

# References

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# **Appendix**

### Spectral data of well-known isolated compounds

**Stigmasterol (2.15):** White solid; 128 mg;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.37 (d, 1H), 5.17 (dd, 1H), 5.04 (dd, 1H), 3.54 (ddd, 1H), 2.32 (ddd, 1H), 2.29 – 2.21 (m, 1H), 2.05 (dd, 3H), 1.90 – 1.82 (m, 3H), 1.77 – 1.65 (m, 1H), 1.63 – 1.45 (m, 10H), 1.30 – 1.26 (m, 1H), 1.25 – 1.16 (m, 3H), 1.16 – 1.06 (m, 4H), 1.04 (d, 6H), 0.94 (d, 4H), 0.90 – 0.77 (m, 9H), 0.71 (d, 3H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  140.8, 138.3, 129.3, 121.7, 71.8, 56.9, 56.8, 51.2, 50.2, 42.3, 42.2, 40.5, 39.8, 37.3, 36.5, 33.9, 31.9, 31.7, 29.2, 28.9, 25.4, 24.4, 23.1, 21.2, 21.1, 19.8, 19.4, 12.2, 12.1.

**$\beta$ -sitosterol (2.16):** White needles; 128 mg;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.39 – 5.31 (1 H, m), 3.52 (1 H, ddd), 2.42 – 2.13 (2 H, m), 1.98 (2 H, tdd), 1.89 – 1.77 (3 H, m), 1.74 – 1.38 (11 H, m), 1.33 – 1.22 (5 H, m), 1.21 – 1.03 (6 H, m), 1.03 – 0.96 (4 H, m), 0.93 (4 H, t), 0.87 – 0.74 (8 H, m), 0.75 – 0.64 (3 H, m);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  140.9, 121.9, 72.0, 56.9, 56.2, 50.3, 46.0, 42.5, 39.9, 37.4, 36.7, 36.3, 34.1, 32.1, 31.8, 29.9, 29.3, 28.4, 26.2, 24.5, 23.2, 21.2, 20.0, 19.5, 19.2, 18.9, 12.1, 12.0.

**Apigenin (2.18):** Yellow solid; 98 mg;  $^1\text{H}$  NMR (500 MHz, DMSO)  $\delta$  12.96 (s, 1H), 10.49 (br, 2H), 7.99 – 7.87 (m, 2H), 6.96 – 6.91 (m, 2H), 6.78 (s, 1H), 6.50 (dd, 1H), 6.20 (t, 1H);  $^{13}\text{C}$  NMR (125 MHz, DMSO)  $\delta$  182.2, 164.6, 164.2, 161.9, 161.6, 157.8, 128.9, 121.6, 116.4, 104.2, 103.3, 99.3, 94.4.

**6-Methoxy salicylic acid (3.1):** 37 mg;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  12.19 (s, 1H), 11.36 (brs, 1H), 7.43 (t,  $J = 8.4$  Hz, 1H), 6.74 (d,  $J = 8.5$  Hz, 1H), 6.52 (d,  $J = 8.2$  Hz, 1H), 4.09 (s, 3H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  170.9, 164.3, 158.5, 135.7, 112.4, 101.5, 101.3, 57.1.

**Caffeic acid (3.14):** 28mg;  $^1\text{H}$  NMR (500 MHz, DMSO- $D_6$ )  $\delta$  12.05 (s, 1H), 9.28 (d, 2H), 7.37 (d,  $J = 14.9$  Hz, 1H), 6.98 (s, 1H), 6.92 (d,  $J = 8.2$  Hz, 1H), 6.72 (s, 1H), 6.13

(d,  $J = 15.9$  Hz, 1H).  $^{13}\text{C}$  NMR (125 MHz, DMSO- $D_6$ )  $\delta$  168.5, 148.6, 146.1, 145.1, 126.2, 121.7, 116.3, 115.6, 115.1.

# **List of Publications**

## LIST OF PUBLICATIONS

### List of publications from thesis

1. **Bharat Goel**, Biswajit Dey, Essha Chatterjee, Nancy Tripathi, Nivedita Bhardwaj, Sanjay Kumar, Santosh Kumar Guru, and Shreyans K. Jain. Antiproliferative Potential of Gloriosine: A Lead for Anticancer Drug Development. *ACS Omega*, **2022**, 7 (33), 28994-29001.
2. **Bharat Goel**, Nancy Tripathi, Nivedita Bhardwaj, Amit Kumar & Shreyans K. Jain. Iodine-mediated one-step synthesis of ipomone from gibberellic acid. *Natural Product Research*, **2022**, DOI: 10.1080/14786419.2022.2065487.
3. **Bharat Goel**, Essha Chatterjee, Biswajit Dey, Nancy Tripathi, Nivedita Bhardwaj, Arun Khattri, Santosh Kumar Guru, and Shreyans K. Jain. Identification and Evaluation of Apoptosis-Inducing Activity of Ipomone from Ipomoea nil: A Novel, Unusual Bicyclo-[3.2.1] Octanone Containing Gibberic Acid Diterpenoid. *ACS Omega*, **2021**, 6 (12), 8253-8260.
4. **Bharat Goel**, Ved Vyas, Nancy Tripathi, Ajit Kumar Singh, Prashanth W. Menezes, Arindam Indra, Shreyans K. Jain. Amidation of Aldehydes with Amines under Mild Conditions Using Metal-Organic Framework Derived NiO@Ni Mott-Schottky Catalyst. *ChemCatChem*, **2020**, 12, 5743.

### List of publications from other work

1. N Tripathi, **B Goel**, N Bhardwaj, RA Vishwakarma, SK Jain, Exploring the Potential of Chemical Inhibitors for Targeting Post-translational Glycosylation of Coronavirus (SARS-CoV-2). *ACS Omega*, **2022**, 7 (31), 27038-27051.
2. **B Goel**, AK Tiwari, RK Pandey, AP Singh, S Kumar, A Sinha, SK Jain, A Khattri. Therapeutic approaches for the treatment of head and neck squamous cell carcinoma—An update on clinical trials. *Translational Oncology*, **2022**, 21, 101426.

3. B Sahu, N Bhardwaj, E Chatterjee, B Dey, N Tripathi, **B Goel**, B Kumar, B Singh, SK Guru, SK Jain. LCMS-DNP based dereplication of *Araucaria cunninghamii* Mudie gum-resin: identification of new cytotoxic labdane diterpene. *Natural Product Research*, **2022**, DOI: 10.1080/14786419.2021.2024530.
4. N Tripathi, **B Goel**, N Bhardwaj, B Sahu, H Kumar, SK Jain. Virtual screening and molecular simulation study of natural products database for lead identification of novel coronavirus main protease inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2022**, *40* (8), 3655-3667.
5. N Bhardwaj, **B Goel**, N Tripathi, B Sahu, SK Jain. A Comprehensive Review on Chemistry and Pharmacology of Marine Bioactives as Antimetastatic Agents. *European Journal of Medicinal Chemistry Reports*, **2022**, *4*, 100023.
6. **B Goel**, A Sharma, N Tripathi, N Bhardwaj, B Sahu, G Kaur, B Singh, SK Jain. In-vitro antitumor activity of compounds from *Glycyrrhiza glabra* against C6 glioma cancer cells: identification of natural lead for further evaluation. *Natural Product Research*, **2021**, *35* (23), 5489-5492.
7. **B Goel**, N Tripathi, N Bhardwaj, B Sahu, SK Jain. Therapeutic Potential of Genus *Pongamia* and *Derris*: Phytochemical and Bioactivity. *Mini Reviews in Medicinal Chemistry*, **2021**, *21* (8), 920-951.
8. **B Goel**, N Tripathi, D Mukherjee, SK Jain. Glycorandomization: A promising diversification strategy for the drug development. *European Journal of Medicinal Chemistry*, **2021**, *213*, 113156.
9. N Bhardwaj, N Tripathi, **B Goel**, SK Jain. Anticancer Activity of Diosgenin and its Semi-synthetic Derivatives: Role in Autophagy Mediated Cell Death and Induction of Apoptosis. *Mini Reviews in Medicinal Chemistry*, **2021**, *21*(13), 1646 - 1665.
10. N Bhardwaj, AK Singh, N Tripathi, **B Goel**, A Indra, SK Jain. Ni–NiO heterojunctions: A versatile nanocatalyst for regioselective halogenation and

- oxidative esterification of aromatics. *New Journal of Chemistry*, **2021**, 45 (31), 14177-14183.
11. **B Goel**, N Bhardwaj, N Tripathi, SK Jain. Drug discovery of small molecules for the treatment of COVID-19: A review on clinical studies. *Mini Reviews in Medicinal Chemistry*, **2021**, 21 (12), 1431-1456.
12. **B Goel**, N Tripathi, N Bhardwaj, SK Jain. Small Molecule CDK Inhibitors for the Therapeutic Management of Cancer. *Current Topics in Medicinal Chemistry*, **2020**, 20(17), 1535-1563.
13. M Kushwaha, **B Goel**, S Jaglan, SK Jain. LC-MS/MS profile of an active pharmaceutical ingredient and its impurities in commercial preparation. *Journal of Liquid Chromatography Related Technologies*, **2020**, 43 (3-4), 131-137.
14. R Singh, K Mandrah, A Asati, DK Patel, **B Goel**, RA Vishwakarma, SK Roy, SK Jain. Transformation of santonin to a naproxen analogue with anti-inflammatory activity. *Journal of Natural Products*, **2019**, 82 (6), 1710-1713.