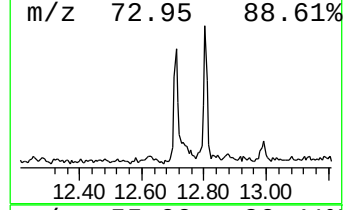
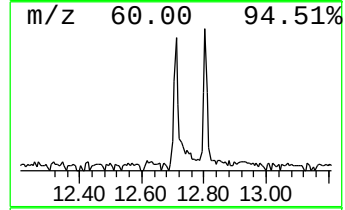
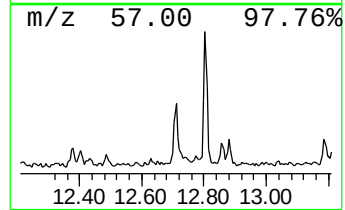
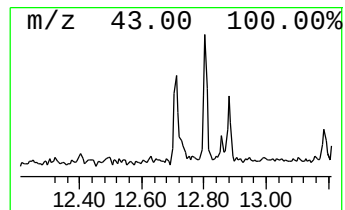
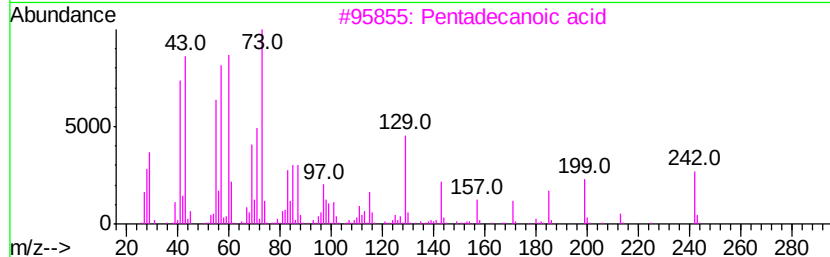
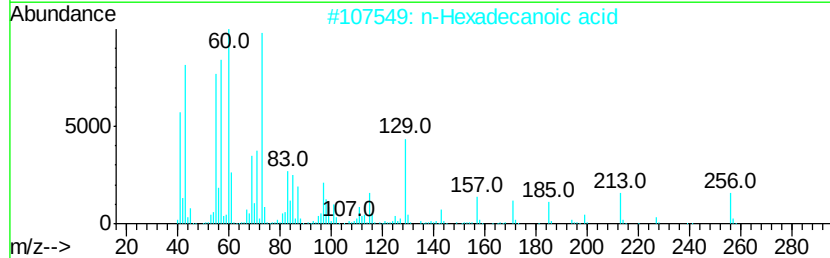
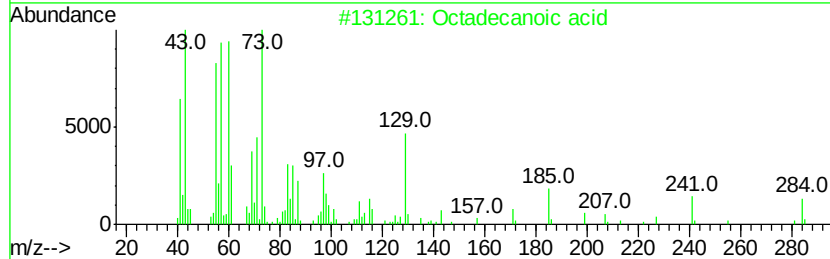
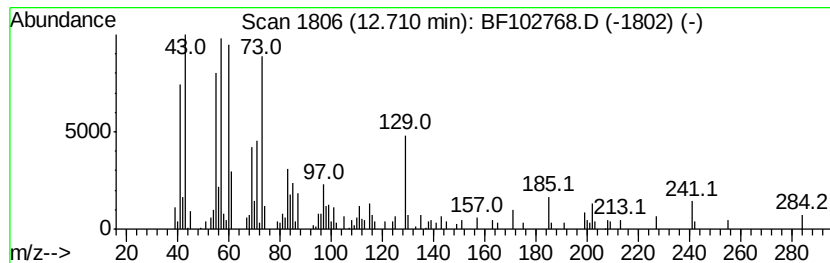
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.09 ng	158029	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4		Dodecanoic acid	200	C12H24O2	000143-07-7	58
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58



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Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
8-SAN-7-EW(4-7)

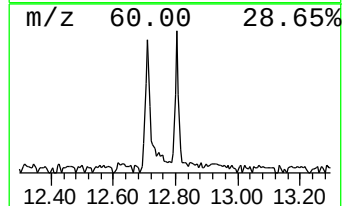
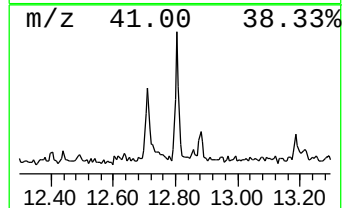
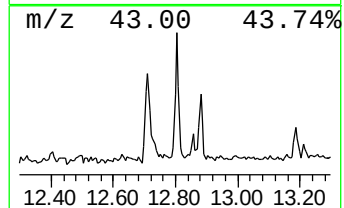
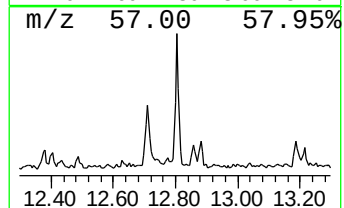
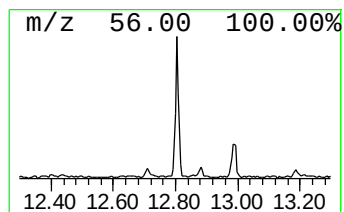
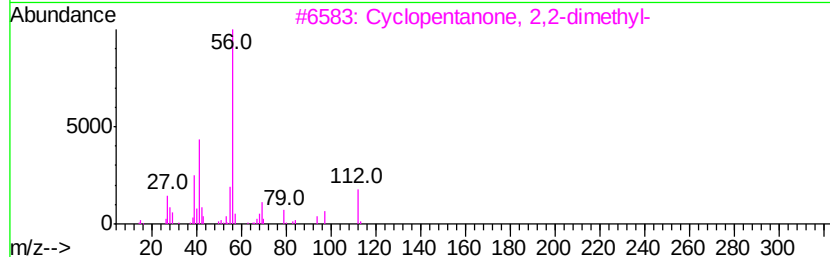
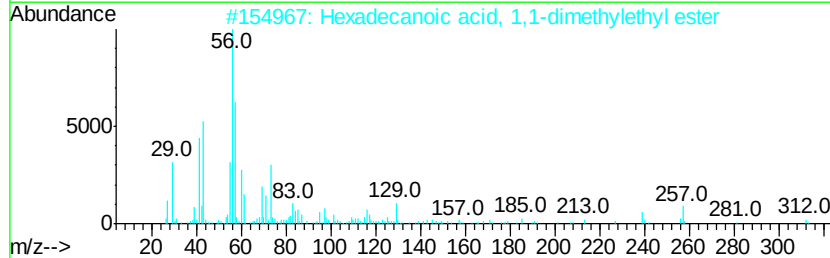
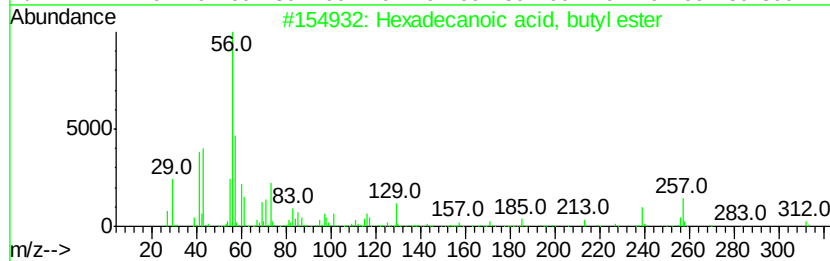
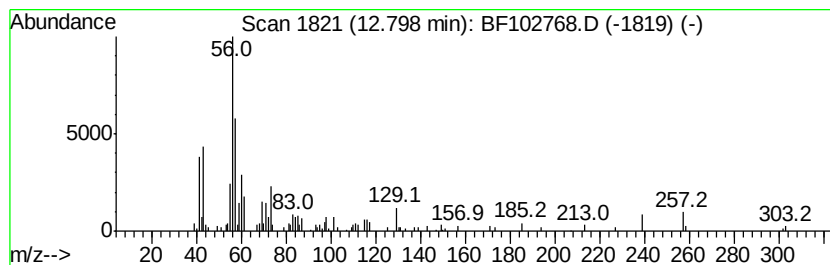
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	3.33 ng	177147	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	87
3		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
4		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	38
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	35



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Sample : J1454-08
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Instrument :
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8-SAN-7-EW(4-7)

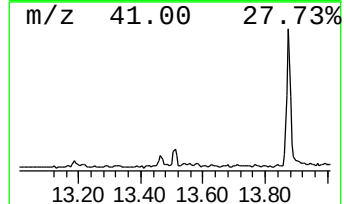
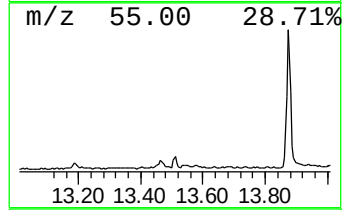
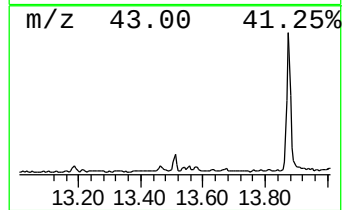
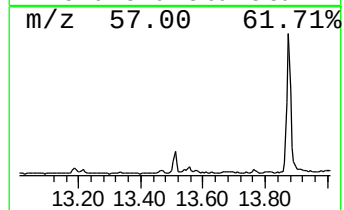
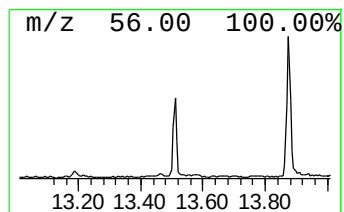
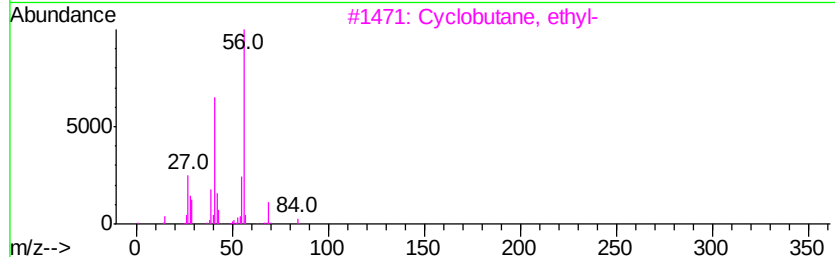
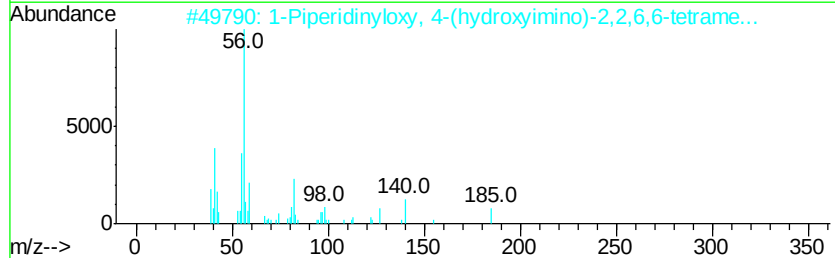
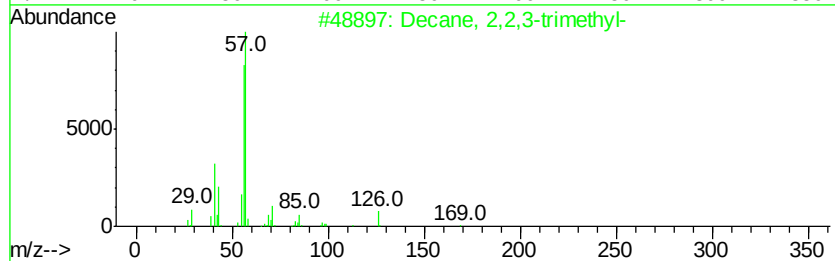
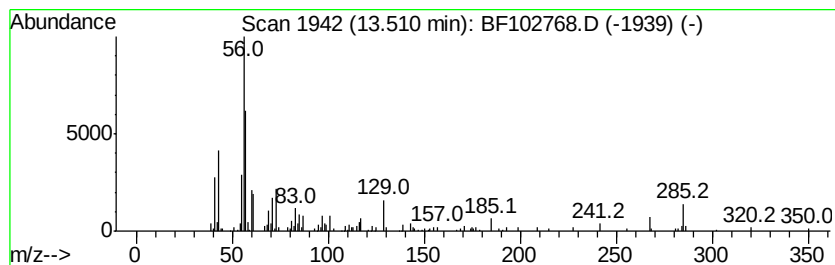
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.51 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.51	2.03 ng	108152	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
2		1-Piperidinyloxy, 4-(hydroximin...	185	C9H17N2O2	003229-75-2	35
3		Cyclobutane, ethyl-	84	C6H12	004806-61-5	35
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



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Instrument :
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ClientSampleId :
8-SAN-7-EW(4-7)

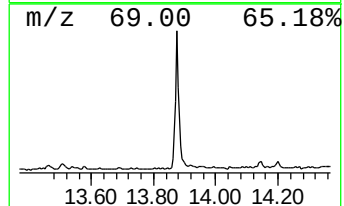
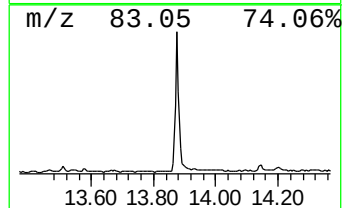
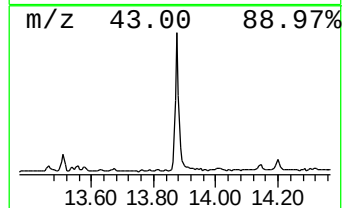
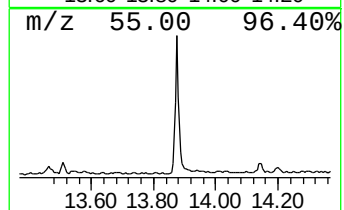
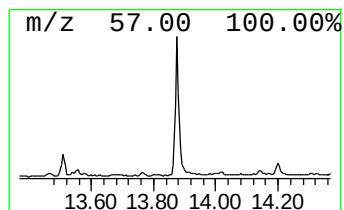
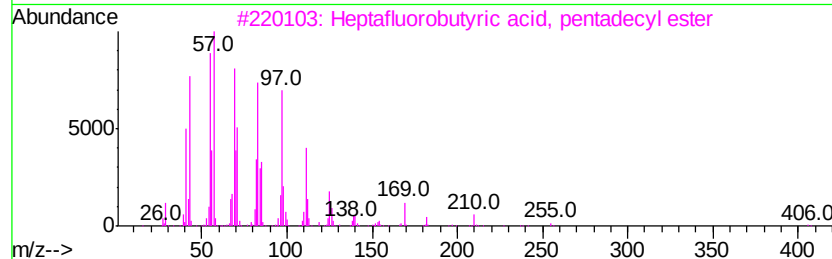
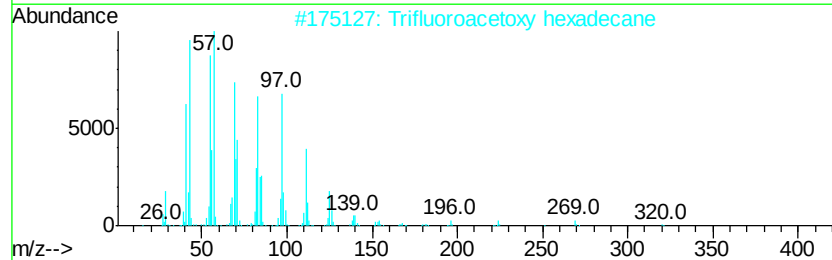
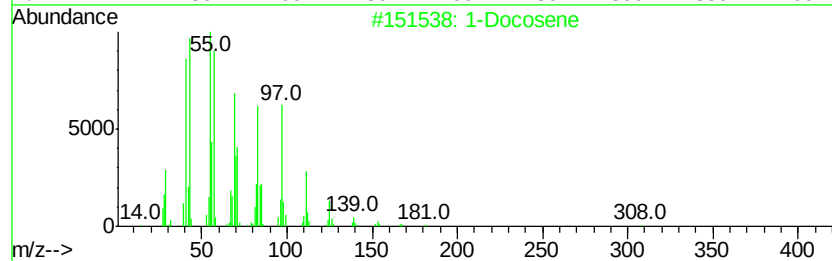
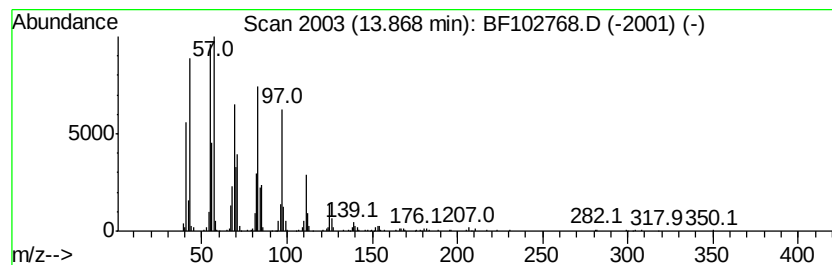
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	15.92 ng	846434	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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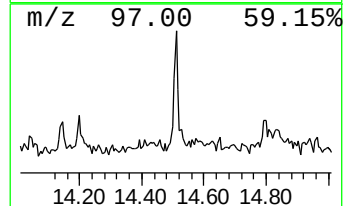
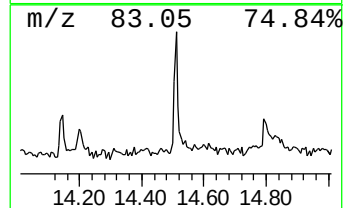
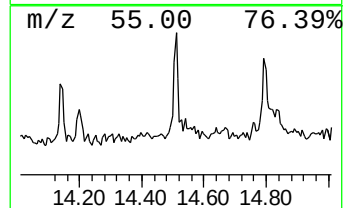
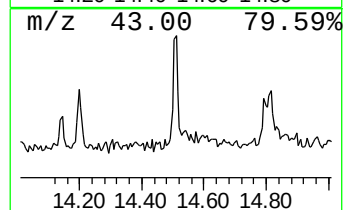
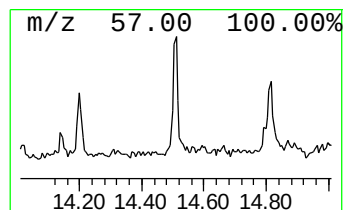
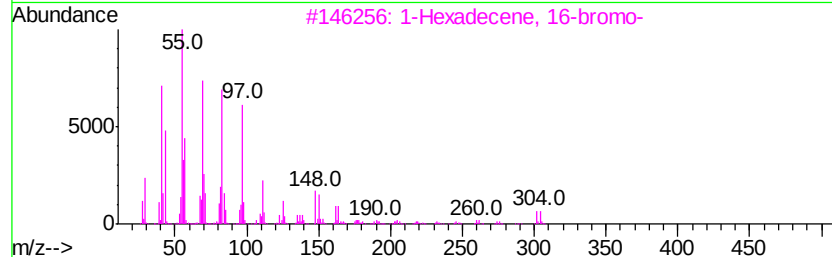
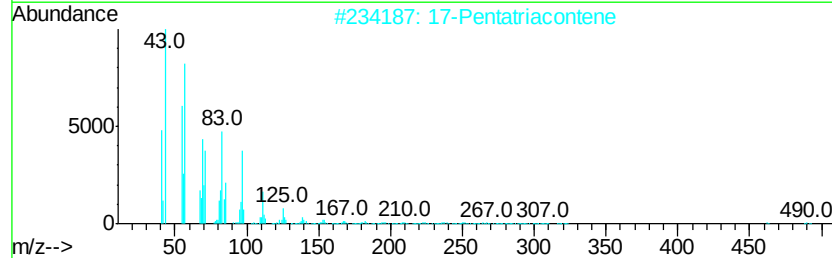
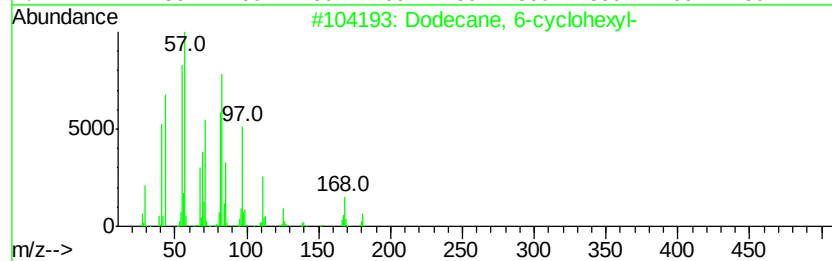
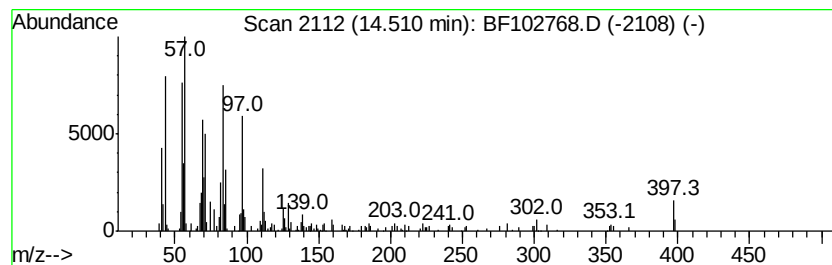
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dodecane, 6-cyclohexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	2.86 ng	152113	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 6-cyclohexyl-	252	C18H36	013151-86-5	80
2		17-Pentatriacontene	491	C35H70	006971-40-0	72
3		1-Hexadecene, 16-bromo-	302	C16H31Br	118625-56-2	70
4		Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	58
5		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	58



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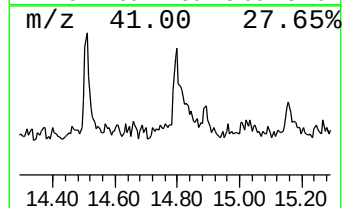
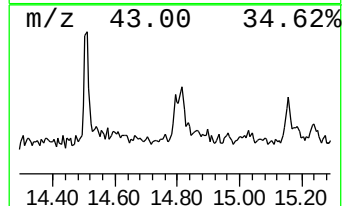
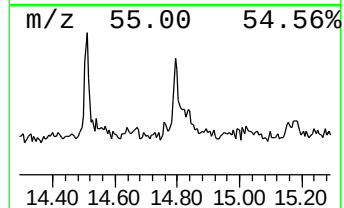
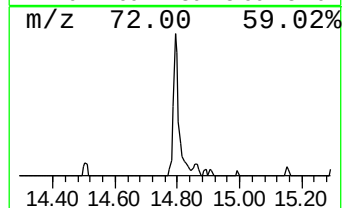
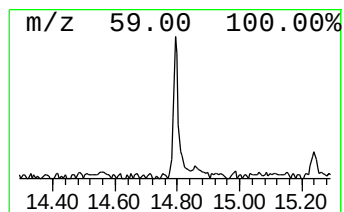
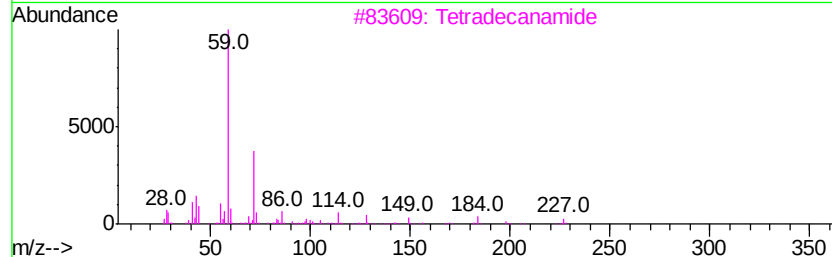
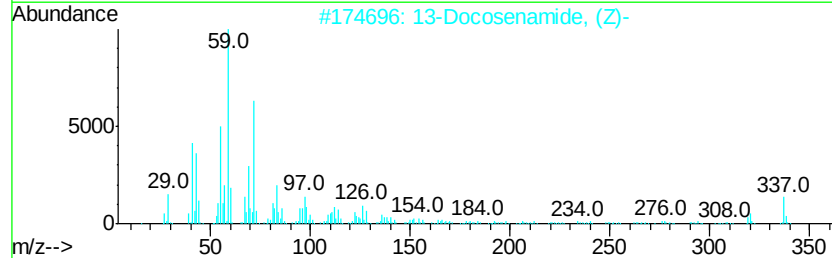
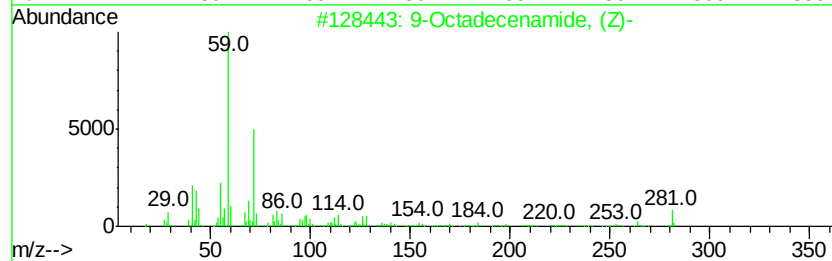
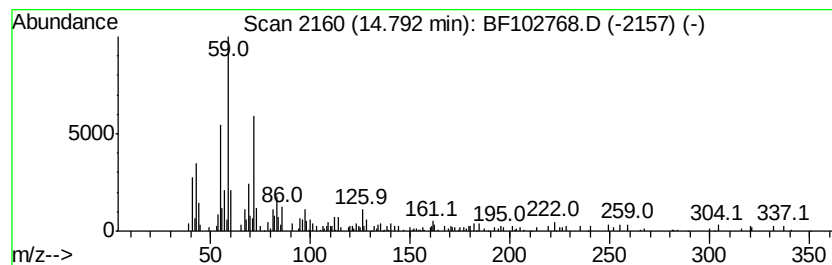
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.28 ng	114276	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	80
3		Tetradecanamide	227	C14H29NO	000638-58-4	53
4		Dodecanamide	199	C12H25NO	001120-16-7	50
5		Propanol, [(butoxymethylethoxy)m...	248	C13H28O4	055934-93-5	38



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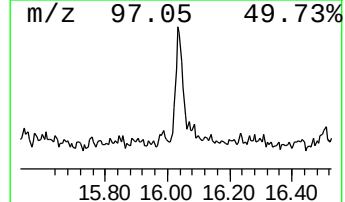
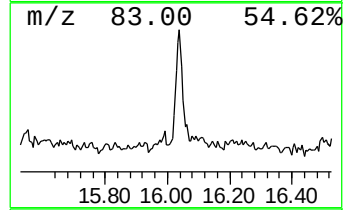
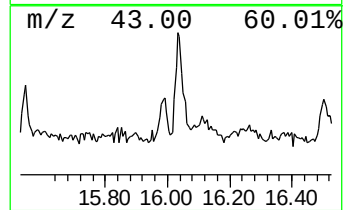
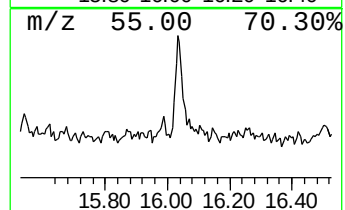
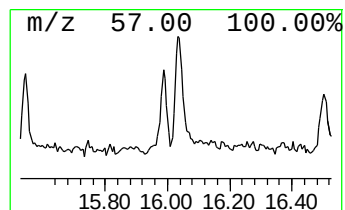
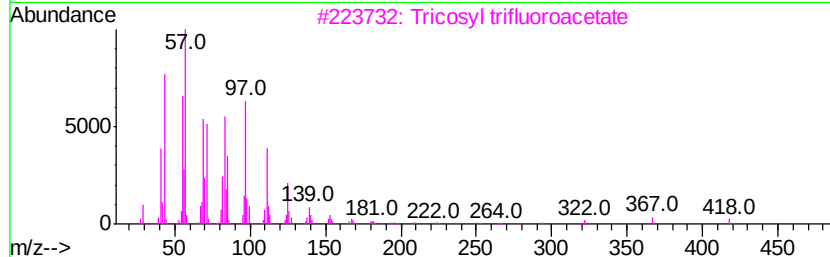
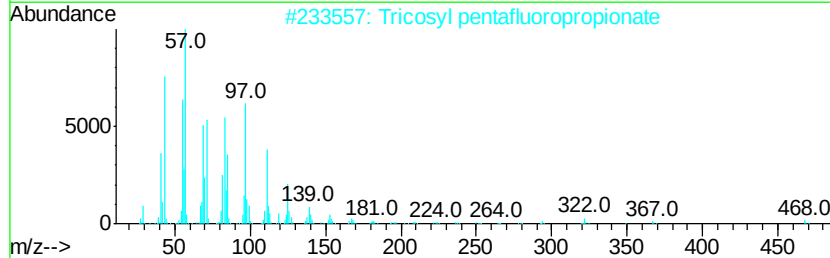
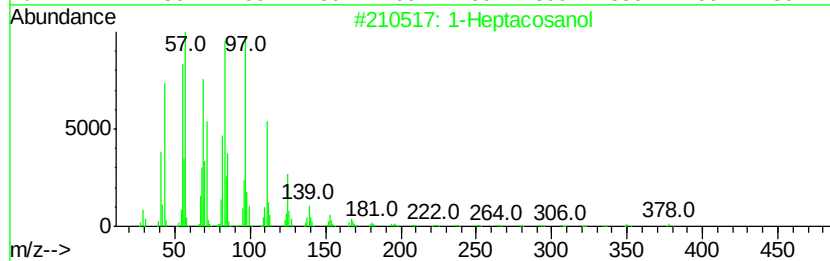
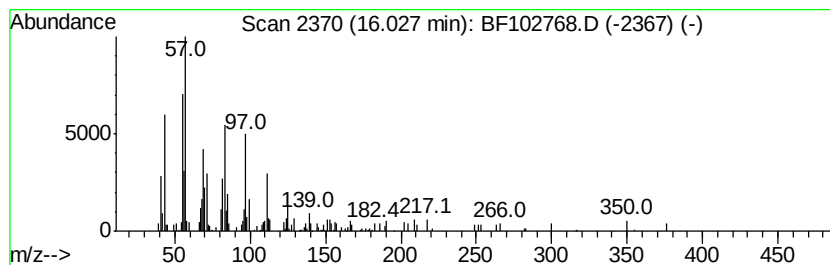
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.03	3.75 ng	188466	Perylene-d12	15.52	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	90
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90



Data Path : U:\HPCHEM1\BNA_F\DATA\BF020518\
Data File : BF102768.D
Acq On : 6 Feb 2018 5:44
Operator : SJ/JU
Sample : J1454-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
8-SAN-7-EW(4-7)

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...	2.19	11.1 ng		735867	1	6.88	1329210	20.0
2-Pentanone, 4-hy...	5.12	3.5 ng		236253	1	6.88	1329210	20.0
unknown6.65	6.65	69.8 ng		4636470	1	6.88	1329210	20.0
Hexadecane	10.82	2.7 ng		205314	4	11.40	1510340	20.0
n-Hexadecanoic acid	11.93	7.2 ng		541370	4	11.40	1510340	20.0
Octadecanoic acid	12.71	2.1 ng		158029	4	11.40	1510340	20.0
Hexadecanoic acid...	12.80	3.3 ng		177147	5	14.04	1063600	20.0
unknown13.51	13.51	2.0 ng		108152	5	14.04	1063600	20.0
1-Docosene	13.87	15.9 ng		846434	5	14.04	1063600	20.0
Dodecane, 6-cyclo...	14.51	2.9 ng		152113	5	14.04	1063600	20.0
9-Octadecenamide, ...	14.79	2.3 ng		114276	6	15.52	1004240	20.0
1-Heptacosanol	16.03	3.8 ng		188466	6	15.52	1004240	20.0