LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUM-15

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	478	481	488	rVB	24327	28516	1.24%	0.163%
2	5.516	544	549	552	rBV	2154478	1920277	83.47%	10.944%
3	6.522	716	720	732	rVB	2117096	2063927	89.71%	11.762%
4	6.887	779	782	786	rBV	808854	677550	29.45%	3.861%
5	7.451	874	878	882	rBV	1415652	1355018	58.90%	7.722%
6	8.075	980	984	992	rBV	75330	97682	4.25%	0.557%
7	8.175	997	1001	1003	rBV	1070692	898799	39.07%	5.122%
8	9.251	1178	1184	1187	rBV	2523876	2300644	100.00%	13.111%
9	9.586	1237	1241	1243	rBV2	29216	29309	1.27%	0.167%
10	9.739	1262	1267	1273	rVB3	24747	36064	1.57%	0.206%
11	9.934	1296	1300	1303	rBV	955322	865457	37.62%	4.932%
12	9.963	1303	1305	1308	rVB	33763	27212	1.18%	0.155%
13	10.245	1348	1353	1356	rBV3	28036	32489	1.41%	0.185%
14	10.328	1363	1367	1368	rBV	31326	31487	1.37%	0.179%
15	10.345	1368	1370	1374	rVB2	38097	34962	1.52%	0.199%
16	10.481	1388	1393	1399	rVB2	22669	28482	1.24%	0.162%
17	10.722	1430	1434	1437	rBV	1395916	1151028	50.03%	6.560%
18	10.828	1449	1452	1457	rVB4	18422	29209	1.27%	0.166%
19	10.928	1464	1469	1475	rBV8	15336	27643	1.20%	0.158%
20	11.269	1524	1527	1529	rBV3	26421	25362	1.10%	0.145%
21	11.363	1540	1543	1546	rVB	54949	43278	1.88%	0.247%
22	11.422	1549	1553	1555	rVV	828785	671669	29.19%	3.828%
23	11.445	1555	1557	1560	rVV	337037	252311	10.97%	1.438%
24	11.498	1563	1566	1568	rVV	43646	34961	1.52%	0.199%
25	11.528	1568	1571	1577	rVB4	15418	25811	1.12%	0.147%
26	11.580	1577	1580	1586	rBV2	31001	46346	2.01%	0.264%
27	11.651	1588	1592	1595	rBV3	30749	36077	1.57%	0.206%
28	11.922	1635	1638	1641	rBV	51719	58268	2.53%	0.332%
29	11.951	1641	1643	1645	rVB	71559	50322	2.19%	0.287%
30	12.033	1654	1657	1660	rBV2	70171	75392	3.28%	0.430%
31	12.216	1686	1688	1691	rBV	30917	30668	1.33%	0.175%
32	12.245	1691	1693	1698	rVB2	42139	37802	1.64%	0.215%
33	12.475	1728	1732	1734	rBV	40122	39920	1.74%	0.228%
34	12.563	1744	1747	1751	rBV2	33116	36676	1.59%	0.209%
35	12.639	1756	1760	1763	rBV	469483	405763	17.64%	2.312%
36	12.786	1779	1785	1788	rBV4	25681	42282	1.84%	0.241%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.869	1796	1799	1805	rVB	409149	349704	15.20%	1.993%
38	13.010	1819	1823	1826	rBV	1409870	1284270	55.82%	7.319%
39	13.086	1832	1836	1839	rVB4	24652	36450	1.58%	0.208%
40	13.174	1847	1851	1852	rBV4	25848	34119	1.48%	0.194%
41	13.192	1852	1854	1857	rVB	44064	42765	1.86%	0.244%
42	13.263	1863	1866	1868	rVB	27848	25099	1.09%	0.143%
43	13.298	1868	1872	1875	rBV2	44509	55056	2.39%	0.314%
44	13.392	1885	1888	1890	rBV	30748	27709	1.20%	0.158%
45	13.704	1938	1941	1946	rVB	41244	41743	1.81%	0.238%
46	13.816	1955	1960	1963	rBV3	50364	79357	3.45%	0.452%
47	13.910	1973	1976	1985	rVB2	102863	148359	6.45%	0.846%
48	14.069	1998	2003	2005	rBV2	548698	606499	26.36%	3.456%
49	14.092	2005	2007	2014	rVB	201033	176966	7.69%	1.009%
50	14.210	2025	2027	2030	rBV3	18646	25255	1.10%	0.144%
51	14.980	2156	2158	2163	rVB5	43065	43331	1.88%	0.247%
52	15.121	2178	2182	2185	rBV	147011	225770	9.81%	1.287%
53	15.233	2198	2201	2205	rBV3	53425	83609	3.63%	0.476%
54	15.433	2232	2235	2241	rVB	119357	170463	7.41%	0.971%
55	15.498	2242	2246	2251	rVB	120730	156461	6.80%	0.892%
56	15.563	2252	2257	2260	rBV	316424	385229	16.74%	2.195%

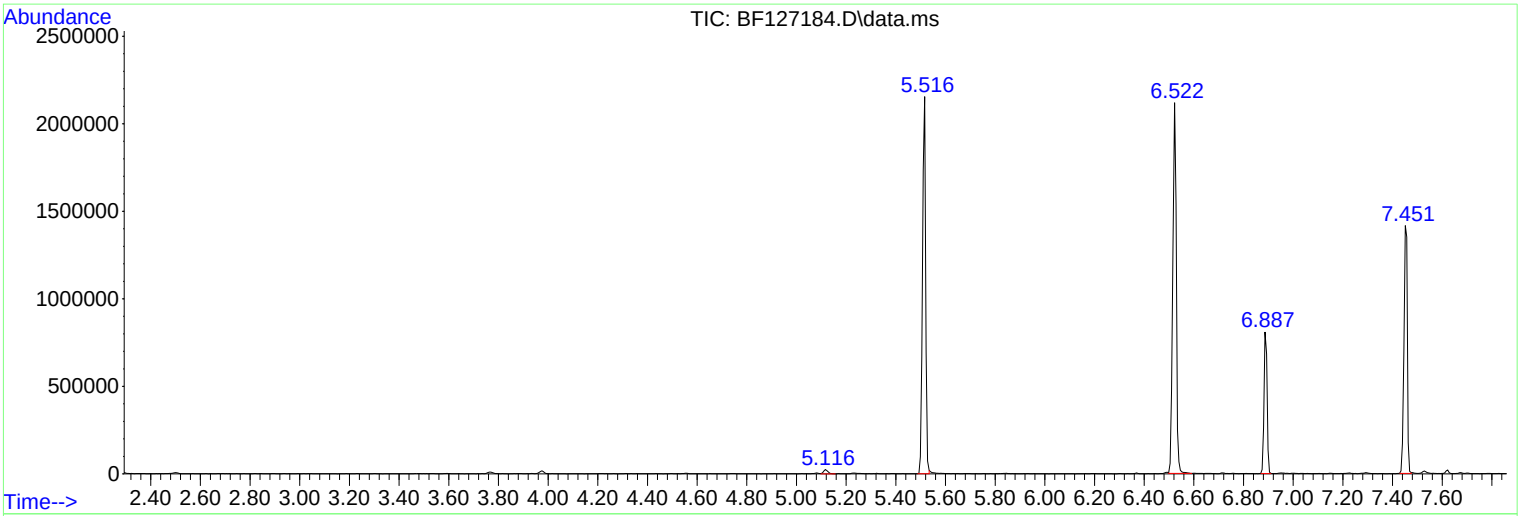
Sum of corrected areas: 17546877

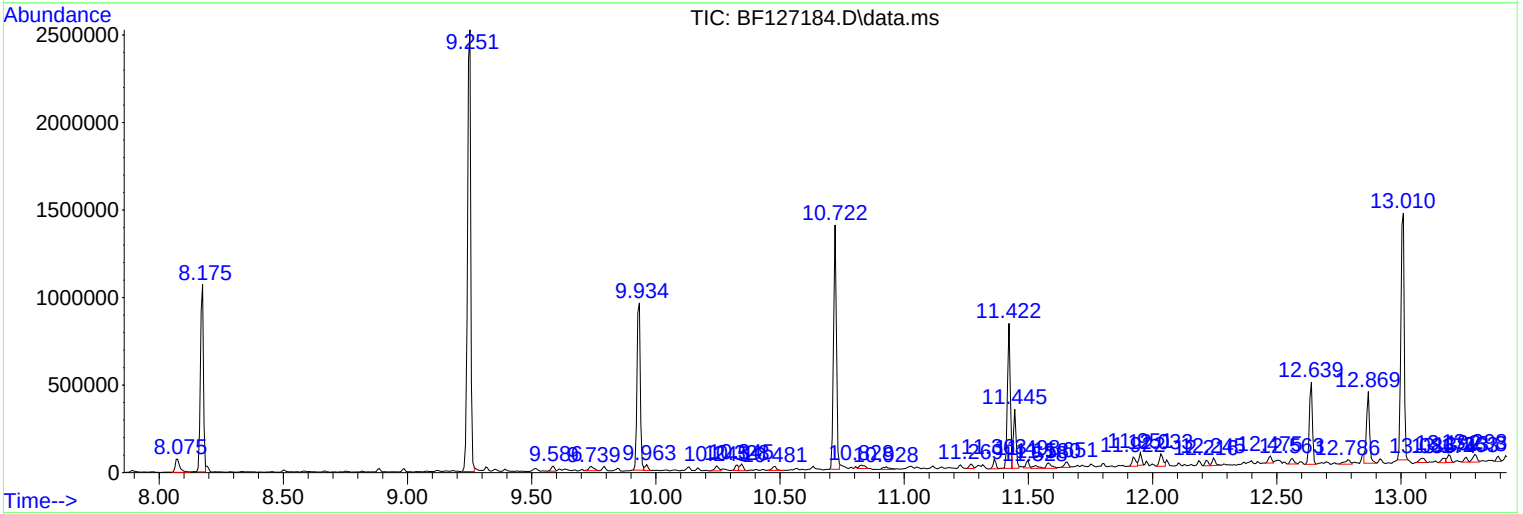
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

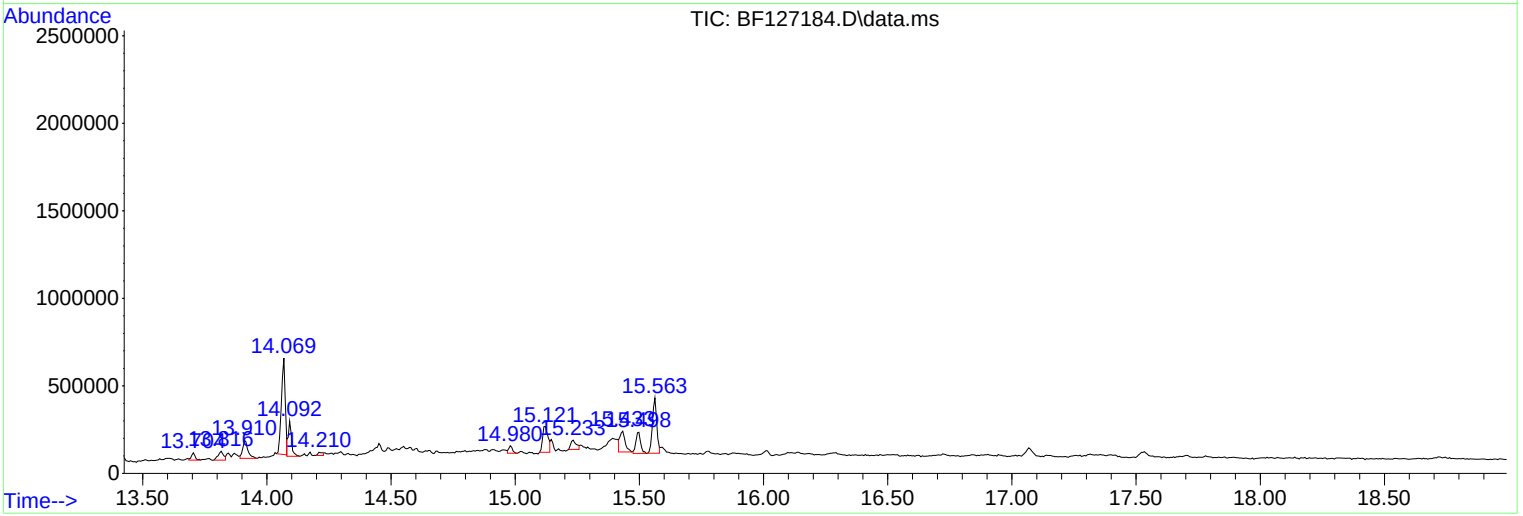
Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

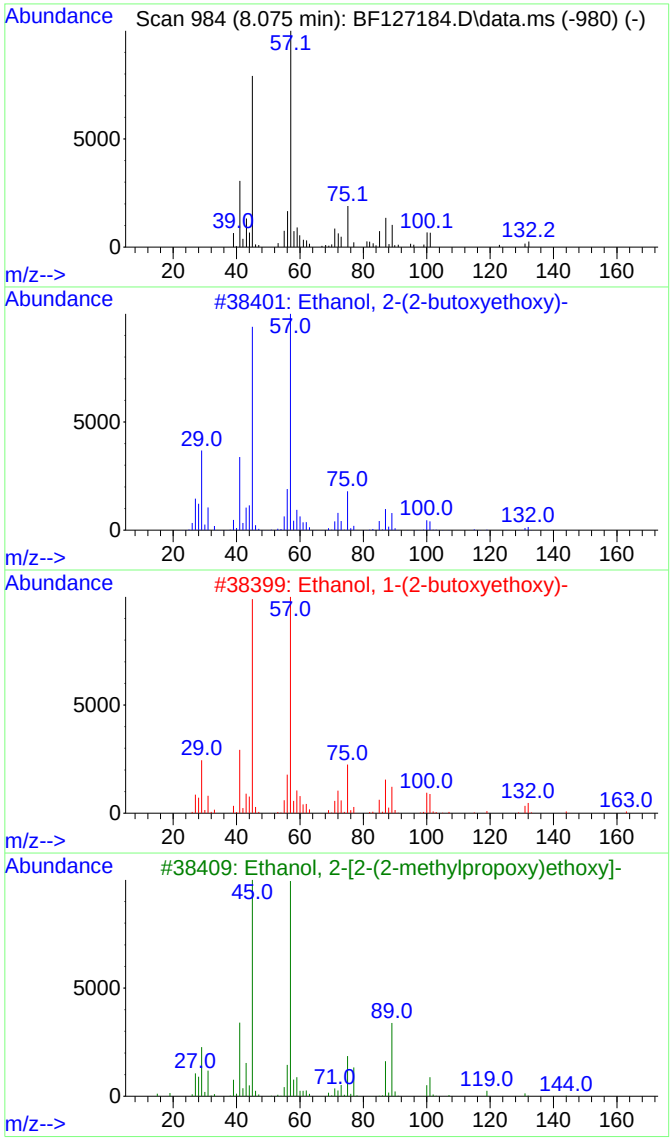
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

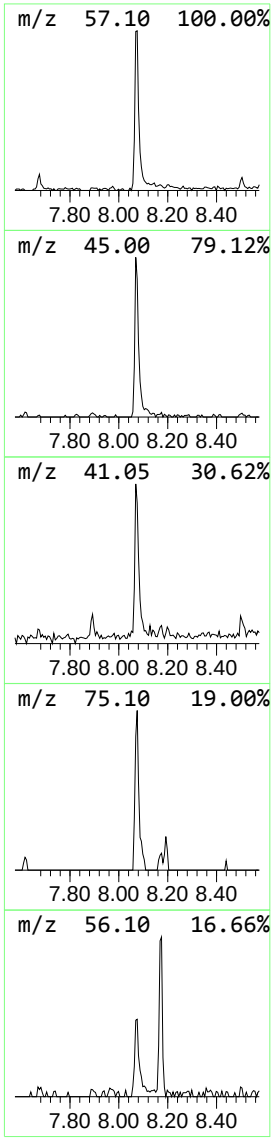
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	2.17 ng	97682	Naphthalene-d8	8.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

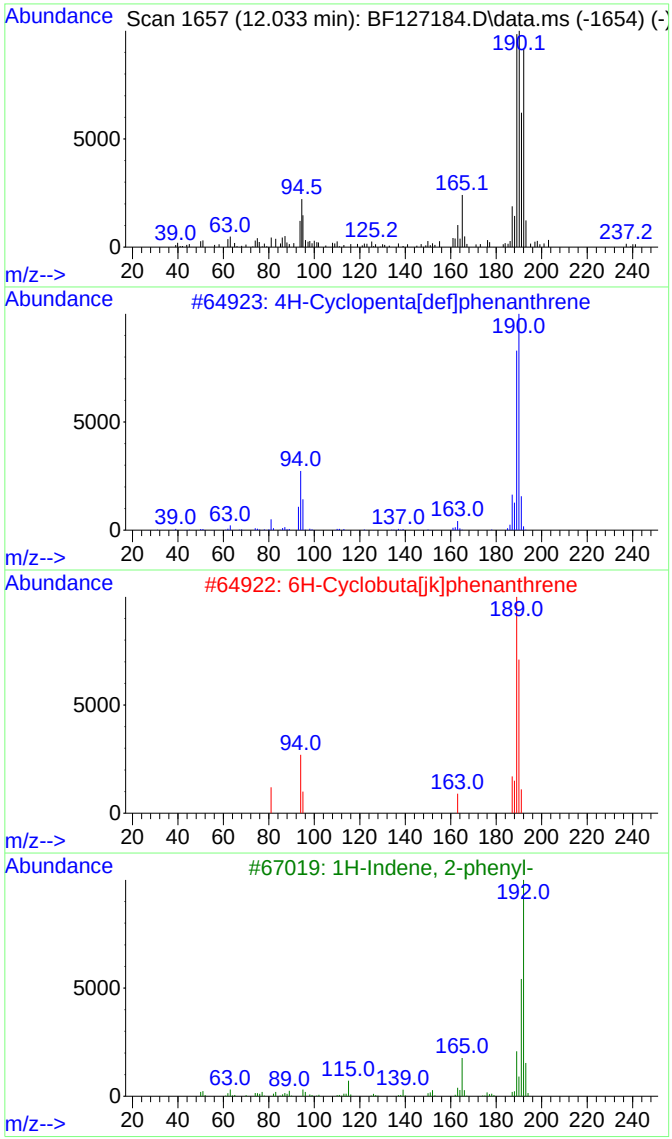
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

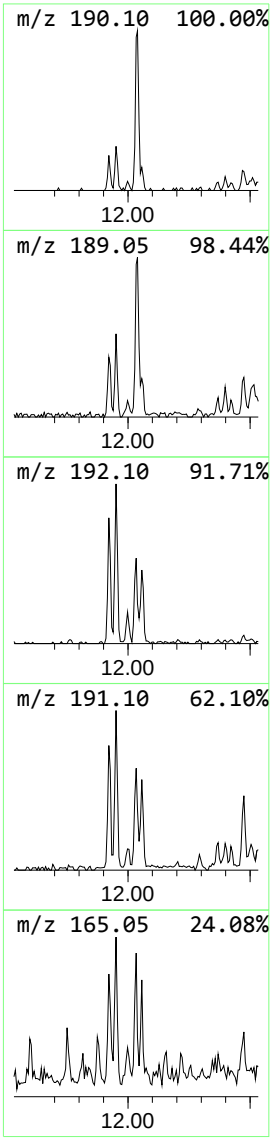
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.24 ng	75392	Phenanthrene-d10	11.422

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	49
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	46
4	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	46
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

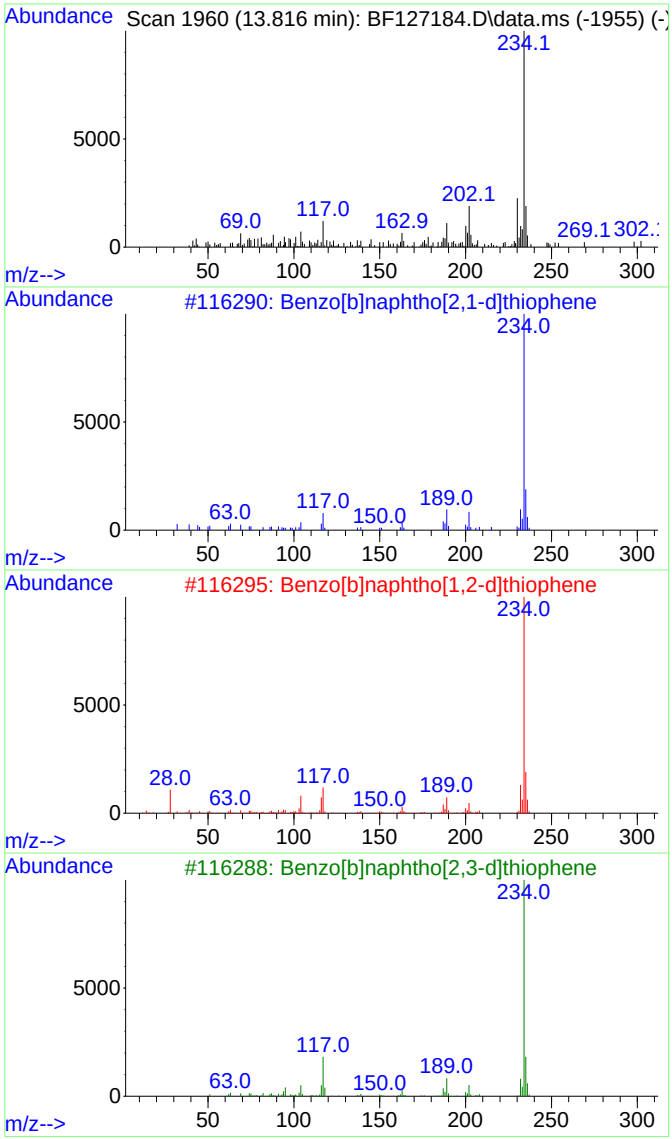
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

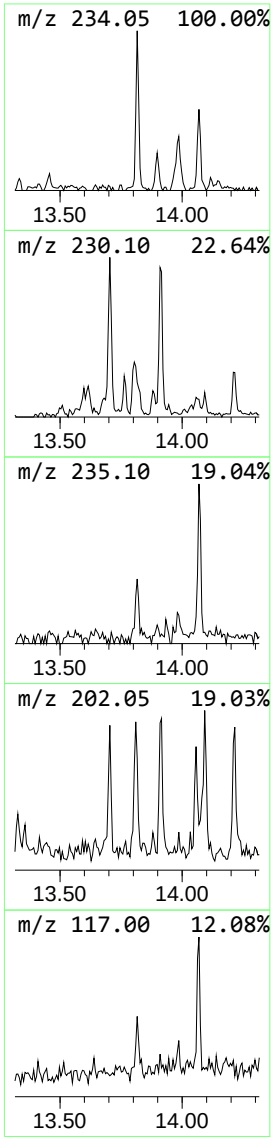
****

Peak Number 3 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	2.62 ng	79357	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	76
2	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	70
3	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	68
4	Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	59
5	Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

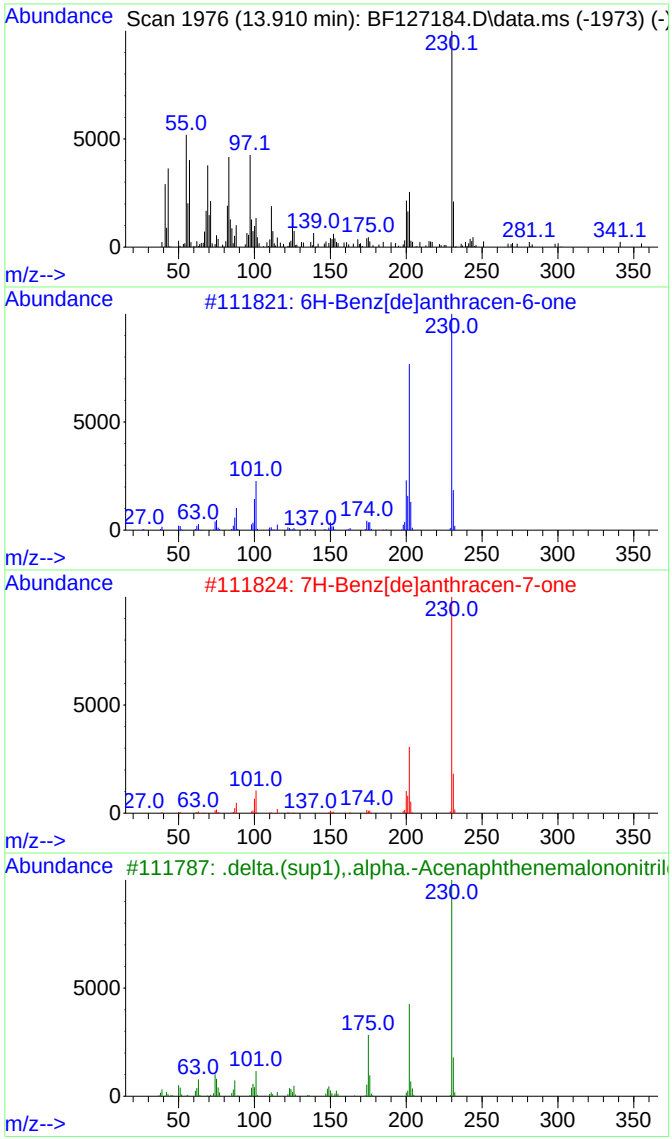
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

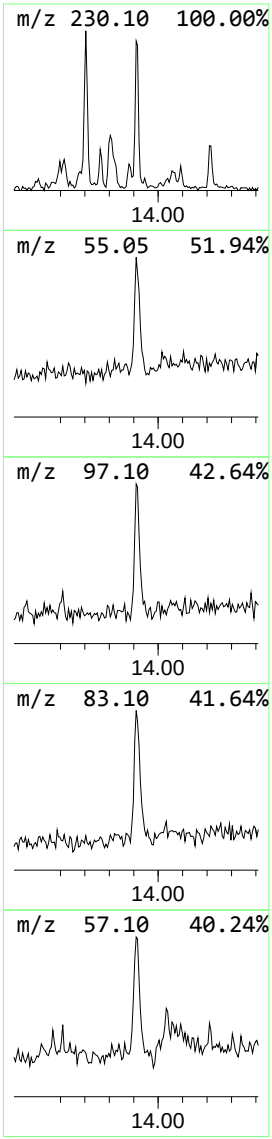
****

Peak Number 4 unknown13.910 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.89 ng	148359	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	43
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	38
3	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	35
4	1-Tetracosene	336	C24H48	010192-32-2	30
5	1-Pentadecanethiol	244	C15H32S	025276-70-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

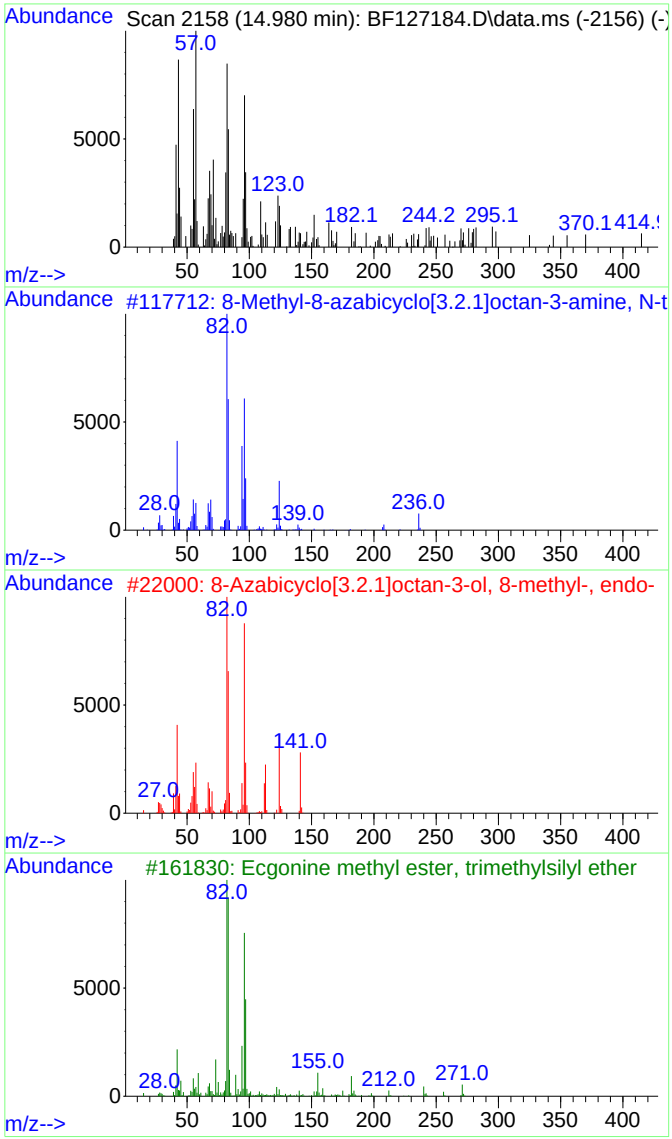
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

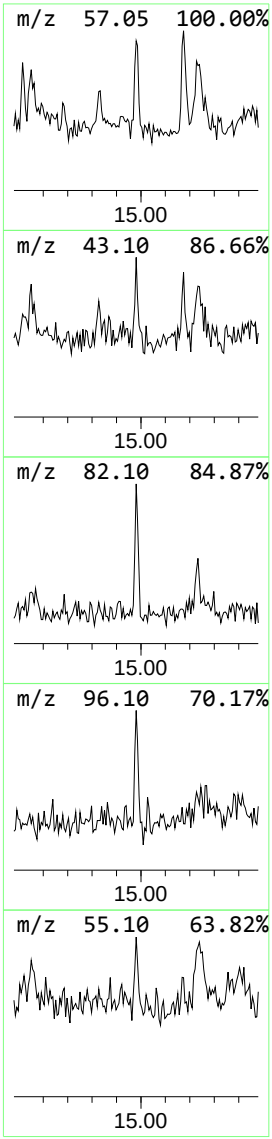
****

Peak Number 5 8-Methyl-8-azabicyclo[3.2.1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	2.25 ng	43331	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	8-Methyl-8-azabicyclo[3.2.1]octa...	236	C10H15F3N2O	1873186-09-4	53
2	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	49
3	Ecgonine methyl ester, trimethyl...	271	C13H25NO3Si	1000417-19-3	49
4	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	46
5	Oxacyclotetradecan-2-one	212	C13H24O2	001725-04-8	43





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

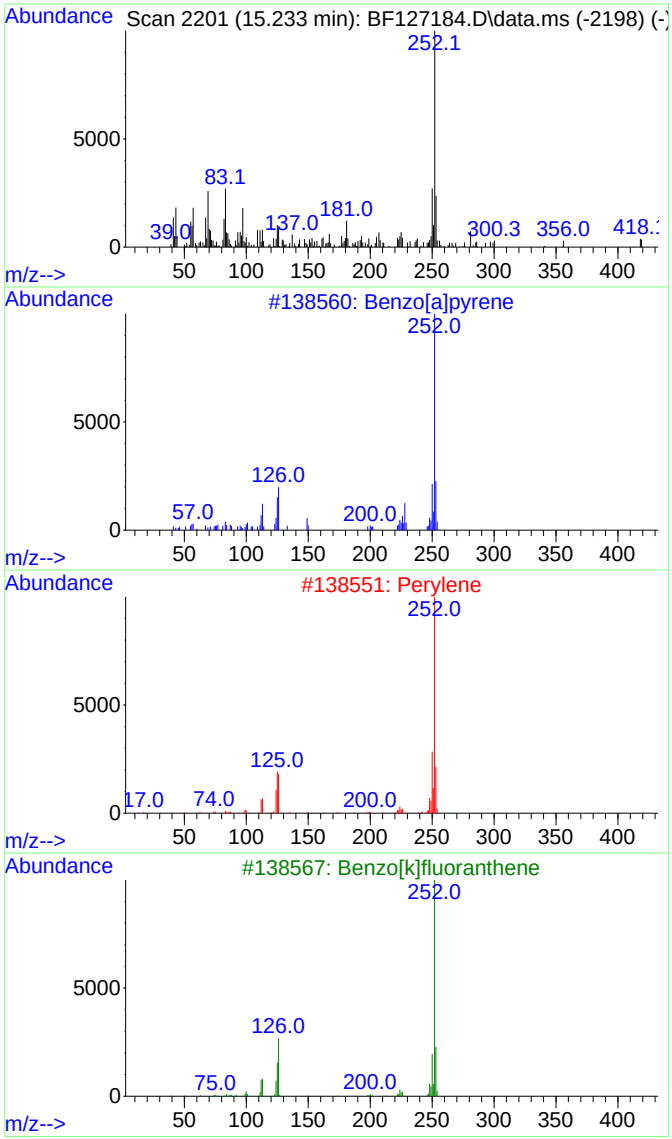
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

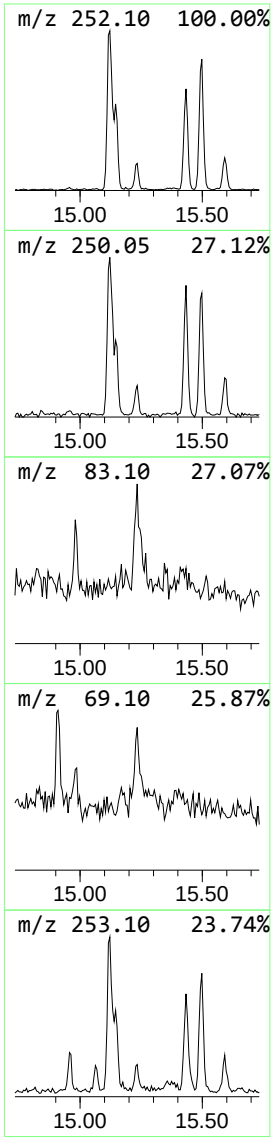
****

Peak Number 6 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	4.34 ng	83609	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	83
2	Perylene	252	C20H12	000198-55-0	76
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	68
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	68
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

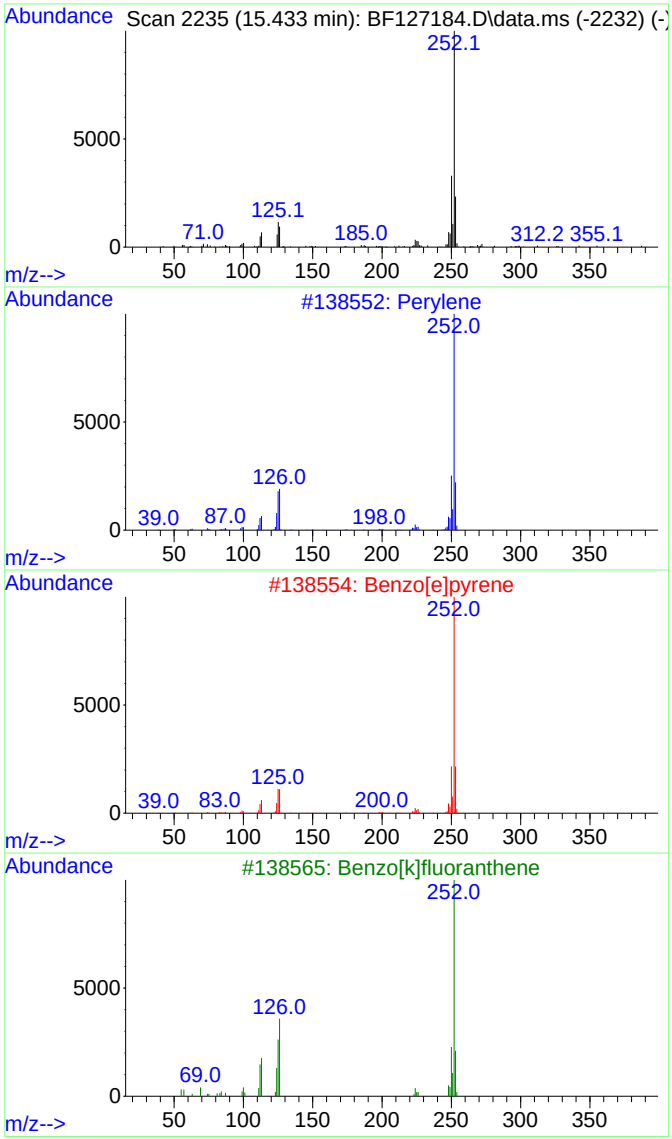
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

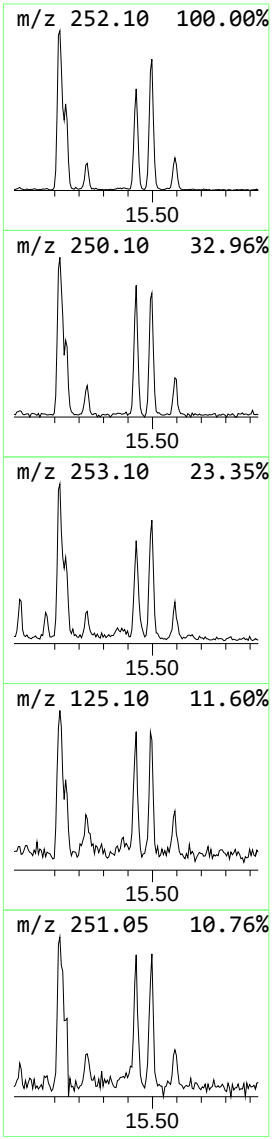
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.433	8.85 ng	170463	Perylene-d12	15.563

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	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030322\
Data File : BF127184.D
Acq On : 03 Mar 2022 21:24
Operator : CG\JU
Sample : N1751-09
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUM-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.075	2.2	ng	97682	2	8.175	898799	20.0
4H-Cyclopenta[d...	12.033	2.2	ng	75392	4	11.422	671669	20.0
Benzo[b]naphtho...	13.816	2.6	ng	79357	5	14.069	606499	20.0
unknown13.910	13.910	4.9	ng	148359	5	14.069	606499	20.0
8-Methyl-8-azab...	14.980	2.3	ng	43331	6	15.563	385229	20.0
Perylene	15.233	4.3	ng	83609	6	15.563	385229	20.0
Benzo[e]pyrene	15.433	8.8	ng	170463	6	15.563	385229	20.0