

# Lipinski Evaluation of Drug Molecules

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2/28/2024

Usage To get started with LipinskiFilters, load the package using:

```
library(LipinskiFilters)
```

```
## Loading required package: cowplot
```

```
## Loading required package: rcdk
```

```
## Loading required package: rcdklibs
```

```
## Warning: package 'rcdklibs' was built under R version 4.1.3
```

```
## Loading required package: rJava
```

```
## Loading required package: ggplot2
```

Set working directory containing co-catenated compounds in SDF format

```
file<-system.file("extdata", "test.sdf", package = "LipinskiFilters")
```

Read sdf molecules

```
mols<-load.molecules(file)
```

Computing Molecular Properties You can compute molecular properties using the compute\_properties function. Here's an example:

```
properties <- compute_properties(mols)
print(properties)
```

```
##           MW nHBDn nHBAcc TopoPSA  ALogP
## 1    356.4180     2      3    54.38 5.8914
## 2    451.5605     2      3    70.50 8.1237
## 3    358.3885     1      3    85.22 3.9521
## 4    472.4570     4      8   159.72 5.6735
## 5    310.3720     1      3    75.99 3.7630
## 6    524.5732     4      4   127.86 6.3384
## 7    406.4993     1      4    90.90 4.8441
```

## 8	637.7222	0	5	107.66	7.0274
## 9	554.5051	0	3	55.84	6.4874
## 10	411.6242	1	4	35.58	4.2339
## 11	390.4999	1	3	79.46	4.1867
## 12	476.0349	0	3	62.90	7.2190
## 13	400.9424	1	3	45.48	3.8604
## 14	384.4878	1	3	35.94	4.0949
## 15	393.4003	1	3	49.77	4.5734
## 16	354.4618	1	3	26.71	4.1113
## 17	571.6646	0	4	54.45	6.8874
## 18	388.5062	2	4	61.02	4.4830
## 19	445.5213	2	4	44.37	4.7031
## 20	218.2522	0	4	41.90	0.9043
## 21	357.7981	1	7	78.66	2.1145
## 22	414.4816	0	5	107.35	4.2277
## 23	400.4549	0	5	107.35	3.7415
## 24	303.3810	2	5	99.33	2.8064
## 25	362.4290	3	7	82.18	3.7992
## 26	362.4326	1	2	15.27	4.3255
## 27	418.5753	0	3	33.53	4.7073
## 28	413.5125	2	3	61.27	4.8044
## 29	479.9994	2	4	62.83	4.5669
## 30	438.8961	1	4	50.80	3.6605
## 31	586.7410	1	5	118.62	5.9067
## 32	425.9519	1	5	48.83	4.6466
## 33	463.9572	0	4	109.53	4.4949
## 34	465.5855	1	4	63.27	4.6322
## 35	462.4235	1	4	44.81	3.1807
## 36	434.5526	1	4	86.88	4.5343
## 37	462.6058	1	4	86.88	4.8900
## 38	448.5792	1	4	86.88	4.5412
## 39	409.5032	1	4	103.68	3.6894
## 40	468.9976	1	4	86.88	5.1987
## 41	391.4820	2	3	48.13	3.9869
## 42	484.5872	1	4	67.87	5.2310
## 43	413.5157	2	5	64.26	3.7656
## 44	398.5011	2	4	61.02	4.6285
## 45	495.0604	2	6	67.50	4.7107
## 46	497.7411	1	6	79.95	4.4994
## 47	458.6204	1	4	78.40	6.0283
## 48	444.5938	1	4	78.40	5.5421
## 49	397.5356	1	5	80.89	3.5364
## 50	493.5983	1	5	90.87	4.6224
## 51	453.5748	1	4	63.27	4.0869
## 52	367.3992	2	6	87.74	2.8245
## 53	456.9675	1	5	58.12	4.3794
## 54	456.9675	1	5	58.12	4.3794
## 55	460.5275	2	2	75.82	6.6530
## 56	459.6084	1	5	81.64	4.6594
## 57	423.4221	1	5	115.94	3.7888
## 58	487.0161	1	6	83.15	3.6188
## 59	420.4806	1	5	121.98	3.4845
## 60	445.5113	1	6	82.71	3.0586
## 61	340.7793	0	3	33.20	4.6625

## 62	367.3992	1	2	86.48	4.0561
## 63	383.4815	1	4	59.00	4.2014
## 64	480.5780	0	5	84.53	5.2072
## 65	395.5197	0	4	83.56	4.6735
## 66	376.4243	1	2	47.17	4.9369
## 67	458.6188	1	4	96.86	4.5785
## 68	450.5735	1	4	77.88	5.4409
## 69	426.5789	1	3	133.00	5.8538
## 70	420.5501	1	3	104.76	5.9004
## 71	425.9519	1	5	48.83	4.7928
## 72	354.8059	2	3	41.13	5.5209
## 73	363.4536	1	4	54.46	4.6697
## 74	405.4904	1	4	63.69	4.8729
## 75	396.9106	1	3	41.57	4.2710
## 76	434.5316	1	5	66.93	4.2618
## 77	341.7193	1	4	55.11	4.4876
## 78	405.4904	0	4	54.90	3.8560
## 79	339.3460	1	2	86.48	3.3585
## 80	389.7904	1	2	95.71	3.5203
## 81	359.7643	1	2	86.48	3.5367
## 82	416.5167	1	5	121.98	3.5627
## 83	384.4937	1	5	74.86	3.8988
## 84	397.4925	1	3	90.68	4.3726
## 85	431.5487	1	3	87.66	7.1551
## 86	510.4217	1	2	38.33	6.6888
## 87	326.4419	0	3	99.56	4.6354
## 88	249.7397	2	3	36.95	2.1546
## 89	292.3325	0	3	41.90	3.7709
## 90	293.3173	0	2	47.89	3.9411
## 91	283.7096	0	2	38.66	4.2731
## 92	273.3276	1	3	49.77	3.0997
## 93	314.4194	1	2	46.53	6.0850
## 94	267.3295	1	4	55.11	3.2326
## 95	368.6529	2	3	49.33	4.3242
## 96	468.3386	0	5	74.30	3.1425
## 97	328.1602	0	2	38.66	4.3571
## 98	420.5034	2	3	58.29	6.8663
## 99	315.6754	2	3	49.33	3.9540
## 100	403.9084	1	5	125.49	4.1159
## 101	327.6927	1	4	55.11	4.0014
## 102	494.5455	2	8	110.98	2.0218
## 103	413.5765	1	2	57.34	6.2161
## 104	559.6258	1	5	53.40	6.4241
## 105	286.3280	0	2	34.89	4.2707
## 106	294.4395	3	6	74.76	4.1261
## 107	592.6492	1	4	67.87	6.9870
## 108	274.3156	1	2	64.36	3.0657
## 109	411.9494	1	3	72.22	5.7612
## 110	301.4050	1	2	67.54	3.8328
## 111	346.4208	2	4	86.44	3.8400
## 112	465.6113	0	2	65.24	7.6743
## 113	377.8626	1	2	56.79	4.3119
## 114	347.8365	1	2	47.56	4.3283
## 115	314.4658	2	2	37.19	4.2308

## 116	353.3726	2	6	87.74	1.6457
## 117	385.8657	1	3	83.64	5.0629
## 118	500.5677	1	6	113.73	5.0774
## 119	460.5468	0	5	86.64	6.0652
## 120	546.5889	1	6	75.71	5.7672
## 121	338.2720	2	2	32.26	4.8755
## 122	479.5309	2	7	98.09	2.7260
## 123	310.4340	2	2	37.19	4.2018
## 124	459.9218	0	3	57.53	6.8199
## 125	309.3167	0	2	57.12	3.5759
## 126	292.5033	1	2	15.27	3.8729
## 127	367.5252	2	3	41.49	4.7391
## 128	281.2700	2	3	96.21	3.2356
## 129	282.5511	1	2	38.33	3.0808
## 130	391.8892	2	2	59.95	4.4488
## 131	343.3794	2	3	67.01	4.0389
## 132	621.7718	0	7	94.76	8.0416
## 133	370.4860	2	4	61.80	3.9713
## 134	659.6837	0	4	91.37	6.4236
## 135	468.0990	0	3	53.26	8.6561
## 136	422.3131	1	2	56.79	4.3959
## 137	357.4043	1	5	75.02	1.7787
## 138	387.4767	1	2	31.92	5.8080
## 139	286.7534	0	1	26.30	4.2597
## 140	377.8626	2	2	59.95	4.1000
## 141	364.4384	1	4	60.45	5.0167
## 142	657.7540	0	5	80.75	7.0971
## 143	338.2720	2	2	32.26	4.9542
## 144	347.8365	2	2	50.72	4.1164
## 145	359.4013	2	6	115.98	1.5991
## 146	494.6477	1	5	96.11	4.7480
## 147	386.4920	0	6	80.29	3.4616
## 148	436.5684	1	4	90.79	5.2410
## 149	335.4435	1	3	46.92	4.1187
## 150	410.4207	2	8	115.22	1.0092
## 151	334.3693	1	2	73.91	3.5003
## 152	322.4447	2	2	37.19	4.4796
## 153	574.2378	2	2	37.19	5.6360
## 154	631.7167	0	4	72.91	6.8546
## 155	496.6825	2	4	76.66	4.9598
## 156	349.8524	2	2	50.72	3.7984
## 157	261.7471	2	2	32.26	3.7257
## 158	337.4179	2	2	40.71	5.3601
## 159	308.4181	2	2	37.19	4.0234
## 160	309.8126	0	3	57.78	3.5043
## 161	419.4755	2	4	67.27	5.7020
## 162	367.2702	2	3	46.42	3.8192
## 163	282.1639	1	2	46.53	2.6255
## 164	312.1899	1	2	55.76	2.6091
## 165	394.4213	1	2	92.37	3.4675
## 166	487.7631	2	4	71.45	6.1295
## 167	453.3181	2	4	71.45	5.4651
## 168	432.8997	2	4	71.45	5.2869
## 169	447.5288	2	4	67.27	6.1951

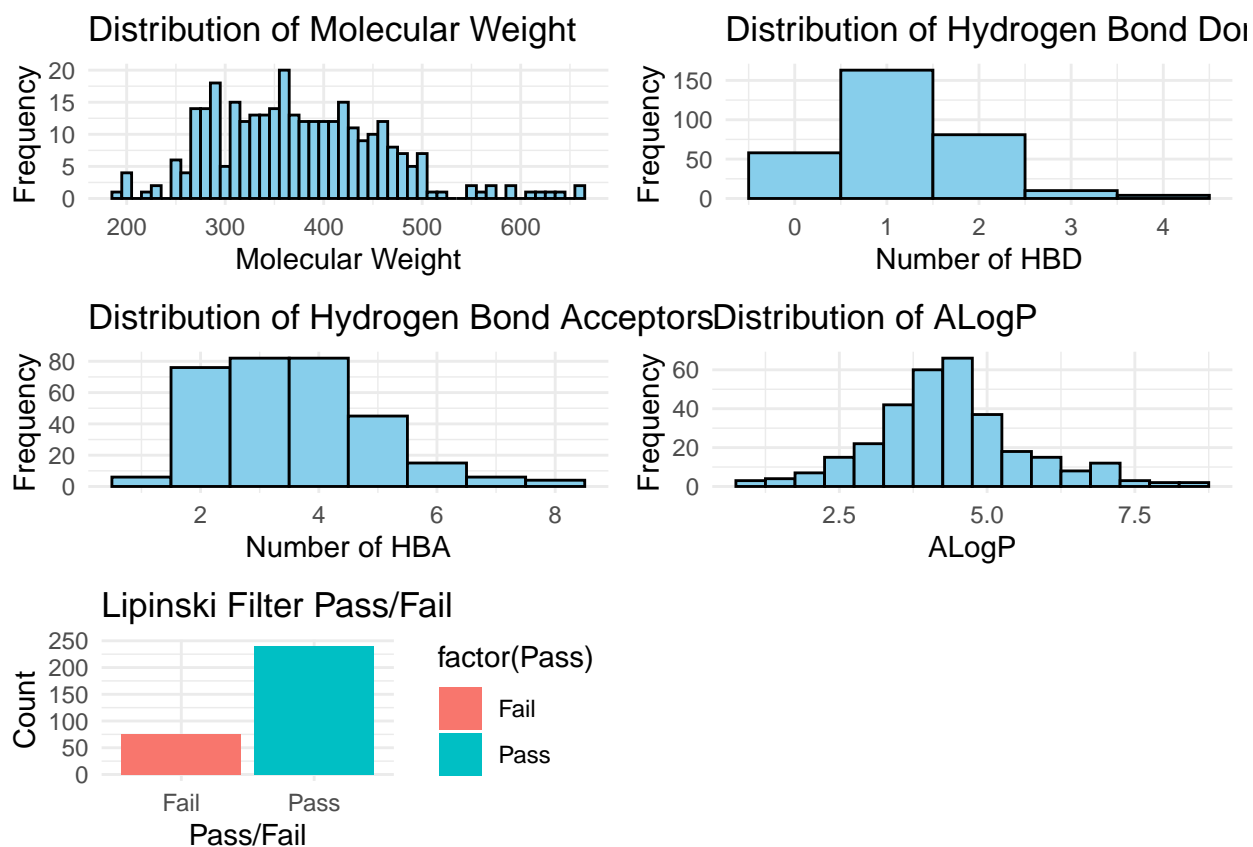
## 170	279.3994	0	2	54.84	3.0059
## 171	395.7213	1	3	26.71	4.5898
## 172	321.7992	2	2	50.72	3.6366
## 173	401.8857	2	3	49.33	5.5740
## 174	354.4021	2	4	62.22	4.1527
## 175	484.9539	1	6	113.73	4.8334
## 176	359.4180	0	2	54.73	5.2512
## 177	398.4547	0	3	51.13	4.5674
## 178	500.1858	1	3	55.87	5.9747
## 179	367.4821	1	3	49.77	4.2540
## 180	334.3859	2	5	67.43	3.5116
## 181	453.5382	1	4	54.57	8.5045
## 182	286.1973	0	2	20.31	4.1286
## 183	371.4535	1	2	63.63	4.8129
## 184	420.3231	1	2	54.40	5.5777
## 185	361.2225	3	3	65.12	4.6665
## 186	332.5052	3	3	76.38	4.5174
## 187	272.3013	0	3	42.85	4.1662
## 188	337.1703	0	3	42.85	4.4284
## 189	293.3173	1	4	55.40	3.1658
## 190	327.4267	1	4	108.42	3.3785
## 191	360.2296	1	4	83.12	3.5851
## 192	415.5751	1	5	98.92	5.1112
## 193	357.4060	2	3	67.01	4.3877
## 194	278.7097	2	3	41.13	3.8790
## 195	422.4364	3	5	100.02	4.2352
## 196	378.4876	1	5	88.00	3.7843
## 197	431.3125	1	4	54.71	4.9098
## 198	265.3917	2	2	41.49	3.4042
## 199	362.2676	2	4	56.84	3.9056
## 200	440.5173	3	7	123.77	3.5500
## 201	329.3726	2	5	66.07	2.4152
## 202	480.5796	2	2	92.67	7.2172
## 203	245.3174	1	2	38.33	3.5255
## 204	358.4355	0	2	24.72	6.4826
## 205	496.0004	1	2	47.67	7.4397
## 206	417.4299	0	2	48.00	5.0091
## 207	256.3865	1	2	27.09	4.9299
## 208	335.8291	1	5	54.46	2.8947
## 209	368.9037	1	4	41.05	4.9191
## 210	470.1598	2	4	49.84	6.9694
## 211	393.4829	2	7	88.86	2.4314
## 212	440.2853	0	5	74.30	2.4449
## 213	466.5579	1	8	112.31	2.0966
## 214	416.2870	1	4	39.60	4.4058
## 215	290.2438	1	4	50.70	4.1130
## 216	290.2438	1	4	51.81	4.4057
## 217	335.3109	0	3	94.35	3.4978
## 218	362.4225	1	4	58.64	3.5192
## 219	372.4174	2	2	67.37	5.0988
## 220	373.4054	2	3	76.24	4.0225
## 221	442.3078	2	3	57.78	5.7121
## 222	427.3140	1	5	88.00	2.3543
## 223	441.3181	1	4	54.71	4.3294

## 224	420.6770	2	5	71.09	4.2420
## 225	383.6675	1	3	45.48	4.3217
## 226	420.5050	1	6	66.93	3.8737
## 227	412.4846	3	5	86.88	4.7220
## 228	382.2433	2	3	57.78	5.3841
## 229	440.4484	4	6	107.89	4.4248
## 230	366.3400	1	4	50.70	5.0847
## 231	434.4846	1	3	87.92	5.5356
## 232	380.4378	1	4	69.68	4.7102
## 233	357.2446	1	2	34.15	4.9298
## 234	430.5048	4	4	109.40	5.1926
## 235	441.8562	1	5	87.07	5.0419
## 236	403.4314	2	3	85.47	4.0061
## 237	307.3697	1	4	101.58	2.0459
## 238	456.5075	0	5	68.31	4.3195
## 239	382.8634	1	5	88.00	2.2703
## 240	381.8130	2	5	80.32	2.8968
## 241	232.7091	0	2	16.13	3.3039
## 242	319.3579	1	3	67.05	3.1872
## 243	349.5168	1	4	108.42	4.4641
## 244	303.7839	0	1	21.70	4.2684
## 245	315.8377	0	1	12.47	5.3364
## 246	312.4153	1	3	108.00	4.3189
## 247	332.3501	0	2	56.51	5.3178
## 248	189.2142	1	3	61.03	1.4288
## 249	200.2800	1	2	27.09	3.1051
## 250	318.3235	0	2	56.51	4.8316
## 251	348.1807	2	3	62.47	4.8811
## 252	341.4098	1	5	63.59	5.1999
## 253	293.5307	0	1	35.53	3.1341
## 254	287.7845	0	1	12.47	4.9084
## 255	287.3591	1	3	51.80	4.4471
## 256	268.1389	1	2	29.10	3.4358
## 257	280.1604	1	2	29.10	3.8341
## 258	201.2648	1	2	29.10	3.0857
## 259	279.3370	1	4	44.70	2.6761
## 260	265.3104	1	4	44.70	2.1899
## 261	320.3890	2	4	59.07	4.3199
## 262	326.3952	2	4	49.84	5.3906
## 263	289.3319	3	3	60.94	3.9204
## 264	273.7180	3	3	60.94	3.6764
## 265	312.4068	1	3	35.94	3.1606
## 266	199.2489	1	2	29.10	2.6950
## 267	252.3149	2	3	57.94	2.6862
## 268	254.3275	0	2	15.71	3.7398
## 269	267.3505	1	3	66.05	4.0883
## 270	298.7674	1	2	34.15	4.4970
## 271	333.5731	2	3	41.13	4.7216
## 272	274.3829	1	3	60.58	3.4279
## 273	319.4203	1	2	75.80	3.5610
## 274	331.4150	0	4	47.57	3.9406
## 275	310.4151	1	3	70.23	4.6406
## 276	245.2743	1	4	55.40	2.3200
## 277	298.7674	1	2	34.15	4.5632

## 278	319.4441	1	3	28.16	4.0719
## 279	348.3959	1	5	68.29	3.9967
## 280	287.3144	1	4	72.28	1.6009
## 281	321.4169	1	3	37.39	4.3436
## 282	280.3218	2	3	54.38	3.5652
## 283	336.3852	1	4	60.45	3.5963
## 284	274.3189	1	4	69.16	4.2202
## 285	308.4423	1	2	53.16	6.2690
## 286	245.2743	1	4	55.40	2.3200
## 287	268.3541	0	2	15.71	4.0886
## 288	268.3110	0	2	24.94	3.5243
## 289	278.3059	1	2	55.13	3.2718
## 290	345.8272	2	5	66.07	2.8741
## 291	275.3085	1	4	55.11	3.2015
## 292	359.4682	0	4	47.57	4.7719
## 293	346.3966	0	5	49.85	3.3648
## 294	228.3333	1	2	27.09	4.0175
## 295	309.4061	0	4	28.07	3.4386
## 296	323.3466	2	4	86.47	2.5607
## 297	368.4751	1	4	31.40	5.0228
## 298	501.3643	3	5	86.88	6.1688
## 299	448.3646	2	4	49.84	7.3572
## 300	291.3908	1	3	28.16	3.9106
## 301	260.3386	2	6	83.24	1.1216
## 302	277.7929	1	3	28.16	3.3257
## 303	288.3008	0	3	52.08	3.6636
## 304	325.5883	2	3	41.13	3.9357
## 305	261.4030	2	2	32.26	4.3590
## 306	355.4332	1	4	37.39	4.3247
## 307	307.4333	1	3	28.16	3.6321
## 308	270.3286	1	1	28.68	4.7890
## 309	293.4067	1	3	28.16	3.5697
## 310	199.2489	1	2	29.10	2.7816
## 311	350.0277	2	3	41.13	5.1805
## 312	281.1344	2	2	40.46	4.0663
## 313	389.5341	1	4	29.95	4.7640
## 314	279.3801	1	3	28.16	3.3630
## 315	608.7247	1	3	72.86	6.9672
## 316	324.4175	1	3	45.59	2.6207

Creating Lipinski Plots Visualize Lipinski Rule of Five parameters using the `create_lipinski_plots` function:

```
create_lipinski_plots(properties)
```



Druglikeness evaluation

```
assess_drug_likeness(properties)
```

##	MW	nHBD	nHBA	TopoPSA	ALogP	DrugLikeness
## 1	356.4180	2	3	54.38	5.8914	Pass
## 2	451.5605	2	3	70.50	8.1237	Fail
## 3	358.3885	1	3	85.22	3.9521	Pass
## 4	472.4570	4	8	159.72	5.6735	Fail
## 5	310.3720	1	3	75.99	3.7630	Fail
## 6	524.5732	4	4	127.86	6.3384	Fail
## 7	406.4993	1	4	90.90	4.8441	Fail
## 8	637.7222	0	5	107.66	7.0274	Fail
## 9	554.5051	0	3	55.84	6.4874	Fail
## 10	411.6242	1	4	35.58	4.2339	Fail
## 11	390.4999	1	3	79.46	4.1867	Pass
## 12	476.0349	0	3	62.90	7.2190	Fail
## 13	400.9424	1	3	45.48	3.8604	Pass
## 14	384.4878	1	3	35.94	4.0949	Fail
## 15	393.4003	1	3	49.77	4.5734	Fail
## 16	354.4618	1	3	26.71	4.1113	Pass
## 17	571.6646	0	4	54.45	6.8874	Fail
## 18	388.5062	2	4	61.02	4.4830	Pass
## 19	445.5213	2	4	44.37	4.7031	Fail
## 20	218.2522	0	4	41.90	0.9043	Fail
## 21	357.7981	1	7	78.66	2.1145	Pass



## 22	414.4816	0	5	107.35	4.2277	Fail
## 23	400.4549	0	5	107.35	3.7415	Pass
## 24	303.3810	2	5	99.33	2.8064	Fail
## 25	362.4290	3	7	82.18	3.7992	Fail
## 26	362.4326	1	2	15.27	4.3255	Pass
## 27	418.5753	0	3	33.53	4.7073	Fail
## 28	413.5125	2	3	61.27	4.8044	Pass
## 29	479.9994	2	4	62.83	4.5669	Fail
## 30	438.8961	1	4	50.80	3.6605	Fail
## 31	586.7410	1	5	118.62	5.9067	Fail
## 32	425.9519	1	5	48.83	4.6466	Fail
## 33	463.9572	0	4	109.53	4.4949	Pass
## 34	465.5855	1	4	63.27	4.6322	Fail
## 35	462.4235	1	4	44.81	3.1807	Fail
## 36	434.5526	1	4	86.88	4.5343	Pass
## 37	462.6058	1	4	86.88	4.8900	Fail
## 38	448.5792	1	4	86.88	4.5412	Pass
## 39	409.5032	1	4	103.68	3.6894	Fail
## 40	468.9976	1	4	86.88	5.1987	Fail
## 41	391.4820	2	3	48.13	3.9869	Pass
## 42	484.5872	1	4	67.87	5.2310	Fail
## 43	413.5157	2	5	64.26	3.7656	Pass
## 44	398.5011	2	4	61.02	4.6285	Fail
## 45	495.0604	2	6	67.50	4.7107	Fail
## 46	497.7411	1	6	79.95	4.4994	Pass
## 47	458.6204	1	4	78.40	6.0283	Fail
## 48	444.5938	1	4	78.40	5.5421	Fail
## 49	397.5356	1	5	80.89	3.5364	Fail
## 50	493.5983	1	5	90.87	4.6224	Fail
## 51	453.5748	1	4	63.27	4.0869	Pass
## 52	367.3992	2	6	87.74	2.8245	Fail
## 53	456.9675	1	5	58.12	4.3794	Pass
## 54	456.9675	1	5	58.12	4.3794	Fail
## 55	460.5275	2	2	75.82	6.6530	Fail
## 56	459.6084	1	5	81.64	4.6594	Pass
## 57	423.4221	1	5	115.94	3.7888	Fail
## 58	487.0161	1	6	83.15	3.6188	Fail
## 59	420.4806	1	5	121.98	3.4845	Fail
## 60	445.5113	1	6	82.71	3.0586	Fail
## 61	340.7793	0	3	33.20	4.6625	Pass
## 62	367.3992	1	2	86.48	4.0561	Fail
## 63	383.4815	1	4	59.00	4.2014	Pass
## 64	480.5780	0	5	84.53	5.2072	Fail
## 65	395.5197	0	4	83.56	4.6735	Fail
## 66	376.4243	1	2	47.17	4.9369	Pass
## 67	458.6188	1	4	96.86	4.5785	Fail
## 68	450.5735	1	4	77.88	5.4409	Fail
## 69	426.5789	1	3	133.00	5.8538	Fail
## 70	420.5501	1	3	104.76	5.9004	Fail
## 71	425.9519	1	5	48.83	4.7928	Pass
## 72	354.8059	2	3	41.13	5.5209	Fail
## 73	363.4536	1	4	54.46	4.6697	Pass
## 74	405.4904	1	4	63.69	4.8729	Fail
## 75	396.9106	1	3	41.57	4.2710	Fail

## 76	434.5316	1	5	66.93	4.2618	Pass
## 77	341.7193	1	4	55.11	4.4876	Fail
## 78	405.4904	0	4	54.90	3.8560	Pass
## 79	339.3460	1	2	86.48	3.3585	Fail
## 80	389.7904	1	2	95.71	3.5203	Fail
## 81	359.7643	1	2	86.48	3.5367	Pass
## 82	416.5167	1	5	121.98	3.5627	Fail
## 83	384.4937	1	5	74.86	3.8988	Pass
## 84	397.4925	1	3	90.68	4.3726	Fail
## 85	431.5487	1	3	87.66	7.1551	Fail
## 86	510.4217	1	2	38.33	6.6888	Fail
## 87	326.4419	0	3	99.56	4.6354	Fail
## 88	249.7397	2	3	36.95	2.1546	Pass
## 89	292.3325	0	3	41.90	3.7709	Fail
## 90	293.3173	0	2	47.89	3.9411	Fail
## 91	283.7096	0	2	38.66	4.2731	Pass
## 92	273.3276	1	3	49.77	3.0997	Fail
## 93	314.4194	1	2	46.53	6.0850	Fail
## 94	267.3295	1	4	55.11	3.2326	Fail
## 95	368.6529	2	3	49.33	4.3242	Fail
## 96	468.3386	0	5	74.30	3.1425	Pass
## 97	328.1602	0	2	38.66	4.3571	Fail
## 98	420.5034	2	3	58.29	6.8663	Fail
## 99	315.6754	2	3	49.33	3.9540	Fail
## 100	403.9084	1	5	125.49	4.1159	Fail
## 101	327.6927	1	4	55.11	4.0014	Pass
## 102	494.5455	2	8	110.98	2.0218	Fail
## 103	413.5765	1	2	57.34	6.2161	Fail
## 104	559.6258	1	5	53.40	6.4241	Fail
## 105	286.3280	0	2	34.89	4.2707	Fail
## 106	294.4395	3	6	74.76	4.1261	Pass
## 107	592.6492	1	4	67.87	6.9870	Fail
## 108	274.3156	1	2	64.36	3.0657	Pass
## 109	411.9494	1	3	72.22	5.7612	Fail
## 110	301.4050	1	2	67.54	3.8328	Fail
## 111	346.4208	2	4	86.44	3.8400	Pass
## 112	465.6113	0	2	65.24	7.6743	Fail
## 113	377.8626	1	2	56.79	4.3119	Pass
## 114	347.8365	1	2	47.56	4.3283	Fail
## 115	314.4658	2	2	37.19	4.2308	Fail
## 116	353.3726	2	6	87.74	1.6457	Pass
## 117	385.8657	1	3	83.64	5.0629	Fail
## 118	500.5677	1	6	113.73	5.0774	Fail
## 119	460.5468	0	5	86.64	6.0652	Fail
## 120	546.5889	1	6	75.71	5.7672	Fail
## 121	338.2720	2	2	32.26	4.8755	Pass
## 122	479.5309	2	7	98.09	2.7260	Fail
## 123	310.4340	2	2	37.19	4.2018	Pass
## 124	459.9218	0	3	57.53	6.8199	Fail
## 125	309.3167	0	2	57.12	3.5759	Fail
## 126	292.5033	1	2	15.27	3.8729	Pass
## 127	367.5252	2	3	41.49	4.7391	Fail
## 128	281.2700	2	3	96.21	3.2356	Pass
## 129	282.5511	1	2	38.33	3.0808	Fail

## 130	391.8892	2	2	59.95	4.4488	Fail
## 131	343.3794	2	3	67.01	4.0389	Pass
## 132	621.7718	0	7	94.76	8.0416	Fail
## 133	370.4860	2	4	61.80	3.9713	Pass
## 134	659.6837	0	4	91.37	6.4236	Fail
## 135	468.0990	0	3	53.26	8.6561	Fail
## 136	422.3131	1	2	56.79	4.3959	Pass
## 137	357.4043	1	5	75.02	1.7787	Fail
## 138	387.4767	1	2	31.92	5.8080	Fail
## 139	286.7534	0	1	26.30	4.2597	Fail
## 140	377.8626	2	2	59.95	4.1000	Fail
## 141	364.4384	1	4	60.45	5.0167	Pass
## 142	657.7540	0	5	80.75	7.0971	Fail
## 143	338.2720	2	2	32.26	4.9542	Pass
## 144	347.8365	2	2	50.72	4.1164	Fail
## 145	359.4013	2	6	115.98	1.5991	Fail
## 146	494.6477	1	5	96.11	4.7480	Pass
## 147	386.4920	0	6	80.29	3.4616	Fail
## 148	436.5684	1	4	90.79	5.2410	Fail
## 149	335.4435	1	3	46.92	4.1187	Fail
## 150	410.4207	2	8	115.22	1.0092	Fail
## 151	334.3693	1	2	73.91	3.5003	Pass
## 152	322.4447	2	2	37.19	4.4796	Fail
## 153	574.2378	2	2	37.19	5.6360	Fail
## 154	631.7167	0	4	72.91	6.8546	Fail
## 155	496.6825	2	4	76.66	4.9598	Fail
## 156	349.8524	2	2	50.72	3.7984	Pass
## 157	261.7471	2	2	32.26	3.7257	Fail
## 158	337.4179	2	2	40.71	5.3601	Fail
## 159	308.4181	2	2	37.19	4.0234	Fail
## 160	309.8126	0	3	57.78	3.5043	Fail
## 161	419.4755	2	4	67.27	5.7020	Pass
## 162	367.2702	2	3	46.42	3.8192	Fail
## 163	282.1639	1	2	46.53	2.6255	Pass
## 164	312.1899	1	2	55.76	2.6091	Fail
## 165	394.4213	1	2	92.37	3.4675	Fail
## 166	487.7631	2	4	71.45	6.1295	Pass
## 167	453.3181	2	4	71.45	5.4651	Fail
## 168	432.8997	2	4	71.45	5.2869	Fail
## 169	447.5288	2	4	67.27	6.1951	Fail
## 170	279.3994	0	2	54.84	3.0059	Fail
## 171	395.7213	1	3	26.71	4.5898	Pass
## 172	321.7992	2	2	50.72	3.6366	Fail
## 173	401.8857	2	3	49.33	5.5740	Fail
## 174	354.4021	2	4	62.22	4.1527	Fail
## 175	484.9539	1	6	113.73	4.8334	Fail
## 176	359.4180	0	2	54.73	5.2512	Pass
## 177	398.4547	0	3	51.13	4.5674	Fail
## 178	500.1858	1	3	55.87	5.9747	Fail
## 179	367.4821	1	3	49.77	4.2540	Fail
## 180	334.3859	2	5	67.43	3.5116	Fail
## 181	453.5382	1	4	54.57	8.5045	Pass
## 182	286.1973	0	2	20.31	4.1286	Fail
## 183	371.4535	1	2	63.63	4.8129	Pass

## 184	420.3231	1	2	54.40	5.5777	Fail
## 185	361.2225	3	3	65.12	4.6665	Fail
## 186	332.5052	3	3	76.38	4.5174	Pass
## 187	272.3013	0	3	42.85	4.1662	Fail
## 188	337.1703	0	3	42.85	4.4284	Pass
## 189	293.3173	1	4	55.40	3.1658	Fail
## 190	327.4267	1	4	108.42	3.3785	Fail
## 191	360.2296	1	4	83.12	3.5851	Pass
## 192	415.5751	1	5	98.92	5.1112	Fail
## 193	357.4060	2	3	67.01	4.3877	Pass
## 194	278.7097	2	3	41.13	3.8790	Fail
## 195	422.4364	3	5	100.02	4.2352	Fail
## 196	378.4876	1	5	88.00	3.7843	Pass
## 197	431.3125	1	4	54.71	4.9098	Fail
## 198	265.3917	2	2	41.49	3.4042	Pass
## 199	362.2676	2	4	56.84	3.9056	Fail
## 200	440.5173	3	7	123.77	3.5500	Fail
## 201	329.3726	2	5	66.07	2.4152	Pass
## 202	480.5796	2	2	92.67	7.2172	Fail
## 203	245.3174	1	2	38.33	3.5255	Pass
## 204	358.4355	0	2	24.72	6.4826	Fail
## 205	496.0004	1	2	47.67	7.4397	Fail
## 206	417.4299	0	2	48.00	5.0091	Pass
## 207	256.3865	1	2	27.09	4.9299	Fail
## 208	335.8291	1	5	54.46	2.8947	Pass
## 209	368.9037	1	4	41.05	4.9191	Fail
## 210	470.1598	2	4	49.84	6.9694	Fail
## 211	393.4829	2	7	88.86	2.4314	Pass
## 212	440.2853	0	5	74.30	2.4449	Fail
## 213	466.5579	1	8	112.31	2.0966	Fail
## 214	416.2870	1	4	39.60	4.4058	Fail
## 215	290.2438	1	4	50.70	4.1130	Fail
## 216	290.2438	1	4	51.81	4.4057	Pass
## 217	335.3109	0	3	94.35	3.4978	Fail
## 218	362.4225	1	4	58.64	3.5192	Pass
## 219	372.4174	2	2	67.37	5.0988	Fail
## 220	373.4054	2	3	76.24	4.0225	Fail
## 221	442.3078	2	3	57.78	5.7121	Pass
## 222	427.3140	1	5	88.00	2.3543	Fail
## 223	441.3181	1	4	54.71	4.3294	Pass
## 224	420.6770	2	5	71.09	4.2420	Fail
## 225	383.6675	1	3	45.48	4.3217	Fail
## 226	420.5050	1	6	66.93	3.8737	Pass
## 227	412.4846	3	5	86.88	4.7220	Fail
## 228	382.2433	2	3	57.78	5.3841	Fail
## 229	440.4484	4	6	107.89	4.4248	Fail
## 230	366.3400	1	4	50.70	5.0847	Fail
## 231	434.4846	1	3	87.92	5.5356	Pass
## 232	380.4378	1	4	69.68	4.7102	Fail
## 233	357.2446	1	2	34.15	4.9298	Pass
## 234	430.5048	4	4	109.40	5.1926	Fail
## 235	441.8562	1	5	87.07	5.0419	Fail
## 236	403.4314	2	3	85.47	4.0061	Pass
## 237	307.3697	1	4	101.58	2.0459	Fail

## 238	456.5075	0	5	68.31	4.3195	Pass
## 239	382.8634	1	5	88.00	2.2703	Fail
## 240	381.8130	2	5	80.32	2.8968	Fail
## 241	232.7091	0	2	16.13	3.3039	Pass
## 242	319.3579	1	3	67.05	3.1872	Fail
## 243	349.5168	1	4	108.42	4.4641	Pass
## 244	303.7839	0	1	21.70	4.2684	Fail
## 245	315.8377	0	1	12.47	5.3364	Fail
## 246	312.4153	1	3	108.00	4.3189	Pass
## 247	332.3501	0	2	56.51	5.3178	Fail
## 248	189.2142	1	3	61.03	1.4288	Pass
## 249	200.2800	1	2	27.09	3.1051	Fail
## 250	318.3235	0	2	56.51	4.8316	Fail
## 251	348.1807	2	3	62.47	4.8811	Pass
## 252	341.4098	1	5	63.59	5.1999	Fail
## 253	293.5307	0	1	35.53	3.1341	Pass
## 254	287.7845	0	1	12.47	4.9084	Fail
## 255	287.3591	1	3	51.80	4.4471	Fail
## 256	268.1389	1	2	29.10	3.4358	Pass
## 257	280.1604	1	2	29.10	3.8341	Fail
## 258	201.2648	1	2	29.10	3.0857	Pass
## 259	279.3370	1	4	44.70	2.6761	Fail
## 260	265.3104	1	4	44.70	2.1899	Fail
## 261	320.3890	2	4	59.07	4.3199	Pass
## 262	326.3952	2	4	49.84	5.3906	Fail
## 263	289.3319	3	3	60.94	3.9204	Pass
## 264	273.7180	3	3	60.94	3.6764	Fail
## 265	312.4068	1	3	35.94	3.1606	Fail
## 266	199.2489	1	2	29.10	2.6950	Pass
## 267	252.3149	2	3	57.94	2.6862	Fail
## 268	254.3275	0	2	15.71	3.7398	Pass
## 269	267.3505	1	3	66.05	4.0883	Fail
## 270	298.7674	1	2	34.15	4.4970	Fail
## 271	333.5731	2	3	41.13	4.7216	Pass
## 272	274.3829	1	3	60.58	3.4279	Fail
## 273	319.4203	1	2	75.80	3.5610	Pass
## 274	331.4150	0	4	47.57	3.9406	Fail
## 275	310.4151	1	3	70.23	4.6406	Fail
## 276	245.2743	1	4	55.40	2.3200	Pass
## 277	298.7674	1	2	34.15	4.5632	Fail
## 278	319.4441	1	3	28.16	4.0719	Pass
## 279	348.3959	1	5	68.29	3.9967	Fail
## 280	287.3144	1	4	72.28	1.6009	Fail
## 281	321.4169	1	3	37.39	4.3436	Pass
## 282	280.3218	2	3	54.38	3.5652	Fail
## 283	336.3852	1	4	60.45	3.5963	Pass
## 284	274.3189	1	4	69.16	4.2202	Fail
## 285	308.4423	1	2	53.16	6.2690	Fail
## 286	245.2743	1	4	55.40	2.3200	Pass
## 287	268.3541	0	2	15.71	4.0886	Fail
## 288	268.3110	0	2	24.94	3.5243	Pass
## 289	278.3059	1	2	55.13	3.2718	Fail
## 290	345.8272	2	5	66.07	2.8741	Fail
## 291	275.3085	1	4	55.11	3.2015	Pass

##	292	359.4682	0	4	47.57	4.7719	Fail
##	293	346.3966	0	5	49.85	3.3648	Pass
##	294	228.3333	1	2	27.09	4.0175	Fail
##	295	309.4061	0	4	28.07	3.4386	Fail
##	296	323.3466	2	4	86.47	2.5607	Pass
##	297	368.4751	1	4	31.40	5.0228	Fail
##	298	501.3643	3	5	86.88	6.1688	Fail
##	299	448.3646	2	4	49.84	7.3572	Fail
##	300	291.3908	1	3	28.16	3.9106	Fail
##	301	260.3386	2	6	83.24	1.1216	Pass
##	302	277.7929	1	3	28.16	3.3257	Fail
##	303	288.3008	0	3	52.08	3.6636	Pass
##	304	325.5883	2	3	41.13	3.9357	Fail
##	305	261.4030	2	2	32.26	4.3590	Fail
##	306	355.4332	1	4	37.39	4.3247	Pass
##	307	307.4333	1	3	28.16	3.6321	Fail
##	308	270.3286	1	1	28.68	4.7890	Pass
##	309	293.4067	1	3	28.16	3.5697	Fail
##	310	199.2489	1	2	29.10	2.7816	Fail
##	311	350.0277	2	3	41.13	5.1805	Pass
##	312	281.1344	2	2	40.46	4.0663	Fail
##	313	389.5341	1	4	29.95	4.7640	Pass
##	314	279.3801	1	3	28.16	3.3630	Fail
##	315	608.7247	1	3	72.86	6.9672	Fail
##	316	324.4175	1	3	45.59	2.6207	Pass

Bioavailability prediction

```
predict_oral_bioavailability(properties)
```

##	MW	nHBDdon	nHBAcc	TopoPSA	ALogP	OralBioavailability
## 1	356.4180	2	3	54.38	5.8914	Low
## 2	451.5605	2	3	70.50	8.1237	Low
## 3	358.3885	1	3	85.22	3.9521	High
## 4	472.4570	4	8	159.72	5.6735	Low
## 5	310.3720	1	3	75.99	3.7630	High
## 6	524.5732	4	4	127.86	6.3384	Low
## 7	406.4993	1	4	90.90	4.8441	High
## 8	637.7222	0	5	107.66	7.0274	Low
## 9	554.5051	0	3	55.84	6.4874	Low
## 10	411.6242	1	4	35.58	4.2339	High
## 11	390.4999	1	3	79.46	4.1867	High
## 12	476.0349	0	3	62.90	7.2190	Low
## 13	400.9424	1	3	45.48	3.8604	High
## 14	384.4878	1	3	35.94	4.0949	High
## 15	393.4003	1	3	49.77	4.5734	High
## 16	354.4618	1	3	26.71	4.1113	High
## 17	571.6646	0	4	54.45	6.8874	Low
## 18	388.5062	2	4	61.02	4.4830	High
## 19	445.5213	2	4	44.37	4.7031	High
## 20	218.2522	0	4	41.90	0.9043	High
## 21	357.7981	1	7	78.66	2.1145	High
## 22	414.4816	0	5	107.35	4.2277	High

## 23	400.4549	0	5	107.35	3.7415	High
## 24	303.3810	2	5	99.33	2.8064	High
## 25	362.4290	3	7	82.18	3.7992	High
## 26	362.4326	1	2	15.27	4.3255	High
## 27	418.5753	0	3	33.53	4.7073	High
## 28	413.5125	2	3	61.27	4.8044	High
## 29	479.9994	2	4	62.83	4.5669	High
## 30	438.8961	1	4	50.80	3.6605	High
## 31	586.7410	1	5	118.62	5.9067	Low
## 32	425.9519	1	5	48.83	4.6466	High
## 33	463.9572	0	4	109.53	4.4949	High
## 34	465.5855	1	4	63.27	4.6322	High
## 35	462.4235	1	4	44.81	3.1807	High
## 36	434.5526	1	4	86.88	4.5343	High
## 37	462.6058	1	4	86.88	4.8900	High
## 38	448.5792	1	4	86.88	4.5412	High
## 39	409.5032	1	4	103.68	3.6894	High
## 40	468.9976	1	4	86.88	5.1987	Low
## 41	391.4820	2	3	48.13	3.9869	High
## 42	484.5872	1	4	67.87	5.2310	Low
## 43	413.5157	2	5	64.26	3.7656	High
## 44	398.5011	2	4	61.02	4.6285	High
## 45	495.0604	2	6	67.50	4.7107	High
## 46	497.7411	1	6	79.95	4.4994	High
## 47	458.6204	1	4	78.40	6.0283	Low
## 48	444.5938	1	4	78.40	5.5421	Low
## 49	397.5356	1	5	80.89	3.5364	High
## 50	493.5983	1	5	90.87	4.6224	High
## 51	453.5748	1	4	63.27	4.0869	High
## 52	367.3992	2	6	87.74	2.8245	High
## 53	456.9675	1	5	58.12	4.3794	High
## 54	456.9675	1	5	58.12	4.3794	High
## 55	460.5275	2	2	75.82	6.6530	Low
## 56	459.6084	1	5	81.64	4.6594	High
## 57	423.4221	1	5	115.94	3.7888	High
## 58	487.0161	1	6	83.15	3.6188	High
## 59	420.4806	1	5	121.98	3.4845	High
## 60	445.5113	1	6	82.71	3.0586	High
## 61	340.7793	0	3	33.20	4.6625	High
## 62	367.3992	1	2	86.48	4.0561	High
## 63	383.4815	1	4	59.00	4.2014	High
## 64	480.5780	0	5	84.53	5.2072	Low
## 65	395.5197	0	4	83.56	4.6735	High
## 66	376.4243	1	2	47.17	4.9369	High
## 67	458.6188	1	4	96.86	4.5785	High
## 68	450.5735	1	4	77.88	5.4409	Low
## 69	426.5789	1	3	133.00	5.8538	Low
## 70	420.5501	1	3	104.76	5.9004	Low
## 71	425.9519	1	5	48.83	4.7928	High
## 72	354.8059	2	3	41.13	5.5209	Low
## 73	363.4536	1	4	54.46	4.6697	High
## 74	405.4904	1	4	63.69	4.8729	High
## 75	396.9106	1	3	41.57	4.2710	High
## 76	434.5316	1	5	66.93	4.2618	High

## 77	341.7193	1	4	55.11	4.4876	High
## 78	405.4904	0	4	54.90	3.8560	High
## 79	339.3460	1	2	86.48	3.3585	High
## 80	389.7904	1	2	95.71	3.5203	High
## 81	359.7643	1	2	86.48	3.5367	High
## 82	416.5167	1	5	121.98	3.5627	High
## 83	384.4937	1	5	74.86	3.8988	High
## 84	397.4925	1	3	90.68	4.3726	High
## 85	431.5487	1	3	87.66	7.1551	Low
## 86	510.4217	1	2	38.33	6.6888	Low
## 87	326.4419	0	3	99.56	4.6354	High
## 88	249.7397	2	3	36.95	2.1546	High
## 89	292.3325	0	3	41.90	3.7709	High
## 90	293.3173	0	2	47.89	3.9411	High
## 91	283.7096	0	2	38.66	4.2731	High
## 92	273.3276	1	3	49.77	3.0997	High
## 93	314.4194	1	2	46.53	6.0850	Low
## 94	267.3295	1	4	55.11	3.2326	High
## 95	368.6529	2	3	49.33	4.3242	High
## 96	468.3386	0	5	74.30	3.1425	High
## 97	328.1602	0	2	38.66	4.3571	High
## 98	420.5034	2	3	58.29	6.8663	Low
## 99	315.6754	2	3	49.33	3.9540	High
## 100	403.9084	1	5	125.49	4.1159	High
## 101	327.6927	1	4	55.11	4.0014	High
## 102	494.5455	2	8	110.98	2.0218	High
## 103	413.5765	1	2	57.34	6.2161	Low
## 104	559.6258	1	5	53.40	6.4241	Low
## 105	286.3280	0	2	34.89	4.2707	High
## 106	294.4395	3	6	74.76	4.1261	High
## 107	592.6492	1	4	67.87	6.9870	Low
## 108	274.3156	1	2	64.36	3.0657	High
## 109	411.9494	1	3	72.22	5.7612	Low
## 110	301.4050	1	2	67.54	3.8328	High
## 111	346.4208	2	4	86.44	3.8400	High
## 112	465.6113	0	2	65.24	7.6743	Low
## 113	377.8626	1	2	56.79	4.3119	High
## 114	347.8365	1	2	47.56	4.3283	High
## 115	314.4658	2	2	37.19	4.2308	High
## 116	353.3726	2	6	87.74	1.6457	High
## 117	385.8657	1	3	83.64	5.0629	Low
## 118	500.5677	1	6	113.73	5.0774	Low
## 119	460.5468	0	5	86.64	6.0652	Low
## 120	546.5889	1	6	75.71	5.7672	Low
## 121	338.2720	2	2	32.26	4.8755	High
## 122	479.5309	2	7	98.09	2.7260	High
## 123	310.4340	2	2	37.19	4.2018	High
## 124	459.9218	0	3	57.53	6.8199	Low
## 125	309.3167	0	2	57.12	3.5759	High
## 126	292.5033	1	2	15.27	3.8729	High
## 127	367.5252	2	3	41.49	4.7391	High
## 128	281.2700	2	3	96.21	3.2356	High
## 129	282.5511	1	2	38.33	3.0808	High
## 130	391.8892	2	2	59.95	4.4488	High



## 131	343.3794	2	3	67.01	4.0389	High
## 132	621.7718	0	7	94.76	8.0416	Low
## 133	370.4860	2	4	61.80	3.9713	High
## 134	659.6837	0	4	91.37	6.4236	Low
## 135	468.0990	0	3	53.26	8.6561	Low
## 136	422.3131	1	2	56.79	4.3959	High
## 137	357.4043	1	5	75.02	1.7787	High
## 138	387.4767	1	2	31.92	5.8080	Low
## 139	286.7534	0	1	26.30	4.2597	High
## 140	377.8626	2	2	59.95	4.1000	High
## 141	364.4384	1	4	60.45	5.0167	Low
## 142	657.7540	0	5	80.75	7.0971	Low
## 143	338.2720	2	2	32.26	4.9542	High
## 144	347.8365	2	2	50.72	4.1164	High
## 145	359.4013	2	6	115.98	1.5991	High
## 146	494.6477	1	5	96.11	4.7480	High
## 147	386.4920	0	6	80.29	3.4616	High
## 148	436.5684	1	4	90.79	5.2410	Low
## 149	335.4435	1	3	46.92	4.1187	High
## 150	410.4207	2	8	115.22	1.0092	High
## 151	334.3693	1	2	73.91	3.5003	High
## 152	322.4447	2	2	37.19	4.4796	High
## 153	574.2378	2	2	37.19	5.6360	Low
## 154	631.7167	0	4	72.91	6.8546	Low
## 155	496.6825	2	4	76.66	4.9598	High
## 156	349.8524	2	2	50.72	3.7984	High
## 157	261.7471	2	2	32.26	3.7257	High
## 158	337.4179	2	2	40.71	5.3601	Low
## 159	308.4181	2	2	37.19	4.0234	High
## 160	309.8126	0	3	57.78	3.5043	High
## 161	419.4755	2	4	67.27	5.7020	Low
## 162	367.2702	2	3	46.42	3.8192	High
## 163	282.1639	1	2	46.53	2.6255	High
## 164	312.1899	1	2	55.76	2.6091	High
## 165	394.4213	1	2	92.37	3.4675	High
## 166	487.7631	2	4	71.45	6.1295	Low
## 167	453.3181	2	4	71.45	5.4651	Low
## 168	432.8997	2	4	71.45	5.2869	Low
## 169	447.5288	2	4	67.27	6.1951	Low
## 170	279.3994	0	2	54.84	3.0059	High
## 171	395.7213	1	3	26.71	4.5898	High
## 172	321.7992	2	2	50.72	3.6366	High
## 173	401.8857	2	3	49.33	5.5740	Low
## 174	354.4021	2	4	62.22	4.1527	High
## 175	484.9539	1	6	113.73	4.8334	High
## 176	359.4180	0	2	54.73	5.2512	Low
## 177	398.4547	0	3	51.13	4.5674	High
## 178	500.1858	1	3	55.87	5.9747	Low
## 179	367.4821	1	3	49.77	4.2540	High
## 180	334.3859	2	5	67.43	3.5116	High
## 181	453.5382	1	4	54.57	8.5045	Low
## 182	286.1973	0	2	20.31	4.1286	High
## 183	371.4535	1	2	63.63	4.8129	High
## 184	420.3231	1	2	54.40	5.5777	Low

## 185	361.2225	3	3	65.12	4.6665	High
## 186	332.5052	3	3	76.38	4.5174	High
## 187	272.3013	0	3	42.85	4.1662	High
## 188	337.1703	0	3	42.85	4.4284	High
## 189	293.3173	1	4	55.40	3.1658	High
## 190	327.4267	1	4	108.42	3.3785	High
## 191	360.2296	1	4	83.12	3.5851	High
## 192	415.5751	1	5	98.92	5.1112	Low
## 193	357.4060	2	3	67.01	4.3877	High
## 194	278.7097	2	3	41.13	3.8790	High
## 195	422.4364	3	5	100.02	4.2352	High
## 196	378.4876	1	5	88.00	3.7843	High
## 197	431.3125	1	4	54.71	4.9098	High
## 198	265.3917	2	2	41.49	3.4042	High
## 199	362.2676	2	4	56.84	3.9056	High
## 200	440.5173	3	7	123.77	3.5500	High
## 201	329.3726	2	5	66.07	2.4152	High
## 202	480.5796	2	2	92.67	7.2172	Low
## 203	245.3174	1	2	38.33	3.5255	High
## 204	358.4355	0	2	24.72	6.4826	Low
## 205	496.0004	1	2	47.67	7.4397	Low
## 206	417.4299	0	2	48.00	5.0091	Low
## 207	256.3865	1	2	27.09	4.9299	High
## 208	335.8291	1	5	54.46	2.8947	High
## 209	368.9037	1	4	41.05	4.9191	High
## 210	470.1598	2	4	49.84	6.9694	Low
## 211	393.4829	2	7	88.86	2.4314	High
## 212	440.2853	0	5	74.30	2.4449	High
## 213	466.5579	1	8	112.31	2.0966	High
## 214	416.2870	1	4	39.60	4.4058	High
## 215	290.2438	1	4	50.70	4.1130	High
## 216	290.2438	1	4	51.81	4.4057	High
## 217	335.3109	0	3	94.35	3.4978	High
## 218	362.4225	1	4	58.64	3.5192	High
## 219	372.4174	2	2	67.37	5.0988	Low
## 220	373.4054	2	3	76.24	4.0225	High
## 221	442.3078	2	3	57.78	5.7121	Low
## 222	427.3140	1	5	88.00	2.3543	High
## 223	441.3181	1	4	54.71	4.3294	High
## 224	420.6770	2	5	71.09	4.2420	High
## 225	383.6675	1	3	45.48	4.3217	High
## 226	420.5050	1	6	66.93	3.8737	High
## 227	412.4846	3	5	86.88	4.7220	High
## 228	382.2433	2	3	57.78	5.3841	Low
## 229	440.4484	4	6	107.89	4.4248	High
## 230	366.3400	1	4	50.70	5.0847	Low
## 231	434.4846	1	3	87.92	5.5356	Low
## 232	380.4378	1	4	69.68	4.7102	High
## 233	357.2446	1	2	34.15	4.9298	High
## 234	430.5048	4	4	109.40	5.1926	Low
## 235	441.8562	1	5	87.07	5.0419	Low
## 236	403.4314	2	3	85.47	4.0061	High
## 237	307.3697	1	4	101.58	2.0459	High
## 238	456.5075	0	5	68.31	4.3195	High

## 239	382.8634	1	5	88.00	2.2703	High
## 240	381.8130	2	5	80.32	2.8968	High
## 241	232.7091	0	2	16.13	3.3039	High
## 242	319.3579	1	3	67.05	3.1872	High
## 243	349.5168	1	4	108.42	4.4641	High
## 244	303.7839	0	1	21.70	4.2684	High
## 245	315.8377	0	1	12.47	5.3364	Low
## 246	312.4153	1	3	108.00	4.3189	High
## 247	332.3501	0	2	56.51	5.3178	Low
## 248	189.2142	1	3	61.03	1.4288	High
## 249	200.2800	1	2	27.09	3.1051	High
## 250	318.3235	0	2	56.51	4.8316	High
## 251	348.1807	2	3	62.47	4.8811	High
## 252	341.4098	1	5	63.59	5.1999	Low
## 253	293.5307	0	1	35.53	3.1341	High
## 254	287.7845	0	1	12.47	4.9084	High
## 255	287.3591	1	3	51.80	4.4471	High
## 256	268.1389	1	2	29.10	3.4358	High
## 257	280.1604	1	2	29.10	3.8341	High
## 258	201.2648	1	2	29.10	3.0857	High
## 259	279.3370	1	4	44.70	2.6761	High
## 260	265.3104	1	4	44.70	2.1899	High
## 261	320.3890	2	4	59.07	4.3199	High
## 262	326.3952	2	4	49.84	5.3906	Low
## 263	289.3319	3	3	60.94	3.9204	High
## 264	273.7180	3	3	60.94	3.6764	High
## 265	312.4068	1	3	35.94	3.1606	High
## 266	199.2489	1	2	29.10	2.6950	High
## 267	252.3149	2	3	57.94	2.6862	High
## 268	254.3275	0	2	15.71	3.7398	High
## 269	267.3505	1	3	66.05	4.0883	High
## 270	298.7674	1	2	34.15	4.4970	High
## 271	333.5731	2	3	41.13	4.7216	High
## 272	274.3829	1	3	60.58	3.4279	High
## 273	319.4203	1	2	75.80	3.5610	High
## 274	331.4150	0	4	47.57	3.9406	High
## 275	310.4151	1	3	70.23	4.6406	High
## 276	245.2743	1	4	55.40	2.3200	High
## 277	298.7674	1	2	34.15	4.5632	High
## 278	319.4441	1	3	28.16	4.0719	High
## 279	348.3959	1	5	68.29	3.9967	High
## 280	287.3144	1	4	72.28	1.6009	High
## 281	321.4169	1	3	37.39	4.3436	High
## 282	280.3218	2	3	54.38	3.5652	High
## 283	336.3852	1	4	60.45	3.5963	High
## 284	274.3189	1	4	69.16	4.2202	High
## 285	308.4423	1	2	53.16	6.2690	Low
## 286	245.2743	1	4	55.40	2.3200	High
## 287	268.3541	0	2	15.71	4.0886	High
## 288	268.3110	0	2	24.94	3.5243	High
## 289	278.3059	1	2	55.13	3.2718	High
## 290	345.8272	2	5	66.07	2.8741	High
## 291	275.3085	1	4	55.11	3.2015	High
## 292	359.4682	0	4	47.57	4.7719	High

## 293	346.3966	0	5	49.85	3.3648	High
## 294	228.3333	1	2	27.09	4.0175	High
## 295	309.4061	0	4	28.07	3.4386	High
## 296	323.3466	2	4	86.47	2.5607	High
## 297	368.4751	1	4	31.40	5.0228	Low
## 298	501.3643	3	5	86.88	6.1688	Low
## 299	448.3646	2	4	49.84	7.3572	Low
## 300	291.3908	1	3	28.16	3.9106	High
## 301	260.3386	2	6	83.24	1.1216	High
## 302	277.7929	1	3	28.16	3.3257	High
## 303	288.3008	0	3	52.08	3.6636	High
## 304	325.5883	2	3	41.13	3.9357	High
## 305	261.4030	2	2	32.26	4.3590	High
## 306	355.4332	1	4	37.39	4.3247	High
## 307	307.4333	1	3	28.16	3.6321	High
## 308	270.3286	1	1	28.68	4.7890	High
## 309	293.4067	1	3	28.16	3.5697	High
## 310	199.2489	1	2	29.10	2.7816	High
## 311	350.0277	2	3	41.13	5.1805	Low
## 312	281.1344	2	2	40.46	4.0663	High
## 313	389.5341	1	4	29.95	4.7640	High
## 314	279.3801	1	3	28.16	3.3630	High
## 315	608.7247	1	3	72.86	6.9672	Low
## 316	324.4175	1	3	45.59	2.6207	High