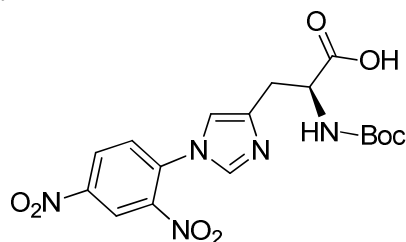


Sample name: **Boc-His(Dnp)-OH isopropanol solvate**

Synonym: N<sub>α</sub>-Boc-N<sub>(im)</sub>-2,4-dinitrophenyl-L-histidine

Sample # **I-0006-BocHistidine**

**Structure:**

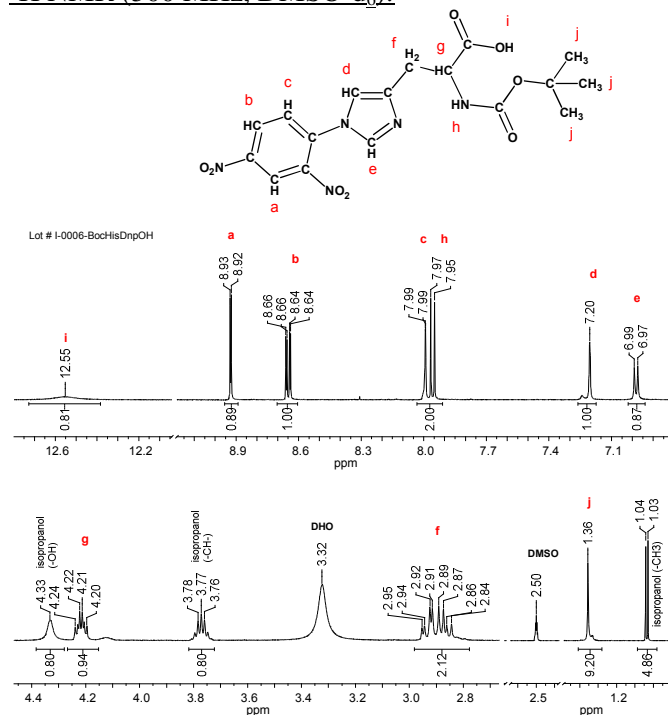


|                    |   |
|--------------------|---|
| CAS Number:        | 25024-53-7  |
| EC Number:         | 246-569-0   |
| Empirical formula: | C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O <sub>8</sub> |
| Molecular weight:  | 421.36  |
| Appearance:        | light yellow powder   |
| Melting point:     | 100 °C  |

Material characterization:

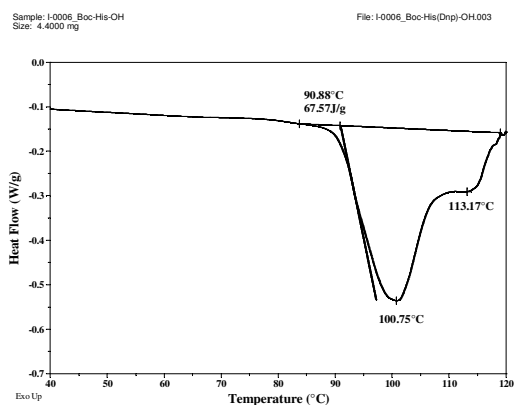
- Proton NMR spectrum was recorded on Bruker Avance III 500 spectrometer at ambient temperature using DMSO-d<sub>6</sub> as the solvent.
- Thermal analysis was performed on TA Instruments Q100 differential scanning calorimeter (DSC) under nitrogen atmosphere.

<sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):



DSC thermograms:

- 1<sup>st</sup> heating scan at 5°C/min (sample decomposes at T>120°C):



- 2<sup>nd</sup> heating scan at 10°C/min in 20°–100°C temp. range (T<sub>g</sub> is also reproducible for 3<sup>rd</sup> heating scan):

