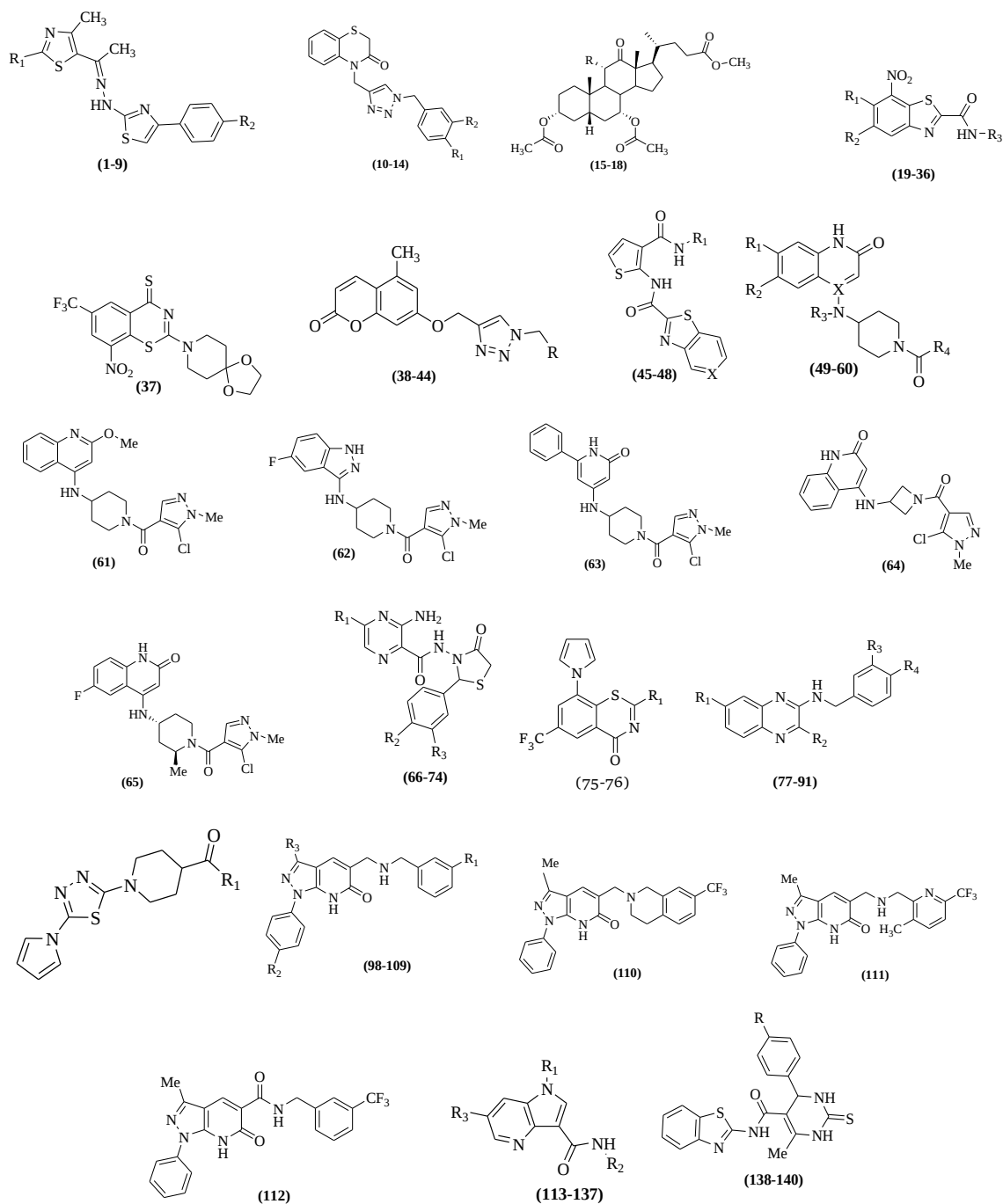
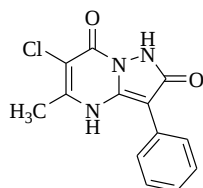


Dataset used for the development of pharmacophore model

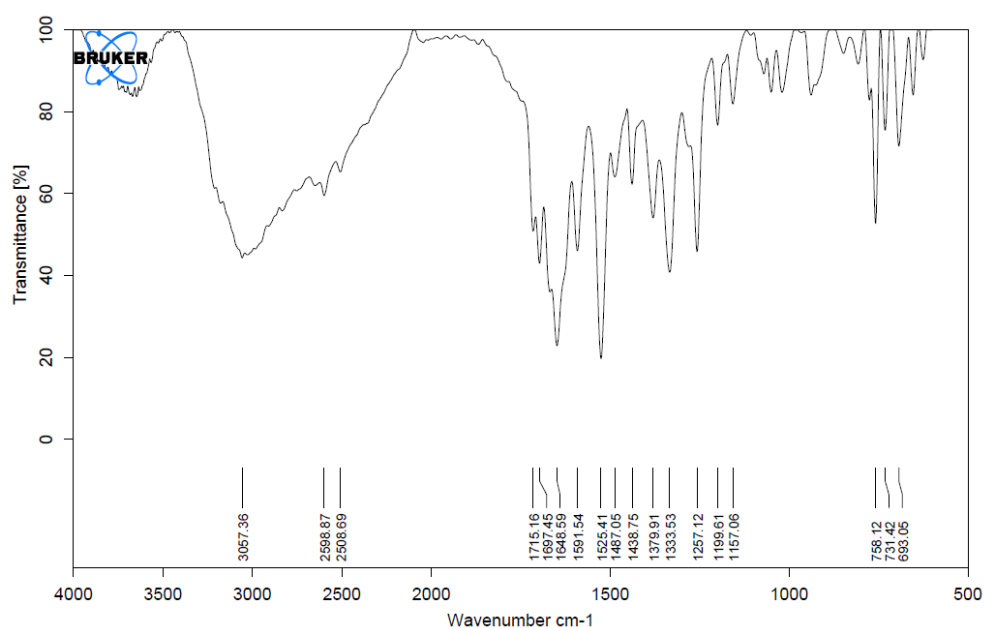


2. Chemical data

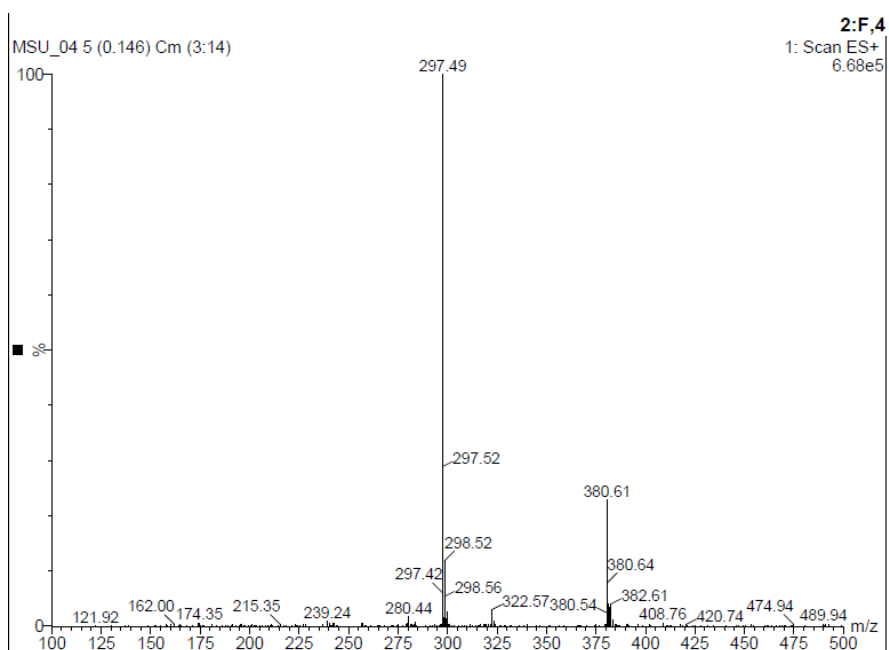
Synthesis of 6-chloro-5-methyl-3-phenylpyrazolo[1,5-*a*]pyrimidine-2,7(1*H*,4*H*)-dione (109)



IR

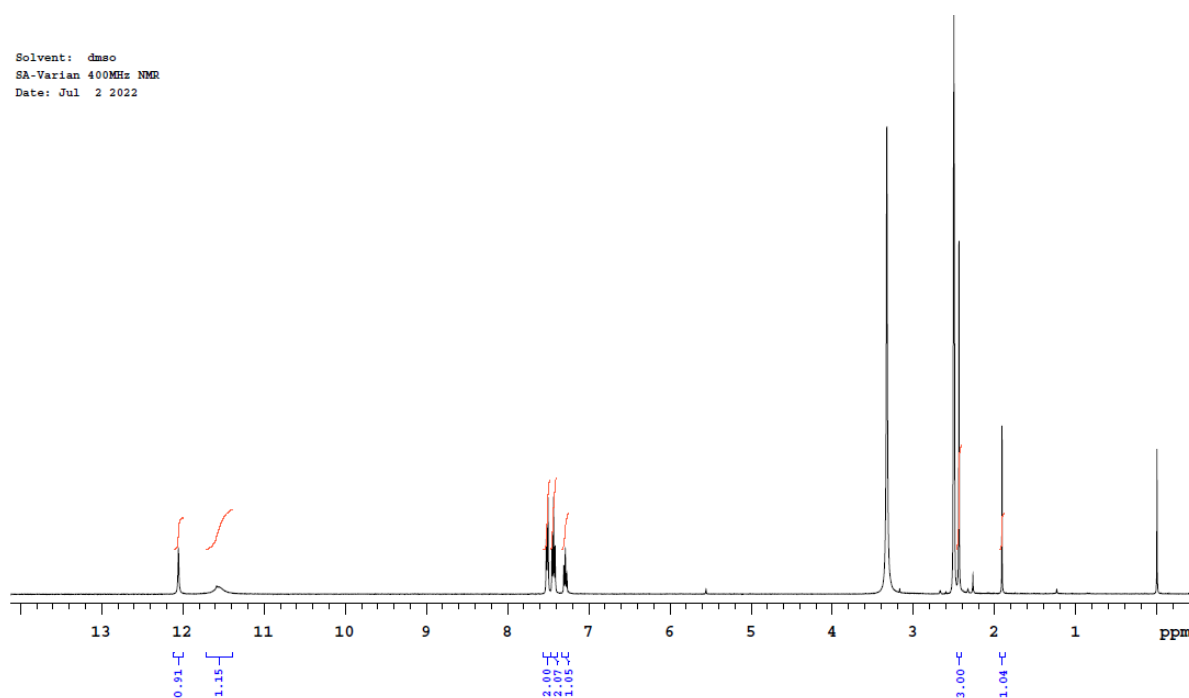
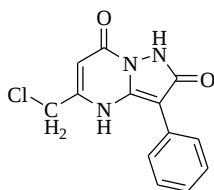
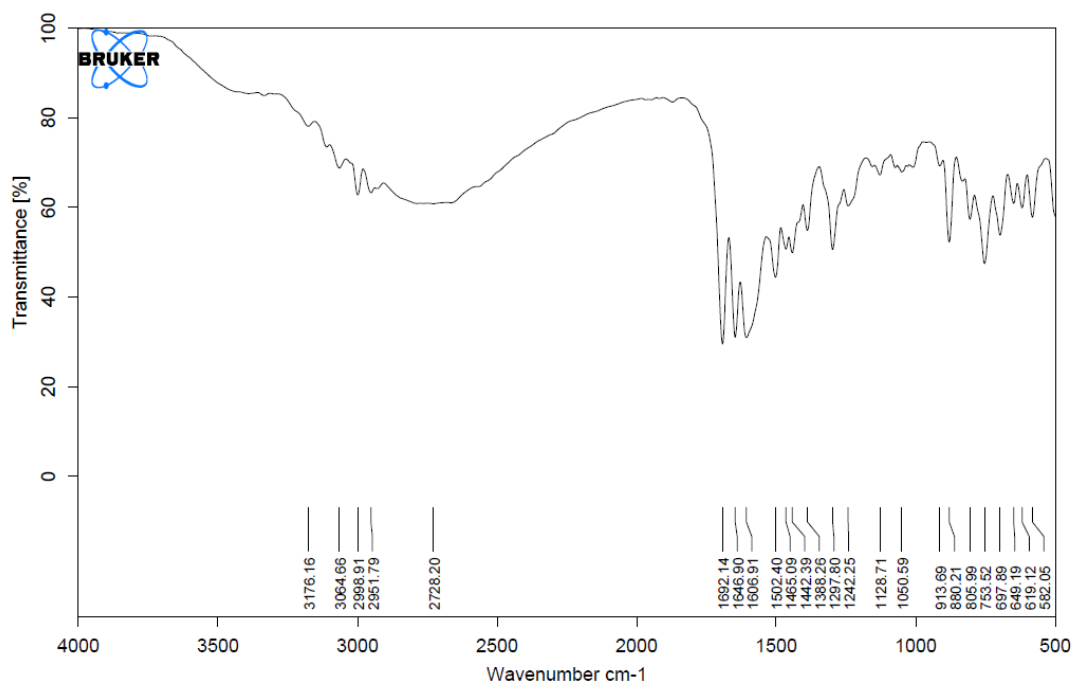


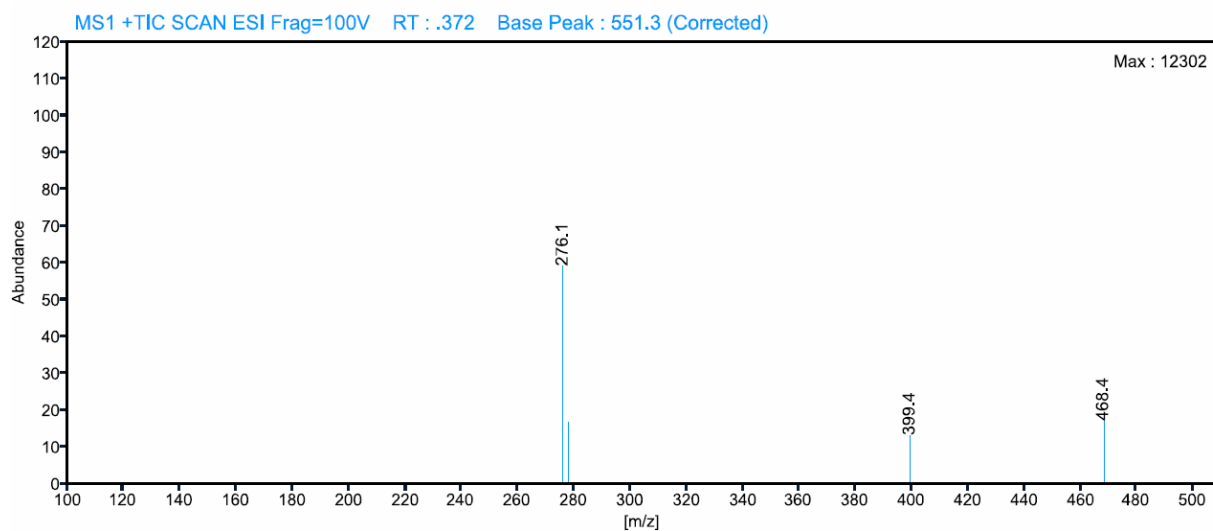
Mass



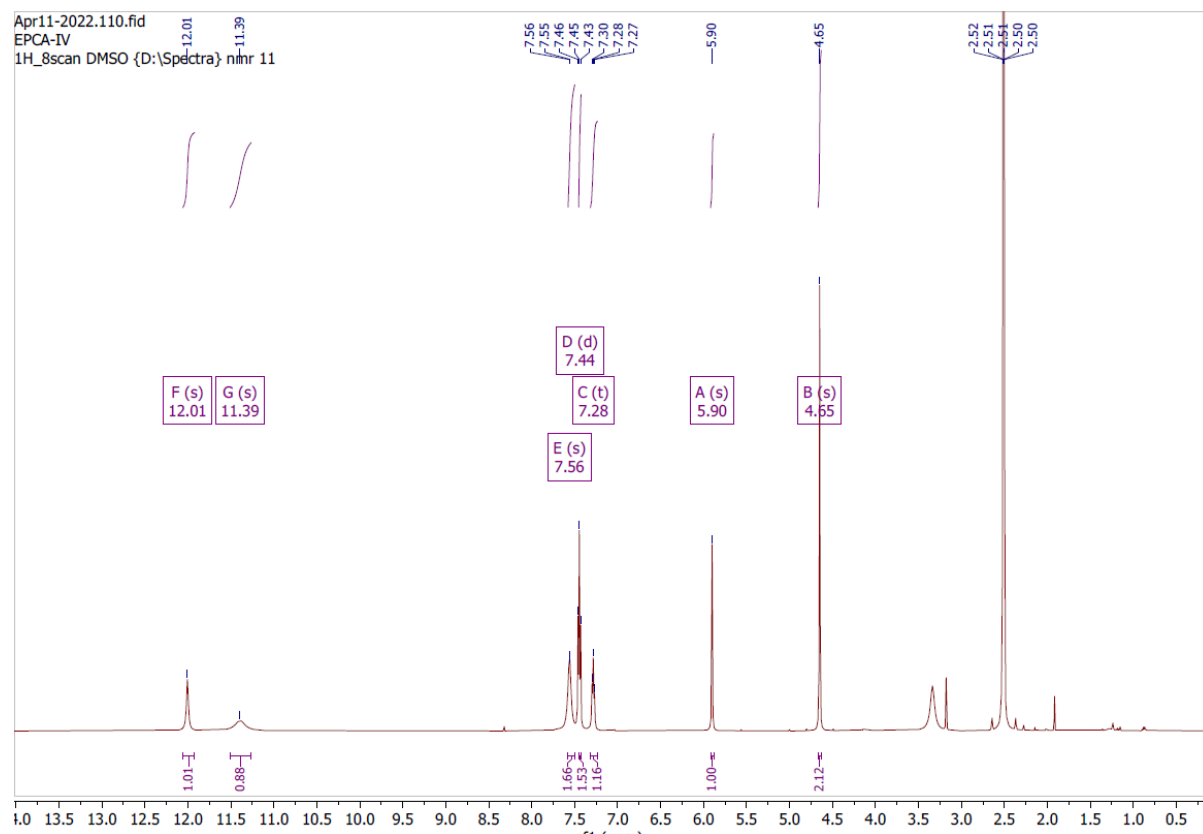
¹H-NMR

Solvent: dmsc
SA-Varian 400MHz NMR
Date: Jul 2 2022

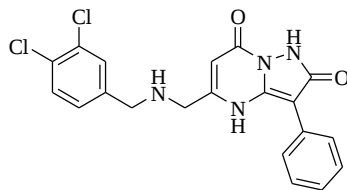
**5-(Chloromethyl)-3-phenylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (110)****IR****MASS**



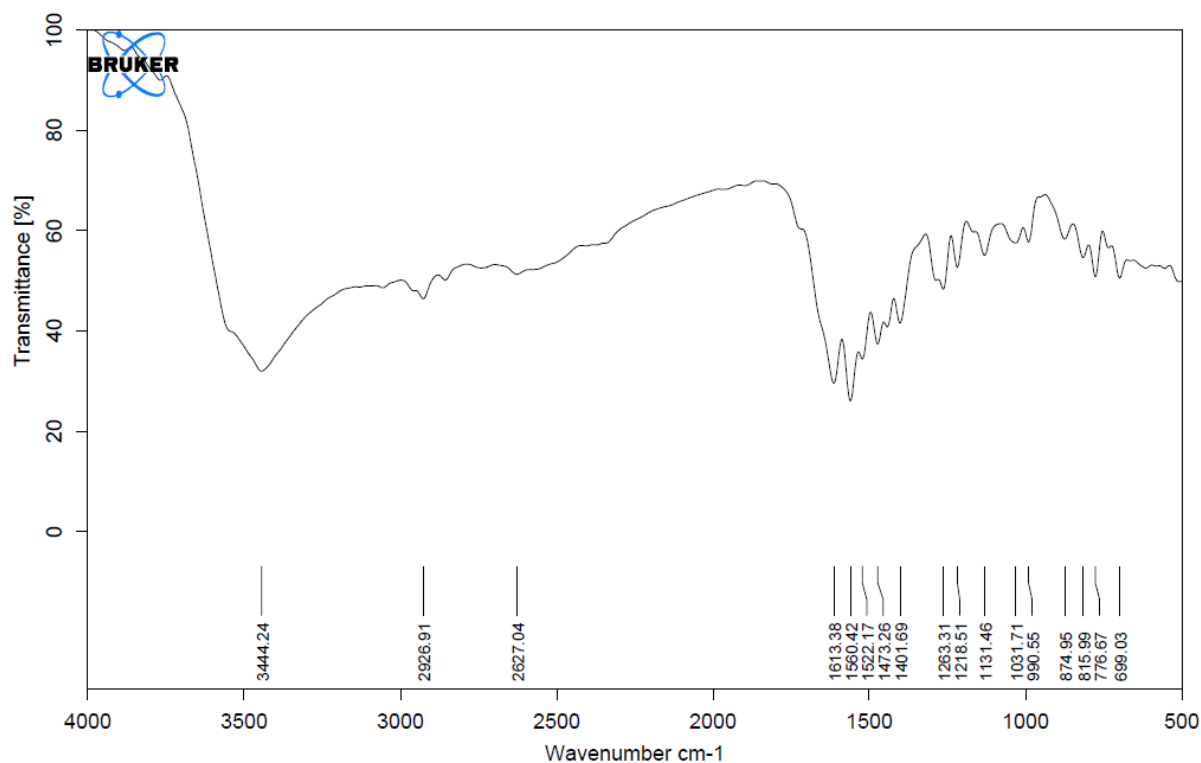
¹H-NMR



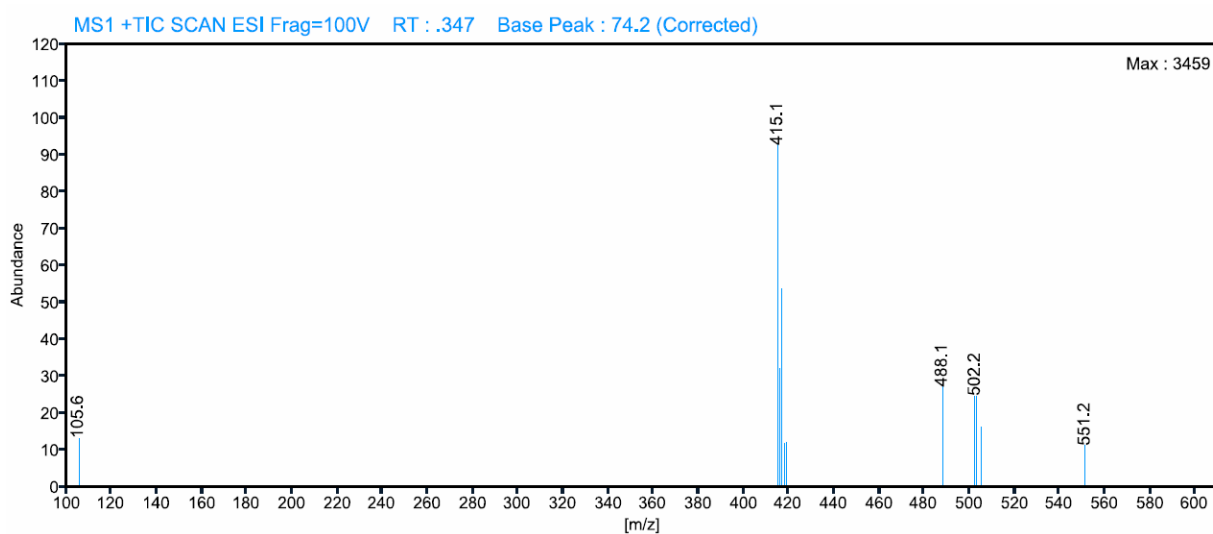
5-((3,4-Dichlorobenzylamino)methyl)-3-phenylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (115)



IR

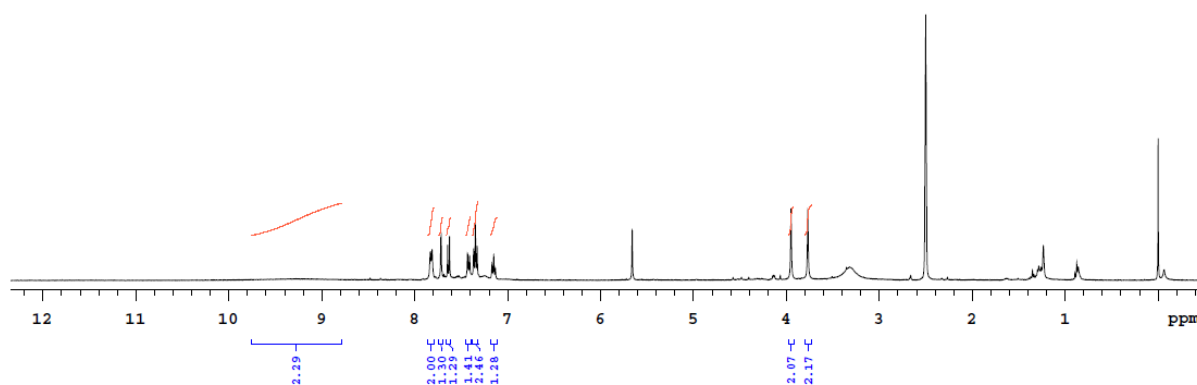


MASS

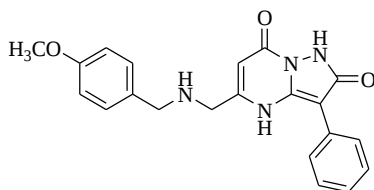


¹H-NMR

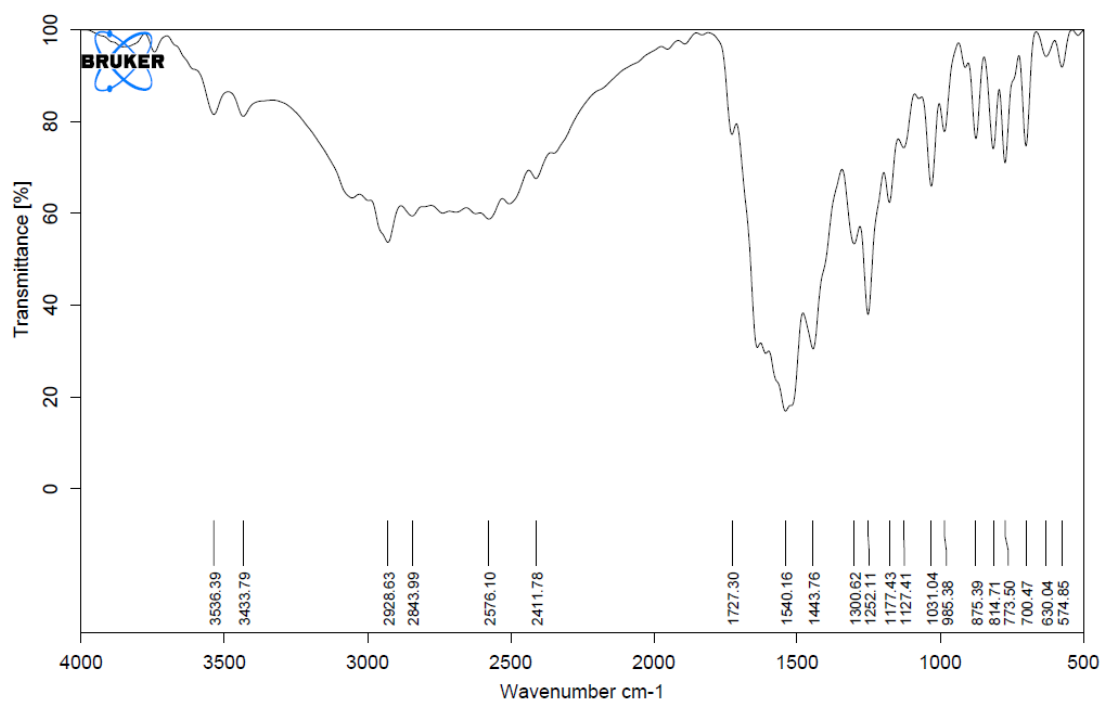
Solvent: dmsc
SA-Varian 400MHz NMR
Date: Jun 27 2022



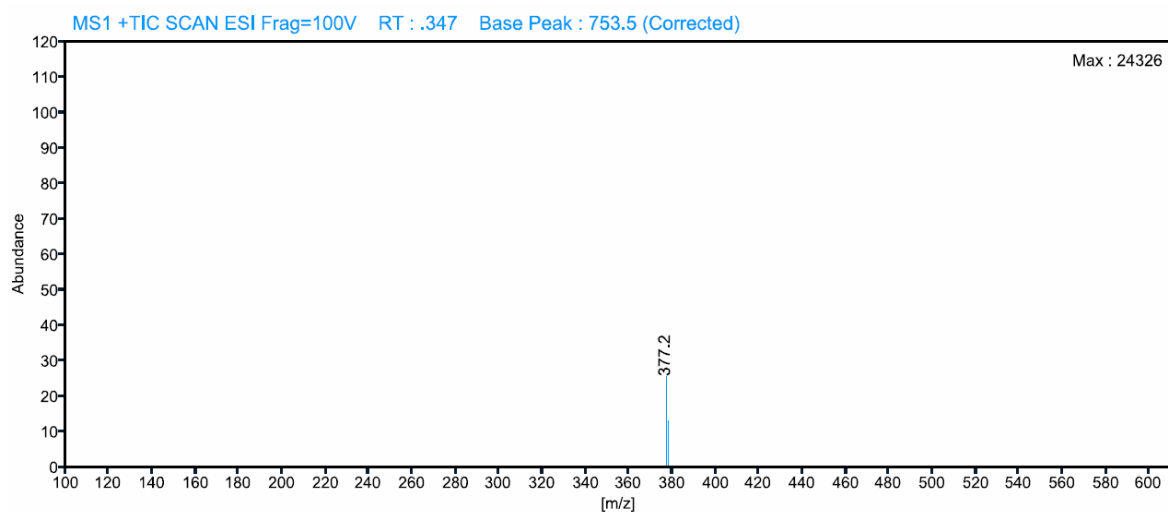
5-((4-Methoxybenzylamino)methyl)-3-phenylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (116)



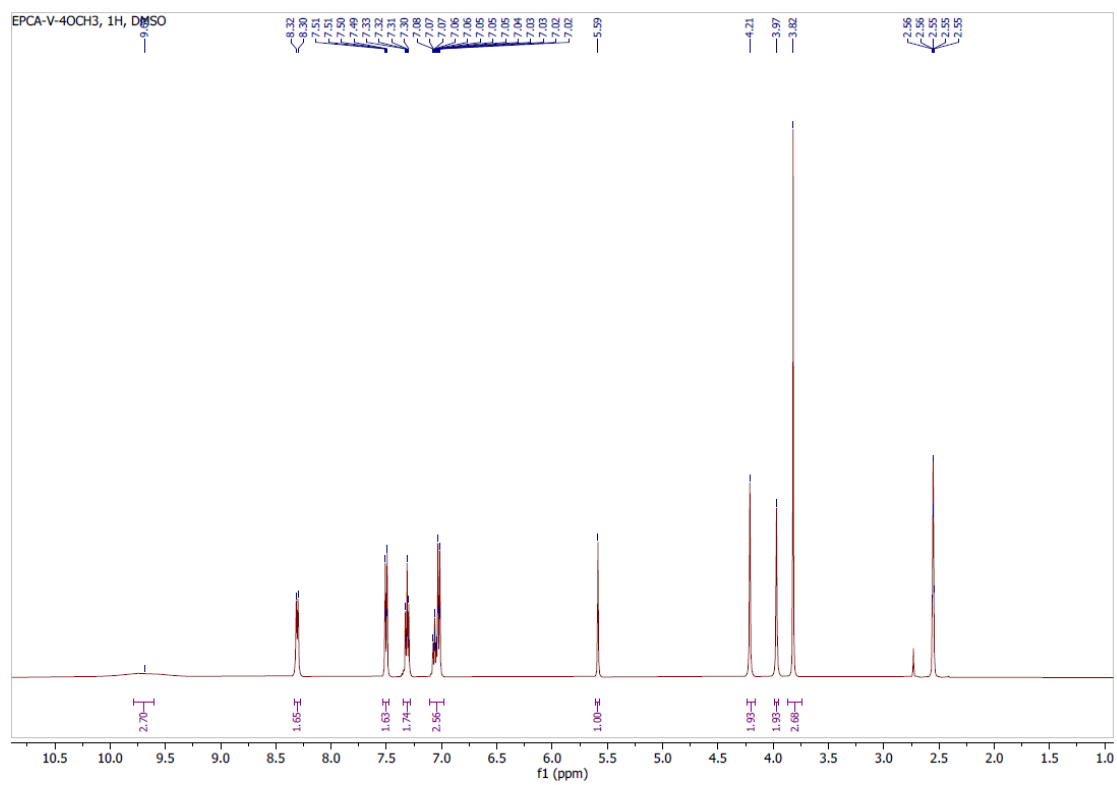
IR

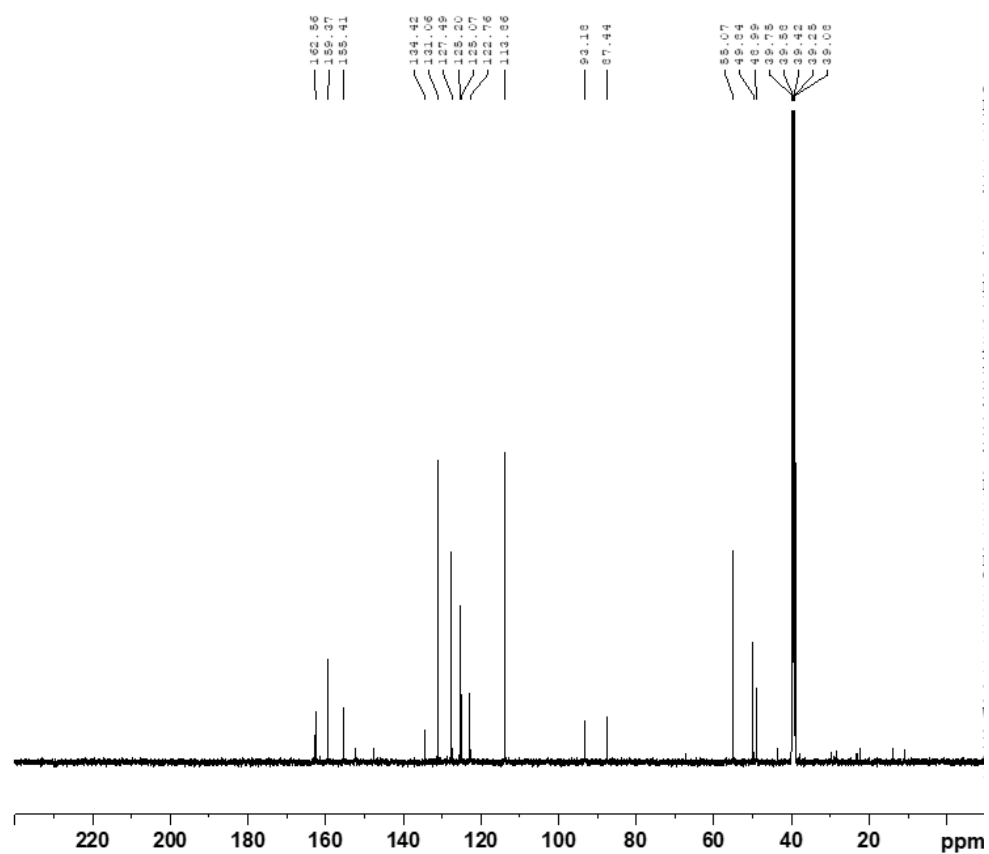


MASS

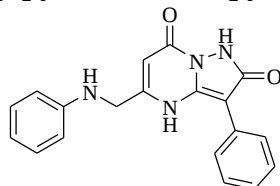


¹H-NMR

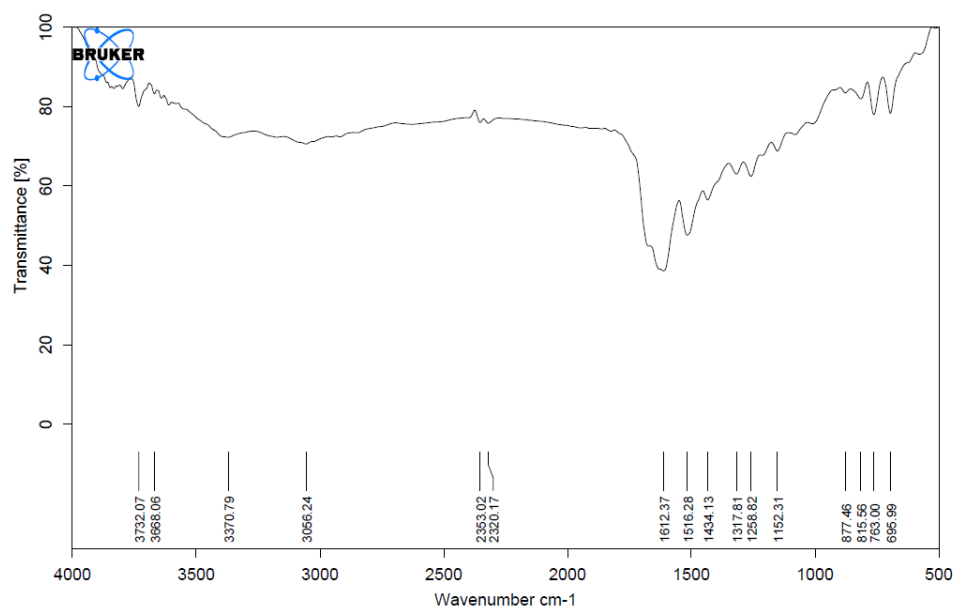


^{13}C -NMR

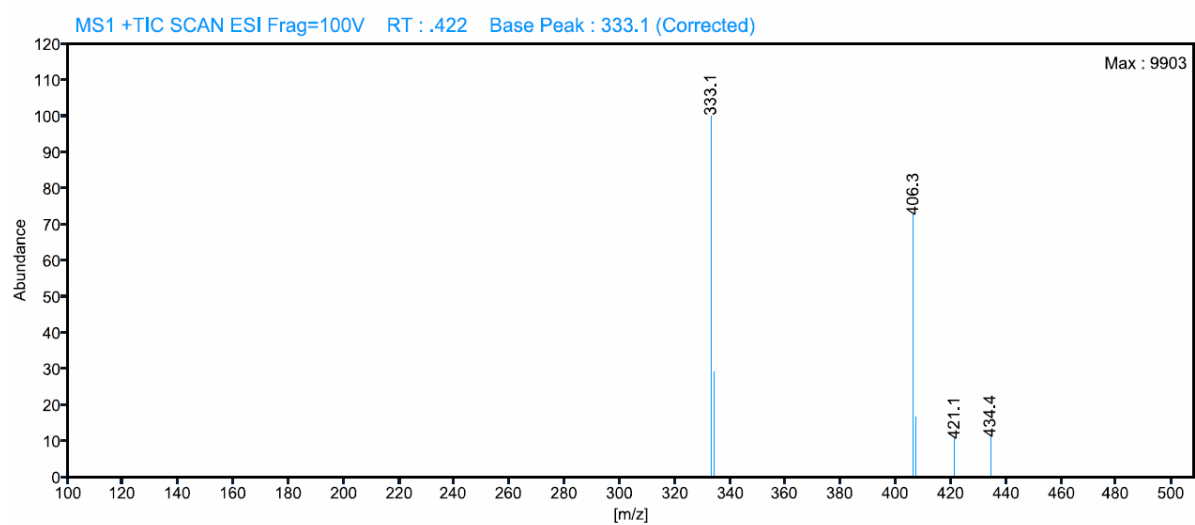
5-((Phenylamino)methyl)-3-phenylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (117)



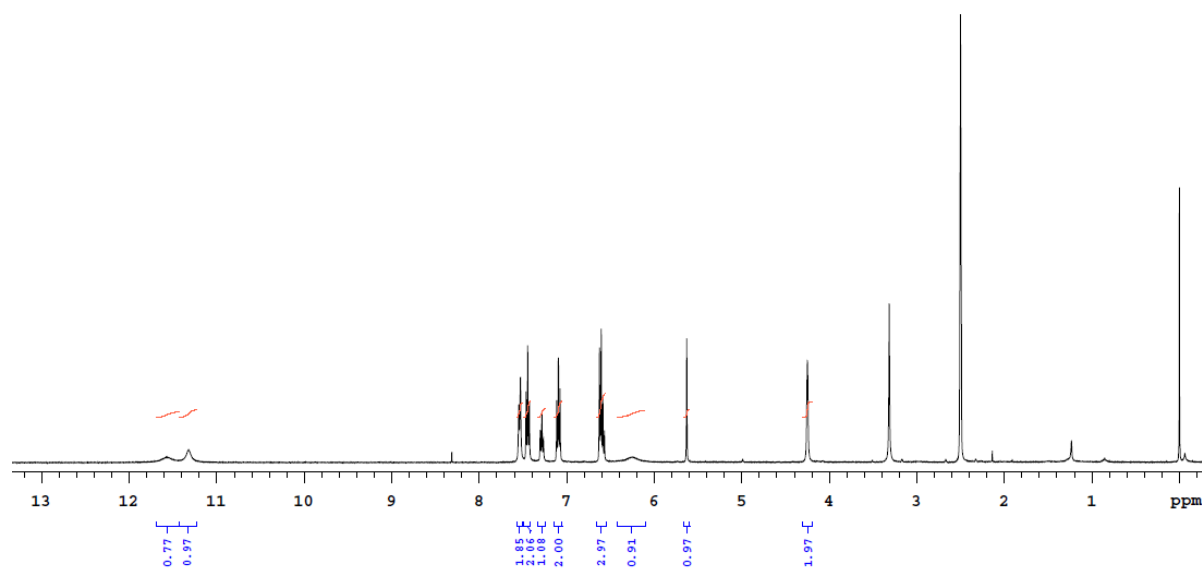
IR



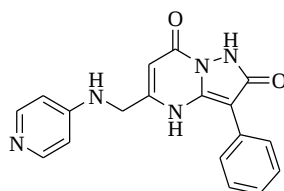
MASS

 $^1\text{H-NMR}$

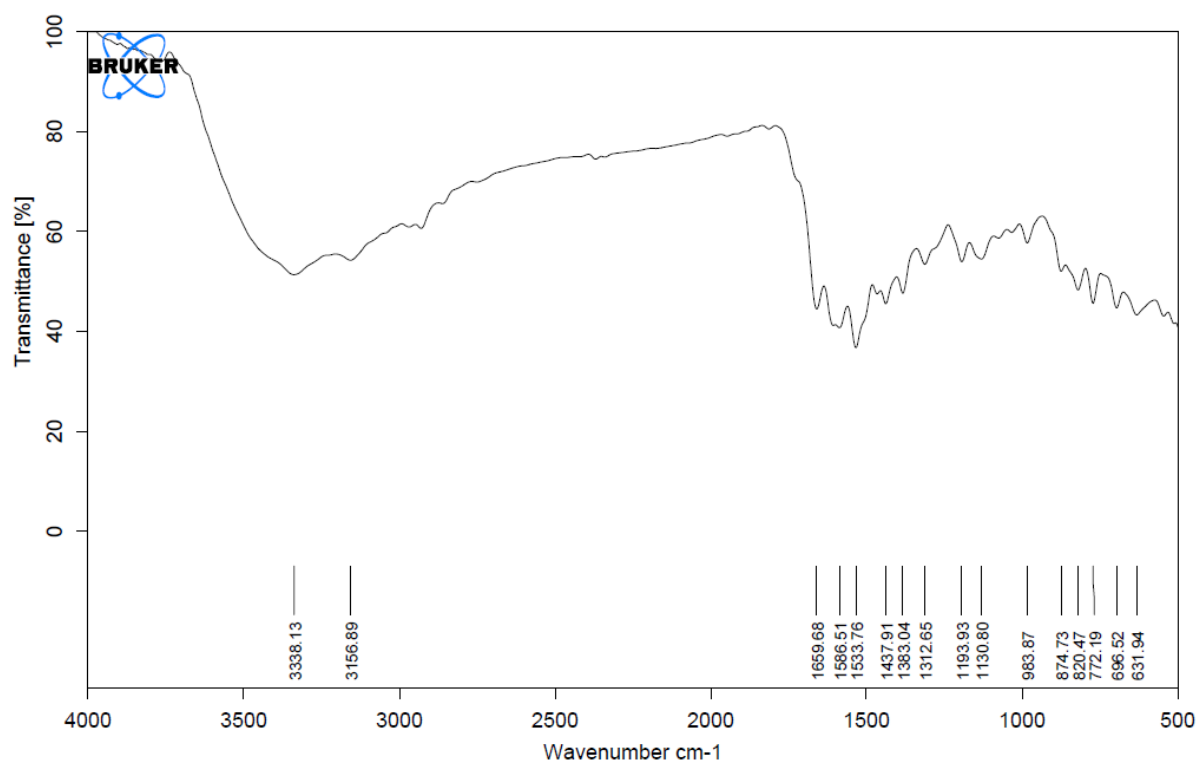
Solvent: dmsc
SA-Varian 400MHz NMR
Date: Jun 27 2022



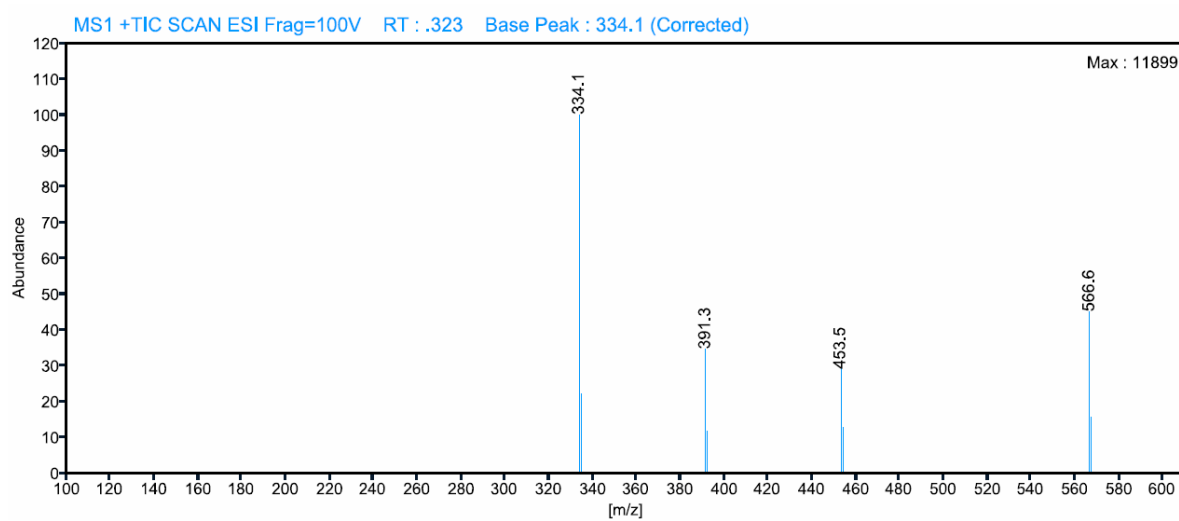
3-Phenyl-5-((pyridin-4-ylamino)methyl)pyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione
(121)



IR

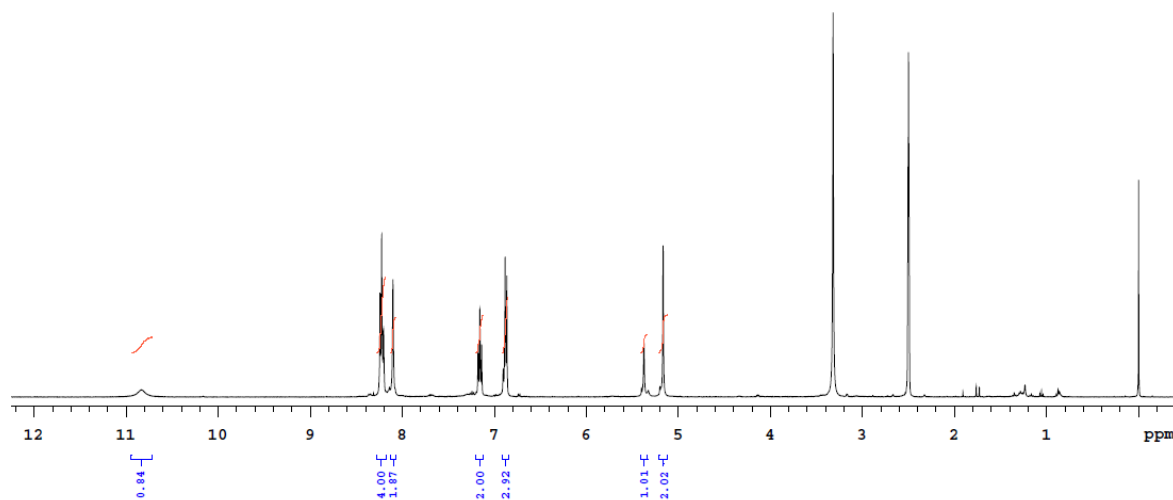
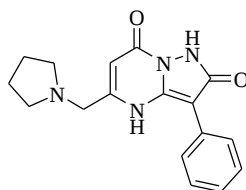
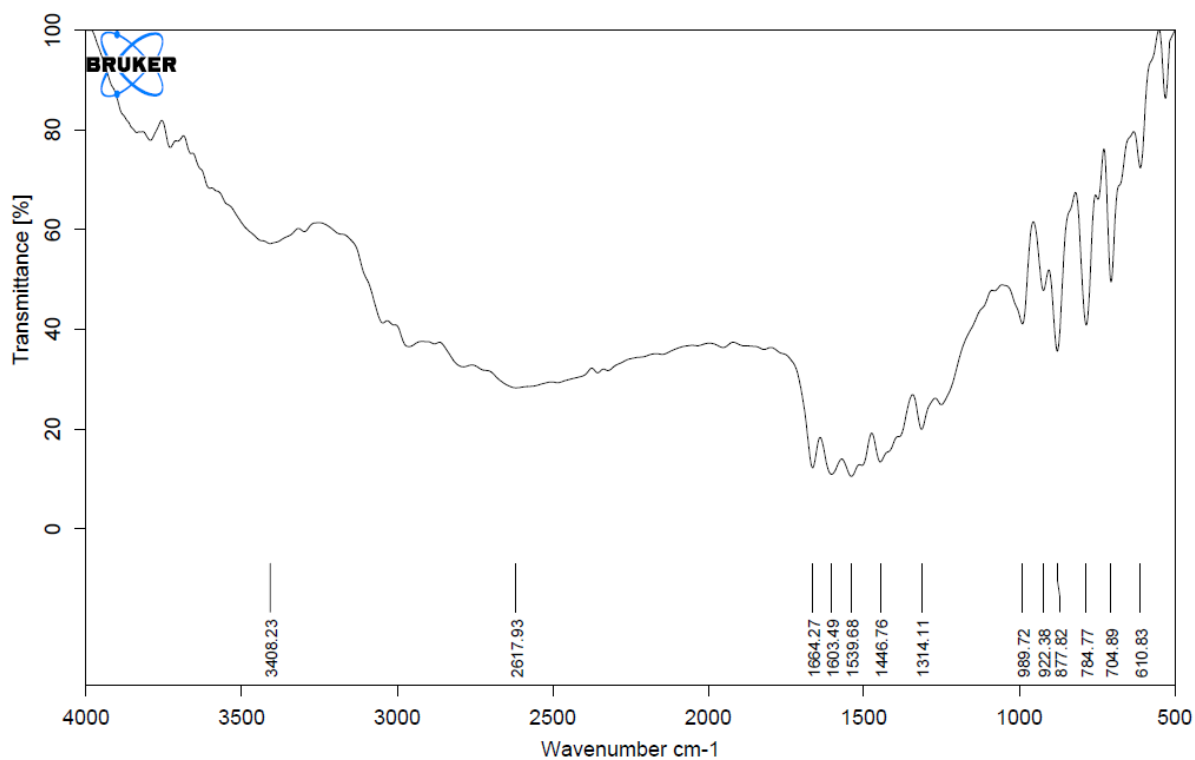


MASS

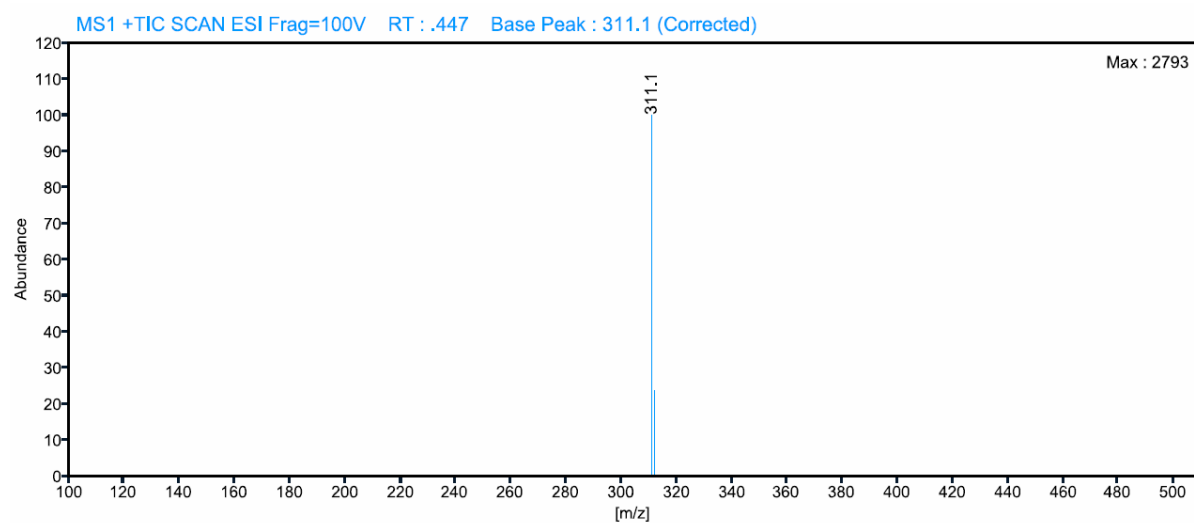
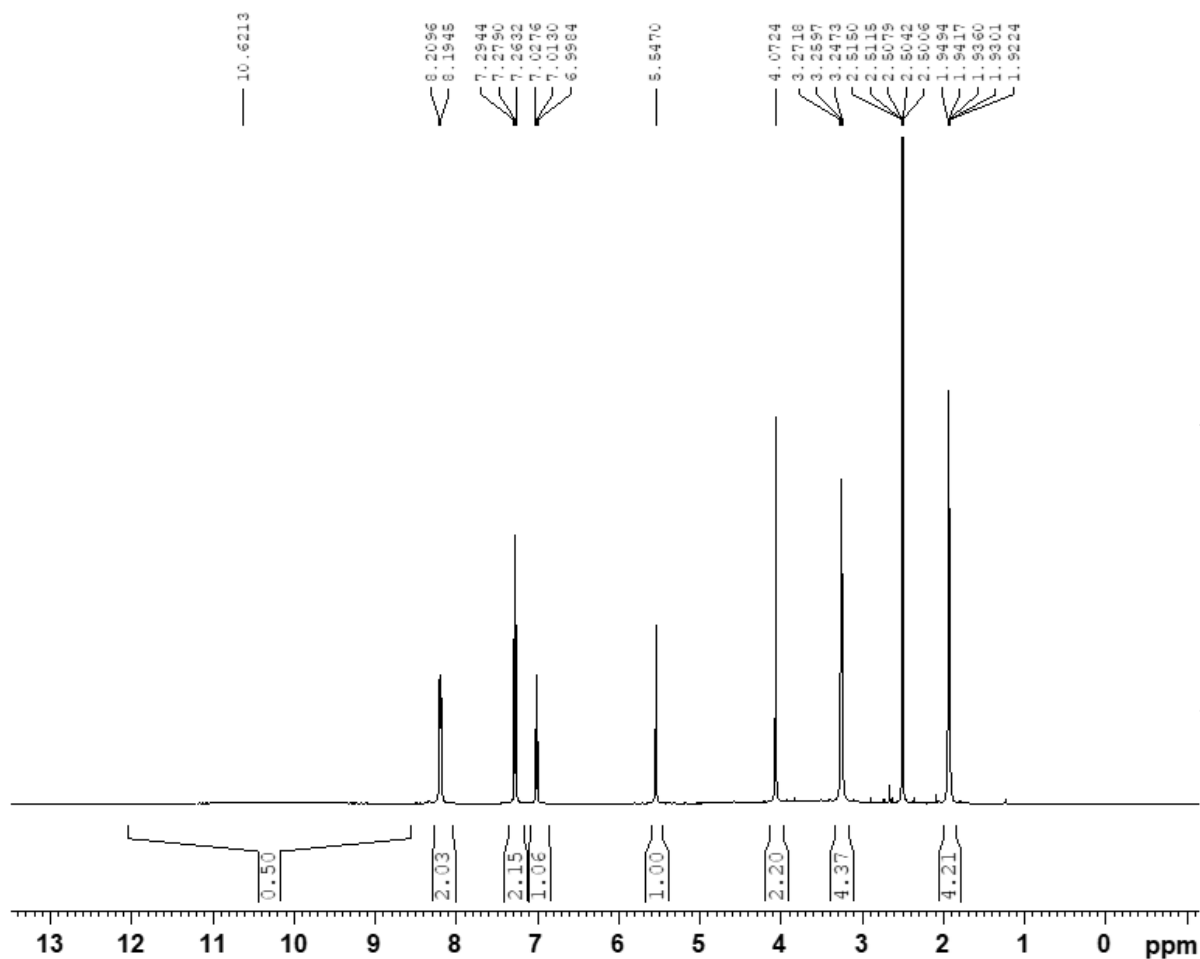


¹H-NMR

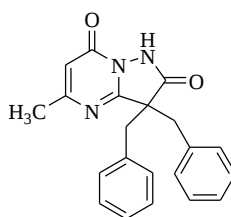
Solvent: dmsc
SA-Varian 400MHz NMR
Date: Jun 27 2022

**3-Phenyl-5-((pyrrolidin-1-yl)methyl)pyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (122)****IR**

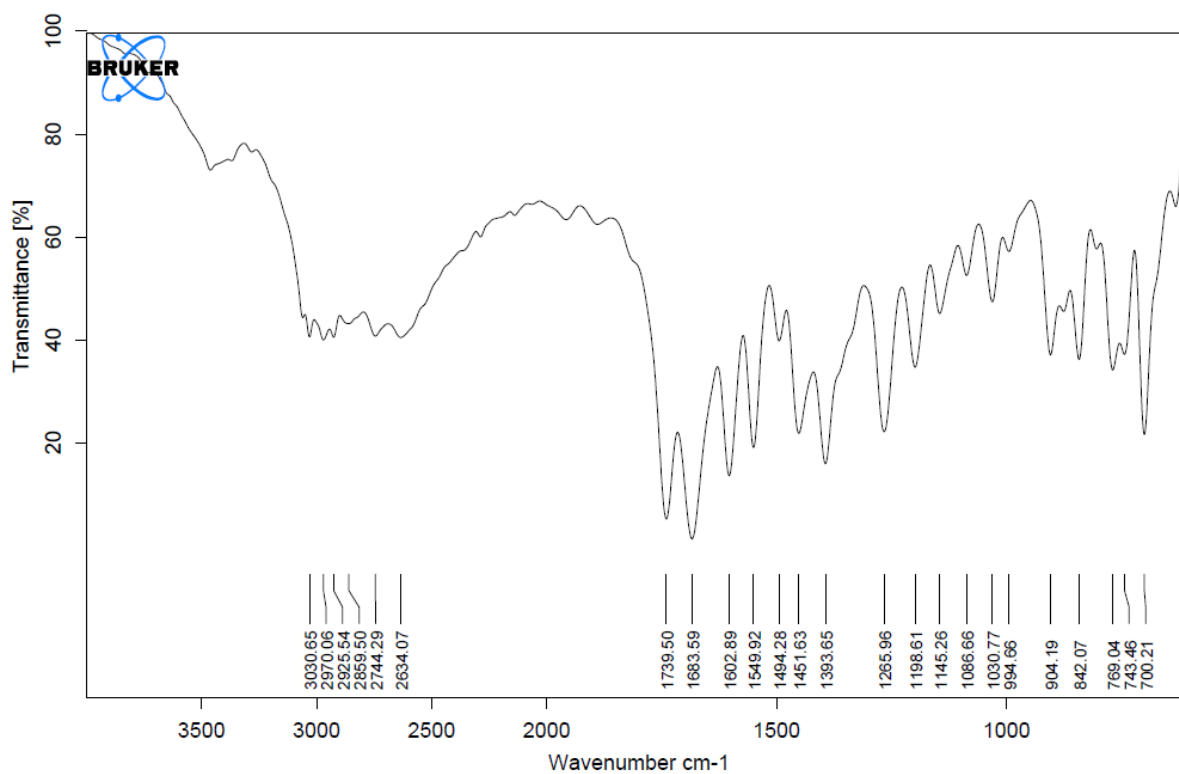
MASS

 $^1\text{H-NMR}$ 

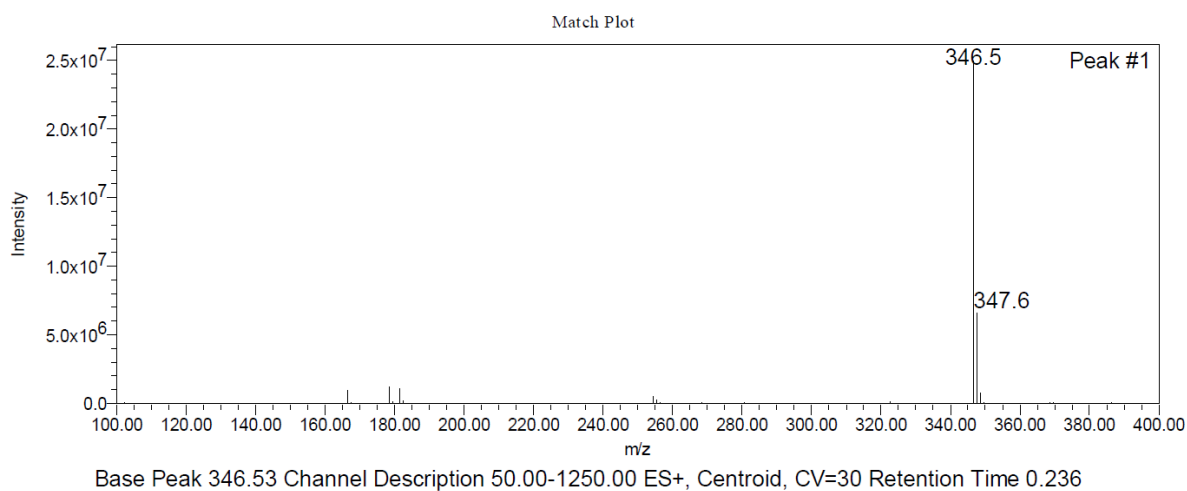
3,3-dibenzyl-5-methylpyrazolo[1,5-a]pyrimidine-2,7(1H,3H)-dione (130)

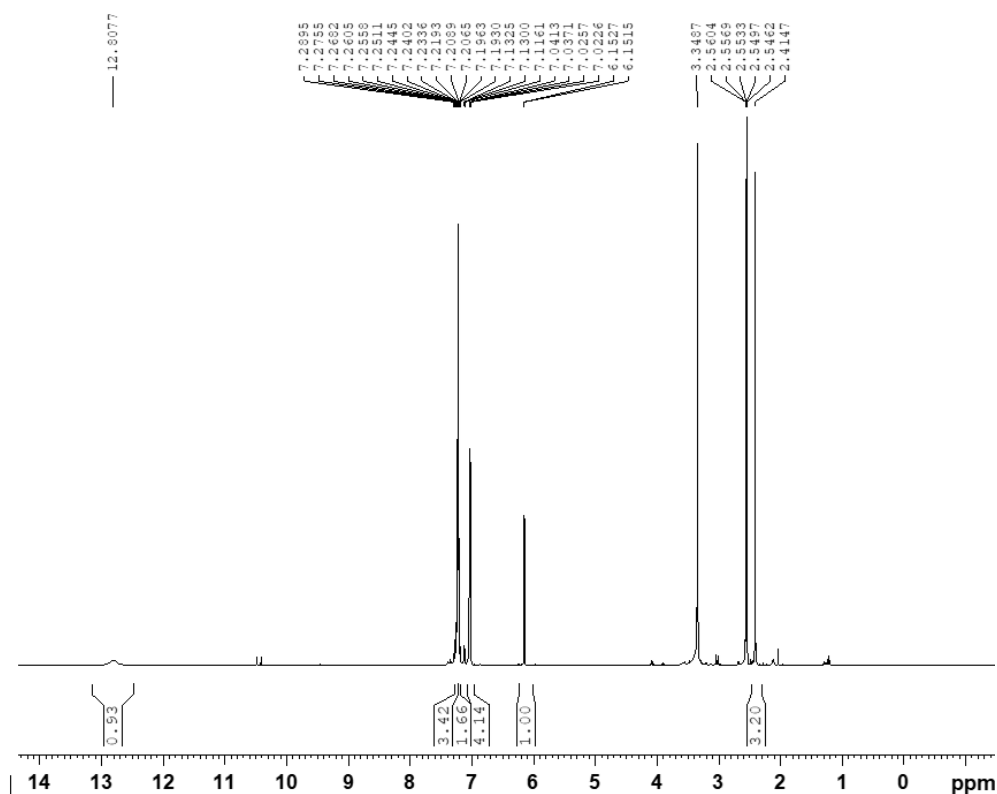
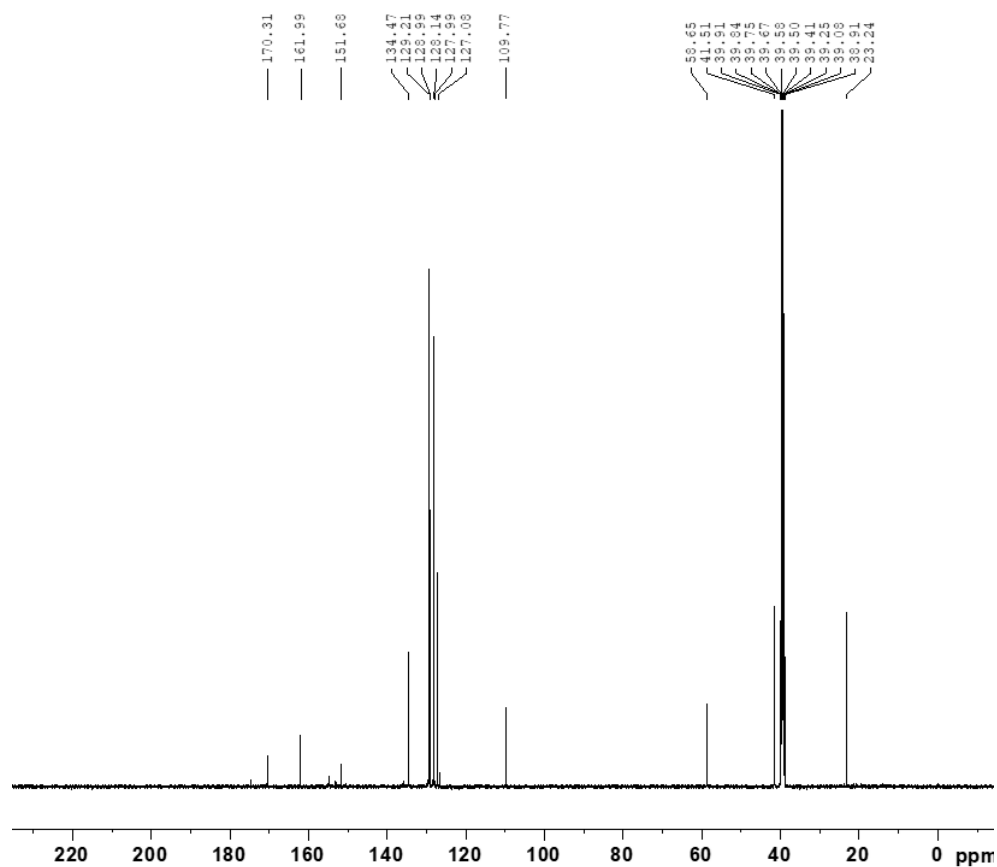


IR

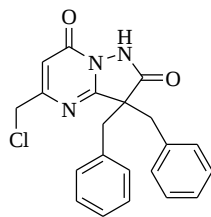


MASS

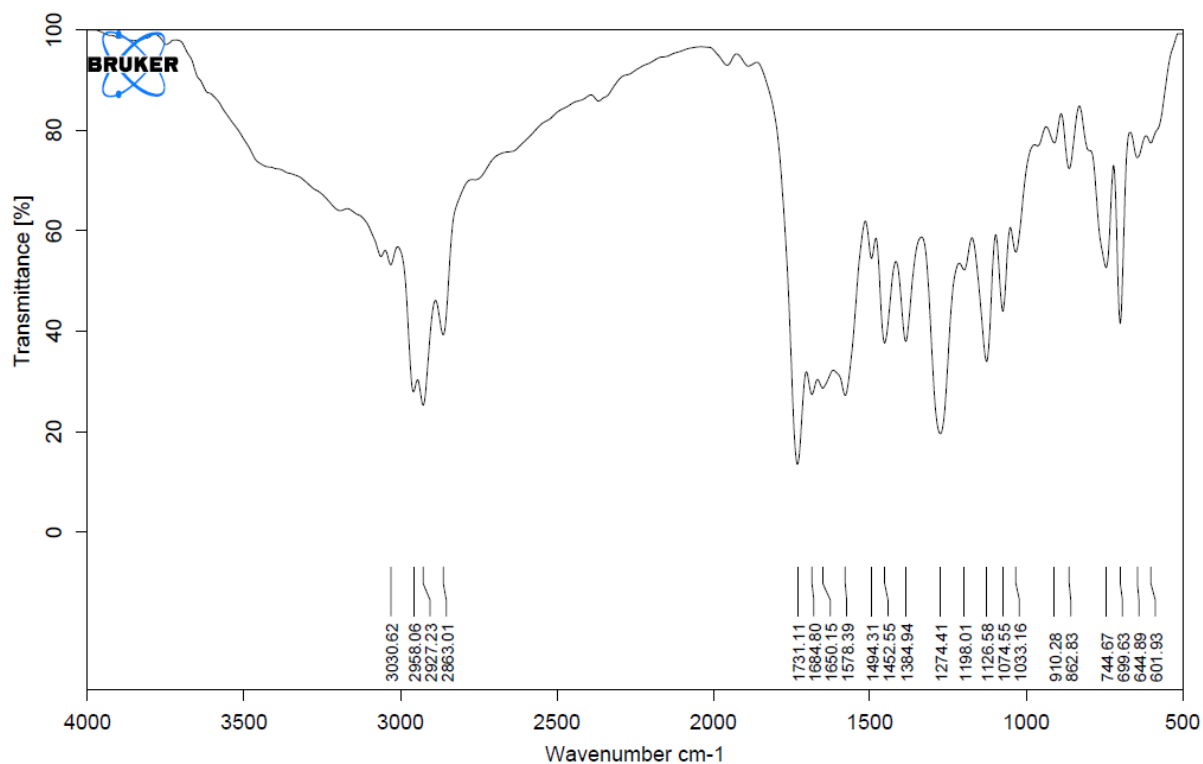


¹H-NMR¹³C NMR

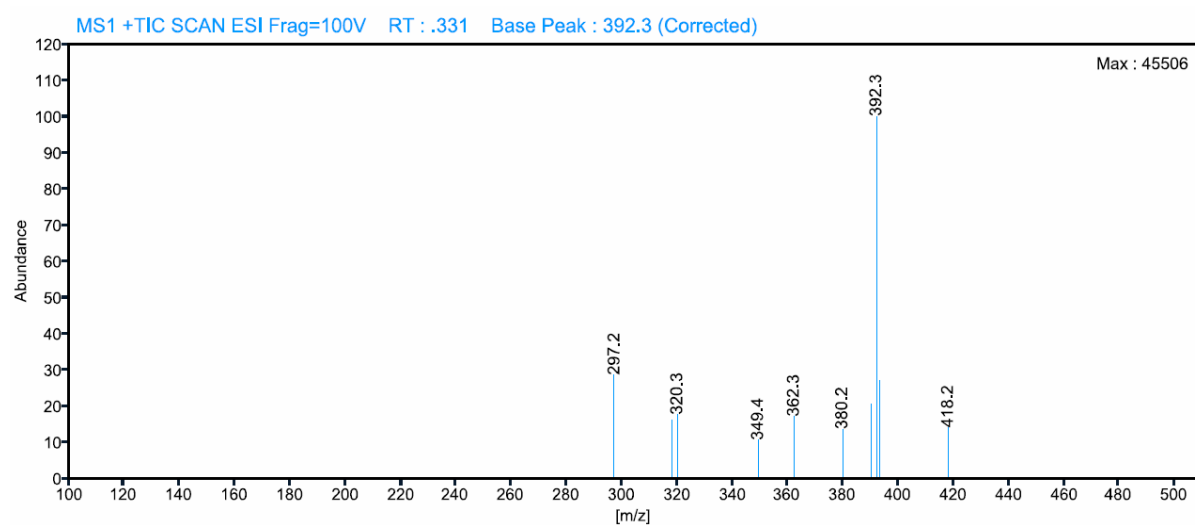
3,3-dibenzyl-5-(chloromethyl)pyrazolo[1,5-a]pyrimidine-2,7(1H,3H)-dione (133)

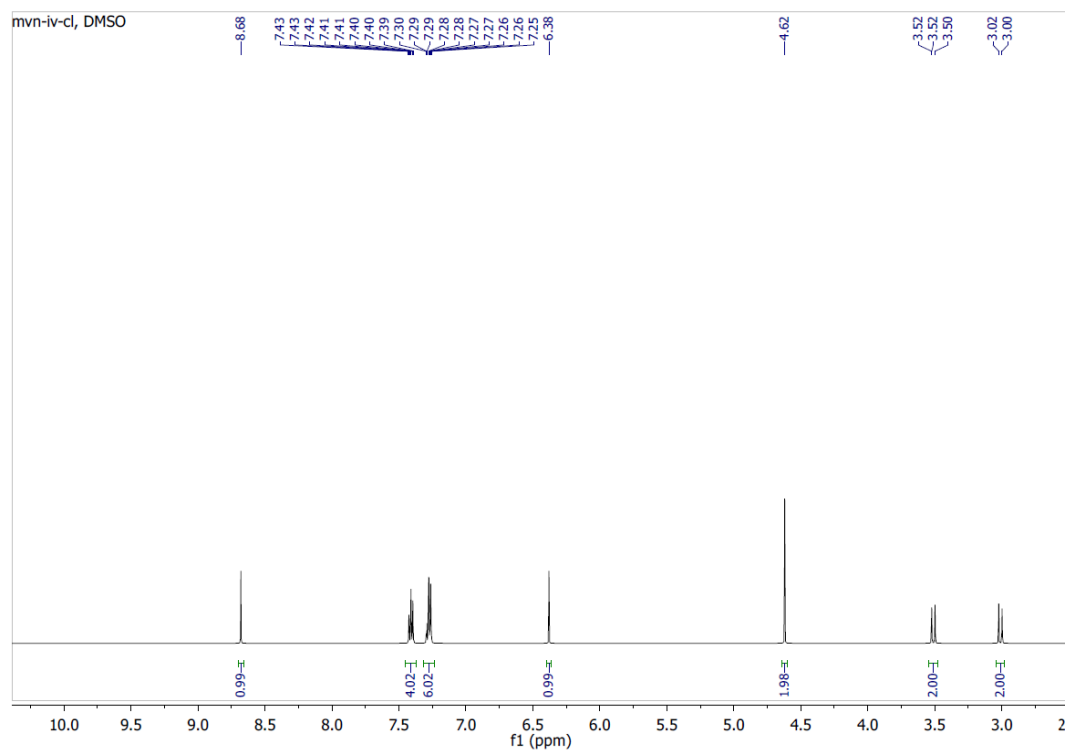


IR

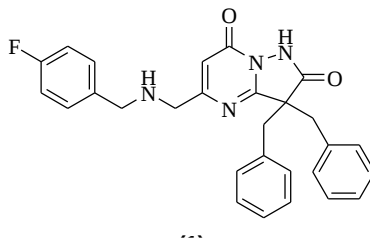


MASS

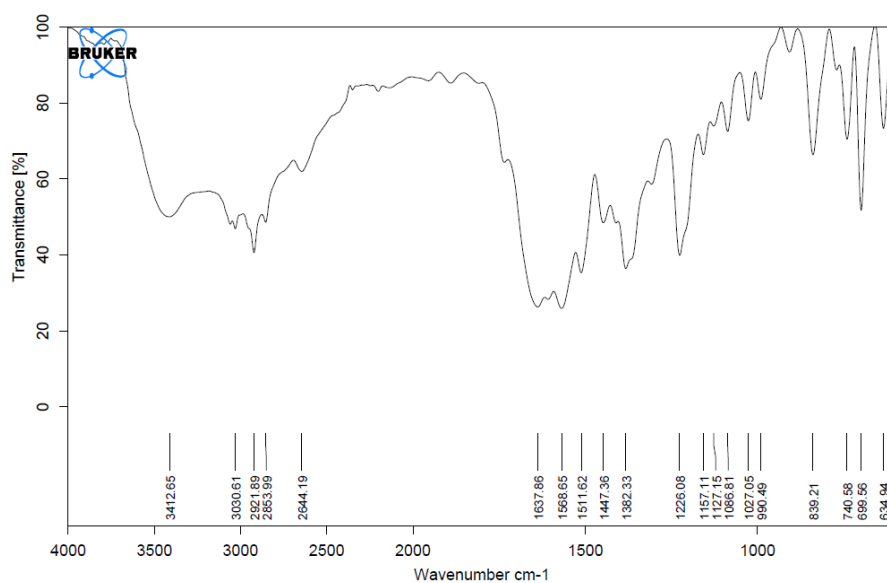
¹H-NMR



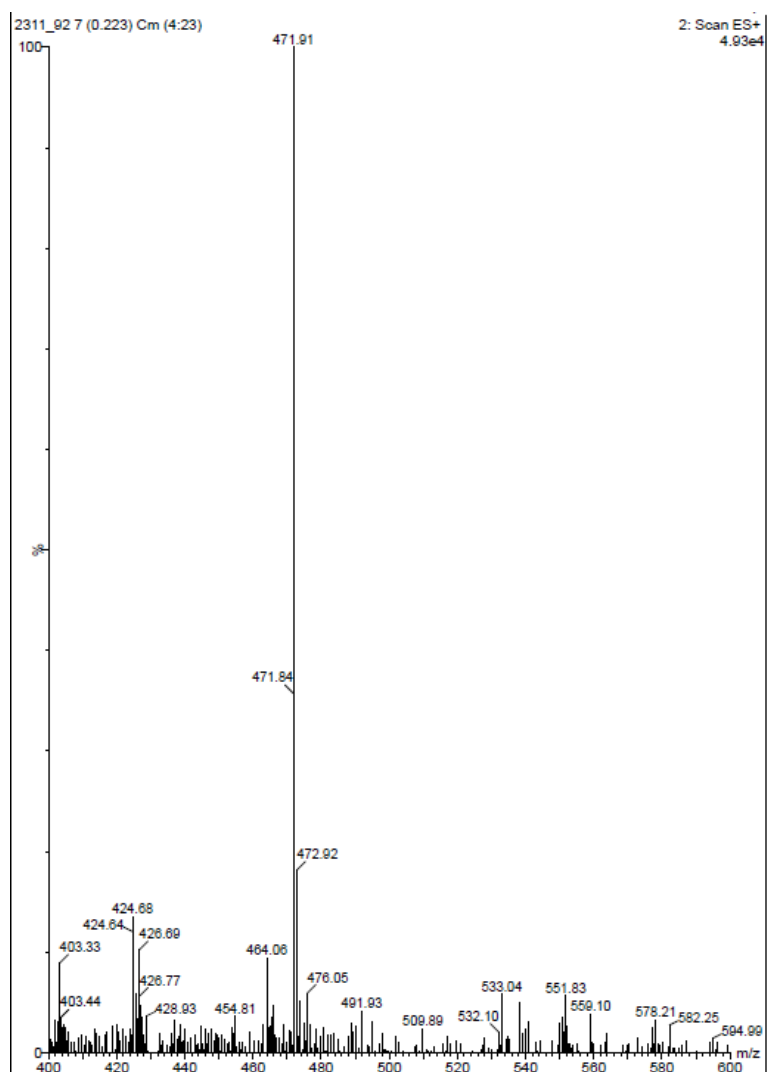
5-((4-Fluorobenzylamino)methyl)-3,3-dibenzylpyrazolo[1,5-a]pyrimidine-2,7(1H,3H)-dione (135)

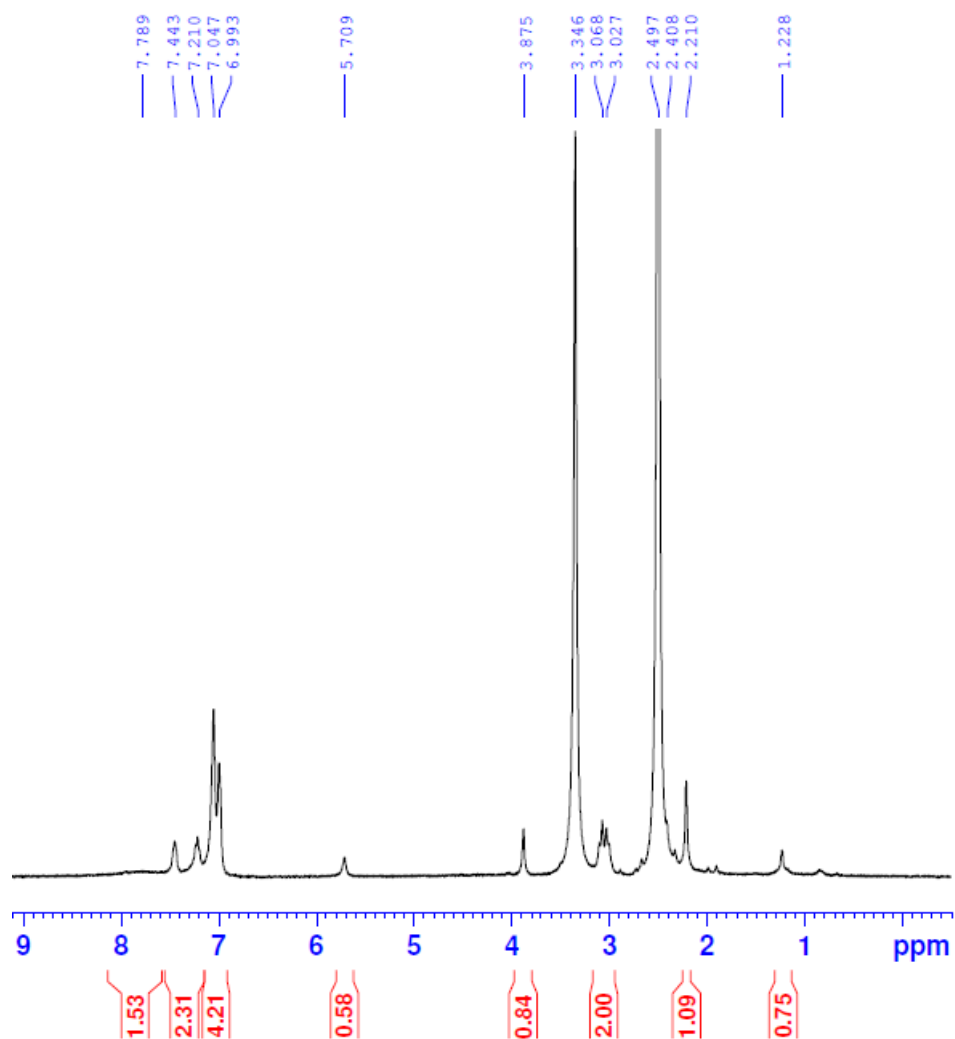


IR

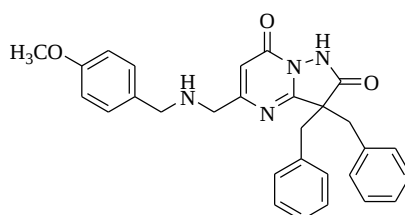


MASS

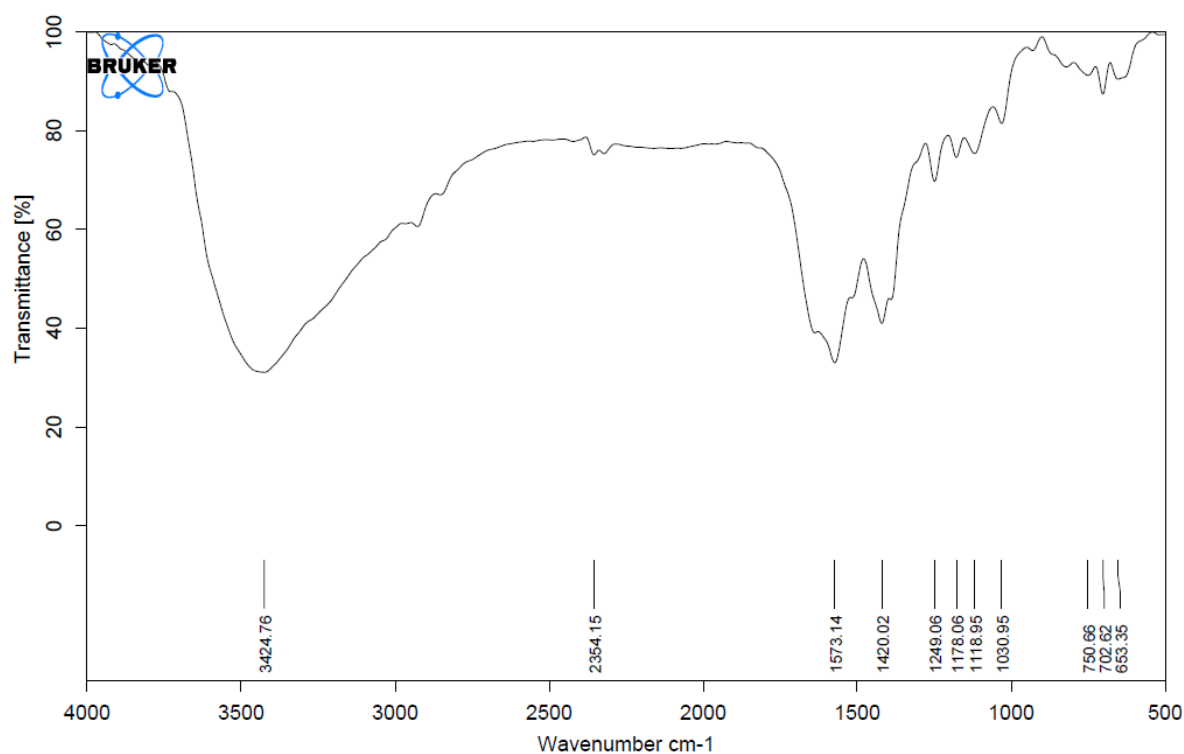
 $^1\text{H-NMR}$



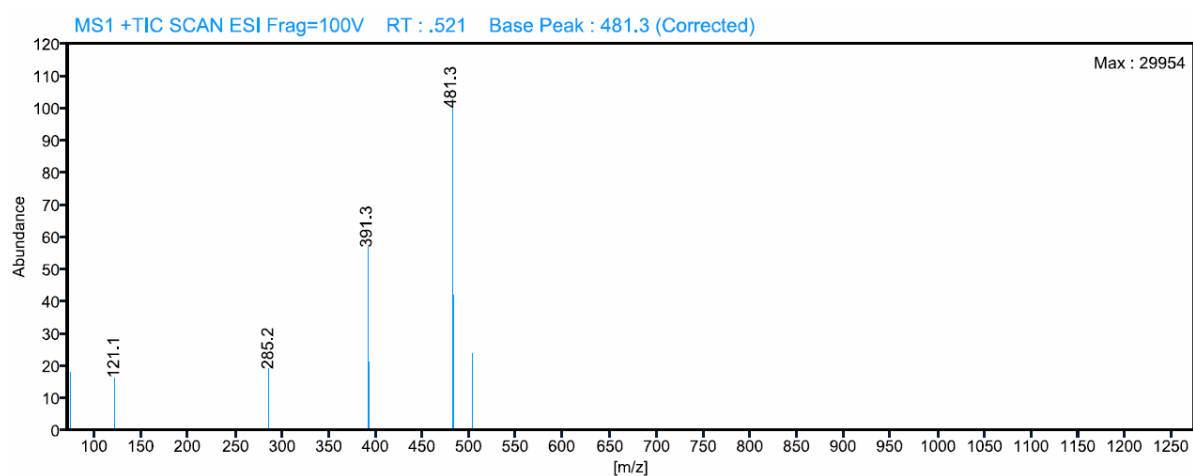
5-((4-Methoxybenzylamino)methyl)-3,3-dibenzylpyrazolo[1,5-*a*]pyrimidine-2,7(1*H*,3*H*)-dione (140)

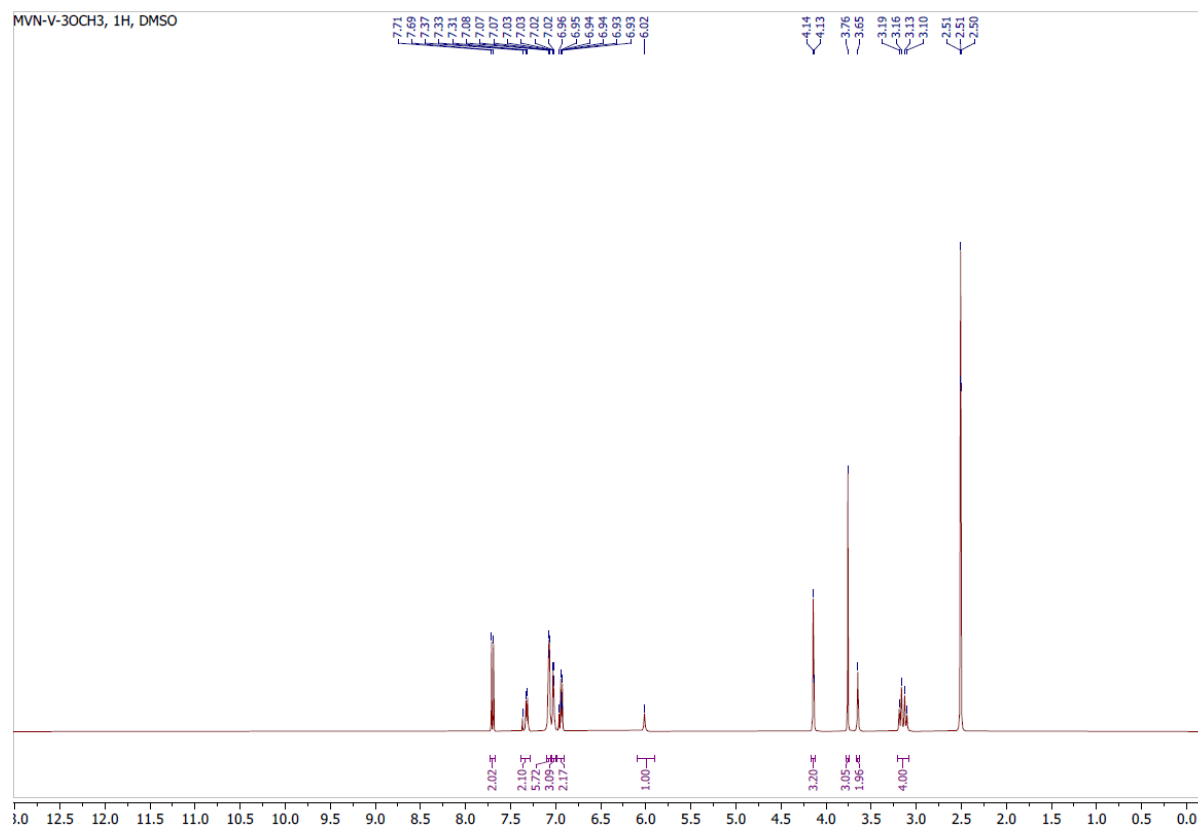


IR

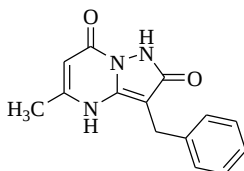


MASS

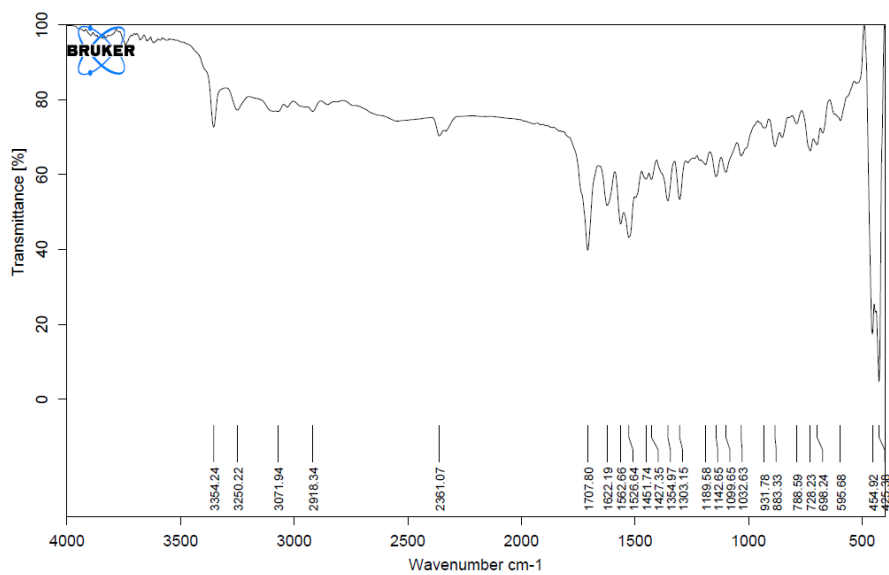


¹H-NMR

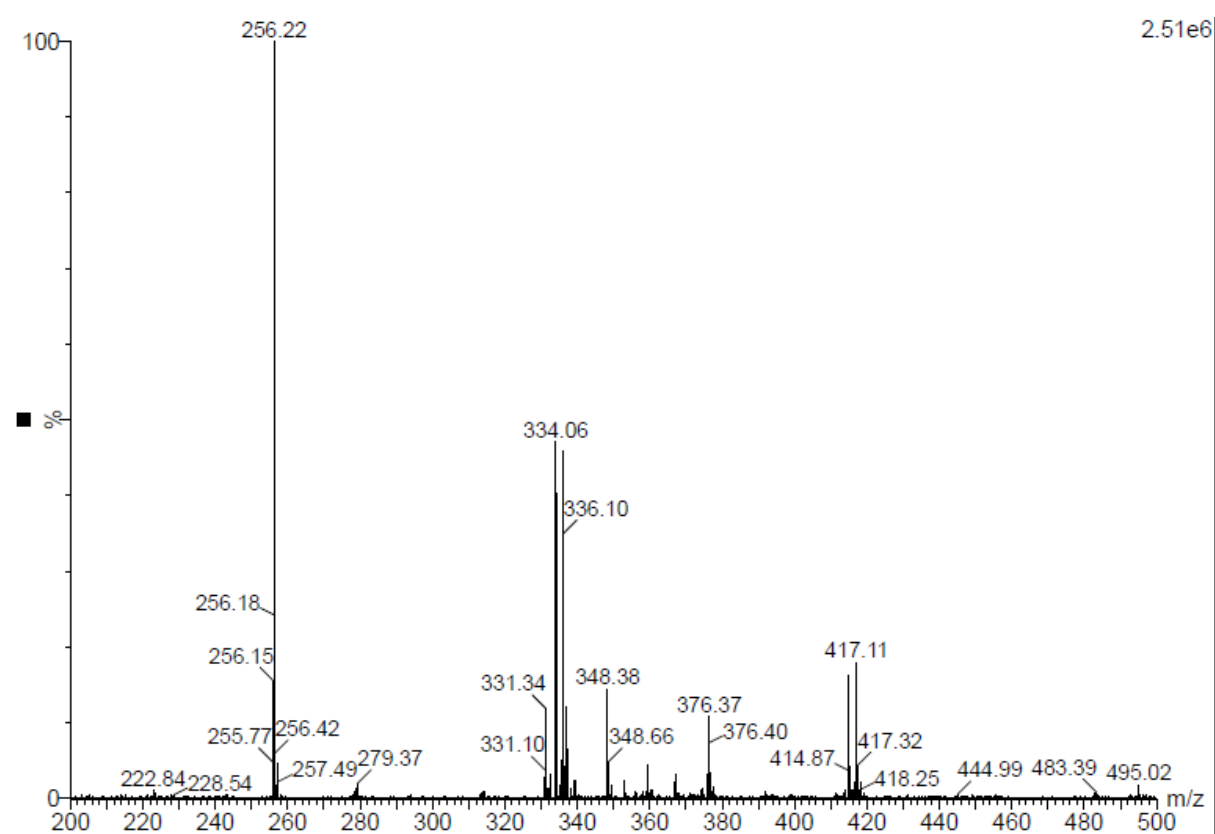
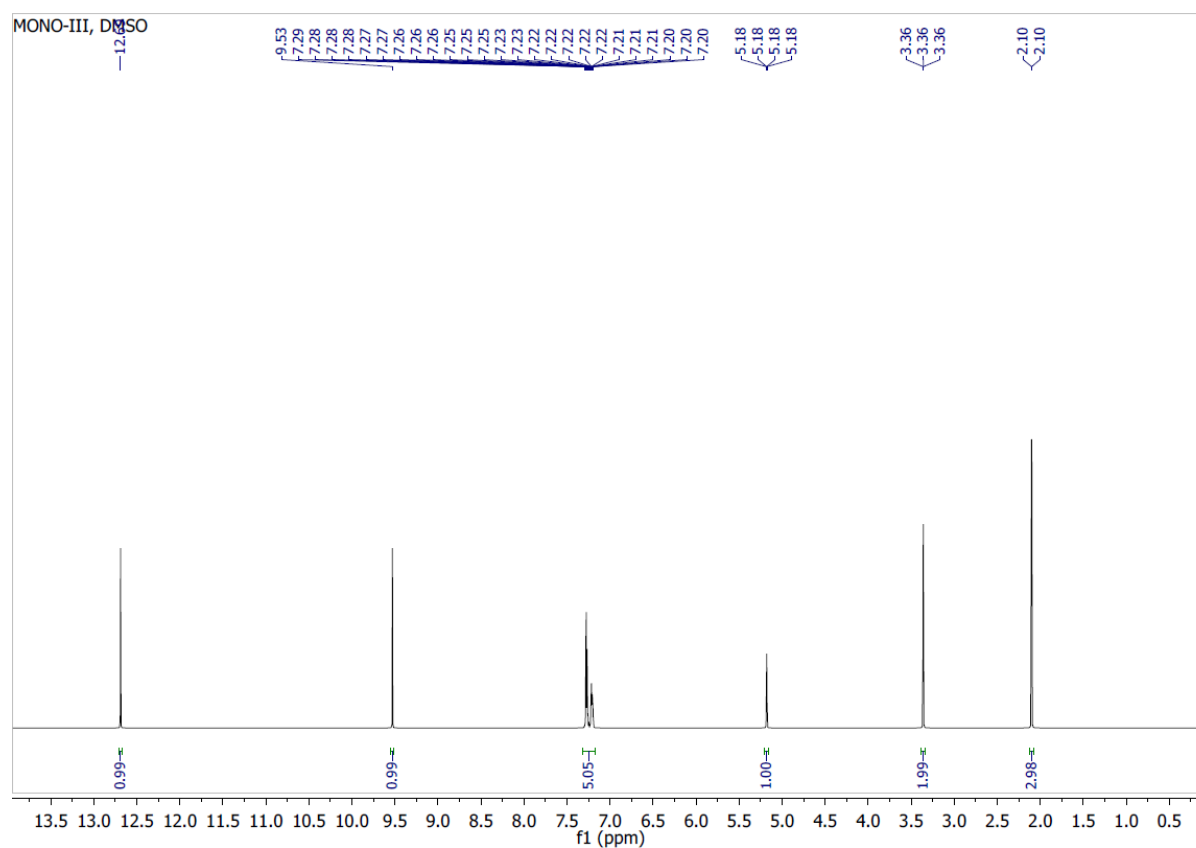
3-benzyl-5-methylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (144)



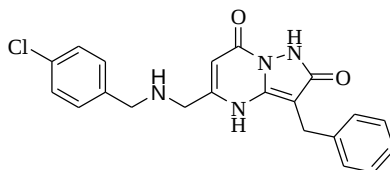
IR



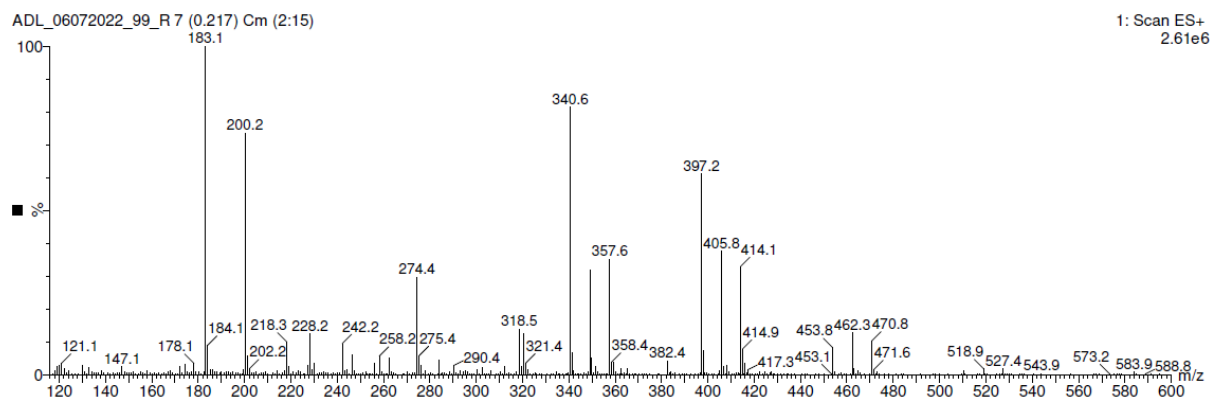
MASS

¹H-NMR

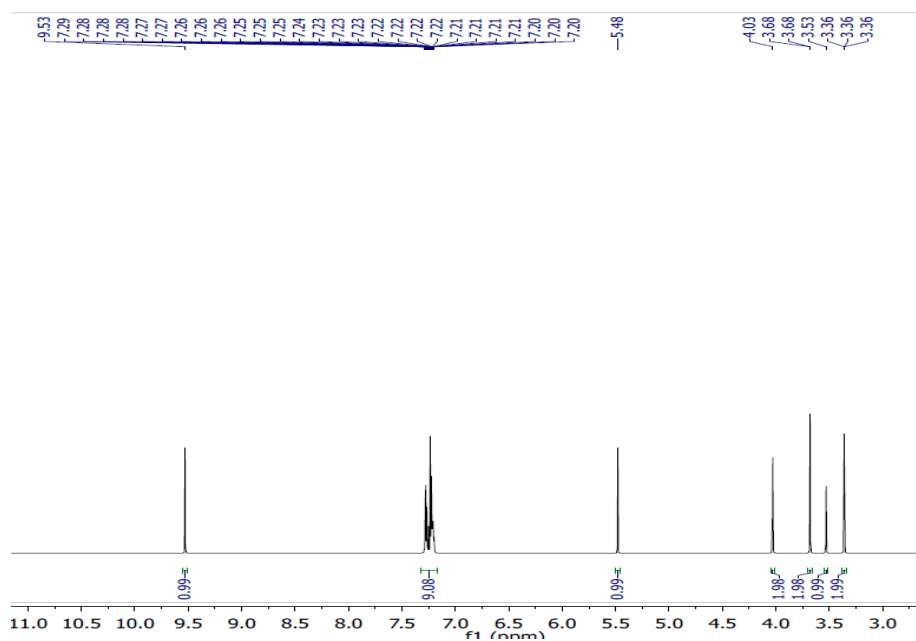
5-((4-Chlorobenzylamino)methyl)-3-benzylpyrazolo[1,5-a]pyrimidine-2,7(1H,4H)-dione (149)



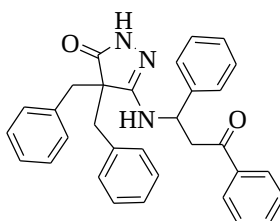
MASS



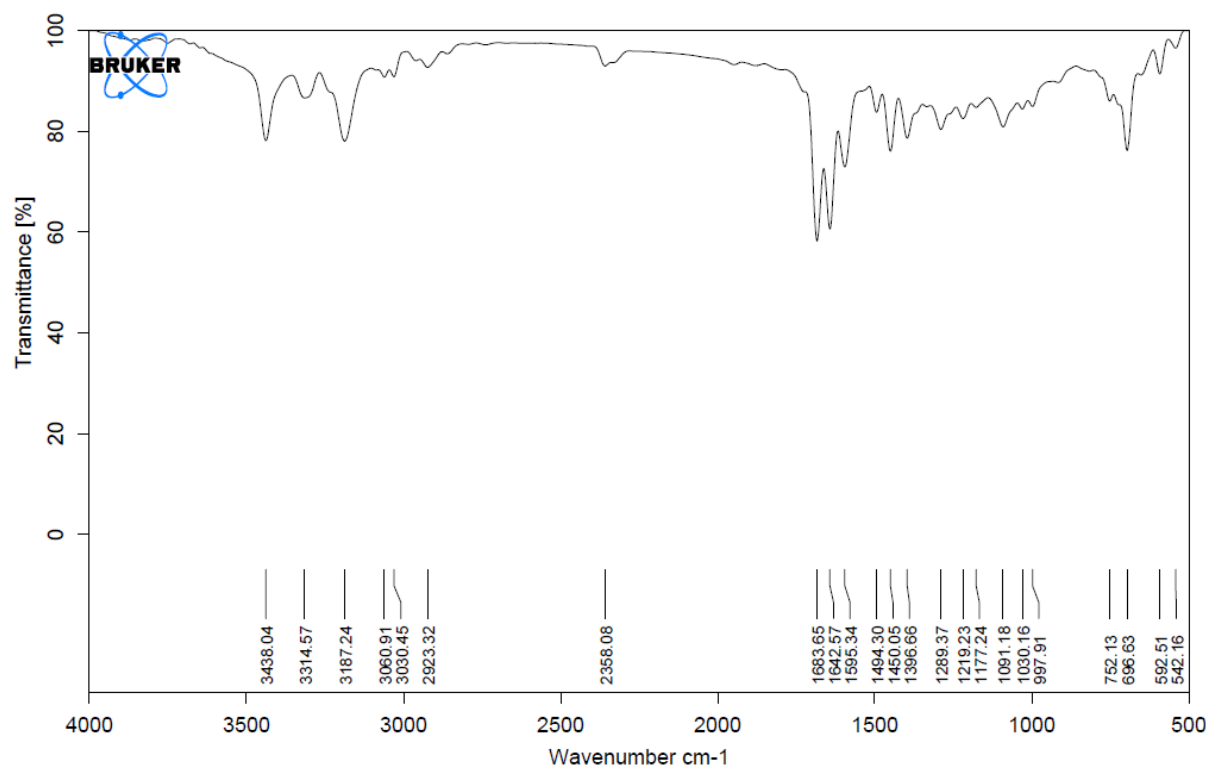
¹H-NMR



3-(3-Oxo-1,3-diphenylpropylamino)-4,4-dibenzyl-1H-pyrazol-5(4H)-one (211)

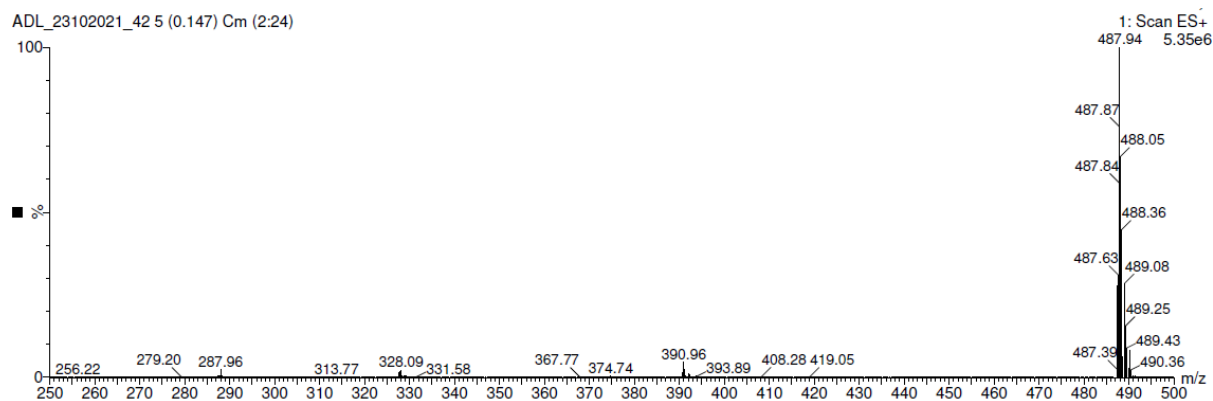


IR

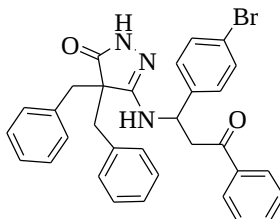


MASS

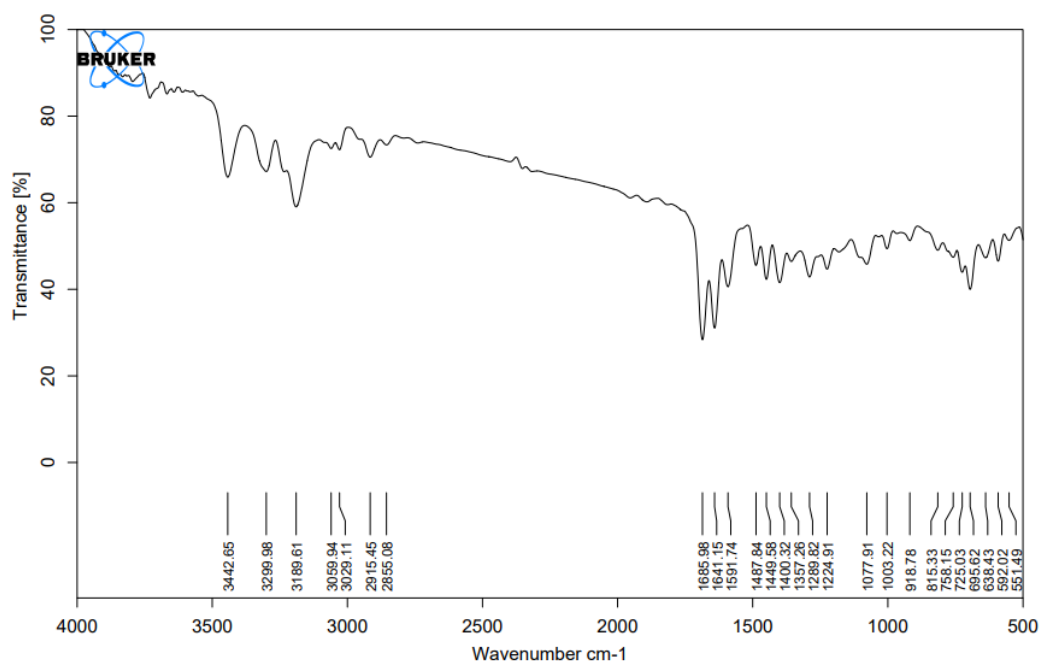
ADL_23102021_42 5 (0.147) Cm (2:24)



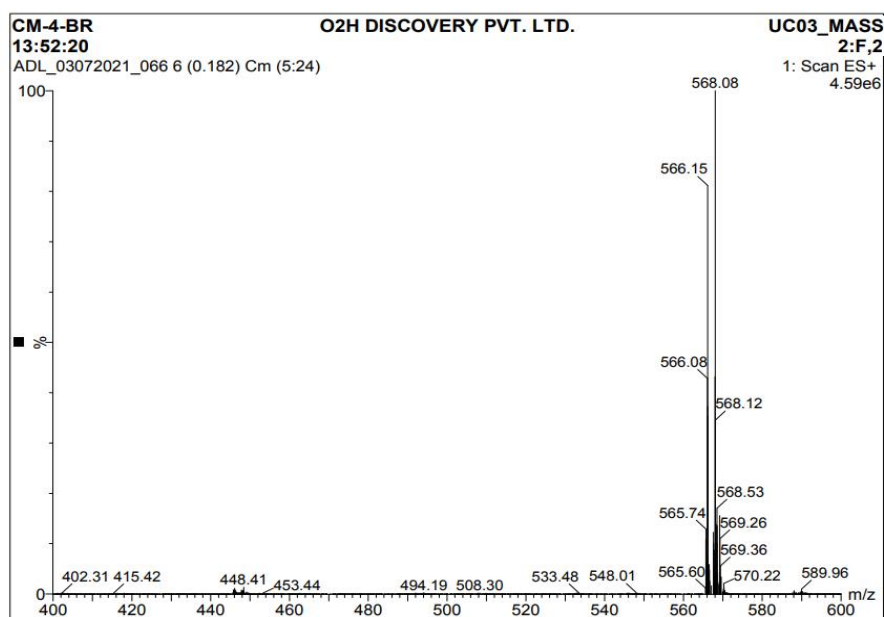
3-(1-(4-bromophenyl)-3-oxo-3-phenylpropylamino)-4,4-dibenzyl-1H-pyrazol-5(4H)-one (215)

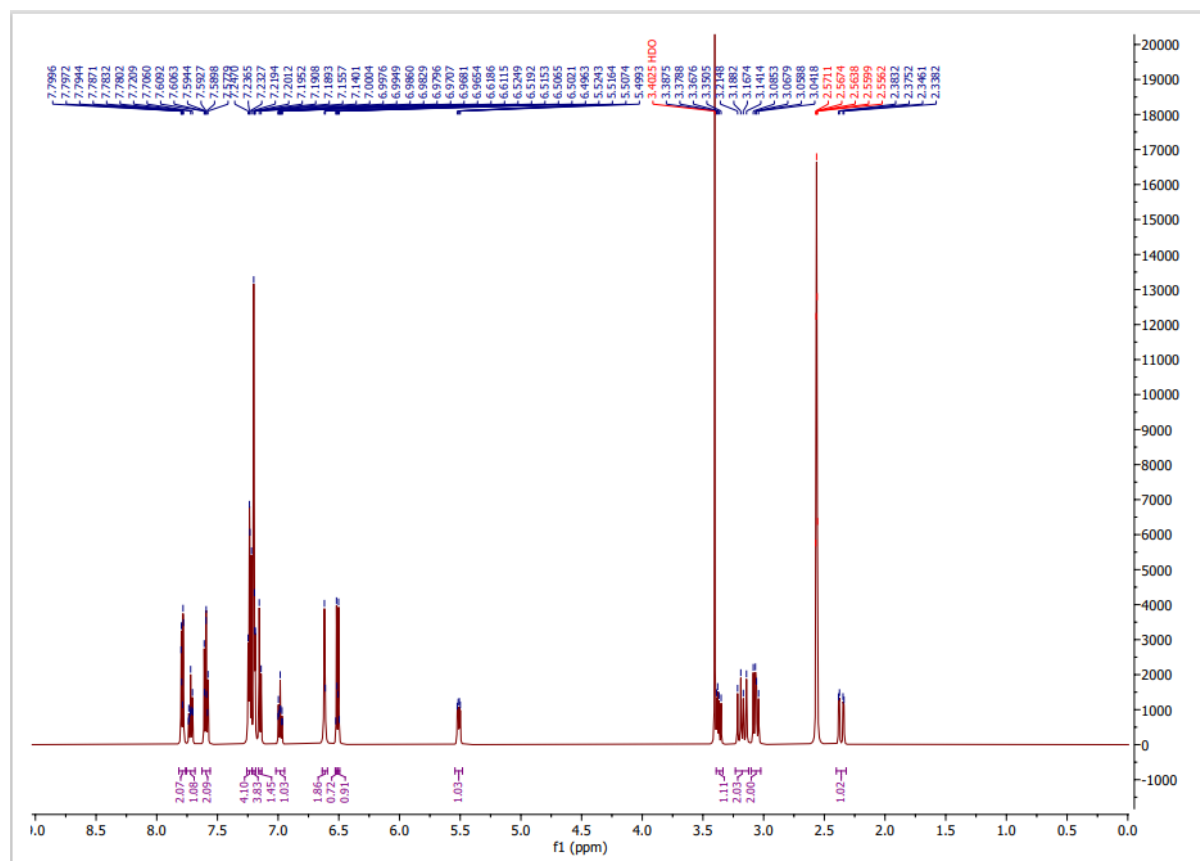


IR

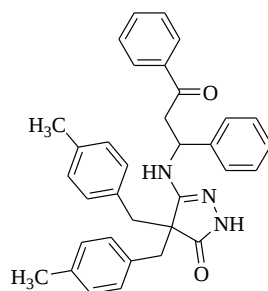


MASS

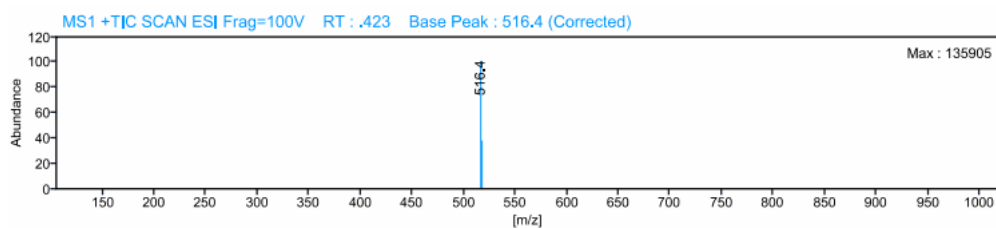


¹H-NMR

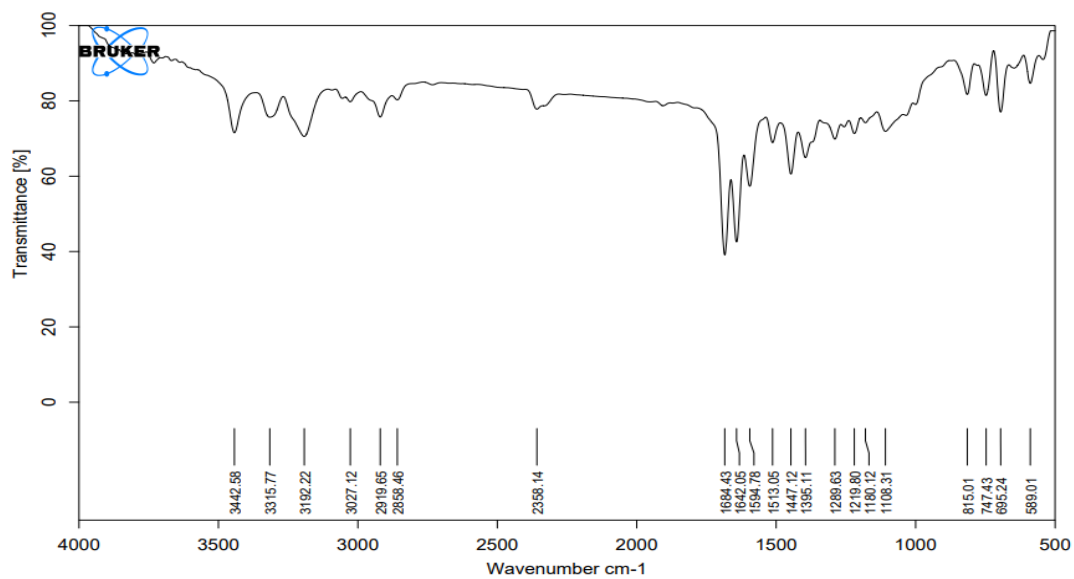
3-(1-Phenyl-3-oxo-3-phenylpropylamino)-4,4-bis(4-methylbenzyl)-1H-pyrazol-5(4H)-one (245)



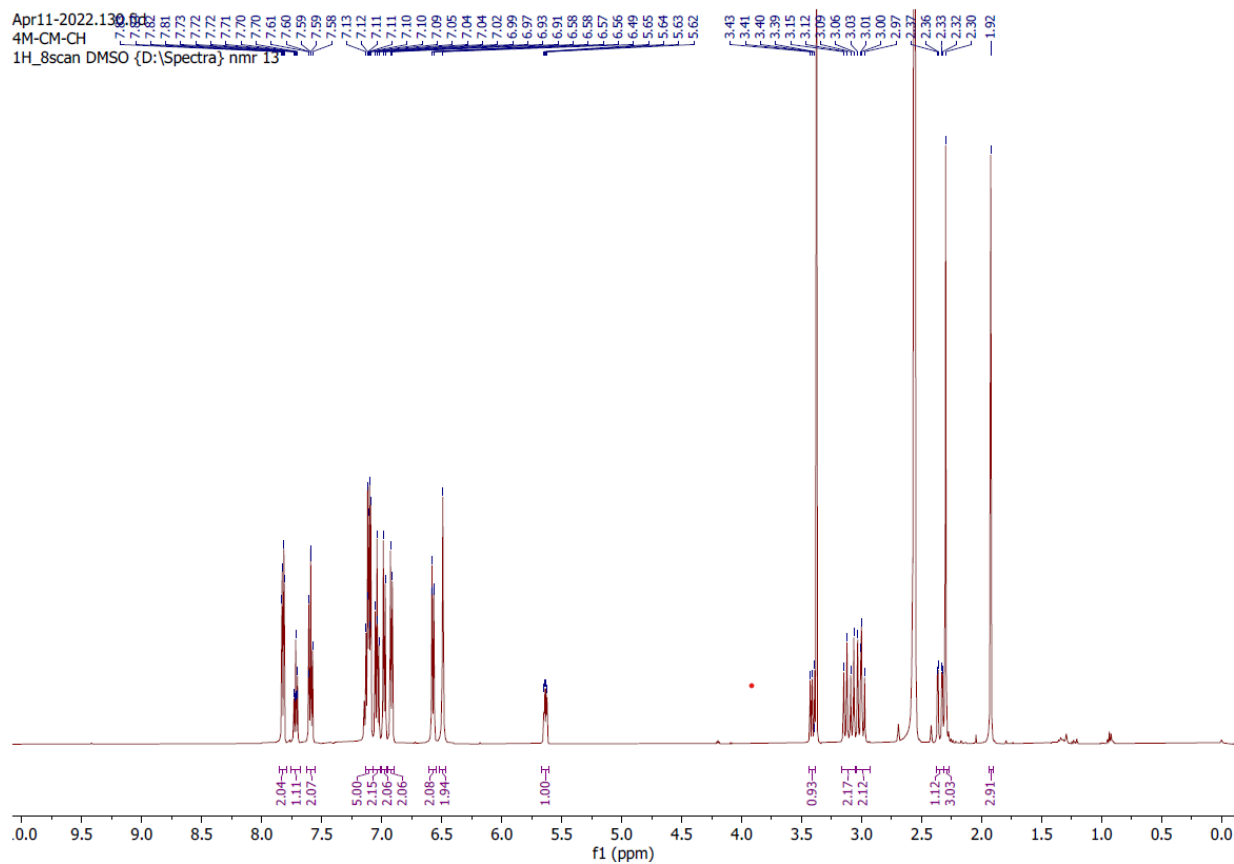
MASS



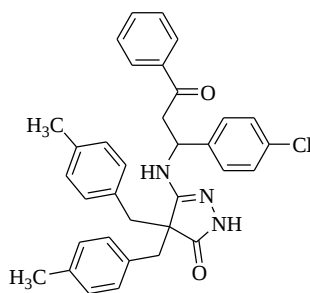
IR



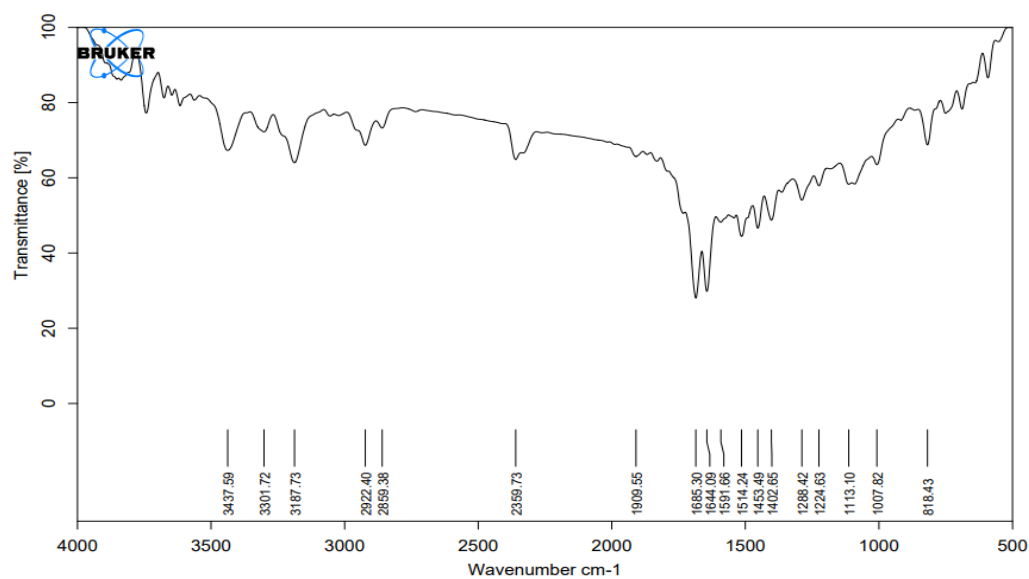
¹H-NMR



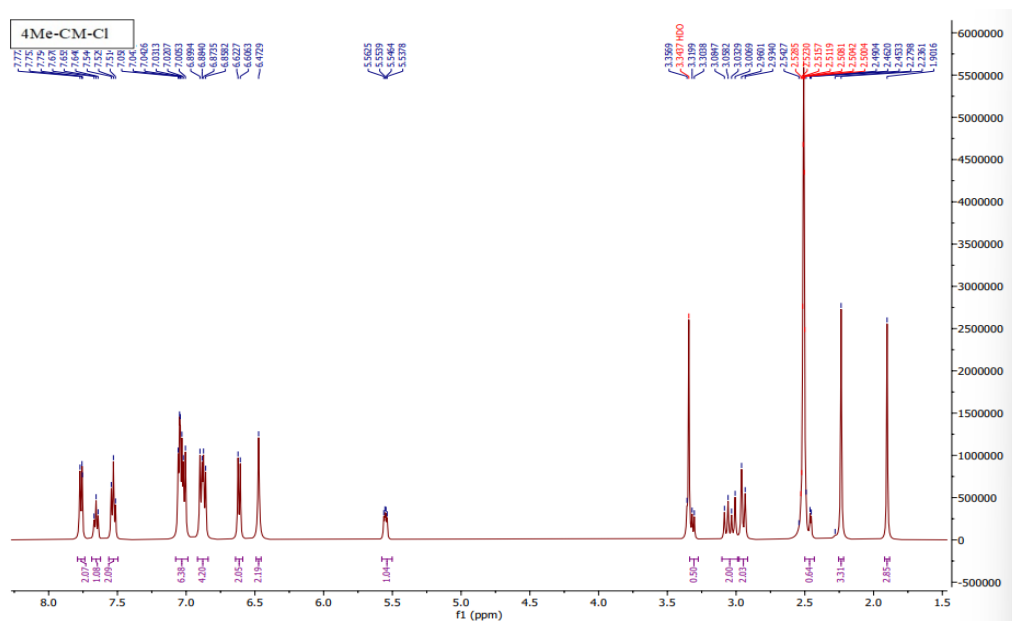
3-(1-(4-Chlorophenyl)-3-oxo-3-phenylpropylamino)-4,4-bis(4-methylbenzyl)-1H-pyrazol-5(4H)-one (246)

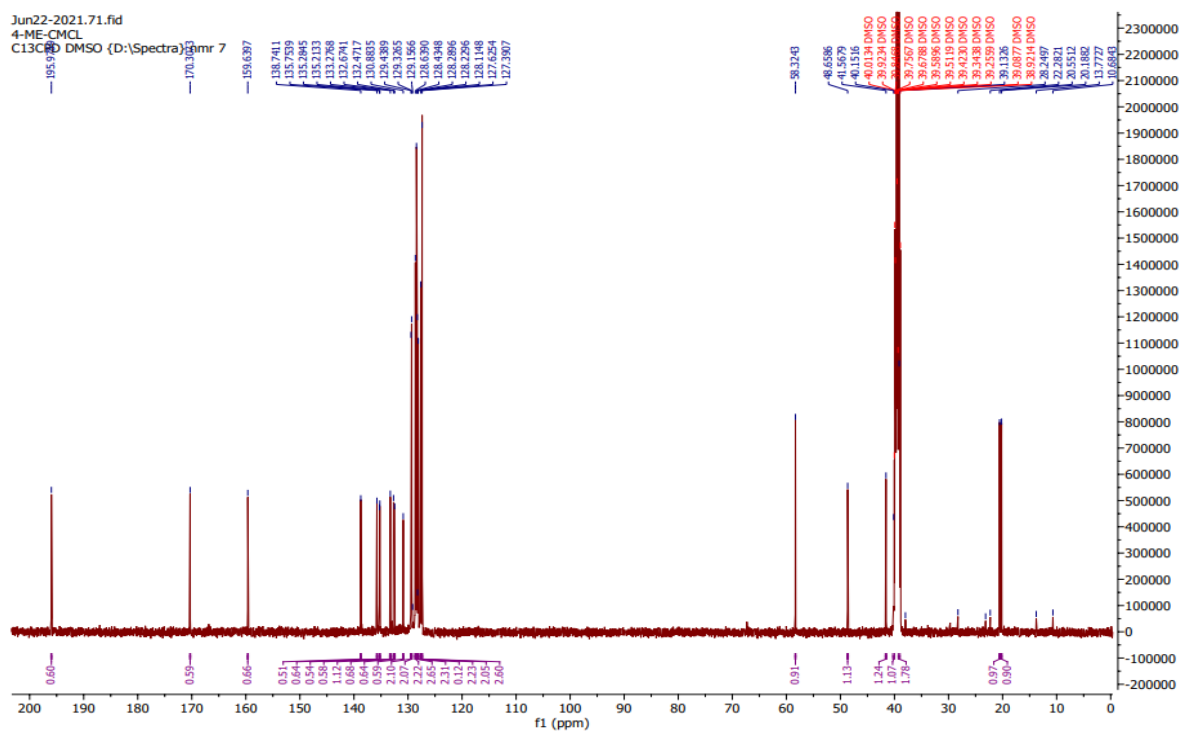


IR

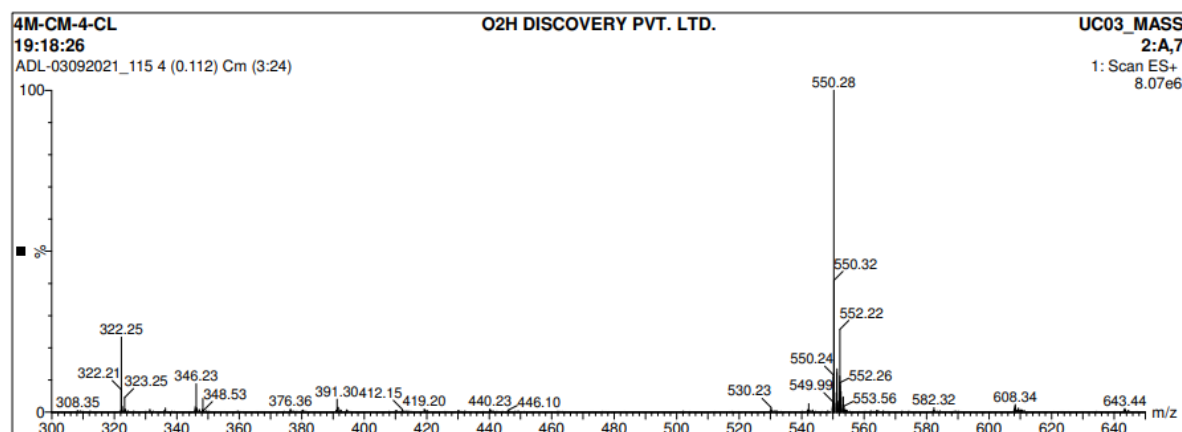


¹H-NMR

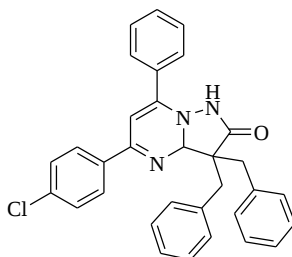


¹³C-NMR

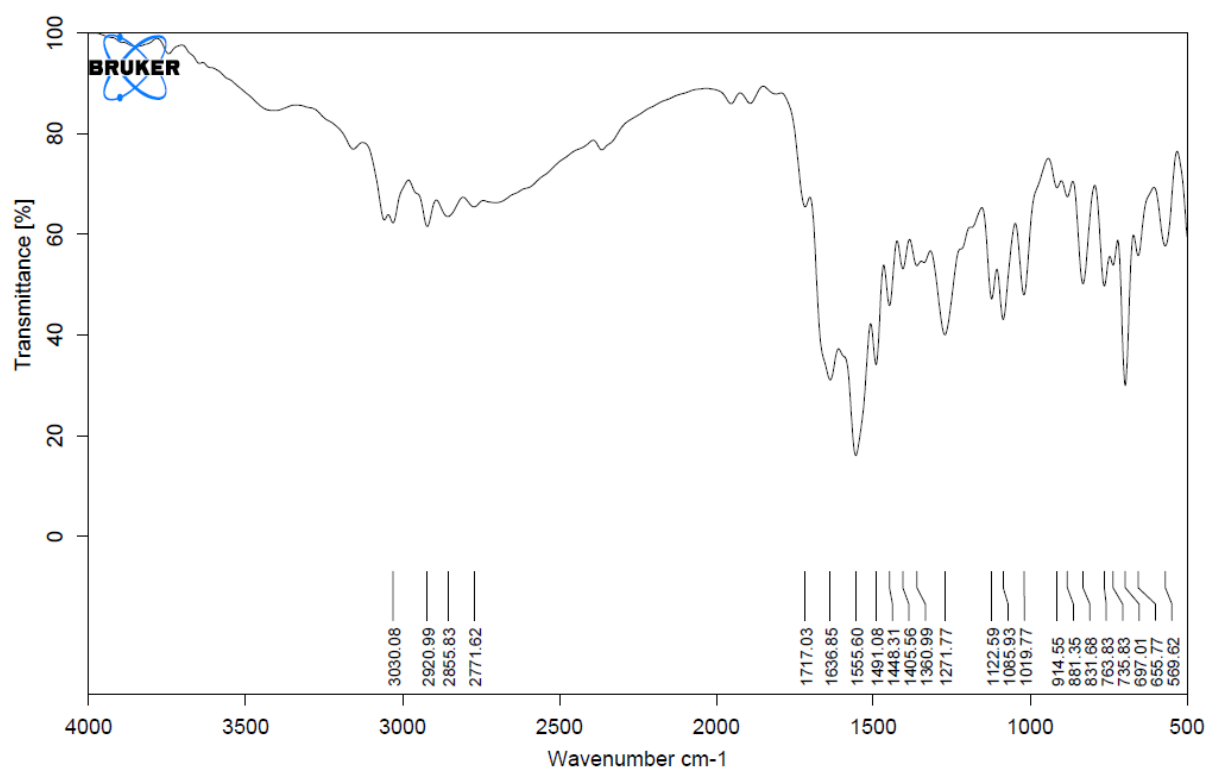
MASS



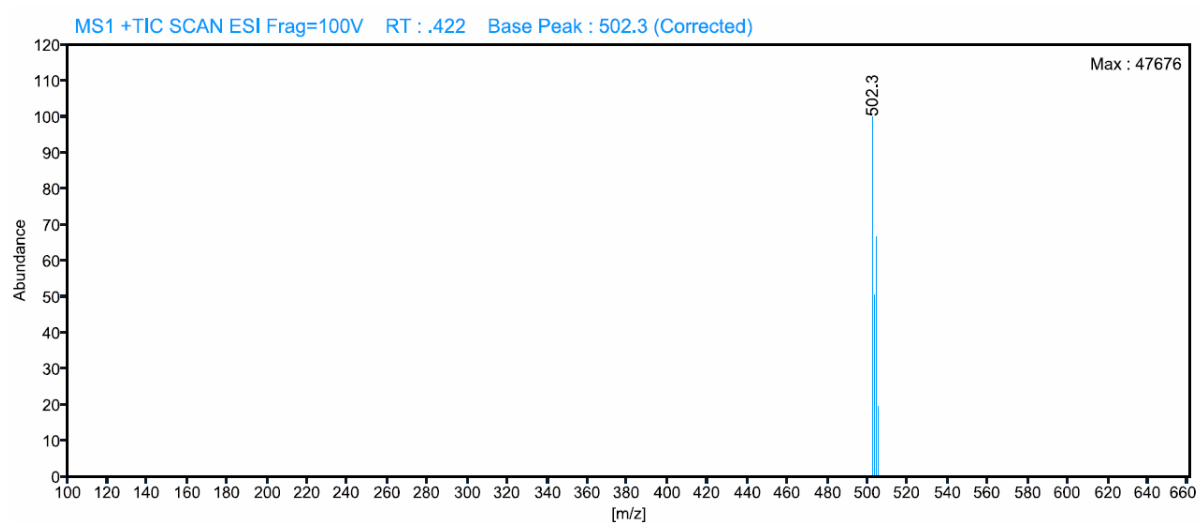
3,3-Dibenzyl-5-(4-chlorophenyl)-3,3a-dihydro-7-phenylpyrazolo[1,5-a]pyrimidin-2(1H)-one (251)

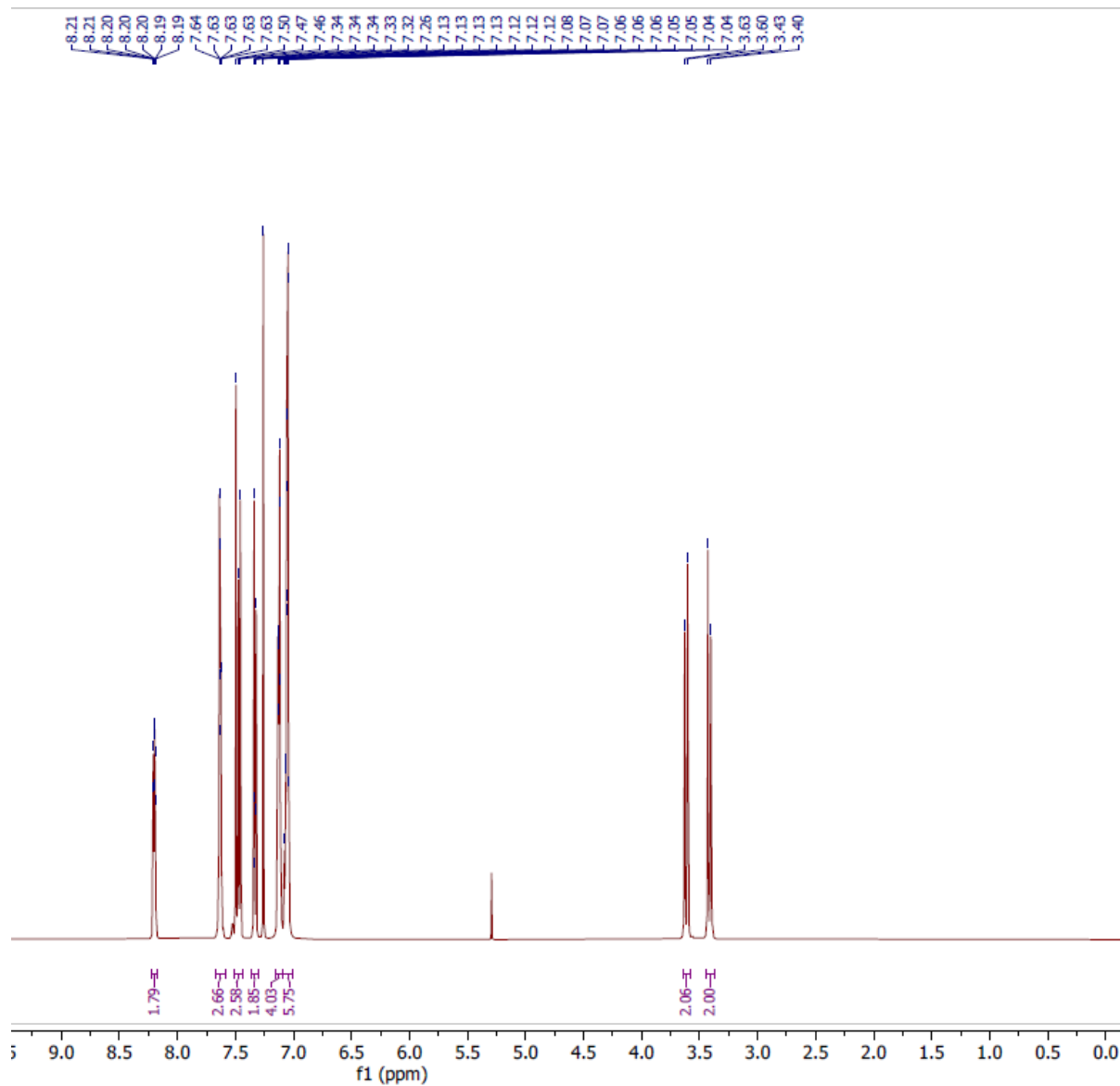


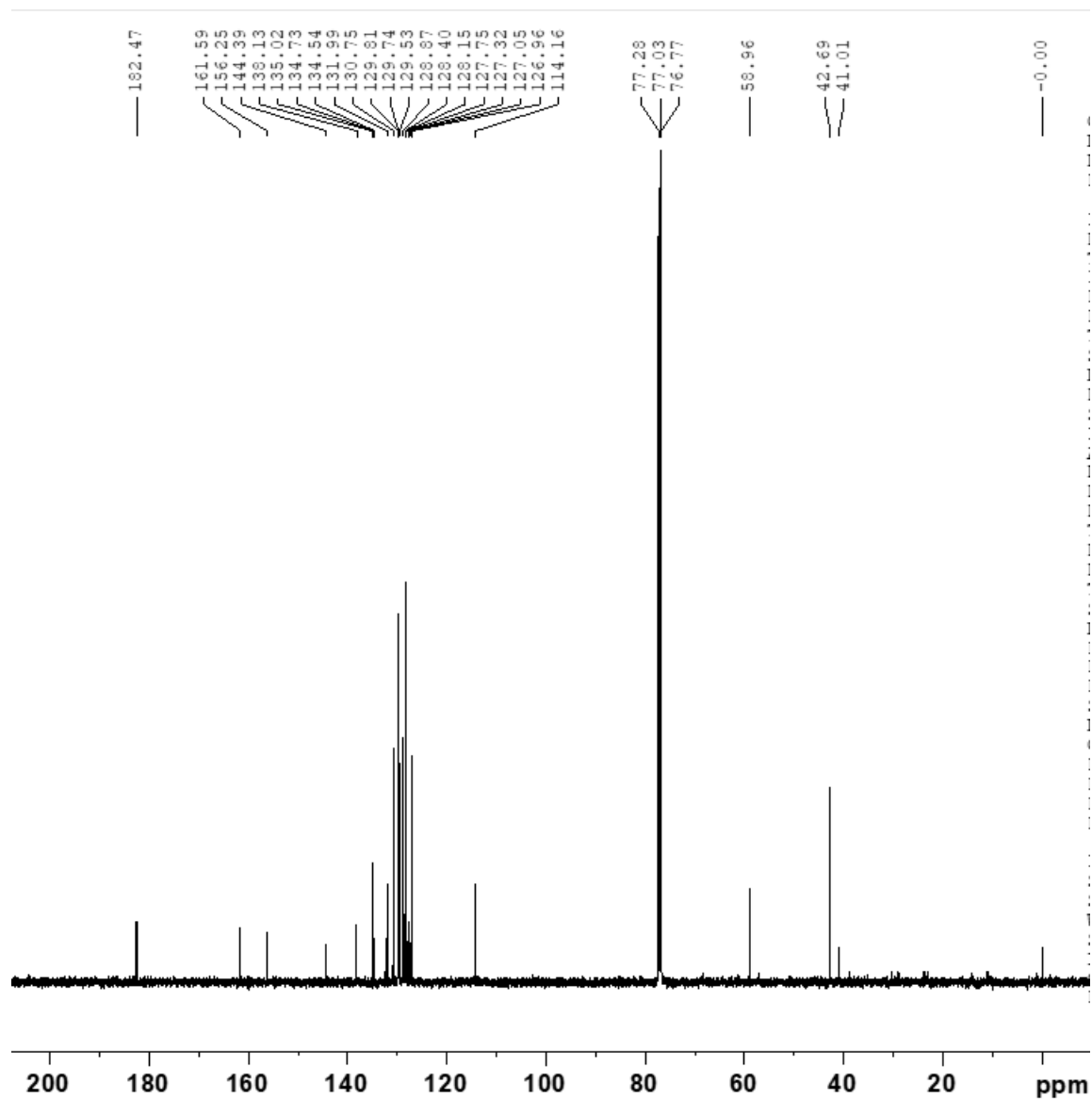
IR



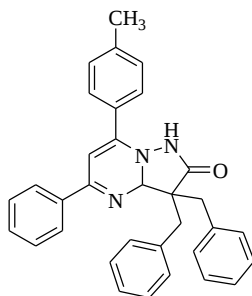
MASS



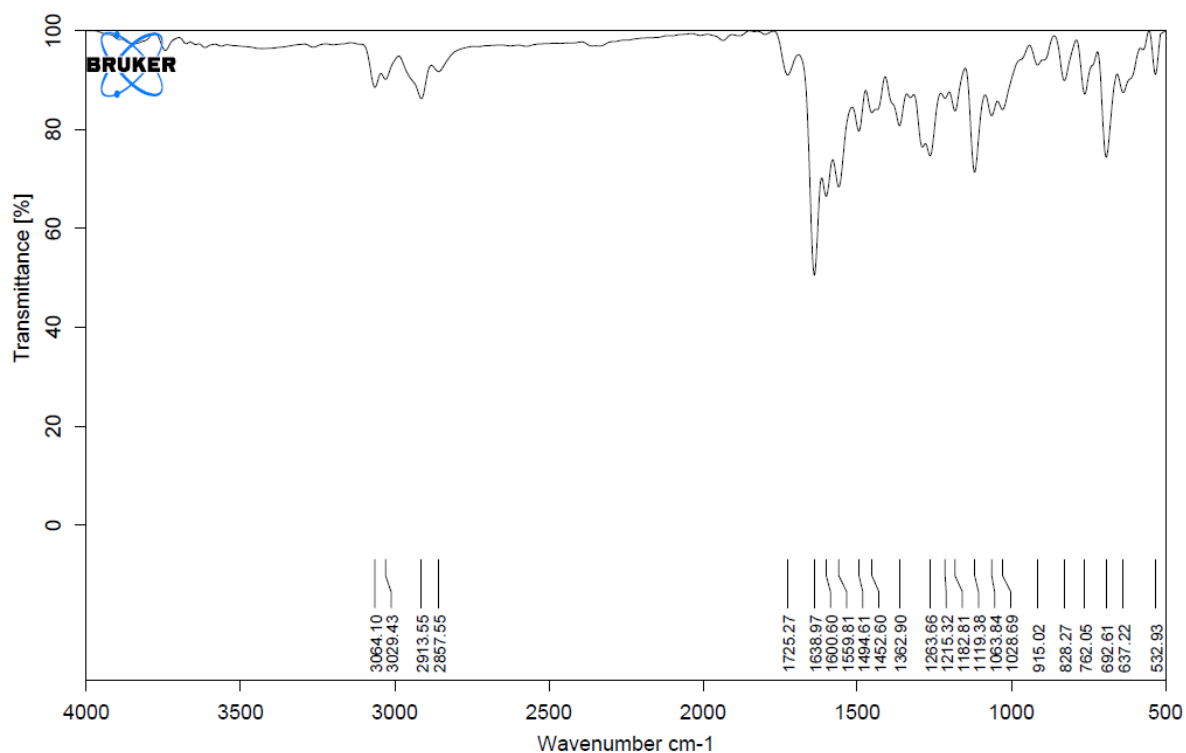
¹H-NMR

^{13}C -NMR

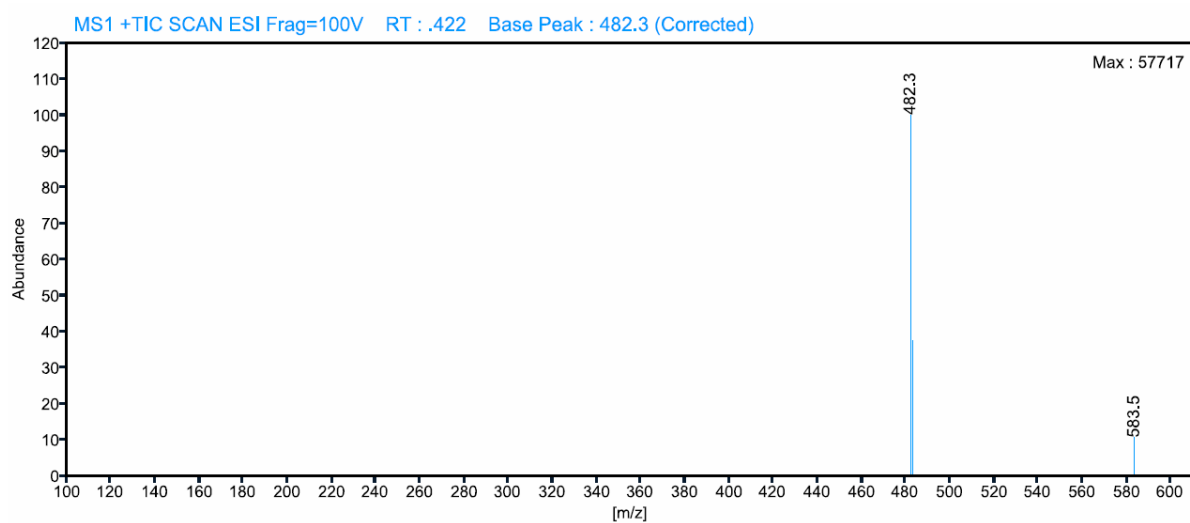
3,3-Dibenzyl-3,3a-dihydro-5-phenyl-7-*p*-tolylpyrazolo[1,5-*a*]pyrimidin-2(1*H*)-one (260)



IR

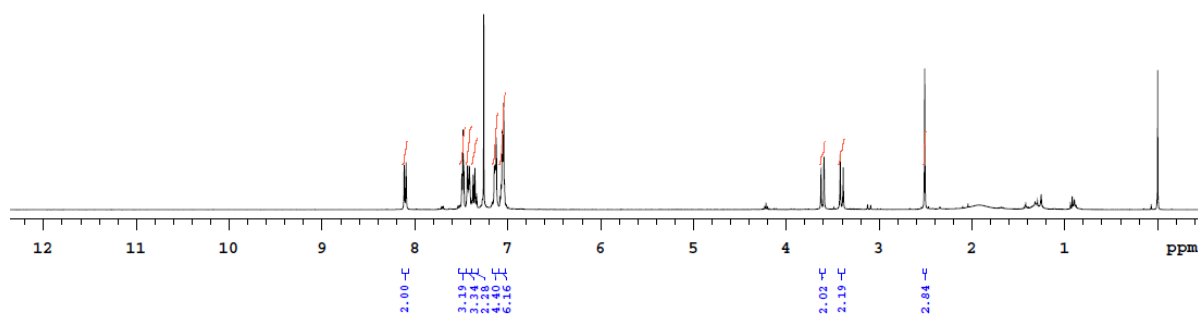


MASS

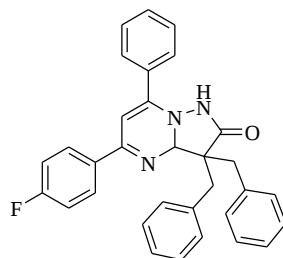
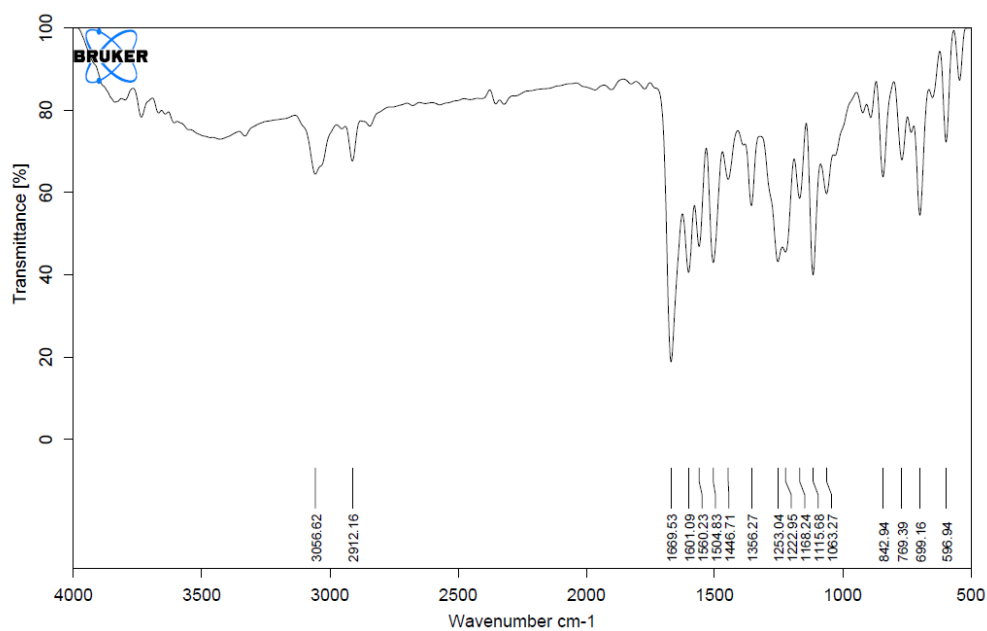


¹H-NMR

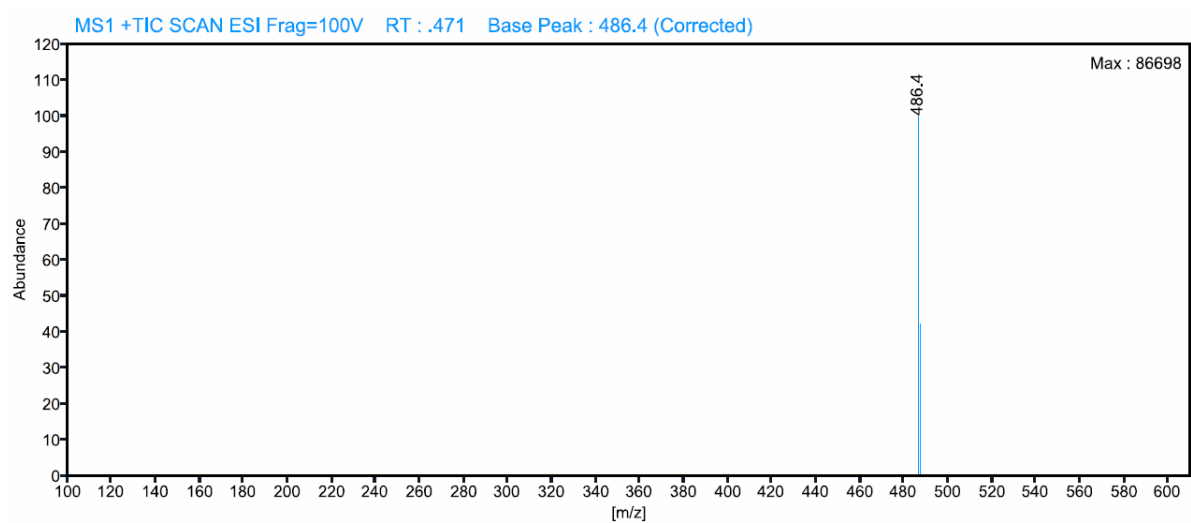
Solvent: cdcl3
SA-Varian 400MHz NMR
Date: Jul 2 2022



3,3-Dibenzyl-5-(4-fluorophenyl)-3,3a-dihydro-7-phenylpyrazolo[1,5-a]pyrimidin-2(1H)-one (254)

**IR**

MASS

 ^1H -NMR