

Supplementary Table S3

List of Publications Supporting the Assessment of Etiological vs. Palliative Drug Mechanisms

Manuscript Title: DruGNNosis-MoA: Elucidating Drug Mechanisms as Etiological or Palliative with Graph Neural Networks Employing a Large Language Model

Publications in both sections are listed in chronological order, with most recent listed first. Multiple publications with the same publication year are sorted secondarily alphabetically by first author's last name.

Key Publications:

Jansen, K., Haugen, D.F., Pont, L. and Ruths, S., 2018. Safety and effectiveness of palliative drug treatment in the last days of life—a systematic literature review. *Journal of Pain and Symptom Management*, 55(2), pp.508-521.

Wang, J., Li, Z.X., Qiu, C.X., Wang, D. and Cui, Q.H., 2012. The relationship between rational drug design and drug side effects. *Briefings in bioinformatics*, 13(3), pp.377-382.

Yildirim, M.A., Goh, K.I., Cusick, M.E., Barabasi, A.L. and Vidal, M., 2007. Drug-target network. *Nature biotechnology*, 25(10), pp.1119-1126.

Lindpaintner, K., 2002. The impact of pharmacogenetics and pharmacogenomics on drug discovery. *Nature Reviews Drug Discovery*, 1(6), pp.463-469.

Additional Publications:

Hong, J.H., Yong, C.H., Heng, H.L., Chan, J.Y., Lau, M.C., Chen, J., Lee, J.Y., Lim, A.H., Li, Z., Guan, P. and Chu, P.L., 2024. Integrative multiomics enhancer activity profiling identifies therapeutic vulnerabilities in cholangiocarcinoma of different etiologies. *Gut*, 73(6), pp.966-984.

Pal, R.S., Pal, Y., Chaitanya, M.V.N.L., Babu, R., Mazumder, R. and Kumar, A., 2024. Multifaceted Understandings of Cancer: A Review of Disease Mechanisms and Therapies. *Current Cancer Therapy Reviews*, 20(5), pp.481-488.

D'Arrigo, J.S., 2023. Vascular Risks, Aging, and Late-Onset Dementia: Overlapping Etiologies Point to 'Scavenger Receptor'-Mediated Therapeutics. *OBM Geriatrics*, 7(3), pp.1-10.

He, Z., Li, Y., Zhao, X. and Li, B., 2022. Dravet syndrome: Advances in etiology, clinical presentation, and treatment. *Epilepsy Research*, 188, p.107041

Bejjani, A.T., Wary, N. and Gu, M., 2021. Hypoplastic left heart syndrome (HLHS): Molecular pathogenesis and emerging drug targets for cardiac repair and regeneration. *Expert opinion on therapeutic targets*, 25(8), pp.621-632.

Fernandez, J., Silván, B., Entrialgo-Cadierno, R., Villar, C.J., Capasso, R., Uranga, J.A., Lombo, F. and Abalo, R., 2021. Antiproliferative and palliative activity of flavonoids in colorectal cancer. *Biomedicine & Pharmacotherapy*, 143, p.112241.

Leggio, L., Vivarelli, S., L'Episcopo, F., Tirolo, C., Caniglia, S., Testa, N., Marchetti, B. and Iraci, N., 2017. microRNAs in Parkinson's disease: From pathogenesis to novel diagnostic and therapeutic approaches. *International journal of molecular sciences*, 18(12), p.2698.

Guney, E., Menche, J., Vidal, M. and Barábasi, A.L., 2016. Network-based in silico drug efficacy screening. *Nature communications*, 7(1), p.10331.

Blasco, H., Mavel, S., Corcia, P. and Gordon, P.H., 2014. The glutamate hypothesis in ALS: Pathophysiology and drug development. *Current medicinal chemistry*, 21(31), pp.3551-3575.

Wood, L.J. and Weymann, K., 2013. Inflammation and neural signaling: Etiologic mechanisms of the cancer treatment-related symptom cluster. *Current opinion in supportive and palliative care*, 7(1), pp.54-59.

Dhillon, K.S., Singh, J. and Lyall, J.S., 2011. A new horizon into the pathobiology, etiology and treatment of migraine. *Medical hypotheses*, 77(1), pp.147-151.

Sakharkar, M.K. and Sakharkar, K.R., 2008. Genetic and pharmacological interaction network of targets and drugs. *Int J Integ Biol*, 4, pp.1-8.

Frolich, L., Fox, J., Padberg, F., Maurer, K., Moller, H.J. and Hampel, H., 2004. Targets of antidementive therapy: Drugs with a specific pharmacological mechanism of action. *Current pharmaceutical design*, 10(3), pp.223-229.

Charney, D.S., Menkes, D.B. and Heninger, G.R., 1981. Receptor sensitivity and the mechanism of action of antidepressant treatment: Implications for the etiology and therapy of depression. *Archives of General Psychiatry*, 38(10), pp.1160-1180.