LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

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-BF083018.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	5.225	488	491	499	rVB2	4975	8657	1.13%	0.109%
2	5.684	559	569	570	rBV4	6401	15064	1.96%	0.190%
3	6.660	729	735	737	rBV3	20050	36270	4.72%	0.457%
4	6.778	750	755	782	rVB	50523	205876	26.79%	2.594%
5	6.995	788	792	811	rBV	115468	307537	40.02%	3.875%
6	7.148	814	818	832	rVB	97184	182605	23.76%	2.301%
7	7.589	884	893	896	rBV3	17377	47724	6.21%	0.601%
8	8.272	1006	1009	1025	rBV	214122	426298	55.48%	5.372%
9	8.836	1102	1105	1110	rBV2	11980	12438	1.62%	0.157%
10	9.342	1188	1191	1199	rBV	182416	268729	34.97%	3.386%
11	9.401	1199	1201	1206	rVB2	22113	29518	3.84%	0.372%
12	9.736	1251	1258	1264	rBV	48454	66483	8.65%	0.838%
13	9.895	1281	1285	1288	rBV3	8572	11065	1.44%	0.139%
14	9.930	1288	1291	1296	rVB2	15036	15119	1.97%	0.191%
15	10.030	1305	1308	1312	rBV2	480807	505731	65.81%	6.373%
16	10.436	1373	1377	1381	rBV	19911	18364	2.39%	0.231%
17	10.589	1399	1403	1407	rBV2	14321	20965	2.73%	0.264%
18	10.648	1411	1413	1416	rVB2	8206	9377	1.22%	0.118%
19	10.783	1433	1436	1439	rVB5	9089	7991	1.04%	0.101%
20	10.830	1441	1444	1455	rVV	86070	173317	22.55%	2.184%
21	10.913	1455	1458	1468	rVB3	23562	44980	5.85%	0.567%
22	11.136	1488	1496	1498	rBV5	8180	13201	1.72%	0.166%
23	11.360	1530	1534	1537	rBV3	15299	18211	2.37%	0.229%
24	11.383	1537	1538	1541	rVB2	14588	10812	1.41%	0.136%
25	11.430	1543	1546	1555	rVB2	11830	24790	3.23%	0.312%
26	11.530	1559	1563	1565	rBV	445399	481388	62.64%	6.066%
27	11.554	1565	1567	1574	rVV	305100	445685	58.00%	5.616%
28	11.613	1574	1577	1584	rVB	51186	97334	12.67%	1.227%
29	11.789	1602	1607	1611	rBV7	23017	37977	4.94%	0.479%
30	12.036	1645	1649	1651	rBV	40000	53081	6.91%	0.669%
31	12.065	1651	1654	1660	rVB	36335	56163	7.31%	0.708%
32	12.113	1660	1662	1664	rBV3	9639	8688	1.13%	0.109%
33	12.148	1664	1668	1670	rBV2	53521	67161	8.74%	0.846%
34	12.330	1695	1699	1704	rBV	18571	34964	4.55%	0.441%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

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-BF083018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.477	1721	1724	1727	rBV2	10173	10858	1.41%	0.137%
36	12.530	1731	1733	1738	rVB5	10652	13368	1.74%	0.168%
37	12.583	1738	1742	1744	rBV	49094	53954	7.02%	0.680%
38	12.683	1755	1759	1767	rVB5	21385	44819	5.83%	0.565%
39	12.748	1767	1770	1780	rBV	425845	607109	79.00%	7.651%
40	12.907	1793	1797	1799	rBV4	19988	22978	2.99%	0.290%
41	12.983	1803	1810	1823	rBV	433125	731516	95.19%	9.218%
42	13.112	1828	1832	1842	rVV	366833	499183	64.96%	6.291%
43	13.195	1842	1846	1853	rVB3	35424	71822	9.35%	0.905%
44	13.289	1859	1862	1863	rBV3	23564	24456	3.18%	0.308%
45	13.312	1863	1866	1871	rVB	56593	60888	7.92%	0.767%
46	13.383	1874	1878	1881	rBV2	29299	47221	6.14%	0.595%
47	13.412	1881	1883	1885	rBV2	25484	24130	3.14%	0.304%
48	13.507	1896	1899	1902	rBV	23829	33336	4.34%	0.420%
49	13.542	1902	1905	1909	rVV2	25663	32988	4.29%	0.416%
50	13.654	1922	1924	1926	rBV2	22998	20462	2.66%	0.258%
51	13.936	1970	1972	1974	rBV2	24205	29419	3.83%	0.371%
52	13.983	1978	1980	1983	rVV3	25083	27904	3.63%	0.352%
53	14.124	2001	2004	2007	rVB2	53671	46996	6.12%	0.592%
54	14.183	2009	2014	2018	rBV2	484900	768450	100.00%	9.684%
55	14.295	2030	2033	2038	rBV3	49846	65278	8.49%	0.823%
56	15.283	2196	2201	2214	rVB2	127091	353228	45.97%	4.451%
57	15.606	2253	2256	2263	rVB	46637	64300	8.37%	0.810%
58	15.677	2265	2268	2274	rVV2	78899	156714	20.39%	1.975%
59	15.742	2274	2279	2291	rVB	194690	360492	46.91%	4.543%

Sum of corrected areas: 7935432

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
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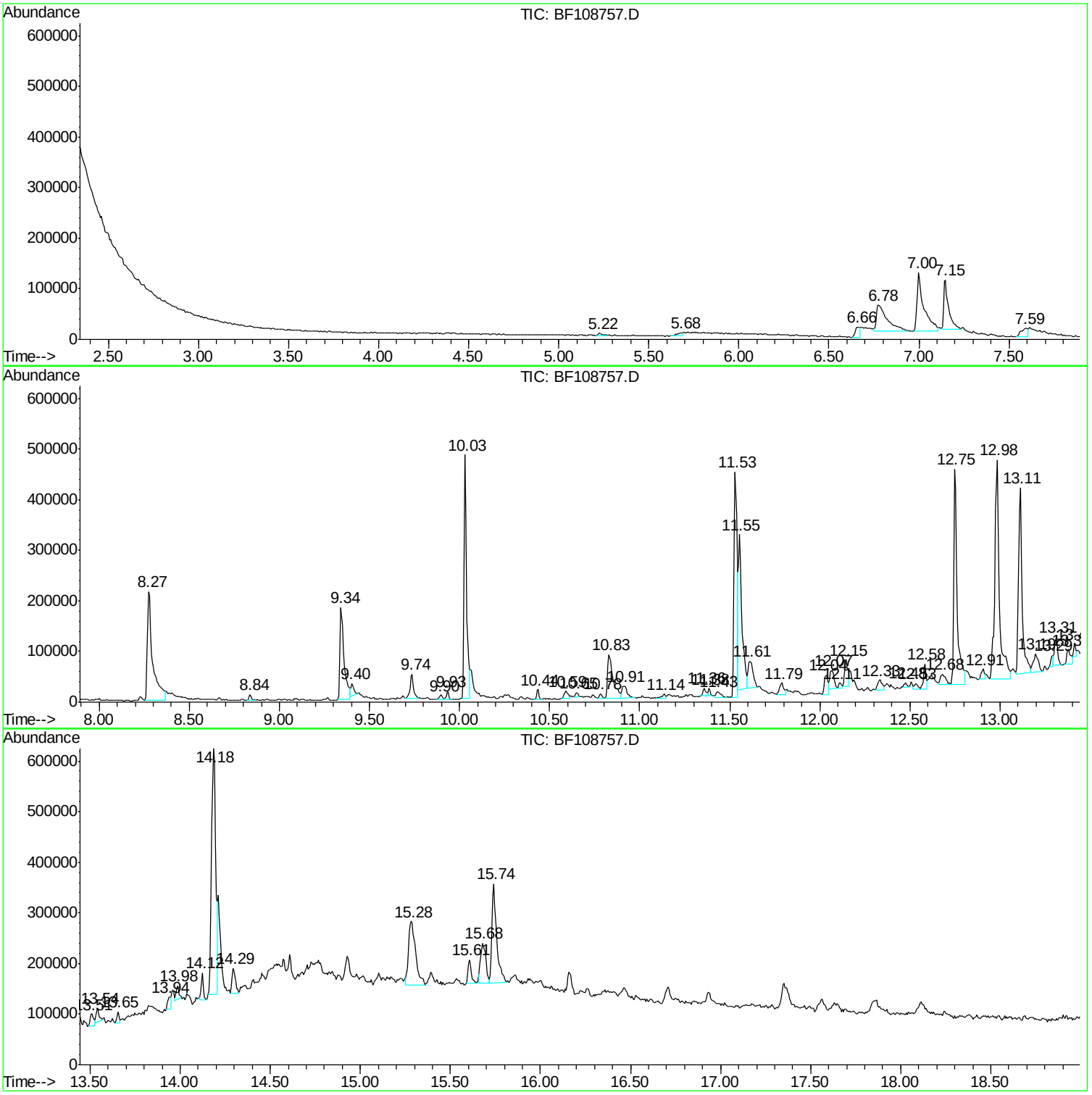
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

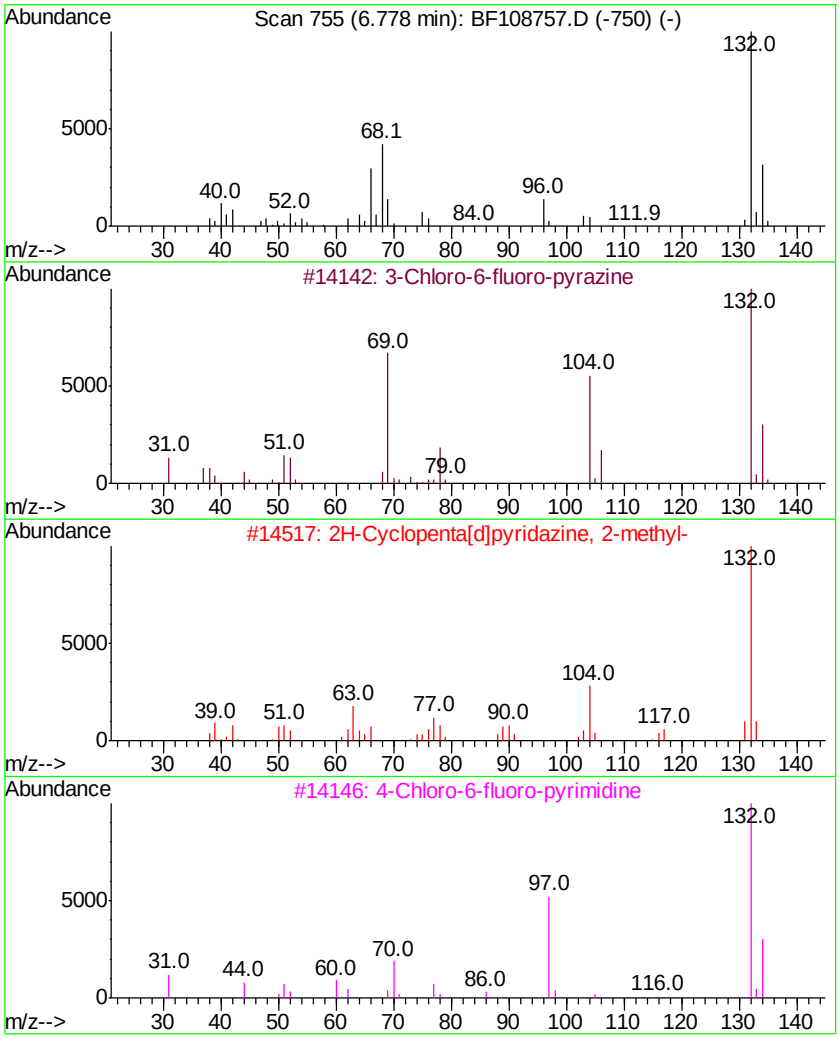
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

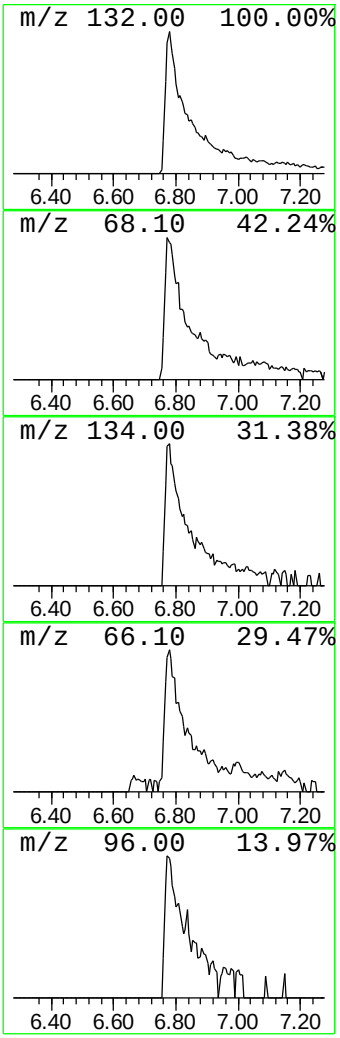
****

Peak Number 1 unknown6.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	13.39 ng	205876	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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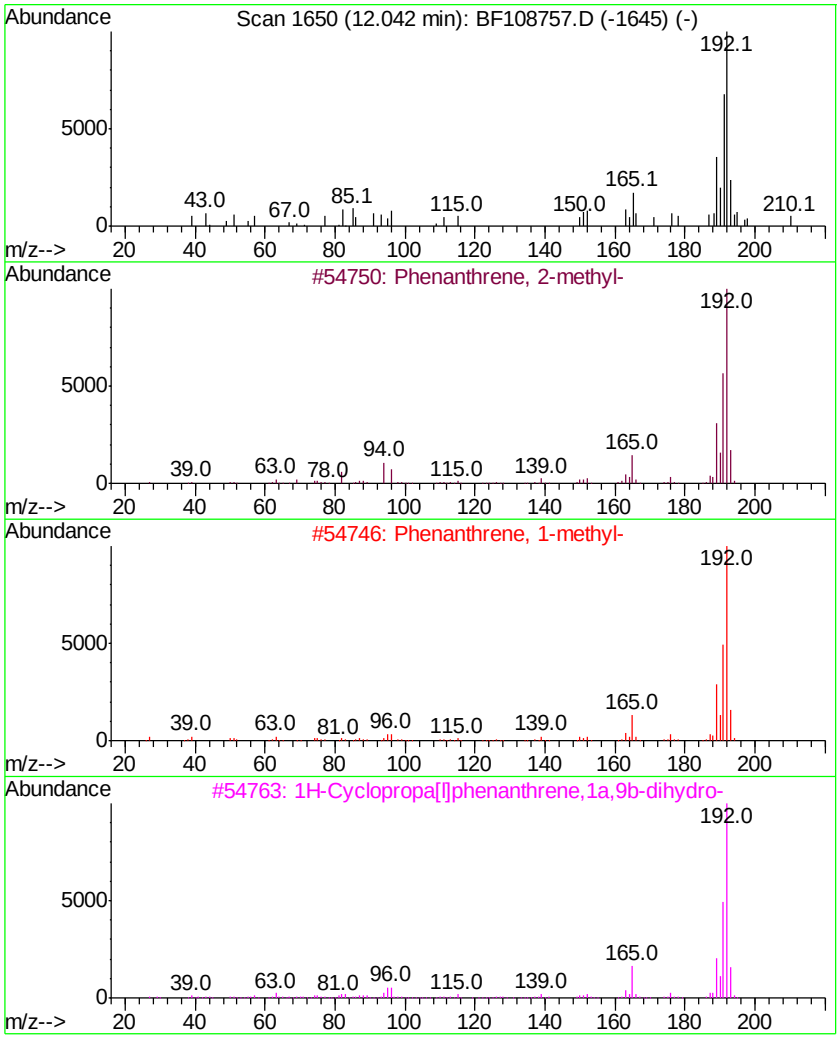
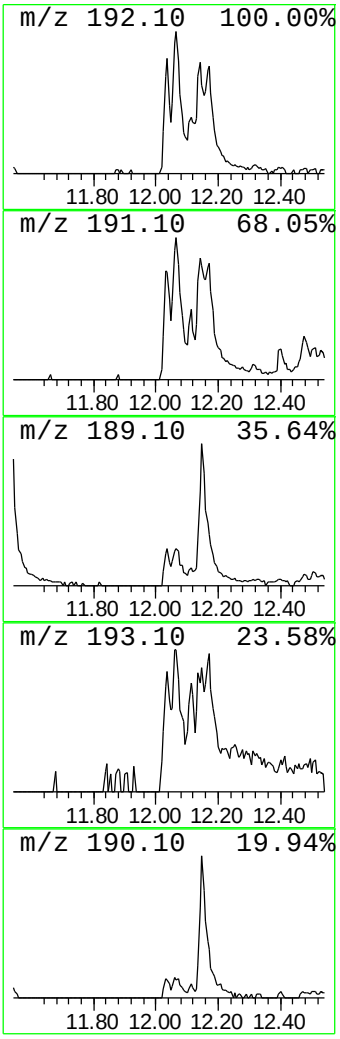
Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.21 ng	53081	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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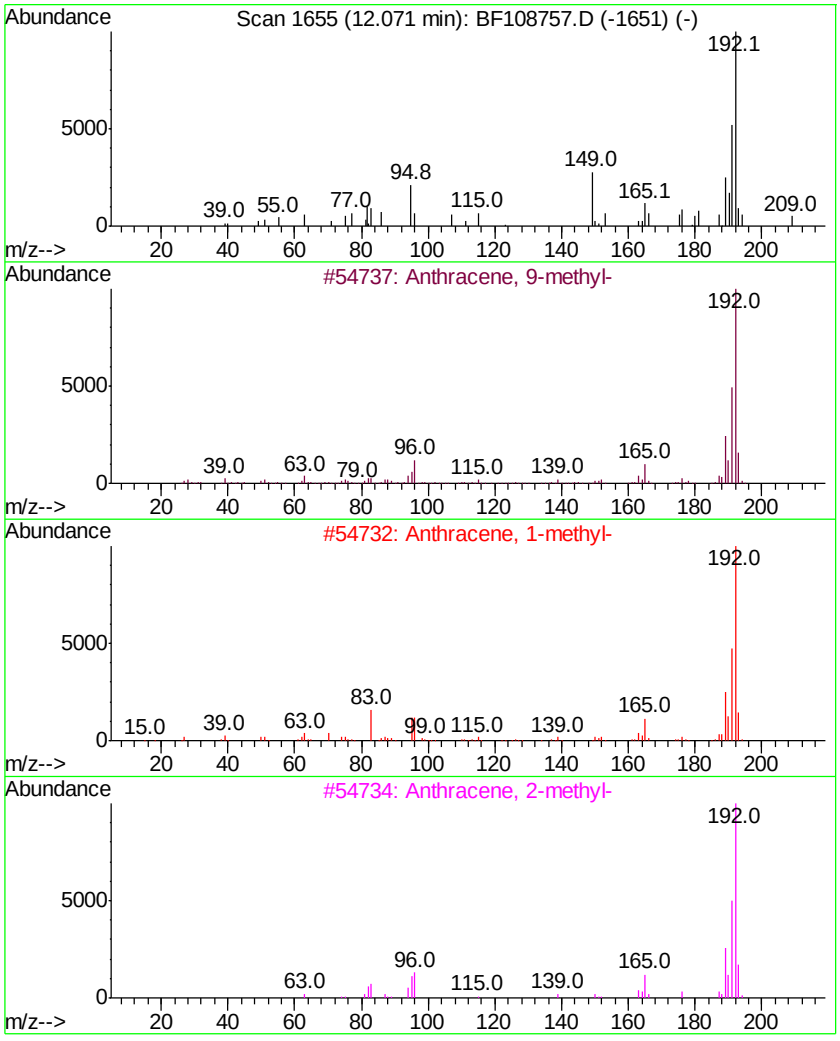
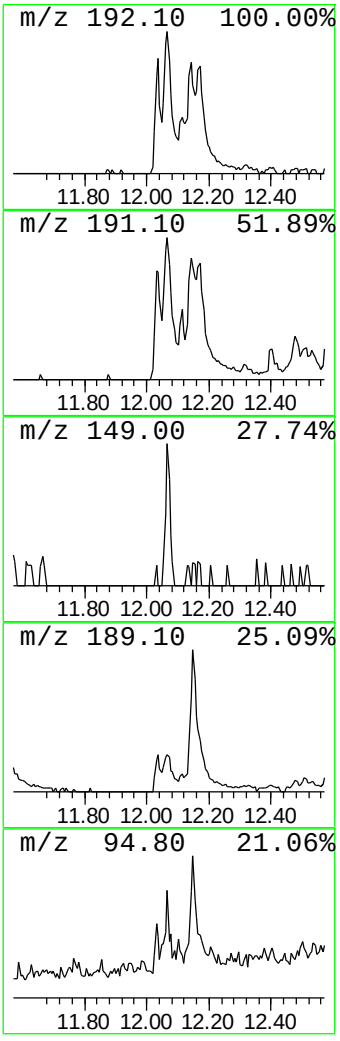
Peak Number 4 Anthracene, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	2.33 ng	56163	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	76
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	76
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	76
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	76
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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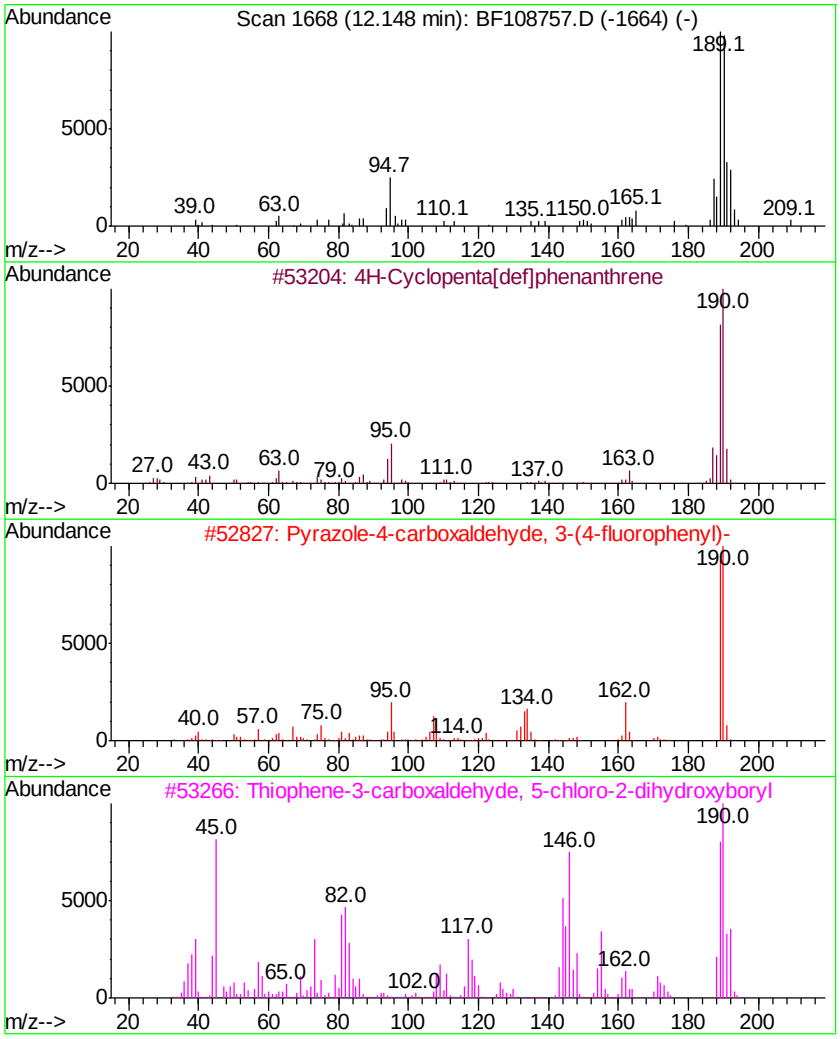
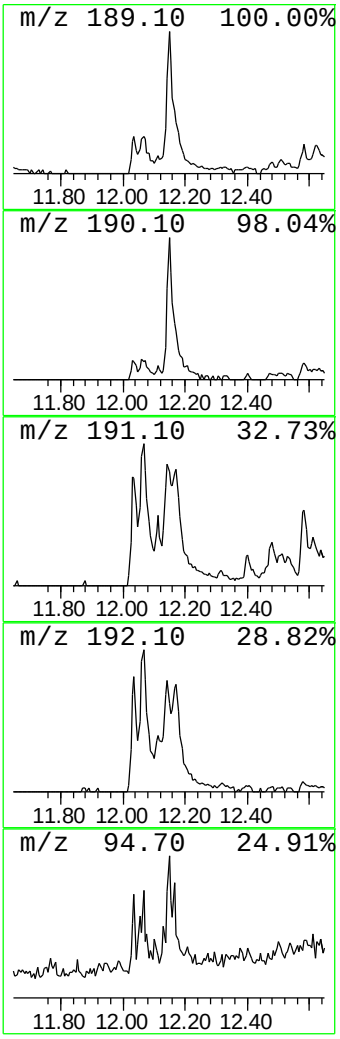
Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	2.79 ng	67161	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	58
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	52
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
5	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

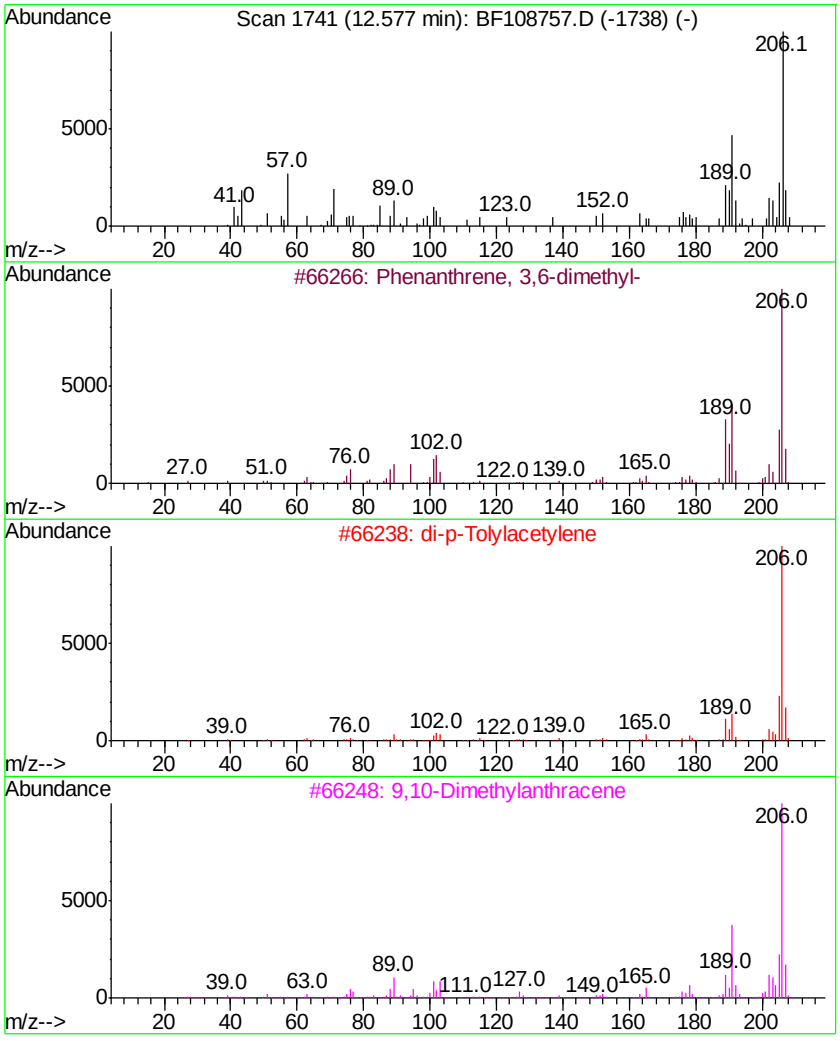
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

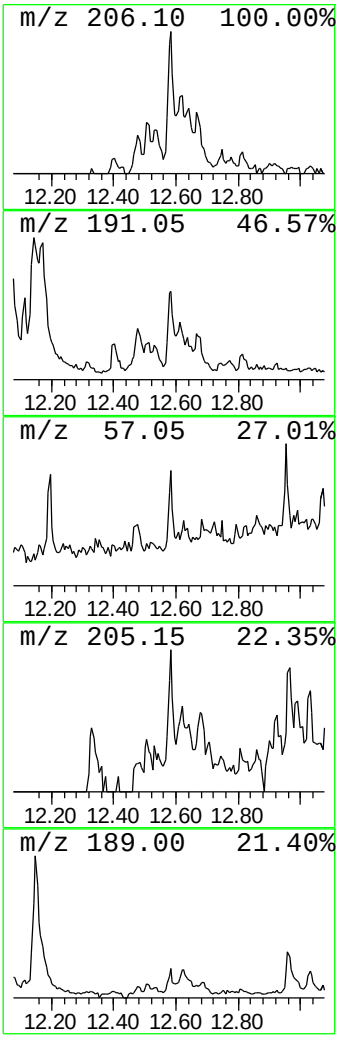
****

Peak Number 6 Phenanthrene, 3,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	2.24 ng	53954	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	93
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	93
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
4	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	87
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

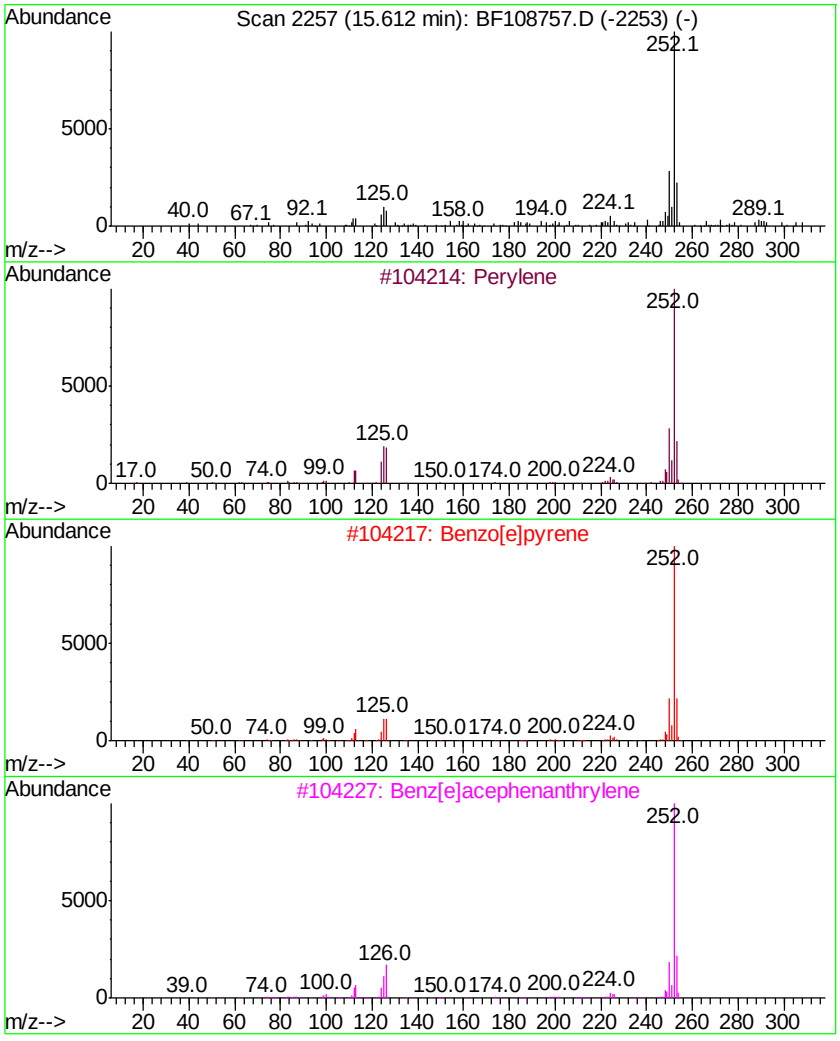
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

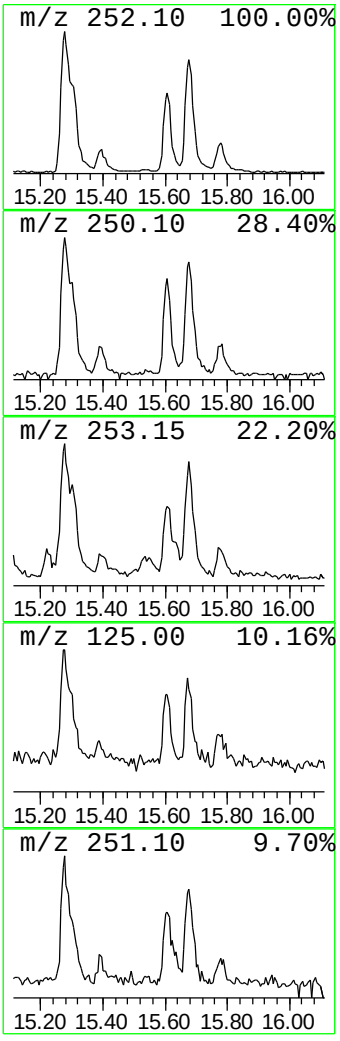
****

Peak Number 7 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	3.57 ng	64300	Perylene-d12	15.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
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	89
5	Benzo[a]pyrene	252	C20H12	000050-32-8	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090418\
Data File : BF108757.D
Acq On : 4 Sep 2018 22:38
Operator : JU/SJ
Sample : J4756-01 4X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WE-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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
unknown6.78	6.78	13.4	ng	205876	1	7.00	307537	20.0
Phenanthrene, 2-m...	12.04	2.2	ng	53081	4	11.53	481388	20.0
Anthracene, 9-met...	12.07	2.3	ng	56163	4	11.53	481388	20.0
4H-Cyclopenta[def...	12.15	2.8	ng	67161	4	11.53	481388	20.0
Phenanthrene, 3,6...	12.58	2.2	ng	53954	4	11.53	481388	20.0
Perylene	15.61	3.6	ng	64300	6	15.74	360492	20.0