

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112988.D
 Acq On : 12 Mar 2019 7:07
 Operator : JU/SJ
 Sample : K1817-06
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EXT-027-SW017-030719

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.328	547	551	562	rBV	1471896	1418232	63.37%	7.921%
2	6.363	723	727	746	rBV	1762127	1589024	71.00%	8.875%
3	6.492	746	749	753	rBV	1622671	1551820	69.34%	8.667%
4	6.728	786	789	798	rBV	501869	400500	17.89%	2.237%
5	6.887	812	816	819	rBV	1311078	1149412	51.36%	6.420%
6	7.287	880	884	899	rBV	1018002	941401	42.06%	5.258%
7	8.010	1004	1007	1014	rBV	508440	481143	21.50%	2.687%
8	8.063	1014	1016	1031	rVB2	17584	39490	1.76%	0.221%
9	9.086	1186	1190	1205	rBV	1923523	1827266	81.64%	10.205%
10	9.481	1253	1257	1263	rBV	181298	171153	7.65%	0.956%
11	9.763	1301	1305	1315	rBV	704270	698771	31.22%	3.903%
12	10.545	1434	1438	1454	rBV	1691101	1597119	71.36%	8.920%
13	11.239	1552	1556	1564	rBV	876160	835596	37.33%	4.667%
14	11.775	1644	1647	1658	rBV	211749	255141	11.40%	1.425%
15	12.445	1758	1761	1763	rBV	27182	23614	1.06%	0.132%
16	12.557	1777	1780	1787	rBV	59501	85977	3.84%	0.480%
17	12.651	1793	1796	1798	rBV	51662	44860	2.00%	0.251%
18	12.816	1820	1824	1835	rBV	2428624	2238144	100.00%	12.500%
19	13.063	1860	1866	1868	rBV3	24752	34206	1.53%	0.191%
20	13.304	1904	1907	1912	rBV2	59260	63749	2.85%	0.356%
21	13.357	1912	1916	1918	rBV	29036	26709	1.19%	0.149%
22	13.727	1975	1979	1990	rBV	159128	228894	10.23%	1.278%
23	13.863	1998	2002	2014	rBV	731446	749425	33.48%	4.186%
24	14.045	2029	2033	2039	rBV	62566	77624	3.47%	0.434%
25	14.357	2081	2086	2099	rVB3	132690	268291	11.99%	1.498%
26	14.639	2131	2134	2137	rBV	70166	70513	3.15%	0.394%
27	14.774	2154	2157	2162	rVB4	25173	25003	1.12%	0.140%
28	14.957	2185	2188	2190	rBV	79946	83587	3.73%	0.467%
29	14.986	2190	2193	2205	rVB	109241	204844	9.15%	1.144%
30	15.268	2236	2241	2245	rBV	372650	496419	22.18%	2.773%
31	15.310	2246	2248	2255	rVB	72167	87502	3.91%	0.489%
32	15.715	2313	2317	2322	rBV	69632	96610	4.32%	0.540%
33	16.180	2394	2396	2402	rVB3	29947	42812	1.91%	0.239%

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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-027-SW017-030719

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

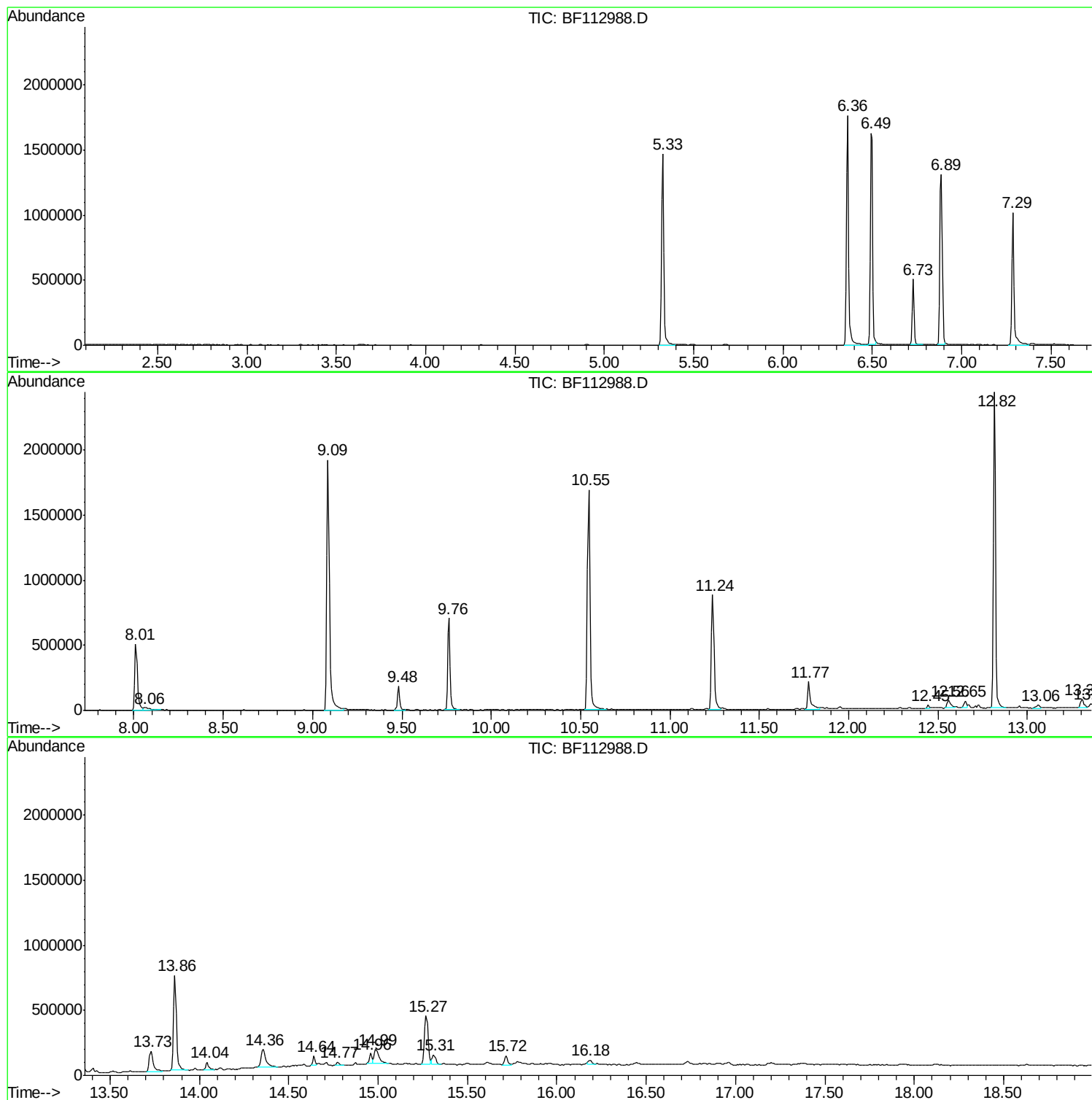
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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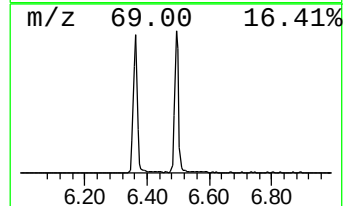
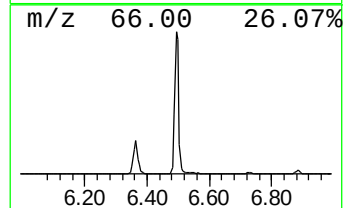
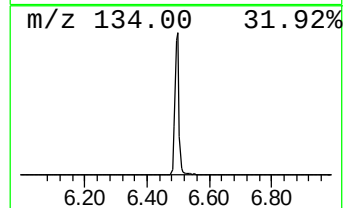
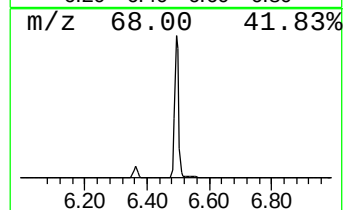
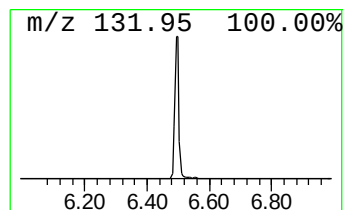
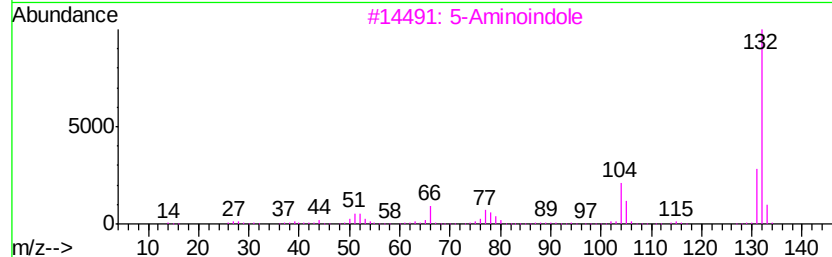
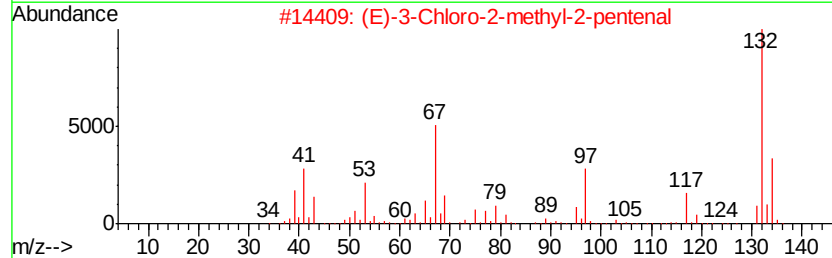
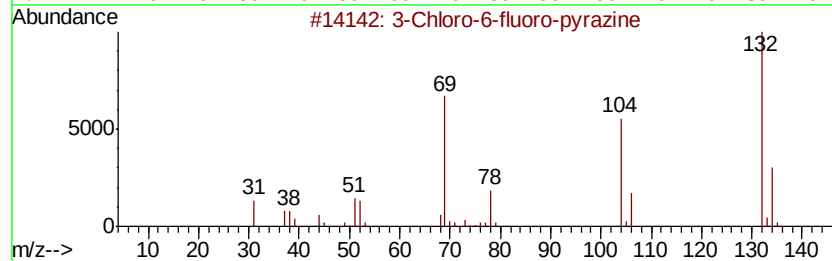
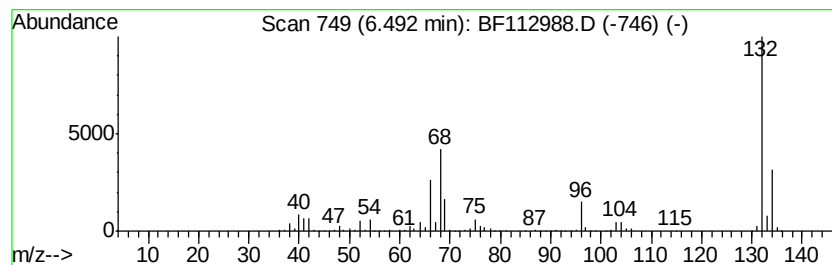
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.49 ng	1551820	1,4-Dichlorobenzene-d4	6.73

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		Amphetaminil	250	C17H18N2	017590-01-1	10



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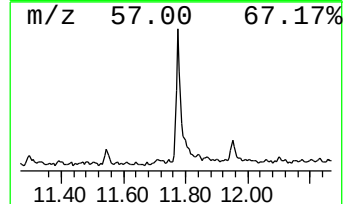
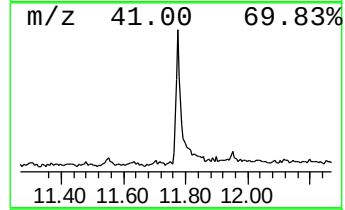
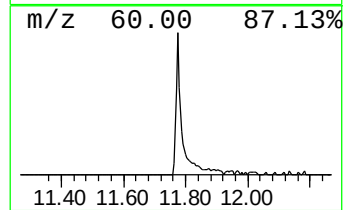
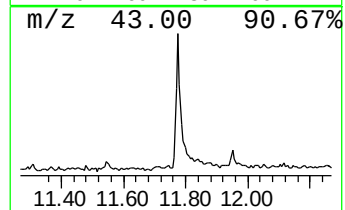
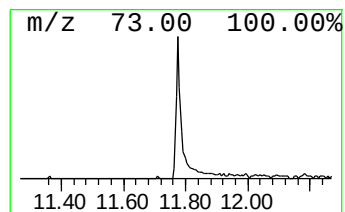
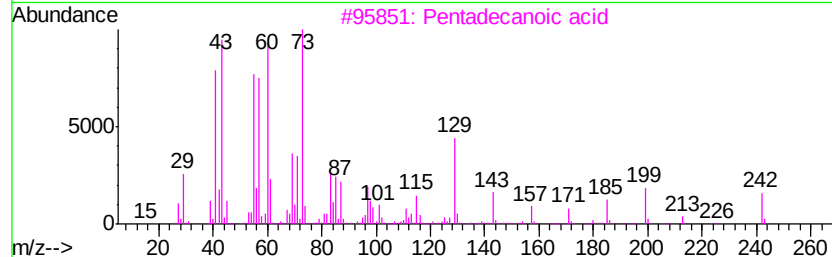
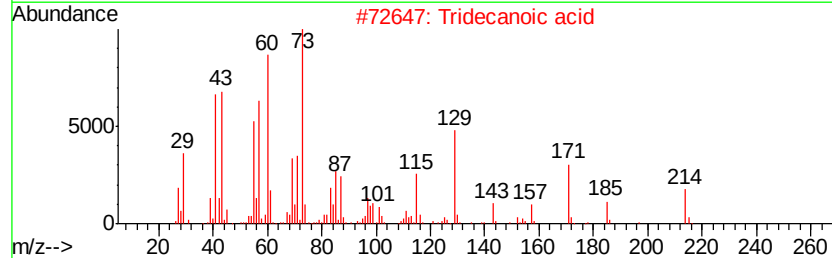
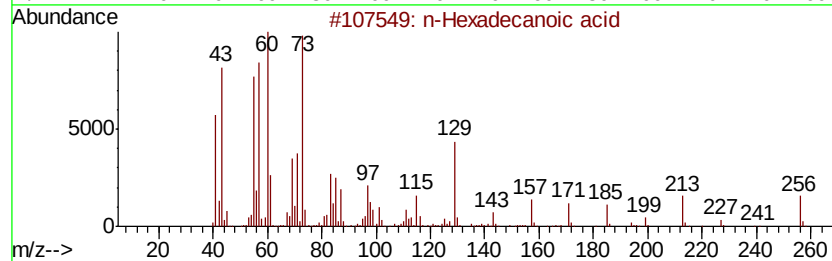
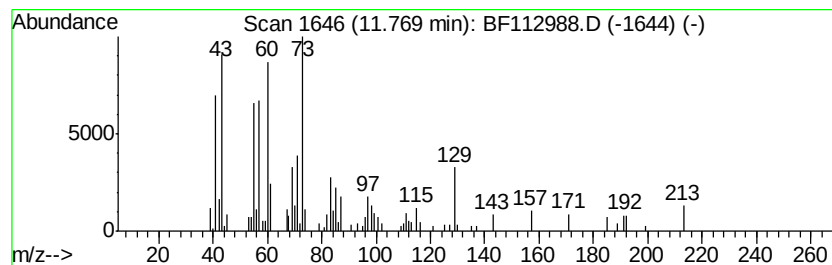
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.77	6.11 ng	255141	Phenanthrene-d10		11.24	
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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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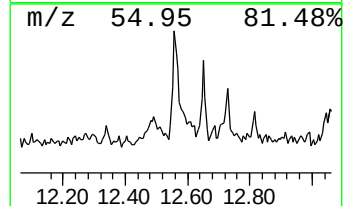
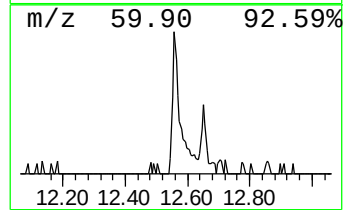
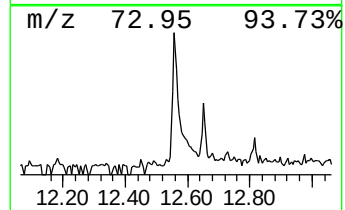
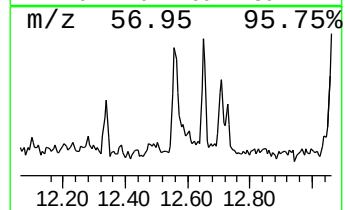
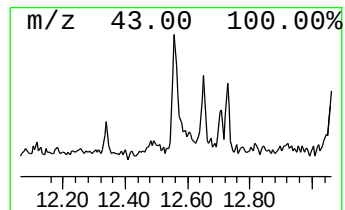
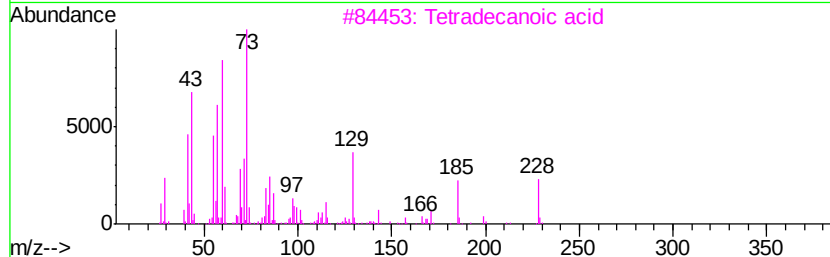
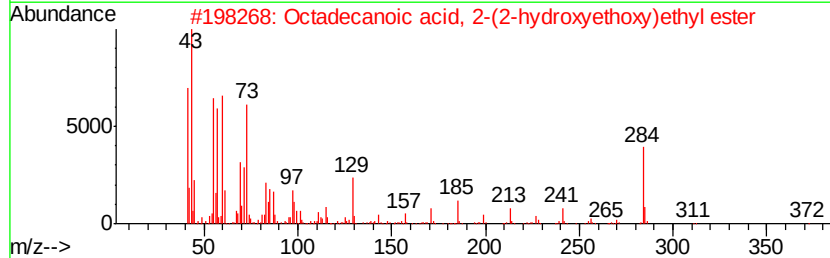
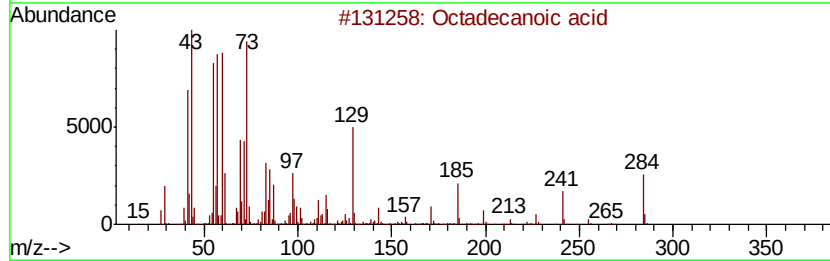
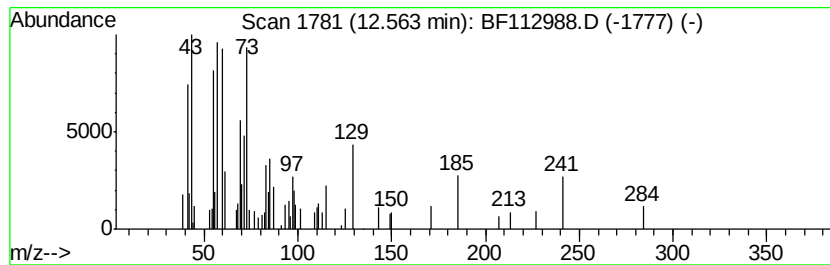
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.56	2.29 ng	85977	Chrysene-d12	13.86		
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	86	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80	
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74	
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64	



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ALS Vial : 34 Sample Multiplier: 1

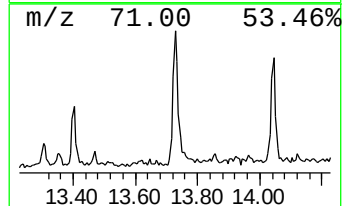
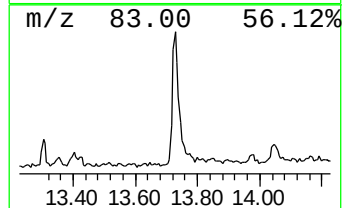
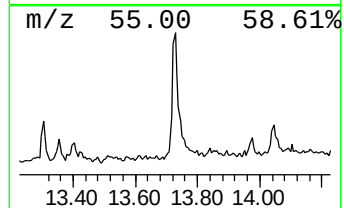
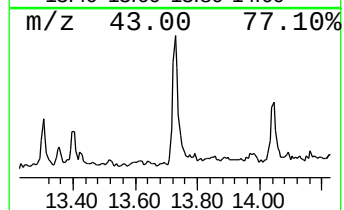
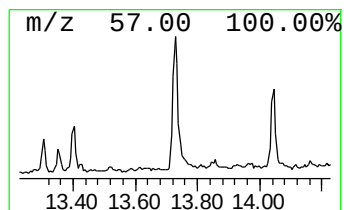
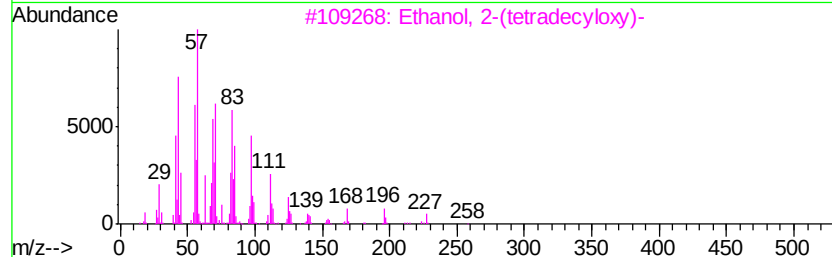
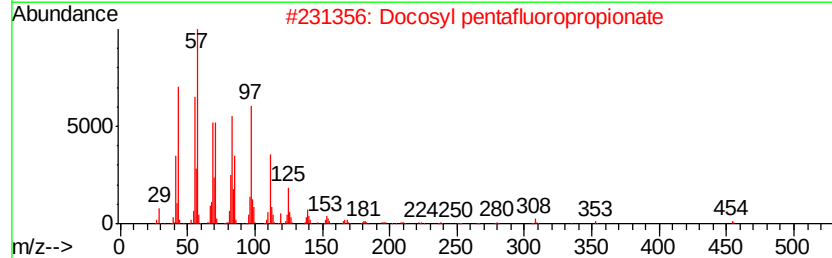
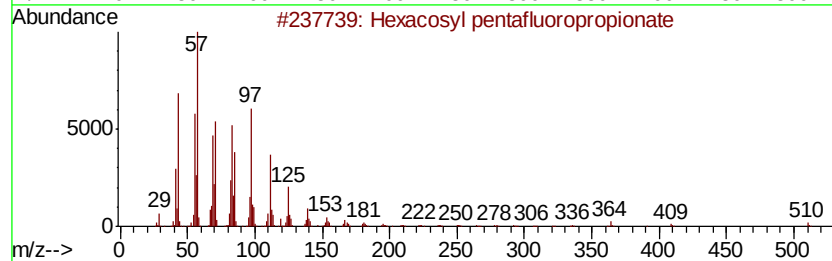
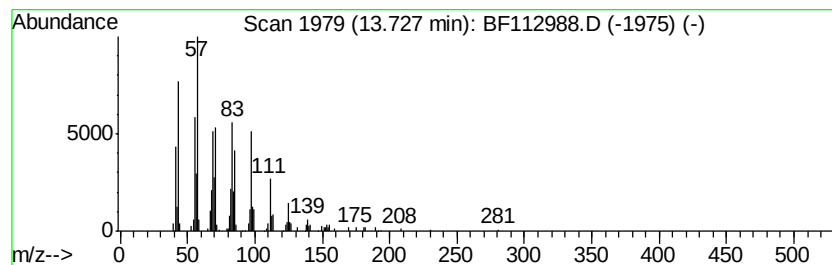
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosyl pentafluoropropio... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.73	6.11 ng	228894	Chrysene-d12		13.86	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl	pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
2	Docosyl	pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Ethanol,	2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Tricosyl	trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5	Octacosyl	heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	90



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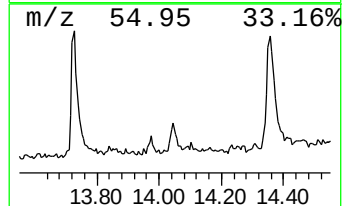
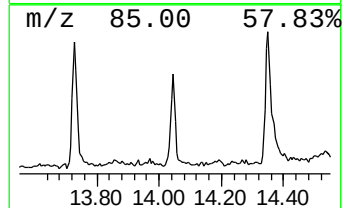
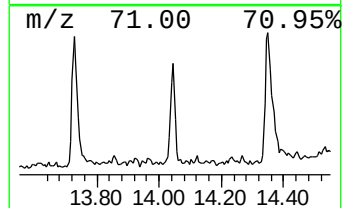
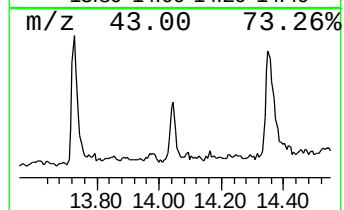
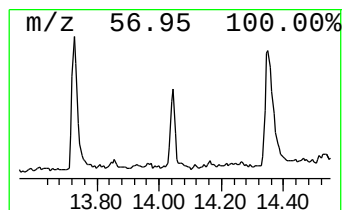
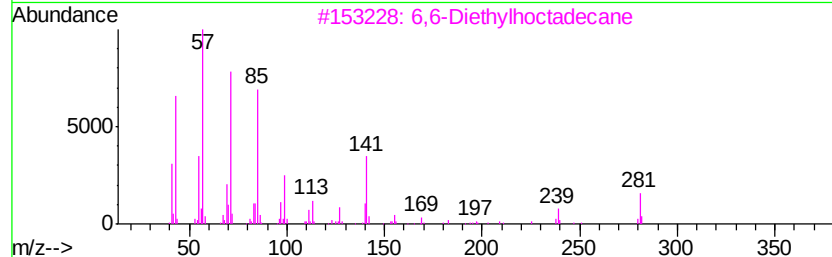
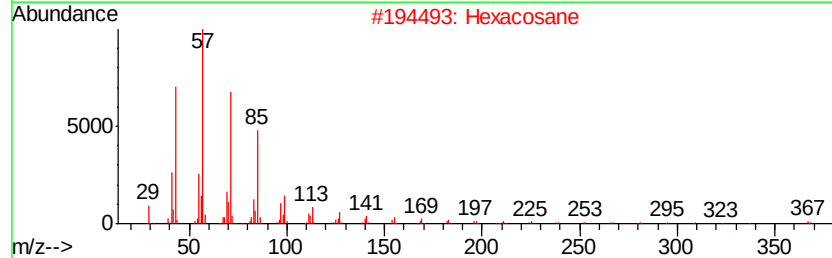
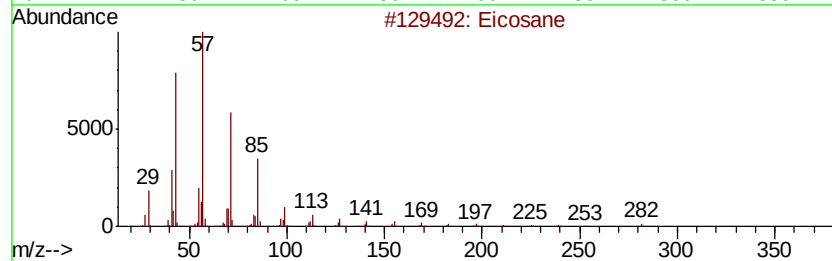
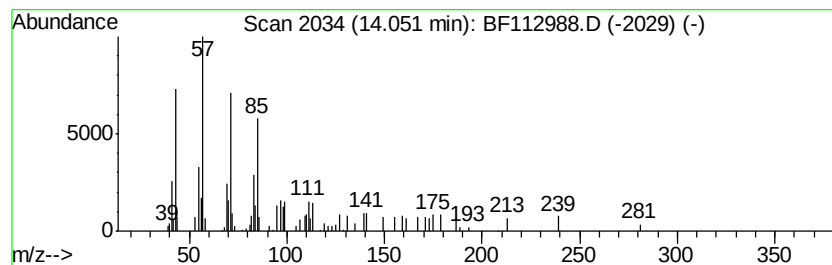
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.07 ng	77624	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	93
2	Hexacosane	366 C26H54	000630-01-3	90
3	6,6-Diethyloctadecane	310 C22H46	1000360-41-8	90
4	Heneicosane	296 C21H44	000629-94-7	87
5	Hexatriacontane	507 C36H74	000630-06-8	87



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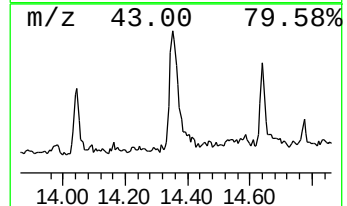
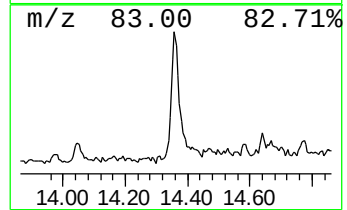
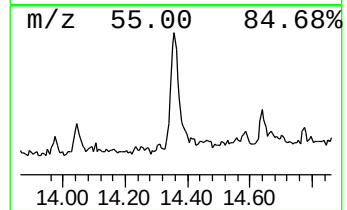
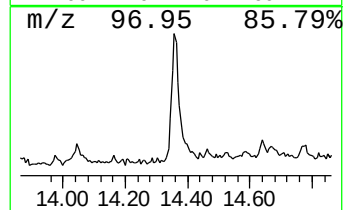
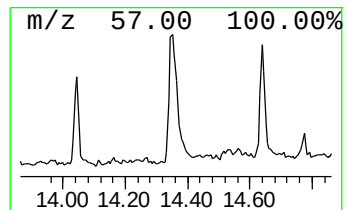
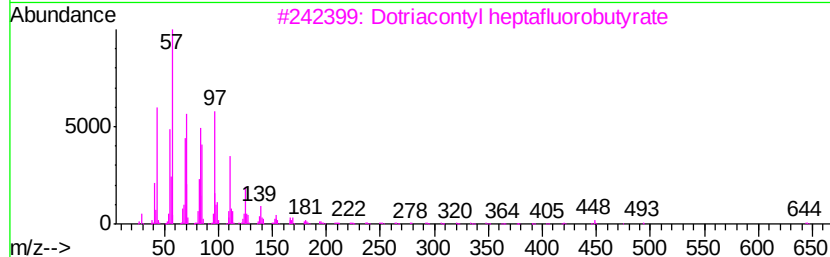
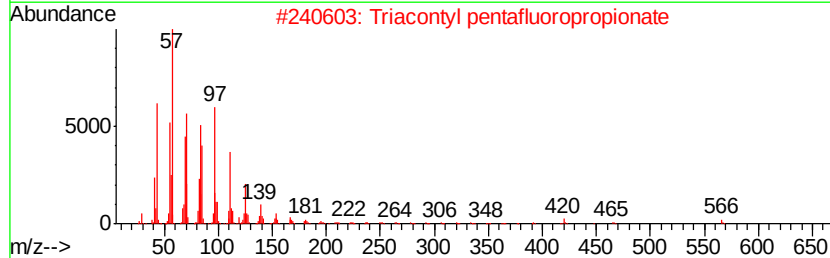
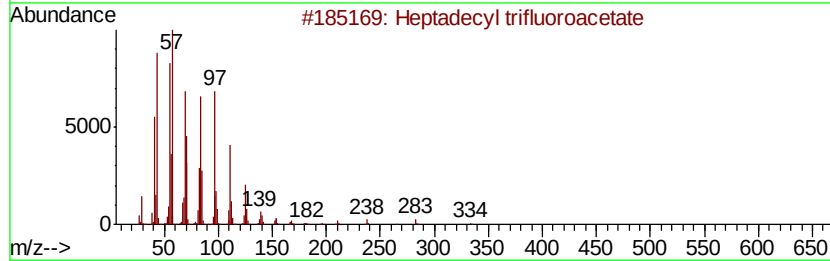
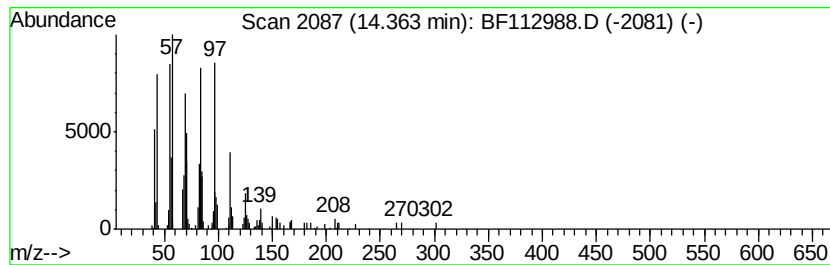
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	7.16 ng	268291	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		Triacetyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	93
3		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	93
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112988.D
Acq On : 12 Mar 2019 7:07
Operator : JU/SJ
Sample : K1817-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EXT-027-SW017-030719

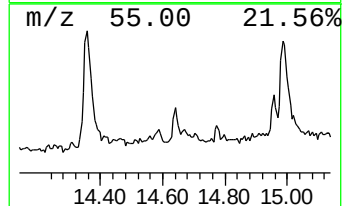
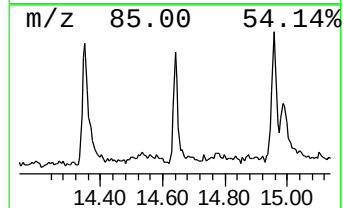
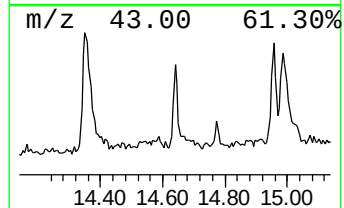
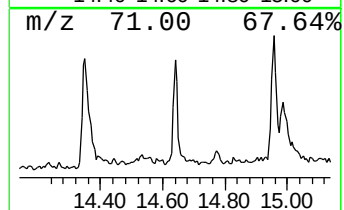
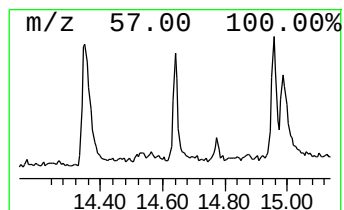
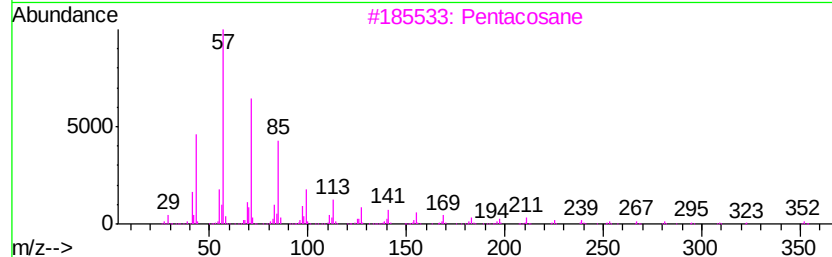
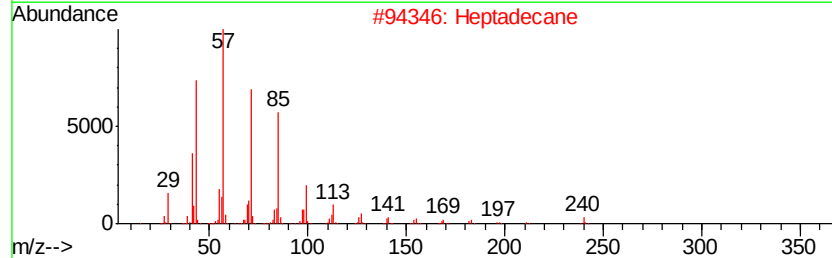
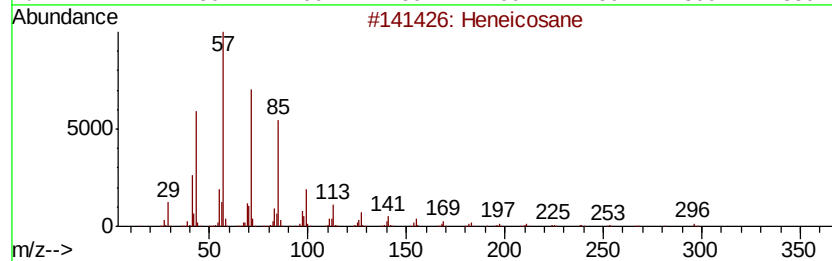
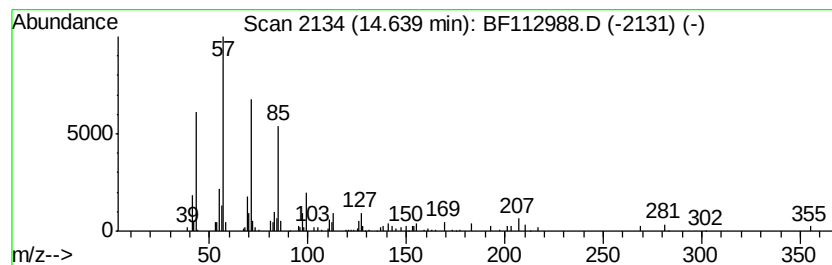
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.84 ng	70513	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Heptadecane	240	C17H36	000629-78-7	87
3		Pentacosane	352	C25H52	000629-99-2	86
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5		Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112988.D
Acq On : 12 Mar 2019 7:07
Operator : JU/SJ
Sample : K1817-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EXT-027-SW017-030719

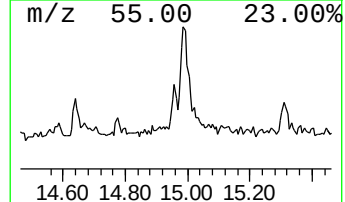
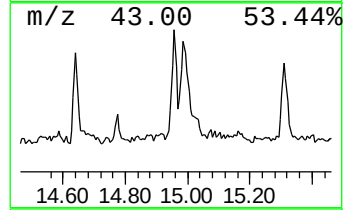
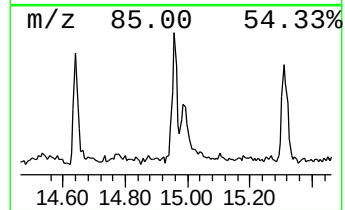
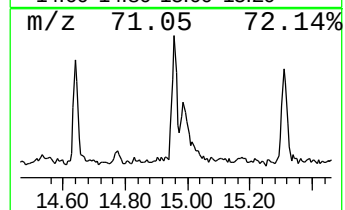
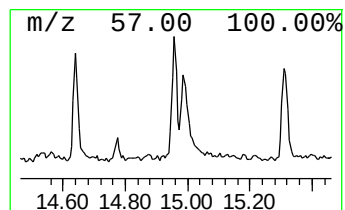
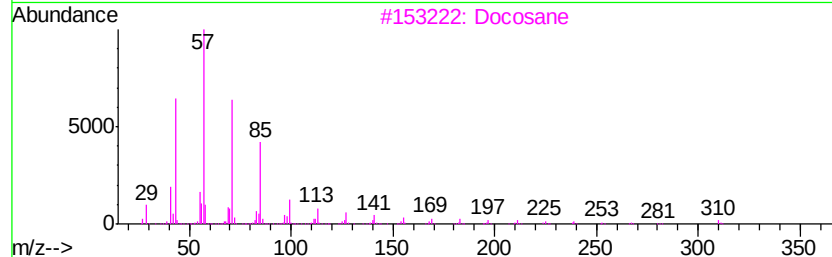
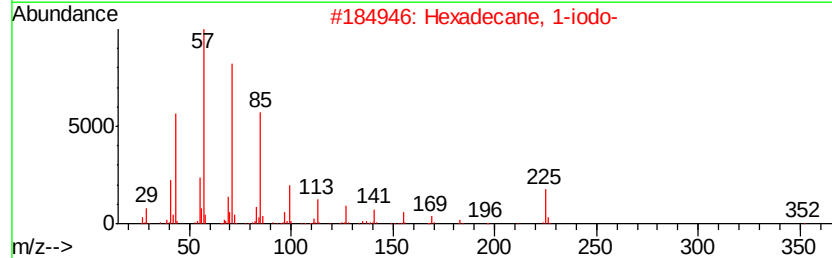
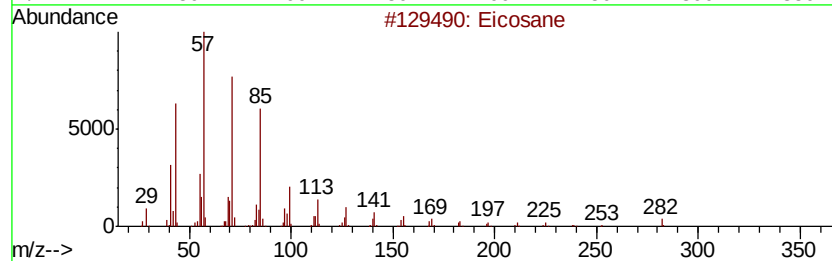
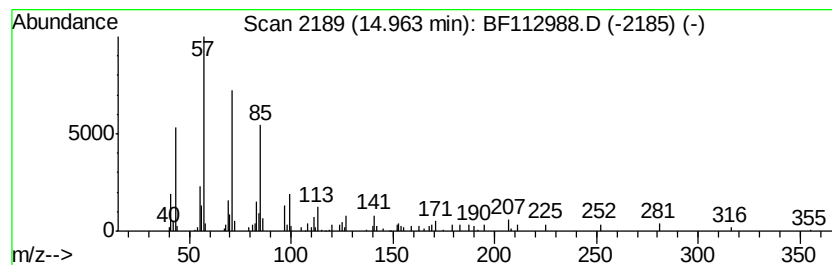
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.96 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.37 ng	83587	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3		Docosane	310	C22H46	000629-97-0	86
4		Tricosane, 2-methyl-	338	C24H50	001928-30-9	86
5		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112988.D
Acq On : 12 Mar 2019 7:07
Operator : JU/SJ
Sample : K1817-06
Misc :
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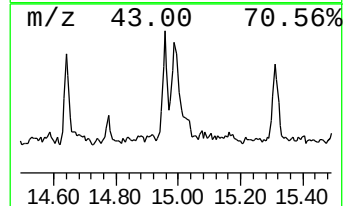
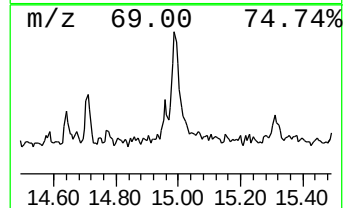
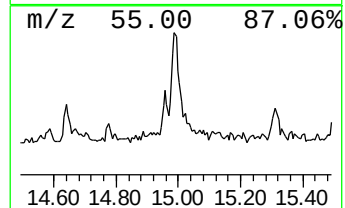
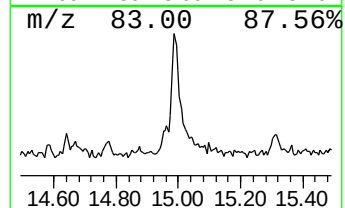
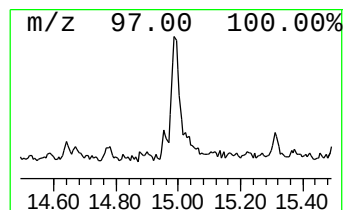
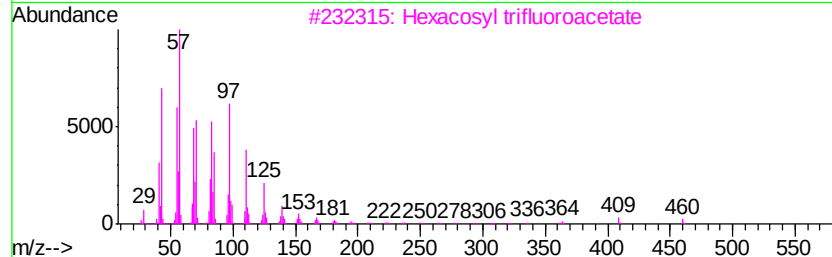
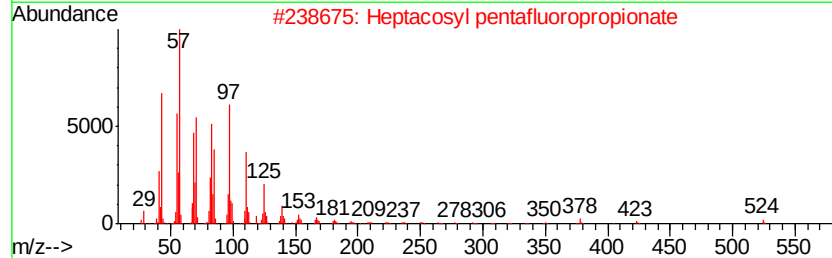
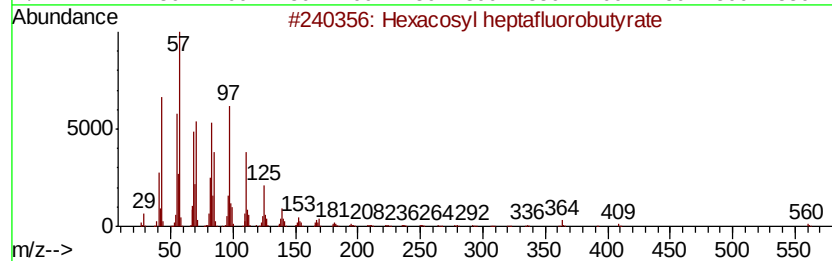
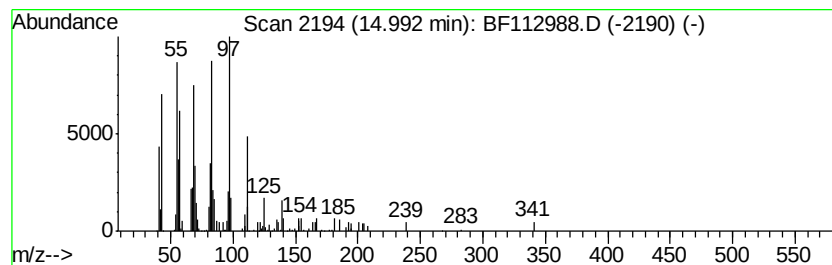
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.99	8.25 ng	204844	Perylene-d12	15.27		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl	heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	68
2	Heptacosyl	pentafluoropropionate	542	C30H55F5O2	1000351-81-6	68
3	Hexacosyl	trifluoroacetate	478	C28H53F3O2	1000351-75-0	68
4	Hexacosyl	pentafluoropropionate	528	C29H53F5O2	1000351-81-2	68
5	Octacosanol		410	C28H58O	000557-61-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
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Operator : JU/SJ
Sample : K1817-06
Misc :
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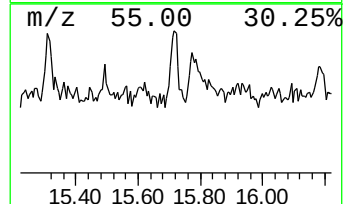
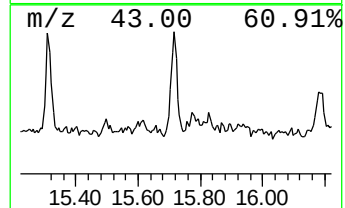
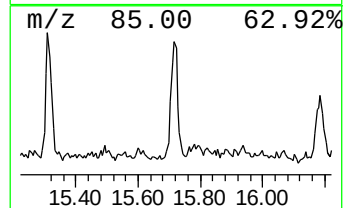
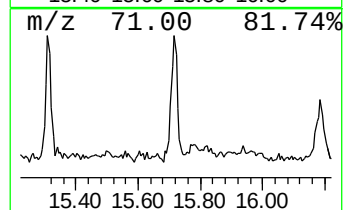
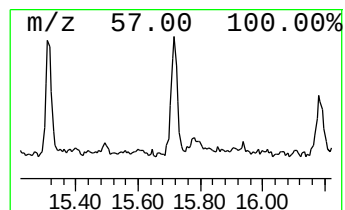
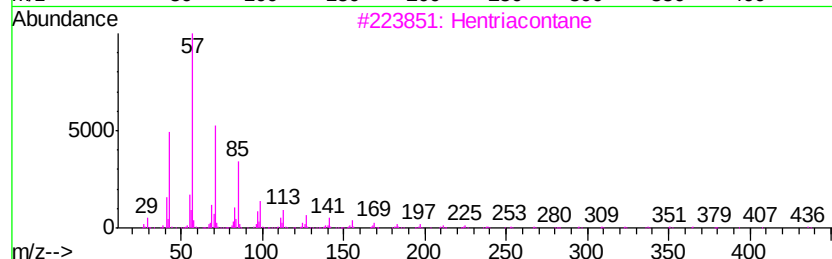
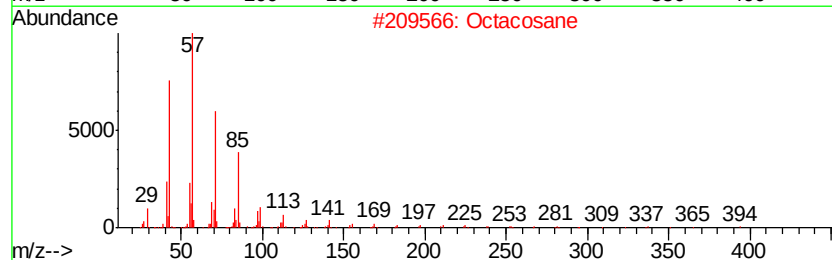
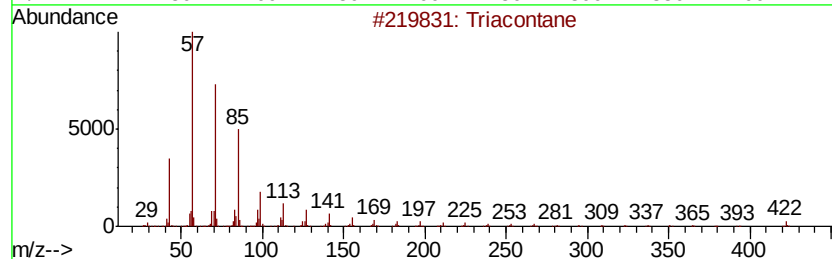
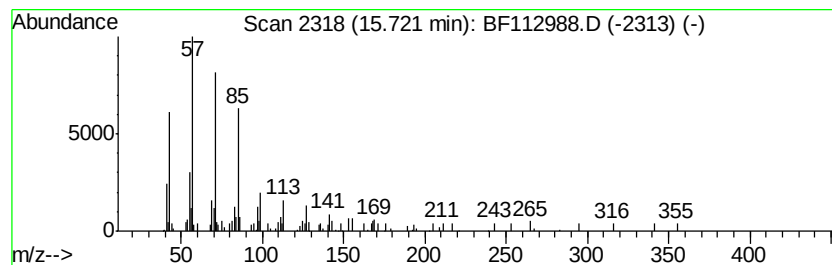
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.72	3.89 ng	96610	Perylene-d12		15.27
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5	Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
 Data File : BF112988.D
 Acq On : 12 Mar 2019 7:07
 Operator : JU/SJ
 Sample : K1817-06
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Octadecanoic acid	12.56	2.3	ng	85977	5	13.86	749425	20.0
Hexacosyl pentafl...	13.73	6.1	ng	228894	5	13.86	749425	20.0
Eicosane	14.05	2.1	ng	77624	5	13.86	749425	20.0
Heptadecyl triflu...	14.36	7.2	ng	268291	5	13.86	749425	20.0
Heneicosane	14.64	2.8	ng	70513	6	15.27	496419	20.0
unknown14.96	14.96	3.4	ng	83587	6	15.27	496419	20.0
Hexacosyl heptafl...	14.99	8.3	ng	204844	6	15.27	496419	20.0
Triacontane	15.72	3.9	ng	96610	6	15.27	496419	20.0