Electronic Supplementary Material (ESI) for RSC Sustainability.


# Supporting Information

## *In Silico* Exploration of Acetic Acid driven Multicomponent Synthesis: Design, Characterization, and Antioxidant Evaluation of Spiroacridines and Spiroquinolines

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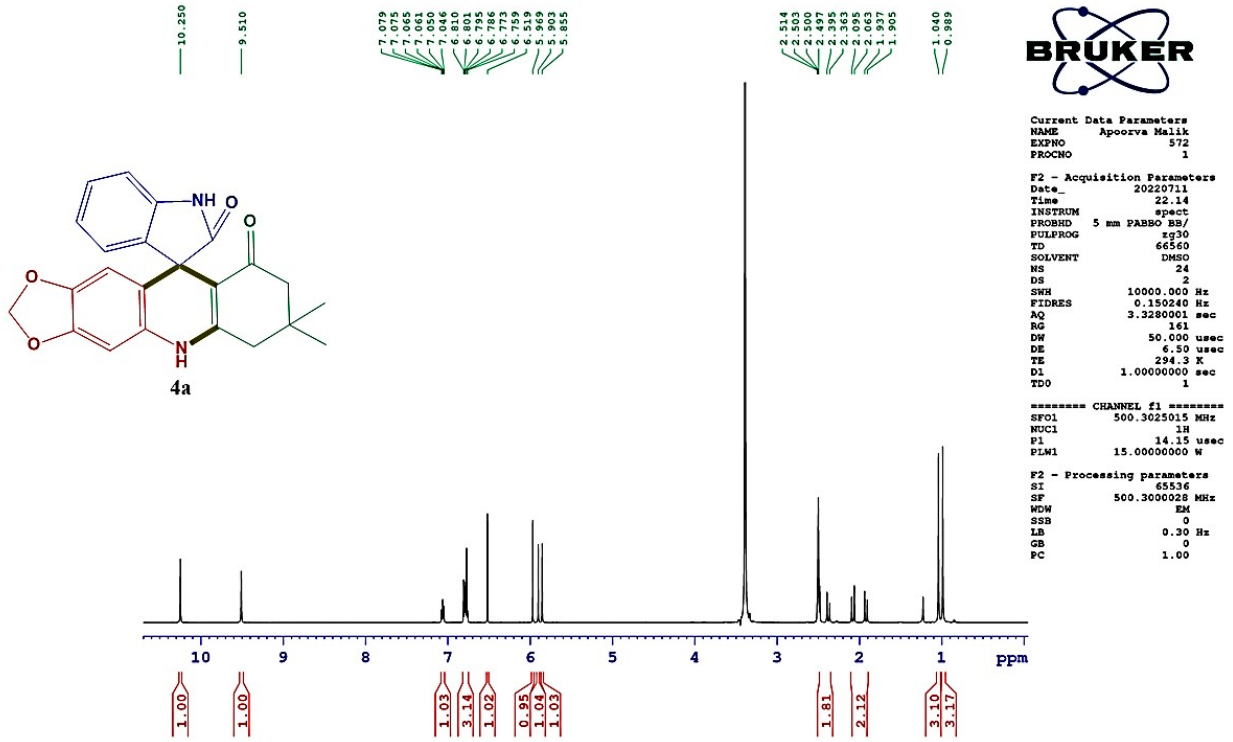
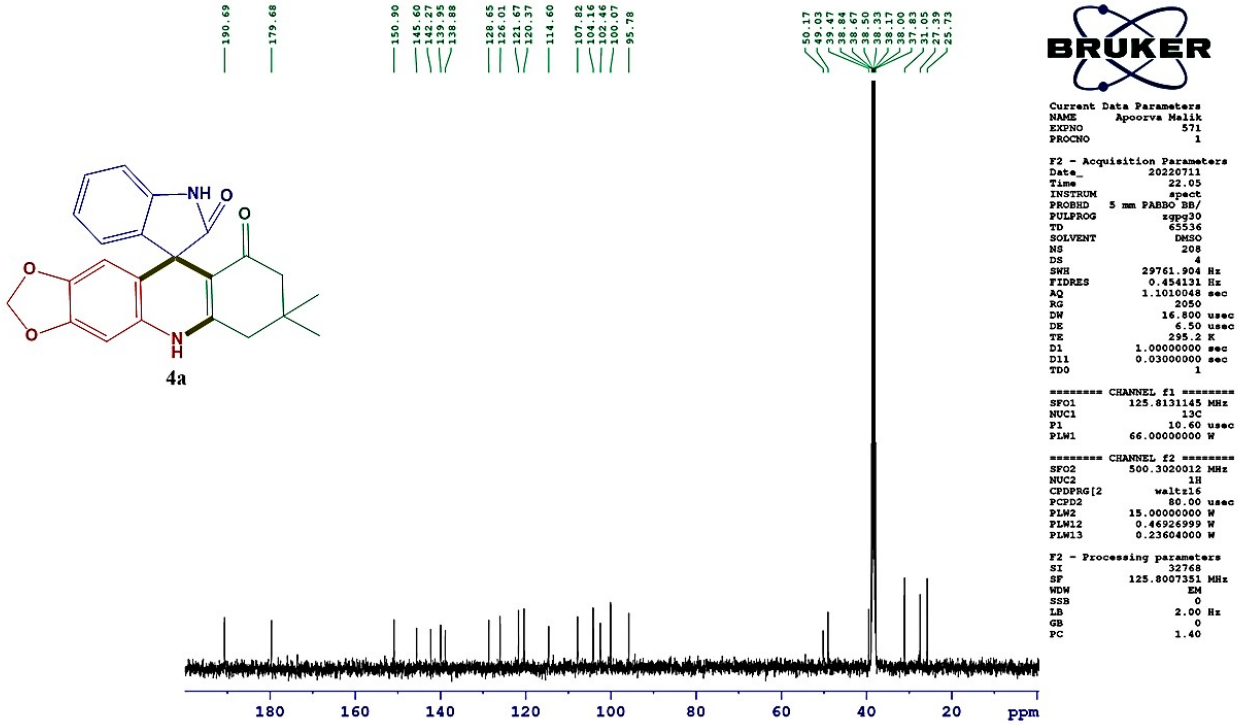



Figure **S2**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4a**.



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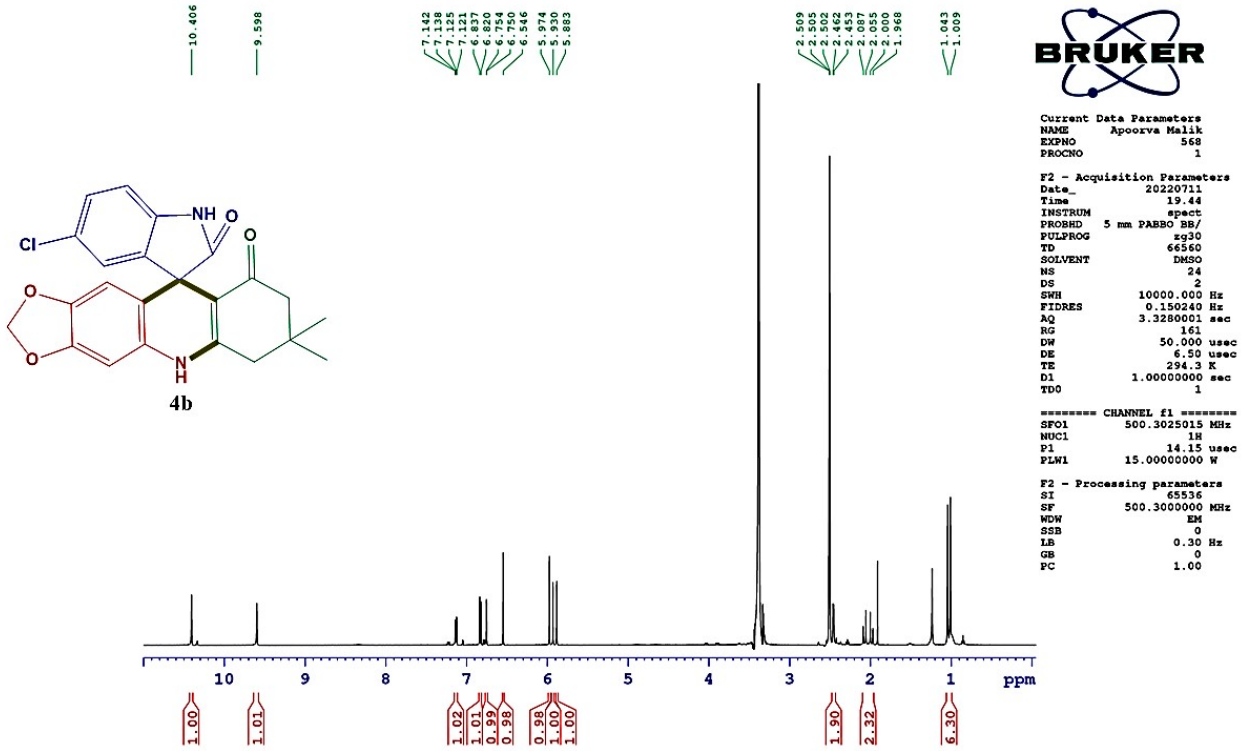


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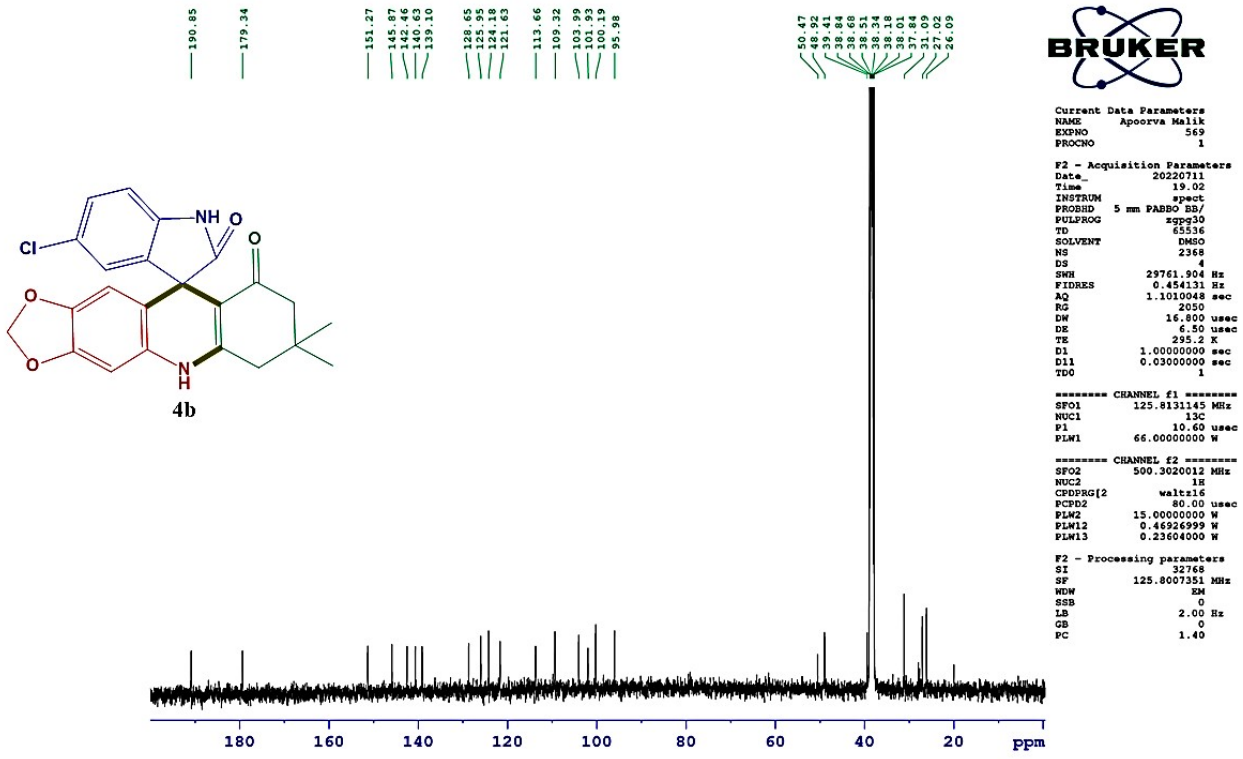

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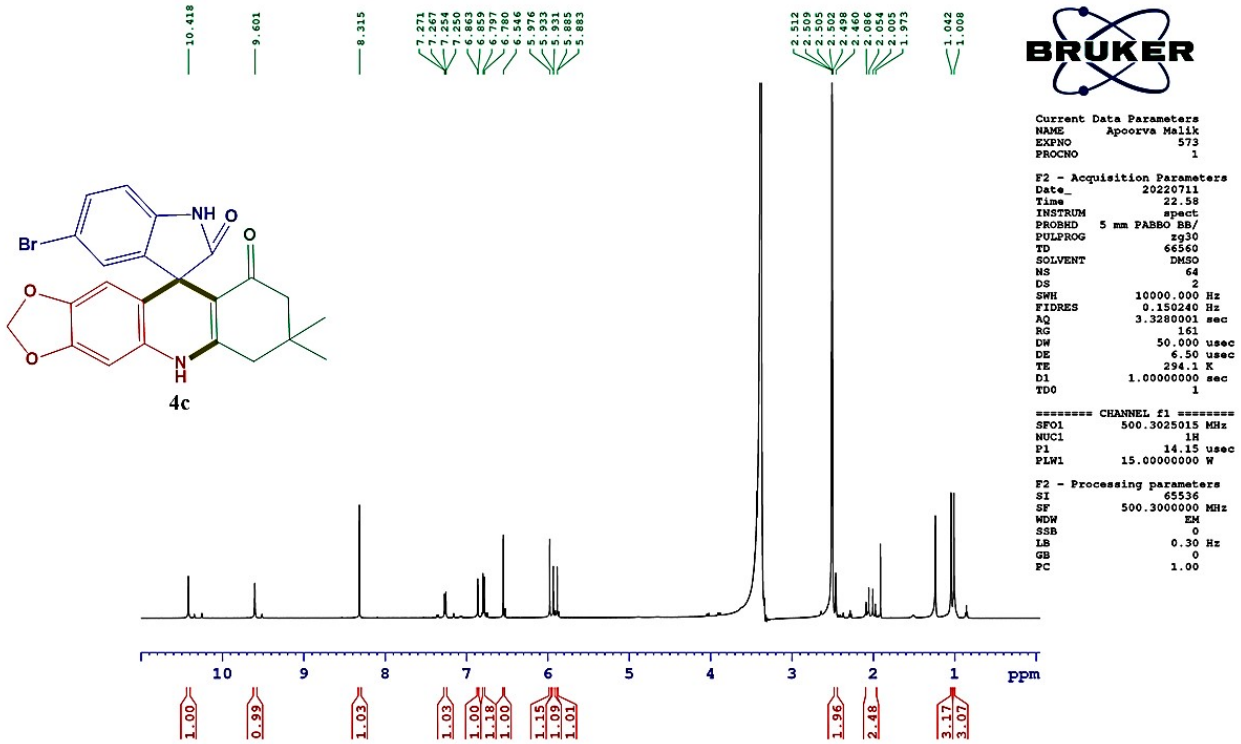


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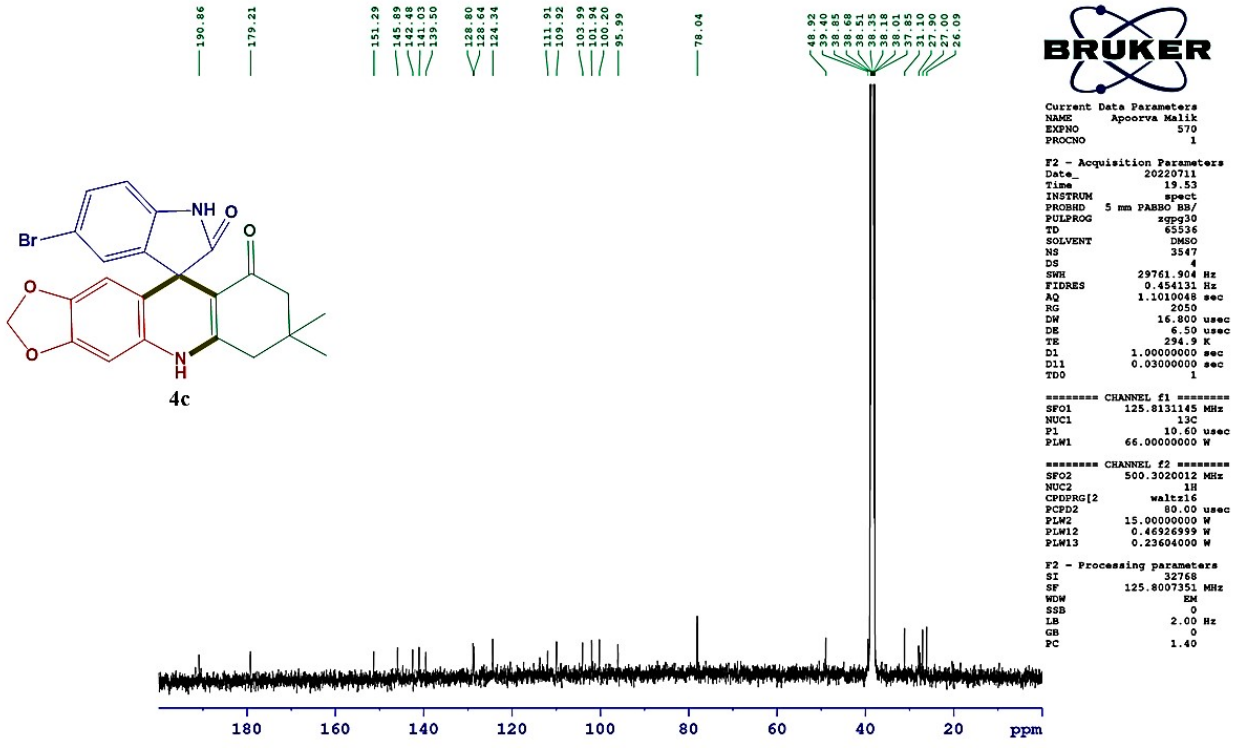

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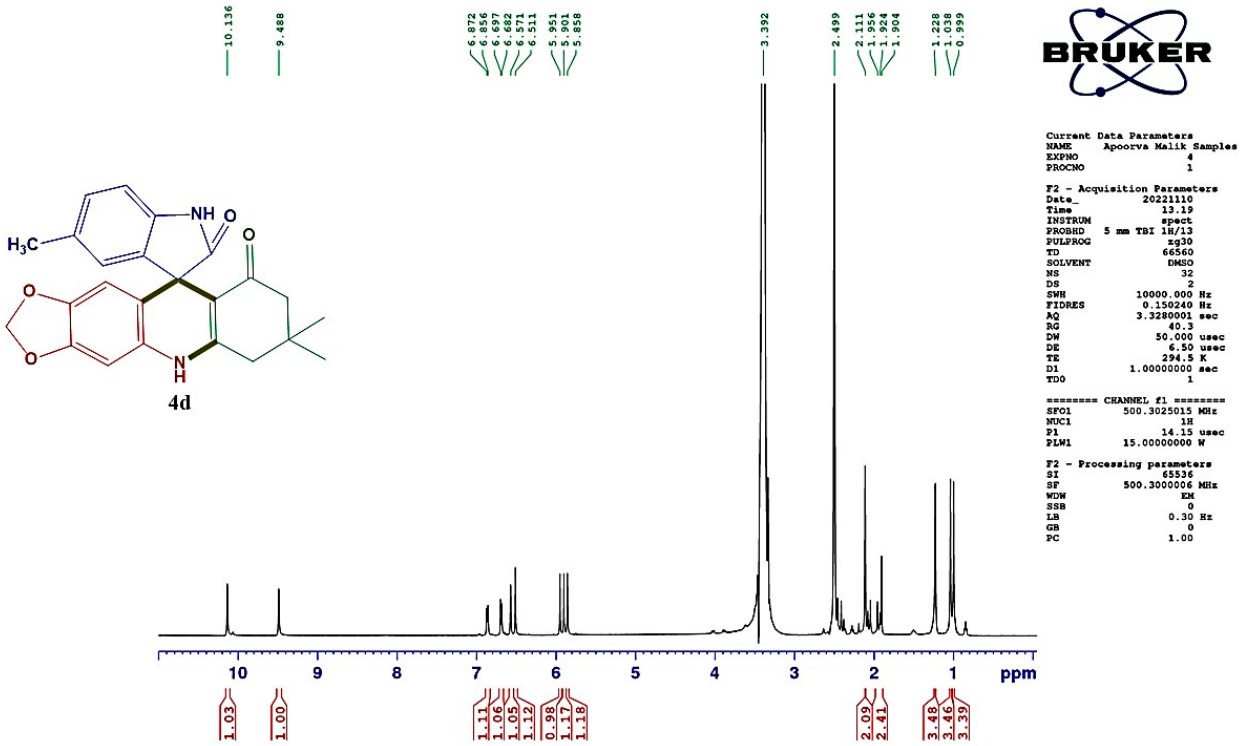


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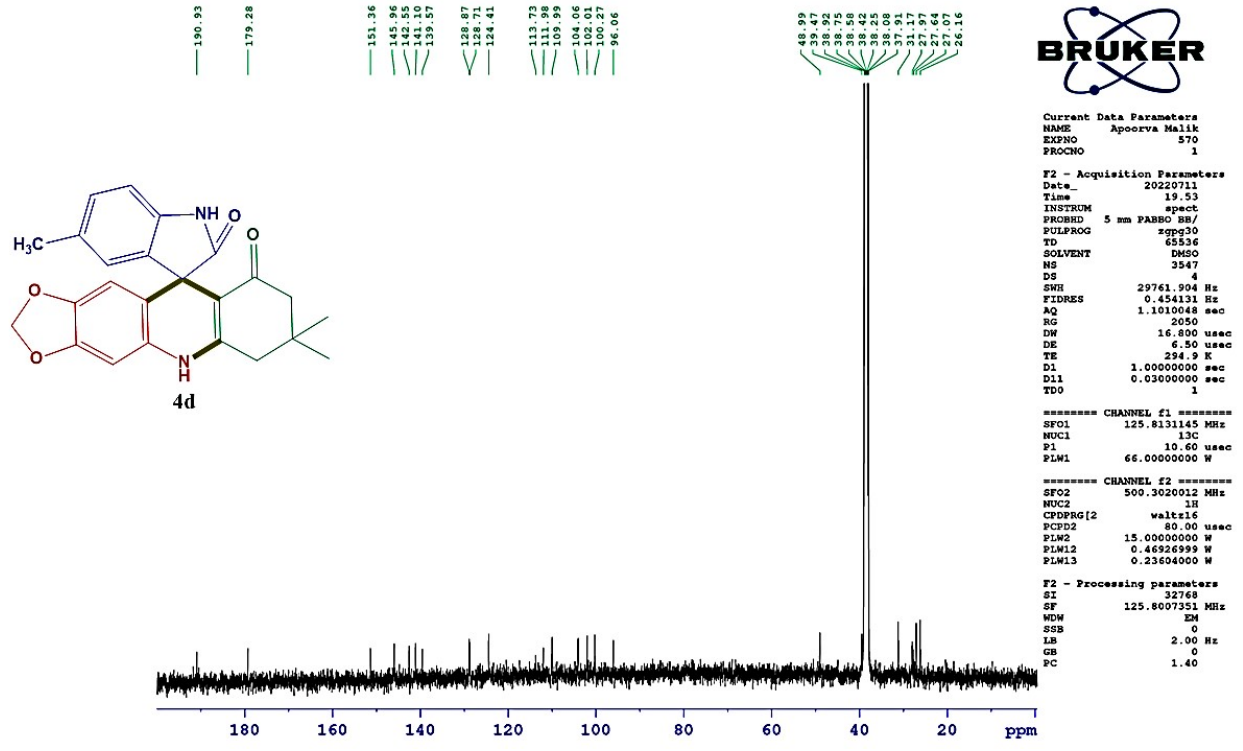

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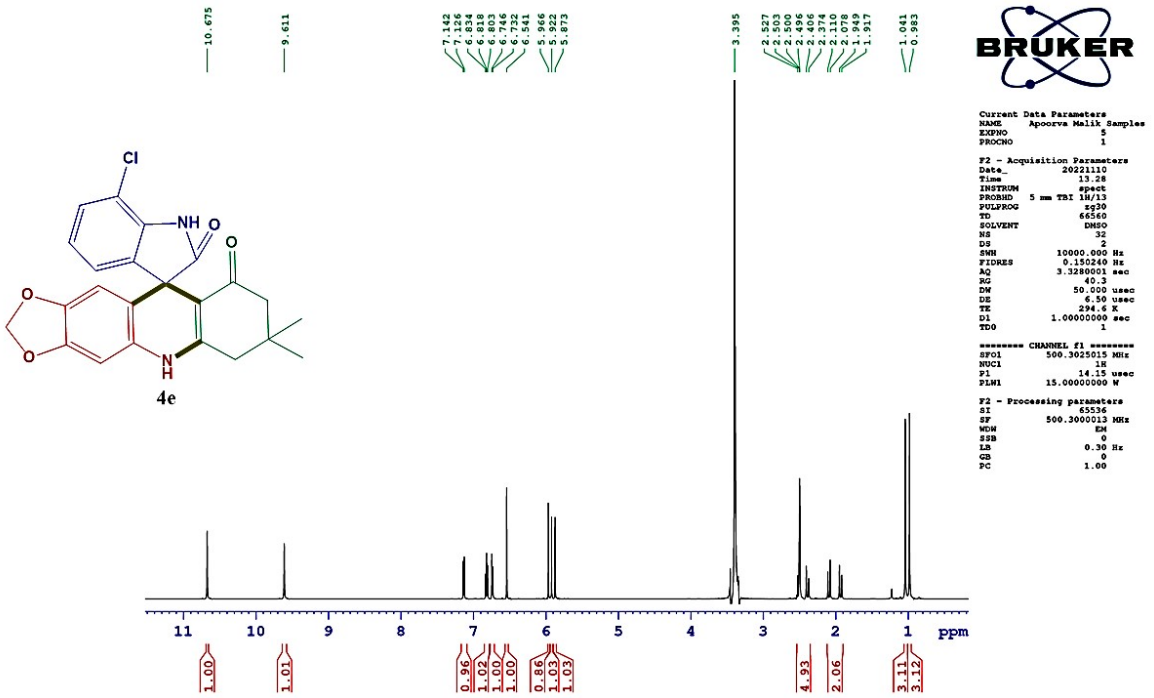


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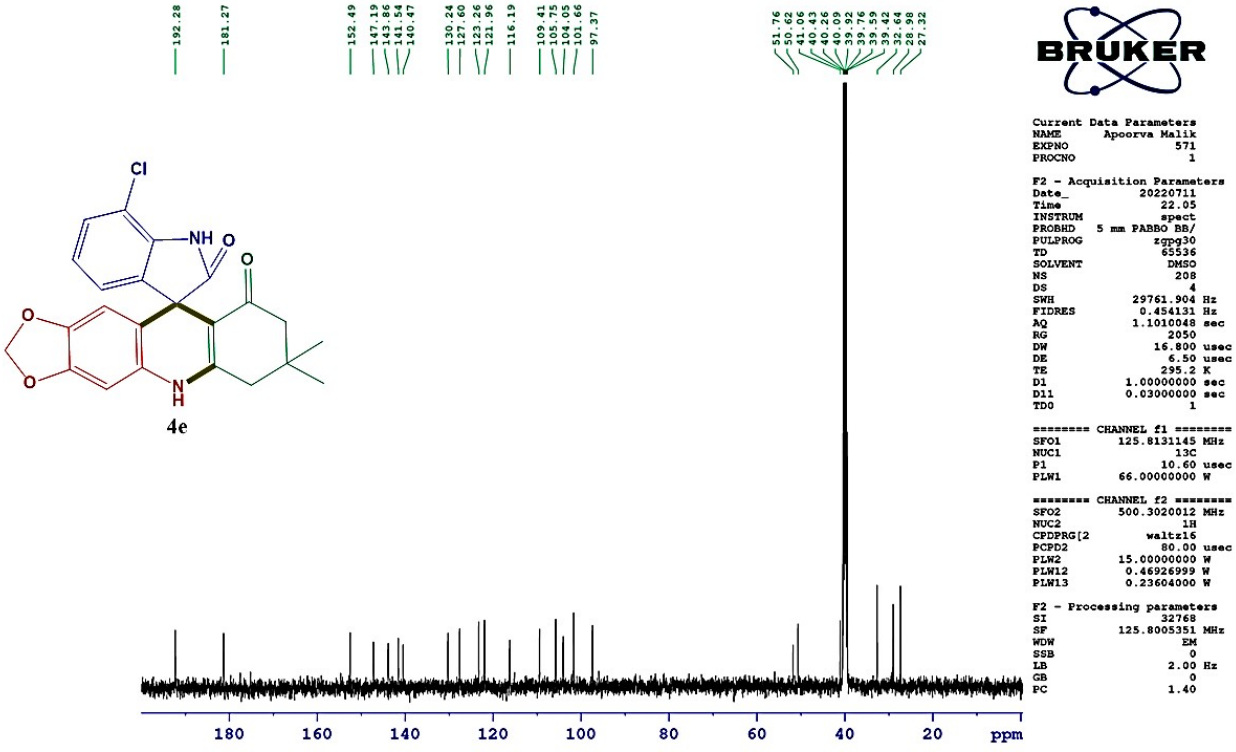

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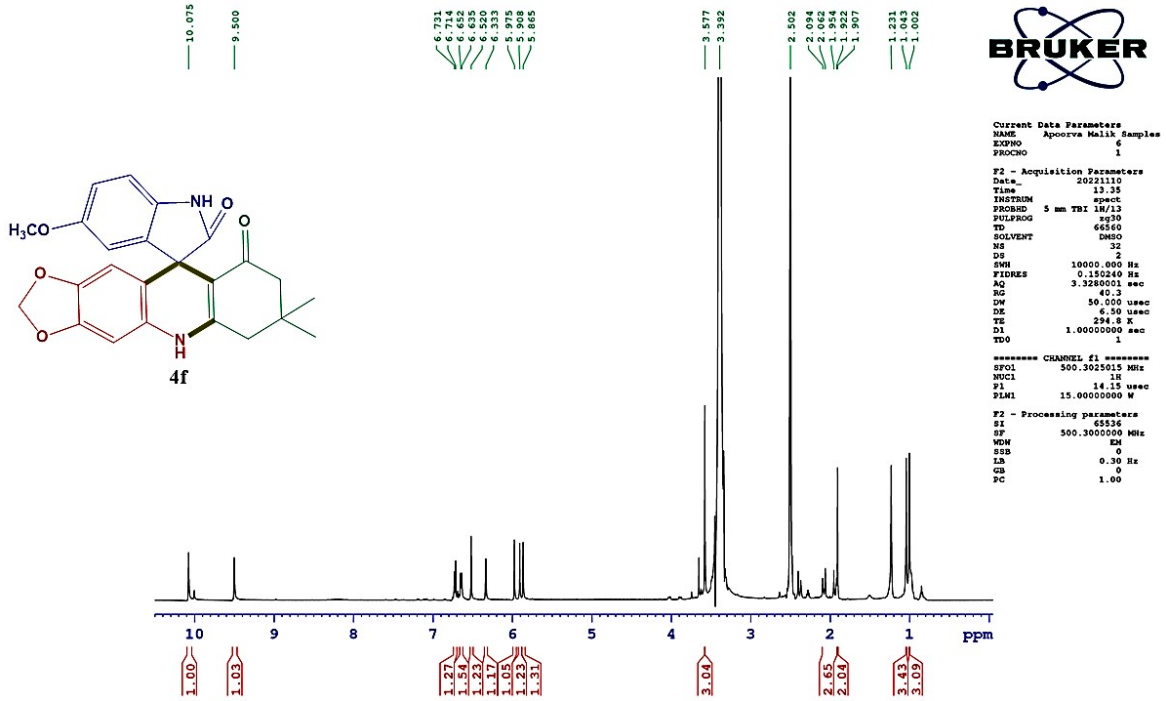


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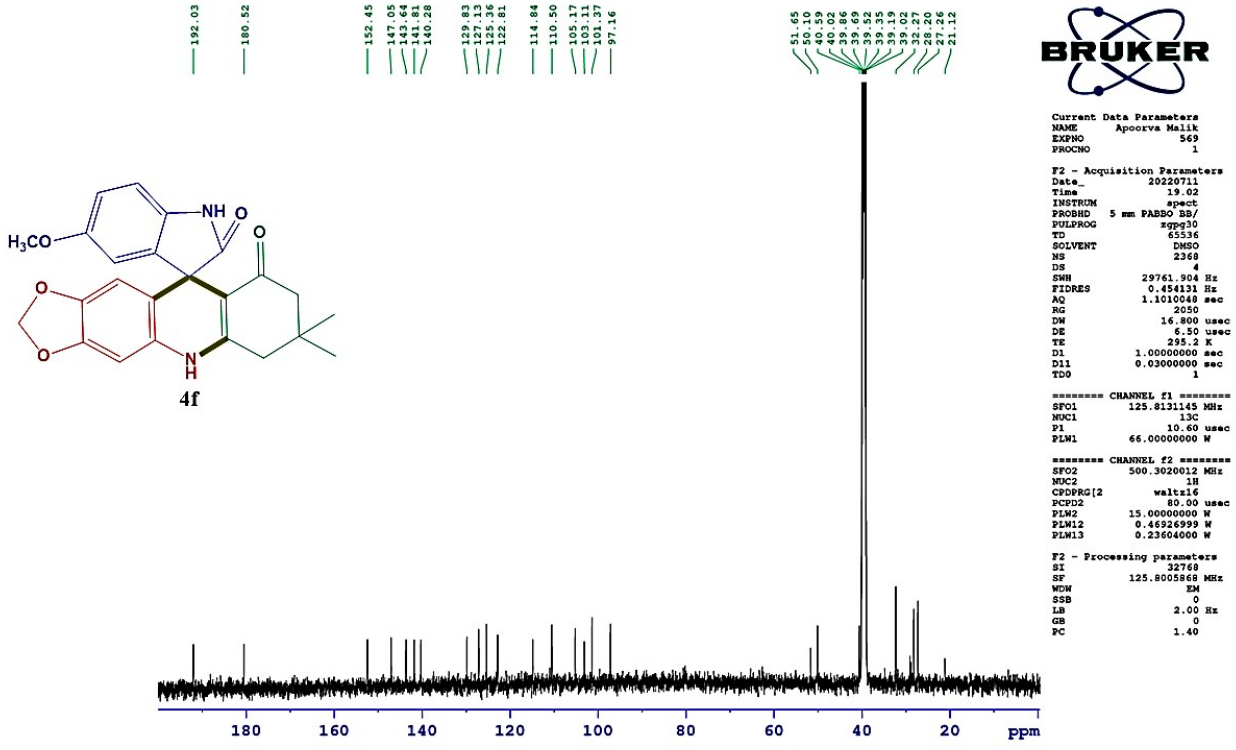

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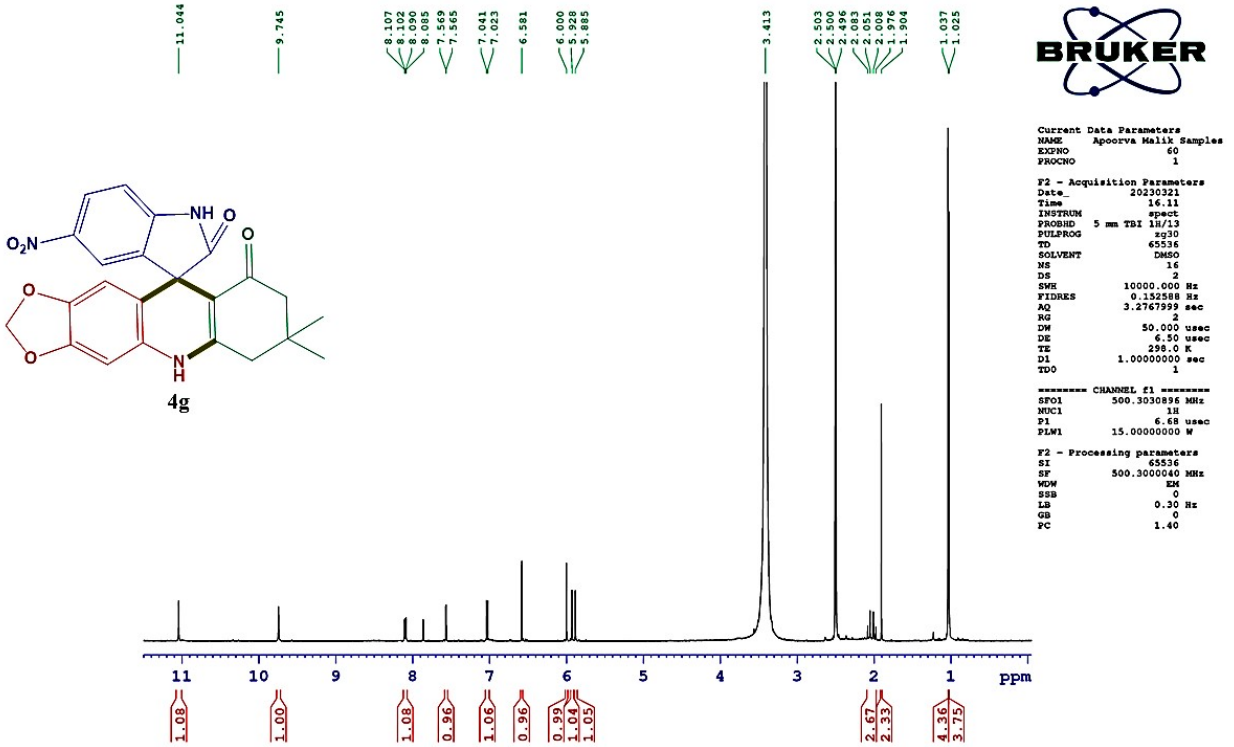


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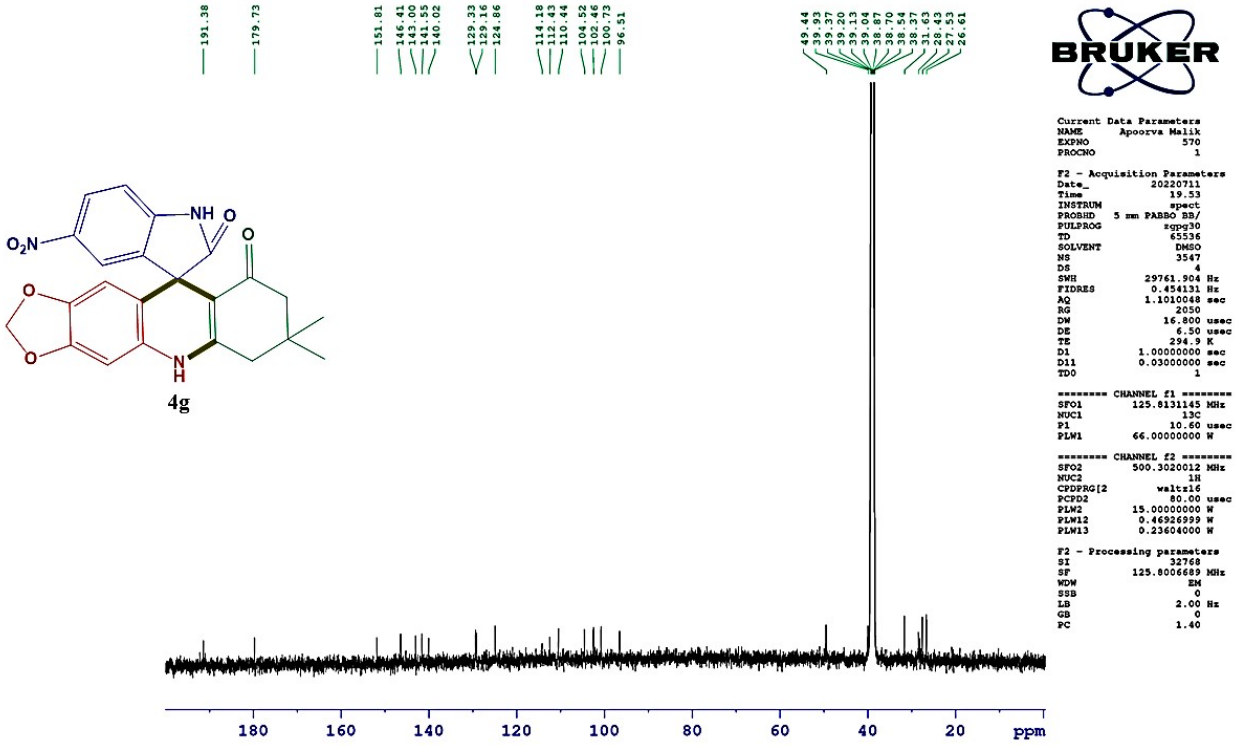

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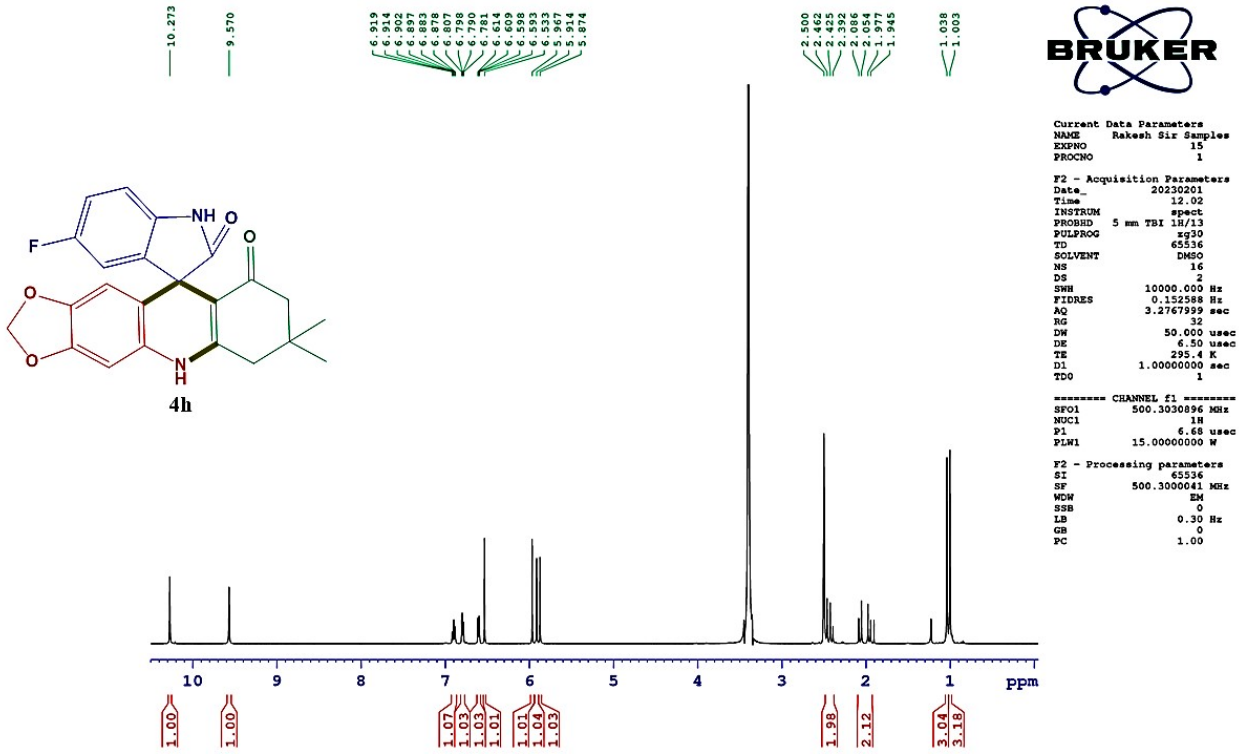


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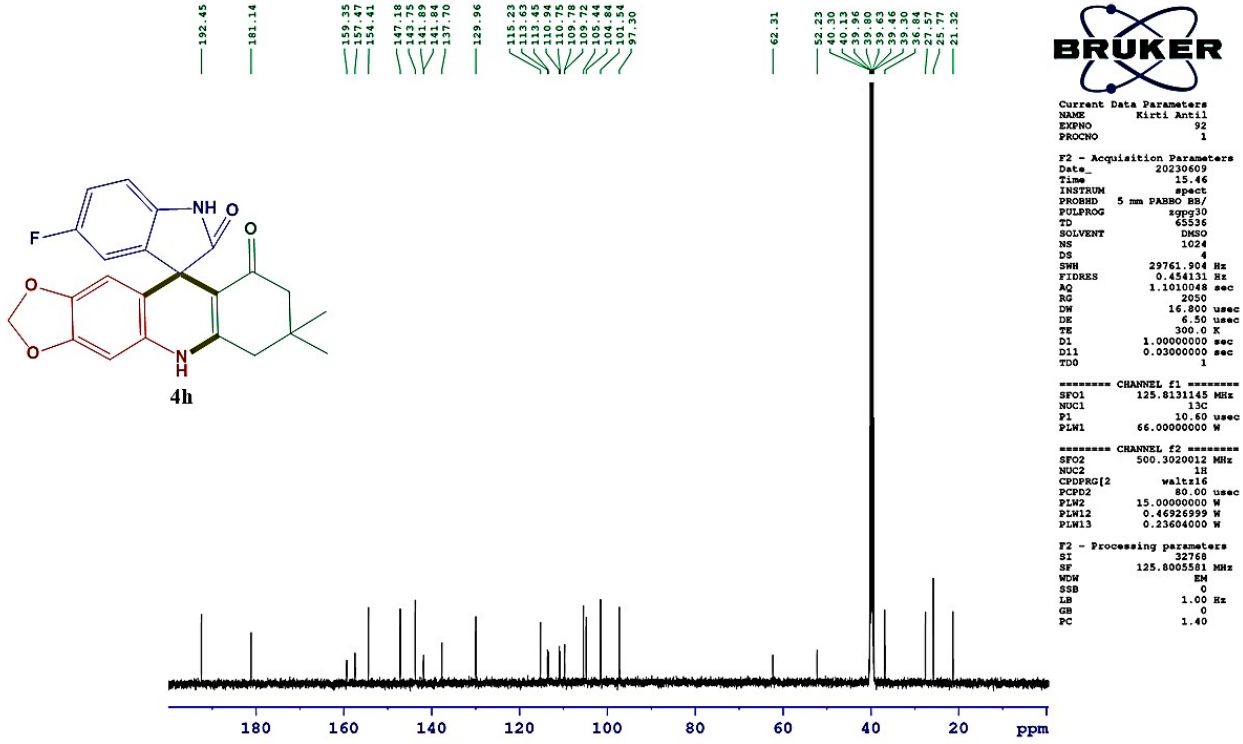

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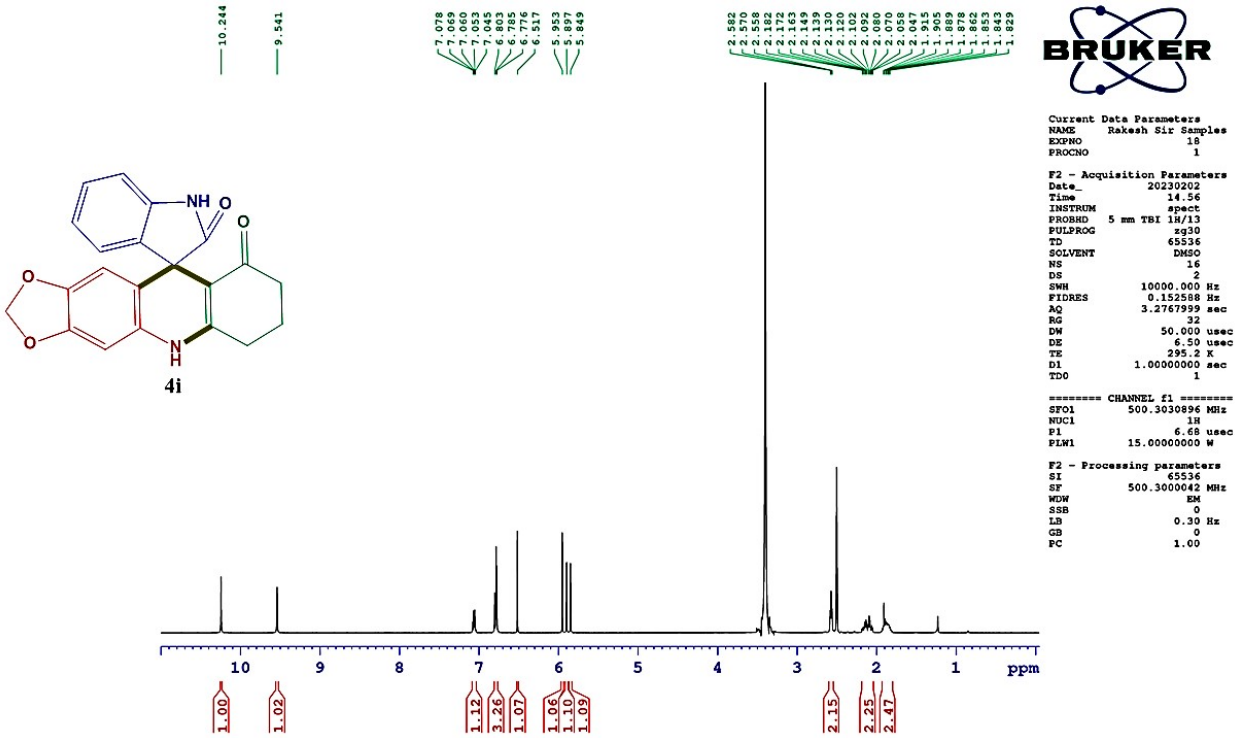


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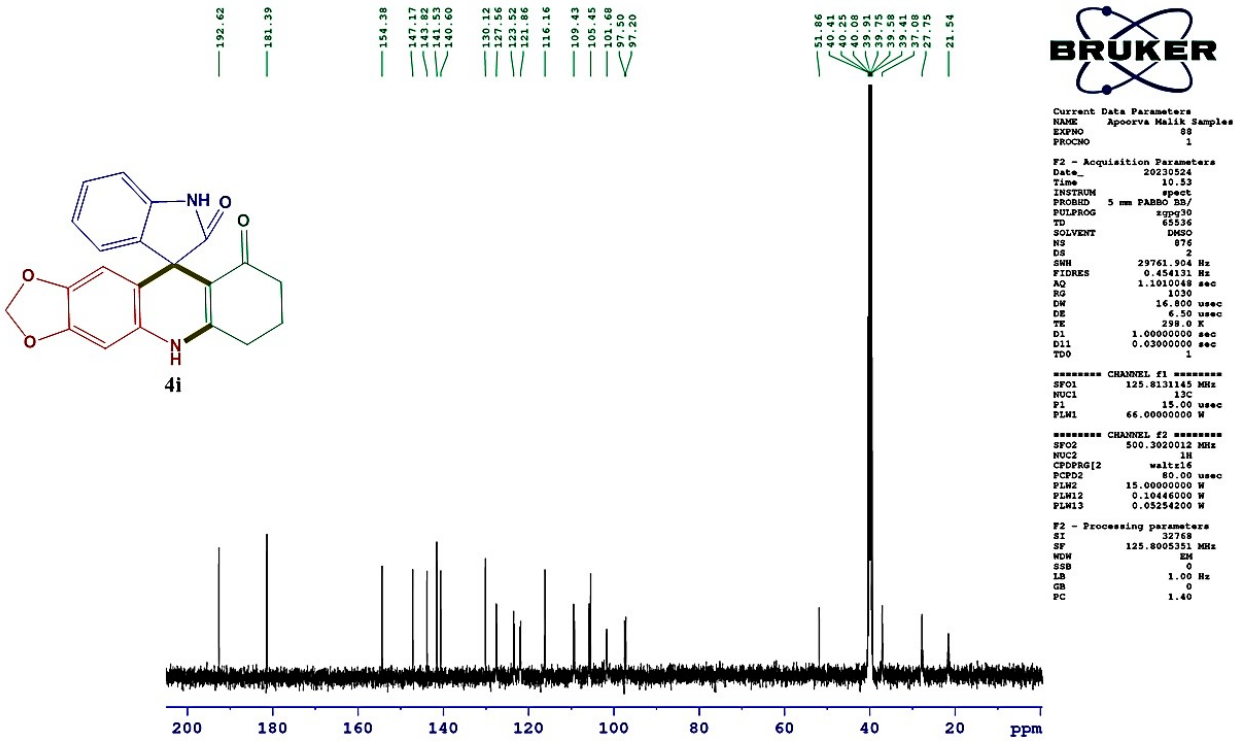

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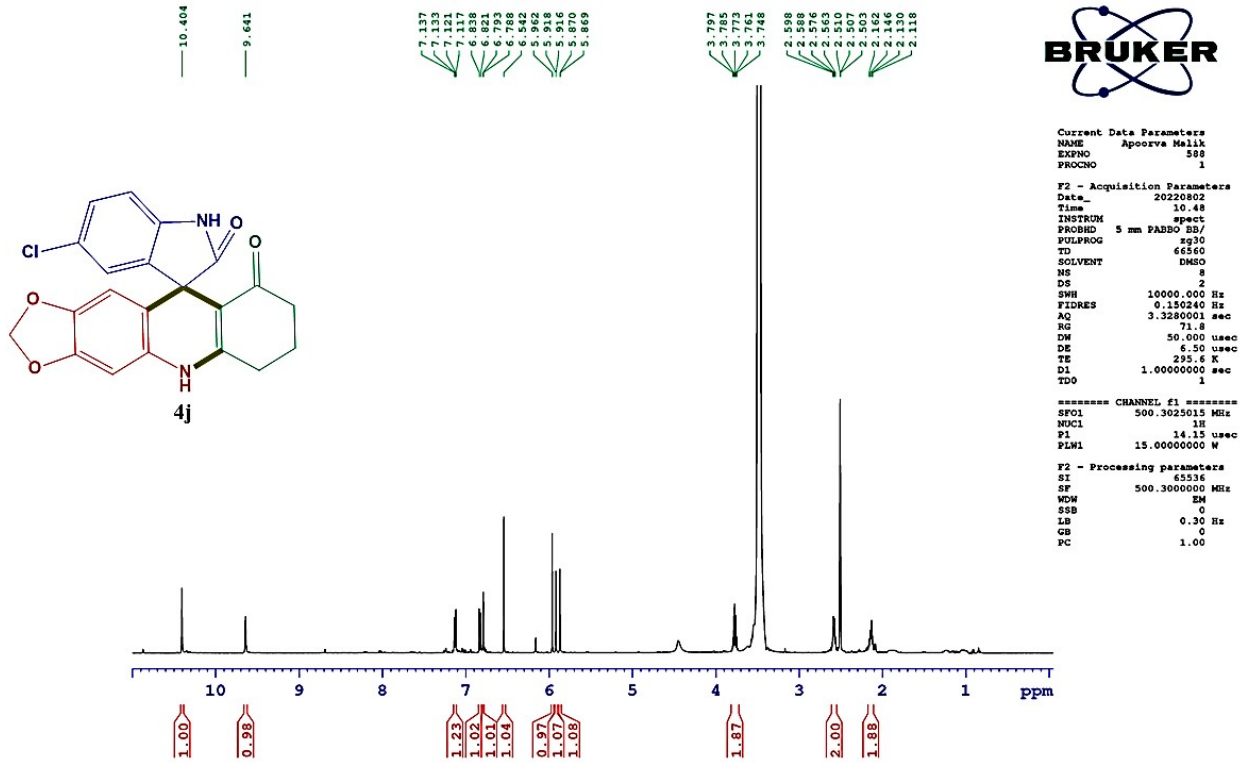
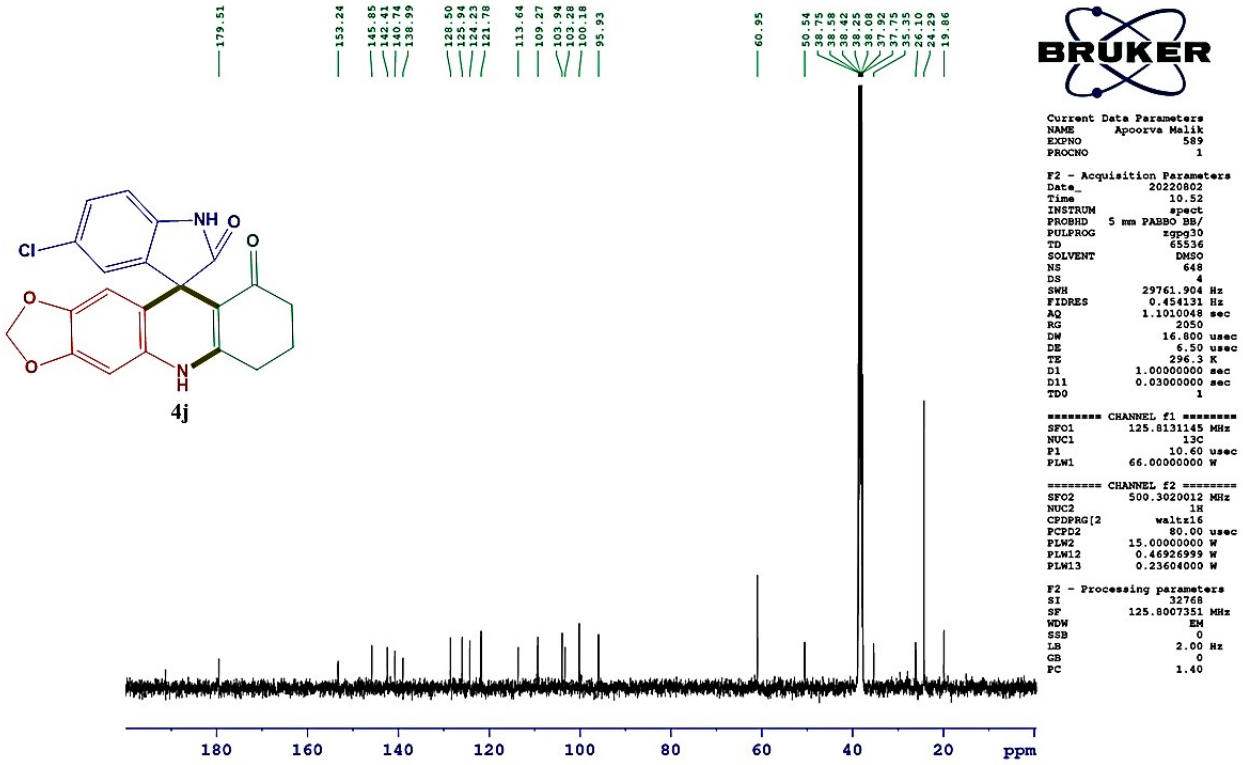



Figure **S20**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4j**.



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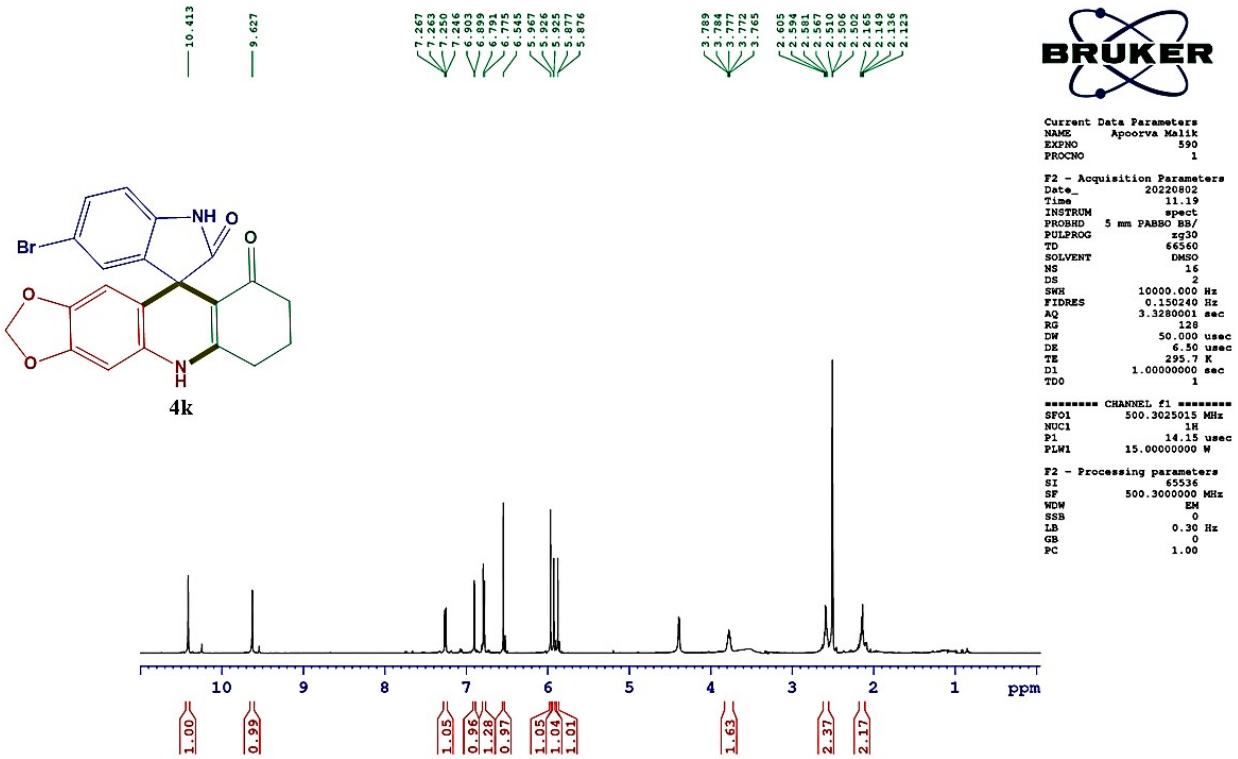


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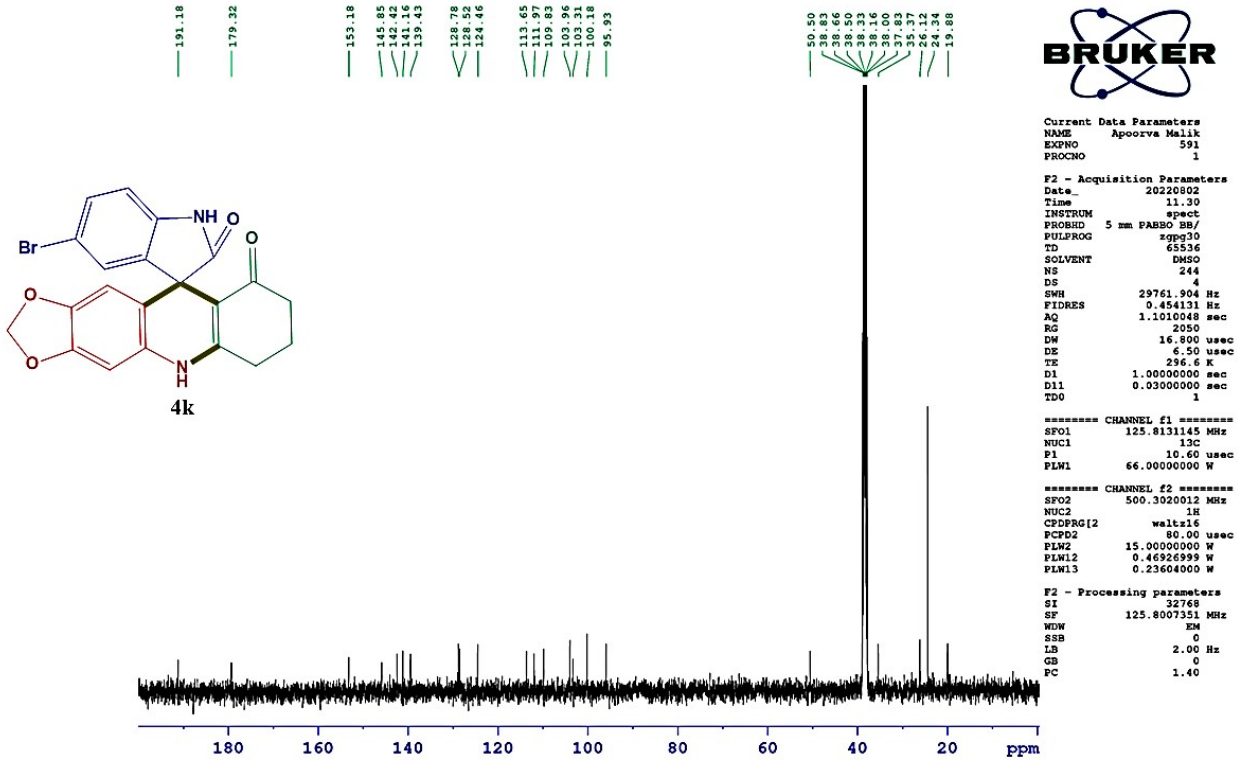
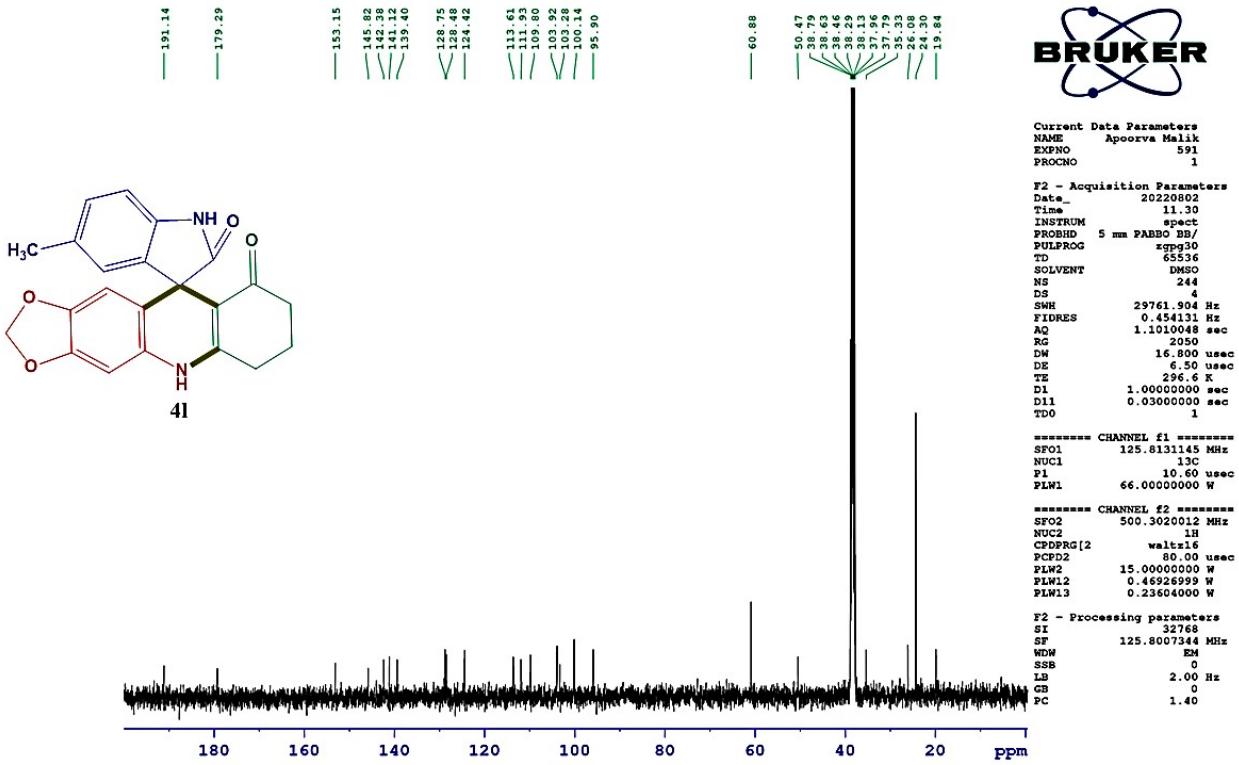


Figure **S23**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4l**.



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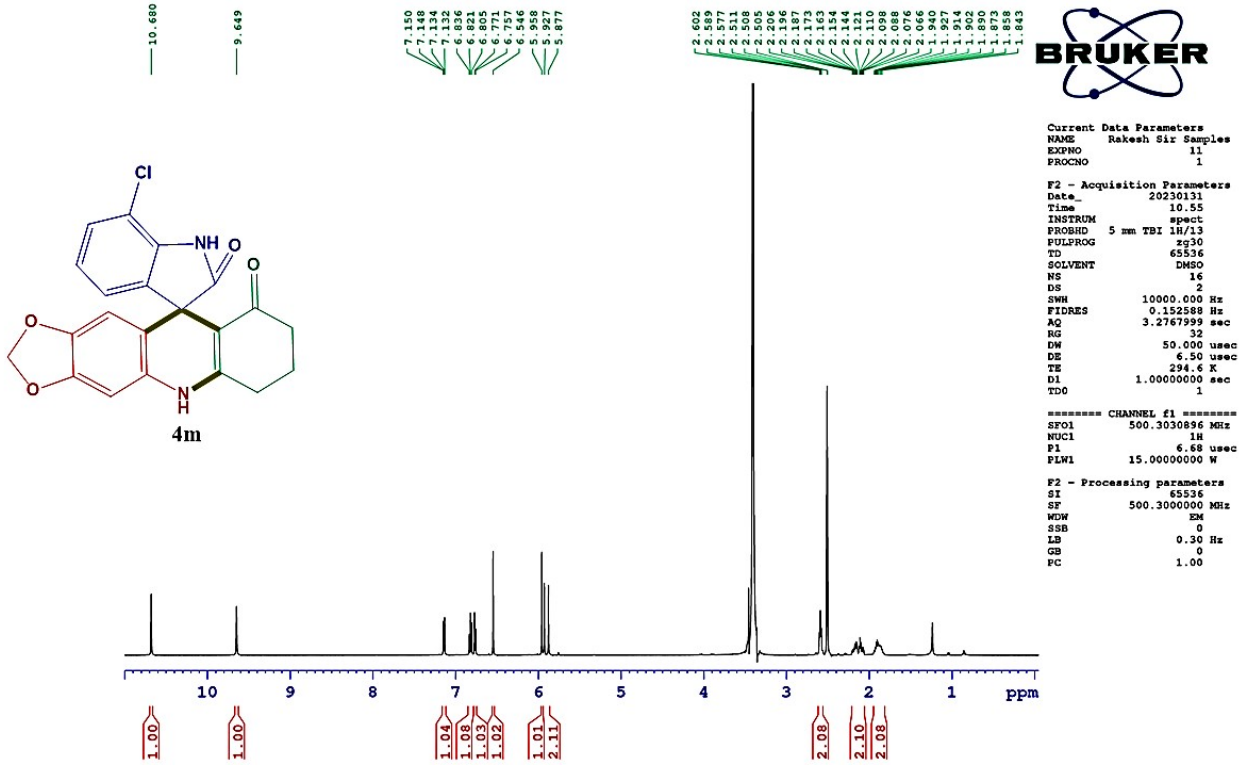


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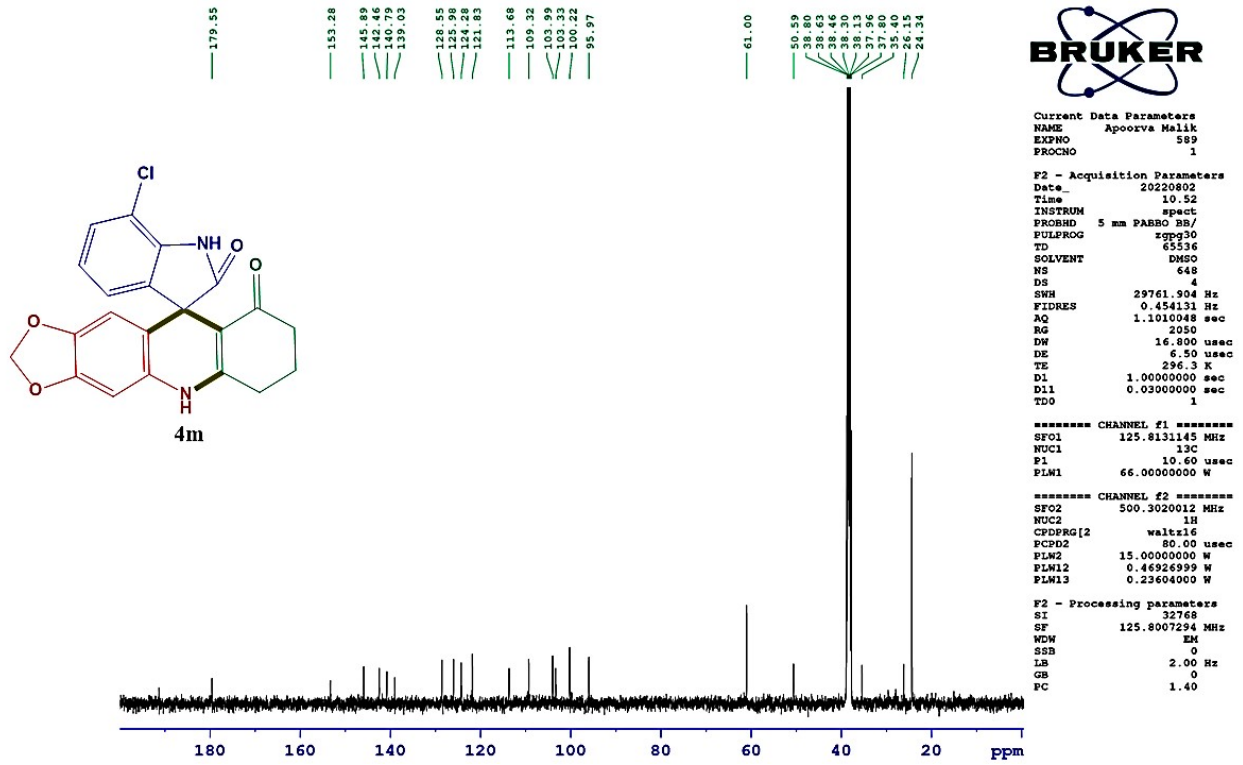

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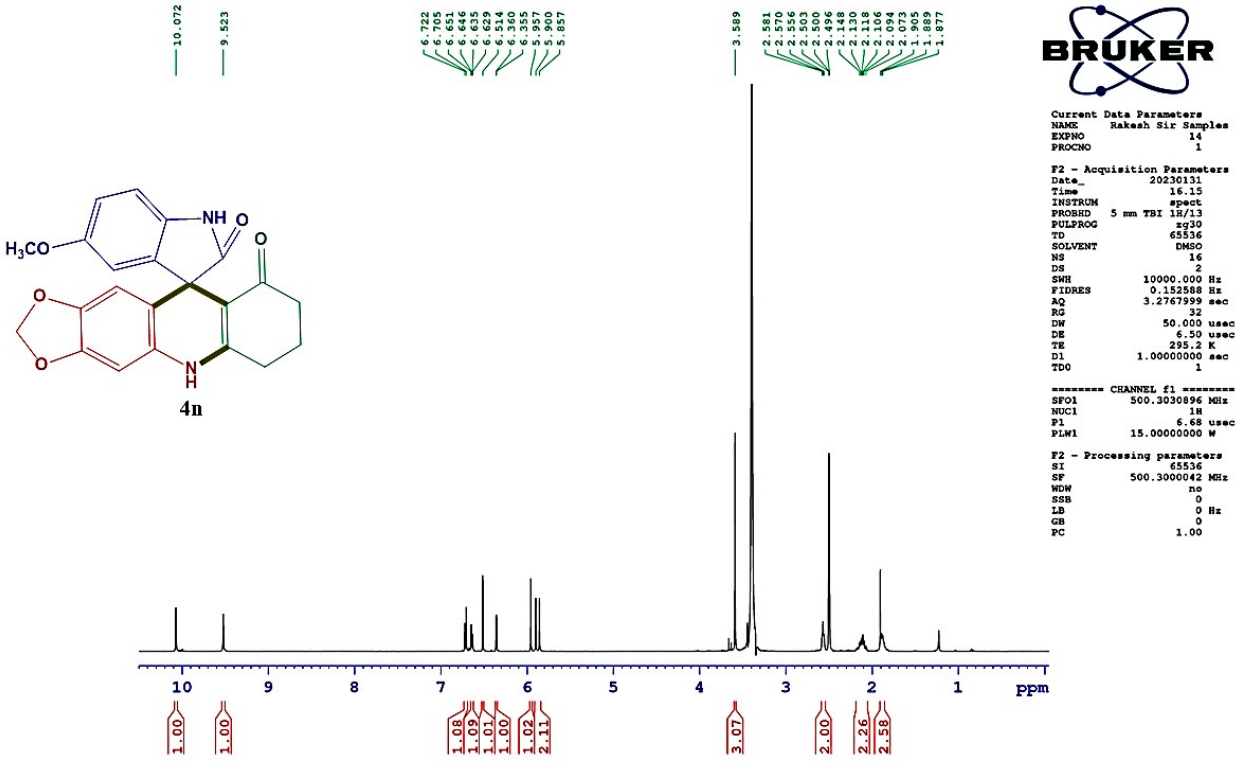
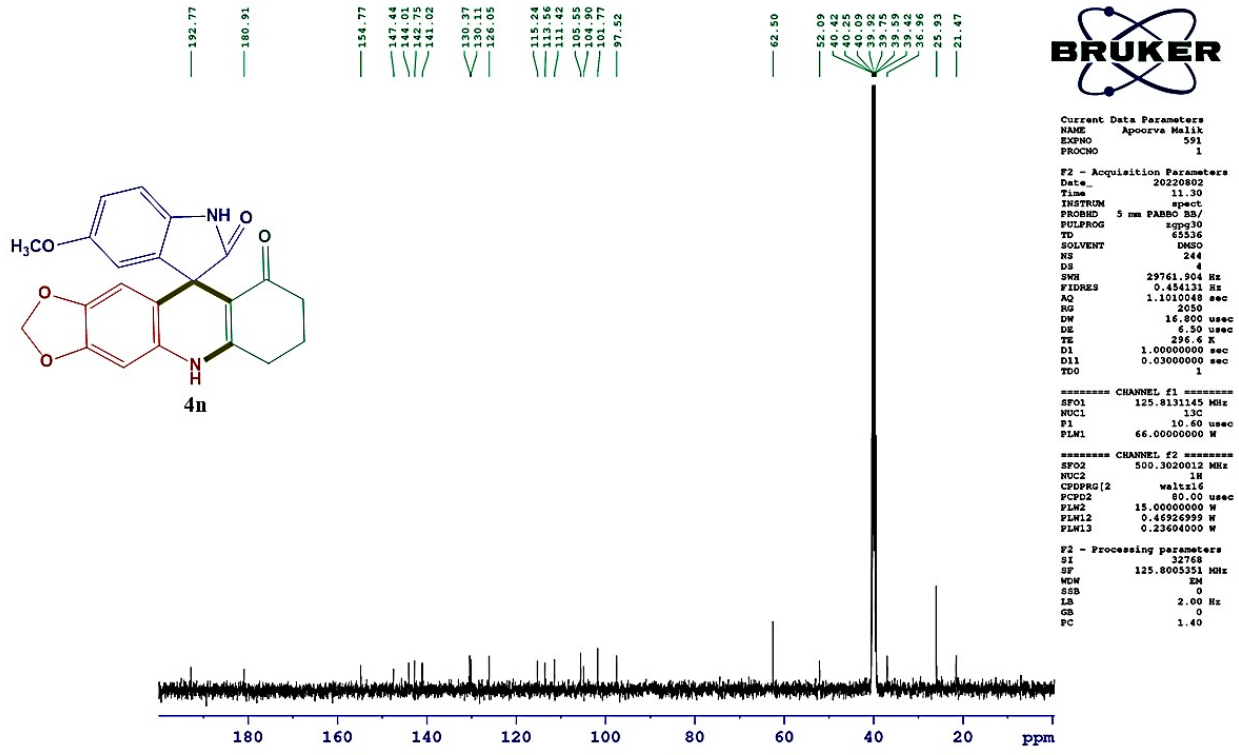



Figure **S27**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4n**.



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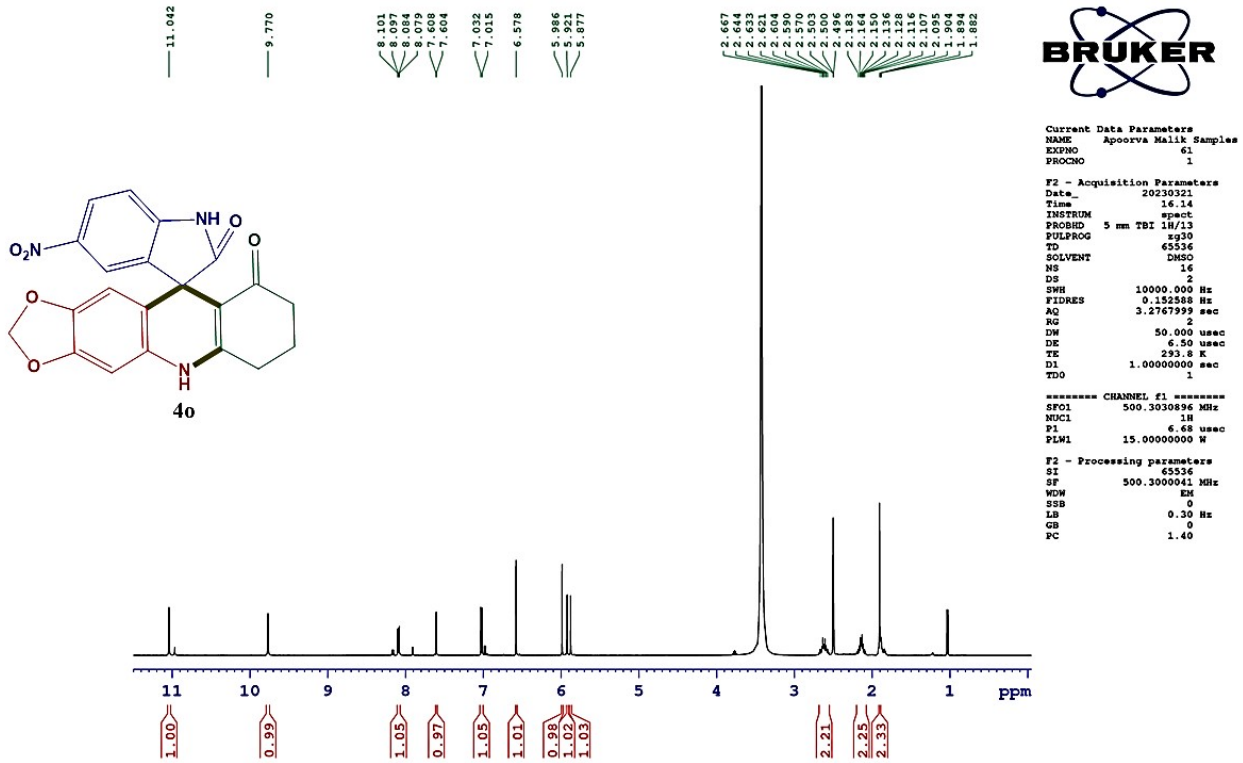


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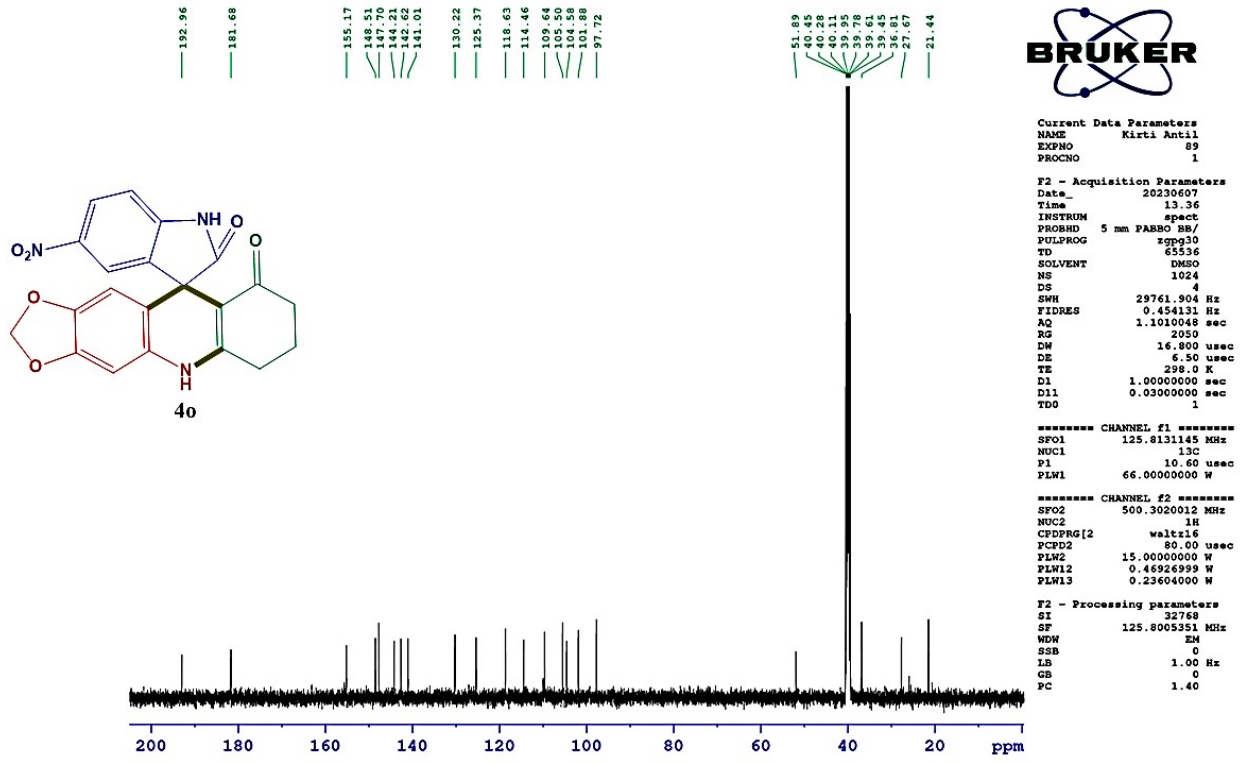


Figure **S30**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4p**.

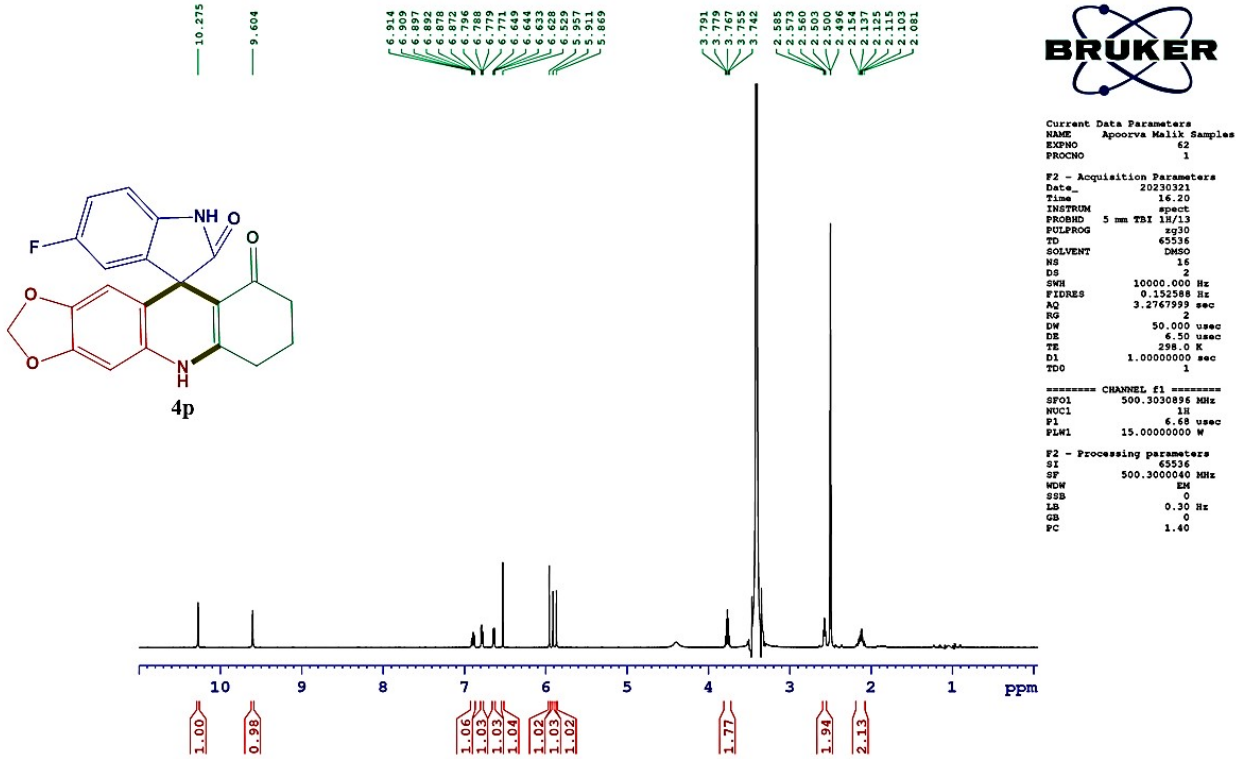



Figure **S31**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4p**.

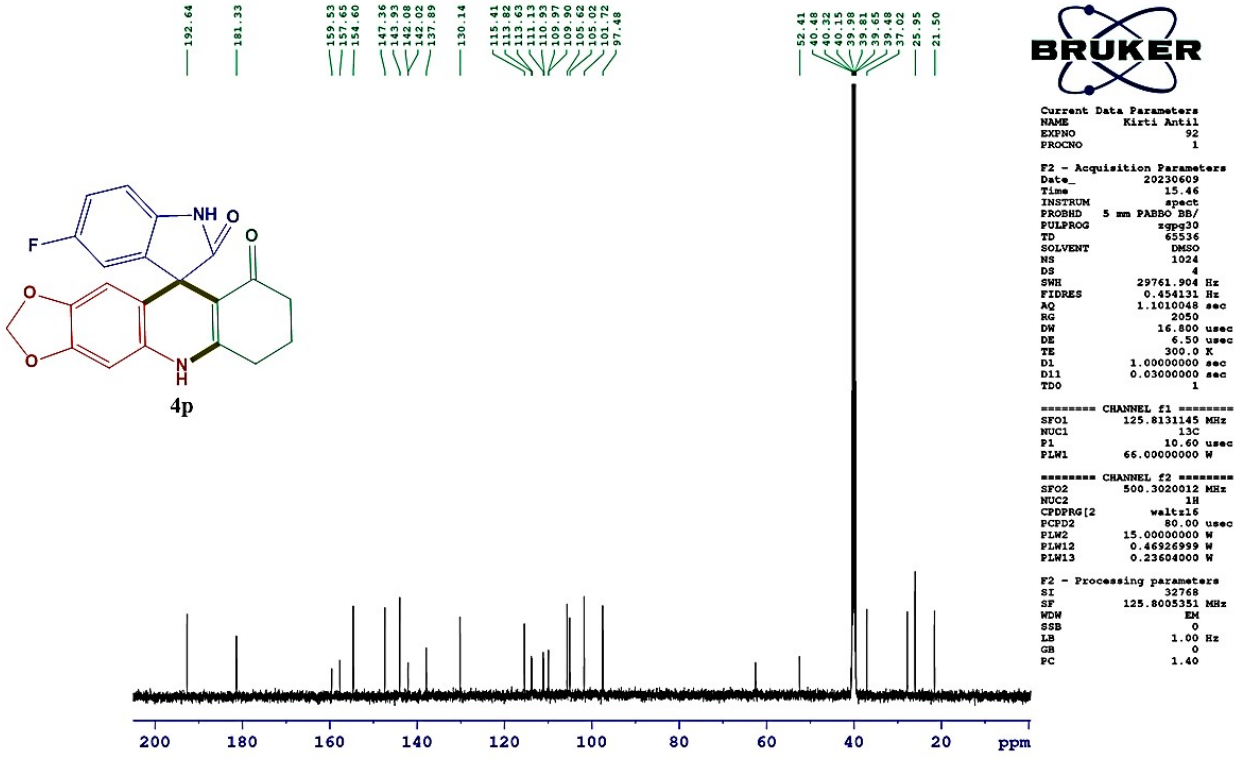


Figure **S32**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4q**.

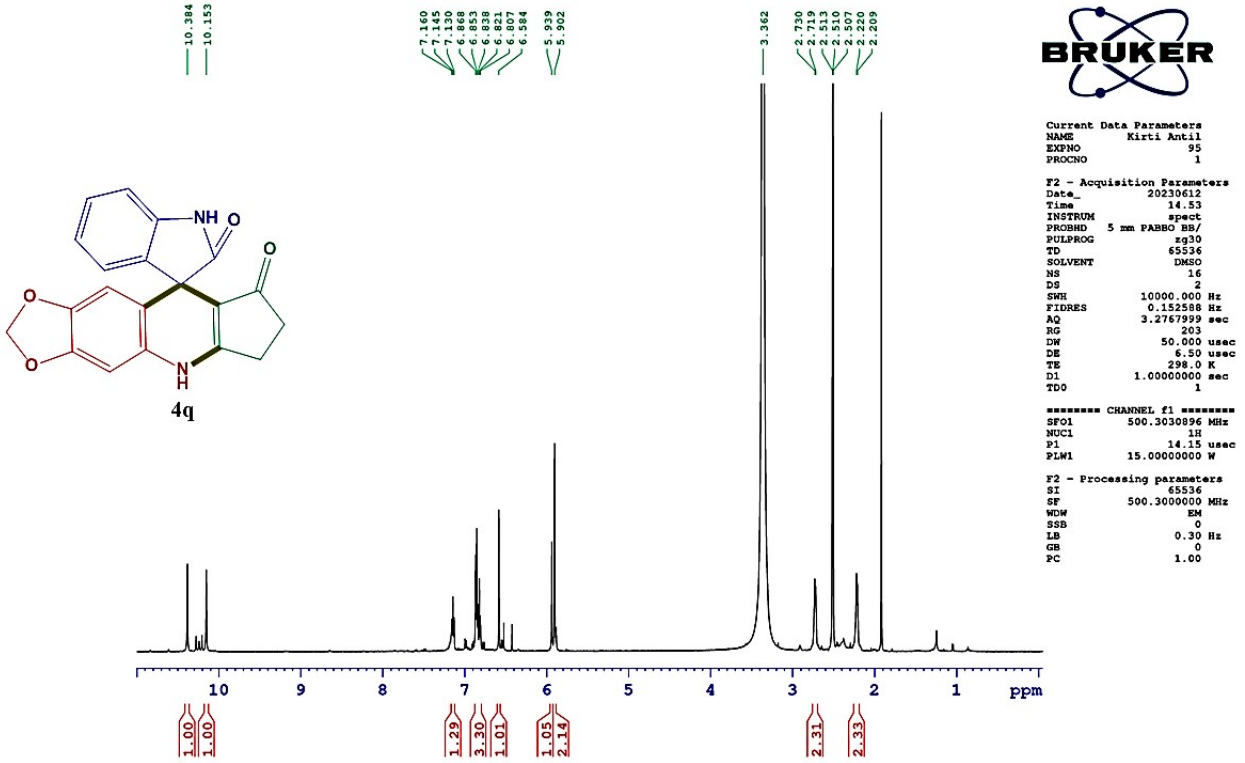



Figure **S33**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4q**.

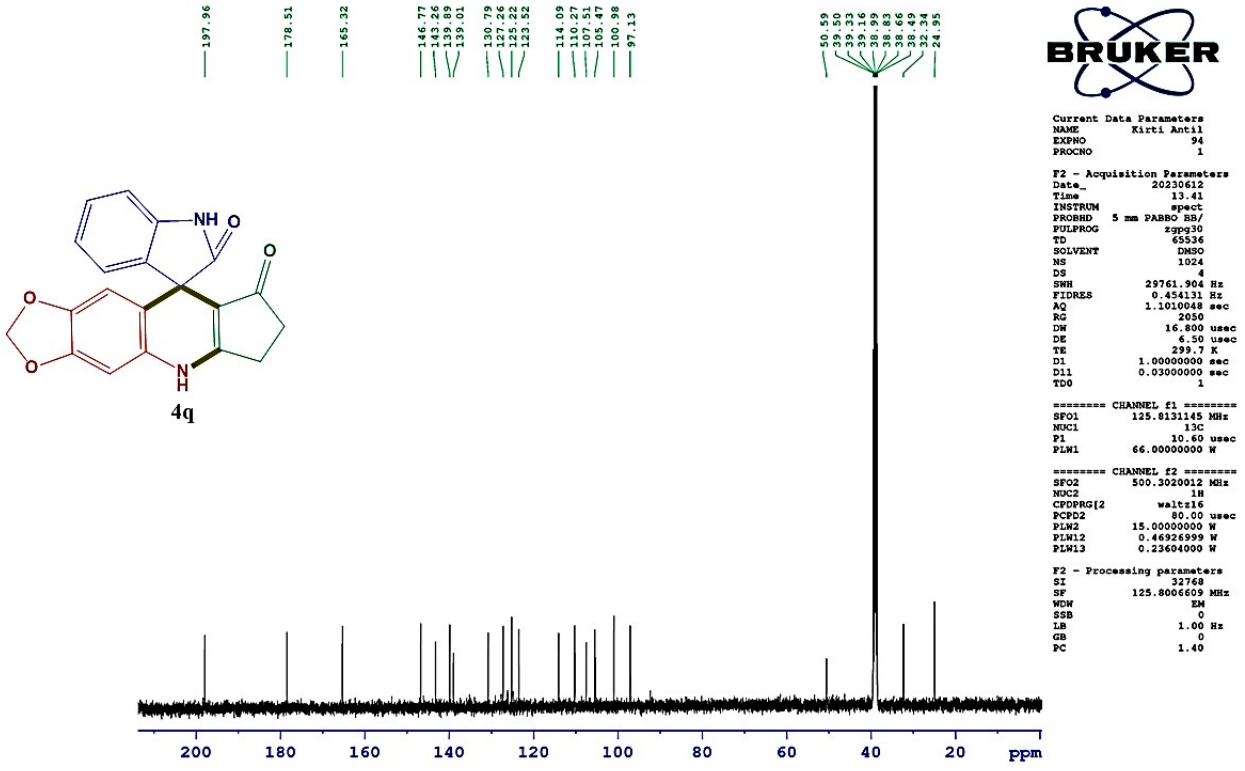
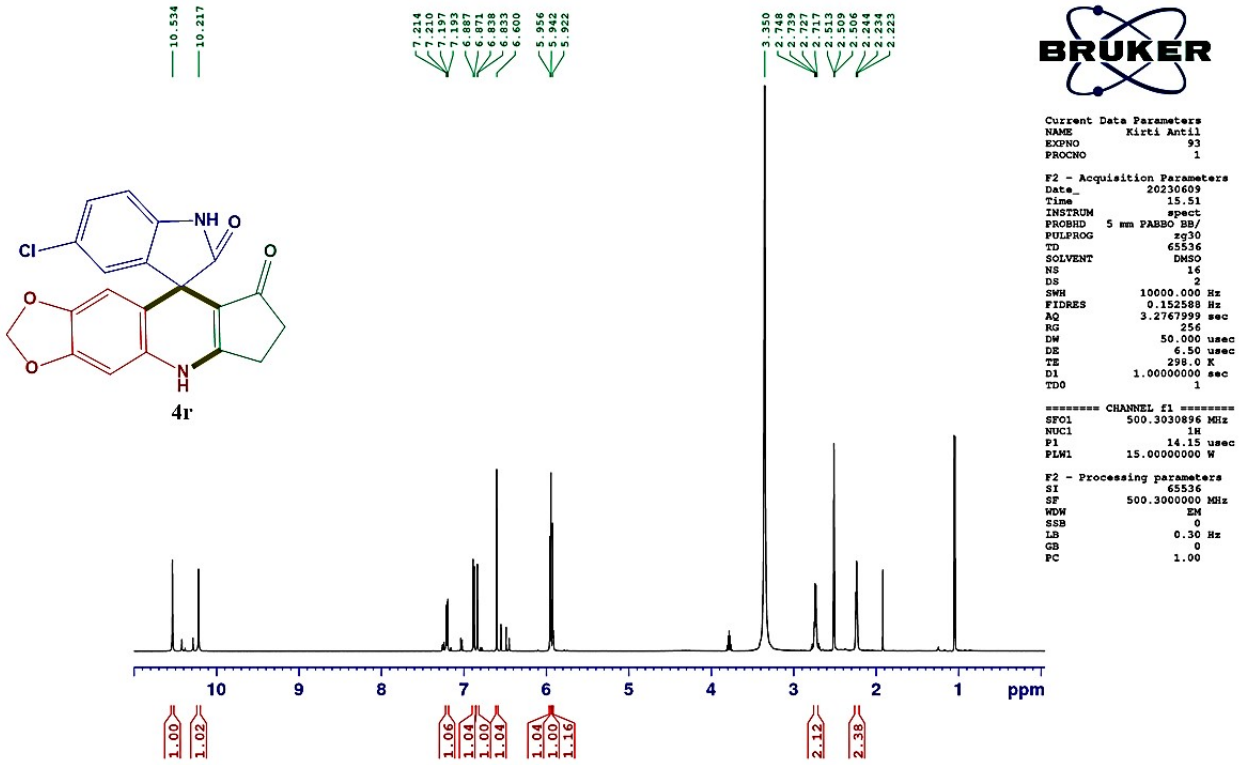


Figure **S34**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4r**.

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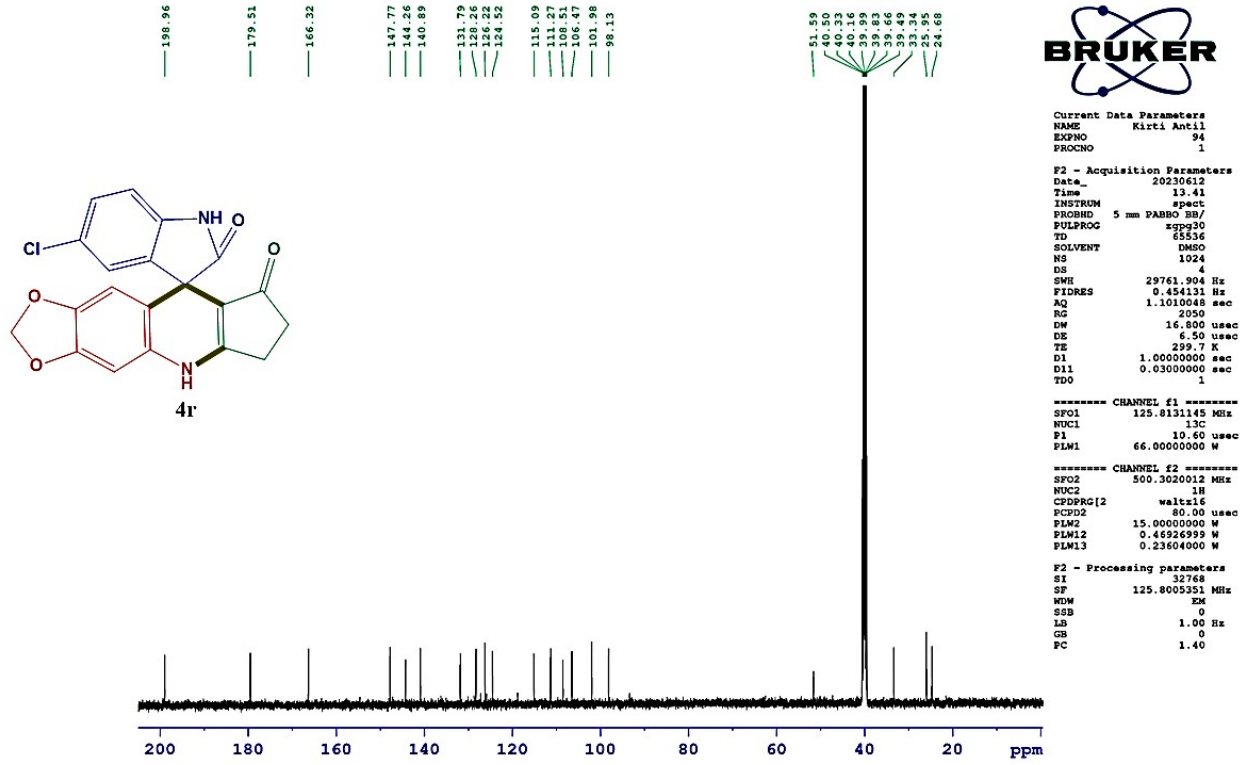
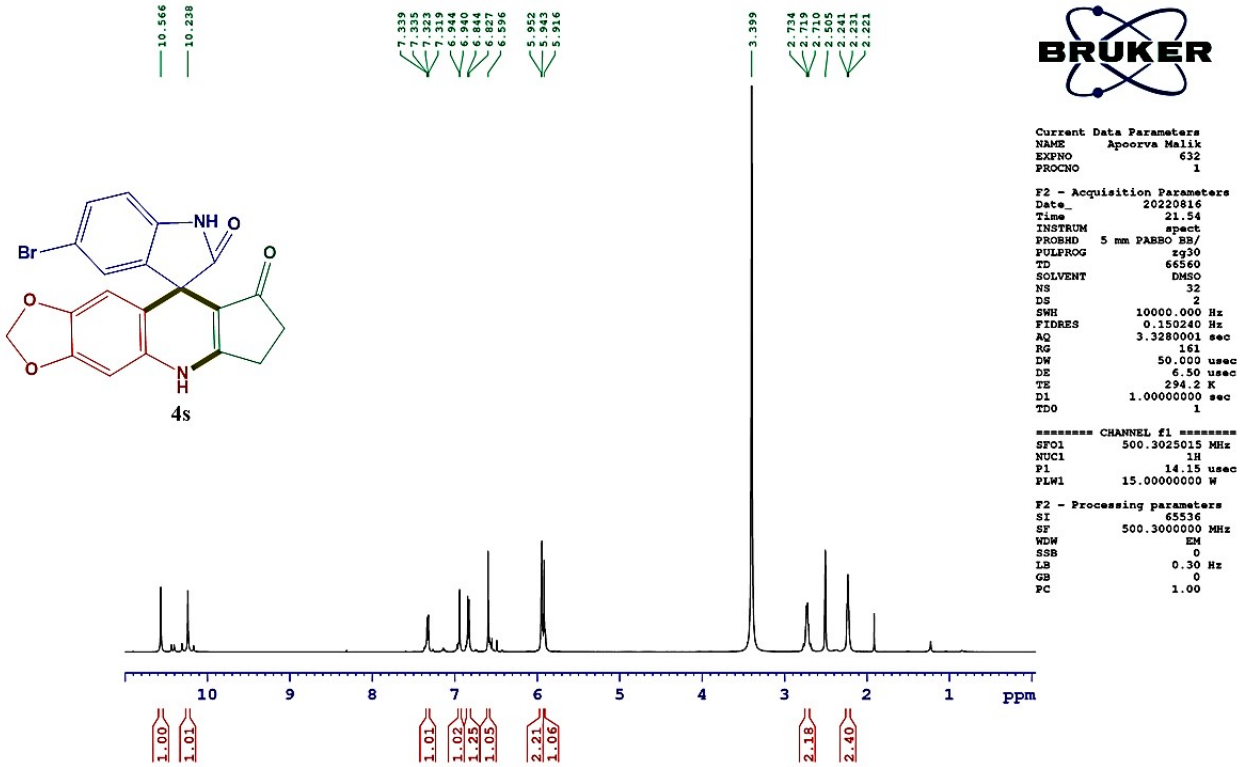


Figure **S36**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4s**.

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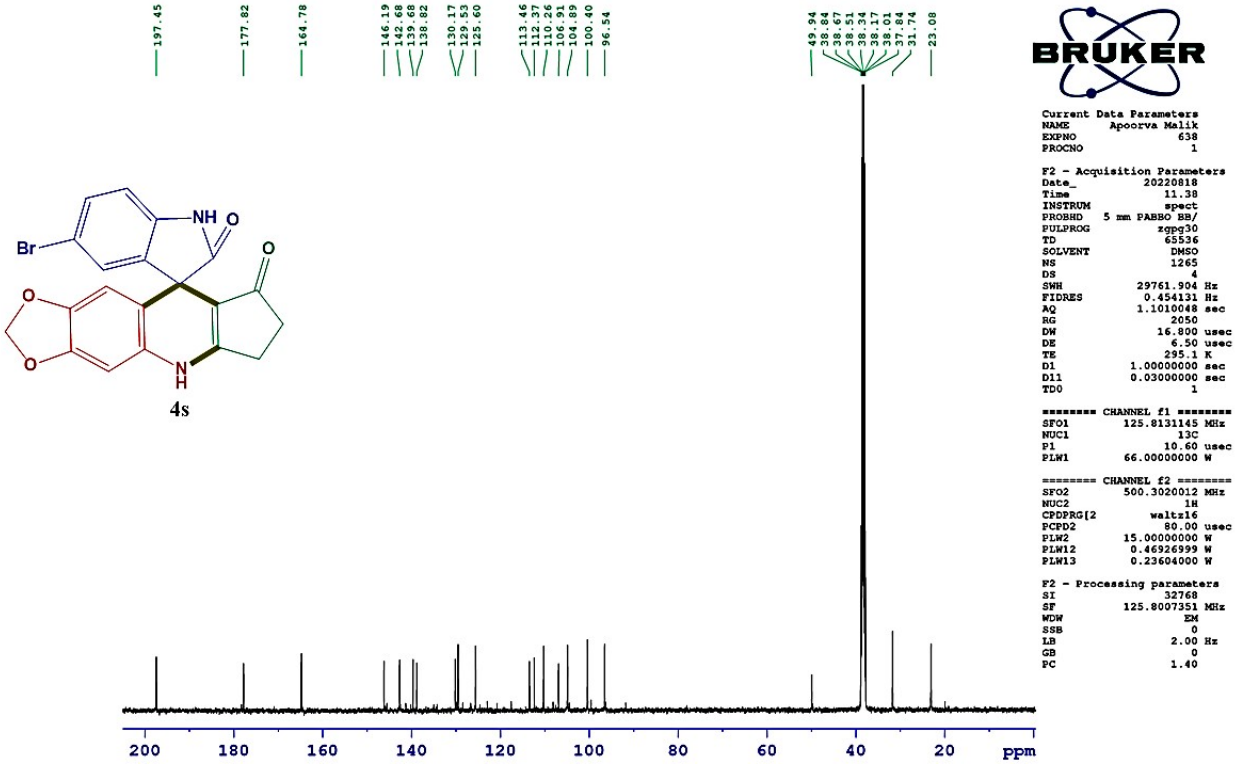

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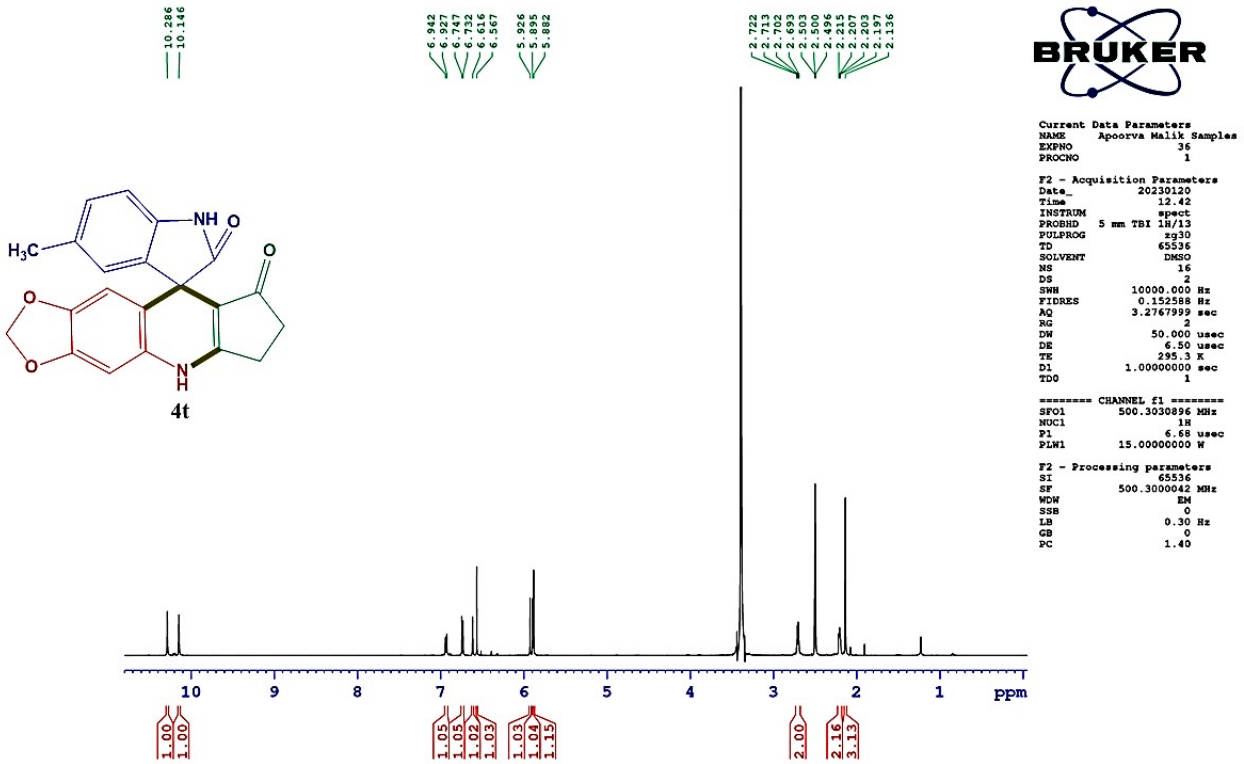


Figure **S39**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4t**.

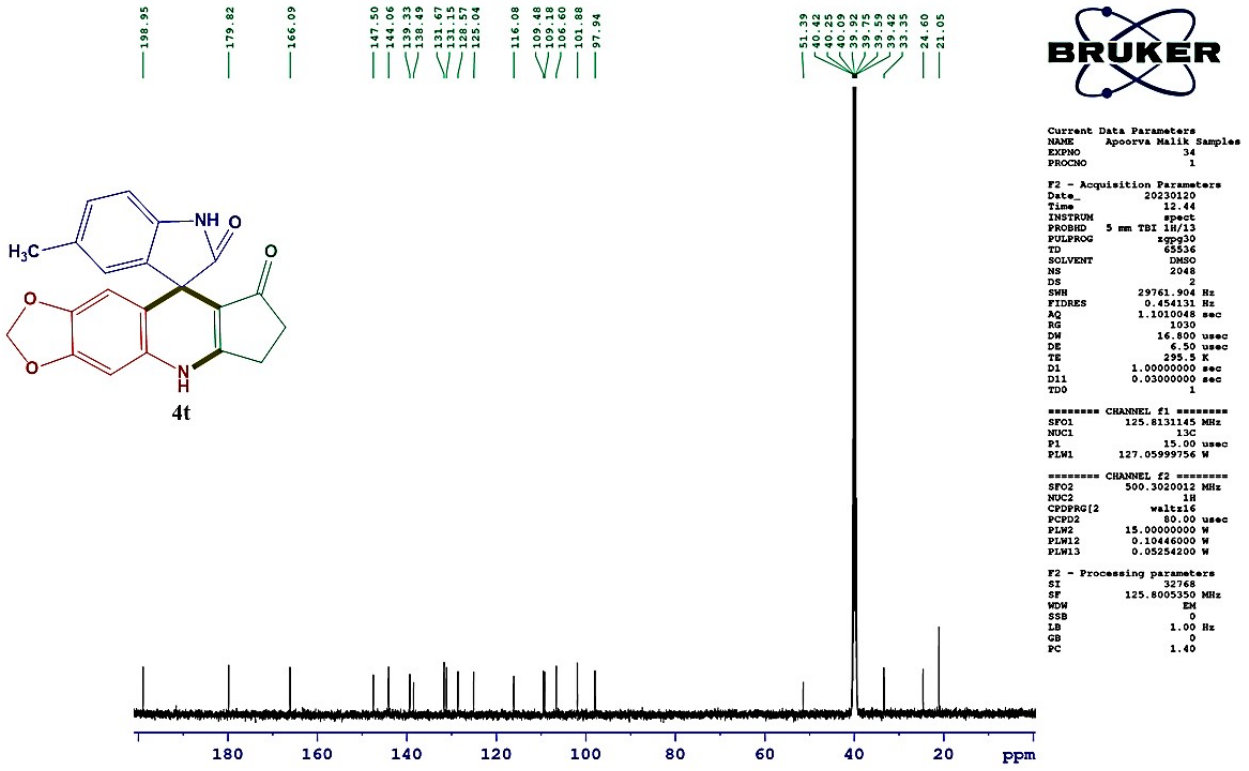

Figure **S40**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4u**.

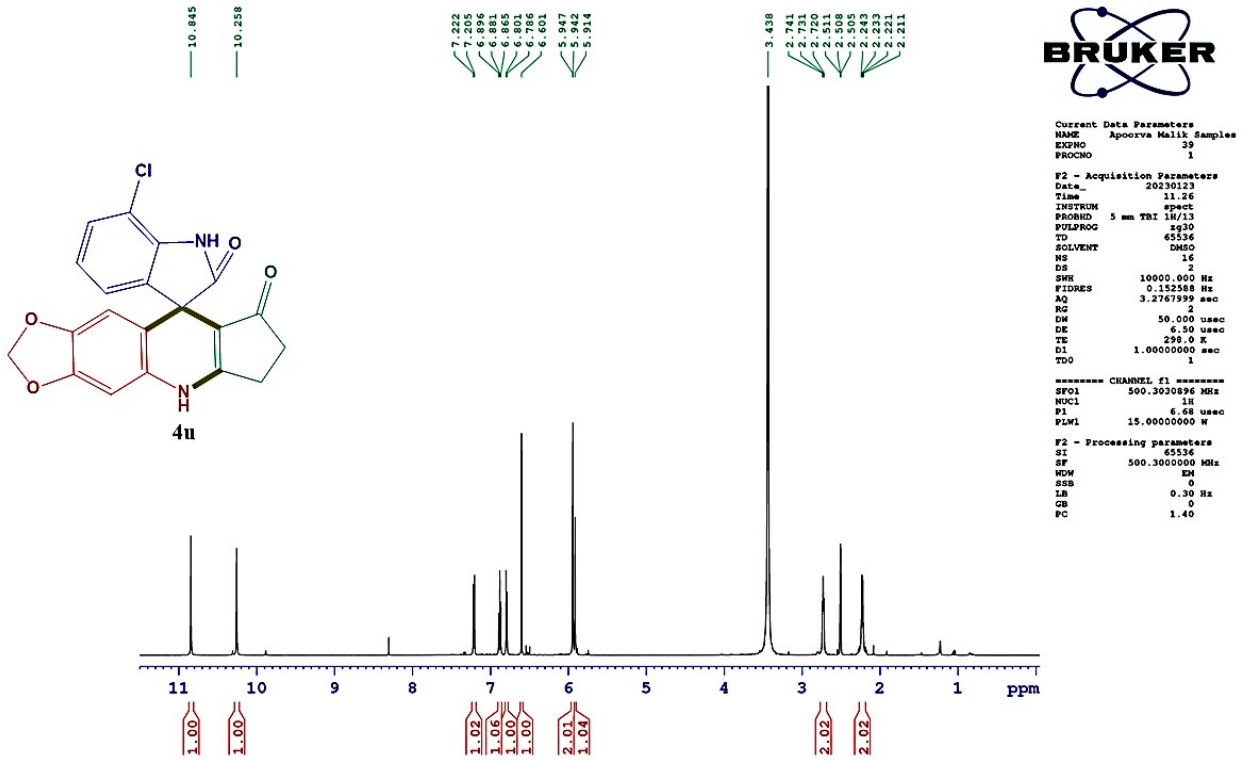


Figure **S41**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4u**.

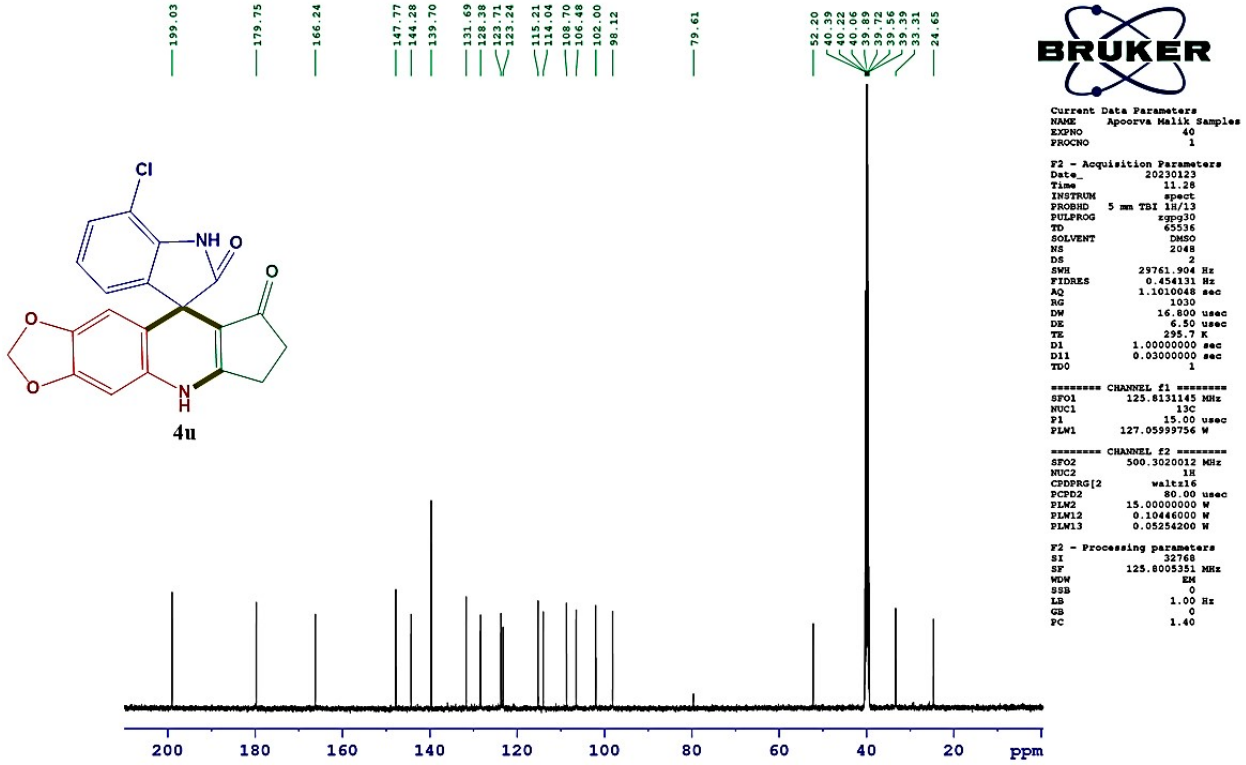

Figure **S42**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4v**.

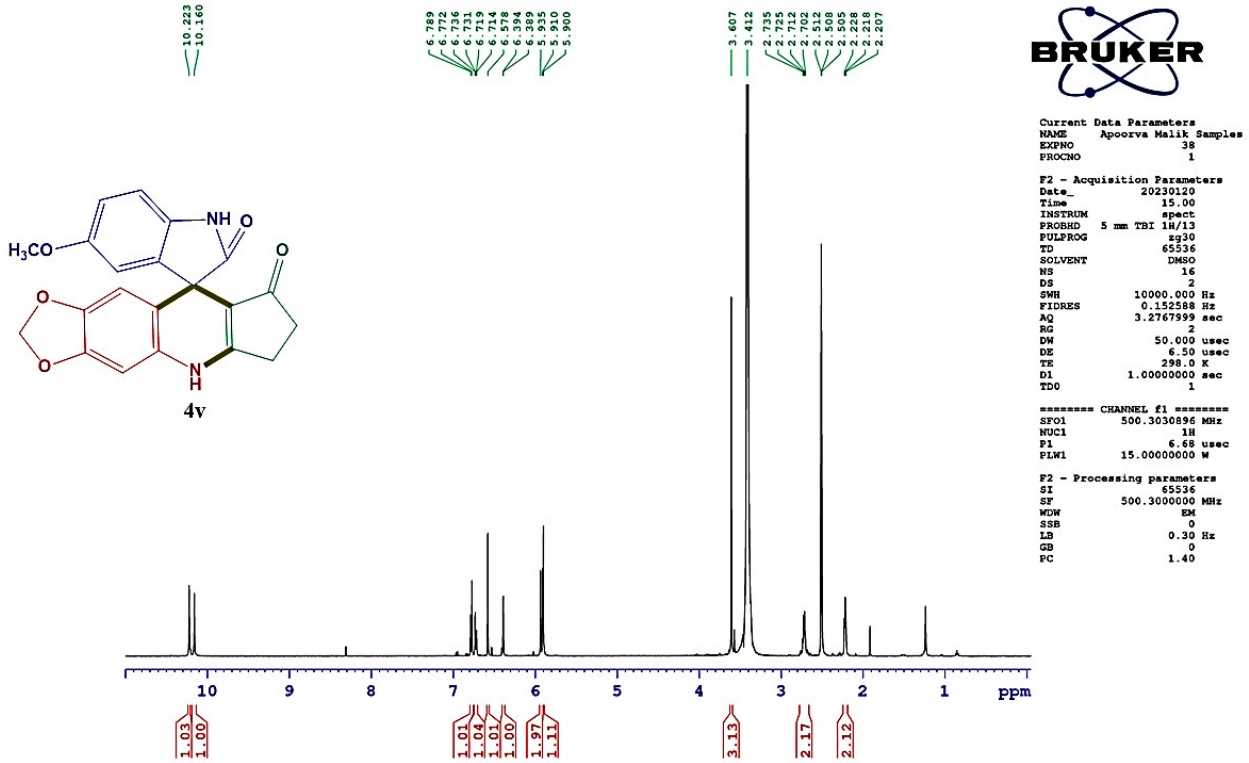


Figure **S43**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4v**.

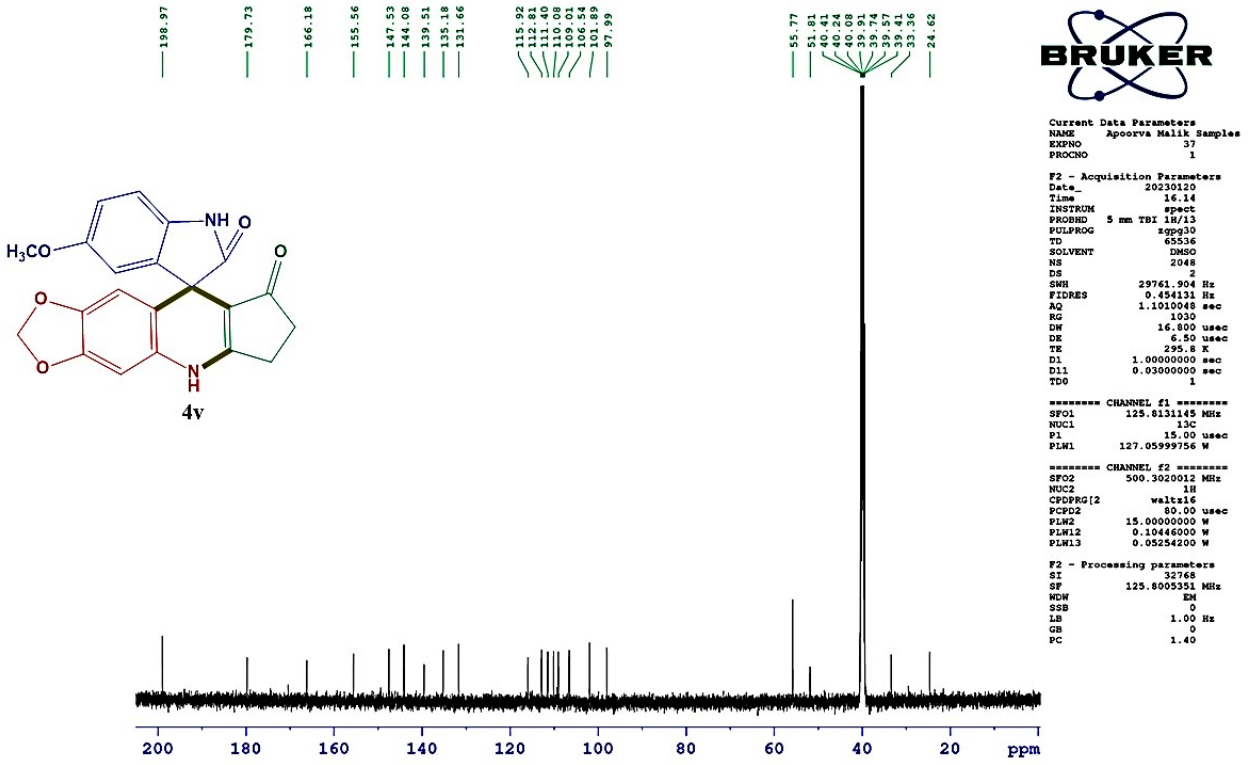

Figure **S44**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4w**.

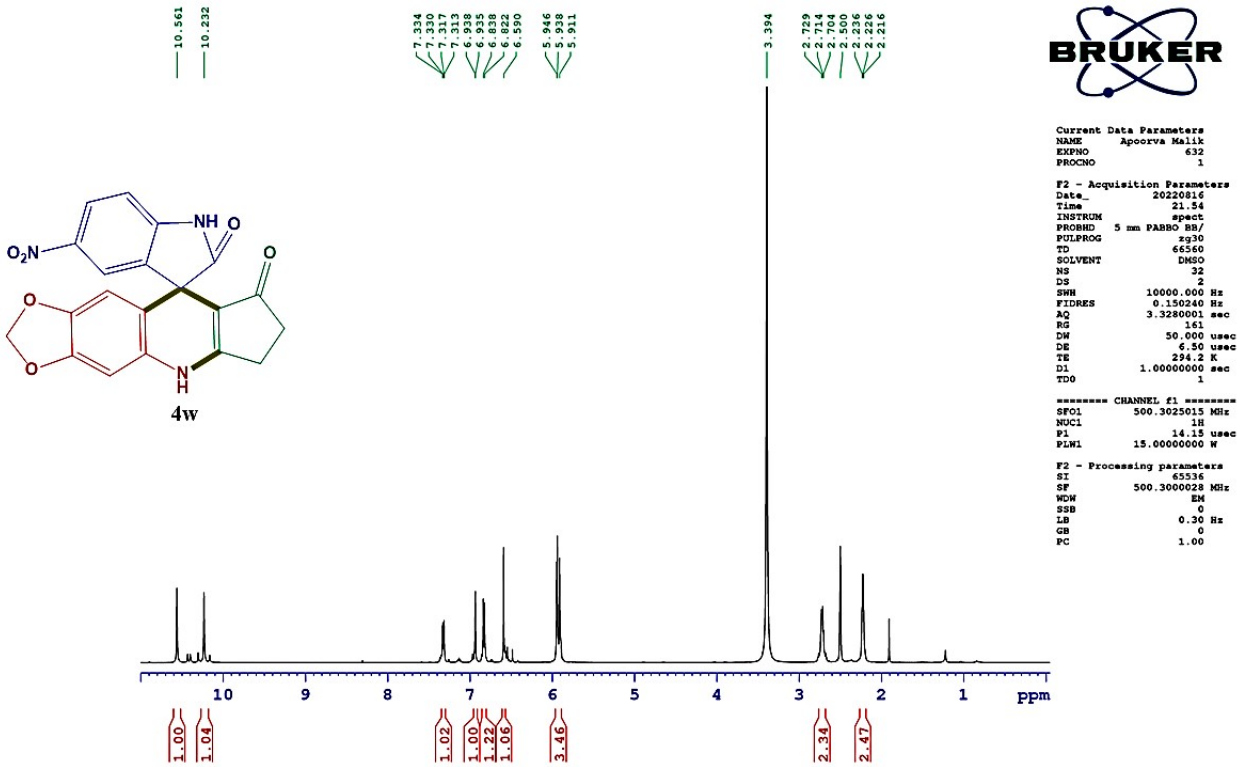


Figure **S45**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4w**.

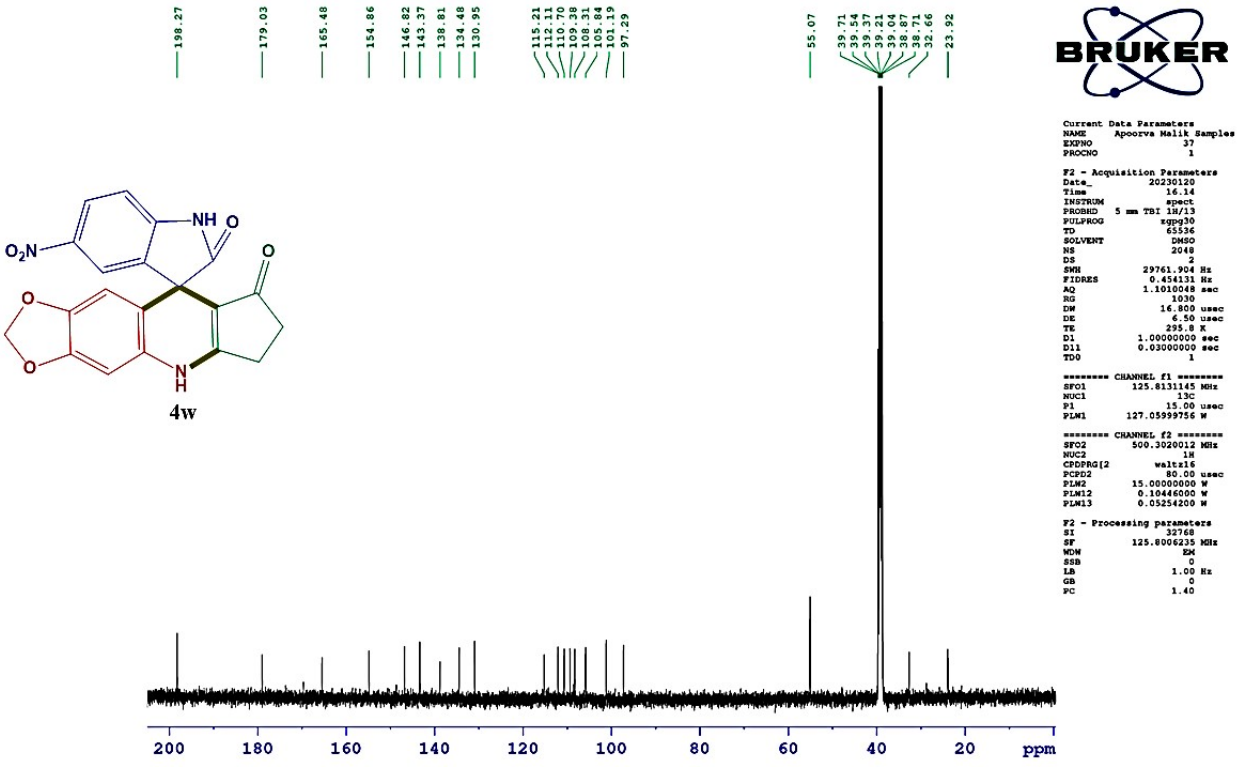

Figure **S46**: $^{1}$H-NMR (500 MHz, DMSO-$d_6$) of Compound **4x**.

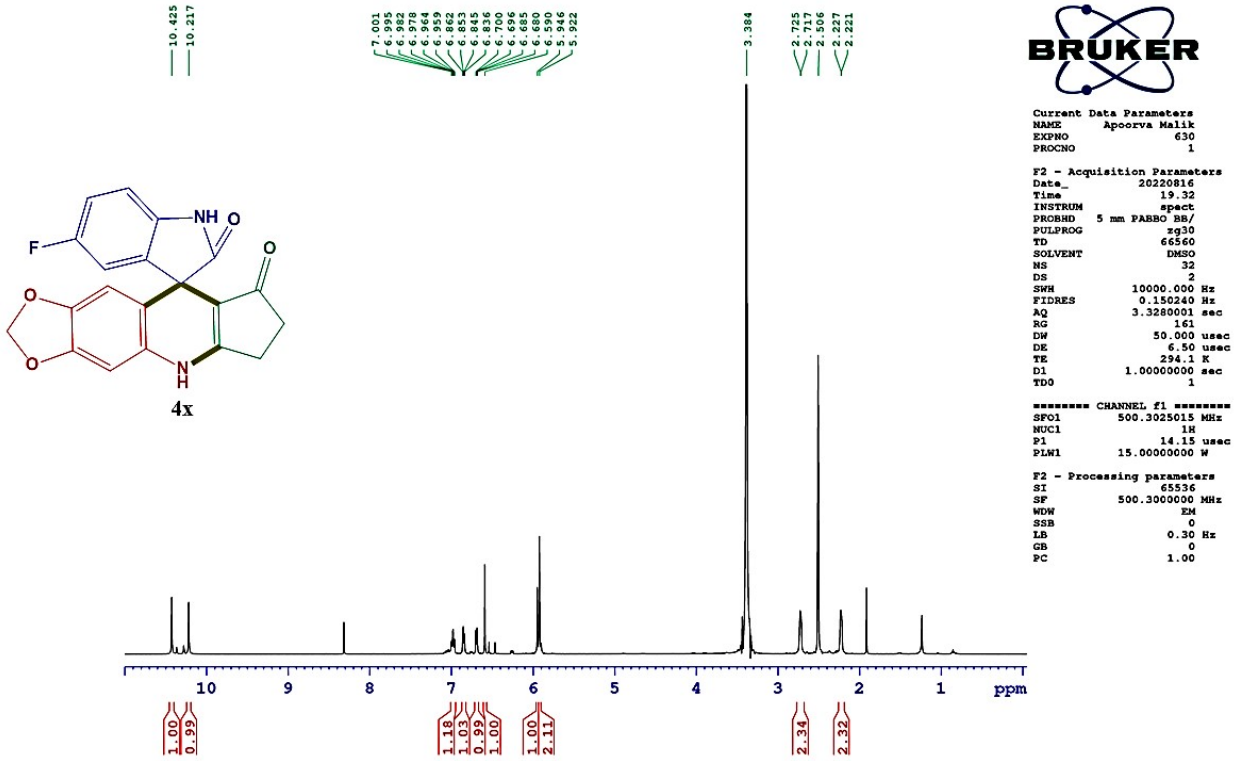


Figure **S47**: $^{13}$C-NMR (125 MHz, DMSO-$d_6$) of Compound **4x**.

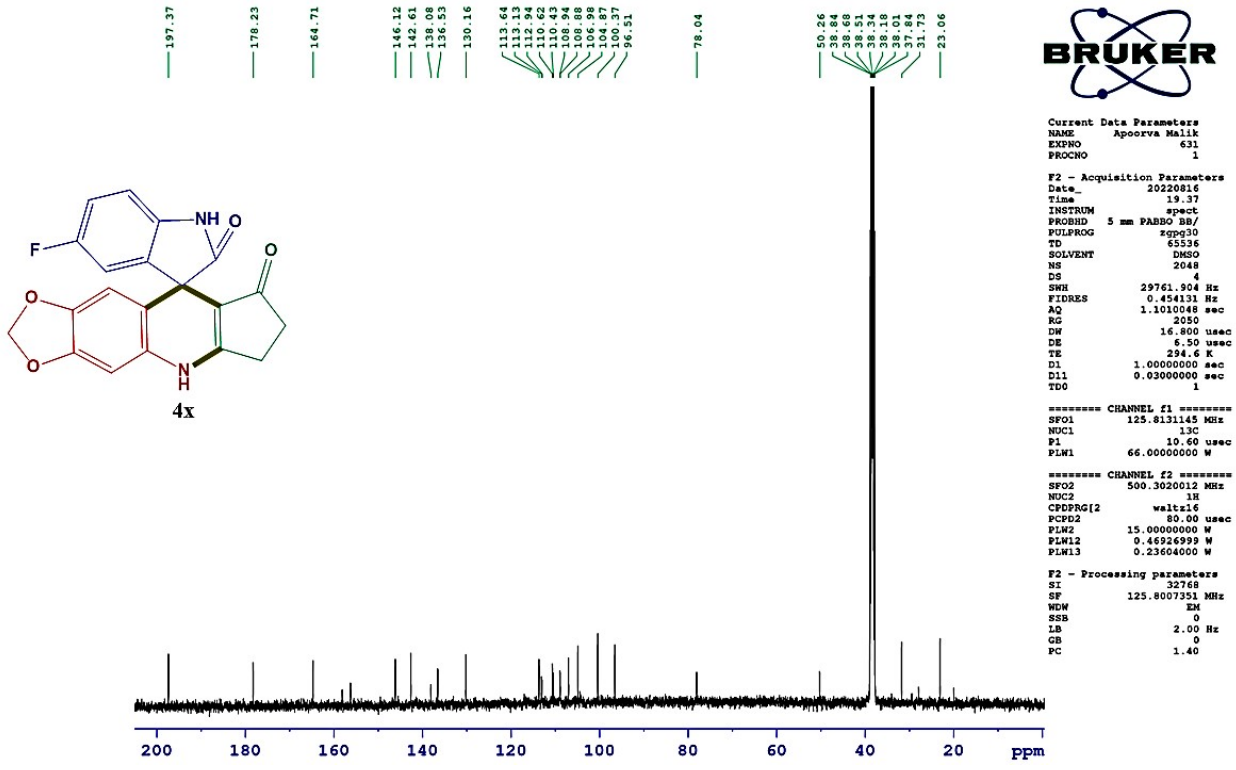

Figure **S48**: HRMS of Compound **4a**.

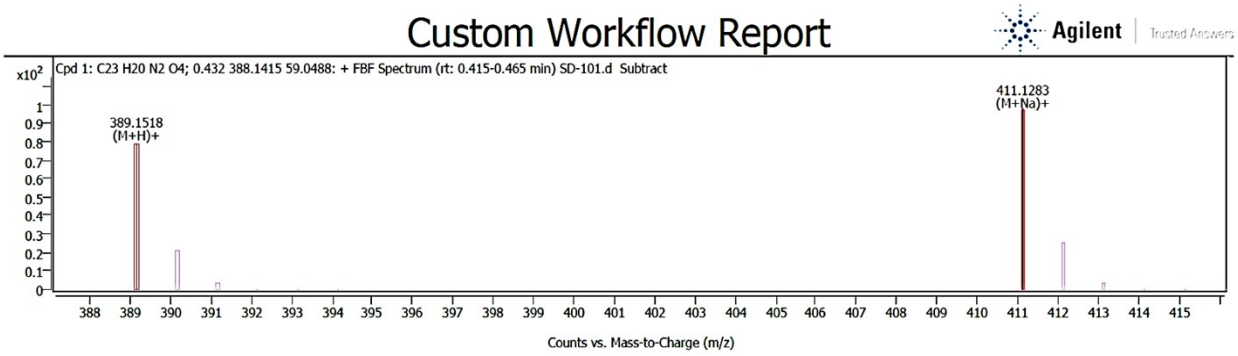


Figure **S49**: HRMS of Compound **4b**.

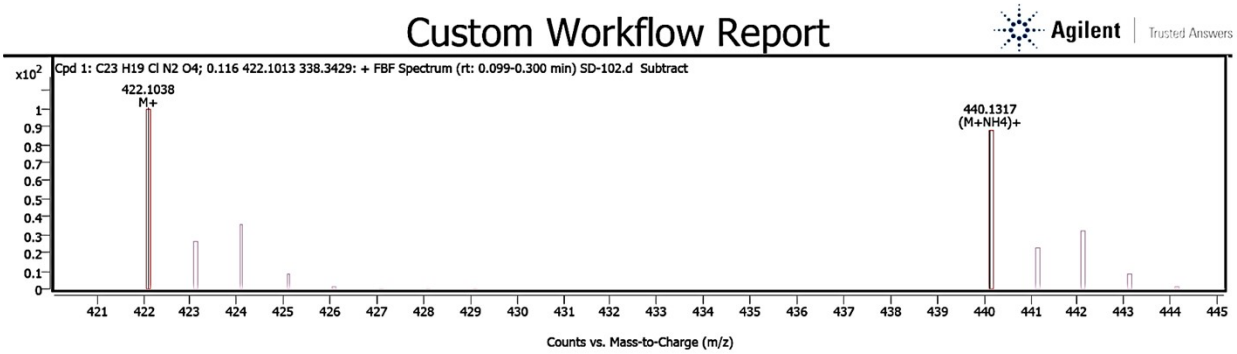


Figure **S50**: HRMS of Compound **4c**.

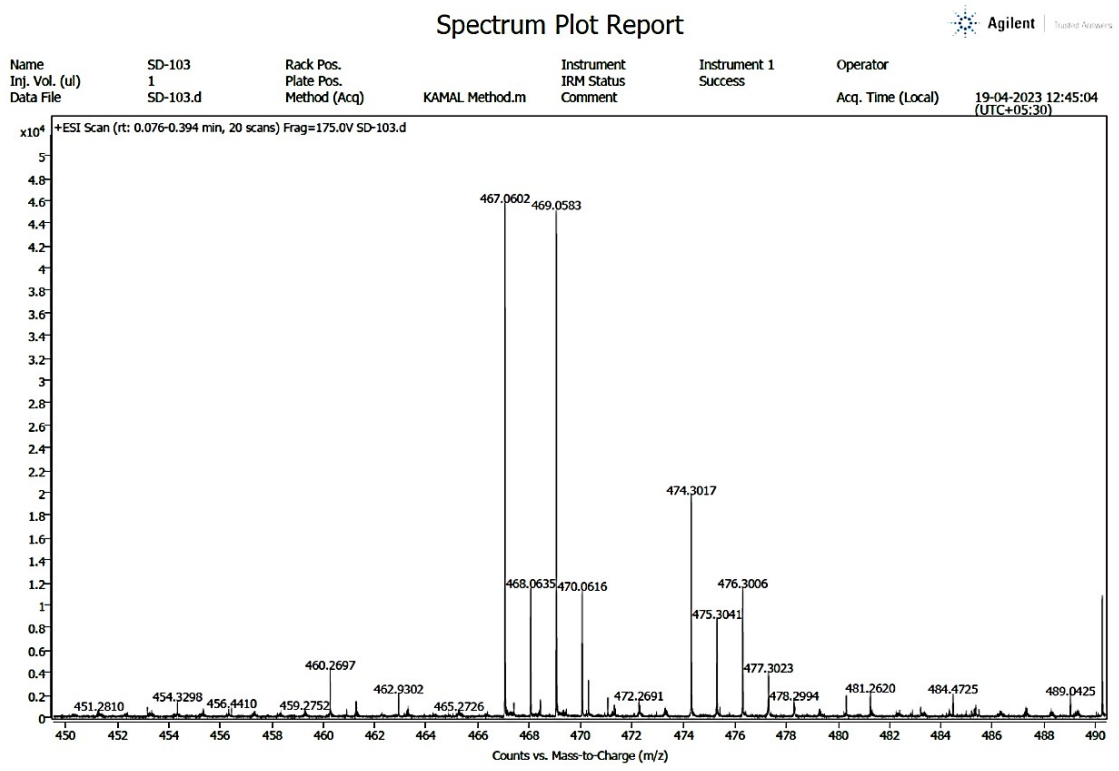

Figure **S51**: HRMS of Compound **4d**.

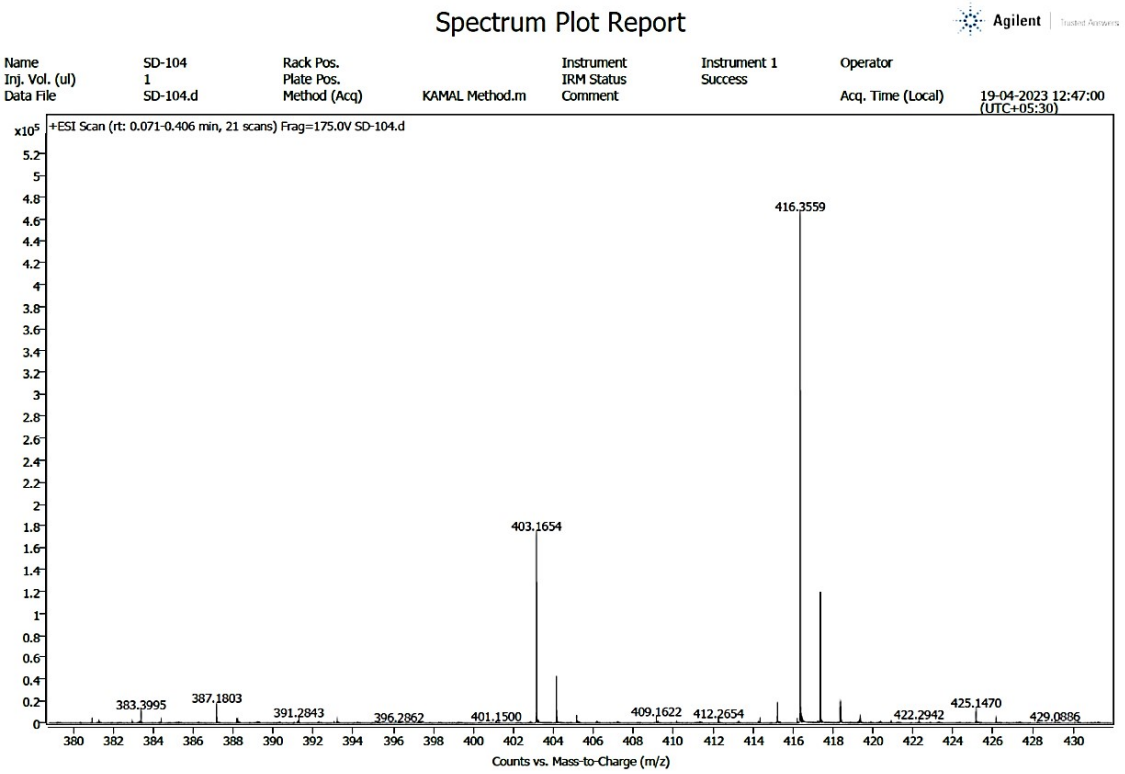


Figure **S52**: HRMS of Compound **4e**.

Figure **S53**: HRMS of Compound **4f**.

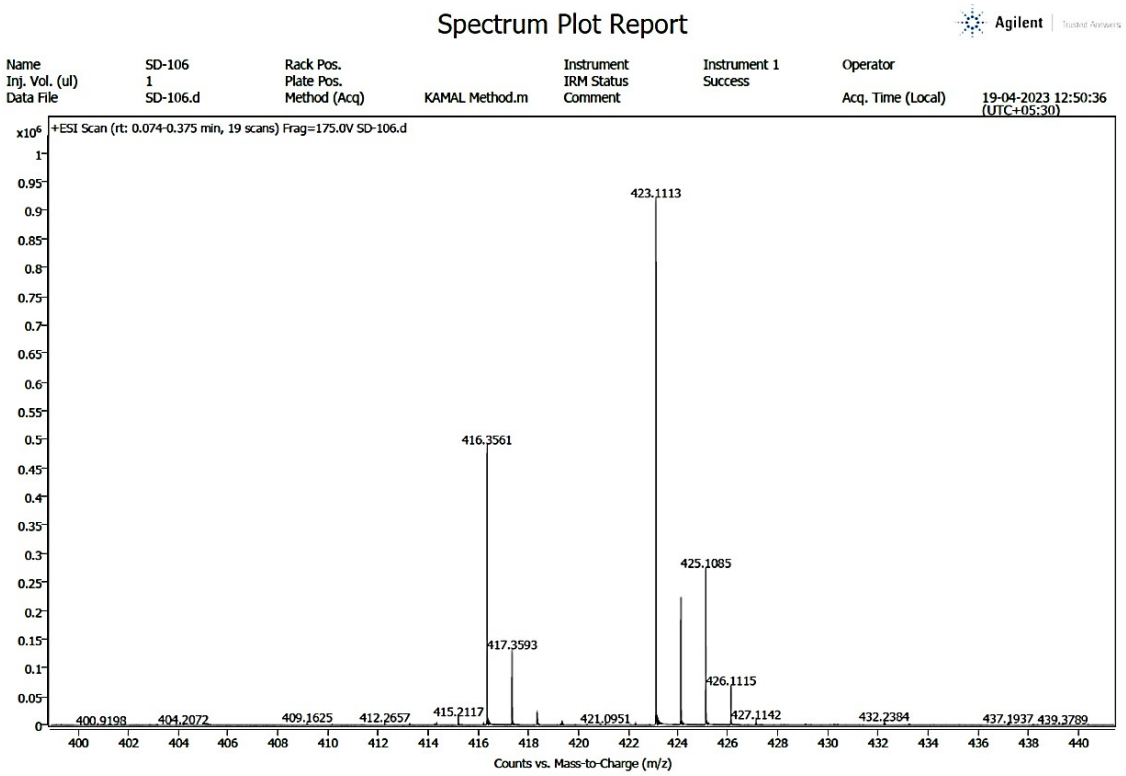


Figure **S54**: HRMS of Compound **4g**.

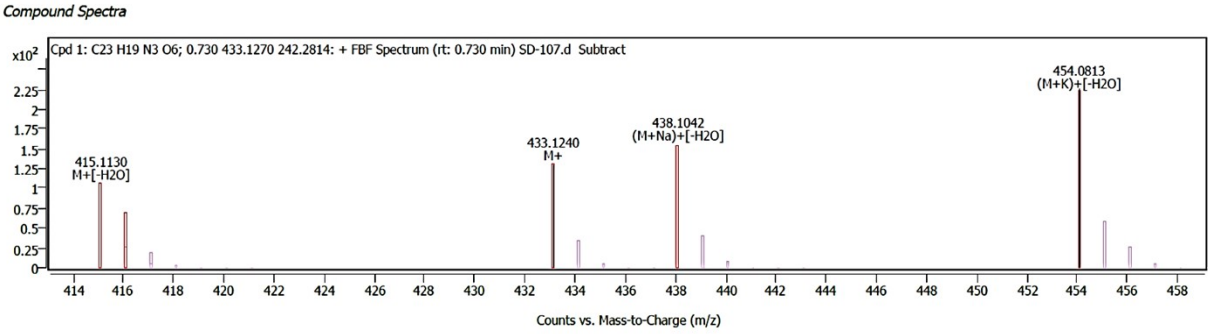


Figure **S55**: HRMS of Compound **4h**.

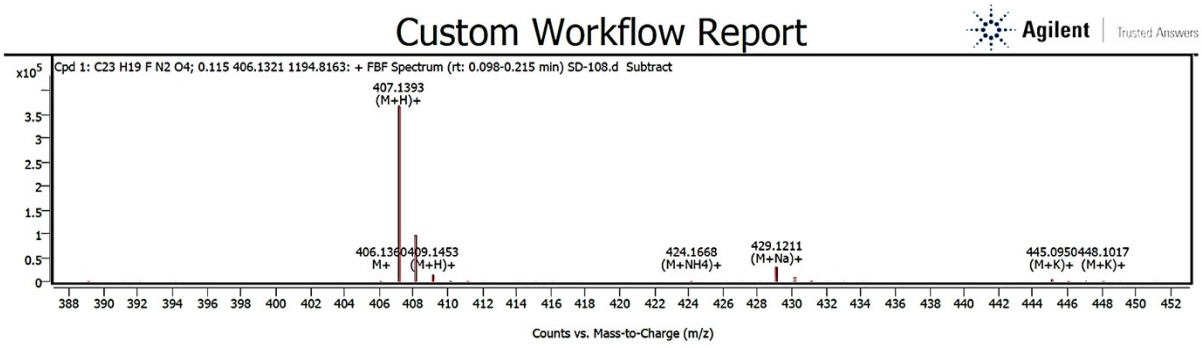

Figure **S56**: HRMS of Compound **4i**.

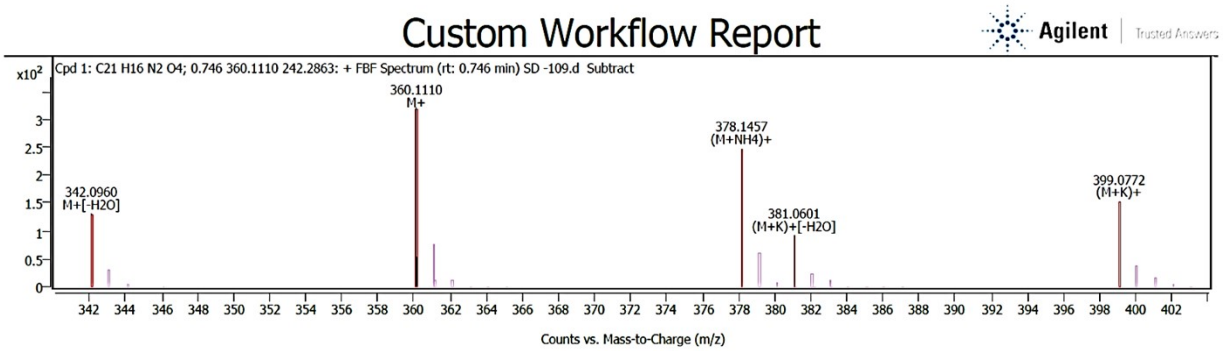


Figure **S57**: HRMS of Compound **4j**.

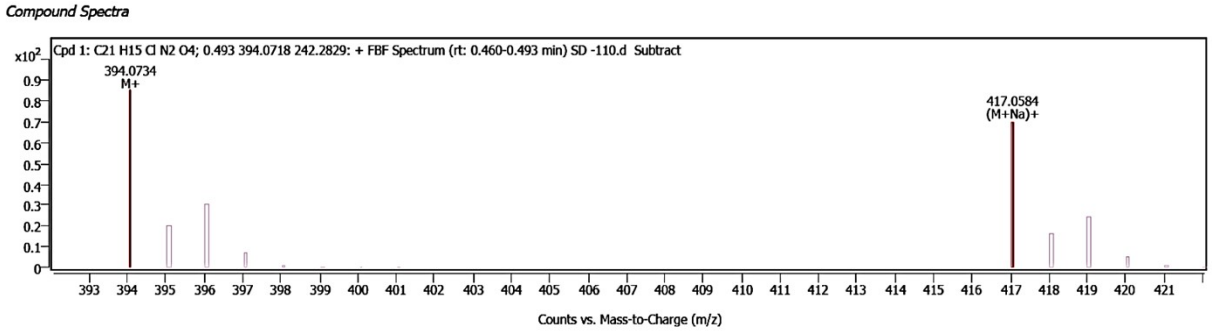


Figure **S58**: HRMS of Compound **4k**.

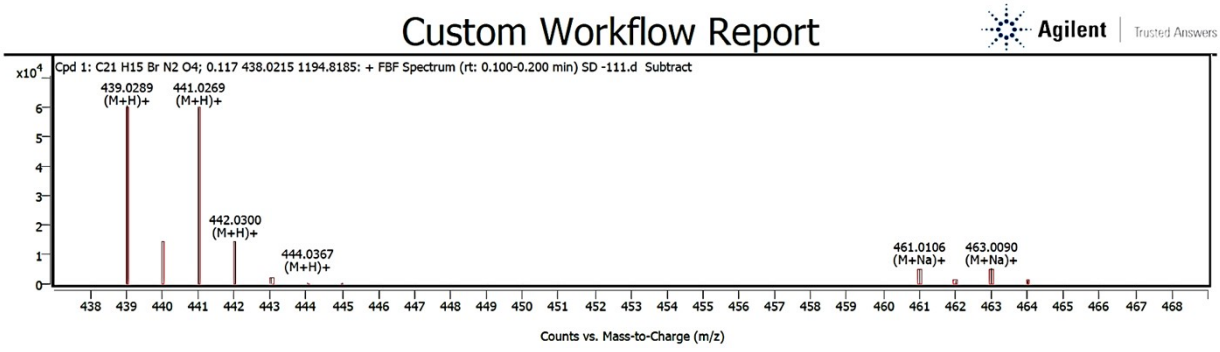

Figure **S59**: HRMS of Compound **4l**.

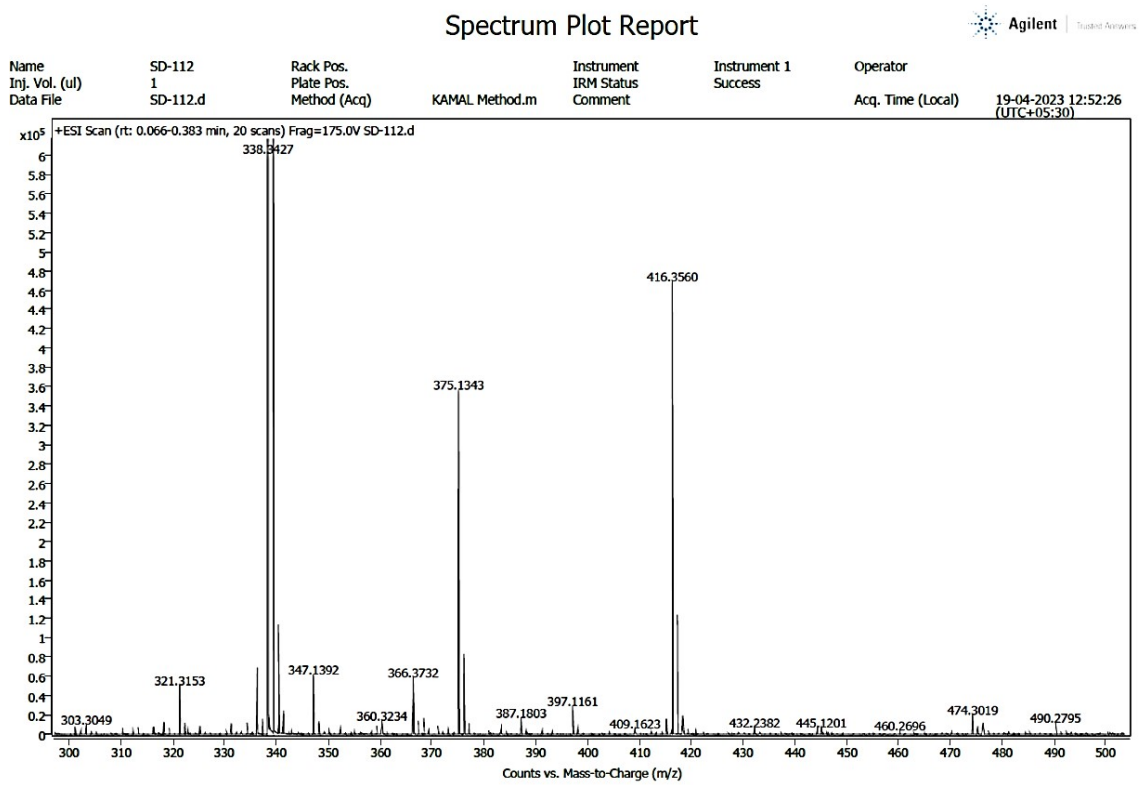


Figure **S60**: HRMS of Compound **4m**.

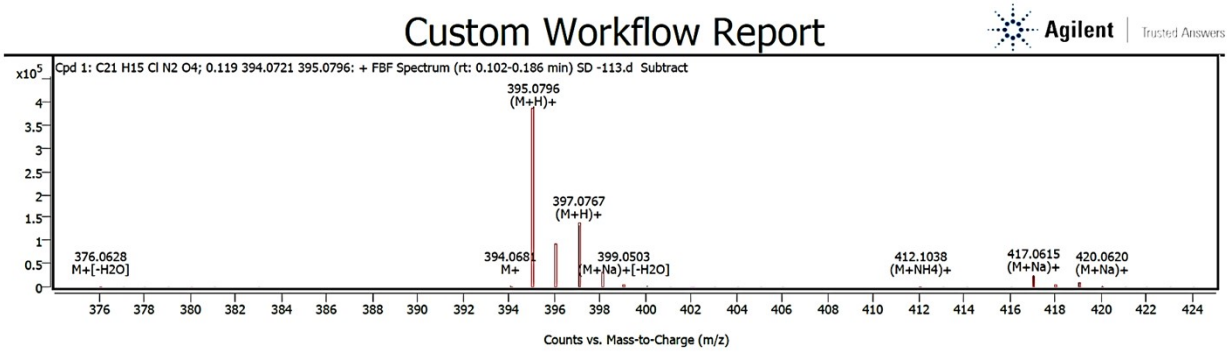


Figure **S61**: HRMS of Compound **4n**.

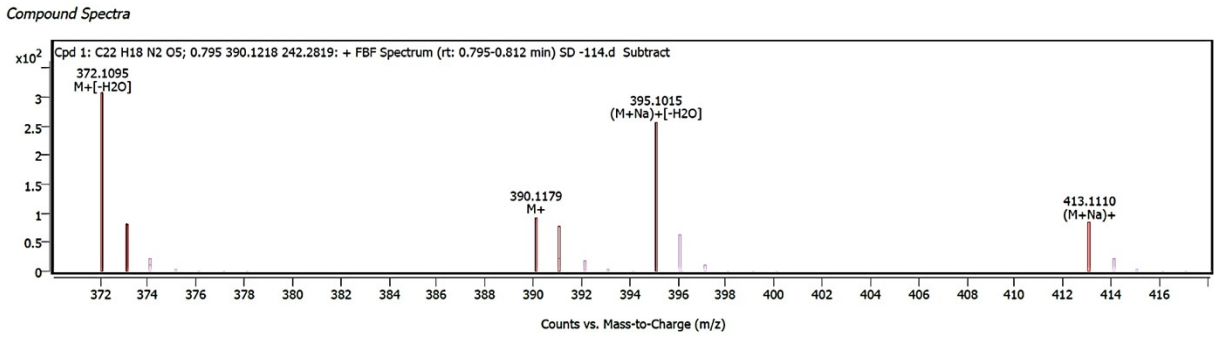

Figure **S62**: HRMS of Compound **4o**.

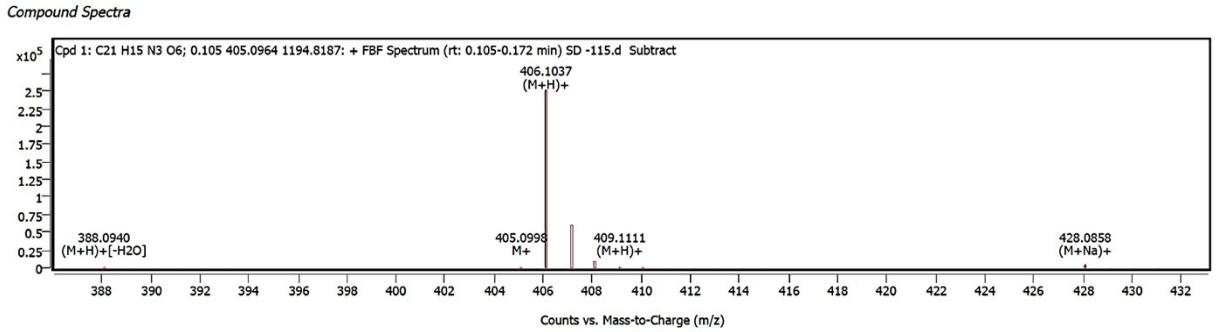


Figure **S63**: HRMS of Compound **4p**.

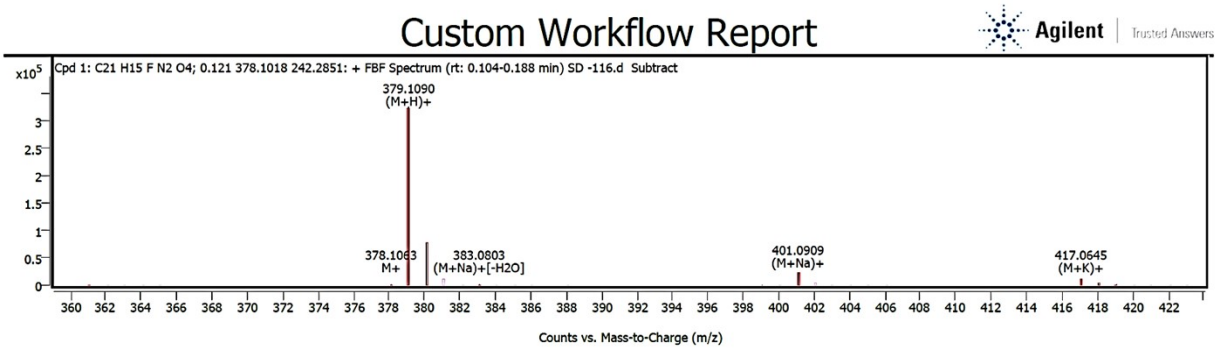


Figure **S64**: HRMS of Compound **4q**.

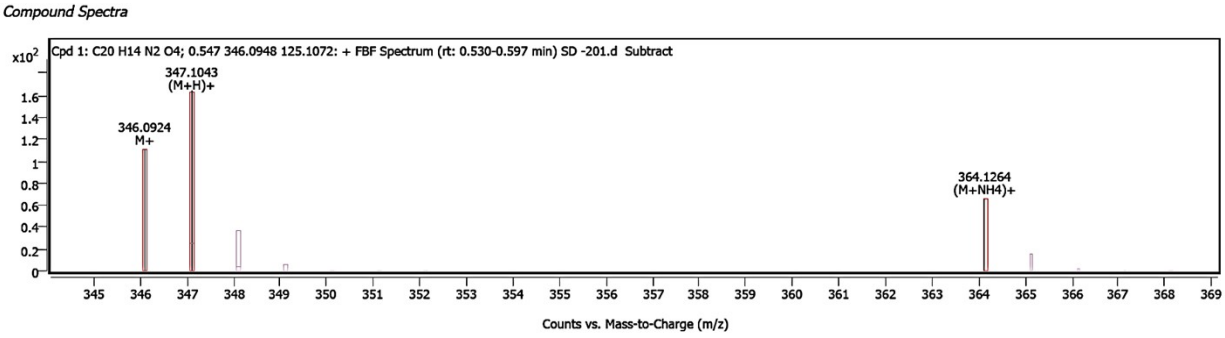


Figure **S65**: HRMS of Compound **4r**.

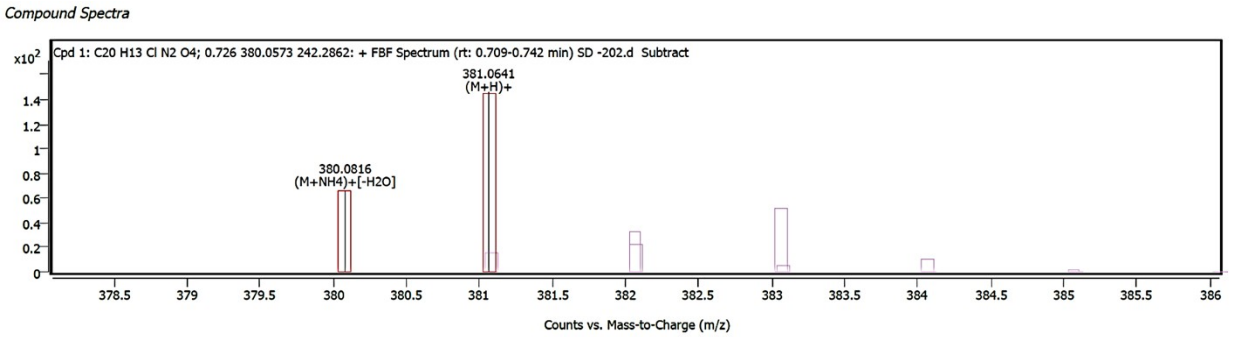

Figure **S66**: HRMS of Compound **4s**.

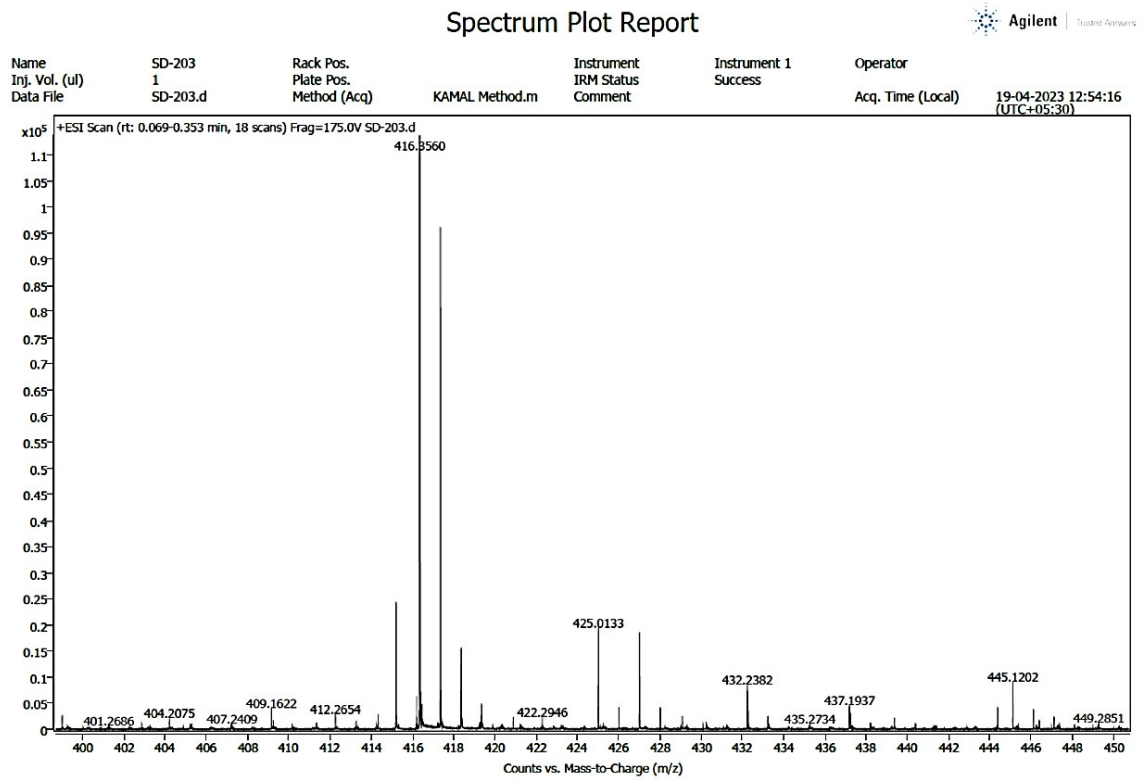


Figure **S67**: HRMS of Compound **4t**.

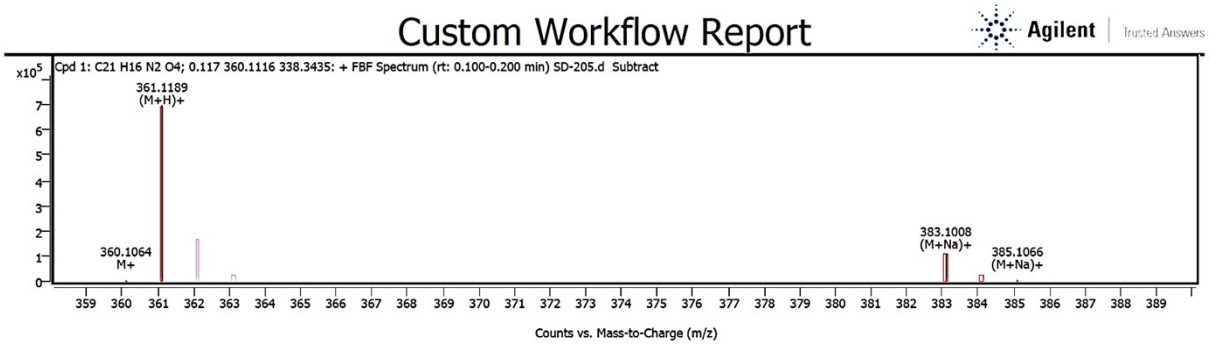


Figure **S68**: HRMS of Compound **4u**.

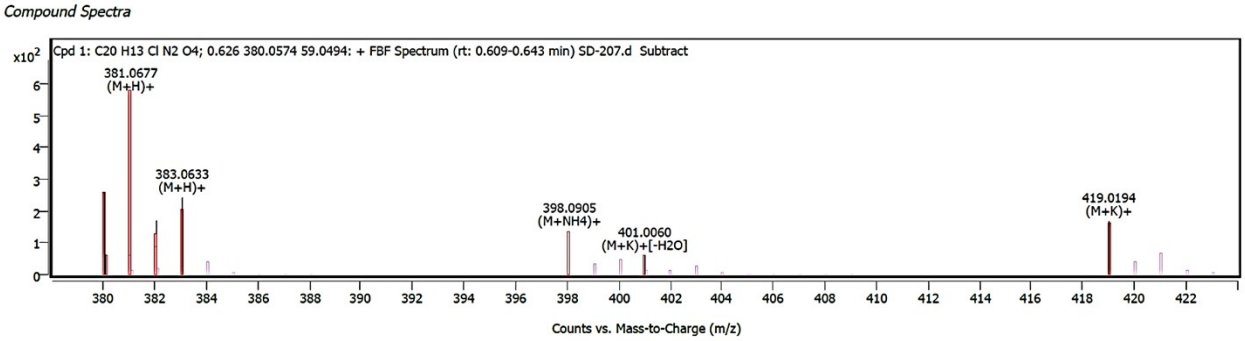

Figure **S69**: HRMS of Compound **4v**.

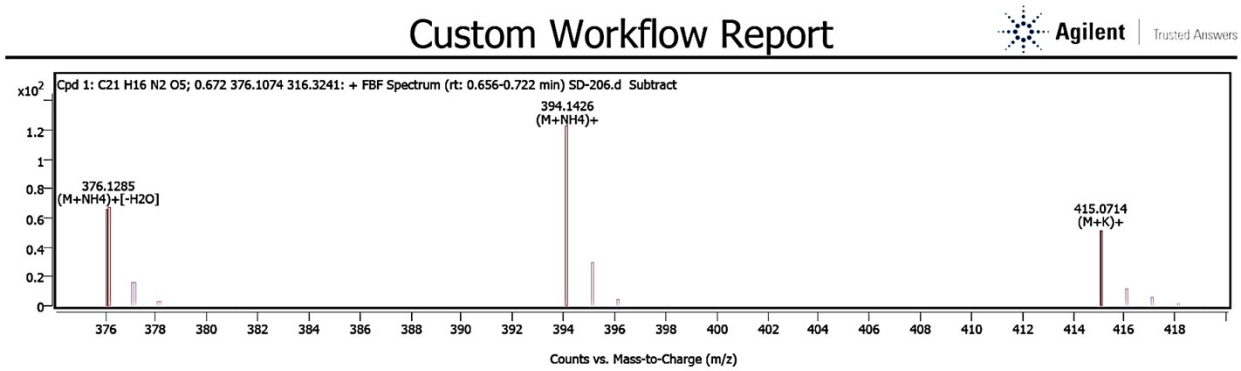


Figure **S70**: HRMS of Compound **4w**.

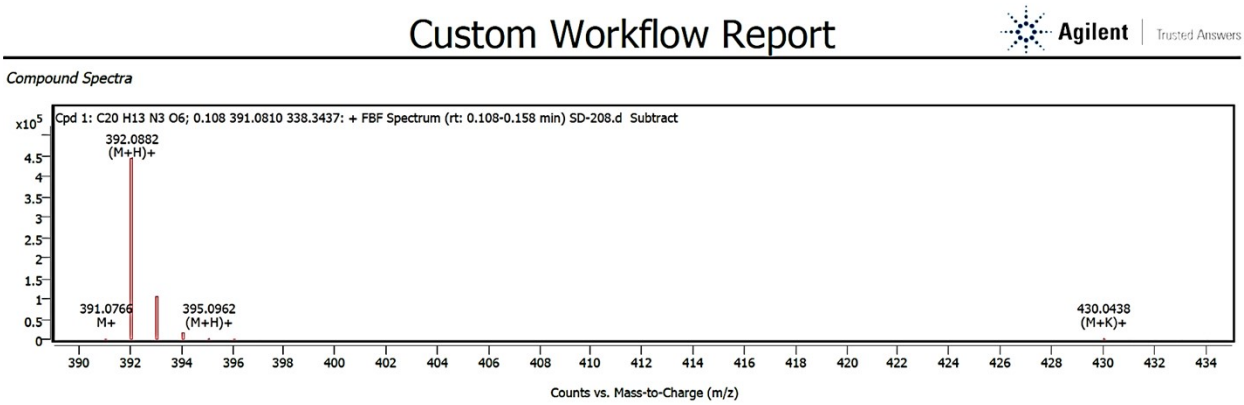


Figure **S71**: HRMS of Compound **4x**.

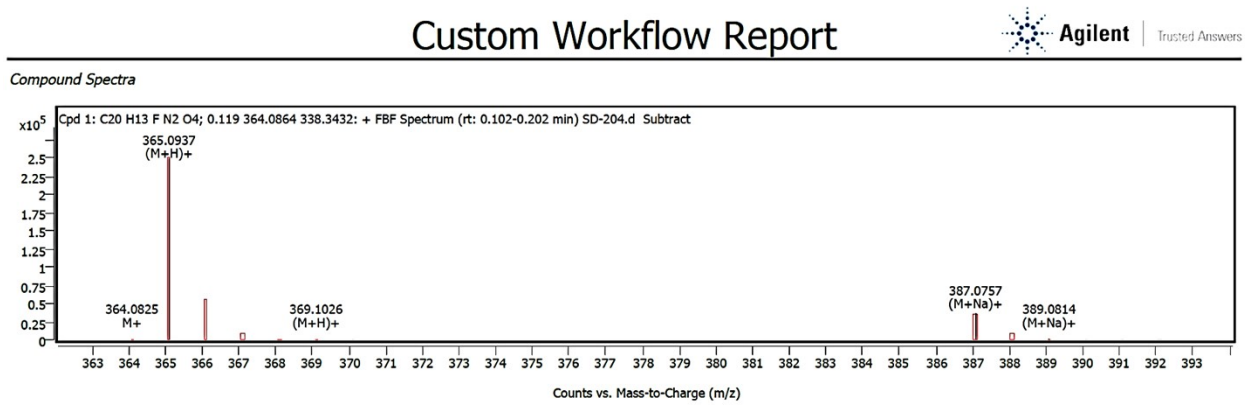

**Table S1** ADMET properties of Compound **4a** and **4v**.

| Sr. No. | Properties | **4a** | **4v** |
|---|---|---|---|
| Physicochemical properties | | | |
| 1 | Molecular weight (g/mol) | 388.42 | 376.36 |
| 2 | Number of rotational bonds | 0 | 1 |
| 3 | Number of H-bond acceptors | 4 | 5 |
| 4 | Number of H-bond donors | 2 | 2 |
| 5 | Molar Refractivity | 113.3 | 105.63 |
| 6 | Topological Polar Surface Area | 76.66 | 85.89 |
| Lipophilicity | | | |
| 7 | XLOGP3 | 2.92 | 1.70 |
| 8 | WLOGP | 2.58 | 1.56 |
| 9 | MLOGP | 2.40 | 1.44 |
| Pharmacokinetics | | | |
| 10 | Gastrointestinal absorption | High | High |
| 11 | BBB permanent | Yes | No |
| 12 | P-gp substrate | Yes | Yes |
| 13 | CYP1A2 inhibitor | Yes | No |
| 14 | CYP2C19 inhibitor | Yes | Yes |
| 15 | CYP2C9 inhibitor | Yes | Yes |
| 16 | CYP2D6 inhibitor | Yes | Yes |
| 17 | CYP3A4 inhibitor | Yes | Yes |
| Drug-likeness | | | |
| 18 | Lipinski | 0 | 0 |
| 19 | Ghose | 0 | 0 |
| 20 | Veber | 0 | 0 |
| 21 | Egan | 0 | 0 |
| 22 | Muegge | 0 | 0 |
| 23 | Bioavailability Score | 0.55 | 0.55 |
| Medicinal Chemistry | | | |
| 24 | PAINS alerts | 0 | 0 |
| 25 | Brenk alerts | 0 | 0 |