

Supporting Information

Design, Synthesis and Molecular Docking Study of Novel Phenylalanine Based Oxadiazole Analogues as Potent Carbonic Anhydrase II Inhibitors

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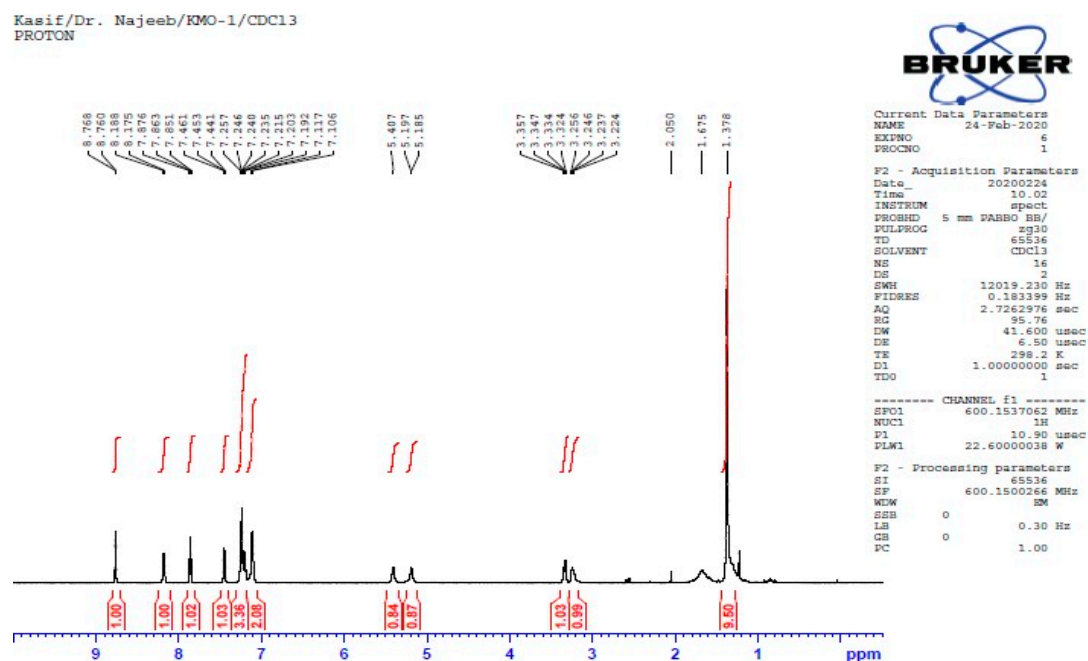
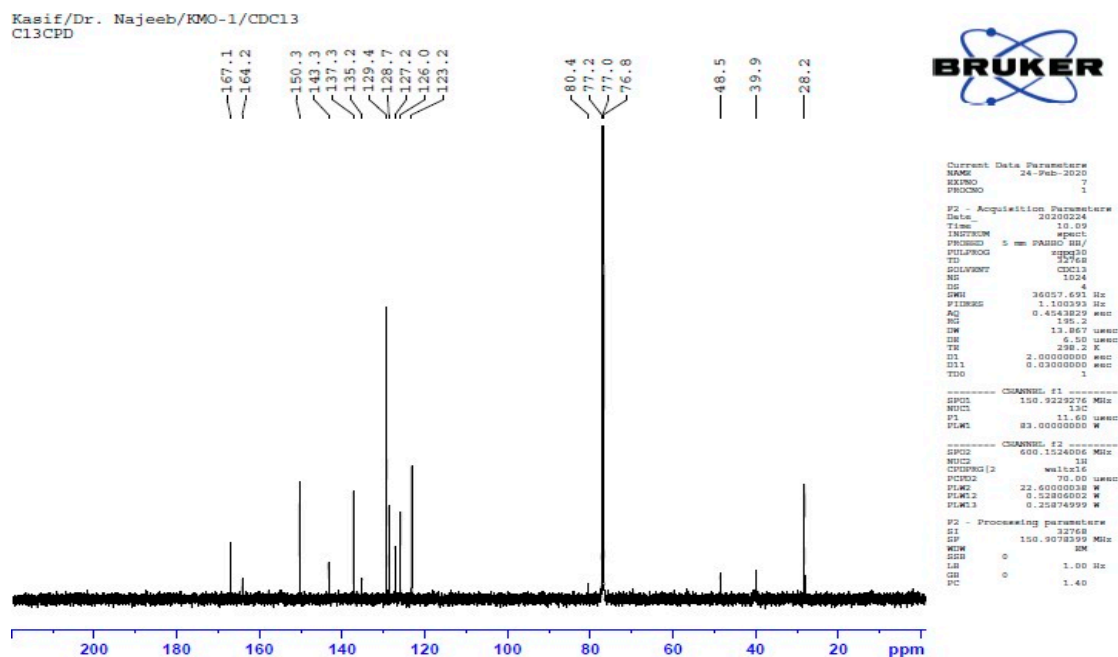
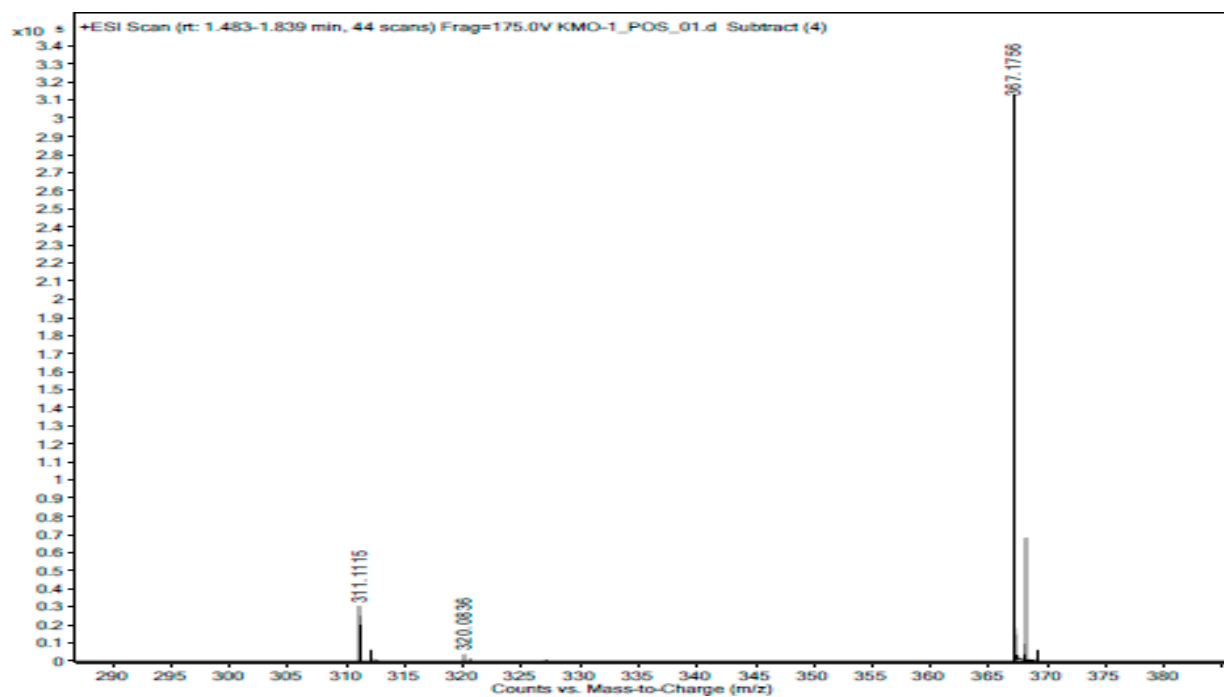


Figure S1. ^1H -NMR (CDCl_3 , 600 MHz) of compound **4a** fix font and size of figure labels.

Figure S2. ¹³C-NMR (CDCl₃, 600 MHz) of compound 4a.Figure S3. HRMS (ESI⁺) of compound 4a.

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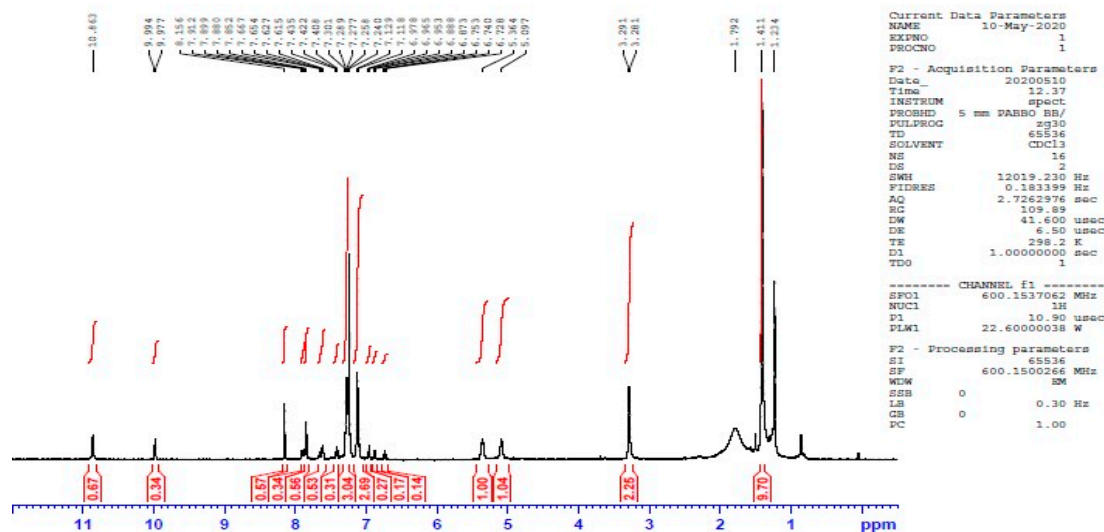


Figure S5. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound **4b**.

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C13CPD

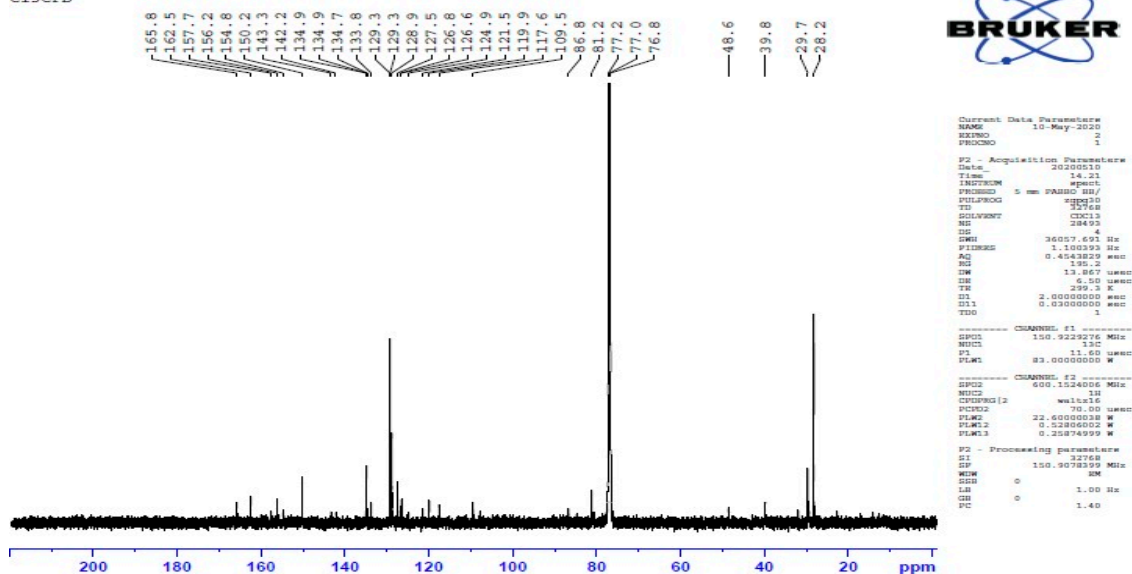
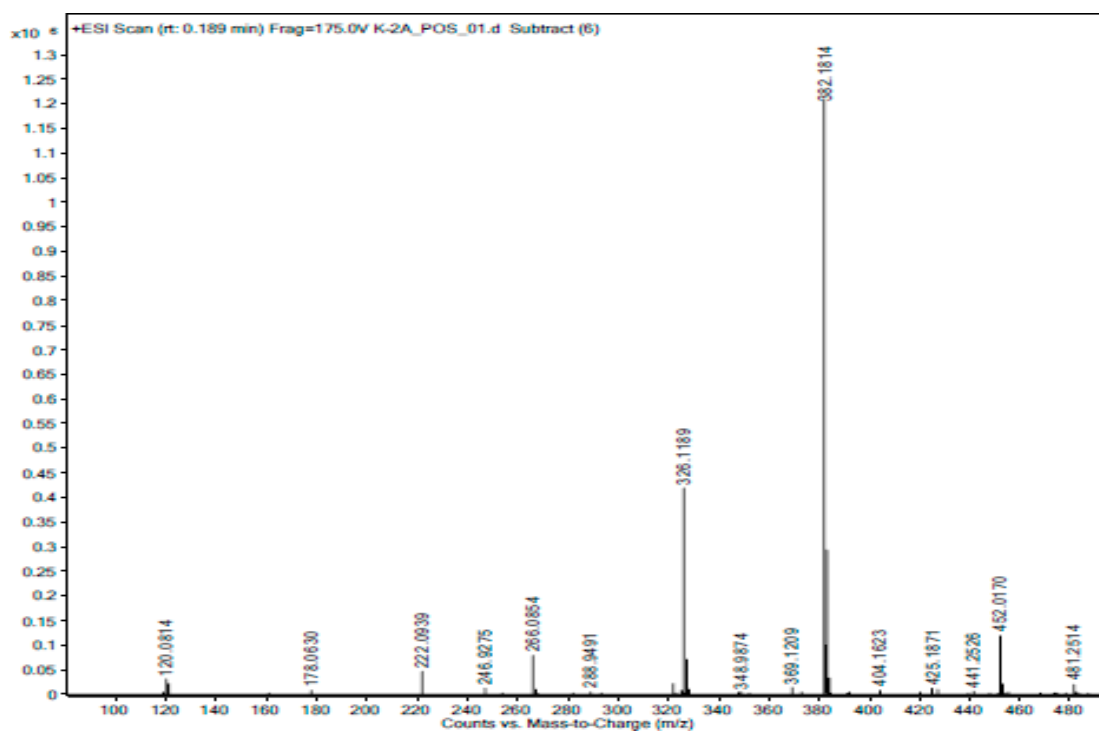
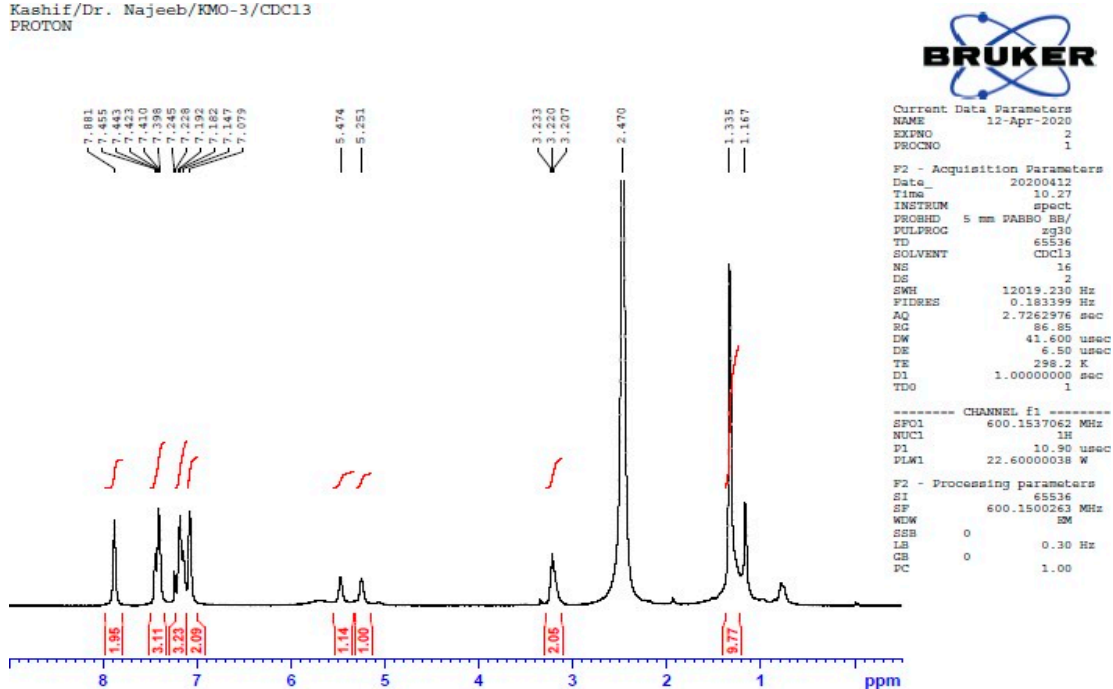
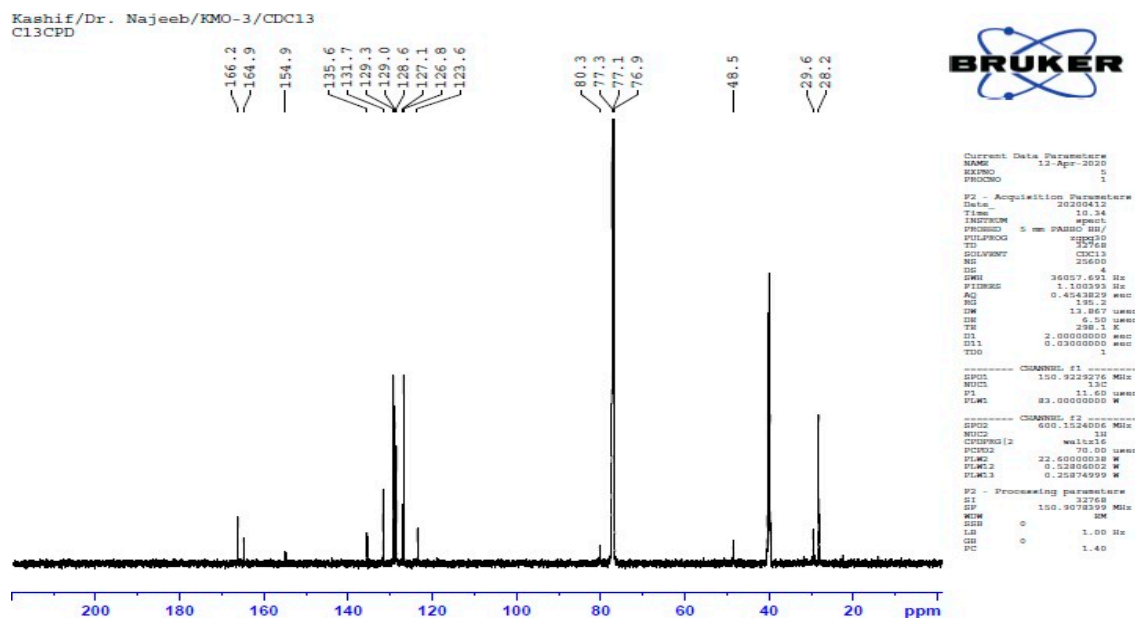
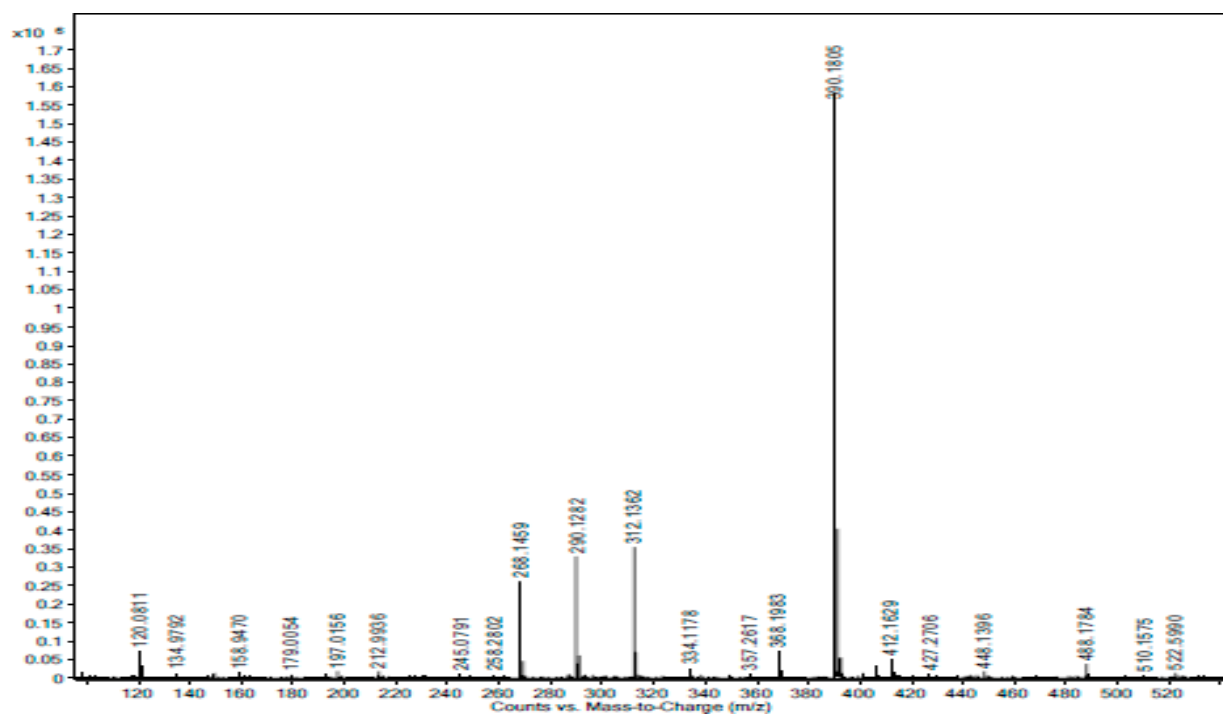


Figure S4. ^1H -NMR (CDCl_3 , 600 MHz) of compound **4b**.

Figure S6. HRMS (ESI⁺) of compound 4b.

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Figure S7. ¹H-NMR (CDCl₃, 600 MHz) of compound 4c.

Figure S8. ¹³C-NMR (CDCl₃, 125 MHz) of compound 4c.Figure S9. HRMS (ESI⁺) of compound 4c.

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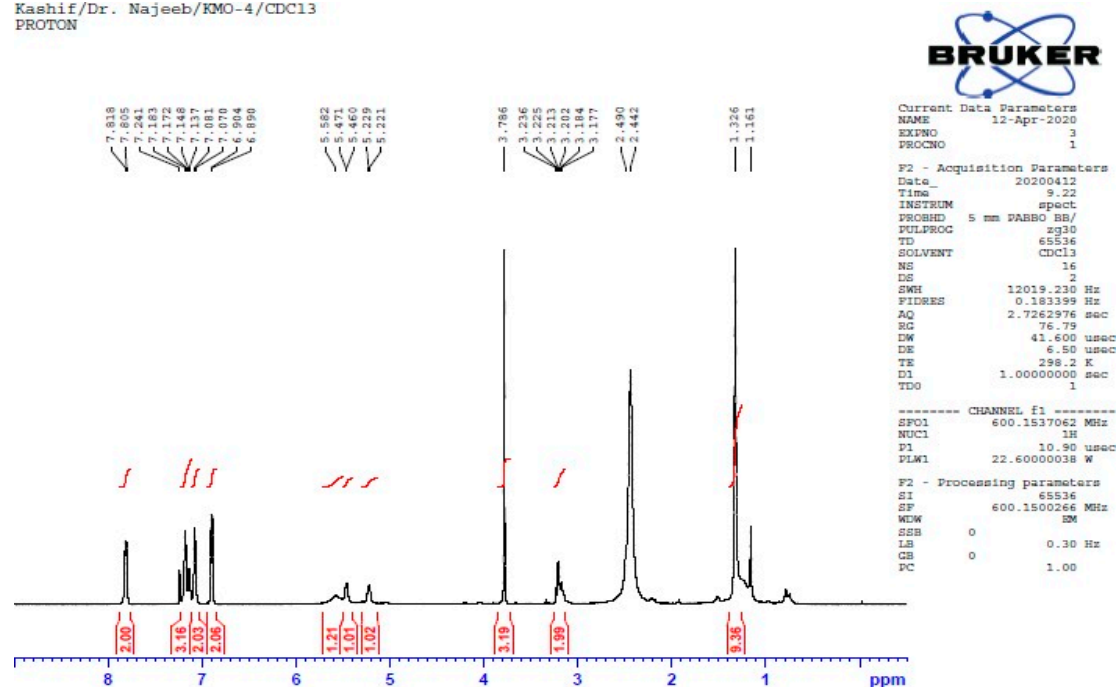


Figure S10. ^1H -NMR (CDCl_3 , 600 MHz) of compound 4d.

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C13CPD

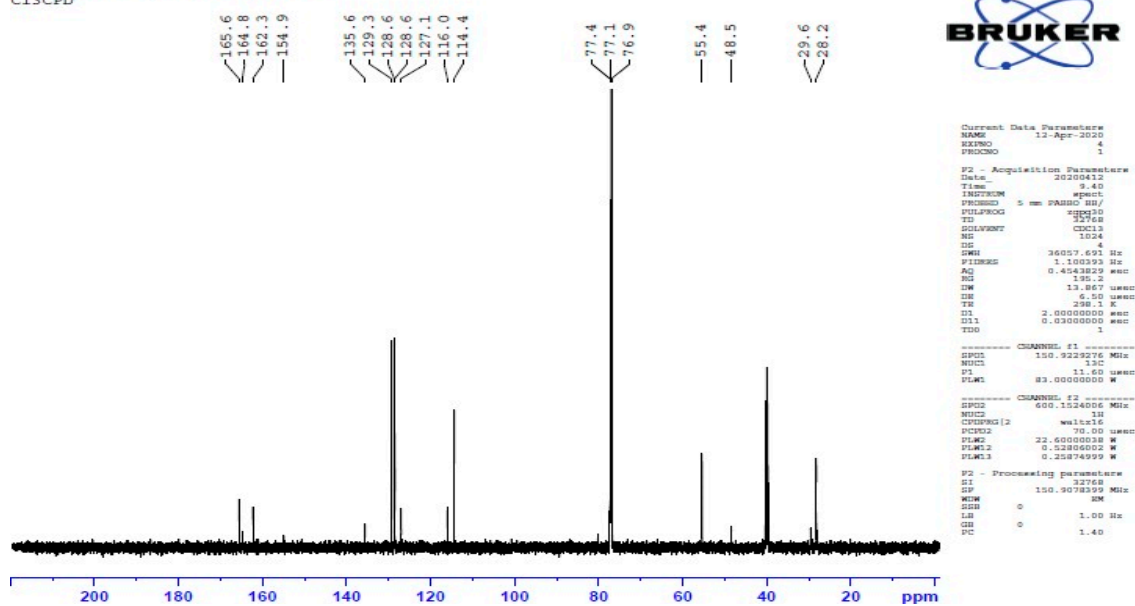
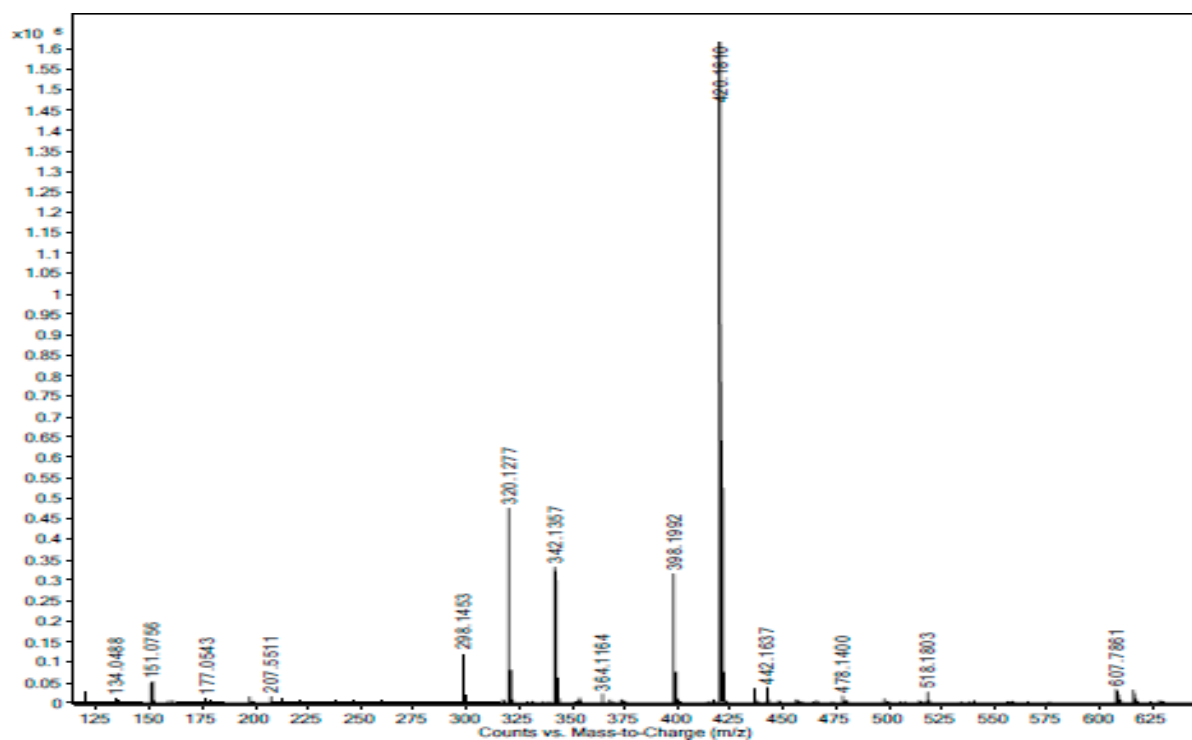
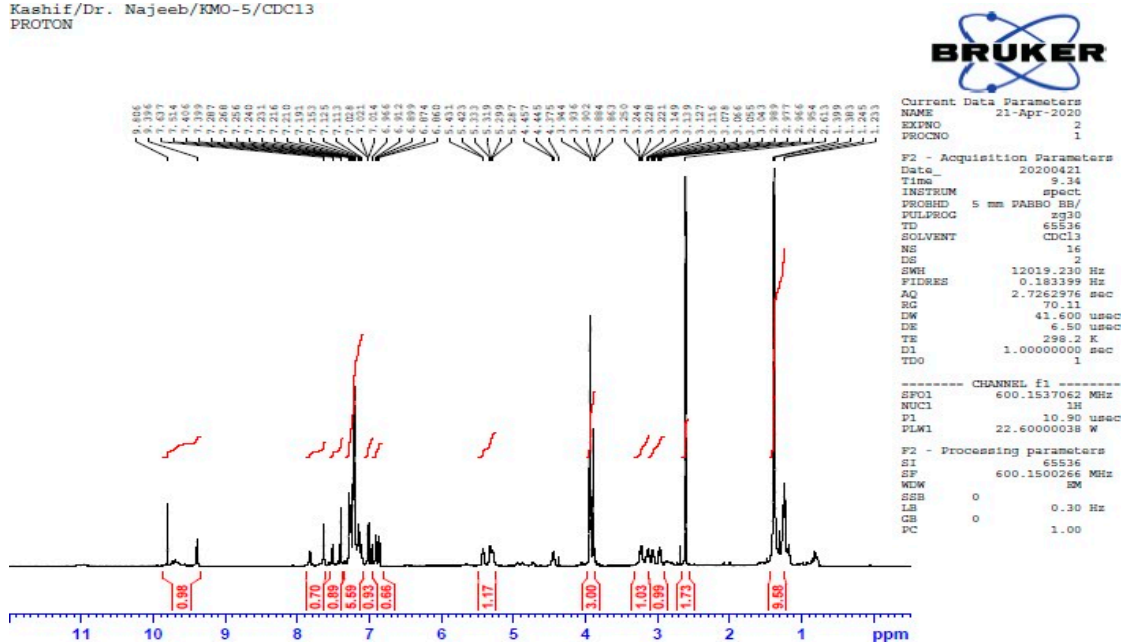
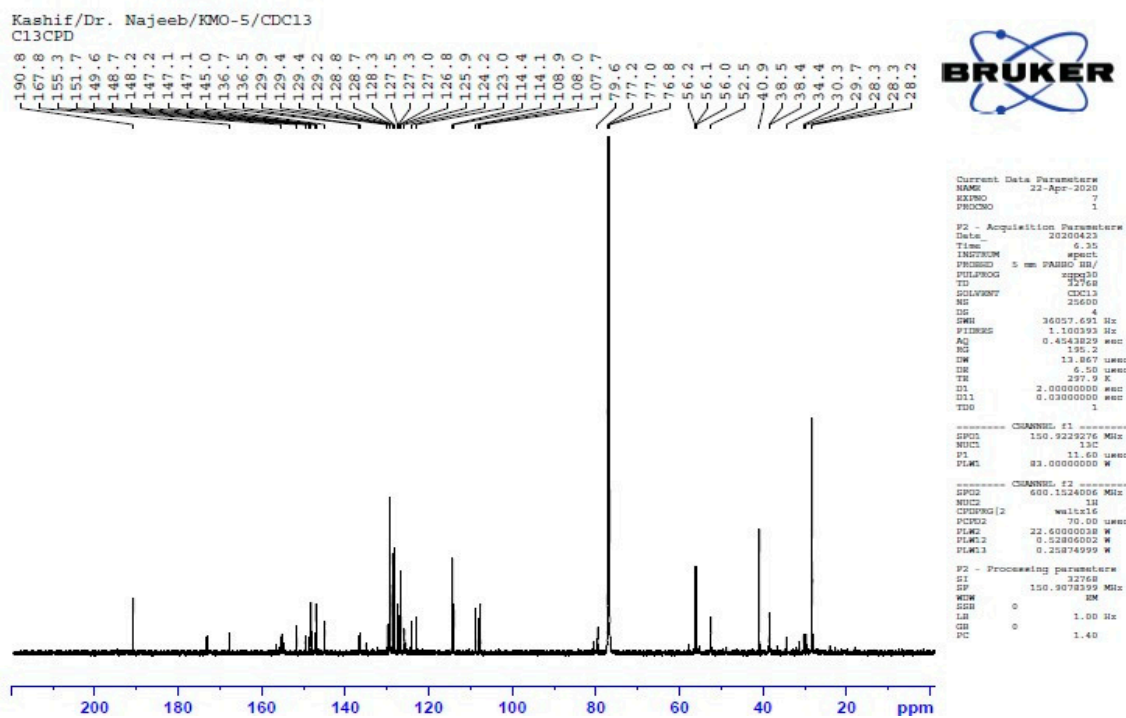
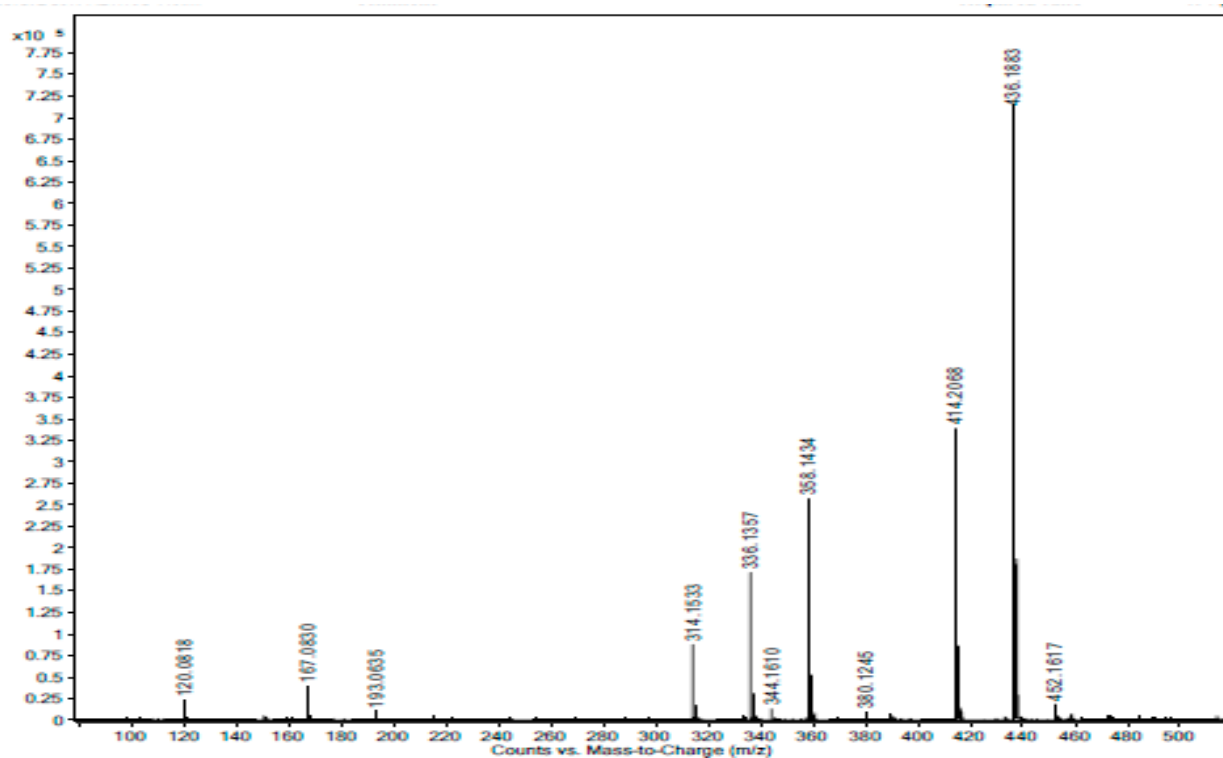


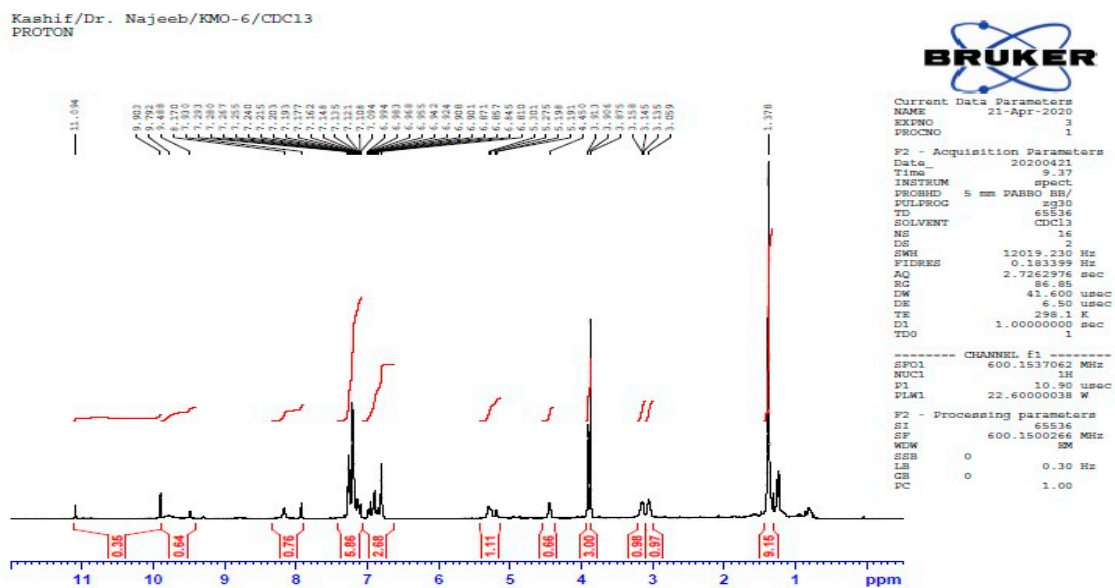
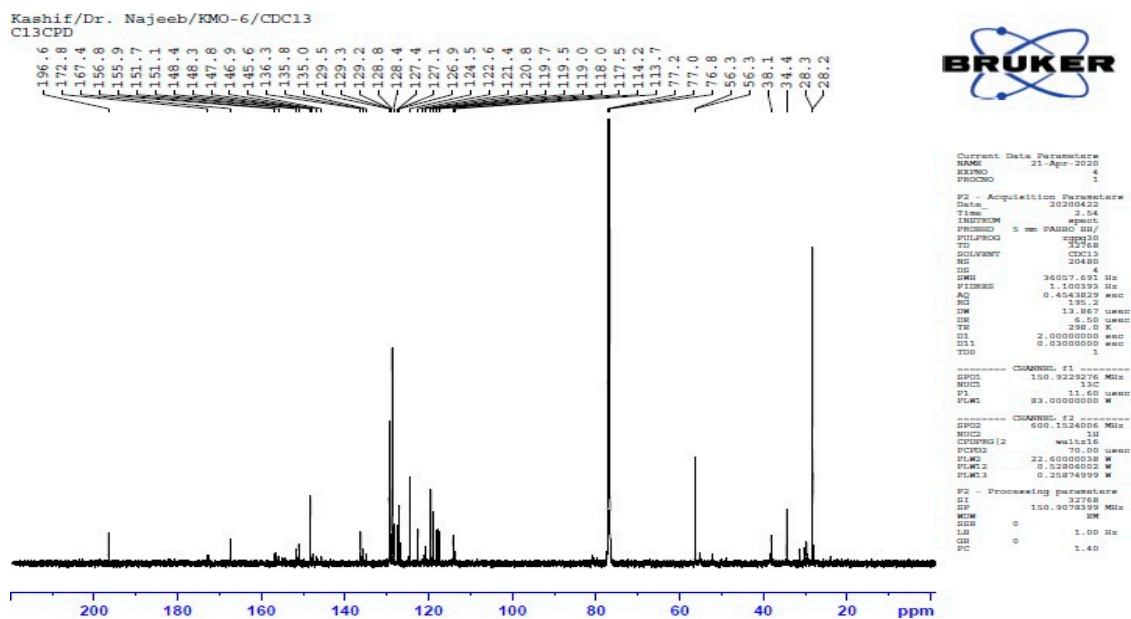
Figure S11. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound 4d.

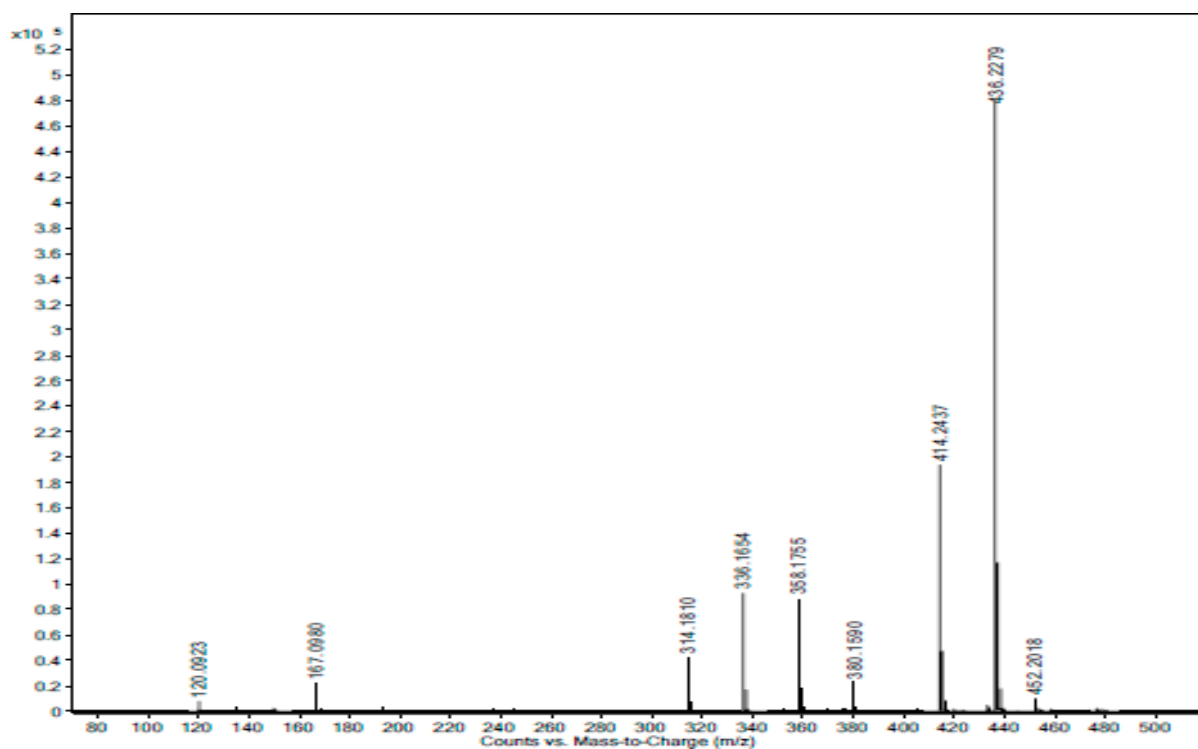
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PROTON

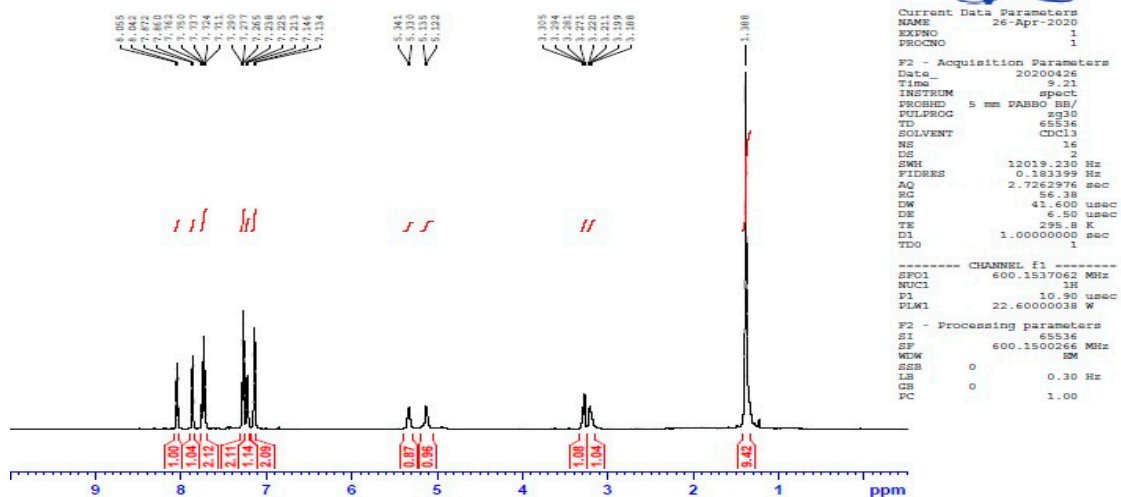
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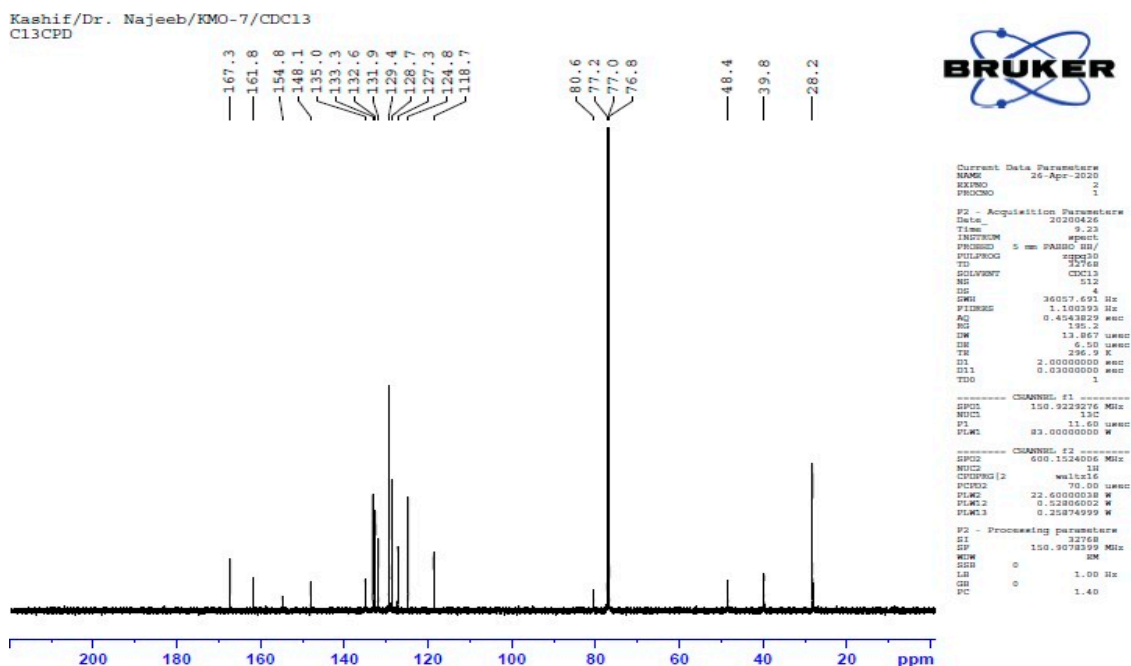
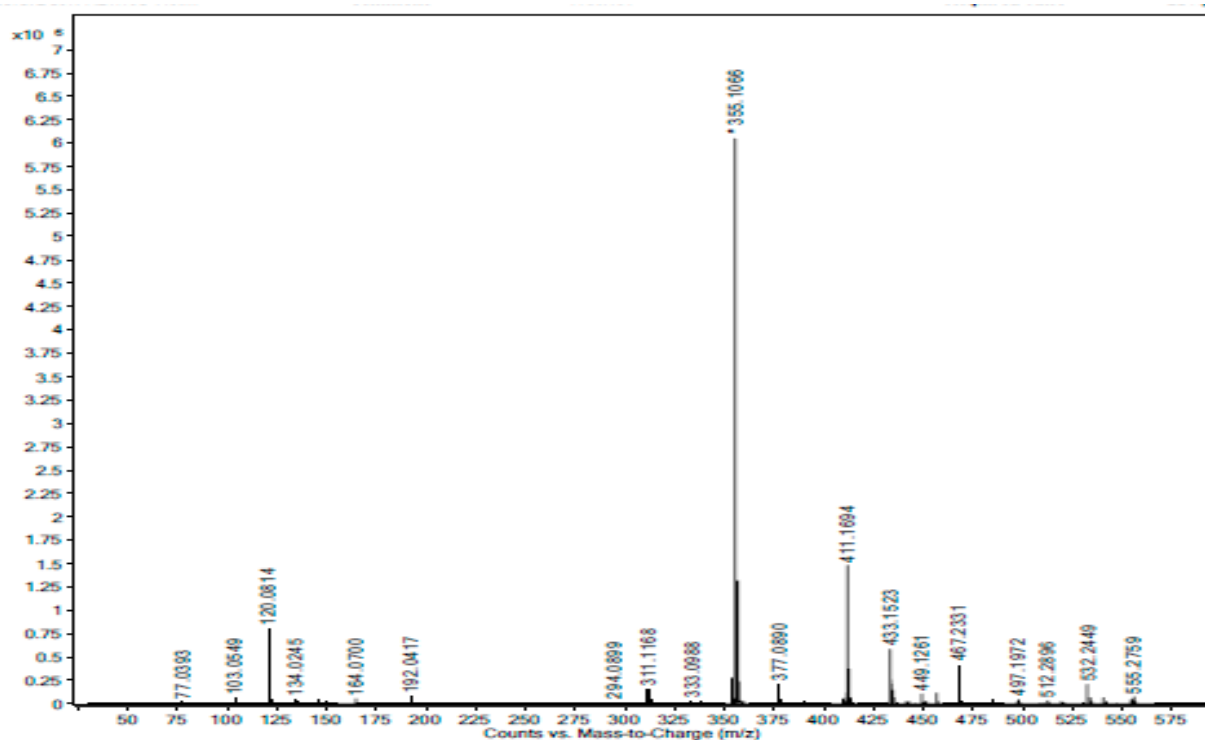
Figure S14. ¹³C-NMR (CDCl₃, 125 MHz) of compound 4e.Figure S15. HRMS (ESI⁺) of compound 4e.

Figure S16. ¹H-NMR (CDCl₃, 600 MHz) of compound 4f.Figure S17. ¹³C-NMR (CDCl₃, 125 MHz) of compound 4f.

Figure S18. HRMS (ESI⁺) of compound 4f.

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Figure S19. ¹H-NMR (CDCl₃, 600 MHz) of compound 4g.

Figure S20. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound **4g**.Figure S21. HRMS (ESI^+) of compound **4g**.

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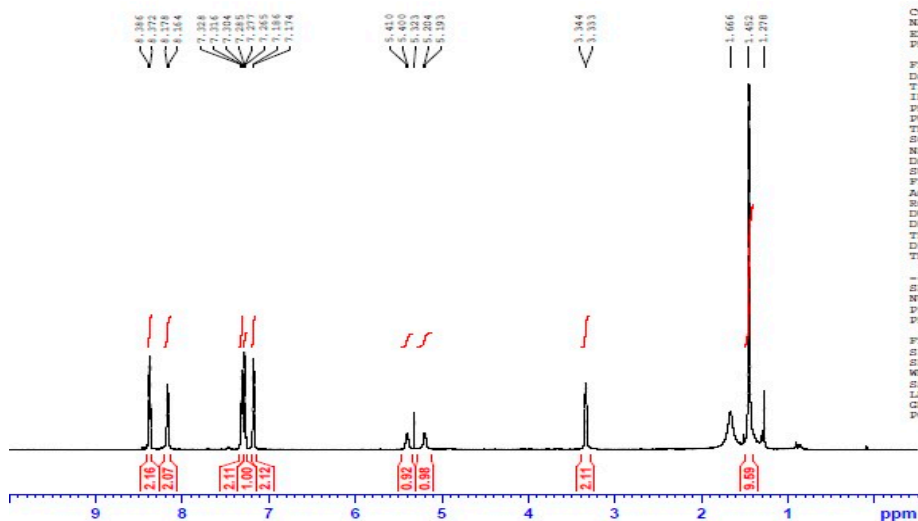


Figure S22. ^1H -NMR (CDCl_3 , 600 MHz) of compound 4h.

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C13CPD

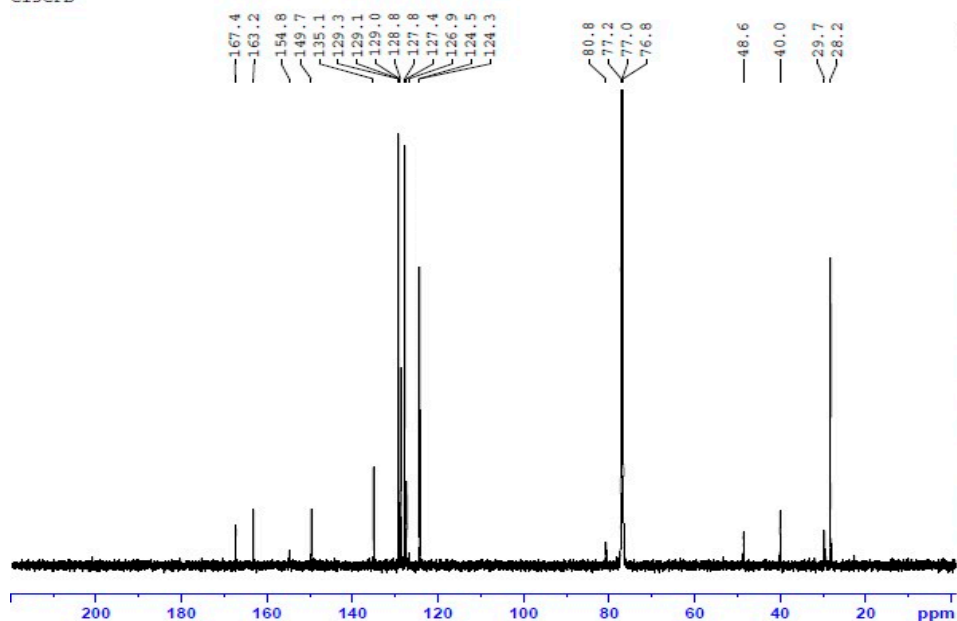
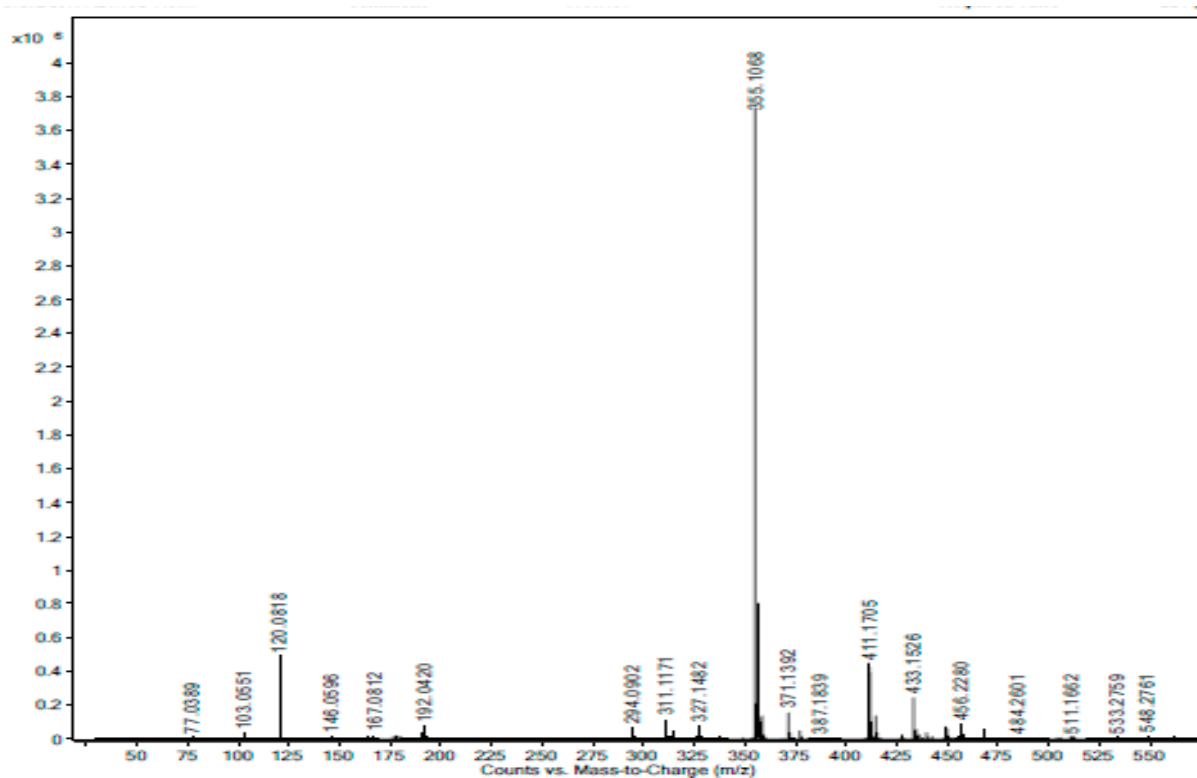
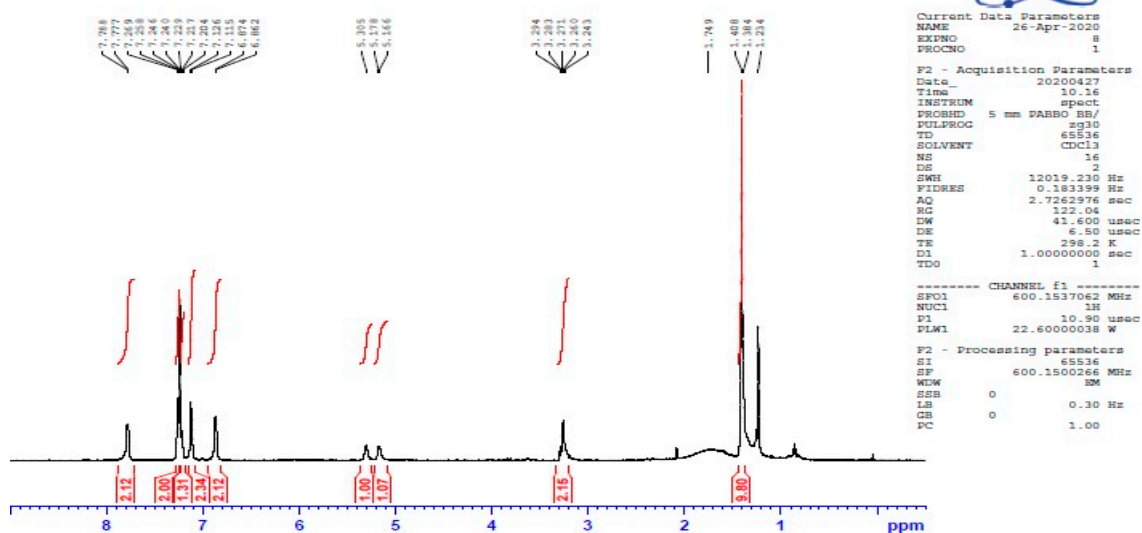
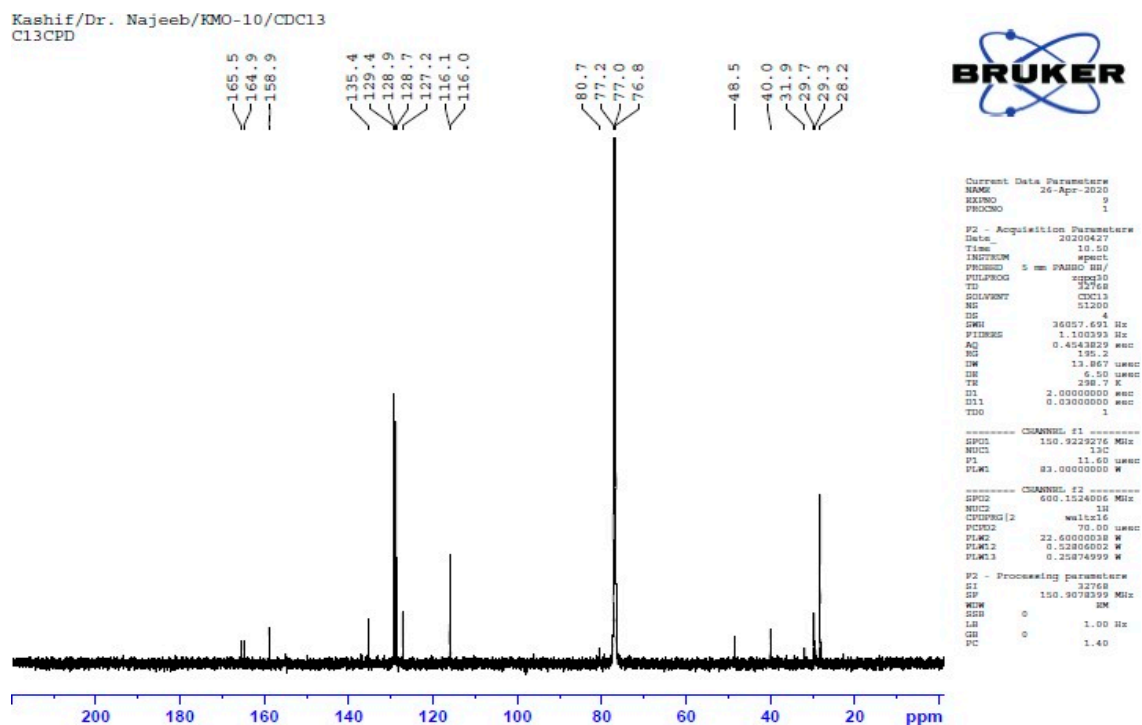
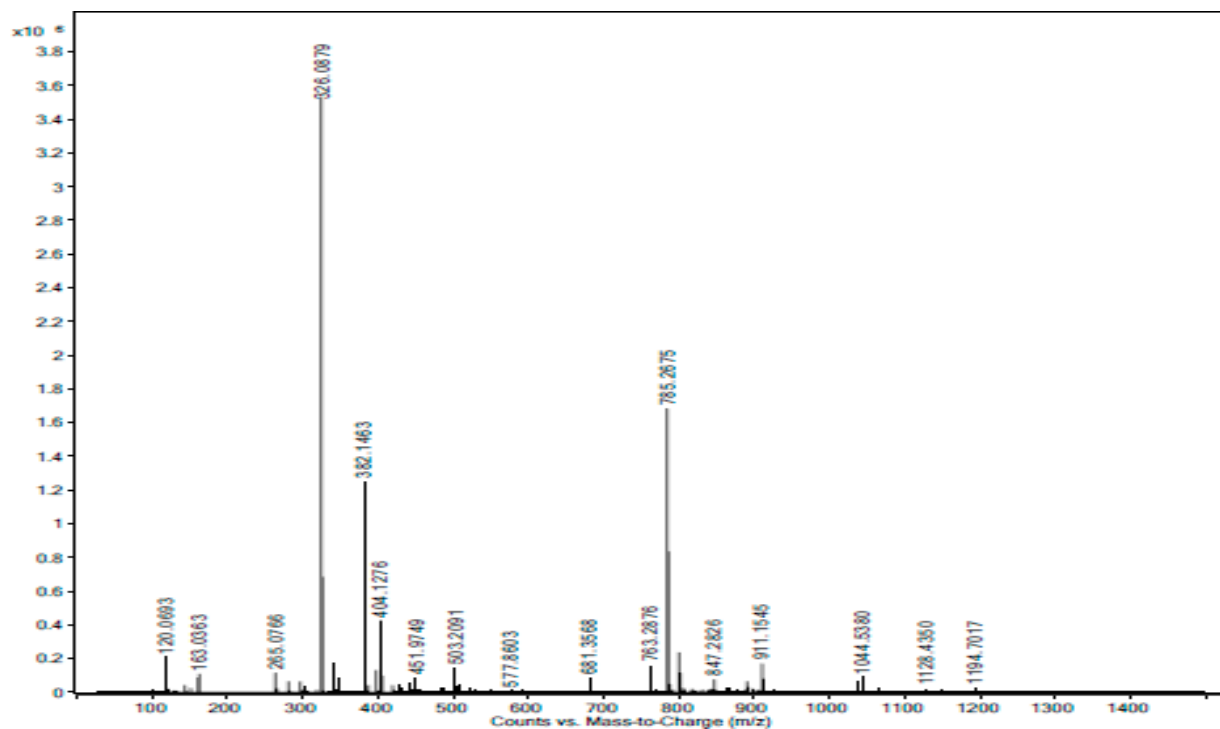


Figure S23. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound 4h.

Figure S24. HRMS (ESI⁺) of compound 4h.

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PROTON

Figure S25. ¹H-NMR (CDCl₃, 600 MHz) of compound 4i.

Figure S26. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound **4i**.Figure S27. HRMS (ESI^+) of compound **4i**.

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PROTON

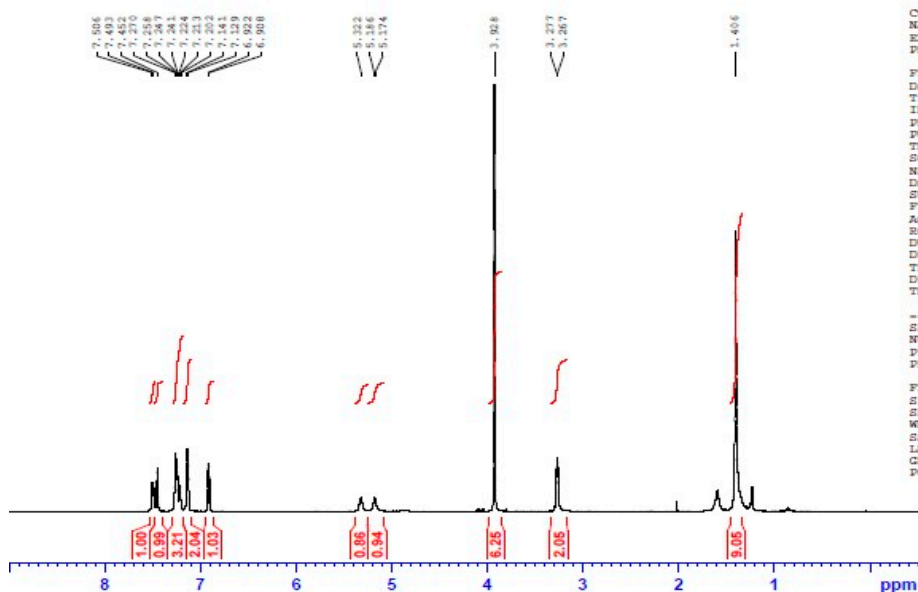


Figure S28. ^1H -NMR (CDCl_3 , 600 MHz) of compound 4j.

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C13CPD

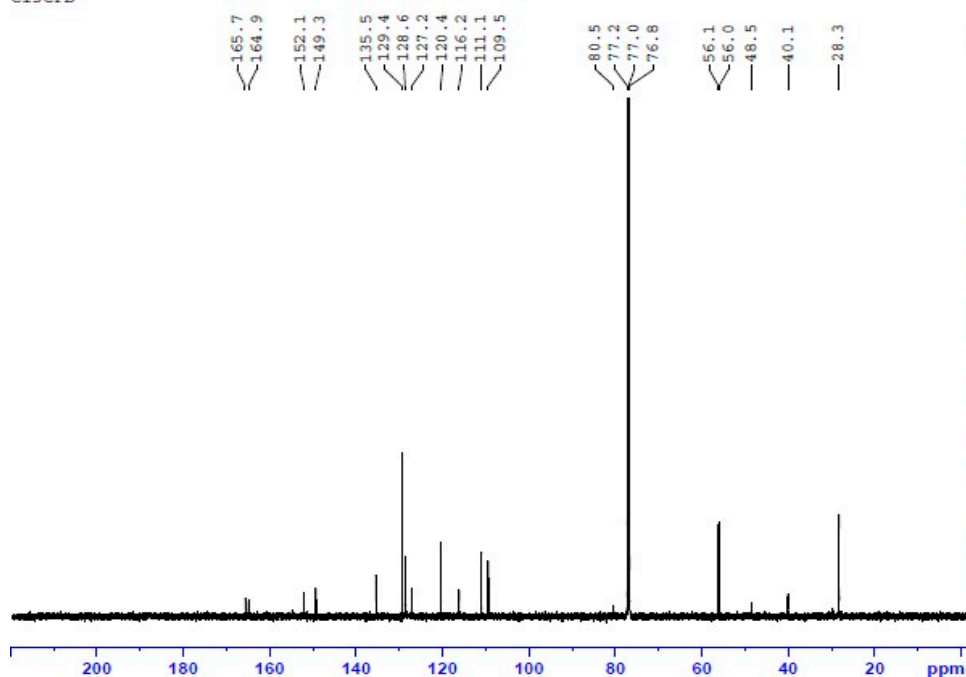


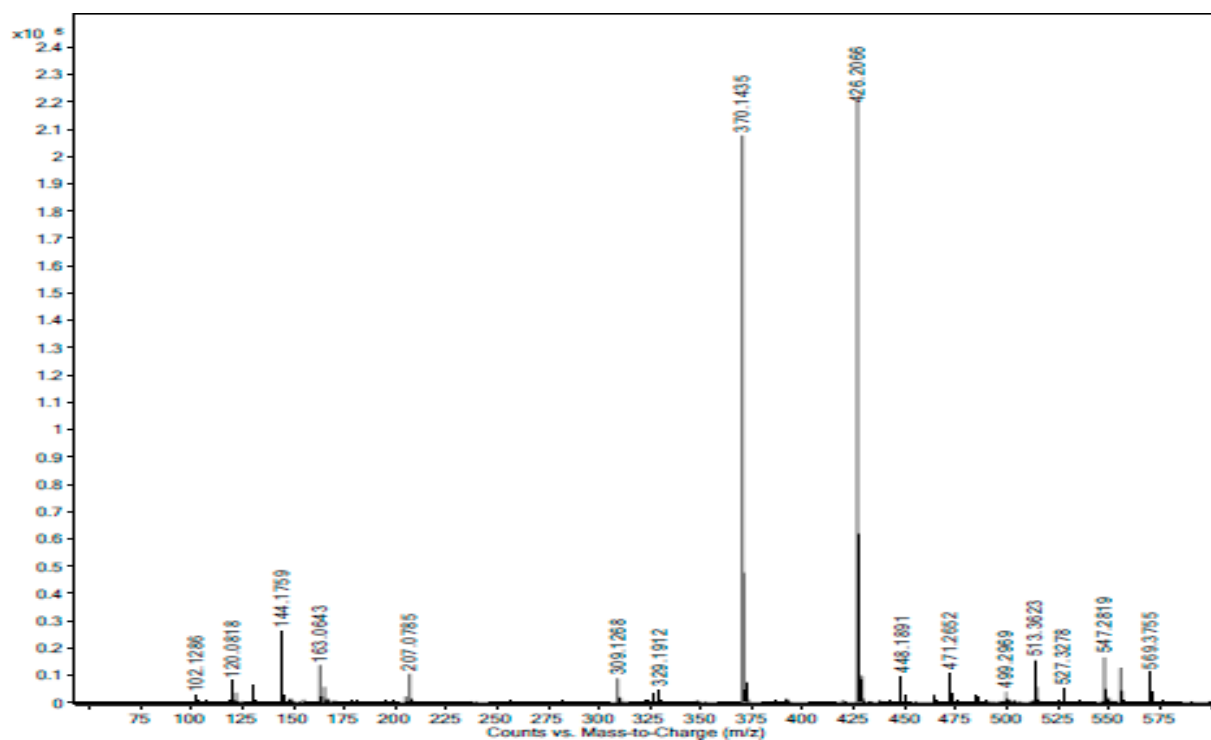
Figure S29. ^{13}C -NMR (CDCl_3 , 125 MHz) of compound 4j.



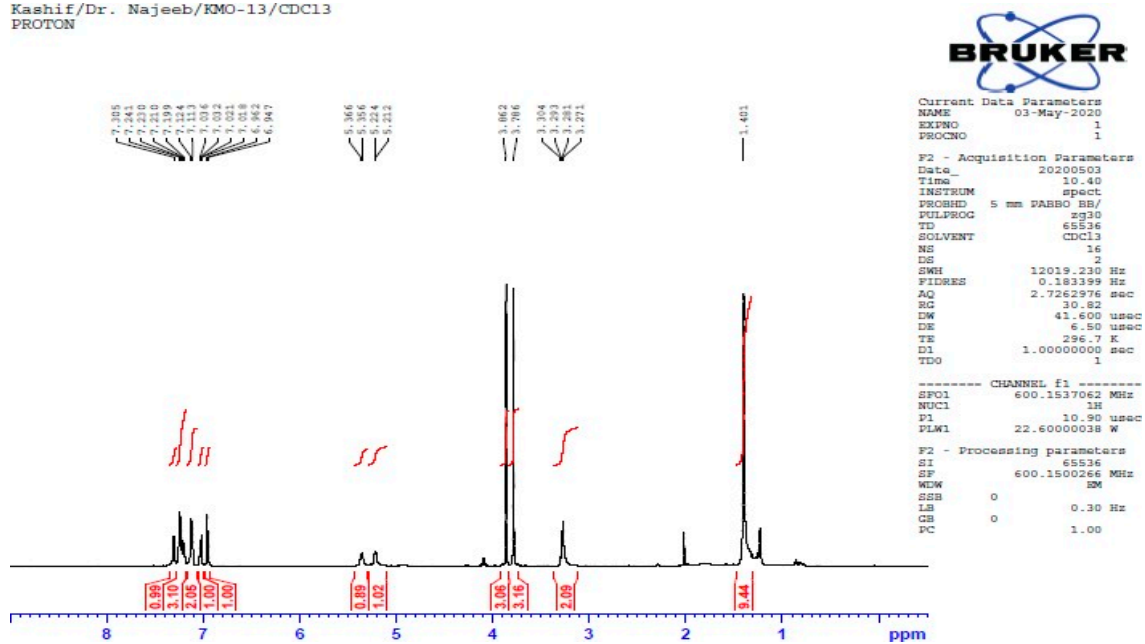
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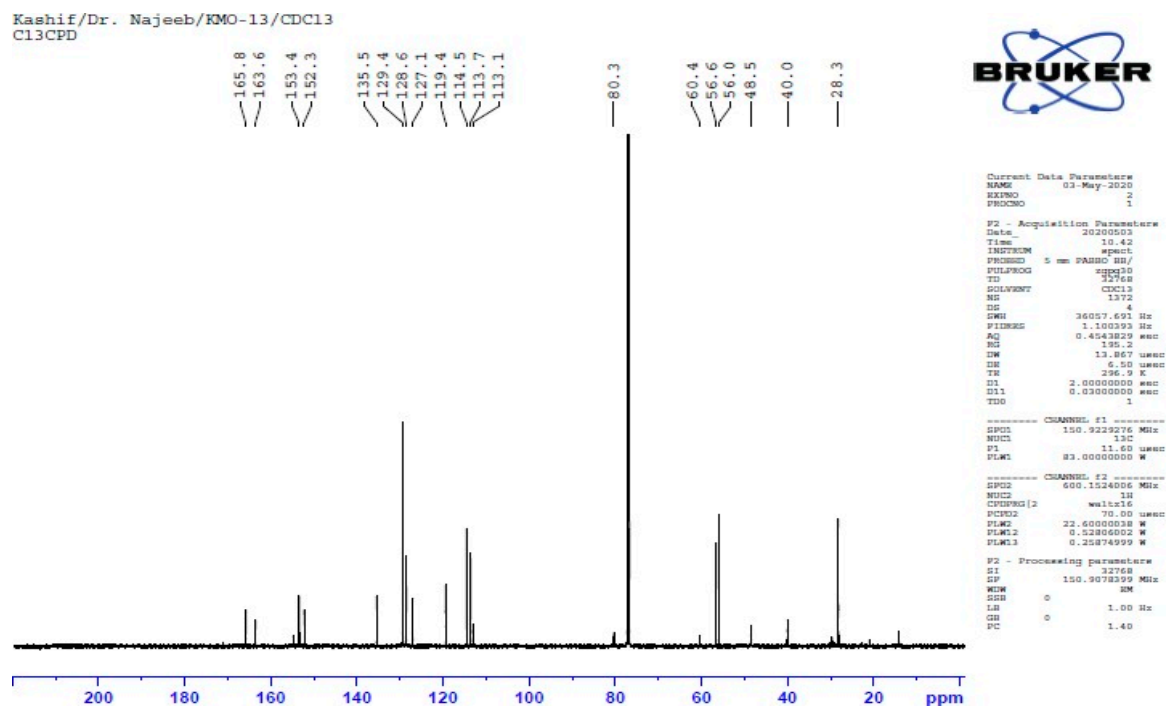
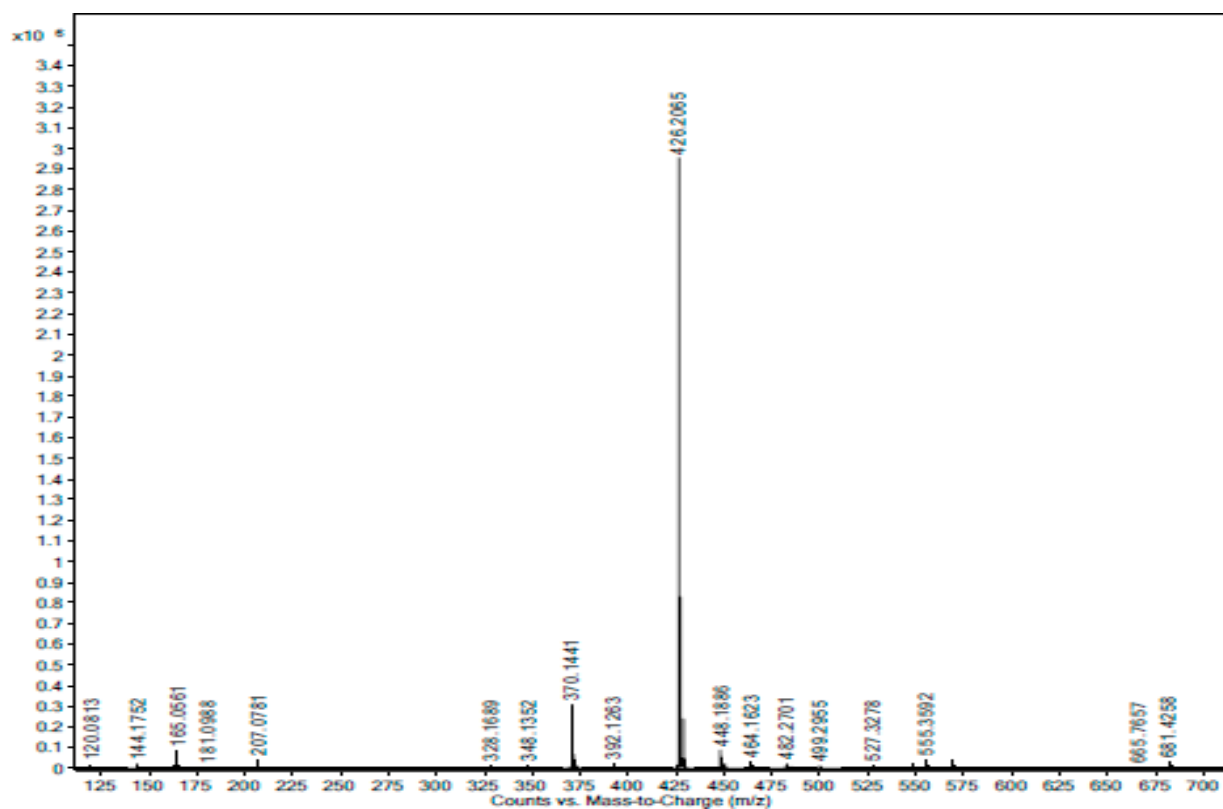


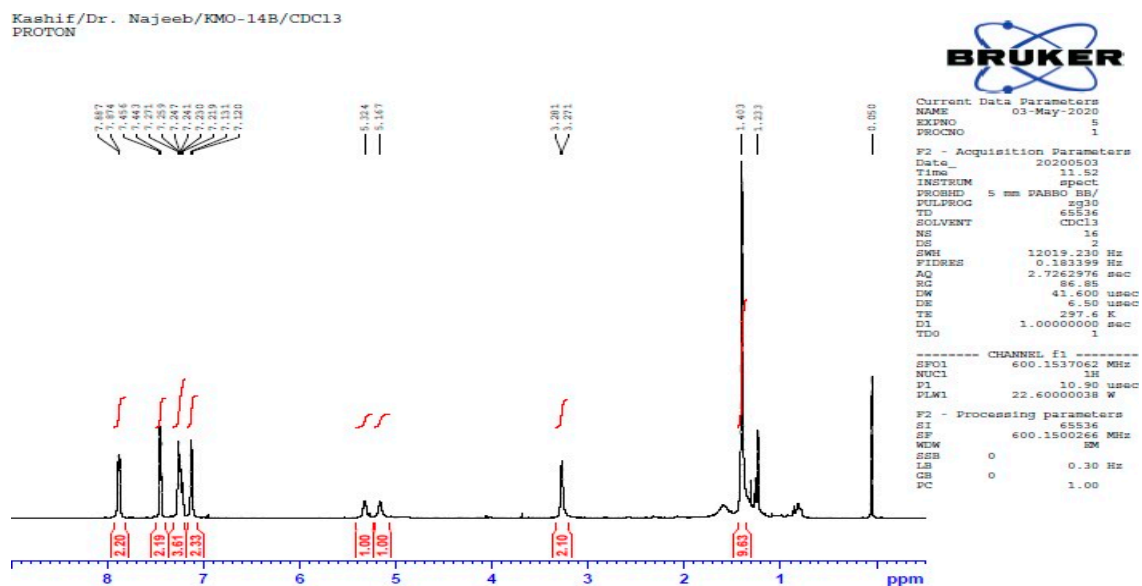
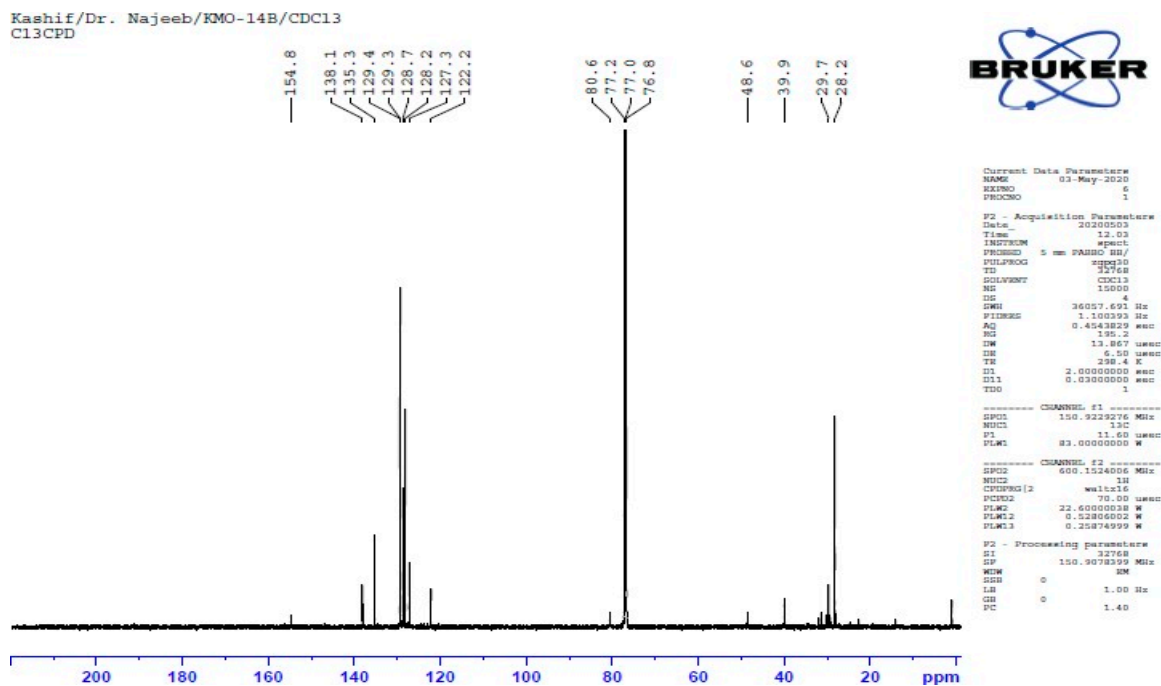
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Figure S30. HRMS (ESI⁺) of compound 4j.

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Figure S31. ¹H-NMR (CDCl₃, 600 MHz) of compound 4k.

Figure S32. ¹³C-NMR (CDCl₃, 125 MHz) of compound 4k.Figure S33. HRMS (ESI⁺) of compound 4k.

Figure S34. ¹H-NMR (CDCl₃, 600 MHz) of compound 4l.Figure S35. ¹³C-NMR (CDCl₃, 125 MHz) of compound 4l.

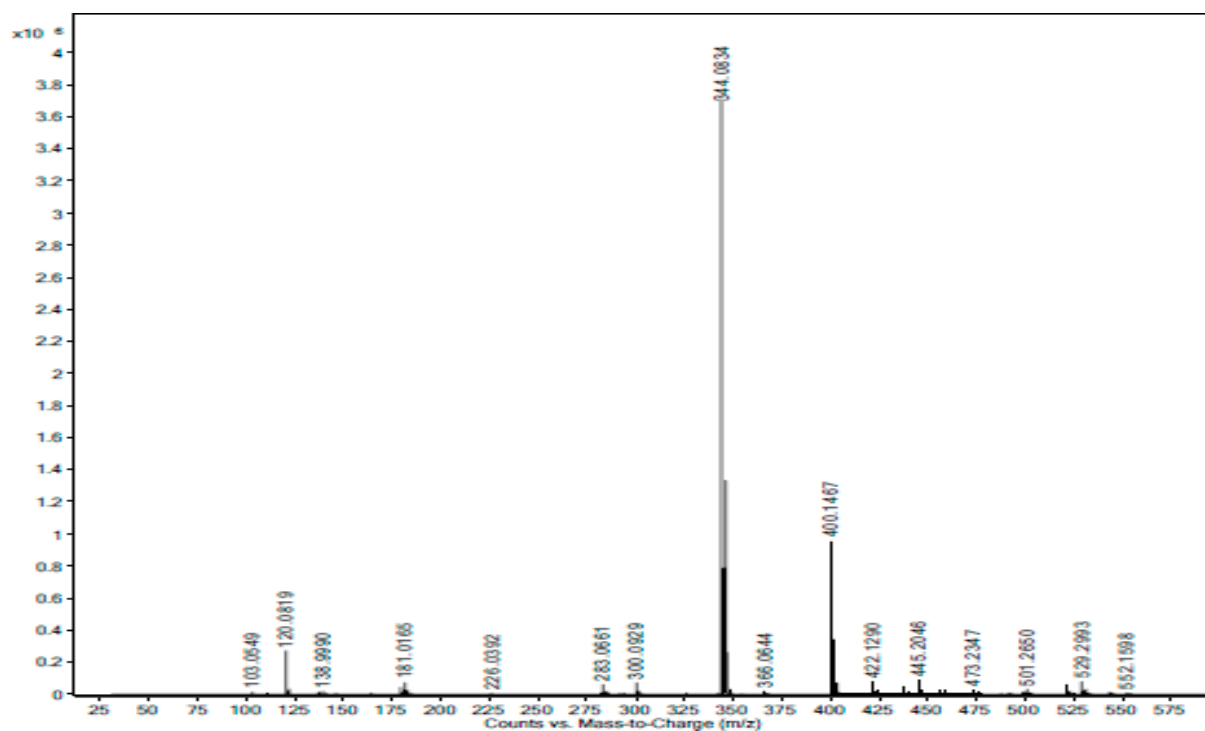


Figure S36. HRMS (ESI⁺) of compound 41.

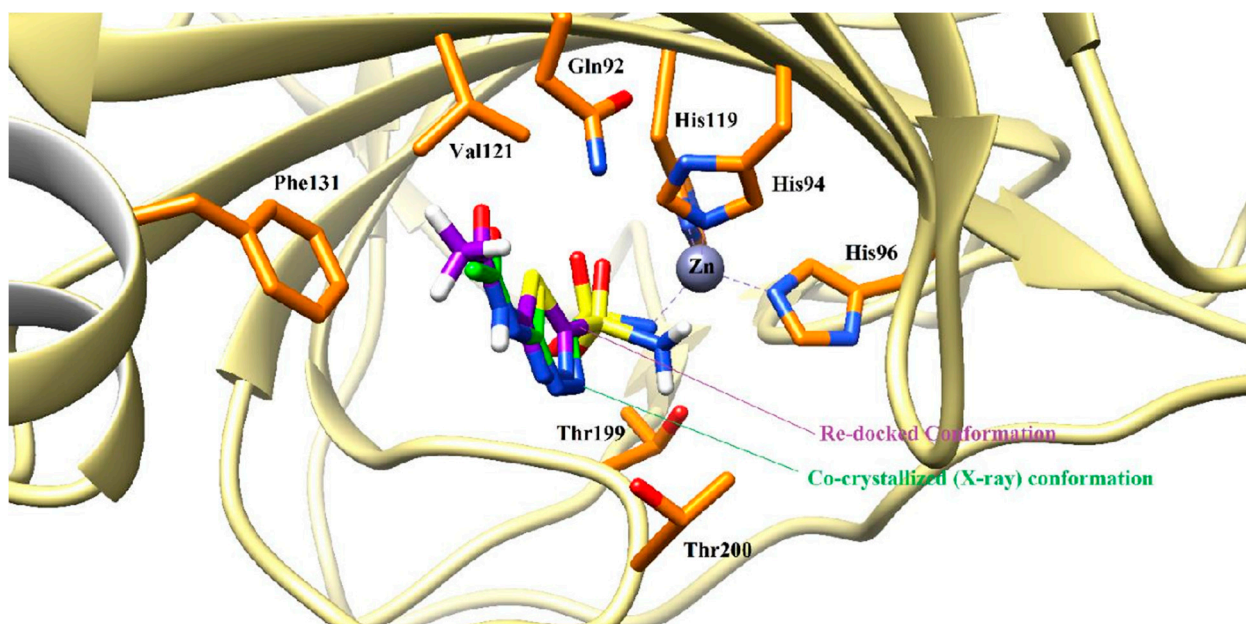


Figure S37. The superimposed view of re-docked orientation of acetazolamide with its reference conformation in the crystal structure (PDB code: 3HS4). The binding residues are shown in orange stick, protein is presented in ribbon model, the X-ray determined conformation and re-docked modes are shown in green and purple stick models, respectively.