|  |  |  |
| --- | --- | --- |
| **ID** | **Structure ↓** | **Normalized Raman spectra ↓** |
| DI-1 → |  |  |
| DI-2 → |  |  |
| DI-3 → |  |  |
| DN-1 → |  |  |
| DN-2 → |  |  |
| DN-3 → |  |  |
| DN-4 → |  |  |
| DN-5 → |  |  |
| DN-6 → |  |  |
| DN-7 → |  |  |
| DN-8 → |  |  |
| DN-9 → |  |  |
| CO-1 → |  |  |
| CO-2 → |  |  |
| CO-3 → |  |  |
| CO-4 → |  |  |
| CO-5 → |  |  |
| CO-6 → |  |  |
| CO-7 → |  |  |
| CO-8 → |  |  |
| CO-9 → |  |  |
|  | Ibuprofen ↓ | Nicotinamide ↓ |
|  |  |  |

**Figure S1.** The fingerprints’ structures and their computed Raman spectra [1-4].

References

1. Khansary, M.A., G. Walker, and S. Shirazian, *Incomplete cocrystalization of ibuprofen and nicotinamide and its interplay with formation of ibuprofen dimer and/or nicotinamide dimer: A thermodynamic analysis based on DFT data.* International Journal of Pharmaceutics, 2020: p. 119992.

2. Khansary, M.A., G.M. Walker, and S. Shirazian. *Correlating Raman Spectra of Ibuprofen, Nicotinamide and their Dimers*. in *Material Science and Engineering Congress*. 2020. Darmstadt, Germany: Deutsche Gesellschaft für Materialkunde e.V.

3. Khansary, M.A., G.M. Walker, and S. Shirazian. *Analysis of Raman spectra signals based on molecular fingerprints from DFT data*. in *European Congress and Exhibition on Advanced Materials and Processes: EUROMAT 2021*. 2021. Graz, Austria: The Austrian Society for Metallurgy and Materials.

4. Asgarpour Khansary, M., S. Shirazian, and G. Walker, *Molecular engineering of cocrystallization process in holt melt extrusion based on kinetics of elementary molecular processes.* International Journal of Pharmaceutics, 2021. **601**: p. 120495.