# Supporting Information File

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## SYNTHESIS OF 2,2-DIMETHYL-2,3-DIHYDROPYRIDO[3',2':4,5]THIENO[3,2-d]PYRIMIDIN-4(1H)-ONES BY REACTION OF 3-AMINOTHIENO[2,3-b]PYRIDIN-2-CARBOXAMIDES WITH ACETONE

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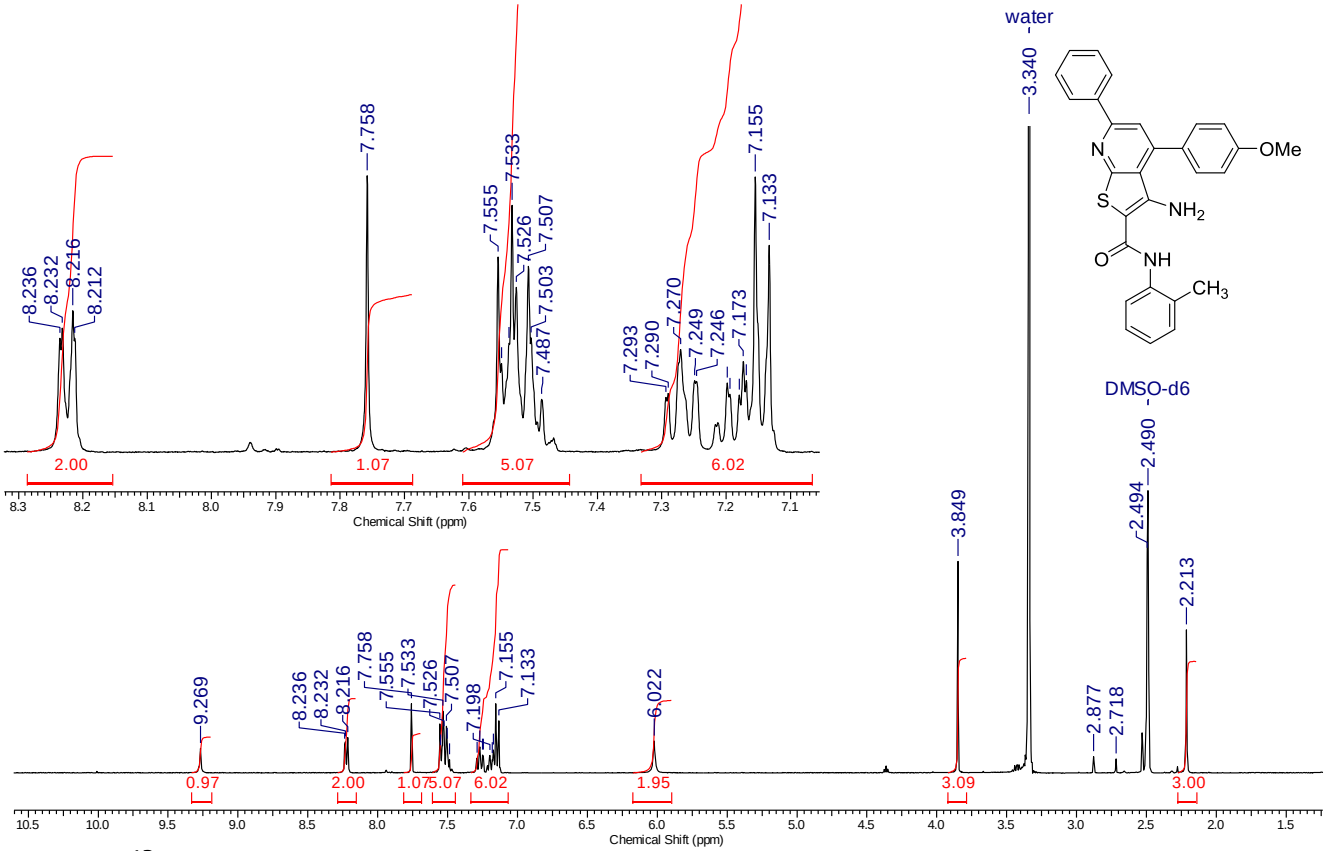
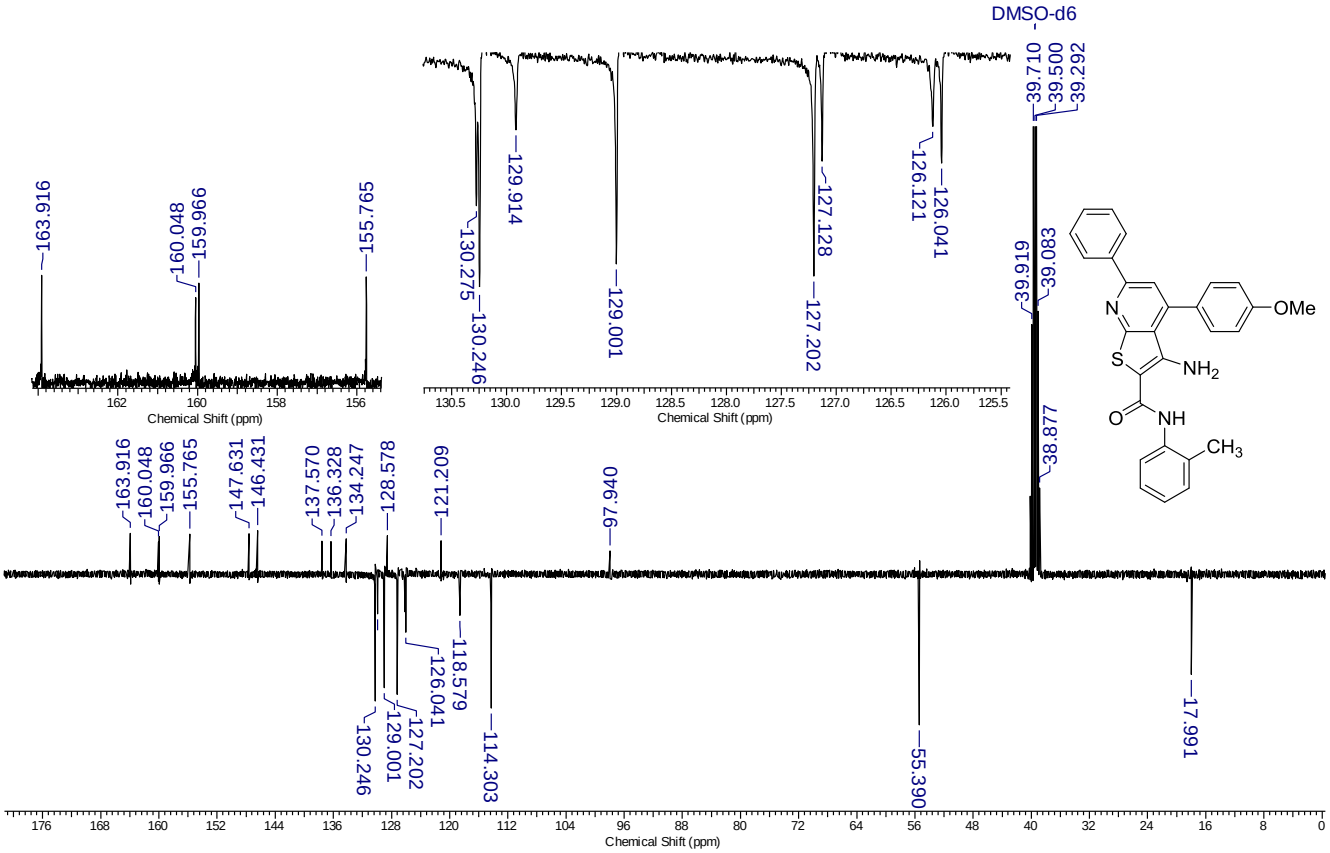
# Contents

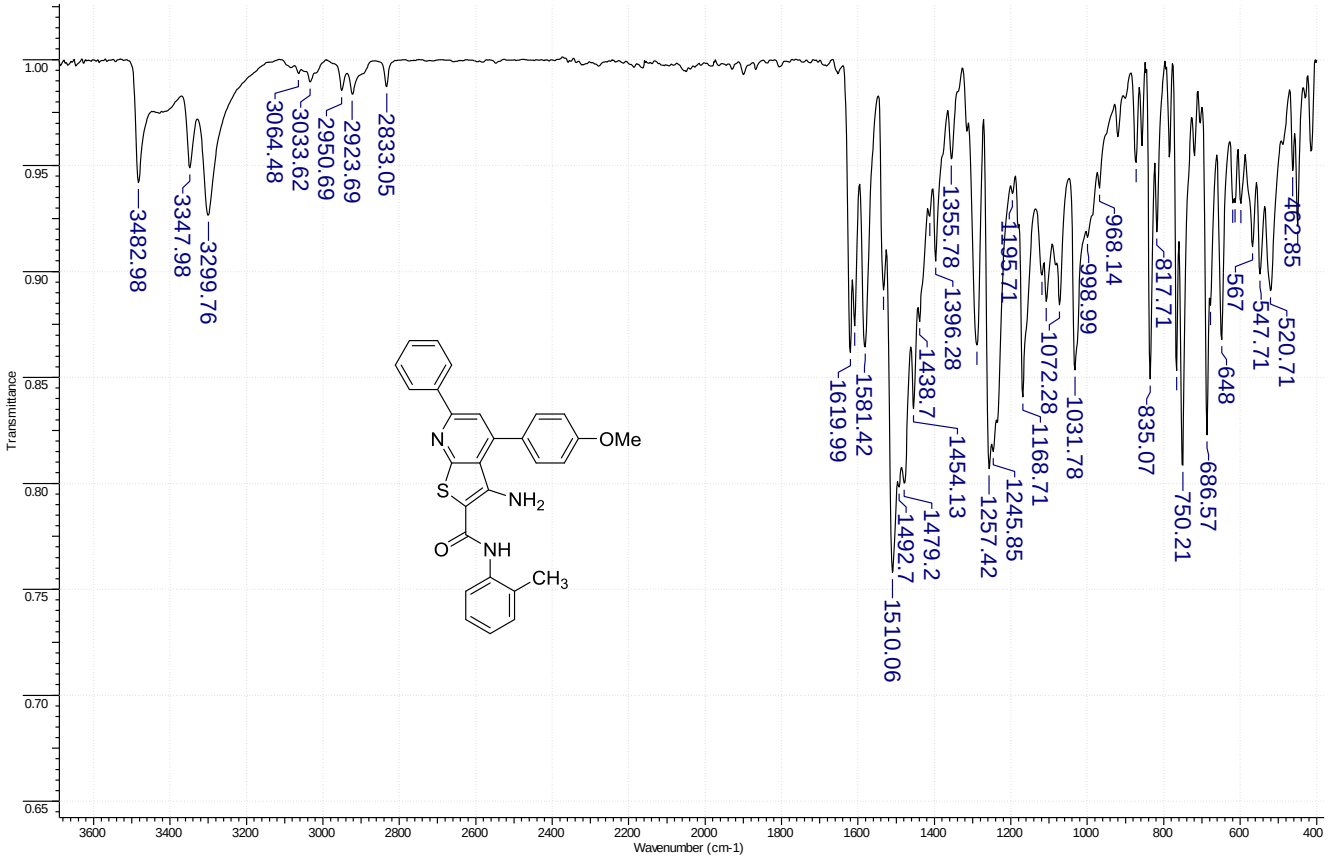
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 7a




## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 7a

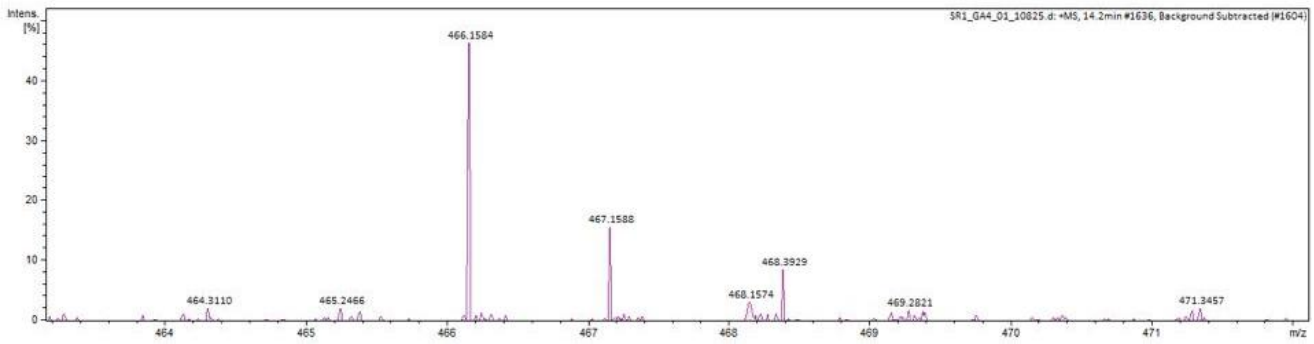


## FT-IR spectrum (ATR mode) of compound 7a

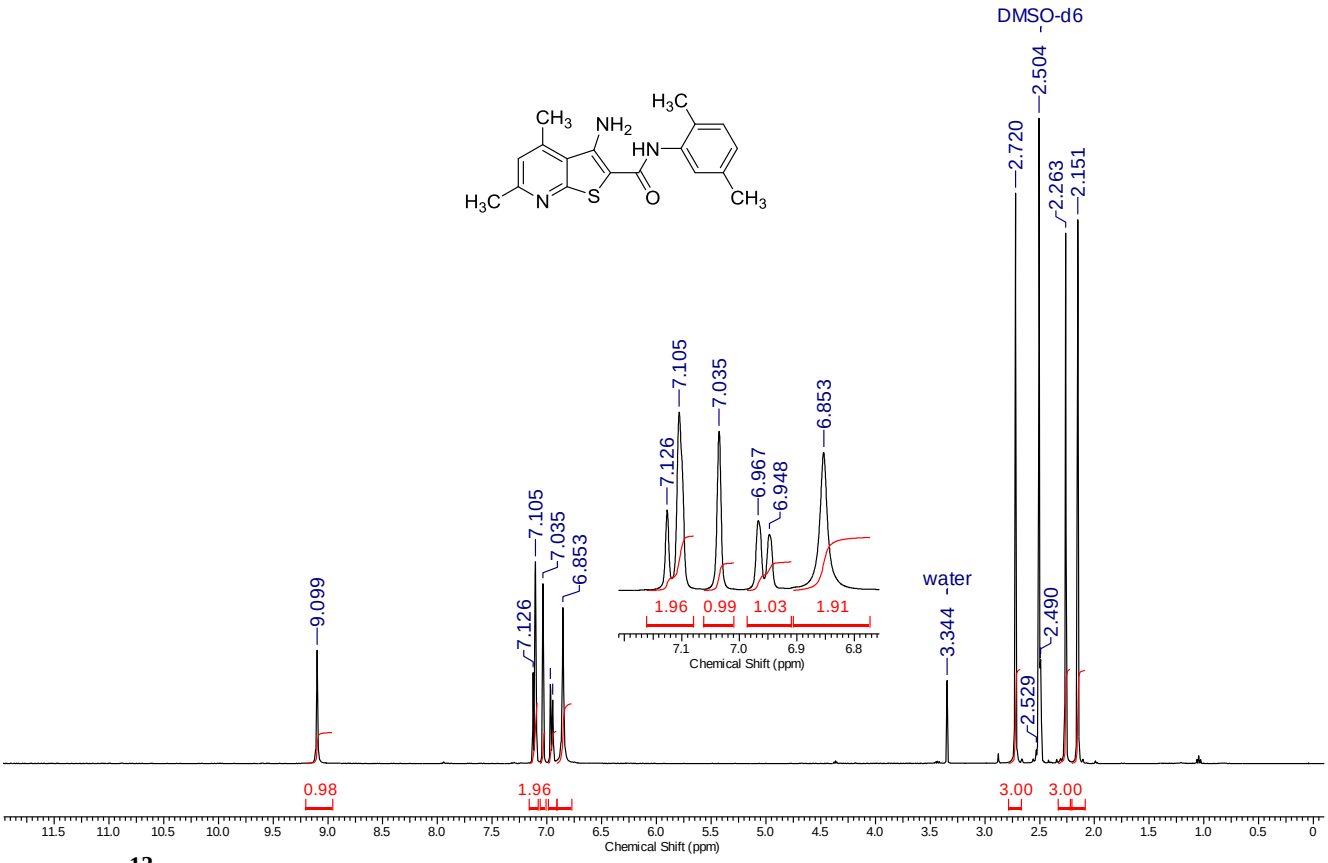



## HRMS spectrum of compound 7a

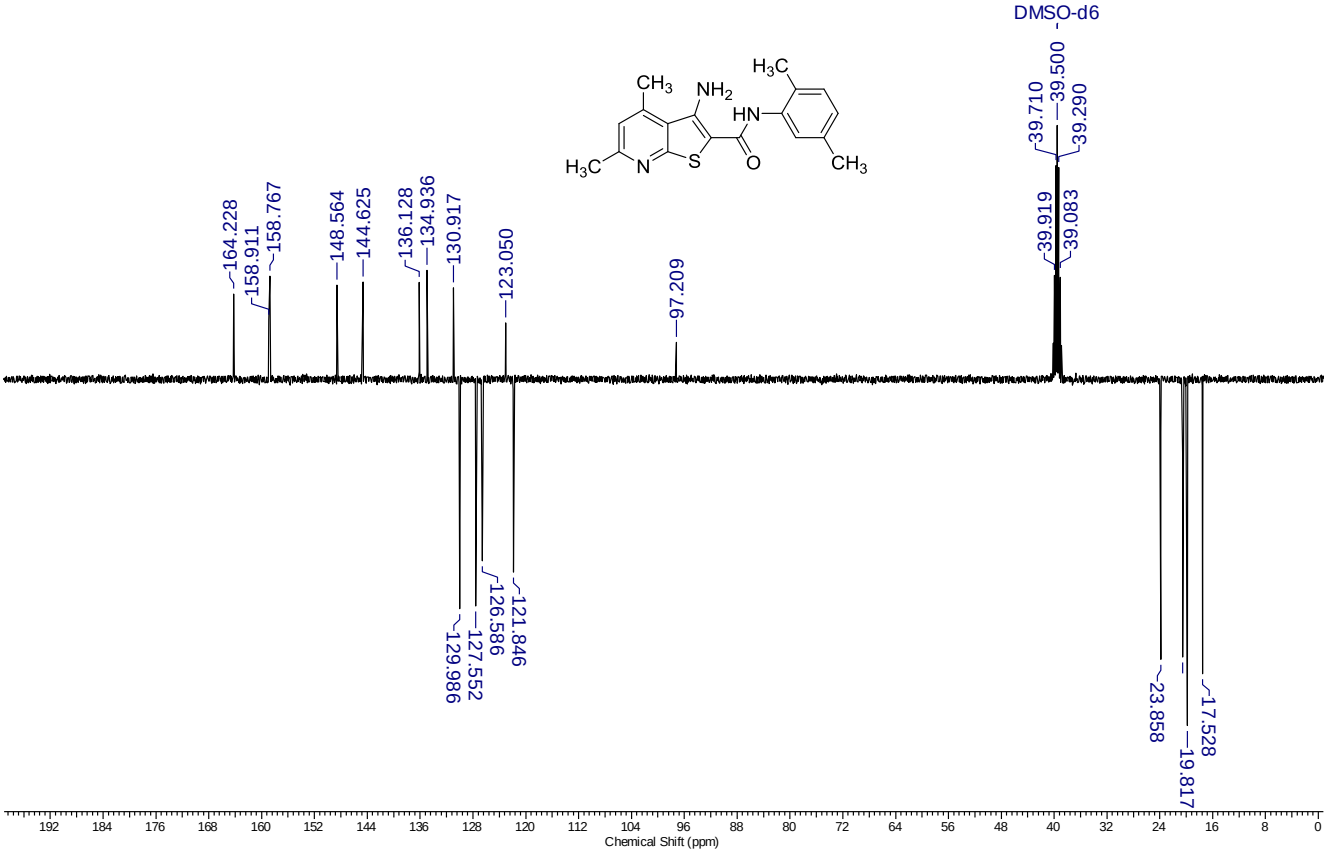
Calculated for $C_{28}H_{24}N_3O_2S$ [M+1]: 466.1589; Found 466.1584, Δ 1.07 ppm



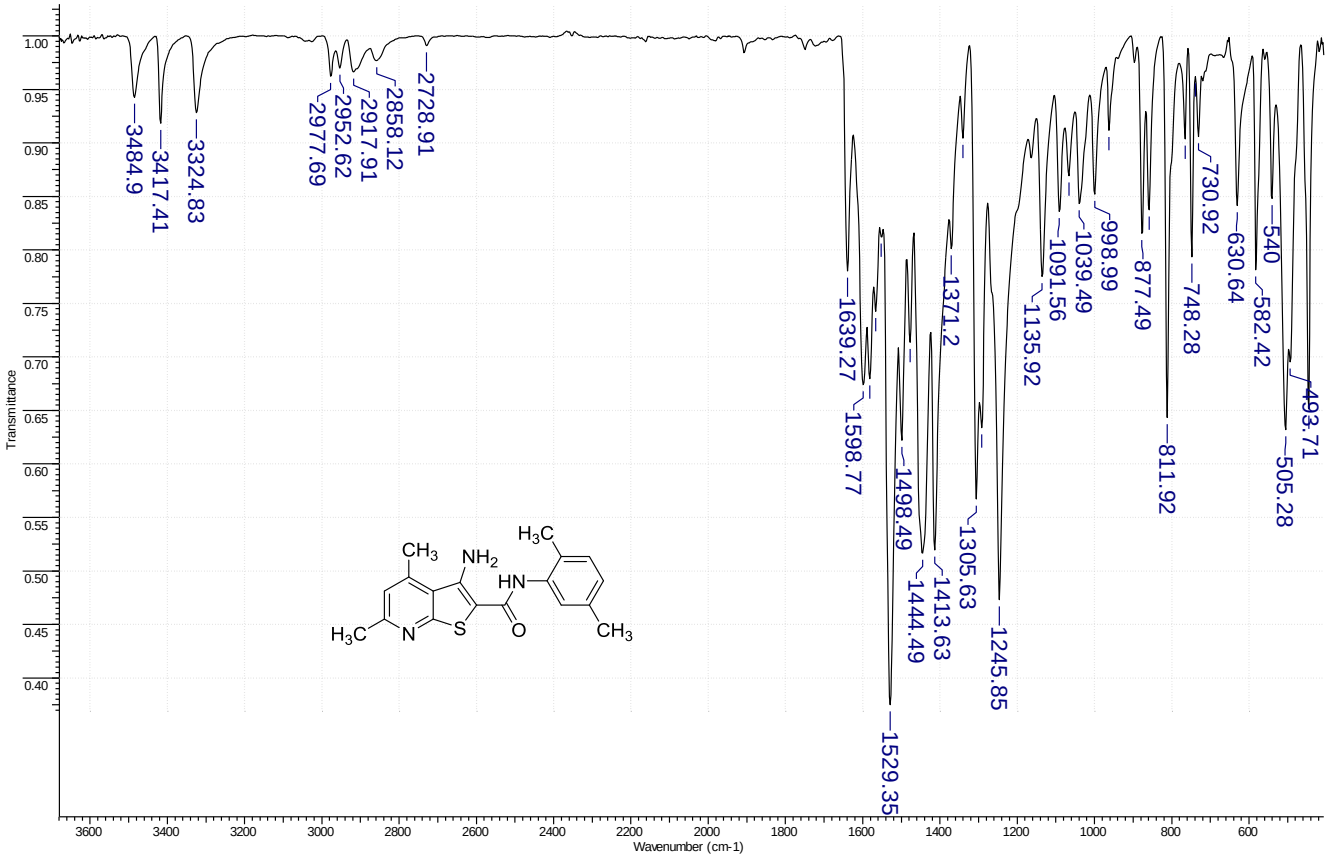
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 7b




## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 7b

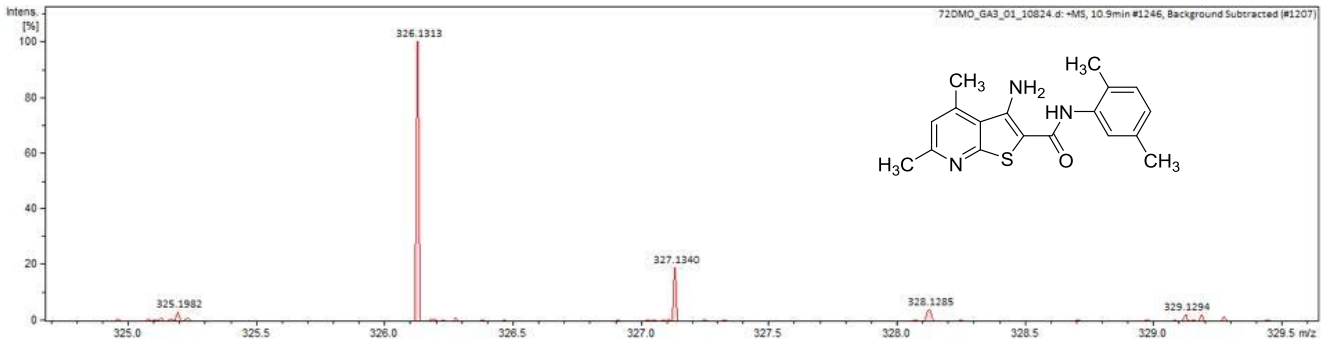


## FT-IR spectrum (ATR mode) of compound 7b

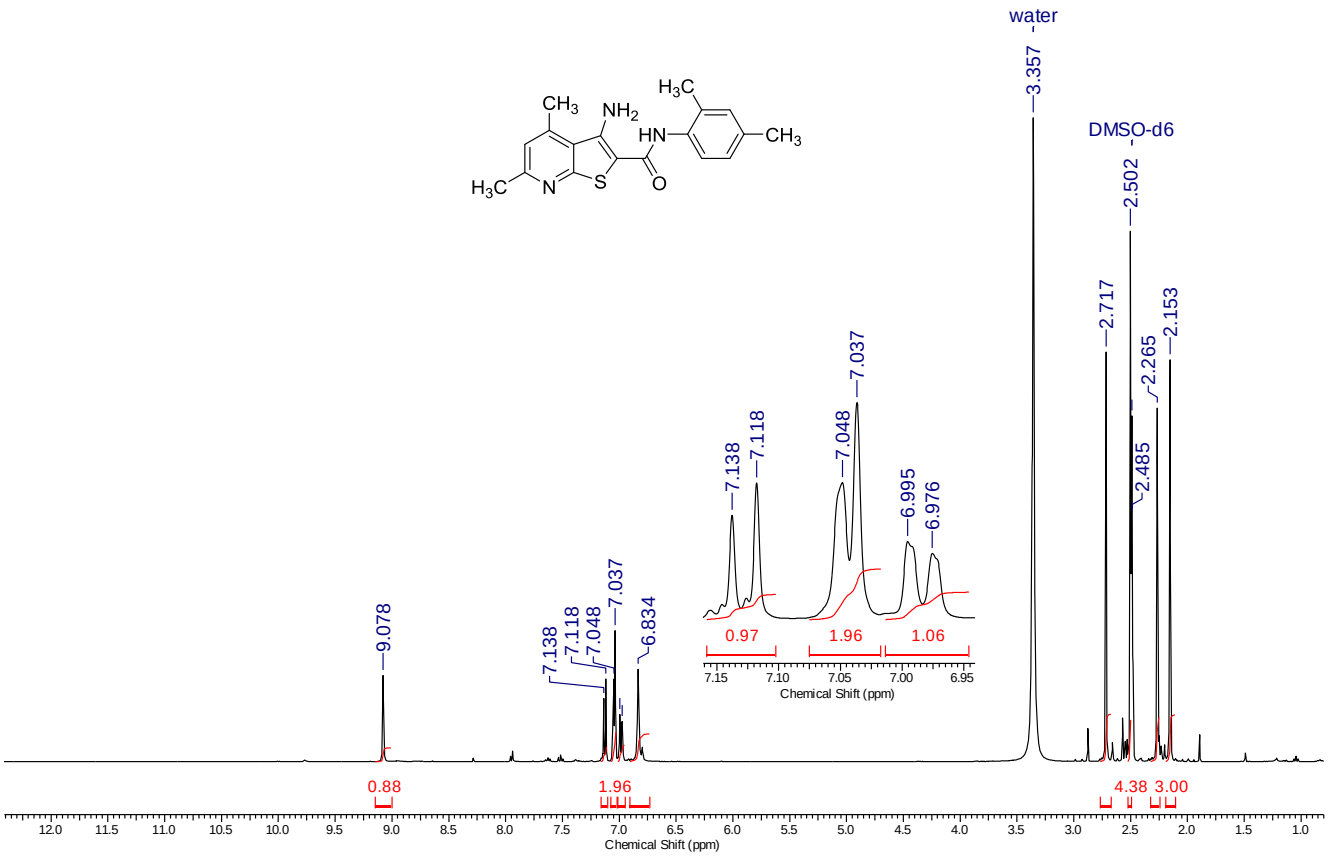



## HRMS spectrum of compound 7b

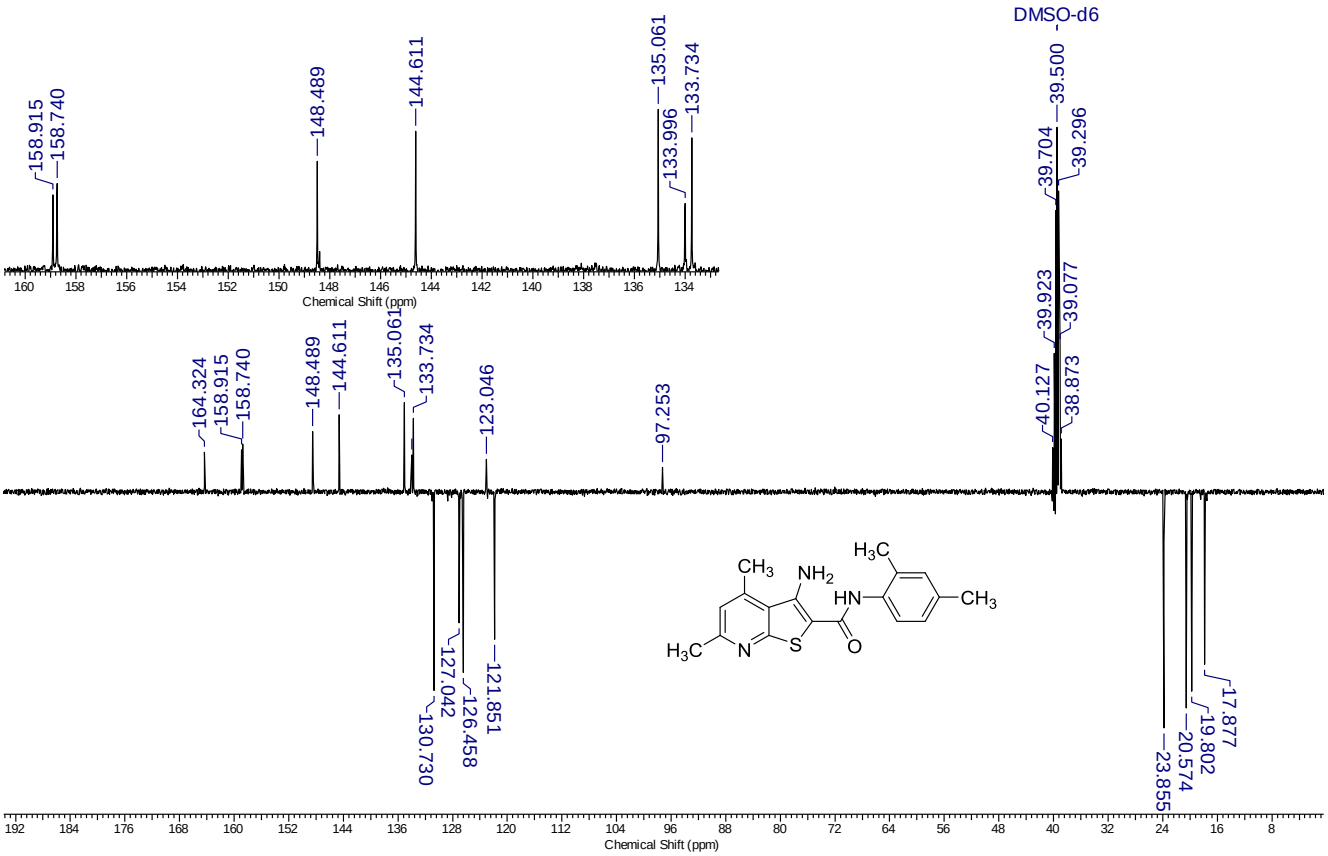
Calculated for $C_{18}H_{20}N_3OS$ [M+1]: 326.1327; Found 326.1313; Δ 4.29 ppm



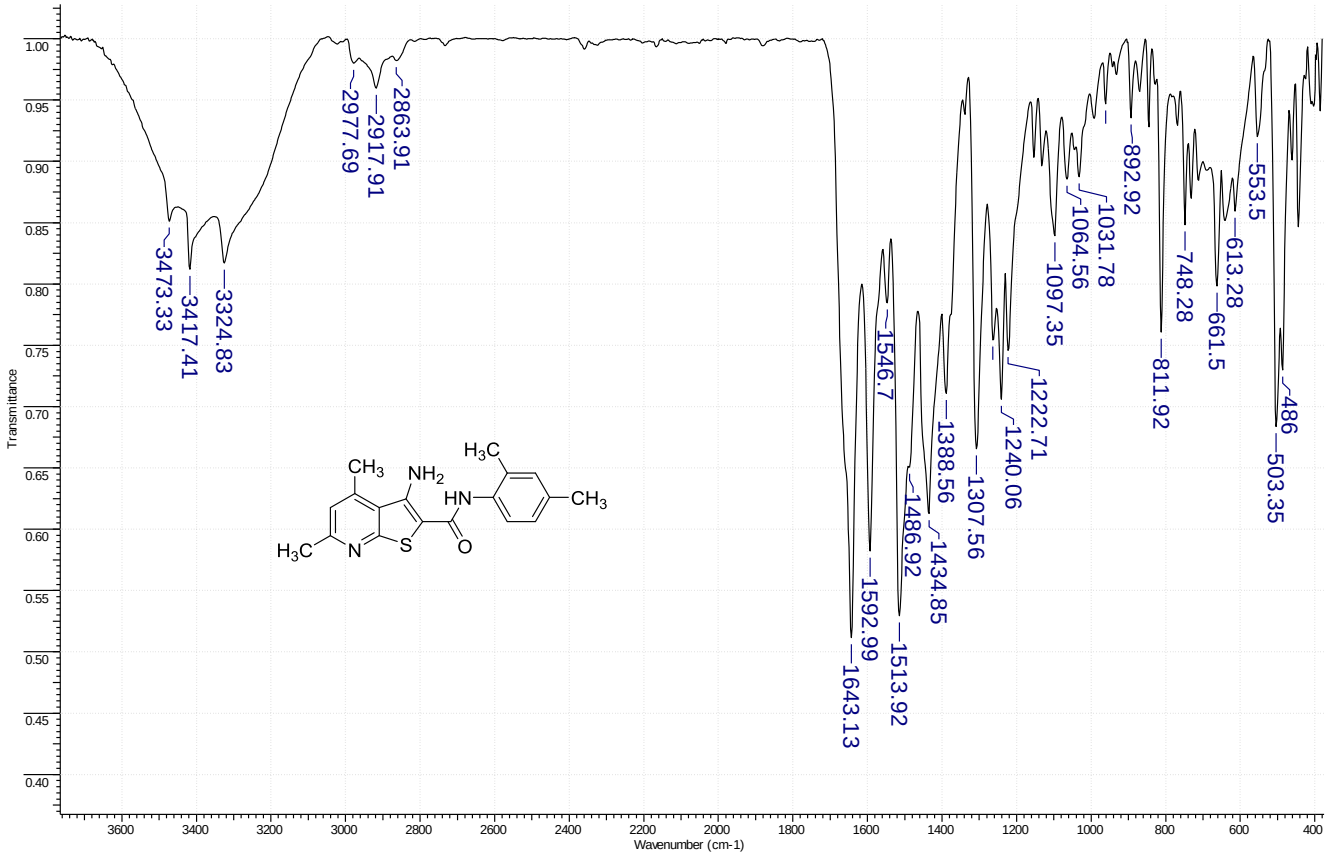
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 7c




## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 7c

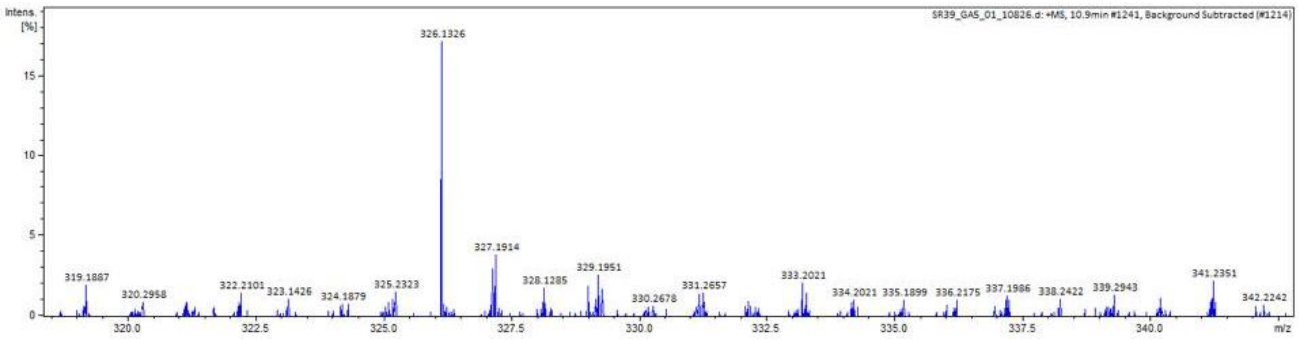


## FT-IR spectrum (ATR mode) of compound 7c

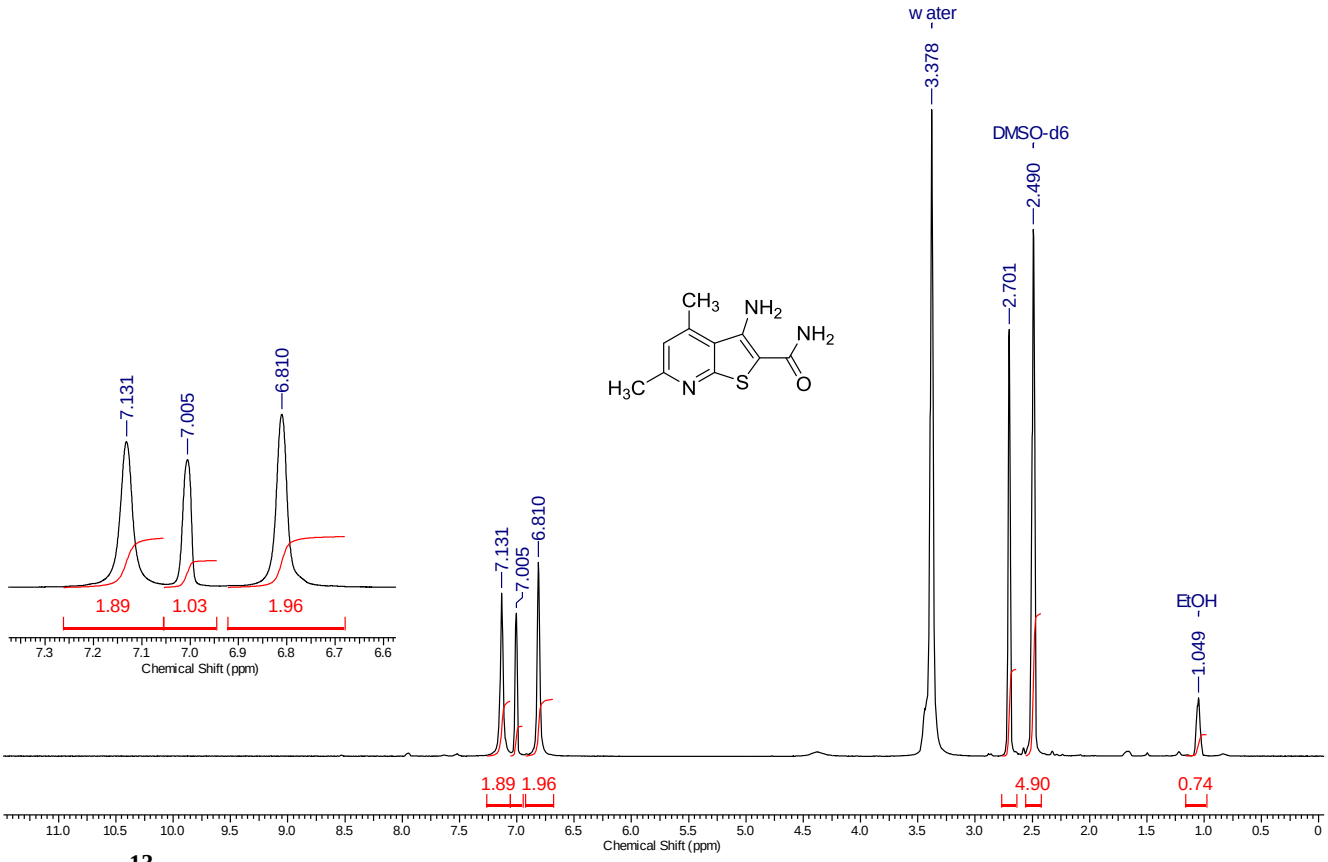



## HRMS spectrum of compound 7c

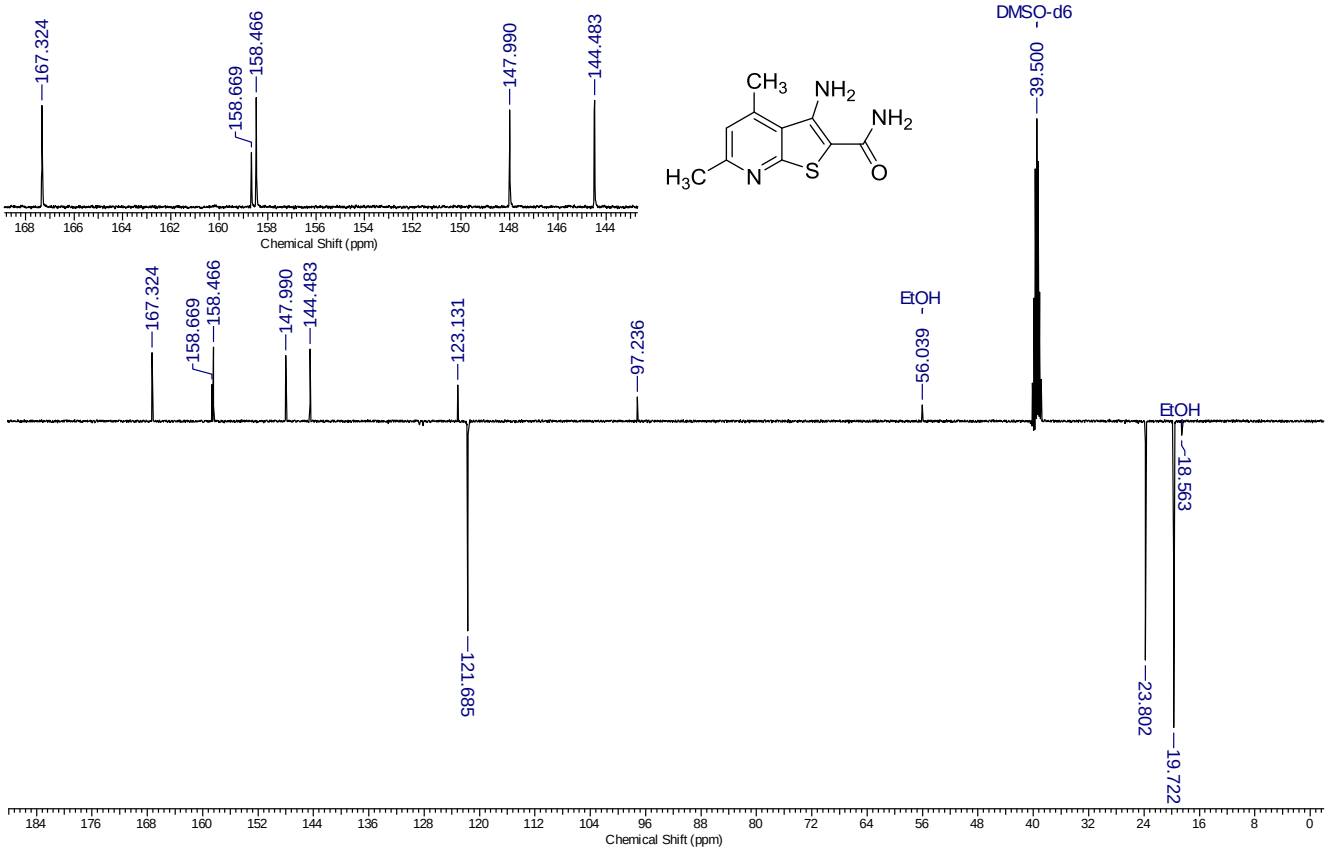
Calculated for $C_{18}H_{20}N_3OS$ [M+1]: 326.1327; Found 326.1326; Δ 0.31 ppm



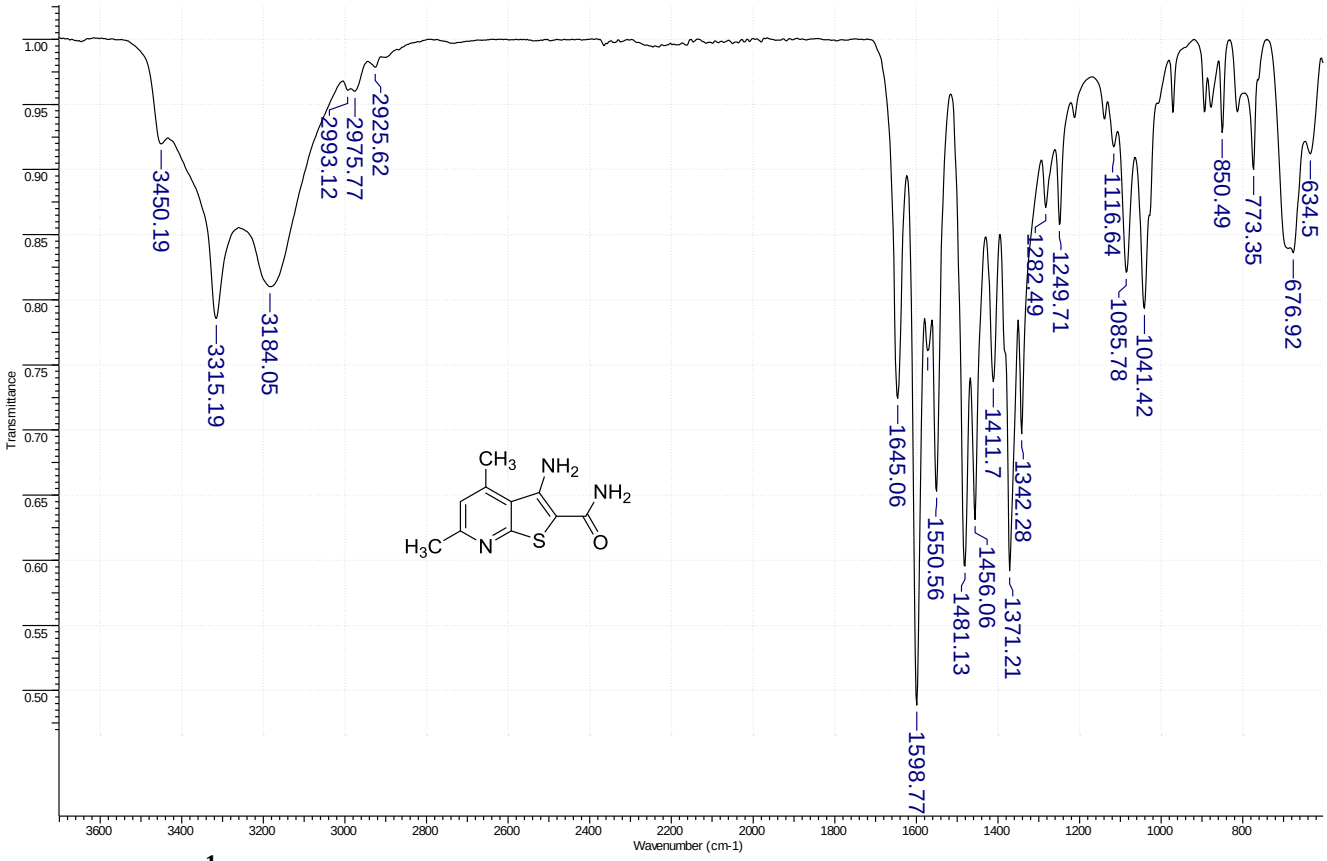
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 7d



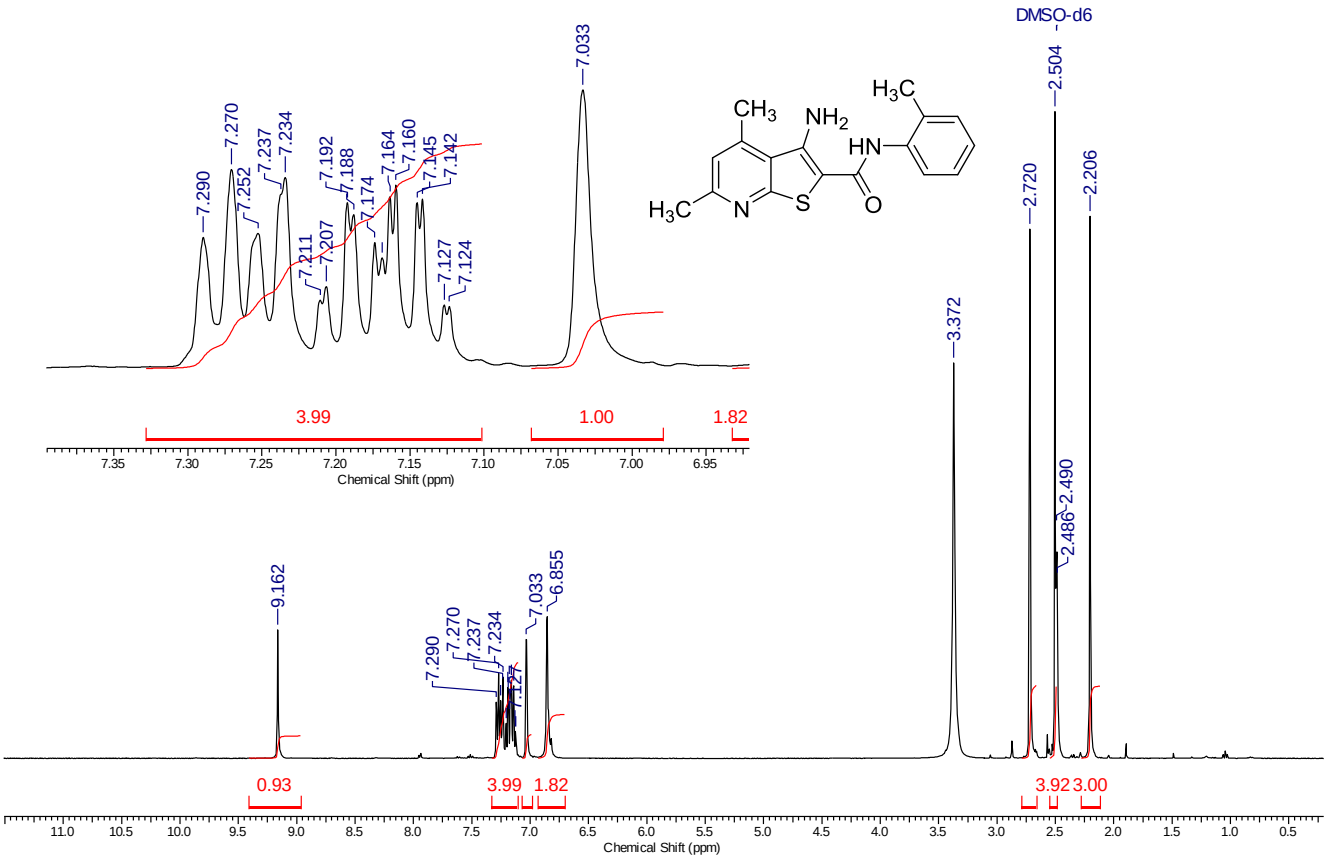

## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 7d



## FT-IR spectrum (ATR mode) of compound 7d




## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 7e



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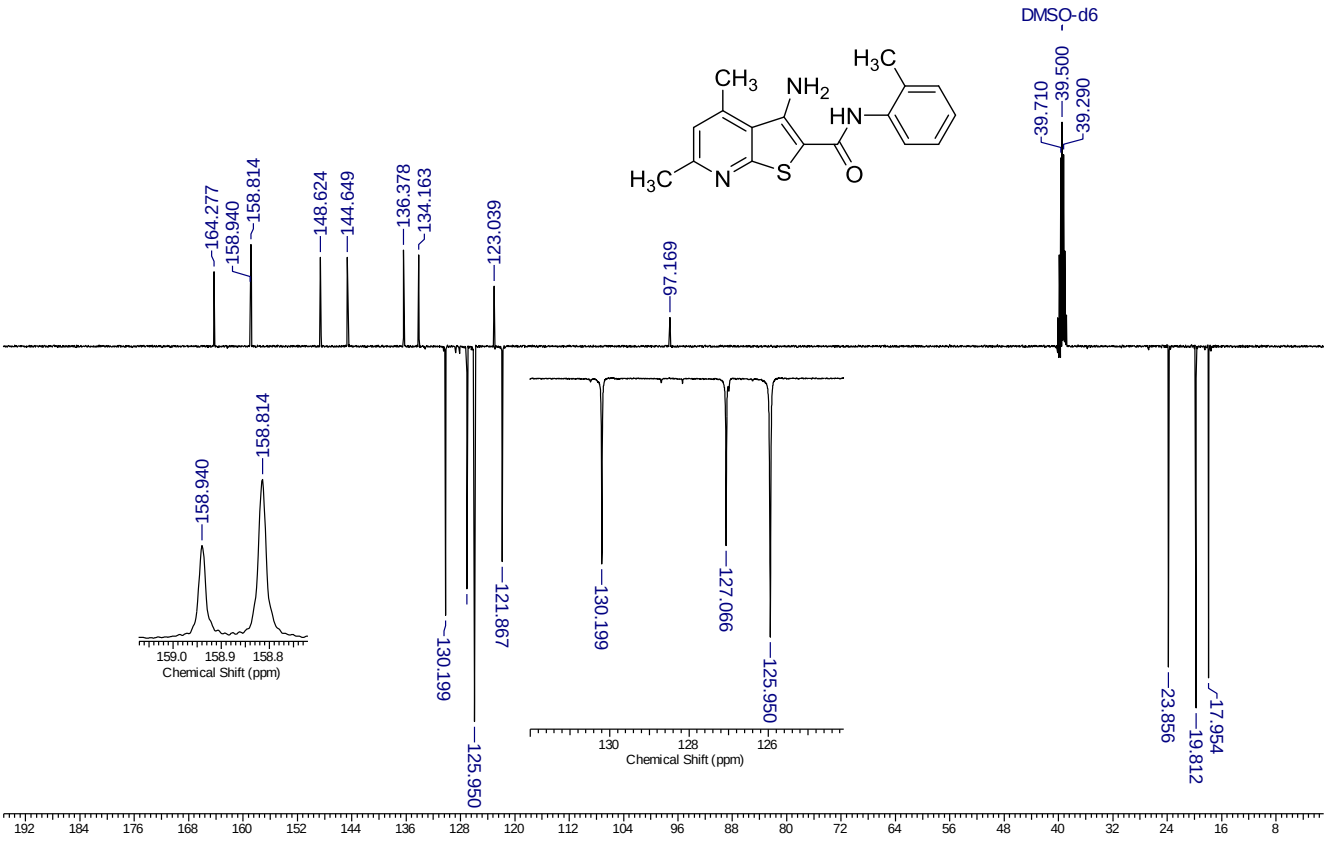
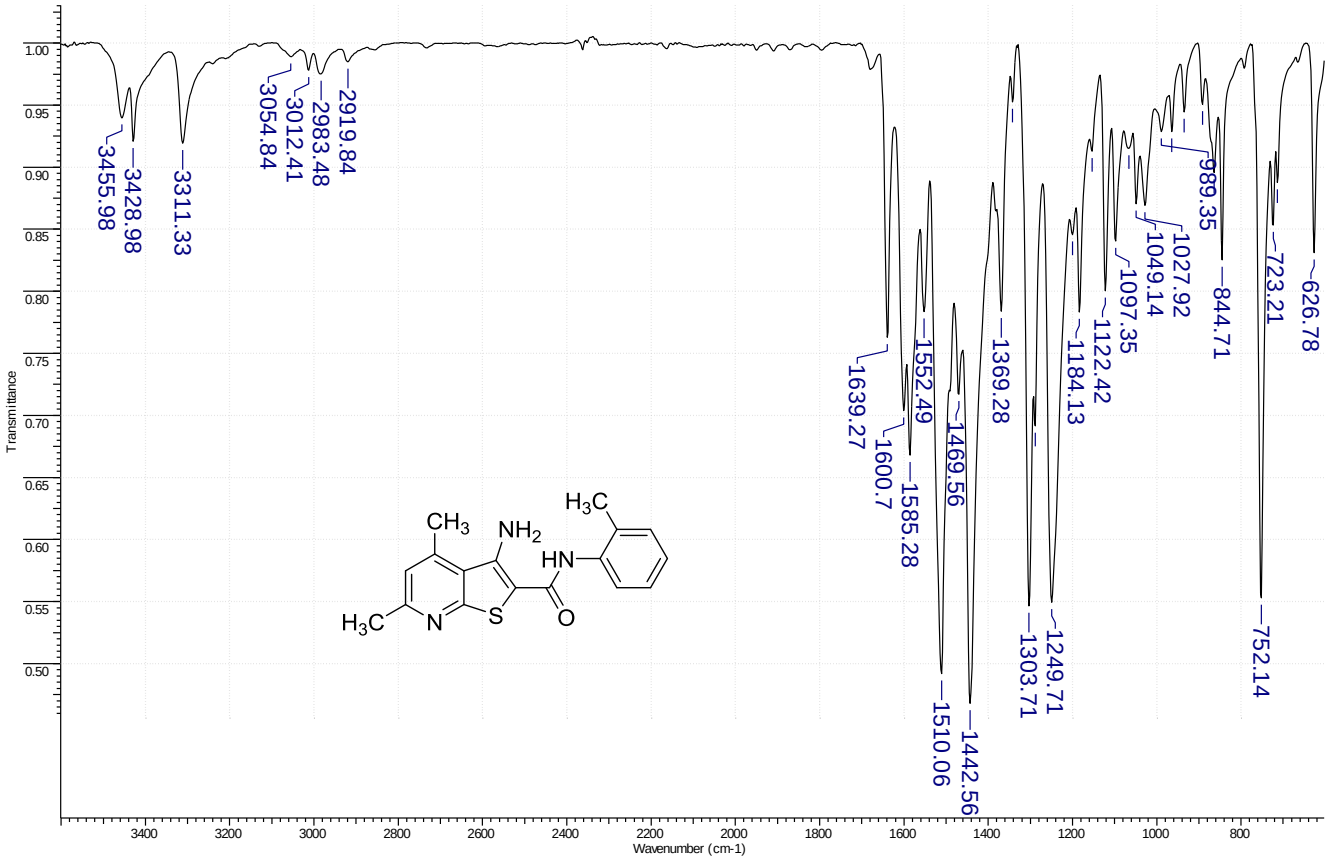
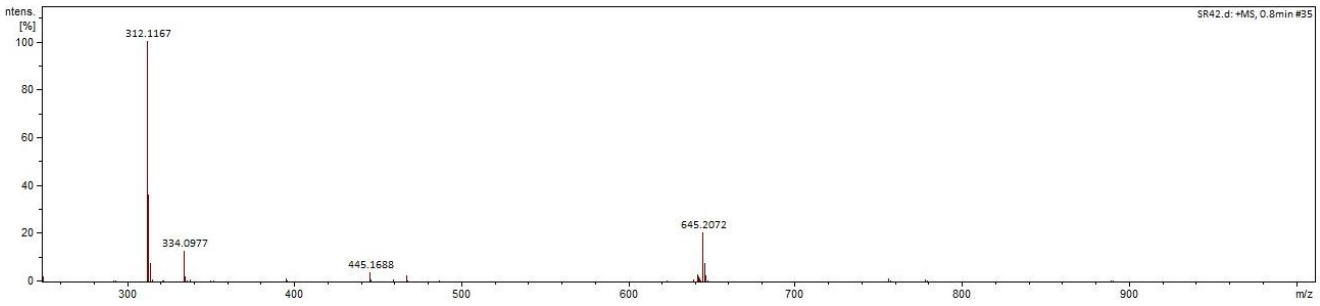


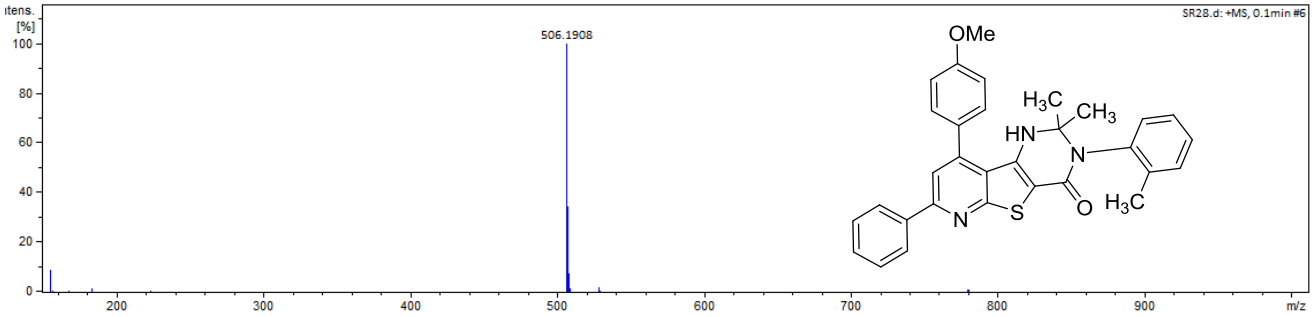
## HRMS spectrum of compound 7e

Calculated for $C_{17}H_{18}N_3OS$ [M+1]: 312.1171
Calculated for $C_{17}H_{17}N_3OSNa$ [M+23]: 334.0990
Calculated for $C_{34}H_{34}N_6O_2S_2Na$ [2M+23]: 645.2082

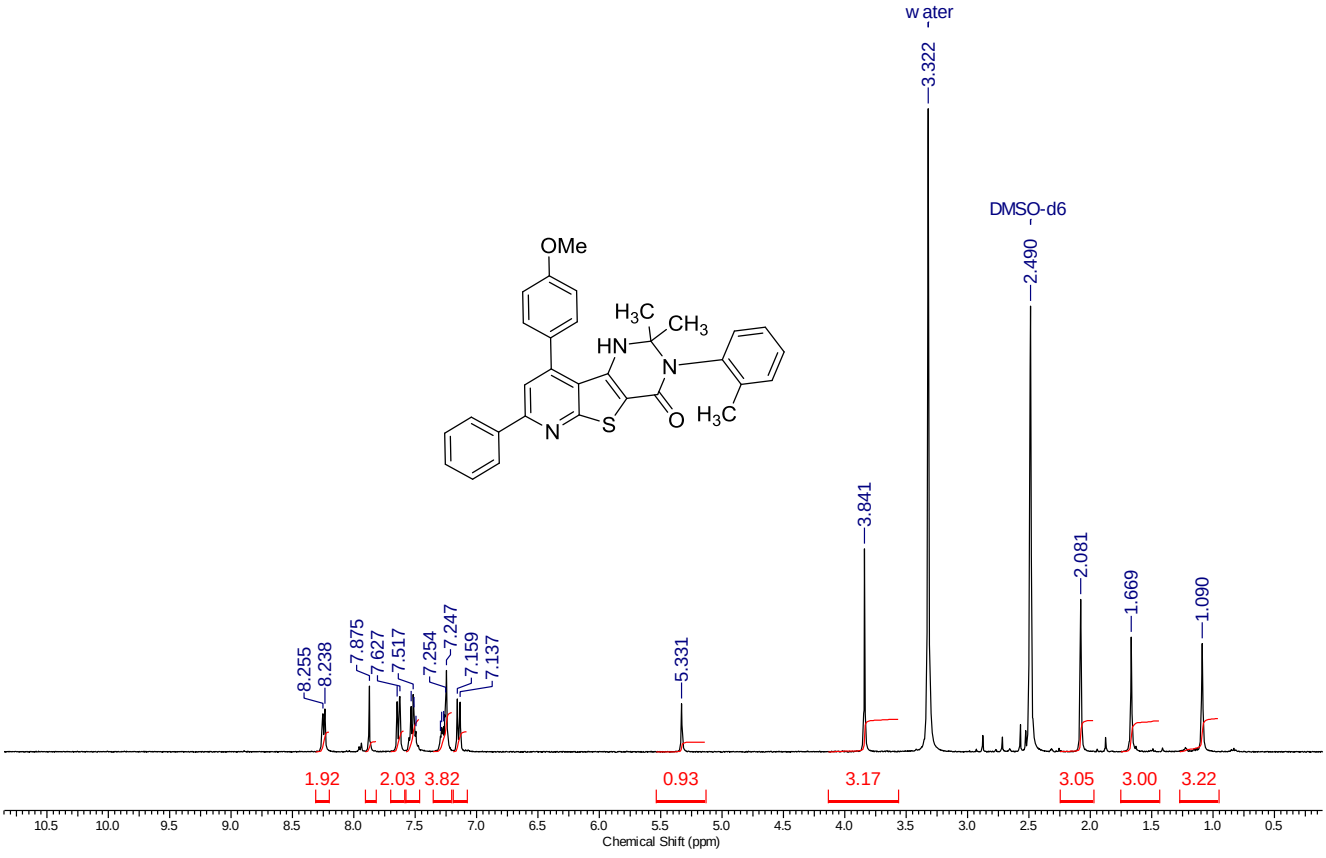



## HRMS spectrum of compound 8a

Calculated for $C_{31}H_{28}N_3O_2S$ [M+1]: 506.1902; Found 506.1908, Δ 1.18 ppm

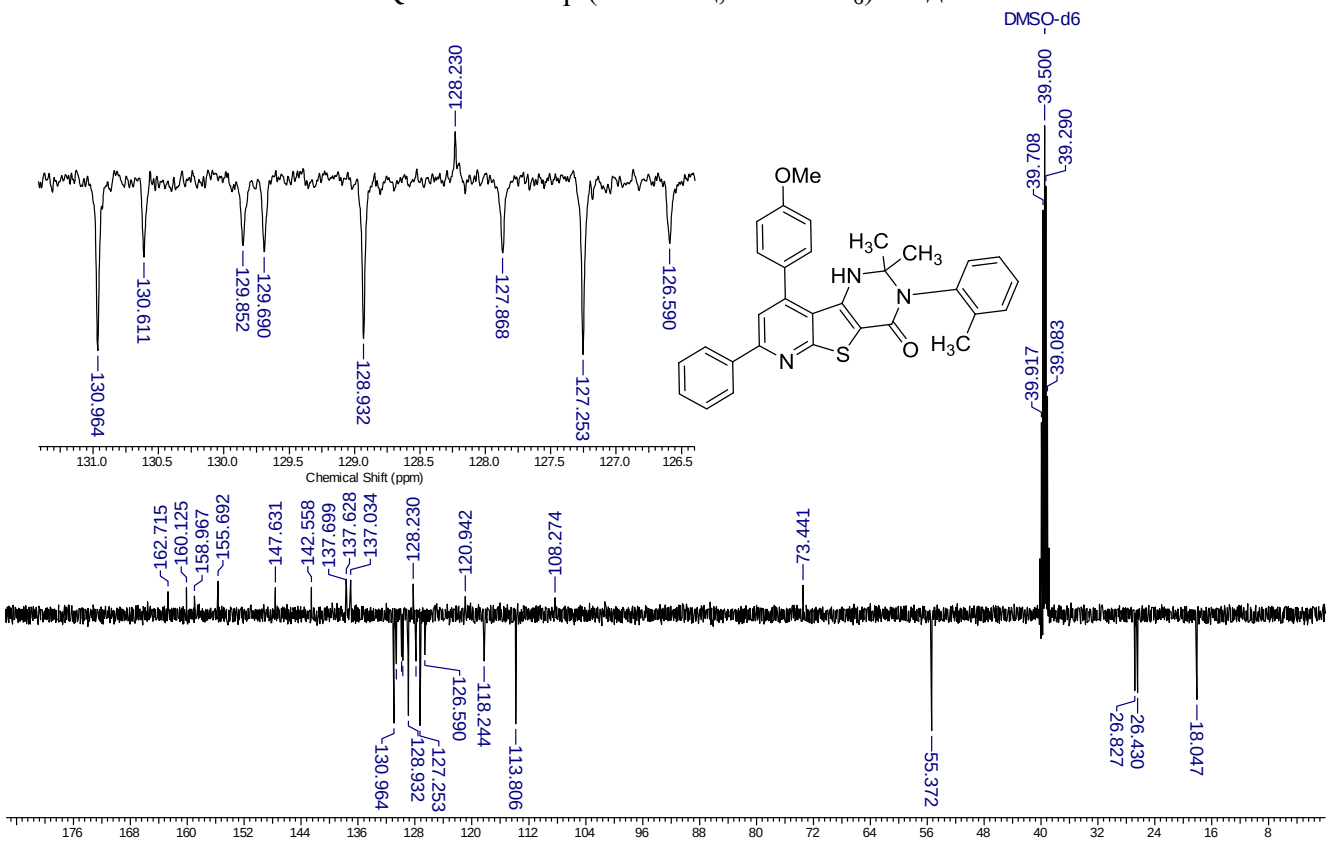


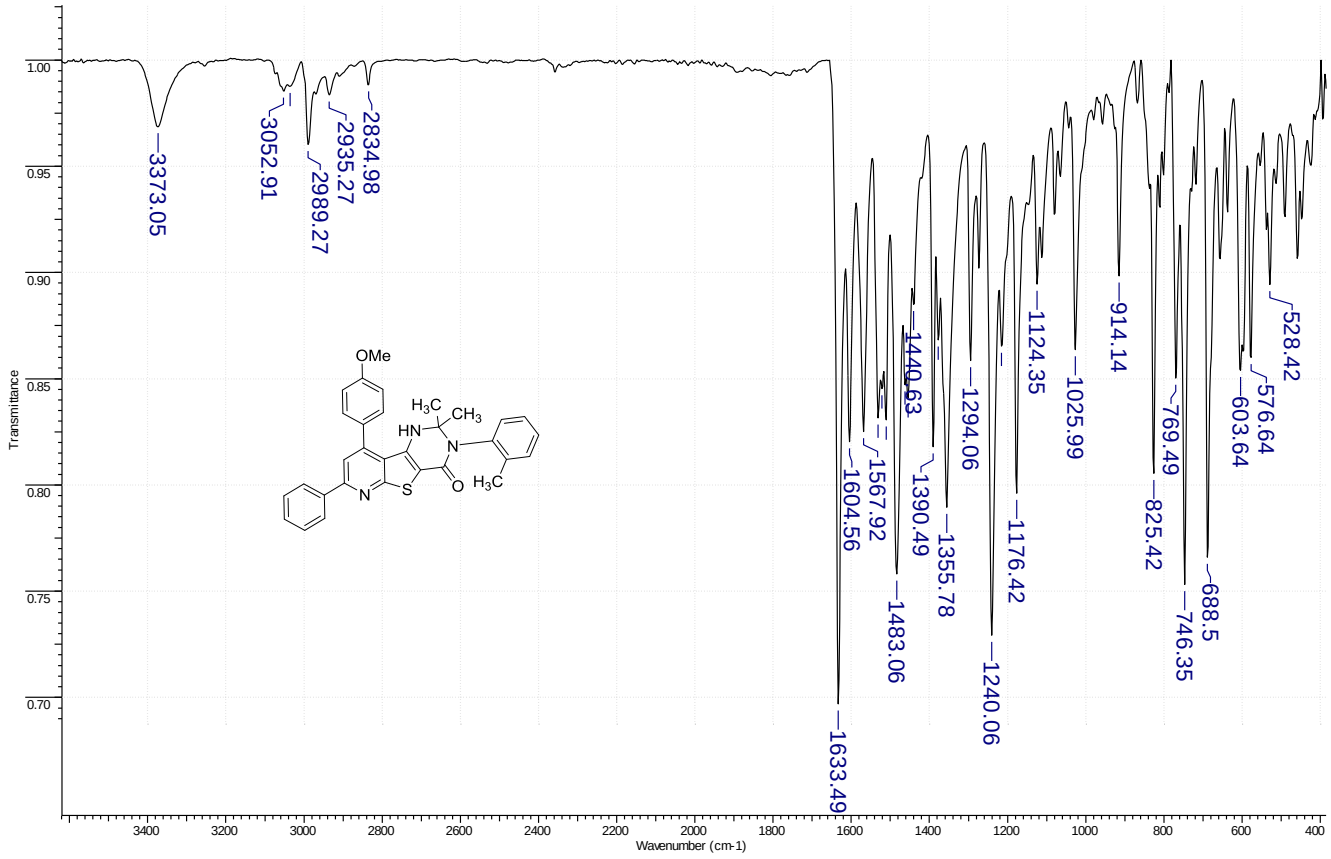

## $^1$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 8a



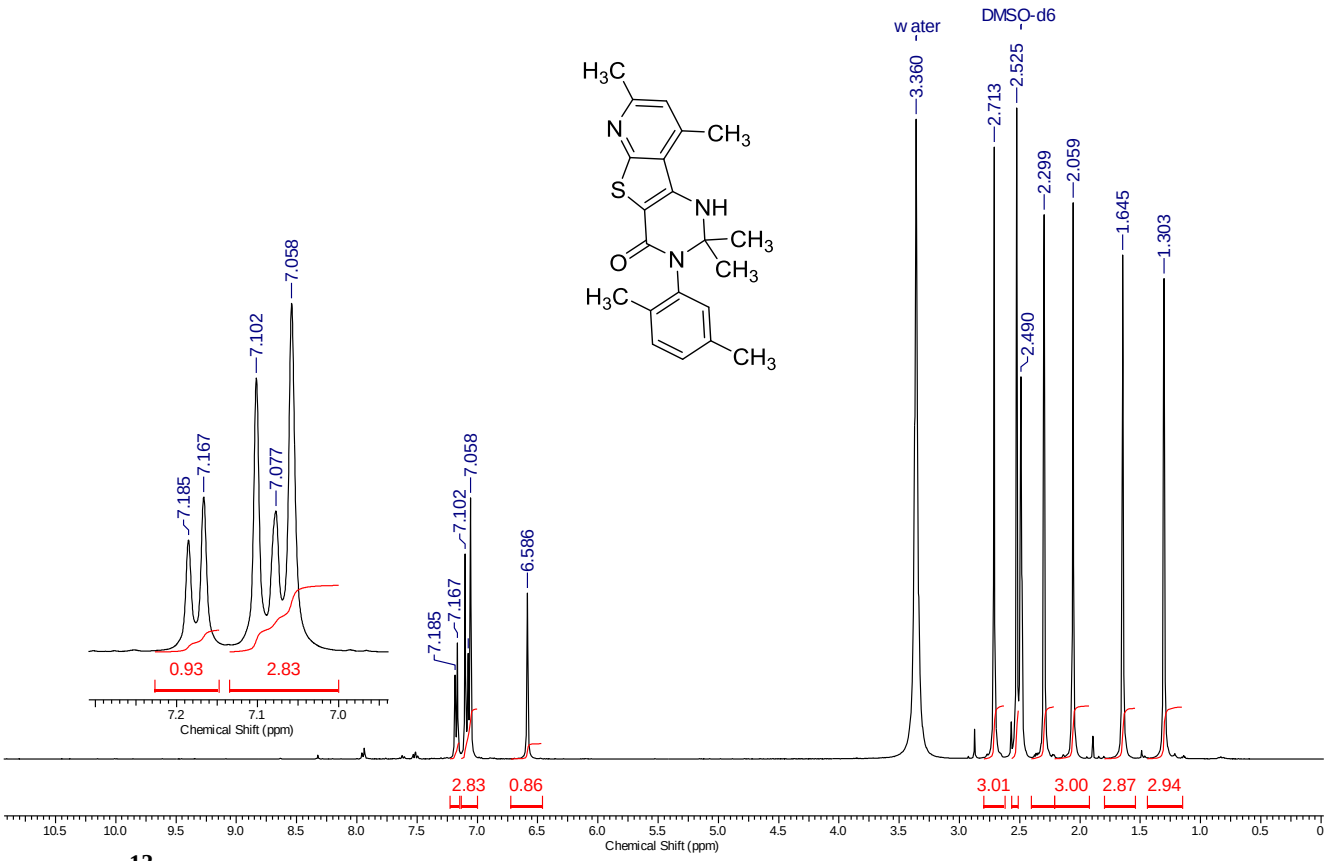
# $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 8a

$^{13}$C DEPTQ ЯМР спектр (101 МГц, DMSO-$d_6$) соединения **8a**

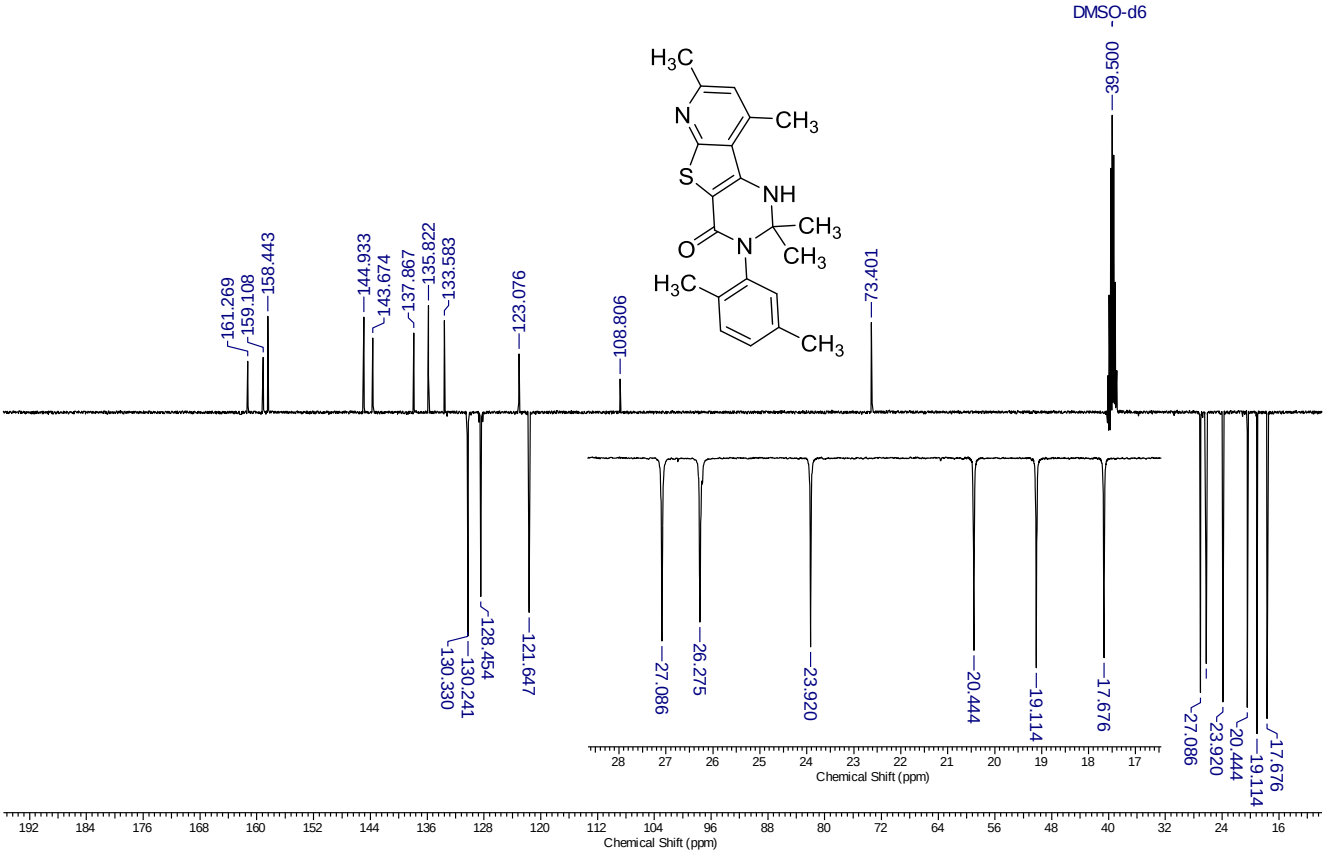


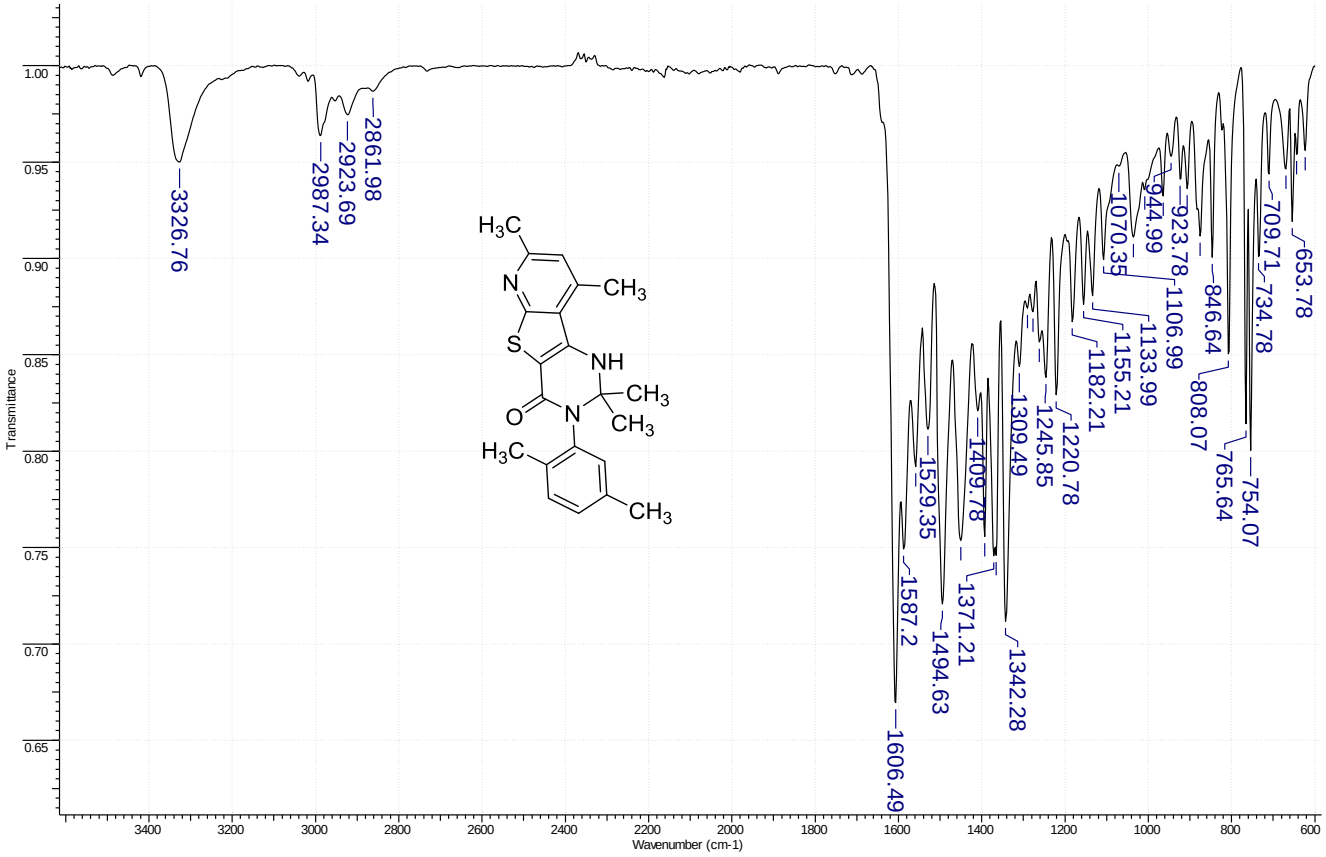
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 8b




## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 8b

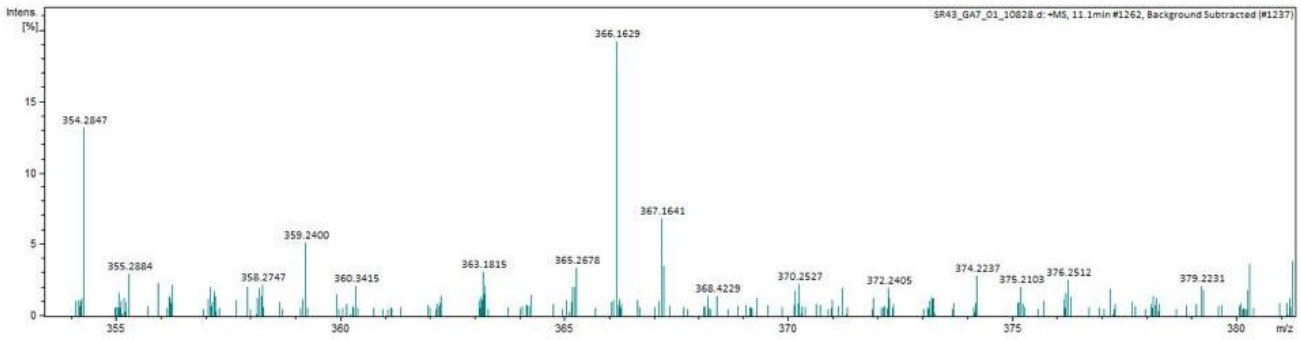


## FT-IR spectrum (ATR mode) of compound 8b

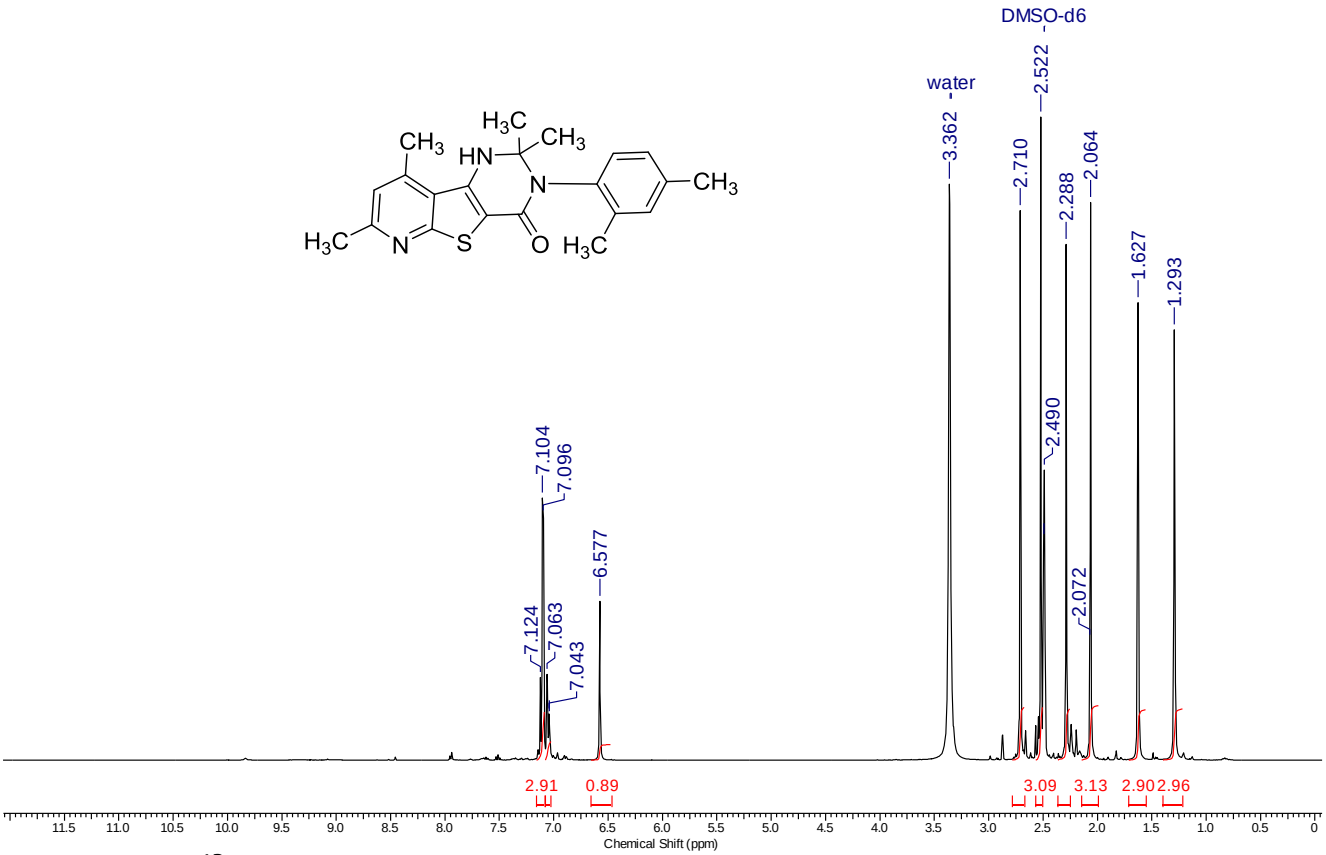



## HRMS spectrum of compound 8b

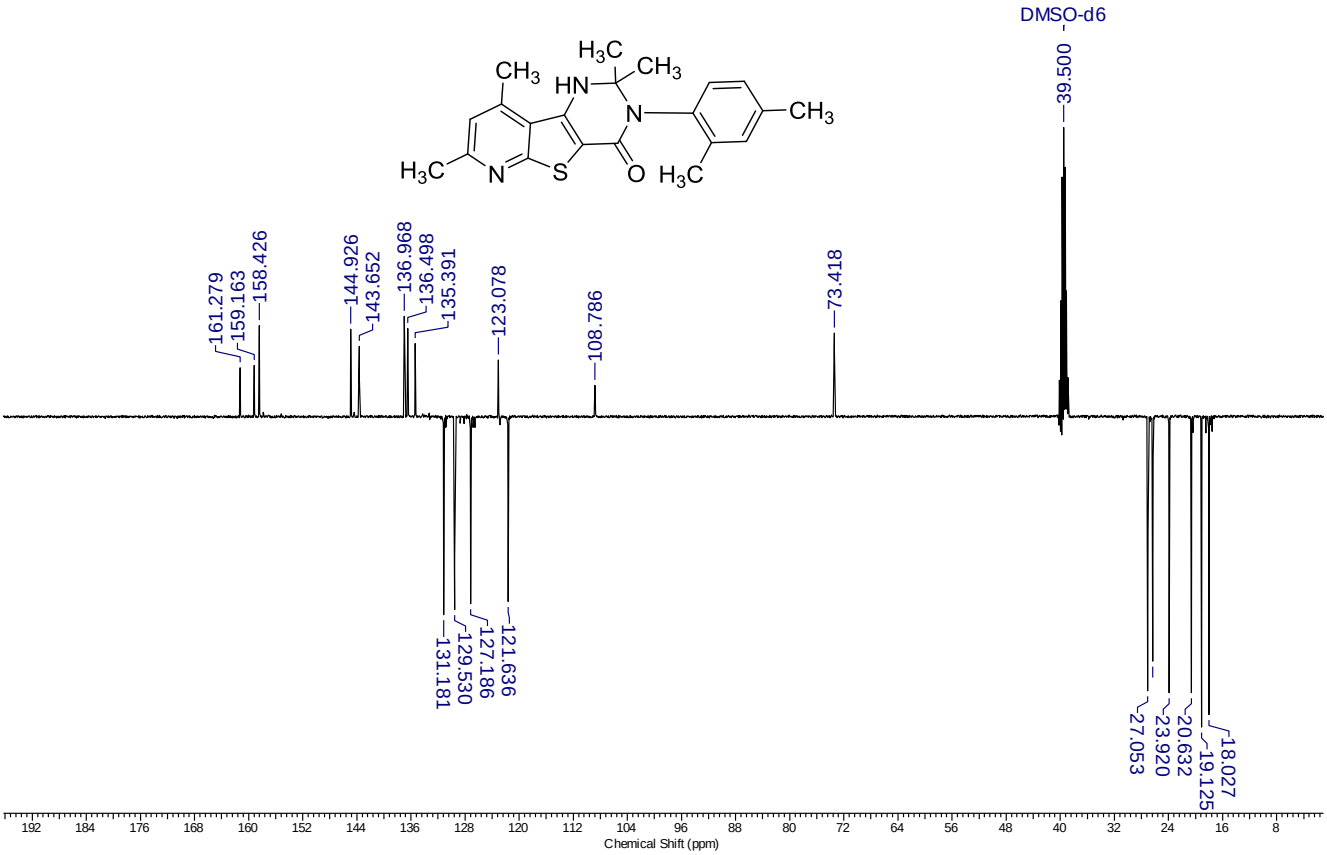
Calculated for $C_{21}H_{24}N_3OS$ [M+1]: 366.1640; Found 366.1629, Δ 3.00 ppm



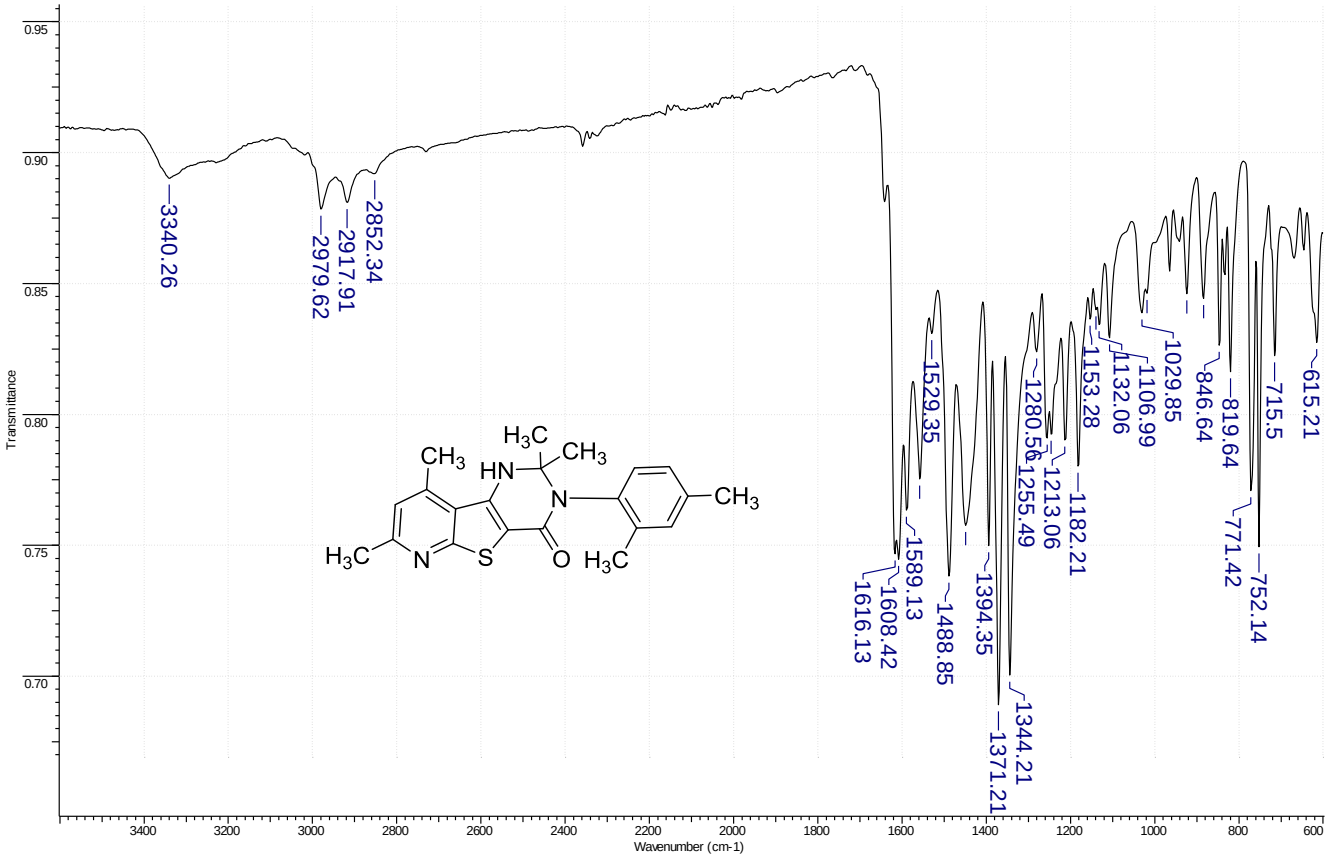
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 8c




## $^{13}$C NMR spectrum (101 MHz, DMSO-$d_6$) of compound 8c

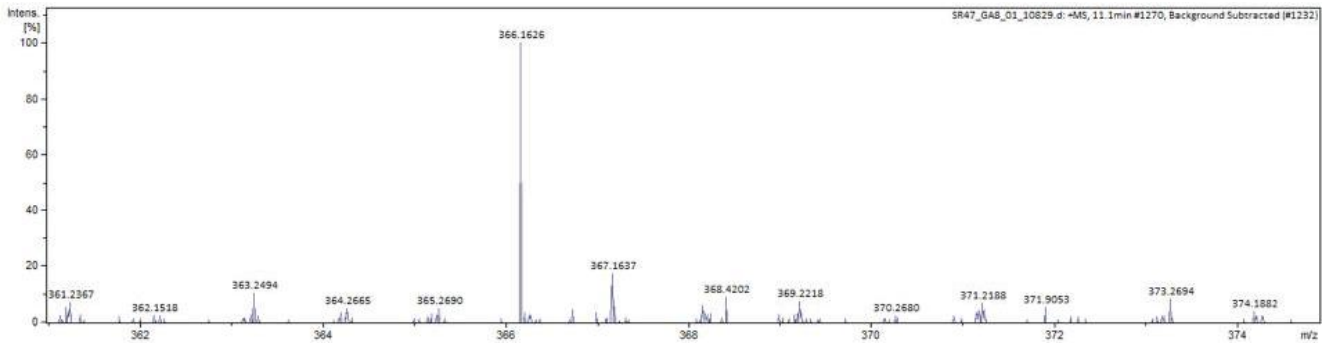


## FT-IR spectrum (ATR mode) of compound 8c

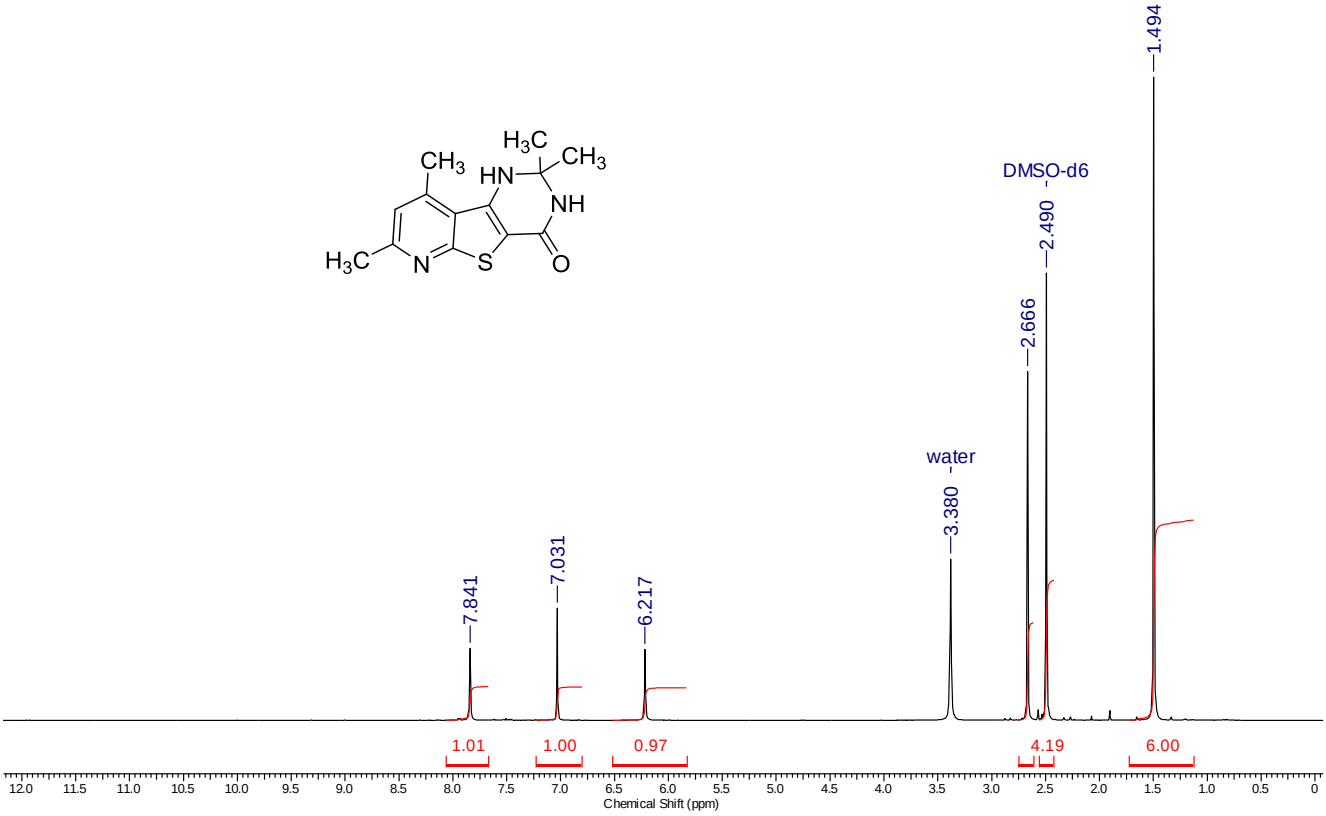



## HRMS spectrum of compound 8c

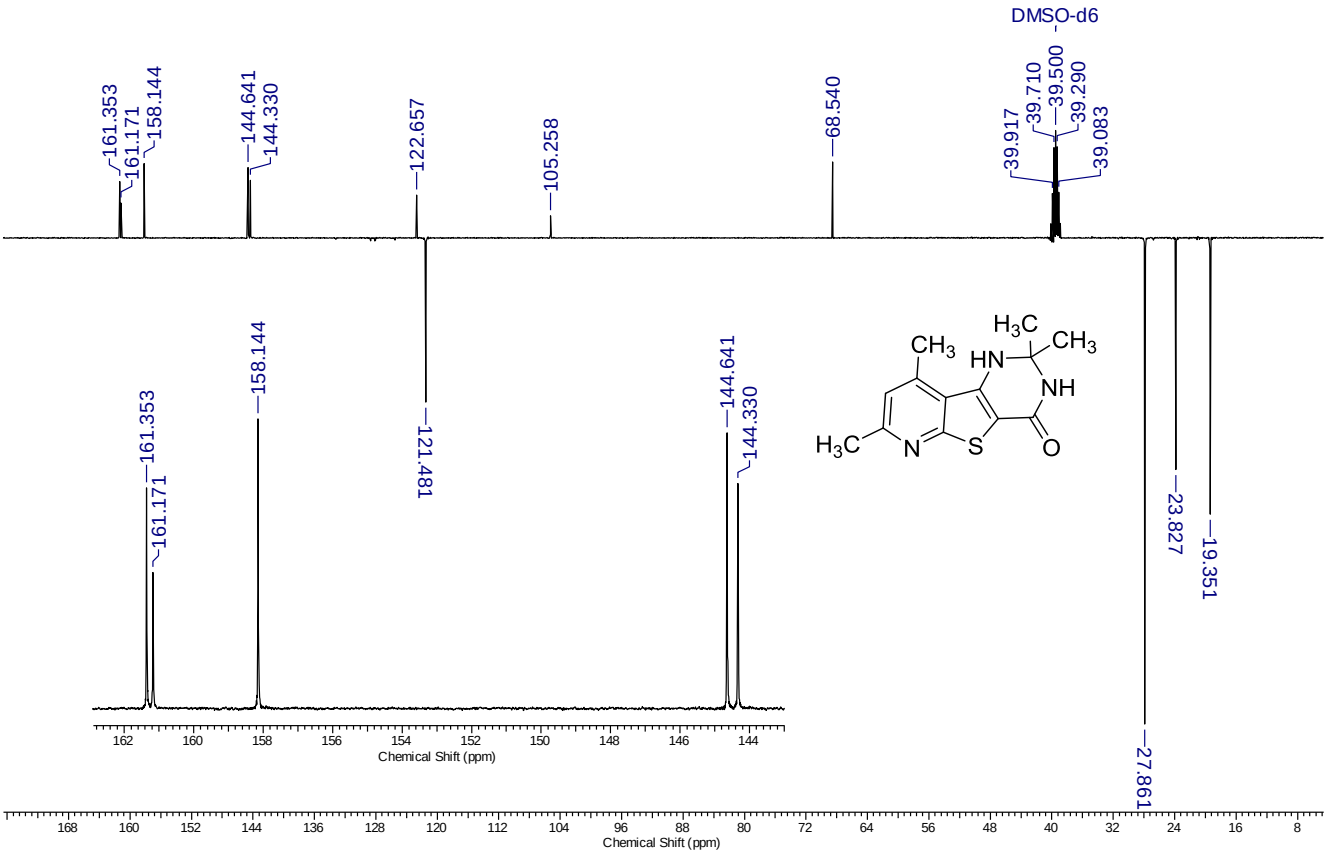
Calculated for $C_{21}H_{24}N_3OS$ [M+1]: 366.1640; Found 366.1626, Δ 3.82 ppm



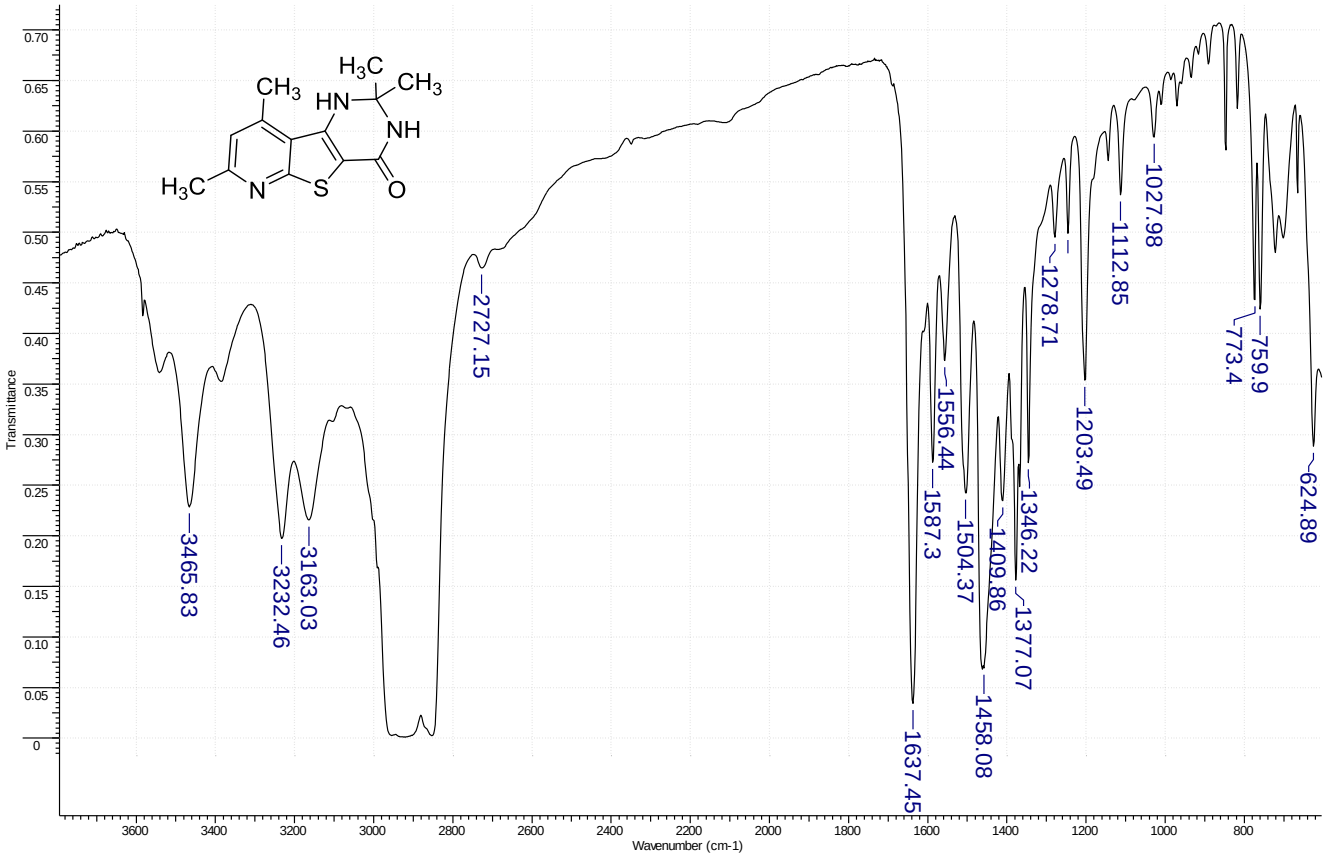
## $^{1}$H NMR spectrum (400 MHz, DMSO-$d_6$) of compound 8d




## $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of compound 8d

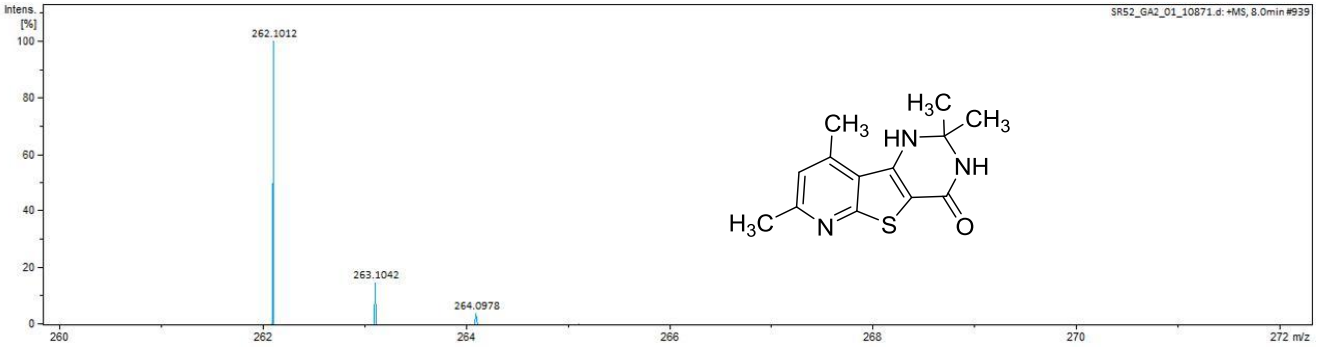


## FT-IR spectrum (nujol mull) of compound 8d

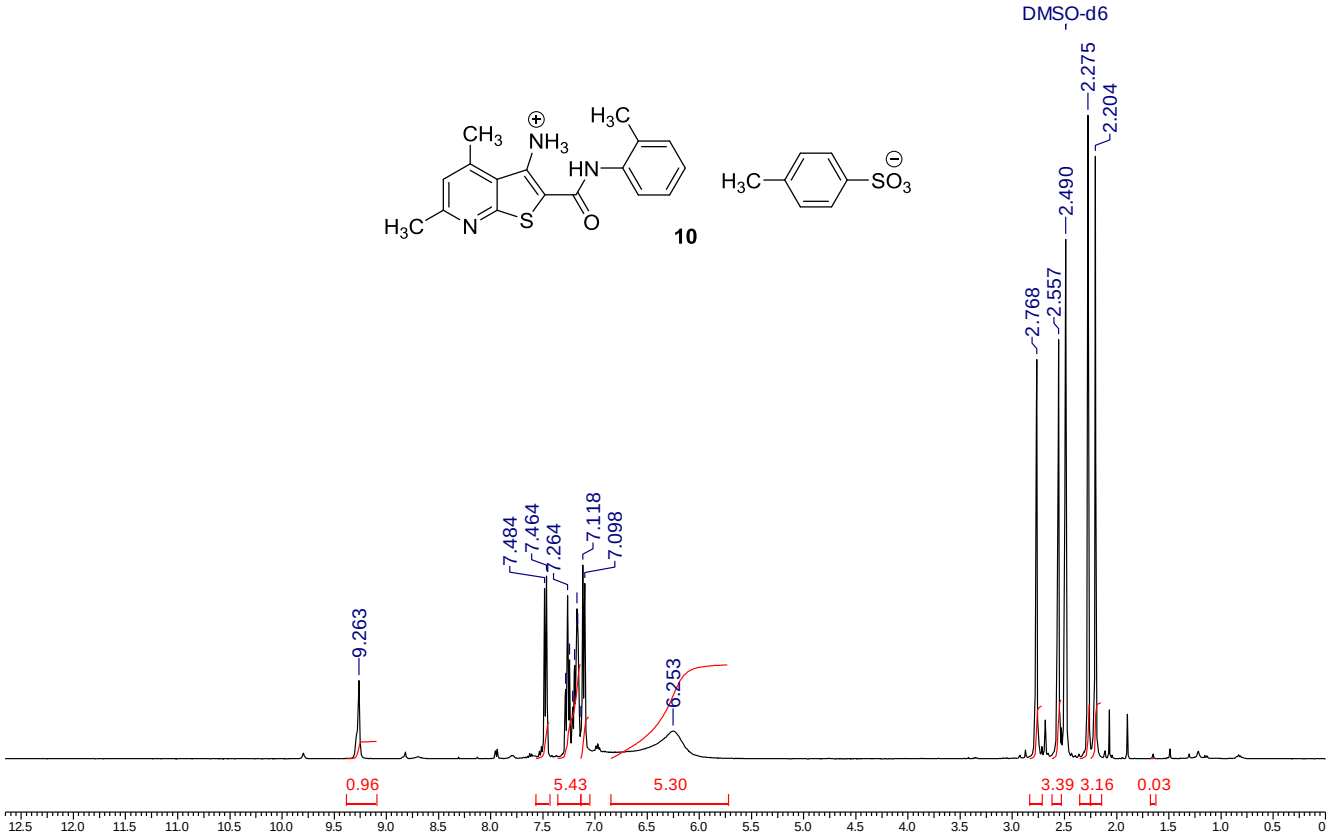


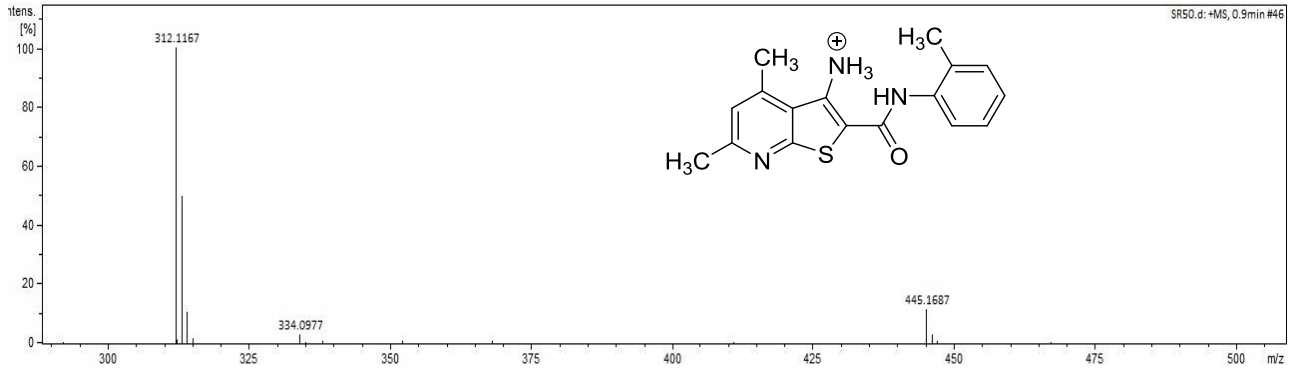

## HRMS spectrum of compound 8d

Calculated for $C_{13}H_{16}N_3OS$ [M+1]: 262.1014; Found 262.1012 (Δ 0.76 ppm)

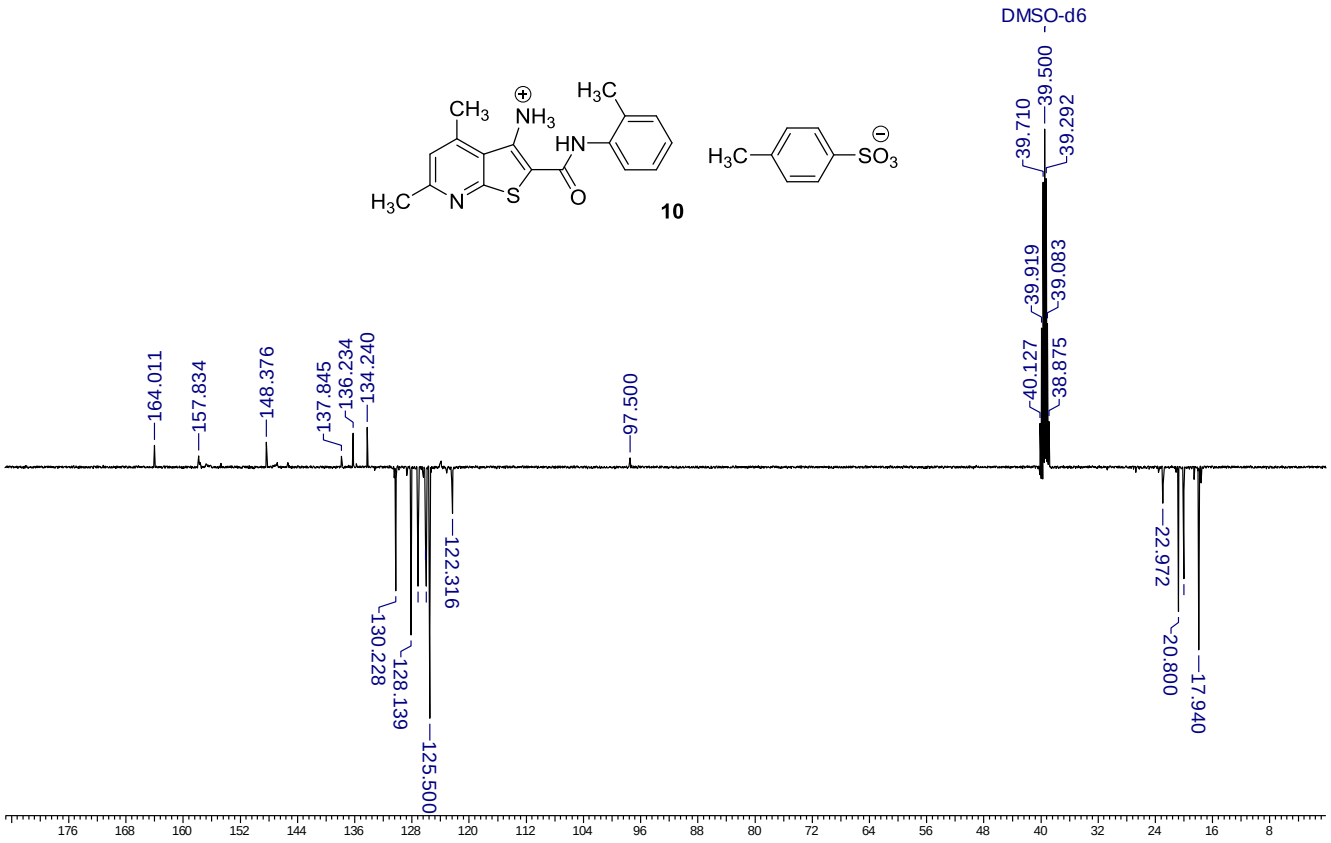


# $^{1}H$ NMR spectrum (400 MHz, DMSO-$d_6$) of crude tosylate 10



# $^{13}$C DEPTQ NMR spectrum (101 MHz, DMSO-$d_6$) of crude tosylate 10



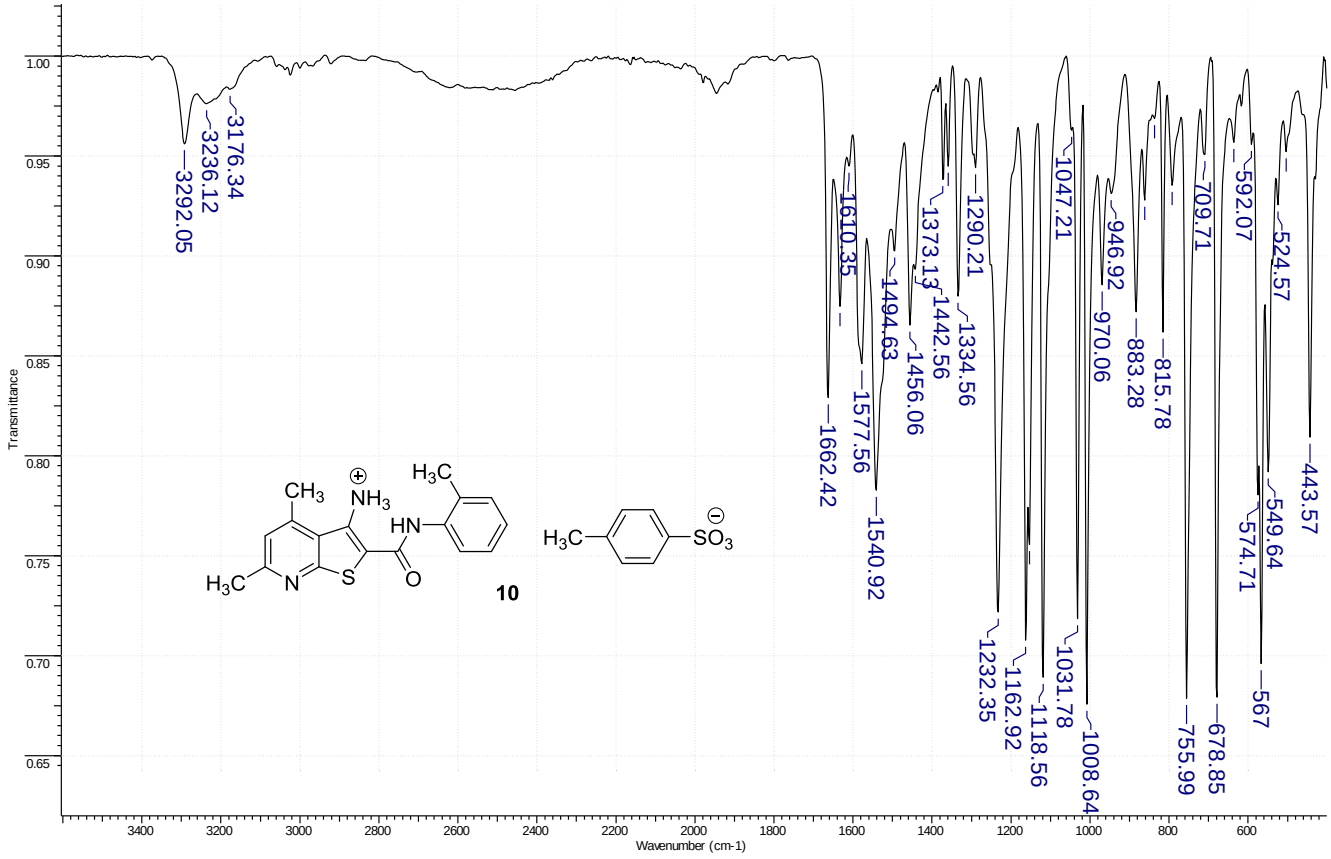



**Table S1. Protein-ligand interaction prediction results for compounds 8a-c,e using the GalaxyWeb Sagittarius-AF molecular docking protocol**

| Compound | Protein PDB ID | Protein UniProt ID | Predock score | Docking score, $\Delta G_{bind}$, kcal\mol | Final score |
|---|---|---|---|---|---|
| **8a** | 2zno_A | P37231 | 0.240 | -26.378 | 0.437 |
| | 8hum_A | P37231-2 | 0.184 | -27.003 | 0.386 |
| | 6lob_A | P51449 | 0.160 | -29.487 | 0.381 |
| | 6p9f_A | Q15788 | 0.150 | -30.435 | 0.378 |
| | 1k7l_G | Q07869 | 0.134 | -29.705 | 0.357 |
| | 7f80_A | Q03181 | 0.136 | -29.370 | 0.356 |
| | 5vql_A | Q15596 | 0.147 | -27.756 | 0.355 |
| | 3gc7_A | Q16539 | 0.142 | -26.293 | 0.339 |
| | 5myv_D | P78362 | 0.104 | -30.730 | 0.335 |
| | Q8NGF1_F1_dom0 | Q8NGF1 | 0.117 | -28.331 | 0.329 |
| **8b** | **4meq_A** | O60885 | 0.196 | -18.948 | 0.339 |
| | **2byi_A** | P07900 | 0.196 | -17.905 | 0.330 |
| | 3u8w_A | Q16539 | 0.166 | -21.806 | 0.329 |
| | 7usi_B | P25440 | 0.168 | -17.550 | 0.299 |
| | **5uch_B** | P08238 | 0.160 | -18.269 | 0.297 |
| | 5l7h_A | P08235 | 0.144 | -19.973 | 0.294 |
| | **7mck_A** | O14757 | 0.141 | -20.064 | 0.292 |
| | 2gvj_A,B | P43490,P43490 | 0.143 | -19.791 | 0.291 |
| | 1uwj_A | P15056 | 0.136 | -19.951 | 0.286 |
| | P08922_F1_dom5 | P08922 | 0.141 | -19.304 | 0.286 |
| **8c** | **4meq_A** | O60885 | 0.196 | -18.712 | 0.337 |
| | 3u8w_A | Q16539 | 0.166 | -21.758 | 0.329 |
| | **2byi_A** | P07900 | 0.196 | -16.727 | 0.321 |
| | 5l7h_A | P08235 | 0.144 | -21.503 | 0.306 |
| | 7usi_B | P25440 | 0.168 | -18.028 | 0.303 |
| | **5uch_B** | P08238 | 0.160 | -18.422 | 0.298 |
| | **7mck_A** | O14757 | 0.141 | -20.375 | 0.294 |
| | 2gvj_A,B | P43490,P43490 | 0.143 | -19.827 | 0.292 |
| | P08922_F1_dom5 | P08922 | 0.141 | -19.108 | 0.284 |
| | 2zno_A | P37231 | 0.111 | -23.032 | 0.284 |
| **8e** | **2byi_A** | P07900 | 0.228 | -16.840 | 0.354 |
| | **4meq_A** | O60885 | 0.215 | -18.388 | 0.353 |
| | **7mck_A** | O14757 | 0.173 | -19.377 | 0.318 |
| | 3poo_A | P17612 | 0.166 | -19.295 | 0.311 |
| | 3nnv_A | Q16539 | 0.170 | -18.714 | 0.311 |
| | 4twp_A | P00519 | 0.169 | -18.655 | 0.309 |
| | 5mwy_A | P08235 | 0.142 | -21.754 | 0.305 |
| | **5uch_B** | P08238 | 0.168 | -17.753 | 0.301 |
| | 1uwj_A | P15056 | 0.150 | -19.804 | 0.299 |
| | P08922_F1_dom5 | P08922 | 0.161 | -18.304 | 0.298 |