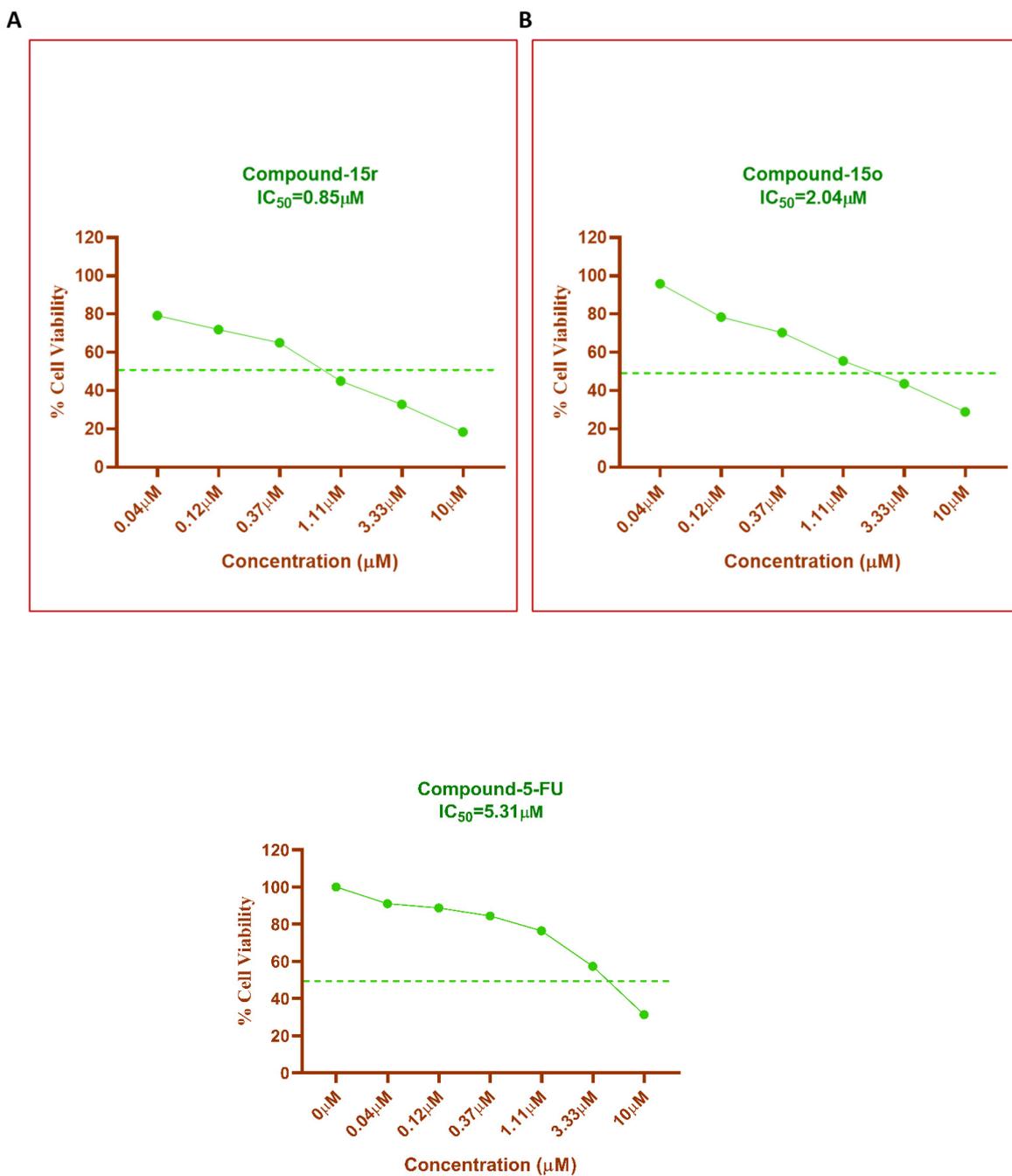
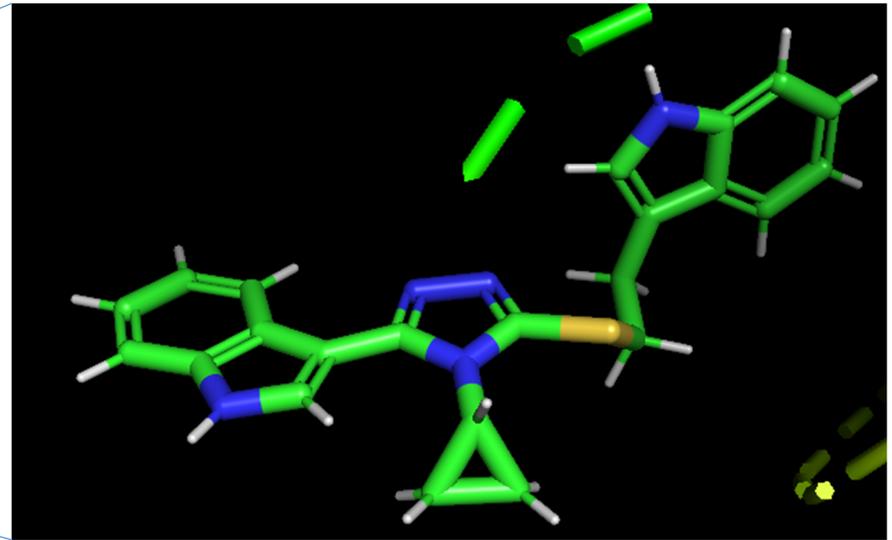
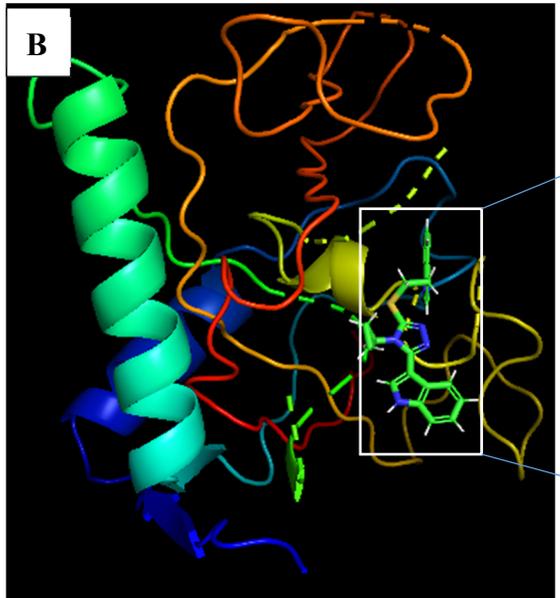
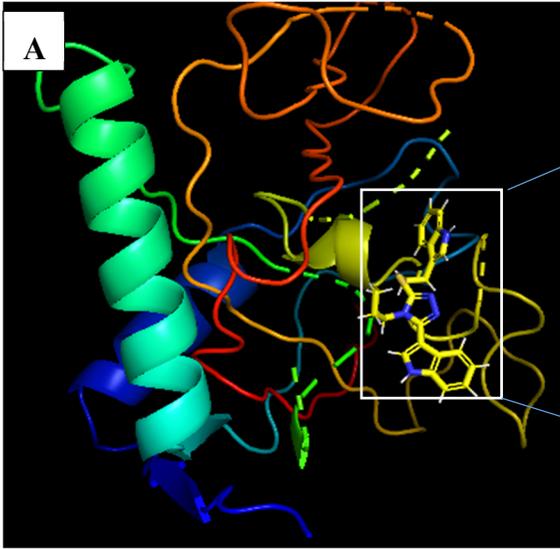


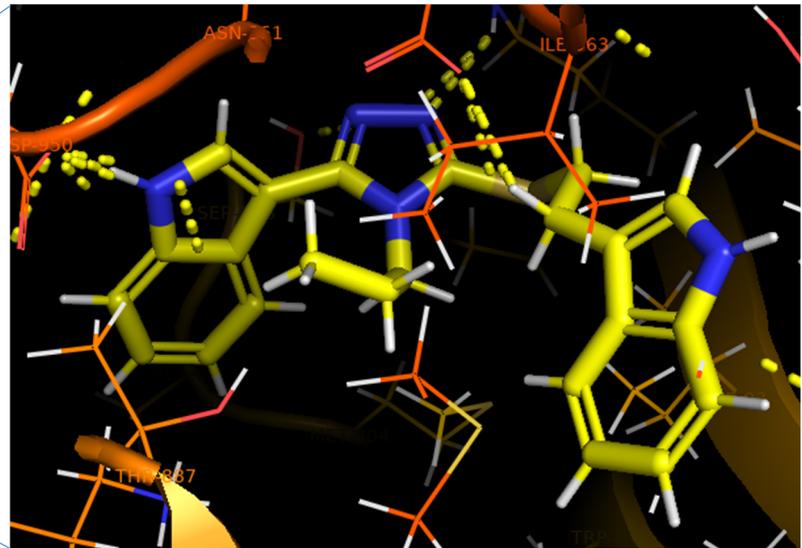
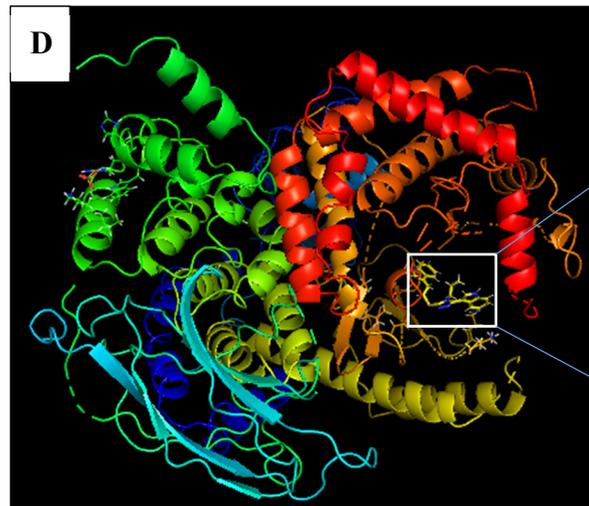
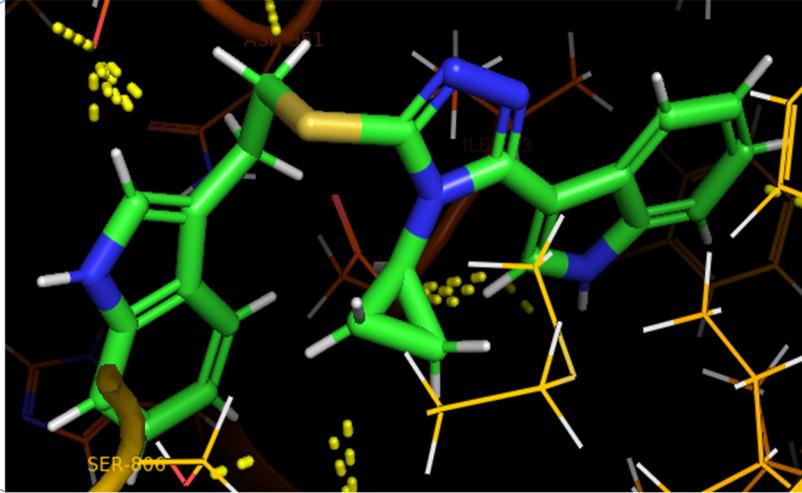
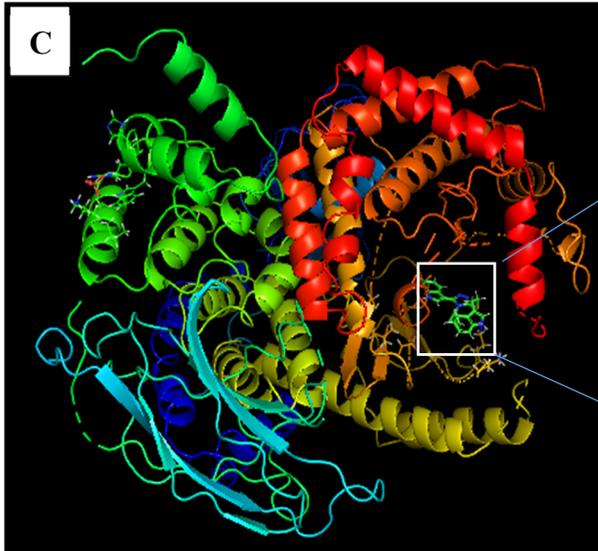
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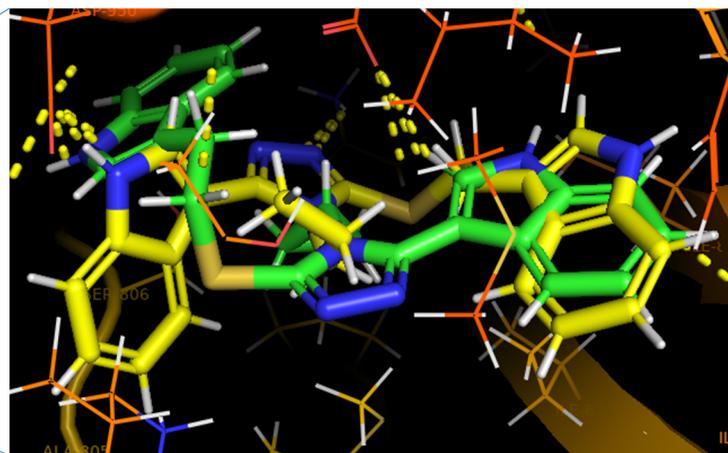
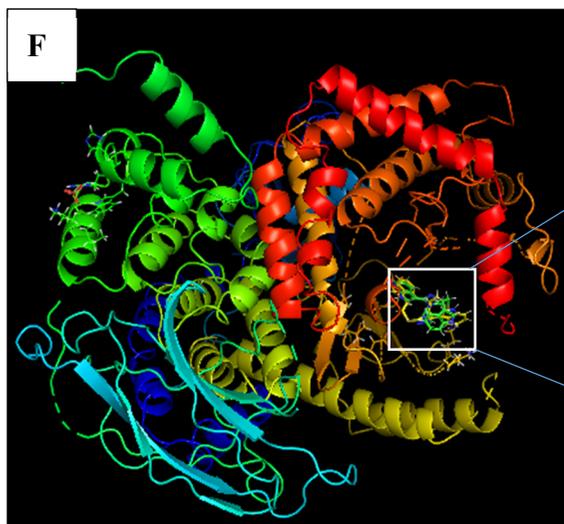
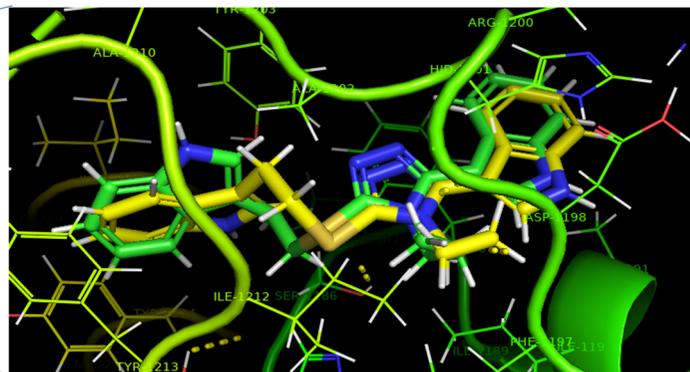
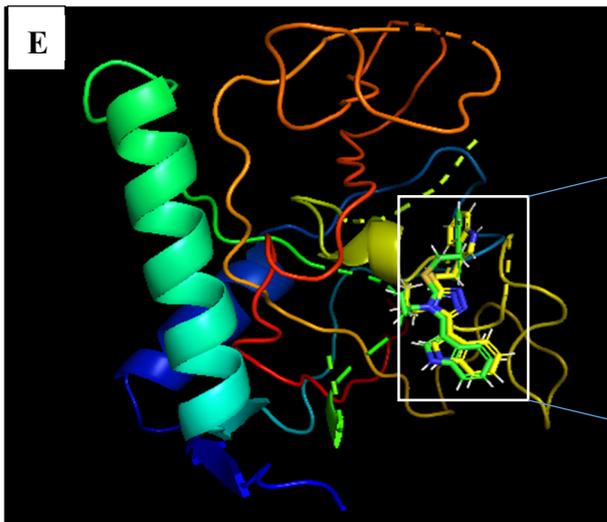
Dose response curve.....	<b>Figure S1</b>
Docking images.....	<b>Figure S2</b>
$^1\text{H}$ , $^{13}\text{C}$ NMR and Mass copies of all products .....	<b>Figure S3</b>



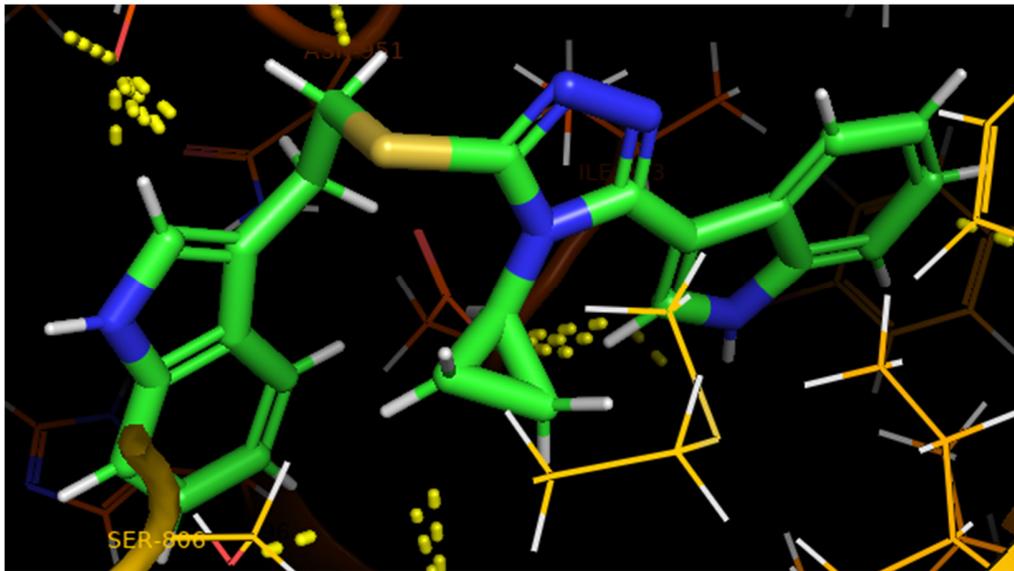
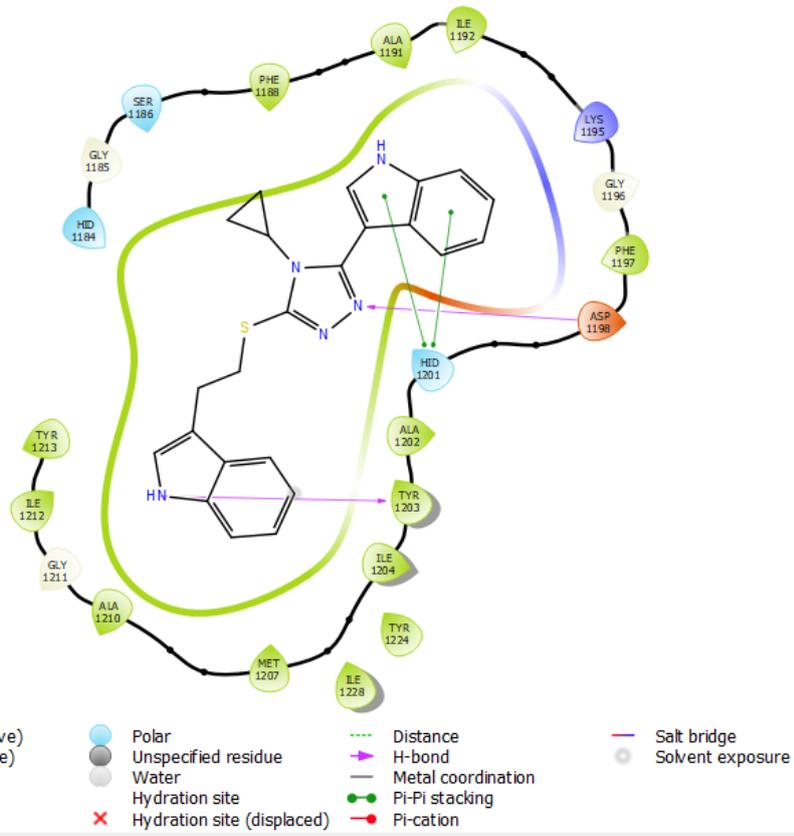
**Figure S1:** Dose Response Curves for 15r, 15o and Standard compounds against HT-29 colon cancer cell lines.



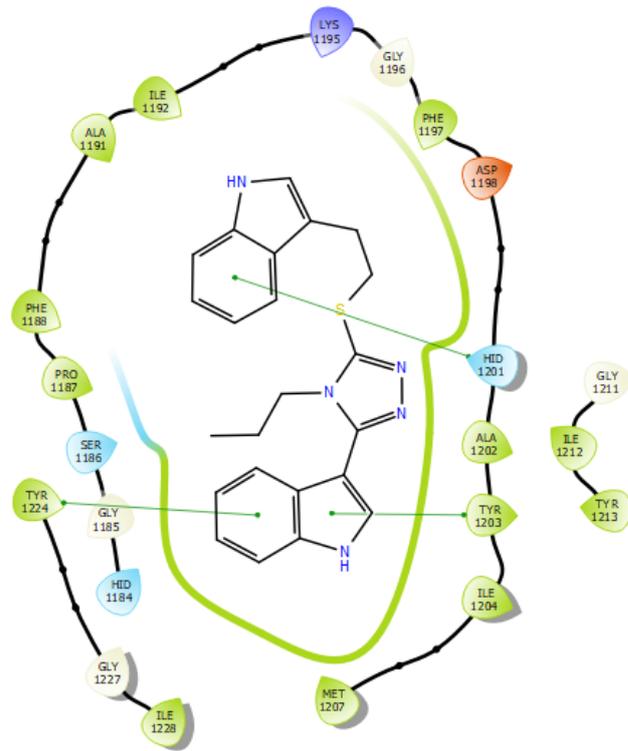




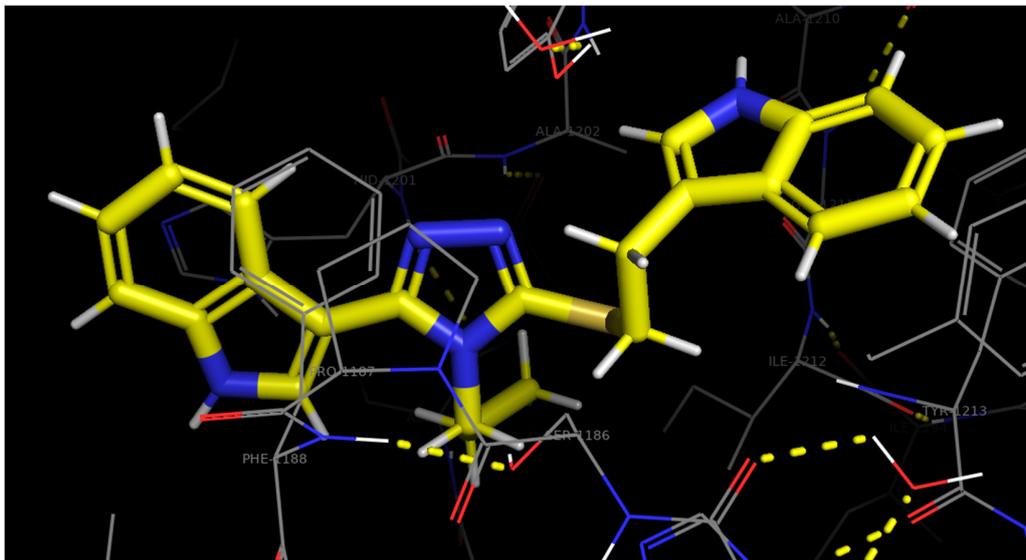
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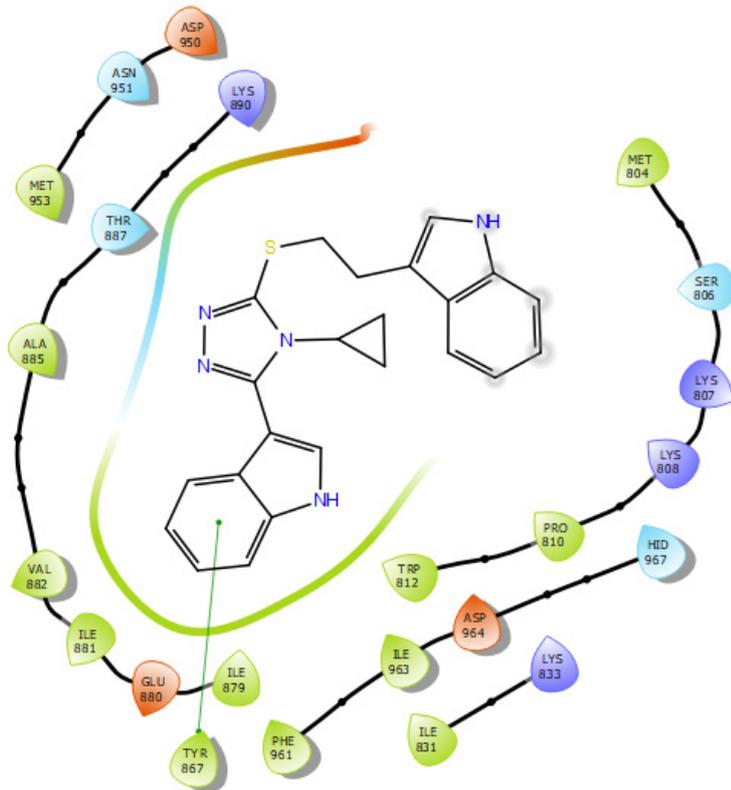
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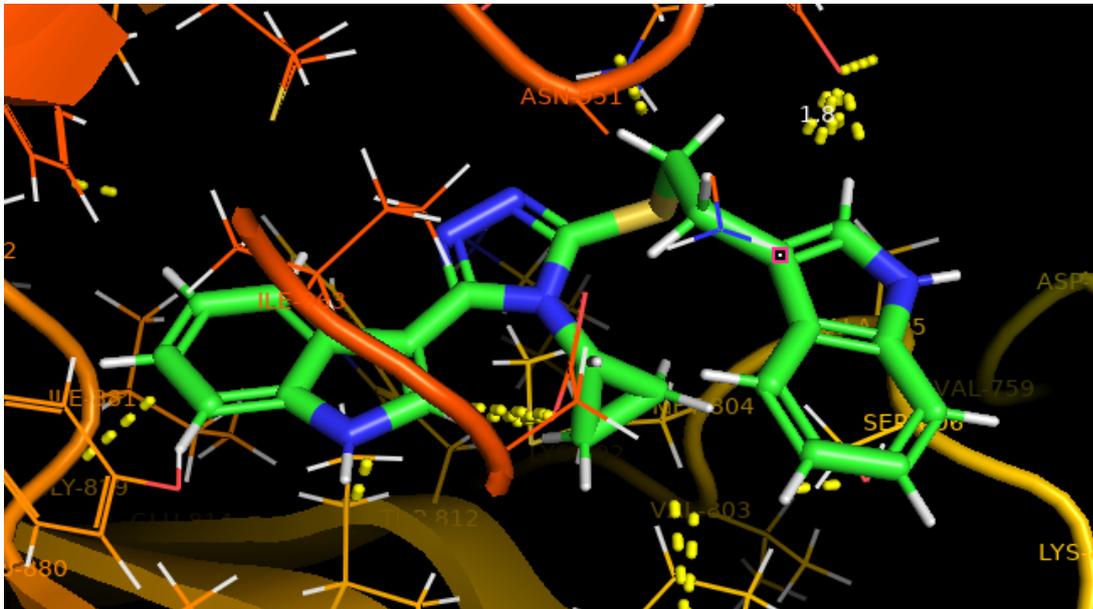
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| Glycine            | Water                      | Metal coordination |                  |
| Hydrophobic        | Hydration site             | Pi-Pi stacking     |                  |
| Metal              | Hydration site (displaced) | Pi-cation          |                  |



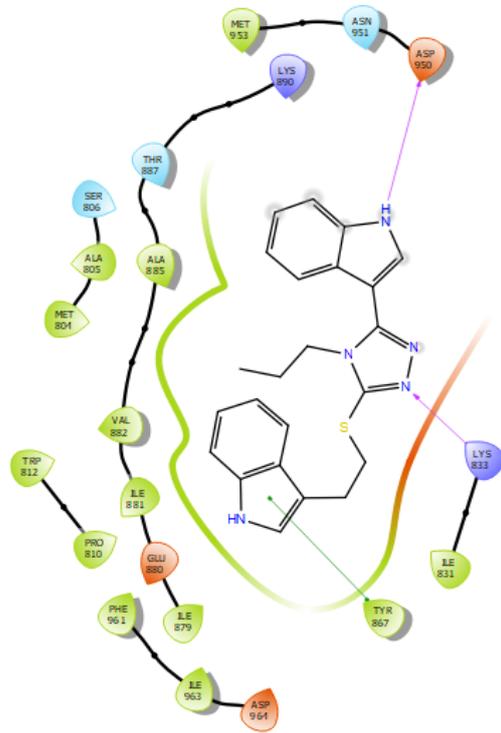
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- |  |   |  |  |
|--|---|--|--|
| <span style="color: orange;">●</span> Charged (negative) | <span style="color: lightblue;">●</span> Polar                | <span style="color: green;">---</span> Distance          | <span style="color: purple;">—</span> Salt bridge    |
| <span style="color: blue;">●</span> Charged (positive)   | <span style="color: grey;">●</span> Unspecified residue       | <span style="color: purple;">—</span> H-bond             | <span style="color: grey;">○</span> Solvent exposure |
| <span style="color: lightgreen;">●</span> Glycine        | <span style="color: grey;">●</span> Water                     | <span style="color: purple;">—</span> Metal coordination |  |
| <span style="color: green;">●</span> Hydrophobic         | <span style="color: grey;">●</span> Hydration site            | <span style="color: green;">●</span> Pi-Pi stacking      |  |
| <span style="color: grey;">●</span> Metal                | <span style="color: red;">×</span> Hydration site (displaced) | <span style="color: red;">●</span> Pi-cation             |  |



J

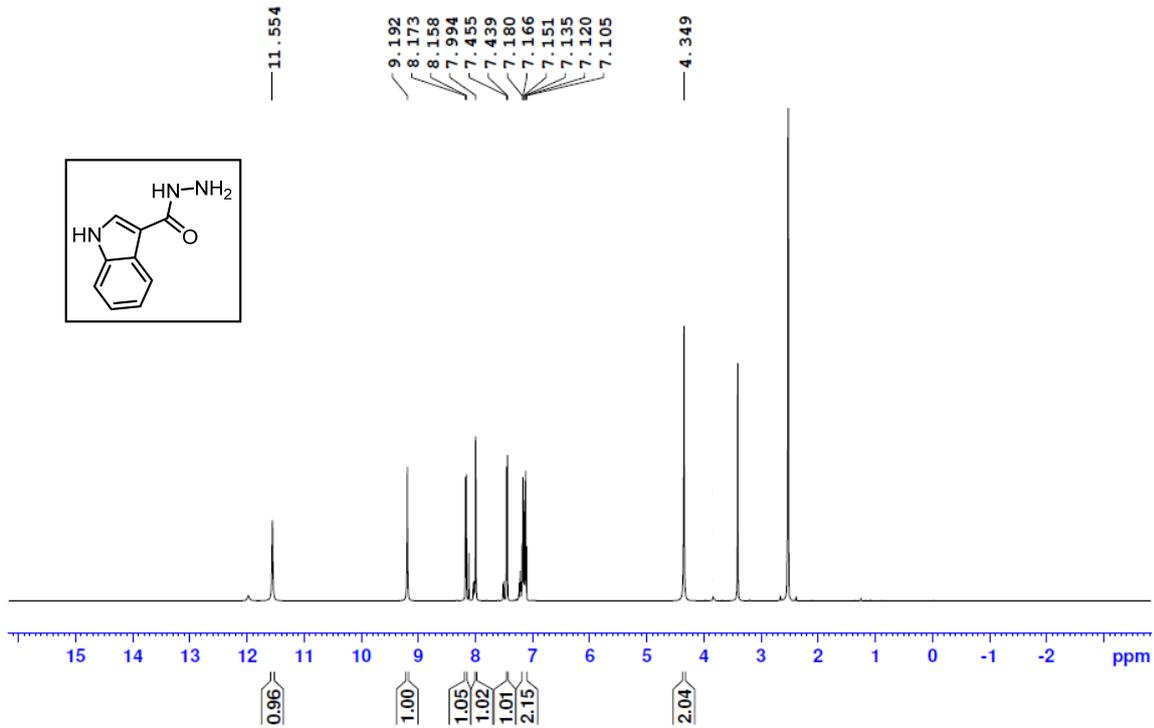


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| Charged (positive) | Unspecified residue        | H-bond             | Solvent exposure |
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| Hydrophobic        | Hydration site (displaced) | Pi-Pi stacking     |                  |
| Metal              |                            | Pi-cation          |                  |

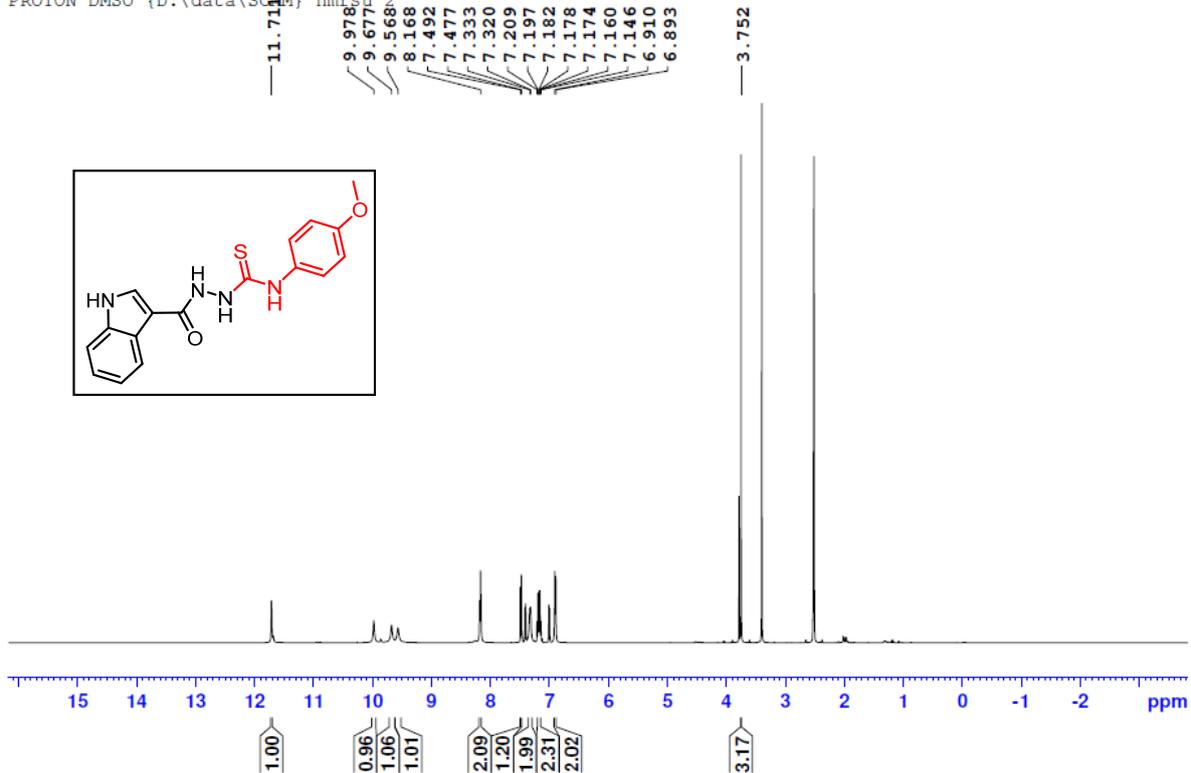


**Figure S2.** (A) Docking pose of 15o in PDB ID 4OA7 is shown in a 3D structure; (B) Docking pose of 15r in PDB ID 4OA7 is shown in a 3D structure. (C) Docking pose of 15r in PDB ID 3L54 is shown in a 3D structure; (D) Docking pose of 15o in PDB ID 3L54 is shown in a 3D structure. (E) Docking pose of 15o & 15r in PDB ID 4OA7 is shown in a 3D structure; (F) Docking pose of 15o & 15r in PDB ID 3L54 is shown in a 3D structure. (G) Docking pose of **15r** in PDB ID 4OA7 is shown in a 2D structure where indole NH bind with TYR 1203 *via* H-bonding is represented by pink arrow line similarly triazole N was formed with ASP 1198. On the other hand, the indole was shown a Pi-Pi staking with HID 1201 represented by a green line; (H) Docking pose of **15o** in PDB ID 4OA7 are shown in a 2D structure where both indoles was shown a Pi-Pi staking with HID 1201, TYR 1203, and TYR 1224 represented by green line; (I) Docking pose of **15r** in PDB ID 3L54 is shown in a 2D structure where indole was shown Pi-Pi staking with TYR 867 represented by green line; (J) Docking pose of **15o** in PDB ID 3L54 is shown in a 2D structure where indole NH and triazole N bind with LYS 833 and ASP 950 respectively *via* H-bonding is represented by pink arrow line. On the other hand, indole was shown Pi-Pi staking with TYR 867 represented by the green line.

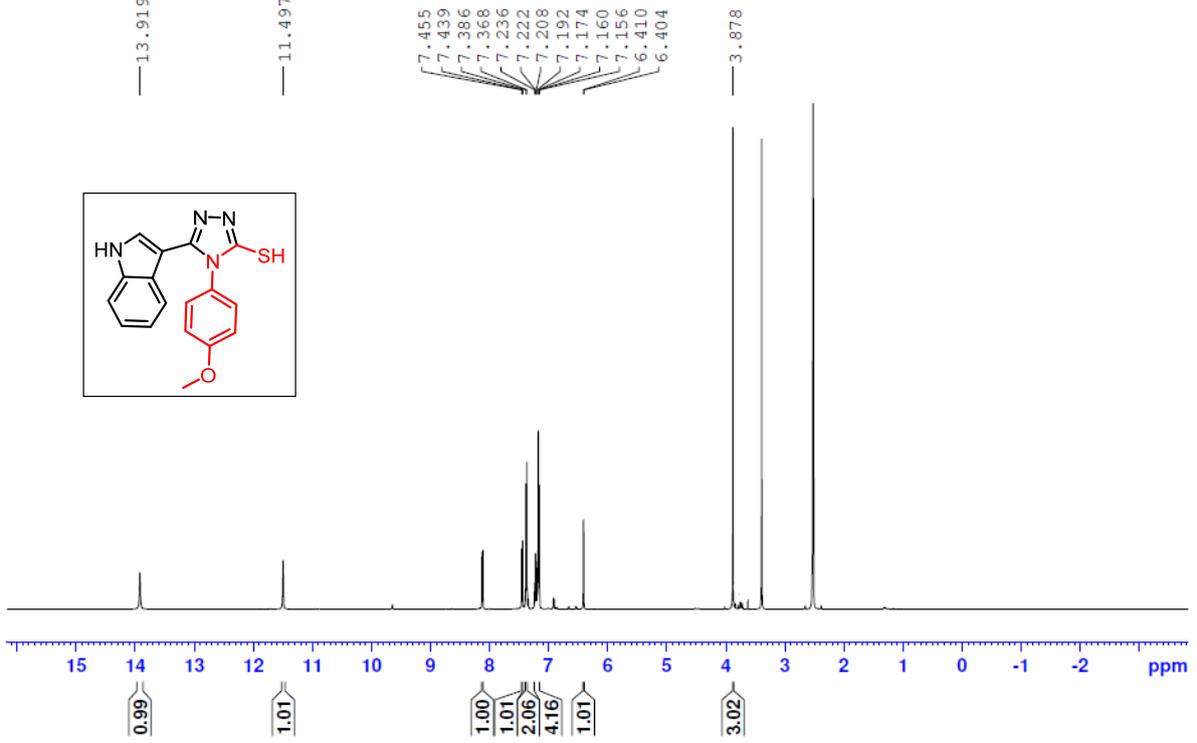
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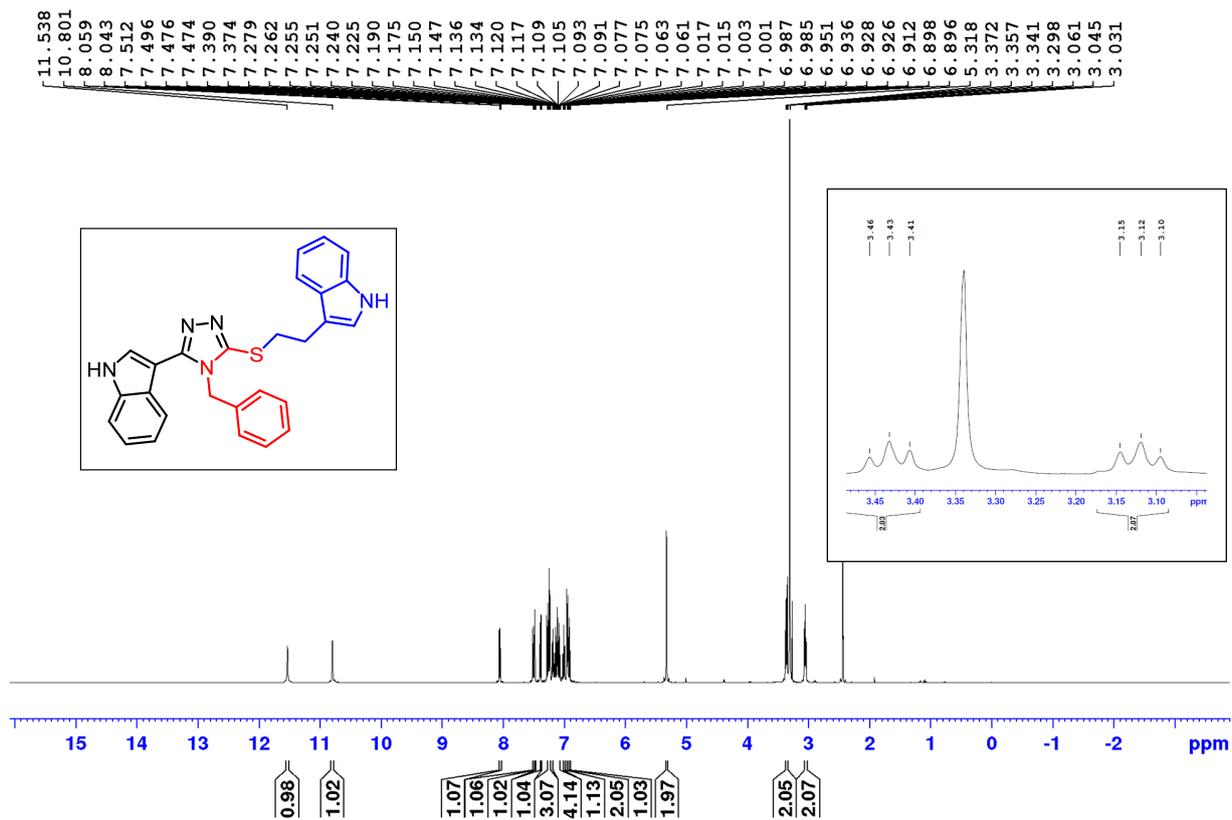


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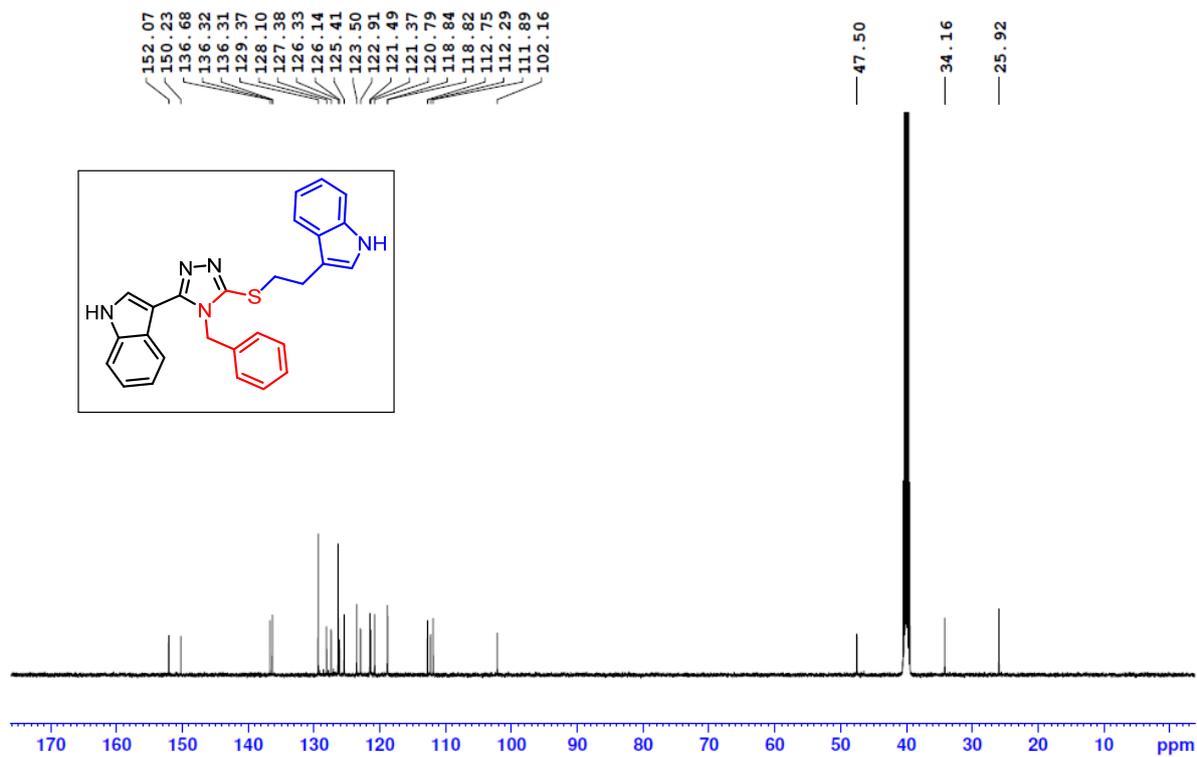


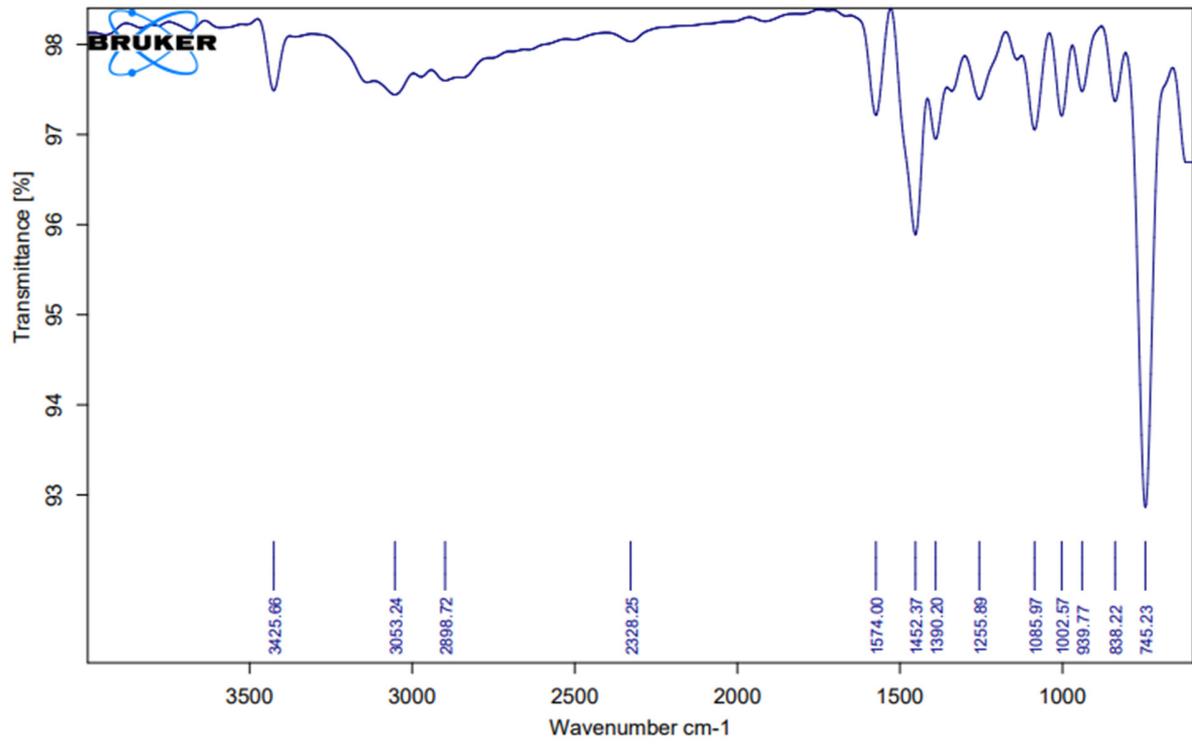
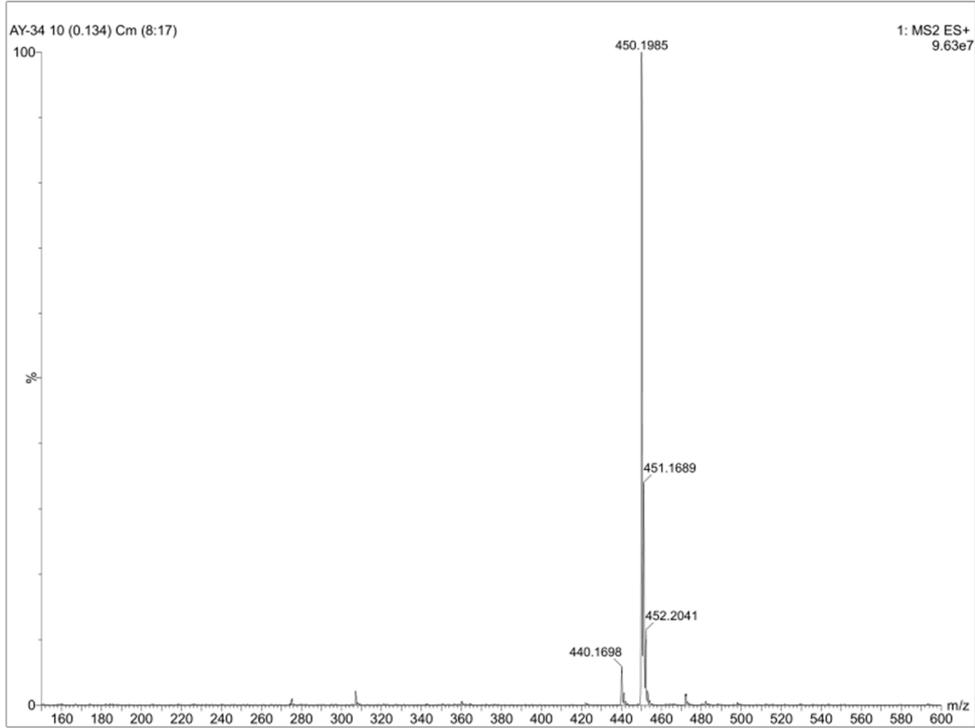
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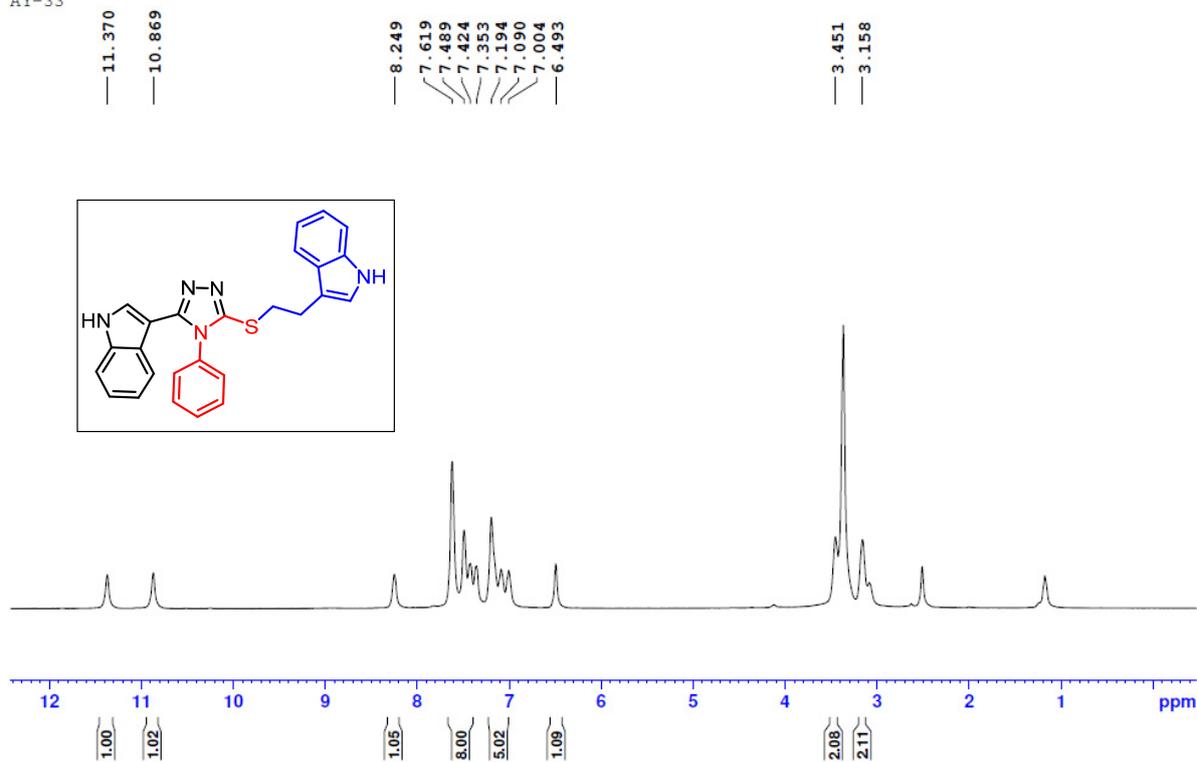
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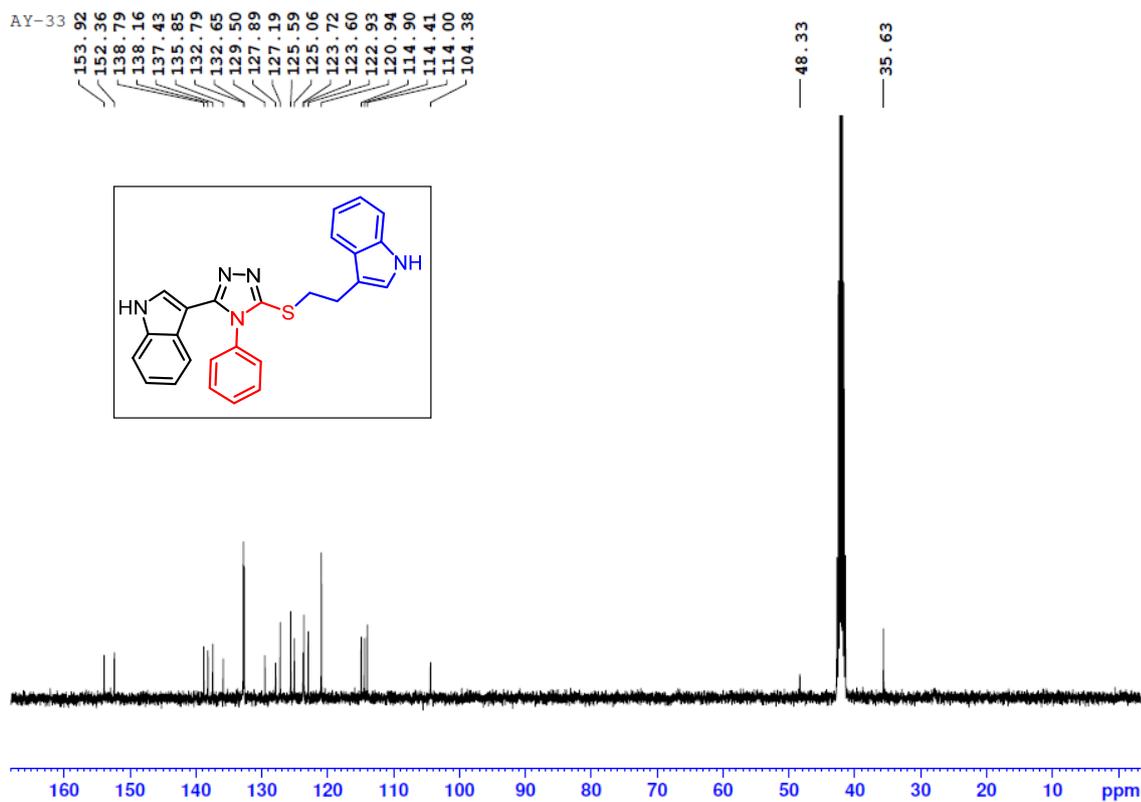


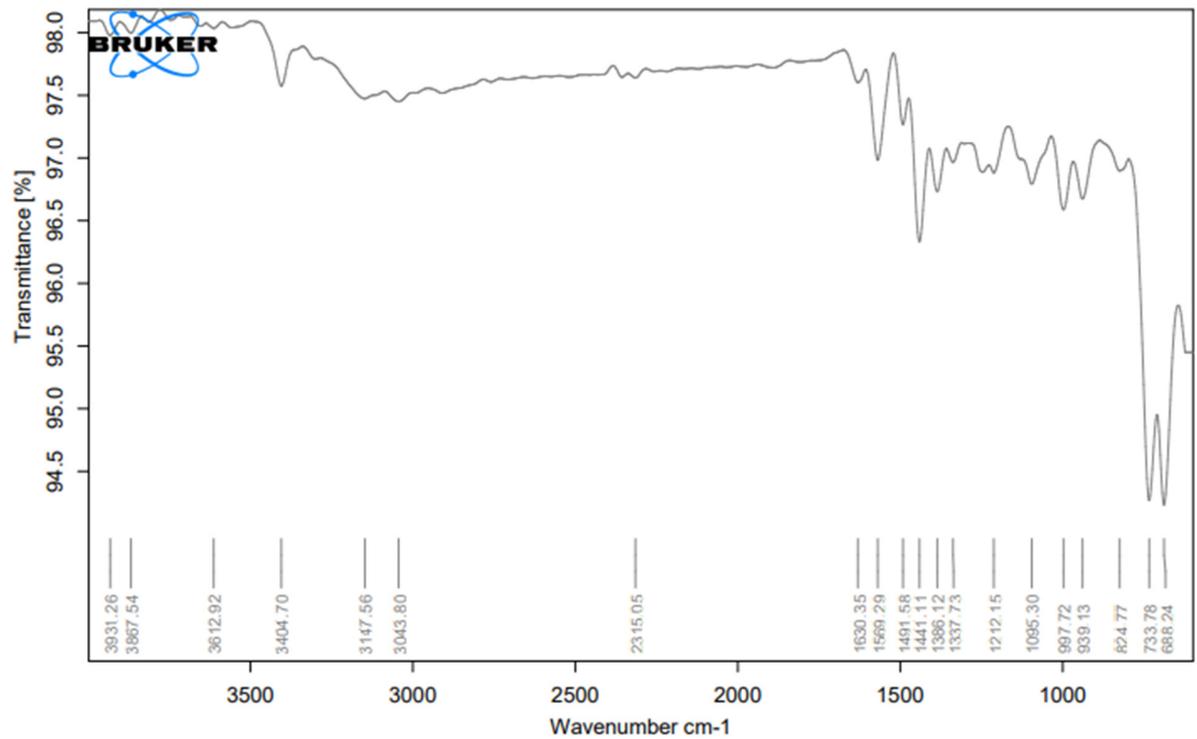
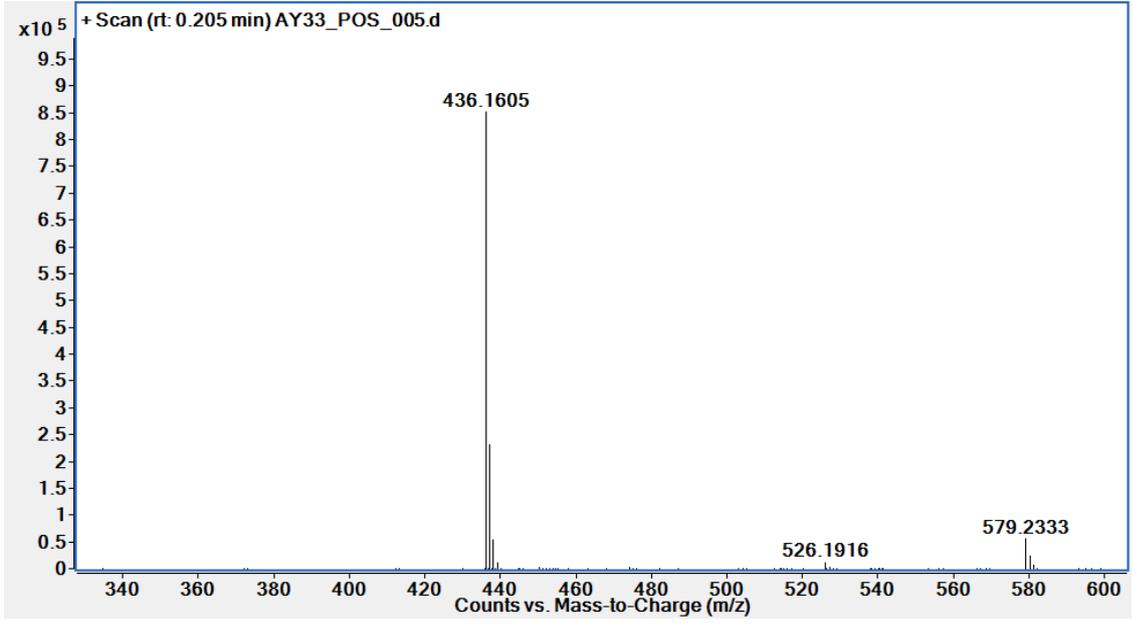
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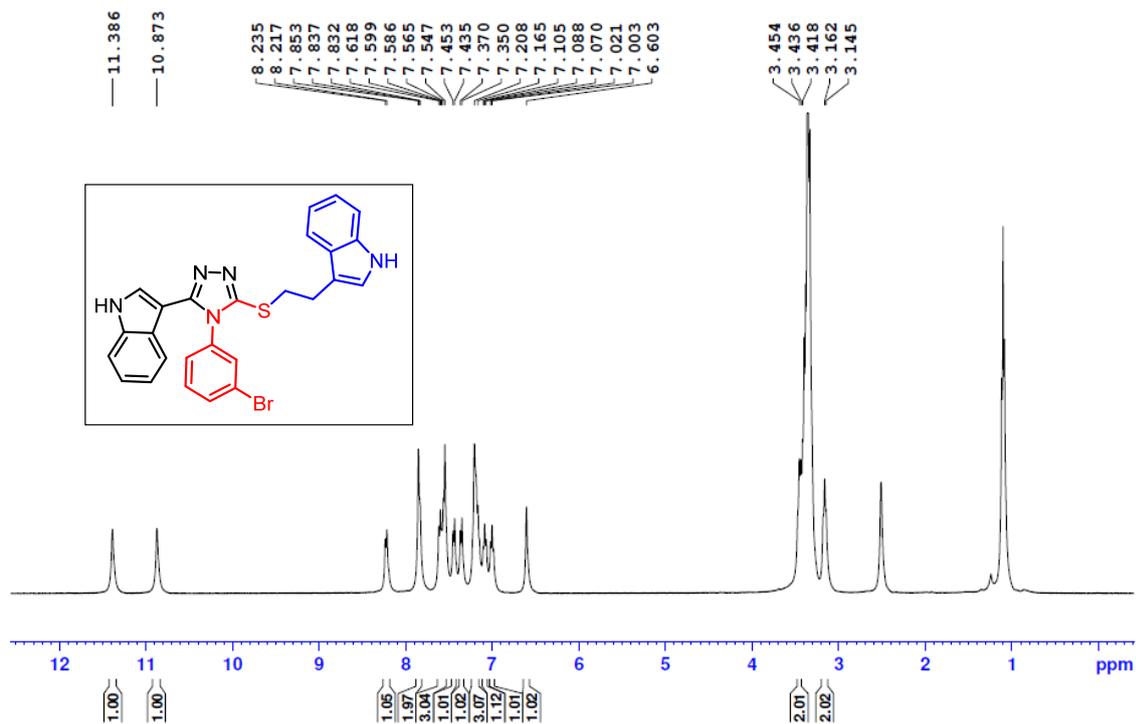
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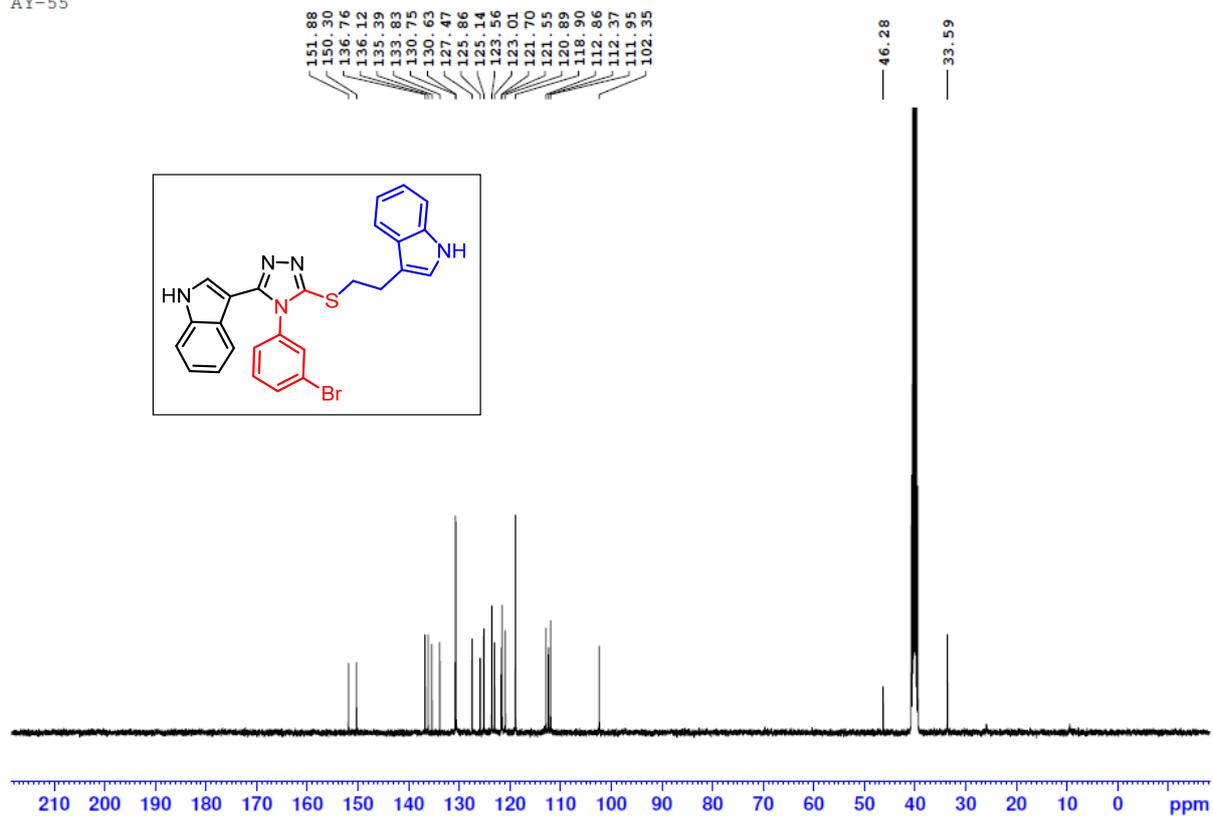


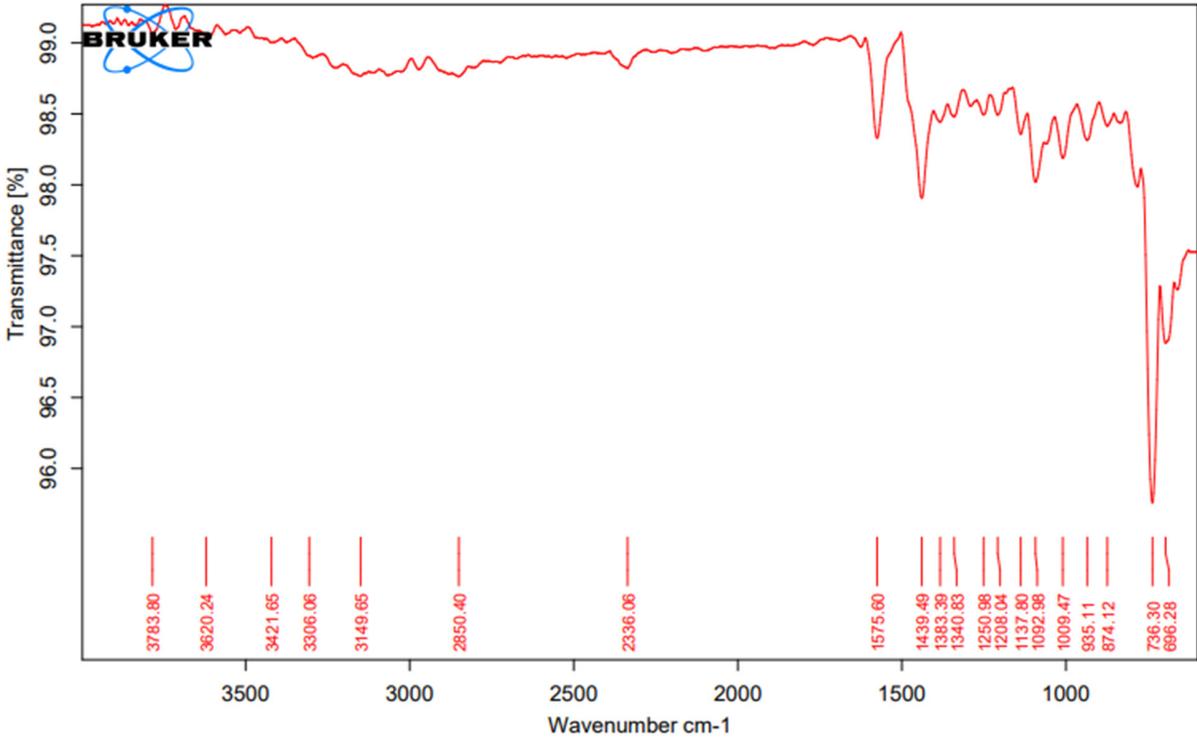
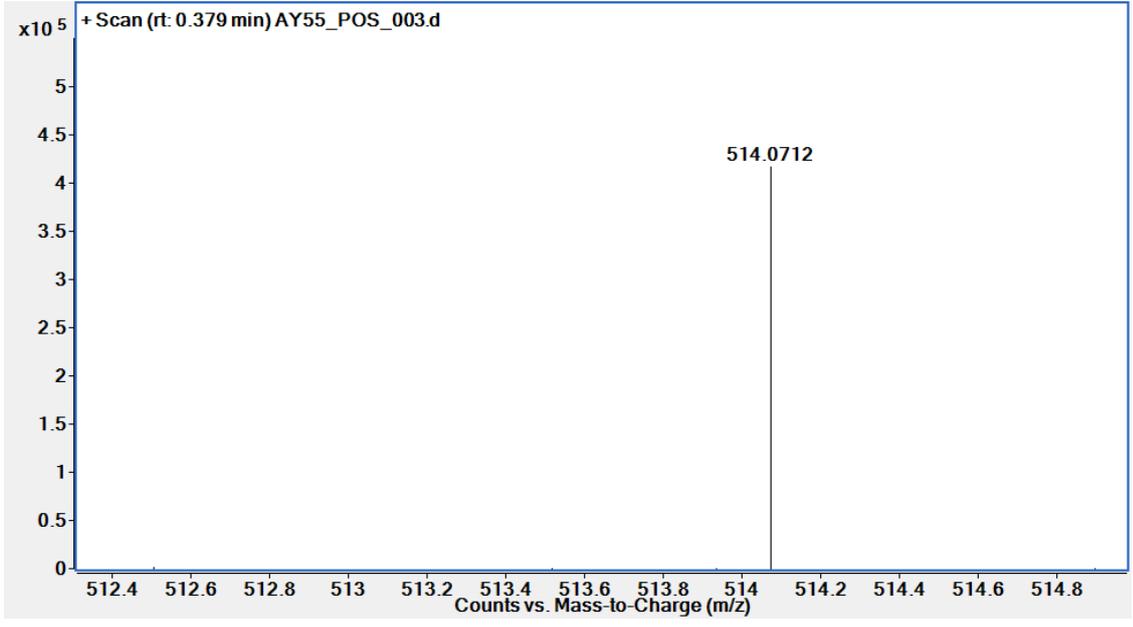
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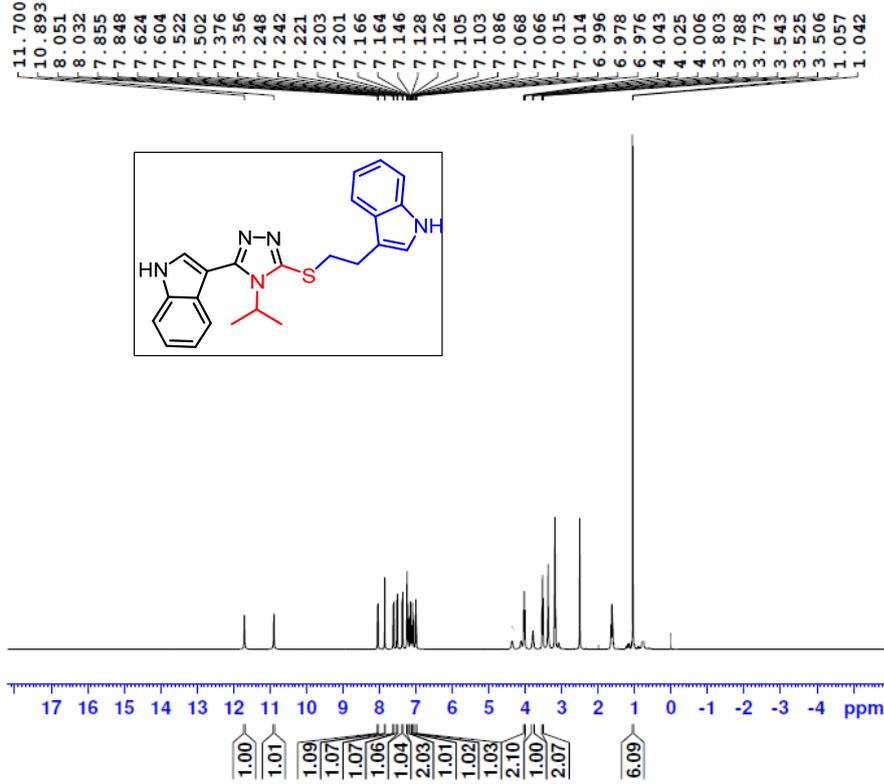
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A4-159



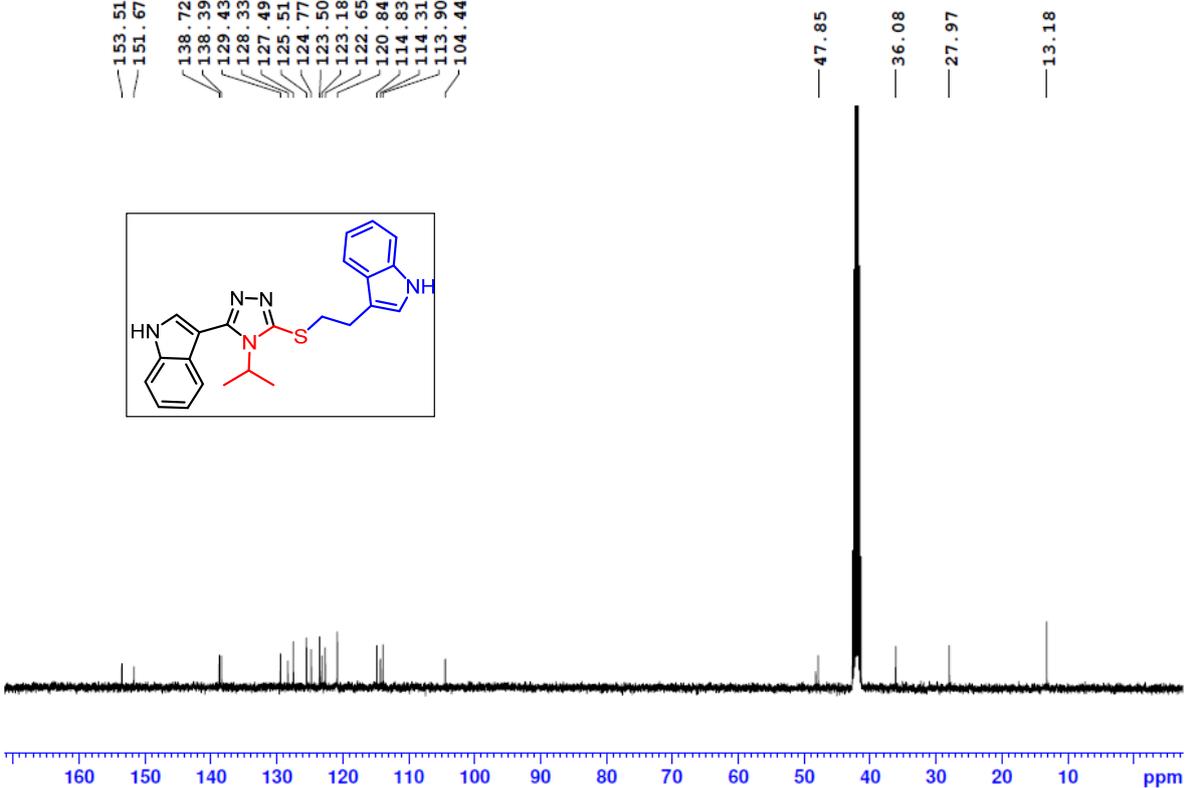
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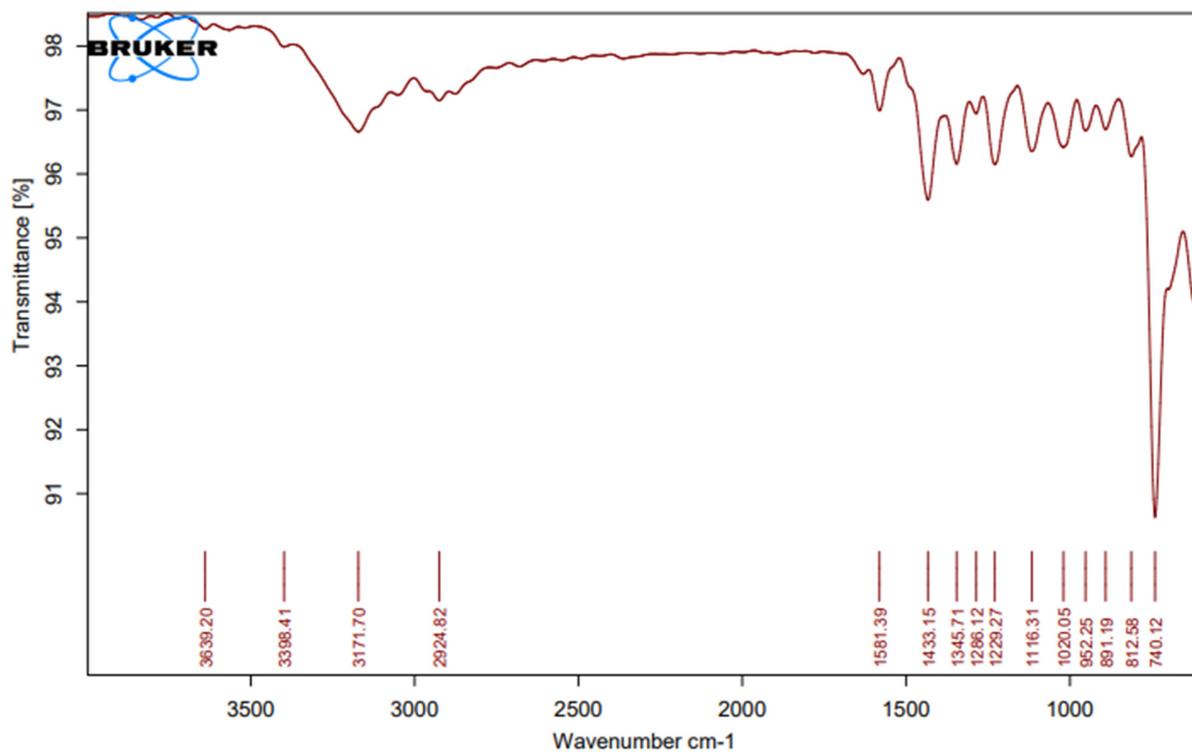
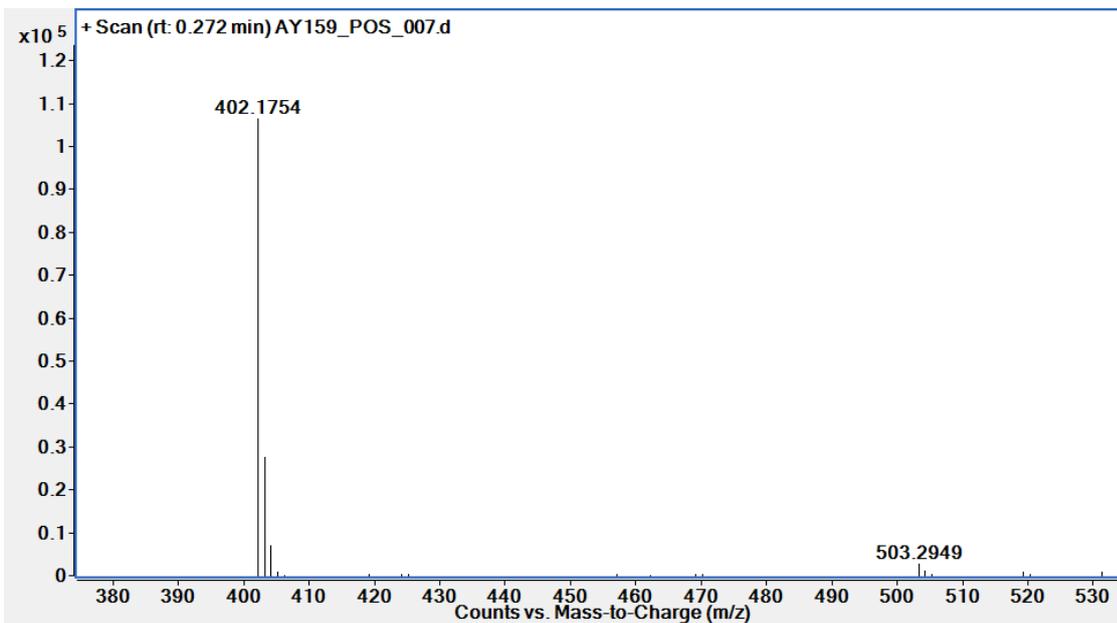
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RG 58.68  
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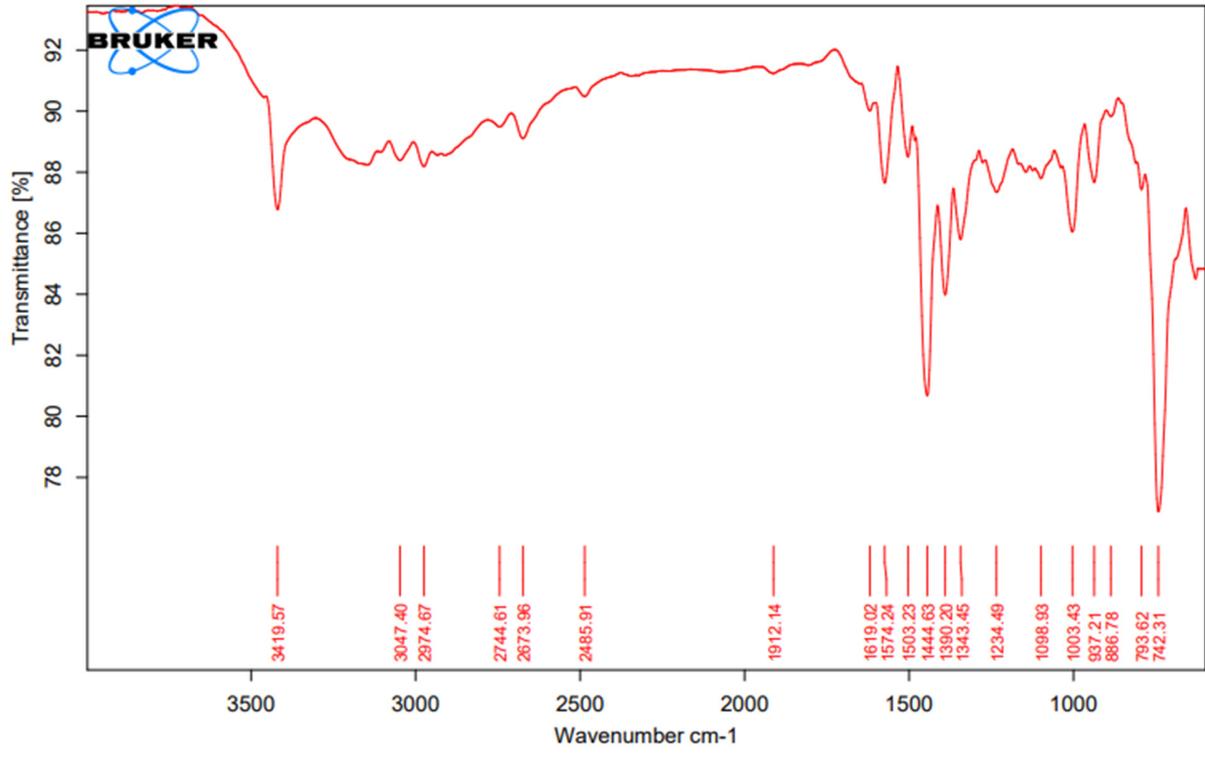
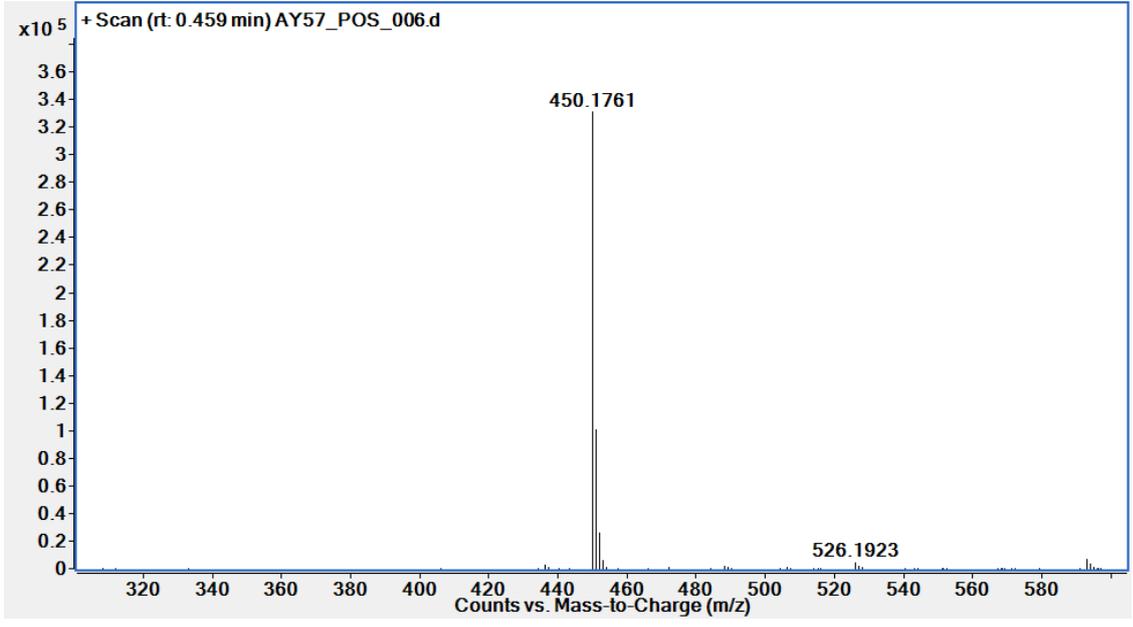
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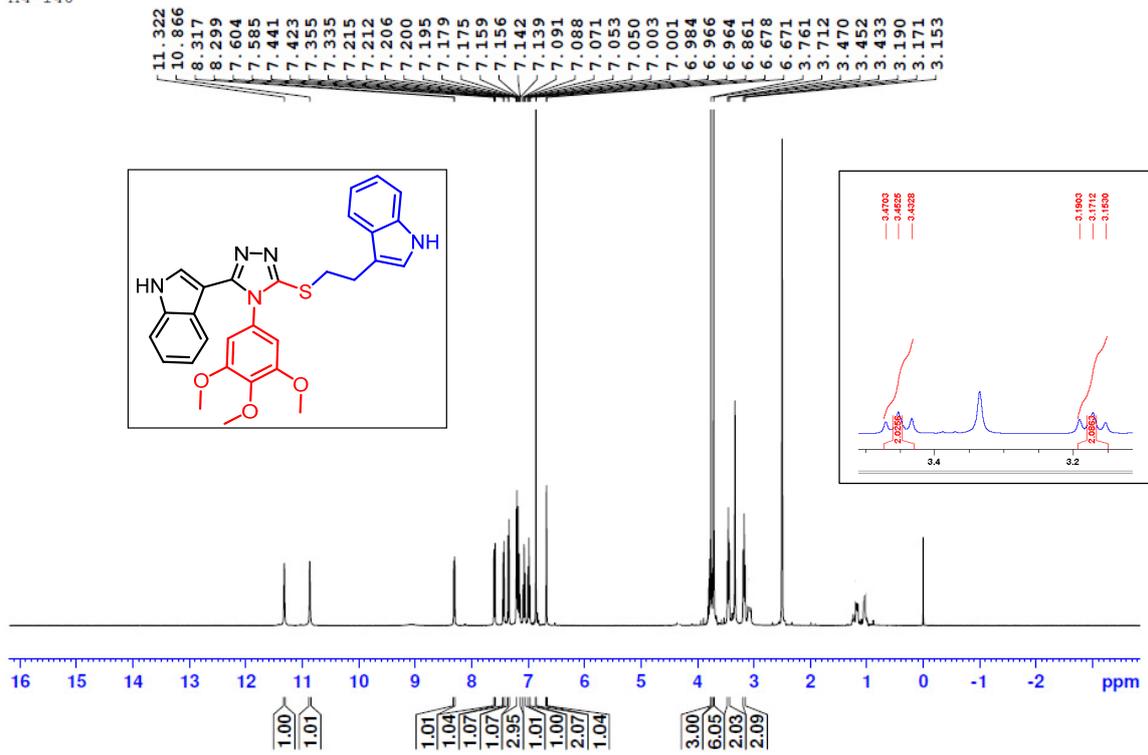
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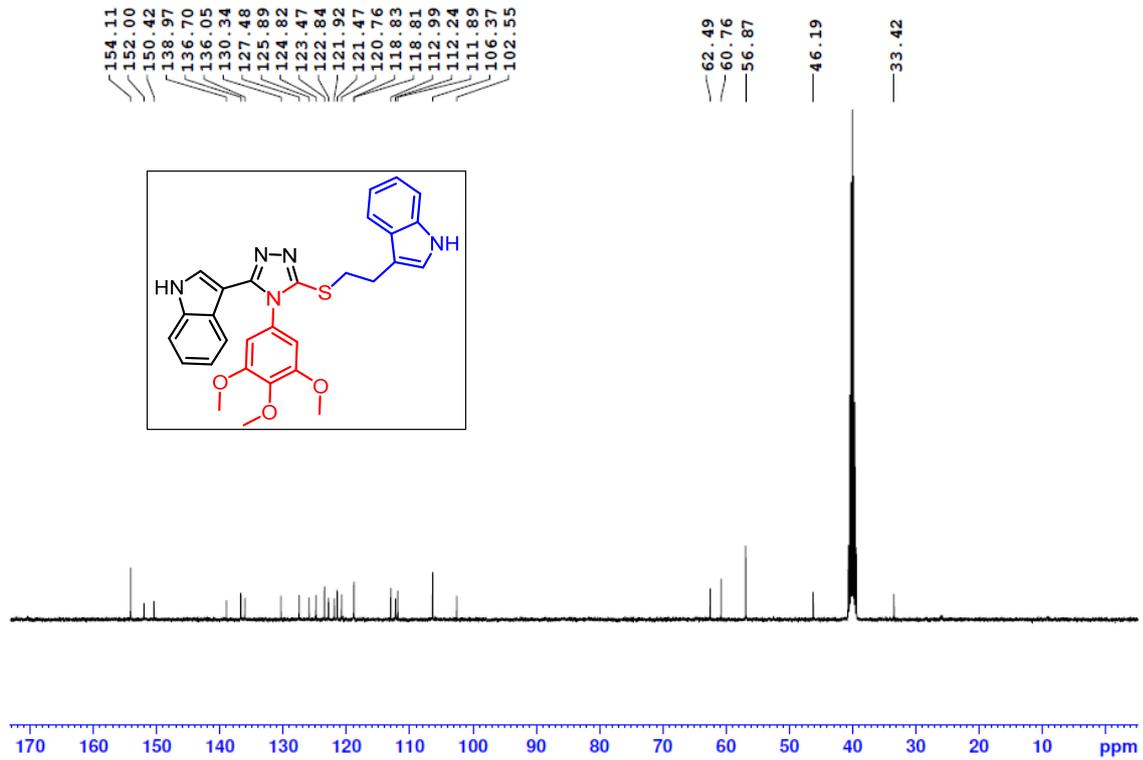


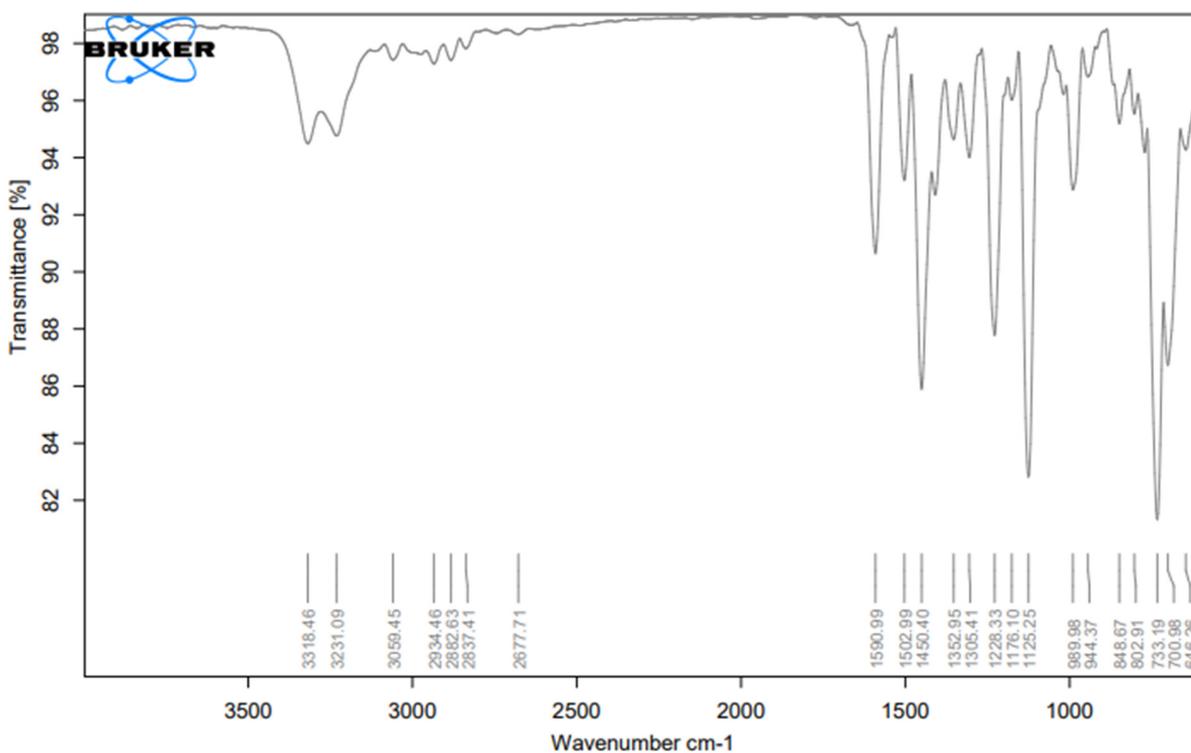
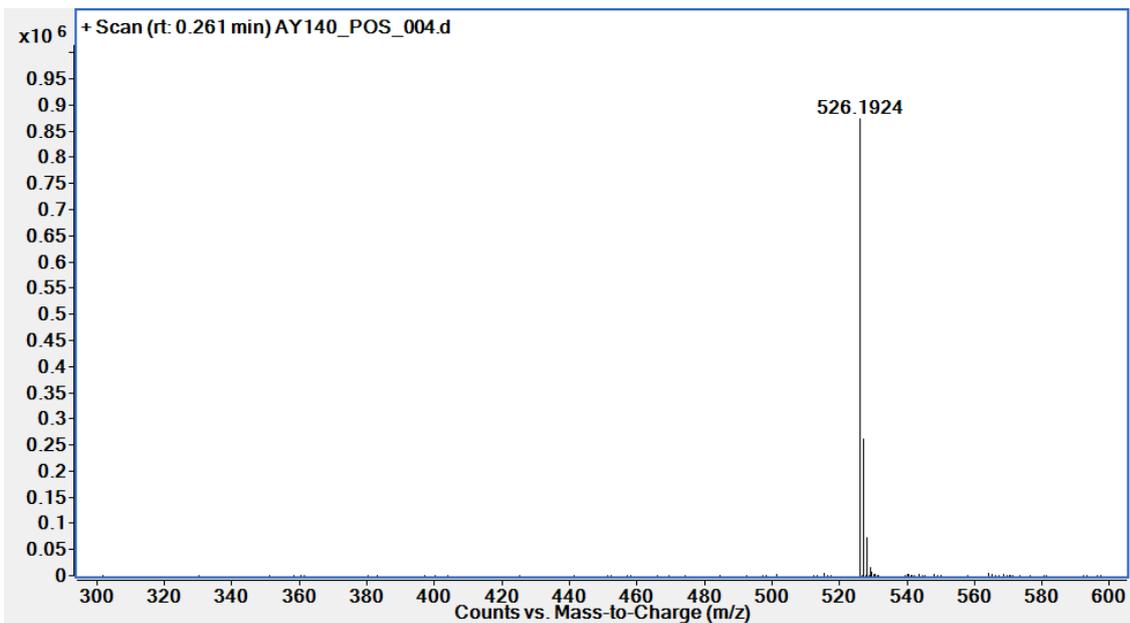
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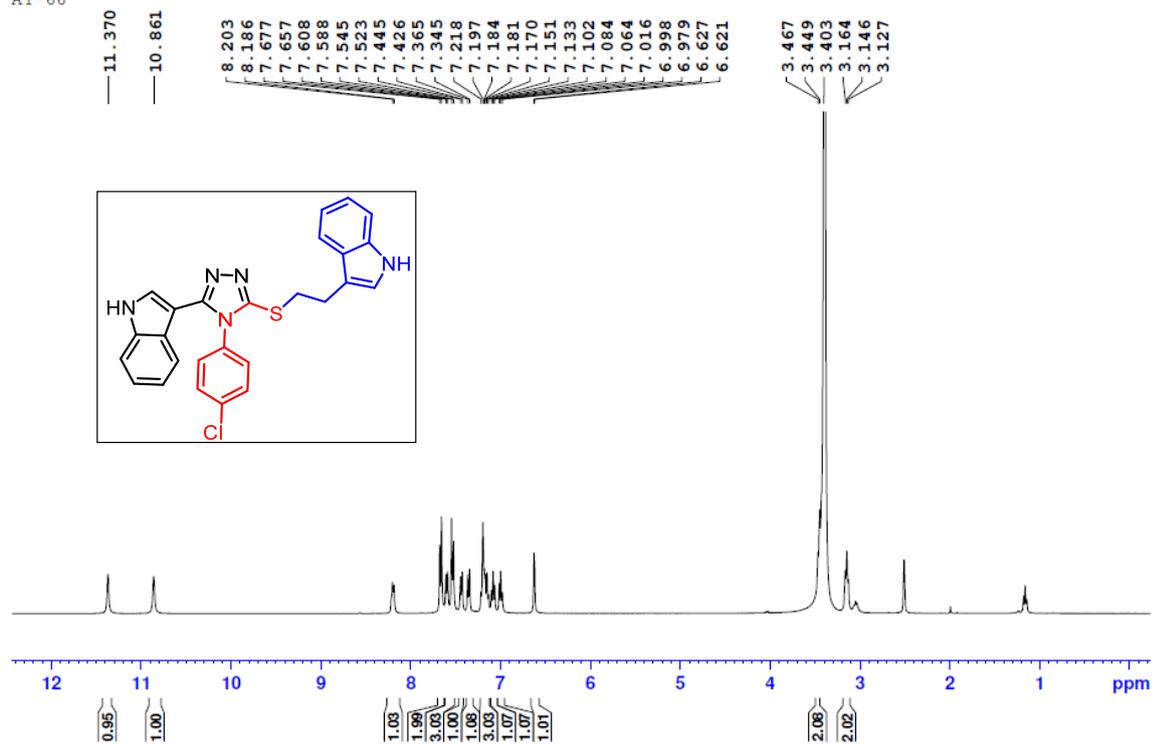
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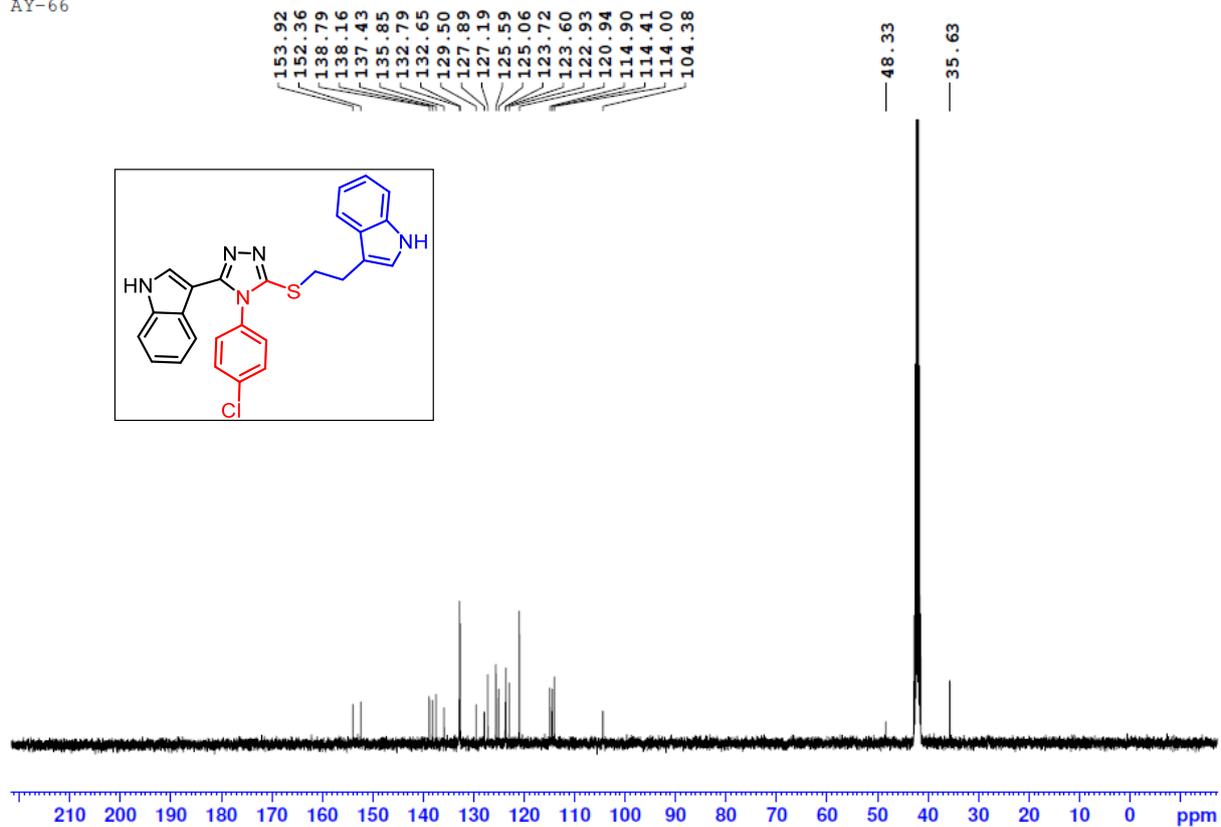


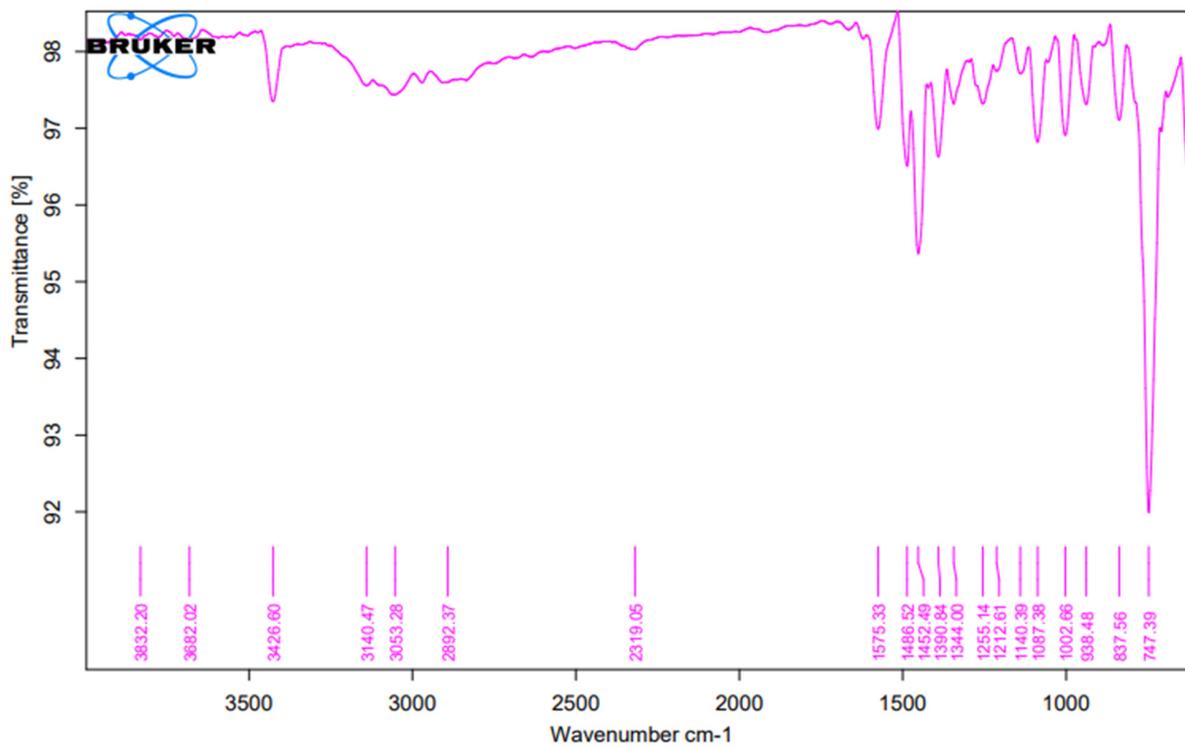
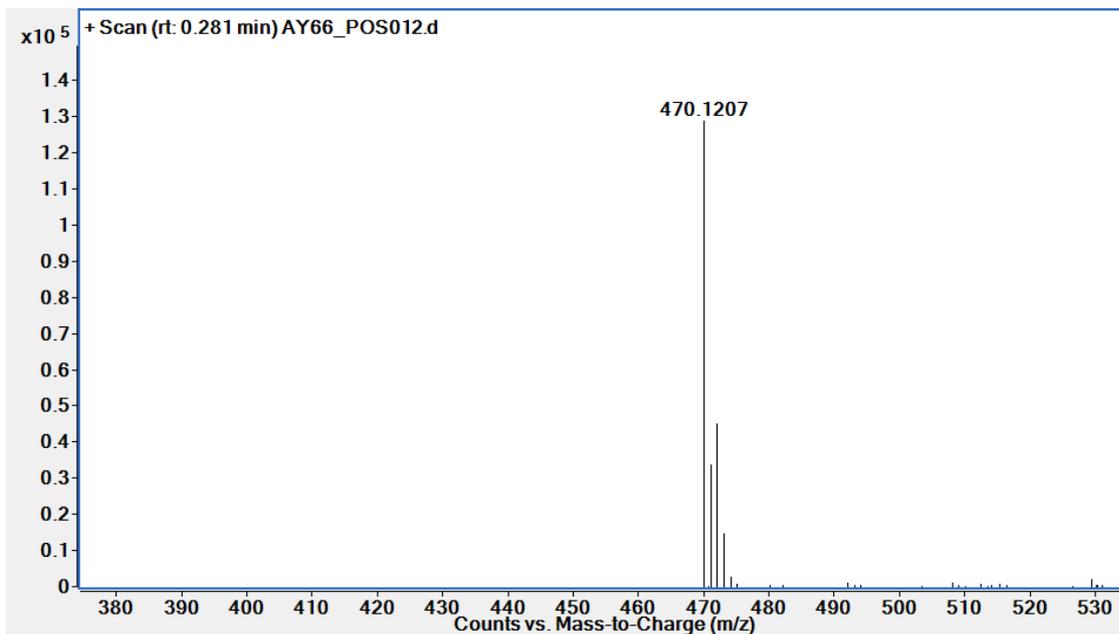
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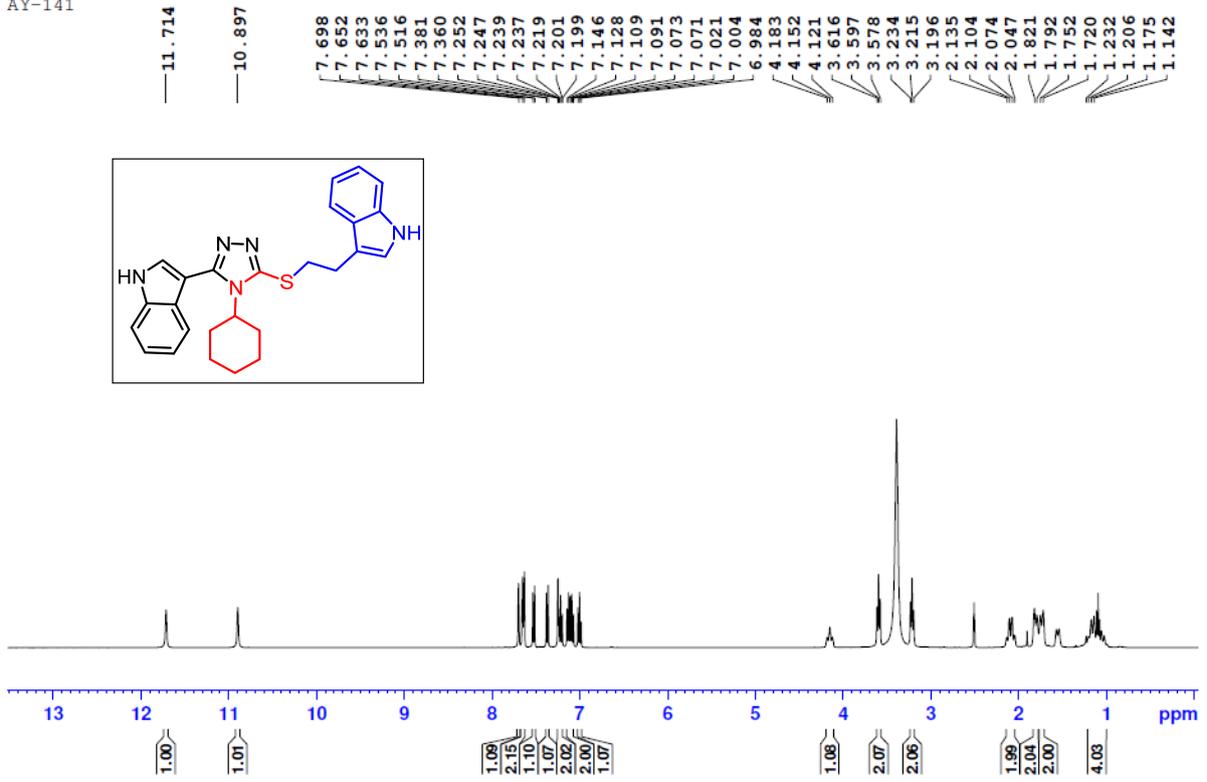
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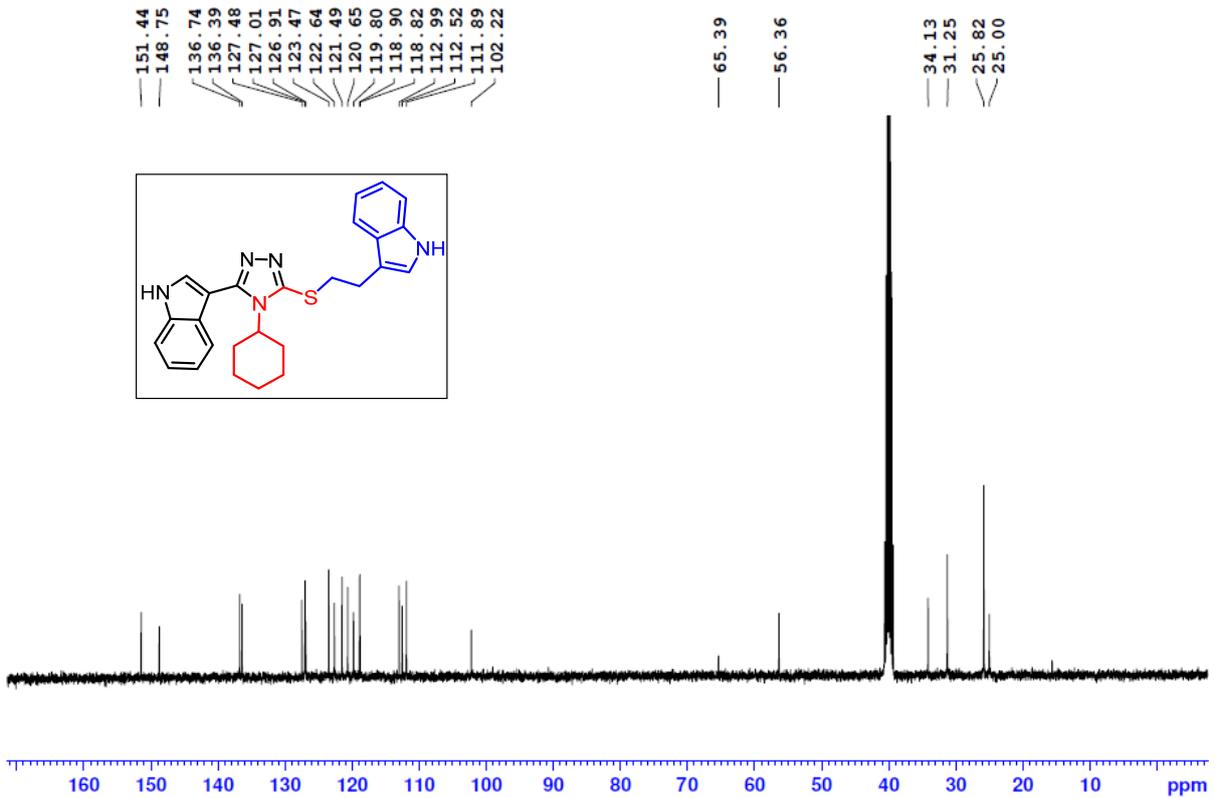


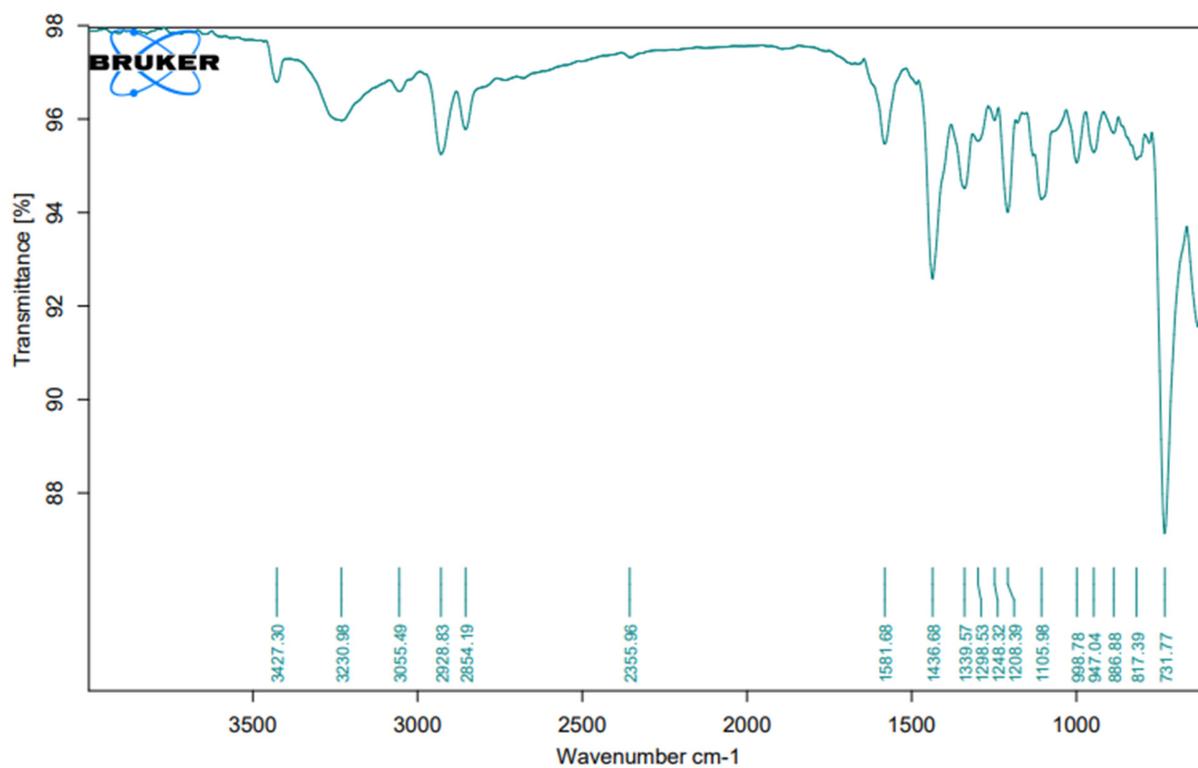
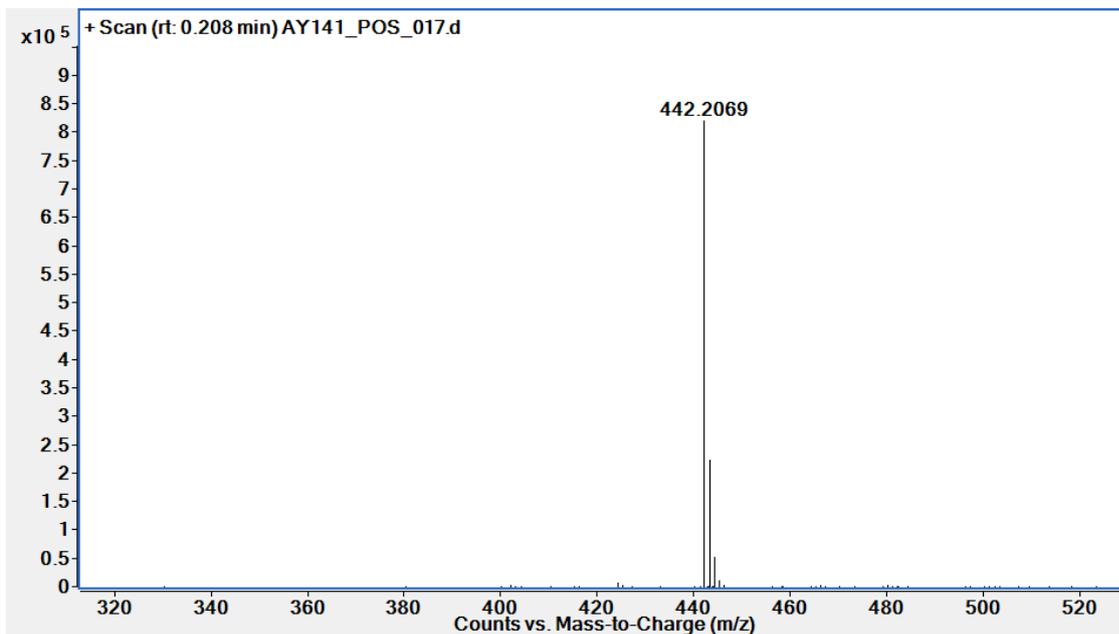
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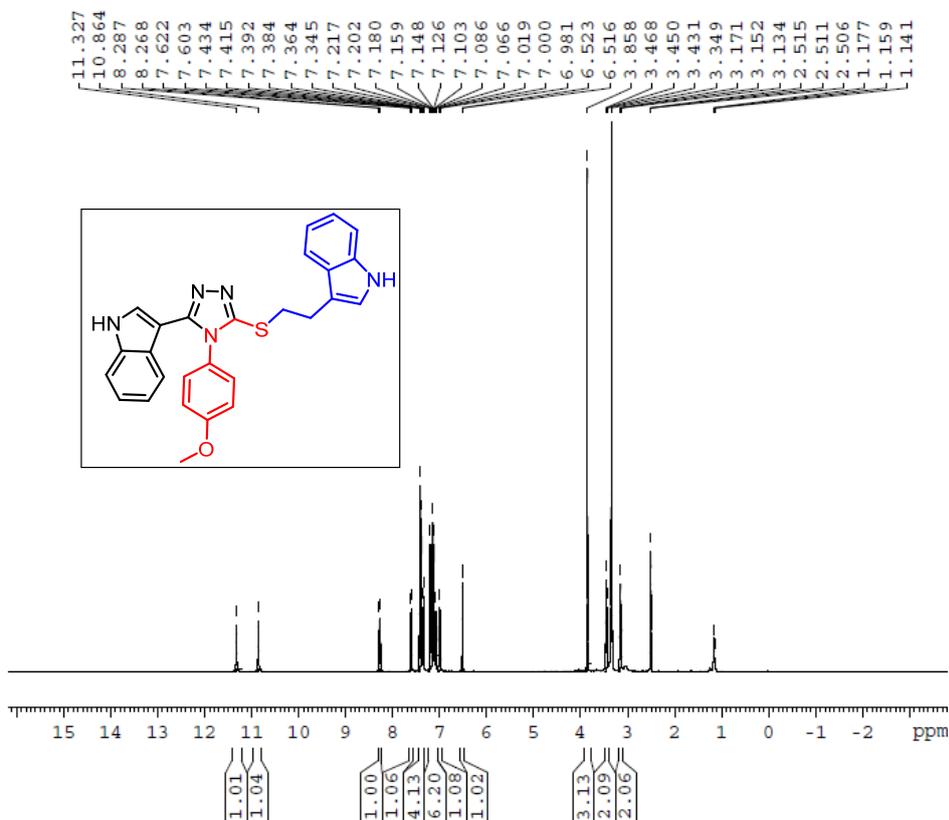
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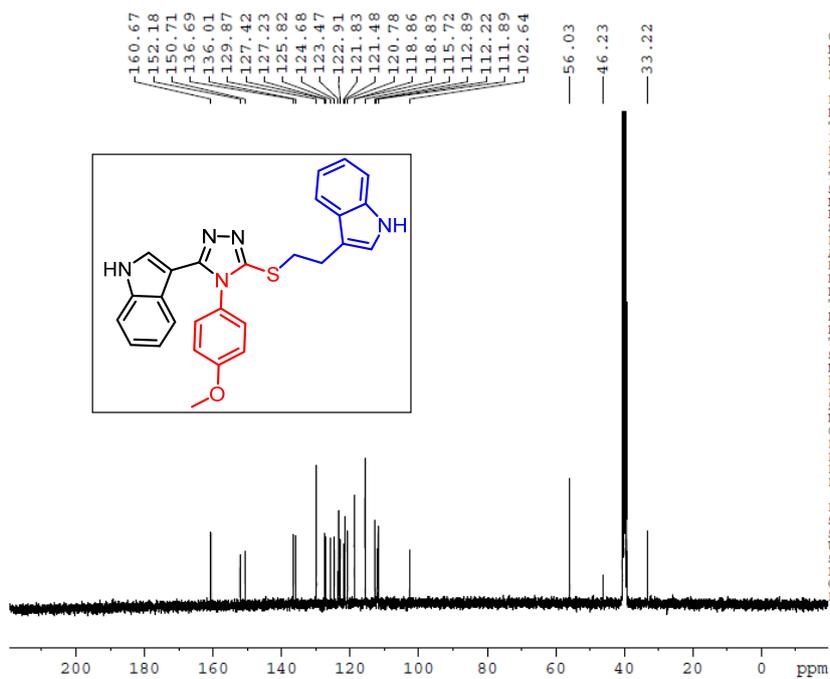


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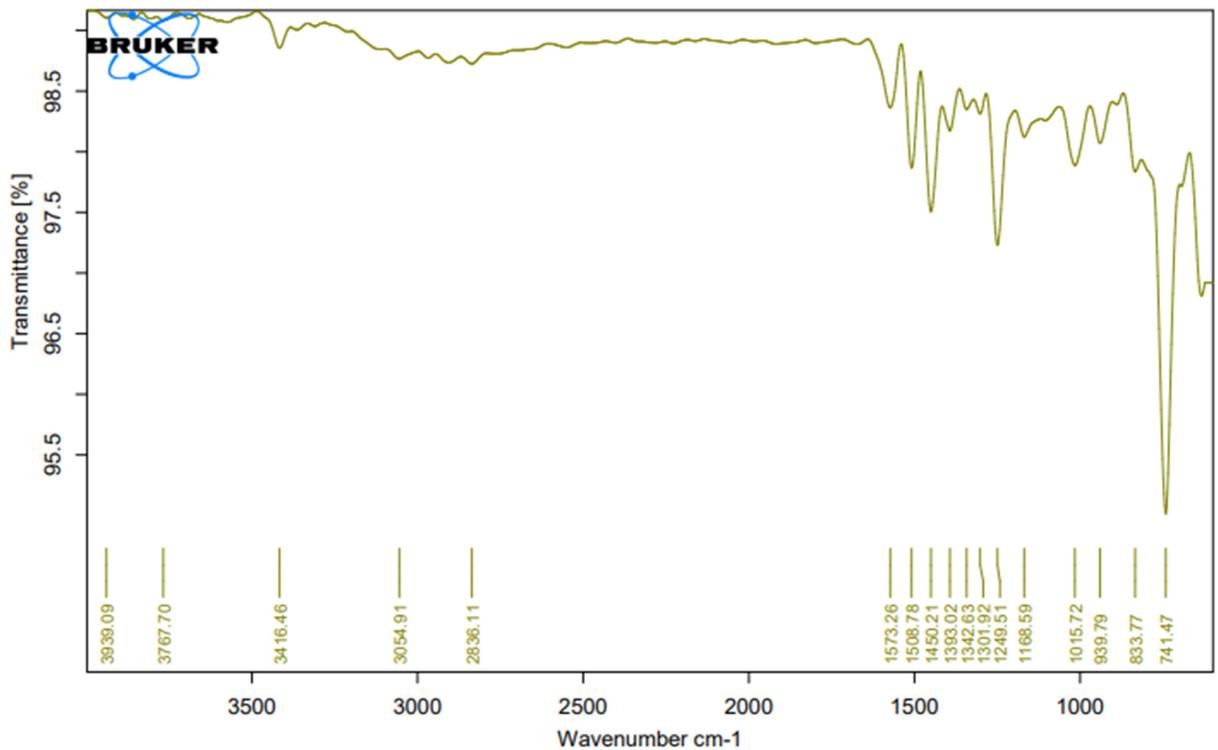
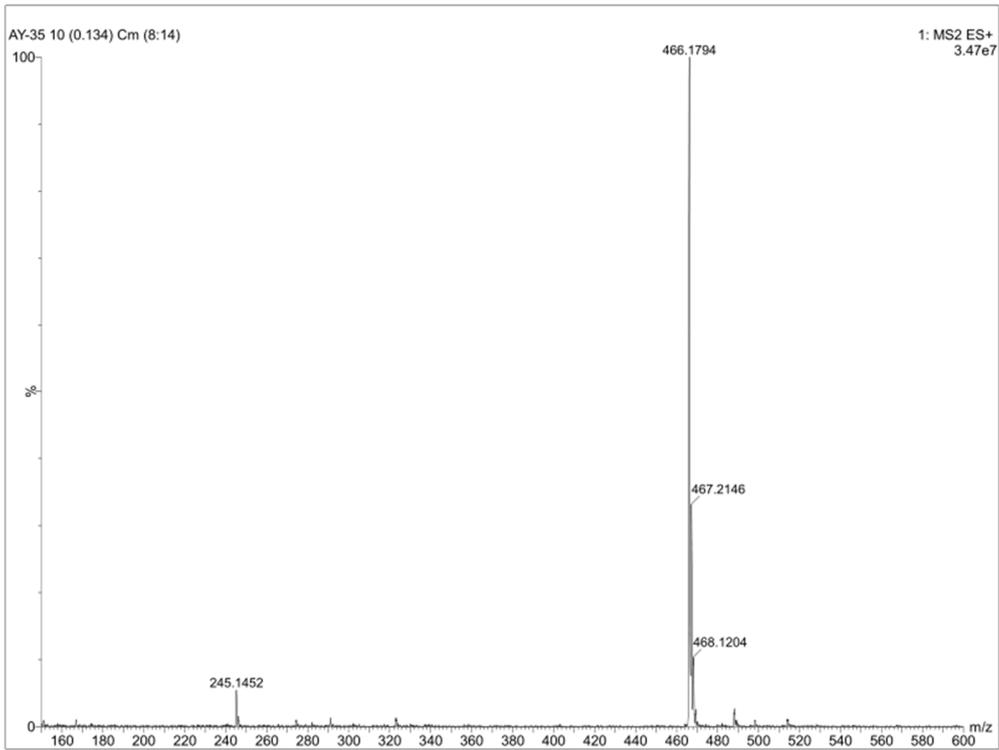
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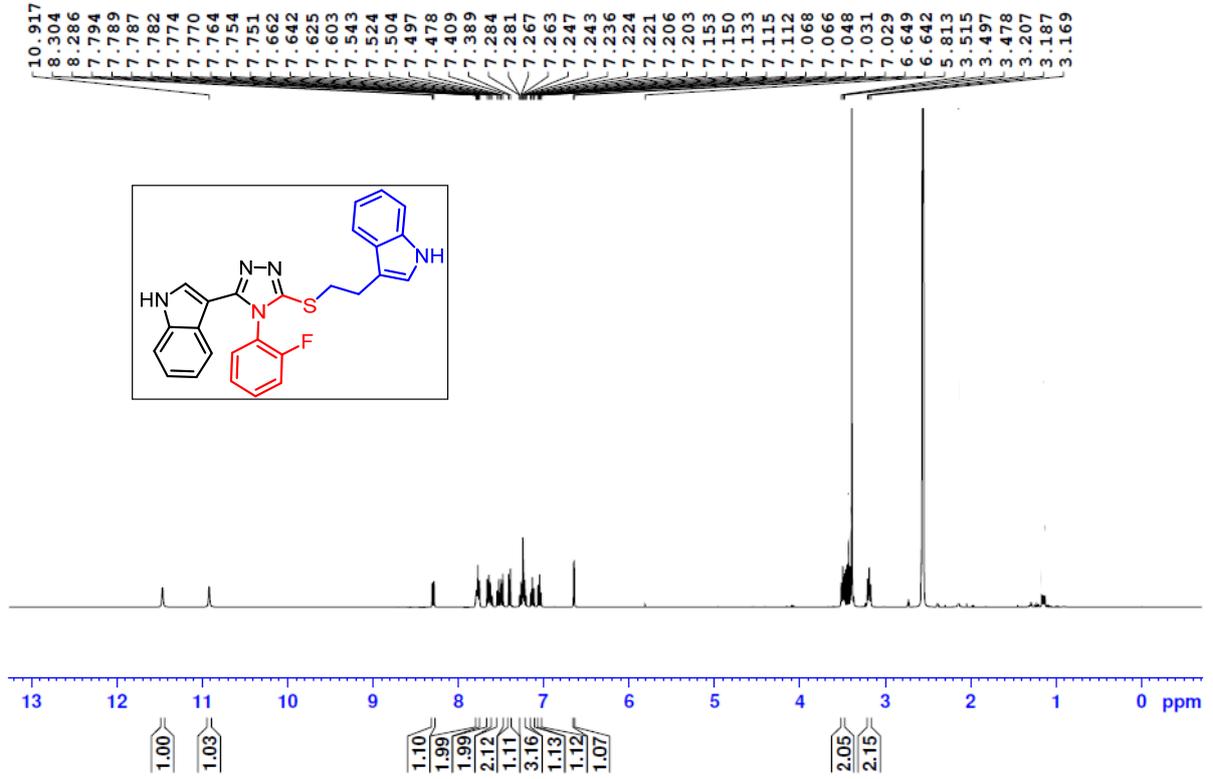
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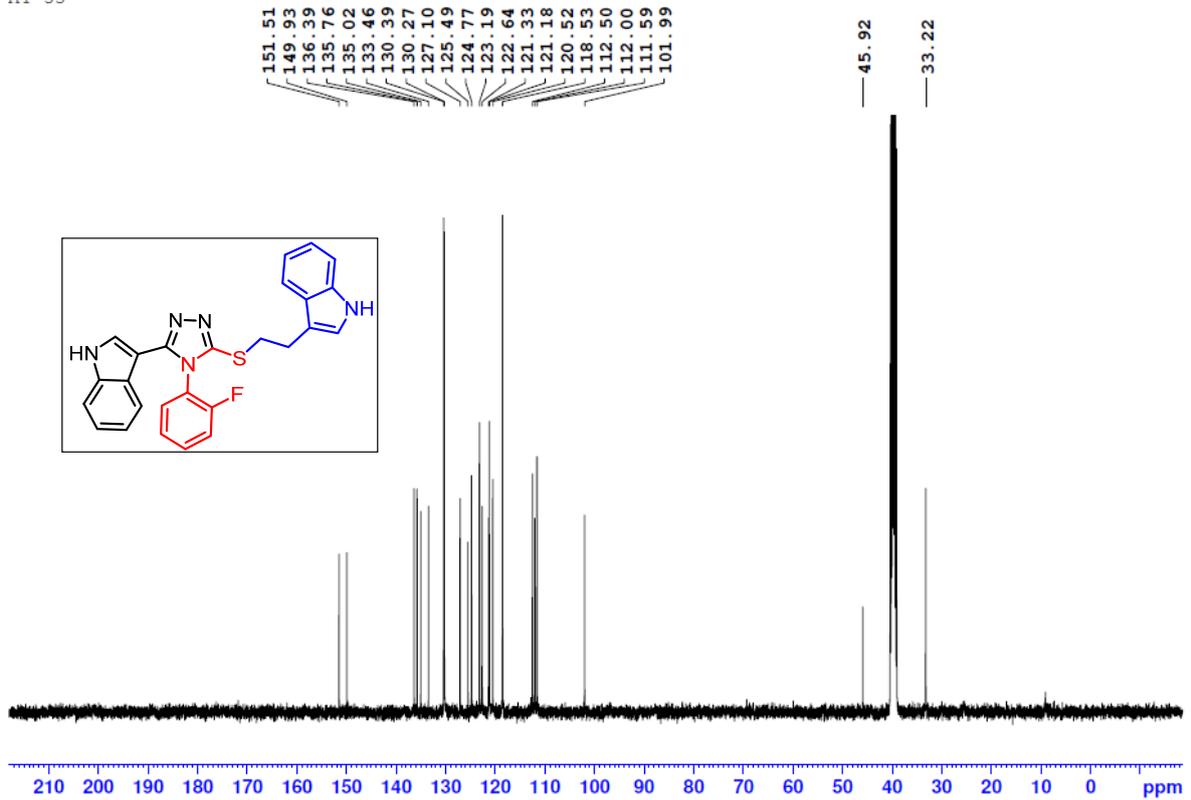


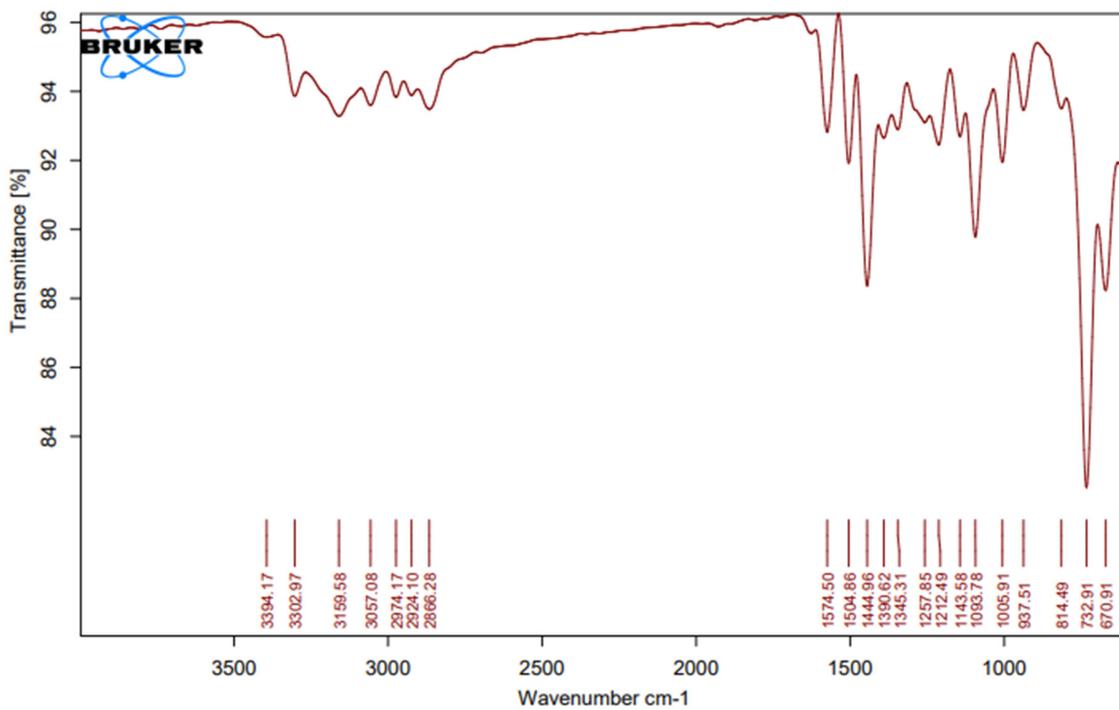
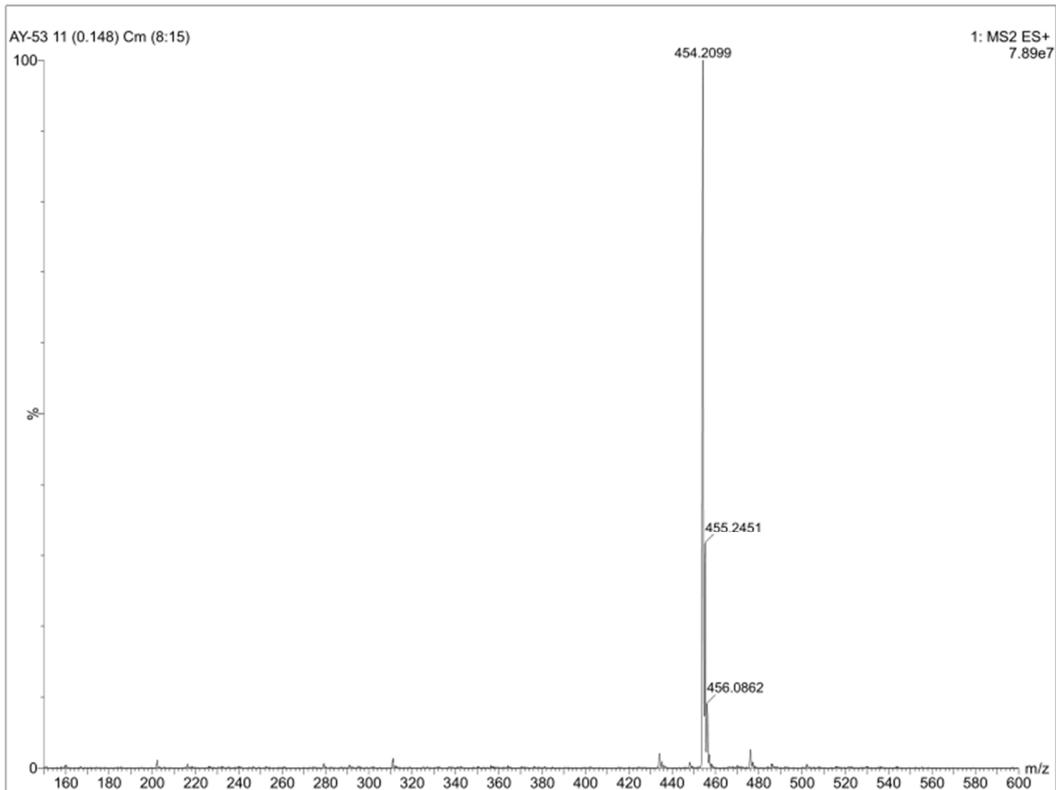
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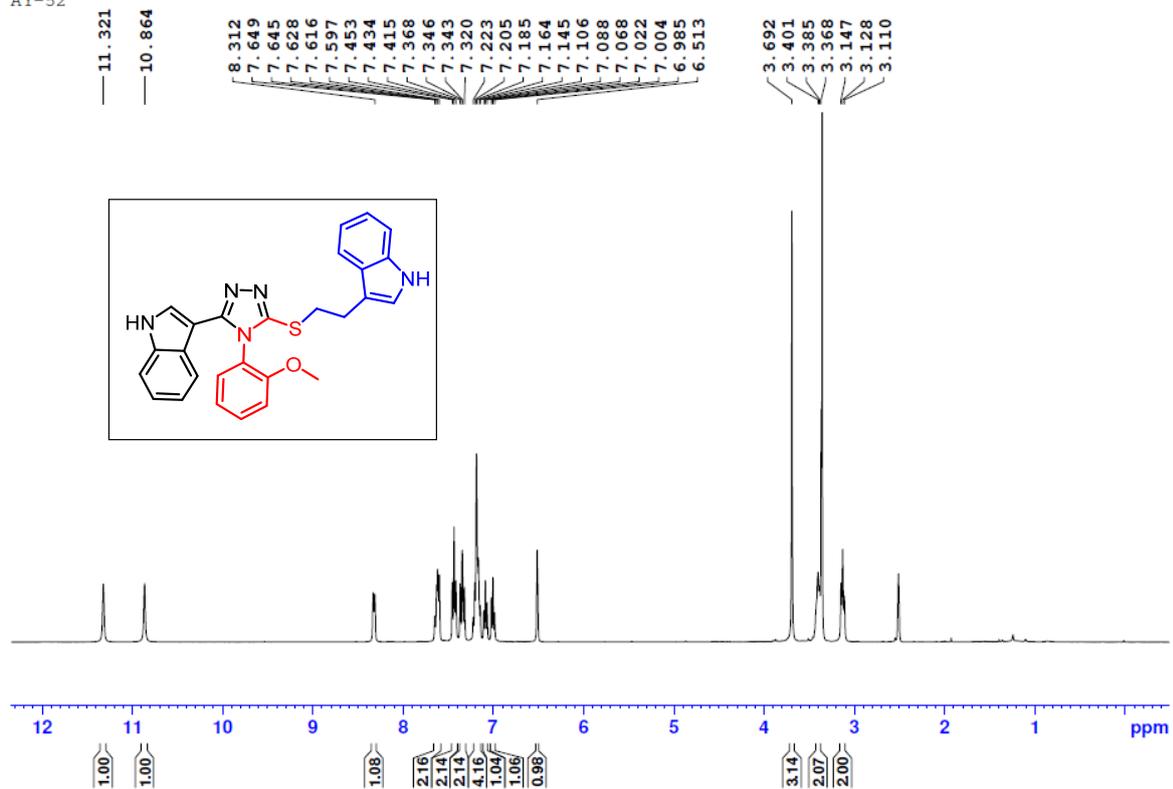
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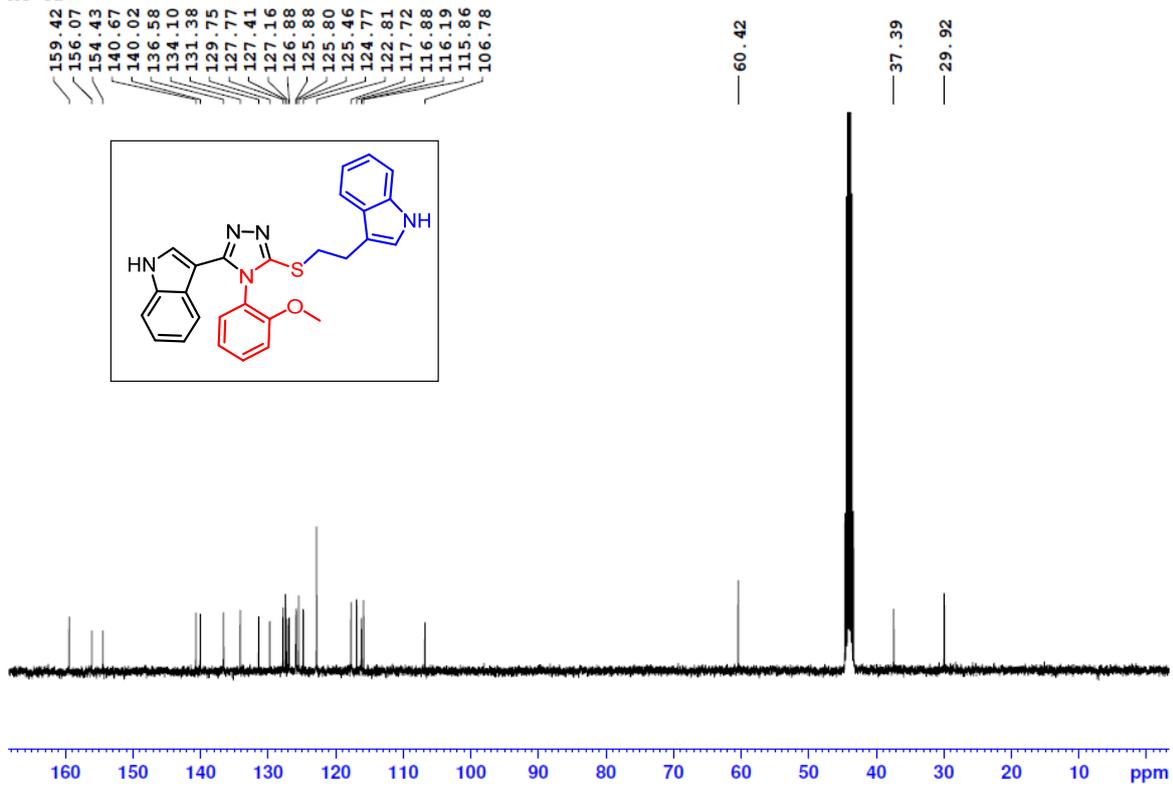


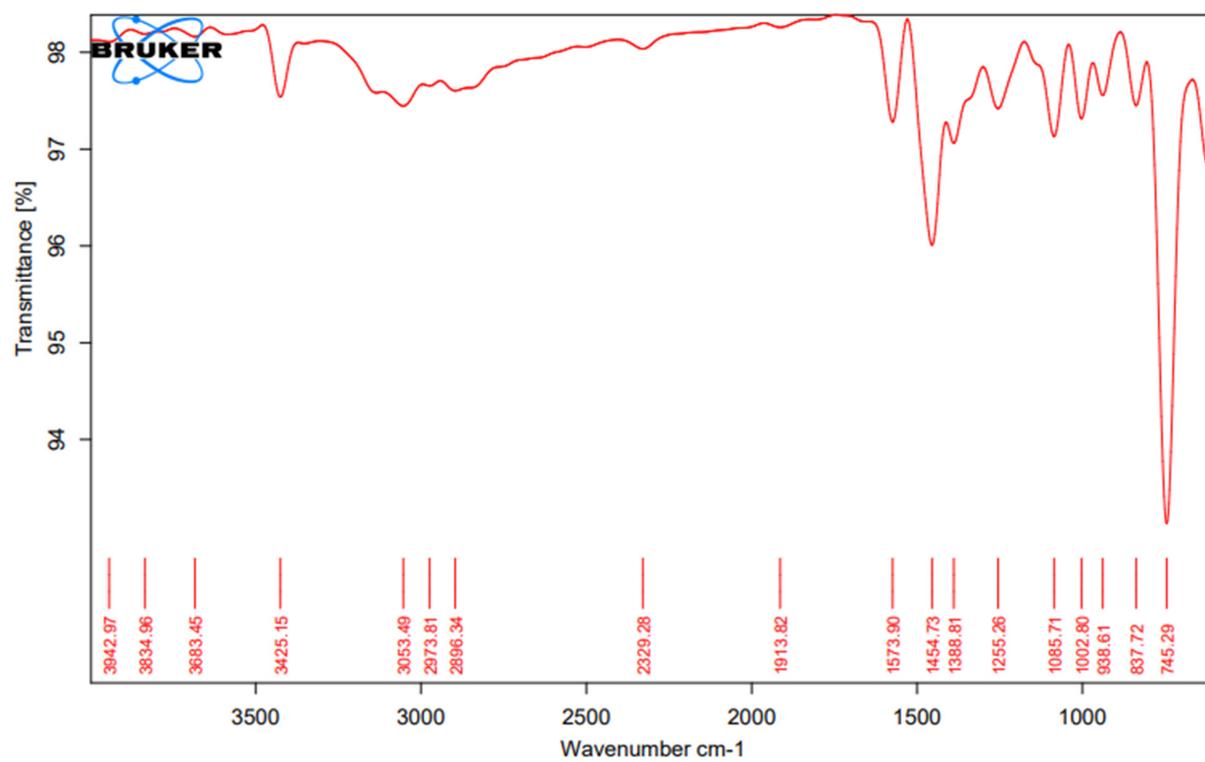
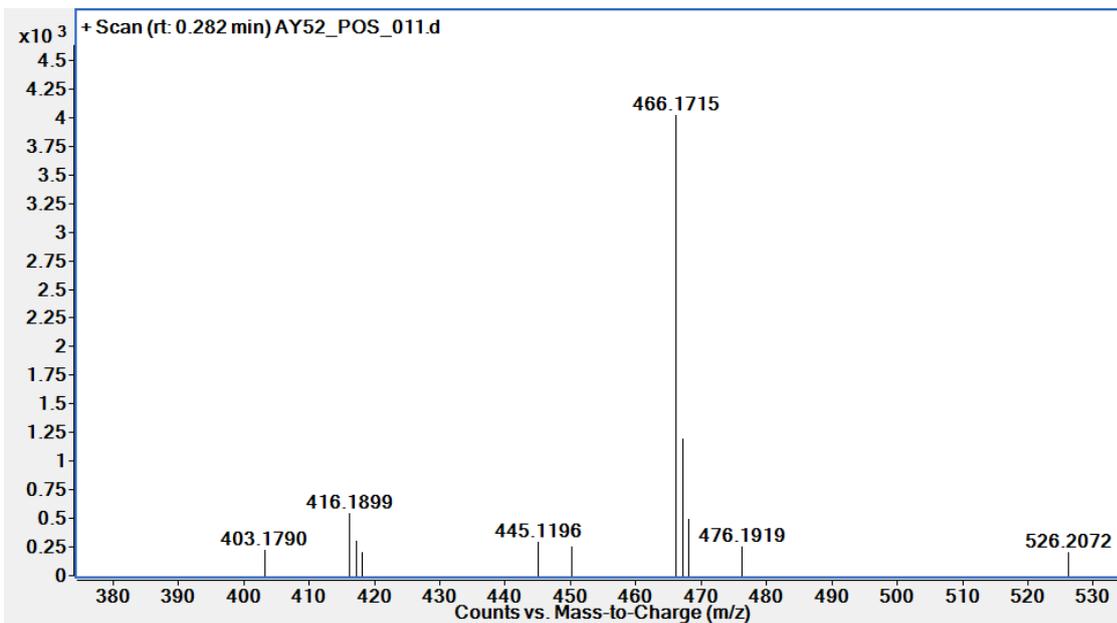
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AY-52



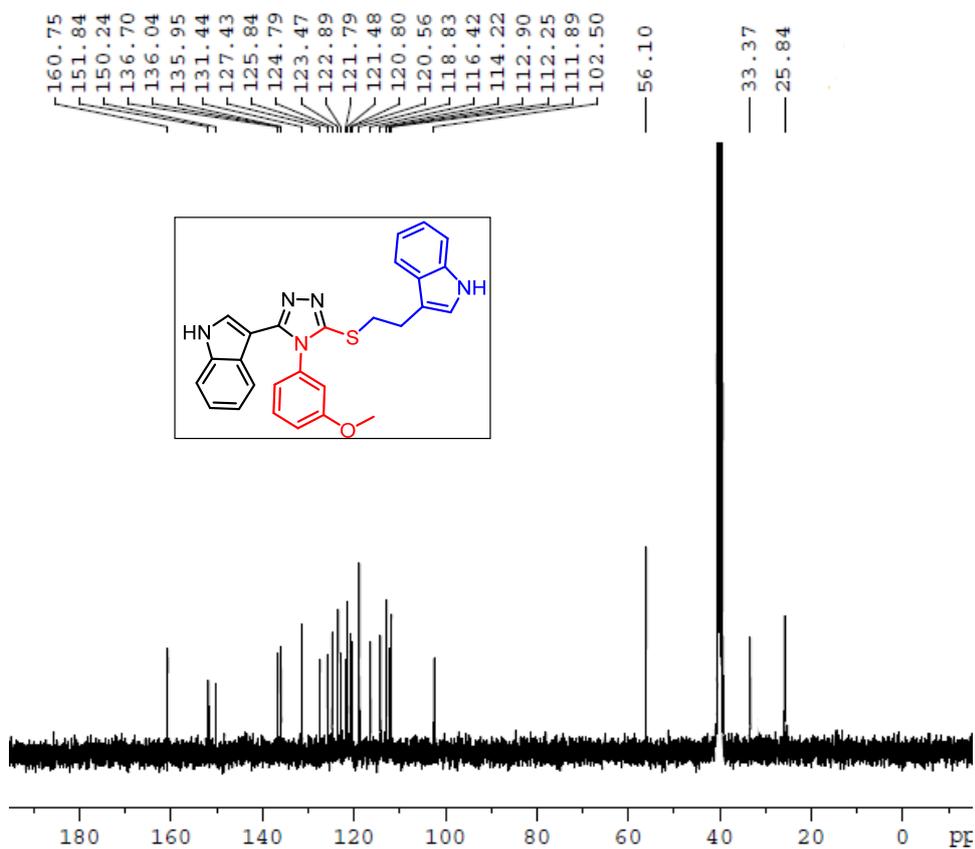
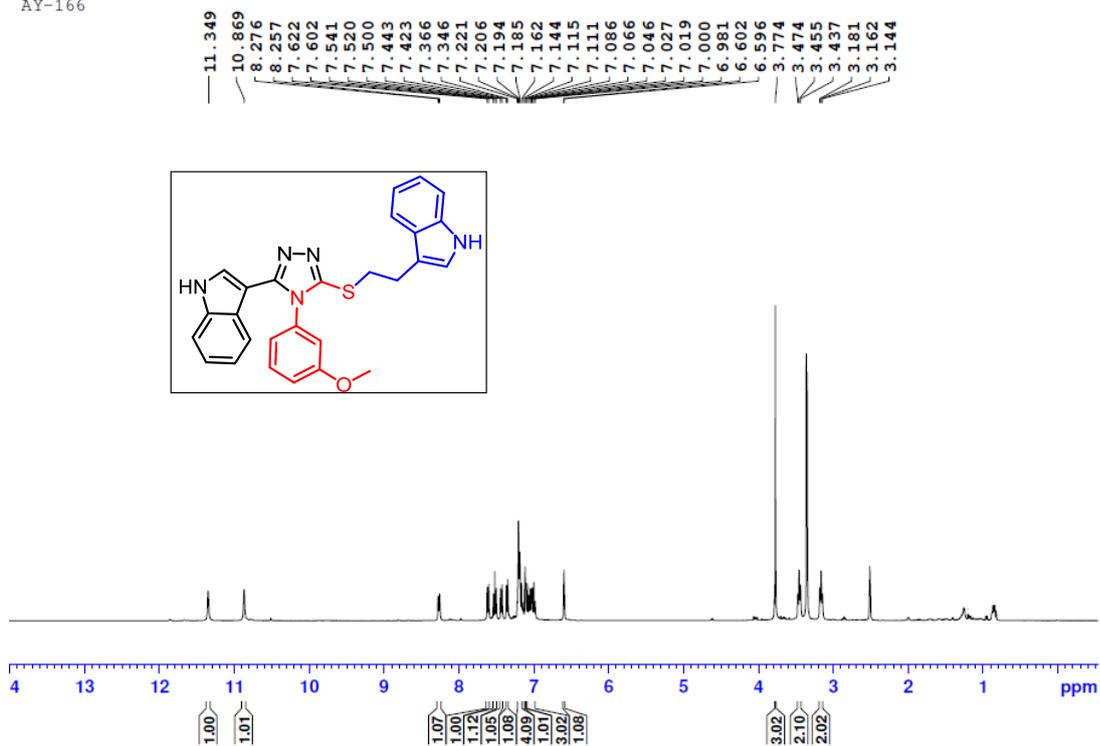
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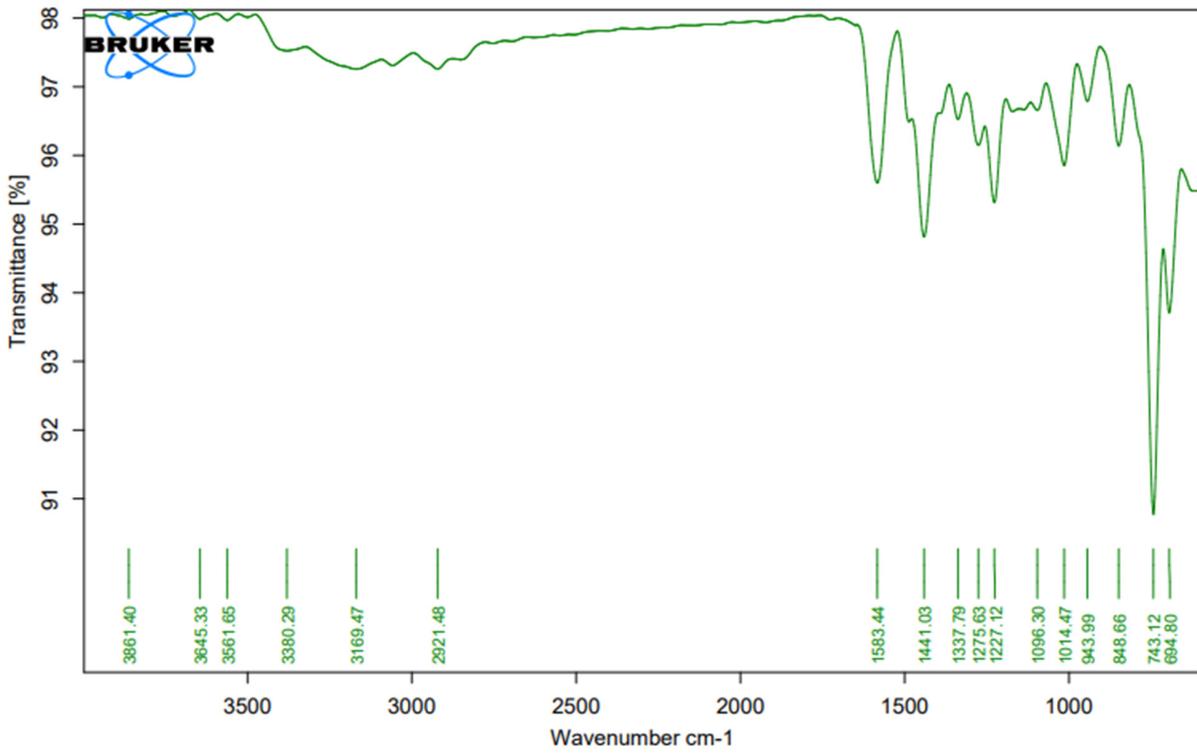
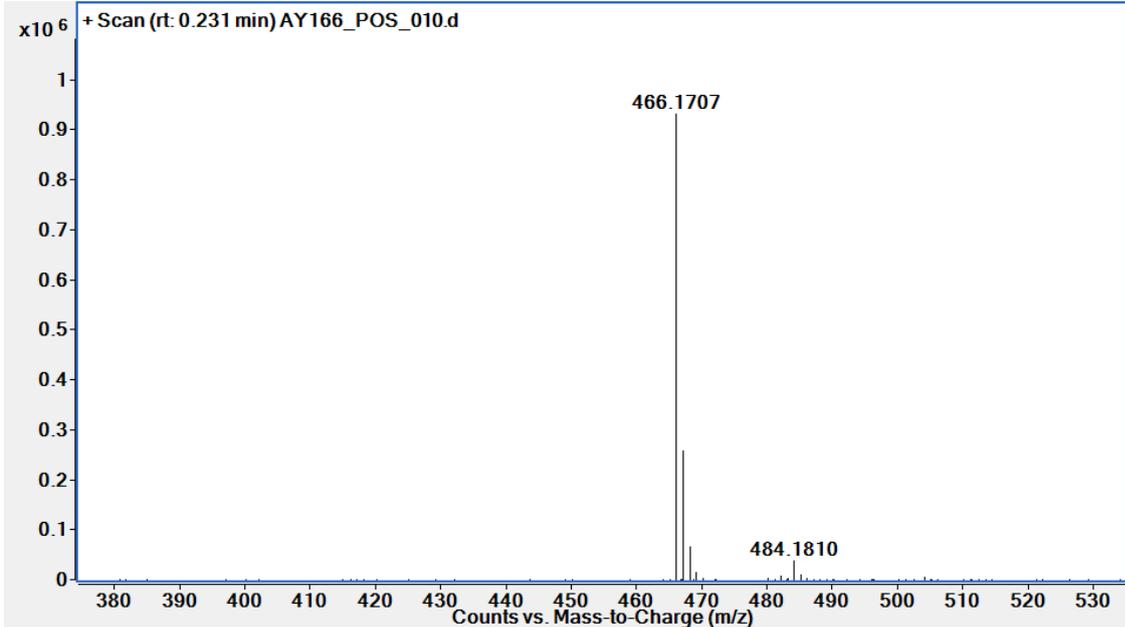




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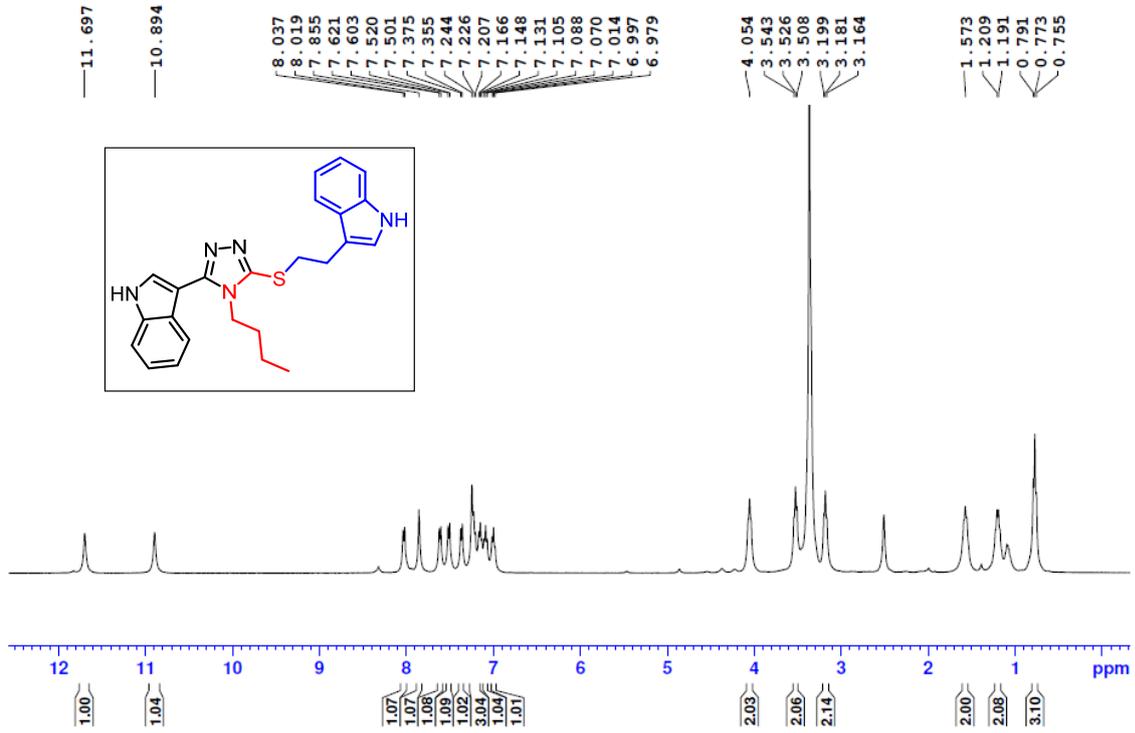
AY-166





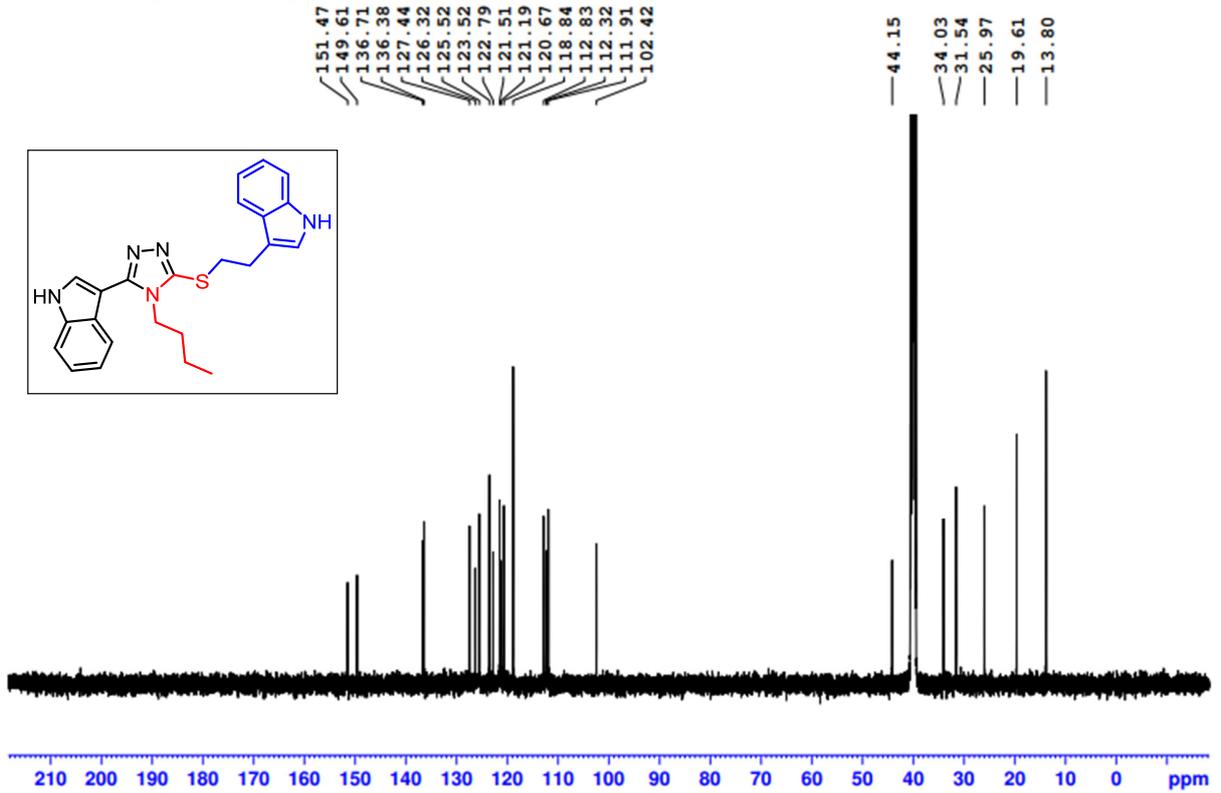
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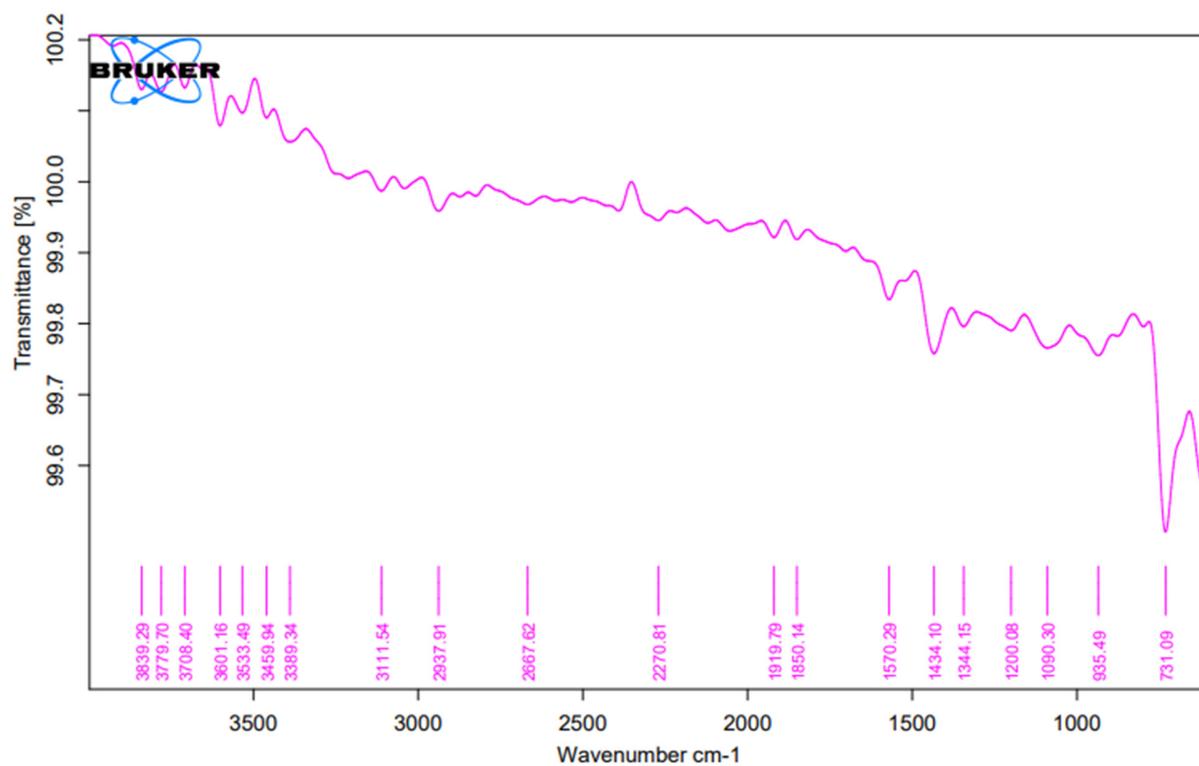
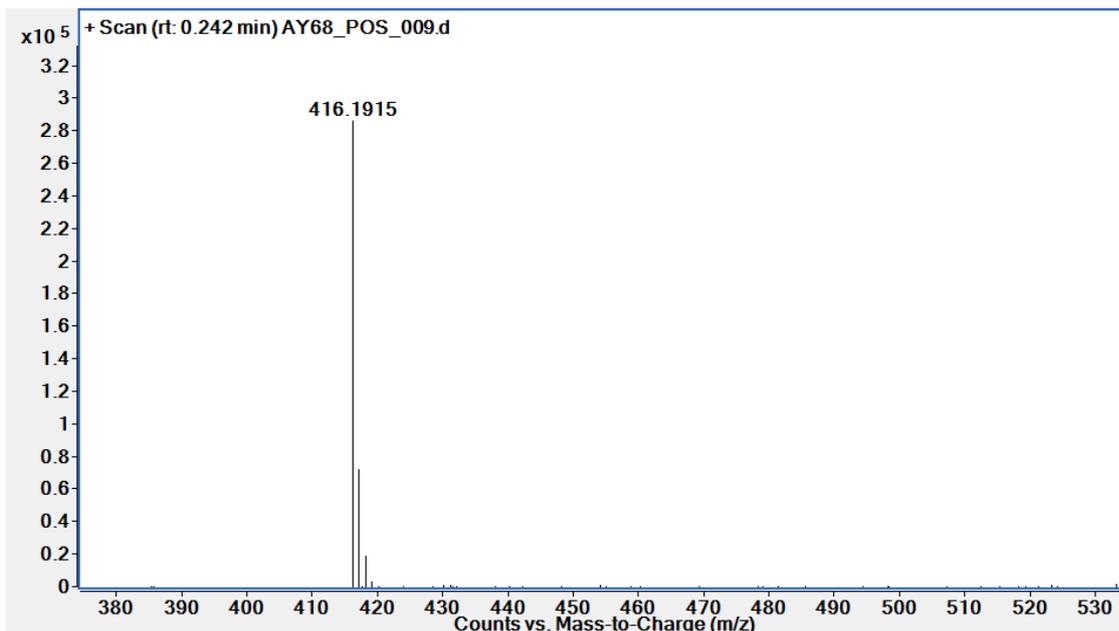
AY-68



AY-68

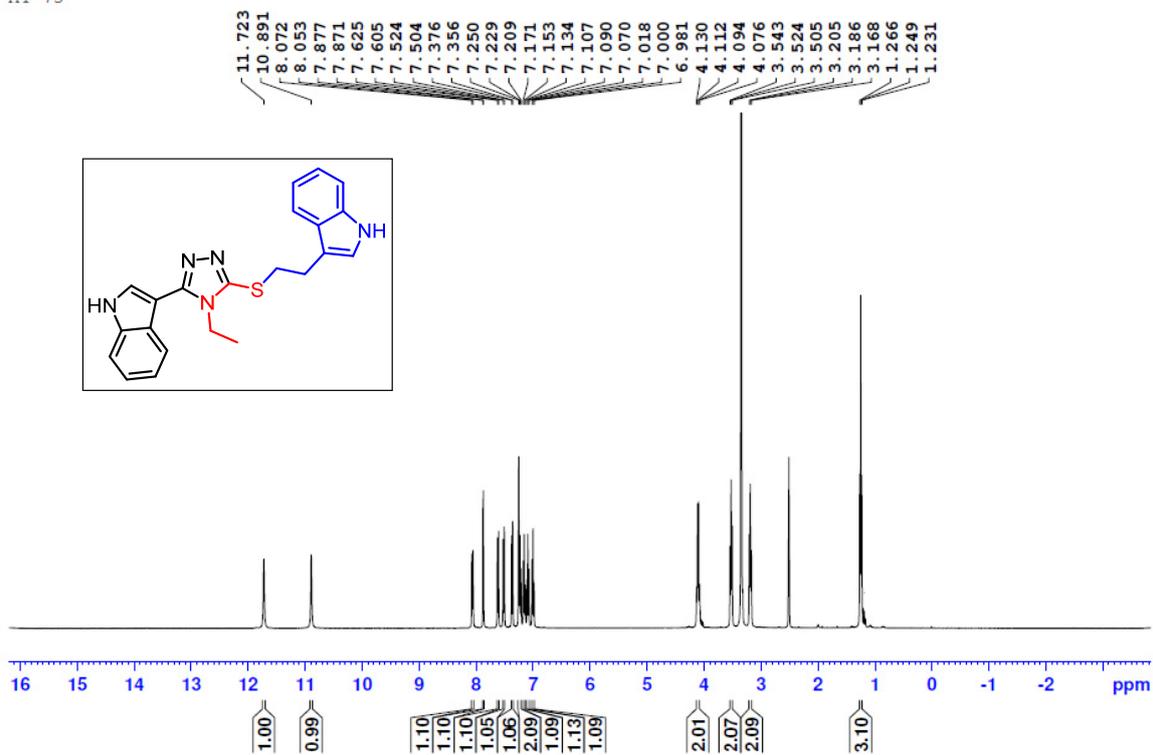
C13CPD DMSO (D:\data\SPS) nmrsu 2



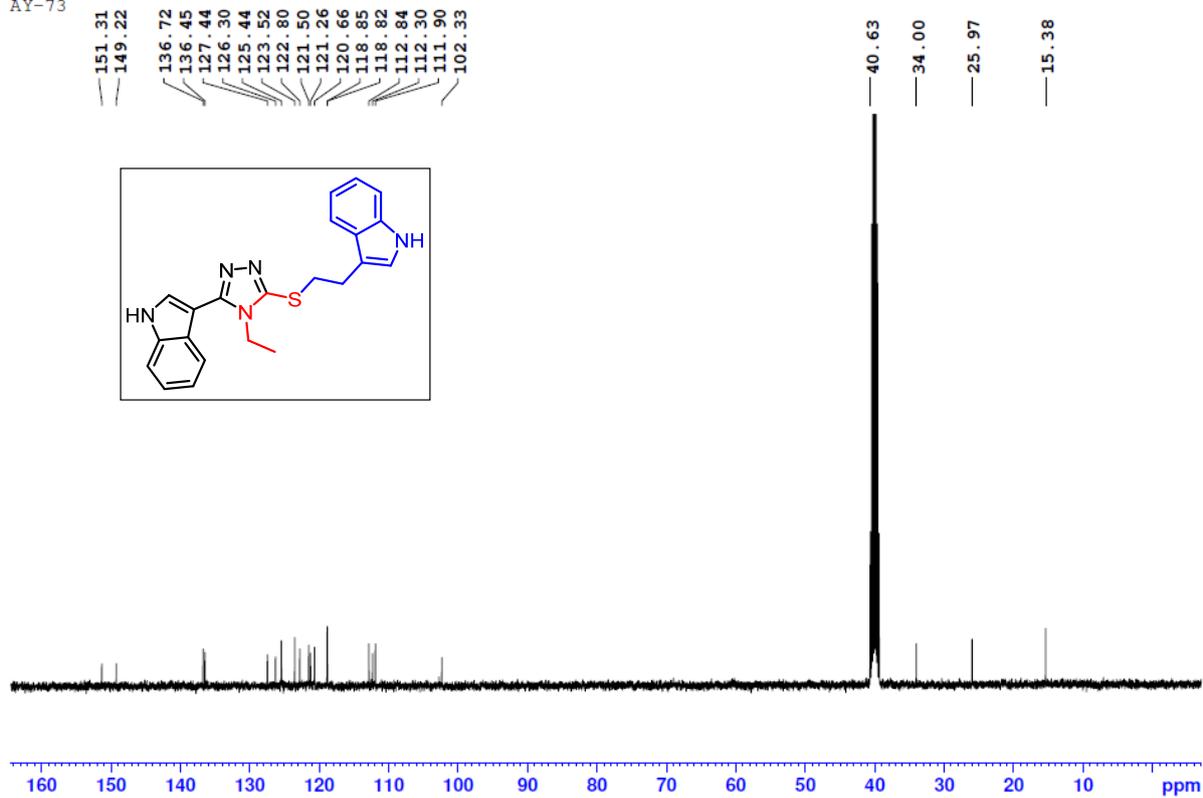


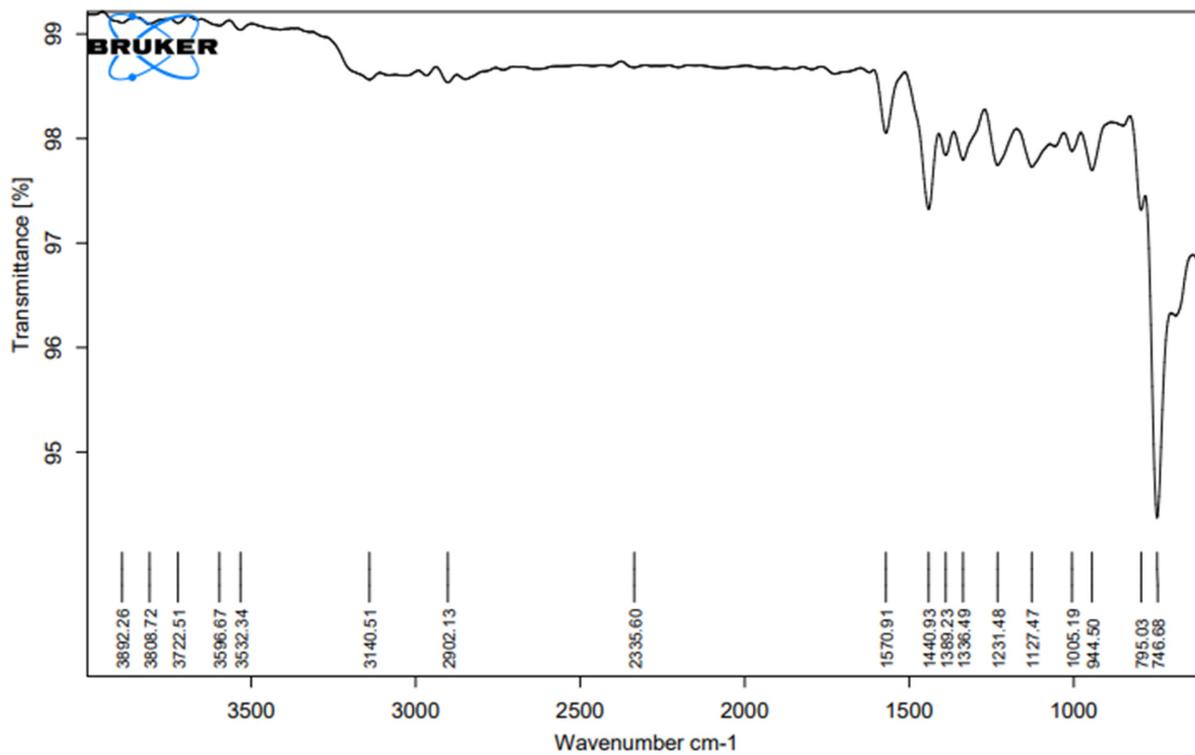
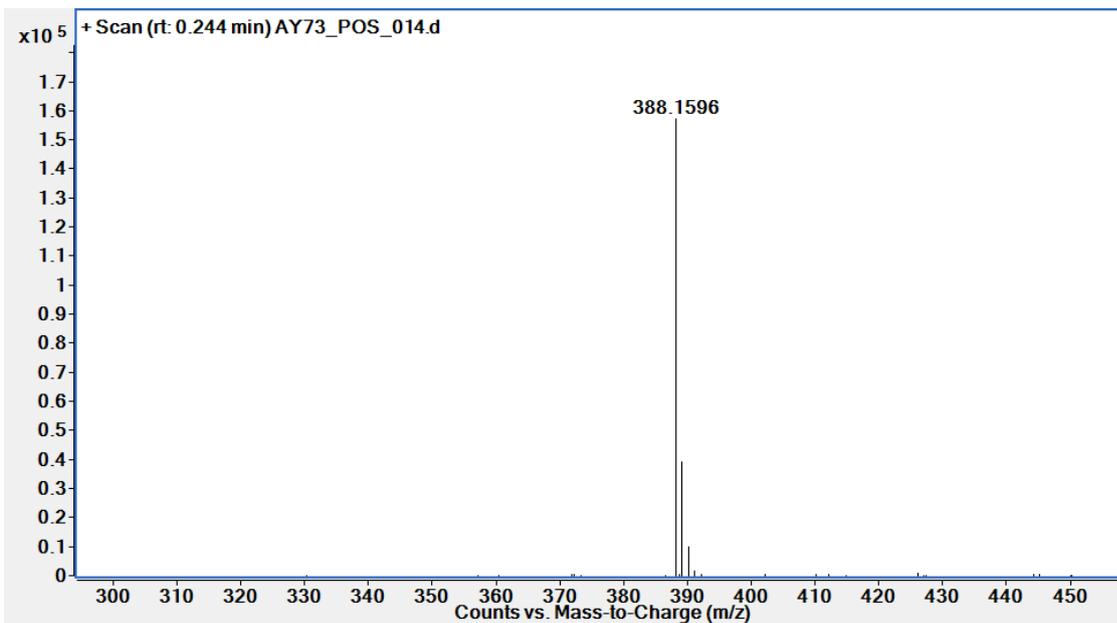
C:\Users\NIPERG\Desktop\Daya\AY\AY-68.0	AY-68	Instrument type and / or accessory	01-11-2022
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AY-73



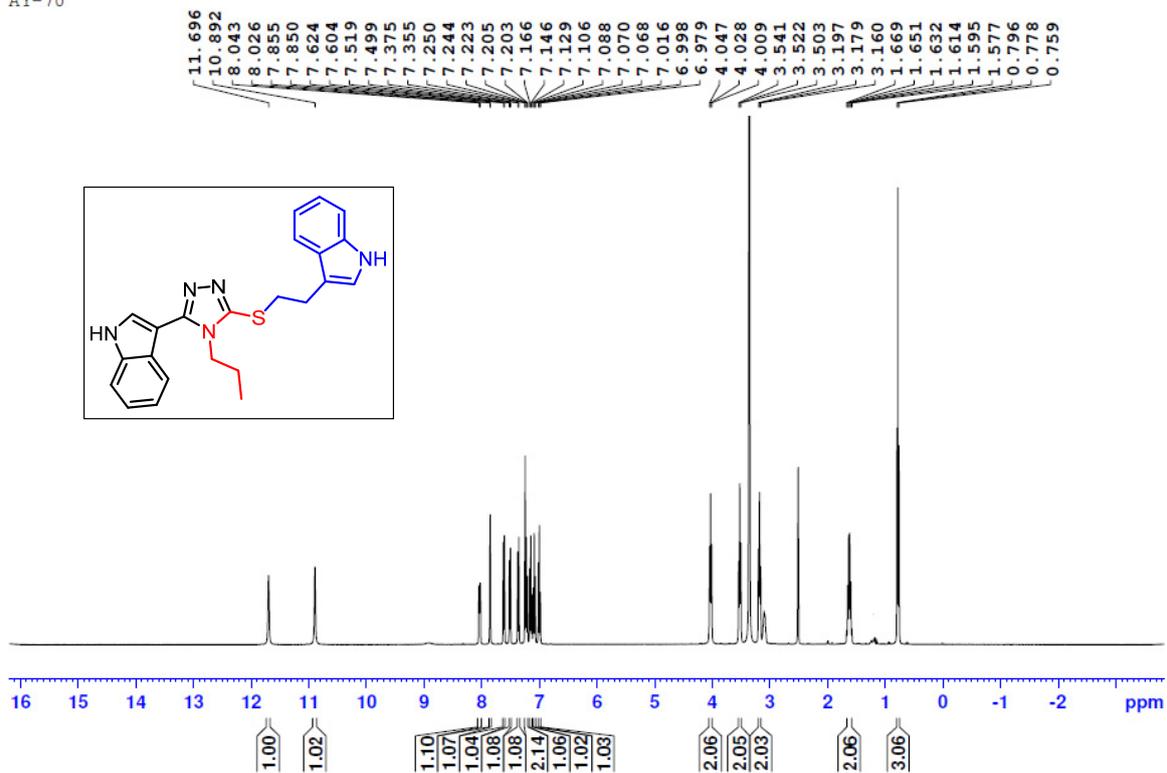
AY-73



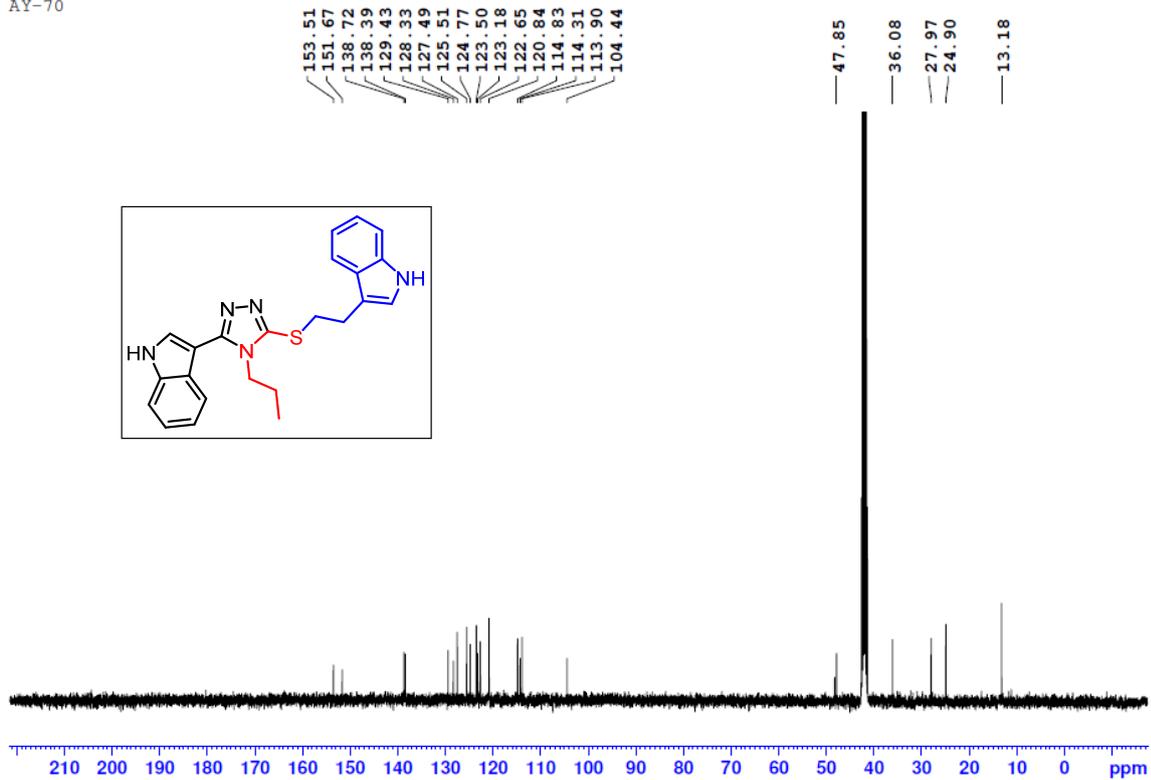


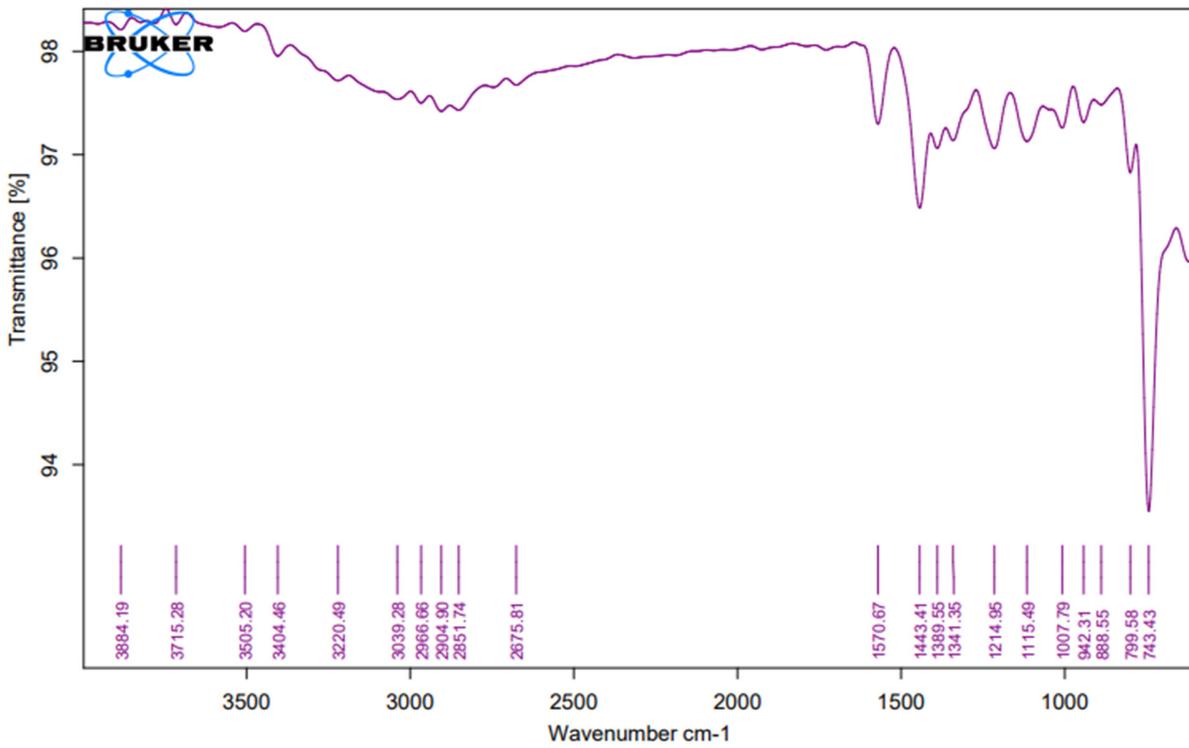
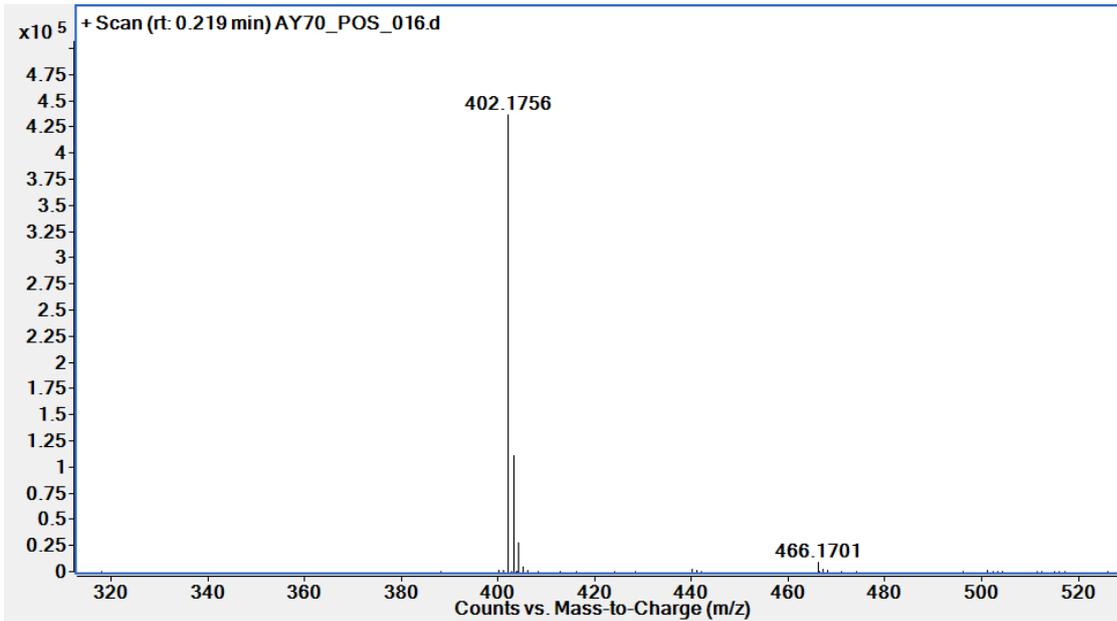
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AY-70



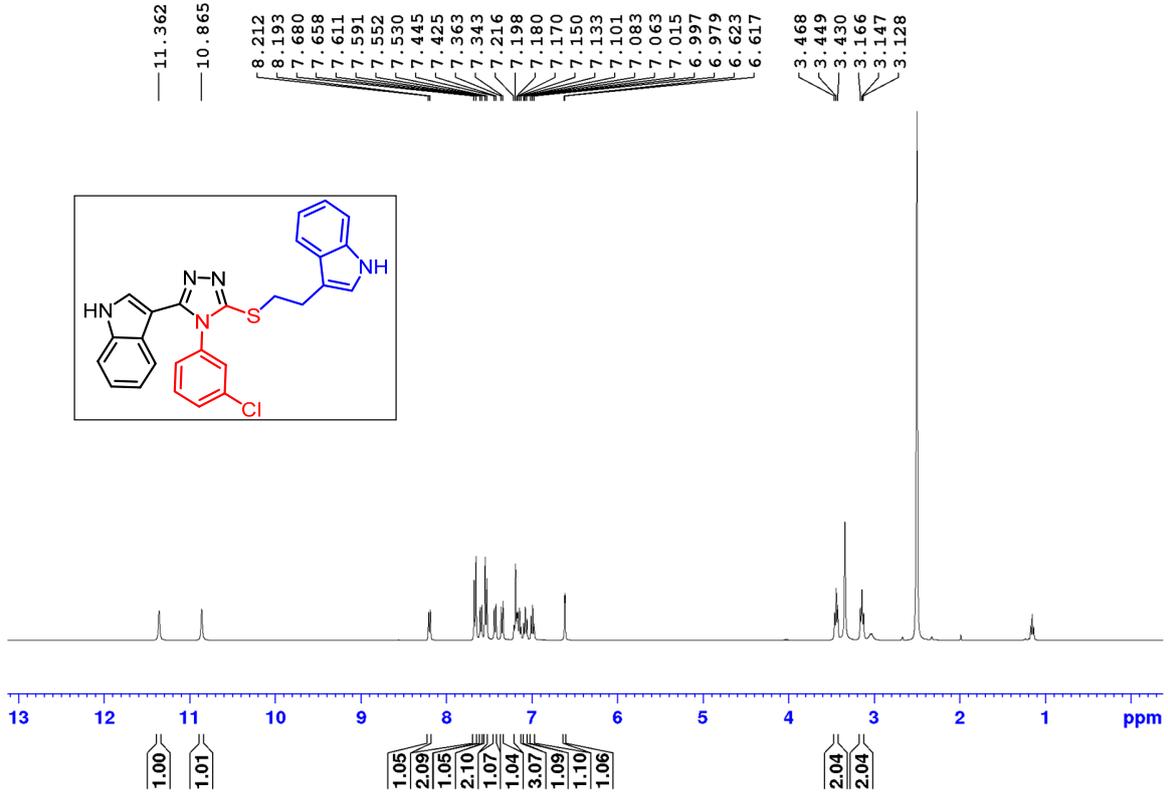
AY-70



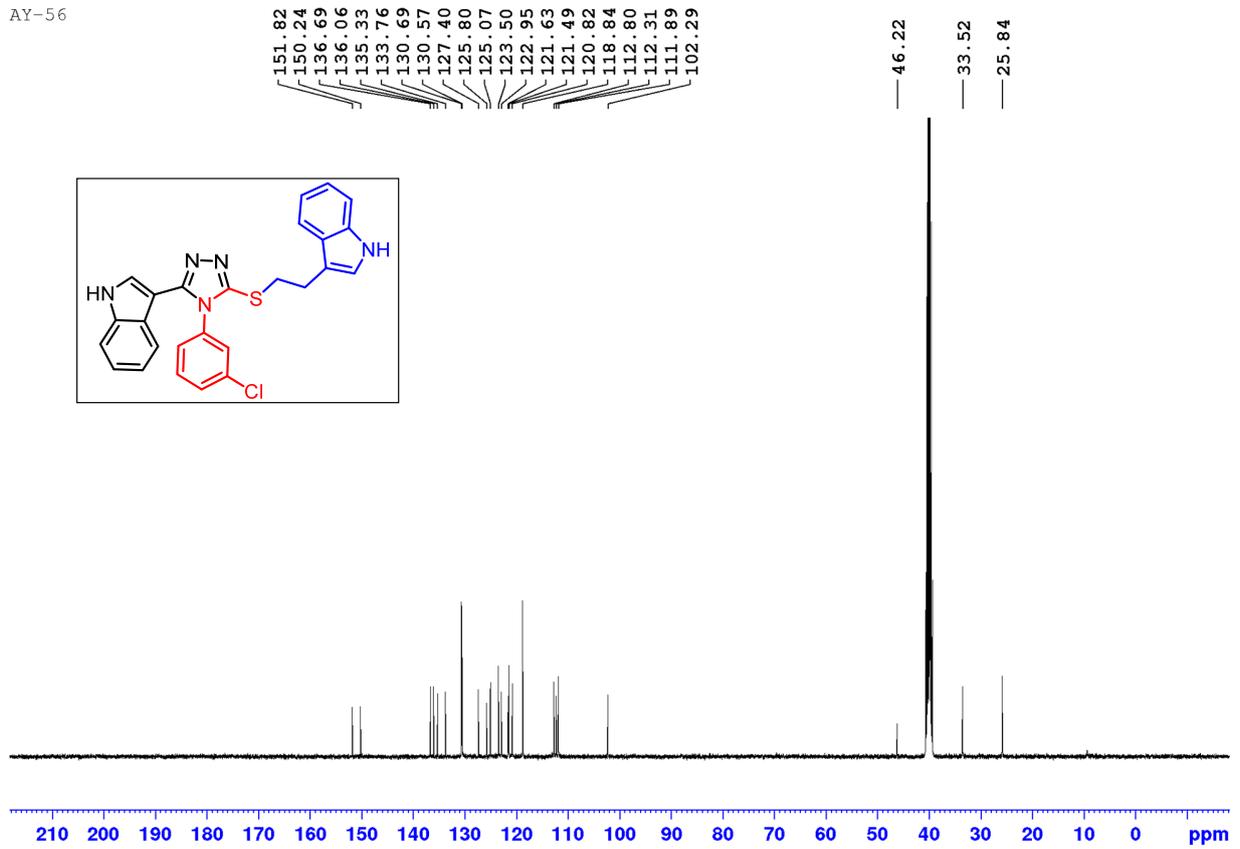


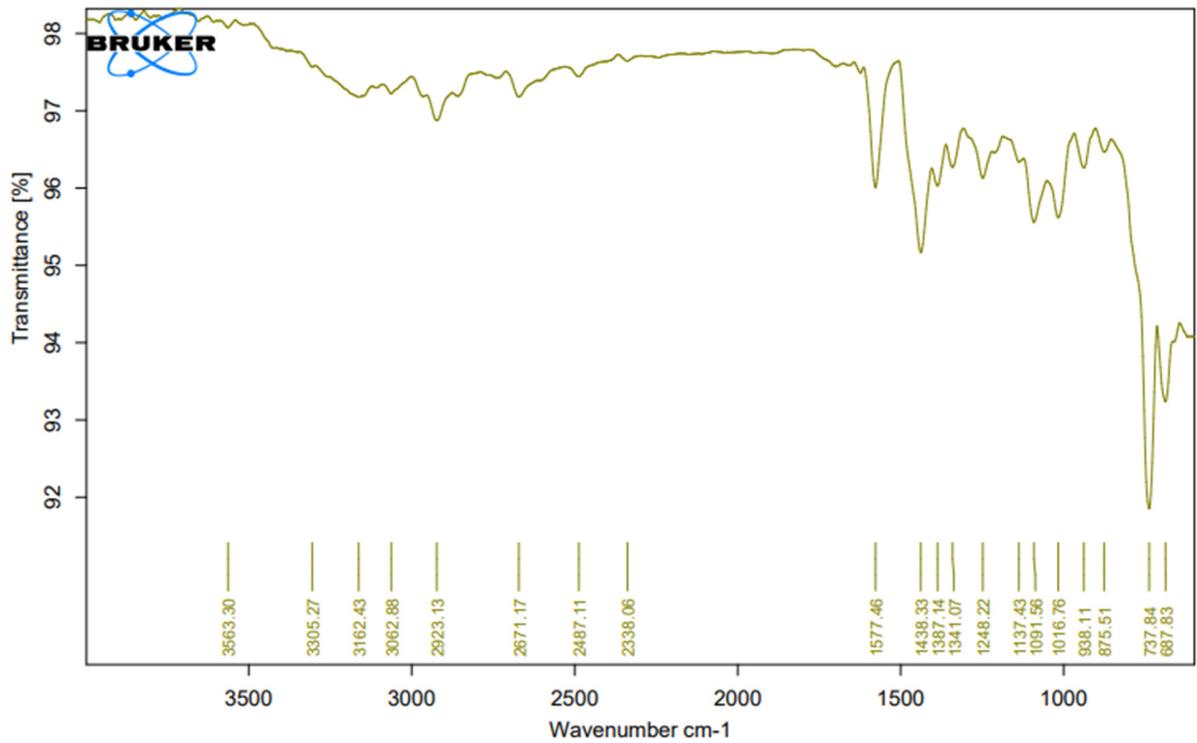
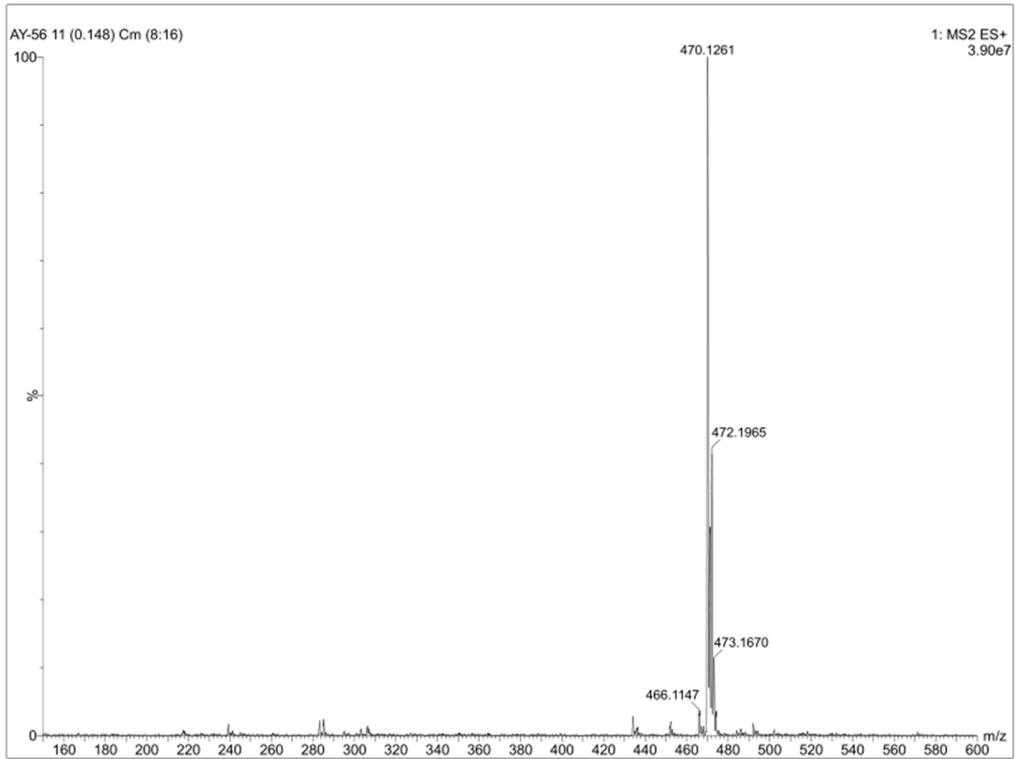
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AY-56



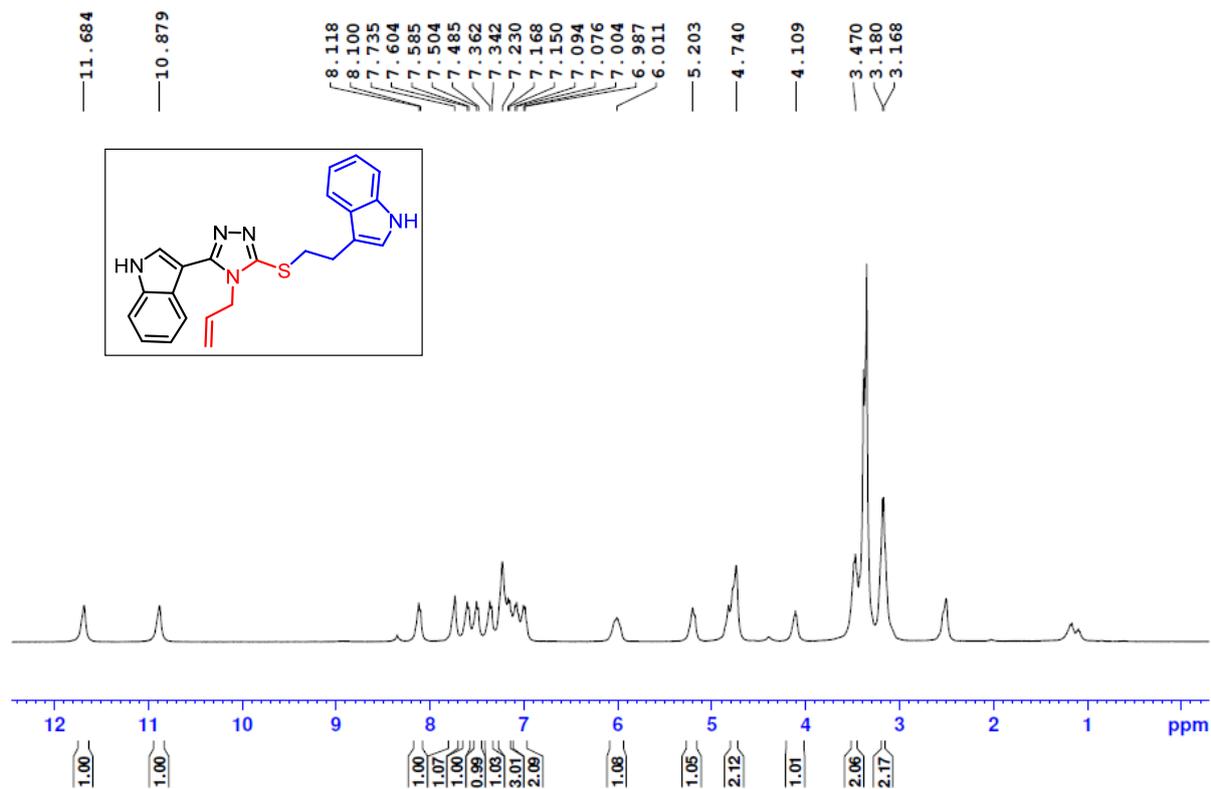
AY-56



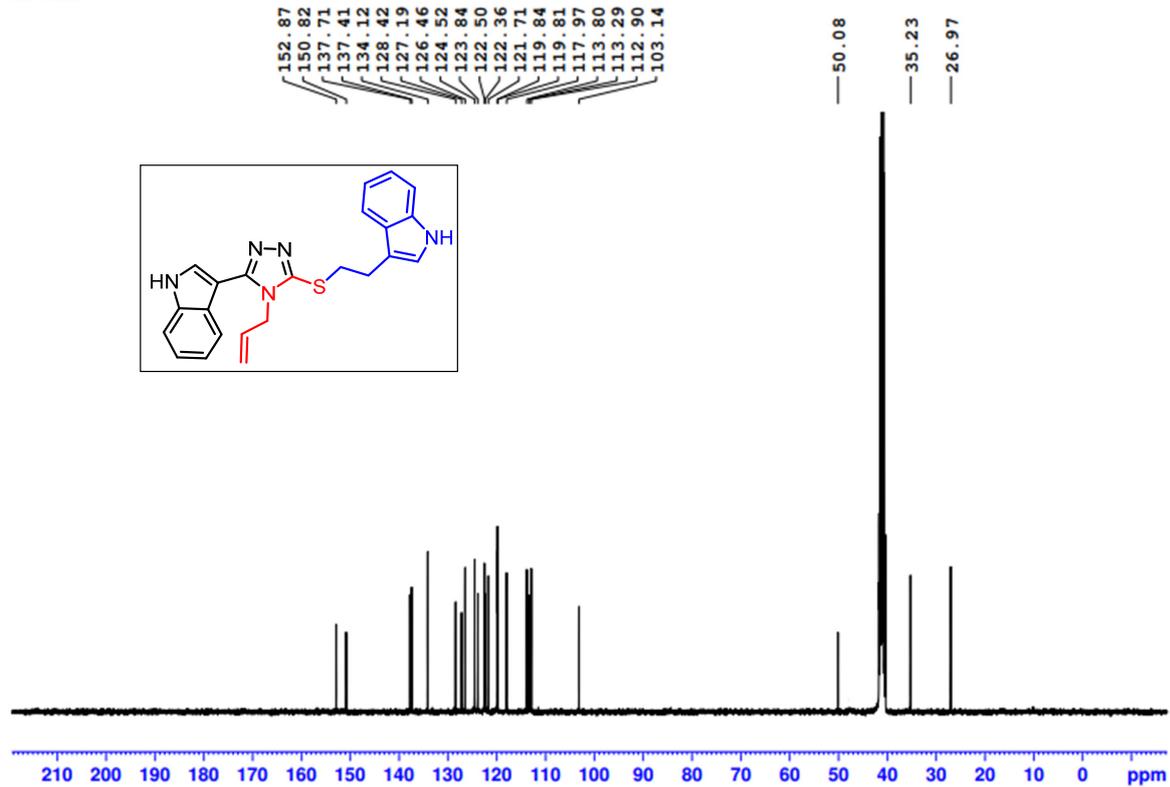


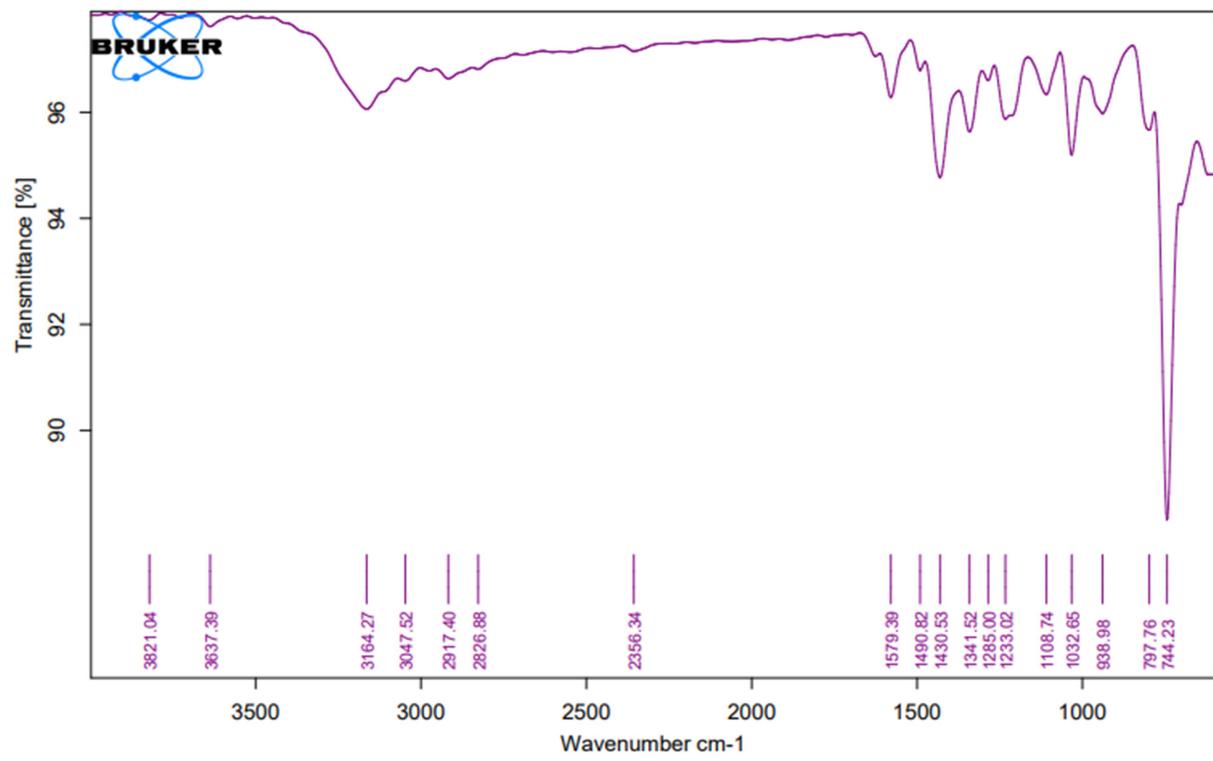
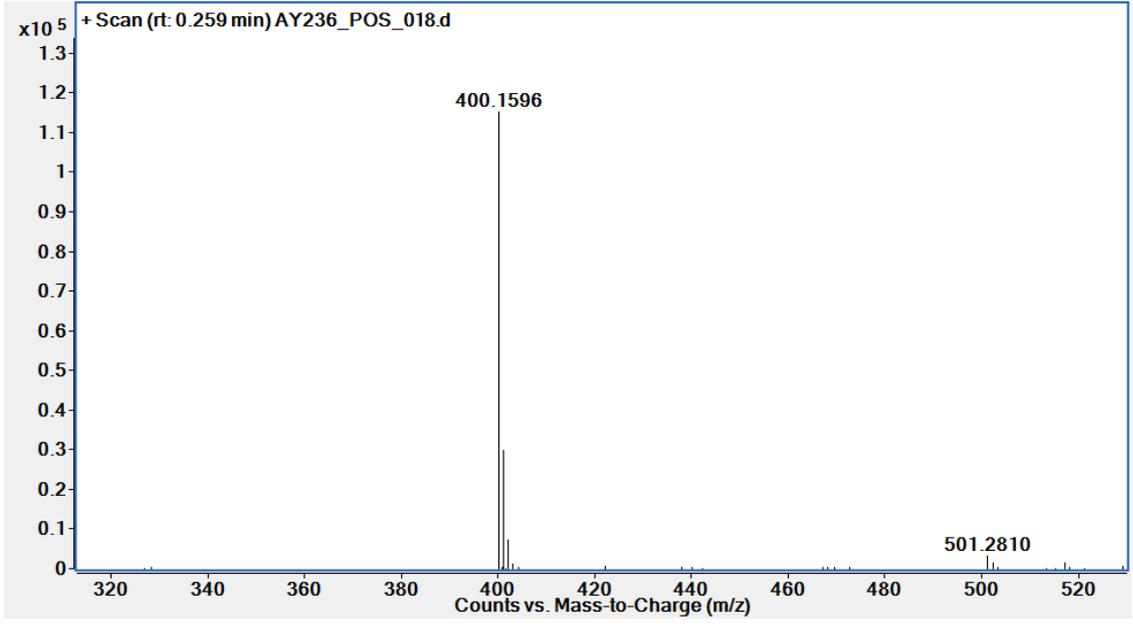
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AY-236



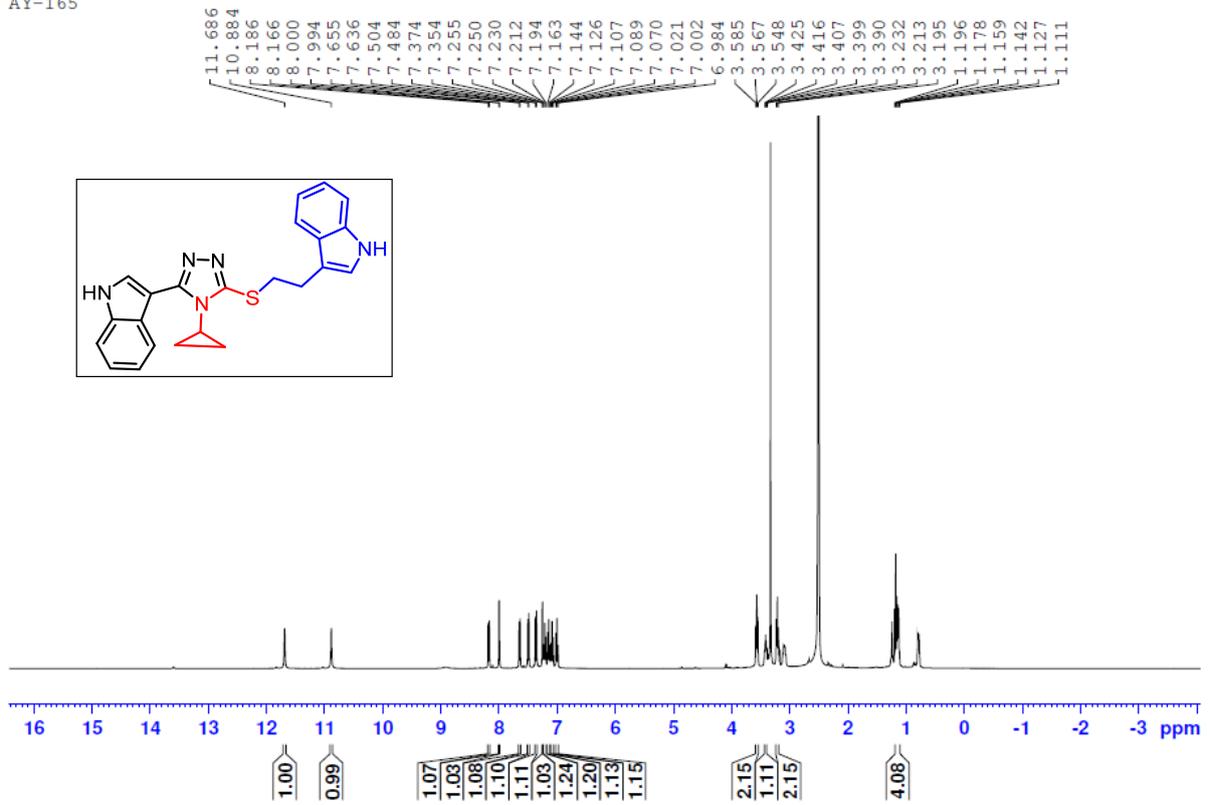
AY-236



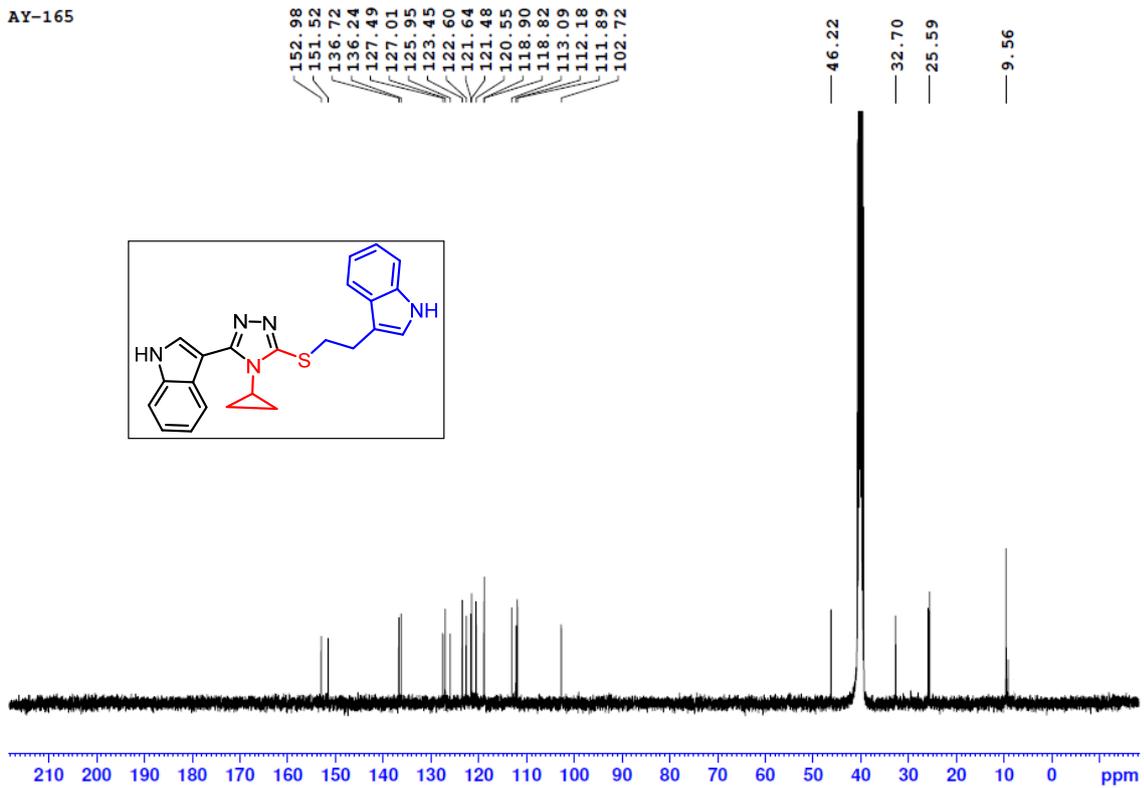


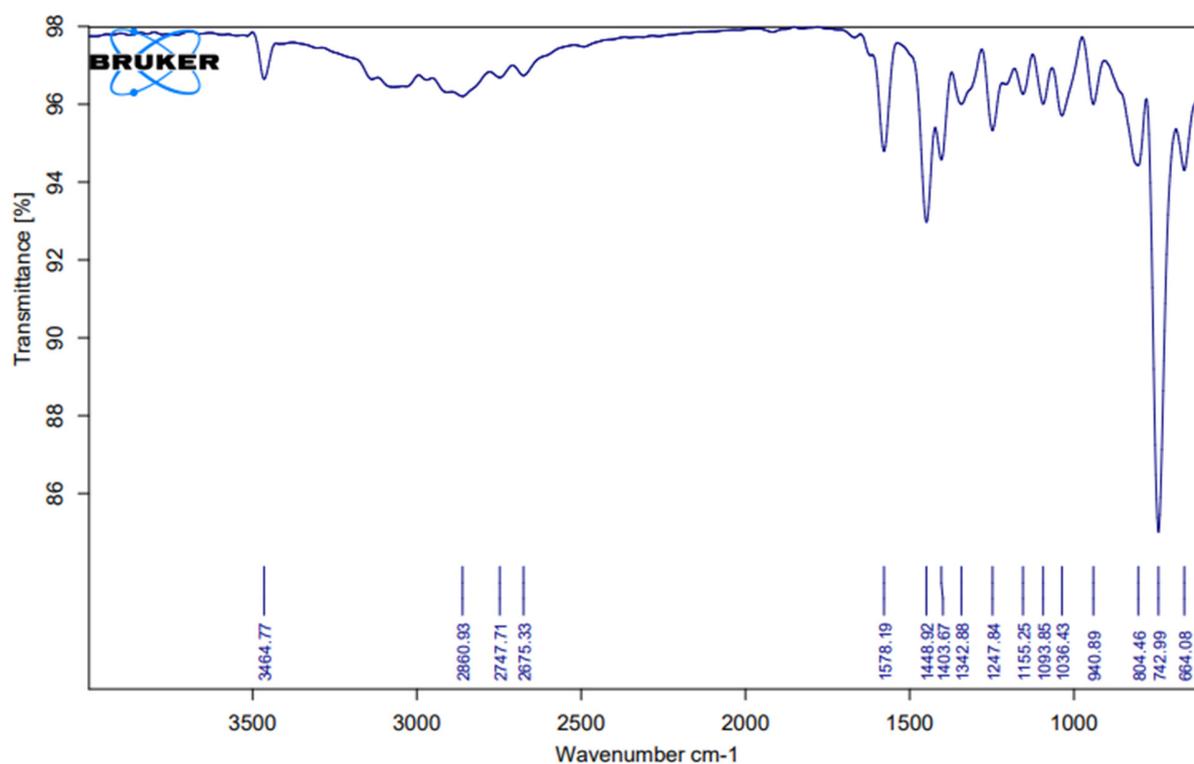
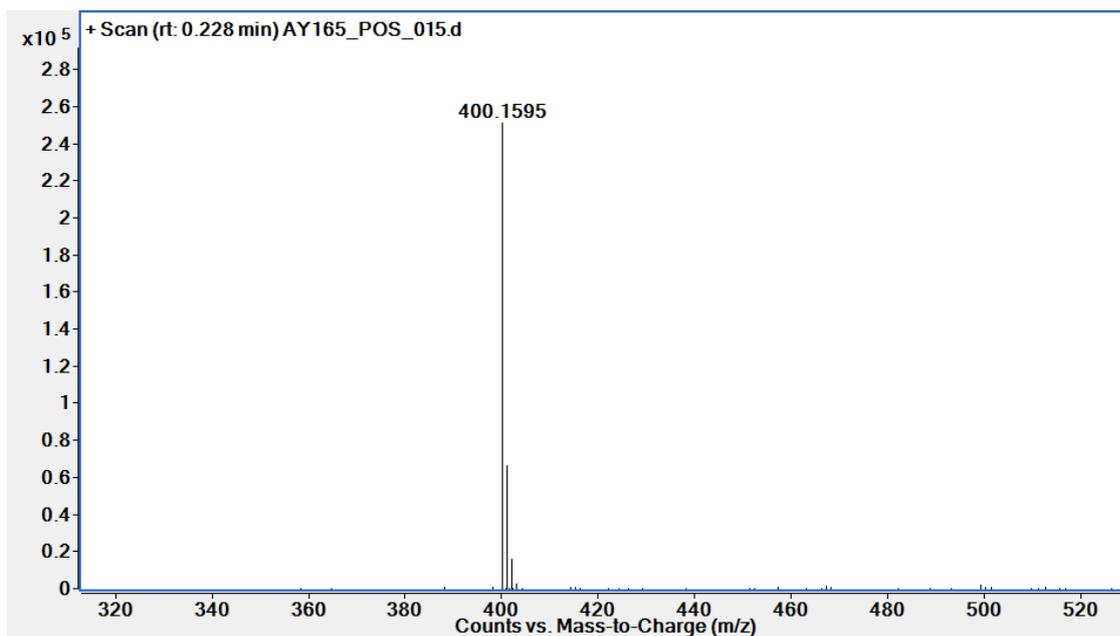
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AY-165



AY-165





C:\Users\NIPERG\Desktop\Dayal\AYAY-165.0	AY-165	Instrument type and / or accessory	01-11-2022
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Figure S3:  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and Mass copies of all products.