

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
 Data File : BF100147.D
 Acq On : 3 Nov 2017 20:59
 Operator : SJ/JU
 Sample : I6079-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4-FILL(3-4)

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-BF102317.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	4.987	490	493	516	rBV	180815	288928	16.71%	1.659%
2	5.393	559	562	581	rBV	1033421	1358189	78.55%	7.799%
3	6.416	733	736	754	rBV	1313640	1493344	86.37%	8.575%
4	6.545	754	758	763	rVB	1533080	1519291	87.87%	8.724%
5	6.769	793	796	806	rBV	548354	515304	29.80%	2.959%
6	6.922	819	822	838	rVB	1385259	1251065	72.36%	7.184%
7	7.339	890	893	906	rBV	972753	945157	54.66%	5.427%
8	8.051	1011	1014	1030	rVB	781124	752732	43.53%	4.322%
9	8.616	1106	1110	1117	rBV2	41168	51563	2.98%	0.296%
10	8.769	1133	1136	1141	rBV	28694	25694	1.49%	0.148%
11	8.869	1149	1153	1162	rVB2	18241	23479	1.36%	0.135%
12	9.122	1192	1196	1199	rBV	2019167	1729043	100.00%	9.928%
13	9.233	1212	1215	1218	rVB	30732	27222	1.57%	0.156%
14	9.398	1239	1243	1246	rBV	17944	23737	1.37%	0.136%
15	9.463	1251	1254	1257	rBV	25025	26968	1.56%	0.155%
16	9.522	1261	1264	1270	rVB	524533	408993	23.65%	2.348%
17	9.804	1306	1312	1316	rBV	922250	803777	46.49%	4.615%
18	9.845	1316	1319	1324	rVB2	26811	34086	1.97%	0.196%
19	10.016	1343	1348	1351	rBV2	19526	28316	1.64%	0.163%
20	10.216	1374	1382	1386	rBV3	18252	24245	1.40%	0.139%
21	10.363	1400	1407	1412	rVB3	35921	43460	2.51%	0.250%
22	10.516	1430	1433	1440	rVB	193186	158007	9.14%	0.907%
23	10.598	1444	1447	1454	rBV	849246	828550	47.92%	4.758%
24	11.298	1562	1566	1568	rBV	794019	709191	41.02%	4.072%
25	11.322	1568	1570	1575	rVB	258271	227209	13.14%	1.305%
26	11.380	1575	1580	1583	rBV2	37903	41823	2.42%	0.240%
27	11.498	1596	1600	1605	rVB3	15595	22724	1.31%	0.130%
28	11.545	1605	1608	1613	rBV4	18883	26965	1.56%	0.155%
29	11.657	1625	1627	1631	rVB	48921	41559	2.40%	0.239%
30	11.798	1648	1651	1654	rBV	54889	61577	3.56%	0.354%
31	11.827	1654	1656	1661	rVB	69433	72296	4.18%	0.415%
32	11.910	1667	1670	1673	rBV2	50512	53502	3.09%	0.307%
33	11.933	1673	1674	1678	rVB	26474	21648	1.25%	0.124%
34	12.092	1696	1701	1705	rBV2	37807	42957	2.48%	0.247%

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Min Area: 3 % of largest Peak
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	12.351	1742	1745	1748	rBV	32316	36257	2.10%	0.208%
36	12.516	1769	1773	1777	rBV	236179	206896	11.97%	1.188%
37	12.745	1806	1812	1818	rVB2	182034	207799	12.02%	1.193%
38	12.874	1830	1834	1838	rBV	1221117	1078399	62.37%	6.192%
39	12.968	1845	1850	1856	rVB6	14936	28964	1.68%	0.166%
40	13.080	1866	1869	1873	rVB2	32115	33756	1.95%	0.194%
41	13.180	1883	1886	1893	rVB4	17455	30527	1.77%	0.175%
42	13.604	1954	1958	1962	rBV2	15771	29905	1.73%	0.172%
43	13.716	1973	1977	1980	rBV3	23707	36768	2.13%	0.211%
44	13.757	1980	1984	1993	rVB3	68511	101935	5.90%	0.585%
45	13.945	2011	2016	2020	rBV2	461506	528018	30.54%	3.032%
46	13.974	2020	2021	2025	rVB	60689	48281	2.79%	0.277%
47	14.080	2037	2039	2043	rVB4	20582	20584	1.19%	0.118%
48	14.321	2074	2080	2082	rBV5	12913	26998	1.56%	0.155%
49	14.380	2086	2090	2093	rVV4	31136	32516	1.88%	0.187%
50	14.427	2094	2098	2103	rVB6	14070	25870	1.50%	0.149%
51	14.674	2136	2140	2146	rVB5	22069	28619	1.66%	0.164%
52	14.992	2190	2194	2197	rBV2	85966	112763	6.52%	0.647%
53	15.292	2241	2245	2252	rVB	39378	51107	2.96%	0.293%
54	15.357	2252	2256	2261	rBV	98646	118514	6.85%	0.681%
55	15.410	2261	2265	2279	rVV	324579	433703	25.08%	2.490%
56	15.774	2322	2327	2334	rVB2	50743	72467	4.19%	0.416%
57	16.251	2402	2408	2413	rVB	50192	82928	4.80%	0.476%
58	16.809	2496	2503	2510	rBV2	41973	84534	4.89%	0.485%
59	16.898	2512	2518	2526	rVB2	23104	47594	2.75%	0.273%
60	17.345	2587	2594	2604	rBV2	18537	44834	2.59%	0.257%
61	17.474	2608	2616	2625	rBV3	36903	89360	5.17%	0.513%
62	18.250	2741	2748	2758	rVB5	17986	48294	2.79%	0.277%
63	19.192	2902	2908	2918	rVB6	14831	44426	2.57%	0.255%

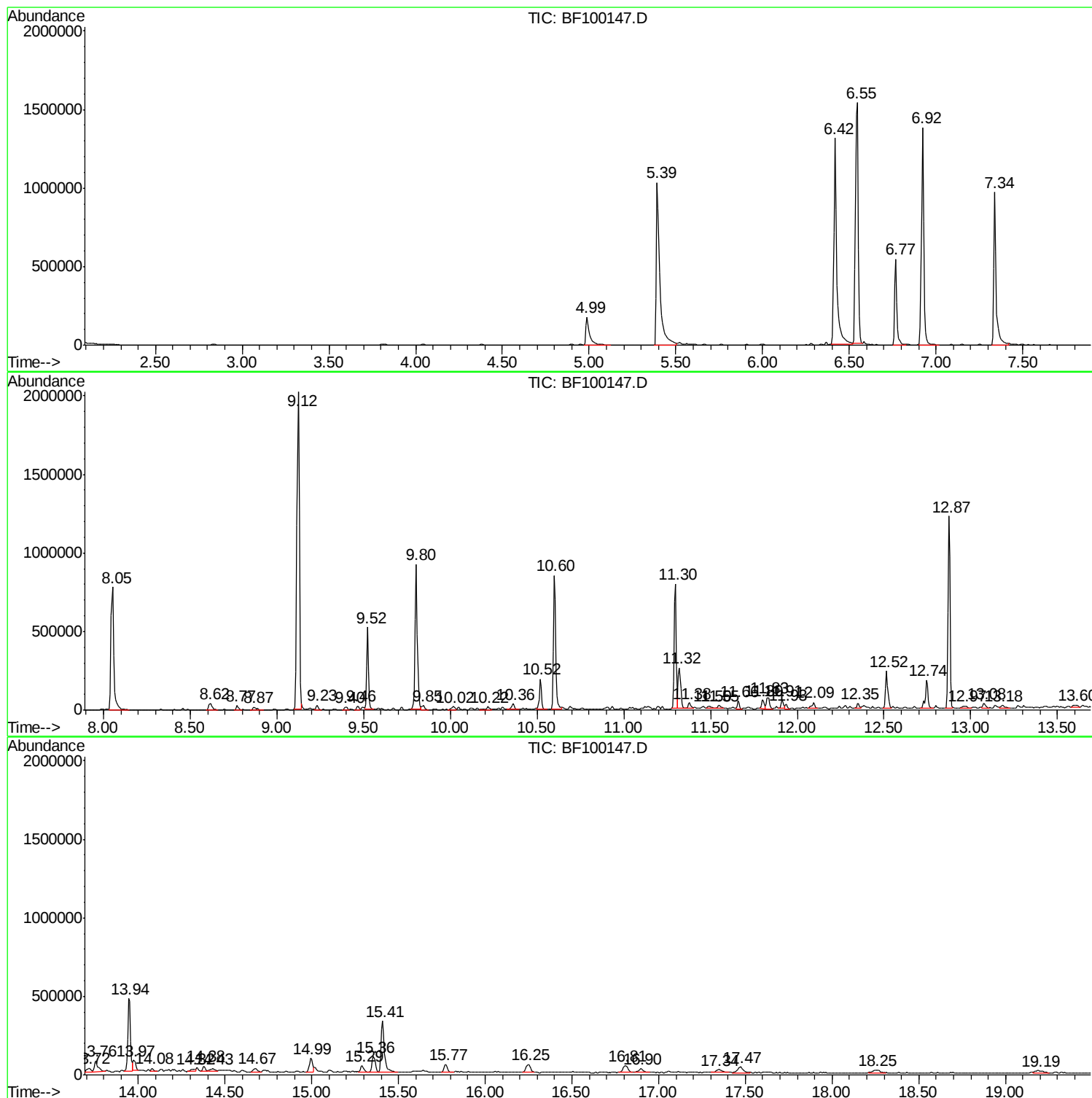
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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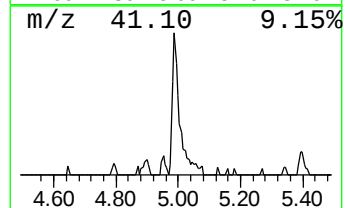
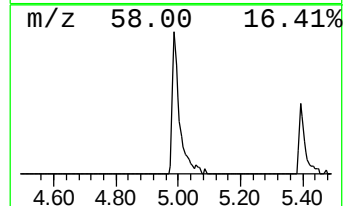
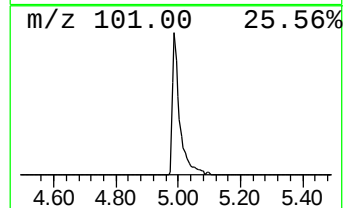
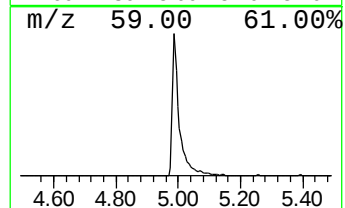
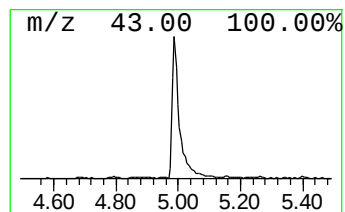
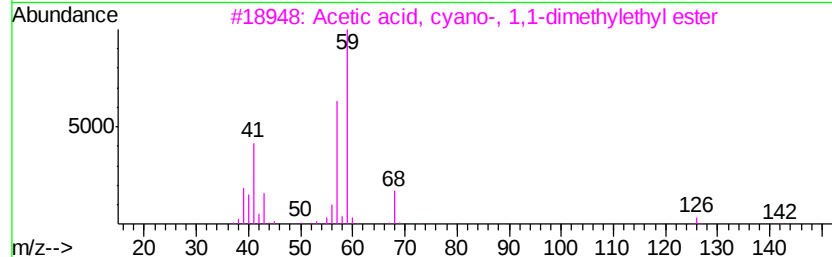
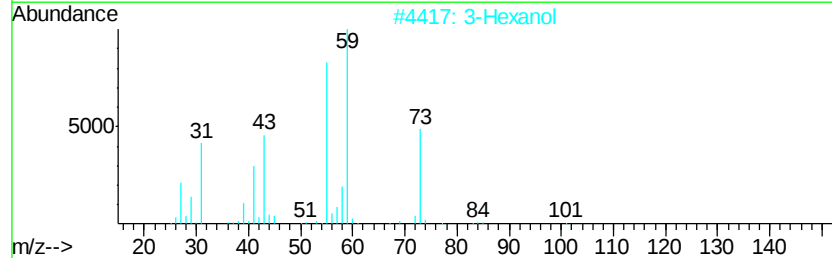
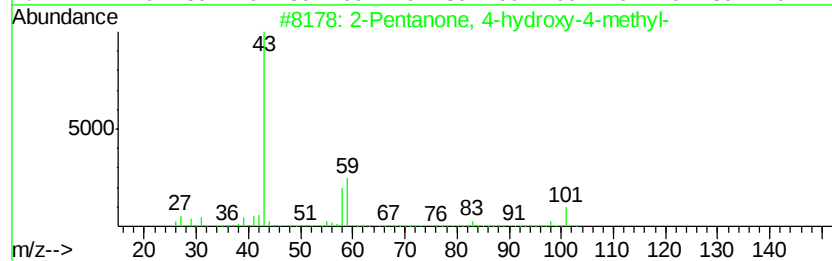
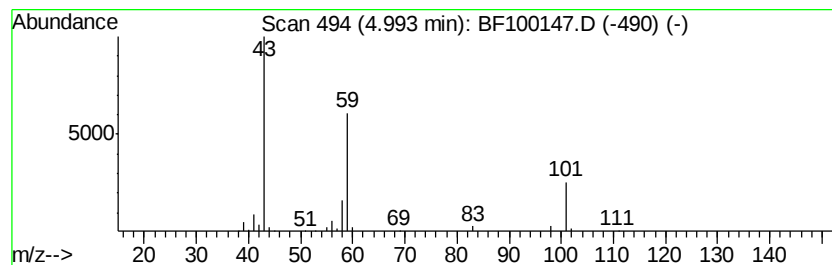
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	11.21 ng	288928	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol	102	C6H14O	000623-37-0	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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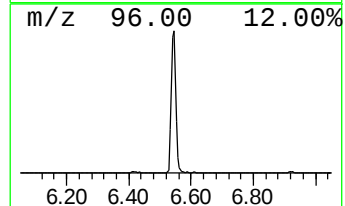
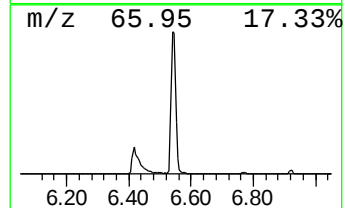
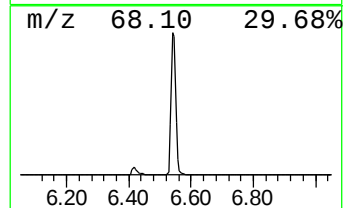
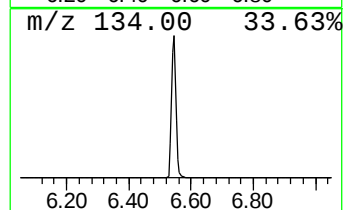
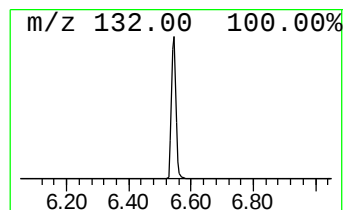
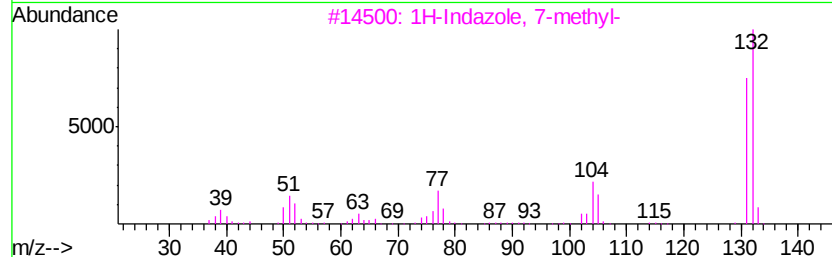
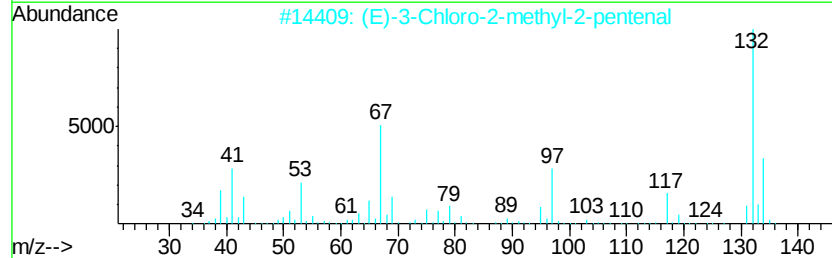
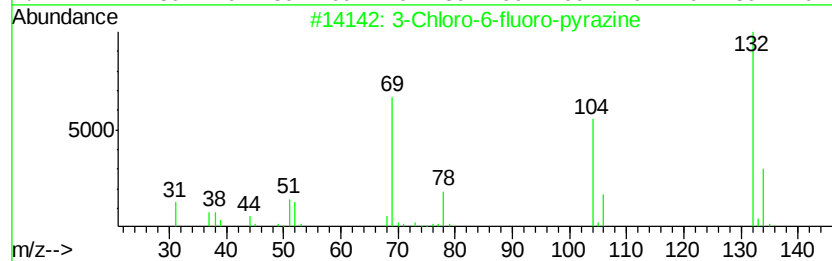
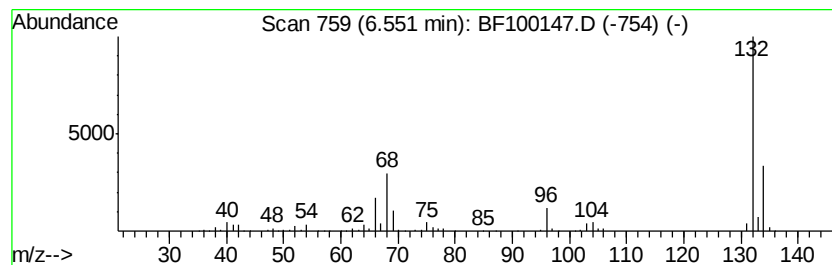
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	58.97 ng	1519290	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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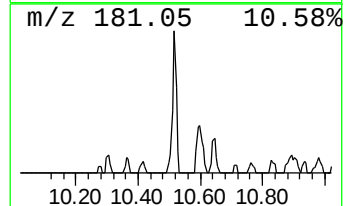
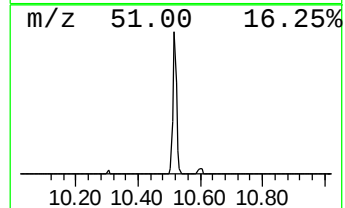
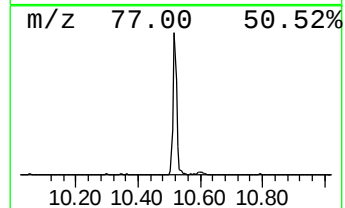
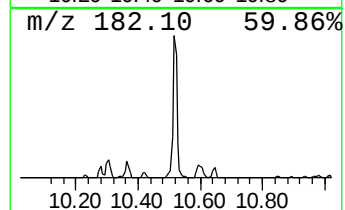
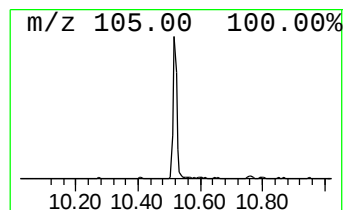
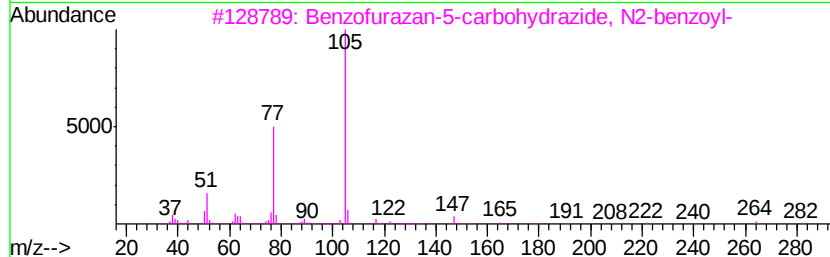
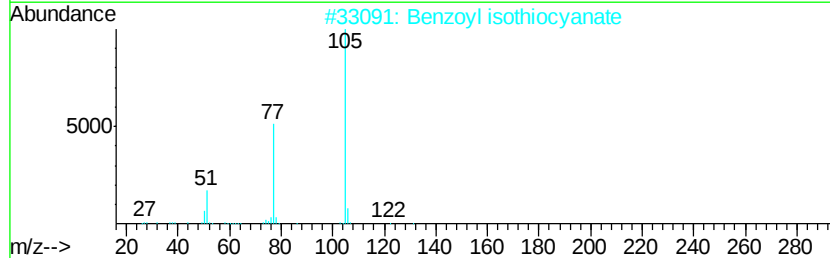
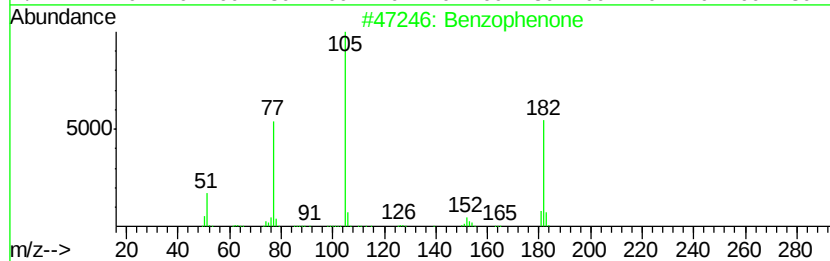
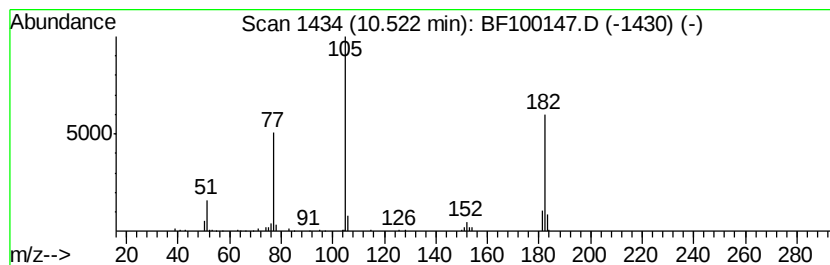
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	3.93 ng	158007	Acenaphthene-d10	9.80
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 96
2		Benzoyl isothiocyanate	163 C8H5NOS	000532-55-8 47
3		Benzofurazan-5-carbohydrazide, N...	282 C14H10N4O3	1000272-94-4 47
4		Vinyl benzoate	148 C9H8O2	000769-78-8 43
5		Cyclobutyl phenyl ketone	160 C11H12O	005407-98-7 43



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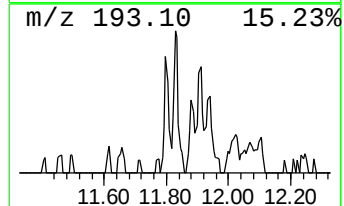
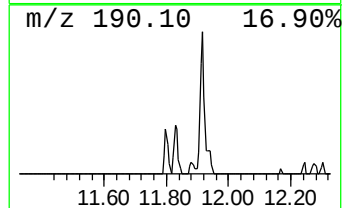
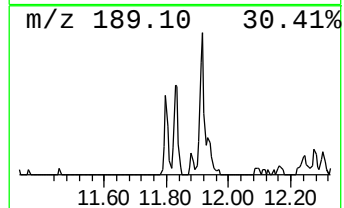
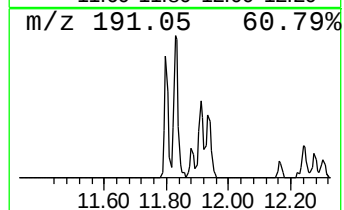
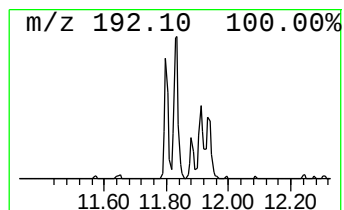
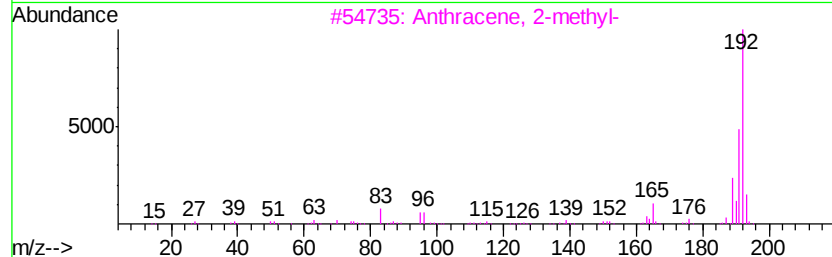
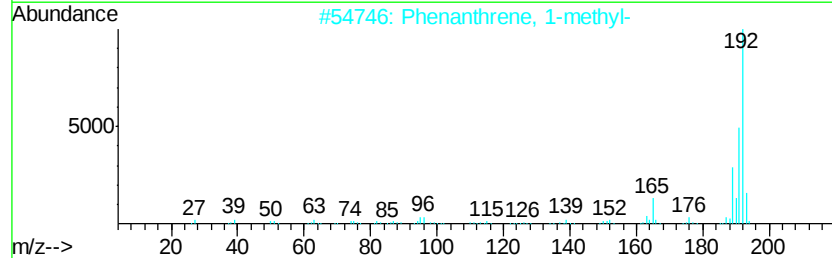
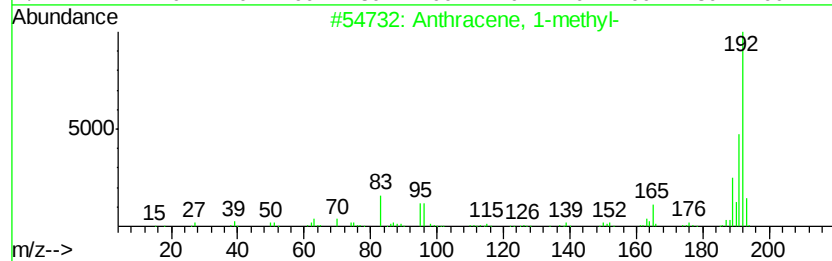
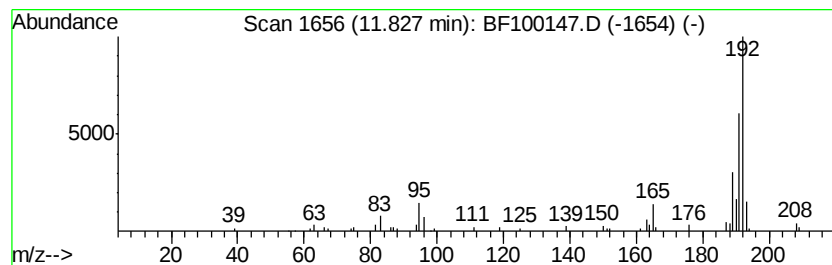
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Anthracene, 1-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.04 ng	72296	Phenanthrene-d10	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4		1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	93
5		Anthracene, 9-methyl-	192	C15H12	000779-02-2	91



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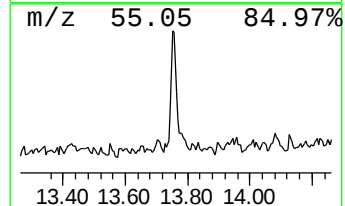
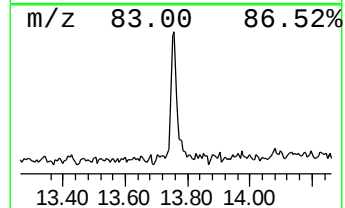
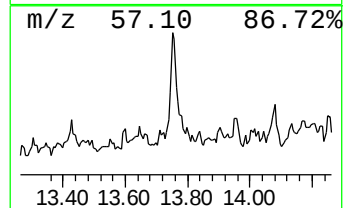
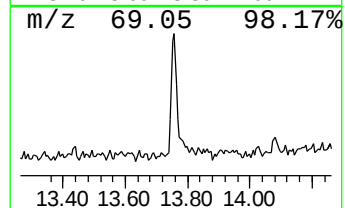
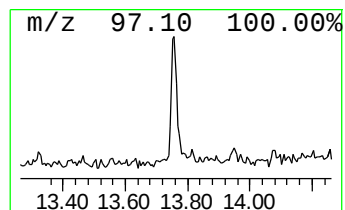
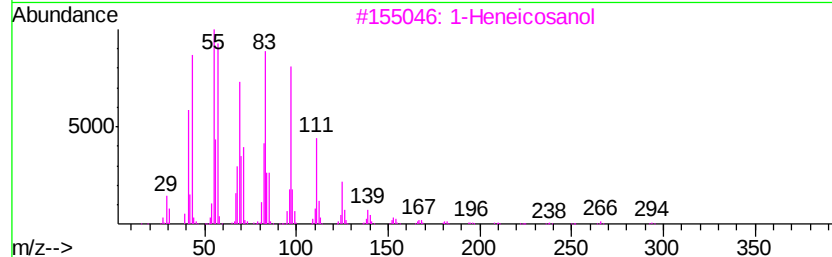
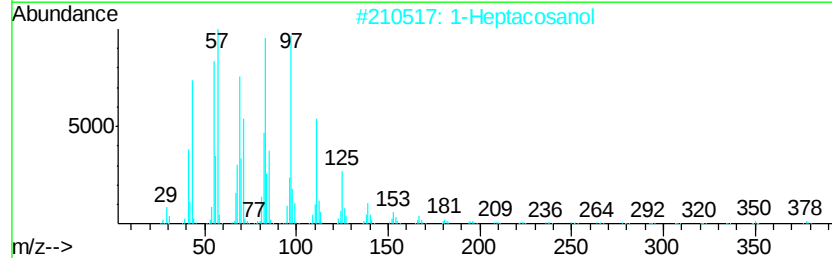
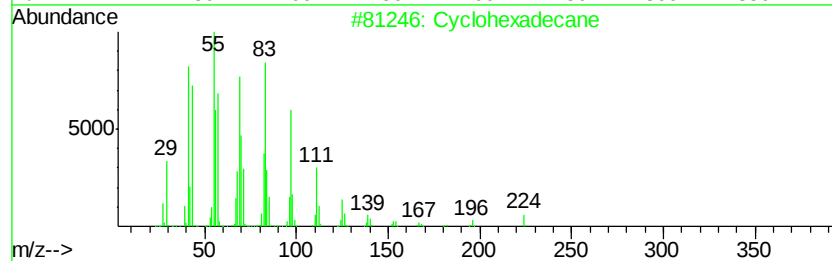
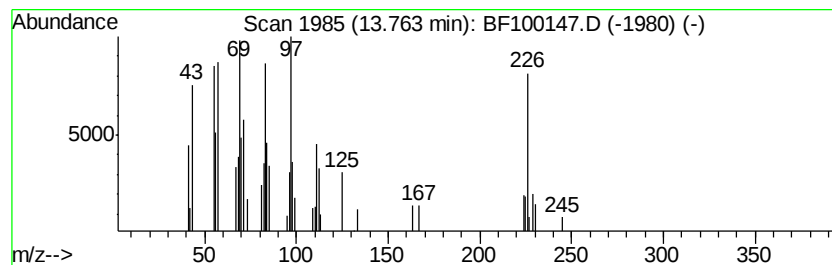
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ClientSampleId :
SB-4-FILL(3-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.86 ng	101935	Chrysene-d12	13.95
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 97
2		1-Heptacosanol	396 C27H56O	002004-39-9 91
3		1-Heneicosanol	312 C21H44O	015594-90-8 91
4		n-Tetracosanol-1	354 C24H50O	000506-51-4 91
5		Behenic alcohol	326 C22H46O	000661-19-8 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
Sample : I6079-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4-FILL(3-4)

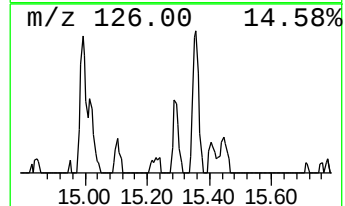
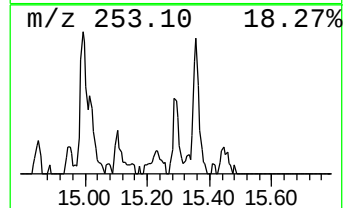
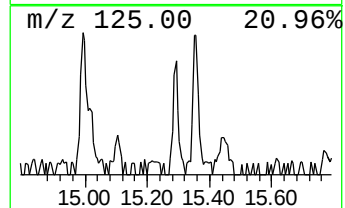
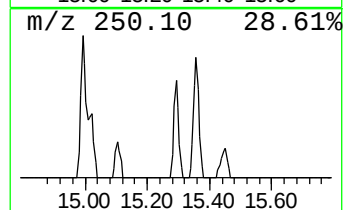
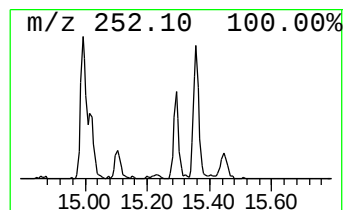
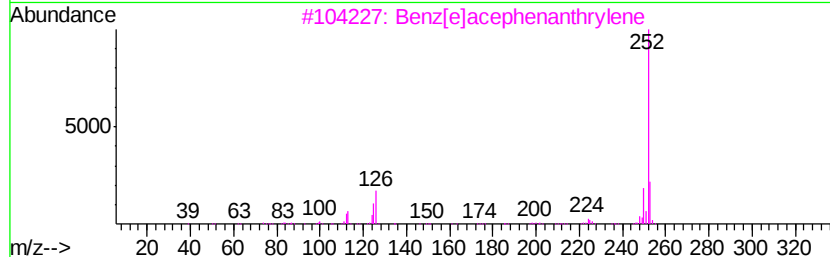
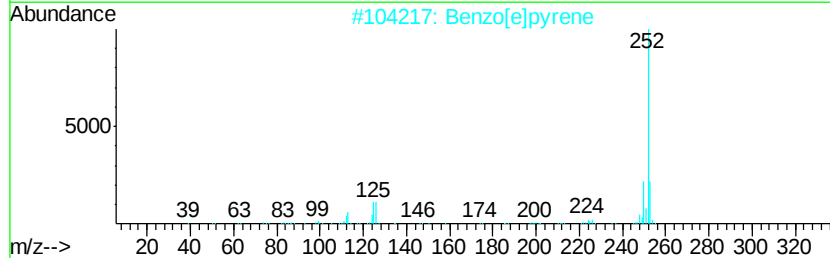
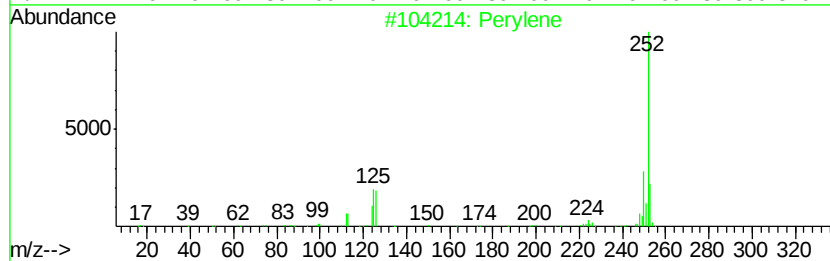
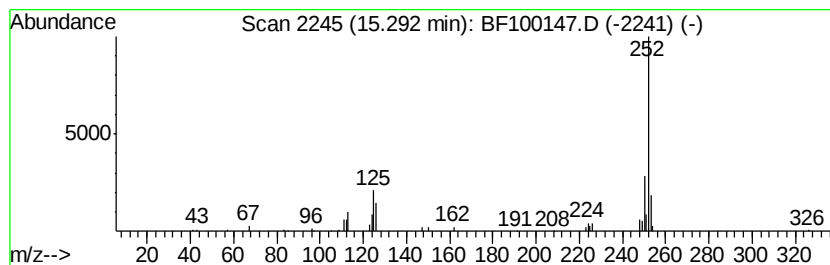
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.36 ng	51107	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	95
2		Benzo[e]pyrene	252	C20H12	000192-97-2	93
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
Sample : I6079-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4-FILL(3-4)

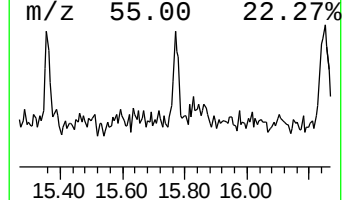
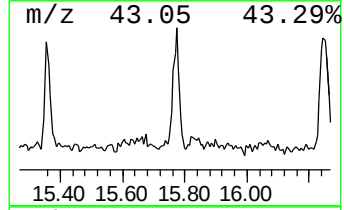
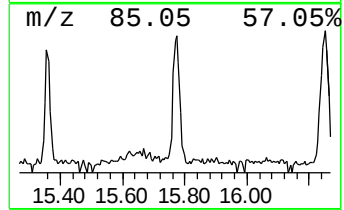
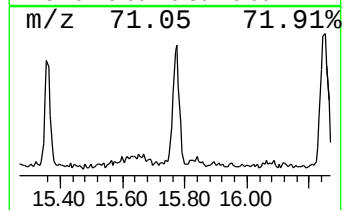
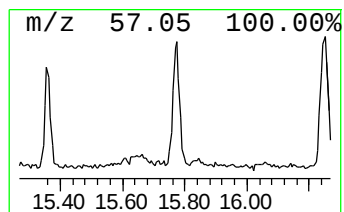
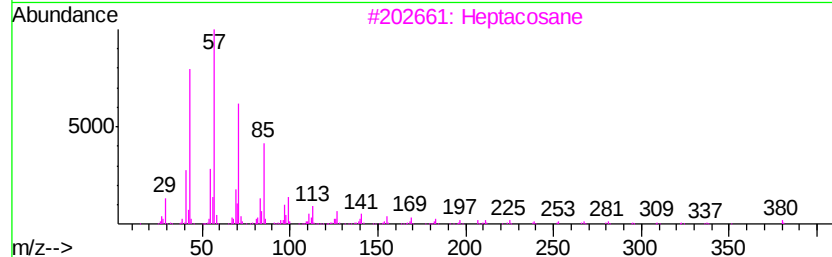
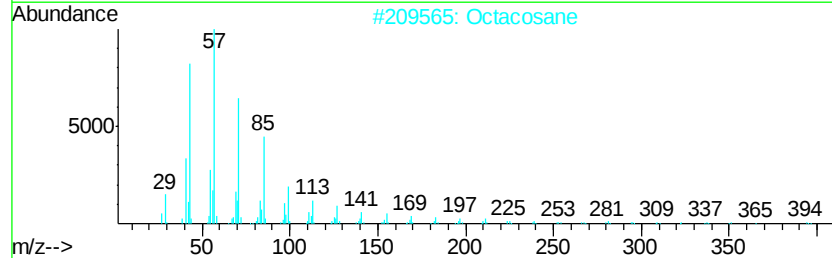
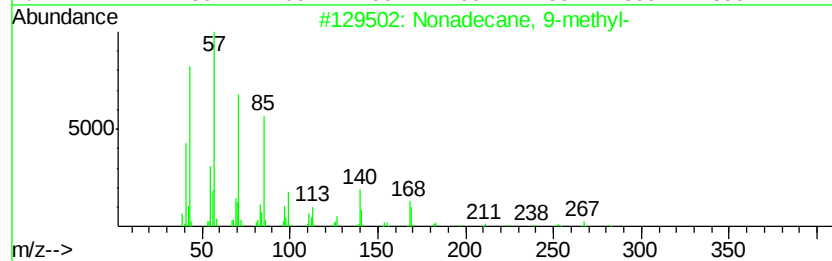
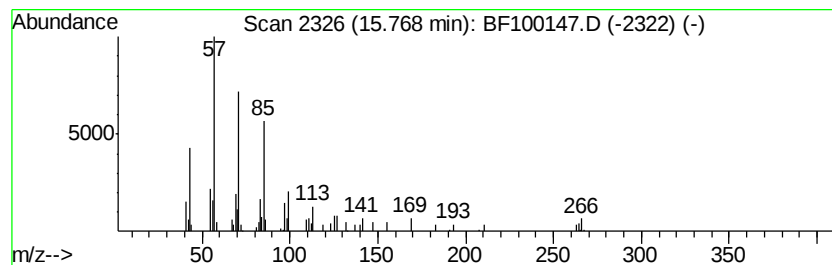
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	3.34 ng	72467	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	95
2		Octacosane	394	C28H58	000630-02-4	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Eicosane	282	C20H42	000112-95-8	91
5		Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
Sample : I6079-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4-FILL(3-4)

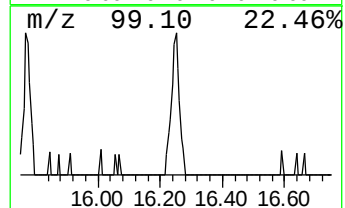
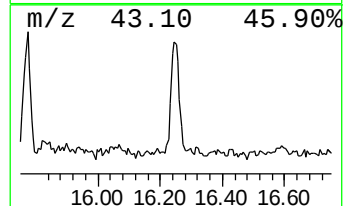
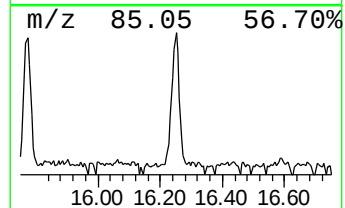
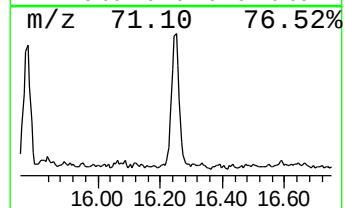
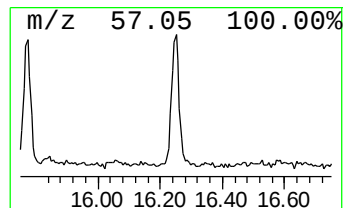
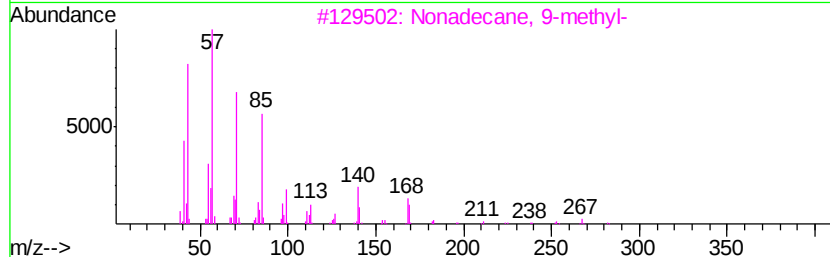
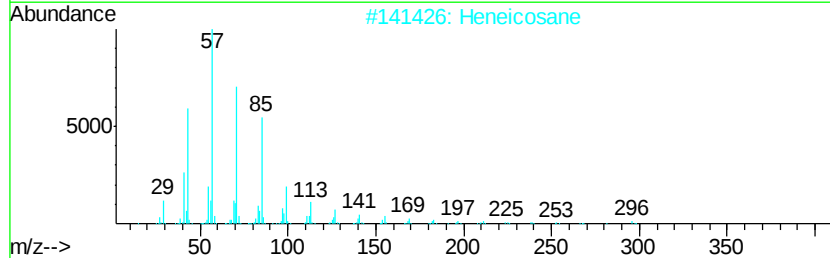
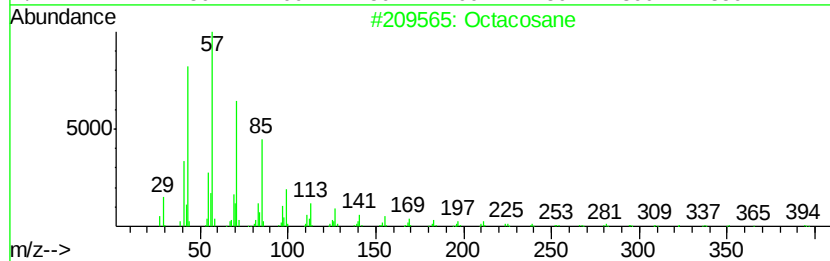
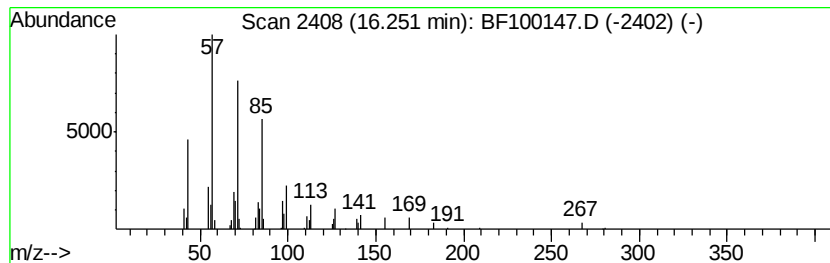
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.82 ng	82928	Perylene-d12	15.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Pentacosane		352	C25H52	000629-99-2	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
Sample : I6079-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4-FILL(3-4)

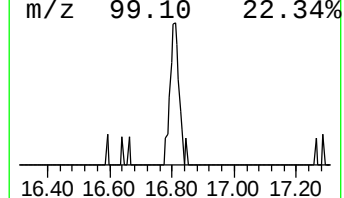
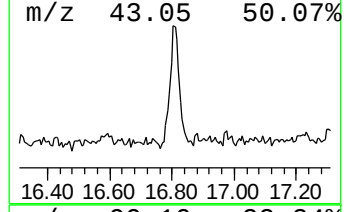
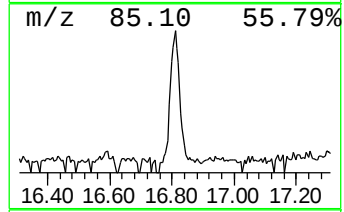
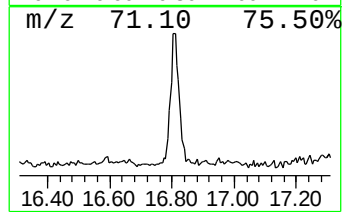
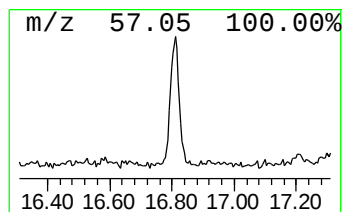
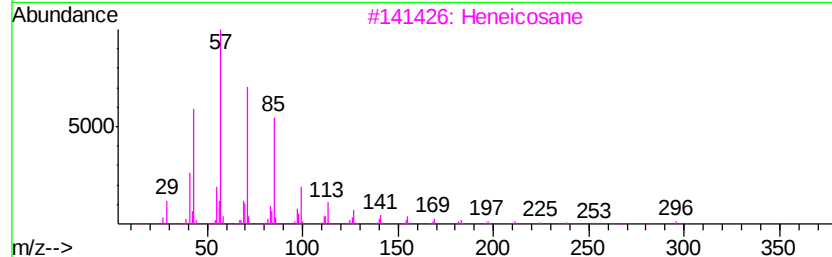
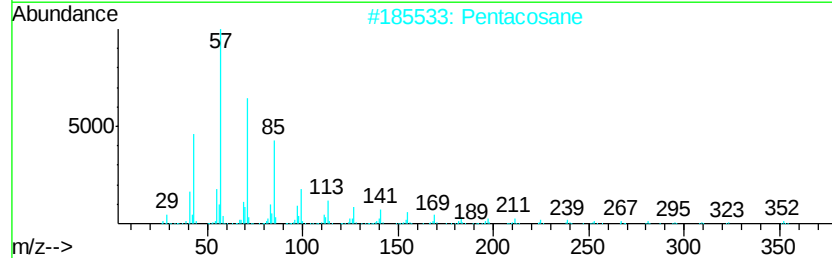
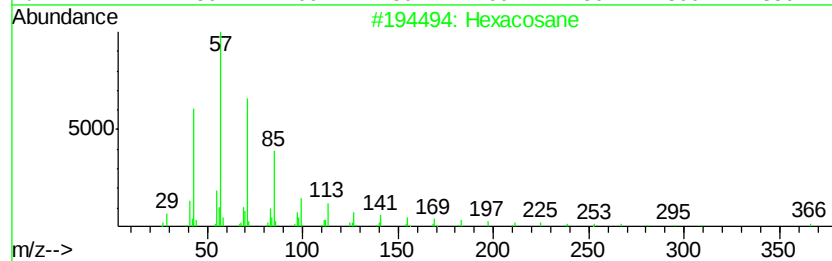
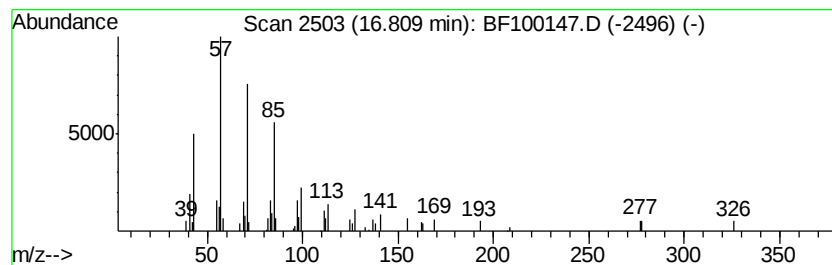
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	3.90 ng	84534	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Pentacosane	352	C25H52	000629-99-2	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Hentriacontane	437	C31H64	000630-04-6	87
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
Sample : I6079-02
Misc :
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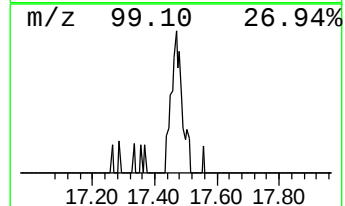
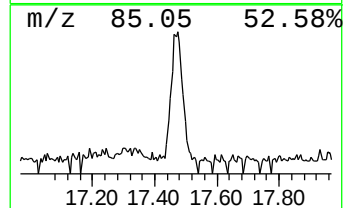
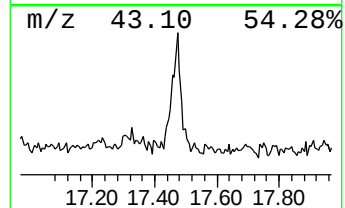
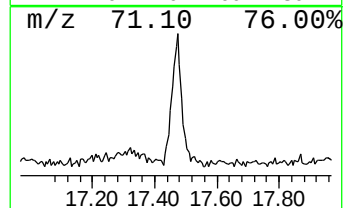
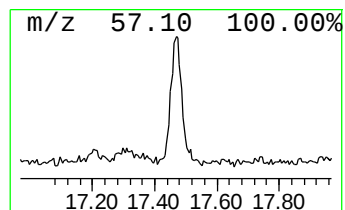
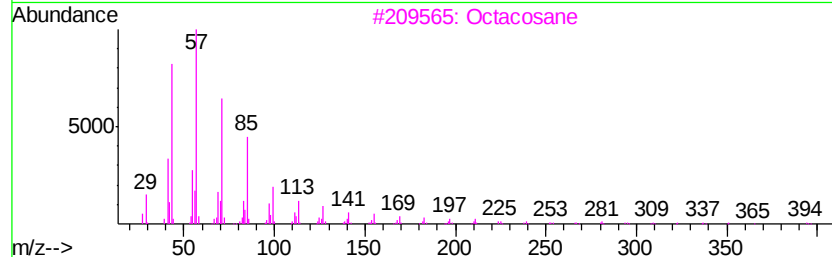
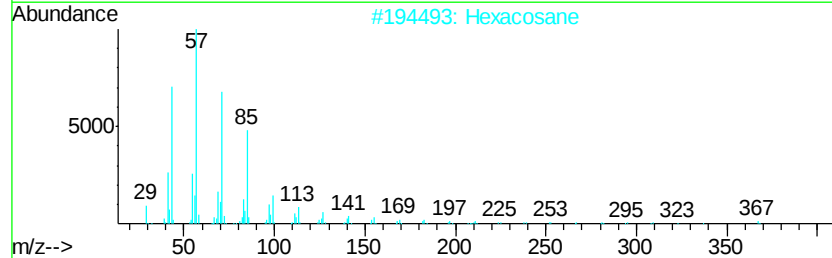
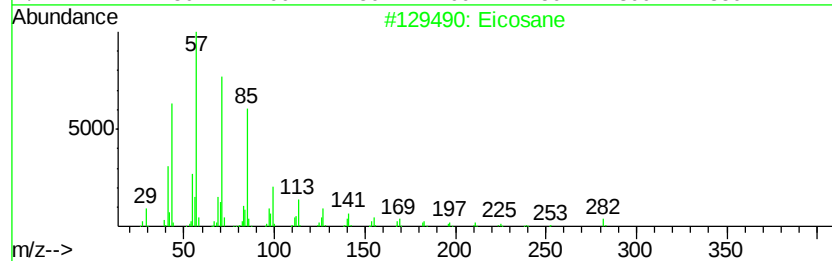
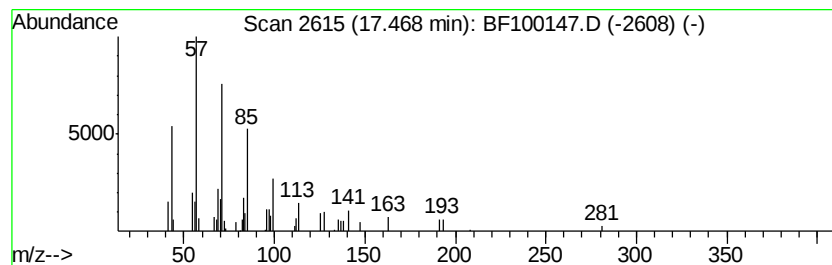
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SB-4-FILL(3-4)

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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 13 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	4.12 ng	89360	Perylene-d12	15.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	97
2	Hexacosane	366 C26H54	000630-01-3	91
3	Octacosane	394 C28H58	000630-02-4	91
4	Hentriacontane	437 C31H64	000630-04-6	91
5	Heptacosane	380 C27H56	000593-49-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
Data File : BF100147.D
Acq On : 3 Nov 2017 20:59
Operator : SJ/JU
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Misc :
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Instrument :
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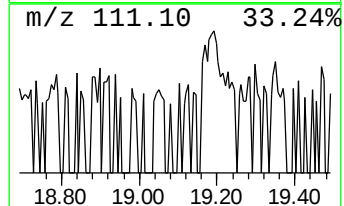
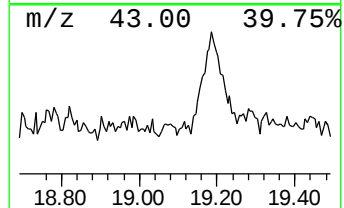
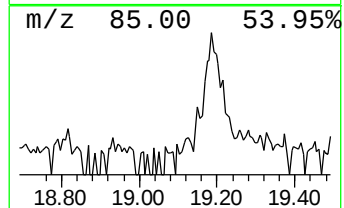
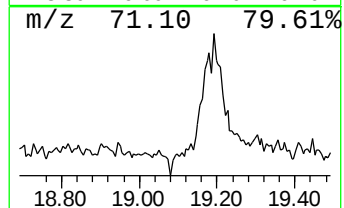
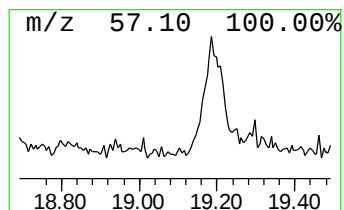
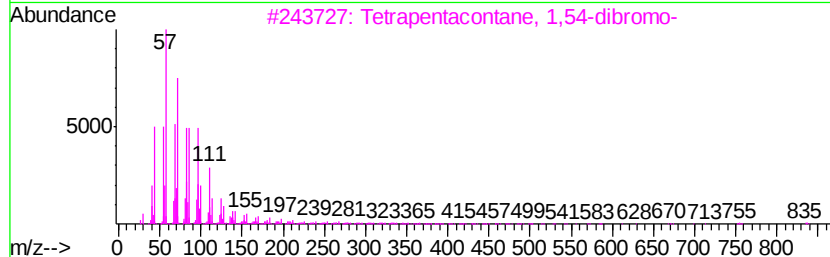
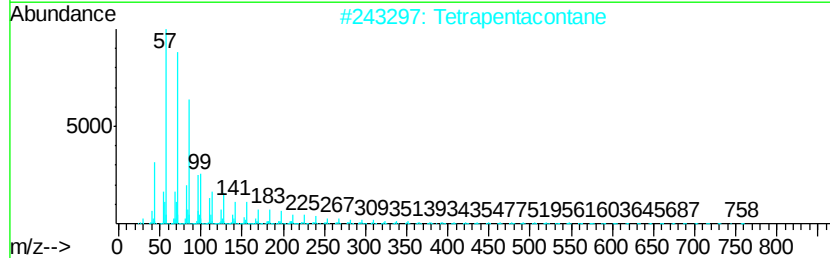
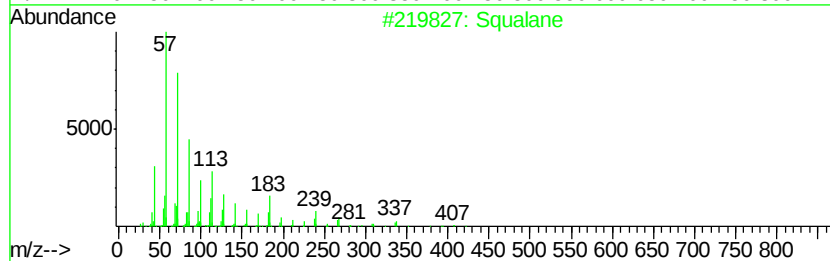
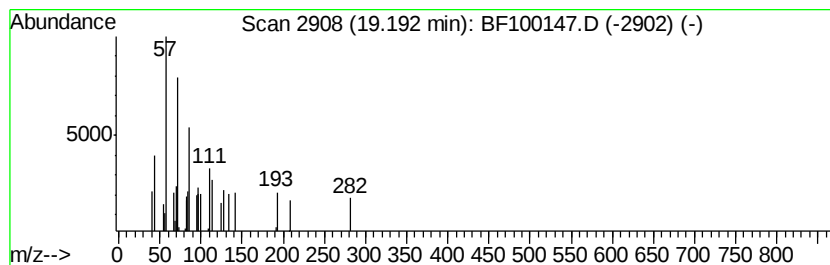
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Squalane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	2.05 ng	44426	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalane	422	C30H62	000111-01-3	50
2		Tetrapentacontane	759	C54H110	005856-66-6	50
3		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	50
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	47
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110317\
 Data File : BF100147.D
 Acq On : 3 Nov 2017 20:59
 Operator : SJ/JU
 Sample : I6079-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4-FILL(3-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	4.99	11.2	ng	288928	1	6.77	515304	20.0
unknown6.55	6.55	59.0	ng	1519290	1	6.77	515304	20.0
Benzophenone	10.52	3.9	ng	158007	3	9.80	803777	20.0
Anthracene, 1-met...	11.83	2.0	ng	72296	4	11.30	709191	20.0
Cyclohexadecane	13.76	3.9	ng	101935	5	13.95	528018	20.0
Perylene	15.29	2.4	ng	51107	6	15.41	433703	20.0
Nonadecane, 9-met...	15.77	3.3	ng	72467	6	15.41	433703	20.0
Octacosane	16.25	3.8	ng	82928	6	15.41	433703	20.0
Hexacosane	16.81	3.9	ng	84534	6	15.41	433703	20.0
Eicosane	17.47	4.1	ng	89360	6	15.41	433703	20.0
Squalane	19.19	2.0	ng	44426	6	15.41	433703	20.0