



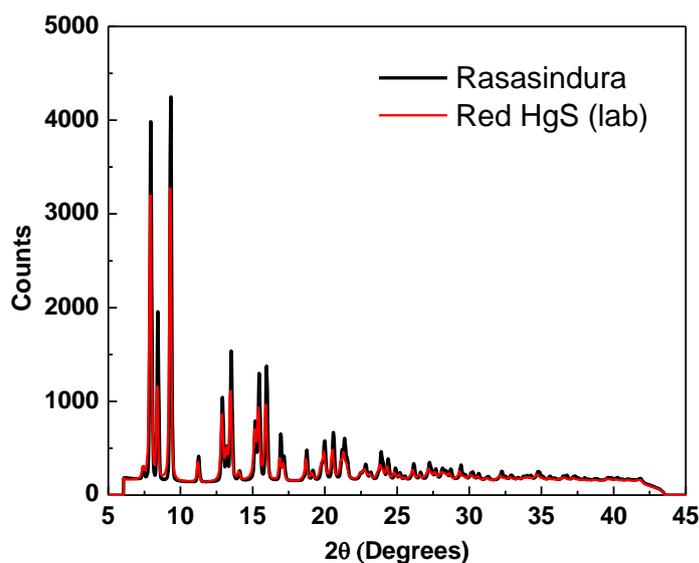
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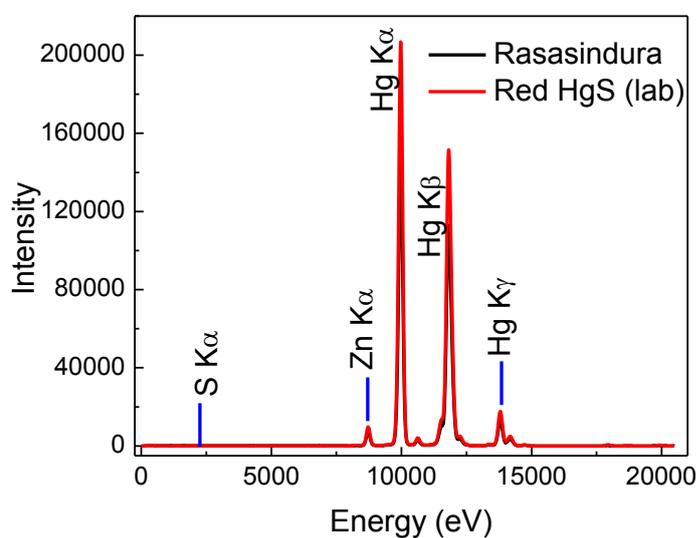
**Supporting information for article:**

**Investigating structural aspects to understand the putative/claimed non-toxicity of the Hg-based Ayurvedic drug *Rasasindura* using XAFS**

**Nitya Ramanan, Debdutta Lahiri, Parasmani Rajput, Ramesh Chandra Varma, A. Arun, T. S. Muraleedharan, K. K. Pandey, Nandita Maiti, S. N. Jha and Surinder M. Sharma**

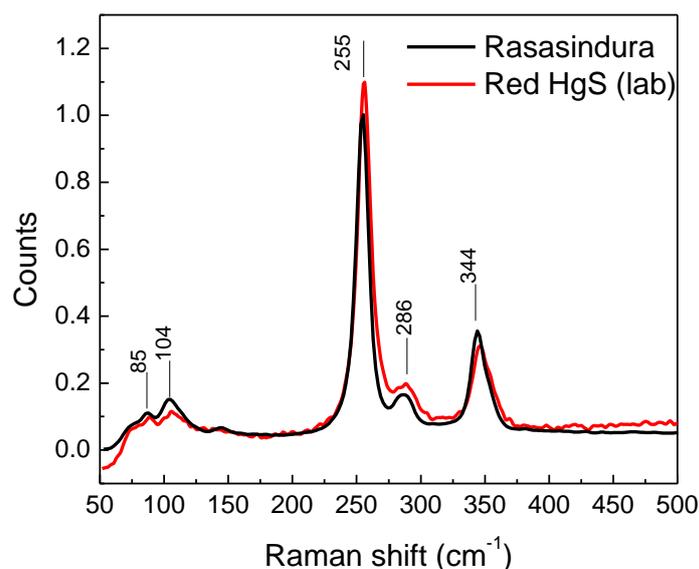


**Figure S1** XRD spectra of *Rasasindura* and Red- *HgS* (lab), recorded at ED-XRD beamline (BL-11), Indus-2 Synchrotron Radiation Source, Raja Ramanna Centre for Advanced Technology (India). Both strongly resemble crystalline  $\alpha$ -*HgS*.  $D_{Rasa} = 24nm$  was obtained from Reitveld refinement of the data, confirming nano-drug status of *Rasasindura*.

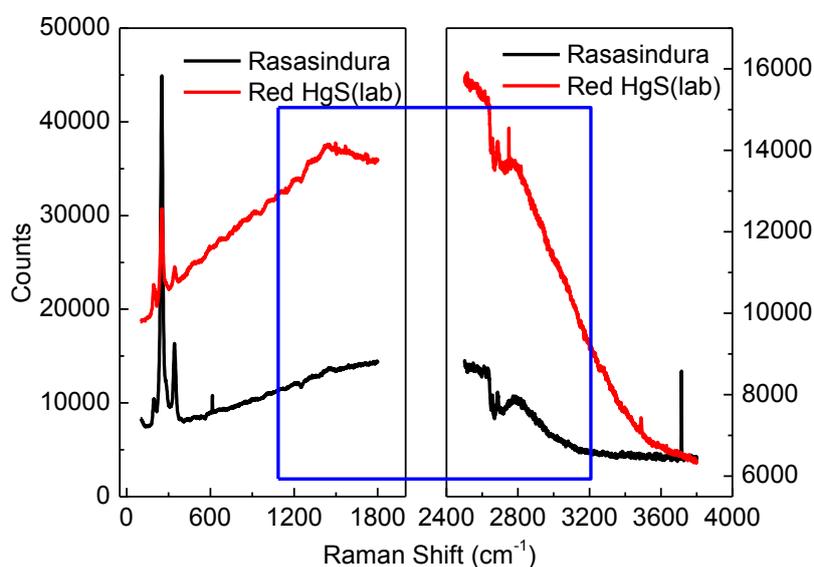


**Figure S2** XRF spectrum of *Rasasindura* and Red *HgS* (lab), recorded at Microprobe X-ray Fluorescence Beamline (BL-16), Indus-2 Synchrotron Radiation Source, Raja Ramanna Centre for Advanced Technology (India). Presence of trace amount of *Zn* was revealed in *Rasasindura*.

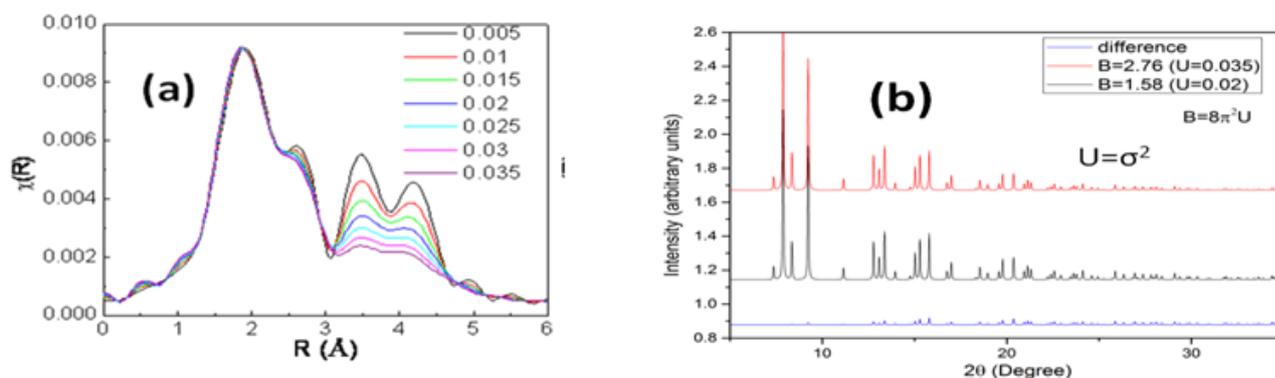
$[x_{Hg} : x_S = 1 : 1]$  for *Rasasindura* [*Zn* is reportedly found as impurity in *Hg*].



**Figure S3** Raman spectrum of *Rasasindura* and Red-*HgS* (lab), recorded using Bruker FT-Raman instrument at Bhabha Atomic Research Centre (India). The spectra clearly matched  $\alpha$ -*HgS* spectrum from literature.

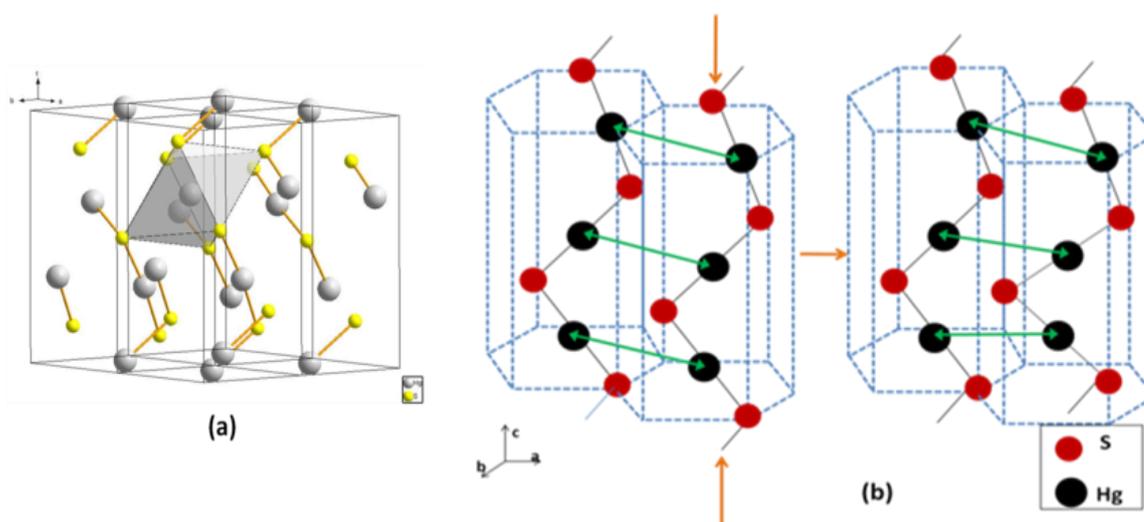


**Figure S4** Surface Enhanced Raman Spectra of *Rasasindura* and Red ( $\alpha$ )-*HgS* (lab) recorded at Bhabha Atomic Research Centre (India). The spectra closely resemble each other in terms of peak positions. No bands were observed between 1000-3000 cm<sup>-1</sup> [area marked by blue box], ruling out presence of organic molecules on the surface.



**Figure S5** Simulations for different values of  $\sigma_{Hg-Hg}^2$ : (a) XAFS simulations (b) XRD simulations.

XRD pattern is insensitive to  $\sigma_{Hg-Hg}^2$  variation up to  $\sigma_{Hg-Hg}^2 = 0.035 \text{ \AA}^2$ . From XAFS simulations,  $Hg-Hg$  features are suppressed for  $\sigma_{Hg-Hg}^2 \geq 0.025 \text{ \AA}^2$ .



**Figure S6** (a) Structure of  $\alpha$ - $HgS$  comprises of parallel  $-S-Hg-S-Hg-S-$  chains along  $c$ -axis. (b) Compression of one of the chains (defect) affects  $Hg-Hg$  (green arrows) substantially.