

Supplementary Material

Ureas as new nucleophilic reagents for S_N^H amination and carbamoyl amination reactions in the 1,3,7-triazapyrene series

Ivan V. Borovlev,* Oleg P. Demidov, Gulminat A. Amangasieva,
Elena K. Avakyan, and Nadezhda A. Kurnosova

North Caucasus Federal University, Pushkin st. 1, Stavropol, 355009, Russia.

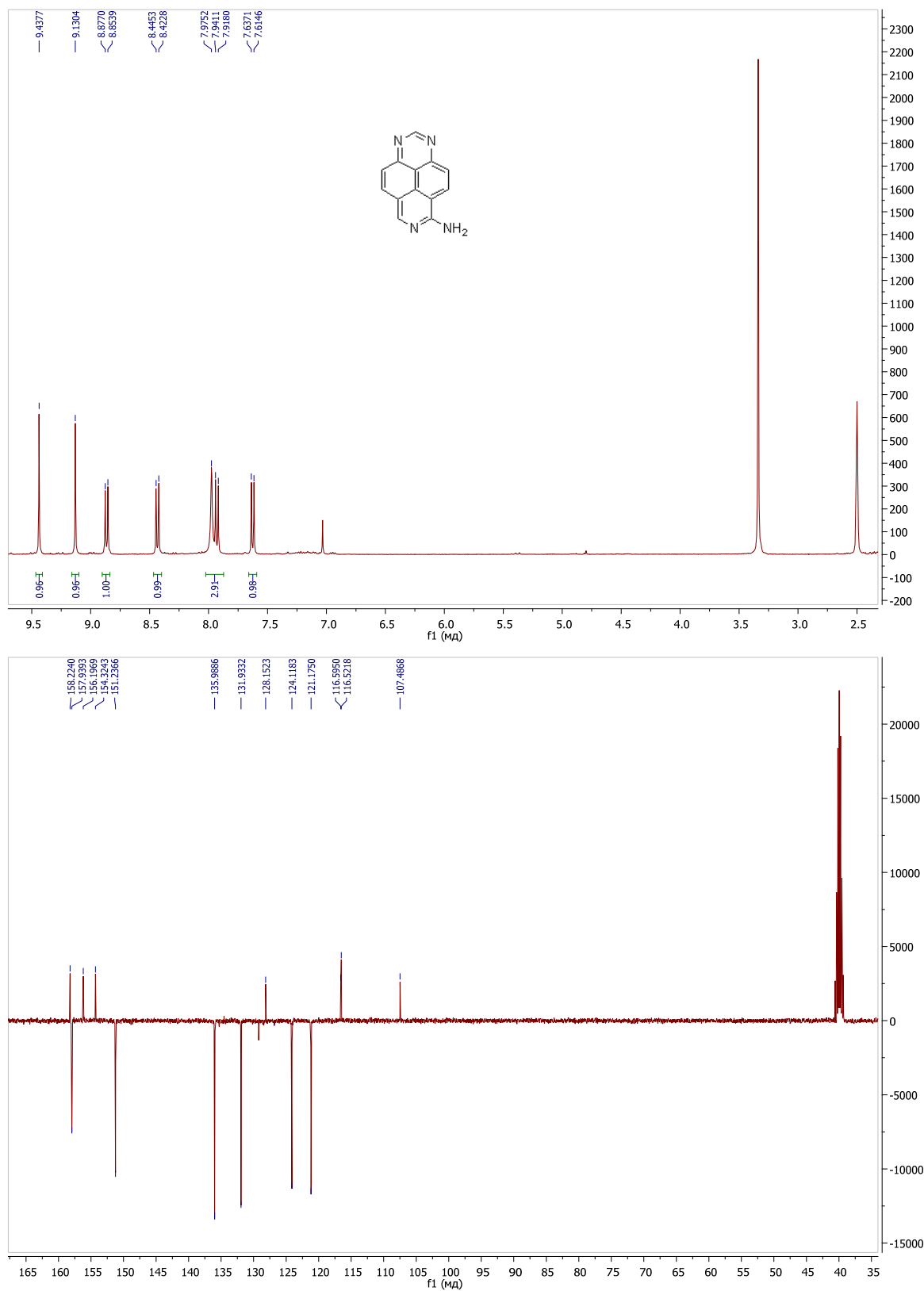
E-mail: ivborovlev@rambler.ru

Table of Contents

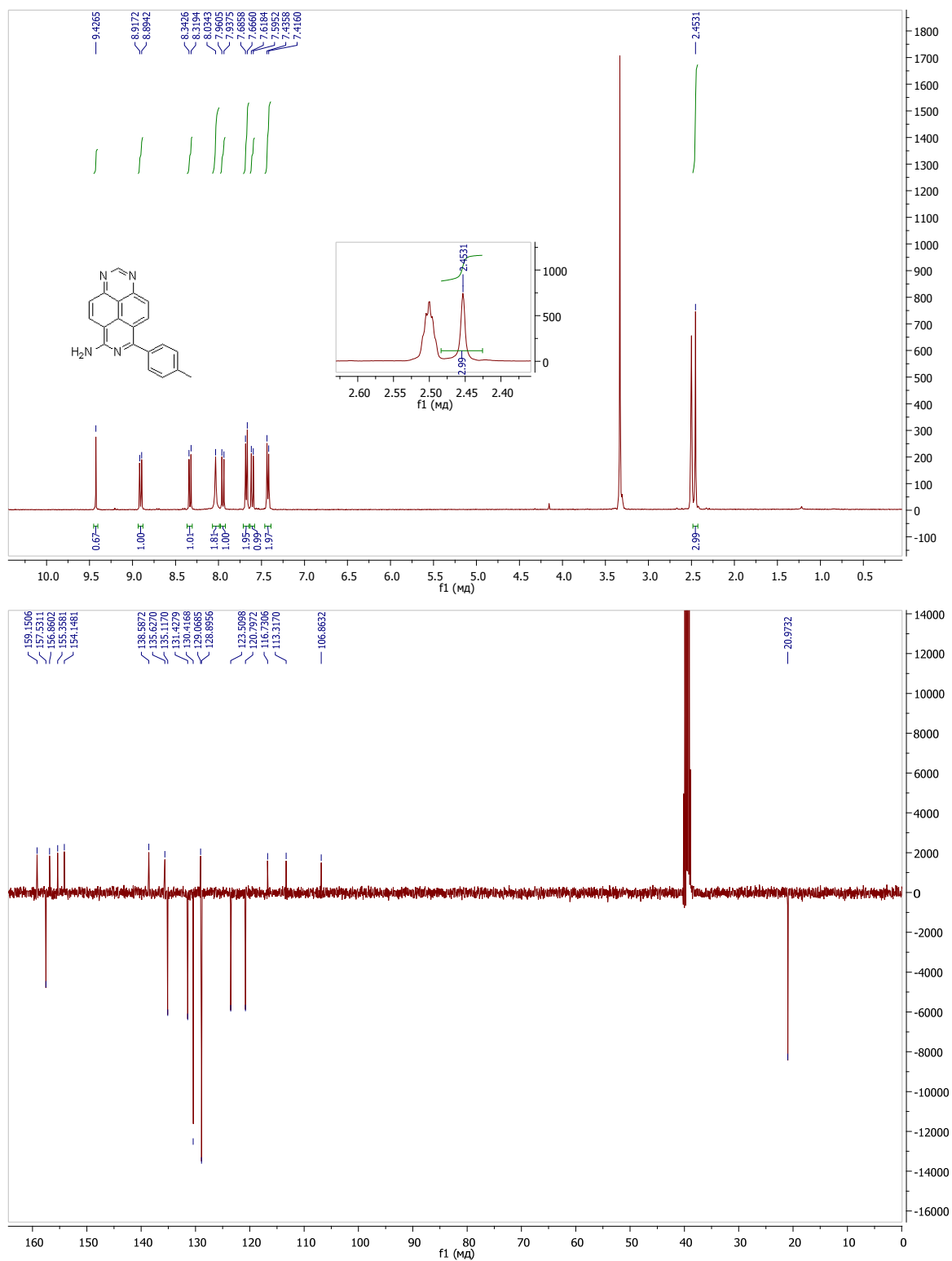
| | |
|---|----|
| NMR-Spectra | 3 |
| 1,3,7-Triazapyrene-6-amine (3a)..... | 3 |
| 8-(4'-Tolyl)-1,3,7-triazapyren-6-amine (3b)..... | 4 |
| 8-(3',4'-Dimethylphenyl)-1,3,7-triazapyren-6-amine (3c)..... | 5 |
| 8-(4'-Methoxyphenyl)-1,3,7-triazapyren-6-amine (3d)..... | 6 |
| 8-(4'-Ethoxyphenyl)-1,3,7-triazapyren-6-amine (3e)..... | 7 |
| N,N-Dimethyl-1,3,7-triazapyren-6,8-diamine (3f)..... | 8 |
| (1,1-Dimethyl-pentyl)-urea..... | 9 |
| 1-(tert-Butyl)-3-(1,3,7-triazapyren-6-yl)-urea (9a)..... | 10 |
| 1-(1,1-dimethyl-pentyl)-3-(1,3,7-triazapyren-6-yl)-urea (9b)..... | 11 |
| IR-Spectra | 12 |
| 6-Amino-1,3,7-triazapyrene (3a)..... | 12 |
| 6-Amino-8-(4'-tolyl)-1,3,7-triazapyrene (3b)..... | 12 |
| 6-Amino-8-(3',4'-dimethylphenyl)-1,3,7-triazapyrene (3c)..... | 13 |
| 6-Amino-8-(4'-methoxyphenyl)-1,3,7-triazapyrene (3d)..... | 13 |
| 6-Amino-8-(4'-ethoxyphenyl)-1,3,7-triazapyrene (3e)..... | 14 |
| 6-Amino-8-dimethylamino-1,3,7-triazapyrene (3f)..... | 14 |
| (1,1-dimethyl-pentyl)-urea..... | 15 |
| 1-(1,1-dimethylpentyl)-3-(1,3,7-triazapyren-6-yl)-urea (9b)..... | 15 |

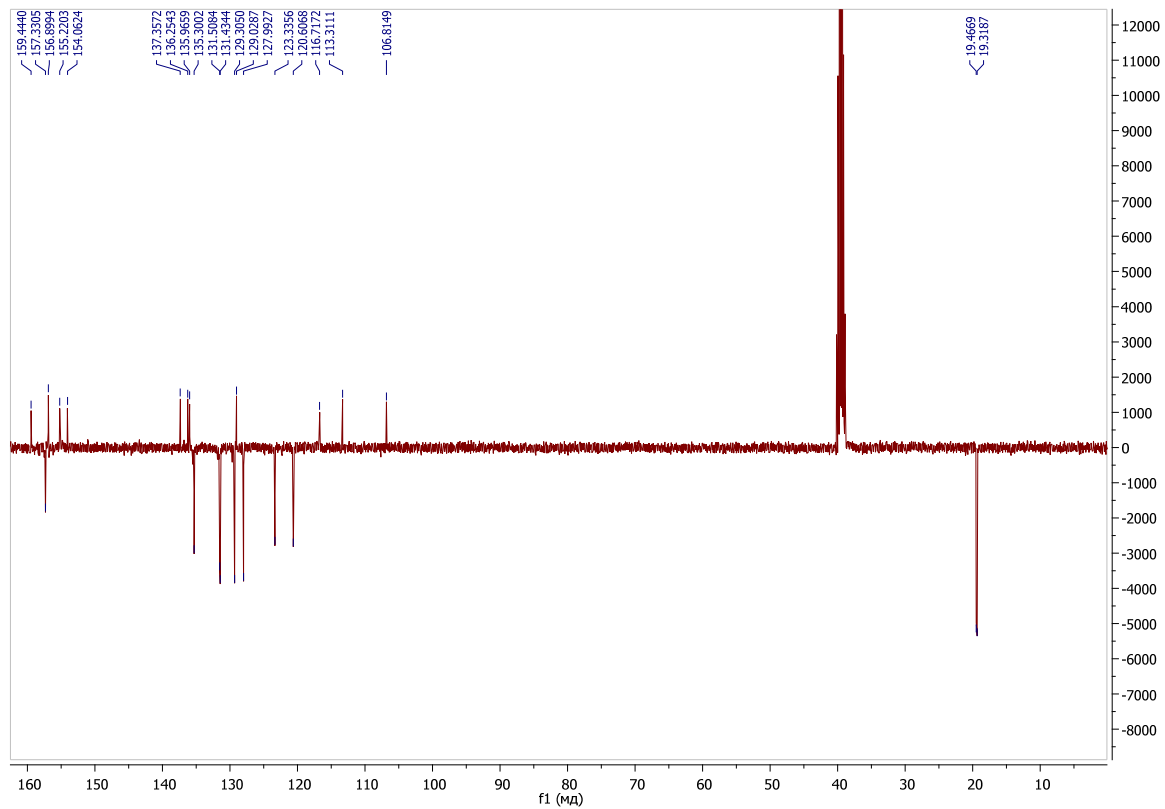
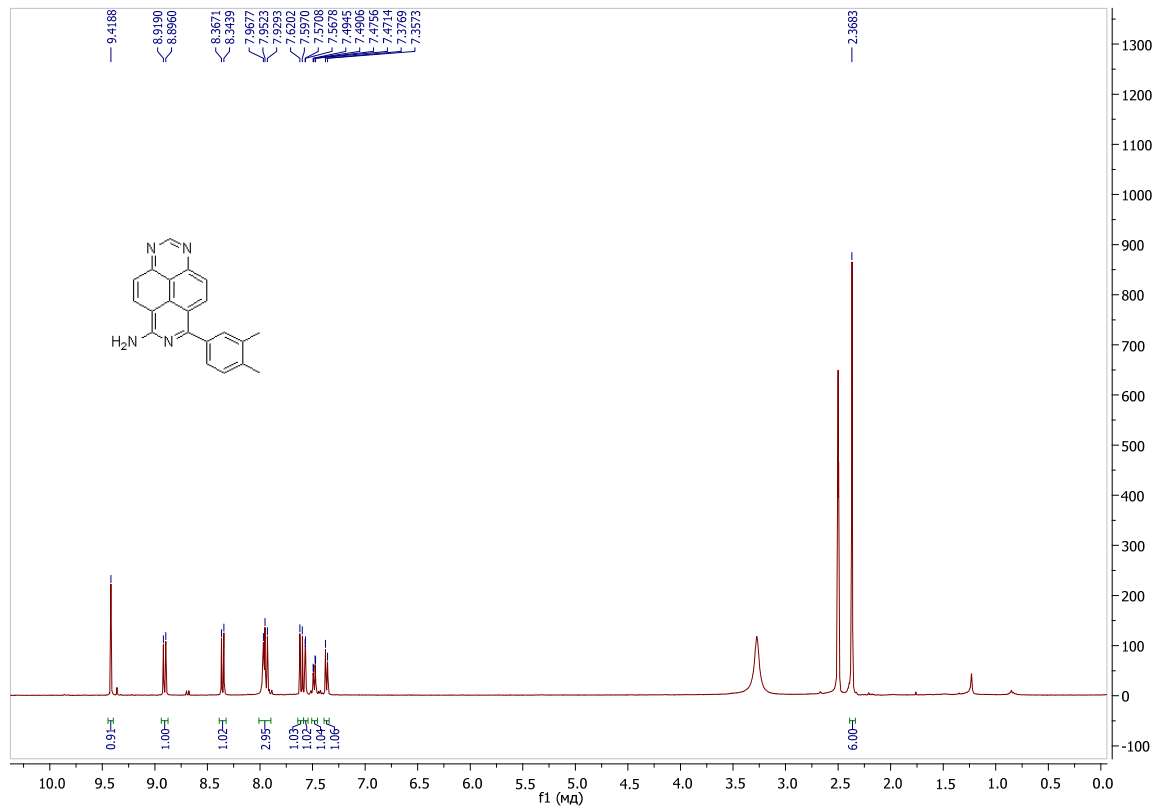
NMR-Spectra

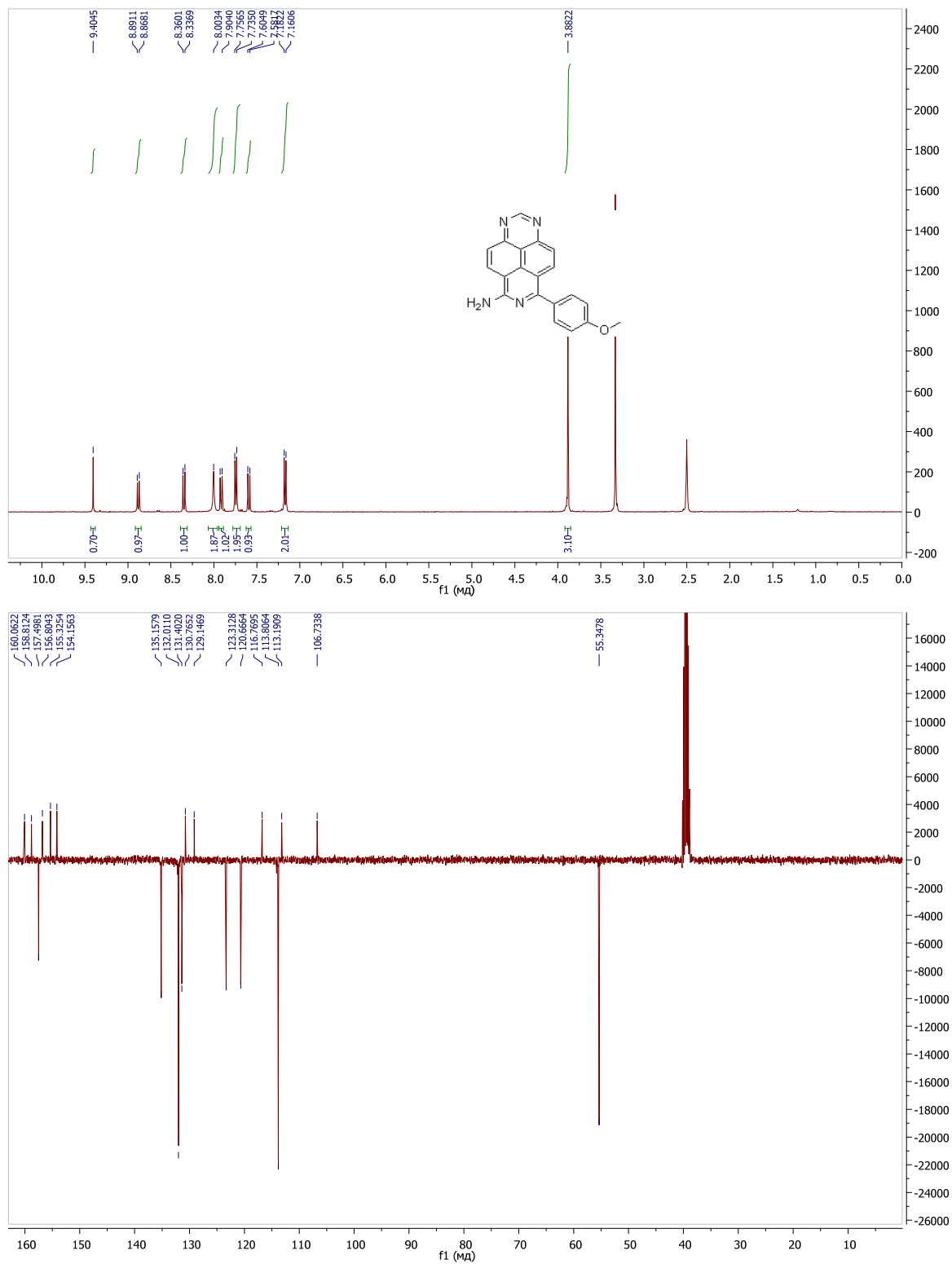
1,3,7-Triazapyrene-6-amine (3a)

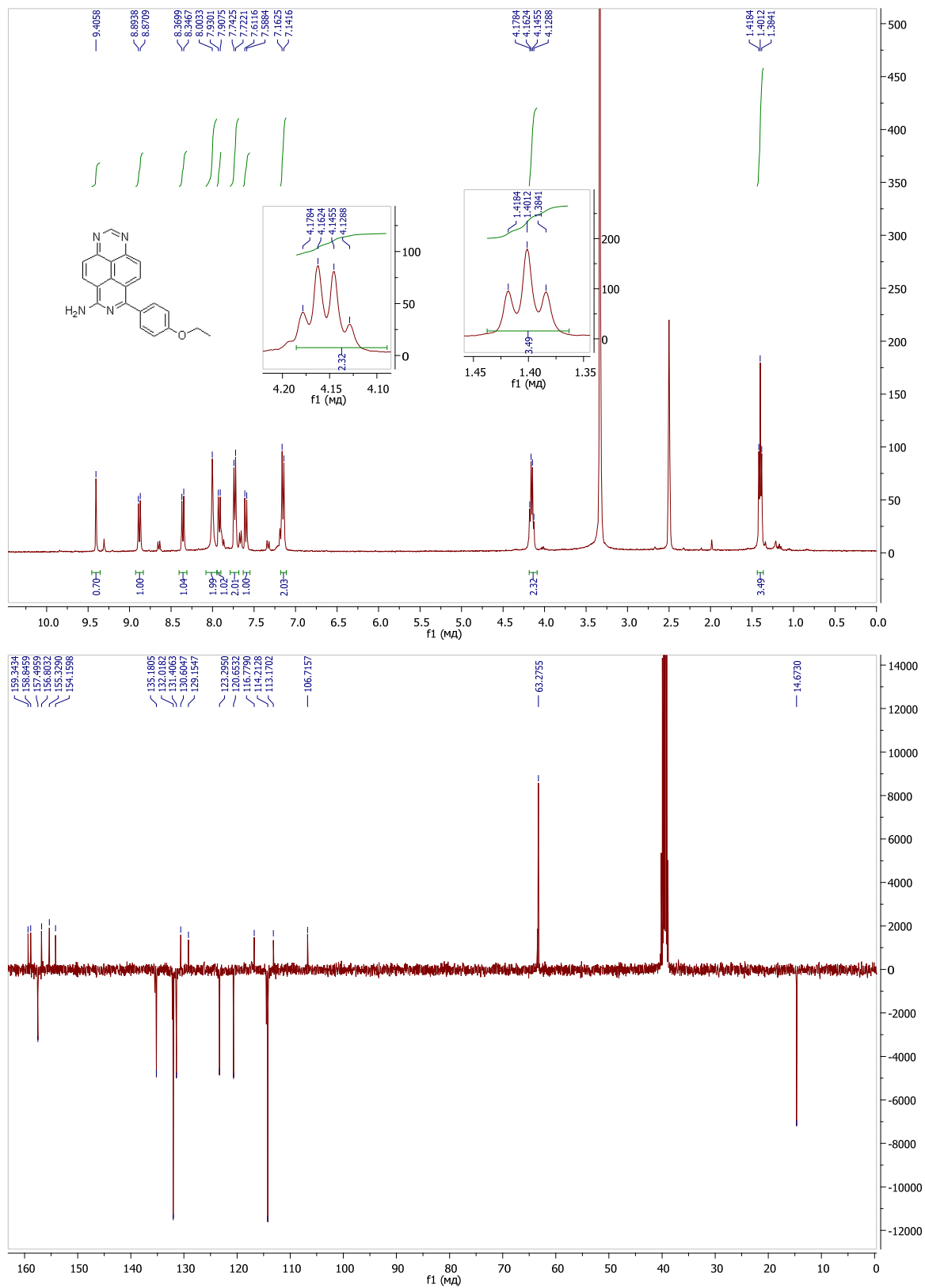


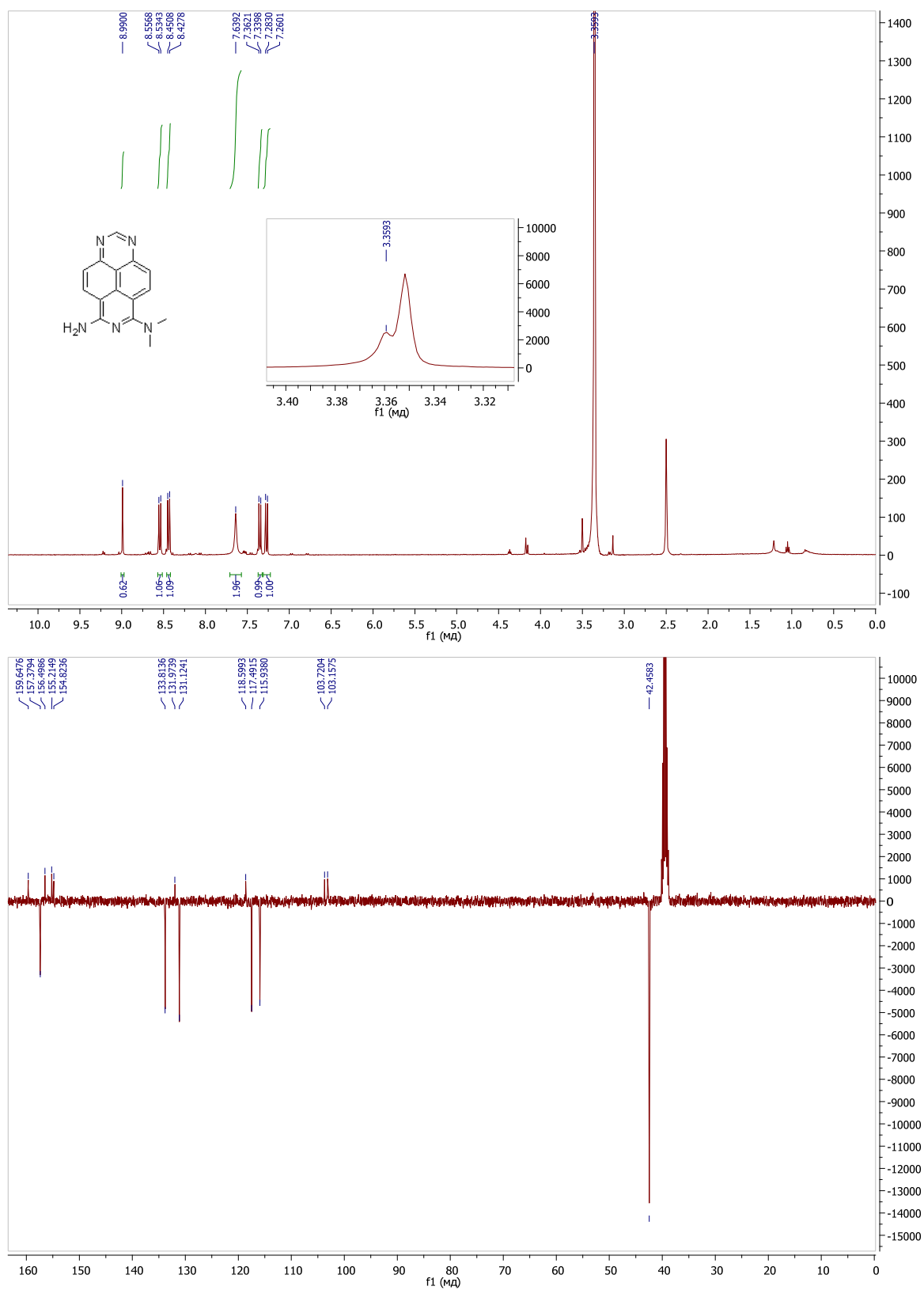
8-(4'-Tolyl)-1,3,7-triazapyren-6-amine (3b)



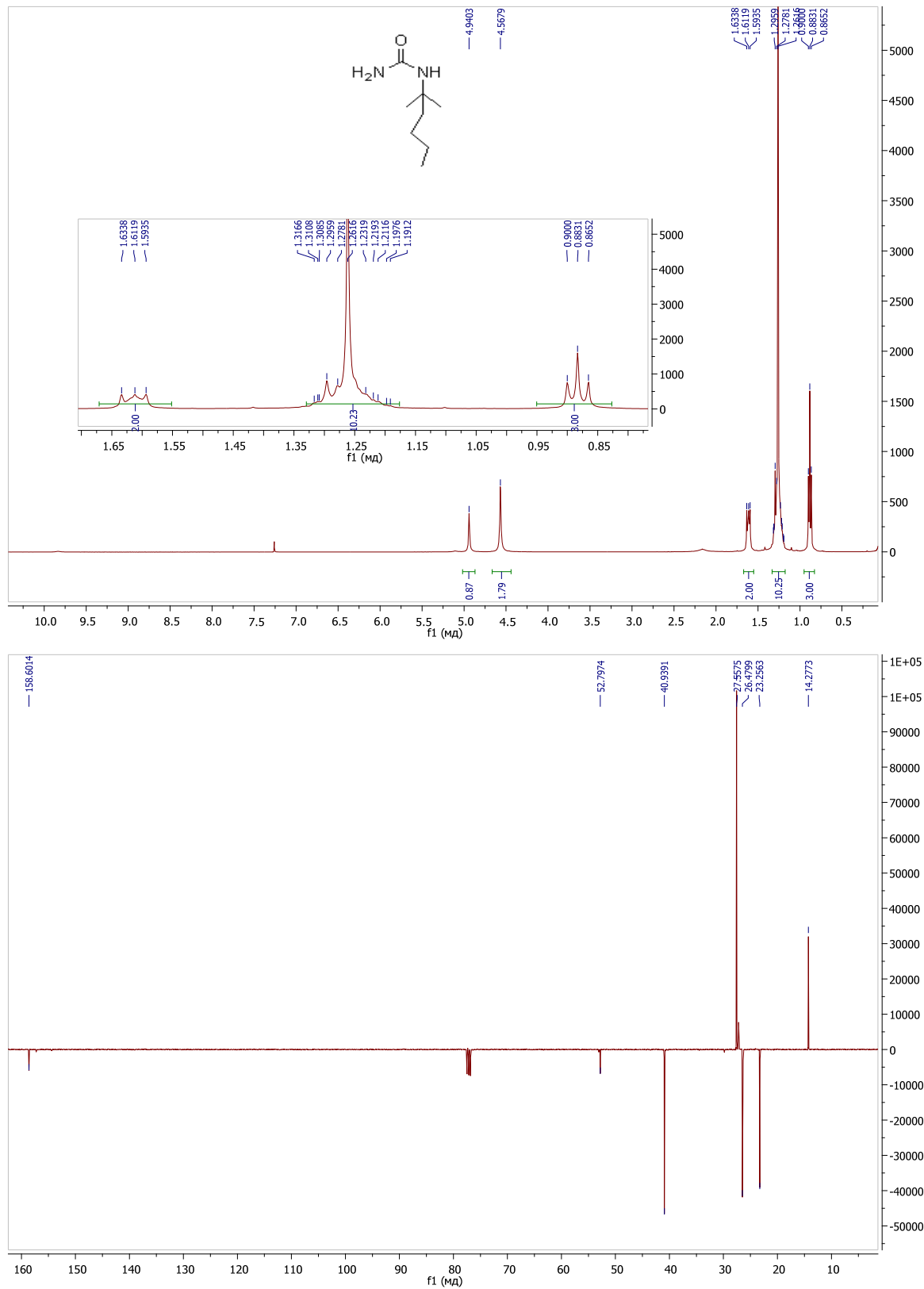
8-(3',4'-Dimethylphenyl)-1,3,7-triazapyren-6-amine (3c)

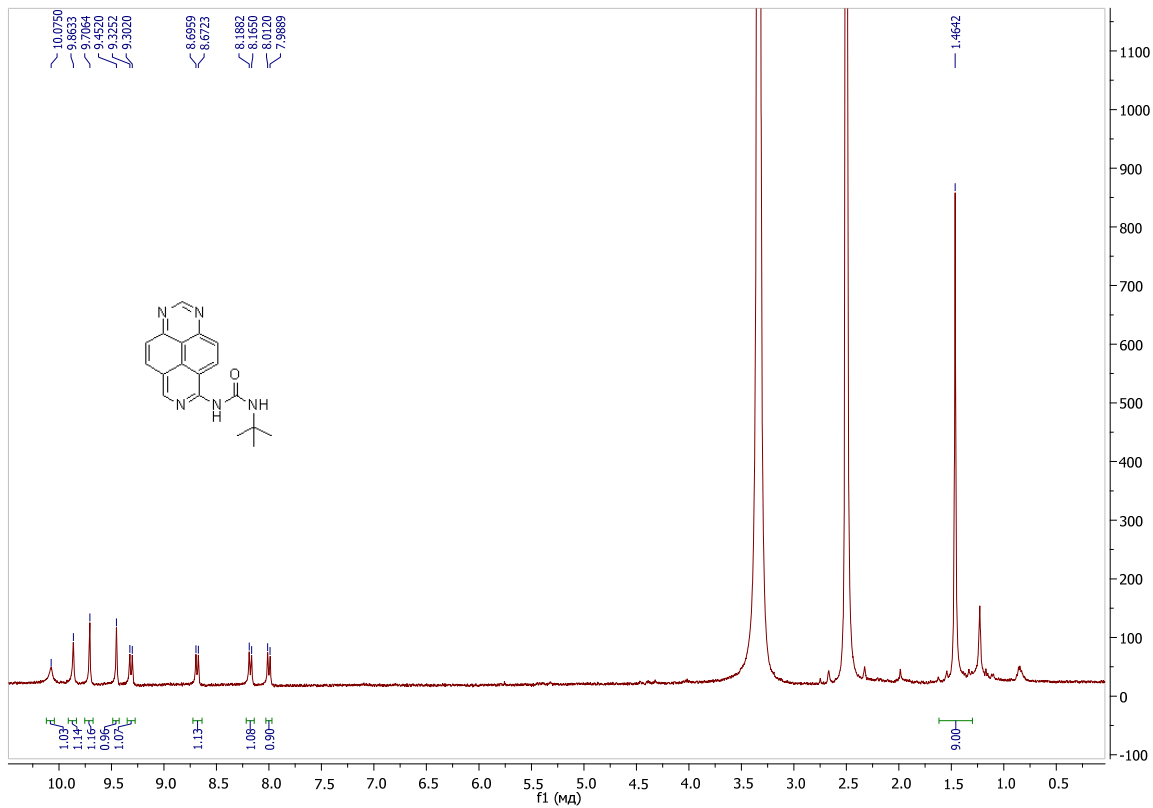
8-(4'-Methoxyphenyl)-1,3,7-triazapyren-6-amine (3d).

8-(4'-Ethoxyphenyl)-1,3,7-triazapyren-6-amine (3e).

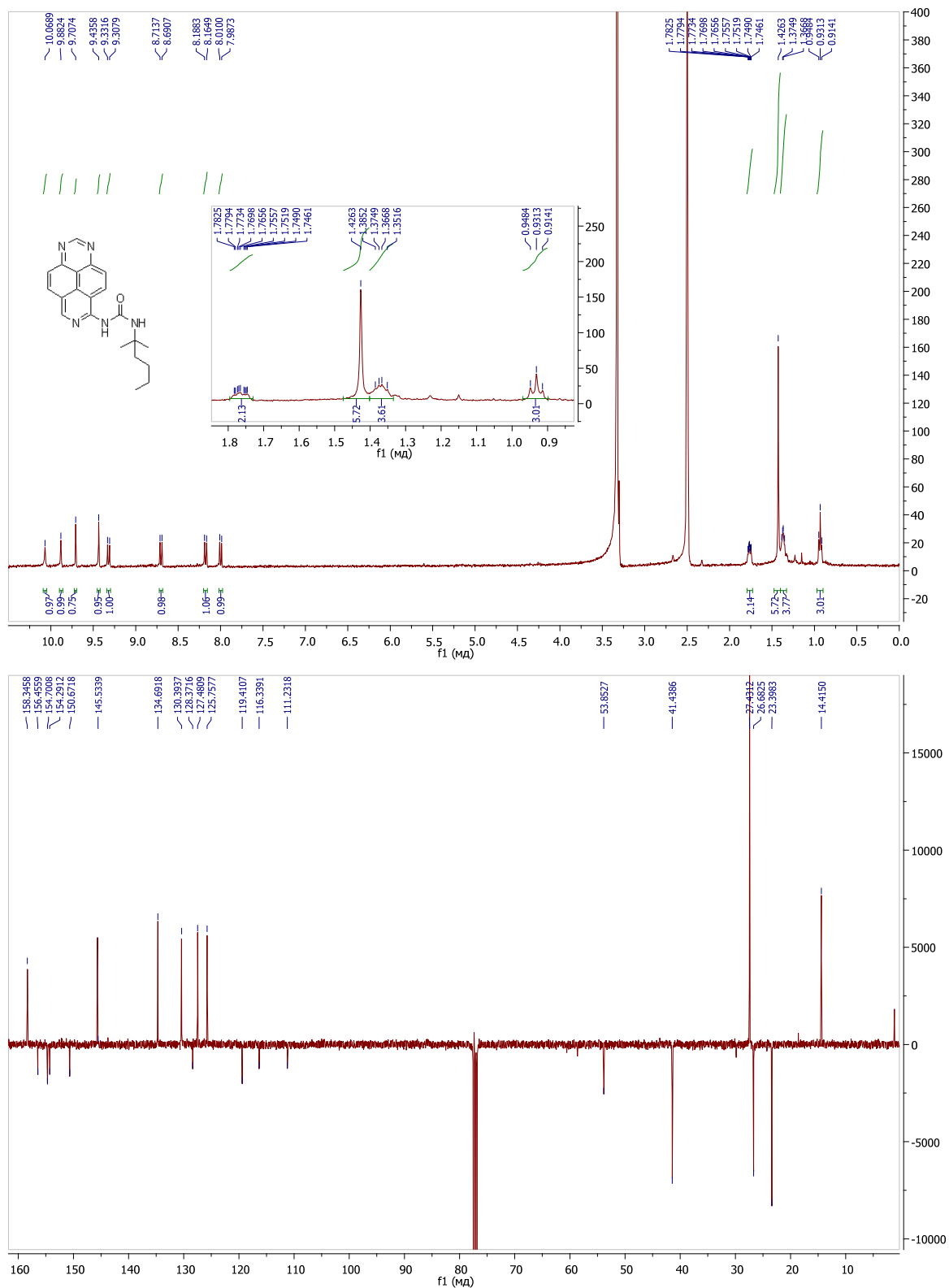
N,N-Dimethyl-1,3,7-triazapyren-6,8-diamine (3f).

(1,1-Dimethyl-pentyl)-urea



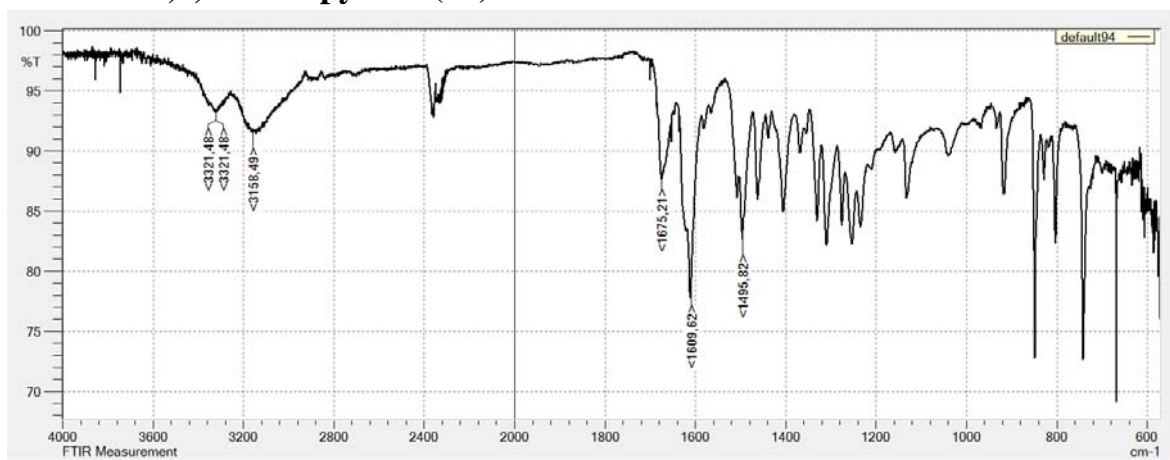
1-(tert-Butyl)-3-(1,3,7-triazapyren-6-yl)-urea (9a)

¹³C NMR spectrum of compound 10a could not be acquired due to insufficient solubility.

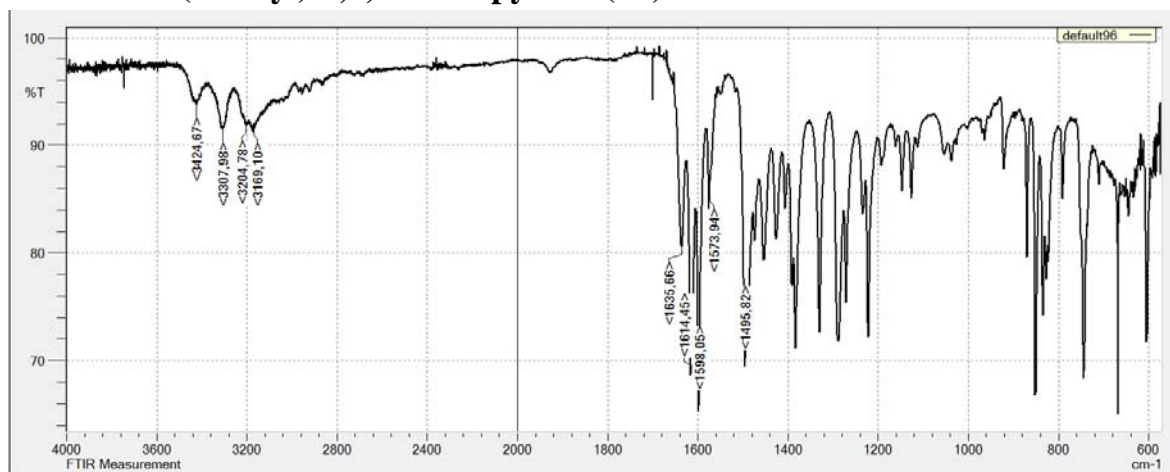
1-(1,1-dimethyl-pentyl)-3-(1,3,7-triazapyren-6-yl)-urea (9b)

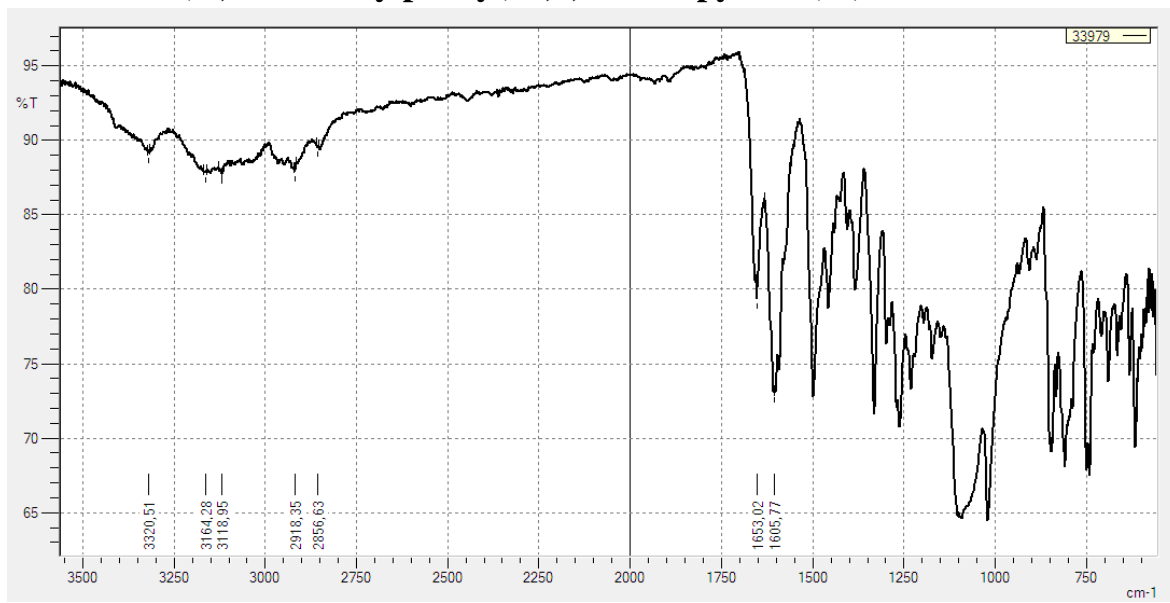
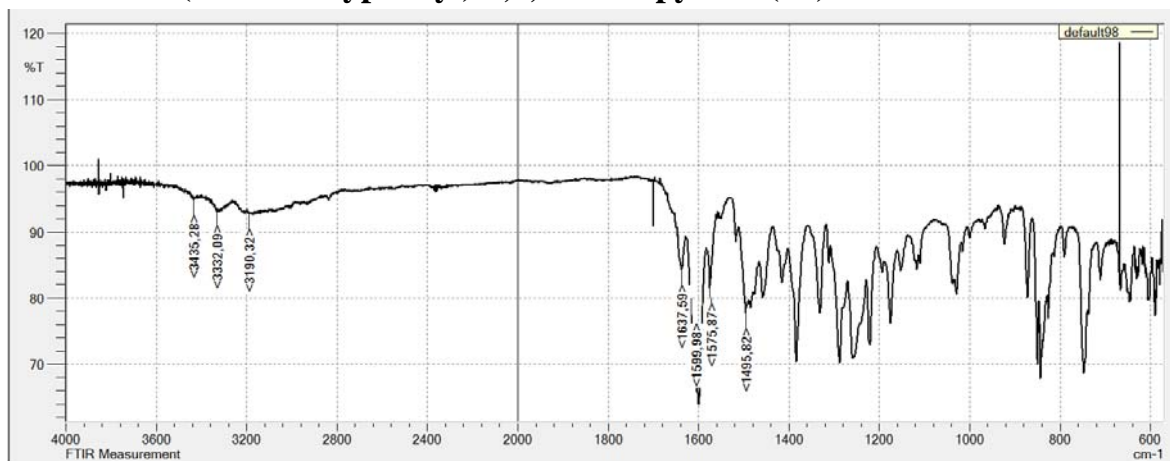
IR-Spectra

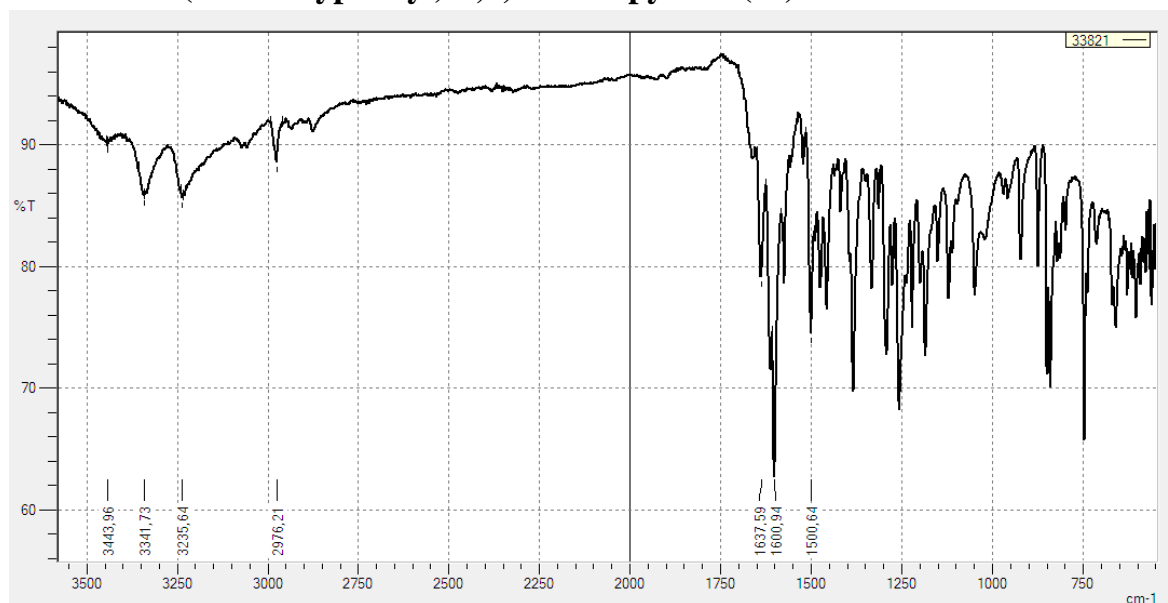
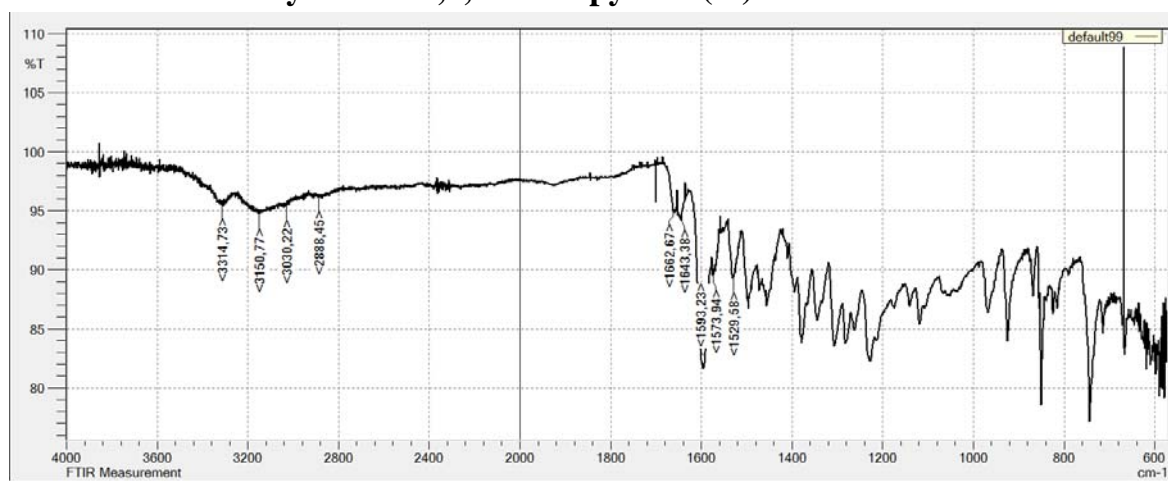
6-Amino-1,3,7-triazapyrene (3a)

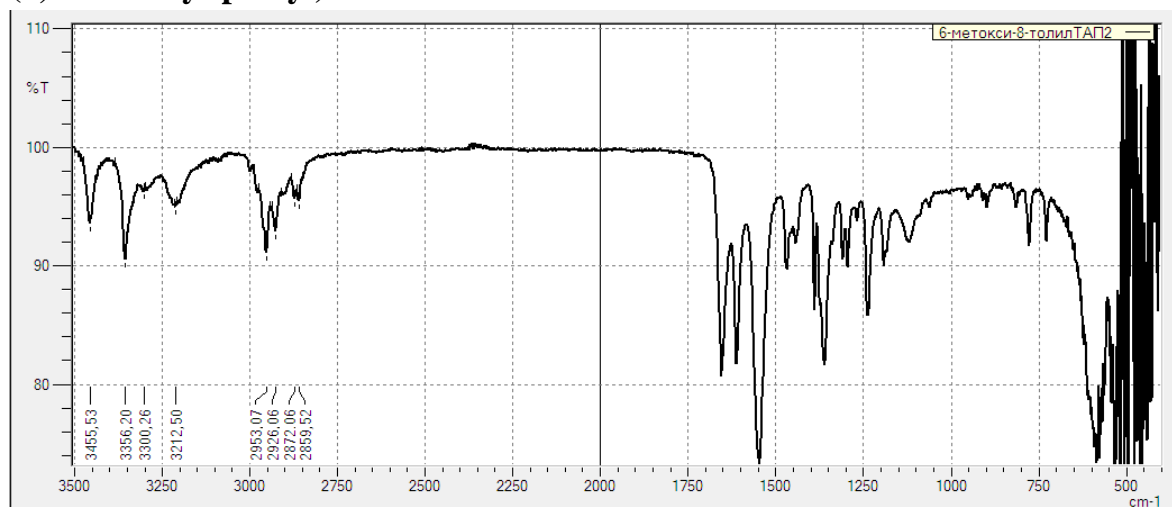
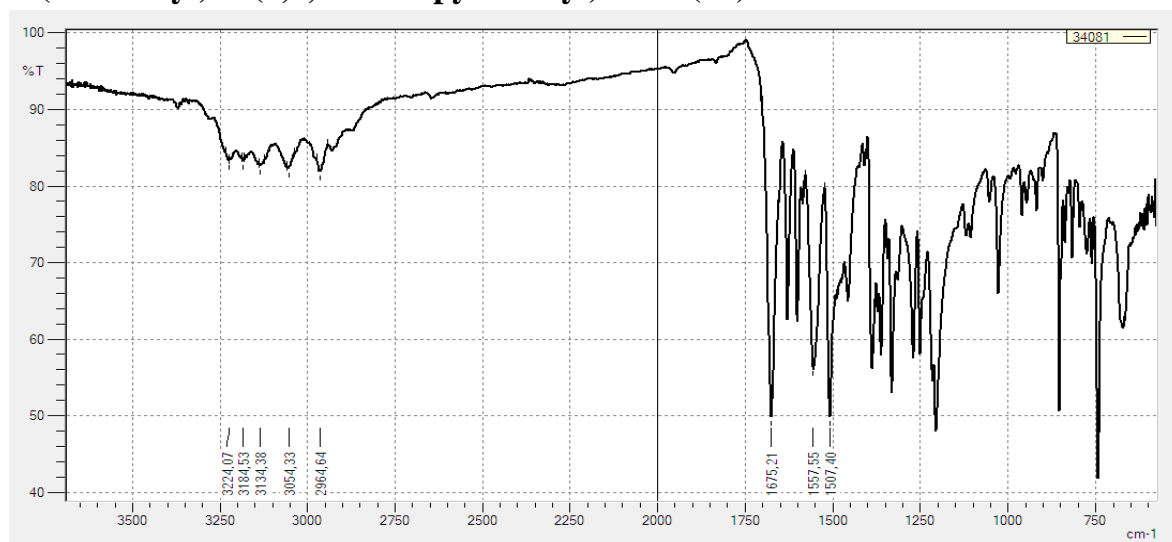


6-Amino-8-(4'-tolyl)-1,3,7-triazapyrene (3b)



6-Amino-8-(3',4'-dimethylphenyl)-1,3,7-triazapyrene (3c)**6-Amino-8-(4'-methoxyphenyl)-1,3,7-triazapyrene (3d)**

6-Amino-8-(4'-ethoxyphenyl)-1,3,7-triazapyrene (3e)**6-Amino-8-dimethylamino-1,3,7-triazapyrene (3f)**

(1,1-dimethyl-pentyl)-urea**1-(tert-Butyl)-3-(1,3,7-triazapyren-6-yl)-urea (9a)****1-(1,1-dimethylpentyl)-3-(1,3,7-triazapyren-6-yl)-urea (9b)**