

Table S1. Docking results of potential MAGL inhibitors. Docking score is given in kcal/mol

SN	Docking score	SN	Docking score	SN	Docking score
1	-15.2	1344	-11.6	2687	-10.5
2	-15.2	1345	-11.6	2688	-10.5
3	-14.6	1346	-11.6	2689	-10.5
4	-14.6	1347	-11.6	2690	-10.5
5	-14.5	1348	-11.6	2691	-10.5
6	-14.5	1349	-11.6	2692	-10.5
7	-14.5	1350	-11.6	2693	-10.5
8	-14.5	1351	-11.6	2694	-10.5
9	-14.5	1352	-11.6	2695	-10.5
10	-14.5	1353	-11.6	2696	-10.5
11	-14.4	1354	-11.6	2697	-10.5
12	-14.4	1355	-11.6	2698	-10.5
13	-14.4	1356	-11.6	2699	-10.5
14	-14.4	1357	-11.6	2700	-10.5
15	-14.4	1358	-11.6	2701	-10.5
16	-14.4	1359	-11.6	2702	-10.5
17	-14.4	1360	-11.6	2703	-10.5
18	-14.4	1361	-11.6	2704	-10.5
19	-14.3	1362	-11.6	2705	-10.5
20	-14.3	1363	-11.6	2706	-10.5
21	-14.2	1364	-11.6	2707	-10.5
22	-14.2	1365	-11.6	2708	-10.5
23	-14.2	1366	-11.6	2709	-10.5
24	-14.2	1367	-11.6	2710	-10.5
25	-14.1	1368	-11.6	2711	-10.5
26	-14.1	1369	-11.6	2712	-10.5
27	-14.1	1370	-11.6	2713	-10.5
28	-14.1	1371	-11.6	2714	-10.5
29	-14.1	1372	-11.6	2715	-10.5
30	-14.1	1373	-11.6	2716	-10.5
31	-14	1374	-11.6	2717	-10.5
32	-14	1375	-11.6	2718	-10.5
33	-14	1376	-11.6	2719	-10.5
34	-14	1377	-11.6	2720	-10.5
35	-14	1378	-11.6	2721	-10.5
36	-14	1379	-11.6	2722	-10.5
37	-14	1380	-11.6	2723	-10.5
38	-14	1381	-11.6	2724	-10.5

39	-14	1382	-11.6	2725	-10.5
40	-14	1383	-11.6	2726	-10.5
41	-13.9	1384	-11.6	2727	-10.5
42	-13.9	1385	-11.6	2728	-10.5
43	-13.9	1386	-11.6	2729	-10.5
44	-13.9	1387	-11.6	2730	-10.5
45	-13.9	1388	-11.6	2731	-10.5
46	-13.9	1389	-11.6	2732	-10.5
47	-13.8	1390	-11.6	2733	-10.5
48	-13.8	1391	-11.6	2734	-10.5
49	-13.8	1392	-11.6	2735	-10.5
50	-13.8	1393	-11.6	2736	-10.5
51	-13.8	1394	-11.6	2737	-10.5
52	-13.8	1395	-11.6	2738	-10.5
53	-13.8	1396	-11.6	2739	-10.5
54	-13.8	1397	-11.6	2740	-10.5
55	-13.7	1398	-11.6	2741	-10.5
56	-13.7	1399	-11.6	2742	-10.5
57	-13.7	1400	-11.6	2743	-10.5
58	-13.7	1401	-11.6	2744	-10.5
59	-13.7	1402	-11.6	2745	-10.5
60	-13.7	1403	-11.6	2746	-10.5
61	-13.7	1404	-11.6	2747	-10.5
62	-13.7	1405	-11.6	2748	-10.5
63	-13.7	1406	-11.6	2749	-10.5
64	-13.7	1407	-11.6	2750	-10.5
65	-13.6	1408	-11.6	2751	-10.5
66	-13.6	1409	-11.6	2752	-10.5
67	-13.6	1410	-11.6	2753	-10.5
68	-13.6	1411	-11.6	2754	-10.5
69	-13.6	1412	-11.6	2755	-10.5
70	-13.6	1413	-11.6	2756	-10.5
71	-13.6	1414	-11.6	2757	-10.5
72	-13.6	1415	-11.6	2758	-10.5
73	-13.6	1416	-11.6	2759	-10.5
74	-13.6	1417	-11.6	2760	-10.5
75	-13.6	1418	-11.6	2761	-10.5
76	-13.5	1419	-11.6	2762	-10.5
77	-13.5	1420	-11.6	2763	-10.5
78	-13.5	1421	-11.6	2764	-10.5
79	-13.5	1422	-11.6	2765	-10.5
80	-13.5	1423	-11.6	2766	-10.5
81	-13.5	1424	-11.6	2767	-10.5

82	-13.5	1425	-11.6	2768	-10.5
83	-13.5	1426	-11.5	2769	-10.5
84	-13.5	1427	-11.5	2770	-10.5
85	-13.5	1428	-11.5	2771	-10.5
86	-13.5	1429	-11.5	2772	-10.5
87	-13.5	1430	-11.5	2773	-10.5
88	-13.5	1431	-11.5	2774	-10.5
89	-13.5	1432	-11.5	2775	-10.5
90	-13.5	1433	-11.5	2776	-10.5
91	-13.5	1434	-11.5	2777	-10.5
92	-13.5	1435	-11.5	2778	-10.5
93	-13.4	1436	-11.5	2779	-10.5
94	-13.4	1437	-11.5	2780	-10.5
95	-13.4	1438	-11.5	2781	-10.5
96	-13.4	1439	-11.5	2782	-10.5
97	-13.4	1440	-11.5	2783	-10.5
98	-13.4	1441	-11.5	2784	-10.5
99	-13.4	1442	-11.5	2785	-10.5
100	-13.4	1443	-11.5	2786	-10.5
101	-13.4	1444	-11.5	2787	-10.5
102	-13.4	1445	-11.5	2788	-10.5
103	-13.4	1446	-11.5	2789	-10.5
104	-13.4	1447	-11.5	2790	-10.5
105	-13.4	1448	-11.5	2791	-10.5
106	-13.4	1449	-11.5	2792	-10.5
107	-13.4	1450	-11.5	2793	-10.5
108	-13.4	1451	-11.5	2794	-10.5
109	-13.4	1452	-11.5	2795	-10.5
110	-13.4	1453	-11.5	2796	-10.5
111	-13.4	1454	-11.5	2797	-10.5
112	-13.4	1455	-11.5	2798	-10.4
113	-13.3	1456	-11.5	2799	-10.4
114	-13.3	1457	-11.5	2800	-10.4
115	-13.3	1458	-11.5	2801	-10.4
116	-13.3	1459	-11.5	2802	-10.4
117	-13.3	1460	-11.5	2803	-10.4
118	-13.3	1461	-11.5	2804	-10.4
119	-13.3	1462	-11.5	2805	-10.4
120	-13.3	1463	-11.5	2806	-10.4
121	-13.3	1464	-11.5	2807	-10.4
122	-13.3	1465	-11.5	2808	-10.4
123	-13.3	1466	-11.5	2809	-10.4
124	-13.3	1467	-11.5	2810	-10.4

125	-13.3	1468	-11.5	2811	-10.4
126	-13.3	1469	-11.5	2812	-10.4
127	-13.3	1470	-11.5	2813	-10.4
128	-13.3	1471	-11.5	2814	-10.4
129	-13.3	1472	-11.5	2815	-10.4
130	-13.3	1473	-11.5	2816	-10.4
131	-13.3	1474	-11.5	2817	-10.4
132	-13.3	1475	-11.5	2818	-10.4
133	-13.3	1476	-11.5	2819	-10.4
134	-13.3	1477	-11.5	2820	-10.4
135	-13.2	1478	-11.5	2821	-10.4
136	-13.2	1479	-11.5	2822	-10.4
137	-13.2	1480	-11.5	2823	-10.4
138	-13.2	1481	-11.5	2824	-10.4
139	-13.2	1482	-11.5	2825	-10.4
140	-13.2	1483	-11.5	2826	-10.4
141	-13.2	1484	-11.5	2827	-10.4
142	-13.2	1485	-11.5	2828	-10.4
143	-13.2	1486	-11.5	2829	-10.4
144	-13.2	1487	-11.5	2830	-10.4
145	-13.2	1488	-11.5	2831	-10.4
146	-13.2	1489	-11.5	2832	-10.4
147	-13.2	1490	-11.5	2833	-10.4
148	-13.2	1491	-11.5	2834	-10.4
149	-13.2	1492	-11.5	2835	-10.4
150	-13.2	1493	-11.5	2836	-10.4
151	-13.2	1494	-11.5	2837	-10.4
152	-13.2	1495	-11.5	2838	-10.4
153	-13.2	1496	-11.5	2839	-10.4
154	-13.2	1497	-11.5	2840	-10.4
155	-13.2	1498	-11.5	2841	-10.4
156	-13.2	1499	-11.5	2842	-10.4
157	-13.2	1500	-11.5	2843	-10.4
158	-13.2	1501	-11.5	2844	-10.4
159	-13.2	1502	-11.5	2845	-10.4
160	-13.2	1503	-11.5	2846	-10.4
161	-13.2	1504	-11.5	2847	-10.4
162	-13.2	1505	-11.5	2848	-10.4
163	-13.2	1506	-11.5	2849	-10.4
164	-13.2	1507	-11.5	2850	-10.4
165	-13.2	1508	-11.5	2851	-10.4
166	-13.2	1509	-11.5	2852	-10.4
167	-13.2	1510	-11.5	2853	-10.4

168	-13.2	1511	-11.5	2854	-10.4
169	-13.2	1512	-11.5	2855	-10.4
170	-13.1	1513	-11.5	2856	-10.4
171	-13.1	1514	-11.5	2857	-10.4
172	-13.1	1515	-11.5	2858	-10.4
173	-13.1	1516	-11.5	2859	-10.4
174	-13.1	1517	-11.5	2860	-10.4
175	-13.1	1518	-11.5	2861	-10.4
176	-13.1	1519	-11.5	2862	-10.4
177	-13.1	1520	-11.5	2863	-10.4
178	-13.1	1521	-11.5	2864	-10.4
179	-13.1	1522	-11.5	2865	-10.4
180	-13.1	1523	-11.5	2866	-10.4
181	-13.1	1524	-11.5	2867	-10.4
182	-13.1	1525	-11.5	2868	-10.4
183	-13.1	1526	-11.5	2869	-10.4
184	-13.1	1527	-11.5	2870	-10.4
185	-13.1	1528	-11.5	2871	-10.4
186	-13.1	1529	-11.5	2872	-10.4
187	-13.1	1530	-11.5	2873	-10.4
188	-13.1	1531	-11.5	2874	-10.4
189	-13.1	1532	-11.5	2875	-10.4
190	-13.1	1533	-11.5	2876	-10.4
191	-13.1	1534	-11.5	2877	-10.4
192	-13.1	1535	-11.5	2878	-10.4
193	-13.1	1536	-11.5	2879	-10.4
194	-13.1	1537	-11.5	2880	-10.4
195	-13.1	1538	-11.5	2881	-10.4
196	-13.1	1539	-11.5	2882	-10.4
197	-13	1540	-11.5	2883	-10.4
198	-13	1541	-11.5	2884	-10.4
199	-13	1542	-11.5	2885	-10.4
200	-13	1543	-11.5	2886	-10.4
201	-13	1544	-11.5	2887	-10.4
202	-13	1545	-11.5	2888	-10.4
203	-13	1546	-11.5	2889	-10.4
204	-13	1547	-11.5	2890	-10.4
205	-13	1548	-11.5	2891	-10.4
206	-13	1549	-11.5	2892	-10.4
207	-13	1550	-11.5	2893	-10.4
208	-13	1551	-11.5	2894	-10.4
209	-13	1552	-11.5	2895	-10.4
210	-13	1553	-11.5	2896	-10.4

211	-13	1554	-11.5	2897	-10.4
212	-13	1555	-11.5	2898	-10.4
213	-13	1556	-11.5	2899	-10.3
214	-13	1557	-11.5	2900	-10.3
215	-13	1558	-11.5	2901	-10.3
216	-13	1559	-11.5	2902	-10.3
217	-13	1560	-11.5	2903	-10.3
218	-13	1561	-11.5	2904	-10.3
219	-13	1562	-11.5	2905	-10.3
220	-13	1563	-11.4	2906	-10.3
221	-13	1564	-11.4	2907	-10.3
222	-13	1565	-11.4	2908	-10.3
223	-13	1566	-11.4	2909	-10.3
224	-13	1567	-11.4	2910	-10.3
225	-13	1568	-11.4	2911	-10.3
226	-12.9	1569	-11.4	2912	-10.3
227	-12.9	1570	-11.4	2913	-10.3
228	-12.9	1571	-11.4	2914	-10.3
229	-12.9	1572	-11.4	2915	-10.3
230	-12.9	1573	-11.4	2916	-10.3
231	-12.9	1574	-11.4	2917	-10.3
232	-12.9	1575	-11.4	2918	-10.3
233	-12.9	1576	-11.4	2919	-10.3
234	-12.9	1577	-11.4	2920	-10.3
235	-12.9	1578	-11.4	2921	-10.3
236	-12.9	1579	-11.4	2922	-10.3
237	-12.9	1580	-11.4	2923	-10.3
238	-12.9	1581	-11.4	2924	-10.3
239	-12.9	1582	-11.4	2925	-10.3
240	-12.9	1583	-11.4	2926	-10.3
241	-12.9	1584	-11.4	2927	-10.3
242	-12.9	1585	-11.4	2928	-10.3
243	-12.9	1586	-11.4	2929	-10.3
244	-12.9	1587	-11.4	2930	-10.3
245	-12.9	1588	-11.4	2931	-10.3
246	-12.9	1589	-11.4	2932	-10.3
247	-12.9	1590	-11.4	2933	-10.3
248	-12.9	1591	-11.4	2934	-10.3
249	-12.9	1592	-11.4	2935	-10.3
250	-12.9	1593	-11.4	2936	-10.3
251	-12.9	1594	-11.4	2937	-10.3
252	-12.9	1595	-11.4	2938	-10.3
253	-12.9	1596	-11.4	2939	-10.3

254	-12.9	1597	-11.4	2940	-10.3
255	-12.9	1598	-11.4	2941	-10.3
256	-12.9	1599	-11.4	2942	-10.3
257	-12.9	1600	-11.4	2943	-10.3
258	-12.9	1601	-11.4	2944	-10.3
259	-12.9	1602	-11.4	2945	-10.3
260	-12.9	1603	-11.4	2946	-10.3
261	-12.9	1604	-11.4	2947	-10.3
262	-12.8	1605	-11.4	2948	-10.3
263	-12.8	1606	-11.4	2949	-10.3
264	-12.8	1607	-11.4	2950	-10.3
265	-12.8	1608	-11.4	2951	-10.3
266	-12.8	1609	-11.4	2952	-10.3
267	-12.8	1610	-11.4	2953	-10.3
268	-12.8	1611	-11.4	2954	-10.3
269	-12.8	1612	-11.4	2955	-10.3
270	-12.8	1613	-11.4	2956	-10.3
271	-12.8	1614	-11.4	2957	-10.3
272	-12.8	1615	-11.4	2958	-10.3
273	-12.8	1616	-11.4	2959	-10.3
274	-12.8	1617	-11.4	2960	-10.3
275	-12.8	1618	-11.4	2961	-10.3
276	-12.8	1619	-11.4	2962	-10.3
277	-12.8	1620	-11.4	2963	-10.3
278	-12.8	1621	-11.4	2964	-10.3
279	-12.8	1622	-11.4	2965	-10.3
280	-12.8	1623	-11.4	2966	-10.3
281	-12.8	1624	-11.4	2967	-10.3
282	-12.8	1625	-11.4	2968	-10.3
283	-12.8	1626	-11.4	2969	-10.3
284	-12.8	1627	-11.4	2970	-10.3
285	-12.8	1628	-11.4	2971	-10.3
286	-12.8	1629	-11.4	2972	-10.3
287	-12.8	1630	-11.4	2973	-10.3
288	-12.8	1631	-11.4	2974	-10.3
289	-12.8	1632	-11.4	2975	-10.3
290	-12.8	1633	-11.4	2976	-10.3
291	-12.8	1634	-11.4	2977	-10.3
292	-12.8	1635	-11.4	2978	-10.3
293	-12.8	1636	-11.4	2979	-10.3
294	-12.8	1637	-11.4	2980	-10.3
295	-12.8	1638	-11.4	2981	-10.3
296	-12.8	1639	-11.4	2982	-10.3

297	-12.8	1640	-11.4	2983	-10.3
298	-12.8	1641	-11.4	2984	-10.3
299	-12.8	1642	-11.4	2985	-10.3
300	-12.8	1643	-11.4	2986	-10.3
301	-12.8	1644	-11.4	2987	-10.3
302	-12.8	1645	-11.4	2988	-10.3
303	-12.8	1646	-11.4	2989	-10.3
304	-12.8	1647	-11.4	2990	-10.3
305	-12.8	1648	-11.4	2991	-10.3
306	-12.8	1649	-11.4	2992	-10.3
307	-12.8	1650	-11.4	2993	-10.3
308	-12.8	1651	-11.4	2994	-10.3
309	-12.8	1652	-11.4	2995	-10.3
310	-12.7	1653	-11.4	2996	-10.3
311	-12.7	1654	-11.4	2997	-10.3
312	-12.7	1655	-11.4	2998	-10.3
313	-12.7	1656	-11.4	2999	-10.3
314	-12.7	1657	-11.4	3000	-10.3
315	-12.7	1658	-11.4	3001	-10.3
316	-12.7	1659	-11.4	3002	-10.3
317	-12.7	1660	-11.4	3003	-10.3
318	-12.7	1661	-11.4	3004	-10.3
319	-12.7	1662	-11.4	3005	-10.3
320	-12.7	1663	-11.4	3006	-10.3
321	-12.7	1664	-11.4	3007	-10.3
322	-12.7	1665	-11.4	3008	-10.3
323	-12.7	1666	-11.4	3009	-10.3
324	-12.7	1667	-11.4	3010	-10.3
325	-12.7	1668	-11.4	3011	-10.3
326	-12.7	1669	-11.4	3012	-10.3
327	-12.7	1670	-11.4	3013	-10.3
328	-12.7	1671	-11.4	3014	-10.3
329	-12.7	1672	-11.4	3015	-10.3
330	-12.7	1673	-11.4	3016	-10.3
331	-12.7	1674	-11.4	3017	-10.3
332	-12.7	1675	-11.4	3018	-10.3
333	-12.7	1676	-11.4	3019	-10.3
334	-12.7	1677	-11.4	3020	-10.3
335	-12.7	1678	-11.4	3021	-10.3
336	-12.7	1679	-11.4	3022	-10.3
337	-12.7	1680	-11.4	3023	-10.2
338	-12.7	1681	-11.4	3024	-10.2
339	-12.7	1682	-11.4	3025	-10.2

340	-12.7	1683	-11.4	3026	-10.2
341	-12.7	1684	-11.4	3027	-10.2
342	-12.7	1685	-11.4	3028	-10.2
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381	-12.6	1724	-11.3	3067	-10.2
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424	-12.6	1767	-11.3	3110	-10.2
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434	-12.5	1777	-11.3	3120	-10.2
435	-12.5	1778	-11.3	3121	-10.2
436	-12.5	1779	-11.3	3122	-10.2
437	-12.5	1780	-11.3	3123	-10.2
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441	-12.5	1784	-11.3	3127	-10.2
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453	-12.5	1796	-11.3	3139	-10.2
454	-12.5	1797	-11.3	3140	-10.2
455	-12.5	1798	-11.3	3141	-10.2
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463	-12.5	1806	-11.3	3149	-10.1
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465	-12.5	1808	-11.3	3151	-10.1
466	-12.5	1809	-11.3	3152	-10.1
467	-12.5	1810	-11.3	3153	-10.1
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473	-12.5	1816	-11.3	3159	-10.1
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478	-12.5	1821	-11.2	3164	-10.1
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615	-12.3	1958	-11.1	3301	-10
616	-12.3	1959	-11.1	3302	-10
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618	-12.3	1961	-11.1	3304	-10
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620	-12.3	1963	-11.1	3306	-10
621	-12.3	1964	-11.1	3307	-10
622	-12.3	1965	-11.1	3308	-10
623	-12.3	1966	-11.1	3309	-10
624	-12.3	1967	-11.1	3310	-10
625	-12.3	1968	-11.1	3311	-10
626	-12.3	1969	-11.1	3312	-10
627	-12.3	1970	-11.1	3313	-10
628	-12.3	1971	-11.1	3314	-10
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653	-12.2	1996	-11.1	3339	-10
654	-12.2	1997	-11.1	3340	-10
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668	-12.2	2011	-11.1	3354	-9.9
669	-12.2	2012	-11.1	3355	-9.9
670	-12.2	2013	-11.1	3356	-9.9
671	-12.2	2014	-11.1	3357	-9.9
672	-12.2	2015	-11.1	3358	-9.9
673	-12.2	2016	-11.1	3359	-9.9
674	-12.2	2017	-11.1	3360	-9.9
675	-12.2	2018	-11.1	3361	-9.9
676	-12.2	2019	-11.1	3362	-9.9
677	-12.2	2020	-11.1	3363	-9.9
678	-12.2	2021	-11.1	3364	-9.9
679	-12.2	2022	-11.1	3365	-9.9
680	-12.2	2023	-11.1	3366	-9.9
681	-12.2	2024	-11.1	3367	-9.9
682	-12.2	2025	-11.1	3368	-9.9
683	-12.2	2026	-11.1	3369	-9.9

684	-12.2	2027	-11.1	3370	-9.9
685	-12.2	2028	-11.1	3371	-9.9
686	-12.2	2029	-11.1	3372	-9.9
687	-12.2	2030	-11.1	3373	-9.9
688	-12.2	2031	-11.1	3374	-9.9
689	-12.2	2032	-11.1	3375	-9.9
690	-12.2	2033	-11.1	3376	-9.9
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696	-12.2	2039	-11.1	3382	-9.9
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706	-12.2	2049	-11.1	3392	-9.9
707	-12.2	2050	-11.1	3393	-9.9
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732	-12.2	2075	-11	3418	-9.9
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734	-12.1	2077	-11	3420	-9.9
735	-12.1	2078	-11	3421	-9.9
736	-12.1	2079	-11	3422	-9.9
737	-12.1	2080	-11	3423	-9.9
738	-12.1	2081	-11	3424	-9.9
739	-12.1	2082	-11	3425	-9.9
740	-12.1	2083	-11	3426	-9.9
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742	-12.1	2085	-11	3428	-9.9
743	-12.1	2086	-11	3429	-9.9
744	-12.1	2087	-11	3430	-9.9
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746	-12.1	2089	-11	3432	-9.8
747	-12.1	2090	-11	3433	-9.8
748	-12.1	2091	-11	3434	-9.8
749	-12.1	2092	-11	3435	-9.8
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751	-12.1	2094	-11	3437	-9.8
752	-12.1	2095	-11	3438	-9.8
753	-12.1	2096	-11	3439	-9.8
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783	-12.1	2126	-11	3469	-9.8
784	-12.1	2127	-11	3470	-9.8
785	-12.1	2128	-11	3471	-9.8
786	-12.1	2129	-11	3472	-9.8
787	-12.1	2130	-11	3473	-9.8
788	-12.1	2131	-11	3474	-9.8
789	-12.1	2132	-11	3475	-9.8
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802	-12.1	2145	-11	3488	-9.8
803	-12.1	2146	-11	3489	-9.8
804	-12.1	2147	-11	3490	-9.8
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818	-12.1	2161	-11	3504	-9.7
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1038	-11.9	2381	-10.8	3724	-9.4
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