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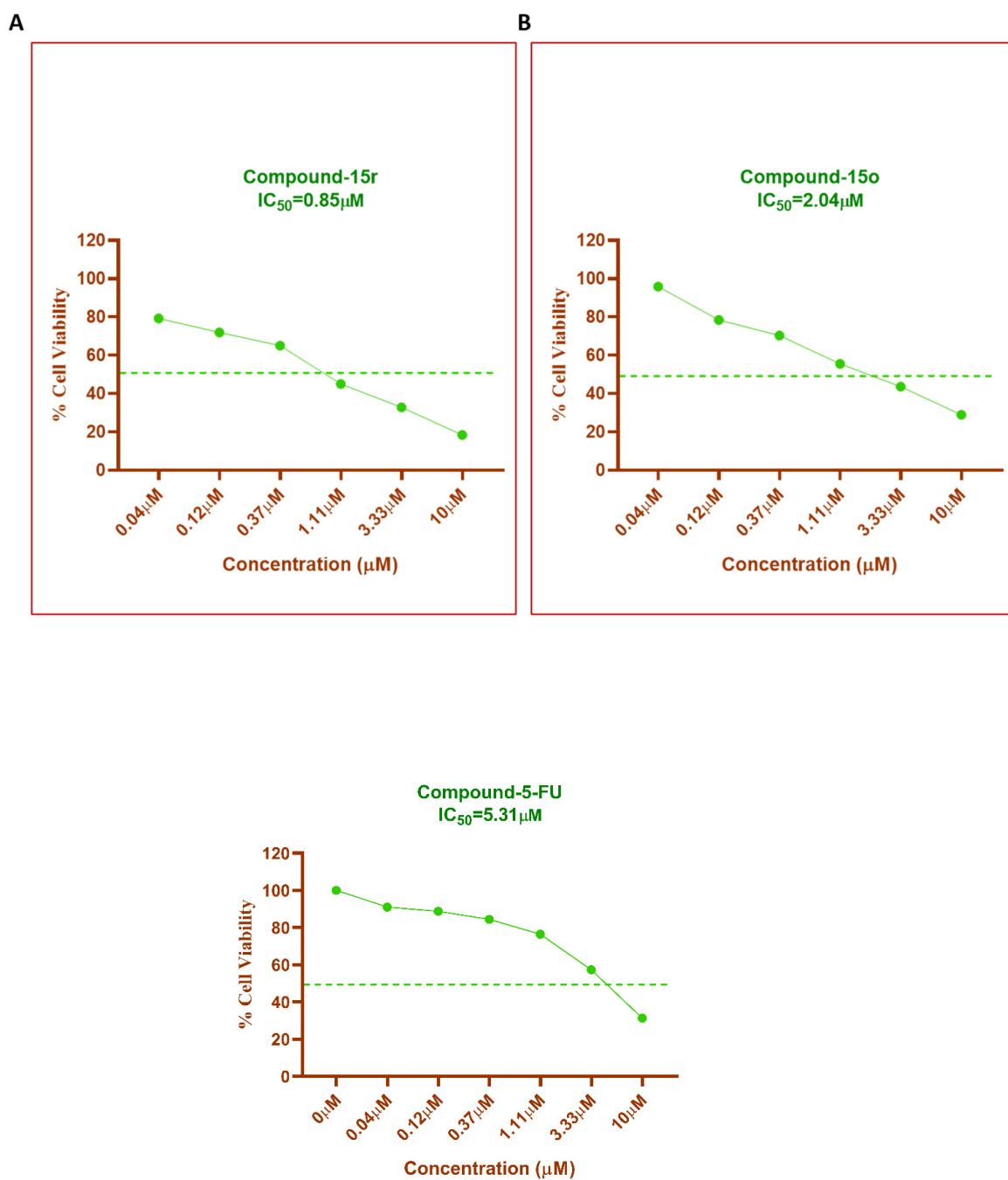
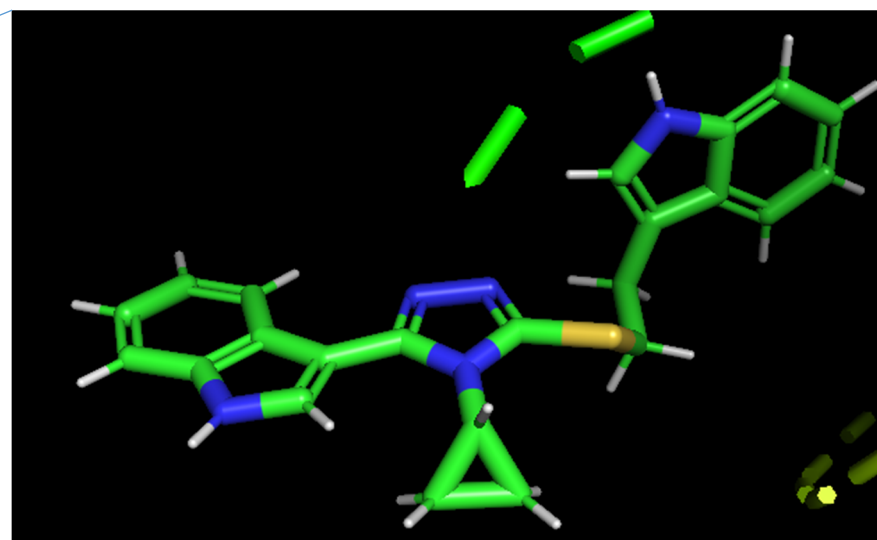
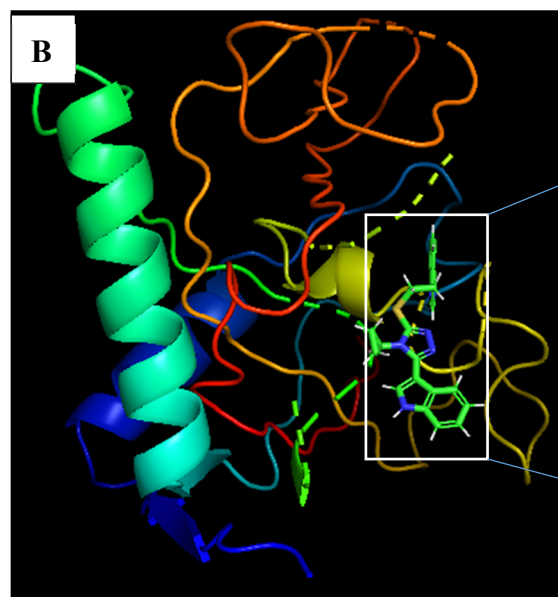
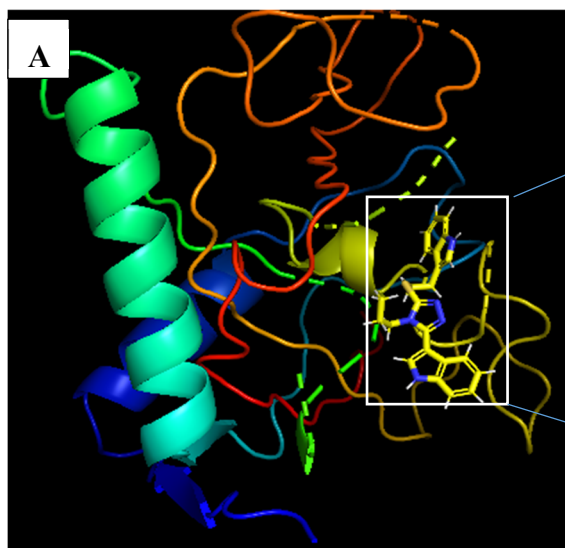
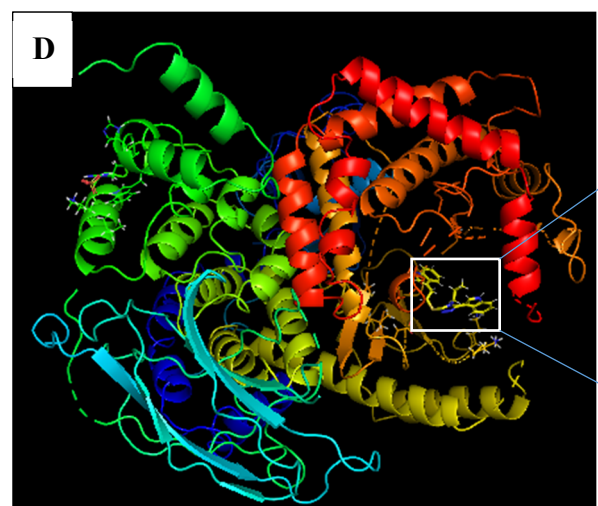
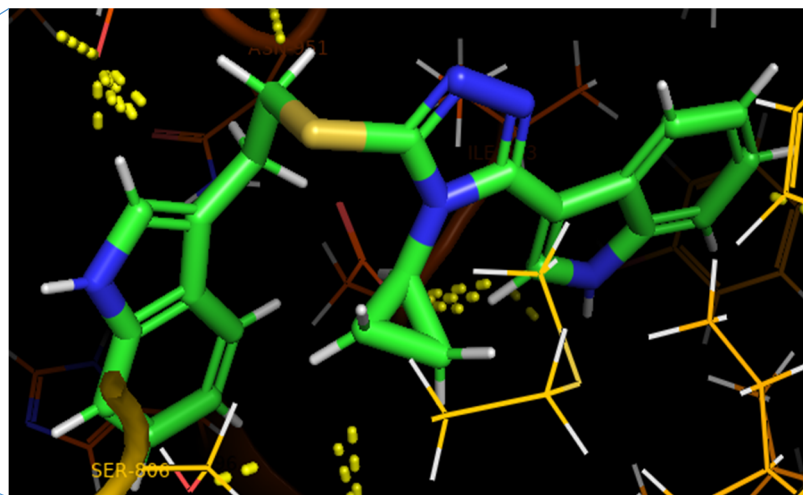
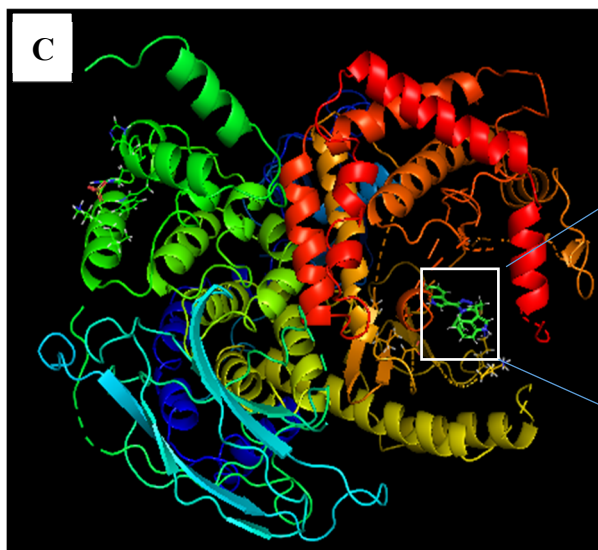
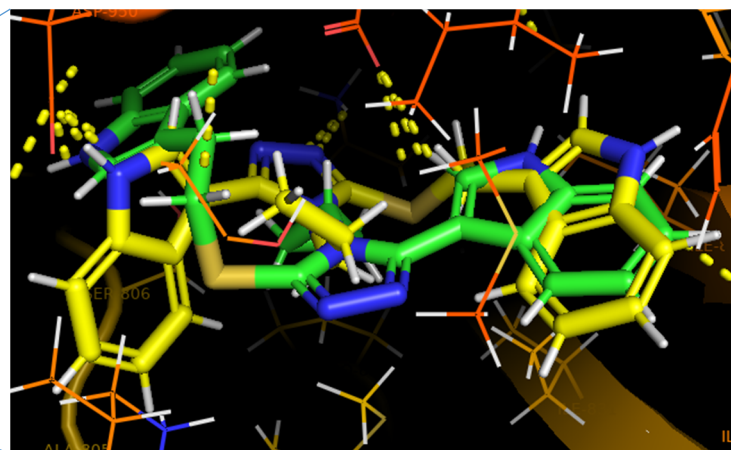
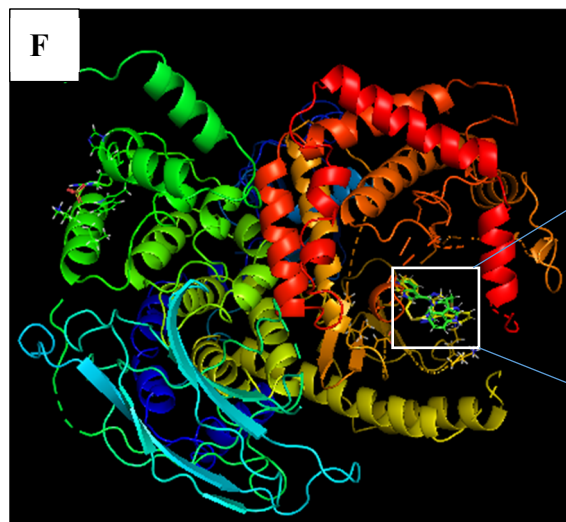
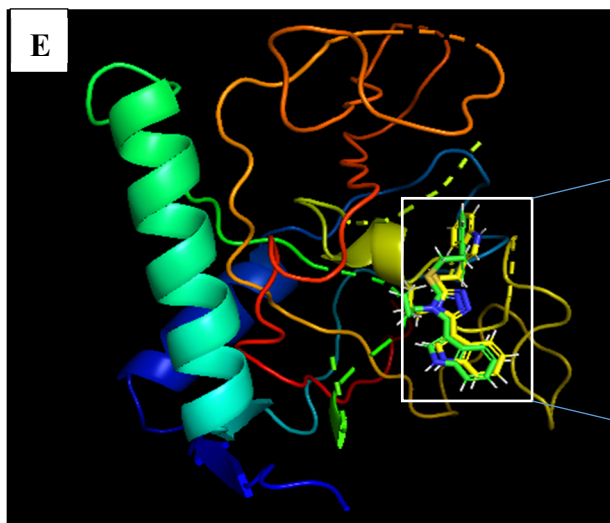


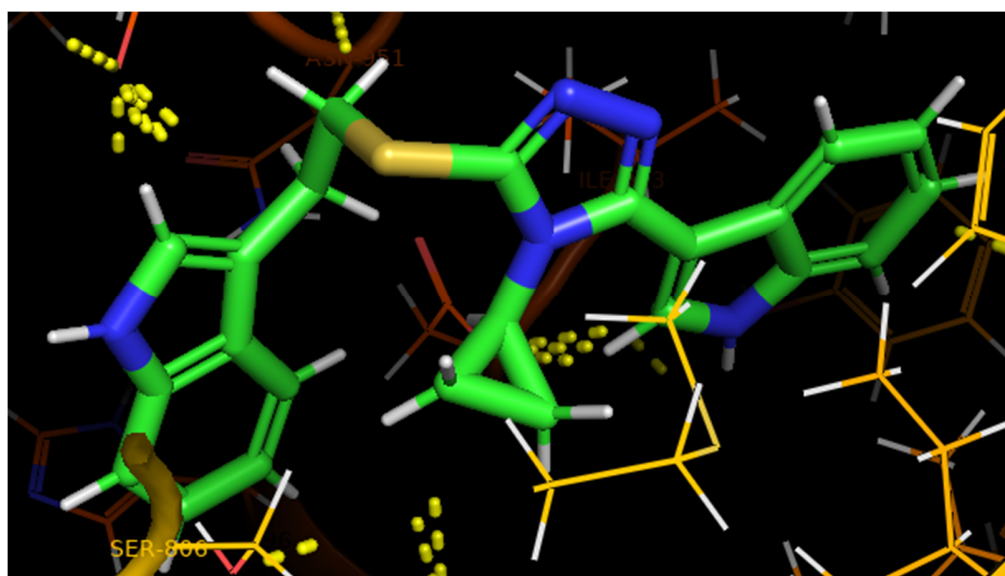
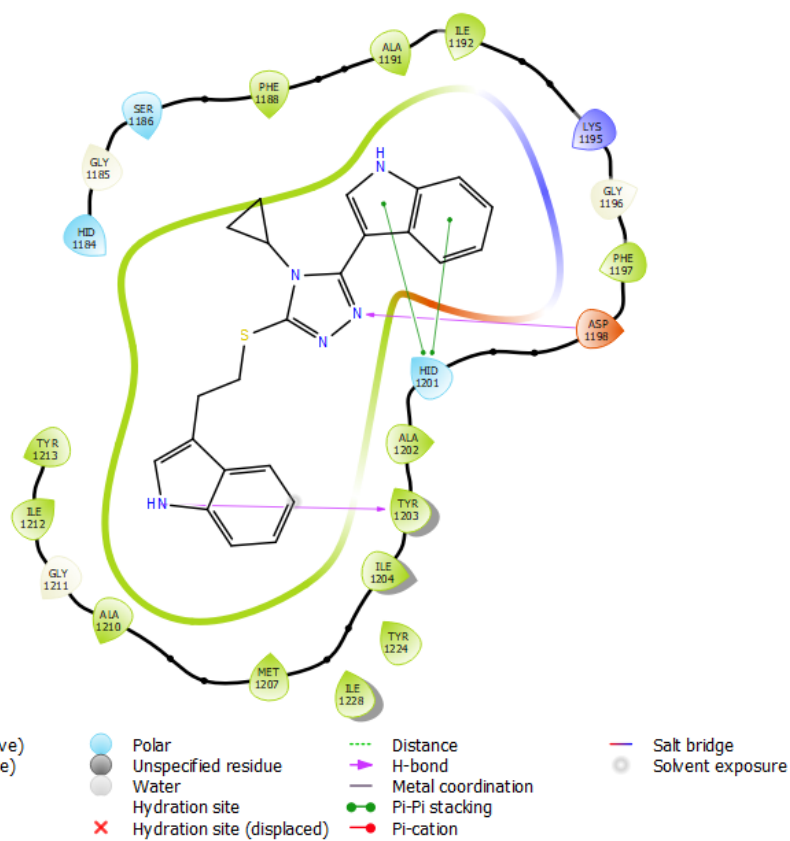
Figure S1: Dose Response Curves for 15r, 15o and Standard compounds against HT-29 colon cancer cell lines.



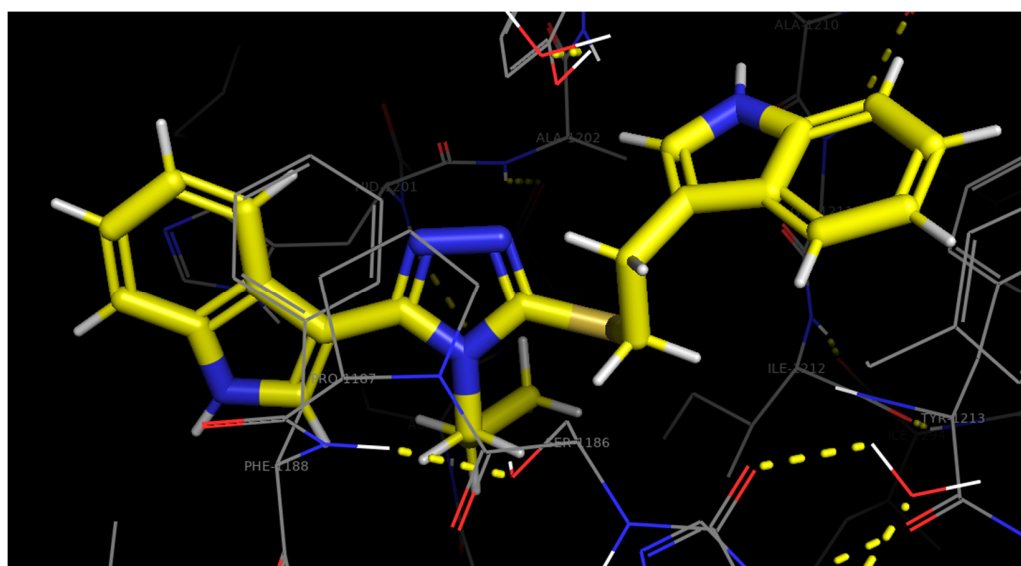
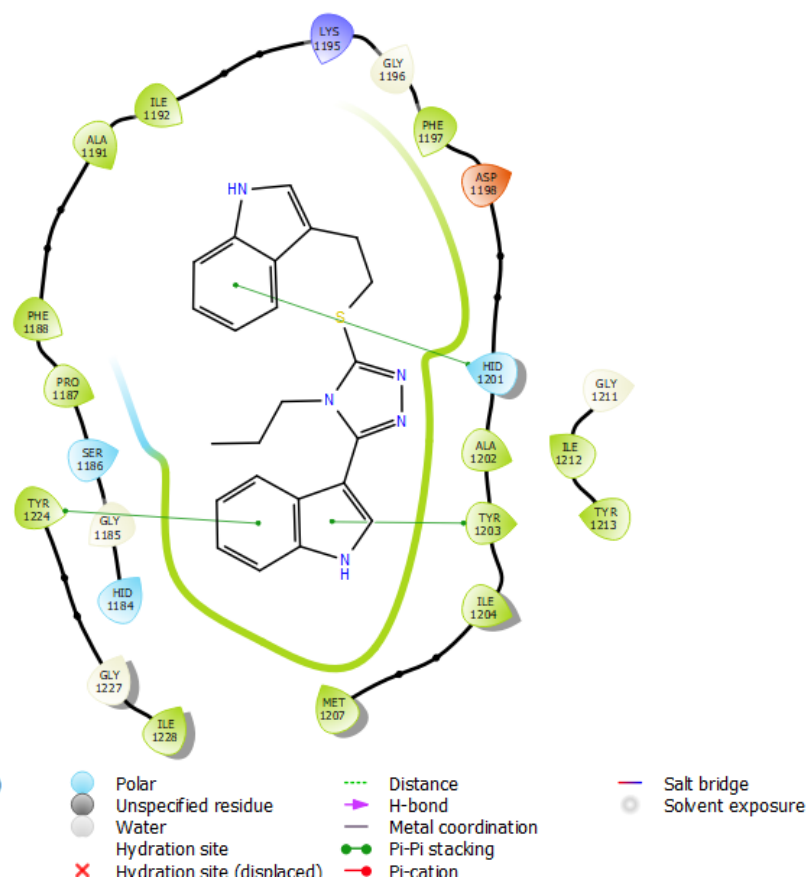




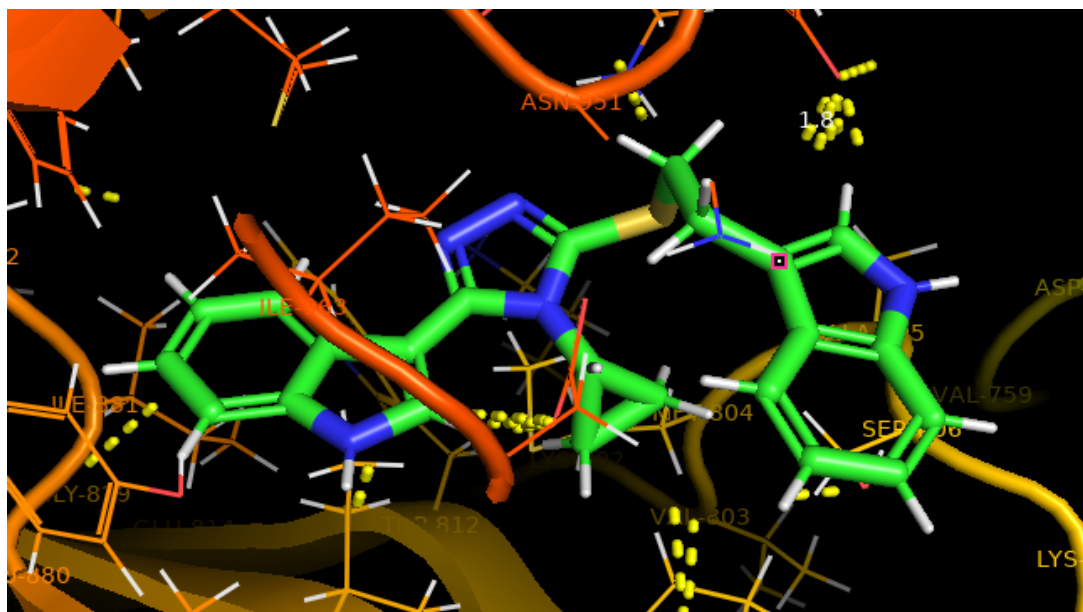
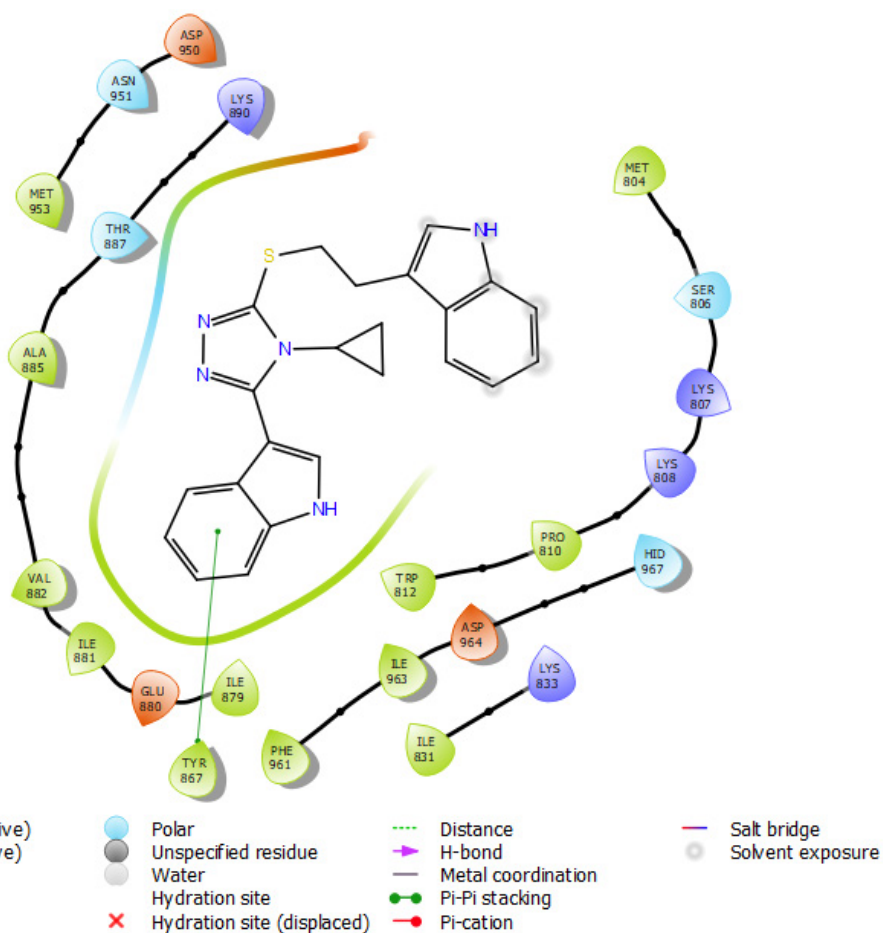
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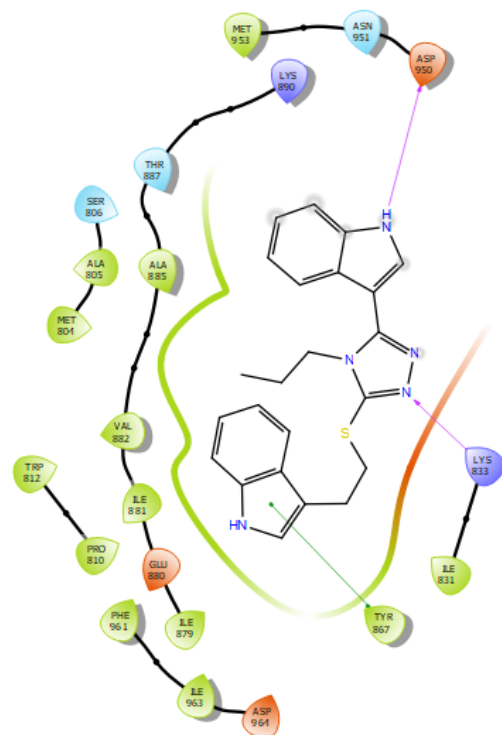
H



I



J



- | | | | |
|----------------------|------------------------------|----------------------|--------------------|
| ● Charged (negative) | ● Polar | --- Distance | — Salt bridge |
| ● Charged (positive) | ● Unspecified residue | → H-bond | ○ Solvent exposure |
| ● Glycine | ● Water | — Metal coordination | |
| ● Hydrophobic | ● Hydration site | ● Pi-Pi stacking | |
| ● Metal | ✗ Hydration site (displaced) | ● Pi-cation | |

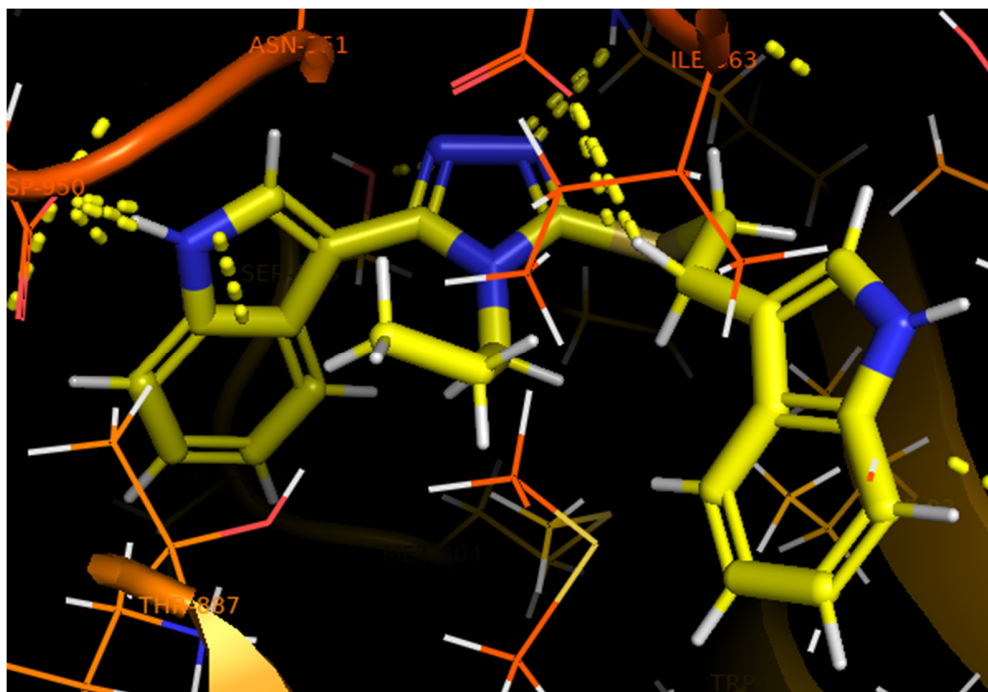
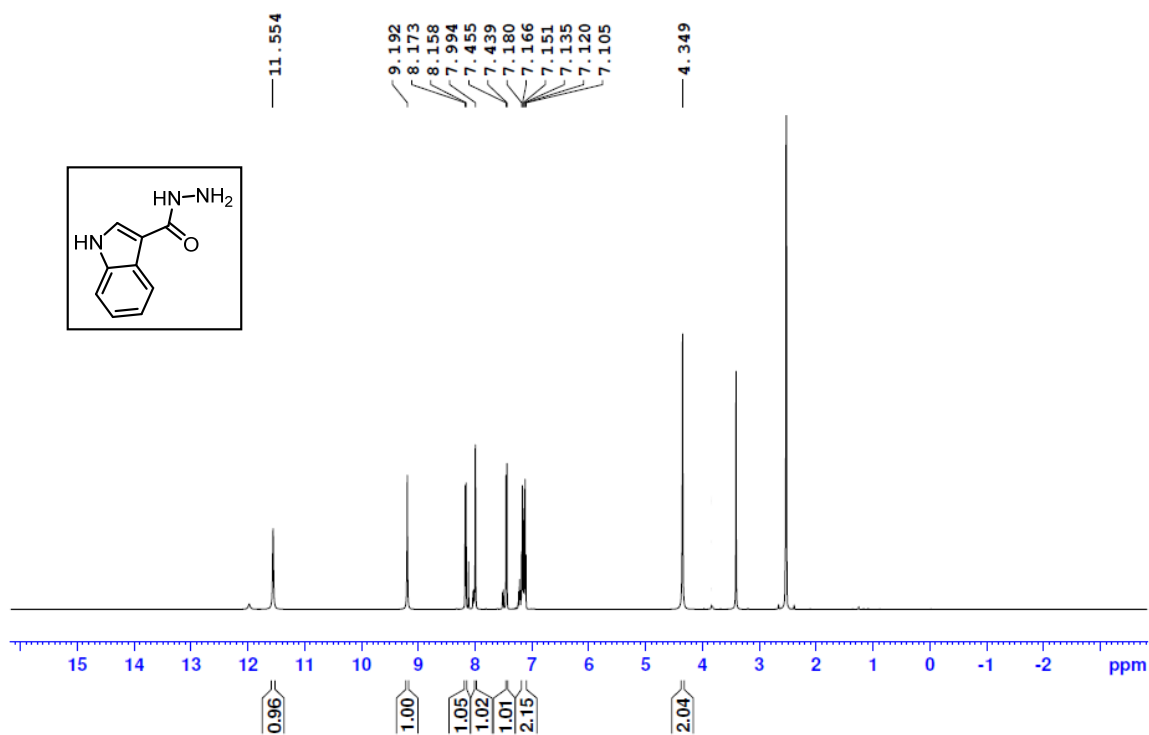
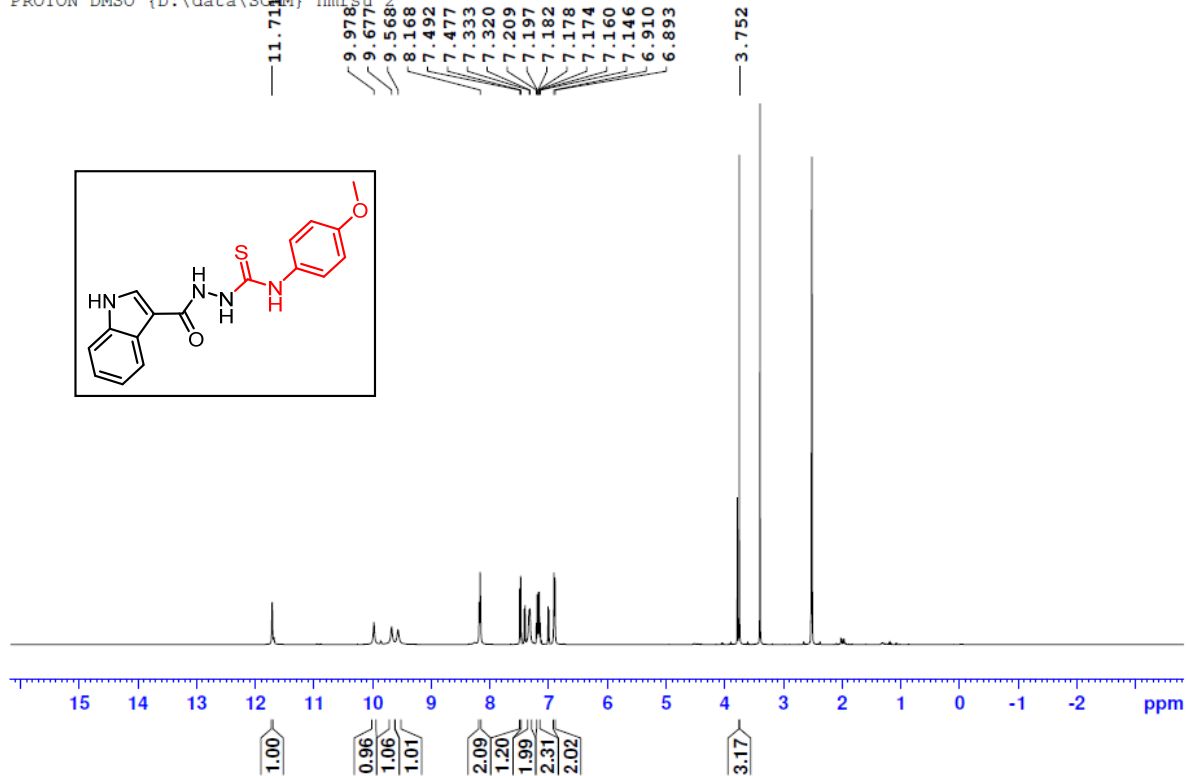


Figure S2. (A) Docking pose of 15o in PDB ID 4OA7 is shown in a 3D structure; (B) Docking pose of 15r in PDB ID 4OA7 is shown in a 3D structure. (C) Docking pose of 15r in PDB ID 3L54 is shown in a 3D structure; (D) Docking pose of 15o in PDB ID 3L54 is shown in a 3D structure. (E) Docking pose of 15o & 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.

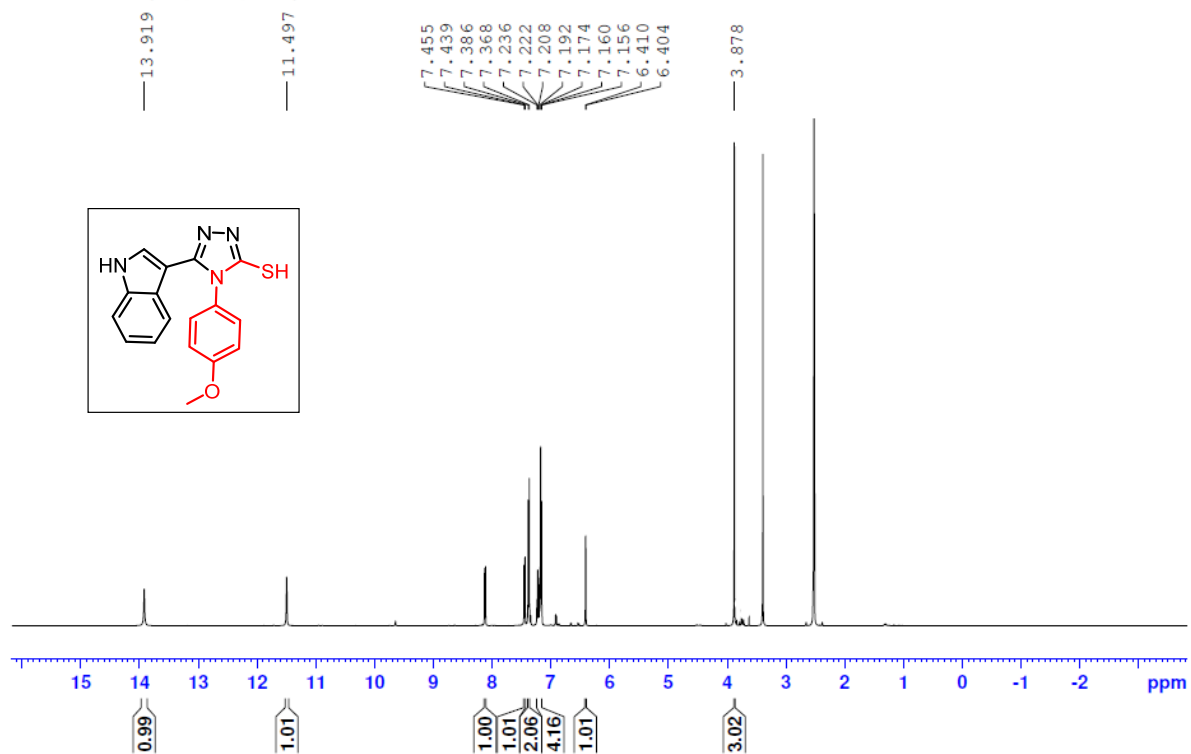
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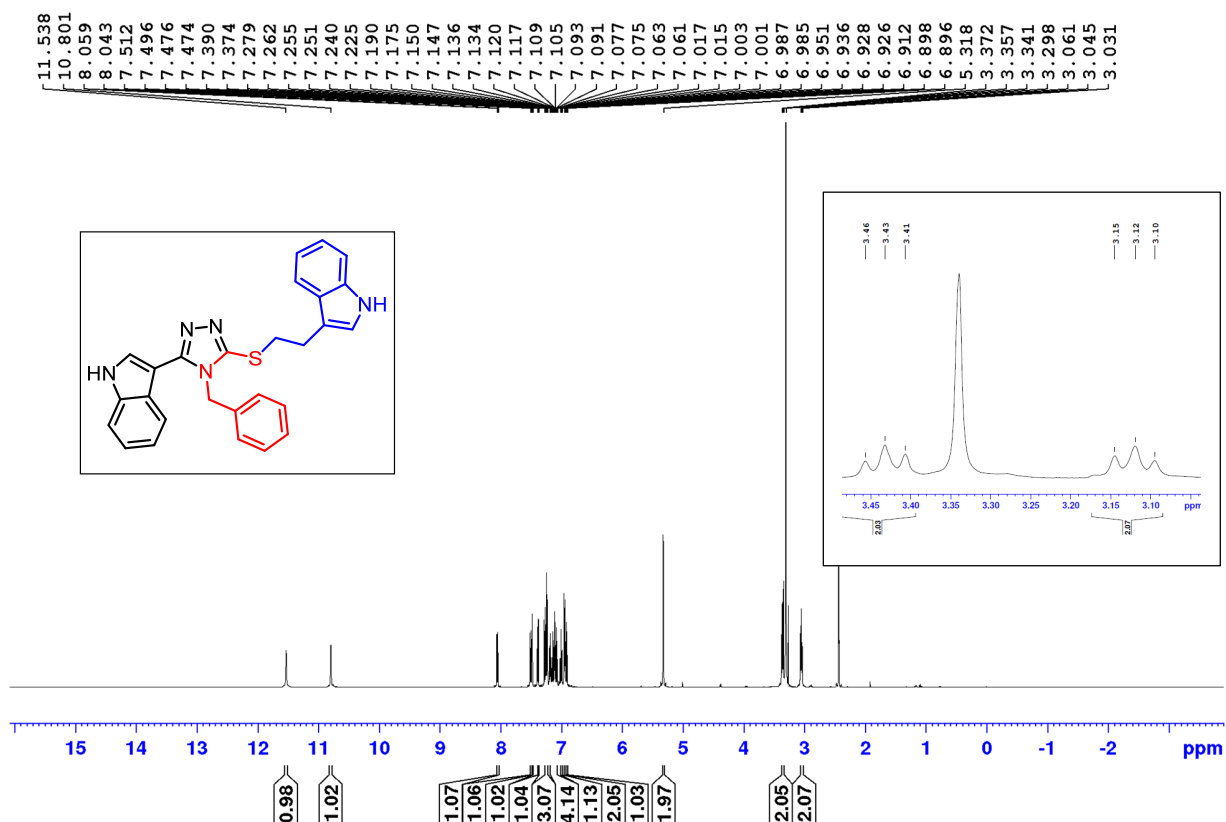


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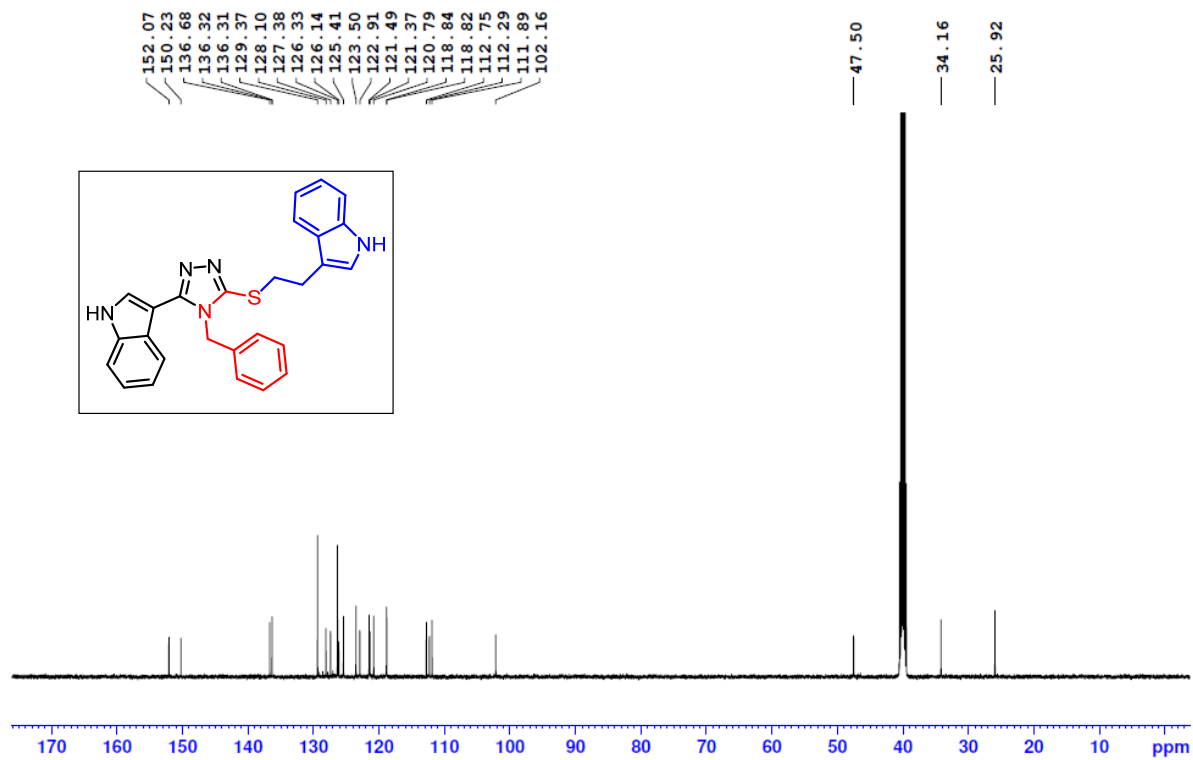


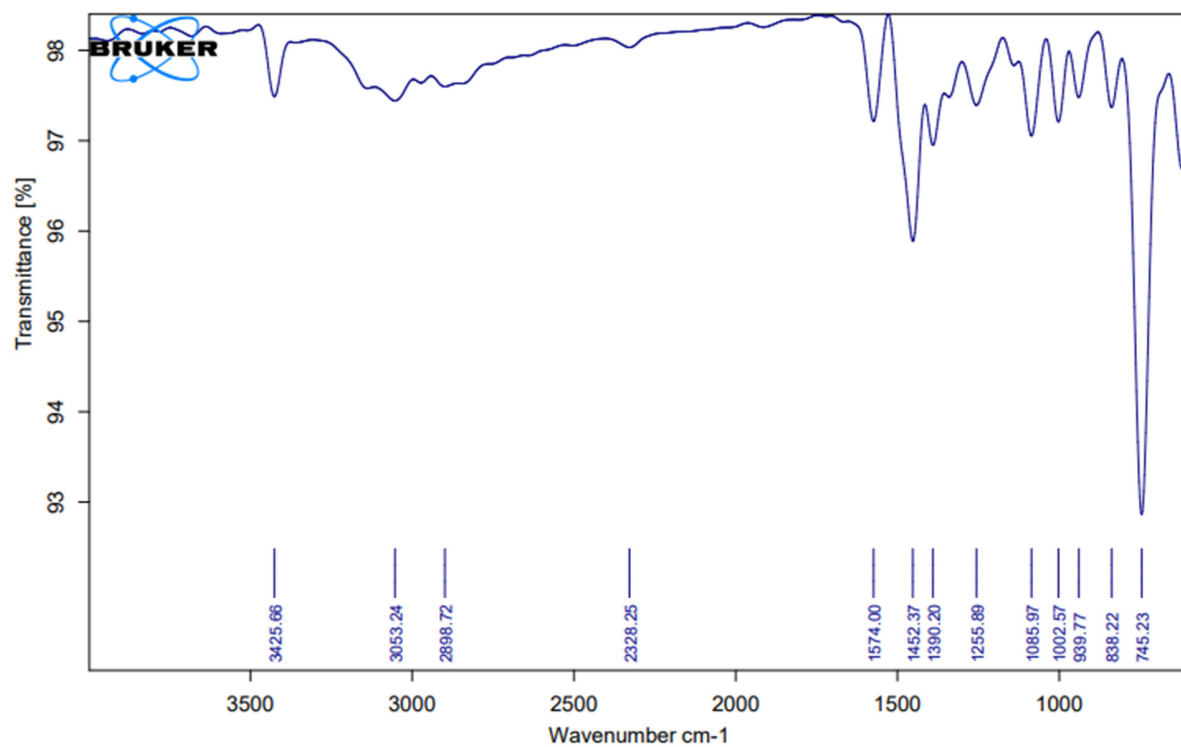
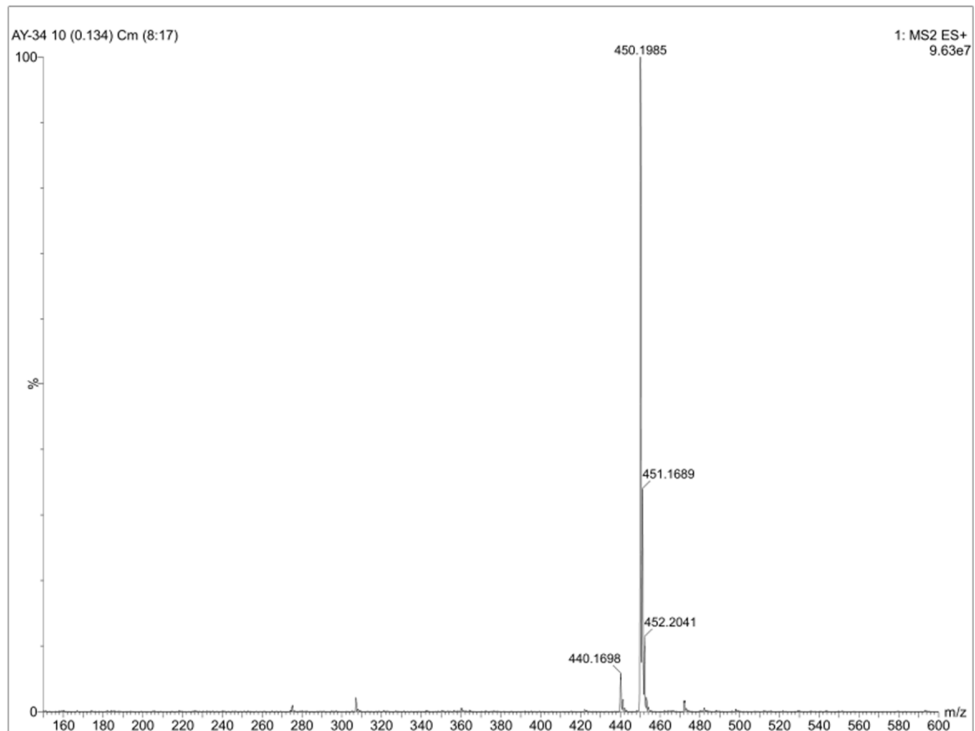
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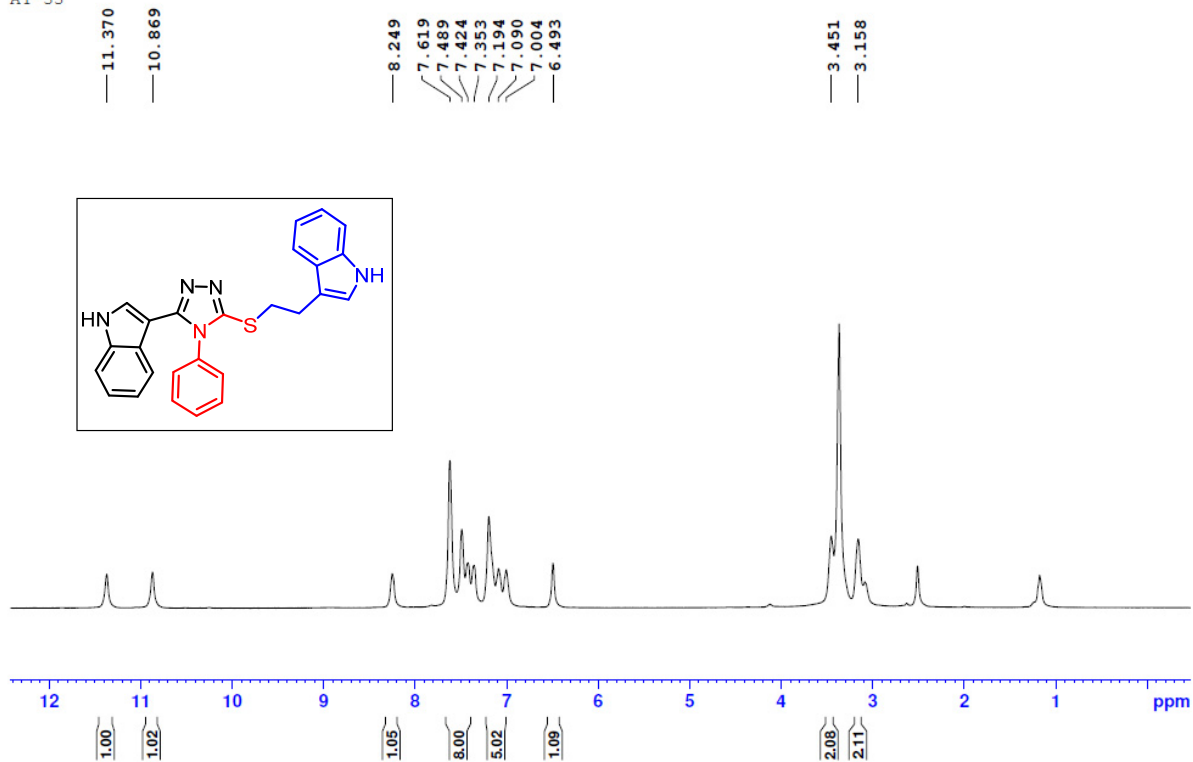
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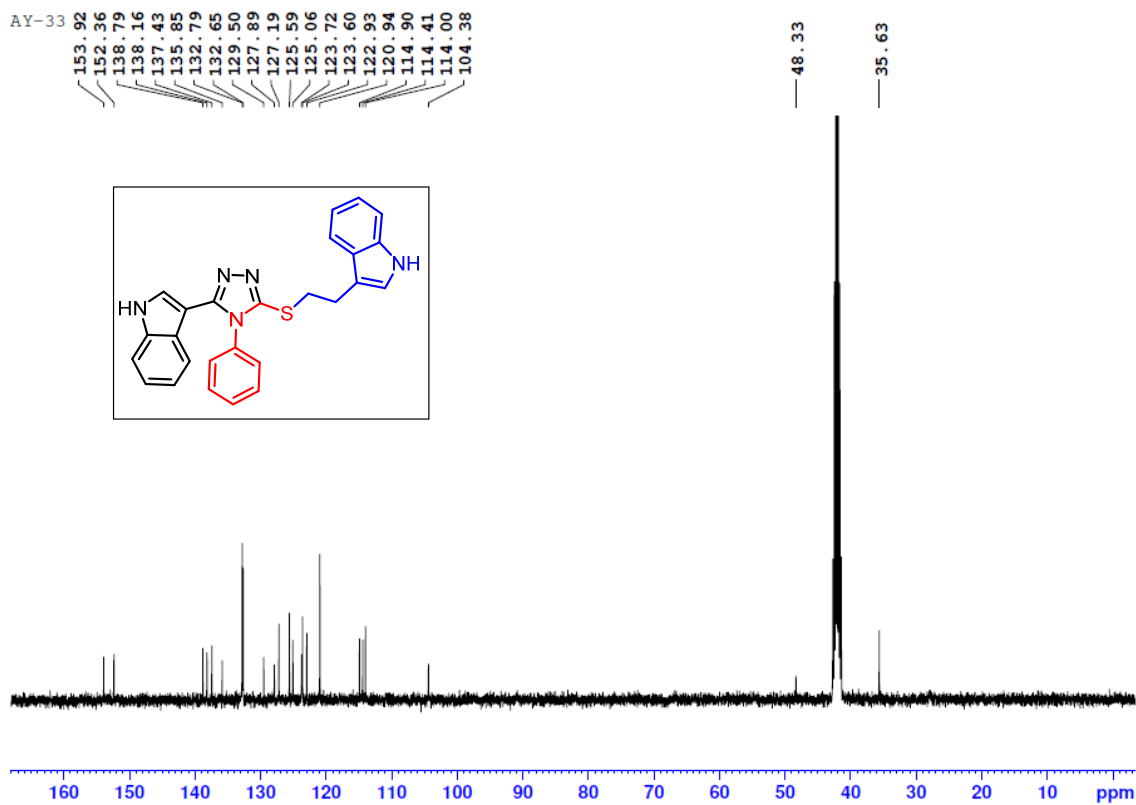
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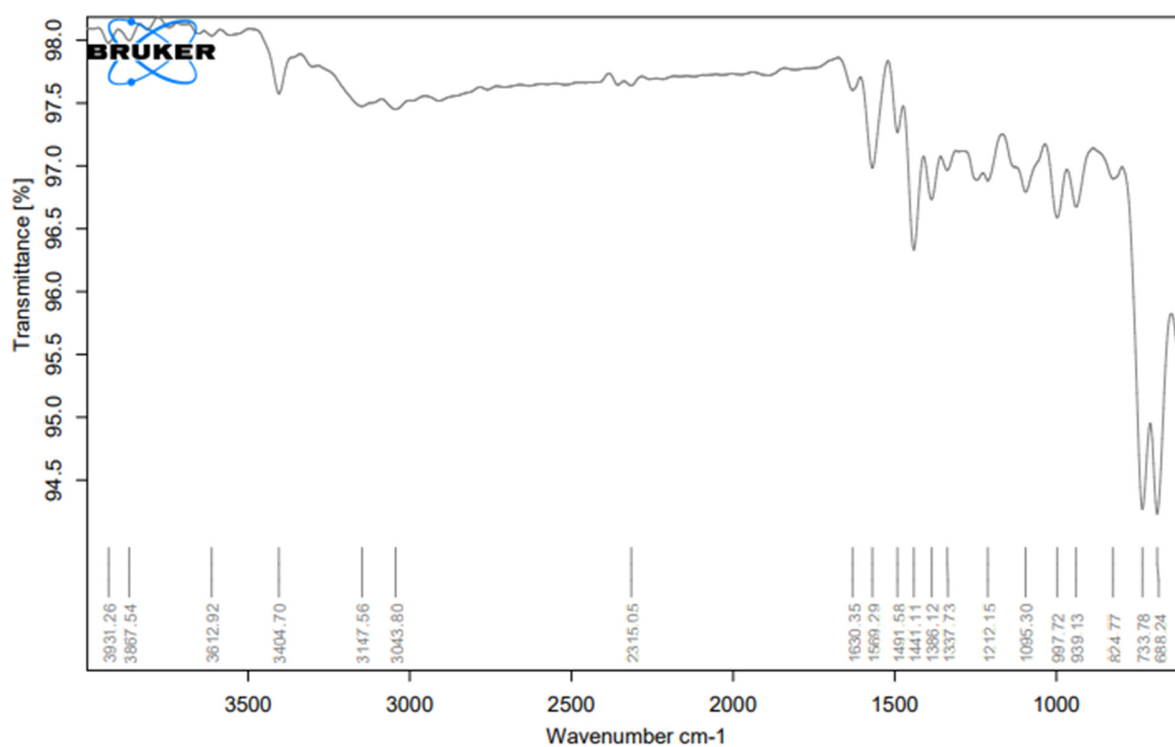
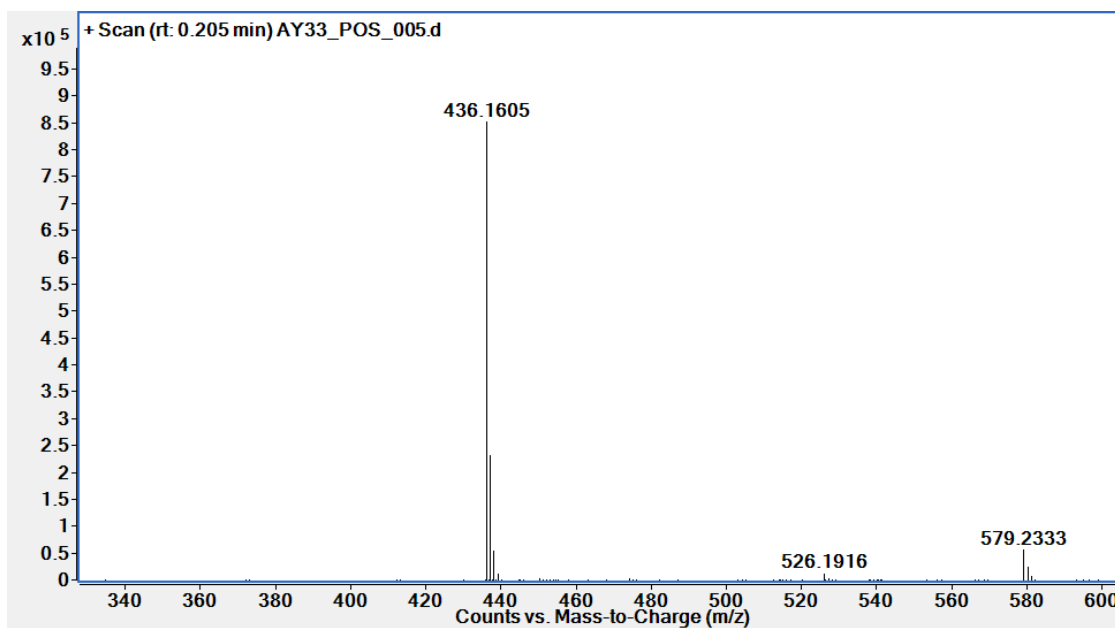
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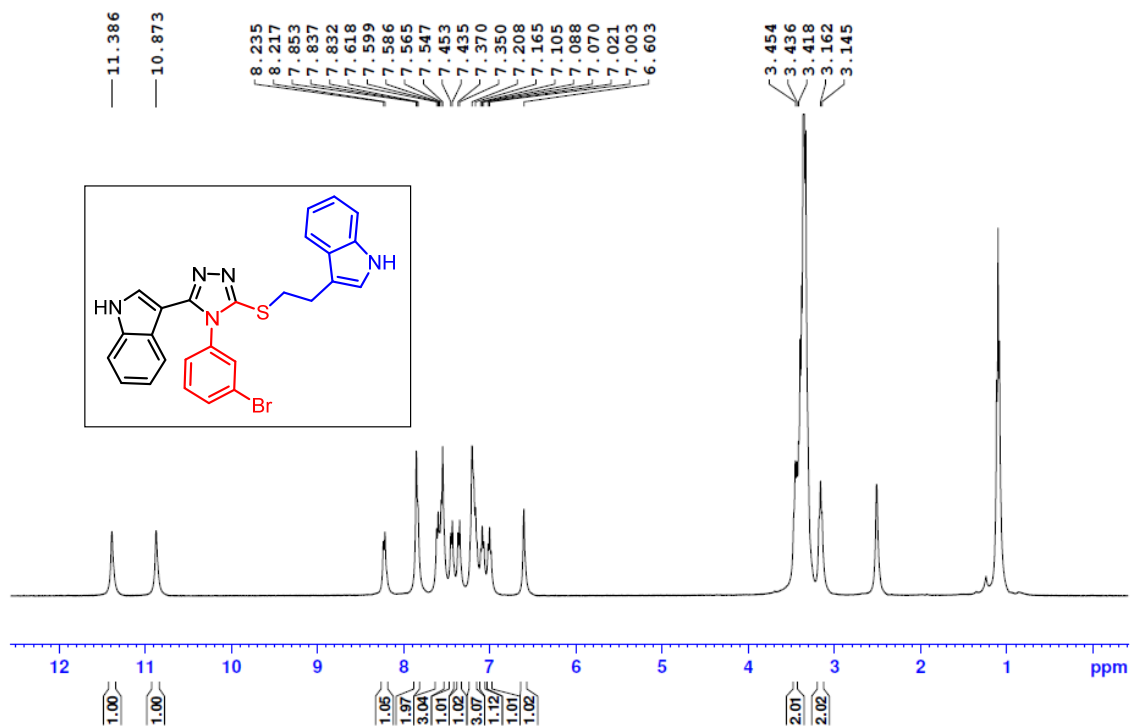
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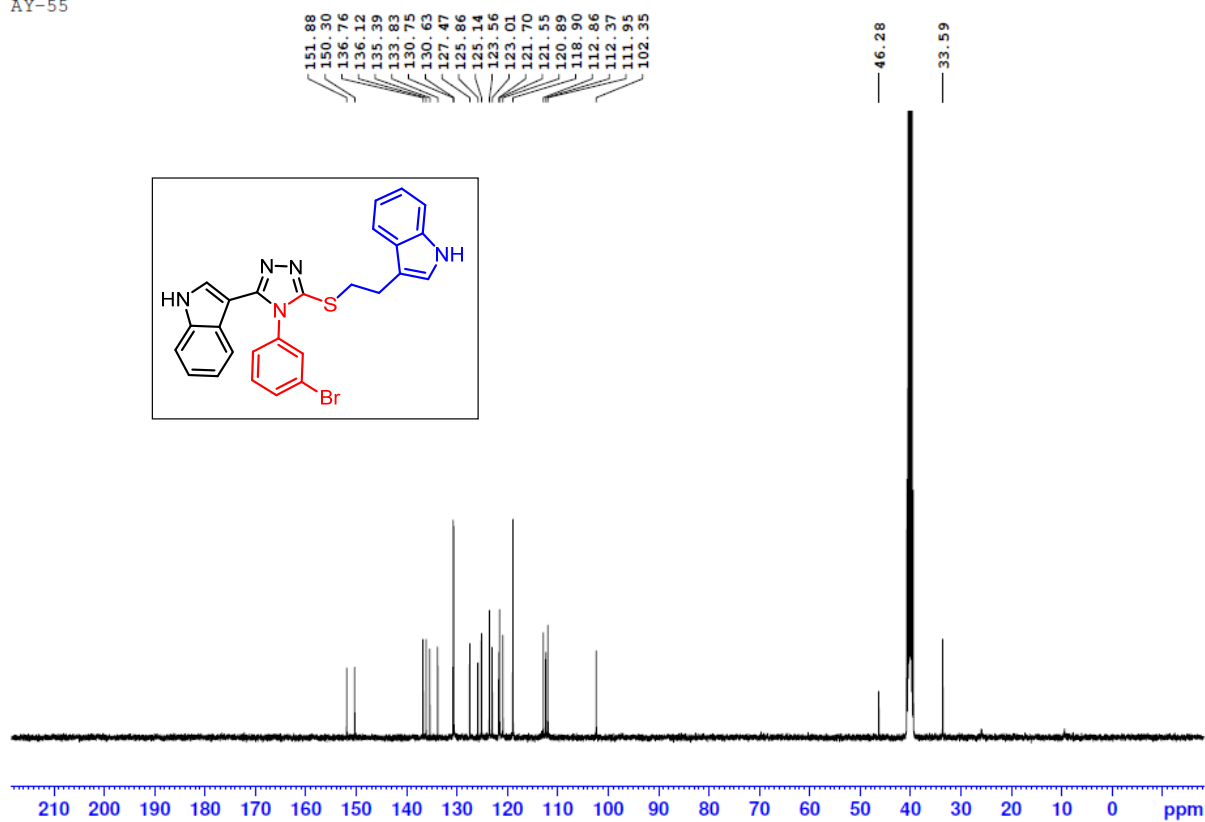
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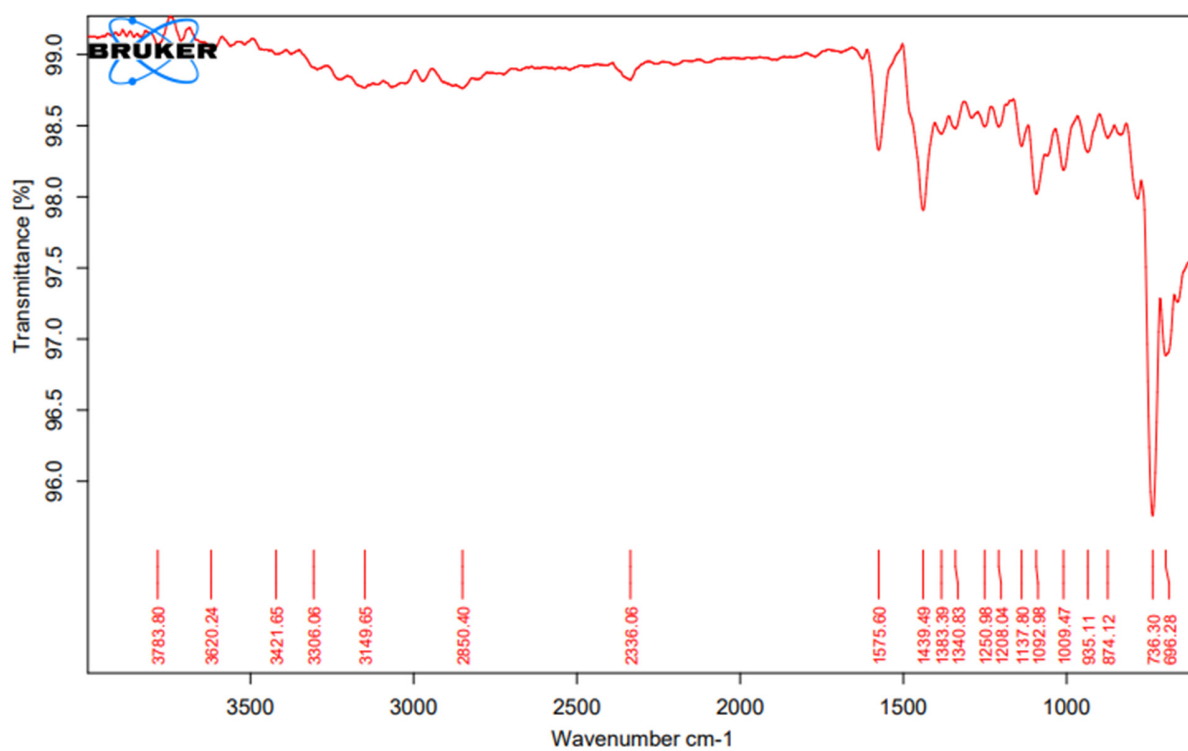
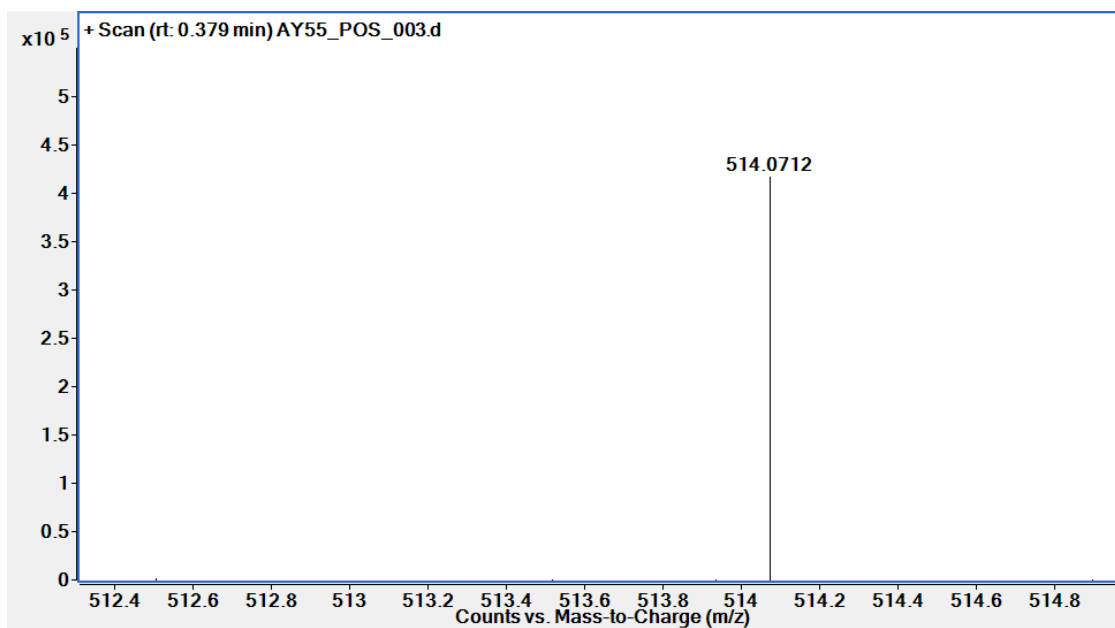
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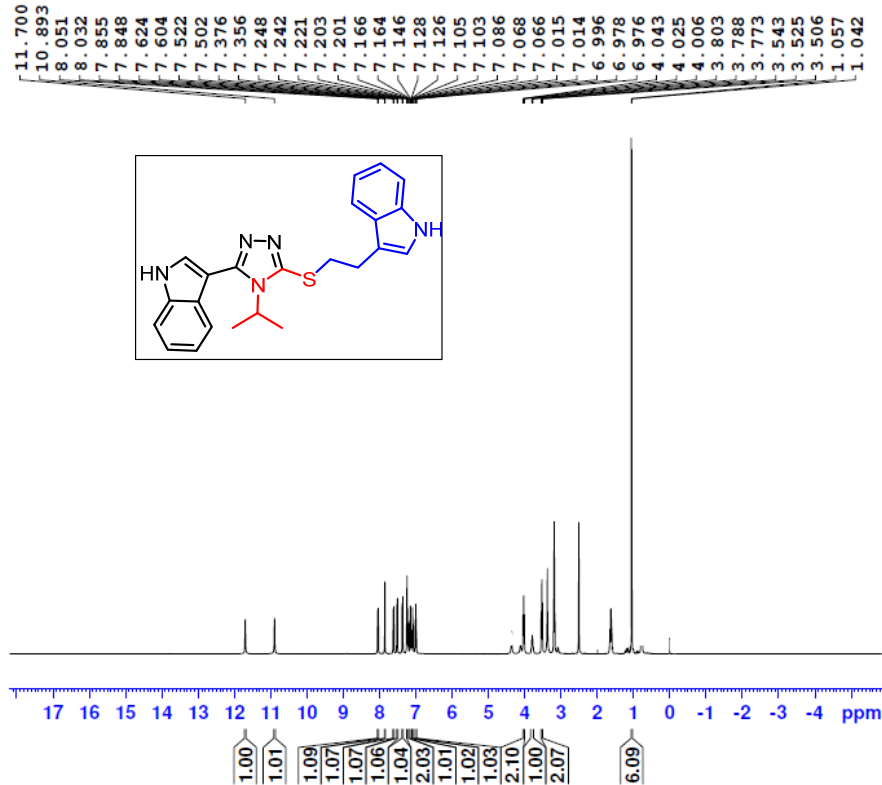
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Instrument type and / or accessory

31-10-2022

A4-159



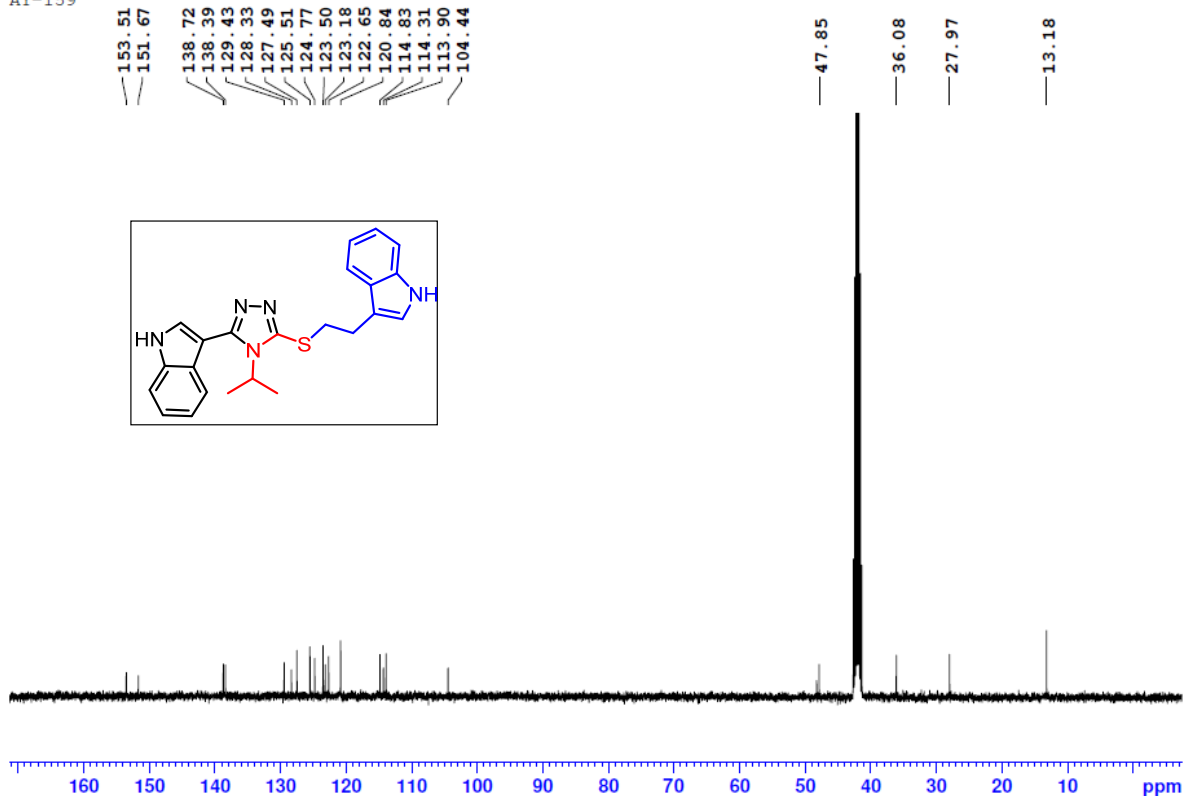
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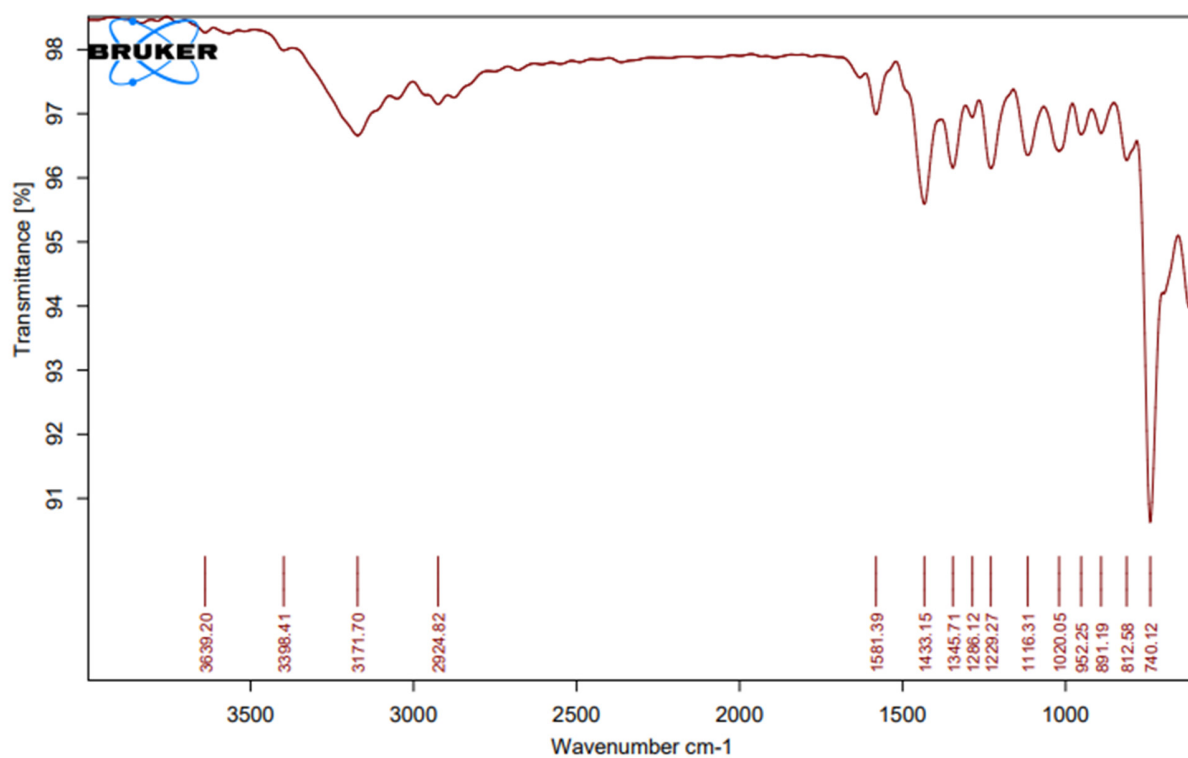
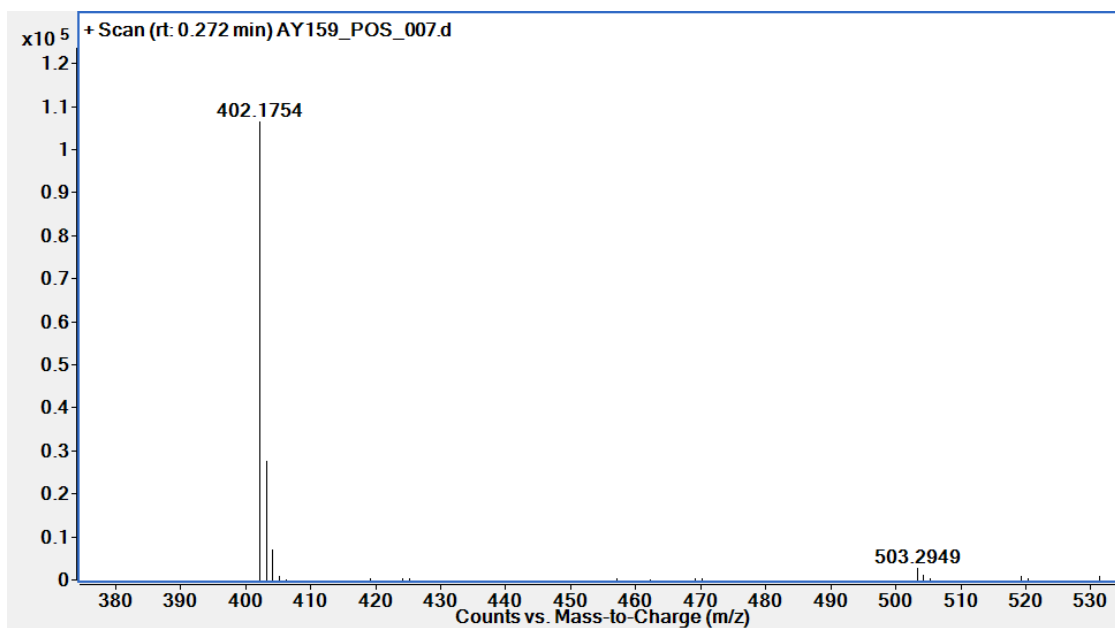
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FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 58.68
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
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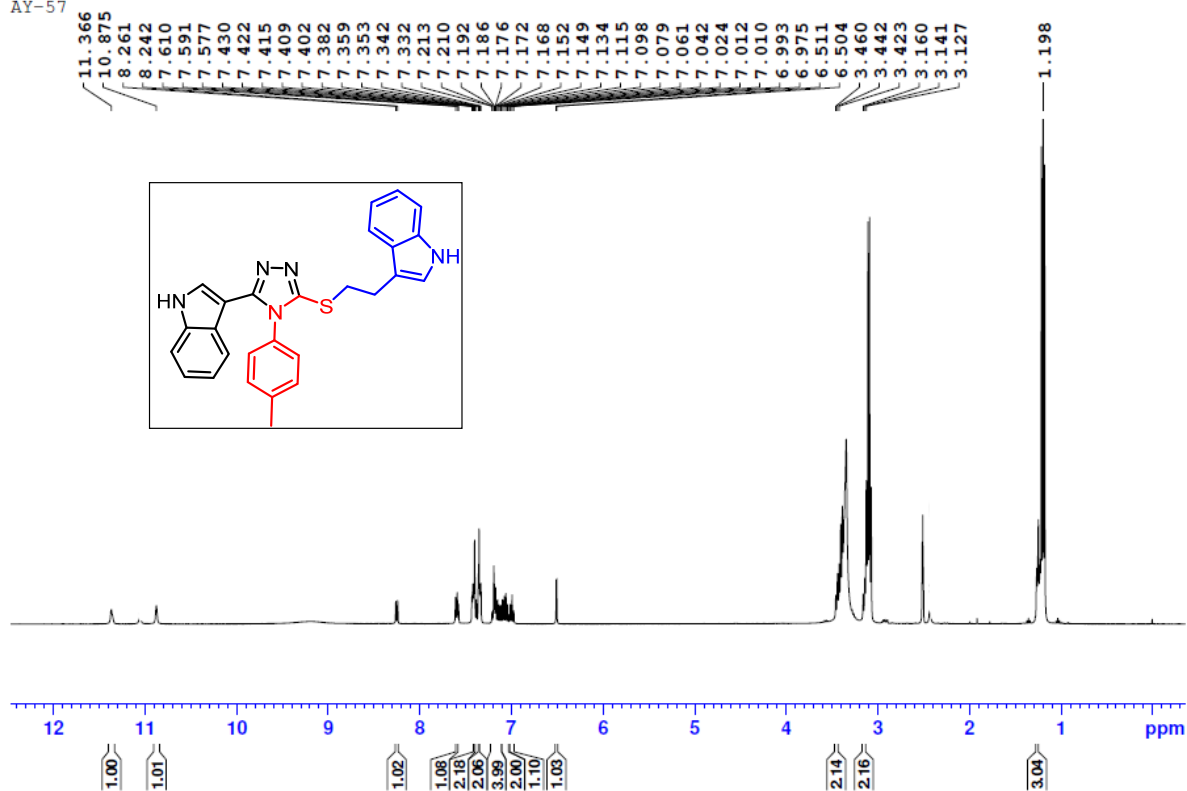
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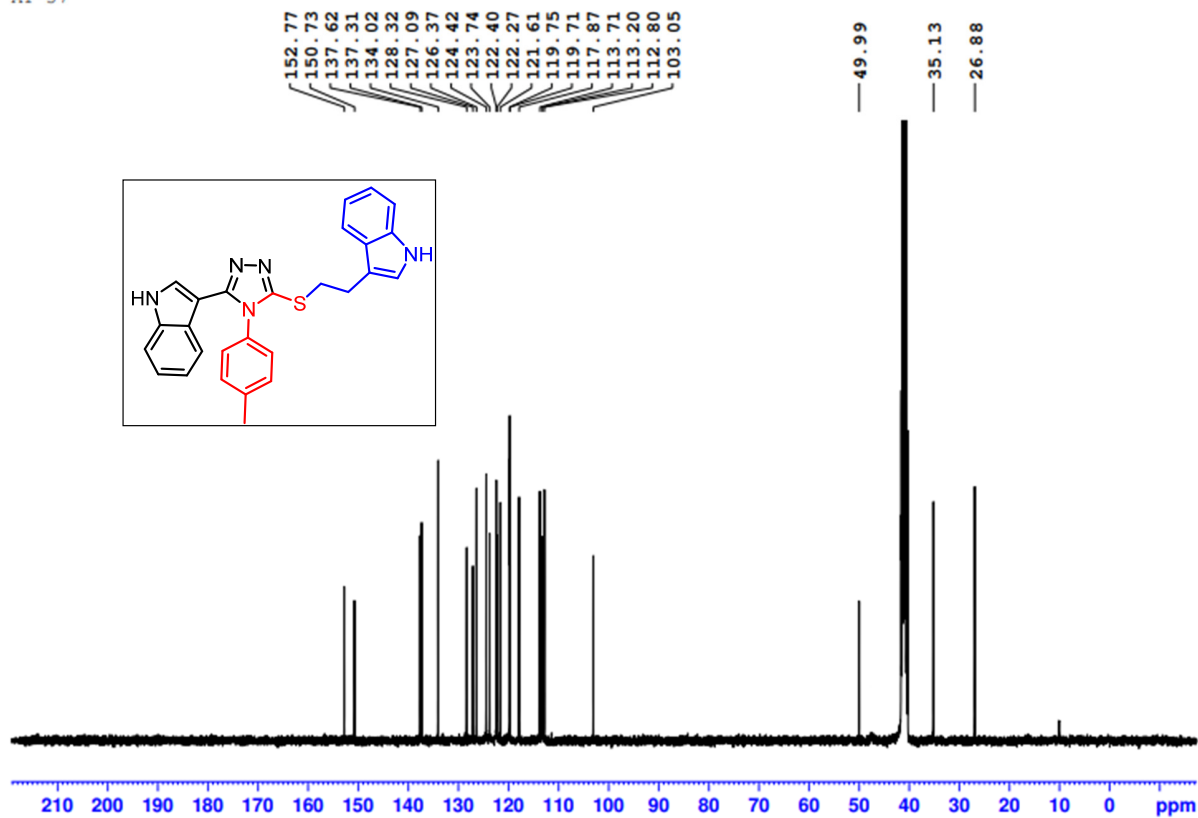
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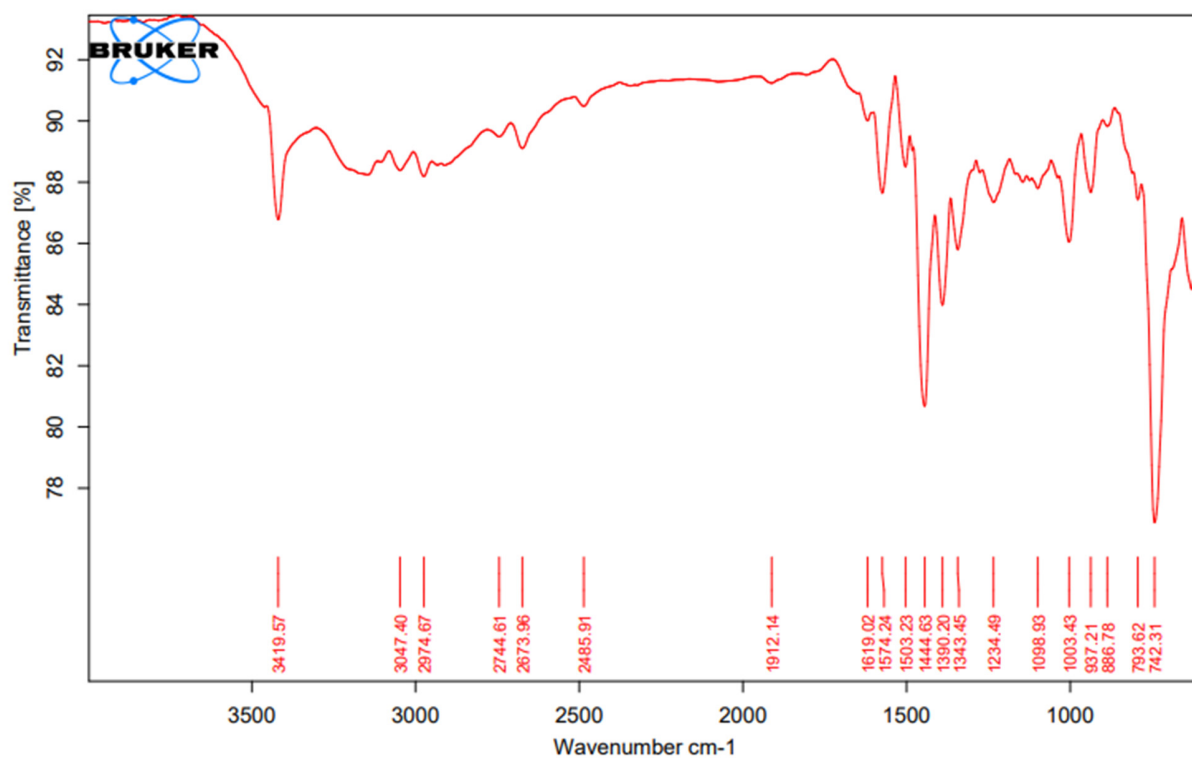
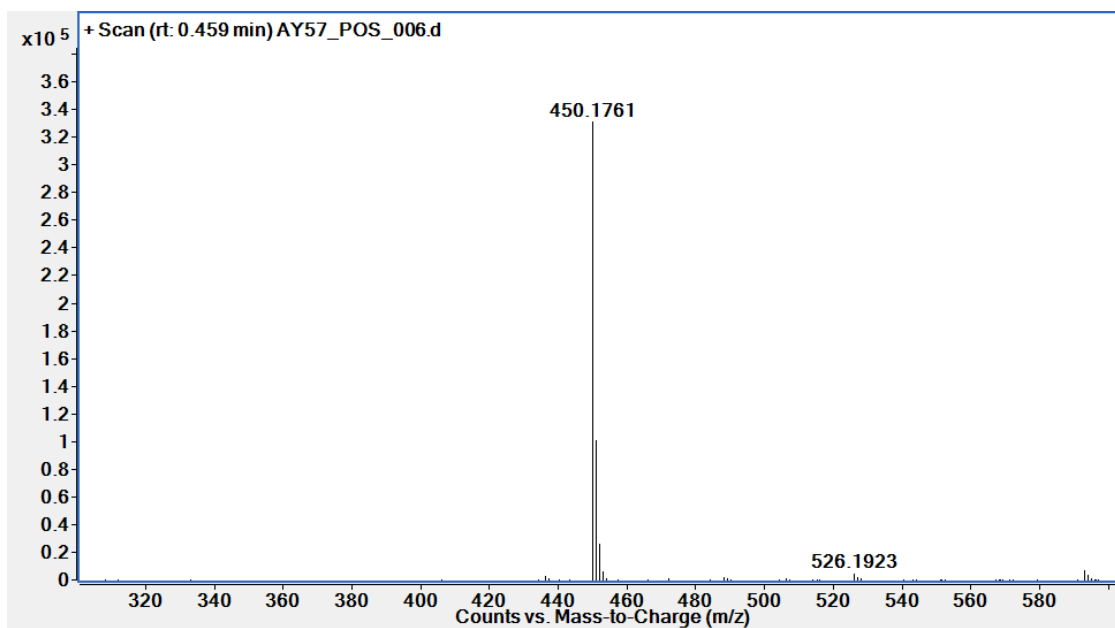
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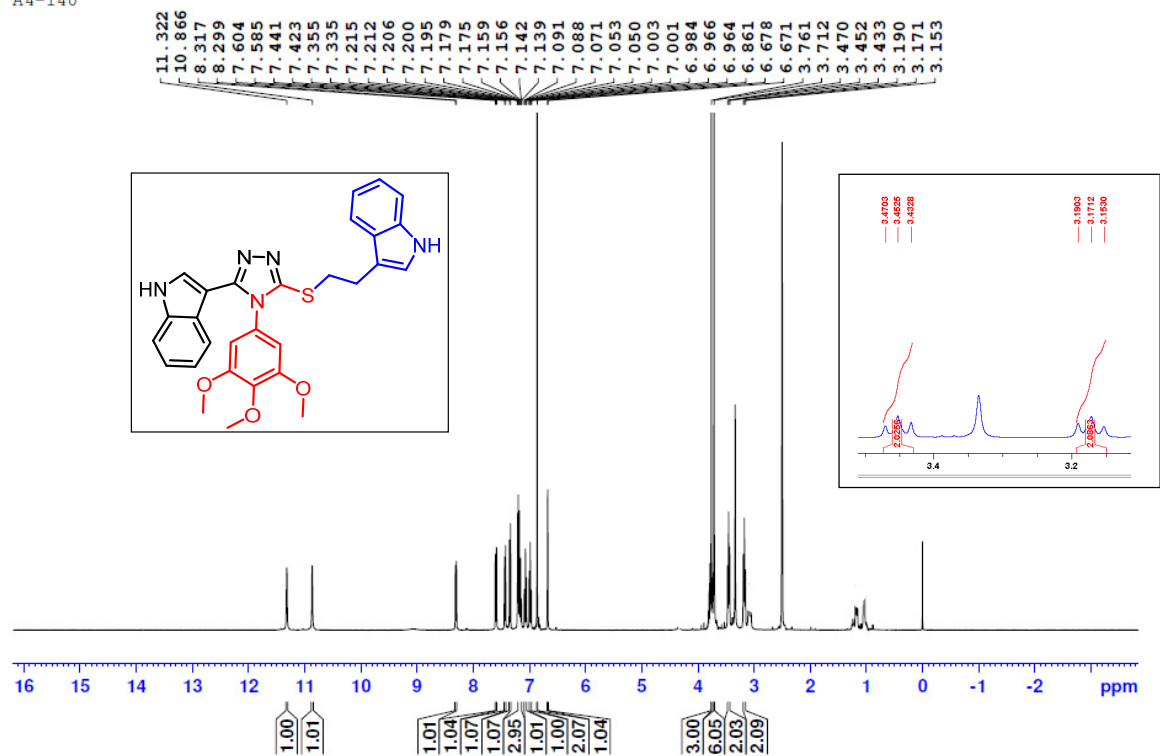
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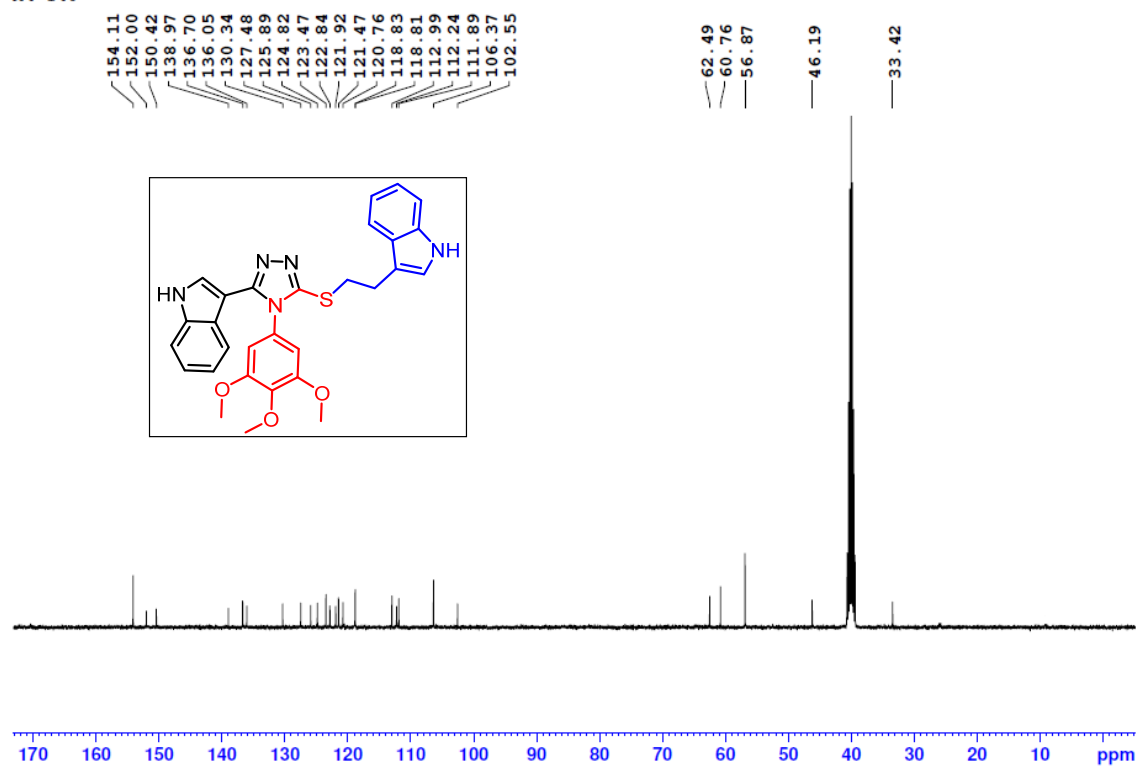
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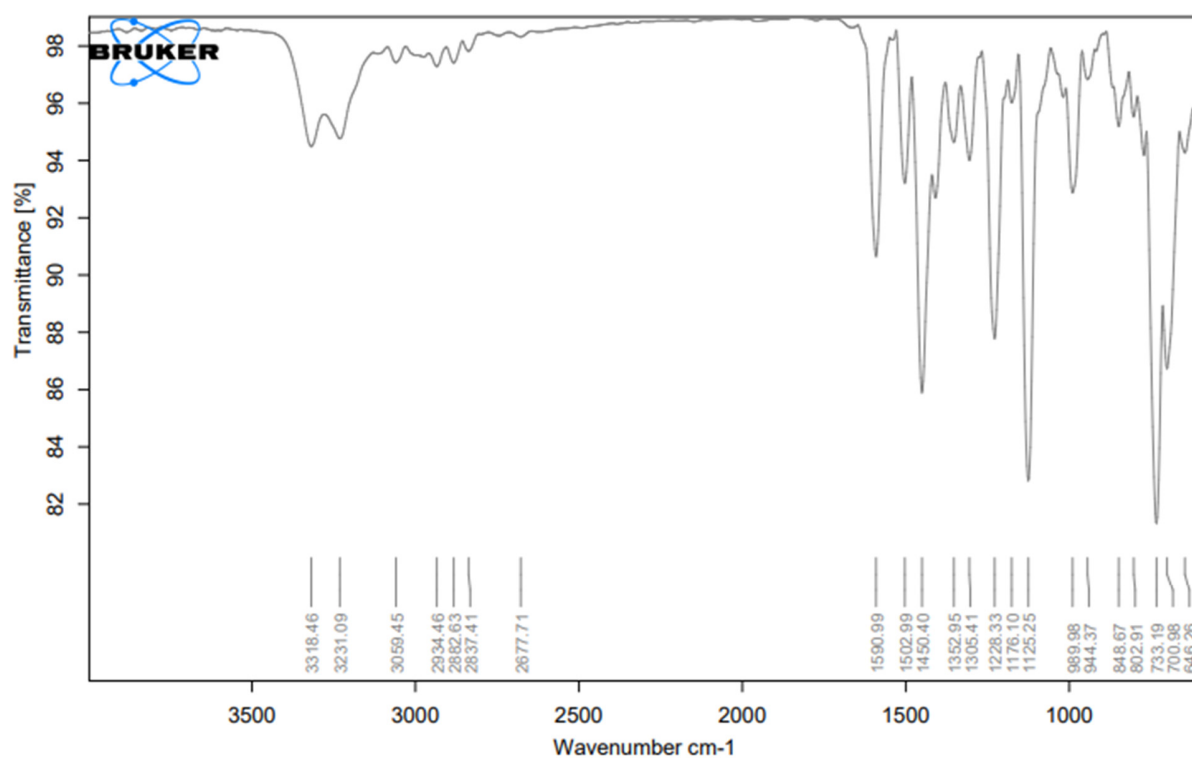
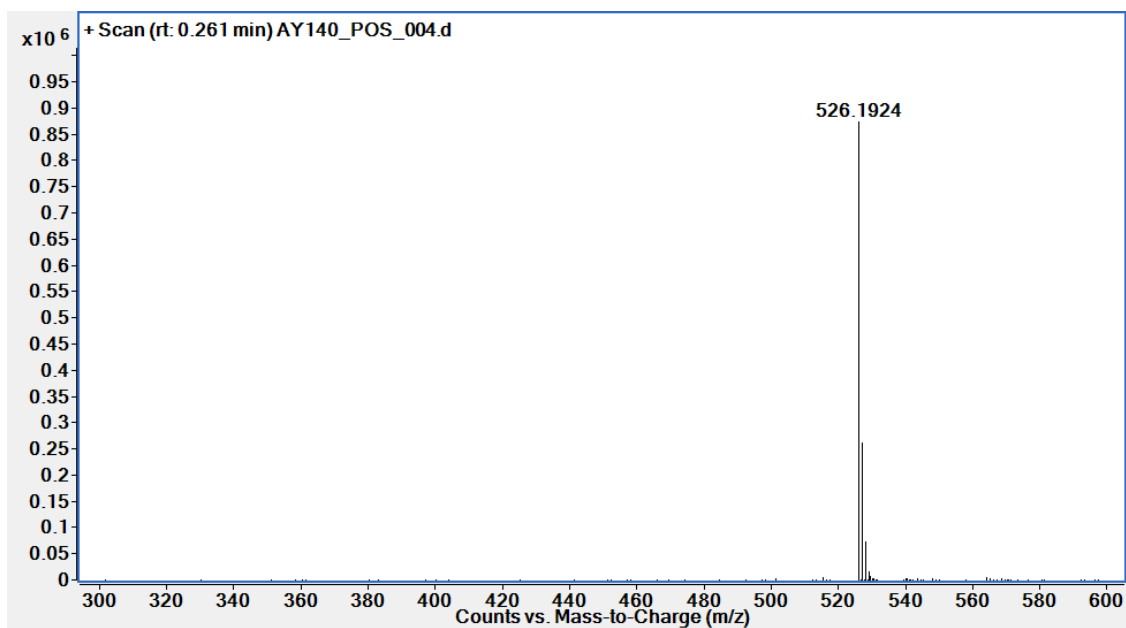
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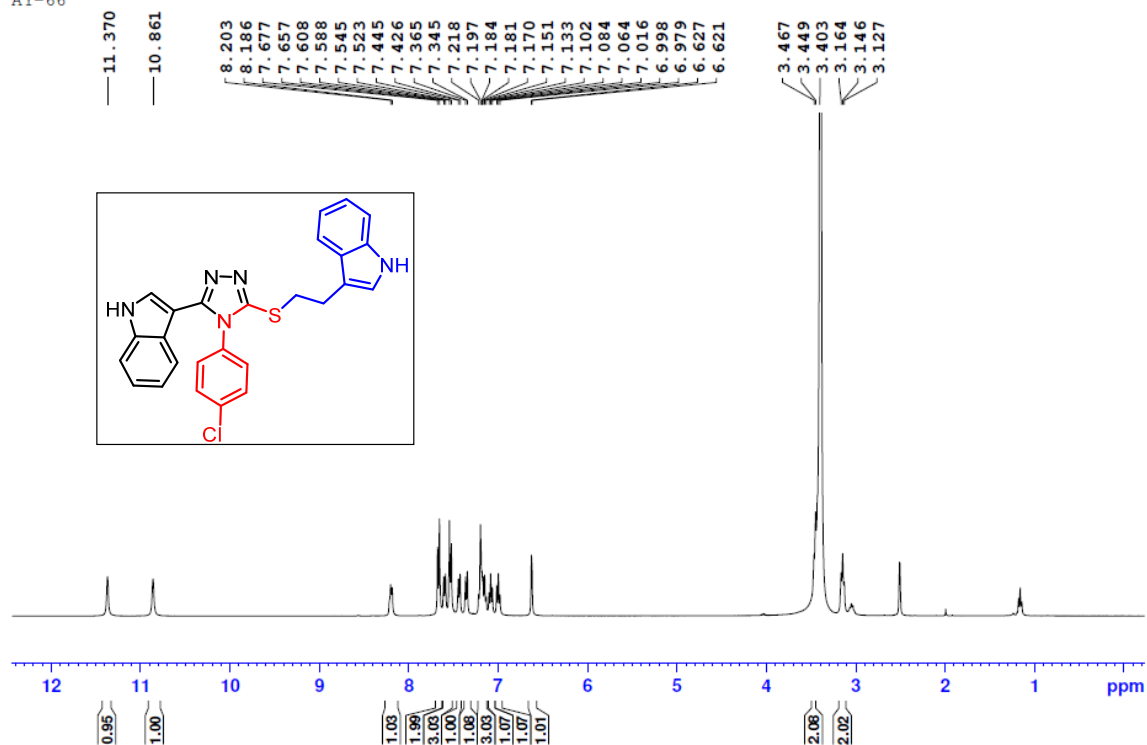
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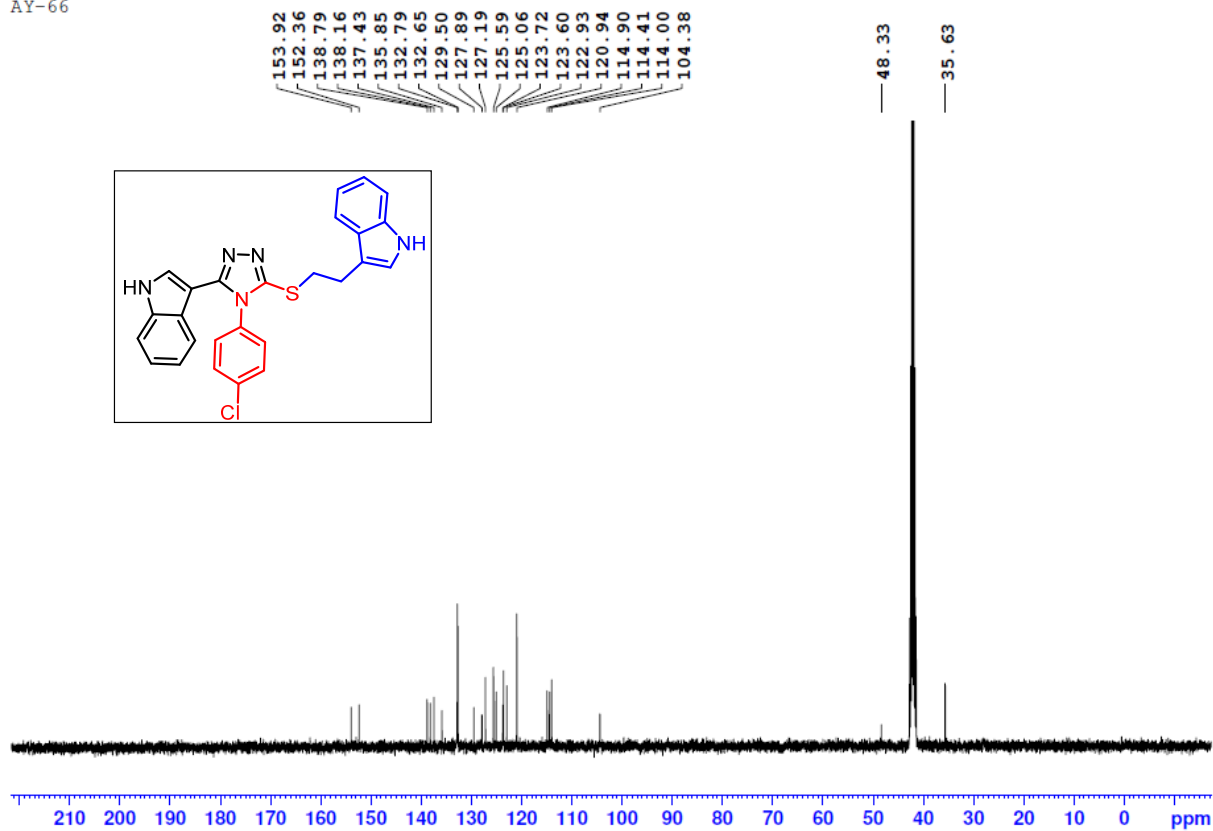


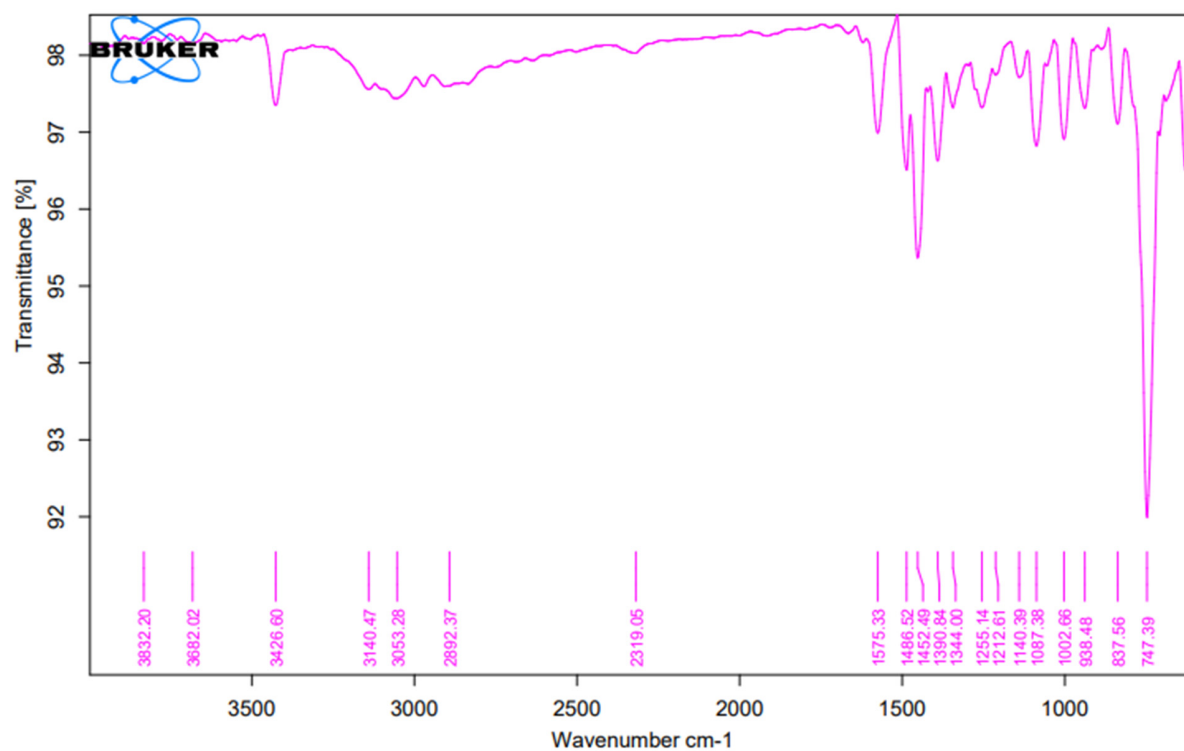
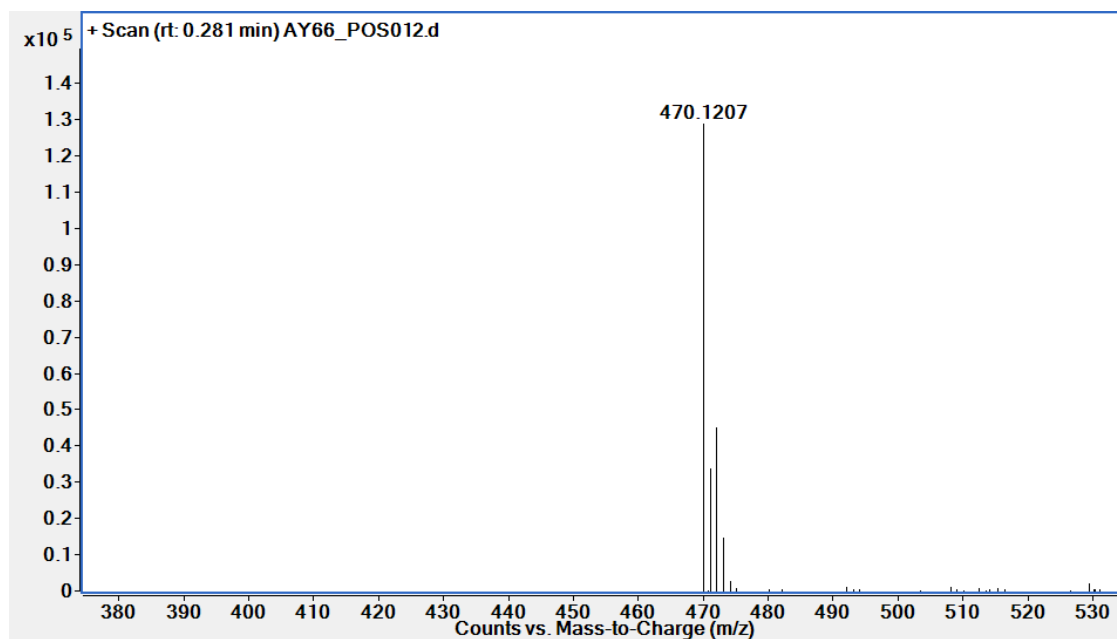
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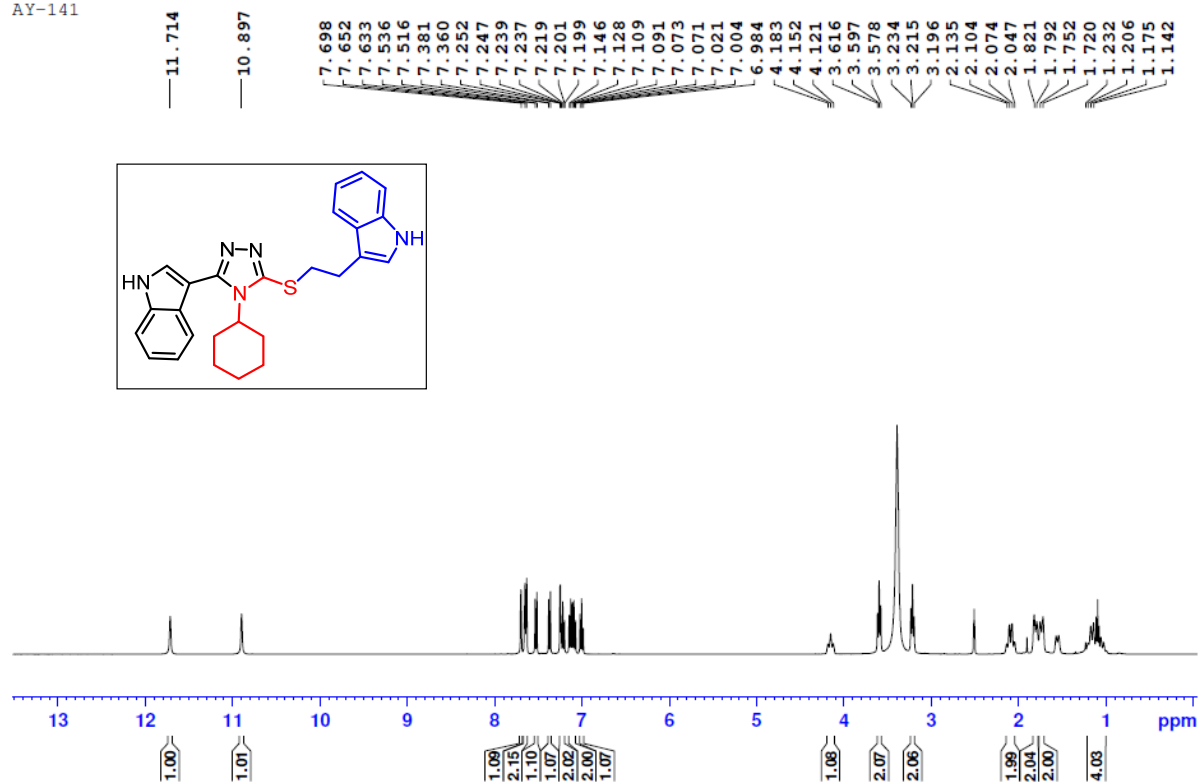
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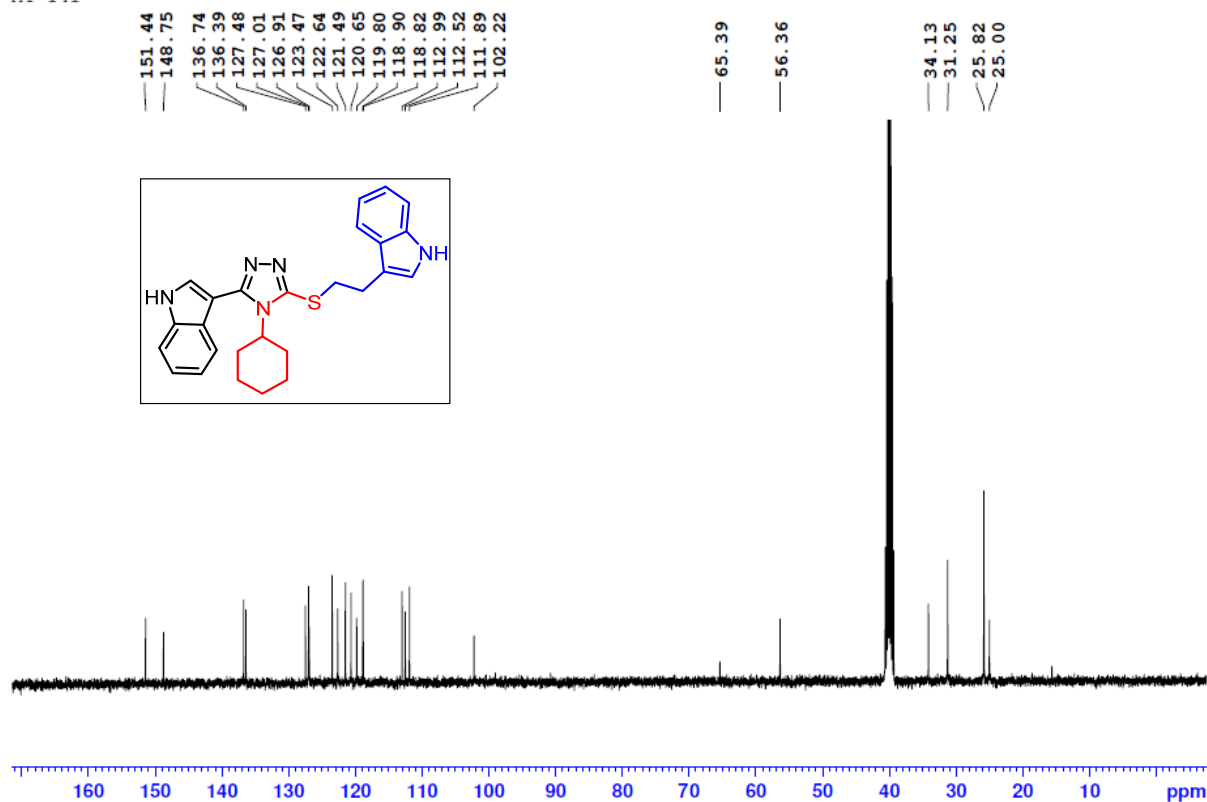


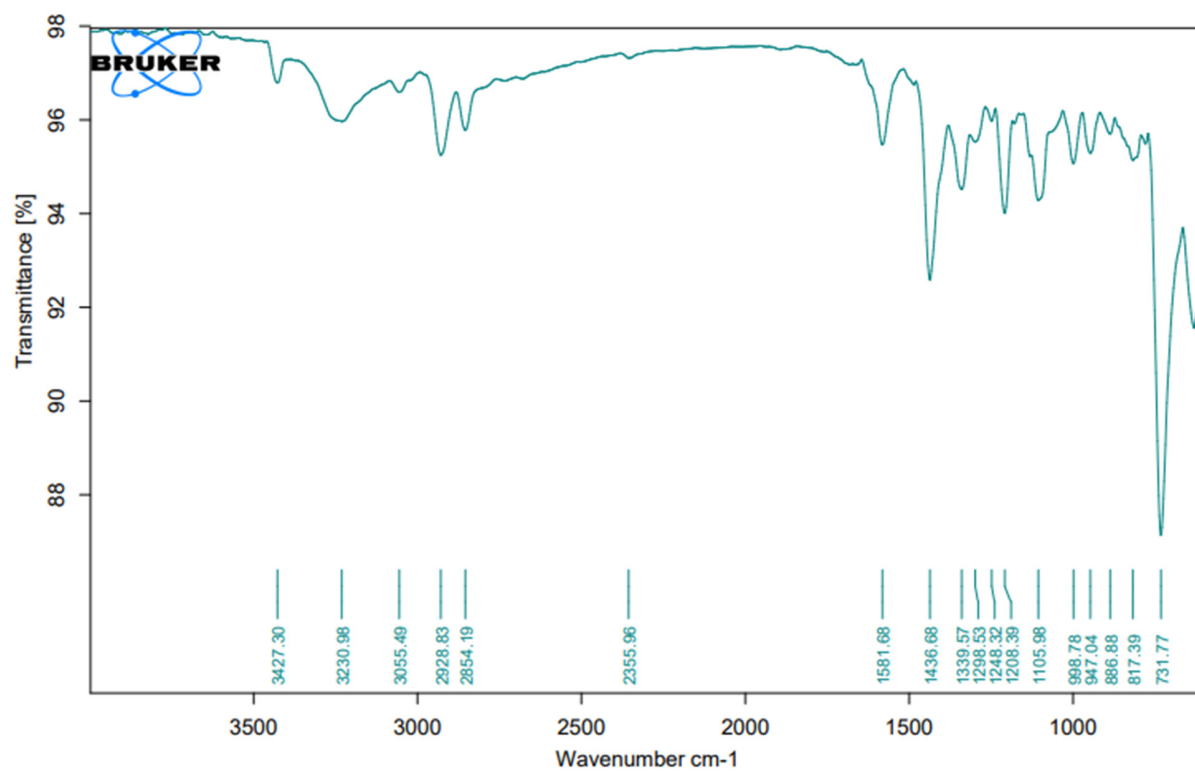
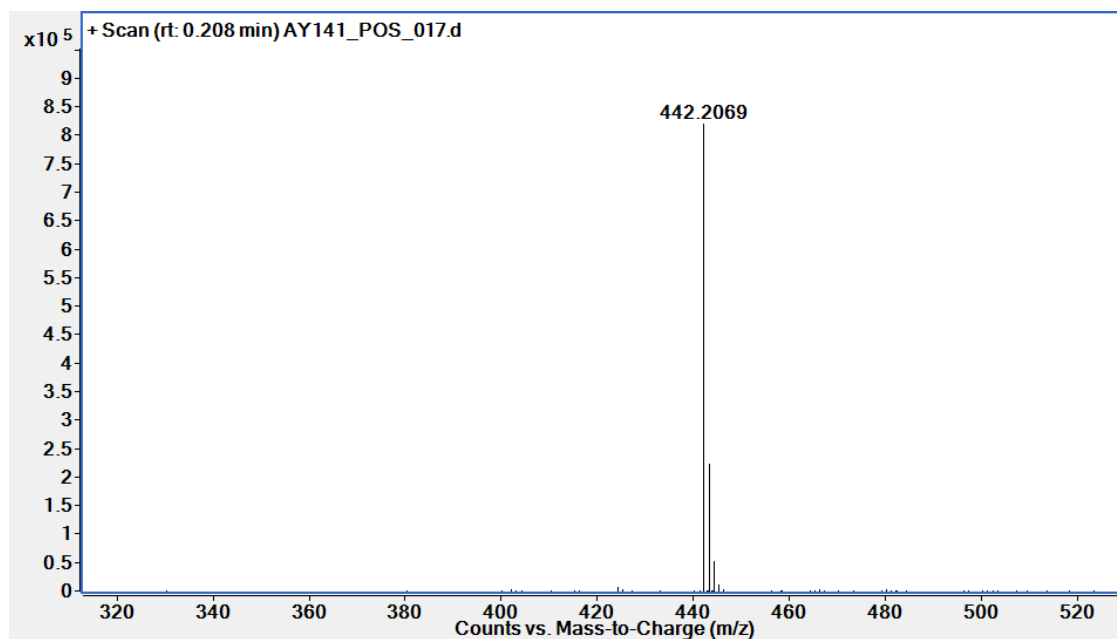
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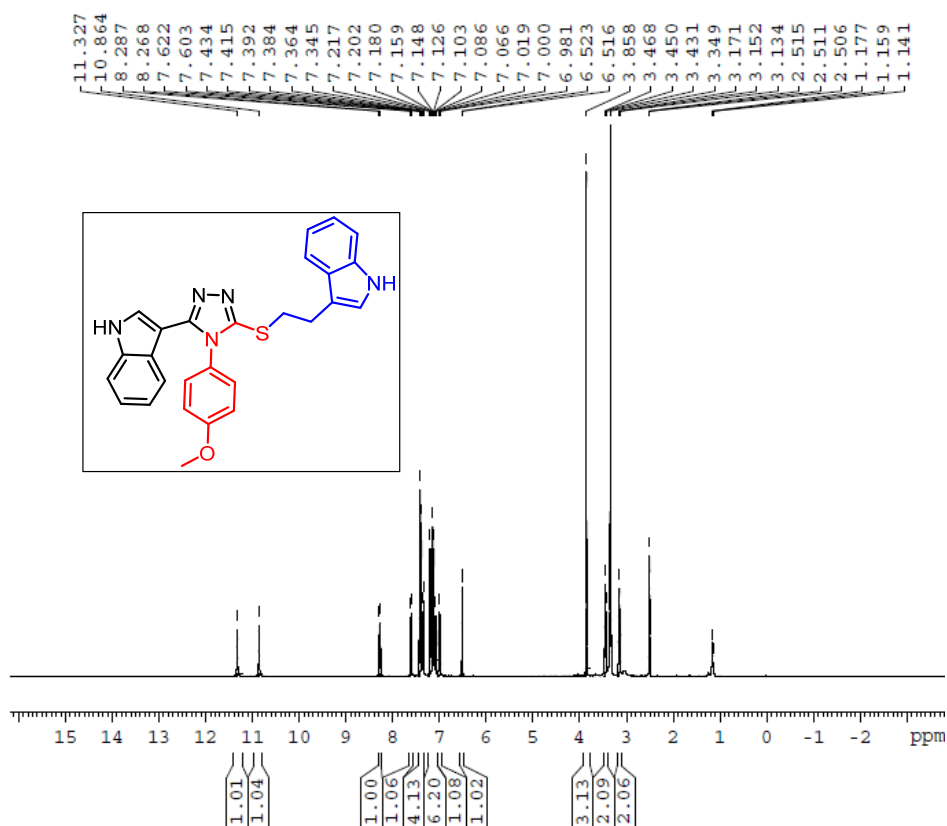
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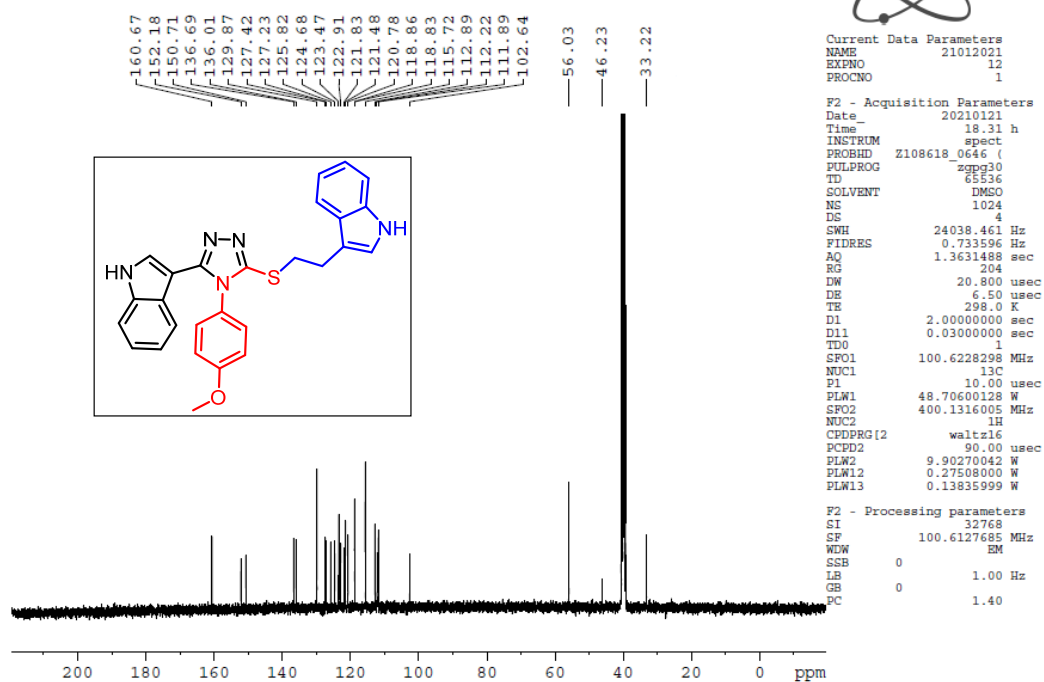
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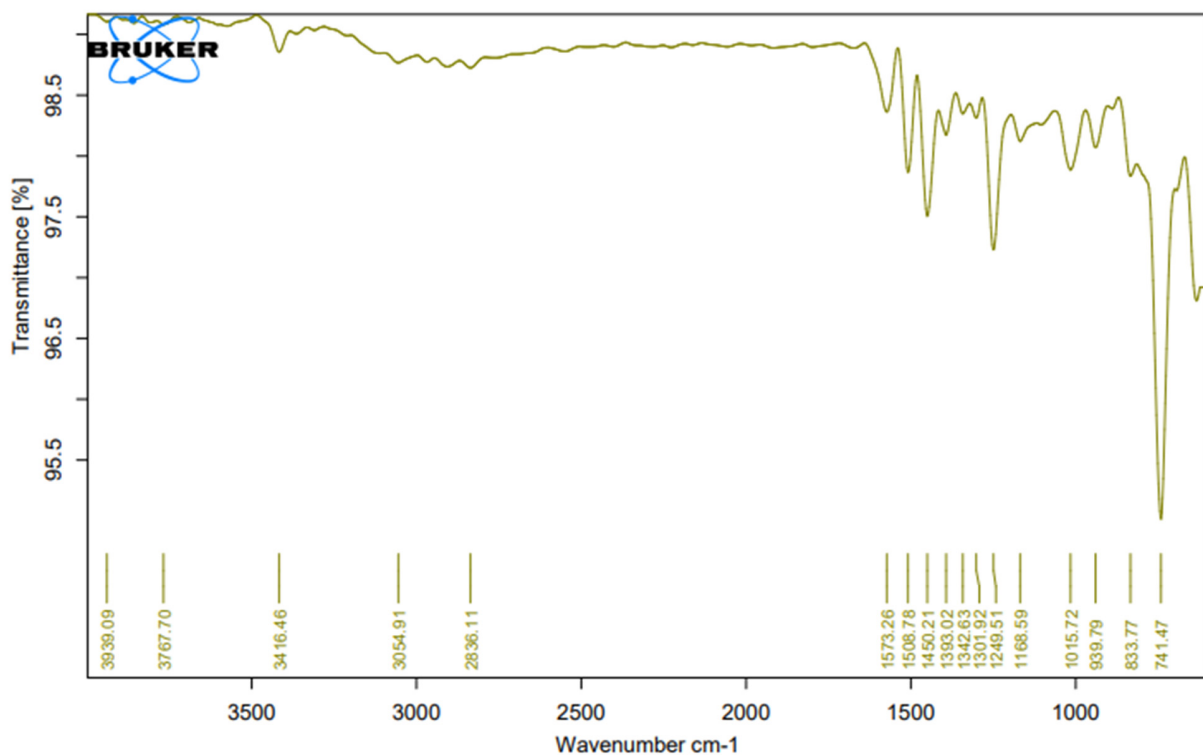
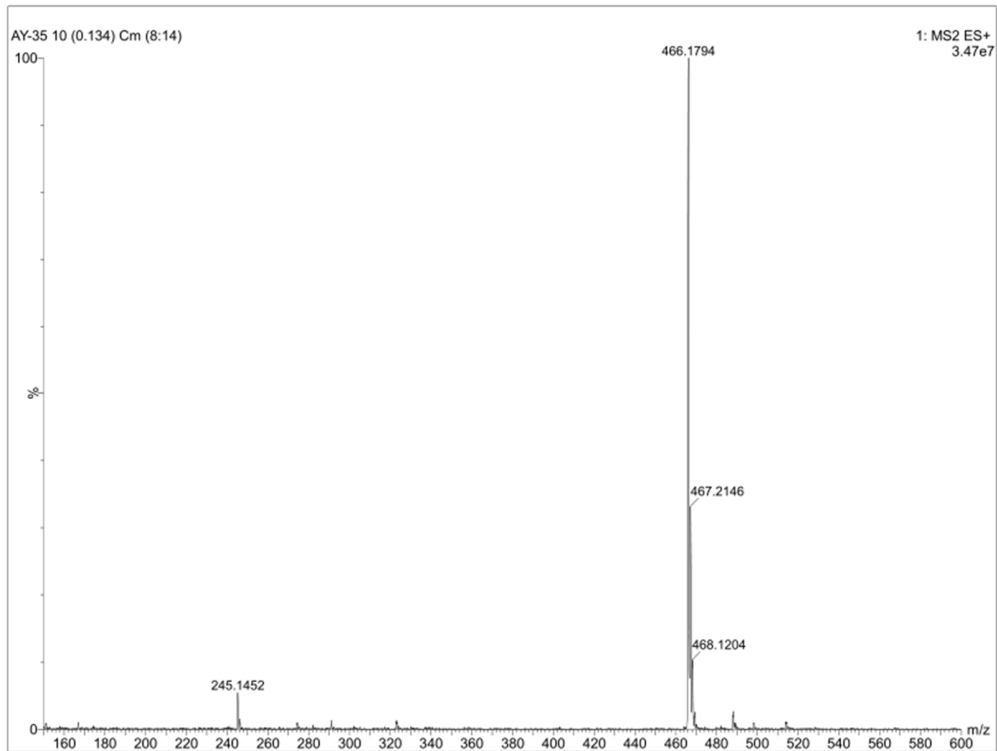
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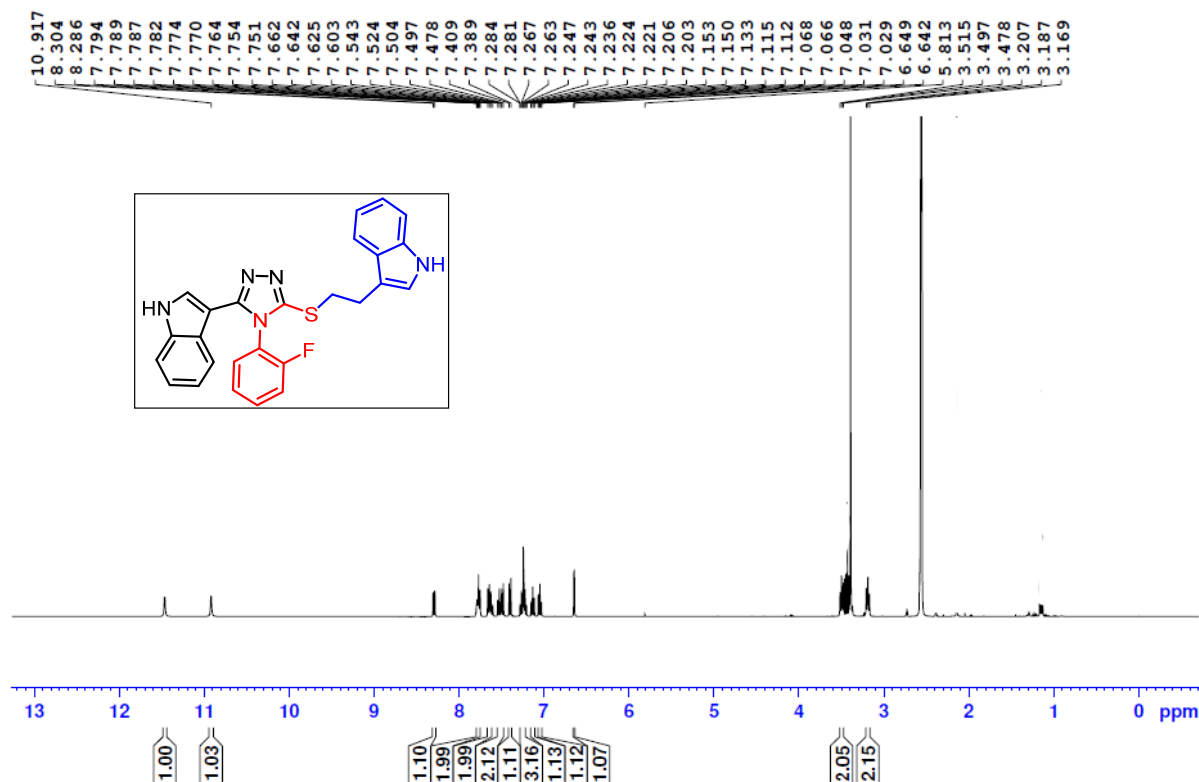
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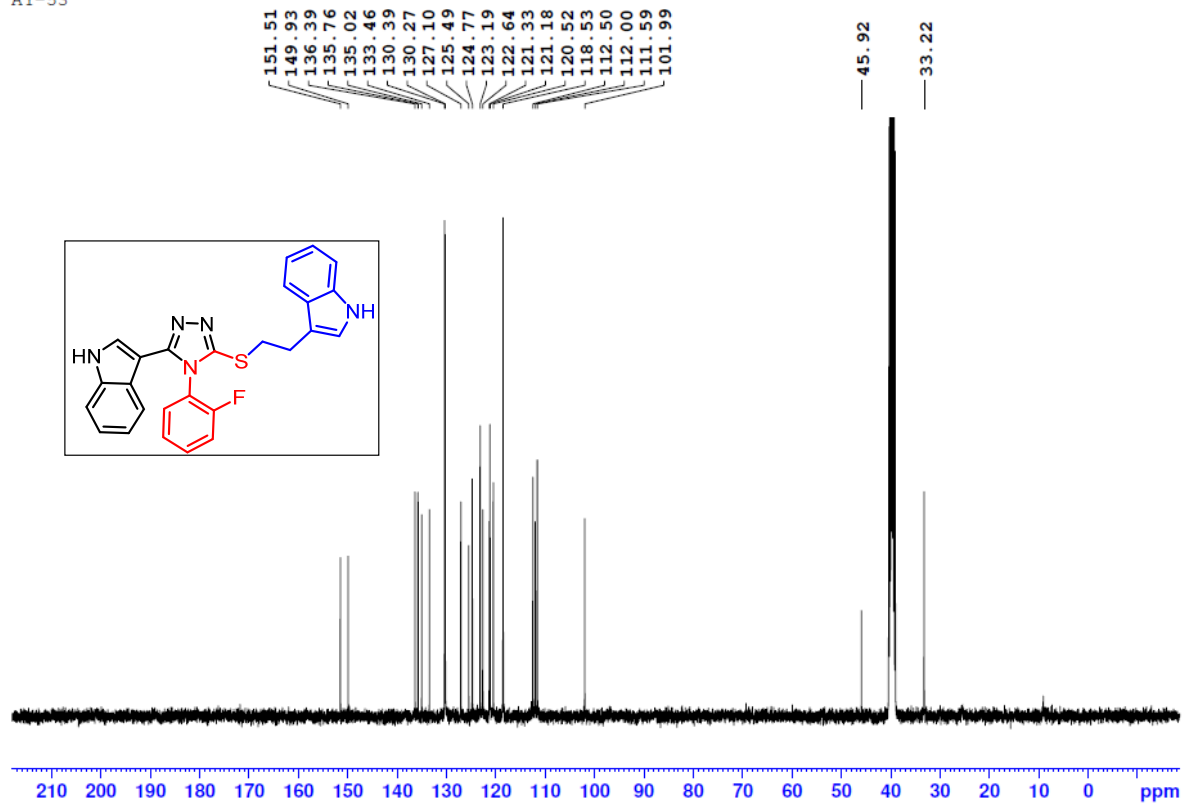
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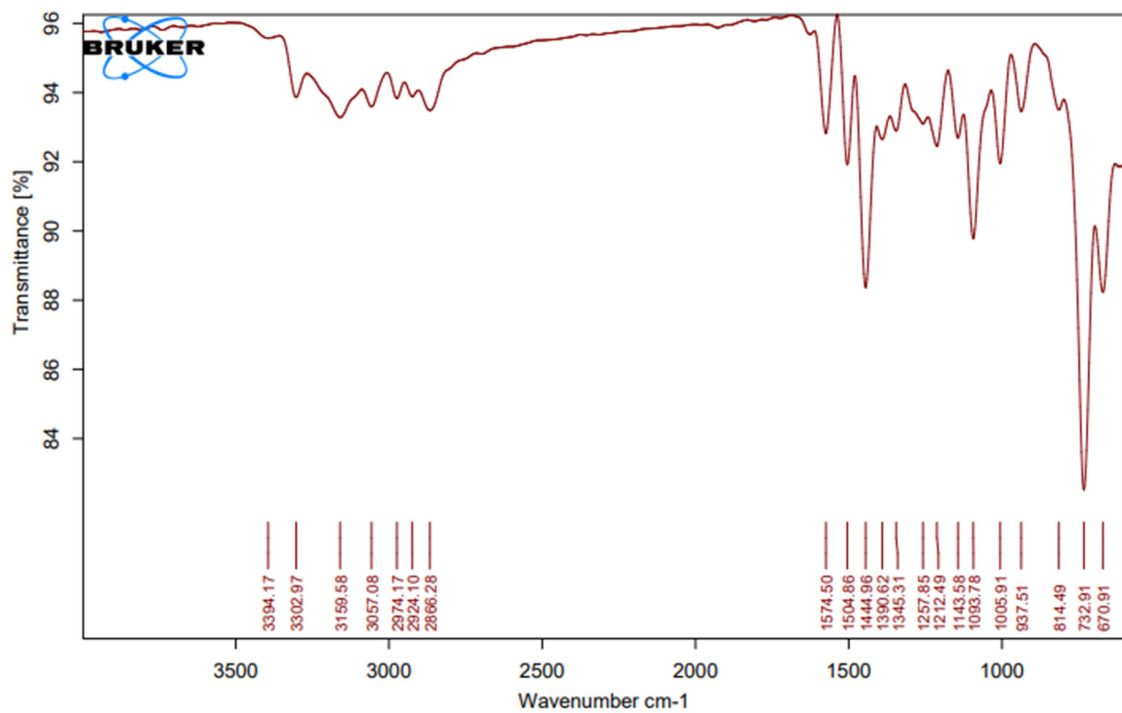
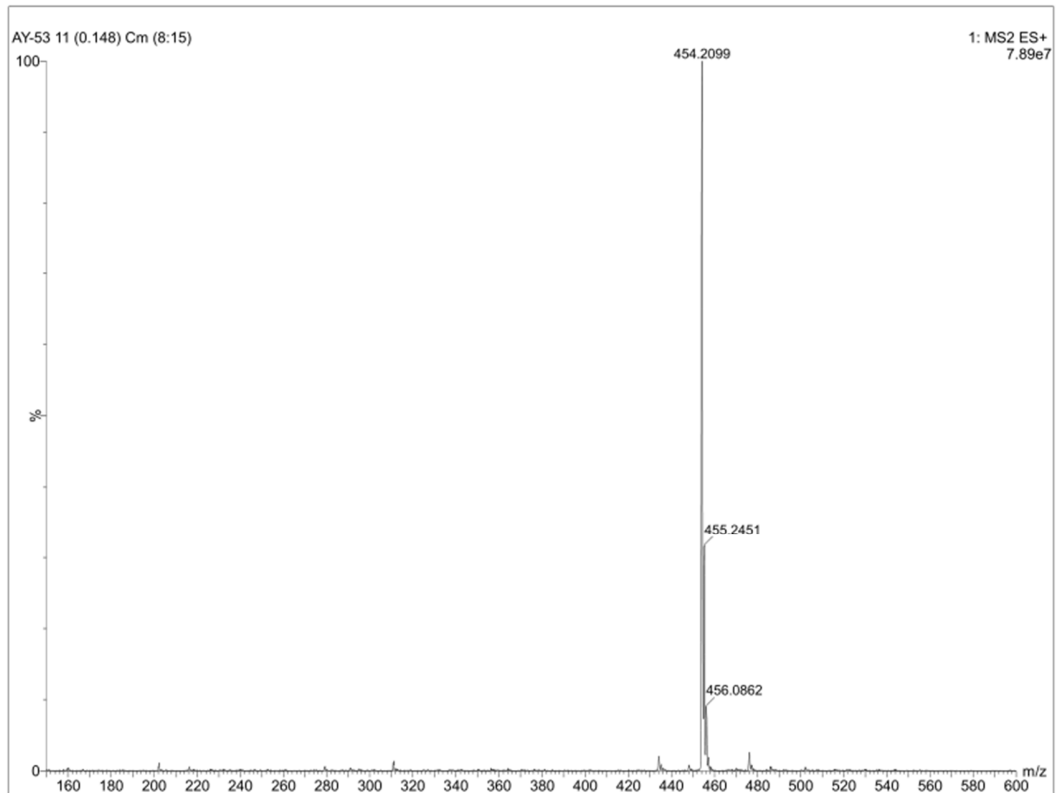
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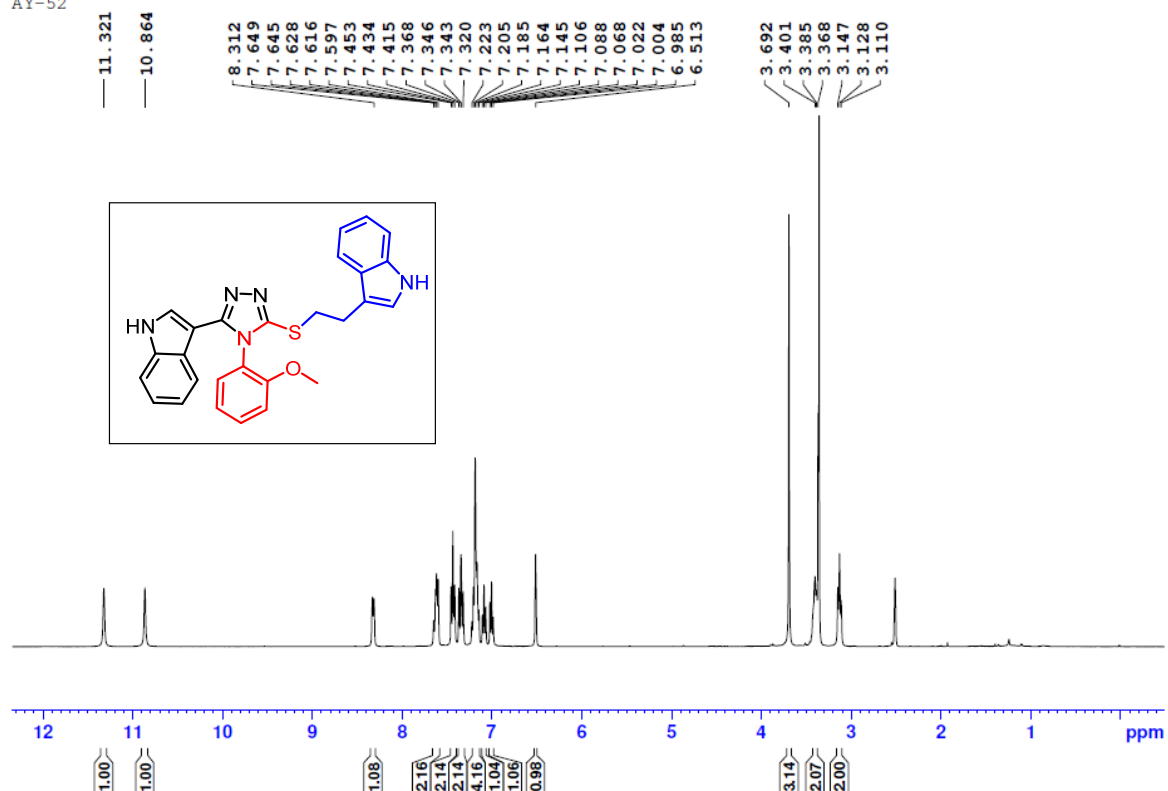
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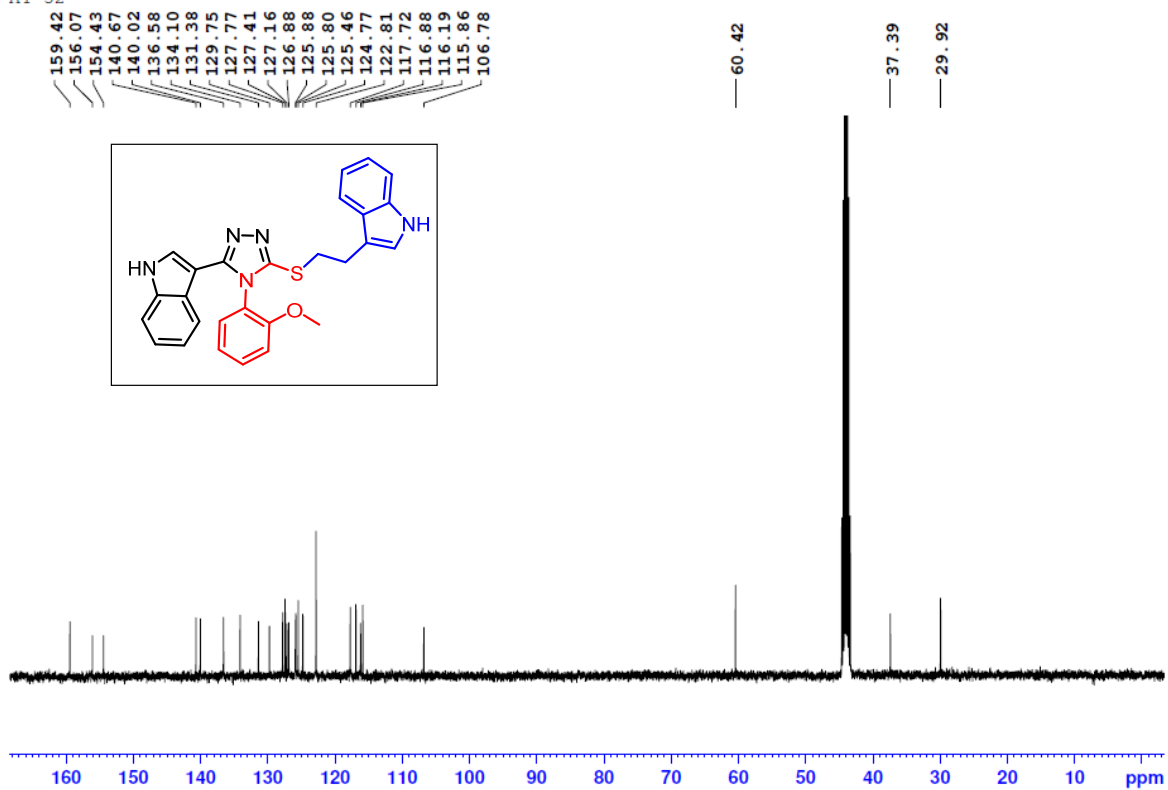
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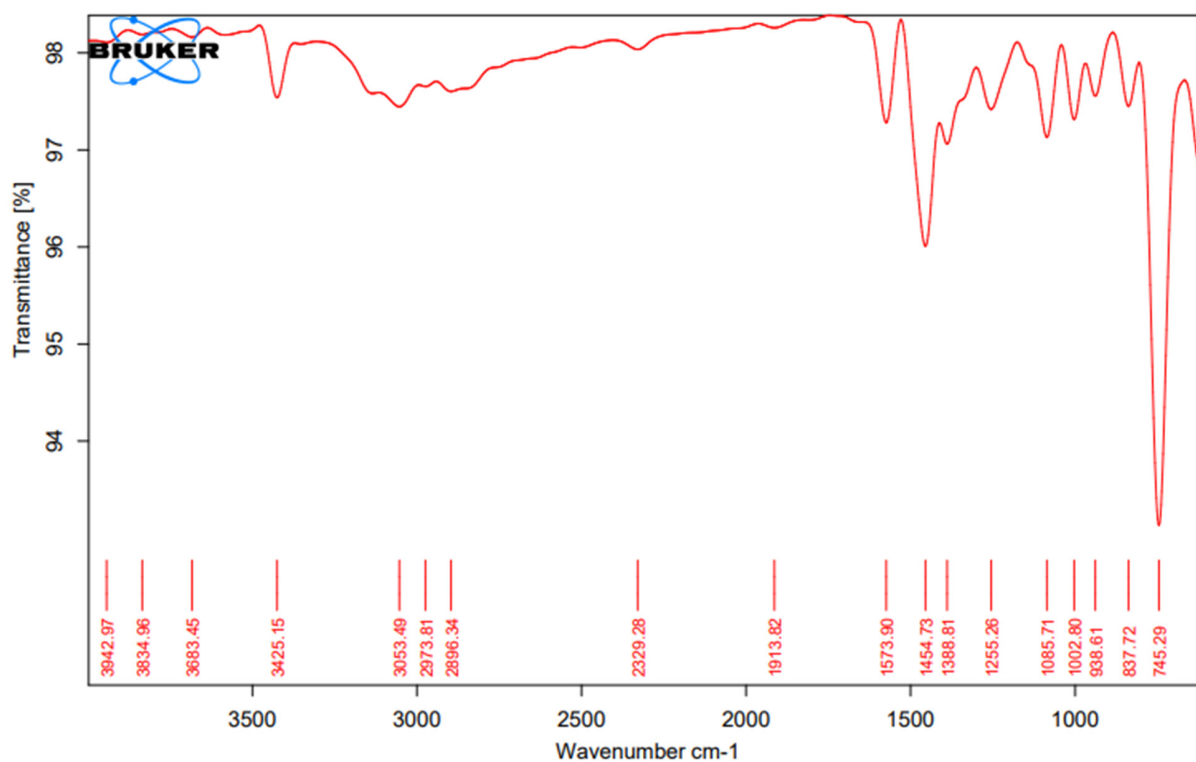
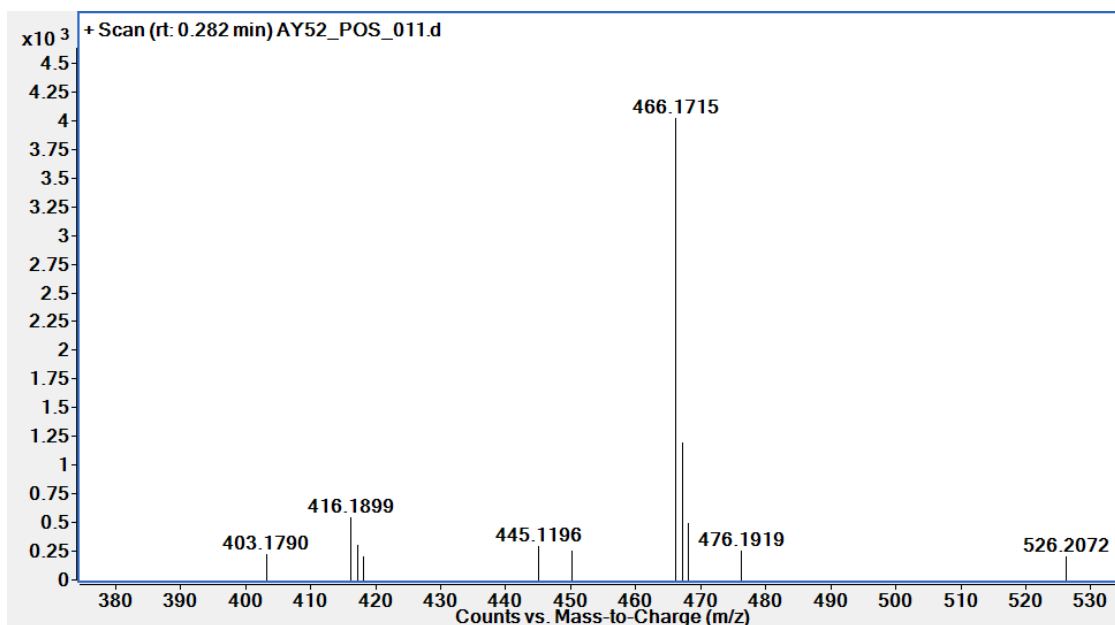
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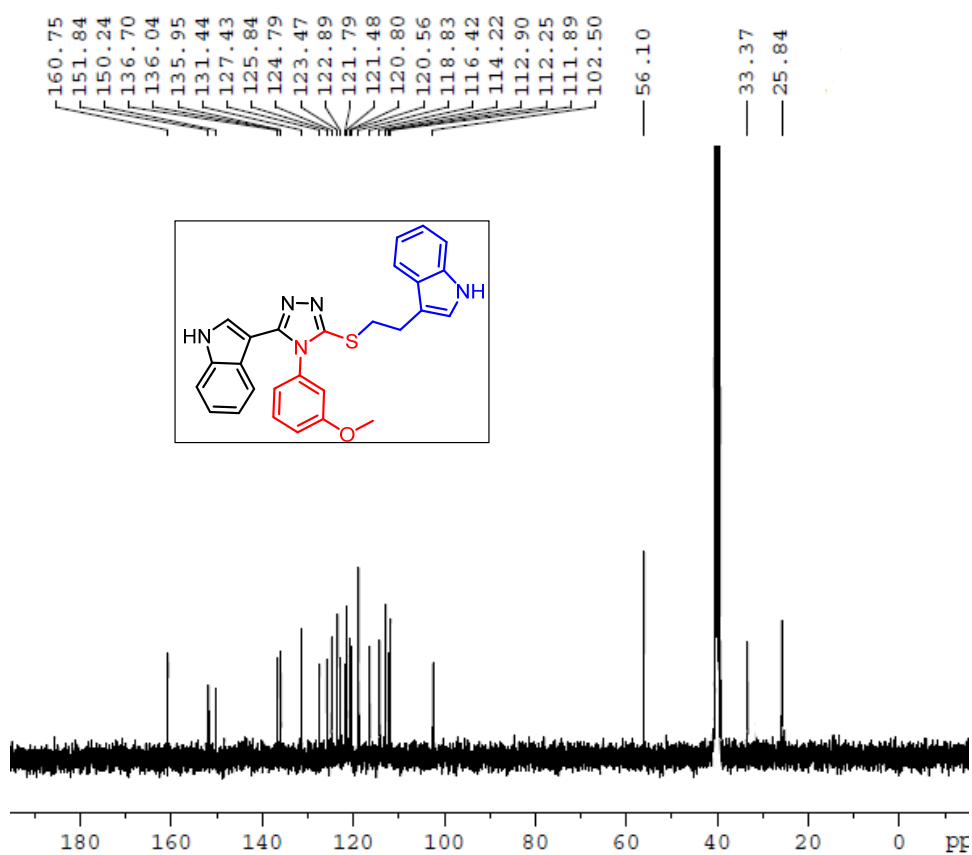
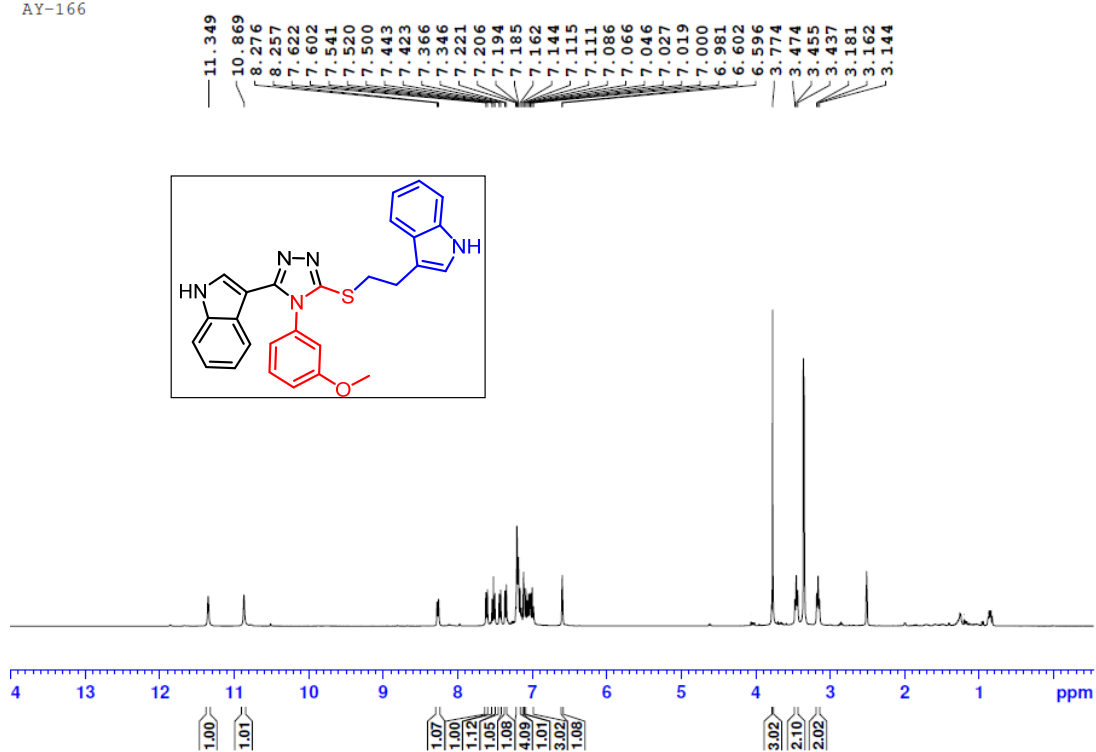
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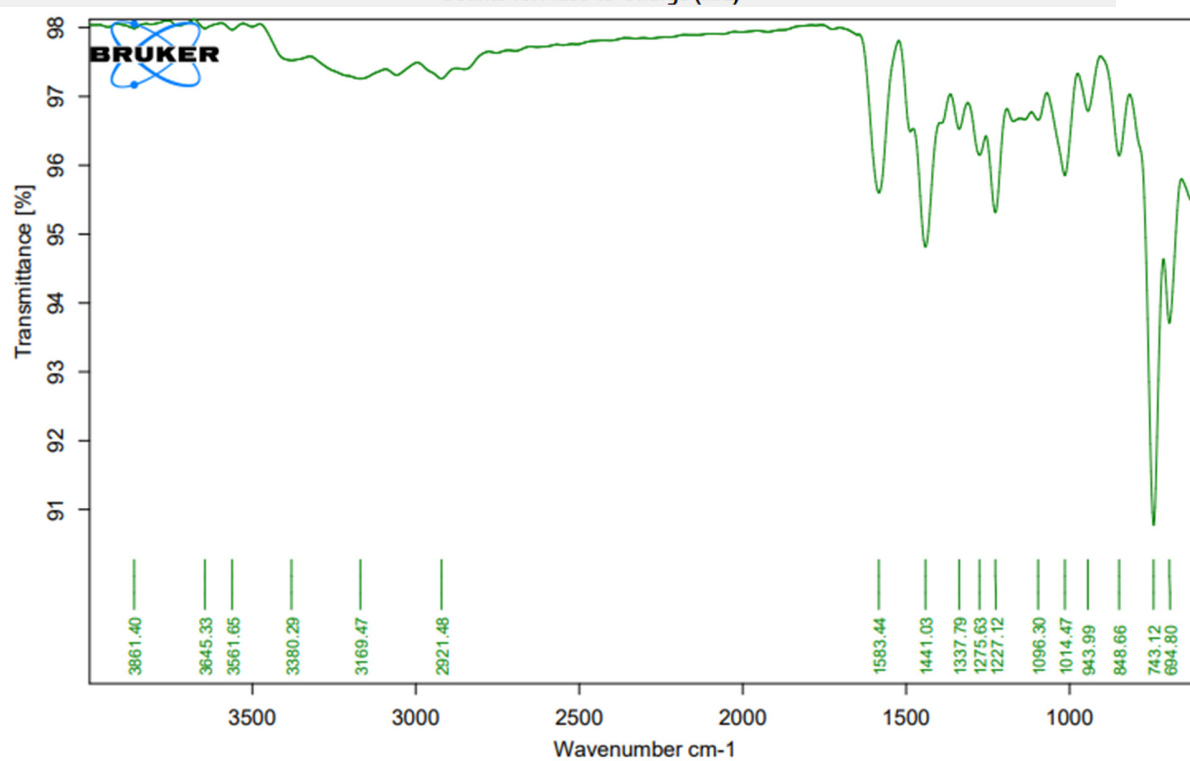
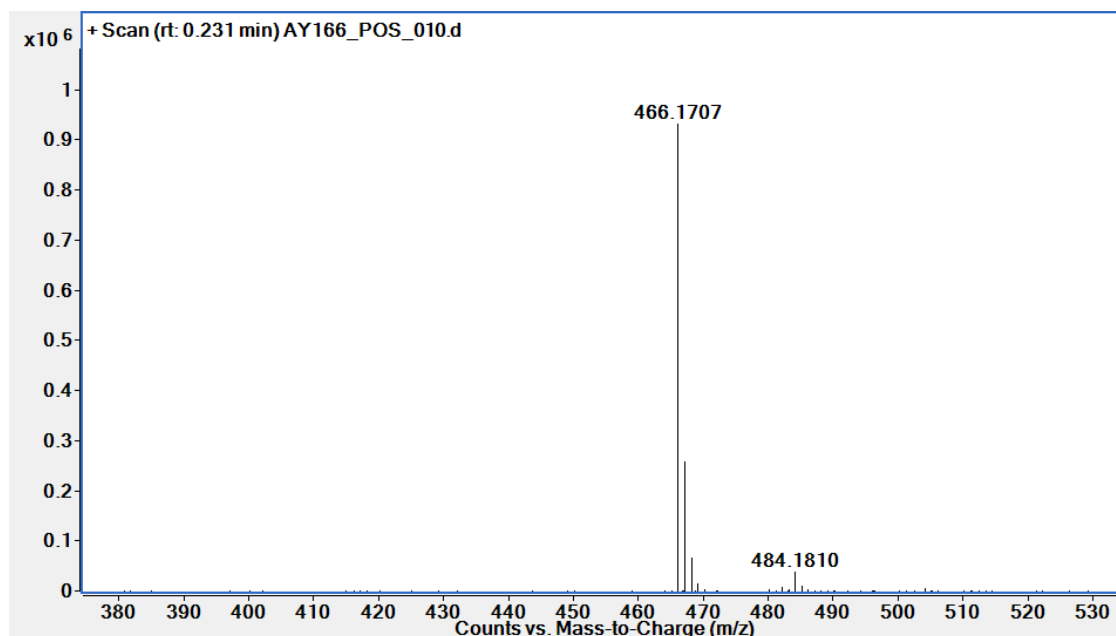
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Instrument type and / or accessory

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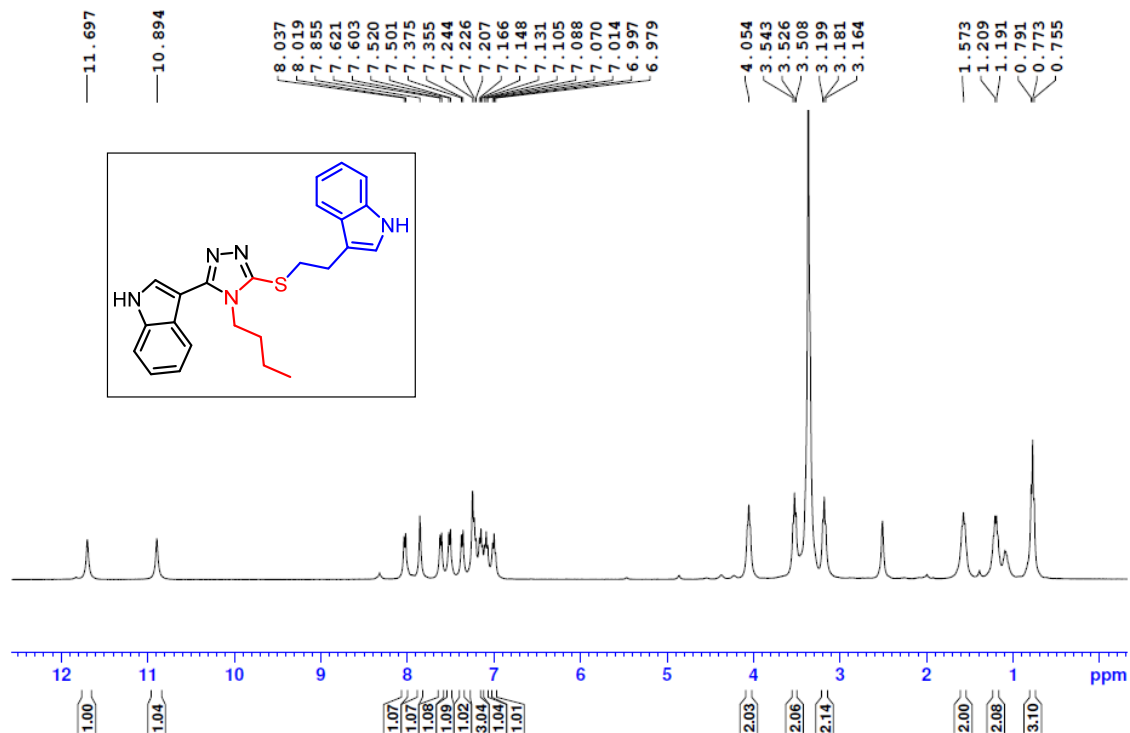
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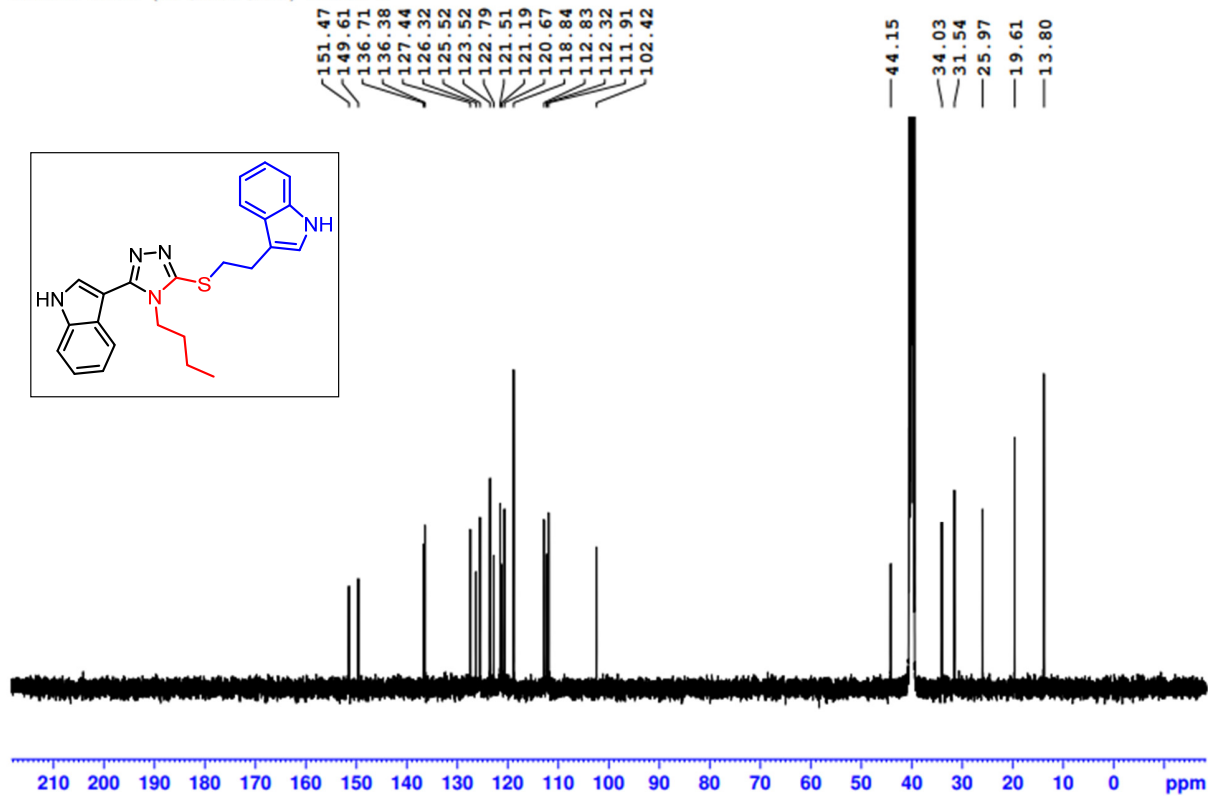
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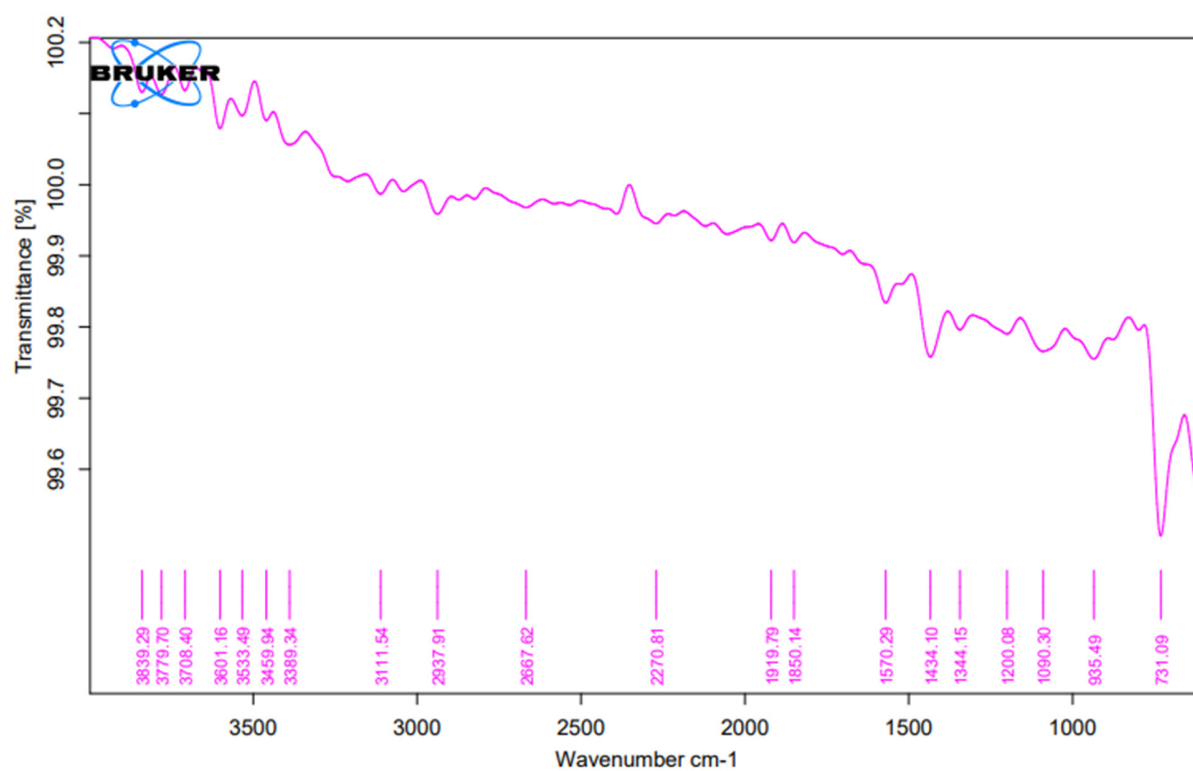
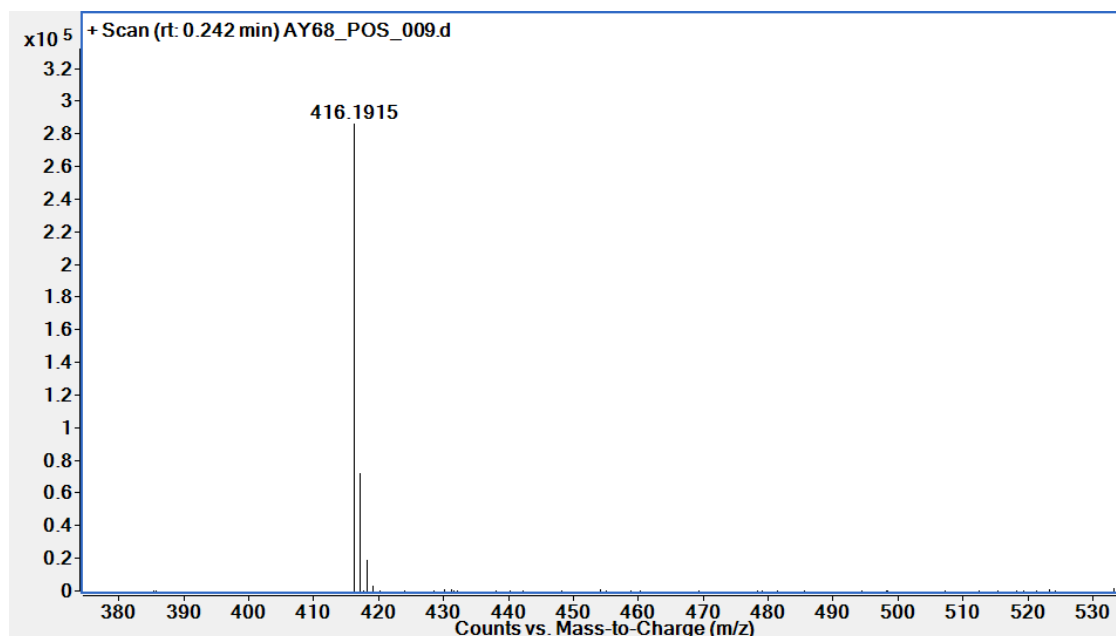
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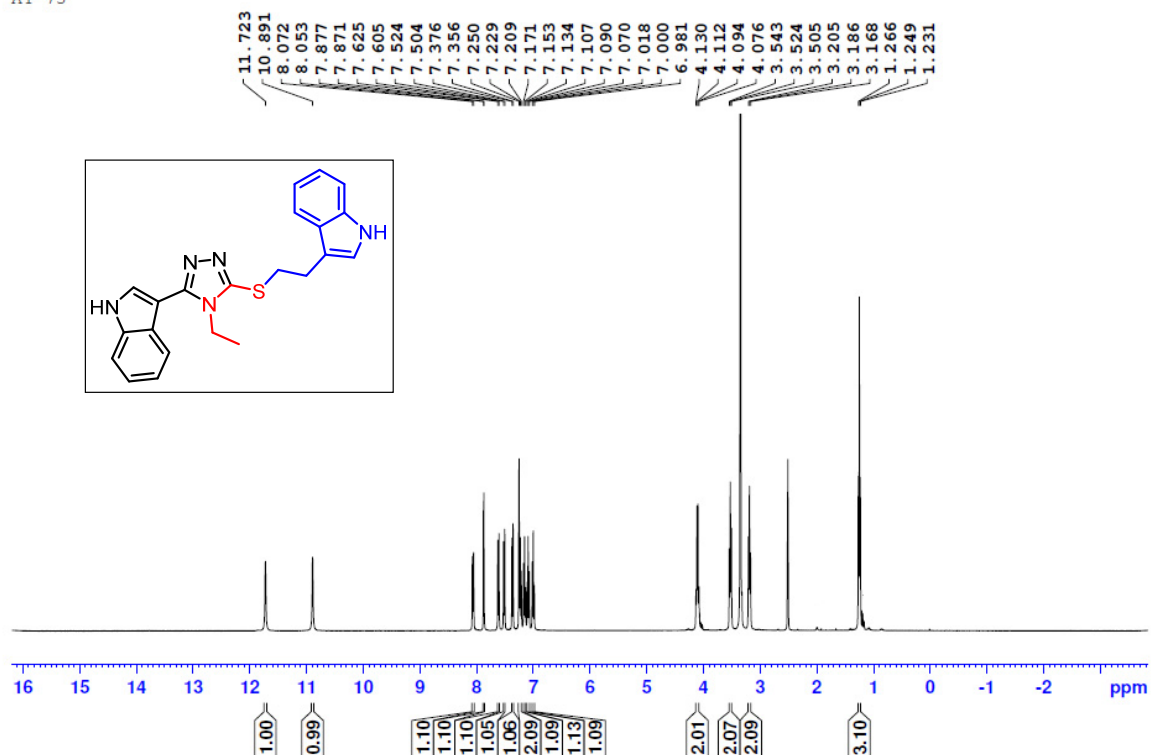
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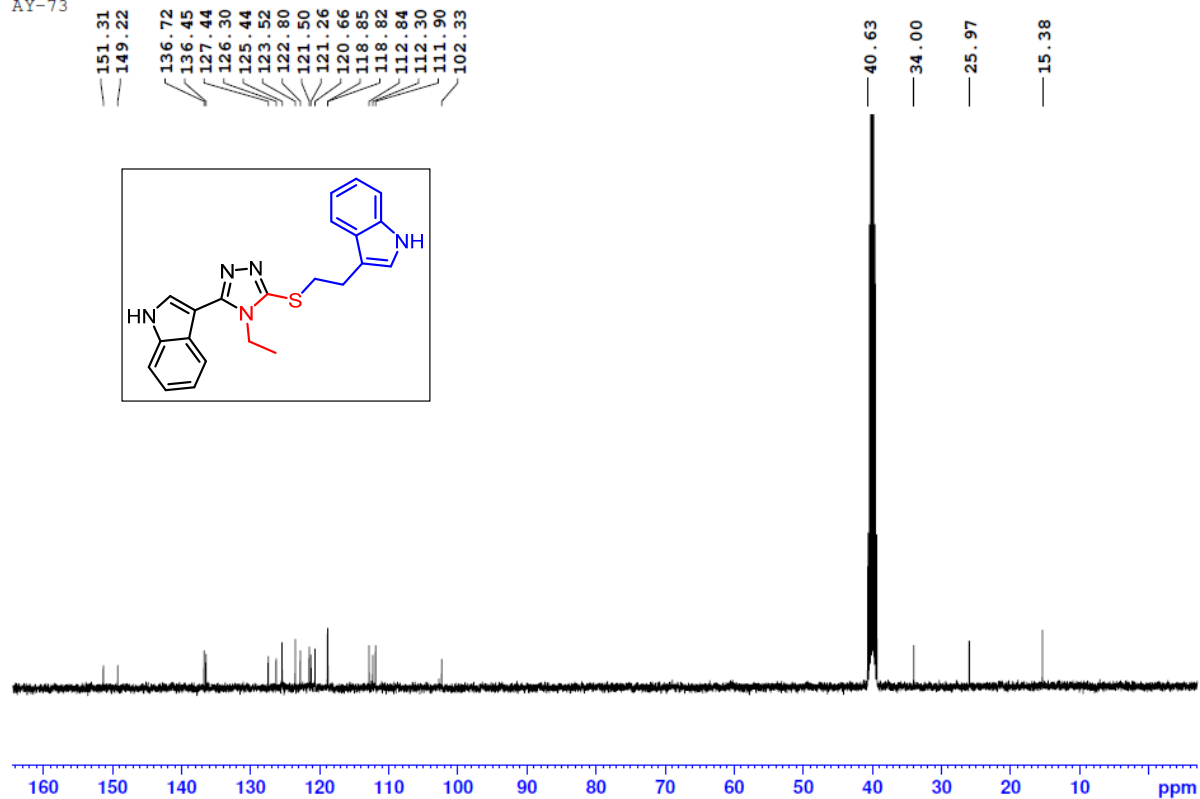
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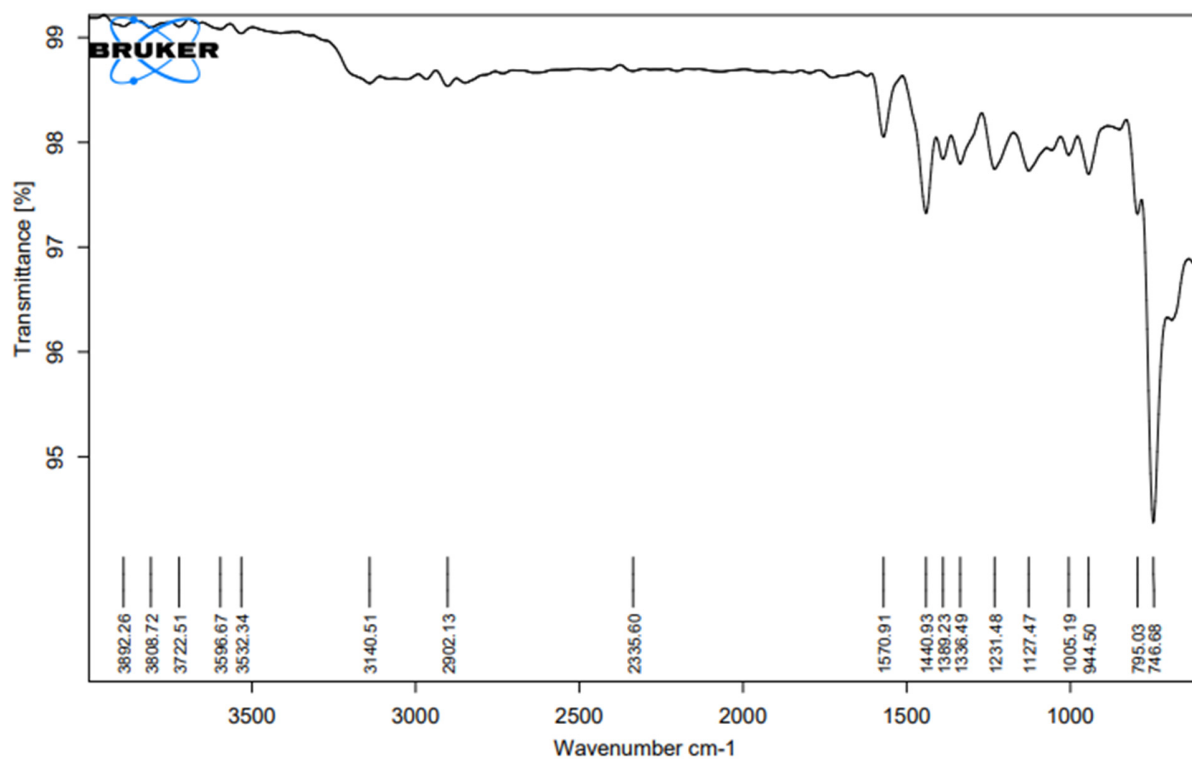
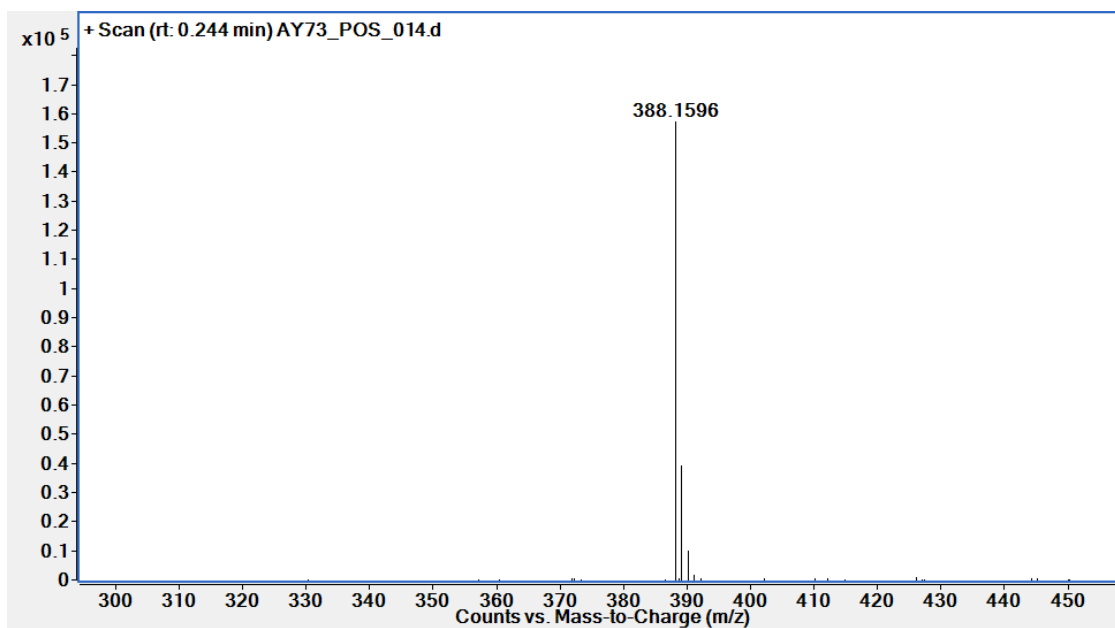
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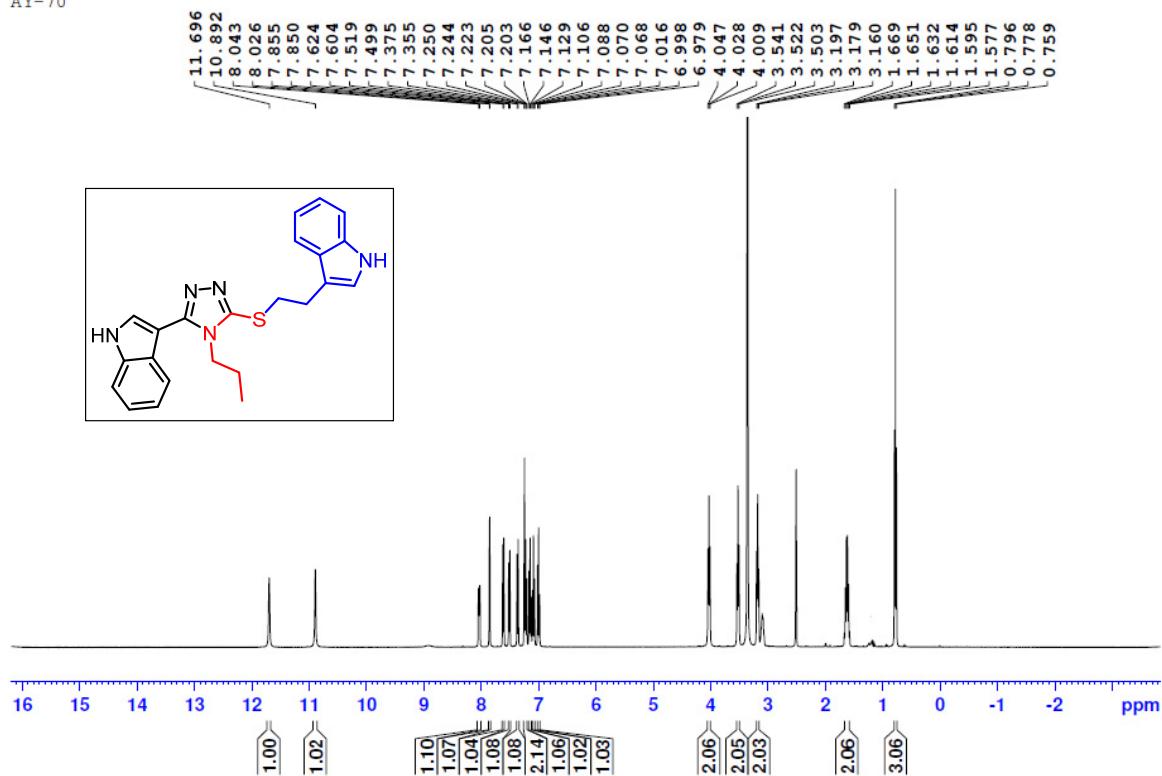
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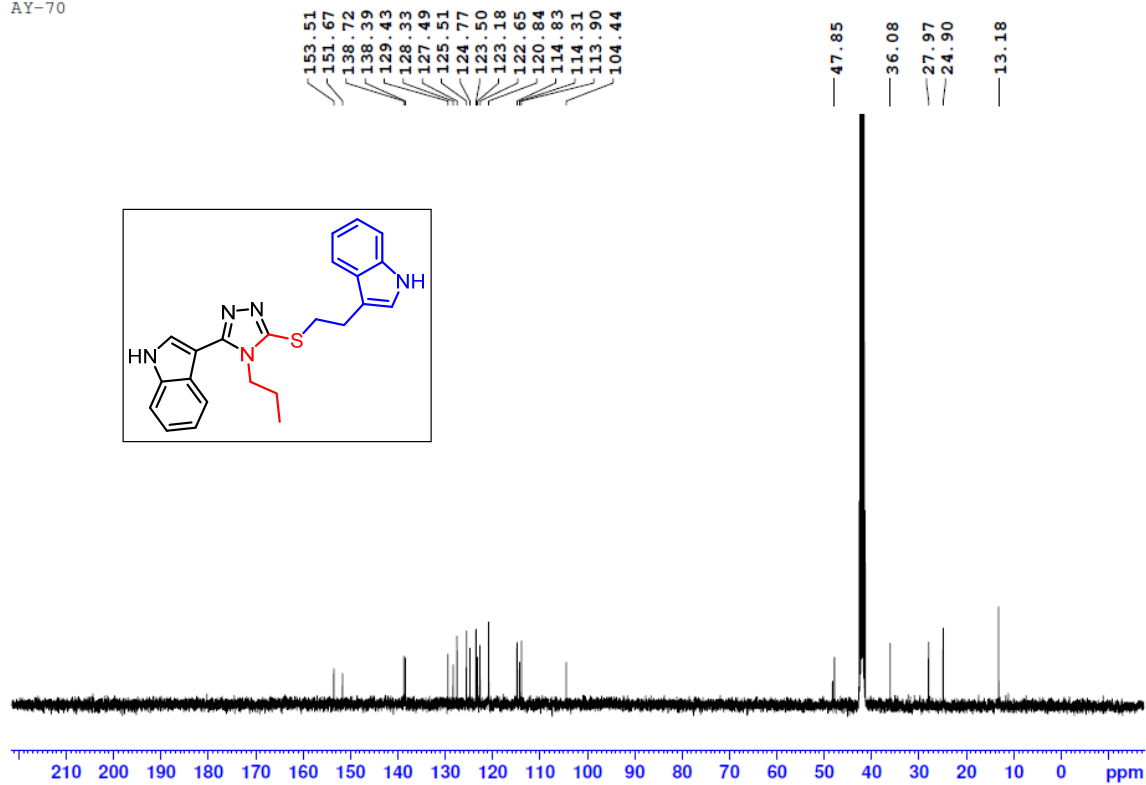
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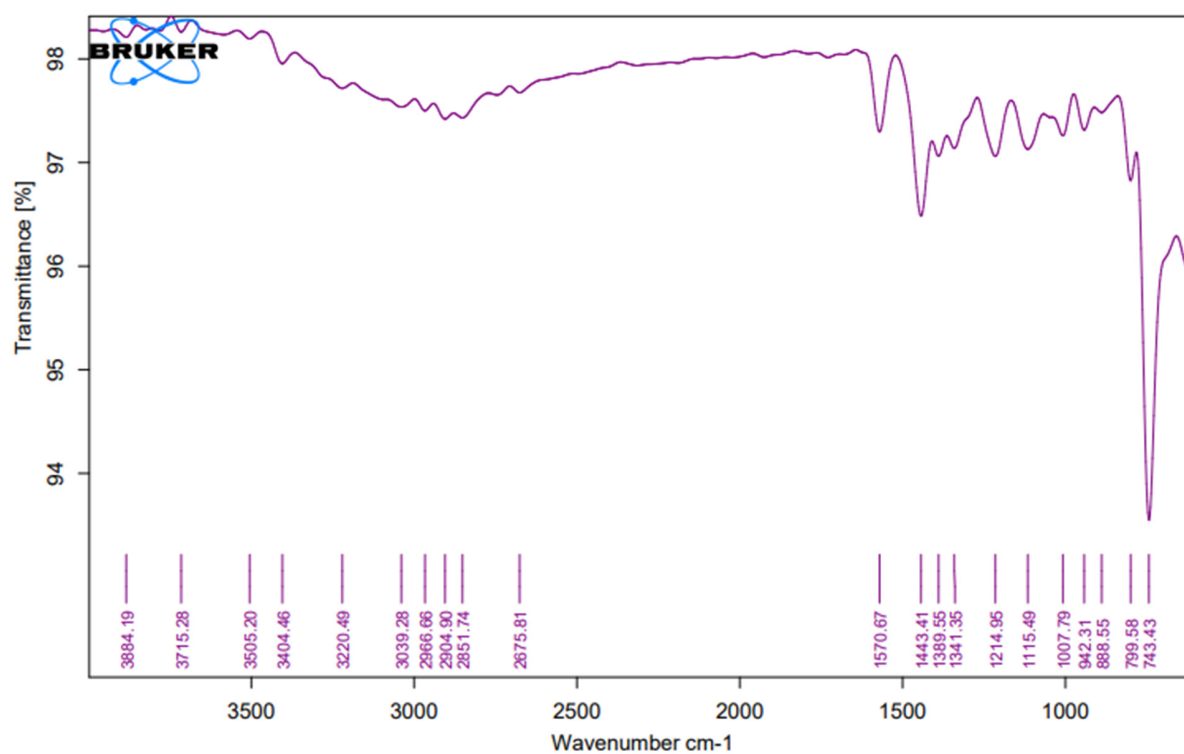
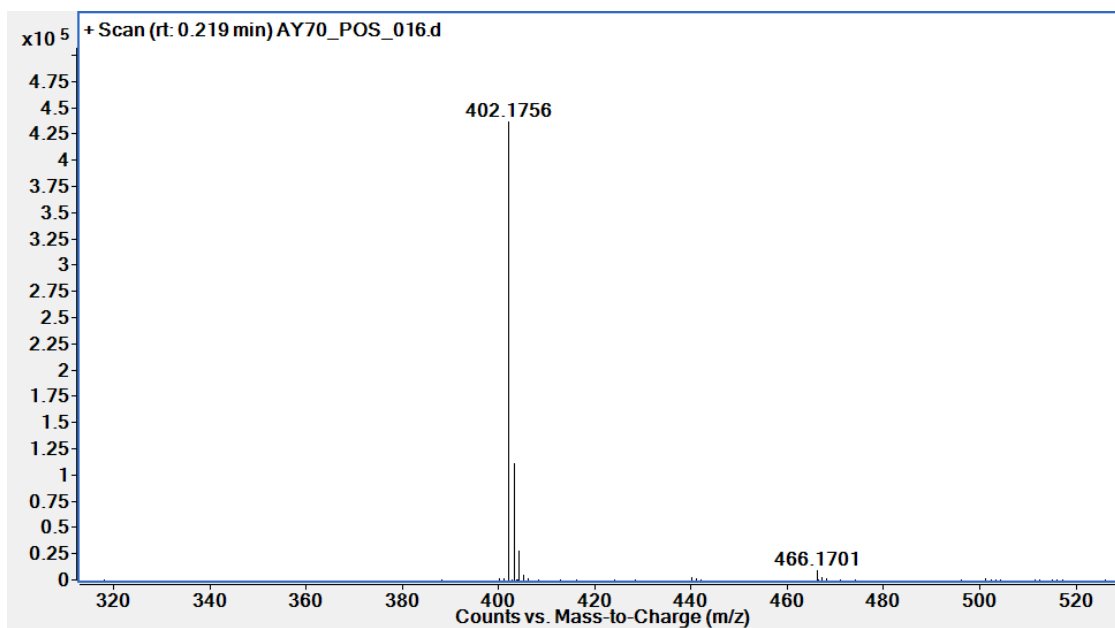
01-11-2022

AY-70



AY-70





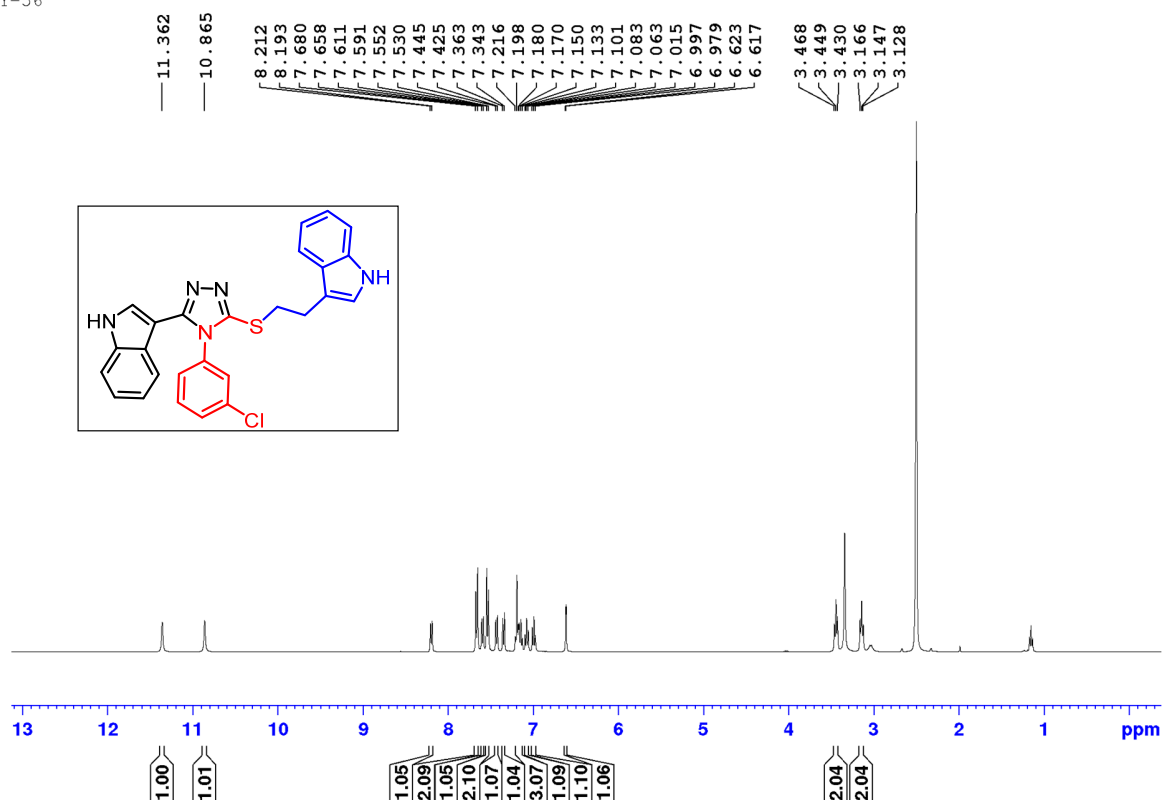
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AY-70

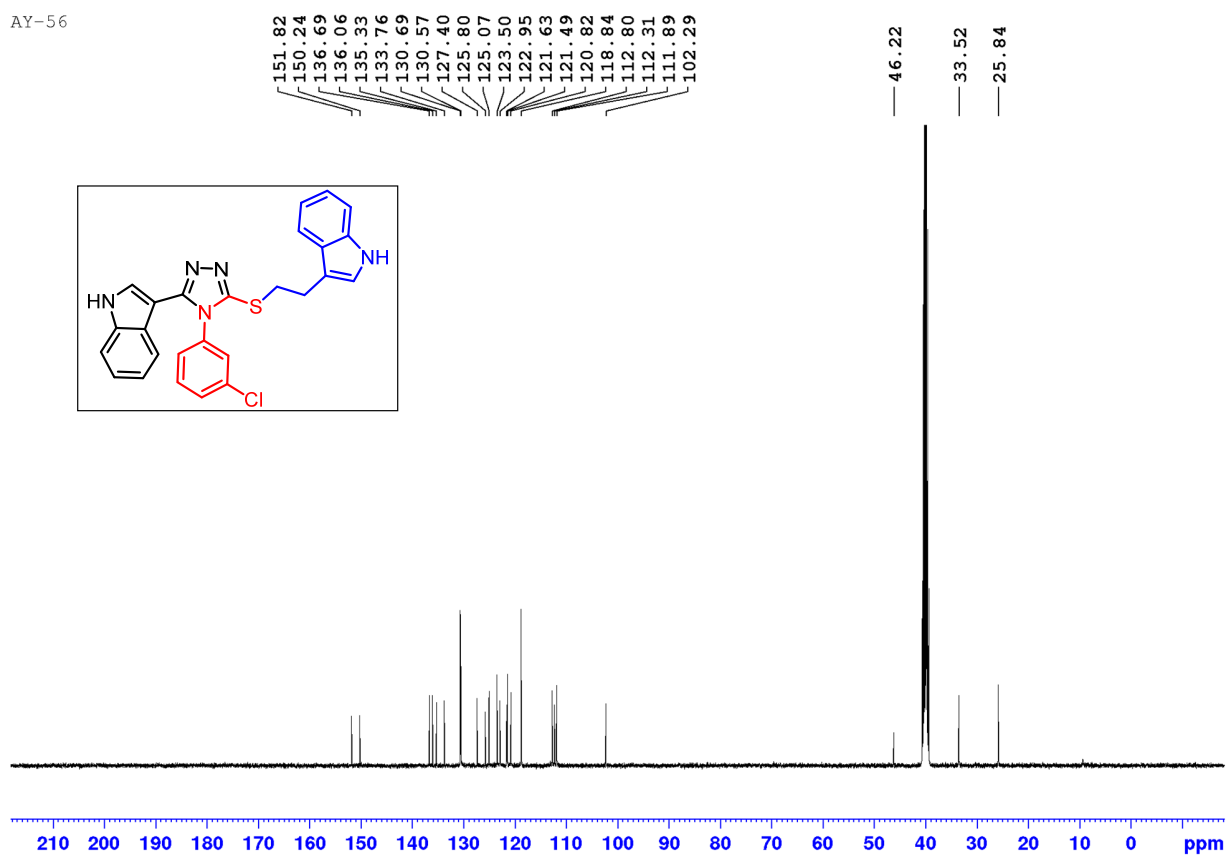
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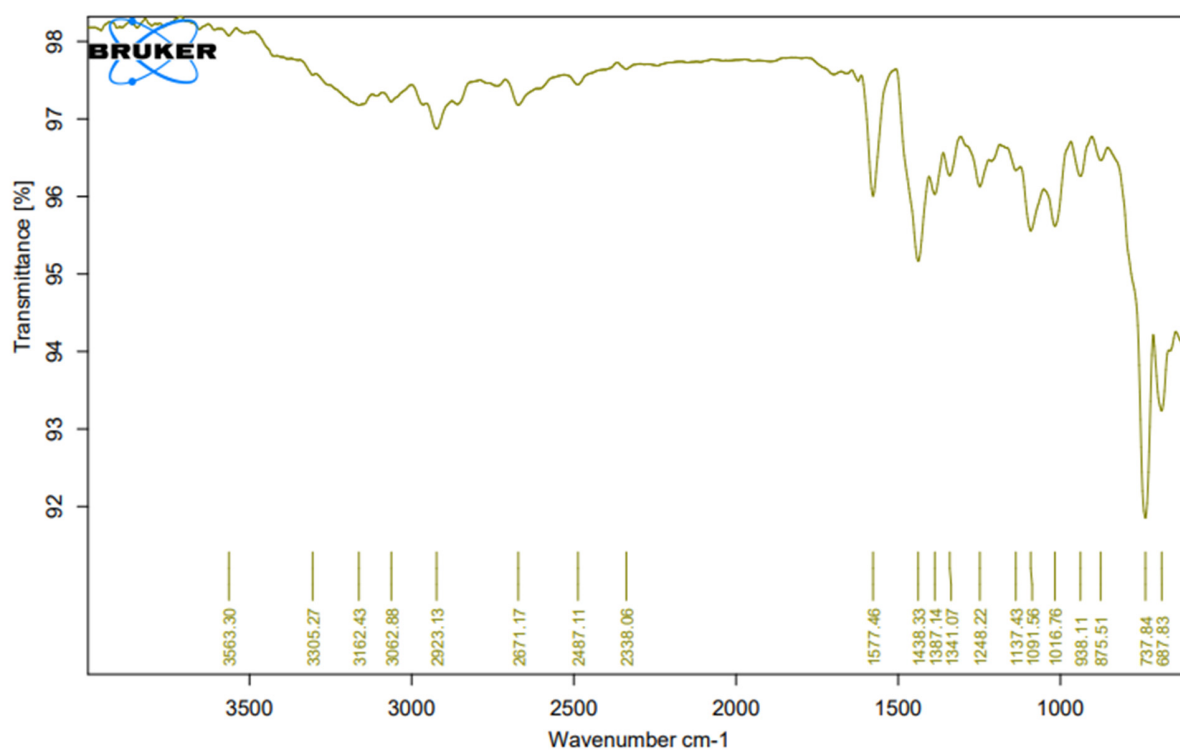
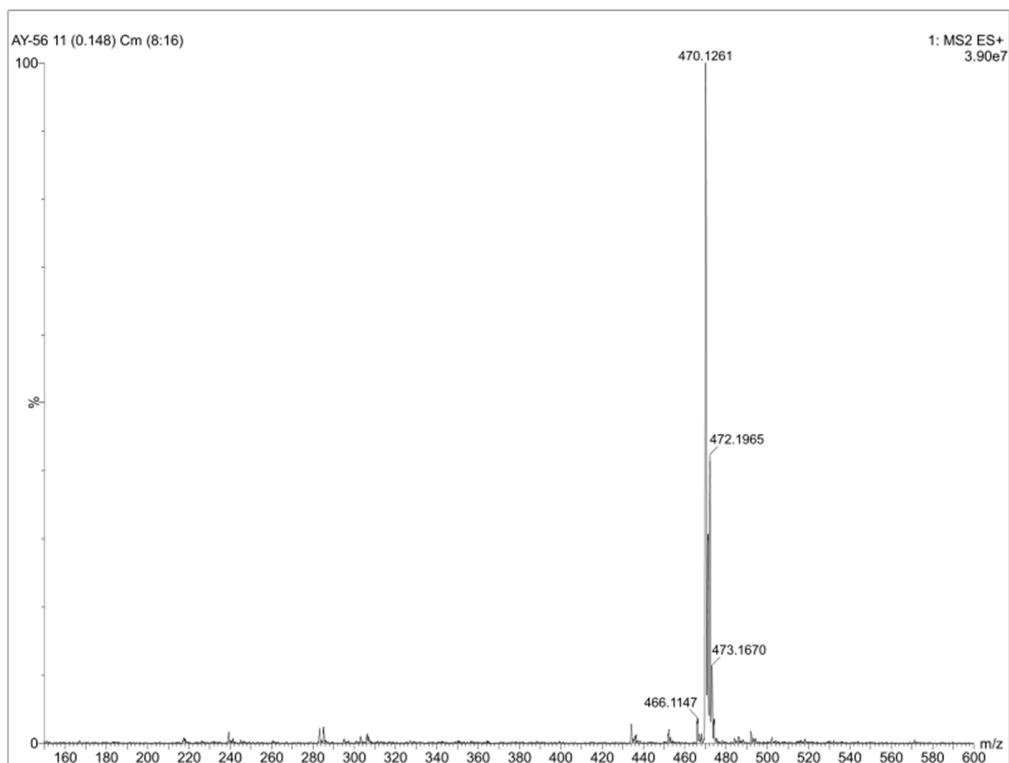
01-11-2022

AY-56



AY-56





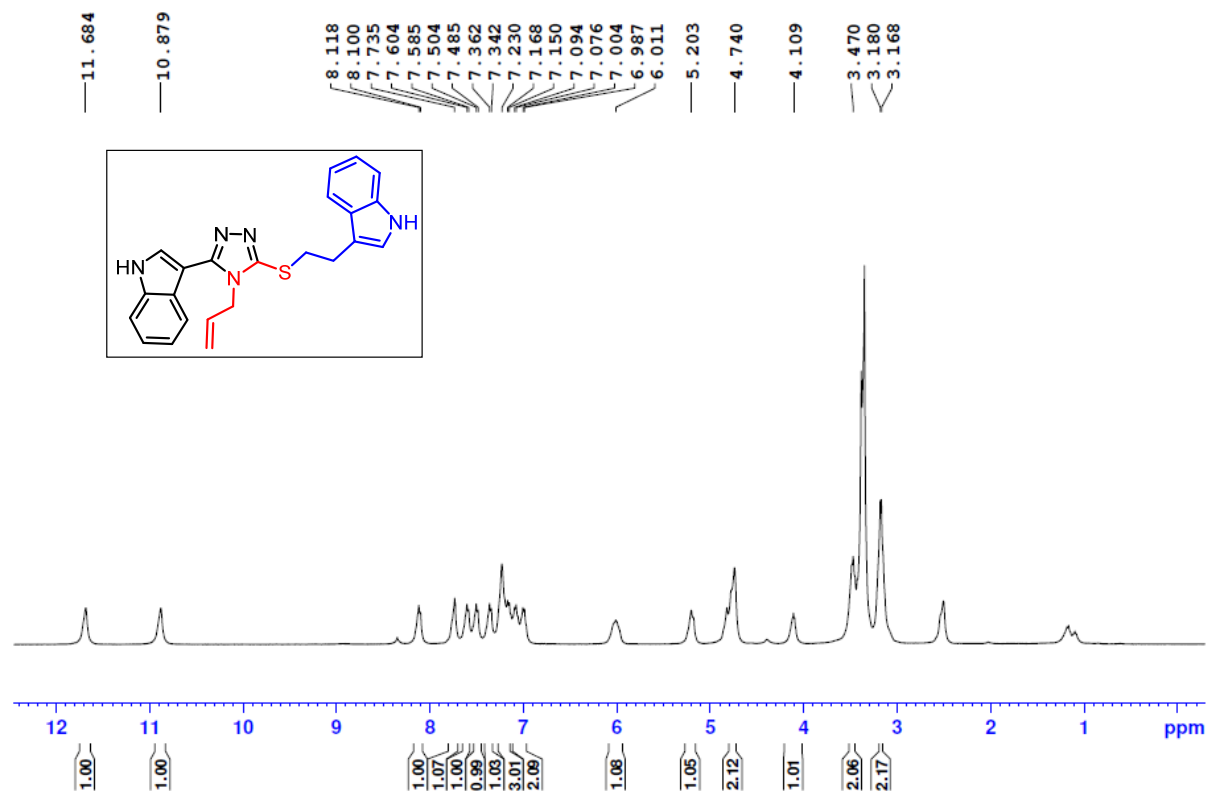
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AY-56

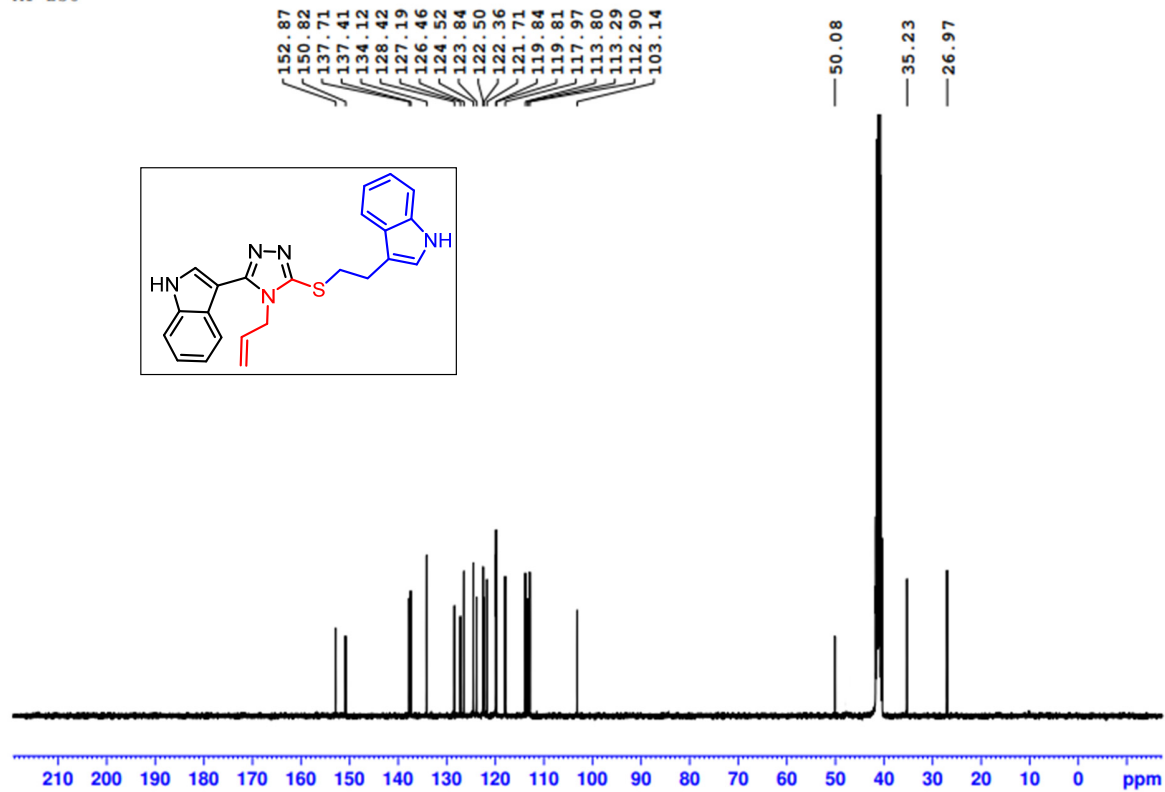
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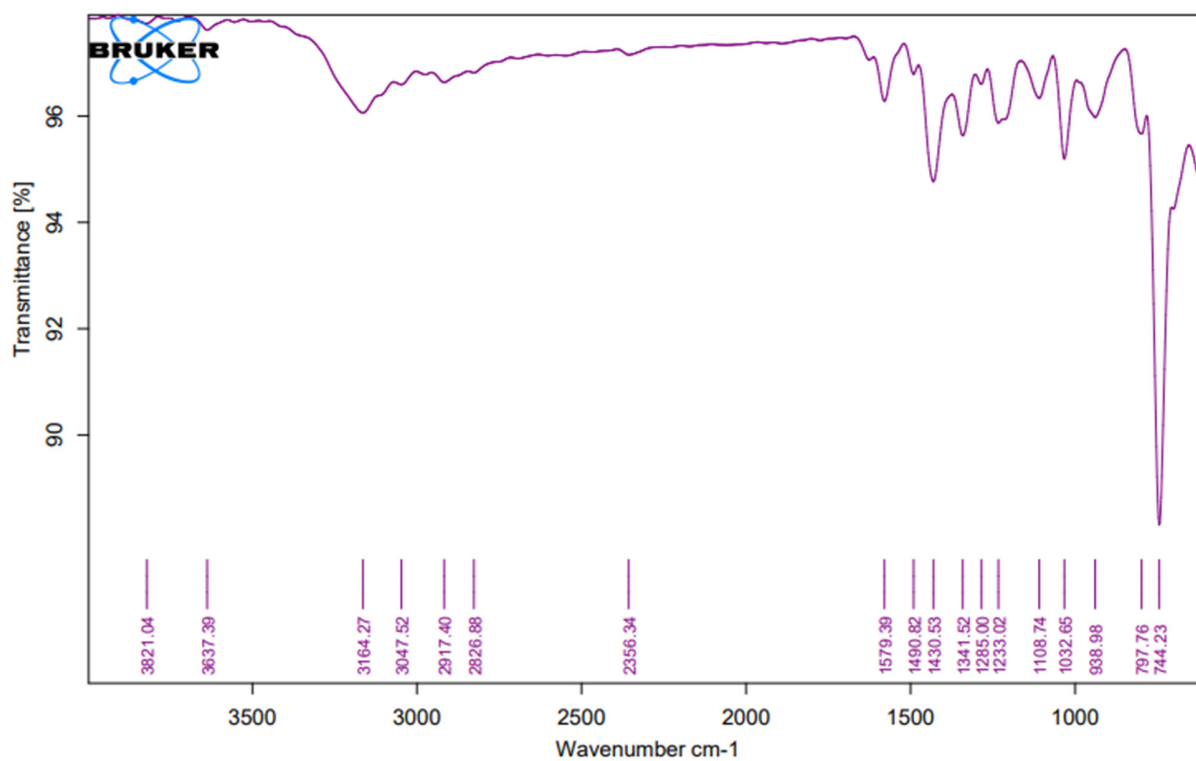
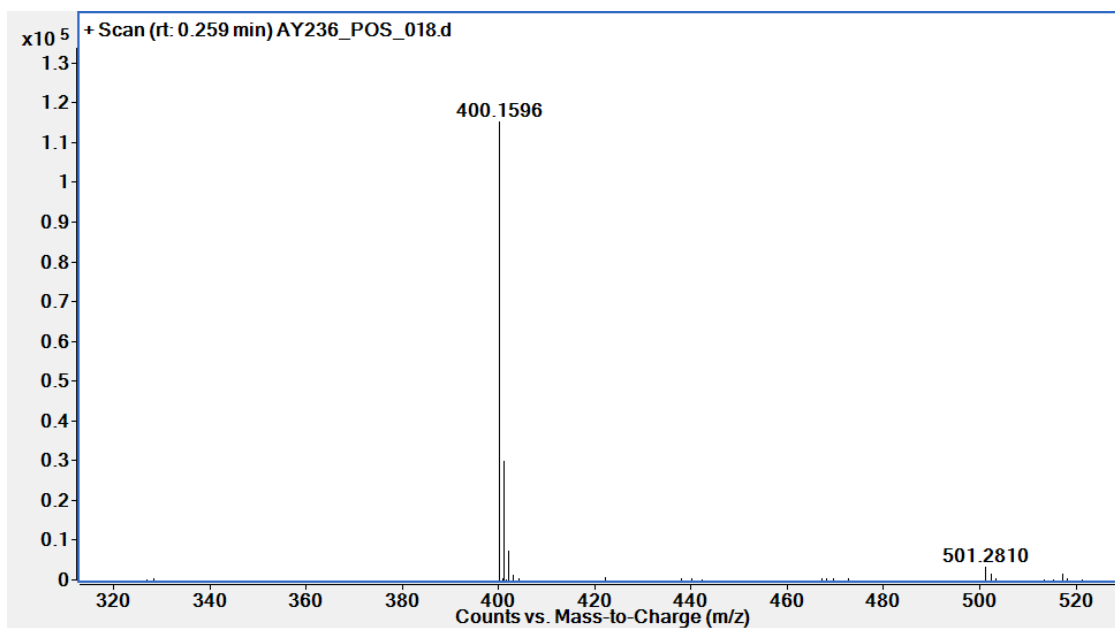
01-11-2022

AY-236



AY-236





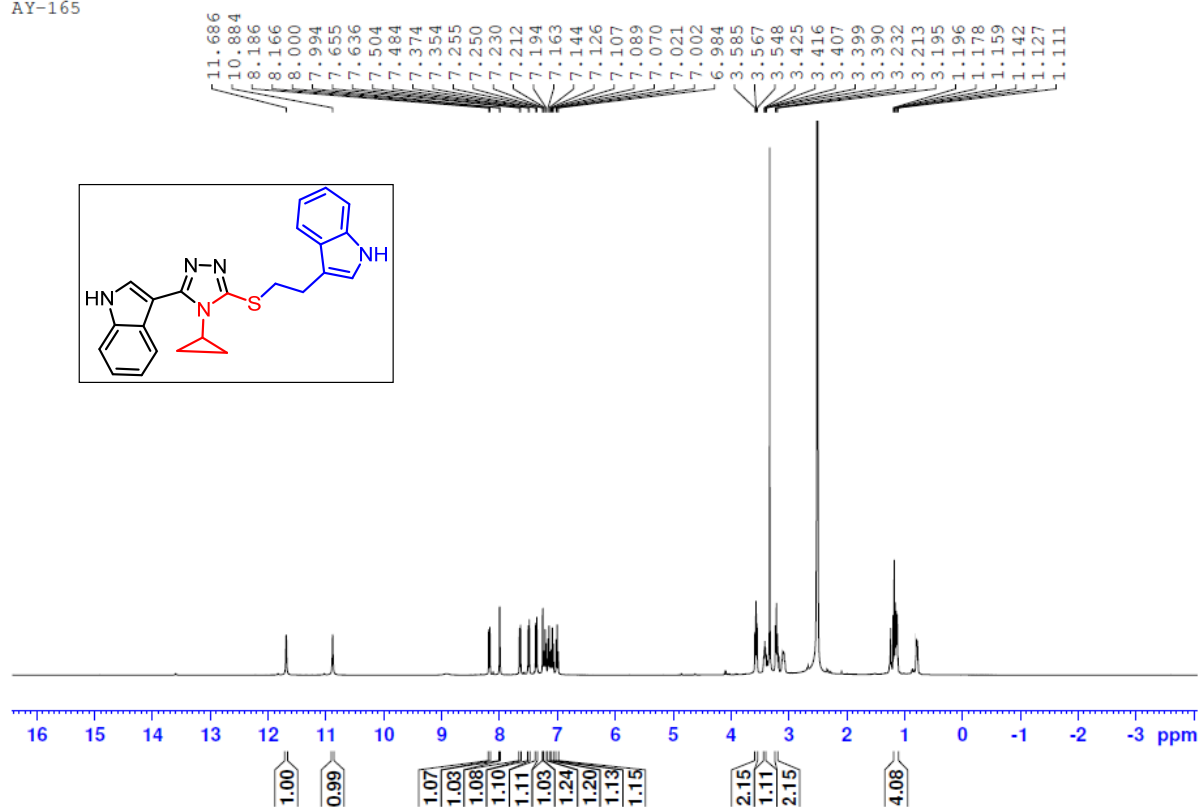
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AY-236

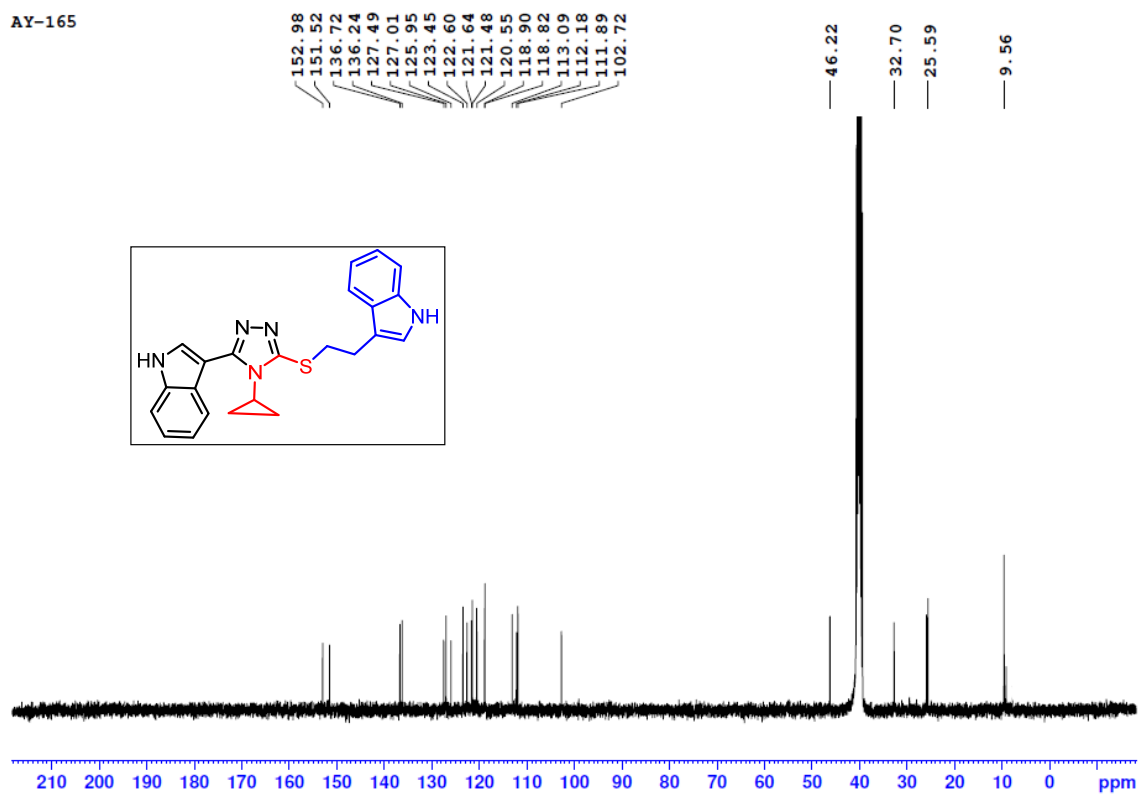
Instrument type and / or accessory

01-11-2022

AY-165



AY-165



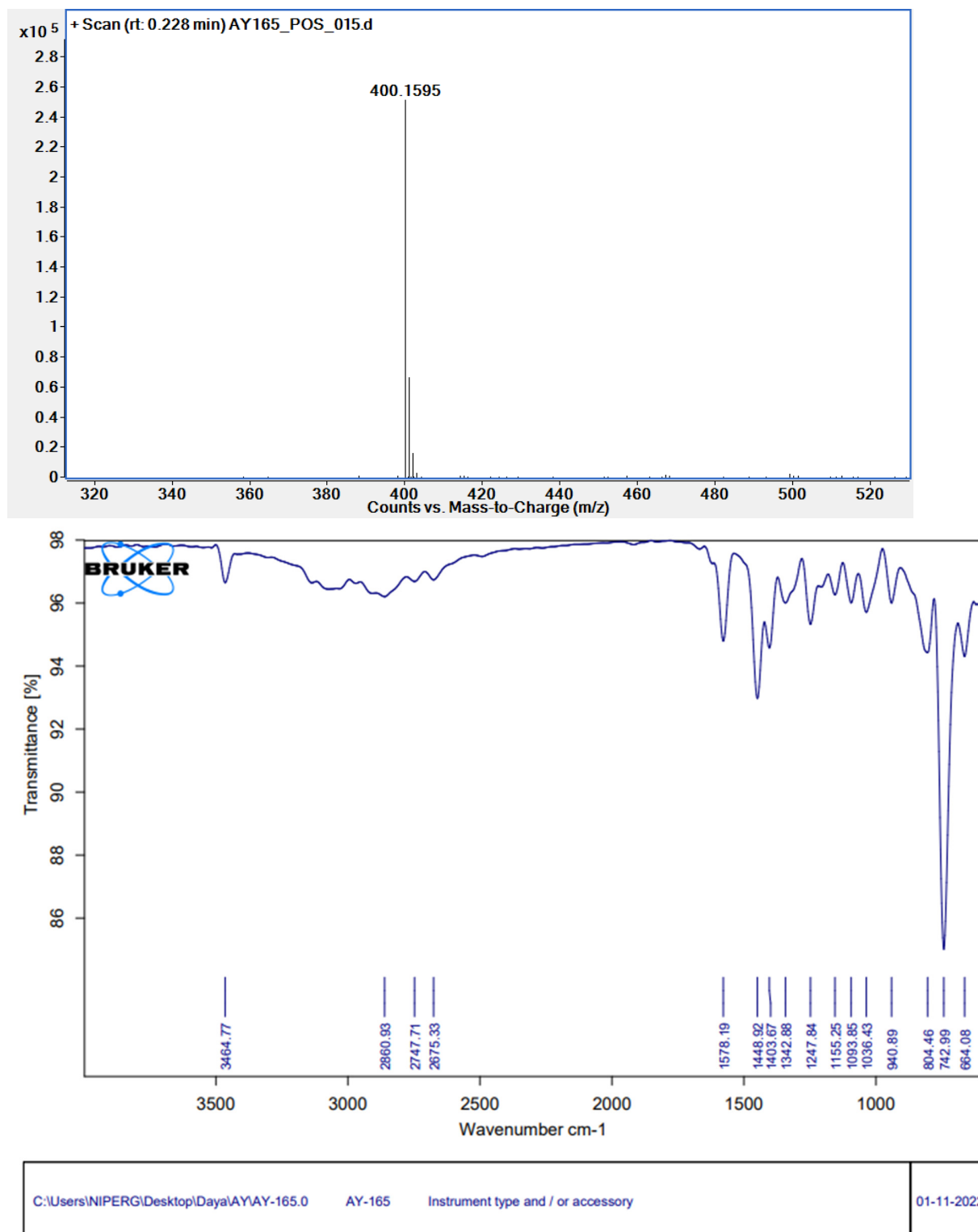


Figure S3: ¹H, ¹³C NMR and Mass copies of all products.