

Appendix OA7. Biomarker peak heights. Numbers in red are poor data quality.											
Sample #	Job #	Seq	C26 data quality	C26 24-nor 20S Ba Dia	C26 24-nor 20R Ba Dia	C26 27-nor 20S Ba Dia	C26 27-nor 20R Ba Dia	C26 24-nor 20S	C26 24-nor 20R aBB	C26 24-nor 20S aBB	C26 21-nor + 24-nor
				Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane
1	96074	002	F								
2	96074	001	F								
3	97016	002	OK	1525	950	1265	1059	863	950	863	1500
4	97016	003	OK	476	410	1434	1014	346	569	346	1420
5	96074	006	F								
6	97012	005	F								
7	97012	001	C	3060	2002	5399	3406	1739	2510	1739	3160
8	97016	001	OK	1746	978	1466	930	880	1108	880	1794
9	97012	002	C	1614	1119	2235	1795	899	1419	899	1600
10	97012	003	D	1540	1135	2309	1571	1041	1203	1041	1548
11	97012	004	C	2252	1615	3892	2855	1816	1912	1816	2622
12	97012	009	OK	4104	3068	6218	4827	2284	3251	2284	4413
13	97012	010	F	1499	653	1527	1141	922	1043	922	1237
14	97012	006	F								
15	97012	008	C	1943	1490	3005	2262	1542	1520	1542	2182
16	97012	007	C	3177	2447	5225	3784	2077	2964	2077	4106
17	97010	026	C	580	441	850	610	347	520	347	569
18	97037	002	OK F	1561	5152	1849	2260	1343	888	1343	936
19	96074	008	F								
20	97037	001									
21	96074	009	C F	1265	5187	1539	2046	922	807	922	537
22(12.1-29	85172	002	OK	4802	3414	2578	1715	1939	2462	1939	2319
23	95069	001	OK	2076	1709	1580	1258	1077	1505	1077	906
24	95069	002	OK	1434	1144	701	679	618	1591	618	1217
25	95069	003	C	791	517	742	415	484	394	484	716
26	95069	007	D	873	628	639	465	425	651	425	832
27	97056	001	F								
28	97035	001	OK F	2646	7168	2567	4454	715	961	715	688
29	97010	027	F	404	373	611	361	254	341	254	341
30	97010	028	D	393	415	1379	746	259	415	259	393
31A	97009	001	D	232	250	447	359	388	272	388	549
31B	97009	008	C	408		564	389	588			704
31C	97009	012	F		282	679	227	309	263	309	542
31D	97009	018									
33A	97009	002	C	3223	2121	2022	1480	841	1113	841	2441
34A	97009	004	F	838	640	1134	923	838			
34B	97009	006	F	793	827	1247	853	814	836	814	663
34C	97009	010	D	598	515	1184	678	617	689		
34D	97009	014	F			579	308	195		195	311
38B	97009	044	F								
42A	97009	025	F	207	164	441	266	269	231	269	347
42B	97009	039	F			712		333			316
42C	97009	053									
42D	97009	065									
43	96074	007									

Appendix OA7. Bior												
Sample #	Job #	Seq	C26 27-nor 20S aaa	C26 27-nor 20R aBB	C26 27-nor 20S aBB	C26 27-nor 20R aaa	File:	C27 data quality	C27 20S Ba Dia	C27 20R Ba Dia	C27 20S aB Dia	C27 20R aB Dia
			Sterane	Sterane	Sterane	Sterane		Sterane	Sterane	Sterane	Sterane	Sterane
1	96074	002					96074602.RST	OK	7238	4738	1543	1777
2	96074	001					96074601.RST	OK	6580	4168	1108	1870
3	97016	002	766	915	944	798	97016602.RST	OK	25639	16984	5061	7381
4	97016	003	1493	1788	1645	1288	97016603.RST	OK	10940	6736	2140	3084
5	96074	006					96074606.RST	OK	6331	4188	1387	1635
6	97012	005					97012605.RST	OK	23414	15550	4169	6320
7	97012	001	1939	2729	2657	1762	97012601.RST	OK	60327	37914	11940	17244
8	97016	001	958	862	811	949	97016601.RST	OK	29117	18450	5377	8172
9	97012	002	1125	1828	1809	1065	97012602.RST	OK	31371	19613	5587	7870
10	97012	003	1342	1256	1350	743	97012603.RST	OK	28285	18399	4990	6565
11	97012	004	1903	2680	2415	1482	97012604.RST	OK	47929	32007	9228	13119
12	97012	009	2477	5137	3452	2593	97012609.RST	OK	92685	61028	17964	25440
13	97012	010	712	964	963	906	97012610.RST	OK	19536	12568	3317	4953
14	97012	006					97012606.RST	OK	15776	10341	2820	4214
15	97012	008	1707	2373	2261	1280	97012608.RST	OK	48063	32086	9169	12713
16	97012	007	2721	4590	3875	2065	97012607.RST	OK	82397	54012	15552	21625
17	97010	026	384	646	575	322	97010626.RST	OK	9849	6487	2121	2696
18	97037	002	880	1459	1181	2930	97037602.RST	F	2050	1826	1088	1974
19	96074	008					96074608.RST	F	699	801	878	694
20	97037	001										
21	96074	009	702	1145	1100	3374	96074609.RST	F	1368	1142	1862	1863
2(12.1-29	85172	002	1042	1040	1413	915	98999701.RST	OK	53323	38246	11271	14732
23	95069	001	229	791	730	220	95069601.RST	OK	36141	22945	7437	9625
24	95069	002	523	1120	489	330	95069602.RST	OK	13135	9167	3001	4049
25	95069	003	309	416	364	350	95069603.RST	OK	8645	5965	1899	2303
26	95069	007	379	339	445	565	95069607.RST	OK	11432	7052	2237	3146
27	97056	001					97056601.RST	OK	7778	4545	1652	1822
28	97035	001	750	704	563	1189	97035601.RST	F	1825	1822	1464	3088
29	97010	027		343	146		97010627.RST	OK	5933	4117	1436	1588
30	97010	028	418	550	566	423	97010628.RST	OK	17535	11460	3432	4839
31A	97009	001	600	511	386	609	97009601.RST	OK	2018	1213	652	823
31B	97009	008	920	824	799	824	97009608.RST	OK	1042	1117	879	1118
31C	97009	012		548	471	525	97009612.RST	C	597	438	574	473
31D	97009	018										
33A	97009	002	739	850	721	949	97009602.RST	OK	51098	30643	8322	11311
34A	97009	004					97009604.RST	OK	13134	7488	1973	2599
34B	97009	006	667		770	507	97009606.RST	OK	11298	6743	2106	2931
34C	97009	010	800	627		540	97009610.RST	OK	7511	5242	1630	2246
34D	97009	014				201	97009614.RST	OK D	2066	1448	464	511
38B	97009	044					97009644.RST	OK	9813	6358	1828	2319
42A	97009	025	221	198	267	129	97009625.RST	OK	2967	2155	749	822
42B	97009	039		263			97009639.RST	OK	1883	1381	611	804
42C	97009	053										
42D	97009	065										
43	96074	007										

Appendix OA7. Bio													
Sample #	Job #	Seq	C27 Dia 1	C27 Dia 2	C27 Dia 3	C27 20S aaa	C27 20R aBB	C27 20S aBB	C27 20R aaa	File:	C28 20S Ba Dia (I)	C28 20S Ba Dia (II)	C28 20R Ba Dia (I)
			Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane		Sterane	Sterane	Sterane
1	96074	002	1455	1404	1123	3394	4345	3808	2810	96074702.RST	3023	3264	1987
2	96074	001	1261	1676	944	2811	3659	3509	2595	96074701.RST	2578	2701	1845
3	97016	002	4146	5167	3178	15124	12656	11407	15088	97016702.RST	17818	18608	12820
4	97016	003	2279	2536	1885	7429	9325	8793	6865	97016703.RST	3863	4203	2735
5	96074	006	1220	1073	733	3167	2598	2426	2758	96074706.RST	3024	2975	2160
6	97012	005	2906	4441	3084	18872	10074	9810	21443	97012705.RST	16424	17401	11319
7	97012	001	10047	11245	6732	27540	26607	26778	27597	97012701.RST	38104	40756	32346
8	97016	001	4581	5888	3600	19492	15332	13767	19095	97016701.RST	19033	20378	13089
9	97012	002	4302	4665	3137	13633	12459	11664	12753	97012702.RST	19303	19622	12975
10	97012	003	3864	4320	2480	11731	12340	11840	9800	97012703.RST	17057	16921	10219
11	97012	004	8555	10042	5286	21842	25531	24729	19994	97012704.RST	30388	31620	24619
12	97012	009	13649	16858	9025	48863	36787	34878	51462	97012709.RST	58849	62171	48925
13	97012	010	2479	2677	1819	7948	8229	7778	6456	97012710.RST	11529	11791	7554
14	97012	006	2327	2621	1523	6989	7759	7055	6138	97012706.RST	9933	10566	6643
15	97012	008	7436	8202	4746	21425	22551	22158	17914	97012708.RST	29171	28494	21189
16	97012	007	13464	15045	8689	39257	33365	31449	36311	97012707.RST	50711	53617	42731
17	97010	026	1808	1946	1310	4951	4911	4471	4471	97010726.RST	5364	5816	3453
18	97037	002	1337	1690	848	1687	1378	981	1216	97037702.RST	1328	1735	1646
19	96074	008	975	1015	930	827	1217	1017	1014	96074708.RST	1043		1107
20	97037	001											
21	96074	009	923	1151	932	1331	1131	994	1179	96074709.RST	1002	949	1288
22(12.1-29)	85172	002	7107	7184	4293	16013	17682	16562	13401	98999801.RST	38667	43336	28743
23	95069	001	4312	4798	3197	6523	10252	10546	1645	95069701.RST	23598	25755	16311
24	95069	002	1480	2117	991	4994	2025	2915	4488	95069702.RST	10570	11461	6901
25	95069	003	1311	1295	872	3664	2978	2775	3491	95069703.RST	6103	6561	4109
26	95069	007	1490	1613	1107	4665	3729	3560	3659	95069707.RST	7398	7879	5251
27	97056	001	955	1209	903	3941	1887	1695	4471	97056701.RST	5047	5413	3581
28	97035	001	1520	1540	1658	1374	1639	1092		97035701.RST	1713	1868	1296
29	97010	027	907	942	679	1930	2175	2148	2104	97010727.RST	3080	3419	2263
30	97010	028	2265	2404	1339	5836	5143	5162	5215	97010728.RST	6945	7687	4901
31A	97009	001	1111	1685	1232	5156	2682	2536	4245	97009701.RST	521	580	441
31B	97009	008	1486	2543	2079	5827	3323	3212	4648	97009708.RST	373	634	449
31C	97009	012	920	1141	1005	1993	2016	1711	1460	97009712.RST	121	379	169
31D	97009	018											
33A	97009	002	4505	6730	3358	23004	7186	5802	24131	97009702.RST	53531	59281	33152
34A	97009	004	1708	1707	1041	3472	3472	3226	2731	97009704.RST	4452	4931	3030
34B	97009	006	1920	1666	1440	3389	3734	3336	2331	97009706.RST	4454	4730	3294
34C	97009	010	1464	1653	1127	2236	2406	2292	1569	97009710.RST	3069	3062	2259
34D	97009	014	304	450	257	540	456	536	390	97009714.RST	643	648	518
38B	97009	044	1248	1577	944	3280	2387	2068	2426	97009744.RST	4986	5516	3510
42A	97009	025	421	693	276	2063	596	431	3325	97009725.RST	1405	1440	901
42B	97009	039	425	875	288	1518	574	560	1542	97009739.RST	866	867	599
42C	97009	053											
42D	97009	065											
43	96074	007											

Appendix OA7. Bio														
Sample #	Job #	Seq	C28 20R Ba Dia (I)	C28 20S aB dia	C28 20R aB Dia	C28 20S aaa (I)	C28 20S aaa (II)	C28 20R aBB	C28 20S aBB	C28 20R aaa	File:	C28 data quality	C29 20S Ba Dia	
			Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane		Sterane	Sterane	
1	96074	002	2079	1075	1060	1335	1736	3286	3272	1923	96074802.RST	OK	7553	
2	96074	001	1868	1187	1023	1628	1412	2507	2763	1740	96074801.RST	OK	6510	
3	97016	002	13999	6952	6590	8910	8474	15186	14762	15668	97016802.RST	OK	18422	
4	97016	003	2995	2406	1842	2497	2721	5765	5942	3640	97016803.RST	OK	10564	
5	96074	006	2584	1354	1223	1286	1618	3135	2537	2327	96074806.RST	OK	9241	
6	97012	005	12892	6725	5612	10583	10805	14411	12359	25026	97012805.RST	OK	21146	
7	97012	001	30417	16415	15859	18906	17054	32897	30901	29288	97012801.RST	OK	55141	
8	97016	001	15393	7437	6695	10022	10396	17015	16200	18061	97016801.RST	OK	18150	
9	97012	002	13911	7431	6500	6831	6821	14552	14262	13549	97012802.RST	OK	27940	
10	97012	003	11766	6241	5301	6204	6160	13379	13230	8799	97012803.RST	OK	22212	
11	97012	004	23839	11623	11424	13714	14133	31122	30863	20841	97012804.RST	OK	42668	
12	97012	009	47895	23033	22979	28410	26240	48255	40936	57779	97012809.RST	OK	85822	
13	97012	010	8388	4243	3679	3543	3884	8785	8268	5590	97012810.RST	OK	16578	
14	97012	006	6941	4211	3322	4140	3922	8491	8386	5789	97012806.RST	OK	14276	
15	97012	008	23019	11148	10568	12970	13264	30426	27847	19510	97012808.RST	OK	42386	
16	97012	007	41780	19018	19421	24718	23149	40549	36959	39116	97012807.RST	OK	78185	
17	97010	026	4302	2359	2159	2767	2816	5031	4948	4183	97010826.RST	OK	7568	
18	97037	002	1450	1140	1566	1271	1352	2279	2299	1642	97037802.RST	F	3164	
19	96074	008		1324	1192		1708	1622		962	96074808.RST	F	4134	
20	97037	001												
21	96074	009		951	1448	1084	2195		1859	1336	96074809.RST	F	3118	
22(12.1-29)	85172	002	29591	14526	13046	10647	11368	25238	24998	14982	98999901.RST	OK	47763	
23	95069	001	18365	9814	8622	3848	1924	15419	14364	2624	95069801.RST	OK	30594	
24	95069	002	7727	4382	3676	2449	2913	2595	3408	4910	95069802.RST	OK	9099	
25	95069	003	4578	2284	2113	1920	1991	4162	3858	3242	95069803.RST	OK	10561	
26	95069	007	6020	2735	2665	2229	2354	5036	4006	4030	95069807.RST	OK	12448	
27	97056	001	4301	2287	1778	2235	2305	3282	2493	5164	97056801.RST	OK	15155	
28	97035	001	2065	2649	2099	1498	1629	2827	2084	2360	97035801.RST	F	4891	
29	97010	027	2392	1418	1152	1203	1117	2140	2149	1573	97010827.RST	OK	6877	
30	97010	028	5468	3228	2755	2276	2318	4443	4578	3288	97010828.RST	OK	20220	
31A	97009	001	611	423	331	1716	1739	1760	1733	2249	97009801.RST	OK	1007	
31B	97009	008	575	517	366	2306	2053	2662	2463	2543	97009808.RST	OK	718	
31C	97009	012	266	582	371	970	840	1375	1175	859	97009812.RST	C	497	
31D	97009	018												
33A	97009	002	37196	16534	13422	11791	12296	12068	9529	24075	97009802.RST	OK	31025	
34A	97009	004	3708	1663	1489	1291	1501	2895	2997	1718	97009804.RST	OK	8703	
34B	97009	006	3377	1820	1520	1331	1595	2933	2660	1540	97009806.RST	OK	8131	
34C	97009	010	2320	1637	1140	1197	1129	2120	1767	1252	97009810.RST	OK	4517	
34D	97009	014	574	442	342	218	259	343	387	334	97009814.RST	D	871	
38B	97009	044	3879	2071	1514	1328	1575	2346	1835	1640	97009844.RST	OK	5249	
42A	97009	025	1145	767	529	439	462	674	527	1425	97009825.RST	C	2411	
42B	97009	039	613	611	412	329	259	524	441	672	97009839.RST	C	1497	
42C	97009	053												
42D	97009	065												
43	96074	007												

Appendix OA7. Bior													
Sample #	Job #	Seq	C29 20R Ba Dia	C29 Dia 1	C29 Dia 2	C29 20S aaa	C29 20R aBB	C29 20S aBB	C29 20R aaa	File:	C30 data quality	C30 20S Ba Dia	C30 20R Ba Dia
			Sterane	Sterane	Sterane	Sterane	Sterane	Sterane	Sterane		Sterane	Sterane	Sterane
1	96074	002	4238	1628	1934	4181	6417	5155	3750	96074902.RST	C	1507	1090
2	96074	001	3706	1233	1856	3483	5897	4551	3212	96074901.RST	C	1349	1076
3	97016	002	11972	4706	5987	13517	17527	13683	15143	97016902.RST	OK	6511	4619
4	97016	003	6868	2354	3278	10520	16271	13726	9402	97016903.RST	OK	1684	1421
5	96074	006	6195	2216	2738	4210	6413	4232	10889	96074906.RST	C	1483	1166
6	97012	005	12836	4734	6227	18575	19272	12685	27767	97012905.RST	OK	6612	4982
7	97012	001	38613	14328	17479	33930	48229	37593	41323	97012901.RST	OK	18038	13141
8	97016	001	11347	4552	6026	16080	17936	14340	17272	97016901.RST	OK	7555	5295
9	97012	002	17733	6788	8102	16598	23723	16053	27224	97012902.RST	OK	7260	5303
10	97012	003	14785	5214	6412	14408	20111	17097	12255	97012903.RST	OK	6795	5373
11	97012	004	28064	9979	12251	29026	41322	35087	25240	97012904.RST	OK	12379	9424
12	97012	009	61510	21397	29291	53858	75598	52161	104155	97012909.RST	OK	25016	19246
13	97012	010	10400	3621	4834	8784	13486	10641	8225	97012910.RST	OK	4956	3273
14	97012	006	9600	3175	4022	8692	12749	10420	8422	97012906.RST	OK	3789	2752
15	97012	008	27678	10680	12728	25273	37391	30638	22222	97012908.RST	OK	13667	10115
16	97012	007	52396	18205	23831	53025	61749	44856	58903	97012907.RST	OK	22253	17625
17	97010	026	4694	2252	2486	5285	6513	5321	4747	97010926.RST	OK	2042	1567
18	97037	002	2614	1521	2211	1428	2352	2013	1303	97037902.RST	F	1210	1479
19	96074	008	3080	2837	2636	1841	4220	2907	1410	96074908.RST	F	2349	2861
20	97037	001											
21	96074	009	2544	2427	1747	1205	2024	2120	2013	96074909.RST	F	922	1136
22(12.1-29)	85172	002	32471	11681	15135	23742	30767	24832	21865	98999001.RST	OK	14215	10582
23	95069	001	20374	7769	9837	7162	24053	17262	0	95069901.RST	OK	9277	7090
24	95069	002	6051	2374	2994	3998	3678	2945	5977	95069902.RST	OK	3129	2205
25	95069	003	6666	2414	3167	6610	10194	6099	15249	95069903.RST	OK	1744	1362
26	95069	007	8045	2836	3706	7598	12095	7854	18266	95069907.RST	OK	2387	1659
27	97056	001	10023	3374	4885	9537	10001	4865	21335	97056901.RST	C	1730	1262
28	97035	001	3803	2785	2314	1760	3887	2852	3149	97035901.RST	F	1476	1813
29	97010	027	4635	2022	2279	3261	4980	3582	4558	97010927.RST	OK	1147	1067
30	97010	028	13923	4847	6516	7526	10029	8871	7312	97010928.RST	OK	3074	2409
31A	97009	001	753	467	509	3539	3078	2197	2921	97009901.RST	OK	277	294
31B	97009	008	539	608	406	4982	4265	2859	3573	97009908.RST	OK	428	342
31C	97009	012	353	391	272	1182	1607	1242	924	97009912.RST	D	369	268
31D	97009	018											
33A	97009	002	17842	6340	7357	13269	12811	6930	17638	97009902.RST	OK	10576	7788
34A	97009	004	4807	1629	1994	2993	4044	3496	2165	97009904.RST	D	1569	1194
34B	97009	006	5126	1750	1898	2775	4133	3145	2127	97009906.RST	D	1529	1221
34C	97009	010	3031	1076	1603	1738	2427	1926	1217	97009910.RST	D	1155	776
34D	97009	014	669	260	391	401	391	231	277	97009914.RST	F		
38B	97009	044	3113	1266	1305	2147	2329	1704	1821	97009944.RST	D	1320	1104
42A	97009	025	1575	700	670	755	1385	532	1790	97009925.RST	C	431	296
42B	97009	039	921	447	612	669	776	398	864	97009939.RST	F	347	320
42C	97009	053											
42D	97009	065											
43	96074	007											

Appendix OA7. Bio																										
Sample #	Job #	Seq	C30 Dia 1	C30 Dia 2	C30 20S aaa	C30 20R aBB	C30 20S aBB	C30 20R aaa	File:	C19 Tricyclic	C20 Tricyclic	C21 Tricyclic	C22 Tricyclic													
			Sterane	Sterane	Sterane	Sterane	Sterane	Sterane		Terpane	Terpane	Terpane	Terpane													
1	96074	002	666	698	1402	1750	2091	1415	96074102.RST	39643	109550	208911	37207													
2	96074	001	677	709	852	1419	1570	1027	96074101.RST	61319	193209	344535	103973													
3	97016	002	2538	2093	5072	6308	7097	7825	97016102.RST	2764	7028	9551	6163													
4	97016	003	604	540	1291	1889	2086	1453	97016103.RST	15983	42771	42504	25231													
5	96074	006	736	649	1093	1386	1915	1350	96074106.RST	74214	216420	329764	162207													
6	97012	005	2563	2069	7057	5018	7540	11160	97012105.RST	22397	54156	207665	114670													
7	97012	001	6098	4524	9937	16554	15228	13505	97012101.RST	56388	133833	291196	118597													
8	97016	001	2994	2055	6539	7702	8383	8881	97016101.RST	3495	6407	10125	4986													
9	97012	002	3173	1922	4670	6384	6568	6355	97012102.RST	59587	158754	488252	206937													
10	97012	003	2330	2171	4075	6271	6519	4509	97012103.RST	114467	213666	519447	183589													
11	97012	004	4623	3489	8908	16693	15439	9766	97012104.RST	7455	44693	176074	89510													
12	97012	009	8596	7619	17808	24278	25162	27555	97012109.RST	51511	179991	516806	228705													
13	97012	010	1763	1396	2508	4148	4331	2948	97012110.RST	24226	49379	153044	79422													
14	97012	006	1437	1143	2289	3786	4097	3054	97012106.RST	12093	57805	190715	80138													
15	97012	008	4622	3158	8047	13837	14634	9633	97012108.RST	74514	236875	819099	382297													
16	97012	007	7798	6301	15131	22551	20710	19387	97012107.RST	77040	170518	526261	247033													
17	97010	026	777	696	1789	2316	2559	2128	97010126.RST	80259	212741	377062	140713													
18	97037	002	1047	1404	1546	1118			97037102.RST	5153	5352	16084	5614													
19	96074	008	1527	1779	1868	2132		2407	96074108.RST		9916	18145	16494													
20	97037	001							97037101.RST	3488	6883	13439	5785													
21	96074	009		1131	964	768		1298	96074109.RST	77696	108242	227651	66378													
2(12.1-29	85172	002	5218	3563	7285	10900	11588	8972	85172102.RST	327	339	317	90													
23	95069	001	3224	2219	5543	6799	7831	8664	95069101.RST	17958	9164	6192	6516													
24	95069	002	1227	1105	1620	1455	2190	2901	95069102.RST	9451	10233	12045														
25	95069	003	719	586	1007	1375	1714	1413	95069103.RST			278														
26	95069	007	821	585	1354	1835	1764	1630	95069107.RST	22188	12614	15037	4293													
27	97056	001	1300	680	1187	1378	897	2092	97056101.RST	6453	5522	7557	2346													
28	97035	001	1246	1270	1425		1272		97035101.RST	21450	11345	23128	9039													
29	97010	027	564	629	794	1032	1067	731	97010127.RST	105982	124512	278354	15219													
30	97010	028	1169	697	1520	2161	2224	1588	97010128.RST	58974	35348	124350	20151													
31A	97009	001	223	471	1196	831	968	1090	97009101.RST	445607	1589647	2532716	554027													
31B	97009	008	265	964	1670	1077	1406	1502	97009108.RST	530872	1815839	3162752	564044													
31C	97009	012	143	429	589	561	681	441	97009112.RST	310155	903955	992829	172450													
31D	97009	018							97009118.RST	146161	262354	65175	17620													
33A	97009	002	3297	2496	5406	4080	4370	8603	97009102.RST	121802	276726	513879	63199													
34A	97009	004	684	730	972	1050	1244	1060	97009104.RST	50393	110755	226182	64082													
34B	97009	006	782	849	870	1013	1310	971	97009106.RST	103351	98510	183604	48724													
34C	97009	010	490	552	469	673	644	436	97009110.RST	106034	84992	83711	22800													
34D	97009	014	305						97009114.RST	59515	41928	18139	11905													
38B	97009	044	632	592	862	844	1010	724	97009144.RST	250040	358020	344662	42525													
42A	97009	025	137	182	219	326	439	487	97009125.RST	161007	162671	236533	37197													
42B	97009	039	178	304	243	175	307	321	97009139.RST	87031	80819	101910	18880													
42C	97009	053							97009153.RST	71595	67603	46154	19530													
42D	97009	065							97009165.RST	25180	16733	1435	7971													
43	96074	007							96074107.RST	63232	70092	93760	33298													

Appendix OA7. Bio												
Sample #	Job #	Seq	C23 Tricyclic	C24 Tricyclic	C25 Tricyclic	C26 22S Tricyclic	C26 22R Tricyclic	C24* Tetracyclic	C28 22S Tricyclic	C28 22R Tricyclic	C29 22S Tricyclic	C29 22R Tricyclic
			Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane
1	96074	002	406682	369472	274965	169478	156304	127822	170557	150123	233908	246871
2	96074	001	933726	700777	433020	276246	252152	232089	262272	264146	356475	369797
3	97016	002	24435	12170	13101	6165	5308	9449	10996	9629	16255	15288
4	97016	003	132423	82195	46416	24627	27343	54168	21961	28532	30982	23538
5	96074	006	1002853	611874	379578	229176	220764	223708	238139	243239	273989	301692
6	97012	005	1050481	750556	601299	349820	316841	351663	467717	437513	573943	649566
7	97012	001	1000266	866389	599439	420668	389987	269529	483509	486370	650266	696219
8	97016	001	30421	19660	17130	7644	8393	7245	7670	6953	7430	10845
9	97012	002	1752837	1328355	806171	534459	493304	433430	568348	505731	767481	827745
10	97012	003	1305398	967358	510258	353952	315782	311120	342971	354286	448280	477672
11	97012	004	755253	579224	390209	249174	234791	203598	267020	270807	364966	375407
12	97012	009	2074816	1490752	1150928	688613	633586	538321	771979	769579	961556	1014377
13	97012	010	900006	798892	802924	575996	542629	387101	758510	773976	1008707	1090519
14	97012	006	654354	479642	263511	210154	183326	231790	211422	189762	262787	276225
15	97012	008	3266534	2435902	1753211	1036108	961556	846308	1087912	1082141	1420042	1514909
16	97012	007	2311874	1711066	1328079	776550	724894	700665	871019	878703	1119930	1208232
17	97010	026	924237	667103	391671	259377	236380	222784	275751	263601	345471	378206
18	97037	002	26581	20728	19799	10224	9691	10561	14253	13826	16961	19906
19	96074	008	69043	48245	51985	35501	31559	52297	18180	57800	27110	45126
20	97037	001	32467	26177	24496	12610	11073	12446	3613	8466	2064	3205
21	96074	009	464088	363204	348393	184069	161389	188287	58011	109507	43013	72401
22(12.1-29)	85172	002	346	338	190	83	93	234	103	97	138	184
23	95069	001	88287	91794	87664	52689	45262	51228	61630	69176	87078	98076
24	95069	002	37252	27745	32607	9388	11562	11839	11515	17997	19116	16666
25	95069	003	353					225				
26	95069	007	37987	26539	21786	17277	9222	25242	13219	18985	27138	24691
27	97056	001	10501	7160	5489	3424	3351	7144	2812	3860	4651	5977
28	97035	001	42588	35493	27556	16943	15675	22226	19391	21388	3015	4028
29	97010	027	501994	449023	277019	212514	168865	265405	200515	242024	285442	306819
30	97010	028	187646	118082	87195	81934	62878	166533	101342	95053	134021	100789
31A	97009	001	2961202	1614862	686996	368568	344064	372465	261408	234625	253405	243728
31B	97009	008	3872711	2931442	1059351	711122	726301	584512	640172	622883	617158	608644
31C	97009	012	1269920	1058747	354819	258073	256758	258676	262393	261118	264760	241277
31D	97009	018	75432	47882	23350	14539	6497	29936	8907	12783	9649	3807
33A	97009	002	815170	403539	543975	203039	184644	241170	498737	278348	287319	378490
34A	97009	004	414286	375383	262487	125723	119526	131125	127899	112266	181936	200557
34B	97009	006	348407	315462	217636	108855	107916	186469	124123	121617	184558	210815
34C	97009	010	136955	121967	80318	44095	45096	128497	64667	50974	77638	77209
34D	97009	014	34525	20927	15695	8931	7740	21326	8493	7468	8702	12140
38B	97009	044	340028	140827	81214	72812	64465	204930	60357	45414	49569	57218
42A	97009	025	252193	121030	60577	53763	45654	100466	42651	38161	27744	39816
42B	97009	039	119821	54875	28447	22322	24012	47217	24605	23244	20092	19899
42C	97009	053	51303	23313	16493	11003	8791	26569	10681	8402	8223	7214
42D	97009	065	6271	5242	4292	3739	1647	2898				
43	96074	007	200900	137202	78353	48529	45166	85551	36696	36995	45574	60940

Appendix OA7. Bior													
Sample #	Job #	Seq	C30 22S Tricyclic	C27 18a Ts	C30 22R Tricyclic	C27 17a Tm	C31 22S Tricyclic	C31 22R Tricyclic	Bisnorhopane	C29 Norhopane	C29 18a Neonorhopane	C29 17B21a Normoretan	
			Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	
1	96074	002	187189	257354	190202	290613	123802	102853	77229	891686	258066	50916	
2	96074	001	281664	375920	274360	515141	190919	177640	123886	1522375	392507	46519	
3	97016	002	13226	18550	12569	21438	5669	7539	13114	66584	19532	10729	
4	97016	003	30442	53484	26262	102045	44336	15539	13038	357602	53125	23637	
5	96074	006	184256	335413	189717	509918	113873	90670	340643	1174502	402482	119012	
6	97012	005	584343	900307	481222	1489544	296312	177646	926529	4747722	1212557	517954	
7	97012	001	649844	906908	475229	702457	258174	182724	660552	2227059	836776	214594	
8	97016	001	25773	16036	5968	30923	1417	5411	4958	85835	20184	7129	
9	97012	002	747335	1059714	569945	903170	338376	252396	841361	3086514	1122640	359909	
10	97012	003	341599	682011	324875	484296	176216	147480	443972	1481139	588447	109036	
11	97012	004	152815	531291	273933	438049	154695	90964	462076	1493337	500709	103072	
12	97012	009	657045	1327746	729546	1567493	432296	302439	1344394	4407778	1471005	507457	
13	97012	010	485736	1185507	775231	901426	459473	364285	849375	2722237	1087681	204687	
14	97012	006	232351	482739	197645	327385	121889	95519	296592	948148	390926	79318	
15	97012	008	1099677	1860964	1061258	1880885	615586	482449	1716654	5113517	1897395	333208	
16	97012	007	981292	1523372	853407	1800164	513538	366473	1401662	5020109	1776780	493988	
17	97010	026	284709	475559	265917	537924	166436	131890	187052	1649405	481630	123803	
18	97037	002		53486	19988	43744	12716	8087	4596	144547	53040	8949	
19	96074	008	58494	781186	138830	361451	147275	170781	316716	140329	623344	229799	
20	97037	001		55097	3332	72330	10542	11389	22096	9288	77635	17760	
21	96074	009	57351	723038	127028	939947	127319	298707	297322	86073	1023803	217135	
22(12.1-29)	85172	002	400	567	155	615	126	32	420	1486	635	160	
23	95069	001	35276	260196	91558	80409	87283	100754	164082	56462	204906	80523	
24	95069	002	8256	61979	12100	66409	13397	9341	22679	177461	56547	22522	
25	95069	003		880		1407	700	300		2197	681	441	
26	95069	007	16899	132504		213295	78174		88602	474089	224697	154490	
27	97056	001		20943		29876	3627	23151	14302	80863	31153	21903	
28	97035	001		46697	7361	34831	15914	37465	170222	1031	56570	14253	
29	97010	027	244342	704349	243998	915403	304746	104102	150838	1952913	560511	346037	
30	97010	028	208763	548500	101690	408794	209215	77713	44273	1404518	795481	167010	
31A	97009	001	140531	153843	139064	673836	132504	71238	37115	1235777	101834	168925	
31B	97009	008	308395	148077	308825	1568823	332586	195576	51437	3063761	132775	427501	
31C	97009	012	145022	57144	146745	758428	160447	97260	19557	1227177	46504	159223	
31D	97009	018	7124	7822	2380	40170	9744	1889	2219	45447		5769	
33A	97009	002	273111	521214	307910	1036950	172515	94164	111808	2015504	543337	452285	
34A	97009	004	108532	317836	120738	381955	62891	38948	41027	886528	328940	50158	
34B	97009	006	119210	374984	129257	536143	83804	49985	33087	1266748	396168	87758	
34C	97009	010	52923	220040	57204	290552	39371	7341	15795	601946	189486	57439	
34D	97009	014	8363	30893	6523	28138	4626	4314	2511	53188	17786	7729	
38B	97009	044	6161	245760	39884	692247	19559	69845	231292	1410824	174848	297059	
42A	97009	025	5668	53902	23546	397585	5554	86396	4650	702983	18275	274321	
42B	97009	039	14151	22698	13051	210843	5144	28163	2907	373496	17501	121080	
42C	97009	053	5285	13105	6150	78136	2860	9666		131853	7353	30116	
42D	97009	065											
43	96074	007	42483	107991	44339	1004917	109541	15421	55804	1471152	132628	663870	

Appendix OA7. Bio											
Sample #	Job #	Seq	C30 Oleanane	C30 Hopane	C30 17B21a Moretane	C31 22S Hopane	C31 22R Hopane	C30 Gammacerane	C32 22S Hopane	C32 22R Hopane	C33 22S Hopane
			Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane	Terpane
1	96074	002		1605135	129732	640093	416538	90583	383520	269698	290498
2	96074	001		2447752	189736	983325	635443	132621	584591	398573	414841
3	97016	002	6924	150743	20823	75720	47934	11243	37738	28593	30967
4	97016	003	6484	318642	28685	115157	83870	33336	80020	34451	62272
5	96074	006	160359	1856495	232777	750020	517755	174118	440422	314446	335800
6	97012	005	424201	5801196	1431762	3741550	2660955	680216	2394100	1647238	1867440
7	97012	001	212418	4682030	607390	1793086	1161590	295529	1034599	746742	757345
8	97016	001	1395	153729	20674	69852	52956	13070	59523	41896	47152
9	97012	002	431226	5482332	994861	2249883	1582575	409106	1319453	955292	991599
10	97012	003	121938	3023076	303383	1122472	736445	168854	681697	485833	507142
11	97012	004	95654	2981914	261527	1172632	773504	165573	725025	510748	535255
12	97012	009	660722	5507634	1241832	3217706	2300201	640835	1879336	1417238	1458818
13	97012	010	246753	5061679	611203	2195456	1439228	370084	1383512	986740	1081351
14	97012	006	85251	1896639	202294	705216	444675	119323	416434	300033	312504
15	97012	008	143120	5504214	1035054	4183998	2799010	602282	2608396	1888428	1992638
16	97012	007	484173	5594408	1335300	3730097	2417170	632190	2261836	1622359	1714823
17	97010	026	40464	3397003	365713	1260724	859466	193102	817045	551071	571372
18	97037	002	5095	411222	59179	132116	83052	24273	82492	54771	57579
19	96074	008	526614	335850	171518	103745	168298	234506	78015	151633	62174
20	97037	001	26657	13645	8892	4849	2646	8403	1031	1253	1343
21	96074	009	340716	145013	65144	68704	84322	154538		76187	35267
22(12.1-29)	85172	002	1803	3921	579	1559	1184	439	1200	799	829
23	95069	001	364339	86322	60254	100094	25139	64107	26049	25150	66635
24	95069	002	13603	376057	82018	166850	116740	34067	74357	66566	52188
25	95069	003	1265	6150	693	1555	1140		718	576	400
26	95069	007	241777	1320590	259874	384172	282380	84716	171229	126063	103980
27	97056	001	38682	178671	51059	63624	41984	20813	32151	22687	22987
28	97035	001	56802	11125	14665	11186	1085	2005	65955	2233	
29	97010	027		3808964	817942	1121154	960631	314663	503908	416686	328567
30	97010	028		3917183	556816	1355126	899602	235900	830261	605817	563832
31A	97009	001		1197337	214597	384534	274742	84027	183693	132819	88421
31B	97009	008		3928949	706330	1007165	706532	209729	477211	367370	261856
31C	97009	012		1681474	294456	370862	273395	92410	215015	165268	117801
31D	97009	018		48466	11206	9087	8879	2226	4974	6802	
33A	97009	002	118105	3062543	752083	1077786	768268	295173	557541	456797	460656
34A	97009	004	6157	1794482	151848	858481	570586	75922	526696	366379	258352
34B	97009	006		2379523	225422	1164957	808452	111032	735197	525470	364110
34C	97009	010		847417	90068	377771	276805	52156	257454	189067	138304
34D	97009	014	3612	76735	9556	31629	22819	2109	19138	15322	10031
38B	97009	044	20170	1266230	438329	361625	267777	127978	173493	136473	105195
42A	97009	025	2810	634698	333531	177061	236448	108004	66686	102179	34038
42B	97009	039		316847	172042	109868	89941	46958	45668	36947	19836
42C	97009	053		98800	52512	31856	23327	12504	16301	12721	8090
42D	97009	065									
43	96074	007	33815	2179203	954891	1350609	950252	454683	356321	269646	180520

Appendix OA7. Bior								
Sample #	Job #	Seq	C33 22R Hopane Terpane	C34 22S Hopane Terpane	C34 22R Hopane Terpane	C35 22S Hopane Terpane	C35 22R Hopane Terpane	
1	96074	002	191766	176952	108269	158589	105195	
2	96074	001	291257	248512	159830	257897	159812	
3	97016	002	22244	21198	15216	21750	20492	
4	97016	003	29906	40372	26895	49779	25595	
5	96074	006	224158	205637	137767	213016	138464	
6	97012	005	1229030	1036978	699854	1209046	843825	
7	97012	001	519112	437012	264123	388986	265457	
8	97016	001	28863	36272	22412	29732	11428	
9	97012	002	669286	547452	353643	523446	331439	
10	97012	003	329159	285546	171978	278563	171124	
11	97012	004	364703	332614	201615	346789	222361	
12	97012	009	998175	853694	565715	881081	559903	
13	97012	010	699371	630165	391691	679840	433924	
14	97012	006	213526	186829	118359	187140	109440	
15	97012	008	1322549	1192495	783891	1328359	829341	
16	97012	007	1090723	1048659	655339	1056948	718225	
17	97010	026	374023	323550	213414	323563	203176	
18	97037	002	37123	33101	21300	26792	18080	
19	96074	008	79154	68918	94590	54245	59573	
20	97037	001	1183		1980	1533	1138	
21	96074	009	33046	29273	16134	18673	6420	
2(12.1-29	85172	002	601	568	440	514	319	
23	95069	001	5787	141962	81390	187752	127830	
24	95069	002	38634	33485	21922	28326	24620	
25	95069	003						
26	95069	007	73836	40250	30868	29661	20375	
27	97056	001	15934	13518	9090	7781	6575	
28	97035	001	1552	1404	1635	995	1189	
29	97010	027	229779	132976	92578	39589	39898	
30	97010	028	373886	330745	218054	154168	95803	
31A	97009	001	50448	39672	26634	19210	8995	
31B	97009	008	168105	124554	86692	66293	45091	
31C	97009	012	81689	54549	37354	31673	17936	
31D	97009	018				1226		
33A	97009	002	333449	236792	170581	250974	184794	
34A	97009	004	149842	132036	79786	108051	67798	
34B	97009	006	234047	208802	131809	177550	114411	
34C	97009	010	93113	79736	53182	72811	46828	
34D	97009	014	6132	5902	4789	3857	3602	
38B	97009	044	70879	33501	23568	38519	25287	
42A	97009	025	45568	16081	20357	10627	12288	
42B	97009	039	17498	8551	7024	5942	4340	
42C	97009	053	5402	3916	2932	2513	2831	
42D	97009	065						
43	96074	007	133726	78165	51033	49177	37874	