

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
 Data File : BF102249.D
 Acq On : 20 Jan 2018 5:59
 Operator : SJ/JU
 Sample : J1113-19
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-20-3.0-3.5

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-BF010918.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	4.922	478	482	491	rVB	176794	250939	7.21%	0.822%
2	5.334	547	552	555	rBV	3352366	3328832	95.69%	10.898%
3	6.363	721	727	730	rBV	3107482	3359445	96.57%	10.998%
4	6.493	744	749	752	rBV	3550248	3391724	97.50%	11.104%
5	6.716	784	787	791	rBV	1037915	882871	25.38%	2.890%
6	6.875	810	814	817	rBV	3058422	2639188	75.87%	8.640%
7	7.287	878	884	887	rBV	2275133	2144279	61.64%	7.020%
8	7.469	912	915	919	rVB	50009	41254	1.19%	0.135%
9	7.998	1001	1005	1009	rBV	1305222	1148869	33.03%	3.761%
10	9.081	1183	1189	1192	rBV	3756367	3478607	100.00%	11.388%
11	9.469	1251	1255	1258	rBV	317016	281121	8.08%	0.920%
12	9.686	1284	1292	1295	rBV	154891	129350	3.72%	0.423%
13	9.751	1299	1303	1307	rVV	1256140	1127953	32.43%	3.693%
14	10.186	1373	1377	1379	rVB	166288	141563	4.07%	0.463%
15	10.404	1409	1414	1416	rBV	47036	52023	1.50%	0.170%
16	10.545	1431	1438	1441	rBV	1850930	1804175	51.86%	5.906%
17	10.657	1454	1457	1462	rBV	139237	142247	4.09%	0.466%
18	10.857	1486	1491	1496	rBV5	14952	37416	1.08%	0.122%
19	11.104	1530	1533	1536	rBV	51818	41877	1.20%	0.137%
20	11.233	1552	1555	1559	rBV	1014222	939721	27.01%	3.076%
21	12.645	1792	1795	1798	rBV	111597	84154	2.42%	0.276%
22	12.822	1821	1825	1829	rBV	2296840	2195939	63.13%	7.189%
23	13.304	1902	1907	1910	rBV4	32145	45373	1.30%	0.149%
24	13.351	1912	1915	1917	rBV	60835	48498	1.39%	0.159%
25	13.716	1973	1977	1988	rBV	414712	428461	12.32%	1.403%
26	13.869	1998	2003	2007	rBV	836958	781930	22.48%	2.560%
27	14.039	2027	2032	2035	rBV3	37580	47004	1.35%	0.154%
28	14.345	2080	2084	2092	rBV3	59039	91707	2.64%	0.300%
29	14.710	2143	2146	2151	rVB2	40402	42456	1.22%	0.139%
30	14.963	2185	2189	2191	rBV	55163	61616	1.77%	0.202%
31	15.292	2240	2245	2252	rBV	675205	826011	23.75%	2.704%
32	15.727	2316	2319	2324	rBV2	33419	53849	1.55%	0.176%
33	15.774	2324	2327	2334	rVB3	71505	101072	2.91%	0.331%
34	15.951	2353	2357	2367	rVB10	59736	143730	4.13%	0.471%

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35	16.233	2403	2405	2410	rVB2	31700	43411	1.25%	0.142%
36	16.704	2482	2485	2490	rVB6	39763	59701	1.72%	0.195%
37	17.209	2566	2571	2580	rVB10	58299	127294	3.66%	0.417%

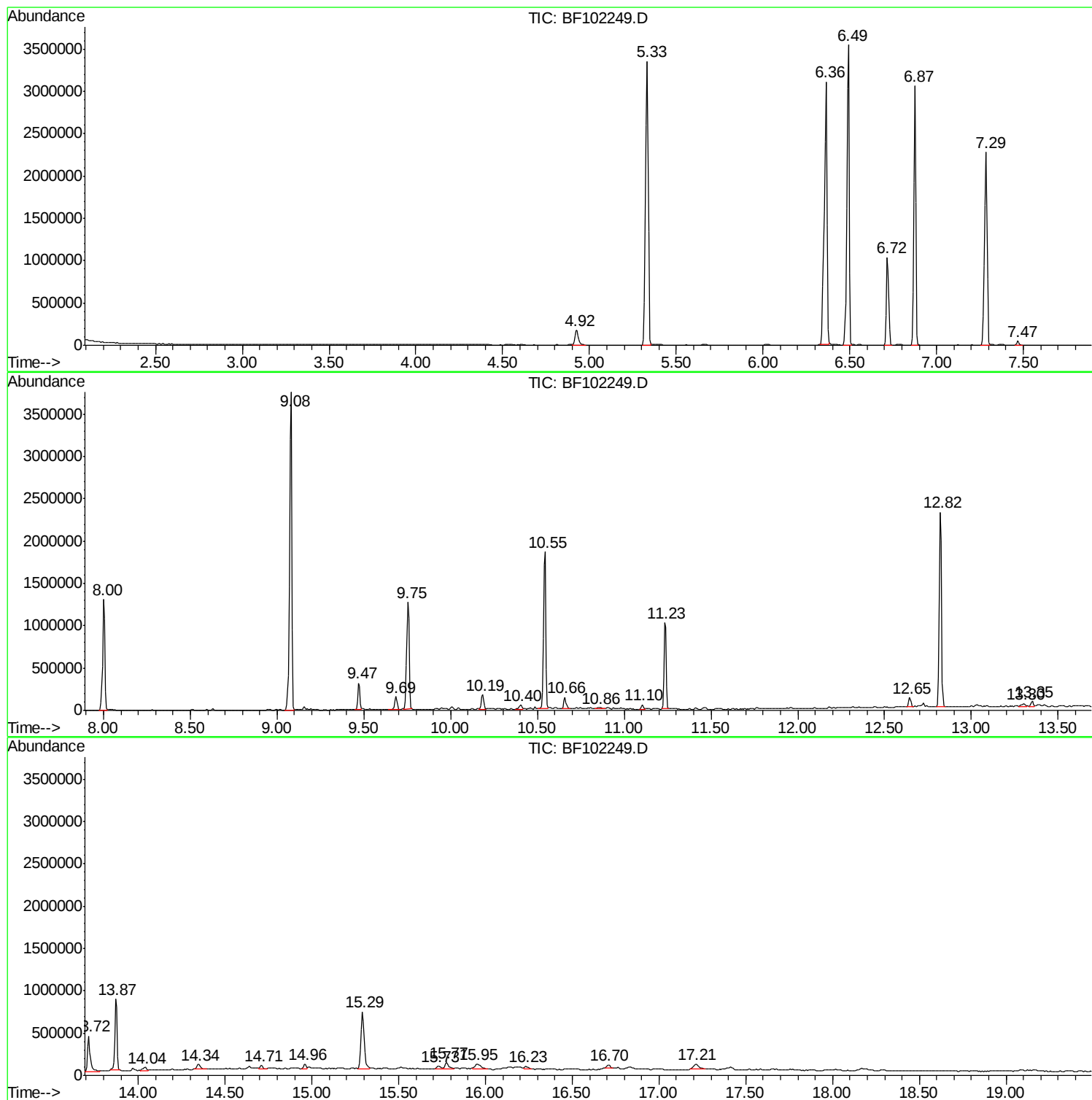
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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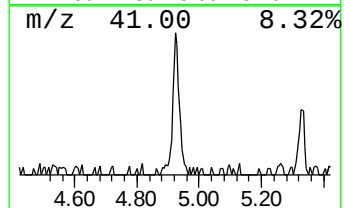
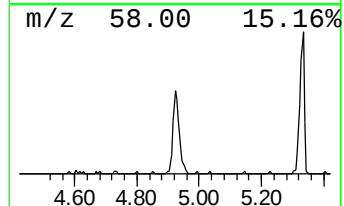
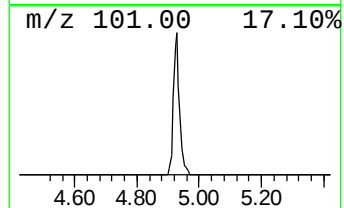
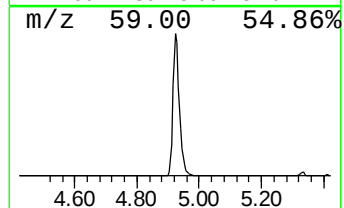
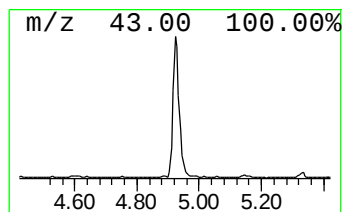
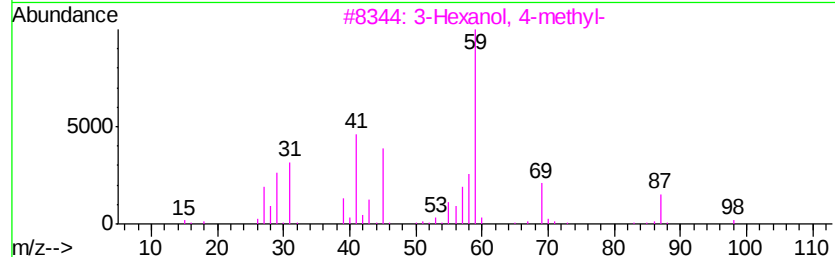
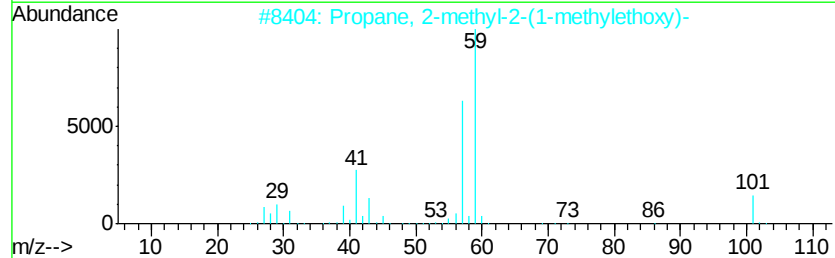
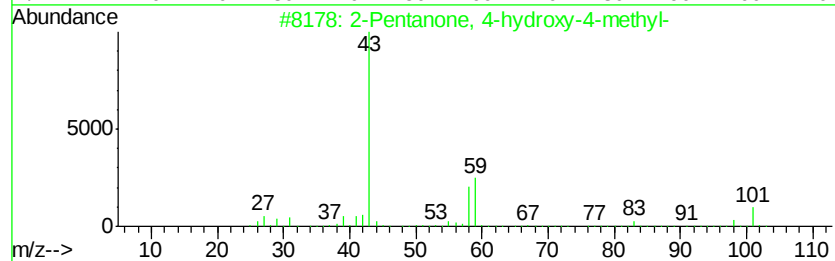
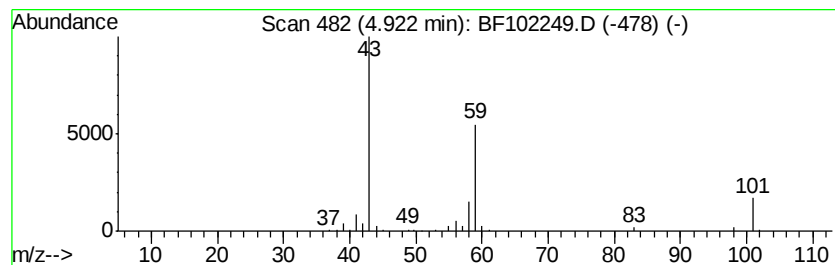
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.68 ng	250939	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42	
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25	



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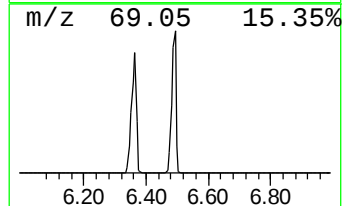
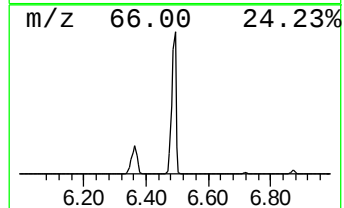
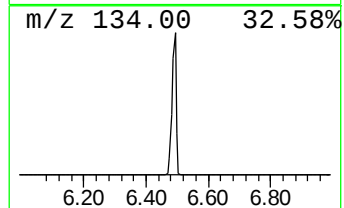
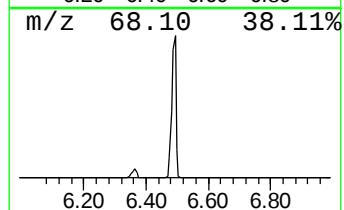
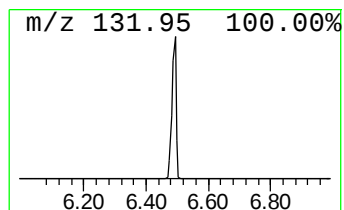
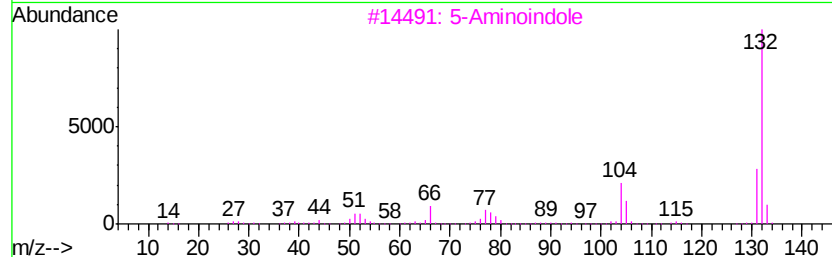
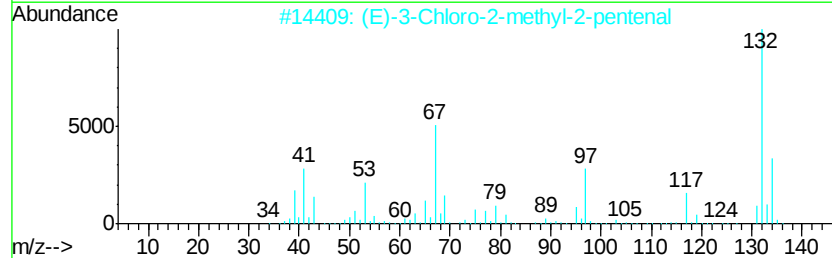
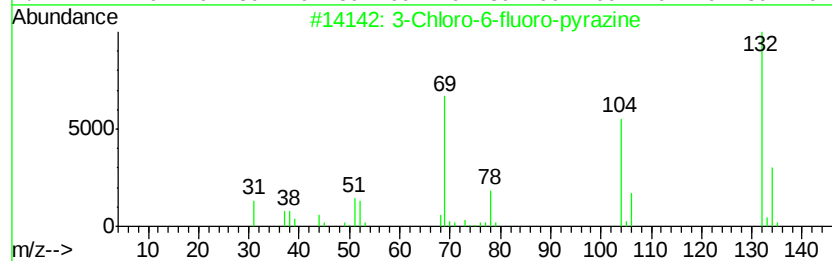
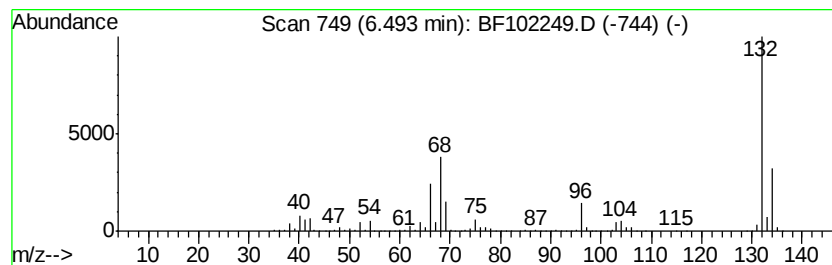
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	76.83 ng	3391720	1,4-Dichlorobenzene-d4	6.72

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		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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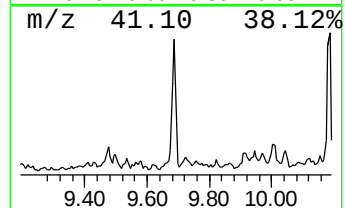
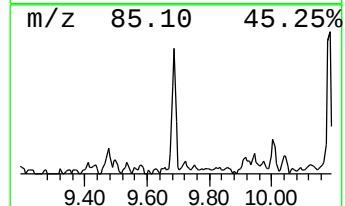
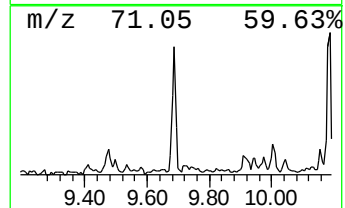
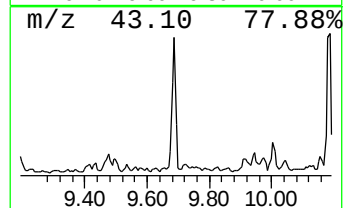
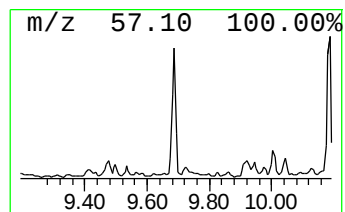
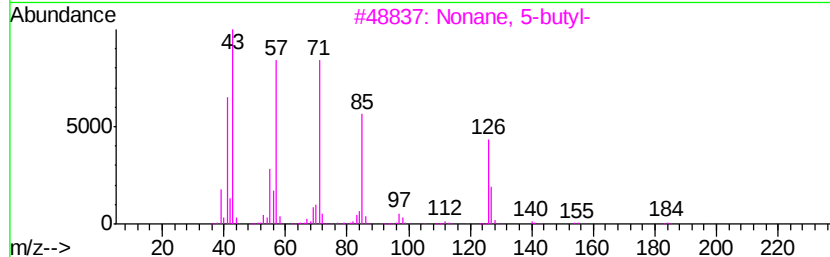
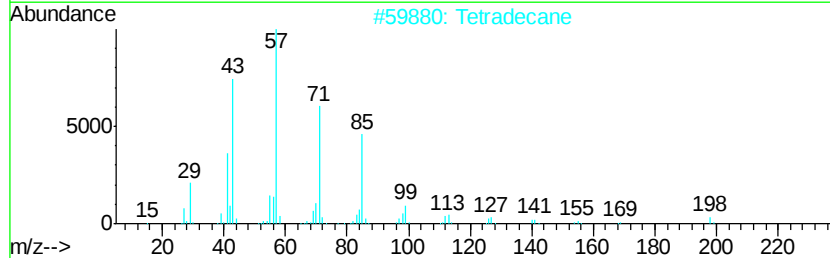
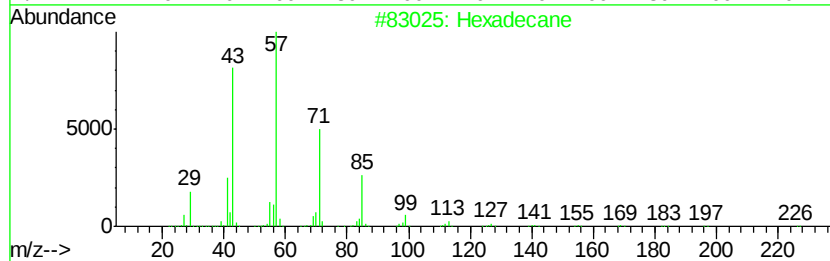
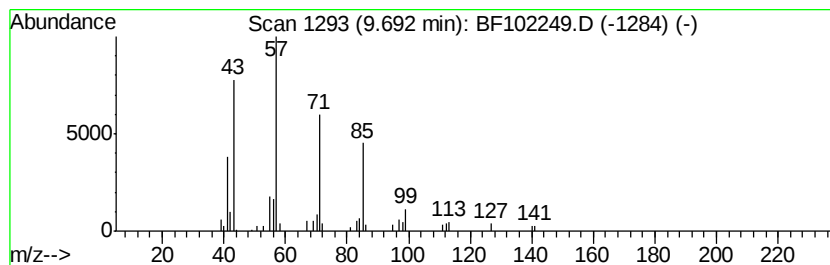
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.29 ng	129350	Acenaphthene-d10	9.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Tetradecane		198	C14H30	000629-59-4	86
3	Nonane, 5-butyl-		184	C13H28	017312-63-9	80
4	Heneicosane		296	C21H44	000629-94-7	78
5	Tridecane		184	C13H28	000629-50-5	78



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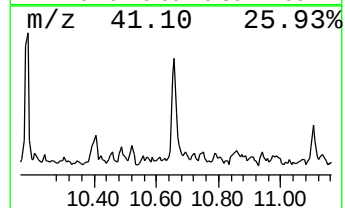
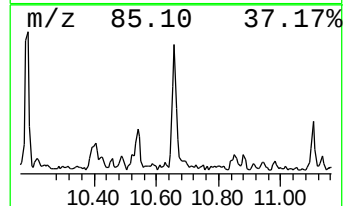
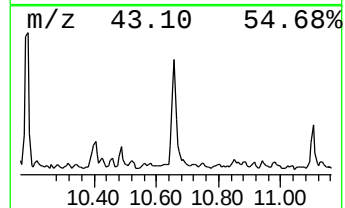
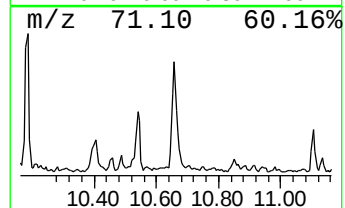
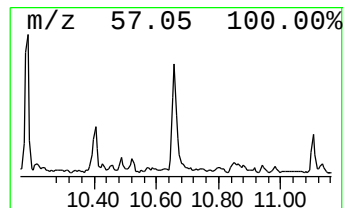
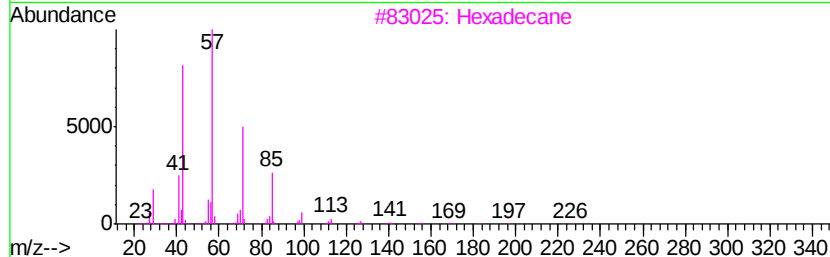
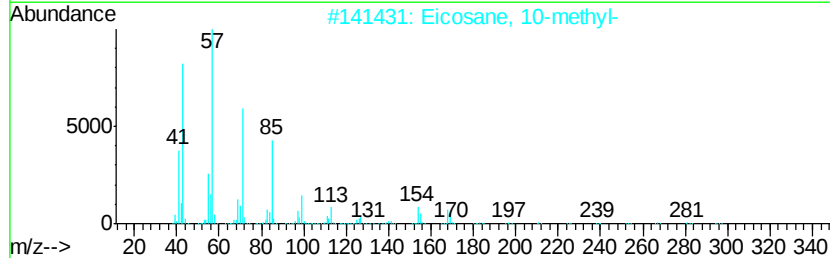
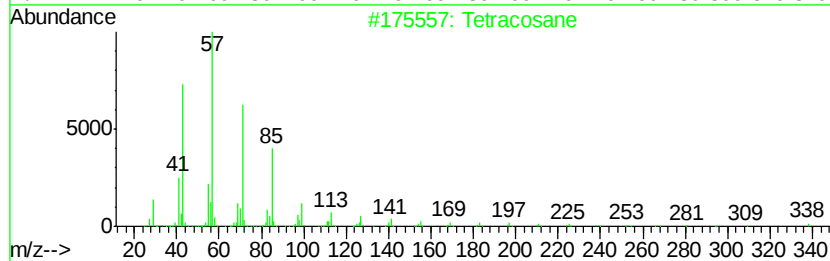
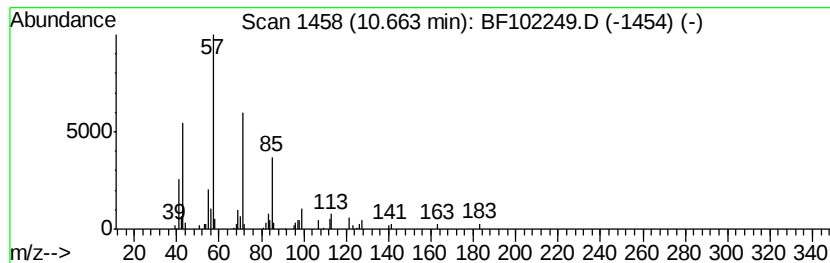
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.03 ng	142247	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane		338	C24H50	000646-31-1	90
2	Eicosane, 10-methyl-		296	C21H44	054833-23-7	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetradecane		198	C14H30	000629-59-4	86
5	Pentadecane		212	C15H32	000629-62-9	86



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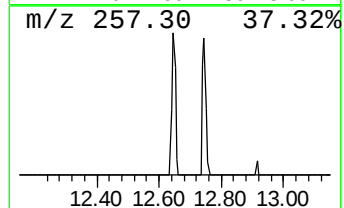
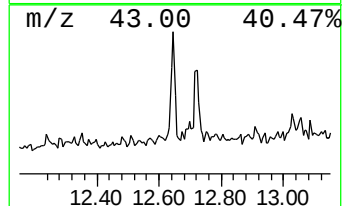
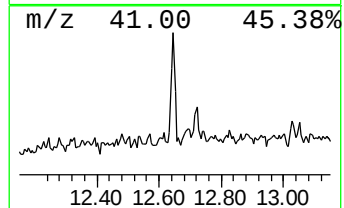
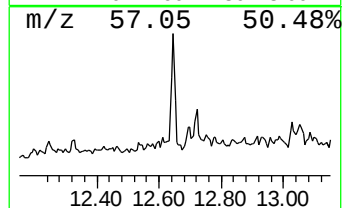
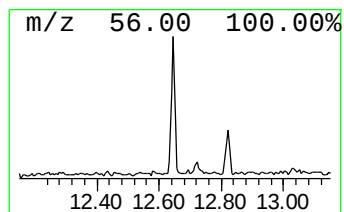
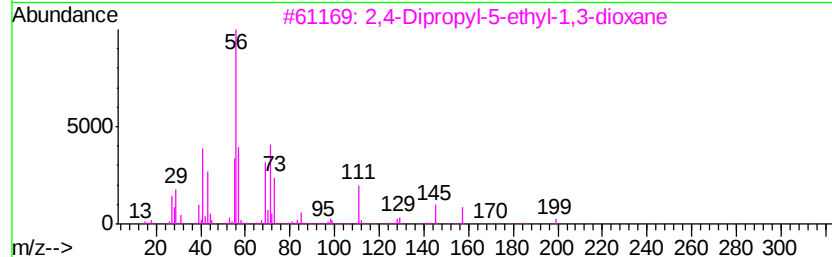
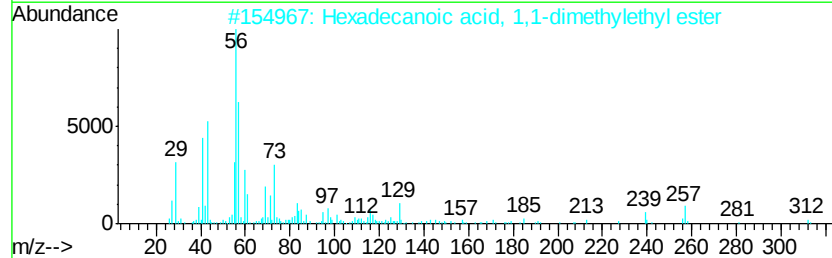
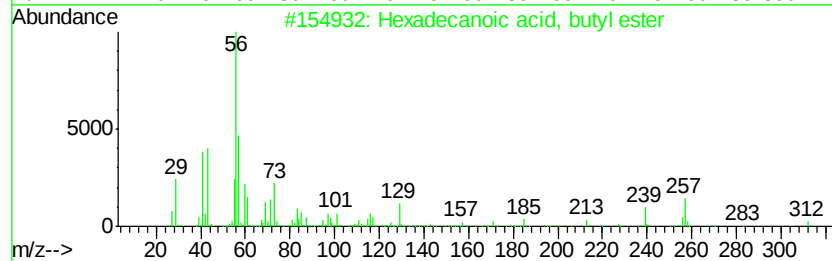
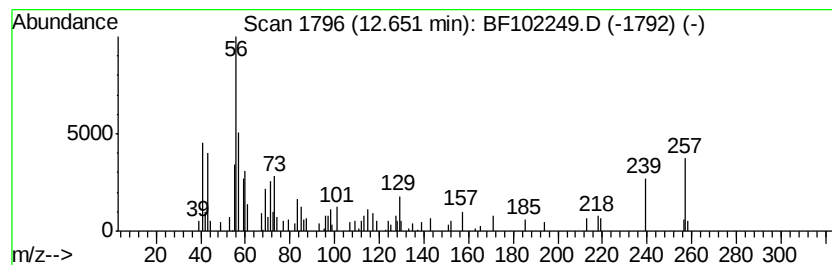
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.15 ng	84154	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	43
5		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102249.D
Acq On : 20 Jan 2018 5:59
Operator : SJ/JU
Sample : J1113-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-3.0-3.5

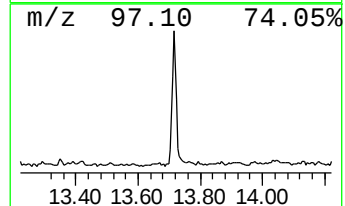
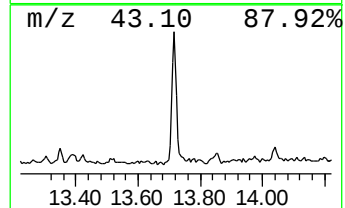
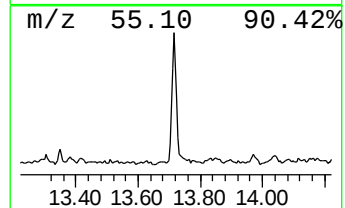
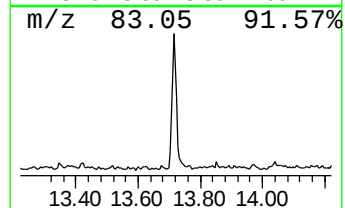
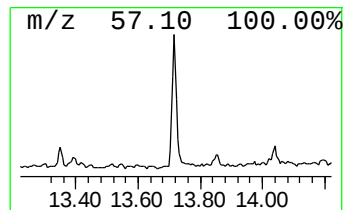
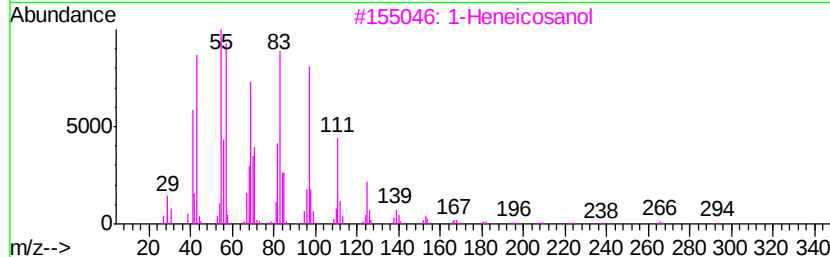
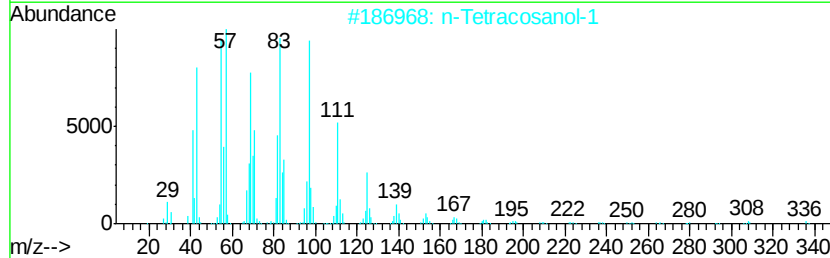
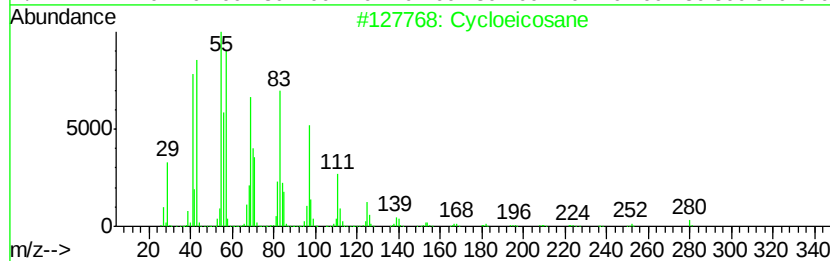
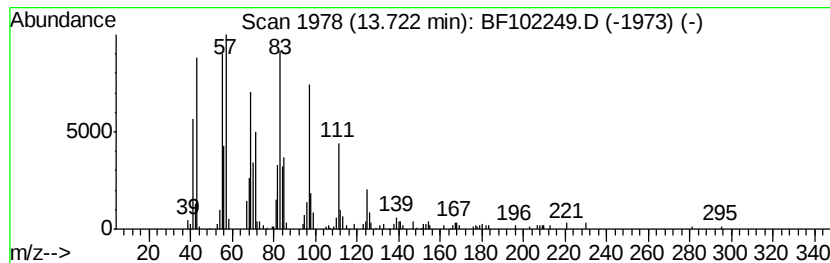
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	10.96 ng	428461	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloeicosane	280	C20H40	000296-56-0	97
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		Behenic alcohol	326	C22H46O	000661-19-8	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102249.D
Acq On : 20 Jan 2018 5:59
Operator : SJ/JU
Sample : J1113-19
Misc :
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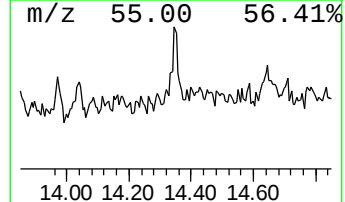
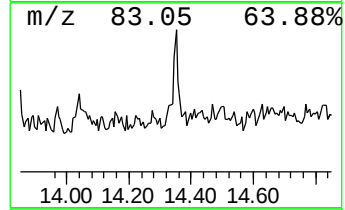
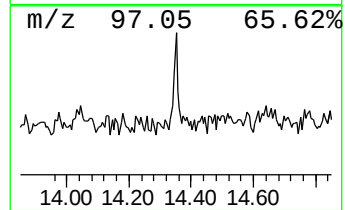
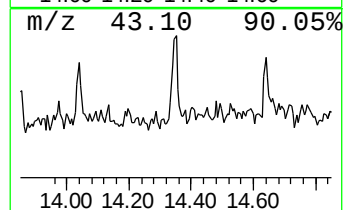
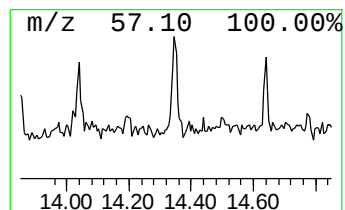
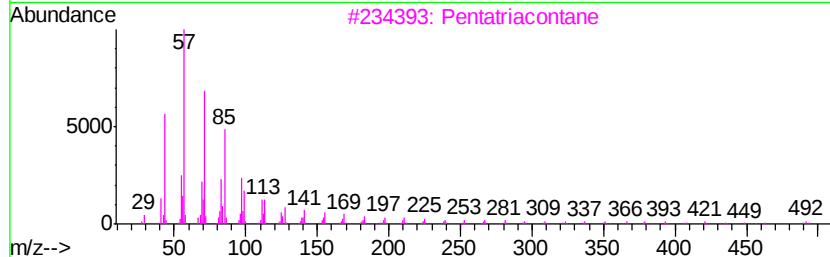
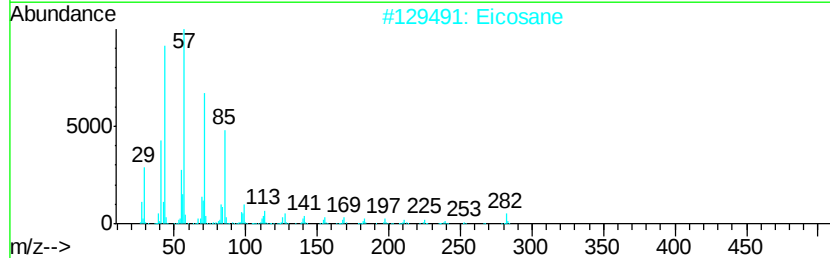
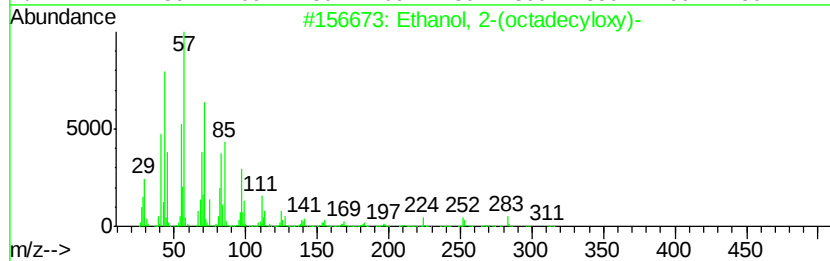
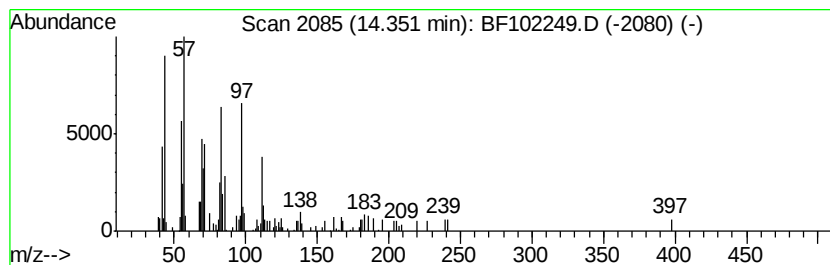
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Ethanol, 2-(octadecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.35	2.35 ng	91707	Chrysene-d12	13.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	68	
2	Eicosane	282	C20H42	000112-95-8	64	
3	Pentatriacontane	493	C35H72	000630-07-9	53	
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	52	
5	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	43	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102249.D
Acq On : 20 Jan 2018 5:59
Operator : SJ/JU
Sample : J1113-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-20-3.0-3.5

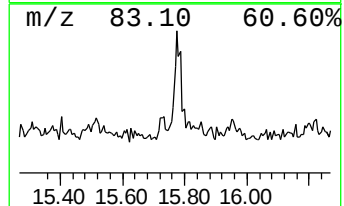
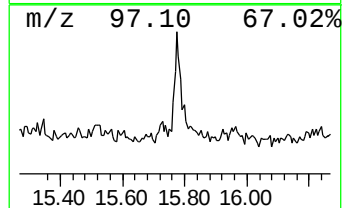
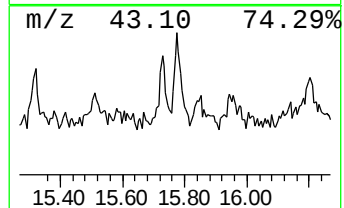
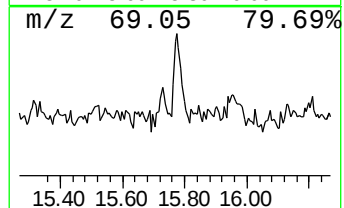
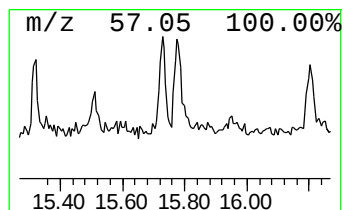
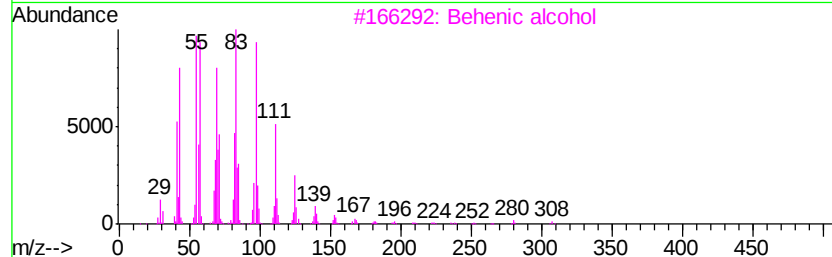
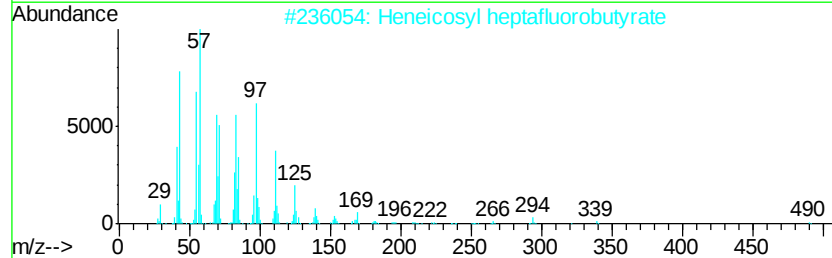
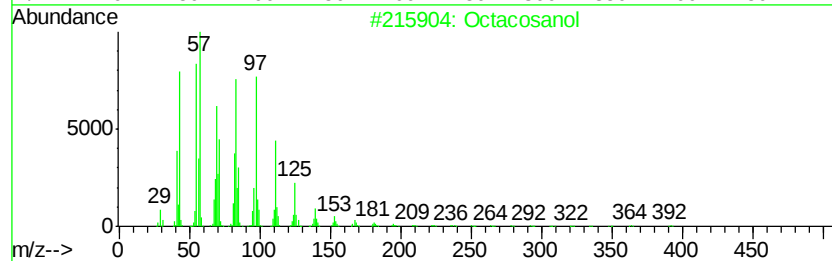
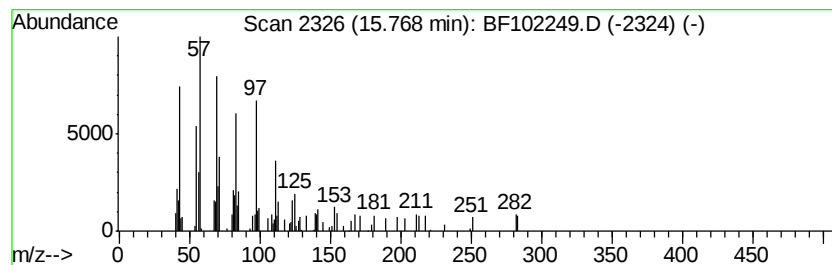
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	2.45 ng	101072	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosanol	410	C28H58O	000557-61-9	80
2		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	72
3		Behenic alcohol	326	C22H46O	000661-19-8	64
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	64
5		1-Heptacosanol	396	C27H56O	002004-39-9	58



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102249.D
Acq On : 20 Jan 2018 5:59
Operator : SJ/JU
Sample : J1113-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-20-3.0-3.5

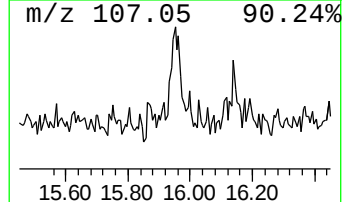
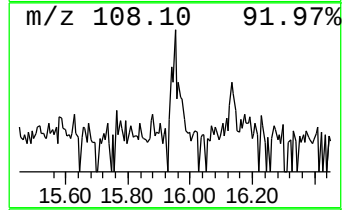
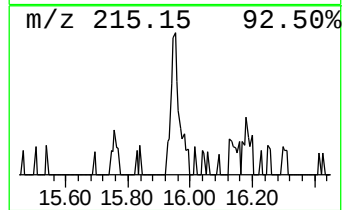
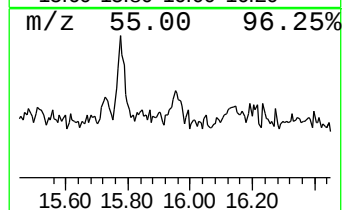
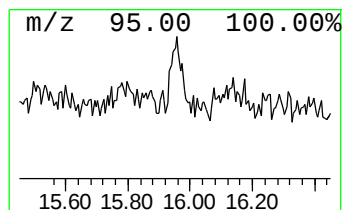
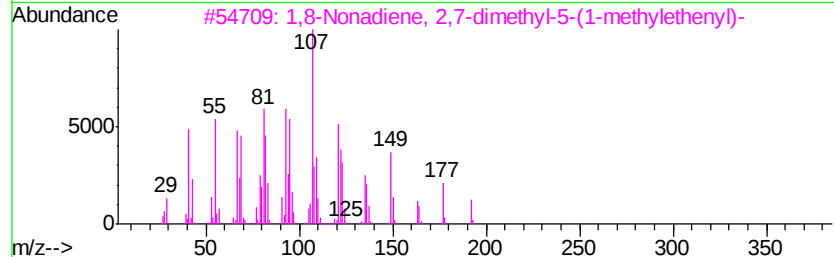
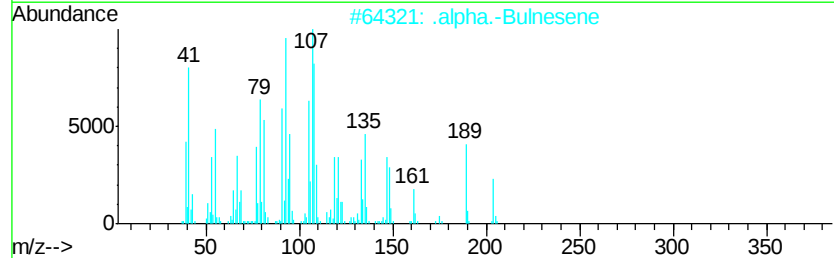
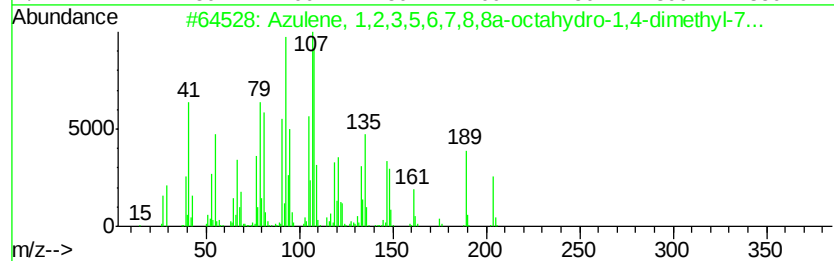
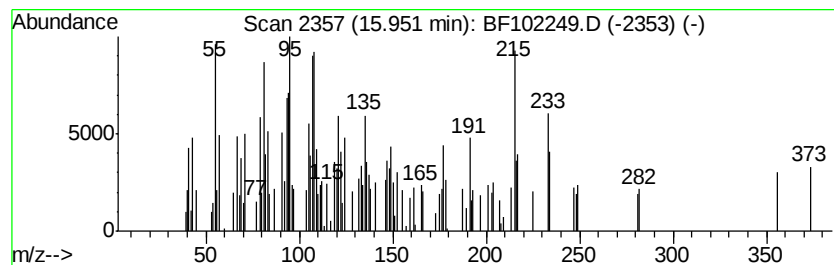
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Azulene, 1,2,3,5,6,7,8,8a-o... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.95	3.48 ng	143730	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Azulene, 1,2,3,5,6,7,8,8a-octahv...	204	C15H24	003691-11-0	81
2		.alpha.-Bulnesene	204	C15H24	1000374-19-9	59
3		1,8-Nonadiene, 2,7-dimethyl-5-(1...	192	C14H24	068702-20-5	47
4		Glaucic acid	234	C15H22O2	087745-30-0	30
5		1,2,4-Methenoazulene, decahydro-...	204	C15H24	001137-12-8	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102249.D
Acq On : 20 Jan 2018 5:59
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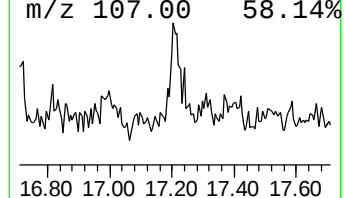
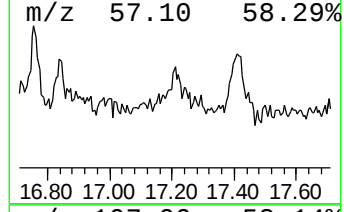
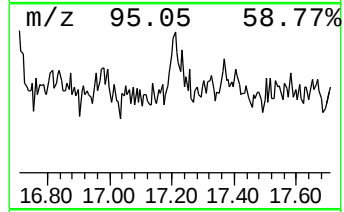
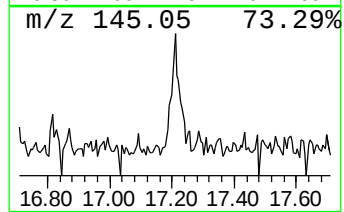
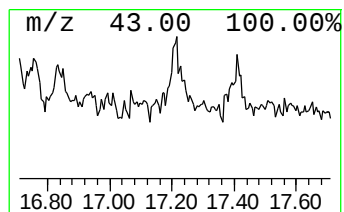
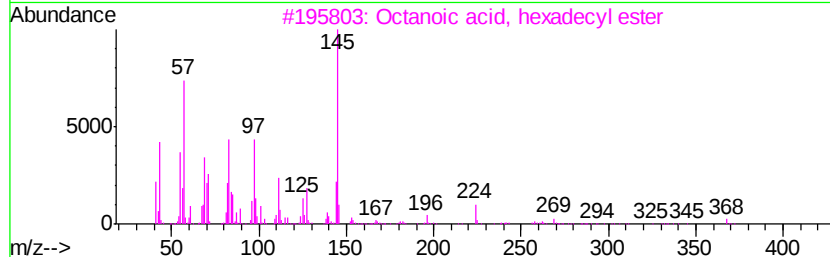
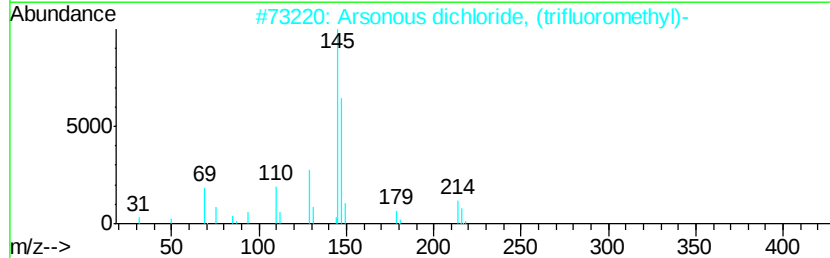
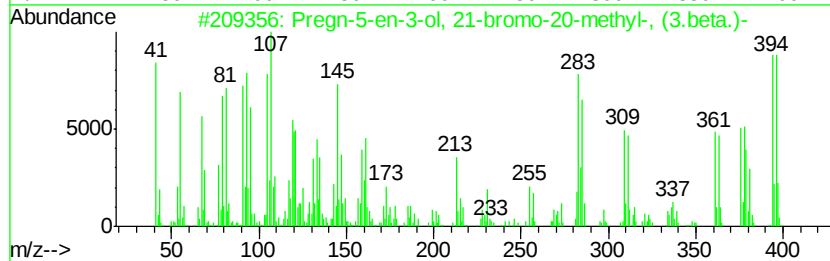
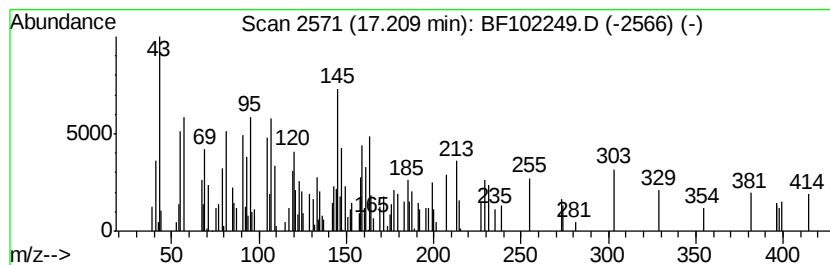
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.21 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.21	3.08 ng	127294	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	35
2		Arsonous dichloride, (trifluorom...	214	CASCl2F3	000421-32-9	22
3		Octanoic acid, hexadecyl ester	368	C24H48O2	029710-31-4	10
4		Clionasterol acetate	456	C31H52O2	004651-54-1	10
5		1,5-Bis[dimethyl(trimethylsilylm...	392	C17H44O2Si4	1000216-99-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
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 Misc :
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Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.92	5.7	ng	250939	1	6.72	882871	20.0
unknown6.49	6.49	76.8	ng	3391720	1	6.72	882871	20.0
Hexadecane	9.69	2.3	ng	129350	3	9.75	1127950	20.0
Tetracosane	10.66	3.0	ng	142247	4	11.23	939721	20.0
Hexadecanoic acid...	12.65	2.1	ng	84154	5	13.87	781930	20.0
Cycloeicosane	13.72	11.0	ng	428461	5	13.87	781930	20.0
Ethanol, 2-(octad...	14.35	2.4	ng	91707	5	13.87	781930	20.0
Octacosanol	15.77	2.5	ng	101072	6	15.29	826011	20.0
Azulene, 1,2,3,5,...	15.95	3.5	ng	143730	6	15.29	826011	20.0
unknown17.21	17.21	3.1	ng	127294	6	15.29	826011	20.0