LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

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-BF061918.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	5.184	481	484	493	rBB	38238	37007	5.82%	0.426%
2	5.601	551	555	566	rBB	562376	502902	79.13%	5.792%
3	6.601	721	725	733	rBV	577132	507240	79.81%	5.842%
4	6.737	744	748	751	rBV	638306	515447	81.11%	5.937%
5	6.960	782	786	789	rBV	459407	347896	54.74%	4.007%
6	7.113	809	812	816	rBV	484704	409309	64.40%	4.714%
7	7.519	877	881	891	rBV	357454	298063	46.90%	3.433%
8	8.242	1000	1004	1021	rBV	517009	429721	67.62%	4.949%
9	9.313	1183	1186	1195	rVB	697190	561755	88.39%	6.470%
10	9.707	1250	1253	1260	rVB	58028	50027	7.87%	0.576%
11	9.866	1277	1280	1283	rBV	16037	14914	2.35%	0.172%
12	9.913	1285	1288	1293	rVB	11434	9774	1.54%	0.113%
13	10.001	1300	1303	1307	rBV	525536	437642	68.86%	5.041%
14	10.031	1307	1308	1311	rVB	12446	9096	1.43%	0.105%
15	10.413	1367	1373	1377	rVB3	16068	18542	2.92%	0.214%
16	10.548	1393	1396	1402	rVB2	20408	22308	3.51%	0.257%
17	10.631	1405	1410	1413	rVB3	7692	10464	1.65%	0.121%
18	10.795	1434	1438	1444	rBV	362184	328043	51.62%	3.778%
19	10.883	1451	1453	1458	rBV	14614	21654	3.41%	0.249%
20	11.101	1484	1490	1493	rBV2	10259	17719	2.79%	0.204%
21	11.336	1527	1530	1532	rBV2	12216	10646	1.68%	0.123%
22	11.389	1537	1539	1542	rVB	15523	11233	1.77%	0.129%
23	11.495	1553	1557	1559	rBV	582765	488526	76.87%	5.627%
24	11.519	1559	1561	1565	rVV	195348	155194	24.42%	1.787%
25	11.572	1567	1570	1572	rVV	36638	34173	5.38%	0.394%
26	11.607	1572	1576	1578	rVB3	10353	11374	1.79%	0.131%
27	11.725	1593	1596	1601	rBV	13746	16158	2.54%	0.186%
28	11.825	1611	1613	1616	rBV	17152	14251	2.24%	0.164%
29	11.907	1624	1627	1630	rVB	11326	11779	1.85%	0.136%
30	11.995	1639	1642	1644	rBV	58658	55771	8.78%	0.642%
31	12.025	1644	1647	1650	rVB	79391	66750	10.50%	0.769%
32	12.072	1652	1655	1658	rVV	22858	22265	3.50%	0.256%
33	12.107	1658	1661	1664	rVV2	81243	95605	15.04%	1.101%
34	12.130	1664	1665	1668	rVB	51976	31853	5.01%	0.367%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.172	1668	1672	1674	rBV4	13048	13849	2.18%	0.160%
36	12.230	1679	1682	1684	rVB2	17407	15591	2.45%	0.180%
37	12.266	1684	1688	1689	rBV3	9427	12539	1.97%	0.144%
38	12.289	1689	1692	1695	rBV	34633	32063	5.05%	0.369%
39	12.319	1695	1697	1703	rVB3	28266	29351	4.62%	0.338%
40	12.366	1703	1705	1708	rBV3	8613	9359	1.47%	0.108%
41	12.419	1712	1714	1716	rBV	17962	18809	2.96%	0.217%
42	12.472	1720	1723	1725	rBV	28142	20764	3.27%	0.239%
43	12.495	1725	1727	1730	rVB	20940	15878	2.50%	0.183%
44	12.548	1732	1736	1739	rBV	69194	88587	13.94%	1.020%
45	12.636	1748	1751	1754	rBV2	42496	53942	8.49%	0.621%
46	12.713	1760	1764	1767	rBV	359802	305607	48.09%	3.520%
47	12.748	1768	1770	1772	rVV2	22187	21436	3.37%	0.247%
48	12.772	1772	1774	1777	rVV3	21965	19163	3.02%	0.221%
49	12.807	1778	1780	1782	rVV	20135	15388	2.42%	0.177%
50	12.866	1787	1790	1792	rBV2	28589	27314	4.30%	0.315%
51	12.942	1797	1803	1808	rBV	385779	440563	69.32%	5.074%
52	12.995	1809	1812	1815	rVV	37353	39203	6.17%	0.452%
53	13.077	1822	1826	1829	rBV	779889	635528	100.00%	7.320%
54	13.154	1836	1839	1845	rBV4	38621	74812	11.77%	0.862%
55	13.336	1868	1870	1872	rVB	37644	28730	4.52%	0.331%
56	13.377	1874	1877	1879	rVB2	45587	45493	7.16%	0.524%
57	13.472	1890	1893	1895	rBV	39177	38188	6.01%	0.440%
58	13.501	1896	1898	1900	rVV	38760	30761	4.84%	0.354%
59	14.148	2003	2008	2010	rBV2	531868	605677	95.30%	6.976%
60	14.171	2010	2012	2019	rVB	152183	148194	23.32%	1.707%
61	15.689	2266	2270	2274	rVB	241882	320509	50.43%	3.691%

Sum of corrected areas: 8682399

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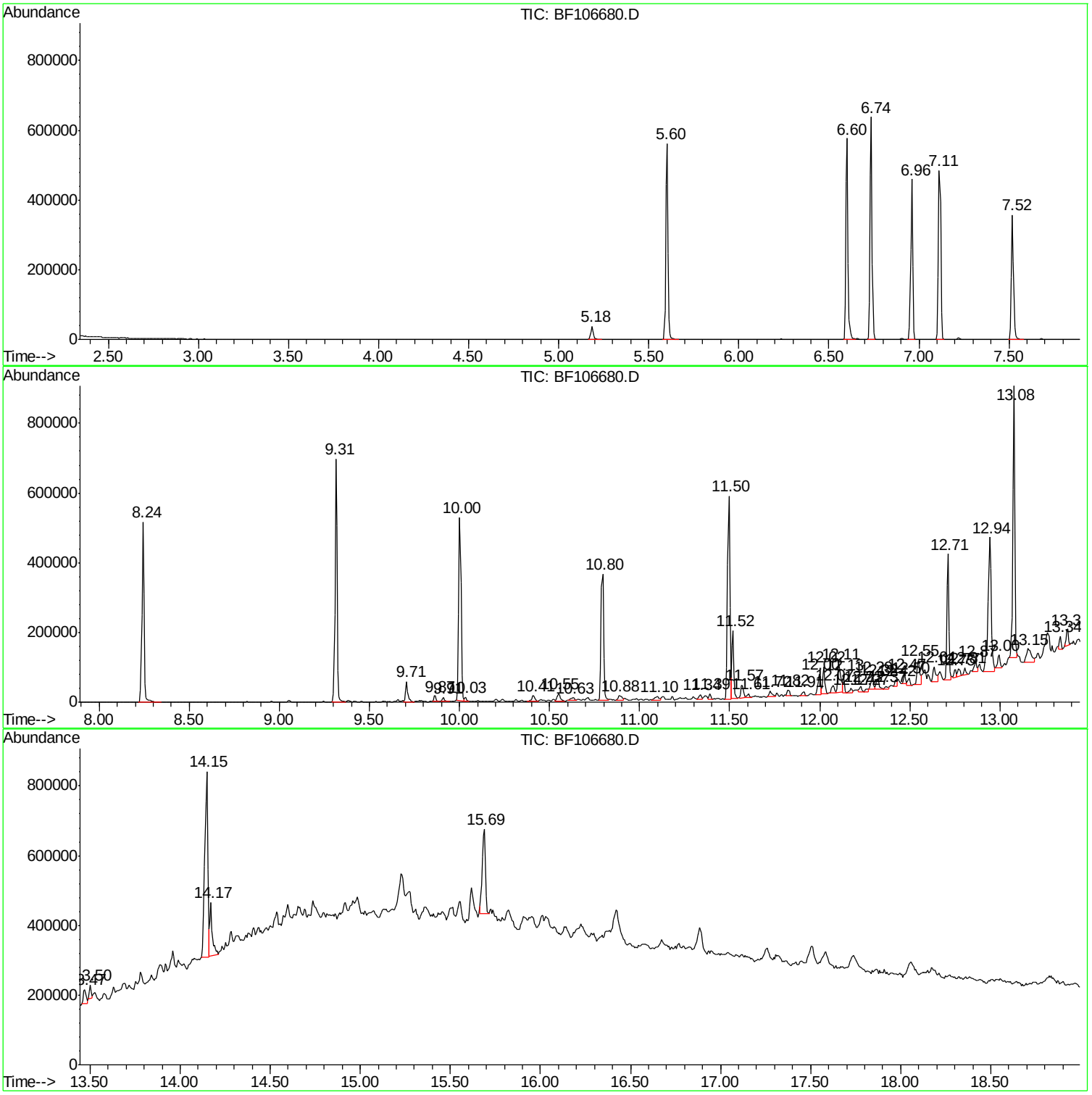
Instrument :
BNA_F
ClientSampleId :
CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

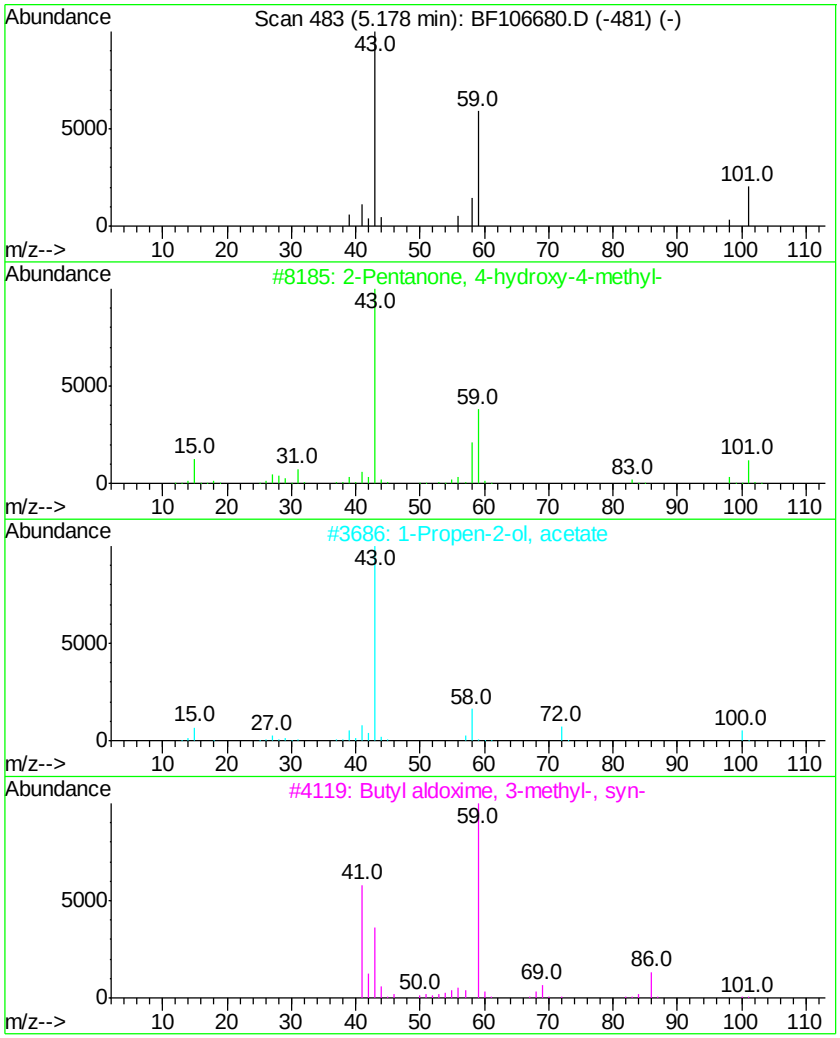
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

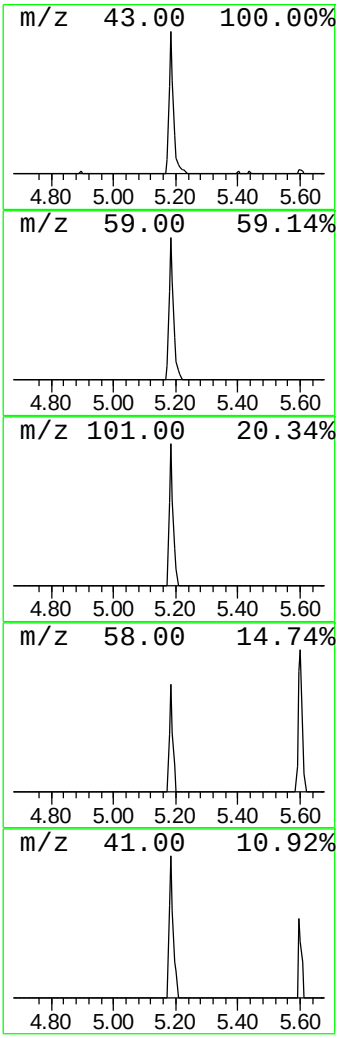
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.13 ng	37007	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

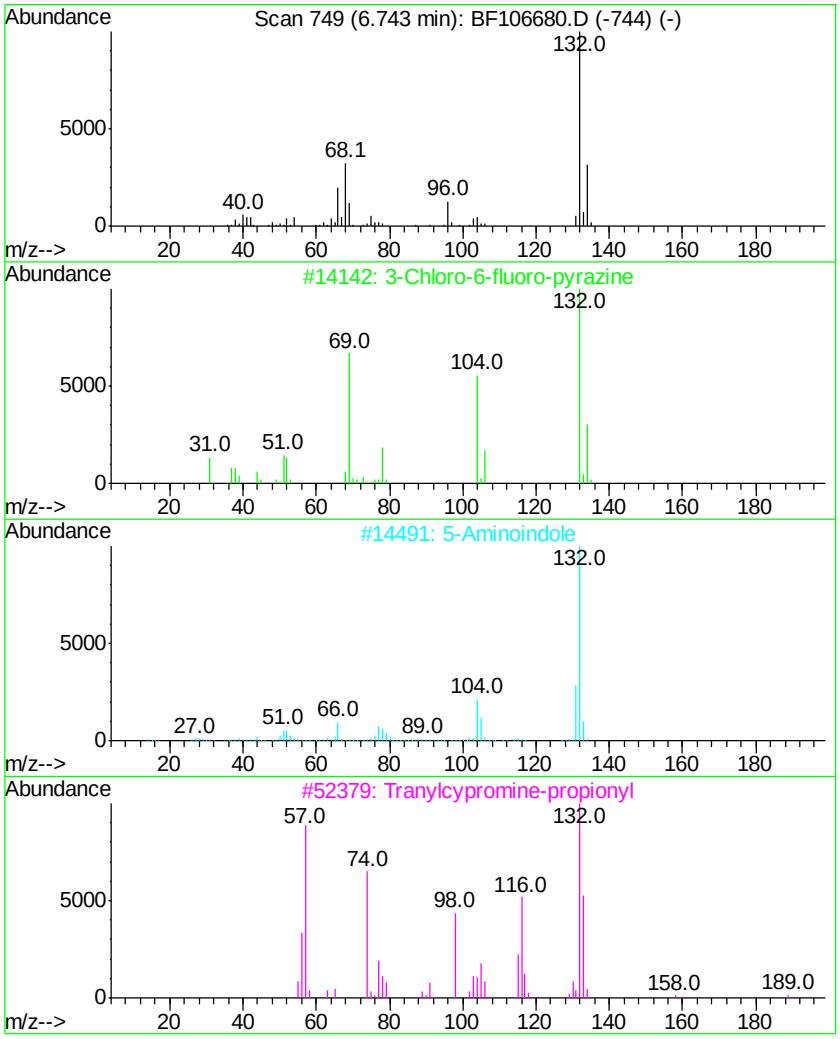
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

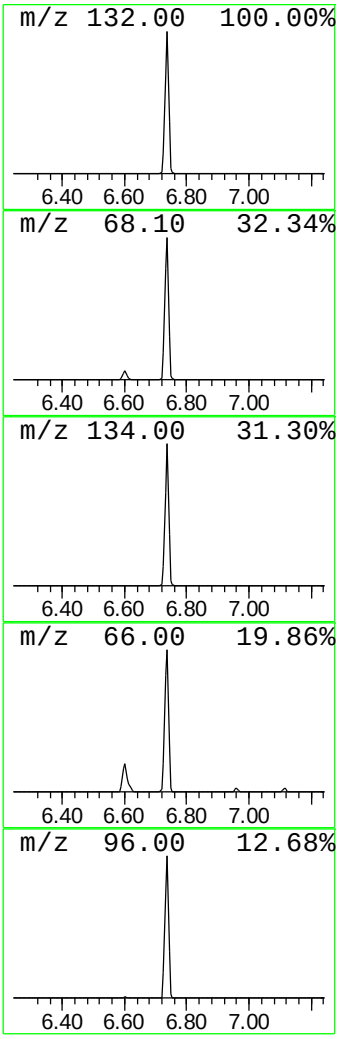
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	29.63 ng	515447	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

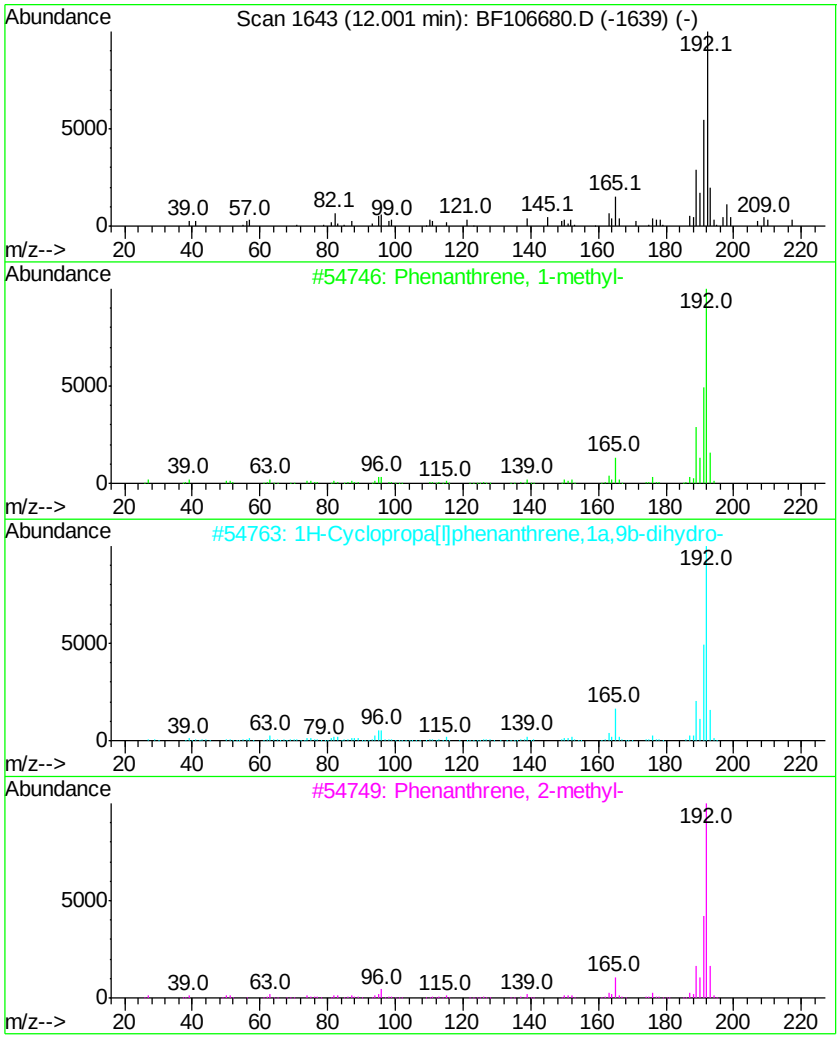
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

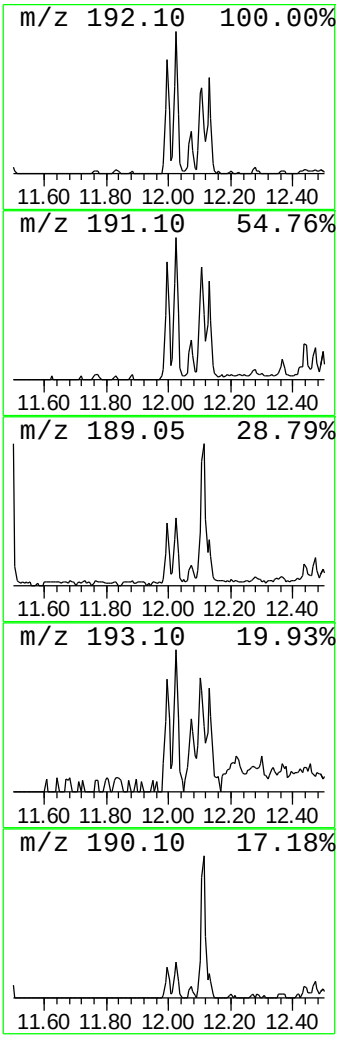
****

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	2.28 ng	55771	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

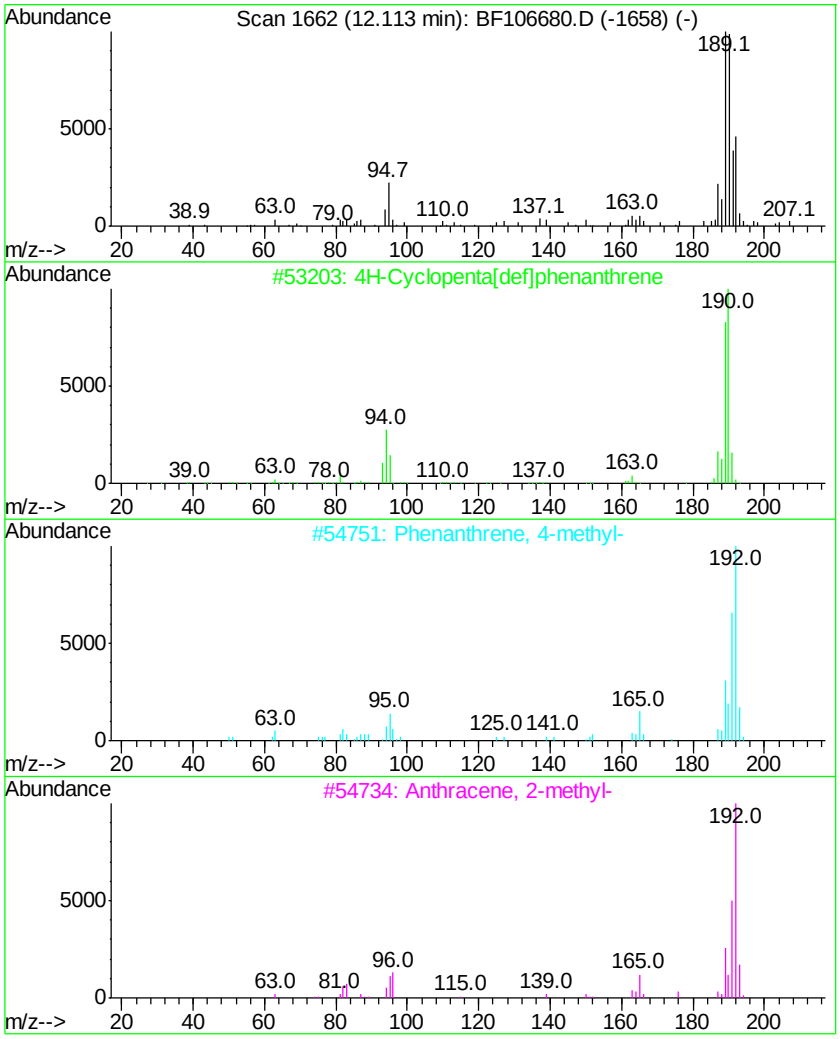
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

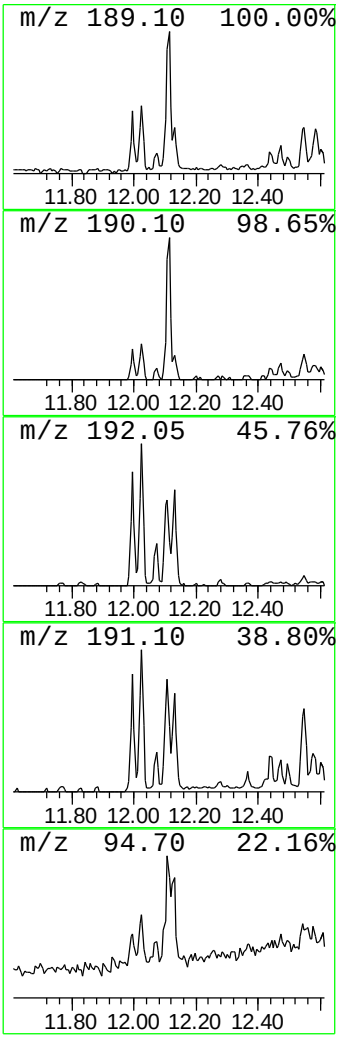
****

Peak Number 6 unknown12.11 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	3.91 ng	95605	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	46
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	45
5	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	43





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Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

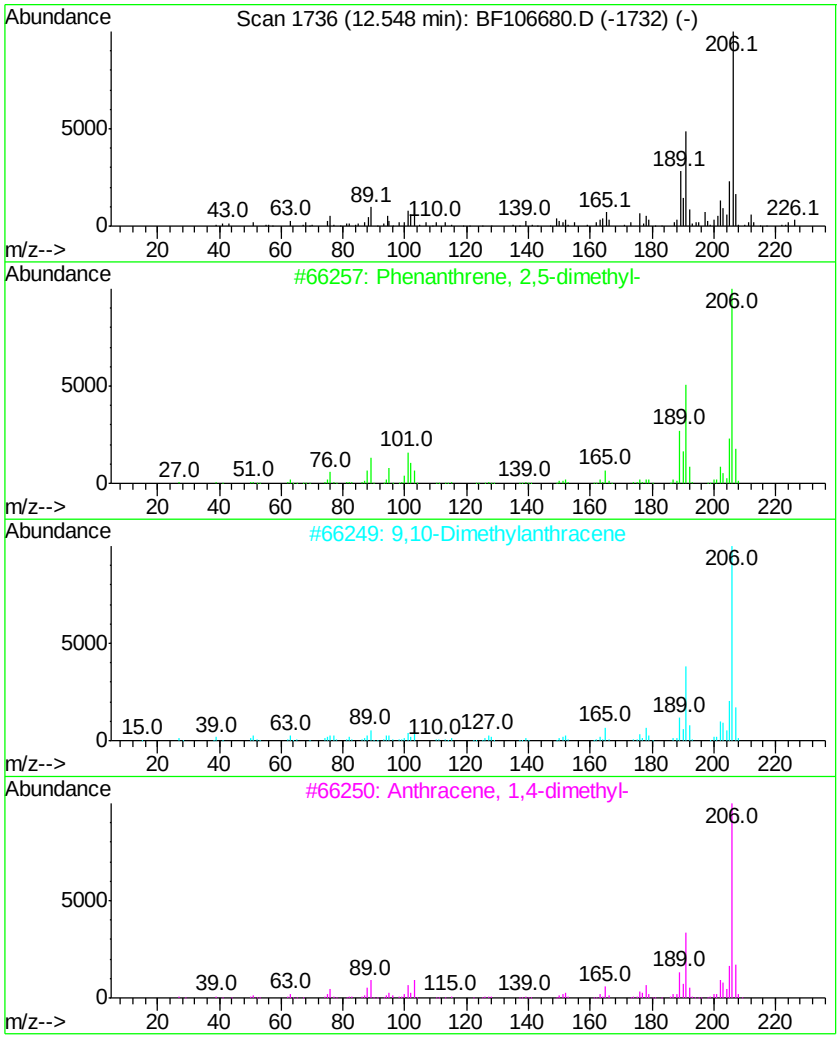
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

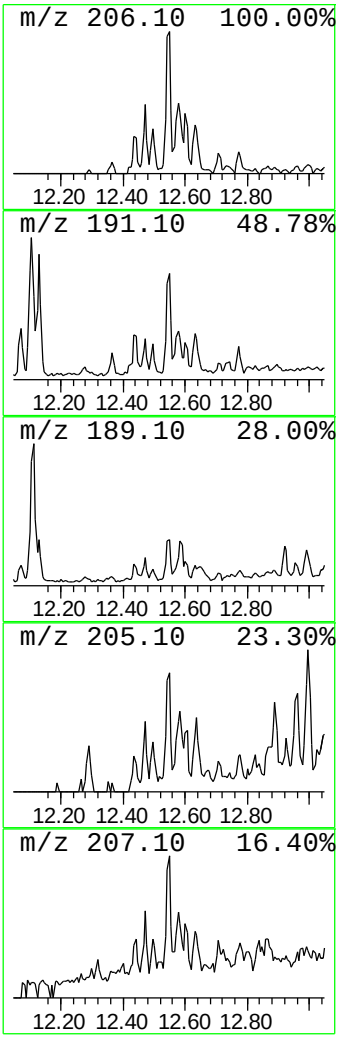
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	3.63 ng	88587	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	86
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	86
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	81





Library Search Compound Report

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Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
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Misc :
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Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

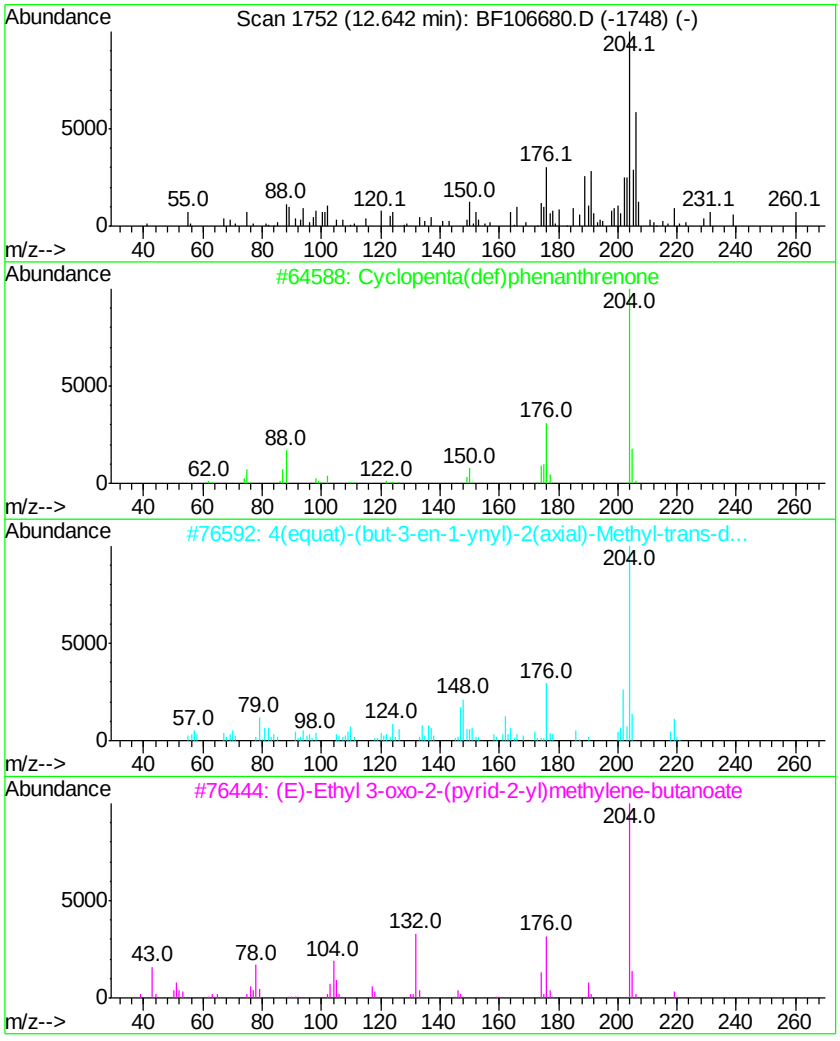
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

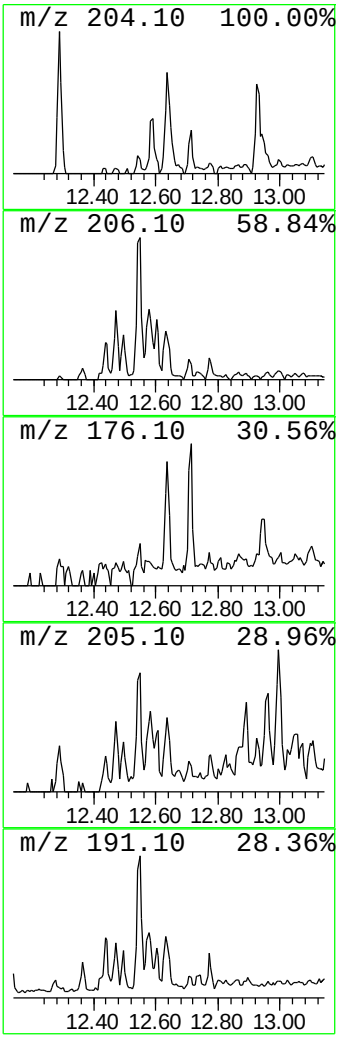
****

Peak Number 8 Cyclopenta(def)phenanthrenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.21 ng	53942	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	55
2	4(equat)-(but-3-en-1-ynyl)-2(axi...	219	C14H21NO	038423-22-2	53
3	(E)-Ethyl 3-oxo-2-(pyrid-2-yl)me...	219	C12H13NO3	1000147-59-7	46
4	3,4-Biphenyldicarbonitrile	204	C14H8N2	004128-63-6	46
5	9,10-Dimethylanthracene	206	C16H14	000781-43-1	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
Operator : JU/SJ
Sample : J3245-11 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

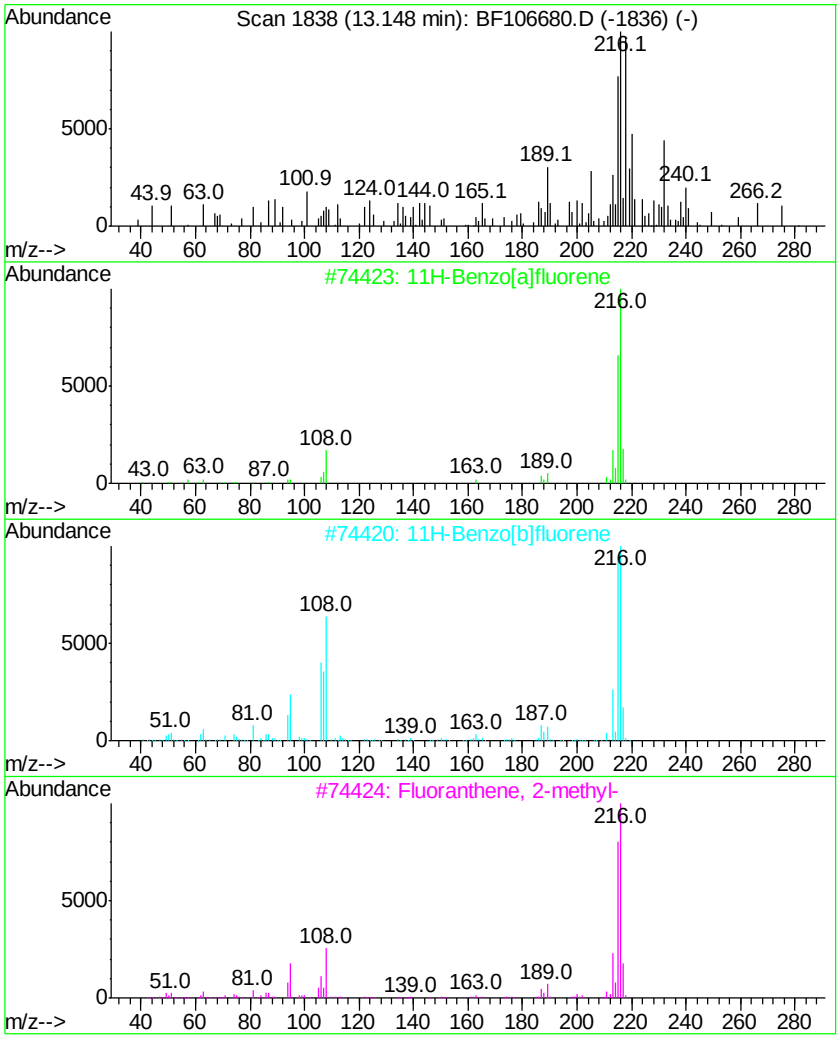
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

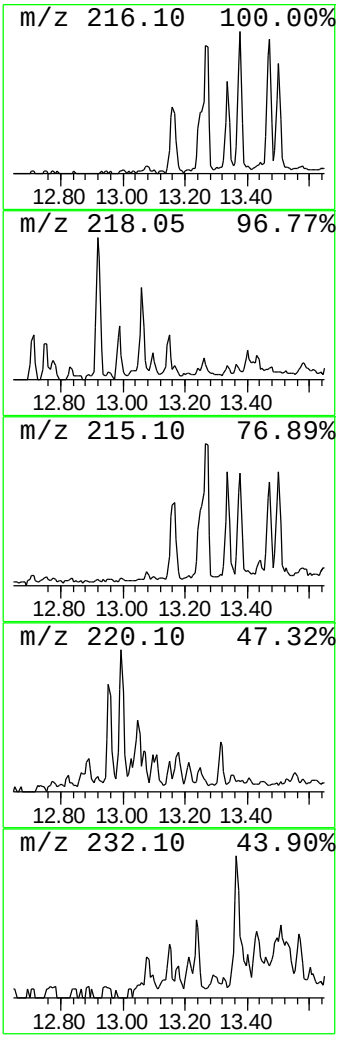
****

Peak Number 9 11H-Benzo[a]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.15	2.47 ng	74812	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	62
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	58
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	53
4	1,3,5-Triazine-2,4,6-triamine, N...	216	C10H12N6	046731-79-7	50
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062118\
Data File : BF106680.D
Acq On : 22 Jun 2018 00:02
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-061918-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	2.1	ng	37007	1	6.96	347896	20.0
unknown6.74	6.74	29.6	ng	515447	1	6.96	347896	20.0
Phenanthrene, 1-m...	12.00	2.3	ng	55771	4	11.50	488526	20.0
unknown12.11	12.11	3.9	ng	95605	4	11.50	488526	20.0
Phenanthrene, 2,5...	12.55	3.6	ng	88587	4	11.50	488526	20.0
Cyclopenta(def)ph...	12.64	2.2	ng	53942	4	11.50	488526	20.0
11H-Benzo[a]fluorene	13.15	2.5	ng	74812	5	14.15	605677	20.0