Supplementary file

1.1. Global chemical reactivity descriptor

In order to understand chemical reactivity of the molecule, global chemical reactivity descriptor is estimated using theoretical estimated HOMO-LUMO, listed below:

Chemical hardness $(\eta = (IP - EA)/2)$ (1)

Electronegativity $(\chi = (IP + EA)/2)$ (2)

Chemical potential $(\mu = -\chi)$ (3)

Chemical softness $(S = 1/2\eta)$ (4)

Electrophilicity index $(\omega = \mu^2/2\eta)$ (5)

Ionization potential, $IP = -E_{HOMO}$ (6)

Electron affinity, $EA = -E_{LUMO}$ (7)

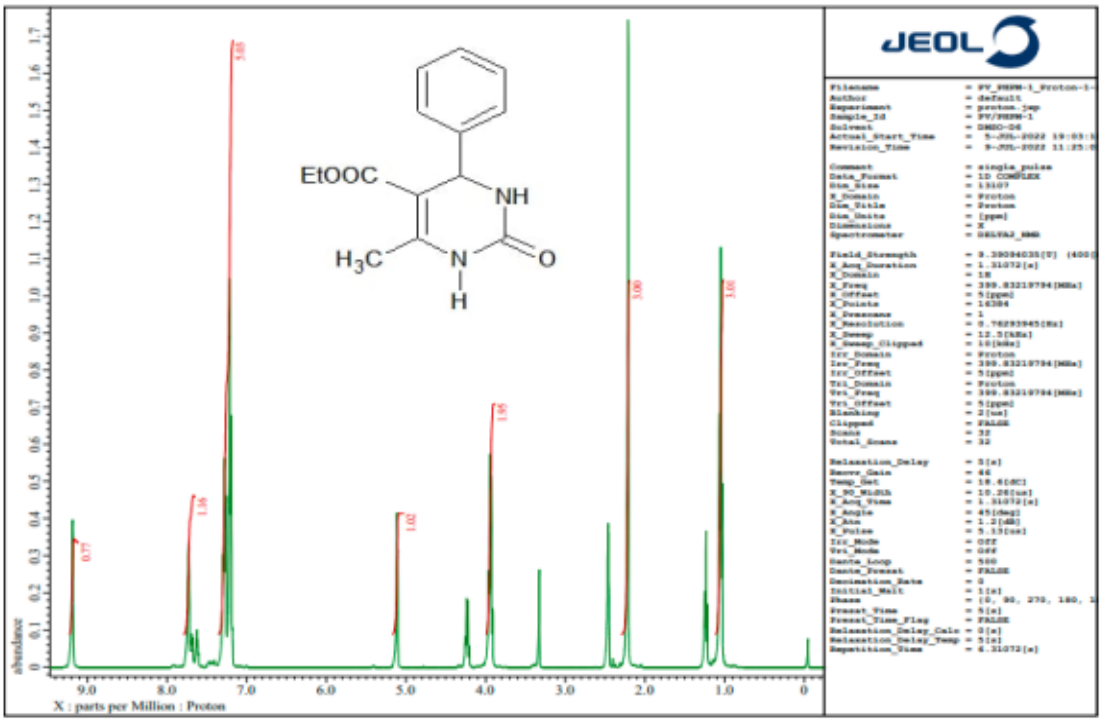


Fig. S1 ^{1}H-NMR spectra of the P1.

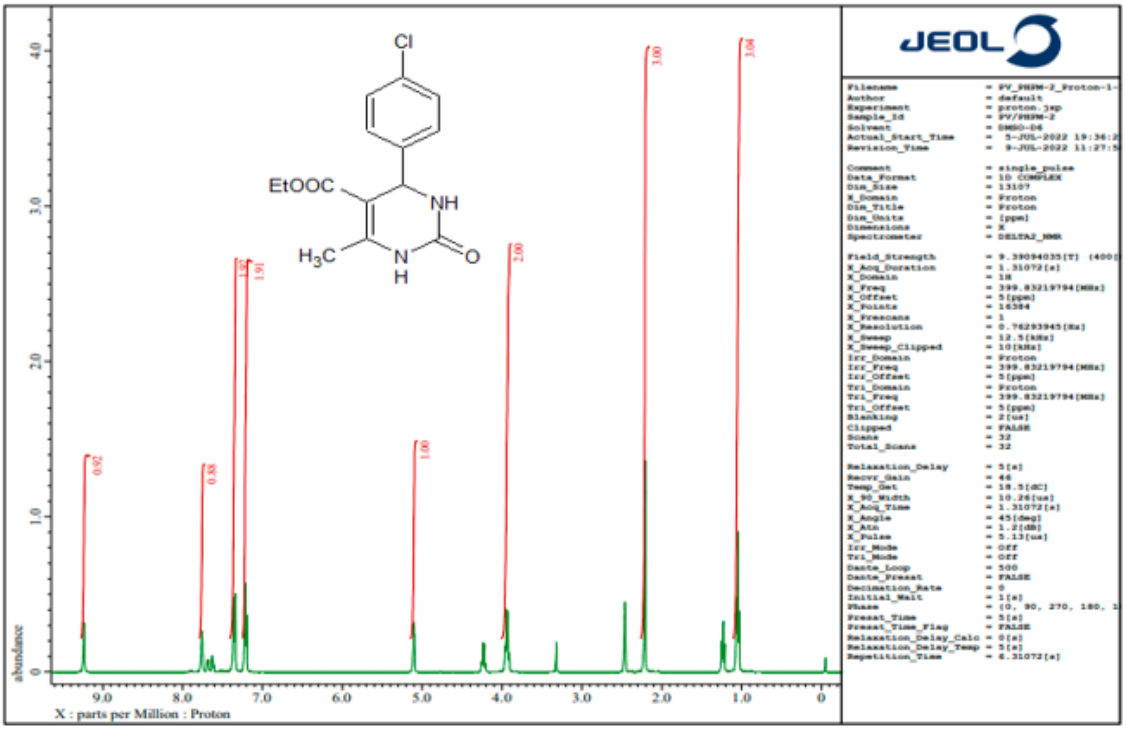


Fig. S2 ^{1}H-NMR spectra of the P2.

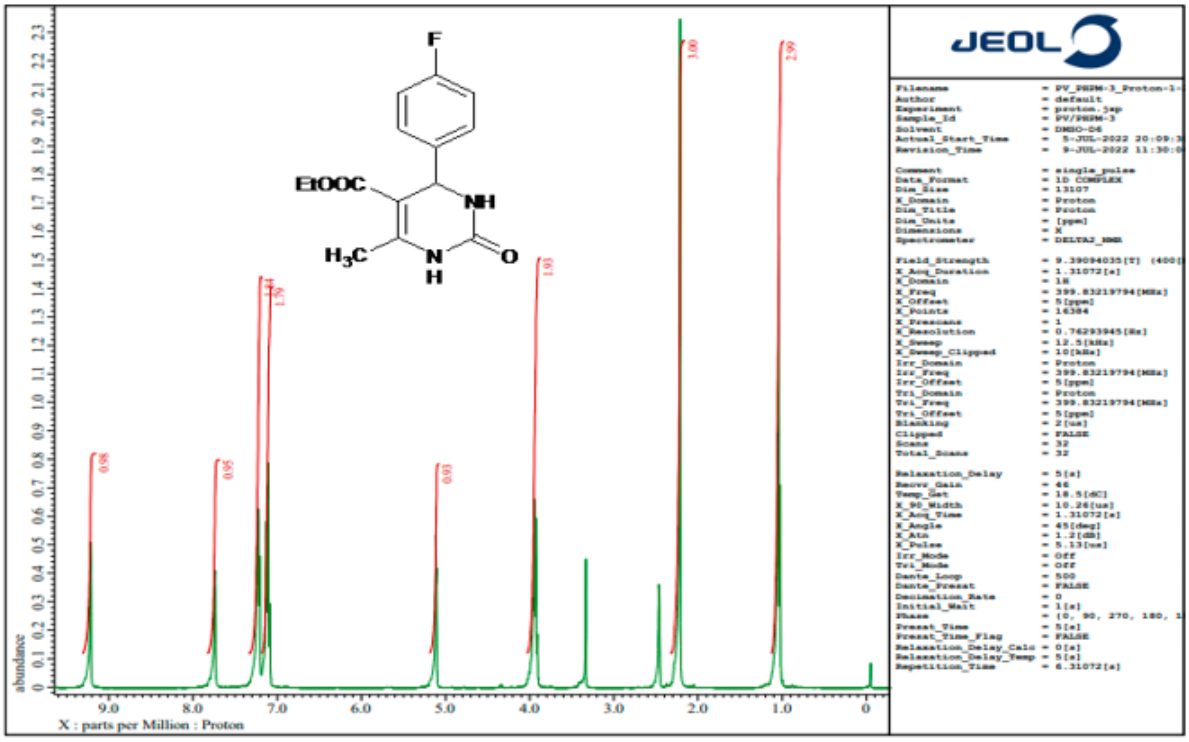


Fig. S3 ^{1}H-NMR spectra of the P3.

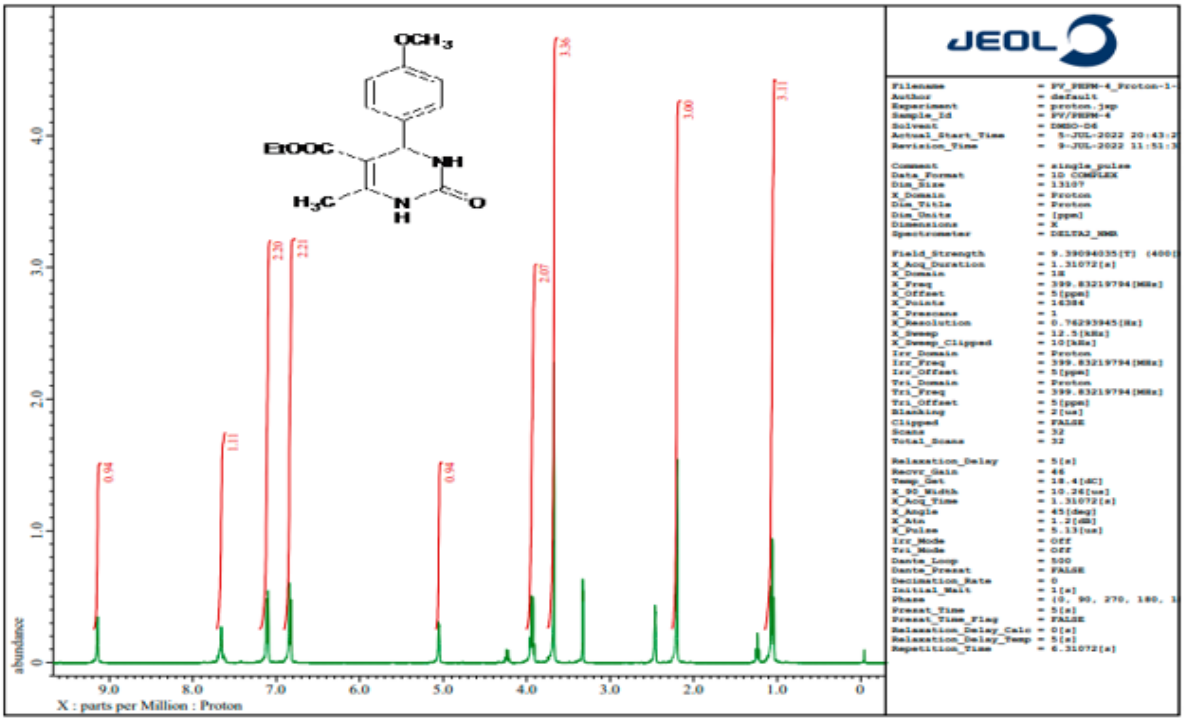


Fig. S4 ^{1}H-NMR spectra of the P4.

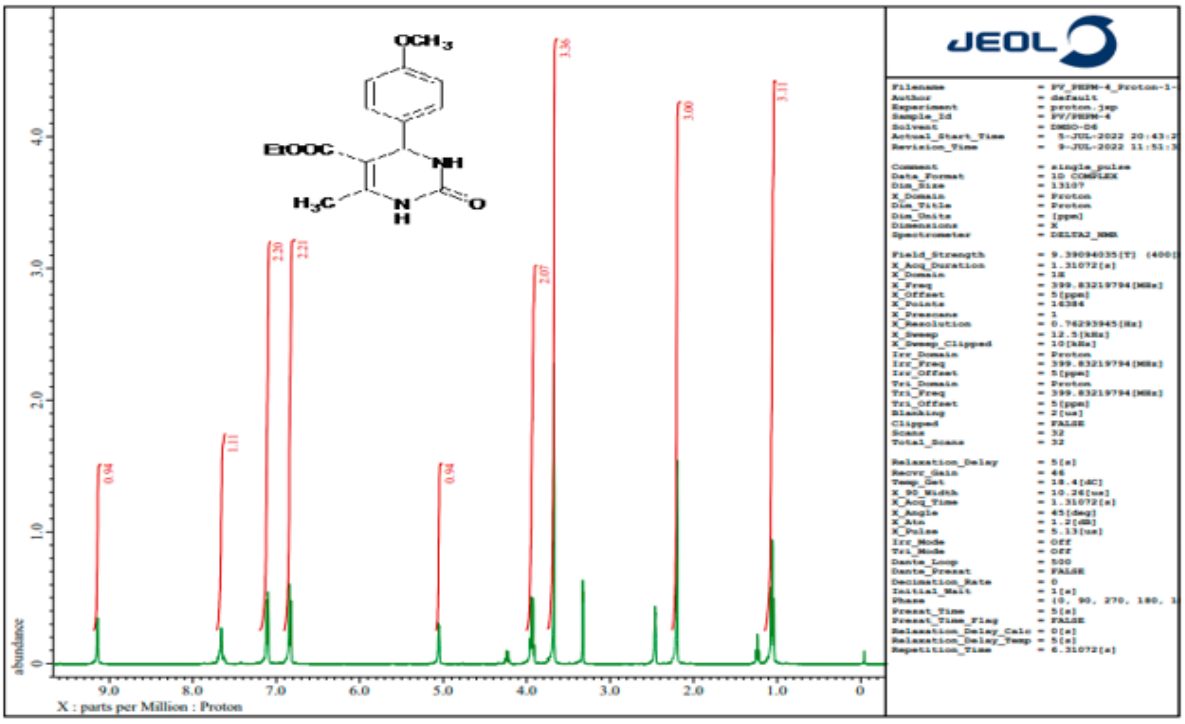


Fig. S5 ^{1}H-NMR spectra of the P5.

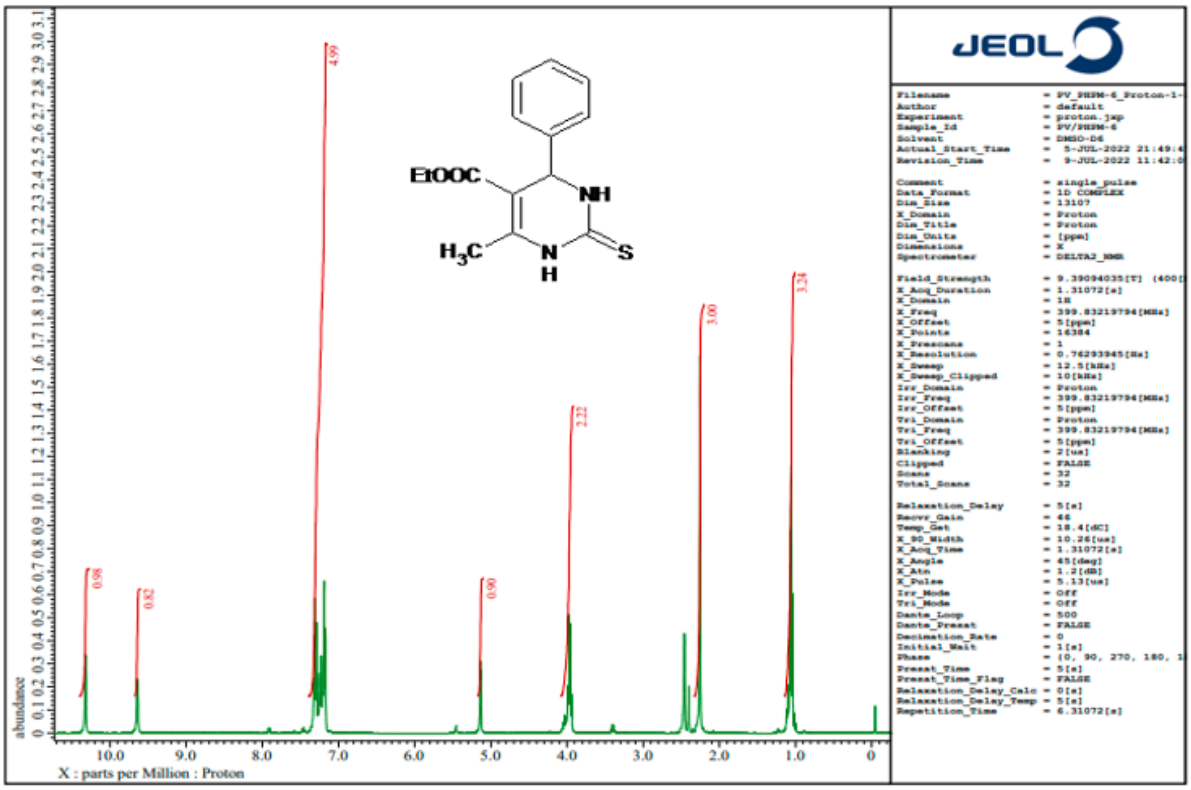


***Figure 5.18**: [1]H NMR Spectra of Ethyl 6-methyl-4-phenyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxyl*

Fig. S6 [1]H-NMR spectra of the P6.

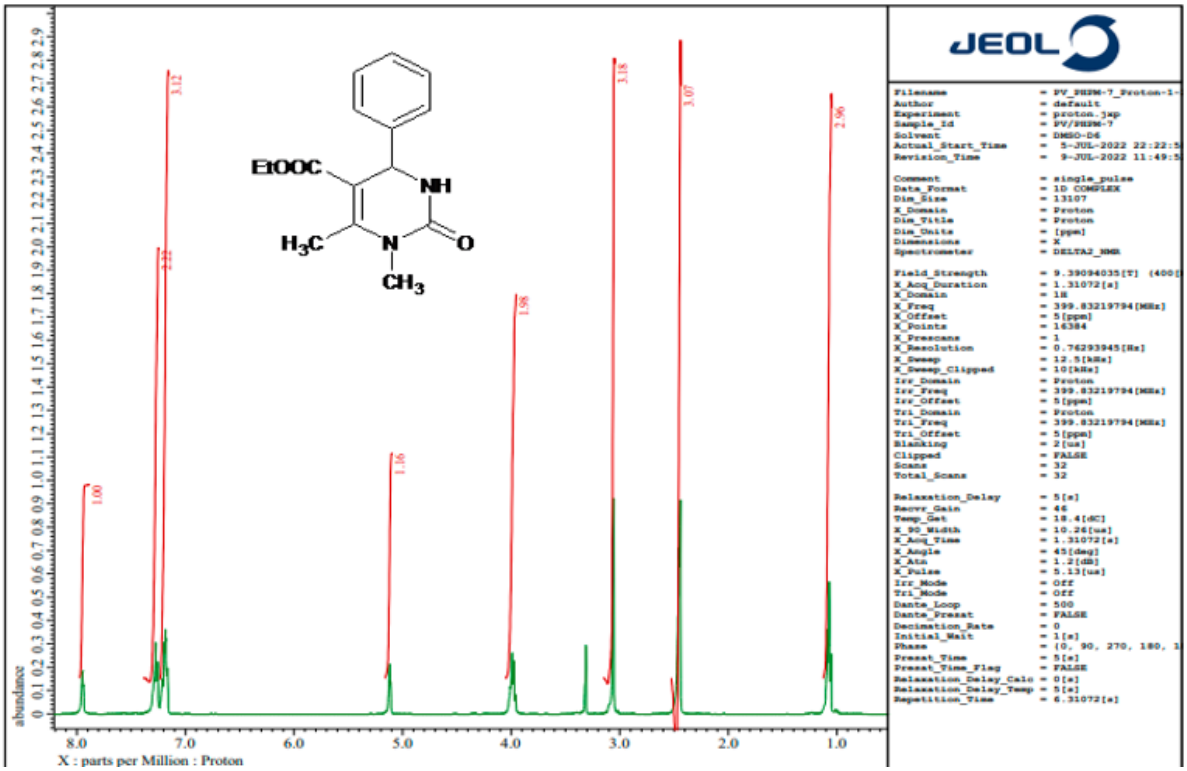


Fig. S7 [1]H-NMR spectra of the P7.

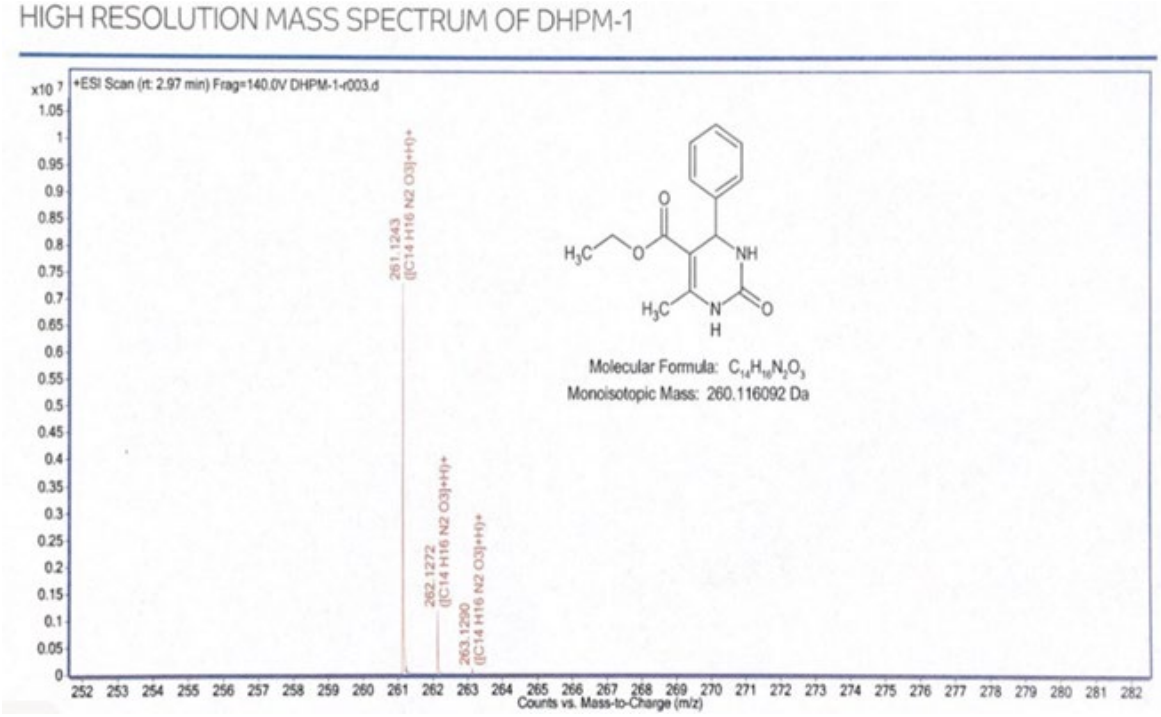


Fig. S8 HPLC spectra of the P1.

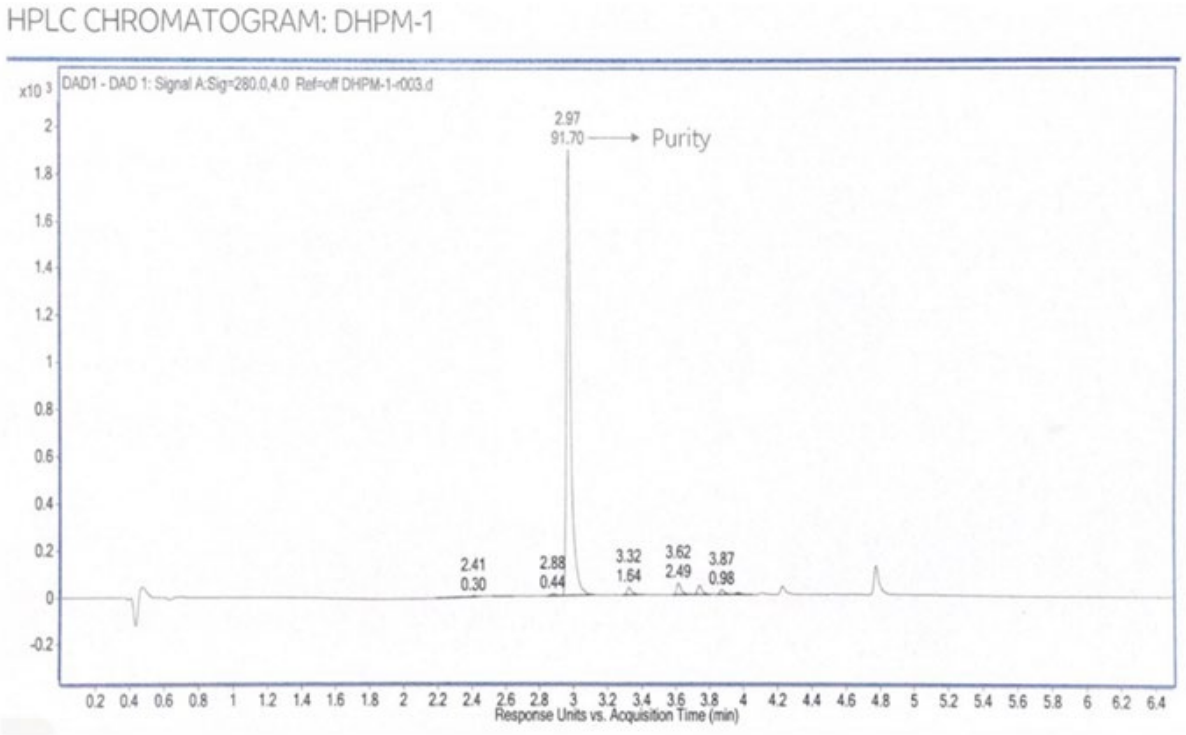


***Figure 5.3**: HPLC Spectra of Ethyl-6-methyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S9 Mass spectra of the P1.

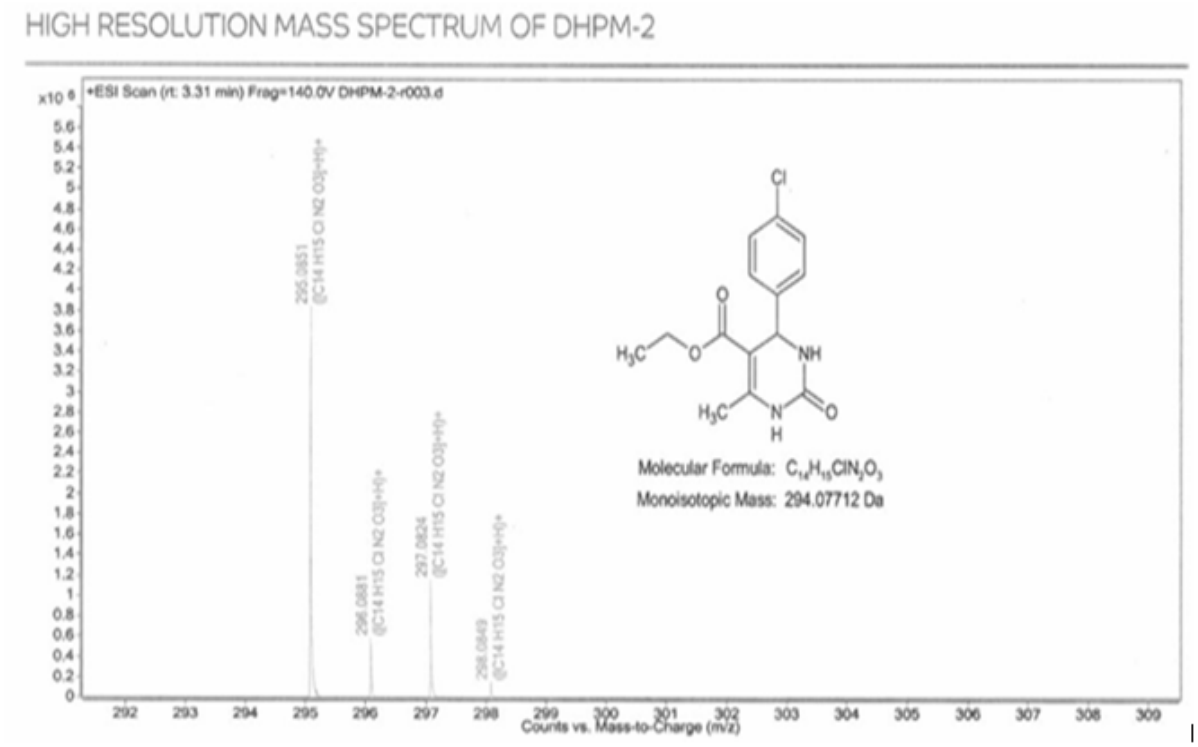


Figure 5.6: *High Resolution MS of Ethyl 4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S10 HPLC spectra of the P2.

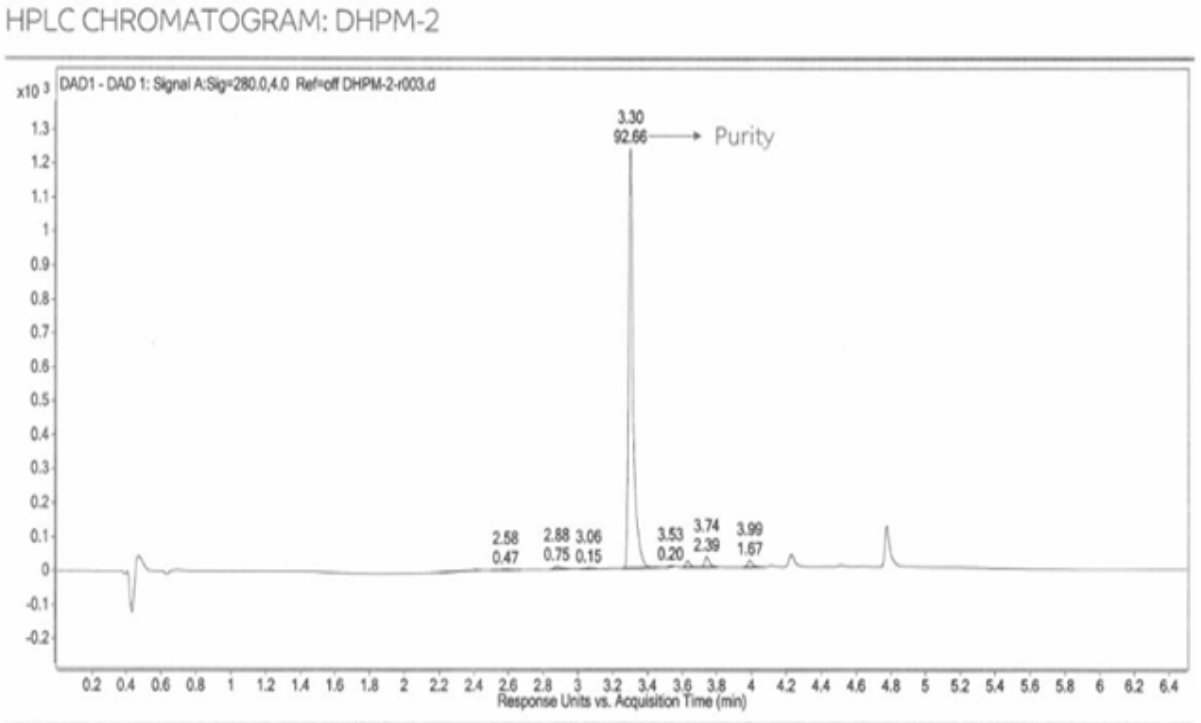


Figure 5.7: *HPLC Spectra of Ethyl 4-(4-chlorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S11 Mass spectra of the P2.

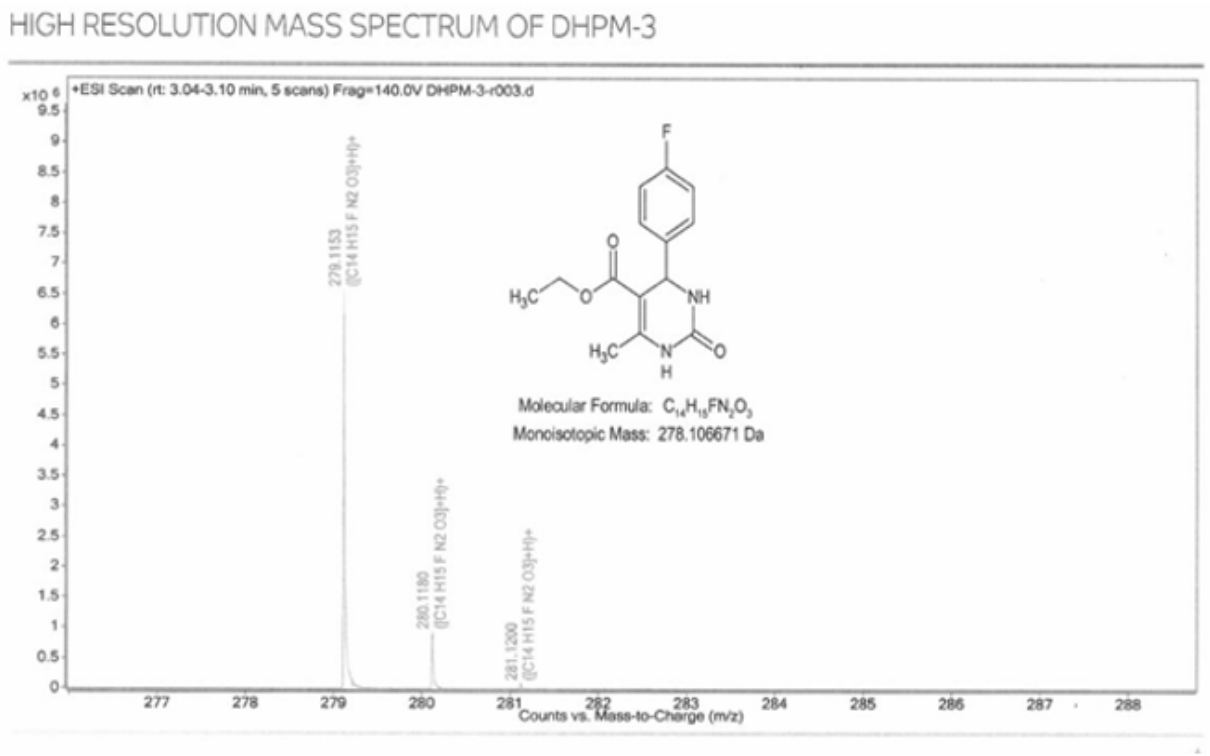


Figure 5.10: *High Resolution MS of Ethyl 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S12 HPLC spectra of the P3.

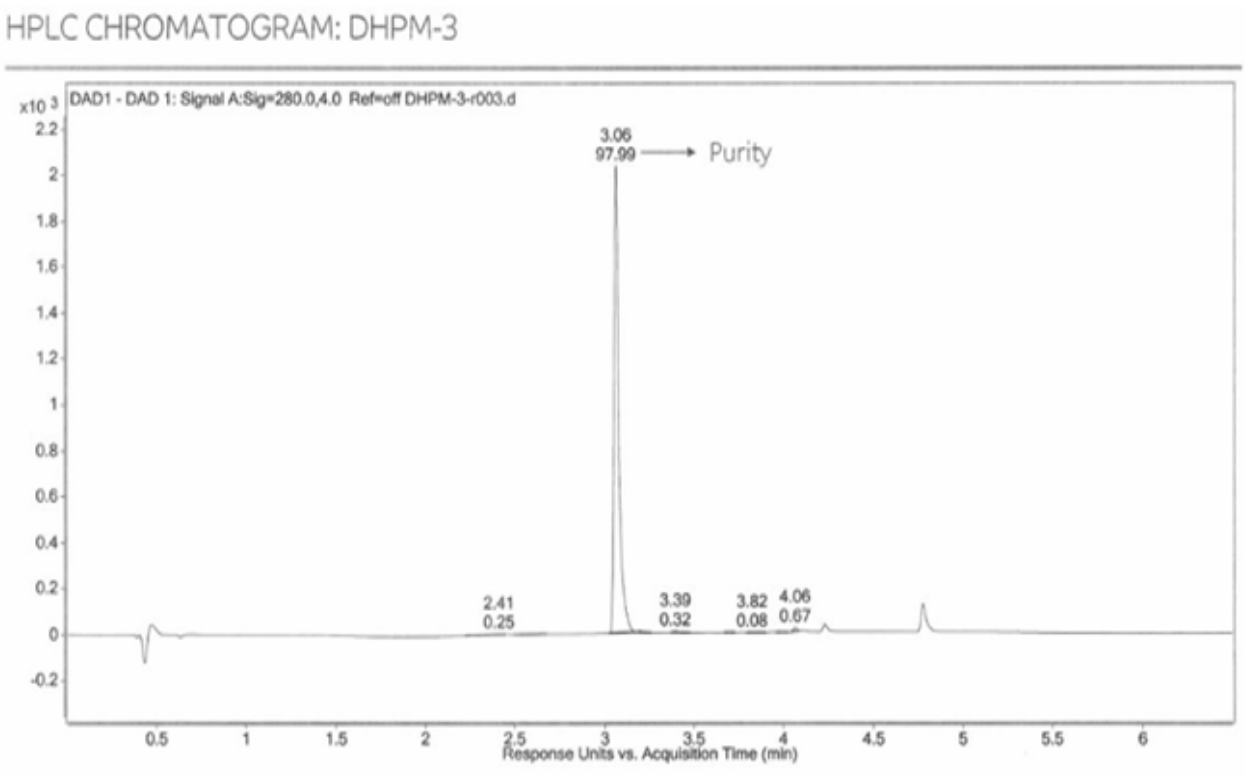


Figure 5.11: *HPLC Spectra of Ethyl 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S13 Mass spectra of the P3.

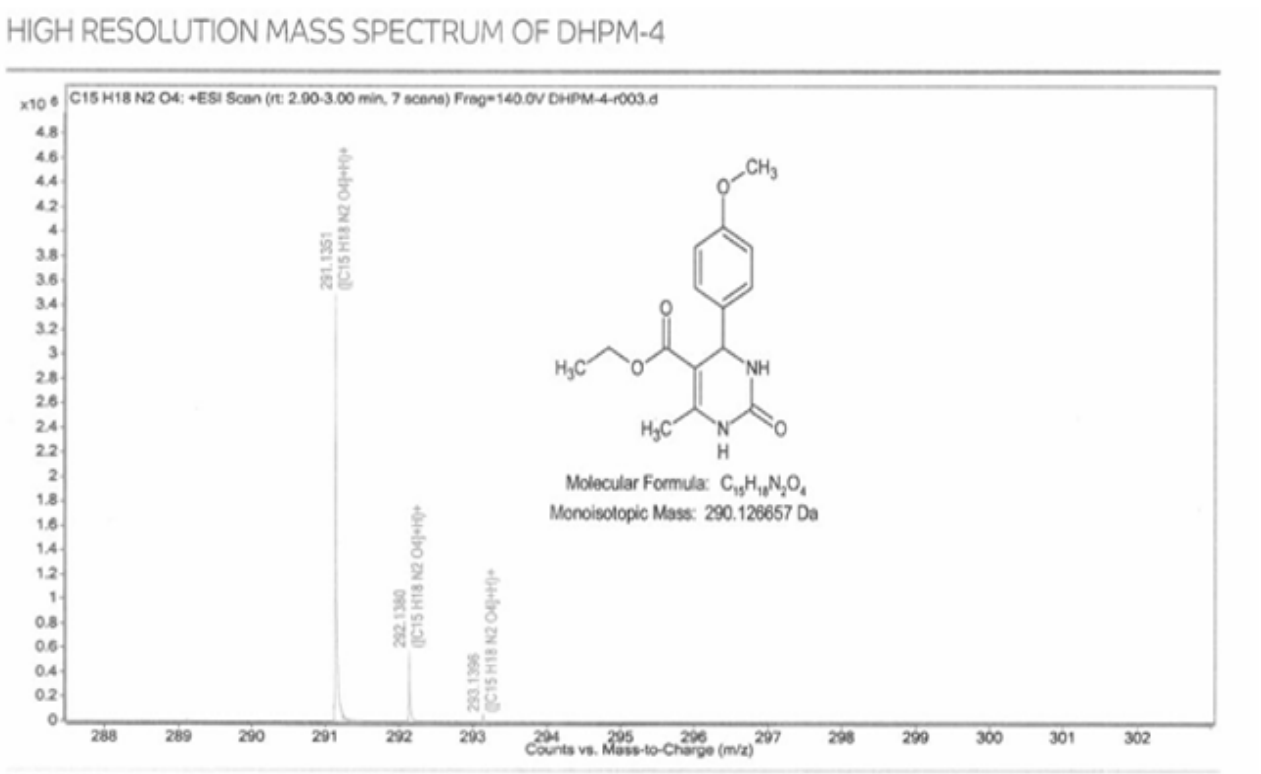


Figure 5.13: *High Resolution MS of Ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S14 HPLC spectra of the P4.

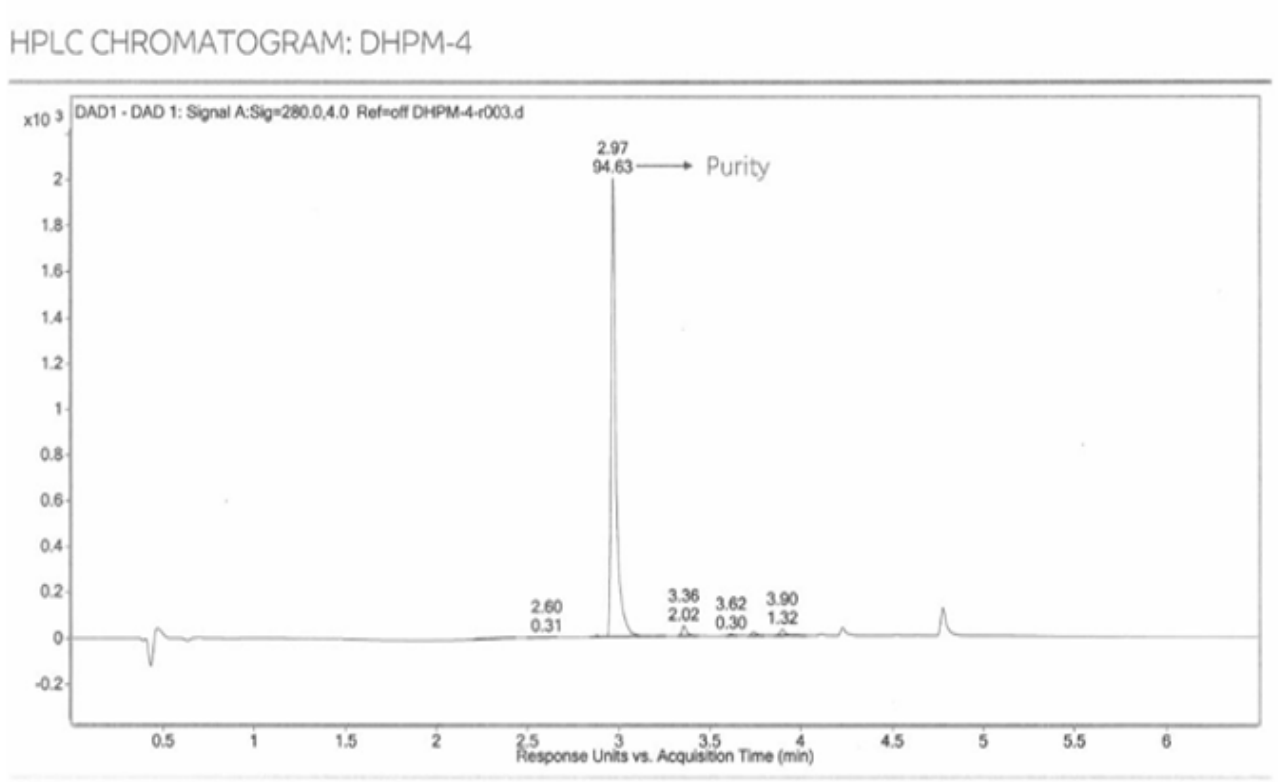


Figure 5.14: *HPLC Spectra of Ethyl 4-(4-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S15 Mass spectra of the P4.

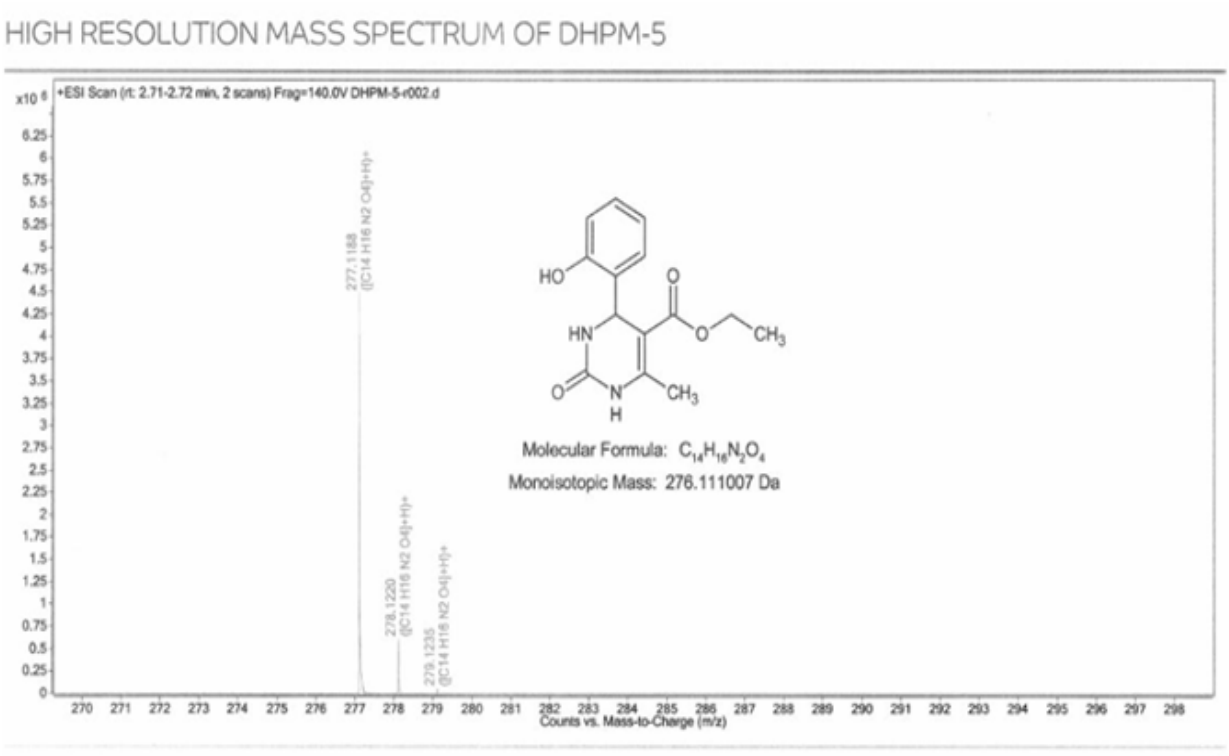


***Figure 5.16**: High Resolution MS of Ethyl 4-(2-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S16 HPLC spectra of the P5.

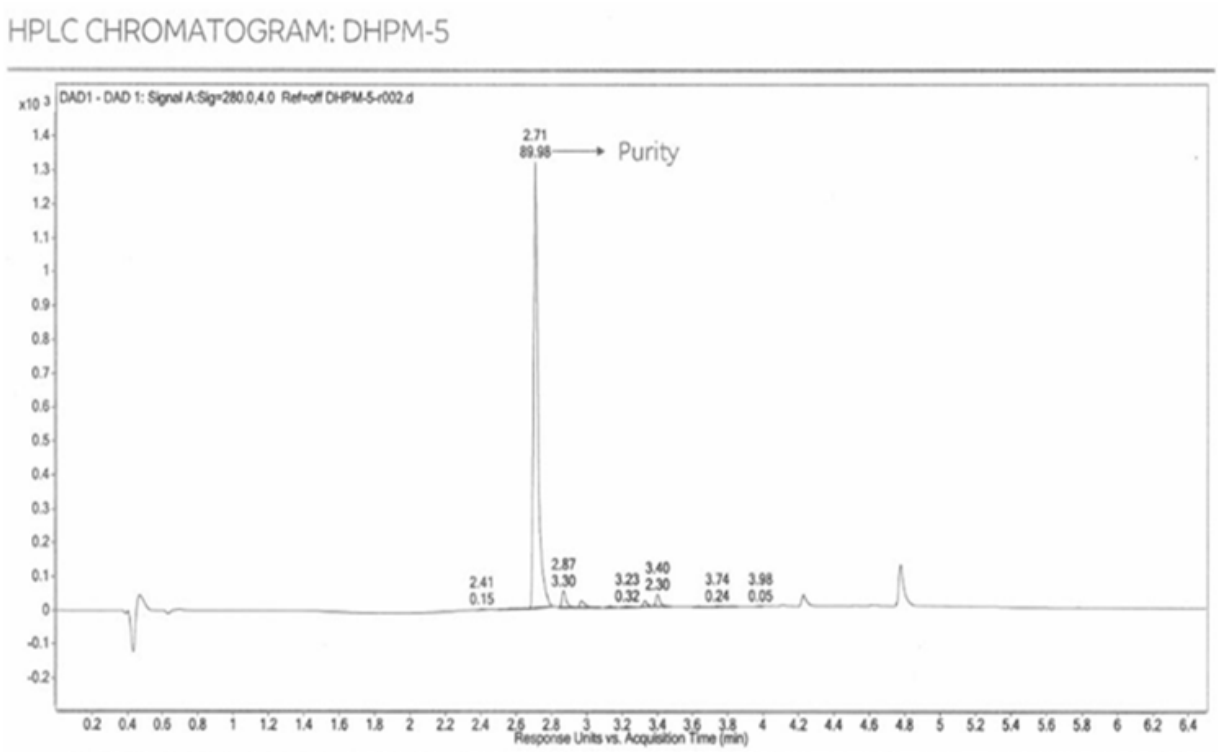


***Figure 5.17**: HPLC Spectra of Ethyl 4-(2-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S17 Mass spectra of the P5.

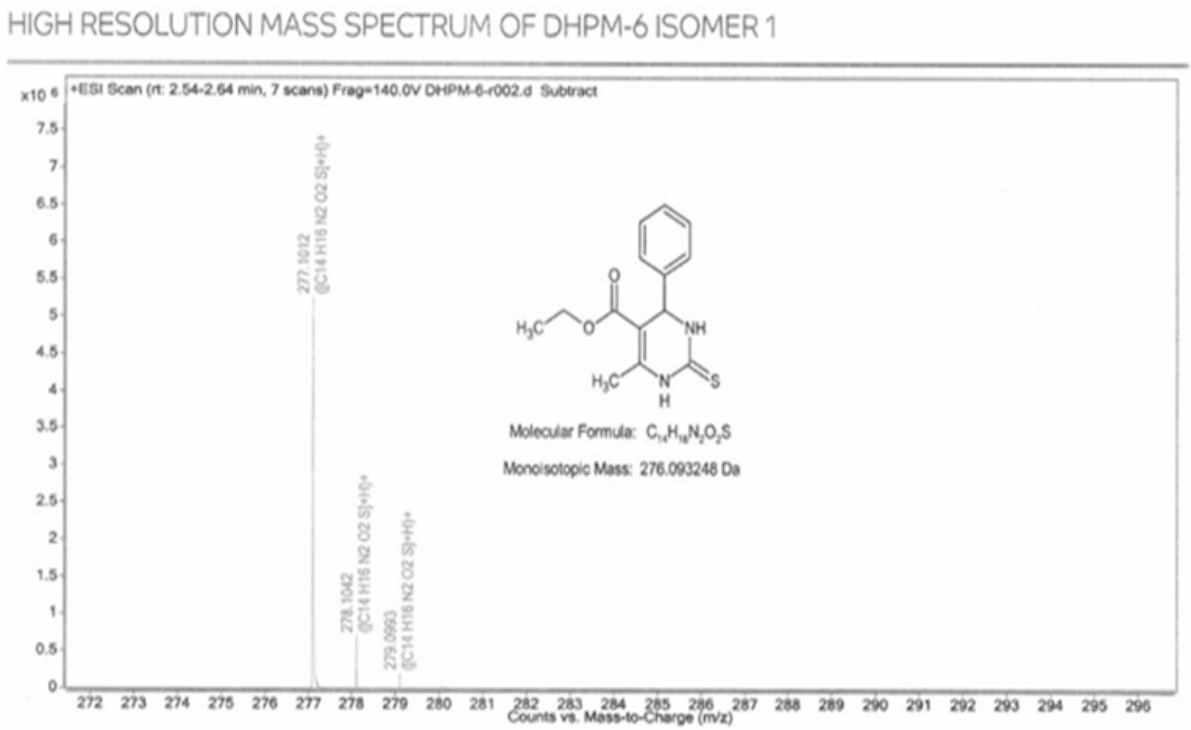


***Figure 5.19**: High Resolution MS of Ethyl 6-methyl-4-phenyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S18 HPLC spectra of the P6.

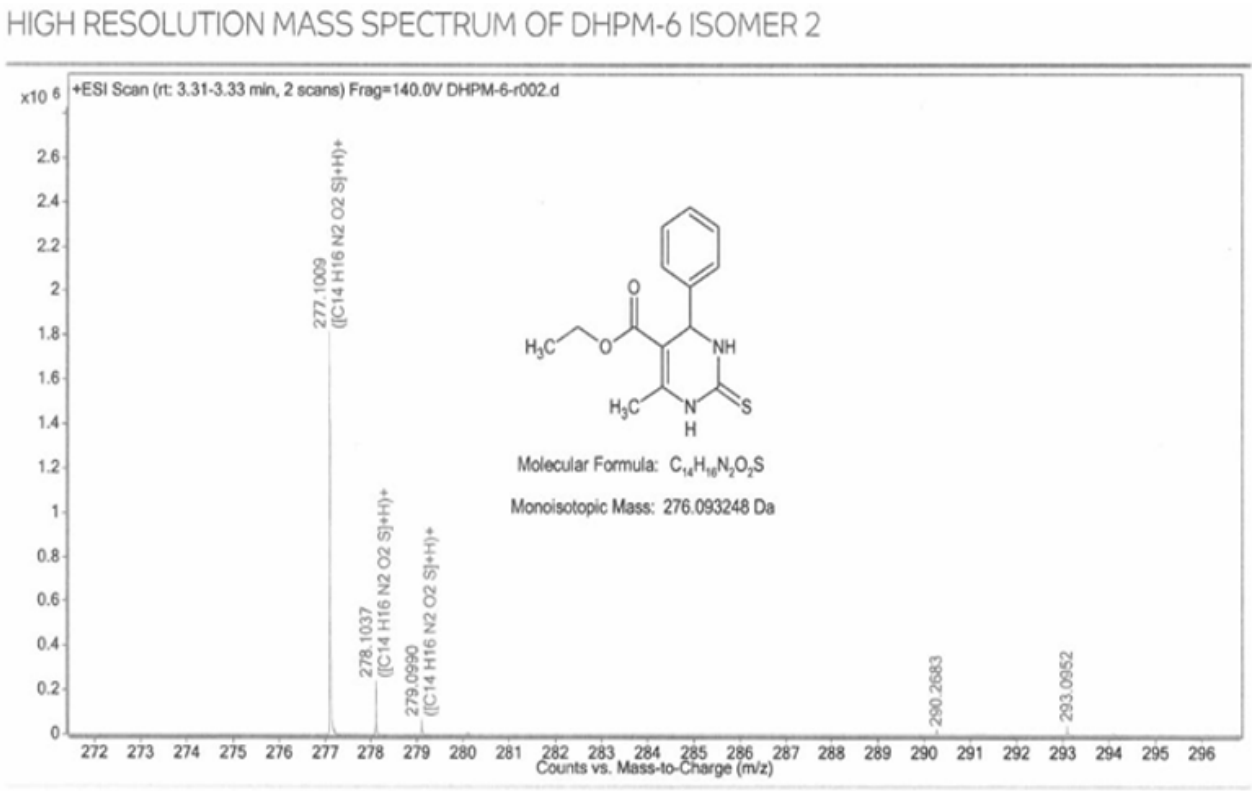


***Figure 5.20**: High Resolution MS of Ethyl 6-methyl-4-phenyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S19 Mass spectra of the P6.

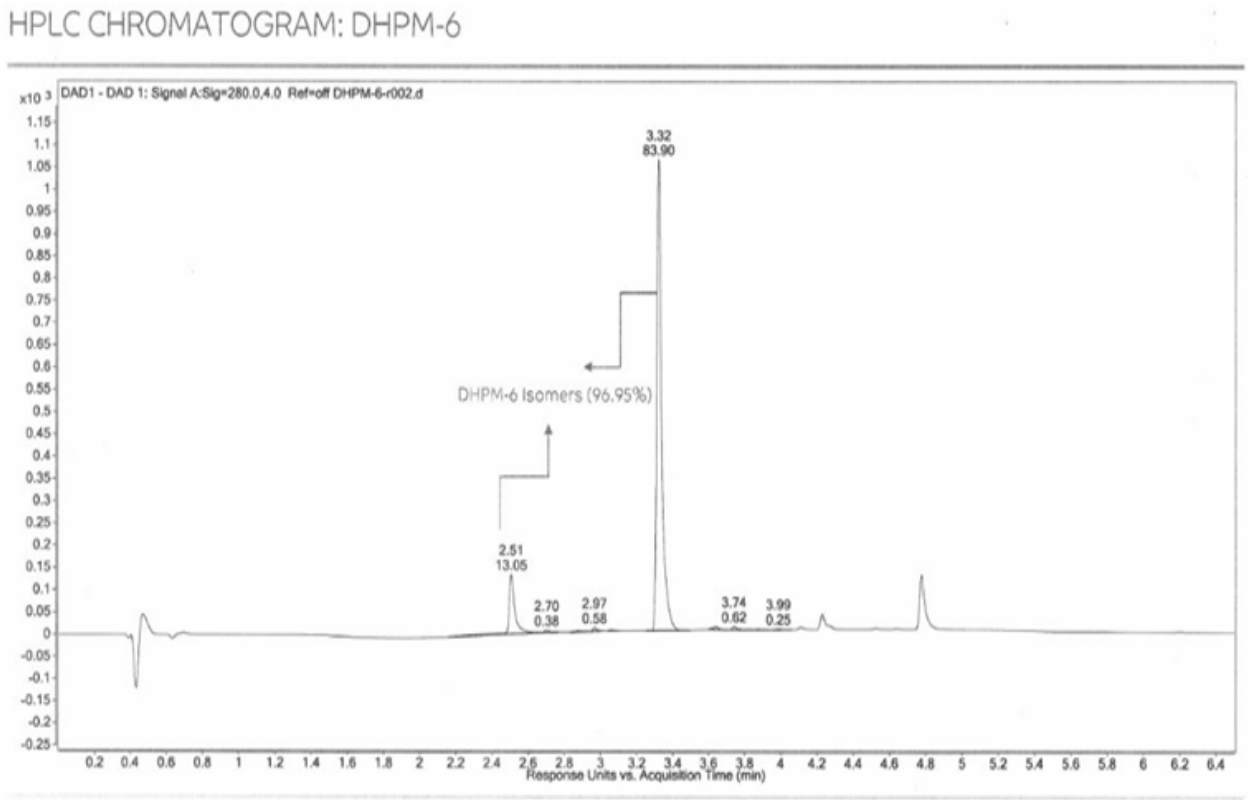


***Figure 5.21**: HPLC Spectra of Ethyl 6-methyl-4-phenyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S20 Mass spectra of the P7.

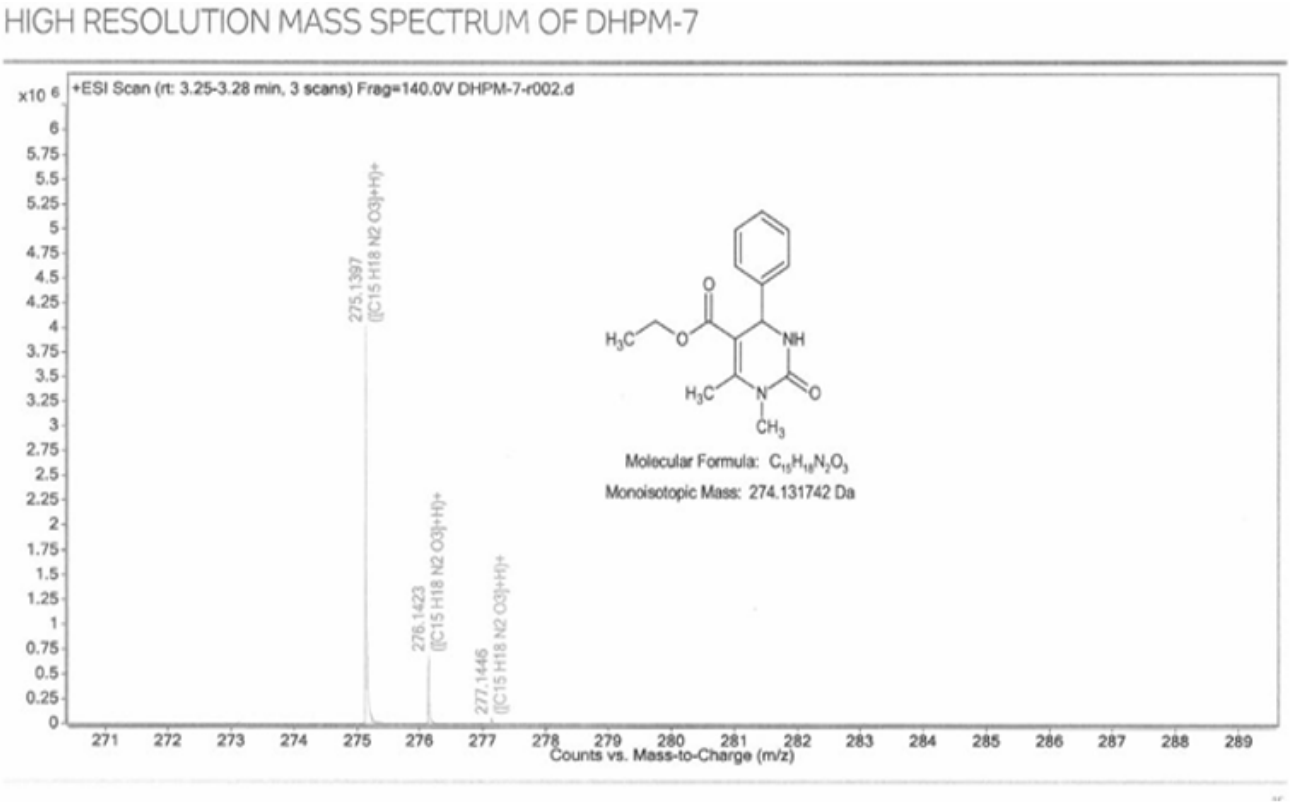


***Figure 5.23**: High Resolution MS of Ethyl 1, 6-dimethyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S21 ^{HPLC} spectra of the P7.

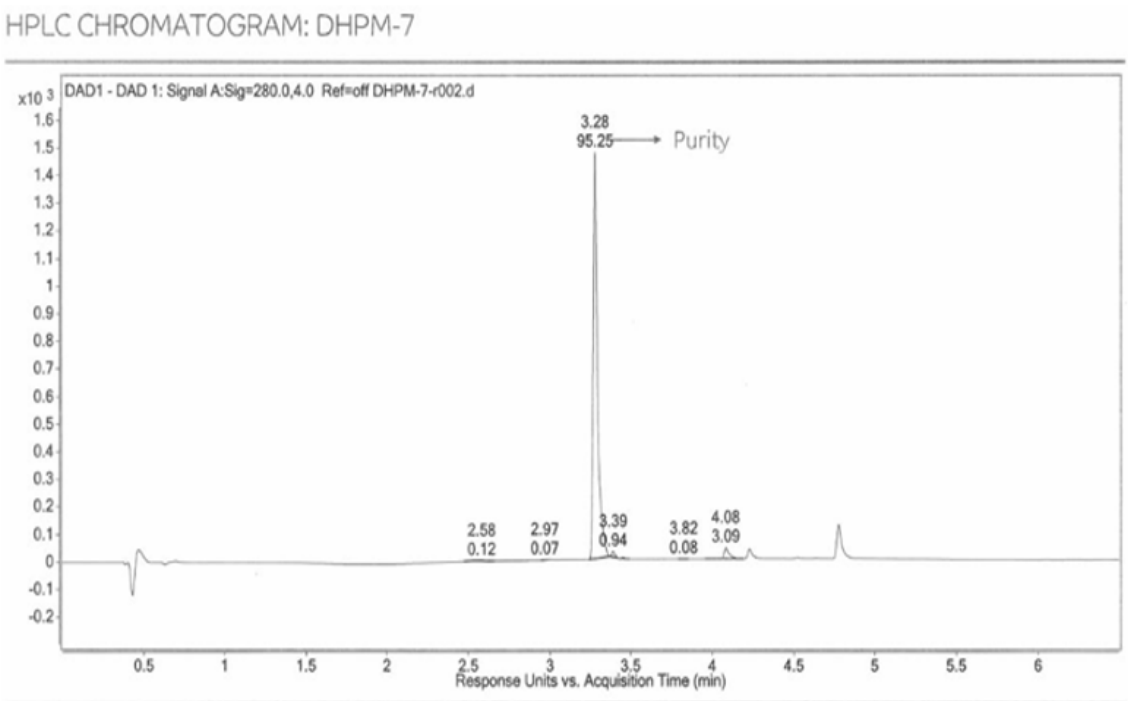


***Figure 5.24**: HPLC Spectra of Ethyl 1,6-dimethyl-2-oxo-4-phenyl-1,2,3,4-tetrahydropyrimidine-5-carboxylate*

Fig. S22 ^{HPLC} spectra of the P7.

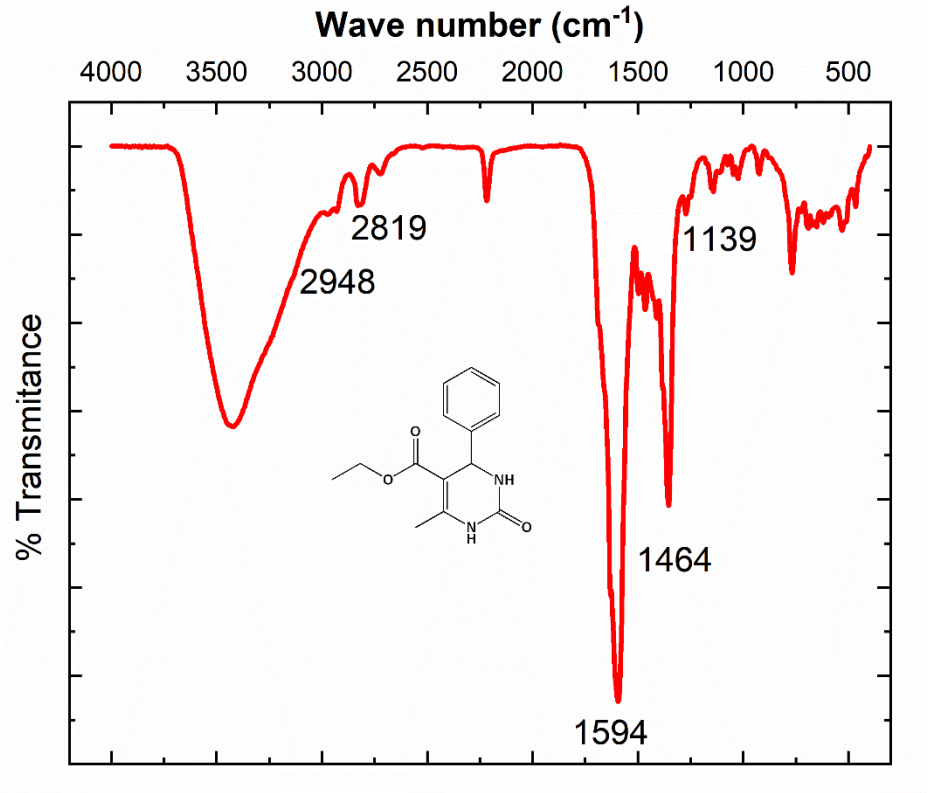


Fig. S23 FT-IR spectra of the P1.

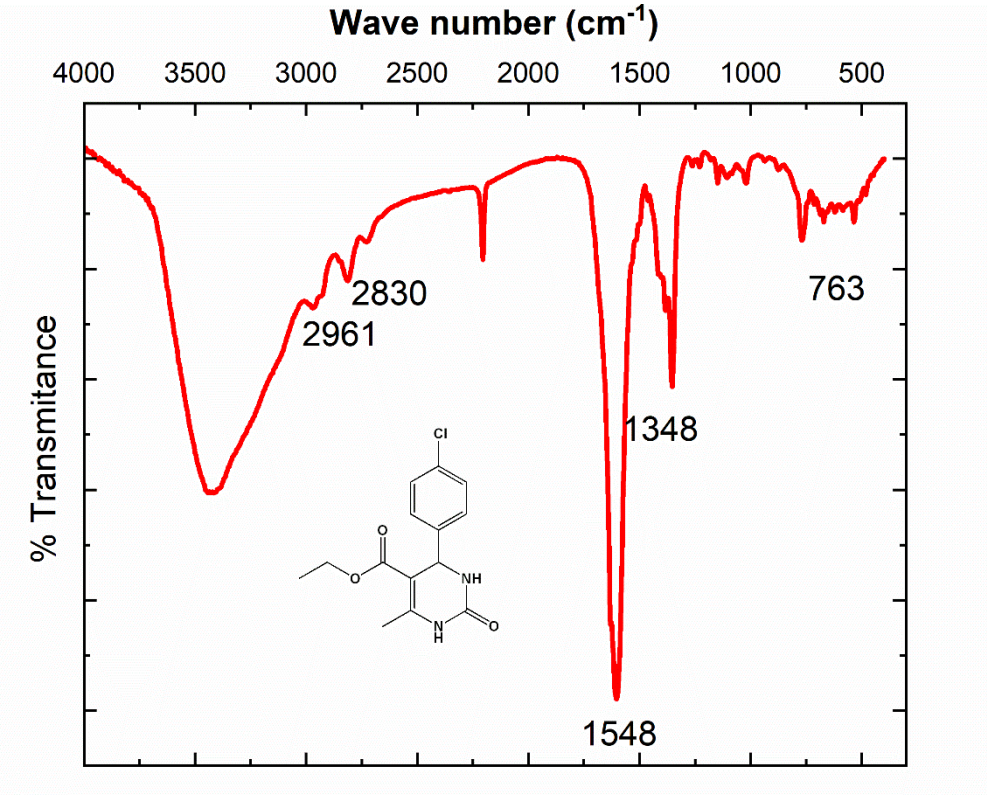


Fig. S24 FT-IR spectra of the P2.

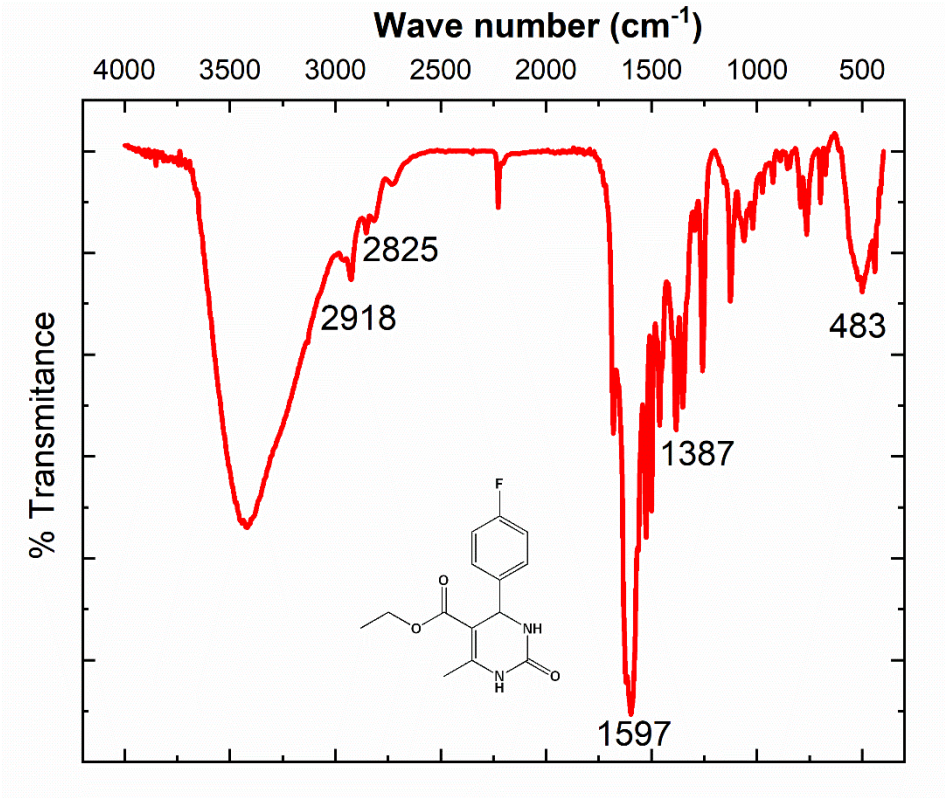


Fig. S25 FT-IR spectra of the P3.

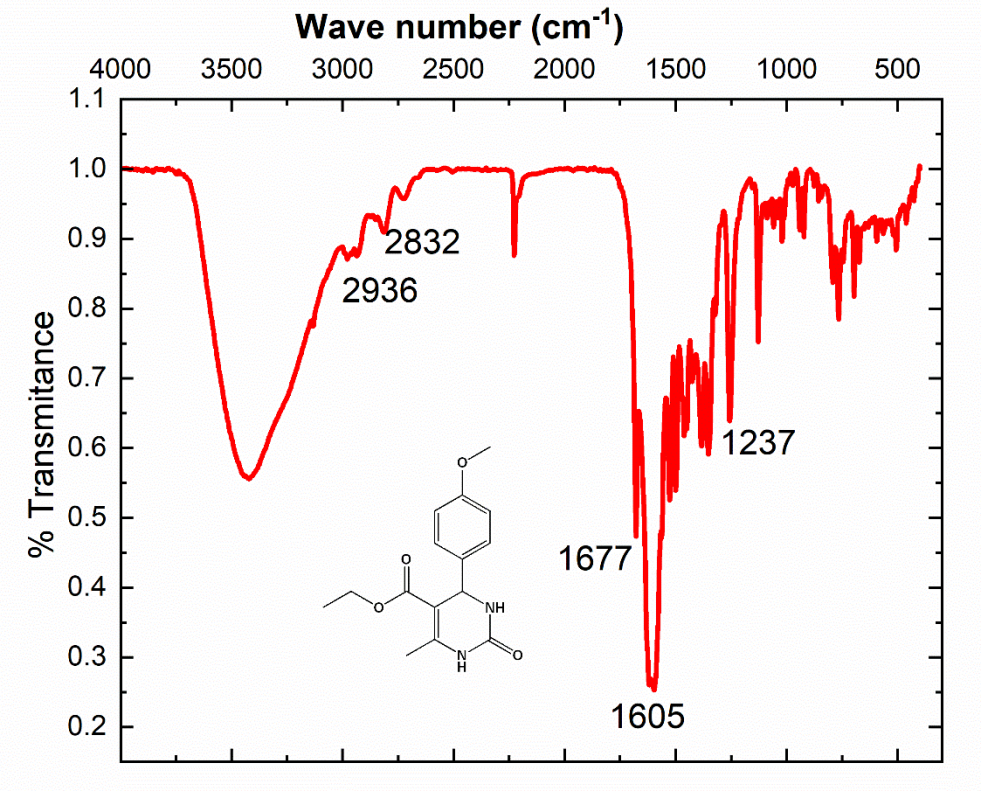


Fig. S26 FT-IR spectra of the P4.

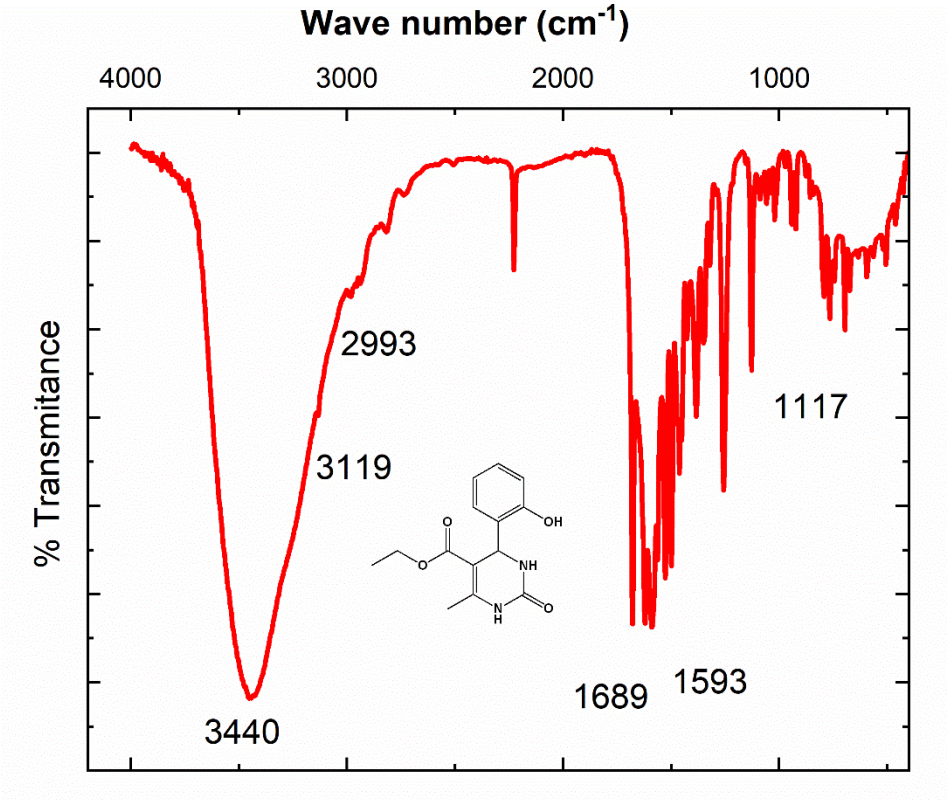


Fig. S27 FT-IR spectra of the P5.

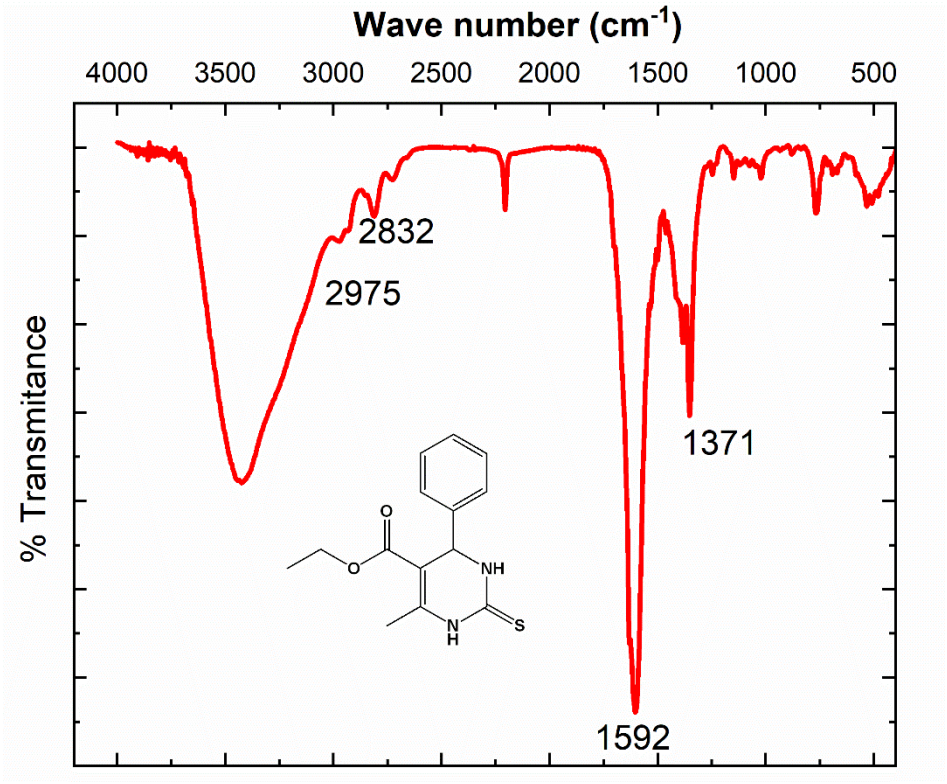


Fig. S27 FT-IR spectra of the P6.

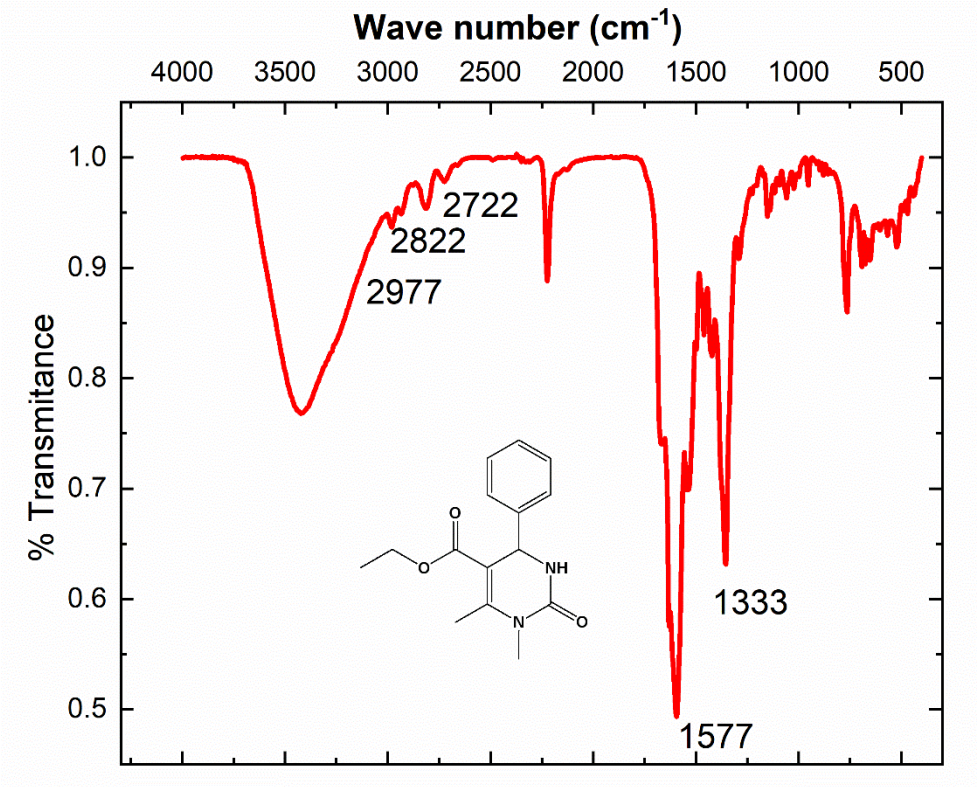
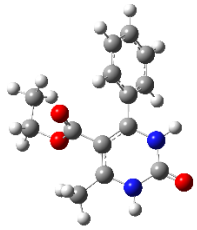
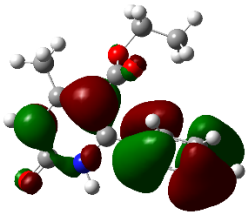
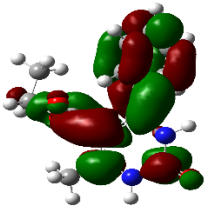
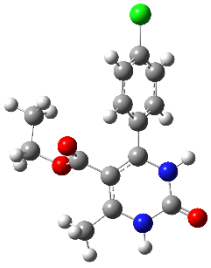
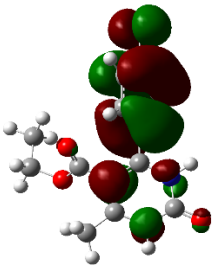
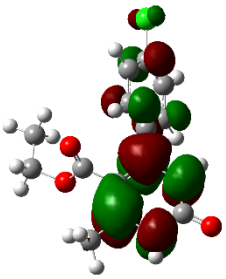
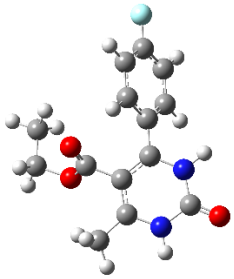
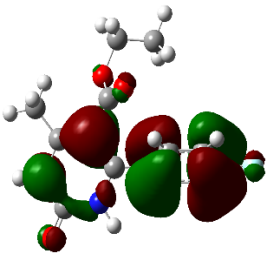
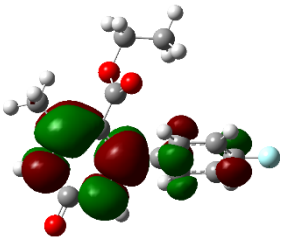
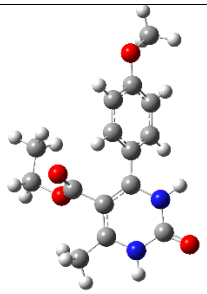
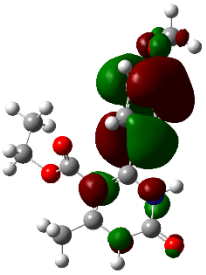
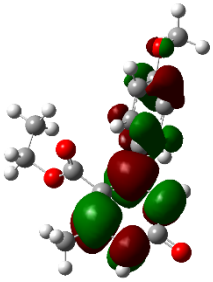
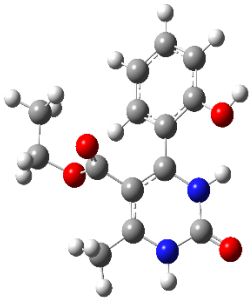
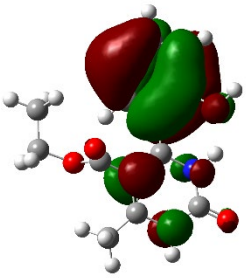
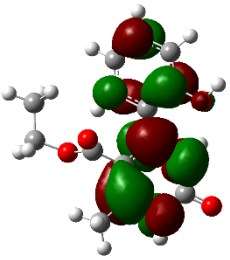
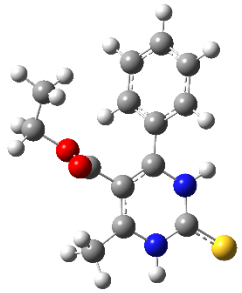
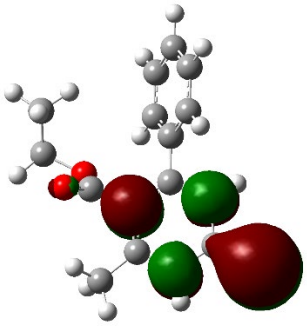
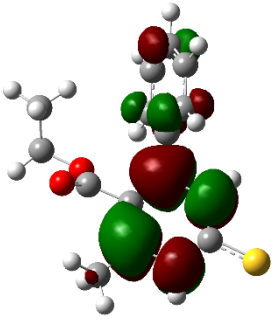


Fig. S28 FT-IR spectra of the P7.

Table S1. Optimized molecular geometry, HOMO and LUMO of newly synthesized molecules (P1-P7).

Compound	Optimised molecular structure	HOMO	LUMO
P1			
P2			
P3			
P4			
P5			

P6			
P7