

(54) Title of the invention : Device for structural elucidation of chemical compounds

(51) International classification	:G01N 33/00, G16C 20/30, G01N 30/72, G01N 27/62, G01N 21/359	(71)Name of Applicant : <b>1)Vels Institute of Science, Technology &amp; Advanced Studies (VISTAS)</b> Address of Applicant :The Registrar, Vels Institute of Science, Technology & Advanced Studies (VISTAS), Pallavaram, Chennai-600117, Tamil Nadu, India
(31) Priority Document No	:NA	(72)Name of Inventor :
(32) Priority Date	:NA	<b>1)Dr.P.Balaji</b>
(33) Name of priority country	:NA	<b>2)Dr. P. Shanmugasundaram</b>
(86) International Application No	:	<b>3)Dr. Shanmuga Priya V</b>
Filing Date	:01/01/1900	<b>4)Mr. E. Joel Mart</b>
(87) International Publication No	: NA	<b>5)Dr. Jaya Vasavi Gurralla</b>
(61) Patent of Addition to Application Number	:NA	<b>6)Mrs.M.Manoyogambiga</b>
Filing Date	:NA	<b>7)Dr. P. Pavazhaviji</b>
(62) Divisional to Application Number	:NA	<b>8)Dr. G. Sharmilaa</b>
Filing Date	:NA	<b>9)Dr. P. Brindha Devi</b>
		<b>10)Dr.S.Arunkumar</b>
		<b>11)Dr.S.Varunraj</b>

(57) Abstract :

**ABSTRACT DEVICE FOR STRUCTURAL ELUCIDATION OF CHEMICAL COMPOUNDS** The device for structural elucidation of chemical compounds is disclosed. The device comprises a data acquisition module configured to receive analytical data associated with a chemical compound, including spectroscopic and mass spectral data. A processing unit executes an analysis engine to process the analytical data and to determine structural features comprising functional groups, molecular connectivity, and stereochemical information. The analysis engine integrates multiple analytical datasets to generate one or more predicted chemical structures. An output interface is configured to display the predicted chemical structure along with confidence metrics and, where applicable, alternative candidate structures ranked based on consistency with the analytical data. The disclosed device enables automated, accurate, and efficient structural elucidation while reducing manual interpretation, time, and subjectivity associated with conventional analytical techniques. Fig 1

No. of Pages : 15 No. of Claims : 4