Regarding the task you assigned to me, ​I have implemented the spectral alignment algorithm by following the details provided in the paper1. I have also tested ​my code by searching the HeLa dataset containing ten files discussed in the paper​. The optimal​ alignments ​obtained, therefore, ​have been provided in an excel file (please see attached *Results.xlsx*). ​Please note that the search parameters include a 50-ppm fragment tolerance and three mass shifts​ only​.

Optimal alignments in **​​File (1-2, 4-8)** reported three mass shifts with **​​23, 32, 27, 29, 17, 21, and ​​13 matched** peaks, respectively. On the other hand, optimal alignments in **​​File (3, 10)** reported two mass shifts with **​​6 and 21 matched** peaks, respectively. **​​File (9)** reported optimal alignment with **​​**​​one mass shift and **four matched** peaks.

However, I could not compare ​these ​results ​with those in the manuscript (Results Table) as the number of peaks ​mentioned ​in the paper does not correspond to the data​set​​ provided alongside​.

​I have attached my code ​as a zip ​file. Moreover, ​to avoid compilation issues, I am including ​an executable file ​as well. Kindly let me know if any part of the implementation needs further explanation.

1.  Frank, A. M., Pesavento, J. J., Mizzen, C. A., Kelleher, N. L. & Pevzner, P. A. Interpreting top-down mass spectra using spectral alignment. *Anal. Chem.* **80,** 2499–2505 (2008).