# Cross-linked poly (dimethylaminoethyl acrylamide) coated magnetic nanoparticles: A high loaded, retrievable, and stable basic catalyst for the synthesis of benzopyranes in water

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## Calculations of CHN

## FT-IR and HNMR of selected compounds:

**1- Calculation of loading amount of MPS on the surface of MNP@MPS**

$$n = \frac{C\%}{100 \times 0.012 \times m}$$

m= The number of carbon atom in MPS

$$n = \frac{3.19}{100 \times 0.012 \times 7} = 0.38\ mmol/g$$

**2- Calculation of loading amount of cross-linker MBA in MNP@PMA**

Since the only source of N atom in MNP@PMA is MBA, it can be calculated by followed;

$$n = \frac{N\%}{100 \times 0.014 \times m}$$

m= The number of nitrogen atom in cross-linker MBA

Note: The nitrogen content in MNP@MPS should be considered in next calculations. However MPS has no N atom but 0.09% can be attributed to $NH_3$ molecule in MNP.

$$n = \frac{(0.87 - 0.09)}{100 \times 0.014 \times 2} = 0.28\ mmol/g$$ (Loading of cross-linker in MNP@PMA)

$$\%MBA\ in\ MNP@PMA = 0.28\left(\frac{mmol}{g}\right) \times 0.154\left(\frac{g}{mmol}\right) \times 100 = 4.3\%$$

**3- Calculation of loading amount of $CO_2Me$ in MNP@PMA**

Amount of methyl acrylate units in PMA and subsequently the loading amount of $CO_2Me$ in MNP@PMA can be calculated by followed:

After subtracting of C% of MPS (from CHN MNP@MPS) and %C of MBA (from calculated loading amount) carbon content of PMA can be concluded.

$$the\ loading\ amount\ for\ MBA = \frac{C\%}{100 \times 0.012 \times m}$$

m= The number of carbon atom in cross-linker MBA

Which;

$$0.28 = \frac{C\%}{100 \times 0.012 \times 7}$$ **and** **%C in MBA=2.35%**

then

13.27= total C% in MNP@PMA

3.19= C% in MNP@MPS

2.35= C% of MBA

Which

%C in poly(methylacrylate) or acrylate units= 13.27-3.19-2.35= 7.73%

$$n = \frac{C\%}{100 \times 0.012 \times m}$$

m= The number of carbon atom in methyl acrylate unite

$$n = \frac{7.73\%}{100 \times 0.012 \times 4}$$ and n=1.61 mmol/g (the loading amount of methyl acrylate acrylate unites or loading amount of $CO_2Me$ unites on the surface of MNP@PMA)

**4- Calculation of loading amount of -$NMe_2$ in MNP@PDMA**

Since the cross-linker amount in MNP@PMA and MNP@PDMA is same, by subtracting N% of MNP@PMA (which is corresponded to MBA) from %N of MNP@PDMA we can calculate the loading amount of dimethylamino ethyl acrylamide and subsequently the loading amount of –$NMe_2$.

5.05= total N% in MNP@PDMA

0.87= total N% in MNP@PMA

Which ;

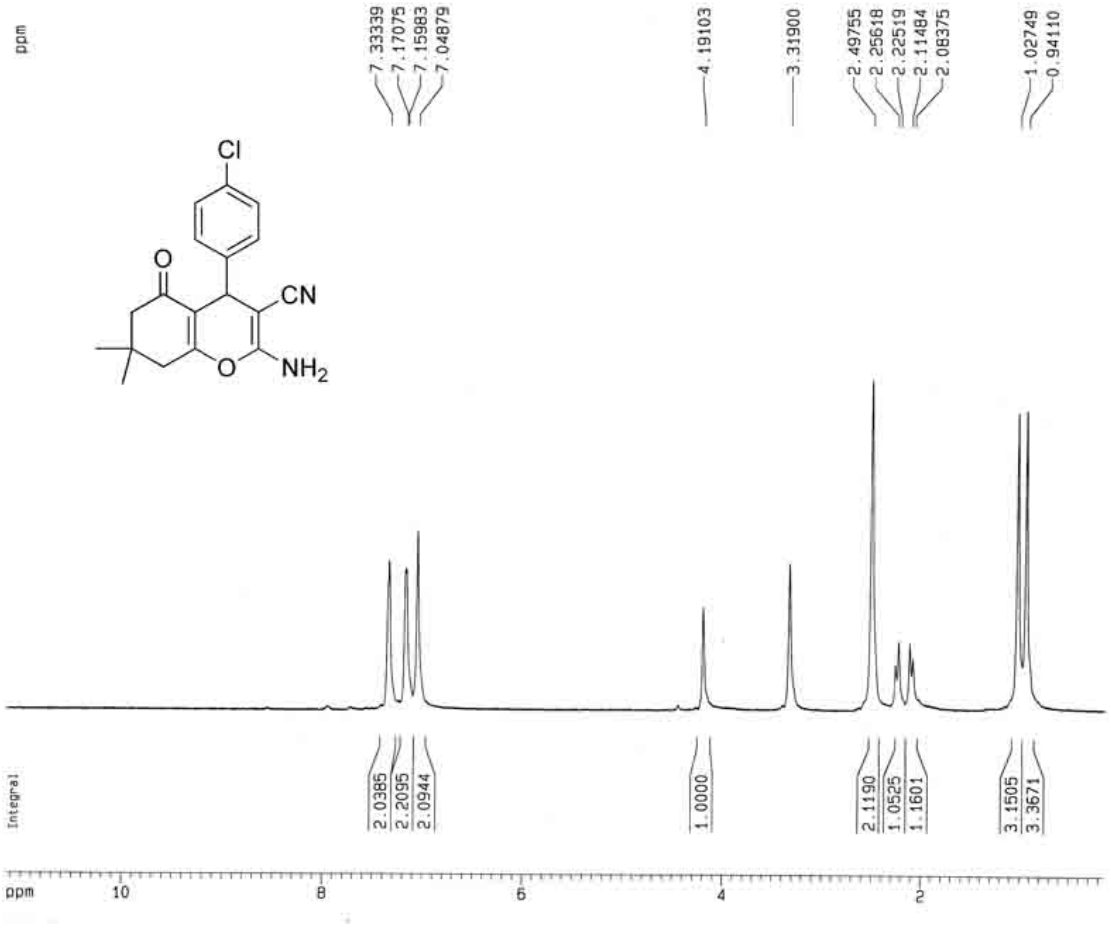
N%= 5.05-0.87=4.18% (N content of dimethylaminoethyl acrylamide units)

$$n = \frac{N\%}{100 \times 0.014 \times m}$$

m= The number of nitrogen atom in dimethylaminoethyl acrylamide unit

$$n = \frac{4.18\%}{100 \times 0.014 \times 2} = 1.49 \left(\frac{mmol}{g}\right)$$

( $Loading\ of dimethylaminoethyl\ acrylamide\ unit\ or - NMe2\ unit$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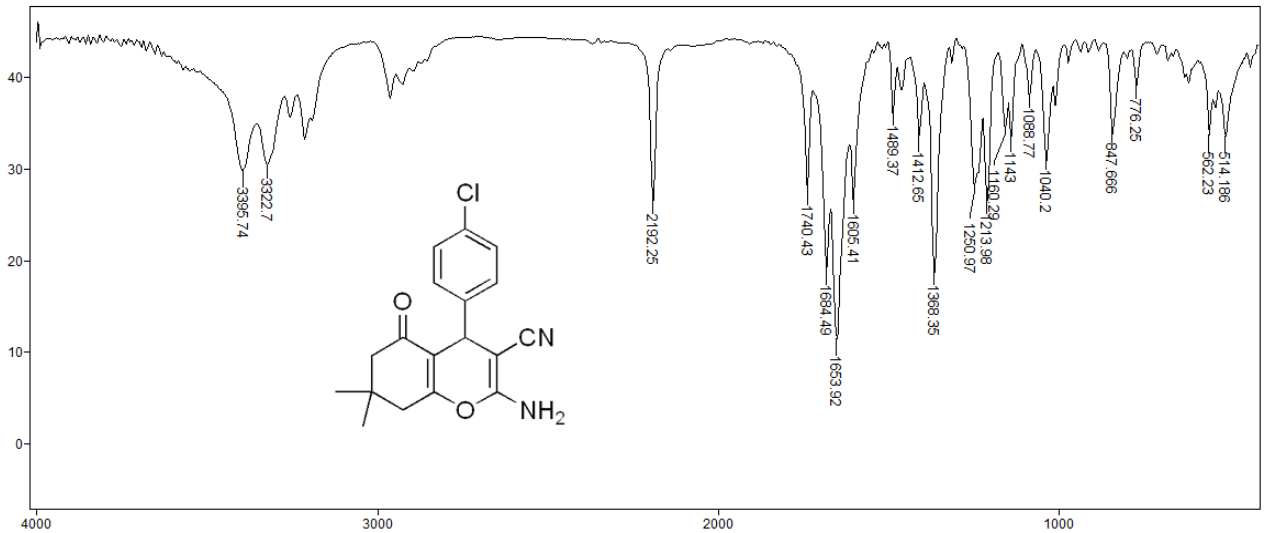
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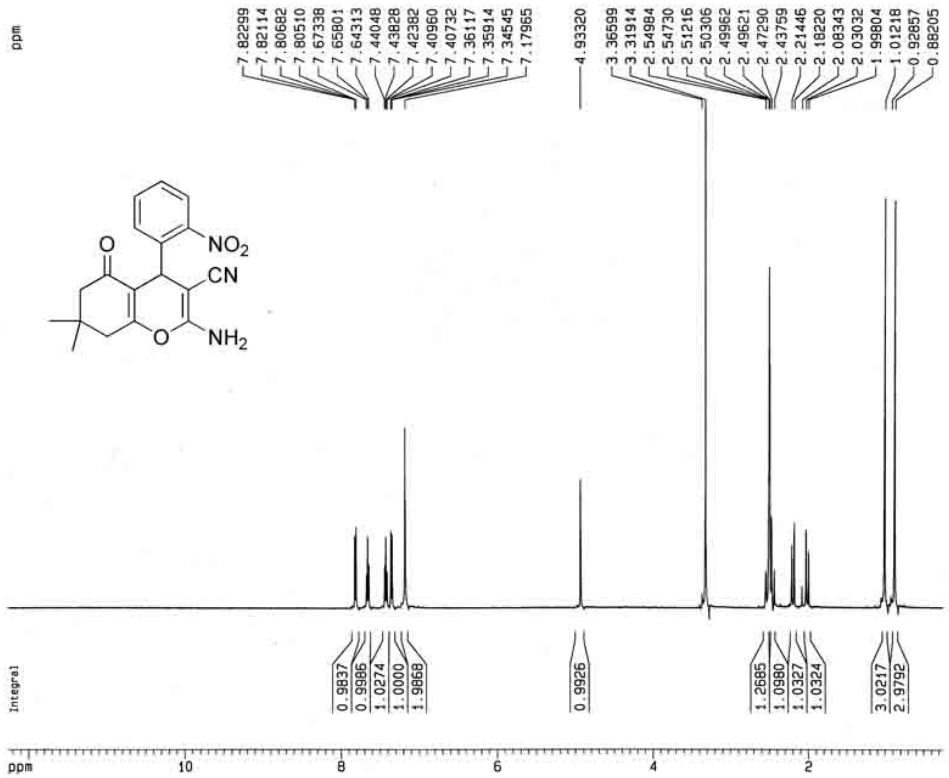
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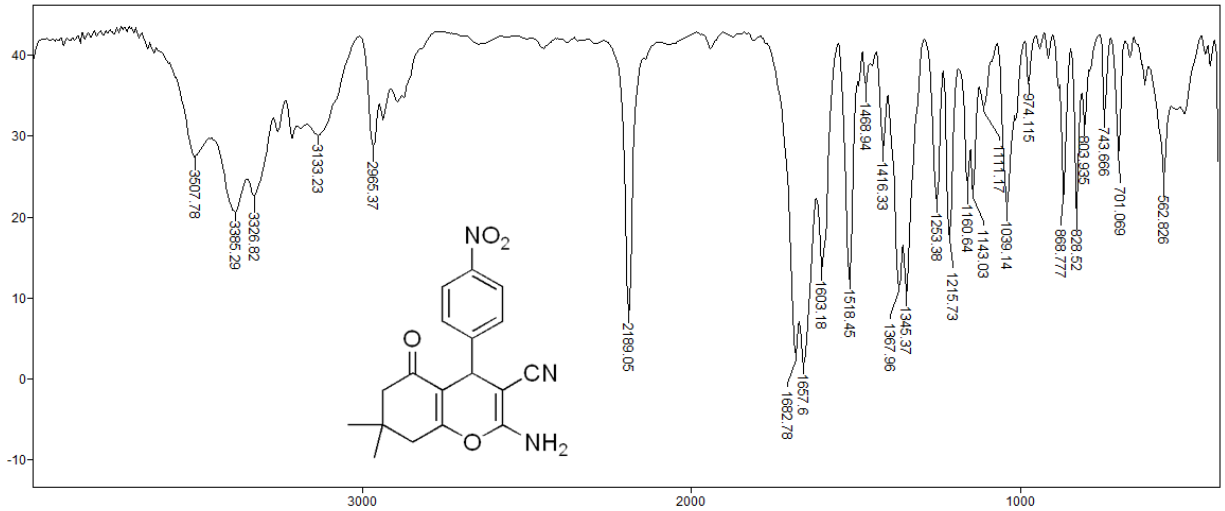
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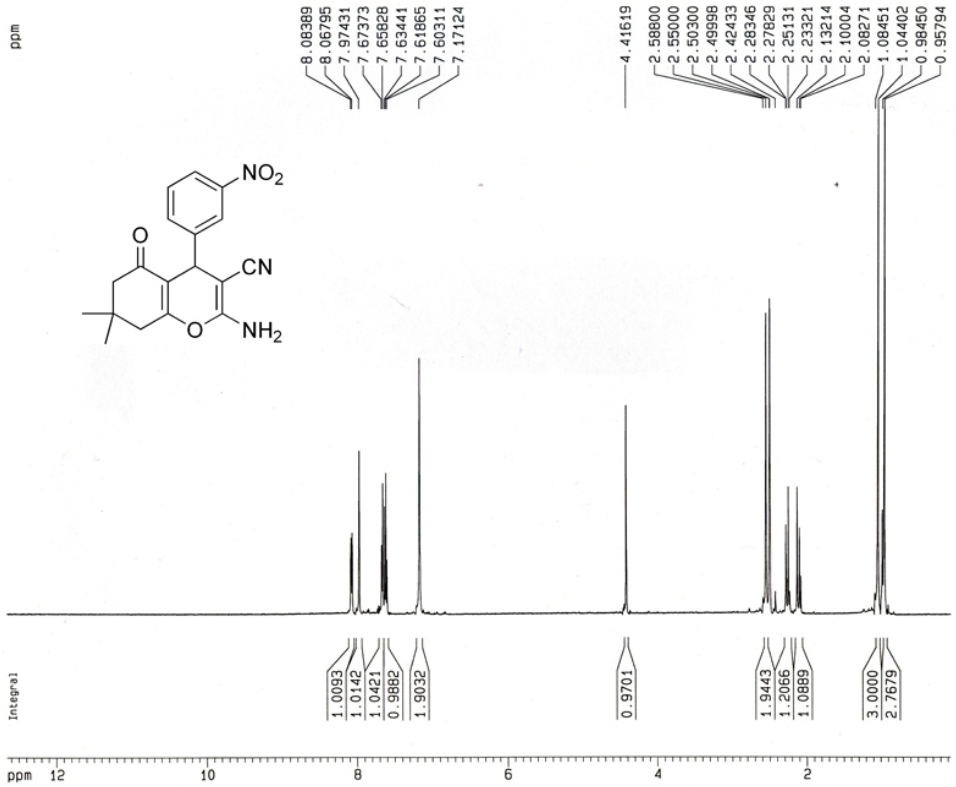
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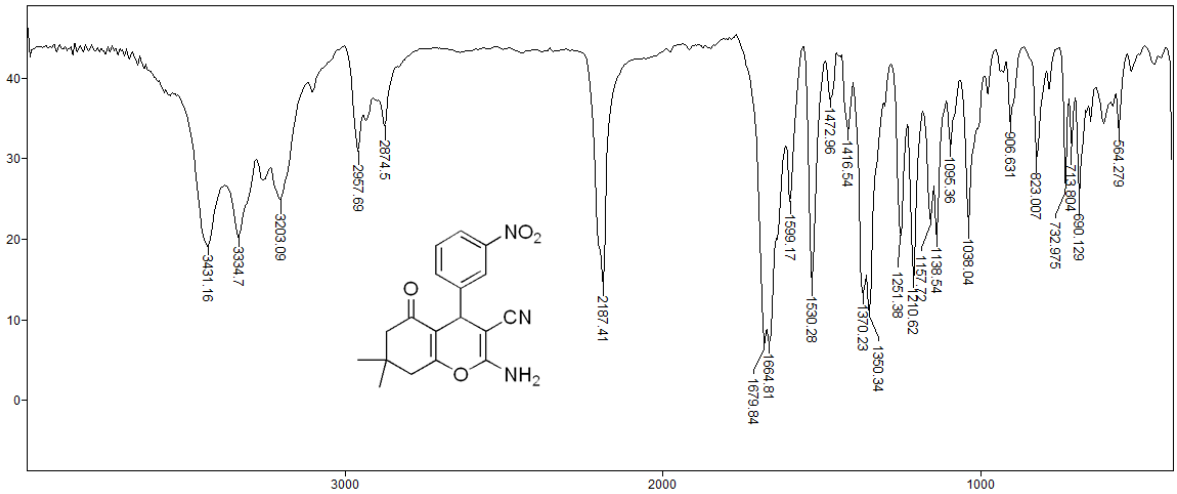
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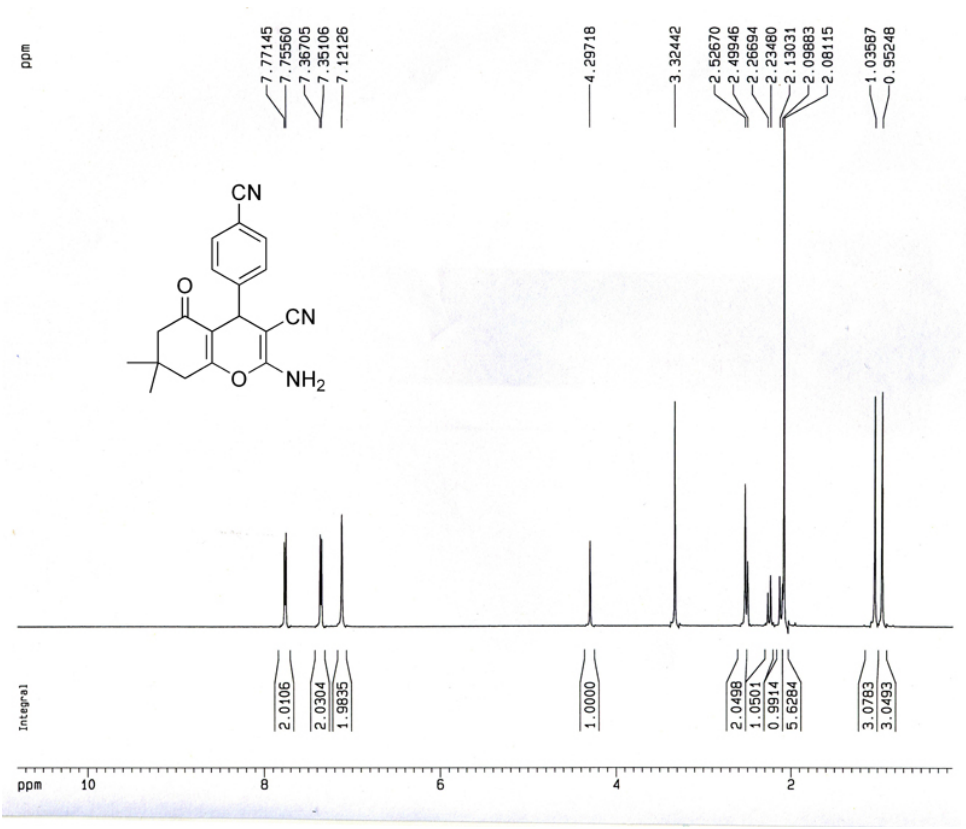
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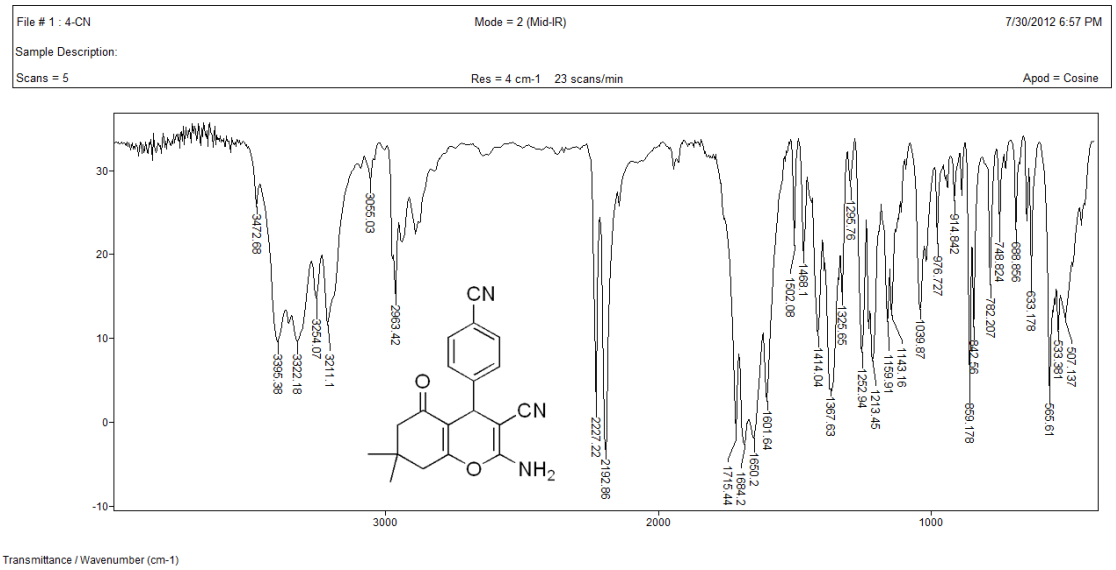
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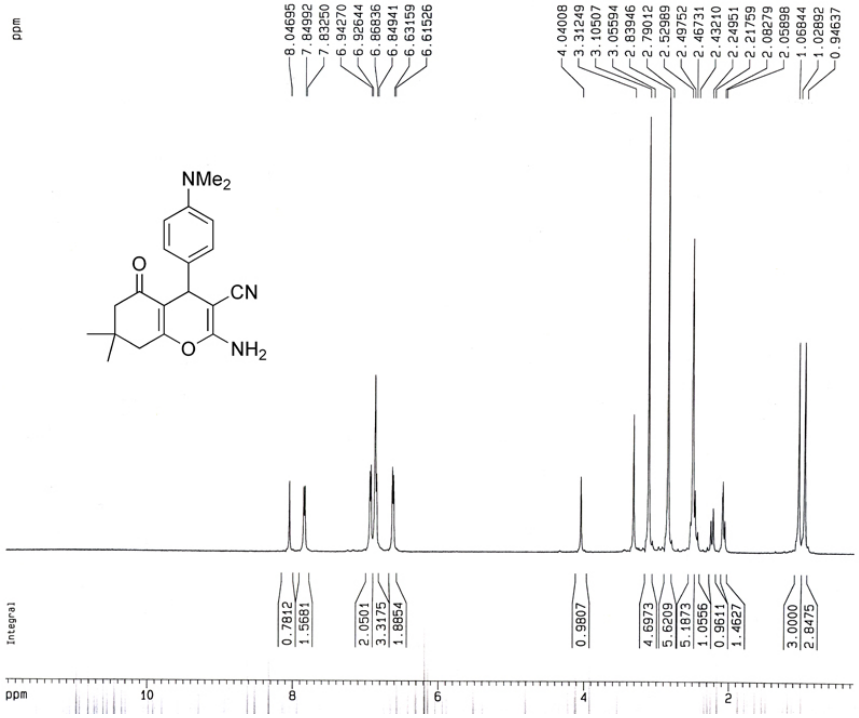
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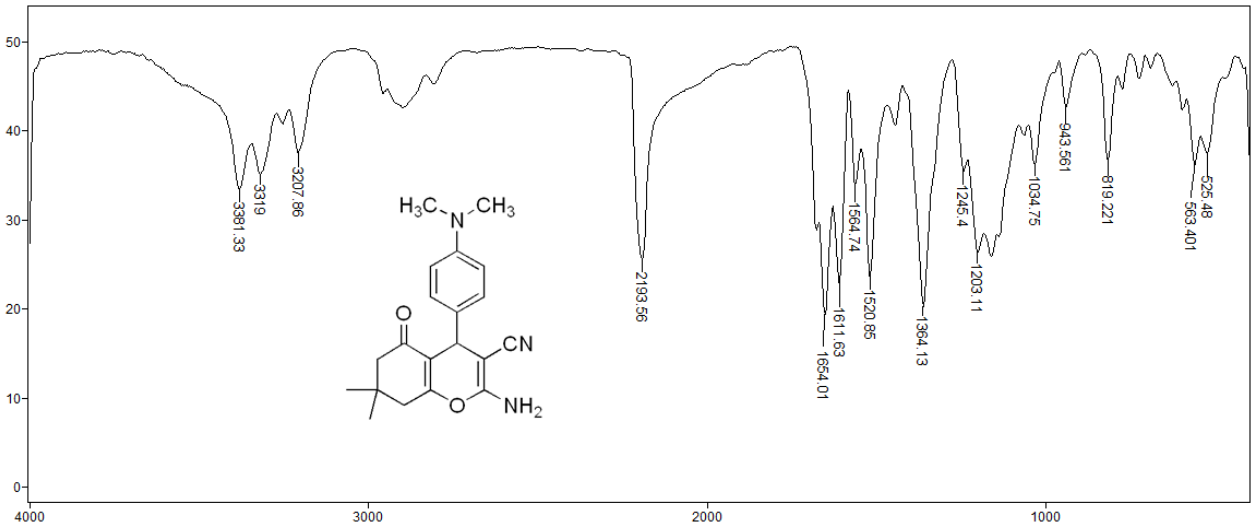
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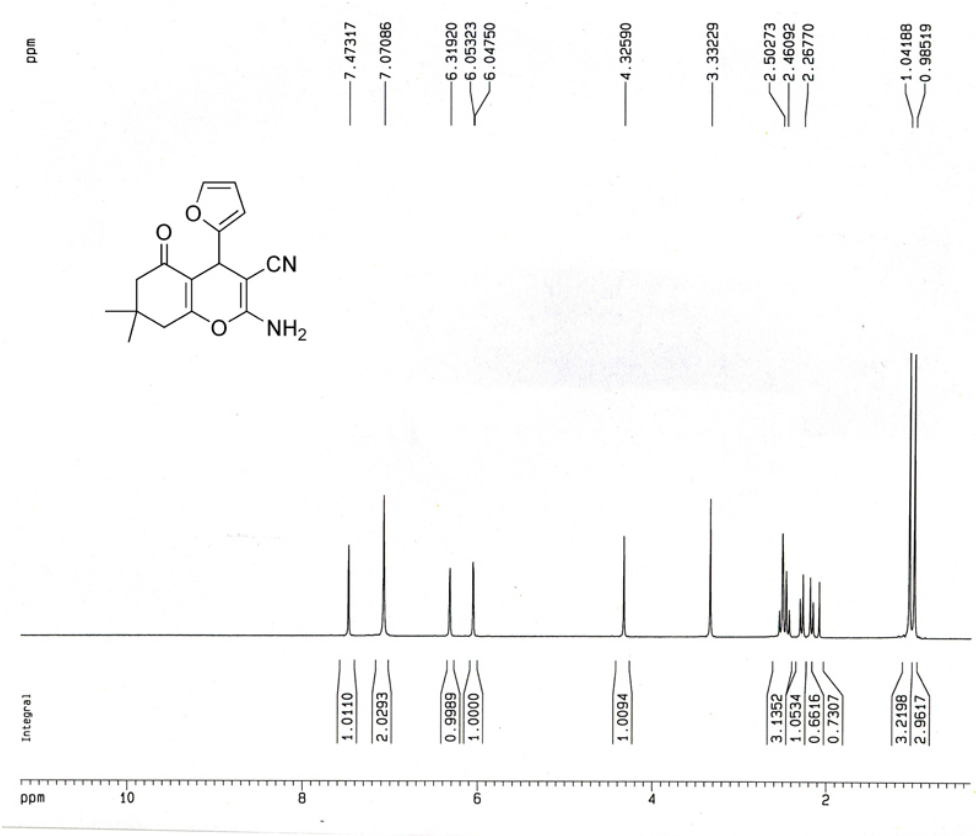
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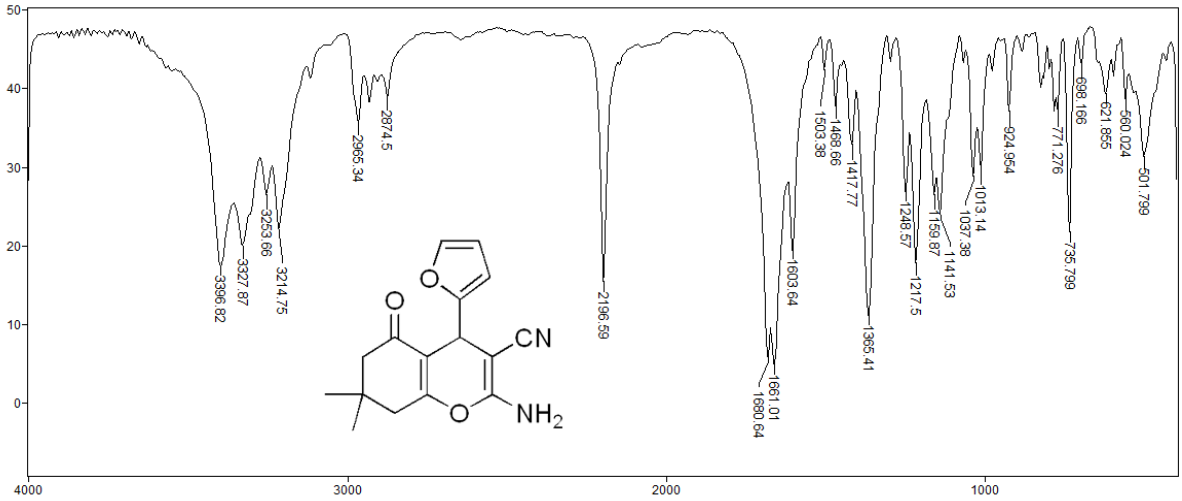
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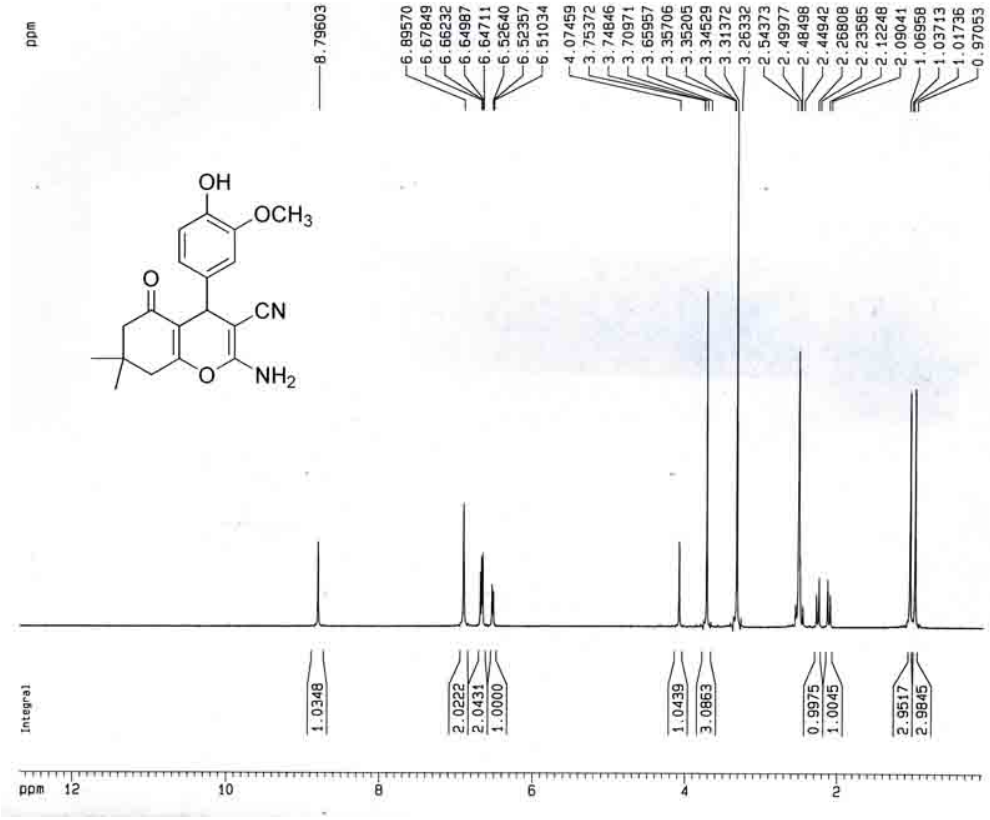
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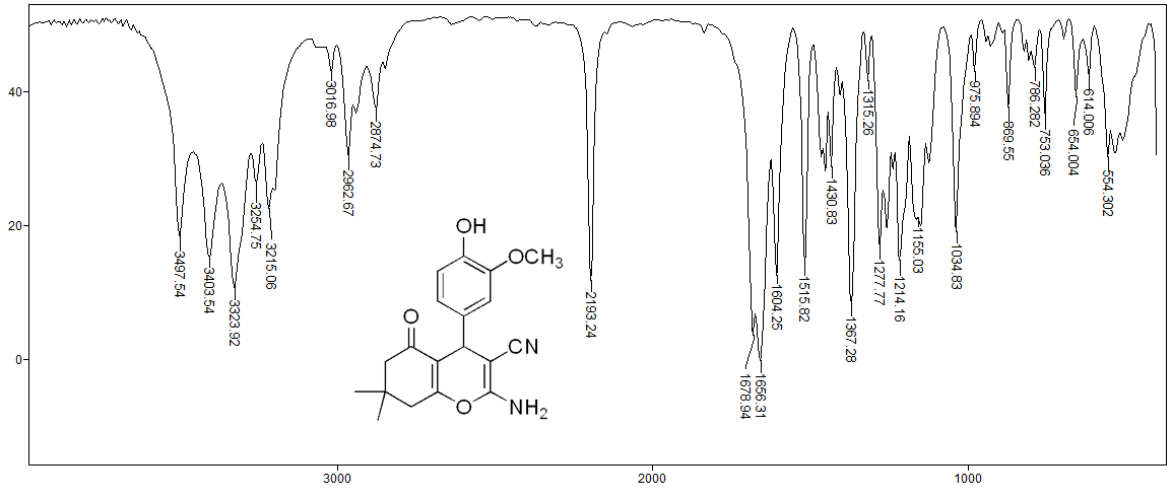
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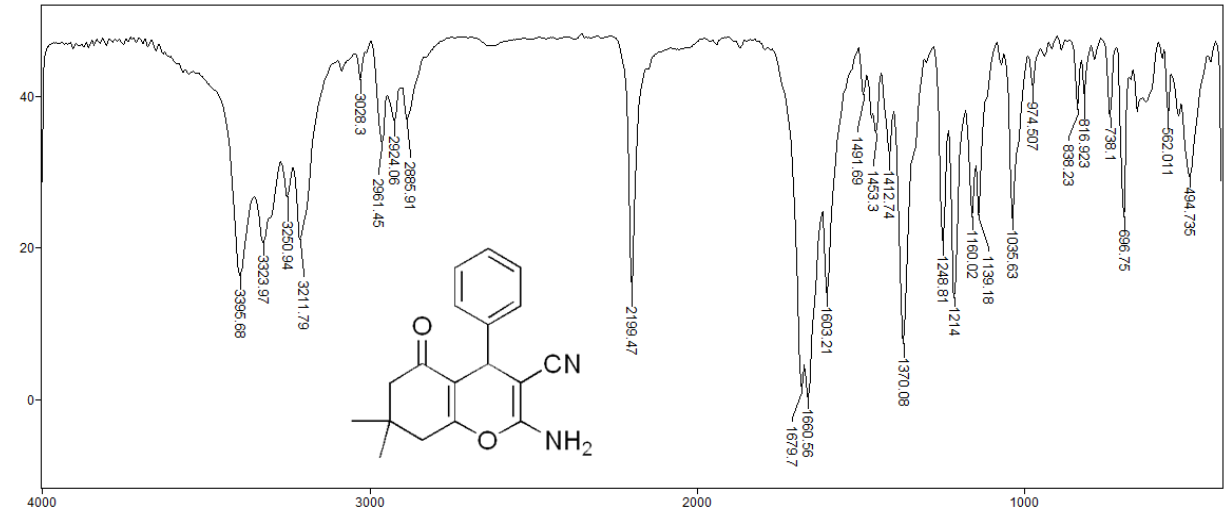
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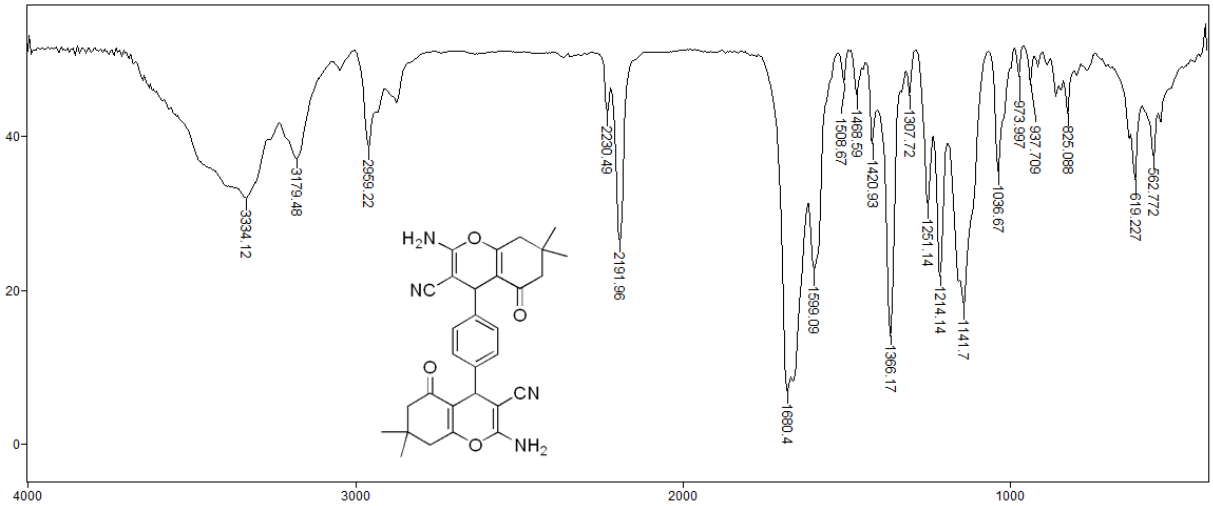
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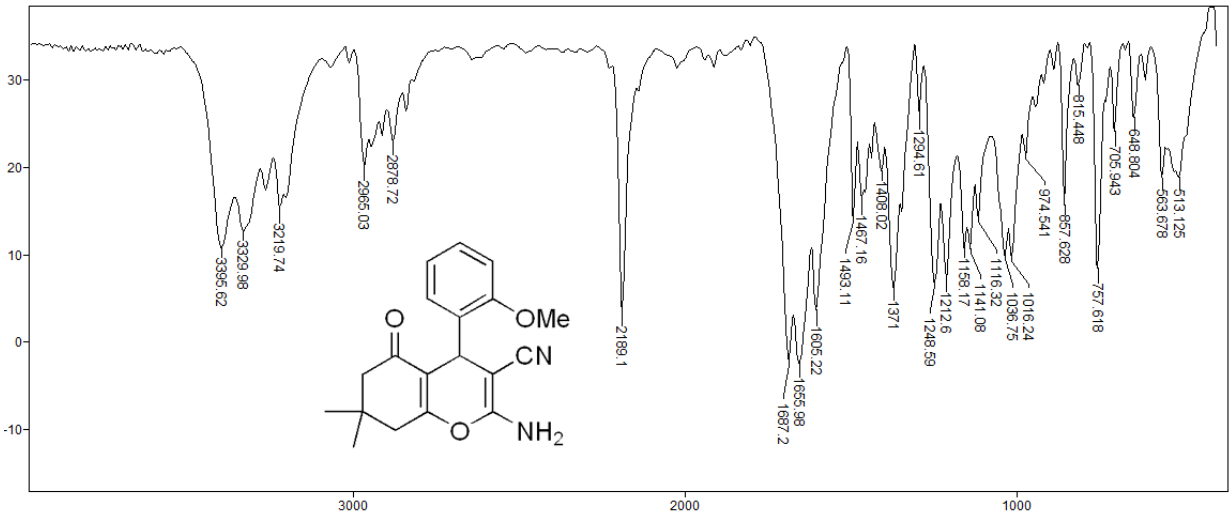
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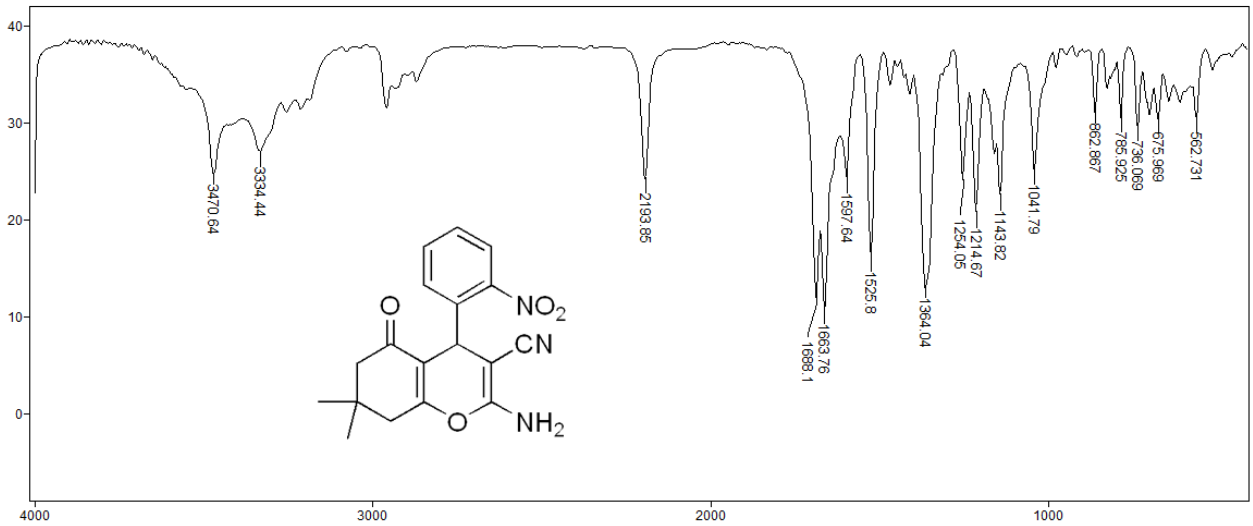
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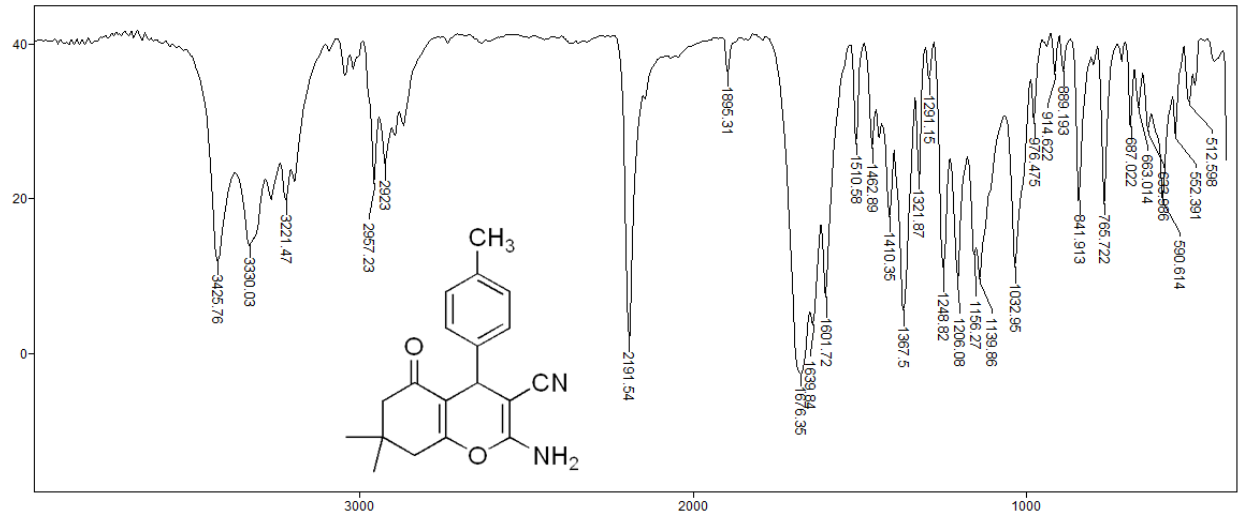
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