

## supplementary materials

### Design and synthesis of multi-target antidepressants: exploration of 1-(4-(7-azaindole)-3,6-dihydropyridin-1-yl)alkyl-3-(1*H*-indol-3-yl)pyrrolidine-2,5-dione derivatives with affinity for the serotonin transporter

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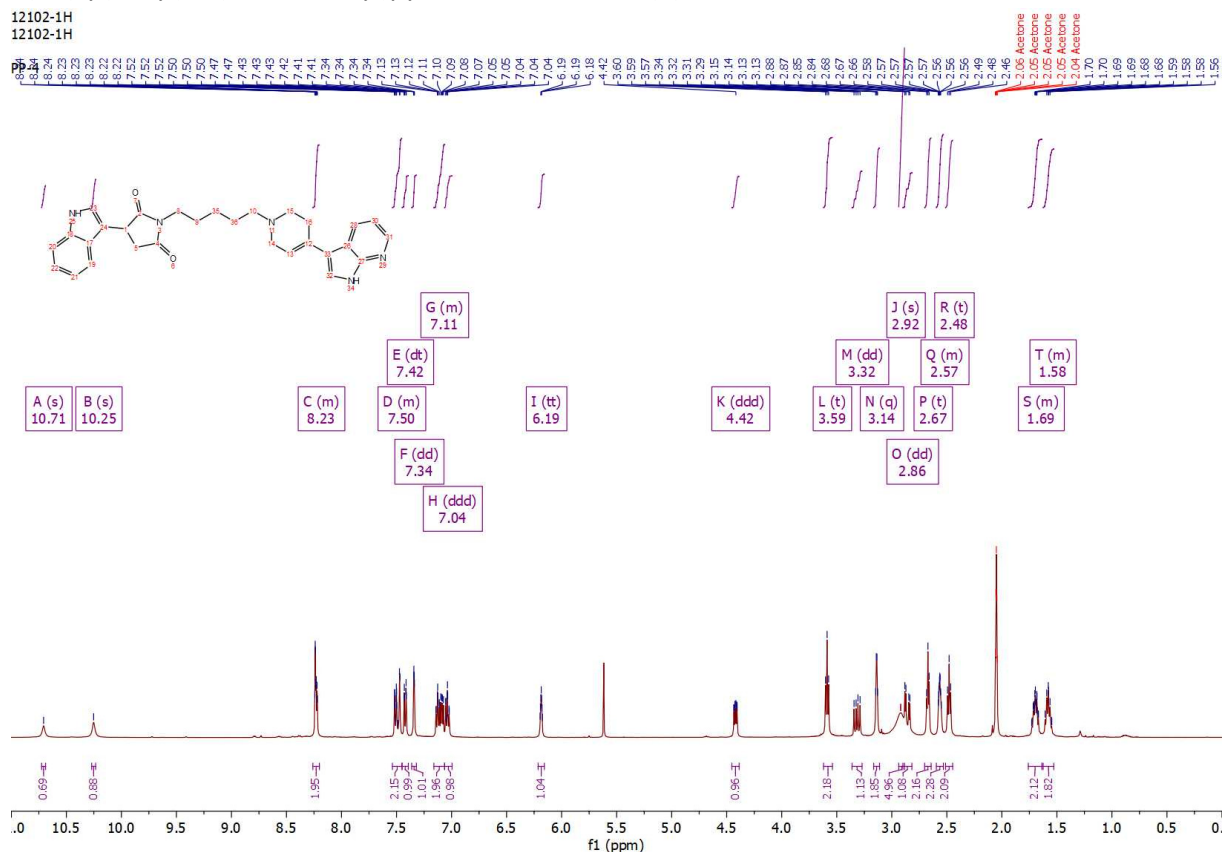
<sup>a</sup>Department of Drug Technology and Pharmaceutical Biotechnology, Faculty of Pharmacy, Medical University of Warsaw, 1 Banacha Street, 02-097 Warszawa, Poland

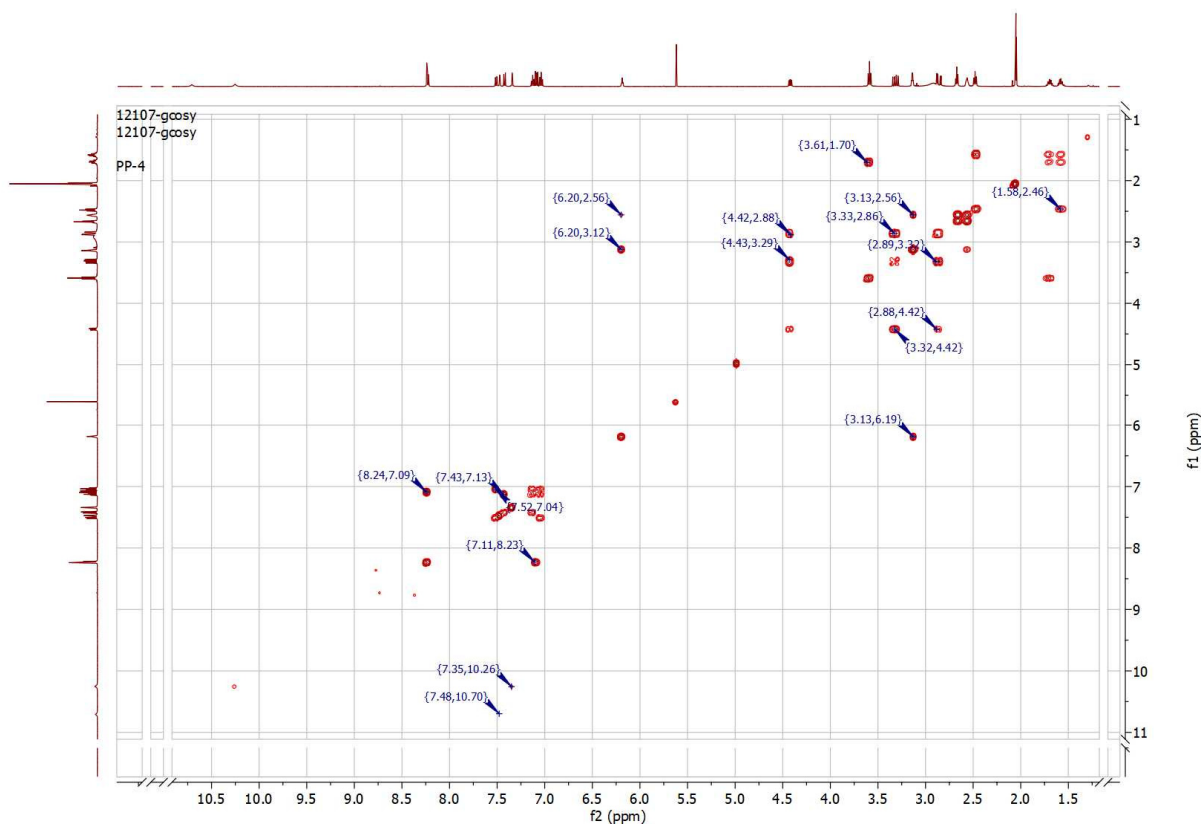
<sup>b</sup>Department of Pharmacobiology, Faculty of Pharmacy, Jagiellonian University Medical College, 9 Medyczna Street, 30-688 Kraków, Poland

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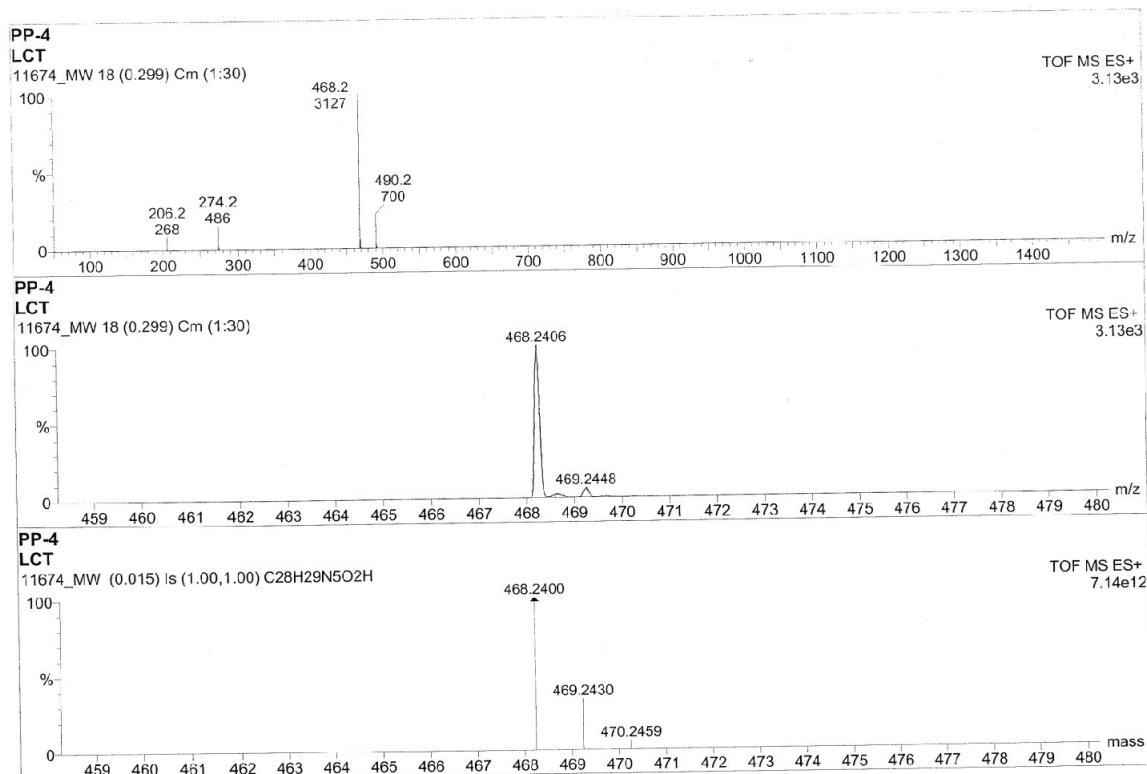
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#### 1. <sup>1</sup>H, <sup>13</sup>C and COSY NMR spectra of 1-(4-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)butyl)-3-(1*H*-indol-3-yl)pyrrolidine-2,5-dione (**4**)

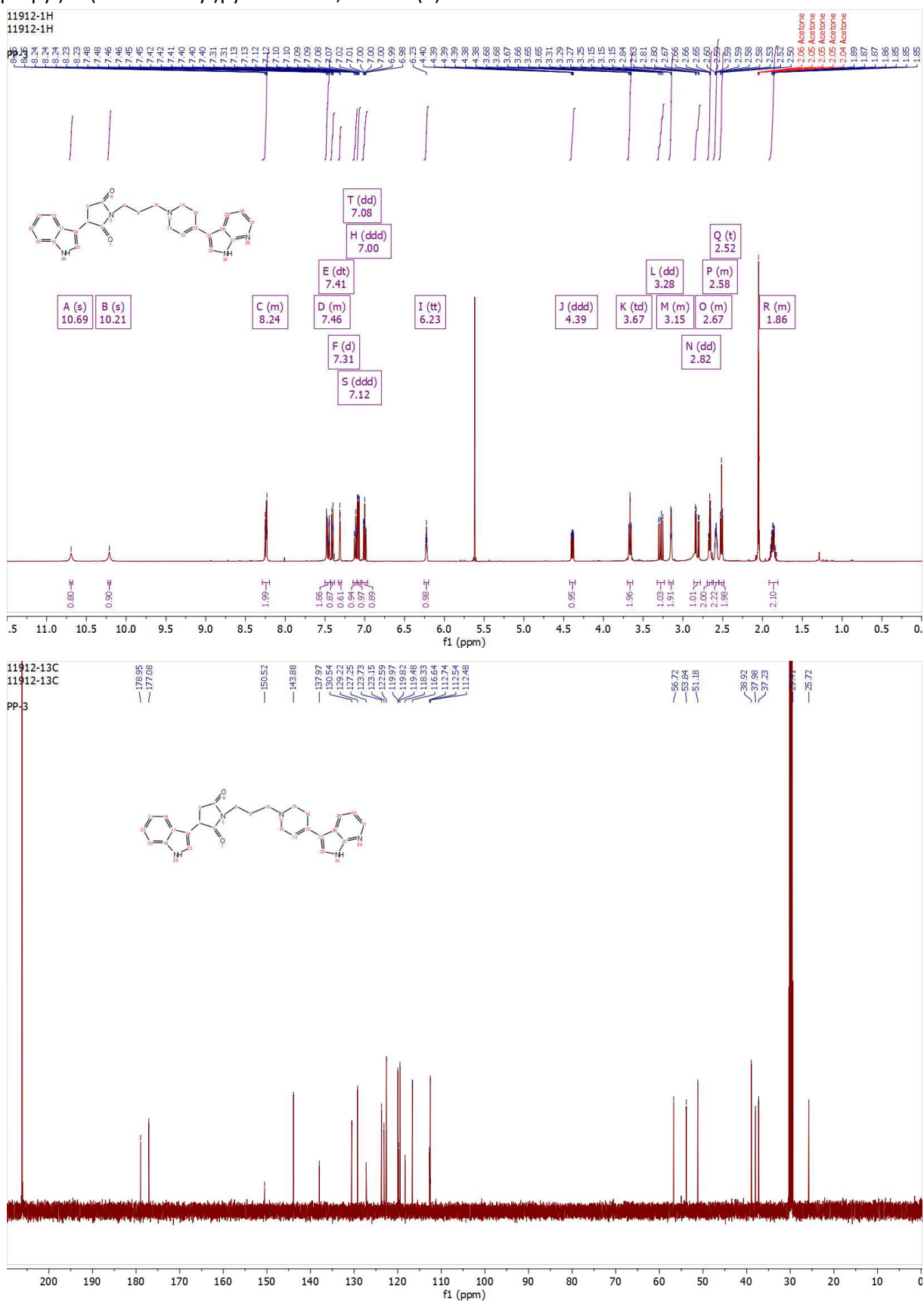




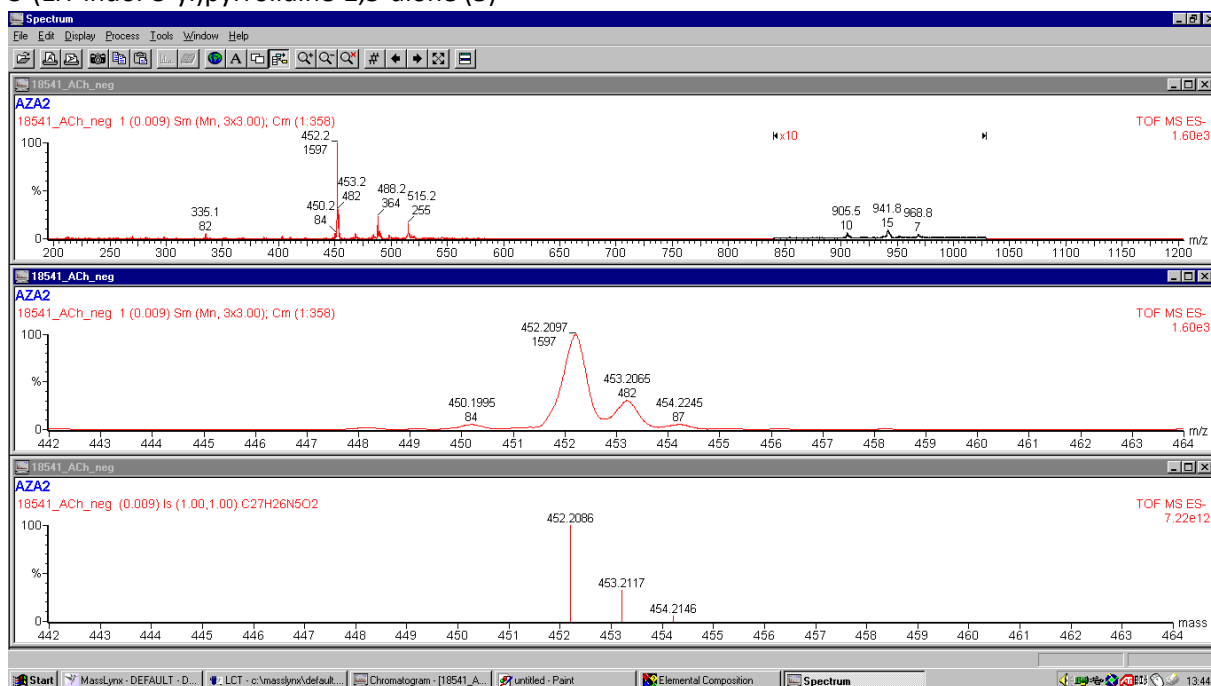
2. HRMS spectra of 1-(4-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)butyl)-3-(1*H*-indol-3-yl)pyrrolidine-2,5-dione (**4**)



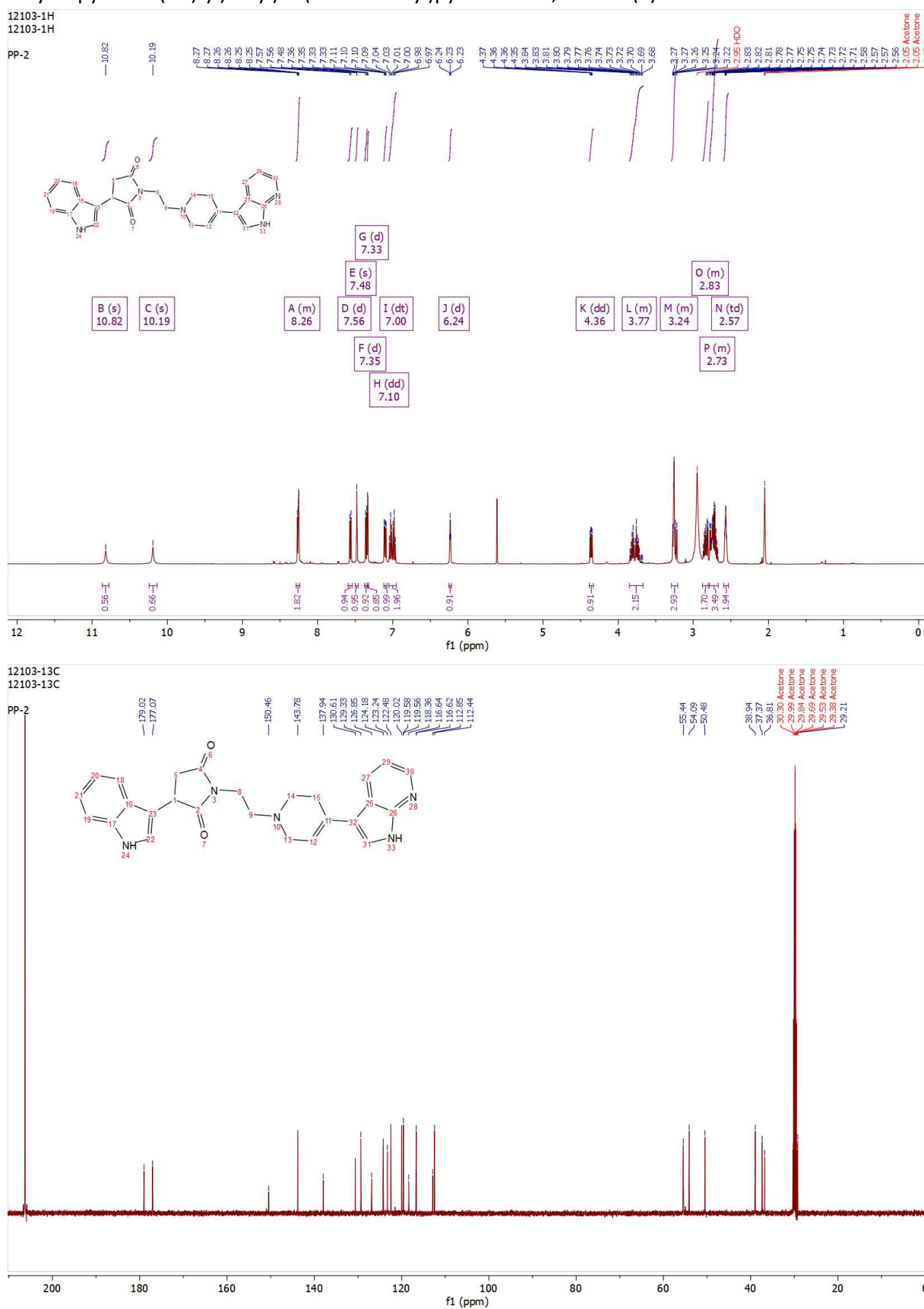
3.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(3-(4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-3,6-dihydropyridin-1(2H)-yl)propyl)-3-(1H-indol-3-yl)pyrrolidine-2,5-dione (**5**)

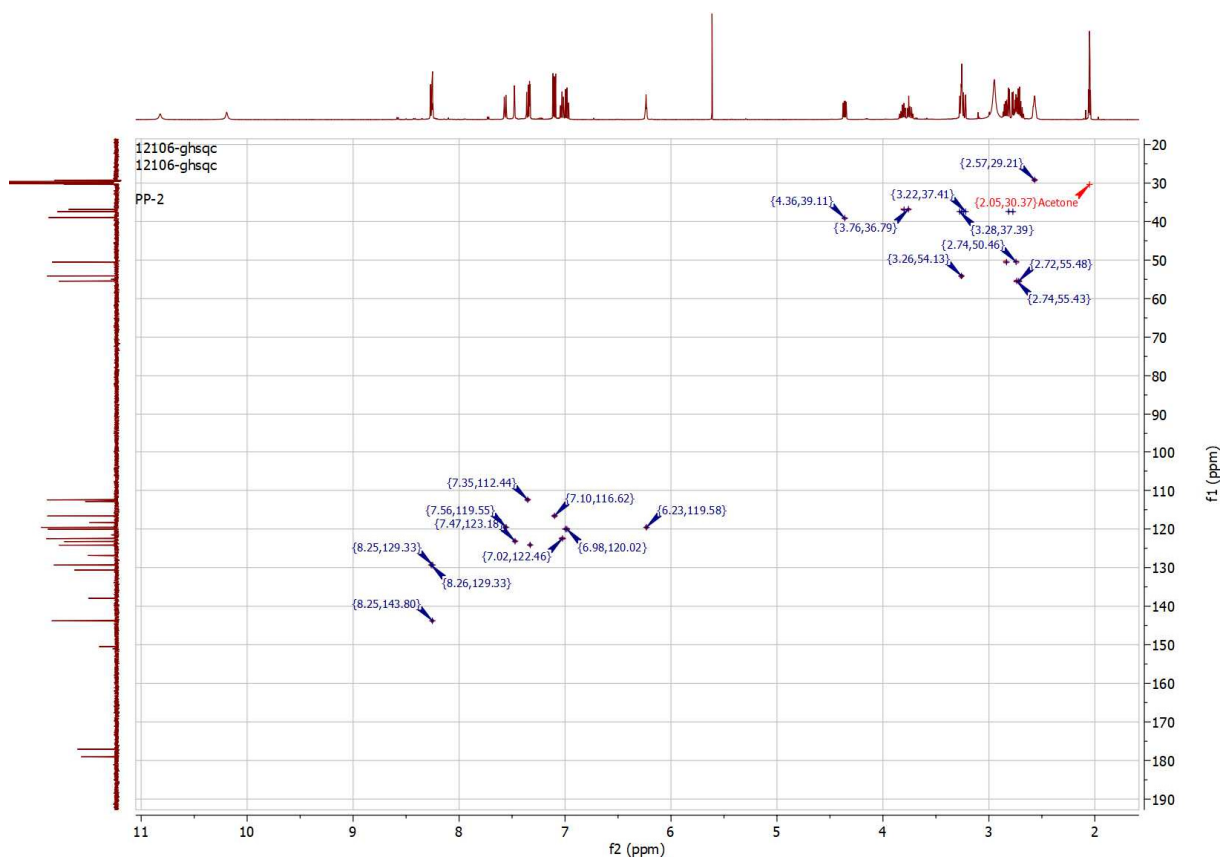
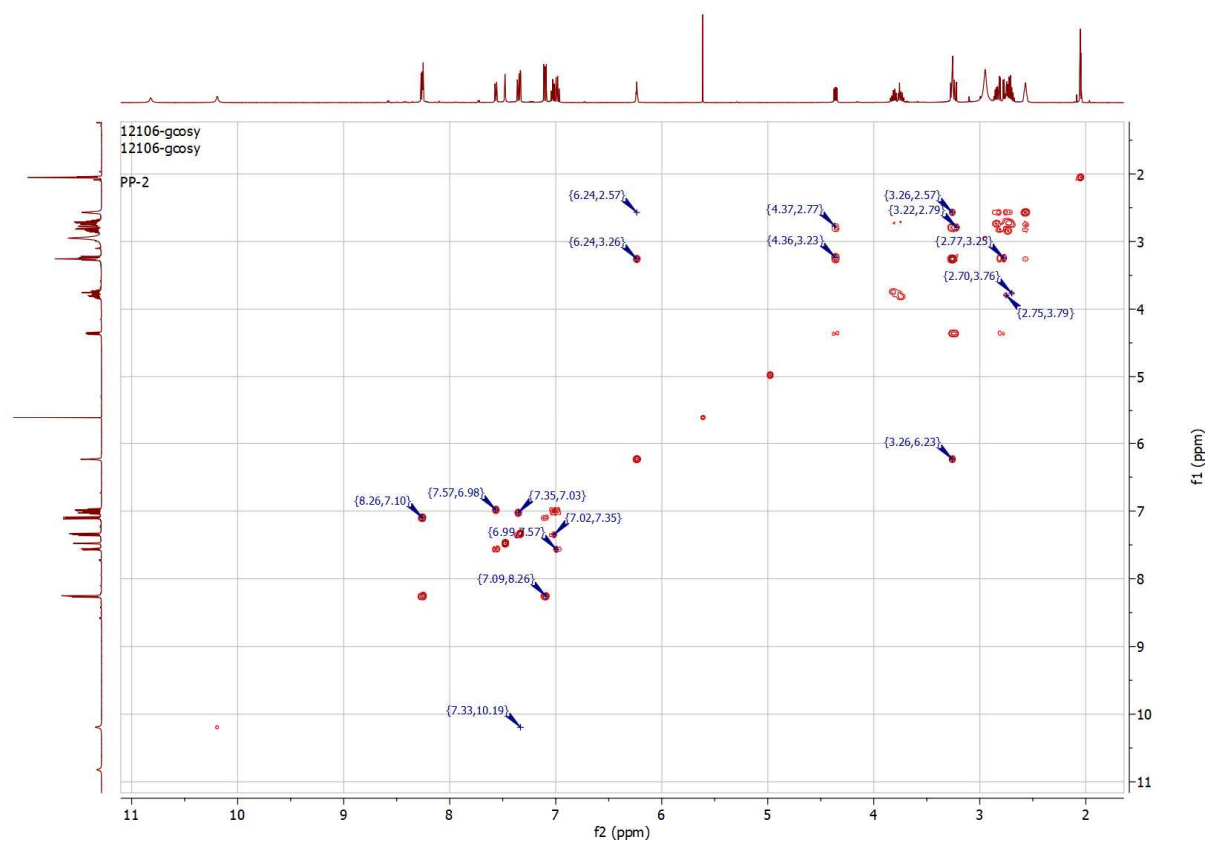


4. HRMS spectra of 1-(3-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)propyl)-3-(1*H*-indol-3-yl)pyrrolidine-2,5-dione (**5**)

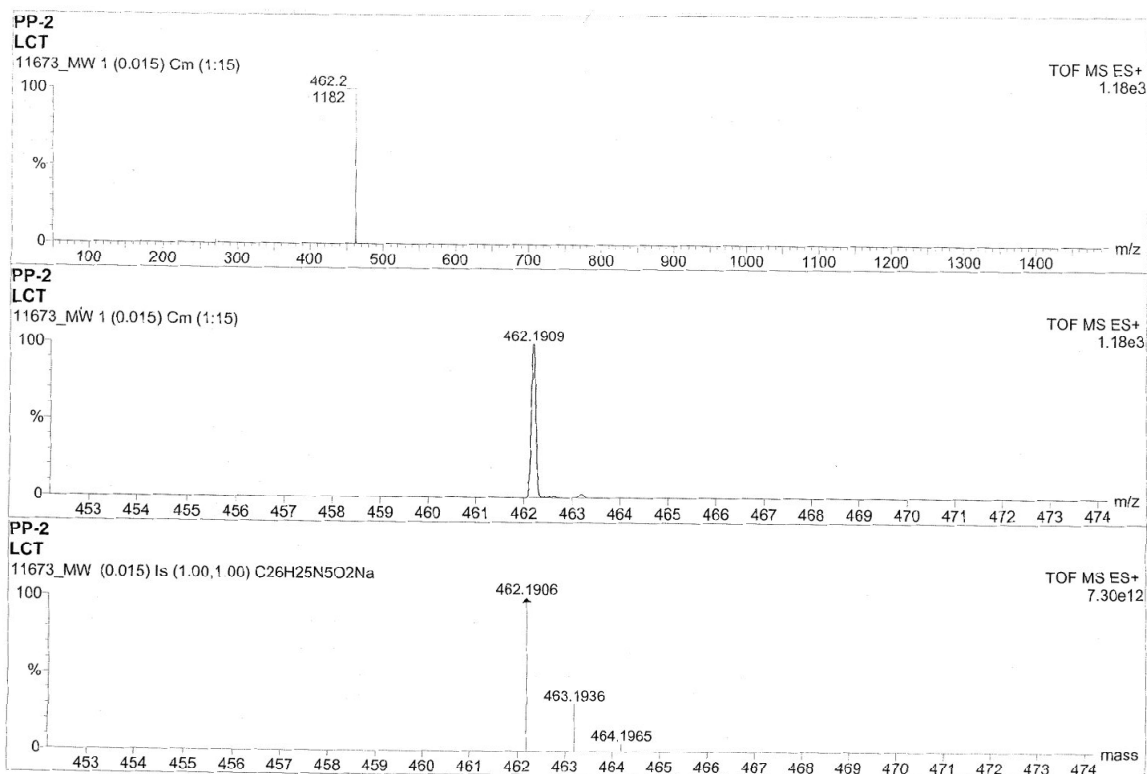


5.  $^1\text{H}$ ,  $^{13}\text{C}$ , COSY and HSQC NMR spectra of 1-(2-(4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-3,6-dihydropyridin-1(2H)-yl)ethyl)-3-(1H-indol-3-yl)pyrrolidine-2,5-dione (6)





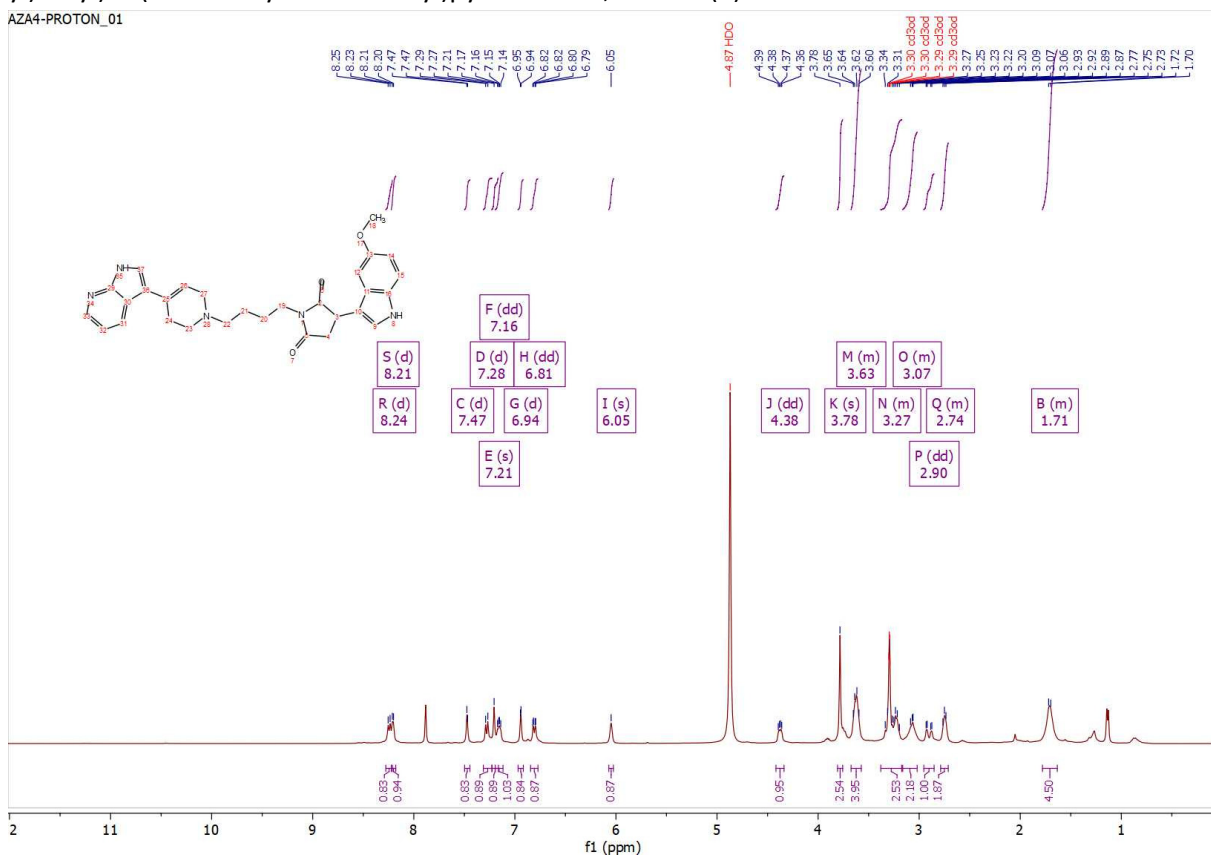
6. HRMS spectra of 1-(2-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)ethyl)-3-(1*H*-indol-3-yl)pyrrolidine-2,5-dione (**6**)



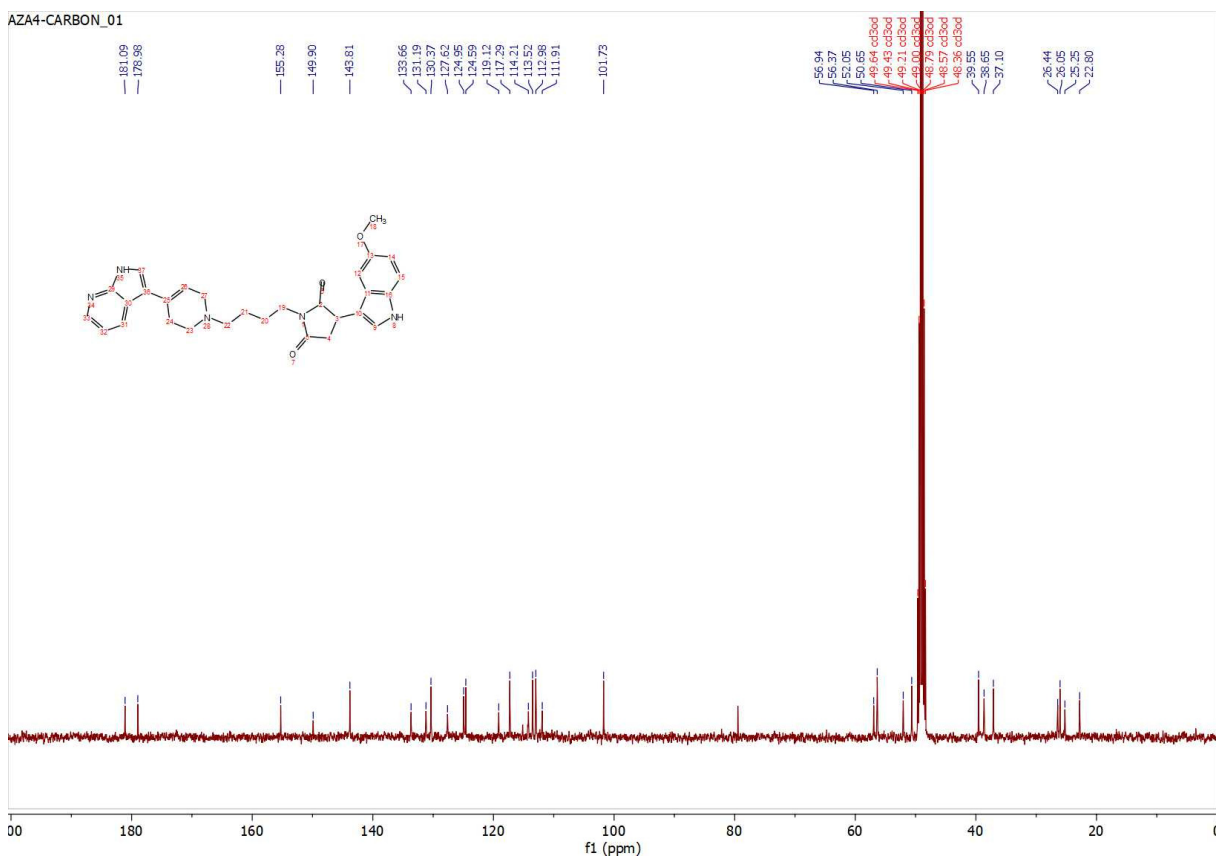


7.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(4-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)butyl)-3-(5-methoxy-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**7**)

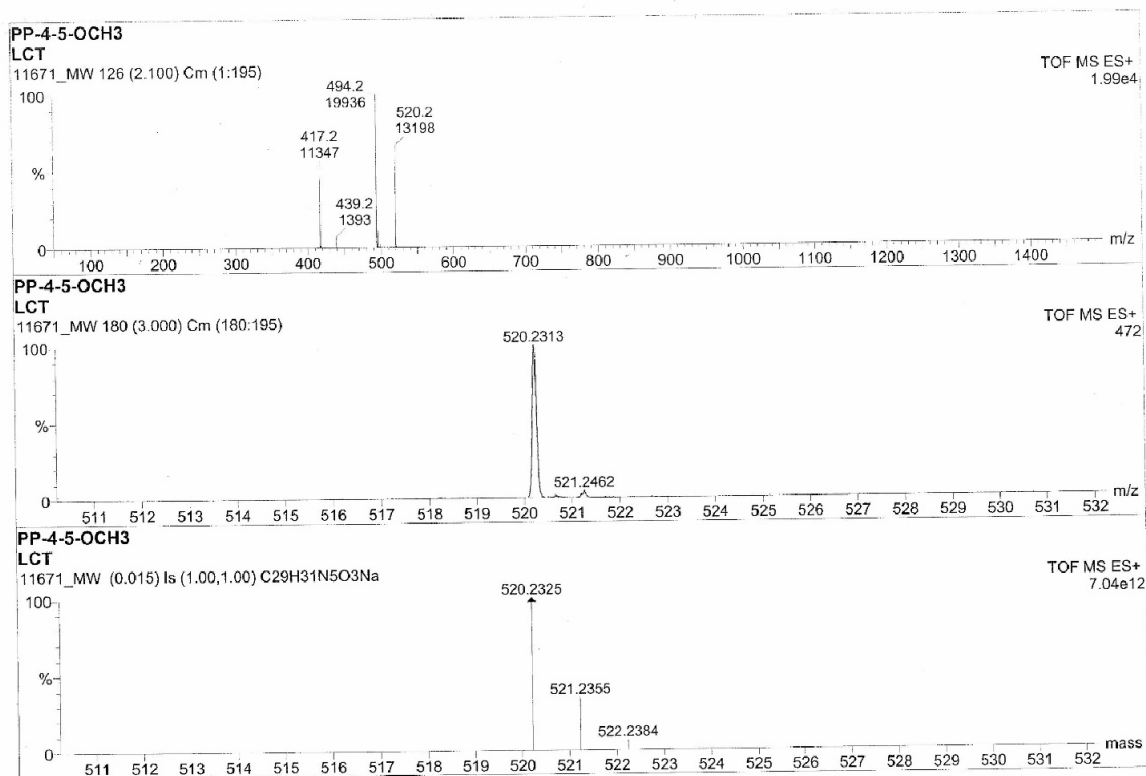
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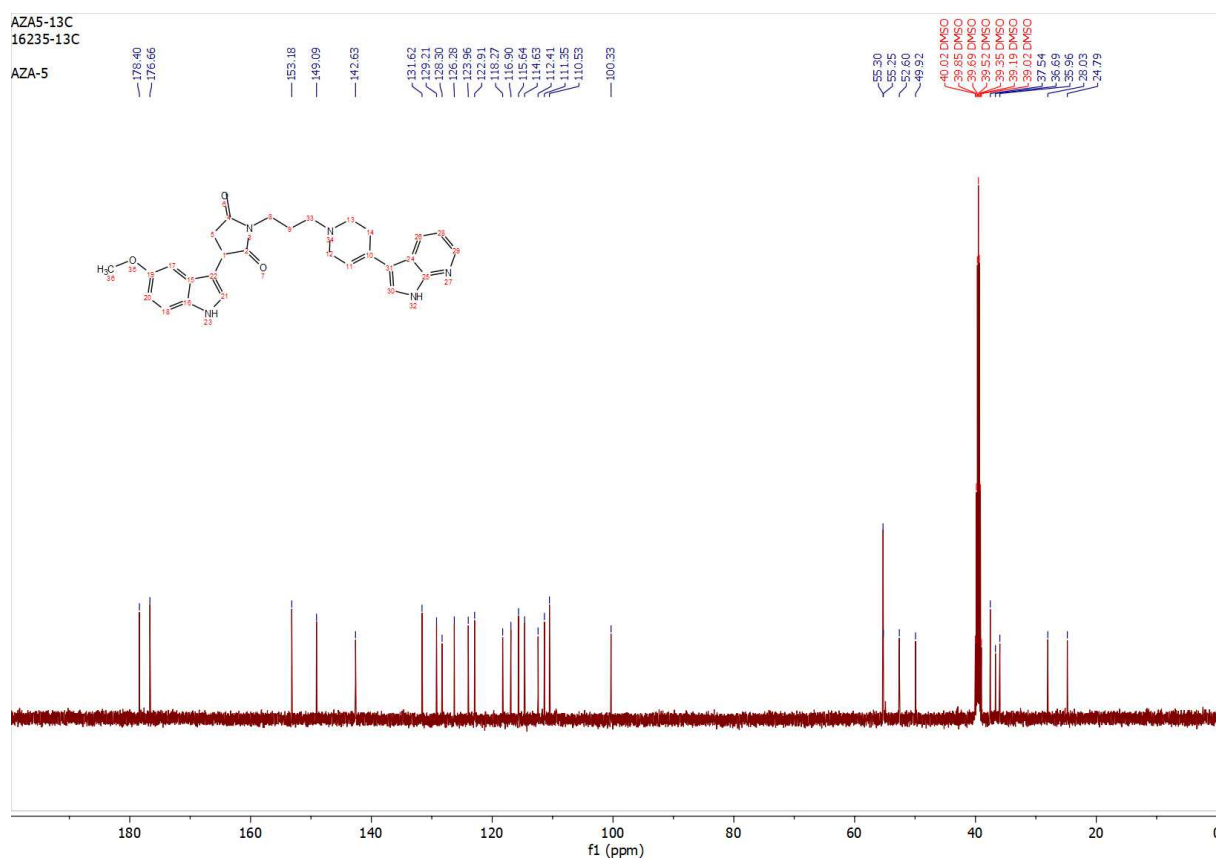
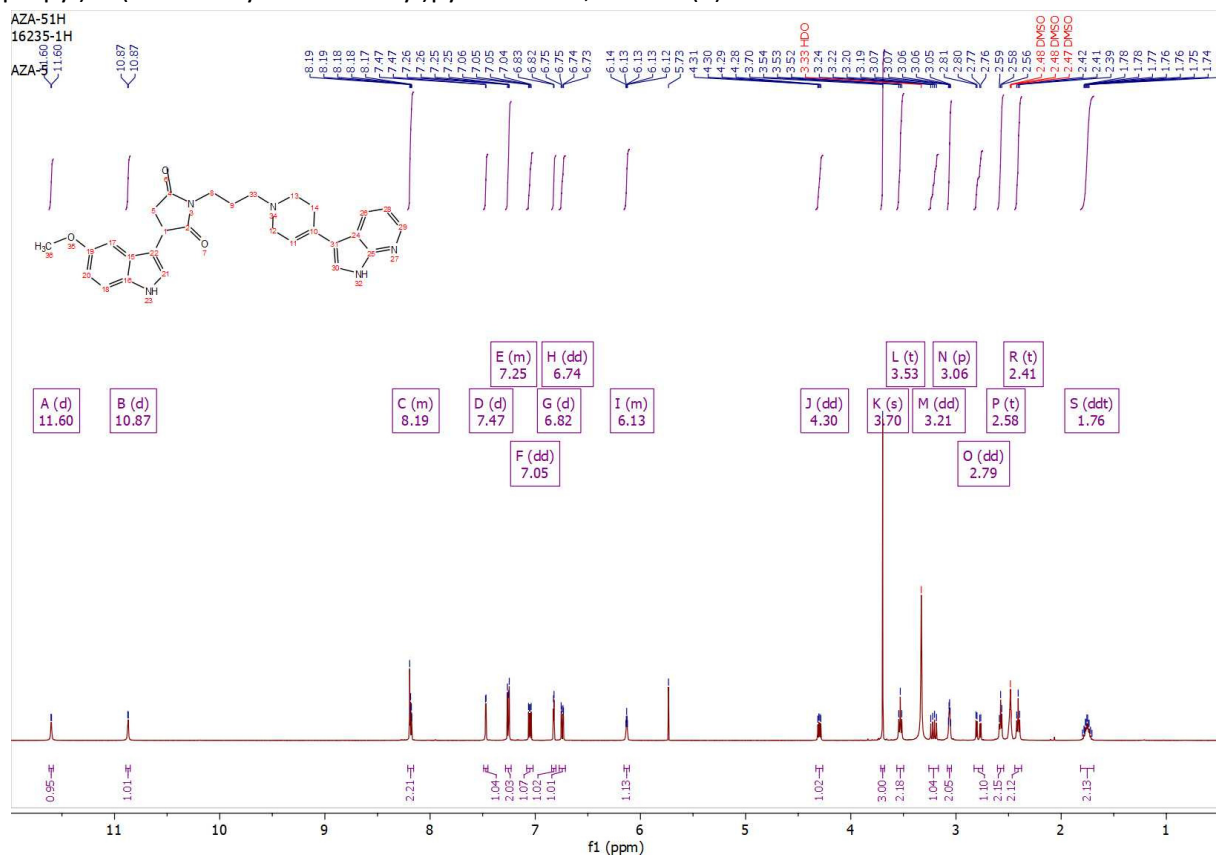
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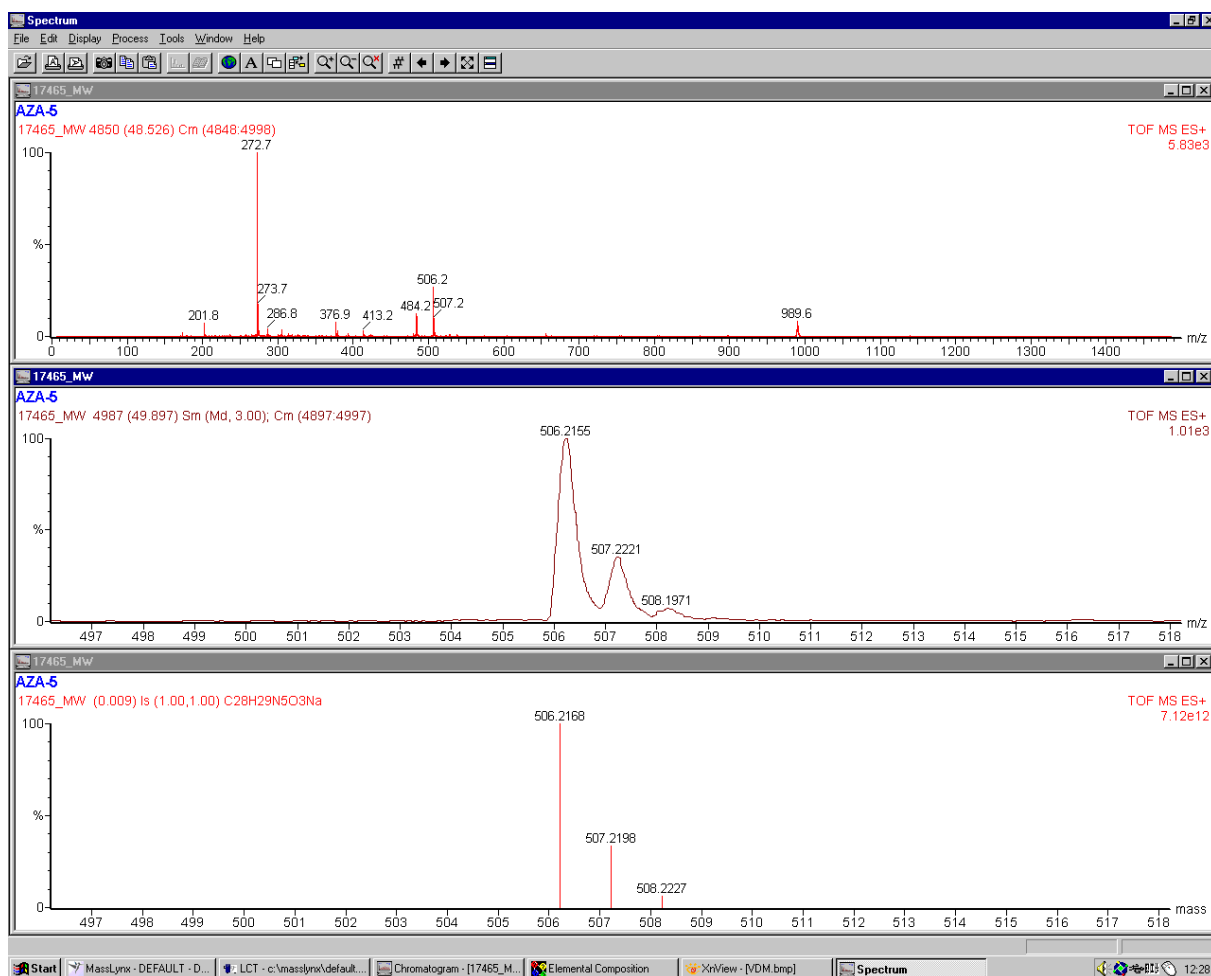
8. HRMS spectra of 1-(4-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)butyl)-3-(5-methoxy-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**7**)



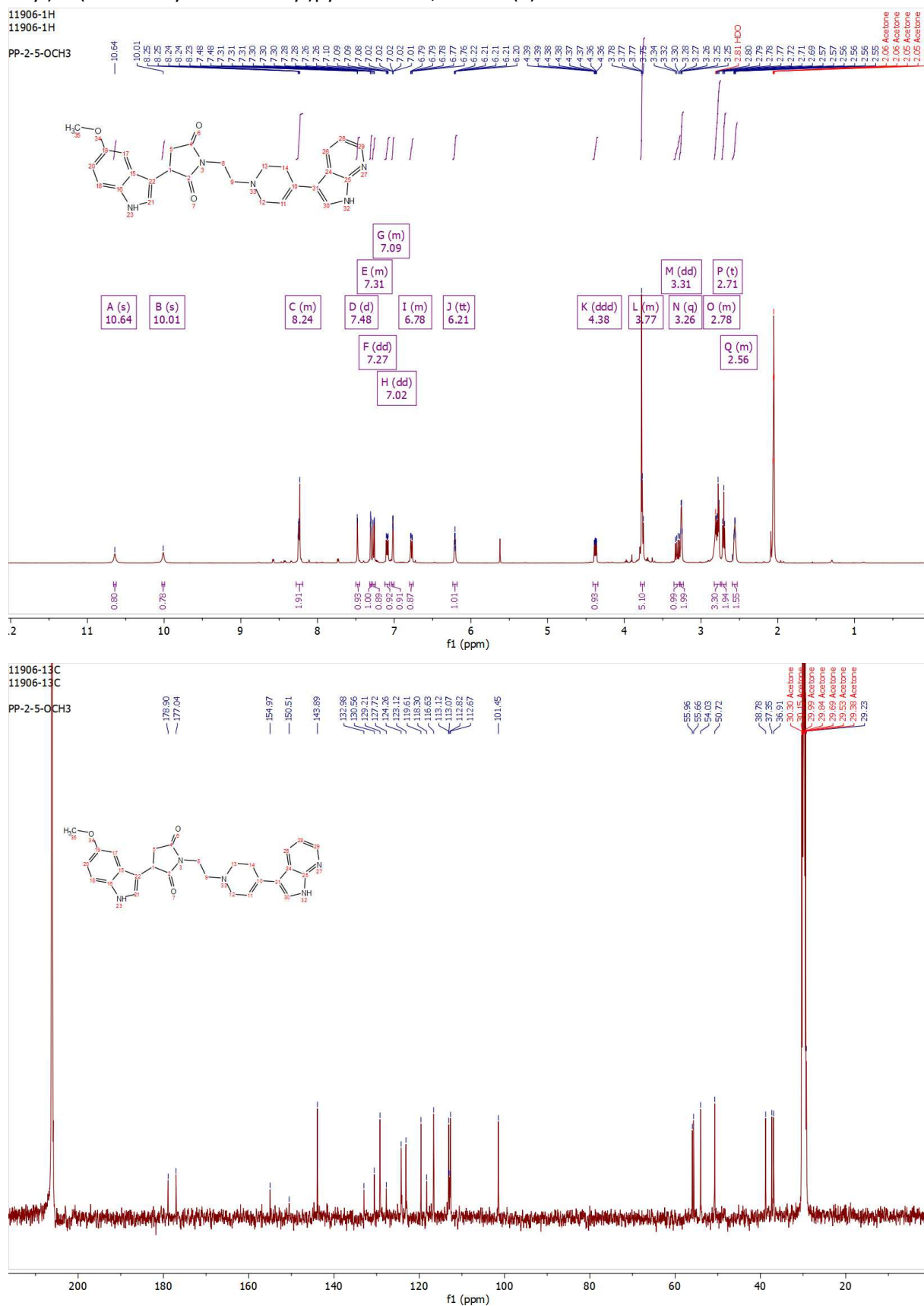
9.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(3-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)propyl)-3-(5-methoxy-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**8**)



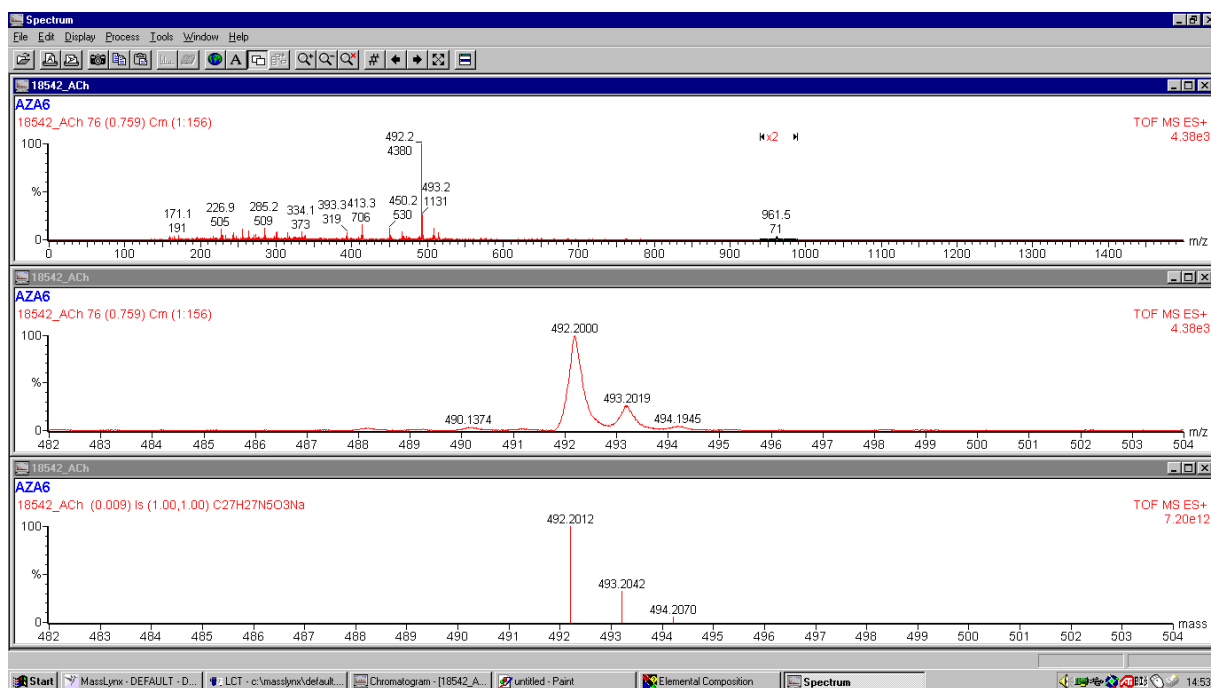
10. HRMS spectra of 1-(3-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)propyl)-3-(5-methoxy-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**8**)



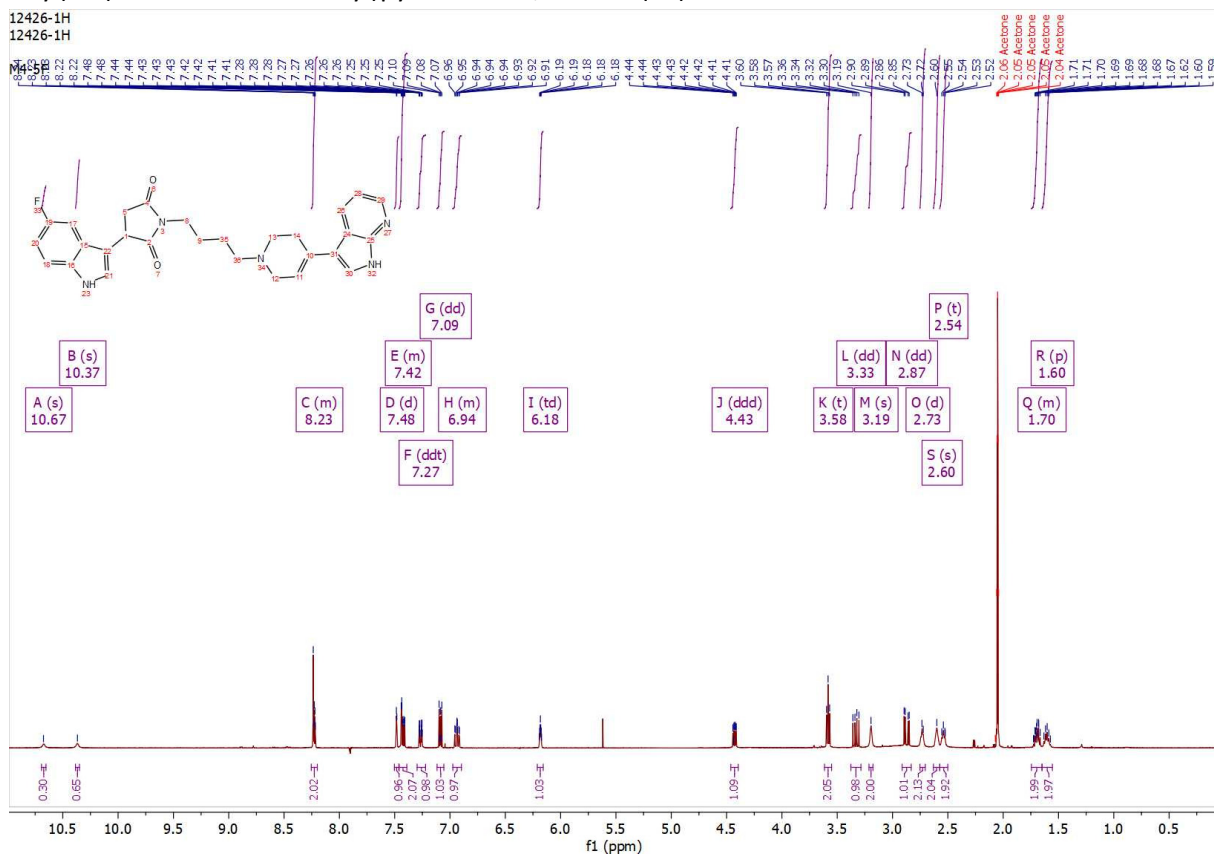
11.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(2-(4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-3,6-dihydropyridin-1(2H)-yl)ethyl)-3-(5-methoxy-1H-indol-3-yl)pyrrolidine-2,5-dione (**9**)

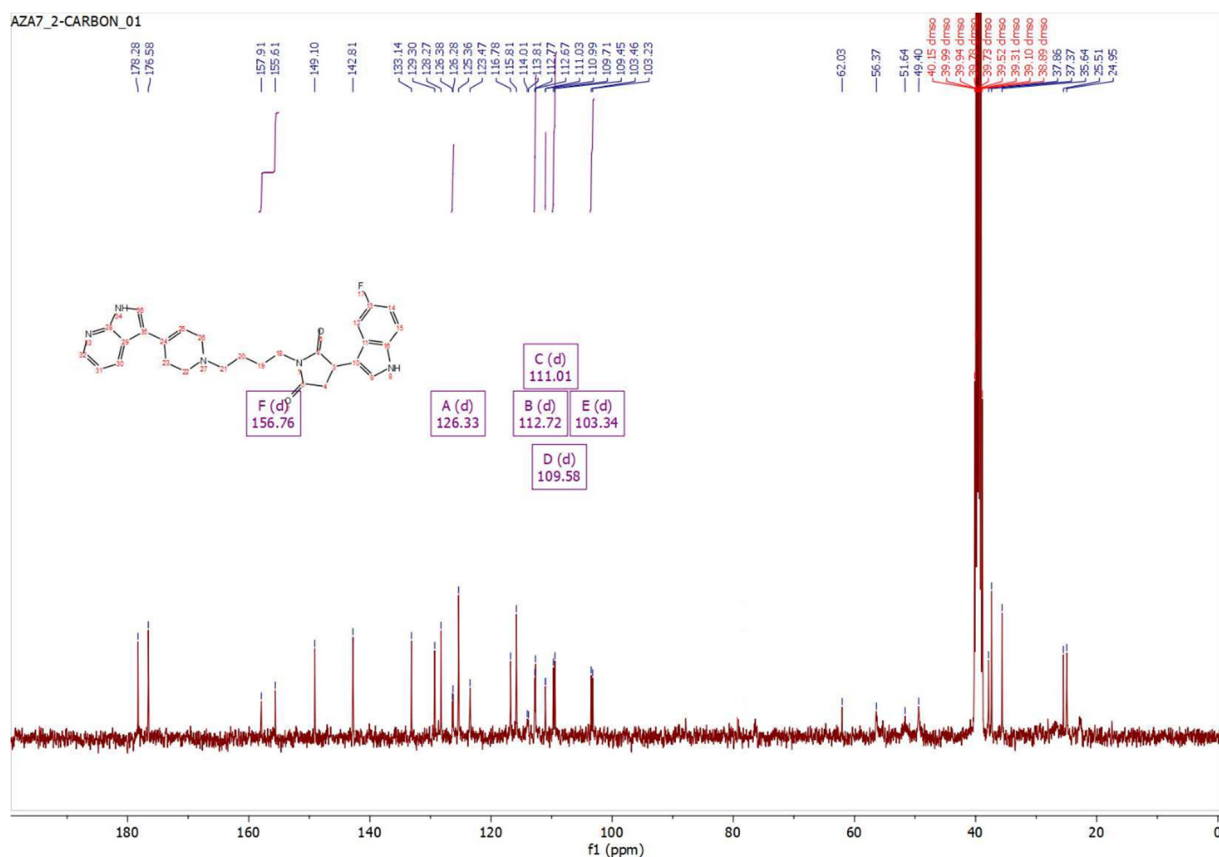


12. HRMS spectra of 1-(2-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)ethyl)-3-(5-methoxy-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**9**)

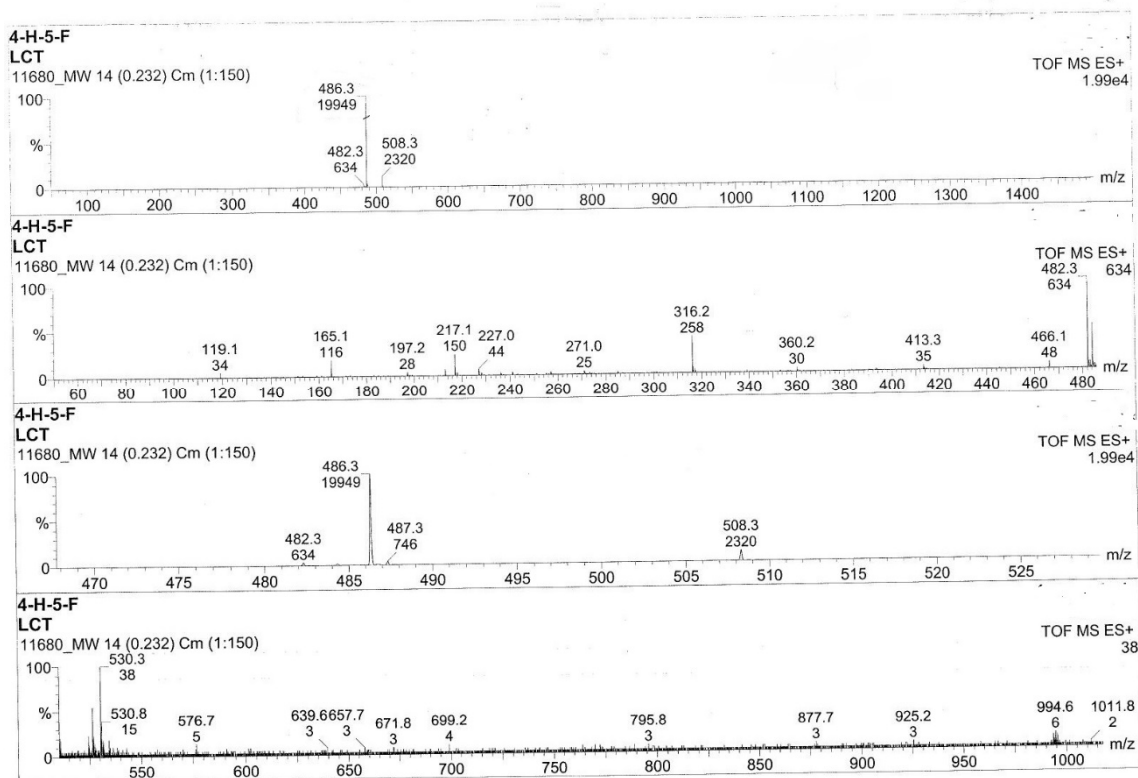


13. <sup>1</sup>H and <sup>13</sup>C NMR spectra of 1-(4-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)butyl)-3-(5-fluoro-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**10**)



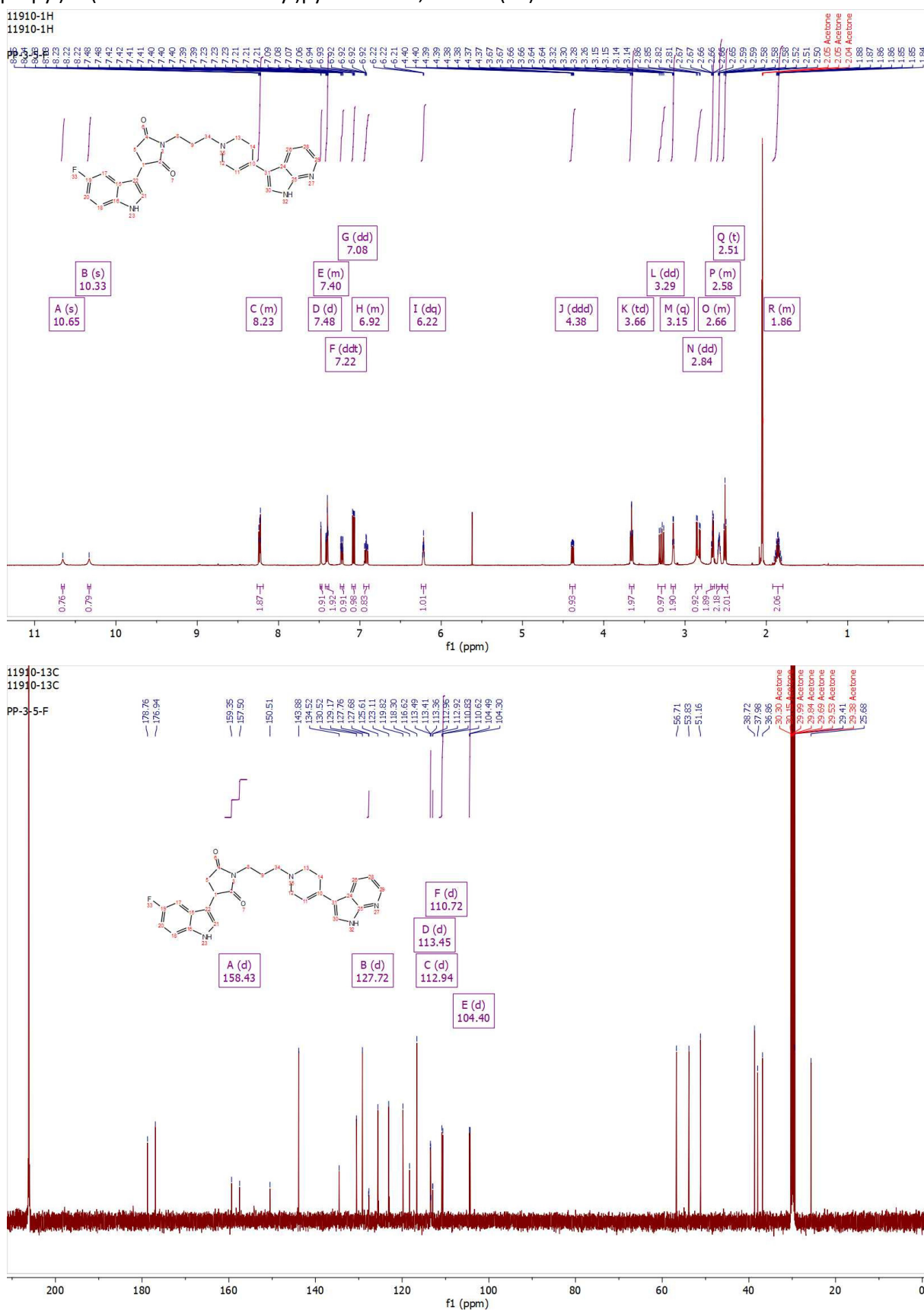


14. HRMS spectra of 1-(4-(4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-3,6-dihydropyridin-1(2H)-yl)butyl)-3-(5-fluoro-1H-indol-3-yl)pyrrolidine-2,5-dione (**10**)



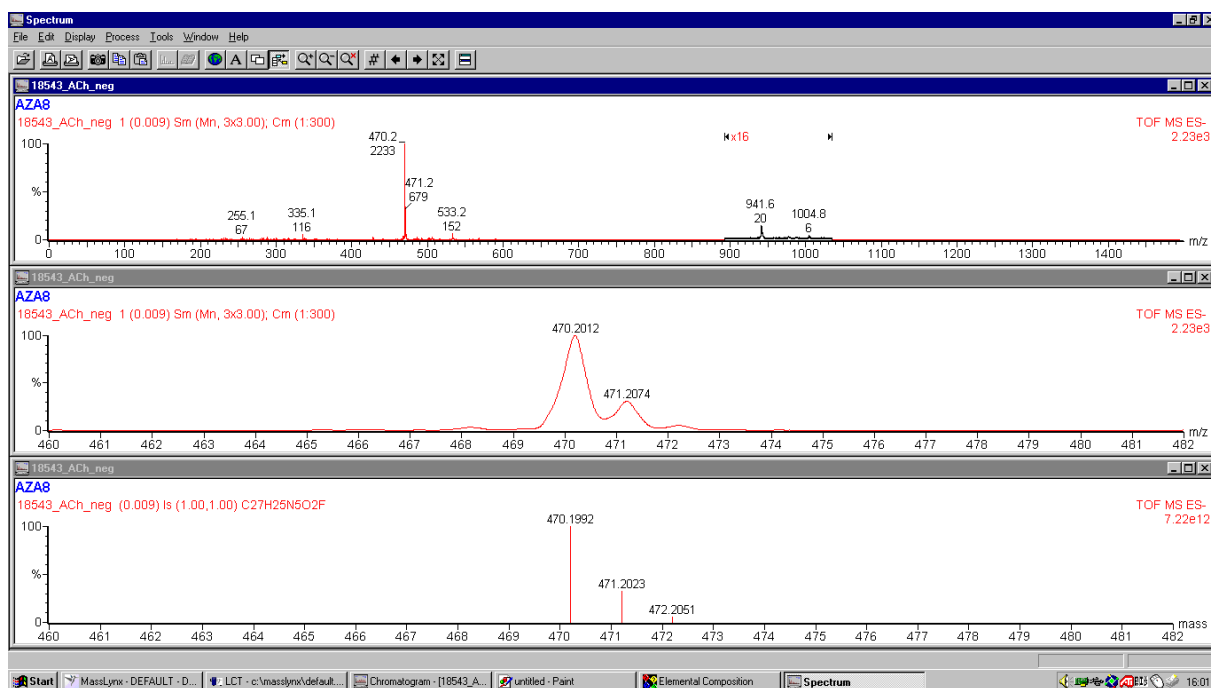


15.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(3-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)propyl)-3-(5-fluoro-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**11**)

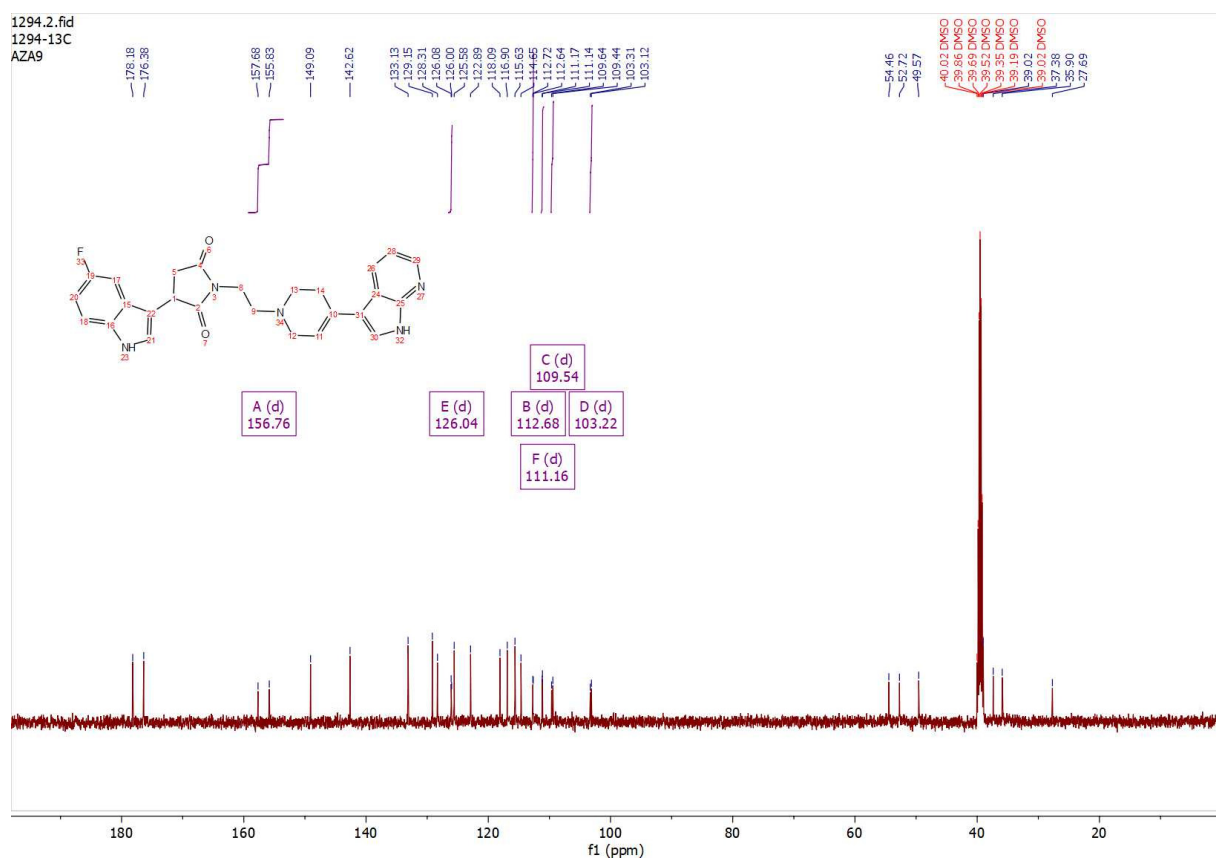
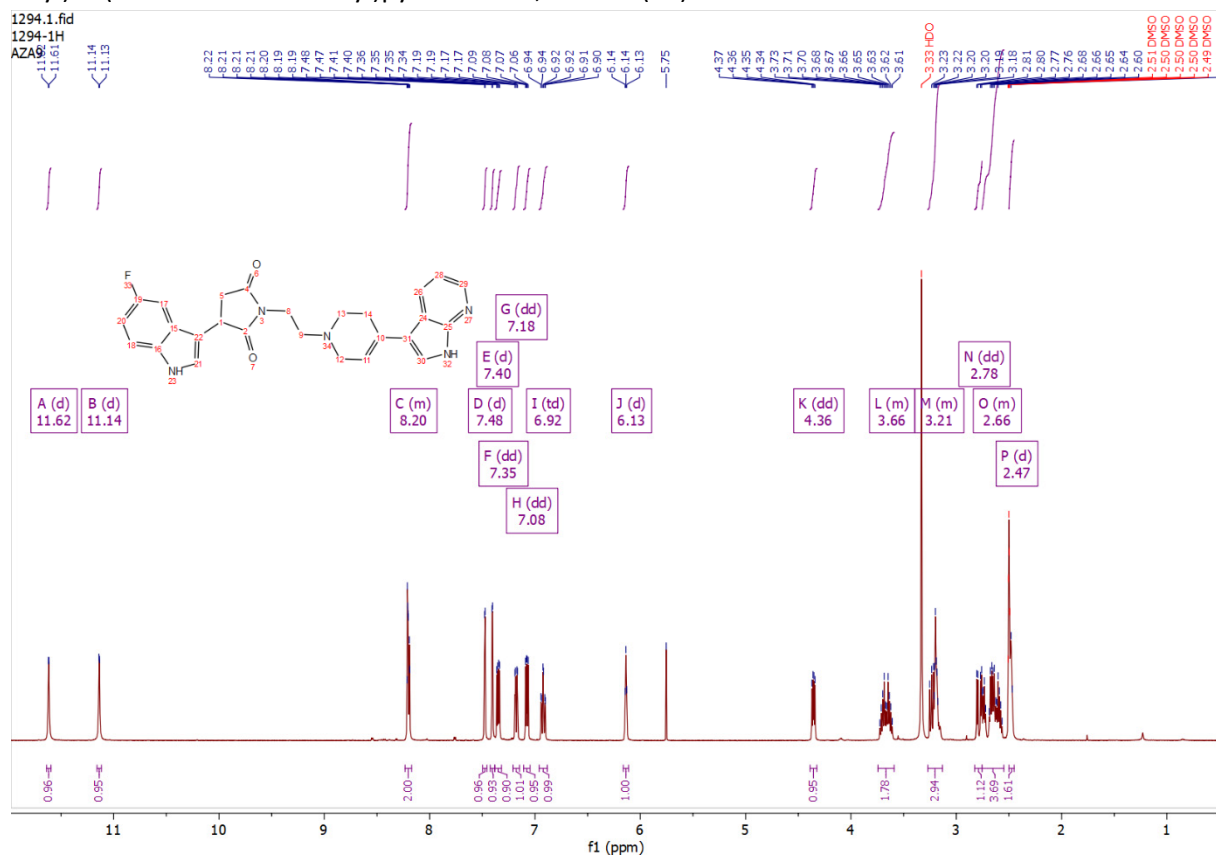




16. HRMS spectra of 1-(3-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)propyl)-3-(5-fluoro-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**11**)



17.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of 1-(2-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)ethyl)-3-(5-fluoro-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**12**)



18. HRMS spectra of 1-(2-(4-(1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)-3,6-dihydropyridin-1(2*H*)-yl)ethyl)-3-(5-fluoro-1*H*-indol-3-yl)pyrrolidine-2,5-dione (**12**)

