Supplementary information

# An analysis of the physicochemical properties of oral drugs from 2000 to 2022

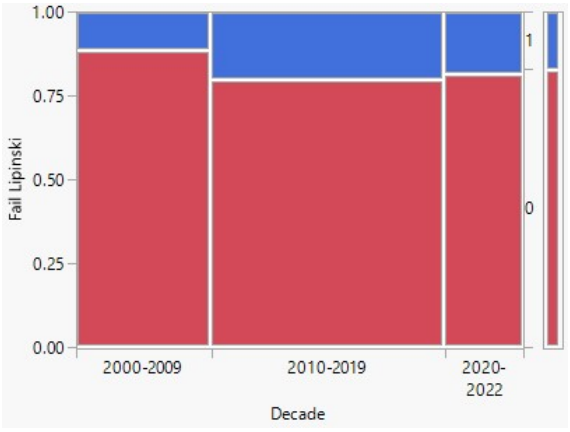
Table S1 – Cross-correlation coefficients ($r^2$) of Lipinski descriptors for the dataset. n = 372

| | HBAs | HBDs | clogP |
|---|---|---|---|
| MWt | 0.69 | 0.27 | 0.65 |
| clogP | 0.12 | -0.14 | |
| HBDs | 0.27 | | |

Table S2 – Analysis of mean clogP values for neutral and charged compounds

| Level | N | Mean | Std Dev | Std Err Mean | Lower 95% | Upper 95% |
|---|---|---|---|---|---|---|
| Neutral | 149 | 3.4301221 | 2.1490323 | 0.1760556 | 3.0822147 | 3.7780295 |
| Charged | 229 | 3.4387821 | 2.0254492 | 0.1338455 | 3.1750499 | 3.7025142 |

Figure S1 – Lipinski fails (blue) and passes (red) over time a) Mosaic plot by decade; b) Table of counts; c) Mosaic plot by year; d) Histogram by year.

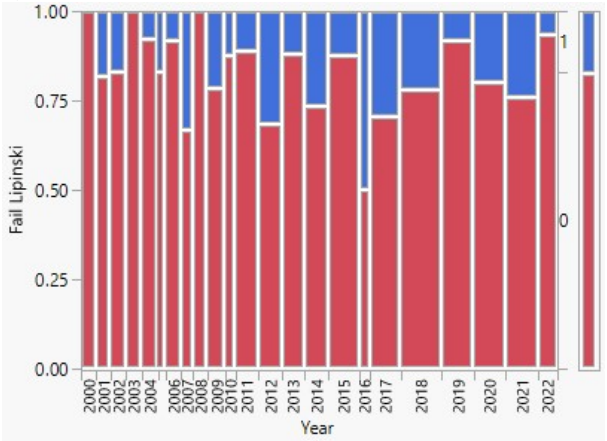



a)

b)

| Count | Pass | Fail | Total |
|---|---|---|---|
| 2000-2009 | 99 (88%) | 13 (12%) | 112 |
| 2010-2019 | 155 (80%) | 39 (20%) | 194 |
| 2020-2022 | 53 (82%) | 12 (18%) | 65 |
| Total | 307 | 64 | 371 |

c)




d)

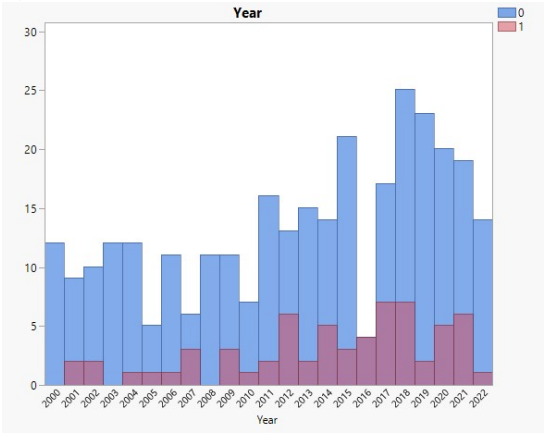
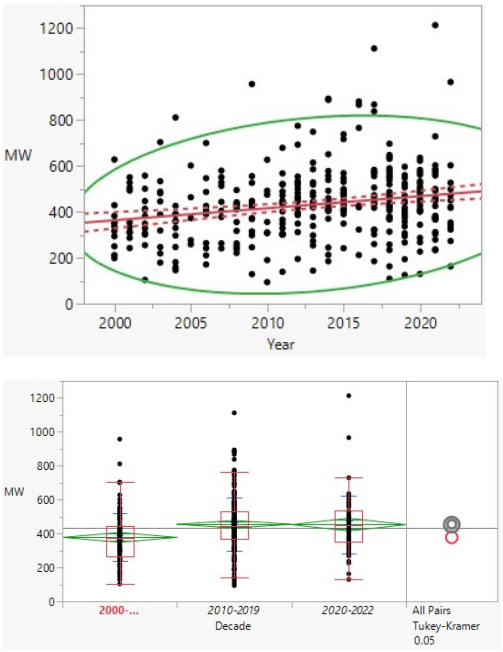
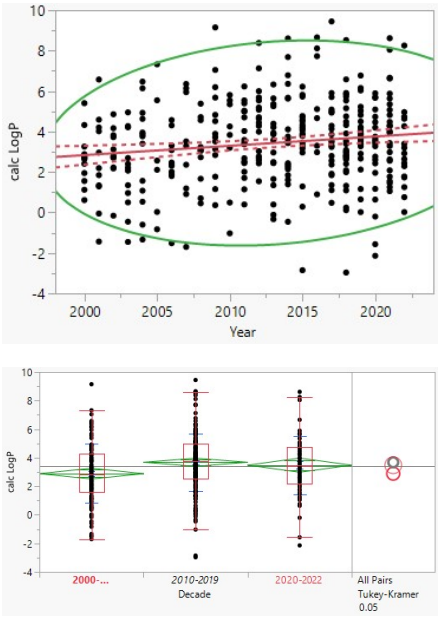
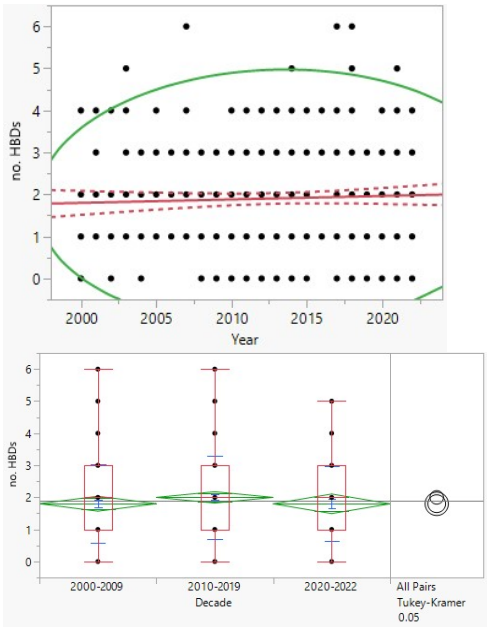
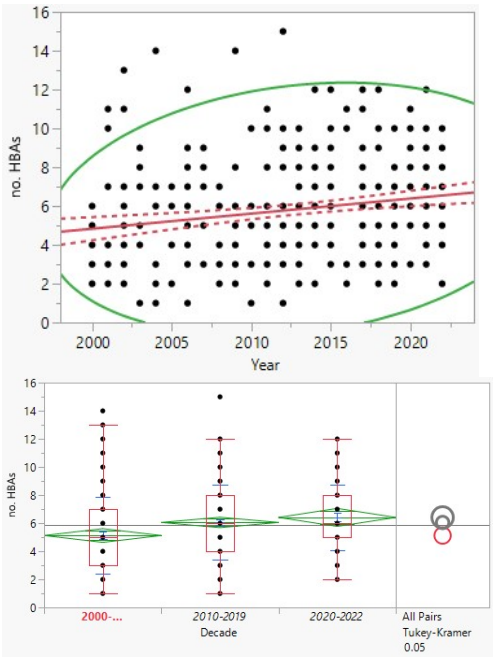


Table S3

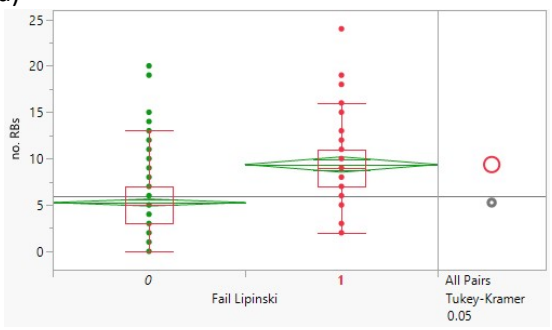
| Mean (std dev) | MWt | clogP |
|---|---|---|
| |  |  |
| 2000-2009 | 378 (139)* | 2.9 (2.1)** |
| 2010-2019 | 455 (156) | 3.7 (2.0) |
| 2020-2022 | 453 (169) | 3.5 (2.0) |

| | HBDs | HBAs |
|---|---|---|
| |  |  |
| 2000-2009 | 2 (1) | 5 (3)* |
| 2010-2019 | 2 (1) | 6 (3) |
| 2020-2022 | 2 (1) | 6 (2) |

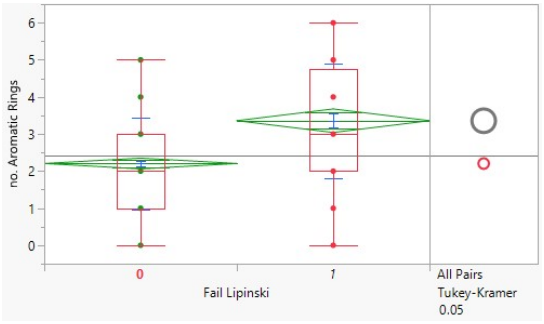
*Value statistically significantly different (Tukey-Kramer method), ** significantly different from 2010-2019 but not 2020-2022.

Figure S2 – Comparison of a) rotatable bond count; b) aromatic ring count; c) $Fsp^3$ between the Lipinski passes and fails.

a)




b)




c)

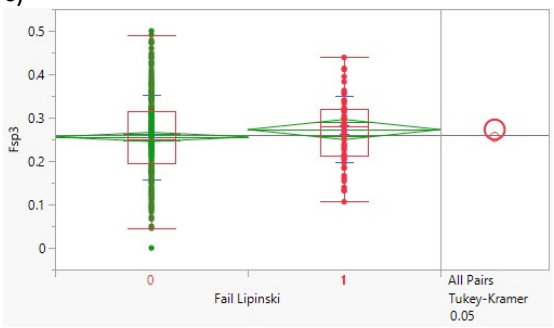
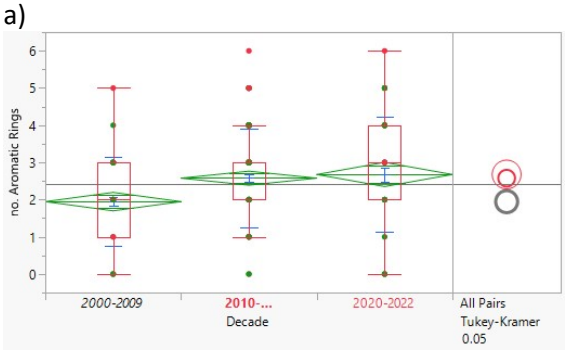



Figure S3 – Variation of a) aromatic ring count; b) $Fsp^3$ by decade.

a)




b)