LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138409.D
Acq On : 01 Jul 2024 18:06
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	21	rVB	2345548	2902842	77.65%	7.380%
2	2.287	30	34	42	rVB	36746	52232	1.40%	0.133%
3	3.404	221	224	254	rBV	110967	333699	8.93%	0.848%
4	5.098	508	512	520	rVB	340452	391903	10.48%	0.996%
5	5.504	576	581	584	rBV	4078391	3631462	97.14%	9.233%
6	5.822	631	635	640	rBV	49433	42795	1.14%	0.109%
7	6.510	747	752	755	rBV	4088294	3738370	100.00%	9.504%
8	6.698	781	784	788	rBV	88497	74964	2.01%	0.191%
9	6.875	810	814	817	rBV	1508071	1263920	33.81%	3.213%
10	7.434	904	909	912	rBV	2578866	2451515	65.58%	6.233%
11	7.686	948	952	959	rVB	170346	129865	3.47%	0.330%
12	8.151	1028	1031	1034	rBV	1836692	1597620	42.74%	4.062%
13	8.369	1063	1068	1074	rVB2	53645	48342	1.29%	0.123%
14	8.463	1080	1084	1093	rVB	261767	234894	6.28%	0.597%
15	9.228	1210	1214	1217	rBV	4188808	3449388	92.27%	8.770%
16	9.563	1267	1271	1273	rBV	43319	41296	1.10%	0.105%
17	9.904	1326	1329	1332	rVB	1826310	1502582	40.19%	3.820%
18	9.939	1332	1335	1338	rVB	181299	141249	3.78%	0.359%
19	10.004	1341	1346	1352	rVB2	130336	173649	4.65%	0.441%
20	10.110	1360	1364	1367	rVB2	72944	69712	1.86%	0.177%
21	10.451	1419	1422	1426	rVB	159673	133161	3.56%	0.339%
22	10.692	1459	1463	1466	rBV	2045916	1704673	45.60%	4.334%
23	10.804	1479	1482	1487	rBV2	39052	57771	1.55%	0.147%
24	10.998	1509	1515	1517	rBV3	42348	51915	1.39%	0.132%
25	11.127	1532	1537	1539	rBV3	29076	40027	1.07%	0.102%
26	11.251	1552	1558	1560	rBV3	40651	55376	1.48%	0.141%
27	11.286	1561	1564	1570	rVB	75118	77403	2.07%	0.197%
28	11.392	1578	1582	1584	rBV	1351330	1230769	32.92%	3.129%
29	11.416	1584	1586	1589	rVV	1218761	919705	24.60%	2.338%
30	11.463	1591	1594	1597	rVB	343179	274572	7.34%	0.698%
31	11.621	1614	1621	1623	rBV2	49170	60310	1.61%	0.153%
32	11.892	1663	1667	1668	rBV	101852	85186	2.28%	0.217%
33	11.916	1668	1671	1676	rVV2	292971	296842	7.94%	0.755%
34	11.963	1676	1679	1682	rVV	71332	77374	2.07%	0.197%
35	12.004	1682	1686	1688	rVV	206355	207784	5.56%	0.528%
36	12.021	1688	1689	1694	rVB	69298	54788	1.47%	0.139%

LSC Area Percent Report

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Data File : BF138409.D
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Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.186	1714	1717	1719	rBV	86679	67876	1.82%	0.173%
38	12.439	1756	1760	1763	rBV	59659	74822	2.00%	0.190%
39	12.474	1763	1766	1772	rVV3	46574	71872	1.92%	0.183%
40	12.521	1772	1774	1780	rVB2	43175	50311	1.35%	0.128%
41	12.604	1784	1788	1791	rBV	1421968	1213549	32.46%	3.085%
42	12.698	1801	1804	1806	rBV2	57318	54524	1.46%	0.139%
43	12.792	1817	1820	1821	rBV	84186	63544	1.70%	0.162%
44	12.833	1821	1827	1832	rVV	1088852	1253956	33.54%	3.188%
45	12.874	1832	1834	1840	rVB3	53362	64203	1.72%	0.163%
46	12.974	1847	1851	1854	rVB	2558934	2159033	57.75%	5.489%
47	13.051	1859	1864	1867	rBV3	55793	97428	2.61%	0.248%
48	13.133	1875	1878	1879	rBV2	45875	45105	1.21%	0.115%
49	13.157	1879	1882	1885	rVB	166967	144000	3.85%	0.366%
50	13.221	1891	1893	1896	rVB	134771	109914	2.94%	0.279%
51	13.257	1896	1899	1902	rBV2	89804	97010	2.59%	0.247%
52	13.351	1913	1915	1918	rVB	50345	44914	1.20%	0.114%
53	13.380	1918	1920	1924	rBV2	50014	53528	1.43%	0.136%
54	13.498	1937	1940	1944	rVB	69687	57140	1.53%	0.145%
55	13.545	1945	1948	1952	rBV3	47224	56374	1.51%	0.143%
56	13.663	1965	1968	1973	rVB	41721	44979	1.20%	0.114%
57	13.774	1984	1987	1990	rBV3	75289	71323	1.91%	0.181%
58	13.804	1990	1992	1994	rVV	83600	64862	1.74%	0.165%
59	13.827	1994	1996	2000	rVV2	68957	91856	2.46%	0.234%
60	13.868	2000	2003	2011	rVB2	292254	338996	9.07%	0.862%
61	14.027	2022	2030	2032	rBV2	1354504	1759763	47.07%	4.474%
62	14.051	2032	2034	2042	rVV	608926	616299	16.49%	1.567%
63	14.133	2045	2048	2051	rVB	138395	120546	3.22%	0.306%
64	14.410	2093	2095	2098	rVB	71717	55232	1.48%	0.140%
65	14.492	2106	2109	2114	rBV3	106320	176882	4.73%	0.450%
66	14.804	2159	2162	2164	rBV	57970	57763	1.55%	0.147%
67	15.062	2202	2206	2209	rBV	348289	501208	13.41%	1.274%
68	15.139	2217	2219	2222	rVV	68223	57008	1.52%	0.145%
69	15.174	2222	2225	2229	rVB	76211	88389	2.36%	0.225%
70	15.368	2254	2258	2264	rBV	194900	305958	8.18%	0.778%
71	15.427	2265	2268	2274	rVB	301972	373988	10.00%	0.951%
72	15.492	2275	2279	2282	rVV	652236	769275	20.58%	1.956%
73	15.521	2282	2284	2291	rVB	127539	157179	4.20%	0.400%
74	16.956	2523	2528	2536	rVB2	94530	199185	5.33%	0.506%
75	17.398	2599	2603	2610	rBV2	57190	103365	2.76%	0.263%

LSC Area Percent Report

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Sample : P3076-13
Misc :
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Instrument :
BNA_F
ClientSampleId :
7-B-1

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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

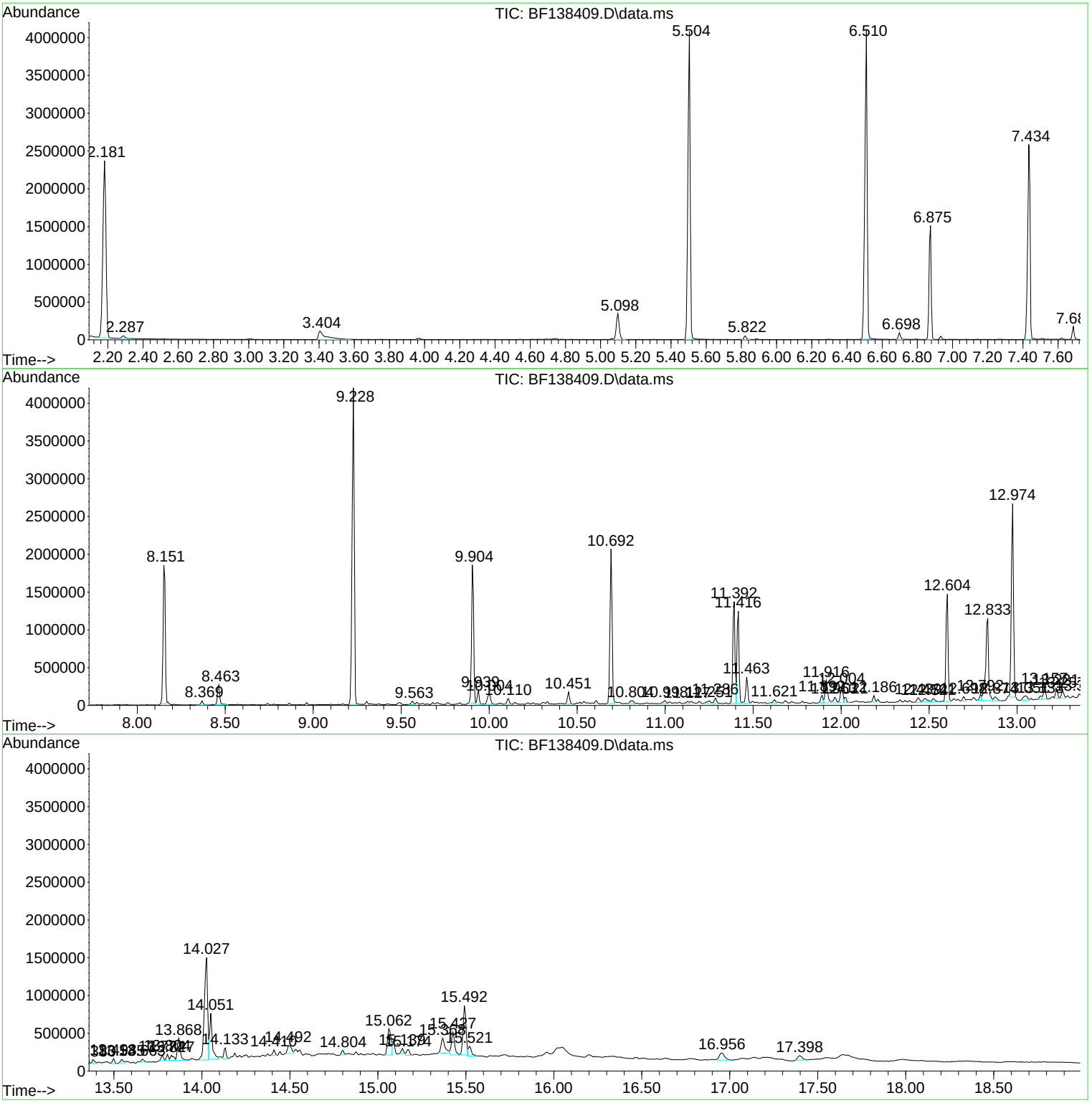
Sum of corrected areas: 39333114

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138409.D
Acq On : 01 Jul 2024 18:06
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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\BF070124\
Data File : BF138409.D
Acq On : 01 Jul 2024 18:06
Operator : CG\JU
Sample : P3076-13
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

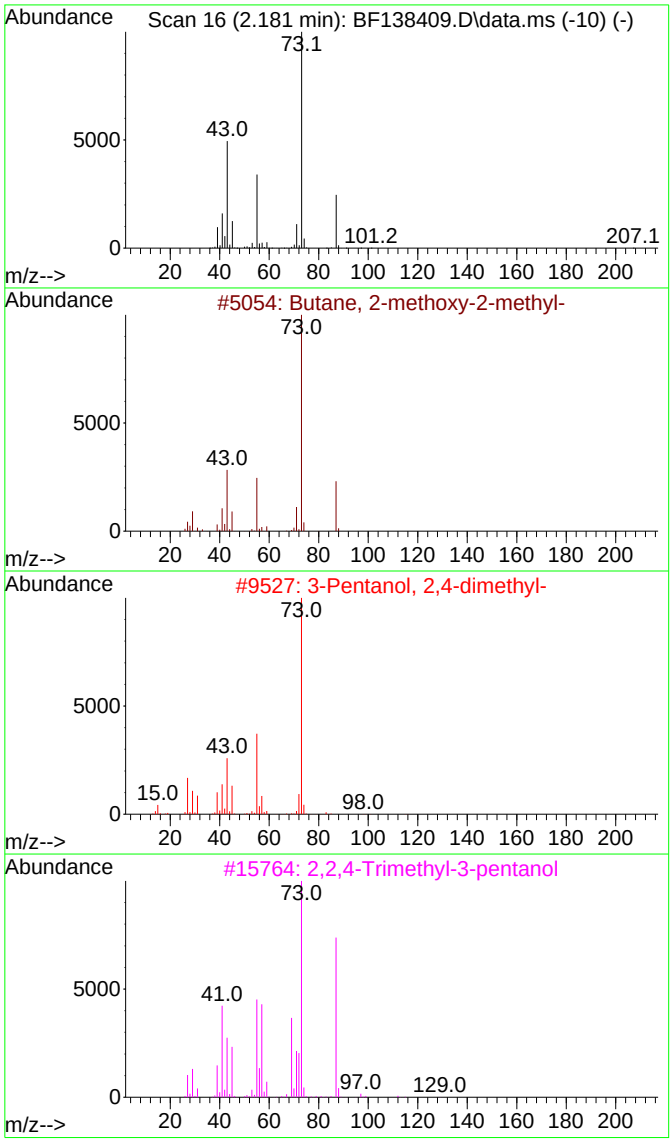
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

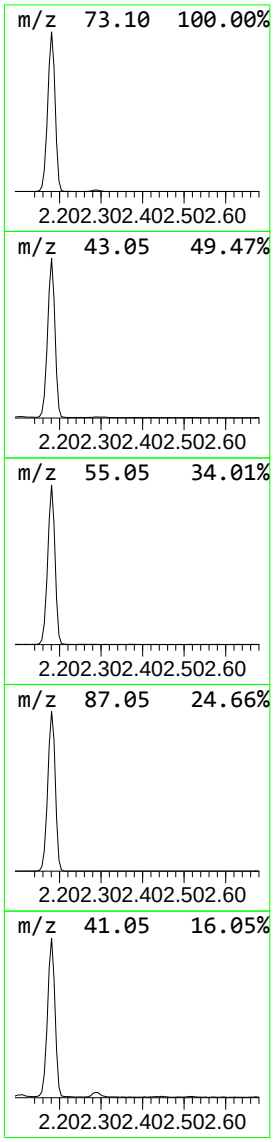
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	45.93 ng	2902840	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138409.D
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Sample : P3076-13
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

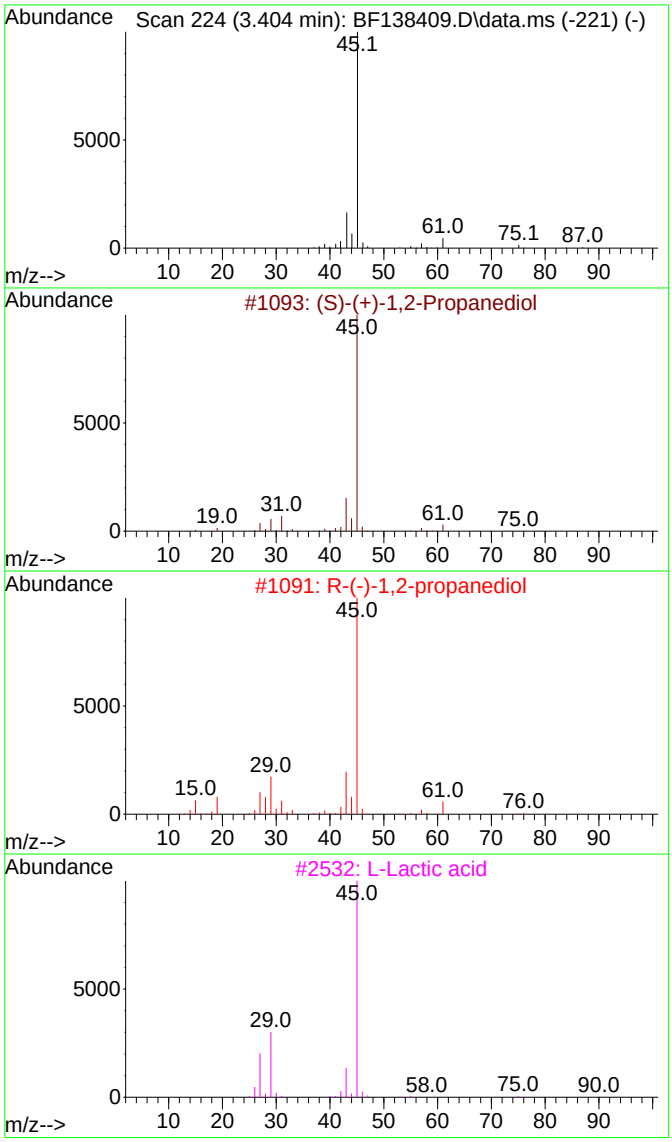
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

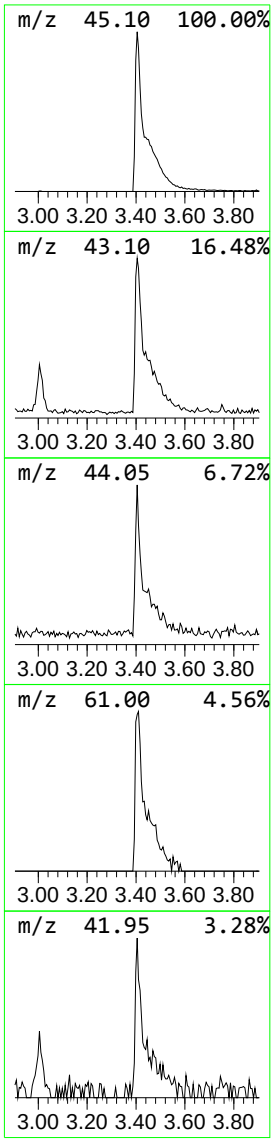
****

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	5.28 ng	333699	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
3	L-Lactic acid	90	C3H6O3	000079-33-4	39
4	Propylene Glycol	76	C3H8O2	000057-55-6	32
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138409.D
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Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

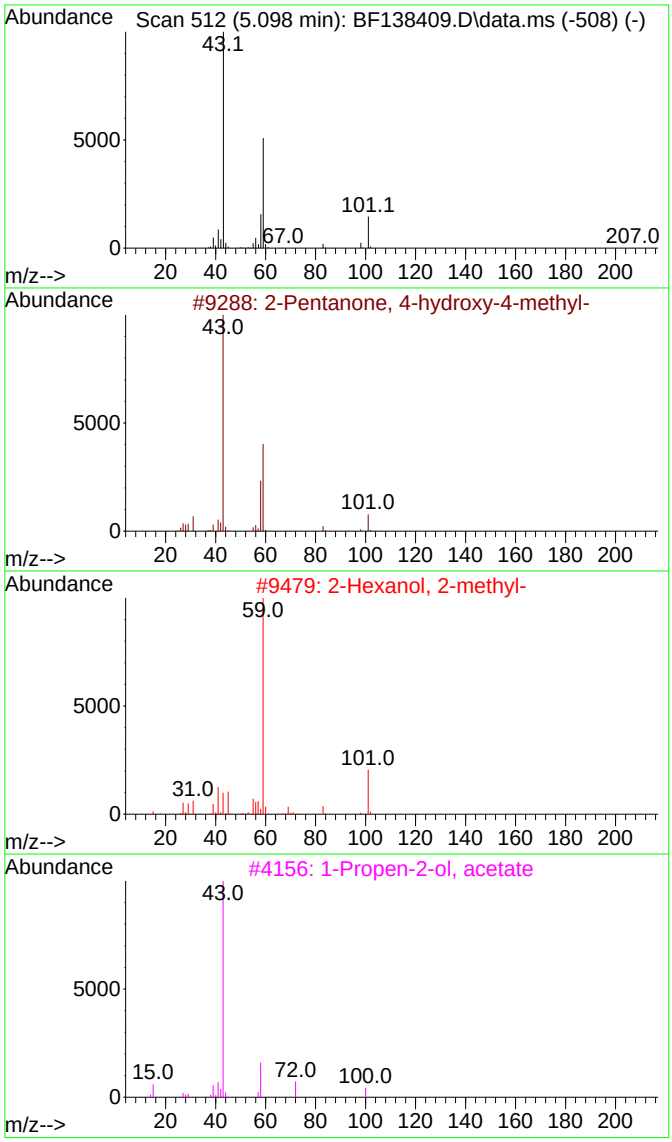
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

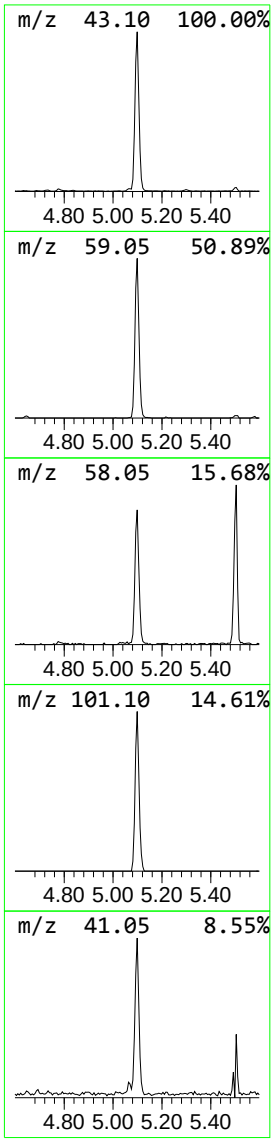
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	6.20 ng	391903	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

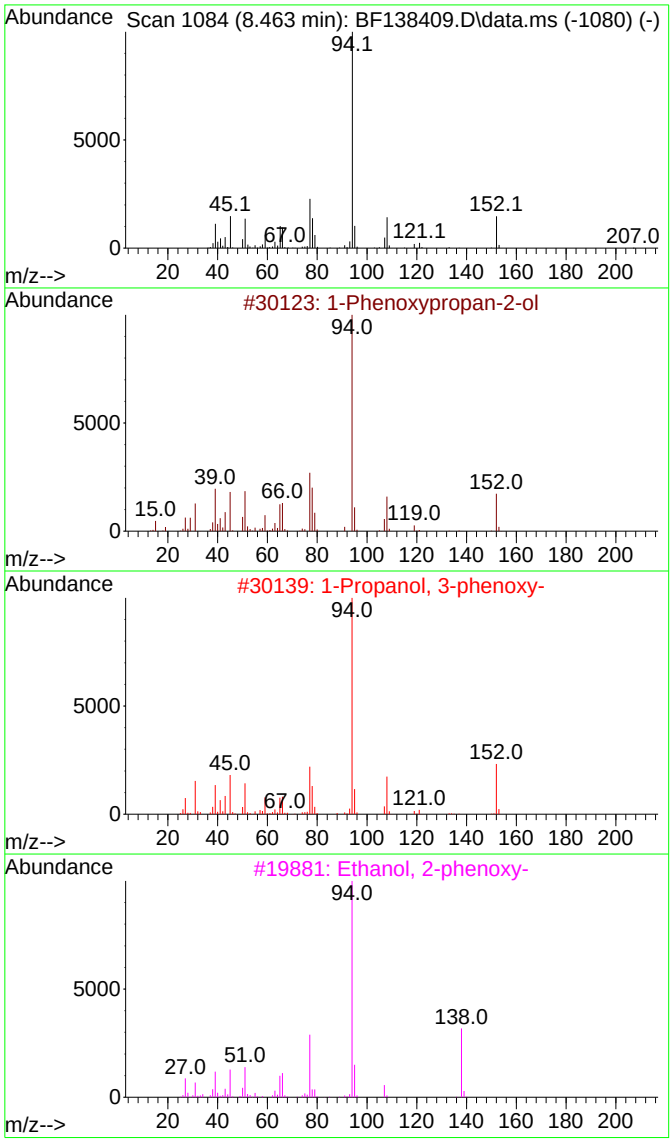
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

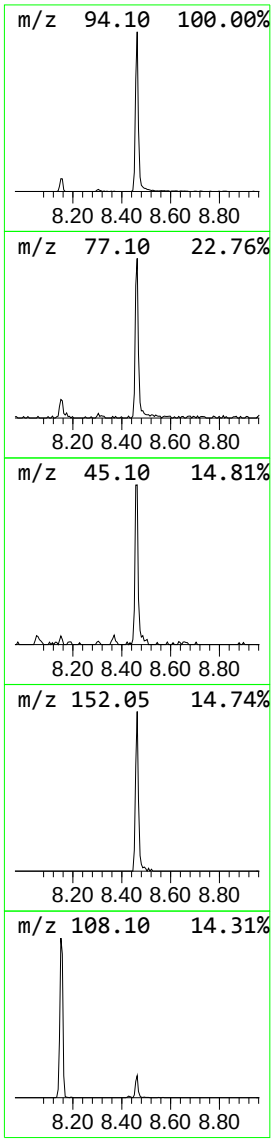
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.94 ng	234894	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

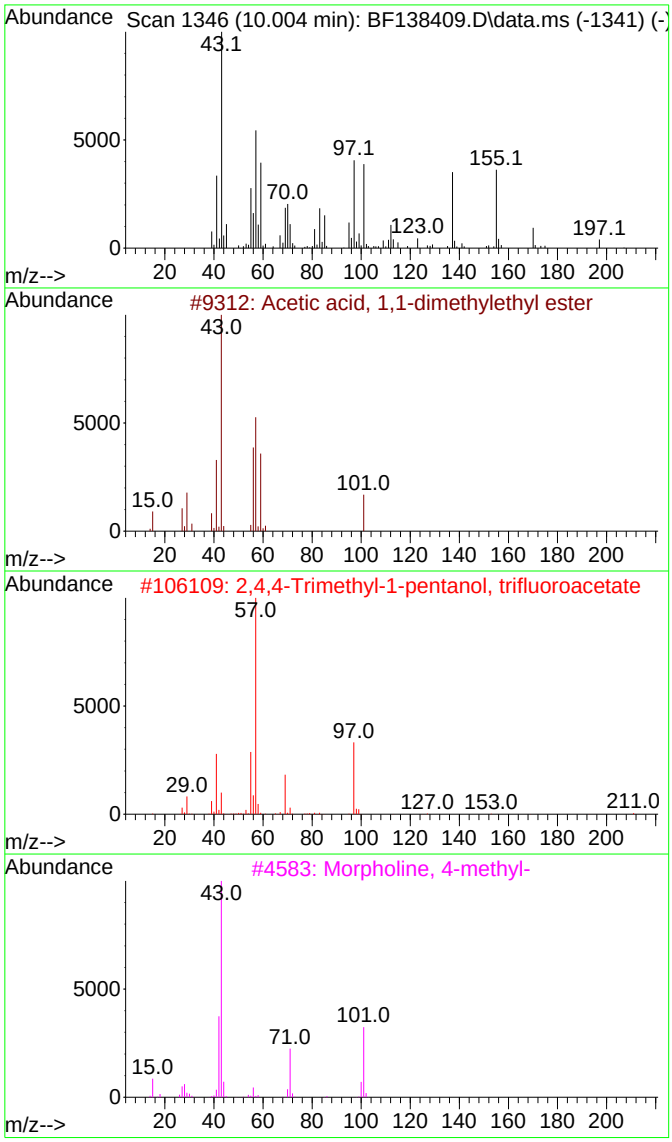
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

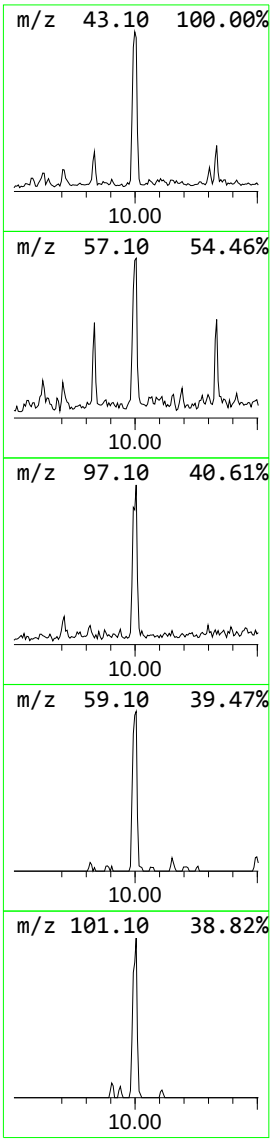
****

Peak Number 5 unknown10.004 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	2.31 ng	173649	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	27
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	10
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	10
4	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10
5	Acetic acid, 3-hydroxy-2-nitroph...	197	C8H7NO5	1000269-41-1	10





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Data File : BF138409.D
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Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

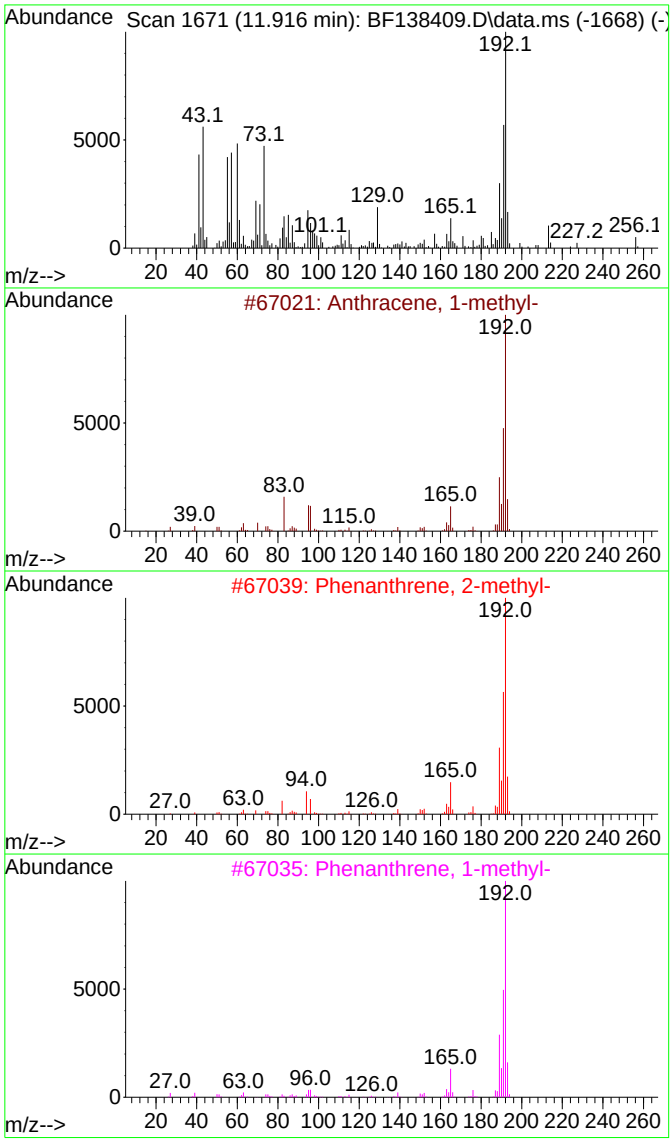
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

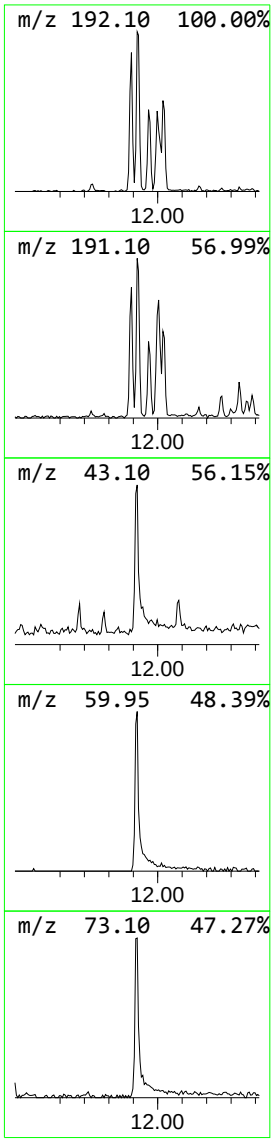
****

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.82 ng	296842	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138409.D
Acq On : 01 Jul 2024 18:06
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

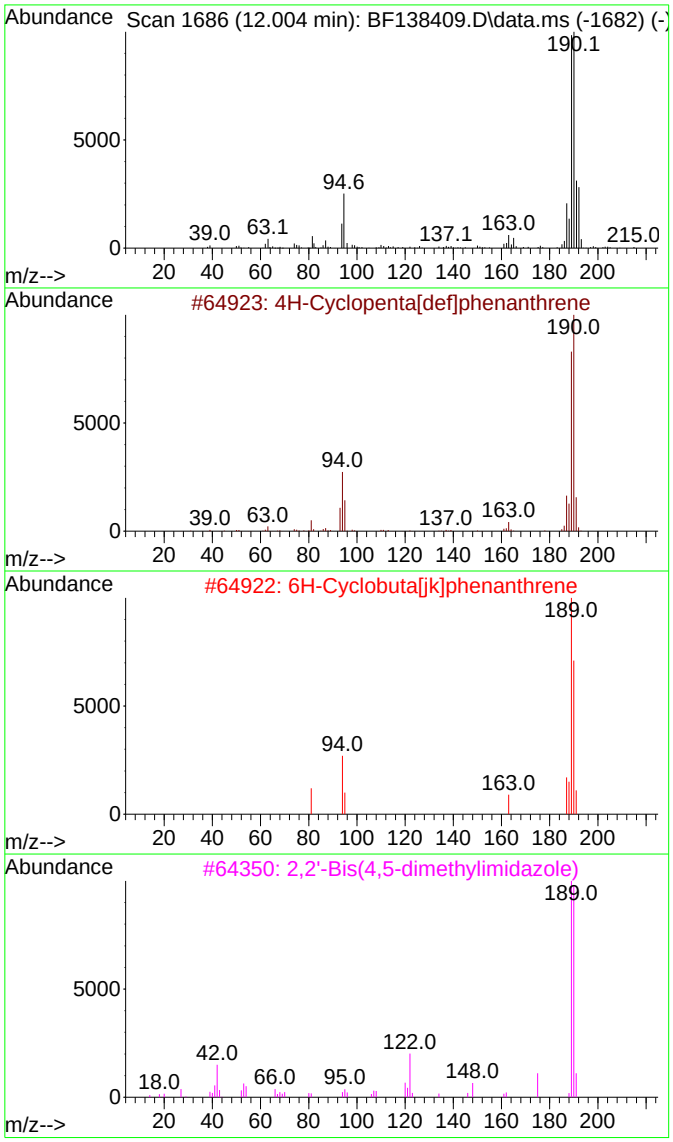
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

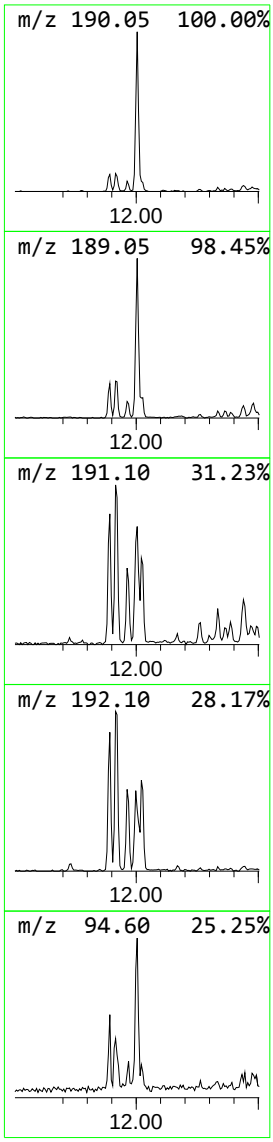
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	3.38 ng	207784	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





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Data File : BF138409.D
Acq On : 01 Jul 2024 18:06
Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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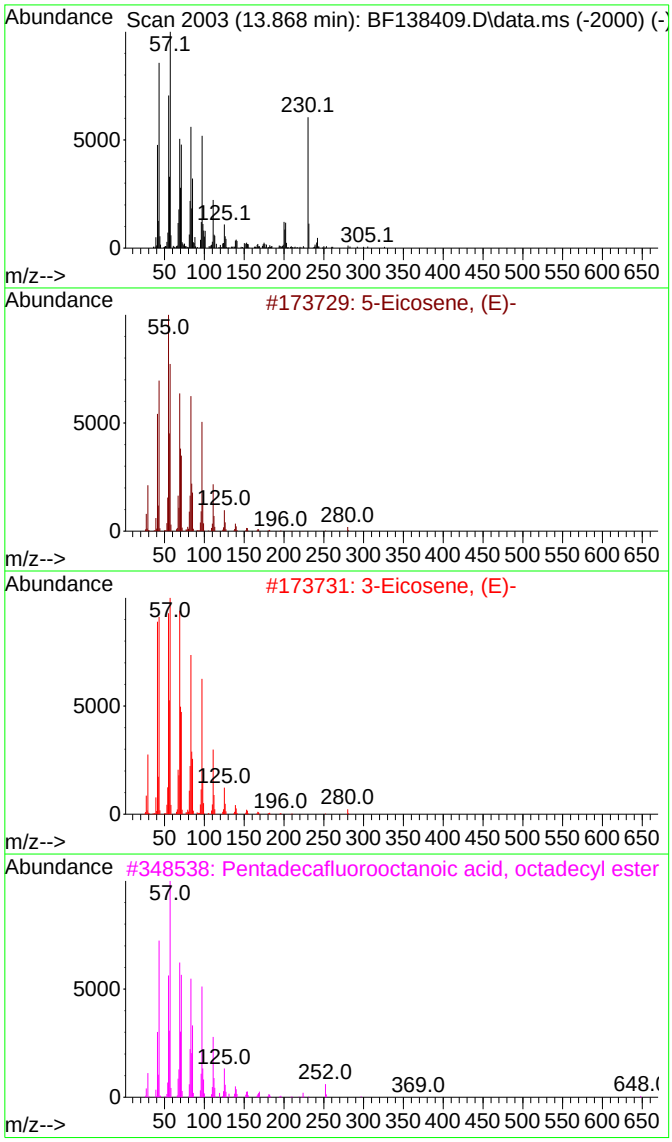
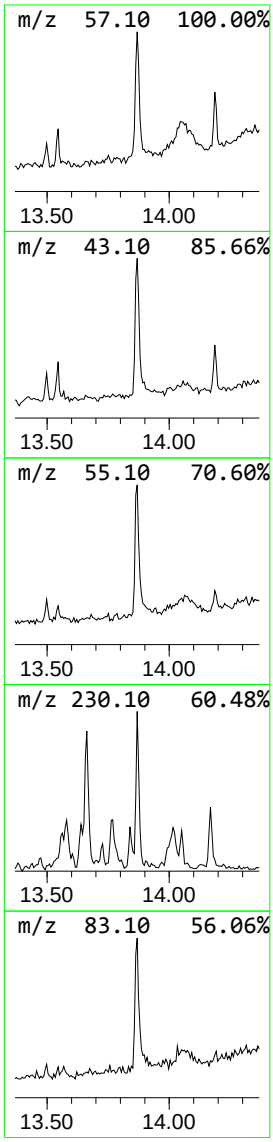
Peak Number 8 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	3.85 ng	338996	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	89
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	86
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	86
4	Cyclopentadecane	210	C15H30	000295-48-7	80
5	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	70





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Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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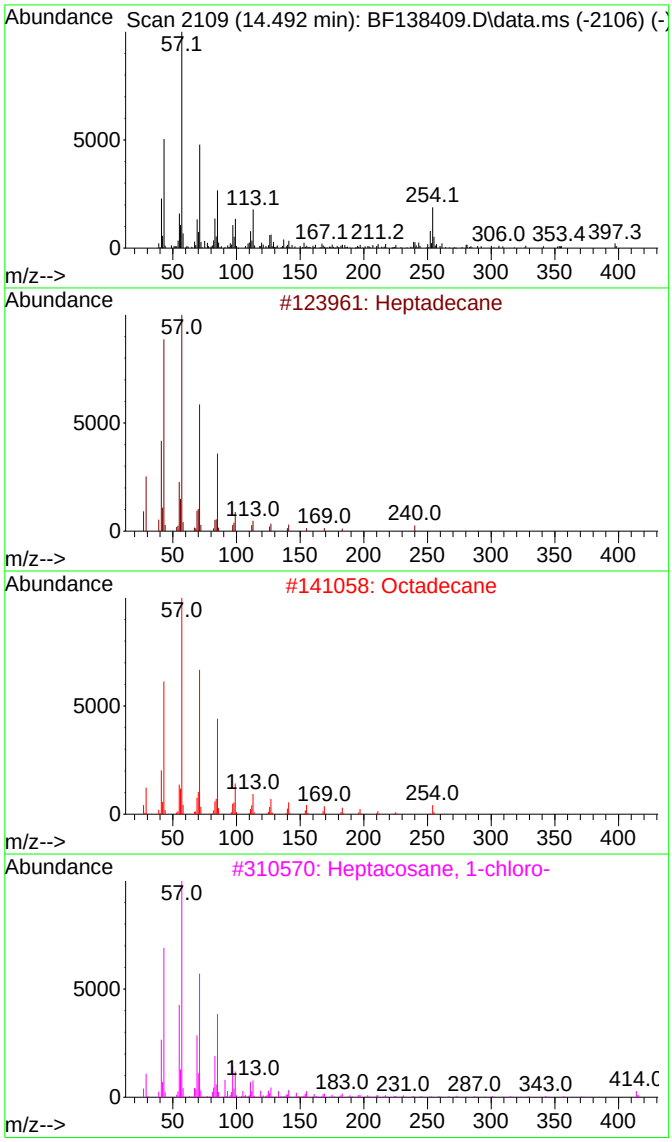
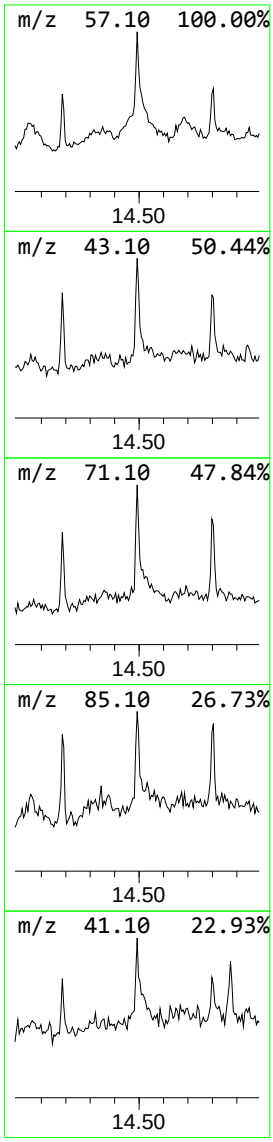
Peak Number 9 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.01 ng	176882	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Octadecane	254	C18H38	000593-45-3	81
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
4	Tetracosane	338	C24H50	000646-31-1	68
5	Tridecane, 5-propyl-	226	C16H34	055045-11-9	64





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Acq On : 01 Jul 2024 18:06
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Sample : P3076-13
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Instrument :
BNA_F
ClientSampleId :
7-B-1

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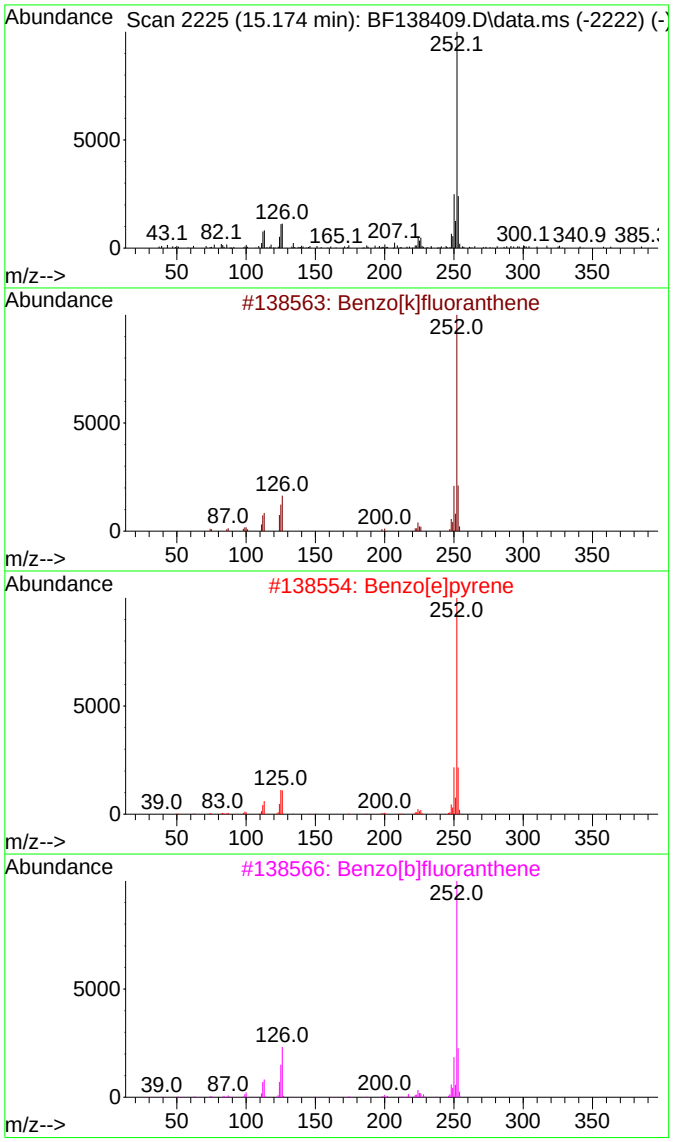
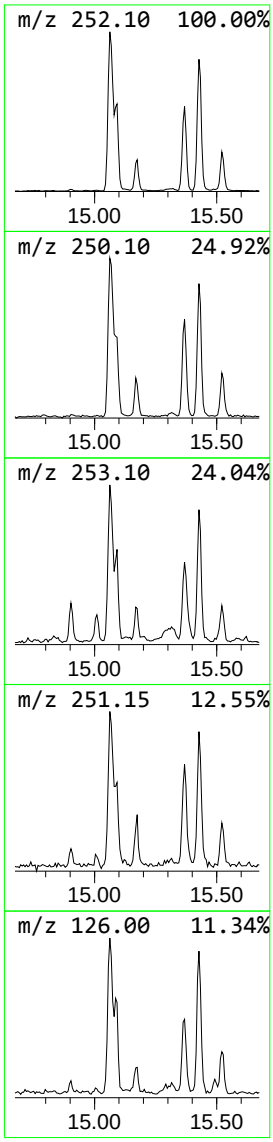
Peak Number 10 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	2.30 ng	88389	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	86
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Perylene	252	C20H12	000198-55-0	81





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Operator : CG\JU
Sample : P3076-13
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
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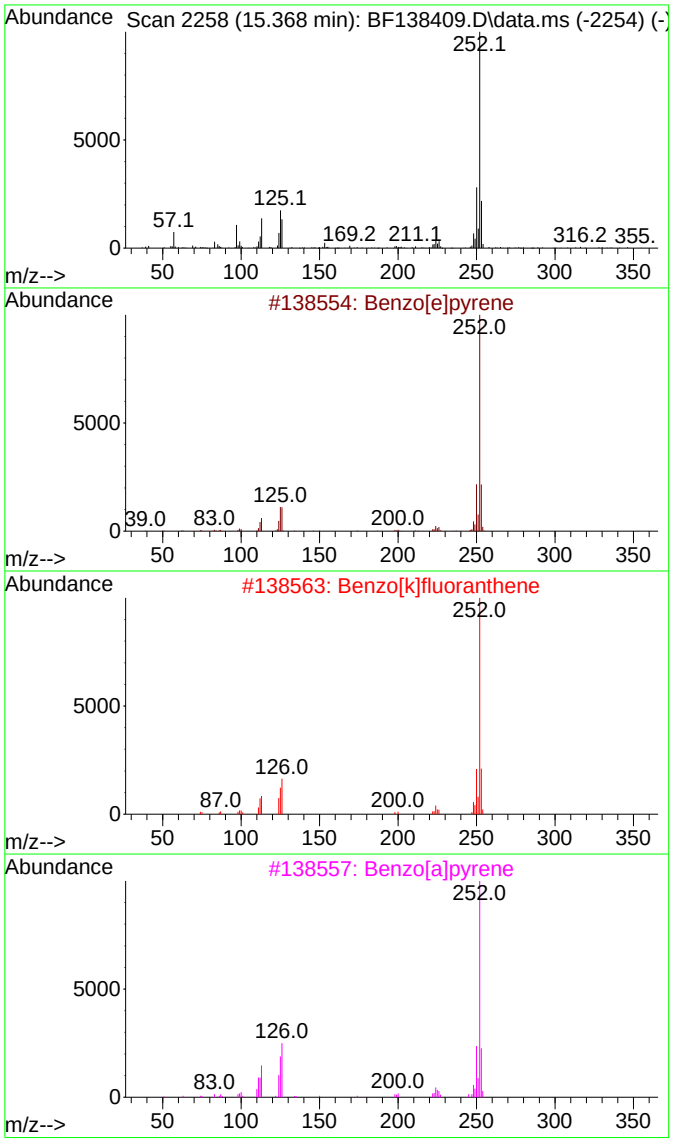
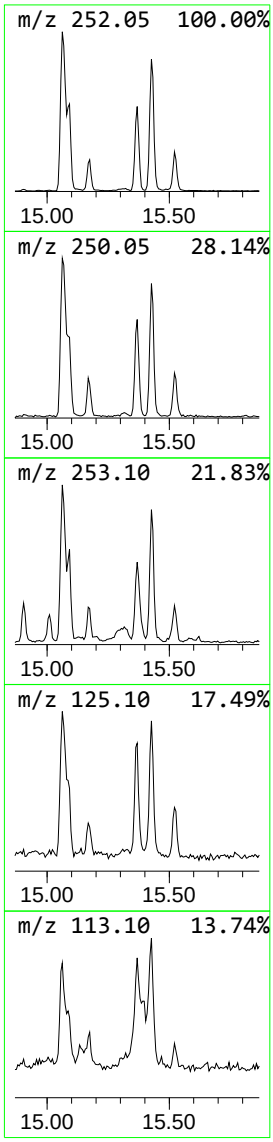
Peak Number 11 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	7.95 ng	305958	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[a]pyrene	252	C20H12	000050-32-8	91
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

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Operator : CG\JU
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BNA_F
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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
Butane, 2-metho...	2.181	45.9	ng	2902840	1	6.875	1263920	20.0
(S)-(+)-1,2-Pro...	3.404	5.3	ng	333699	1	6.875	1263920	20.0
2-Pentanone, 4-...	5.098	6.2	ng	391903	1	6.875	1263920	20.0
1-Phenoxypropan...	8.463	2.9	ng	234894	2	8.151	1597620	20.0
unknown10.004	10.004	2.3	ng	173649	3	9.904	1502580	20.0
Anthracene, 1-m...	11.916	4.8	ng	296842	4	11.392	1230770	20.0
4H-Cyclopenta[d...	12.004	3.4	ng	207784	4	11.392	1230770	20.0
5-Eicosene, (E)-	13.868	3.9	ng	338996	5	14.027	1759760	20.0
Heptadecane	14.492	2.0	ng	176882	5	14.027	1759760	20.0
Benzo[e]pyrene	15.174	2.3	ng	88389	6	15.492	769275	20.0
Benzo[j]fluoran...	15.368	8.0	ng	305958	6	15.492	769275	20.0