

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
 Data File : BF101201.D
 Acq On : 7 Dec 2017 13:27
 Operator : SJ/JU
 Sample : I6615-01 2X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB-2-OW(0-10)

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-BF113017.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	5.057	501	505	513	rBV	31704	37586	4.71%	0.433%
2	5.457	570	573	591	rBV	521462	605816	75.92%	6.974%
3	6.475	743	746	763	rBV	631438	643029	80.58%	7.402%
4	6.610	765	769	773	rBV	798559	662965	83.08%	7.632%
5	6.839	804	808	811	rBV	369553	305312	38.26%	3.515%
6	6.992	830	834	838	rBV	611156	513191	64.31%	5.908%
7	7.251	875	878	882	rBB	16745	15547	1.95%	0.179%
8	7.404	900	904	907	rVB	461796	368001	46.12%	4.236%
9	8.122	1022	1026	1030	rBV	493302	399710	50.09%	4.601%
10	9.198	1204	1209	1212	rBV	1010688	797960	100.00%	9.186%
11	9.592	1272	1276	1278	rBV	38363	29377	3.68%	0.338%
12	9.798	1305	1311	1315	rBV	14110	12117	1.52%	0.139%
13	9.880	1321	1325	1329	rBV	541506	442375	55.44%	5.092%
14	10.298	1393	1396	1399	rVB	18041	13457	1.69%	0.155%
15	10.522	1428	1434	1436	rBV2	6529	9741	1.22%	0.112%
16	10.669	1456	1459	1463	rBV	487434	433745	54.36%	4.993%
17	10.774	1474	1477	1482	rBV	19801	19965	2.50%	0.230%
18	11.221	1550	1553	1555	rBV2	24284	18315	2.30%	0.211%
19	11.369	1575	1578	1581	rBV	503397	443306	55.55%	5.103%
20	11.392	1581	1582	1586	rVV	97090	58792	7.37%	0.677%
21	11.445	1589	1591	1594	rVB	14855	10401	1.30%	0.120%
22	11.886	1661	1666	1674	rBV4	74337	96777	12.13%	1.114%
23	11.986	1680	1683	1685	rBV2	13267	12692	1.59%	0.146%
24	12.057	1691	1695	1699	rBV4	12586	11338	1.42%	0.131%
25	12.586	1782	1785	1788	rBV	126064	105276	13.19%	1.212%
26	12.674	1794	1800	1803	rBV3	31338	34520	4.33%	0.397%
27	12.768	1813	1816	1819	rBV	14904	12466	1.56%	0.144%
28	12.815	1819	1824	1828	rBV	121596	110984	13.91%	1.278%
29	12.957	1840	1848	1851	rBV	712923	630920	79.07%	7.263%
30	13.033	1856	1861	1866	rVV6	7793	14856	1.86%	0.171%
31	13.145	1873	1880	1883	rBV3	14049	20241	2.54%	0.233%
32	13.251	1894	1898	1900	rBV2	15197	14401	1.80%	0.166%
33	13.380	1916	1920	1921	rBV4	8532	10386	1.30%	0.120%
34	13.433	1923	1929	1933	rBV	222797	242563	30.40%	2.792%

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35	13.510	1939	1942	1946	rVB3	15439	20395	2.56%	0.235%
36	13.662	1965	1968	1971	rVB	9155	9954	1.25%	0.115%
37	13.768	1981	1986	1988	rBV2	8448	13653	1.71%	0.157%
38	13.839	1992	1998	2001	rVV3	96263	108091	13.55%	1.244%
39	13.868	2001	2003	2008	rVB3	15776	17941	2.25%	0.207%
40	13.980	2016	2022	2024	rBV	14974	20593	2.58%	0.237%
41	14.015	2024	2028	2031	rVV2	338733	362289	45.40%	4.170%
42	14.045	2031	2033	2036	rVB	42568	36453	4.57%	0.420%
43	14.115	2042	2045	2047	rBV3	12189	15122	1.90%	0.174%
44	14.139	2047	2049	2051	rVB3	15375	12123	1.52%	0.140%
45	14.180	2051	2056	2059	rBV2	26086	34310	4.30%	0.395%
46	14.227	2062	2064	2069	rVB6	12161	15347	1.92%	0.177%
47	14.268	2069	2071	2075	rVB3	17177	18451	2.31%	0.212%
48	14.310	2075	2078	2079	rBV3	19691	20382	2.55%	0.235%
49	14.404	2091	2094	2097	rVB3	20176	22570	2.83%	0.260%
50	14.462	2100	2104	2109	rVB3	28506	49909	6.25%	0.575%
51	14.621	2128	2131	2137	rVB2	33644	50529	6.33%	0.582%
52	14.845	2168	2169	2172	rVB3	15263	10972	1.38%	0.126%
53	15.068	2201	2207	2209	rBV	37186	58925	7.38%	0.678%
54	15.368	2254	2258	2265	rVB	28262	35302	4.42%	0.406%
55	15.433	2265	2269	2273	rBV	37689	44957	5.63%	0.518%
56	15.498	2275	2280	2292	rVB	244403	324957	40.72%	3.741%
57	15.921	2349	2352	2356	rVB5	10684	12524	1.57%	0.144%
58	15.980	2357	2362	2373	rVB9	17315	39023	4.89%	0.449%
59	16.180	2391	2396	2405	rVB9	15552	41457	5.20%	0.477%
60	16.427	2433	2438	2442	rBV8	7837	15529	1.95%	0.179%
61	16.609	2464	2469	2474	rVB8	11617	24945	3.13%	0.287%
62	16.986	2527	2533	2537	rBV3	18421	43670	5.47%	0.503%
63	17.433	2602	2609	2615	rBV	14335	28719	3.60%	0.331%
64	17.698	2650	2654	2659	rBV8	9671	19805	2.48%	0.228%

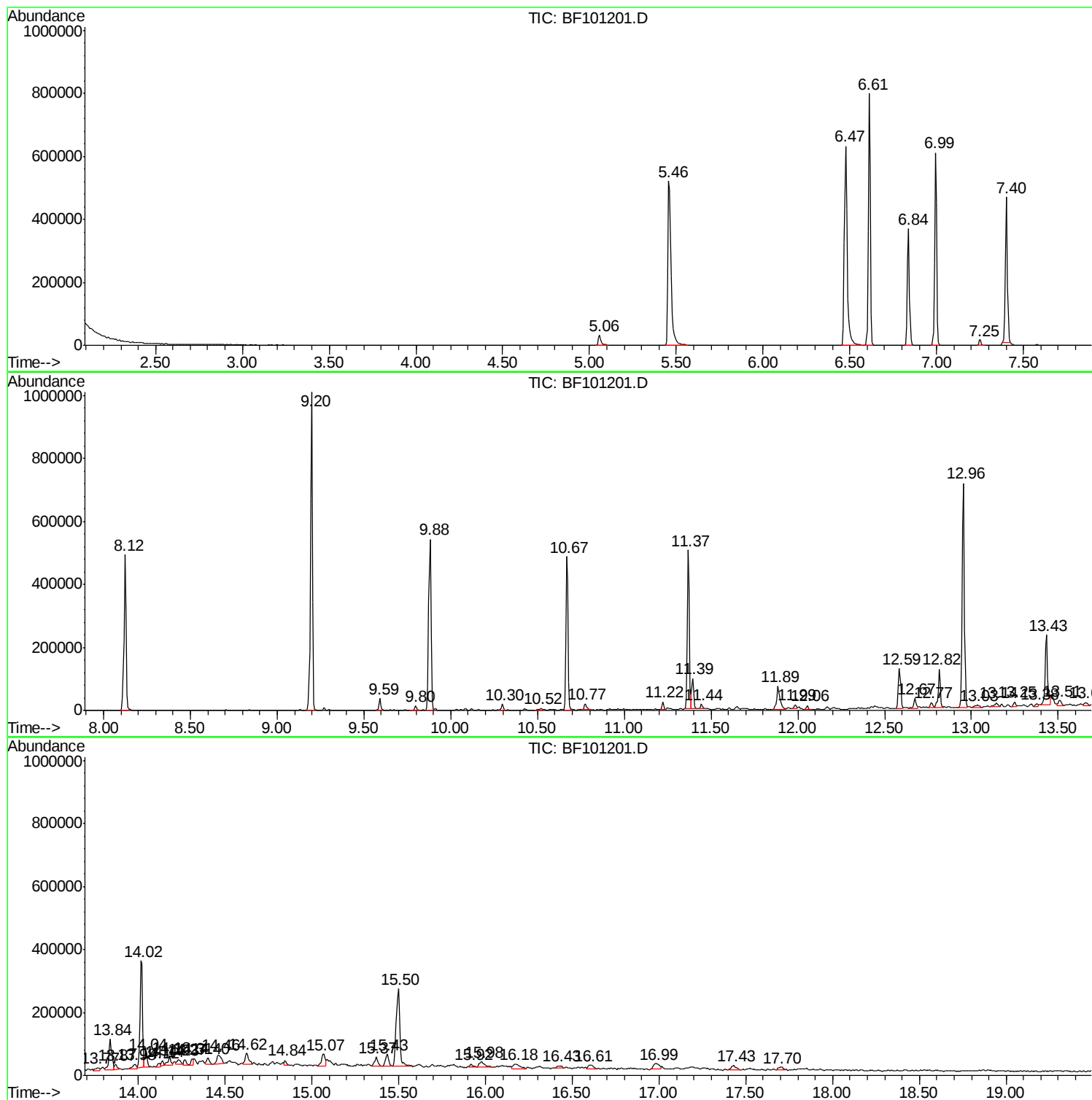
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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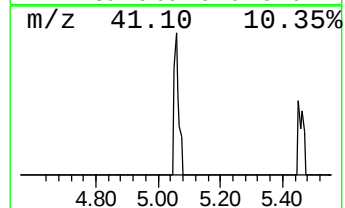
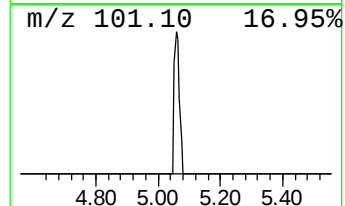
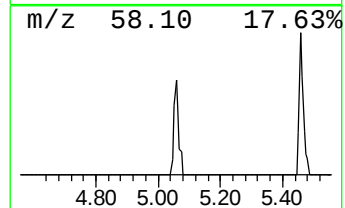
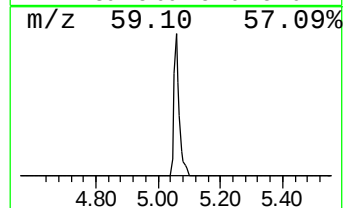
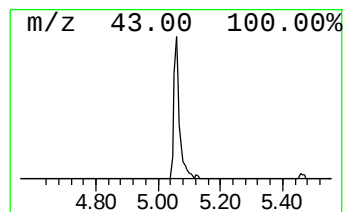
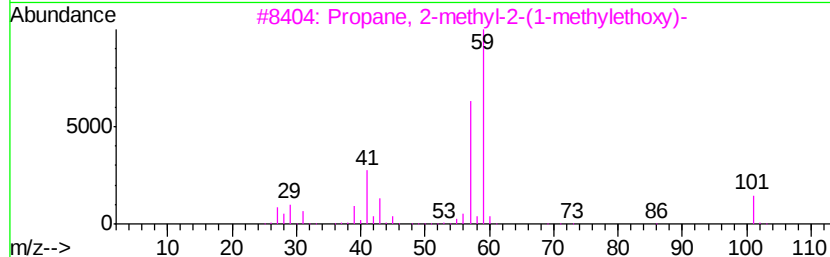
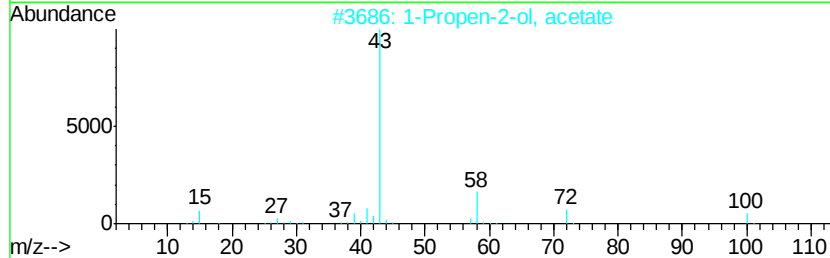
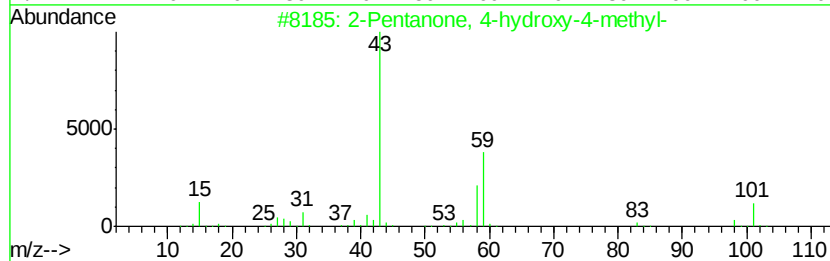
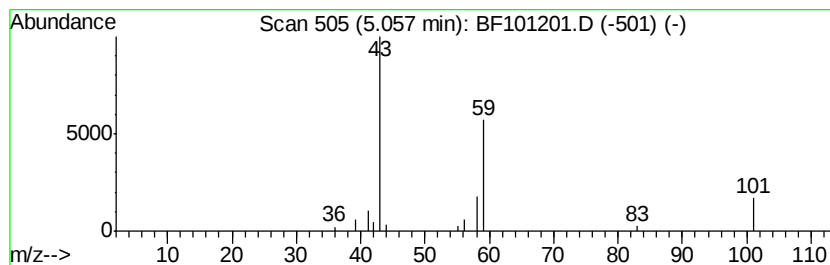
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.46 ng	37586	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	9
4		2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9
5		Acetone	58	C3H6O	000067-64-1	7



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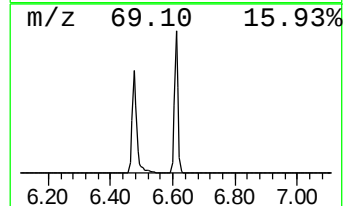
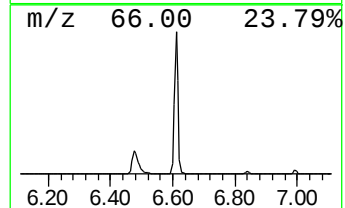
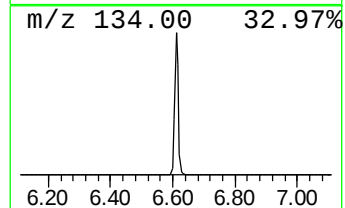
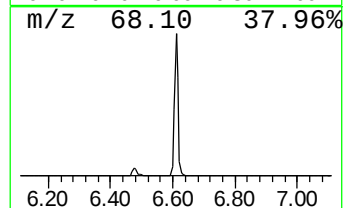
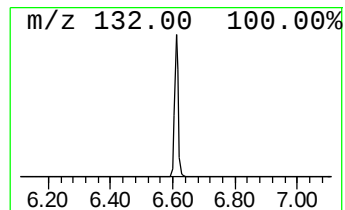
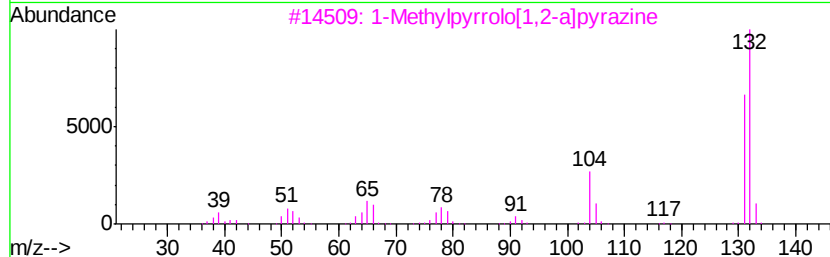
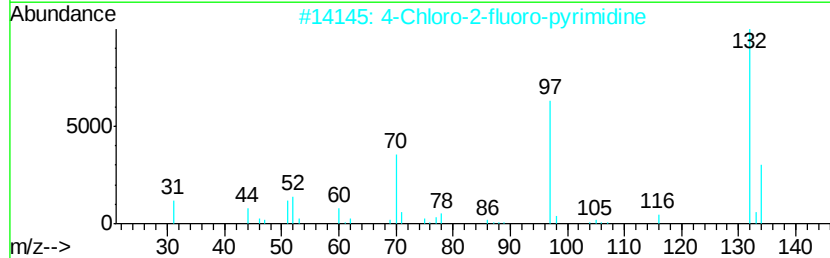
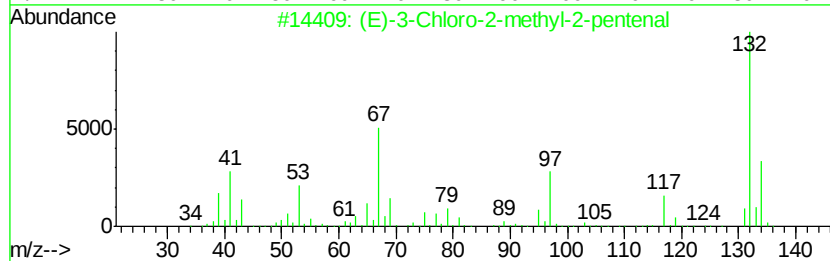
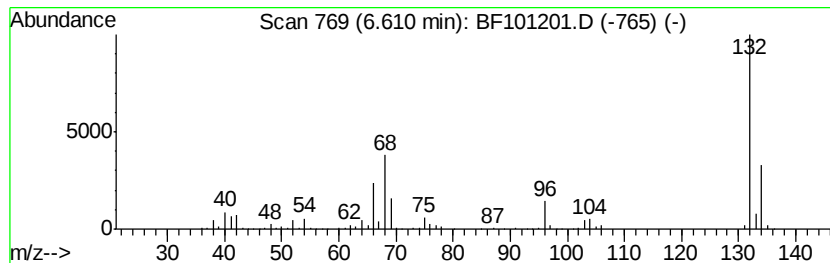
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	43.43 ng	662965	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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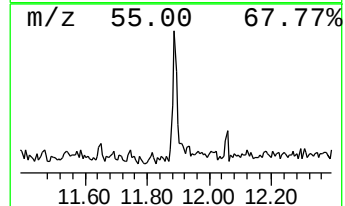
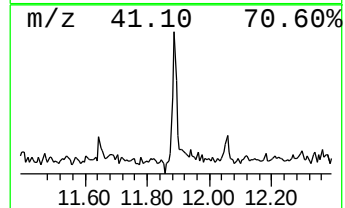
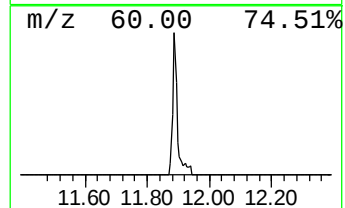
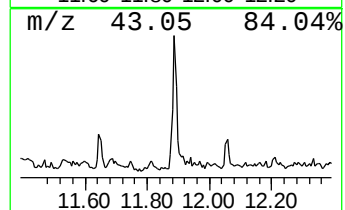
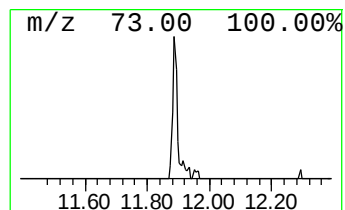
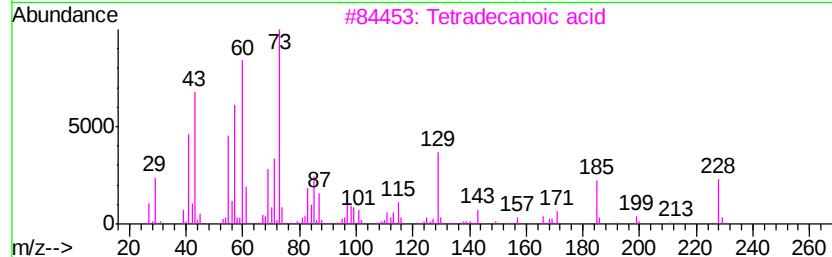
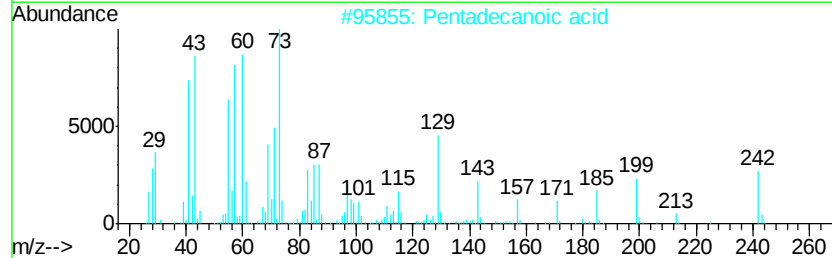
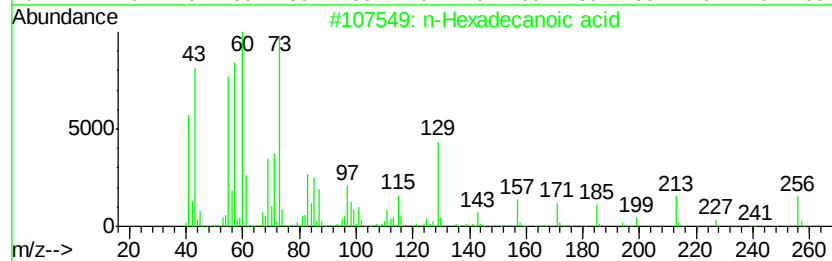
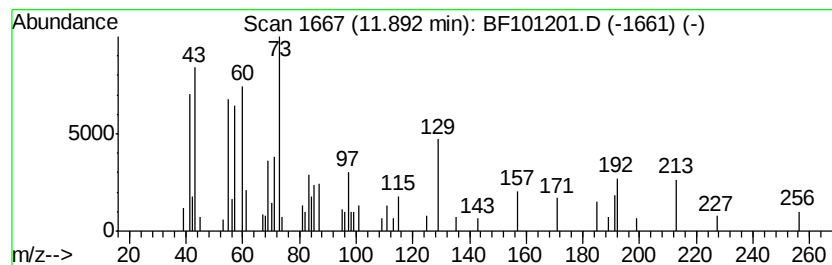
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	4.37 ng	96777	Phenanthrene-d10	11.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	43
5		Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30



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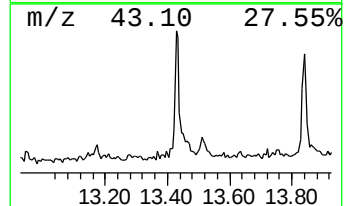
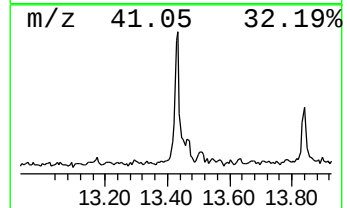
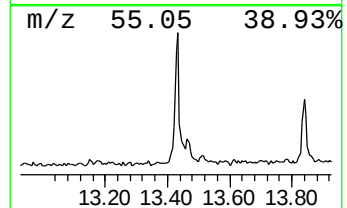
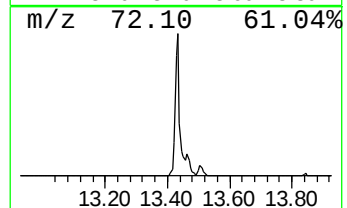
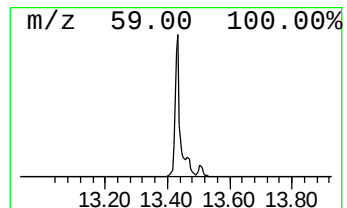
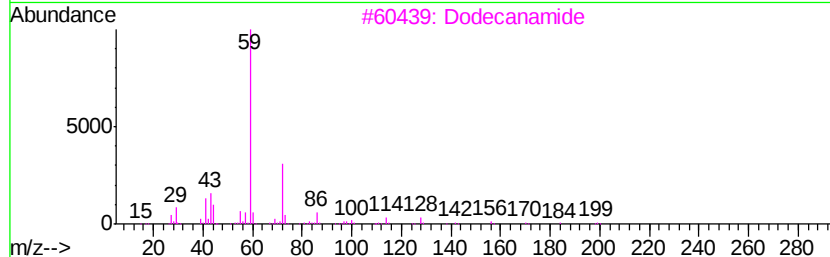
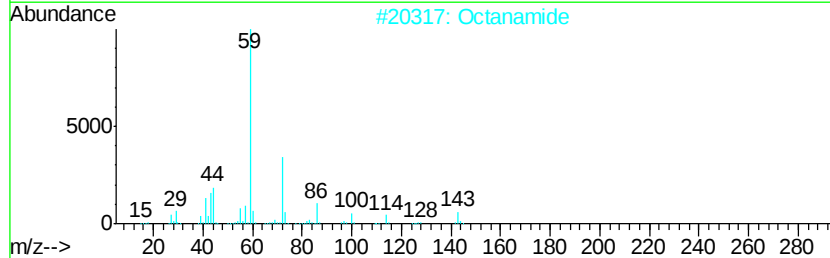
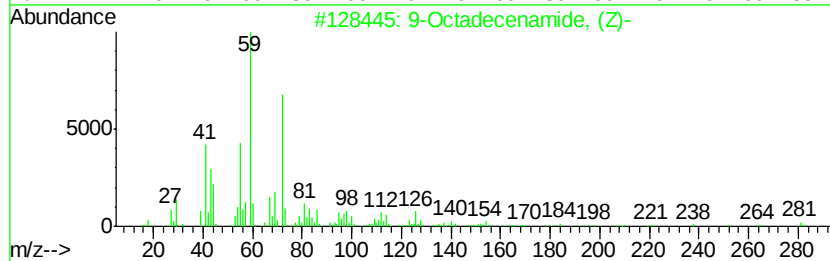
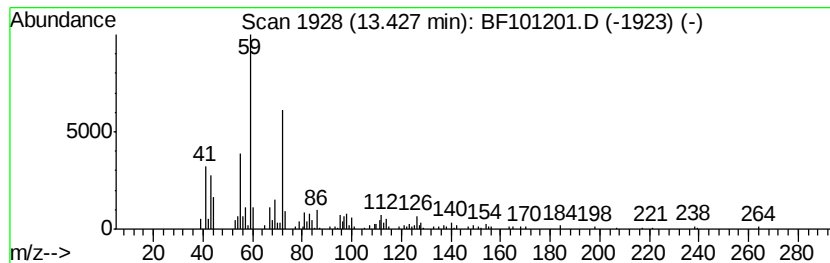
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	13.39 ng	242563	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Octanamide	143	C8H17NO	000629-01-6	59
3		Dodecanamide	199	C12H25NO	001120-16-7	59
4		Nonanamide	157	C9H19NO	001120-07-6	59
5		Pentanamide	101	C5H11NO	000626-97-1	53



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ALS Vial : 5 Sample Multiplier: 1

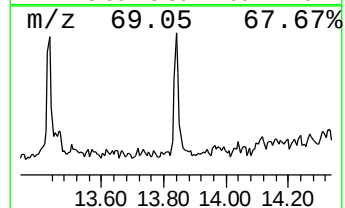
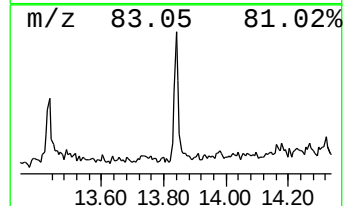
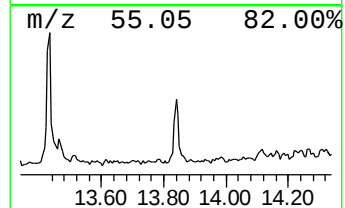
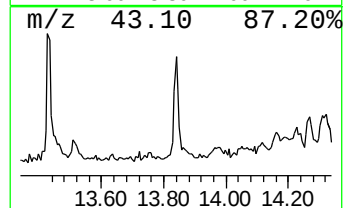
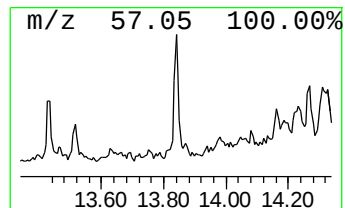
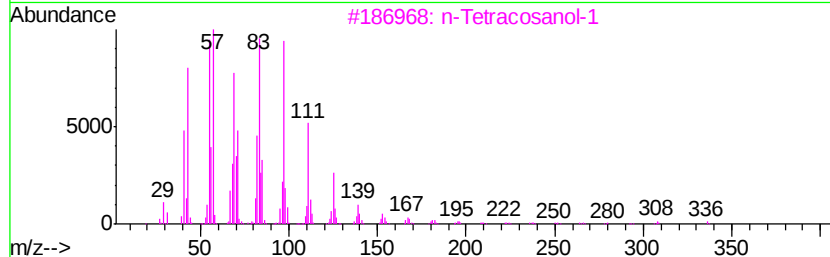
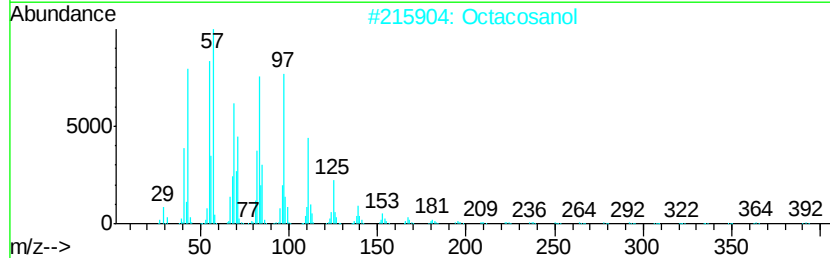
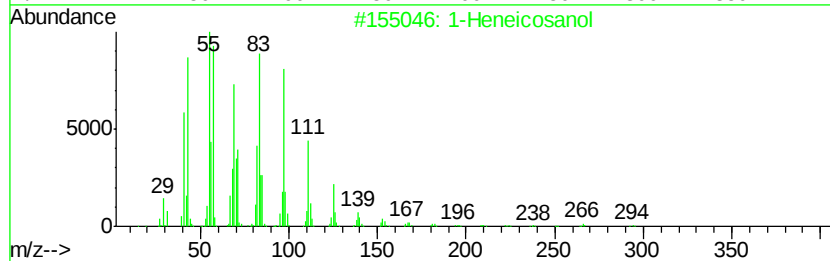
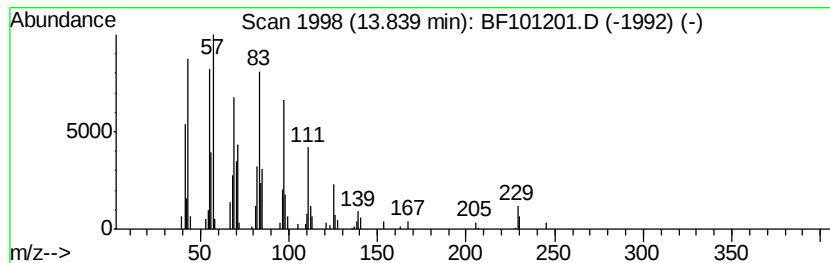
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ClientSampleId :
PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.84	5.97 ng	108091	Chrysene-d12	14.02	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Octacosanol	410	C28H58O	000557-61-9	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120717\
Data File : BF101201.D
Acq On : 7 Dec 2017 13:27
Operator : SJ/JU
Sample : I6615-01 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

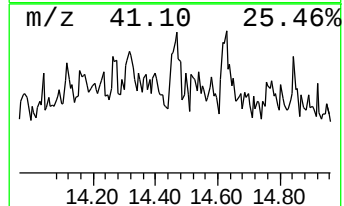
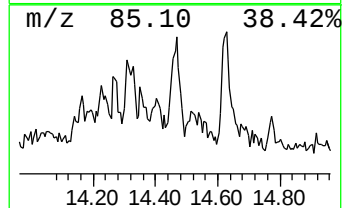
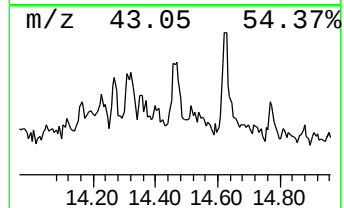
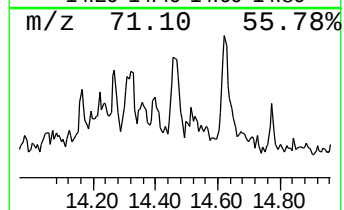
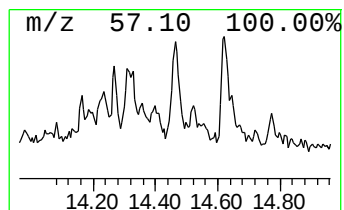
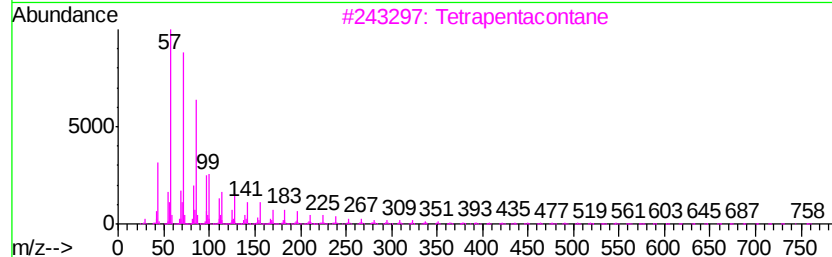
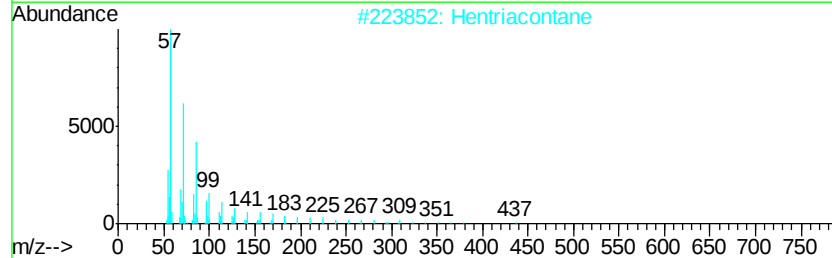
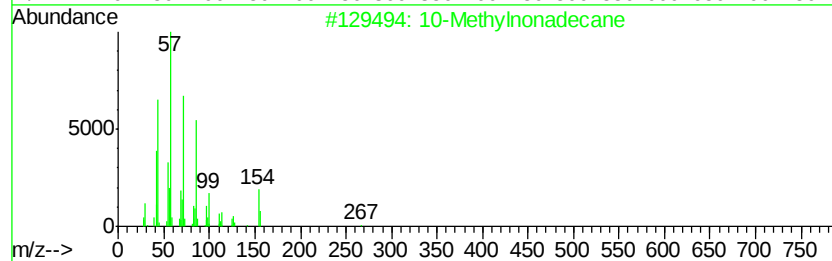
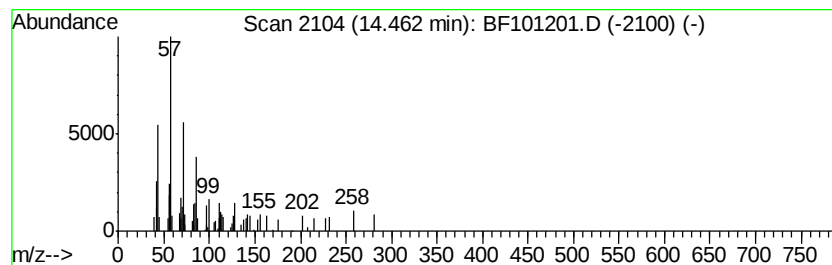
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 10-Methylnonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.46	2.76 ng	49909	Chrysene-d12		14.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	68
2	Hentriacontane	437	C31H64	000630-04-6	64
3	Tetrapentacontane	759	C54H110	005856-66-6	64
4	Octacosane	394	C28H58	000630-02-4	64
5	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101201.D
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Operator : SJ/JU
Sample : I6615-01 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB-2-OW(0-10)

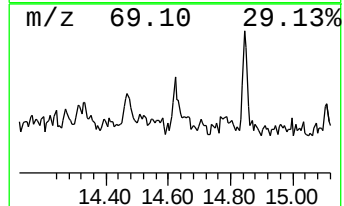
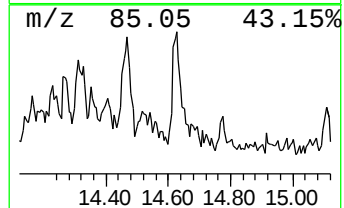
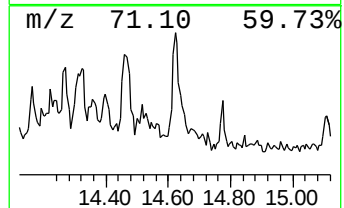
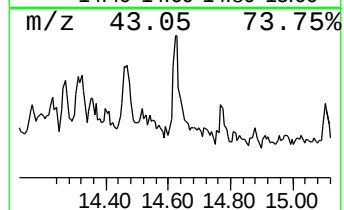
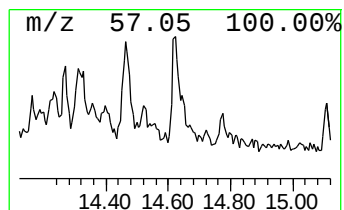
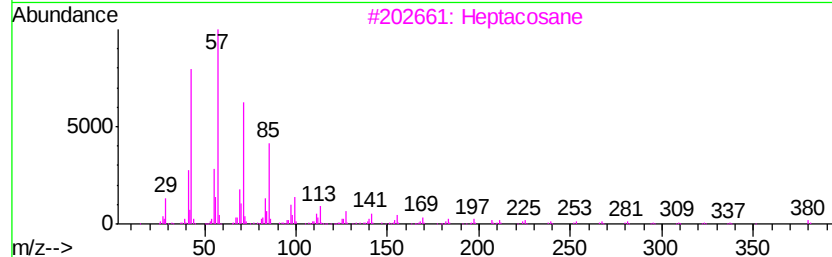
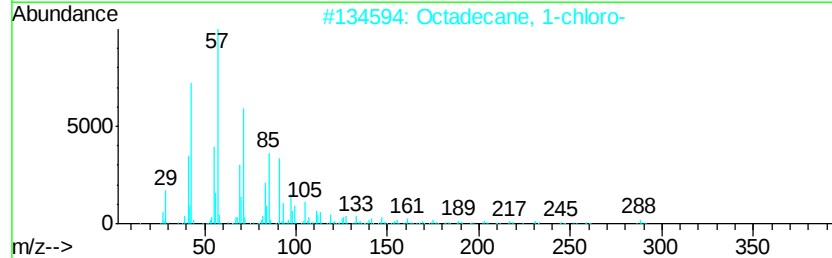
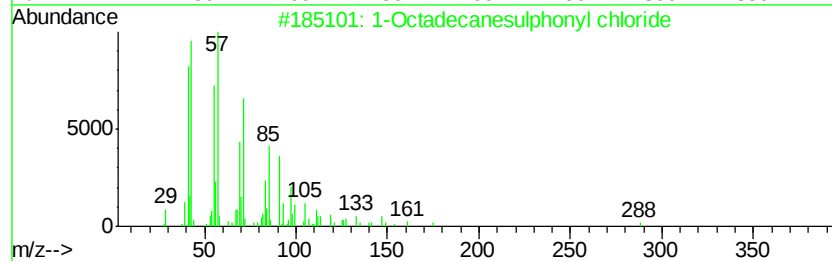
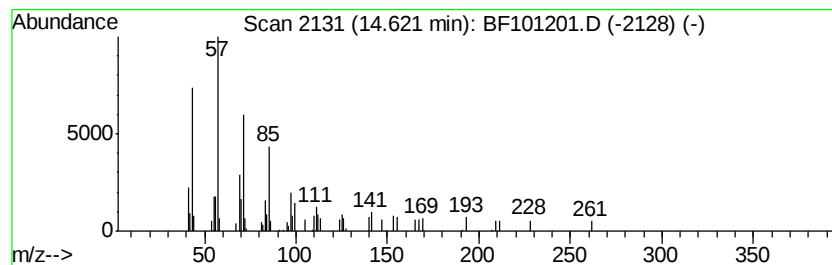
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Octadecanesulphonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.79 ng	50529	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	83
2		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
3		Heptacosane	380	C27H56	000593-49-7	72
4		Hentriacontane	437	C31H64	000630-04-6	64
5		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120717\
Data File : BF101201.D
Acq On : 7 Dec 2017 13:27
Operator : SJ/JU
Sample : I6615-01 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB-2-OW(0-10)

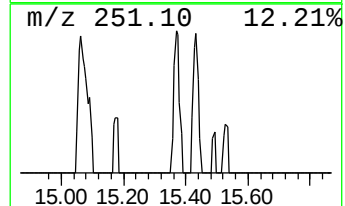
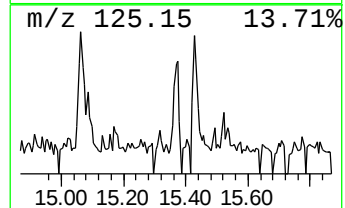
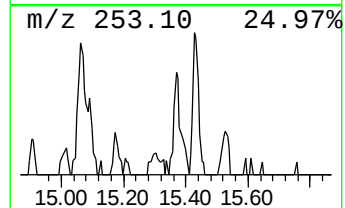
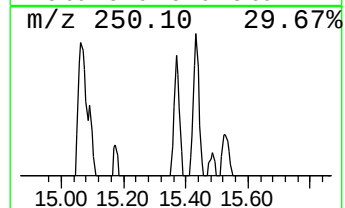
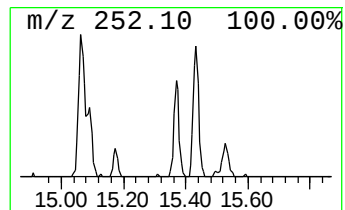
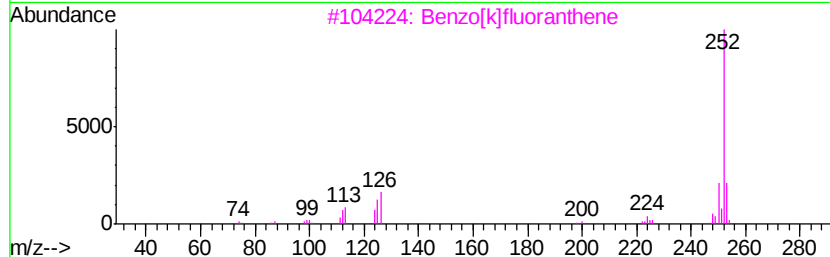
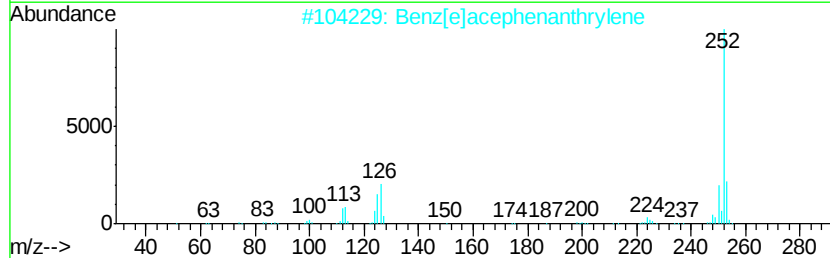
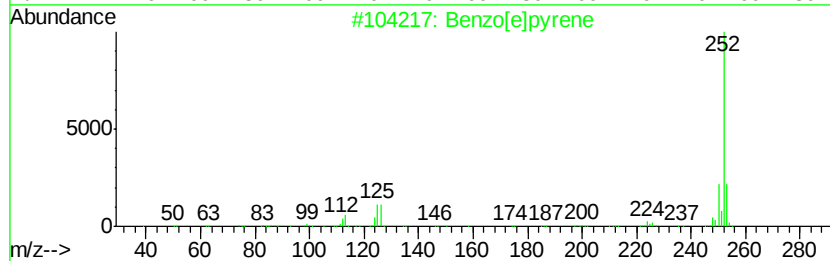
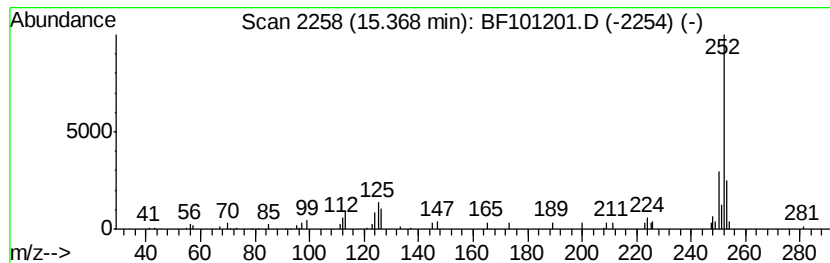
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.17 ng	35302	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	90
3		Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4		Benzo[a]pyrene	252	C20H12	000050-32-8	87
5		(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120717\
Data File : BF101201.D
Acq On : 7 Dec 2017 13:27
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ALS Vial : 5 Sample Multiplier: 1

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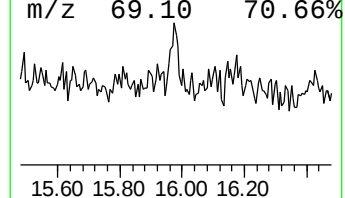
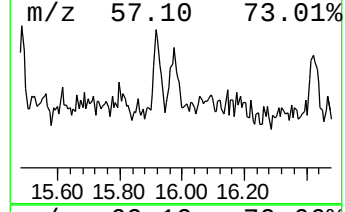
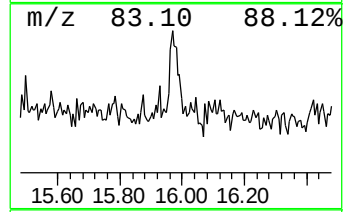
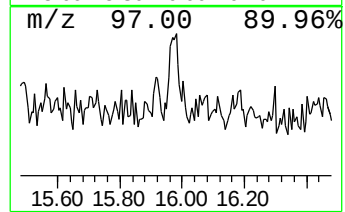
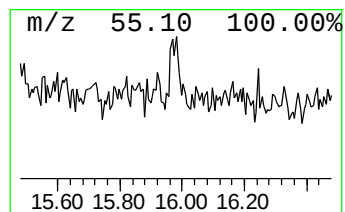
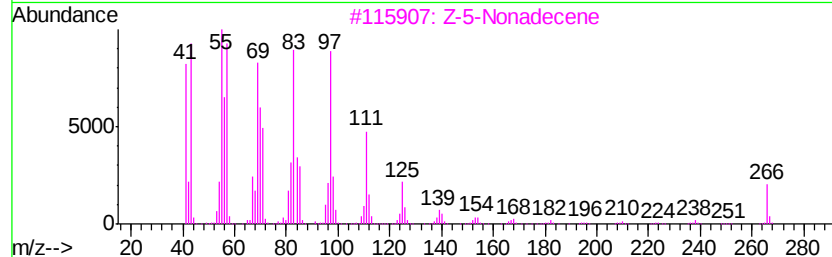
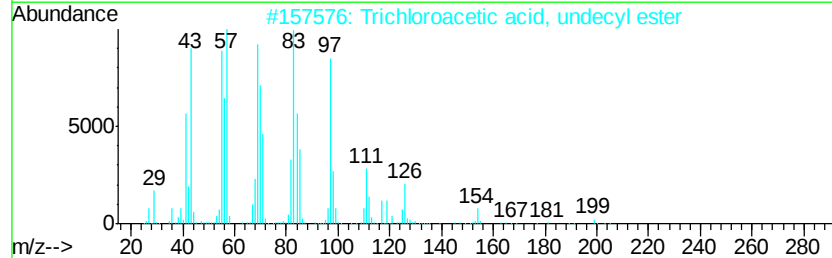
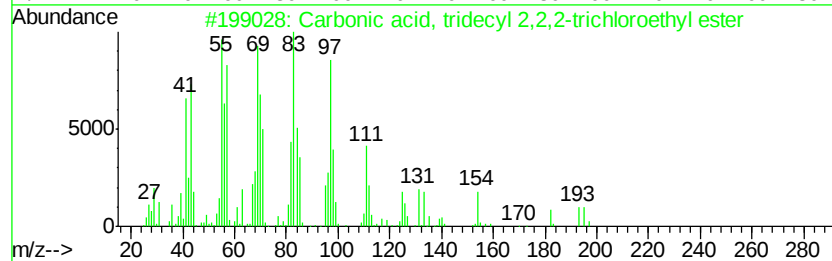
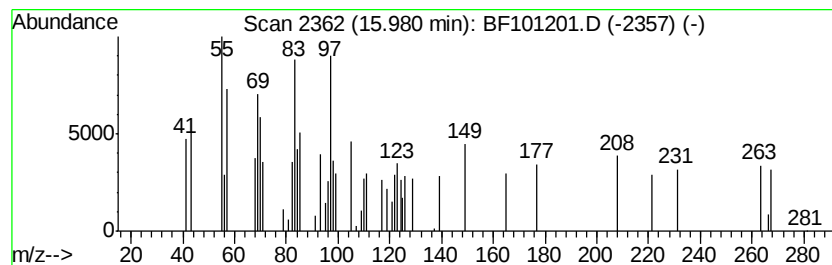
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, tridecyl 2,2... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.40 ng	39023	Perylene-d12	15.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	55
2			Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	46
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	45
4			17-Pentatriacontene	491	C35H70	006971-40-0	43
5			1-Nonadecene	266	C19H38	018435-45-5	43



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101201.D
Acq On : 7 Dec 2017 13:27
Operator : SJ/JU
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB-2-OW(0-10)

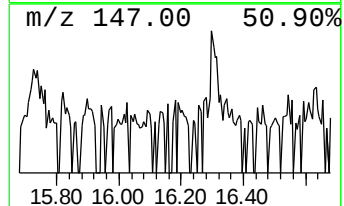
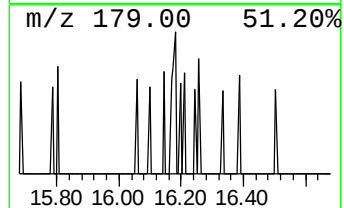
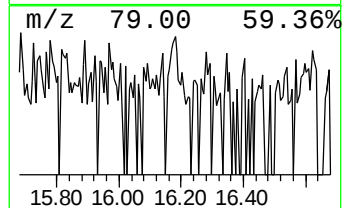
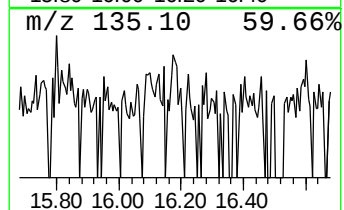
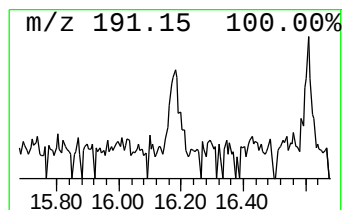
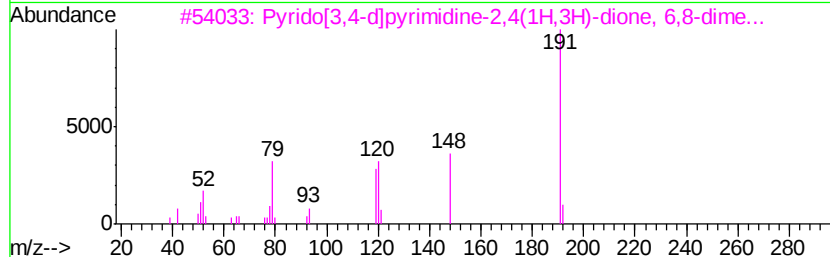
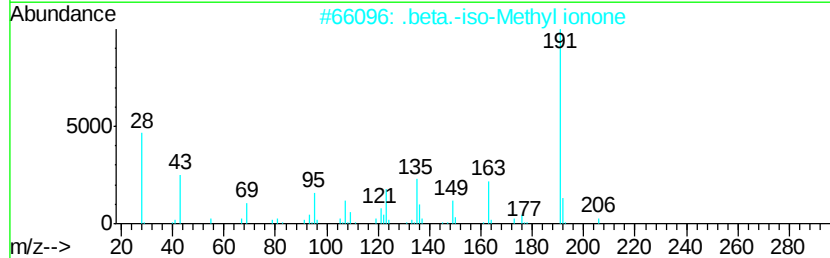
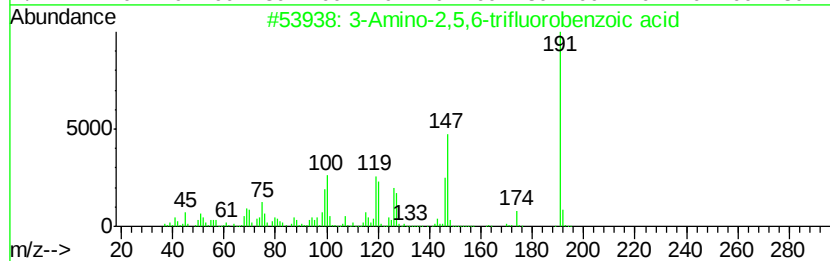
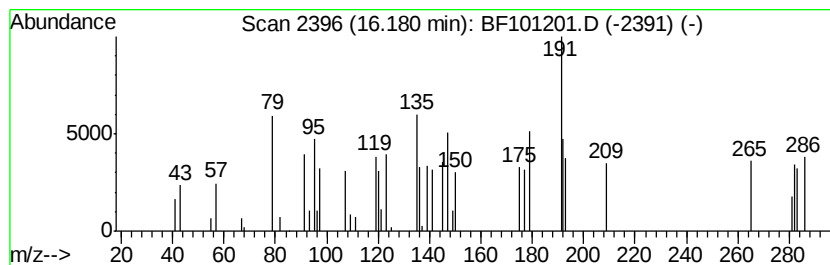
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown16.18 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.55 ng	41457	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Amino-2,5,6-trifluorobenzoic acid	191	C7H4F3NO2	133622-65-8	27
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	25
3		Pyrido[3,4-d]pyrimidine-2,4(1H,3...)	191	C9H9N3O2	022389-87-3	22
4		Silane, diethylethoxy(2-ethoxyvet...)	220	C10H24O3Si	1000363-51-6	17
5		1-Penten-3-one, 1-(2,6,6-trimeth...)	206	C14H22O	000127-43-5	14



Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101201.D
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
PB-2-OW(0-10)

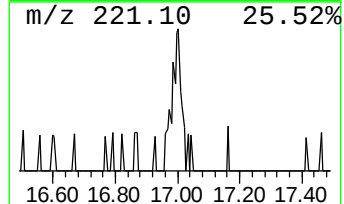
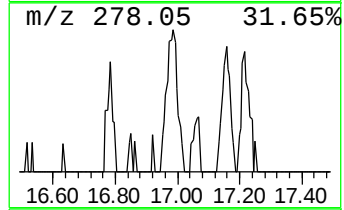
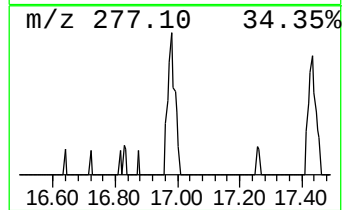
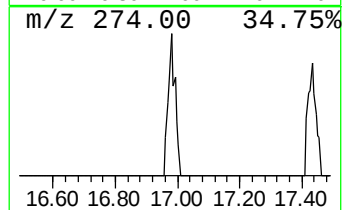
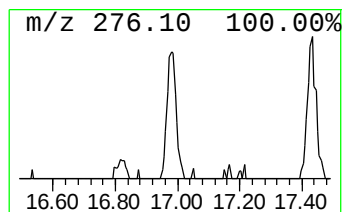
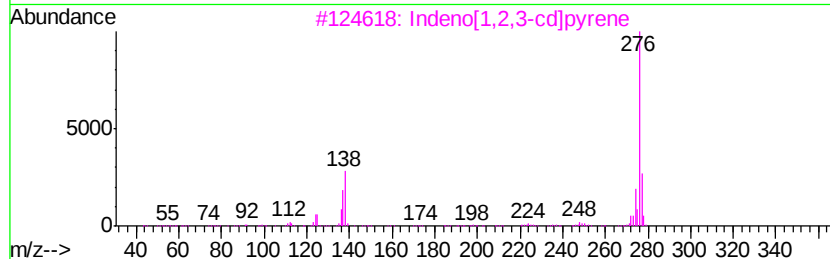
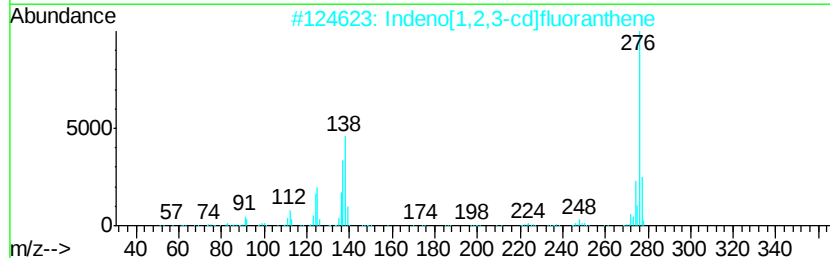
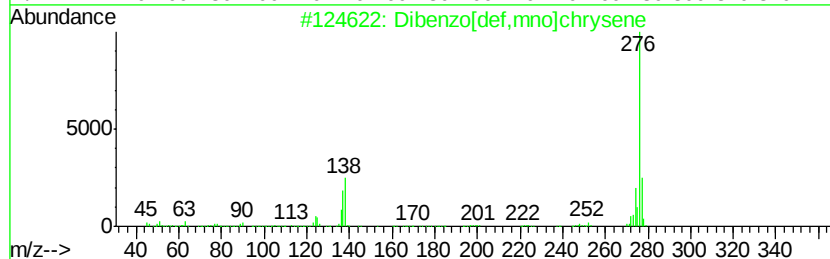
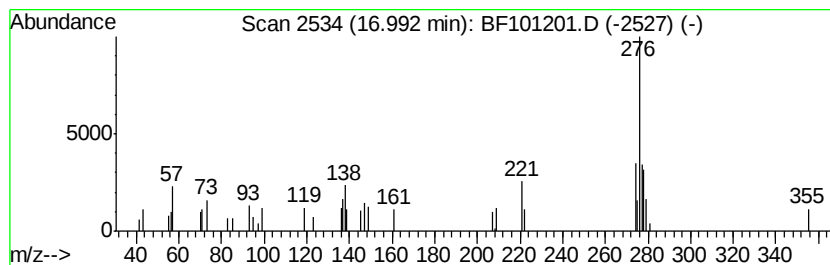
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dibenzo[def,mno]chrysene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	2.69 ng	43670	Perylene-d12	15.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	64
2		Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	53
3		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	52
4		Benzo[ghi]perylene	276	C22H12	000191-24-2	49
5		Phenol, 2-(4-chlorophenyl)iminome...	276	C13H9ClN2O3	1000262-90-3	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120717\
Data File : BF101201.D
Acq On : 7 Dec 2017 13:27
Operator : SJ/JU
Sample : I6615-01 2X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-2-OW(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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...	5.06	2.5	ng	37586	1	6.84	305312	20.0
unknown6.61	6.61	43.4	ng	662965	1	6.84	305312	20.0
n-Hexadecanoic acid	11.89	4.4	ng	96777	4	11.37	443306	20.0
9-Octadecenamamide,...	13.43	13.4	ng	242563	5	14.02	362289	20.0
1-Heneicosanol	13.84	6.0	ng	108091	5	14.02	362289	20.0
10-Methylnonadecane	14.46	2.8	ng	49909	5	14.02	362289	20.0
1-Octadecanesulph...	14.62	2.8	ng	50529	5	14.02	362289	20.0
Benzo[e]pyrene	15.37	2.2	ng	35302	6	15.50	324957	20.0
Carbonic acid, tr...	15.98	2.4	ng	39023	6	15.50	324957	20.0
unknown16.18	16.18	2.5	ng	41457	6	15.50	324957	20.0
Dibenzo[def,mno]c...	16.99	2.7	ng	43670	6	15.50	324957	20.0