Electronic Supporting Information

A Modular Approach Towards Functionalized Highly Stable Self-complementary Quadruple Hydrogen Bonded Systems

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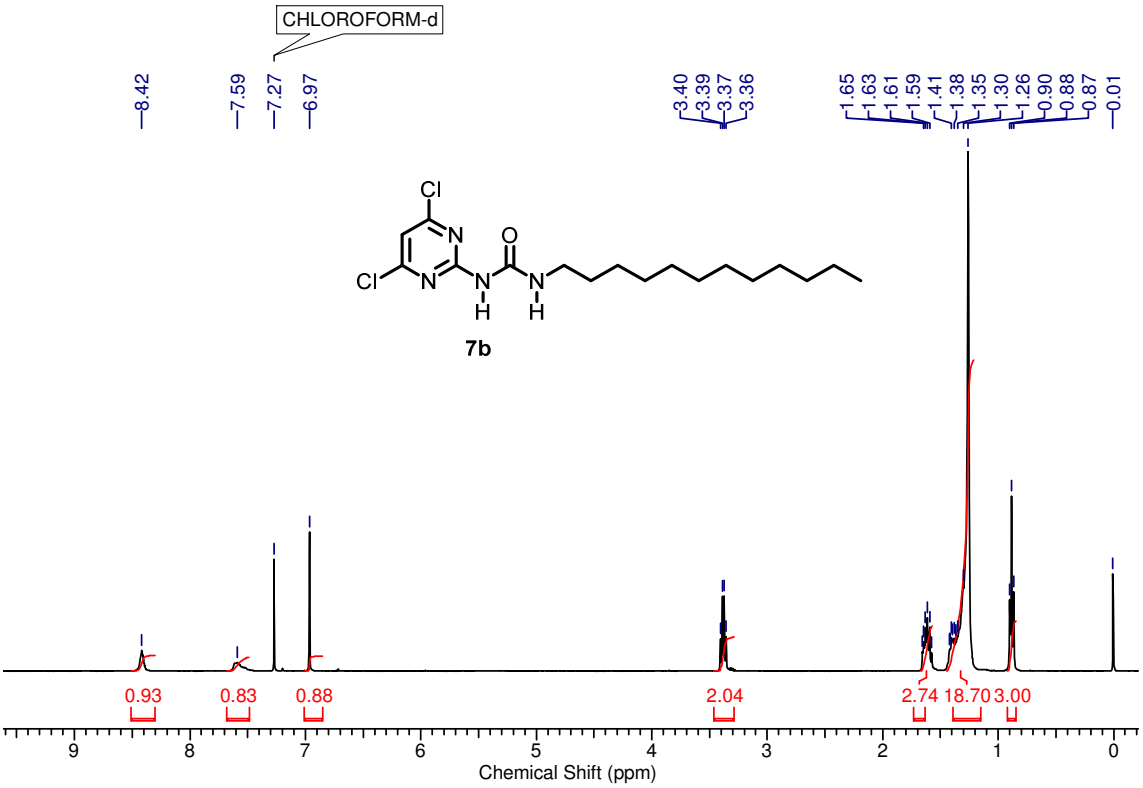
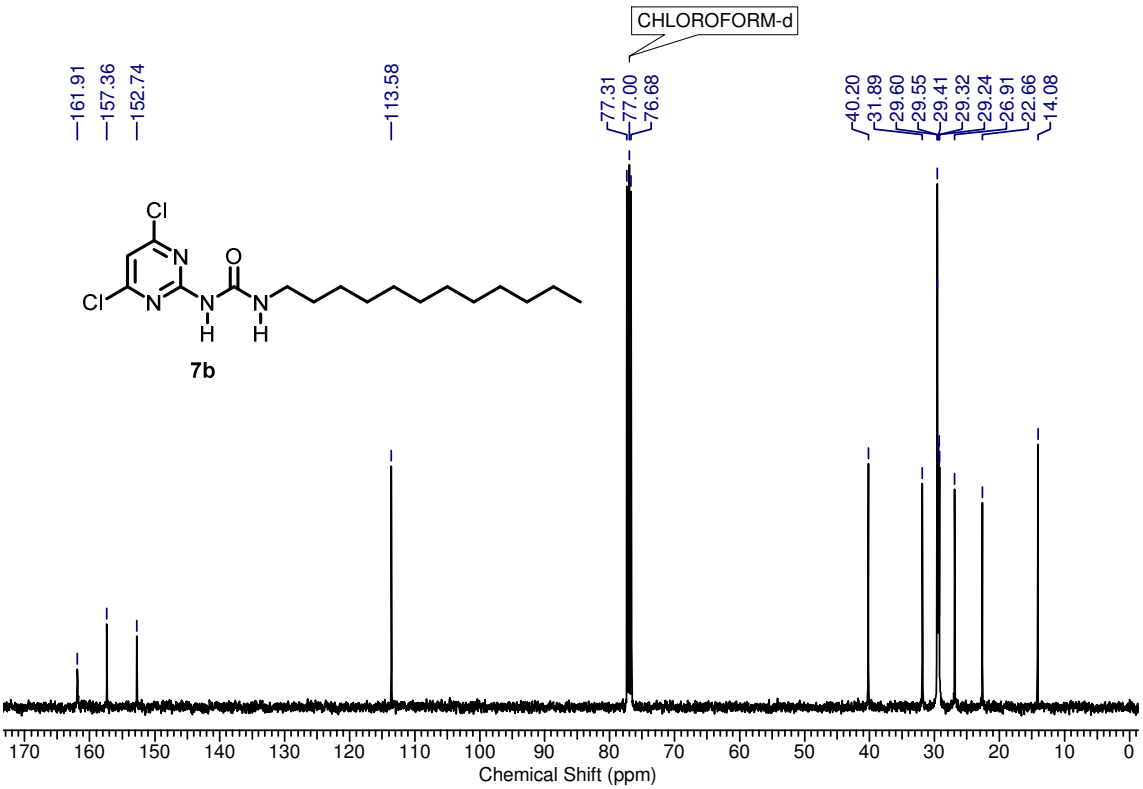
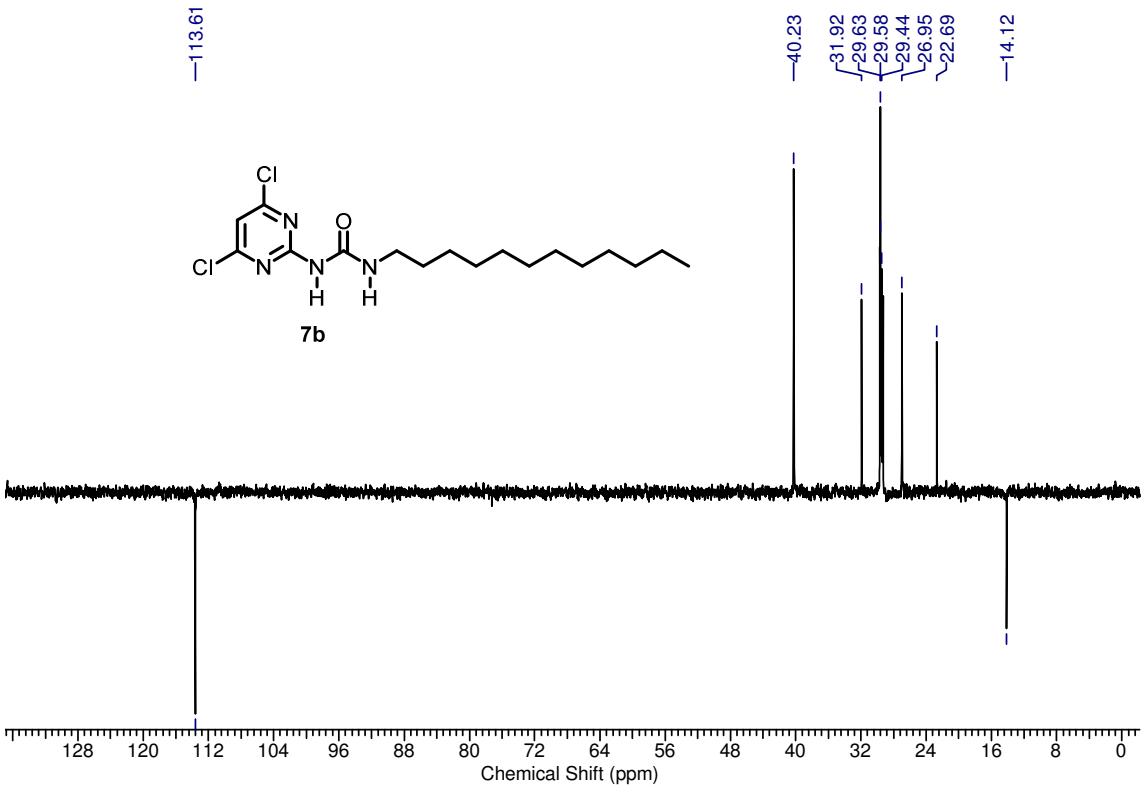


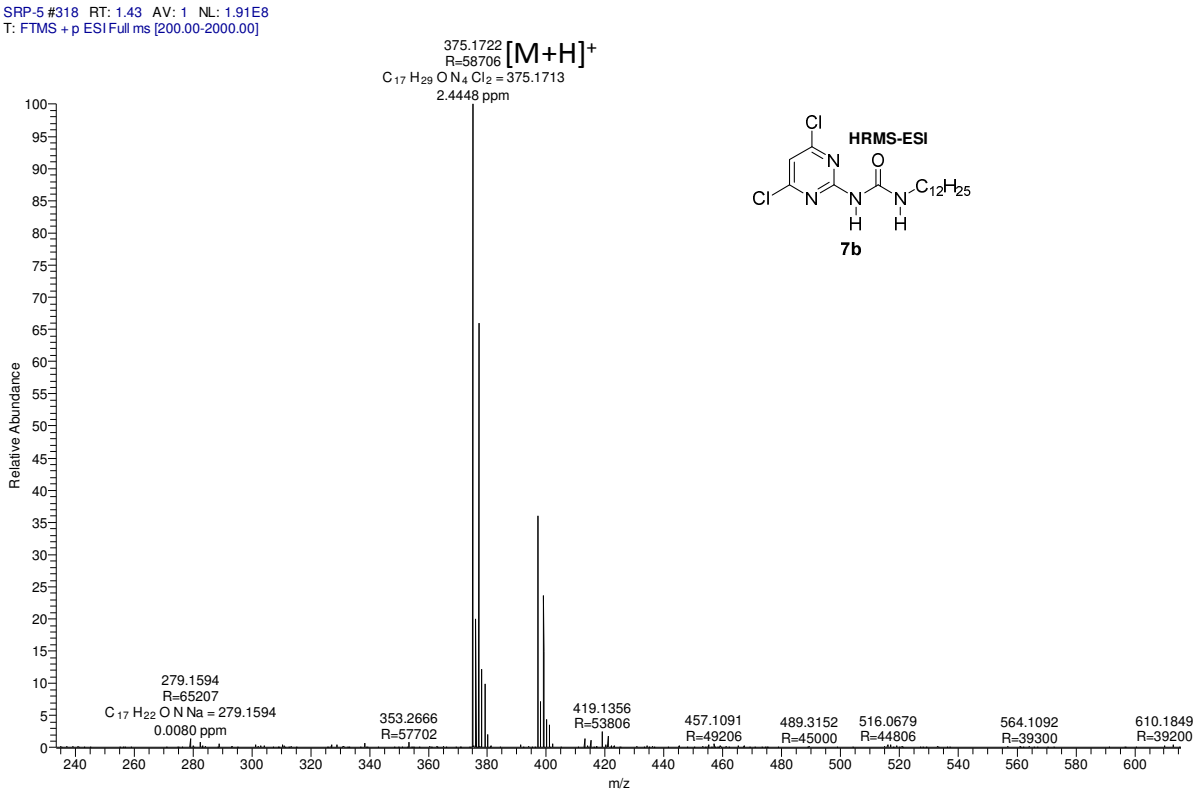
^{1}H NMR spectrum of compound **7b** ($CDCl_3$, 500 MHz, 298 K)

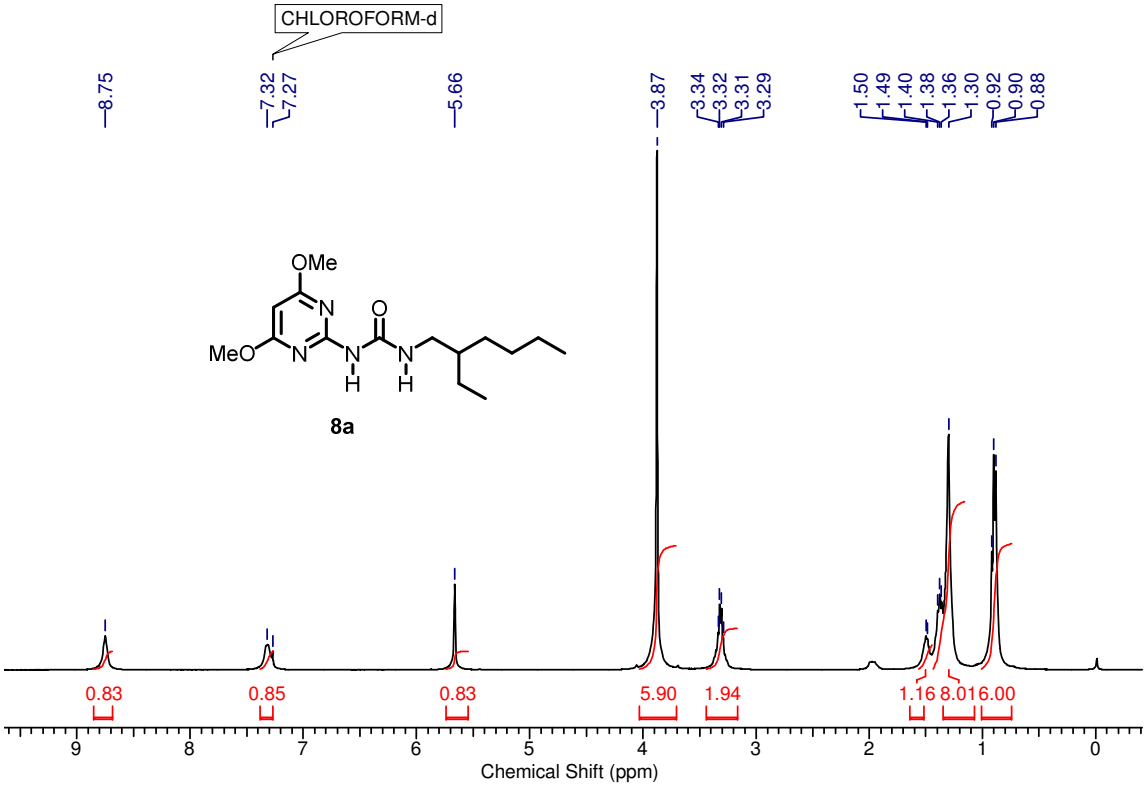


^{13}C NMR spectrum of compound **7b** ($CDCl_3$, 125 MHz, 298 K)

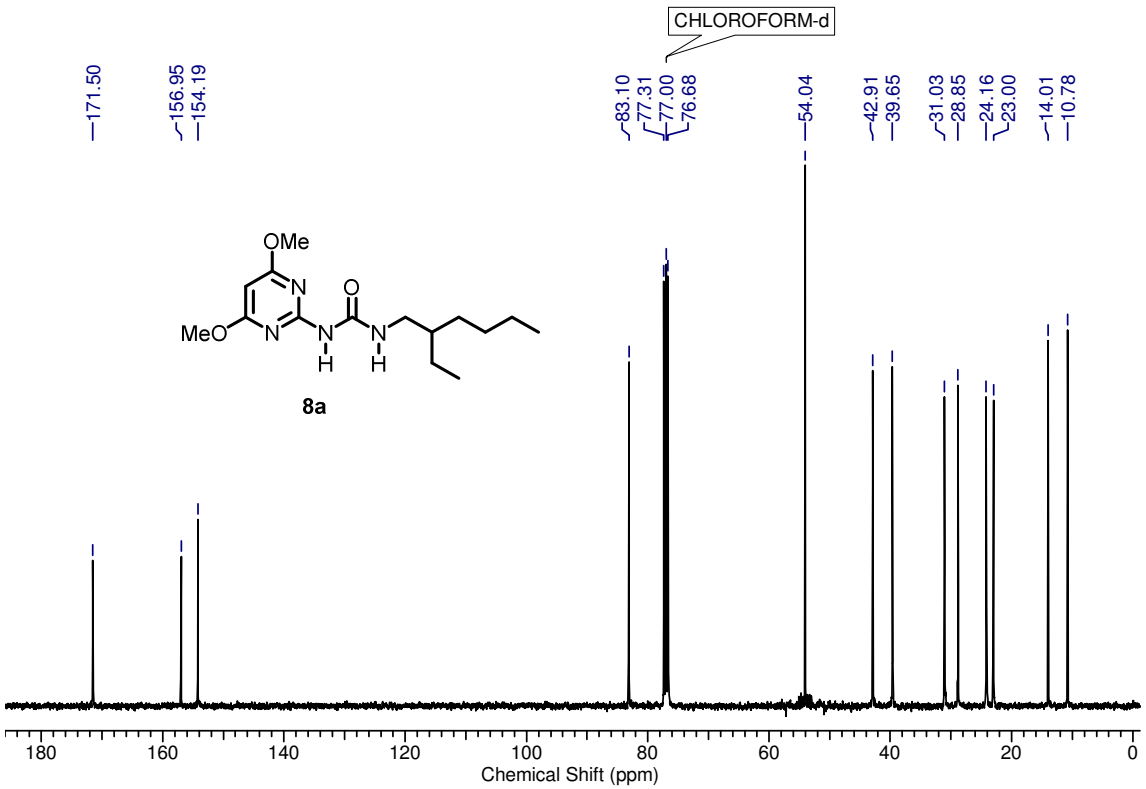


DEPT-135 NMR spectrum of compound **7b** ($CDCl_3$, 125 MHz, 298 K)





^{1}H NMR spectrum of compound **8a** ($CDCl_3$, 400 MHz, 298 K)



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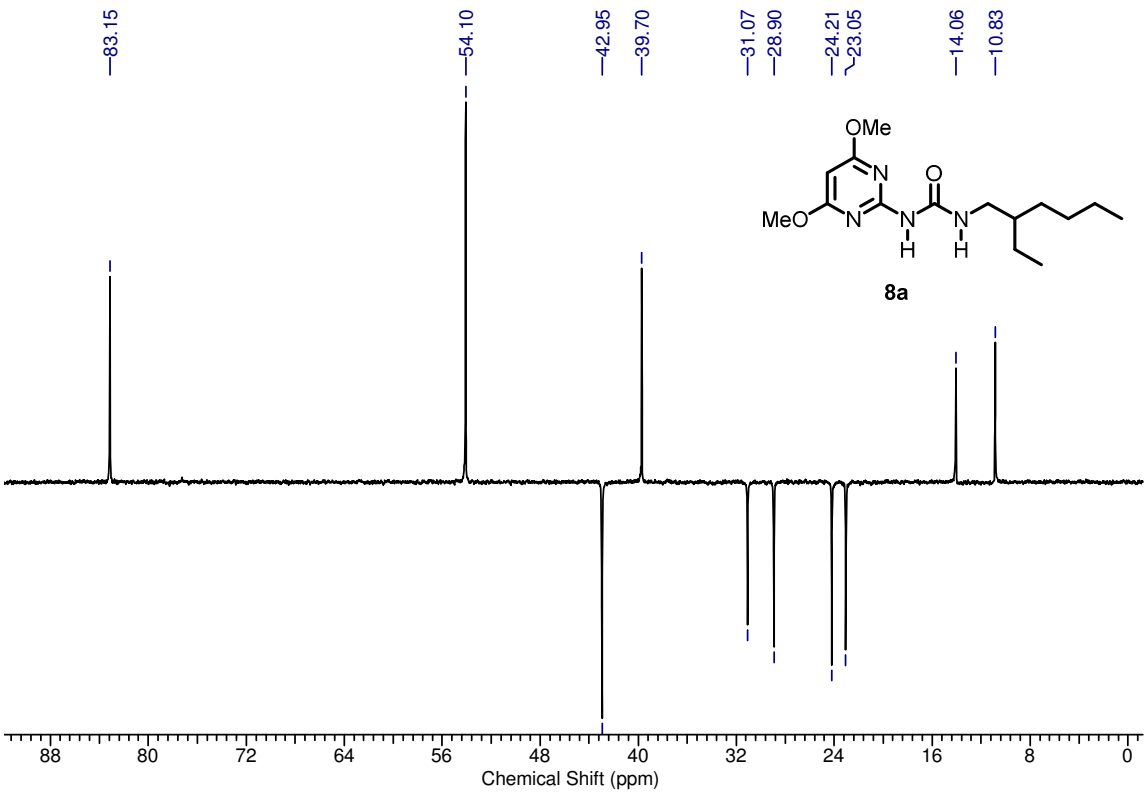
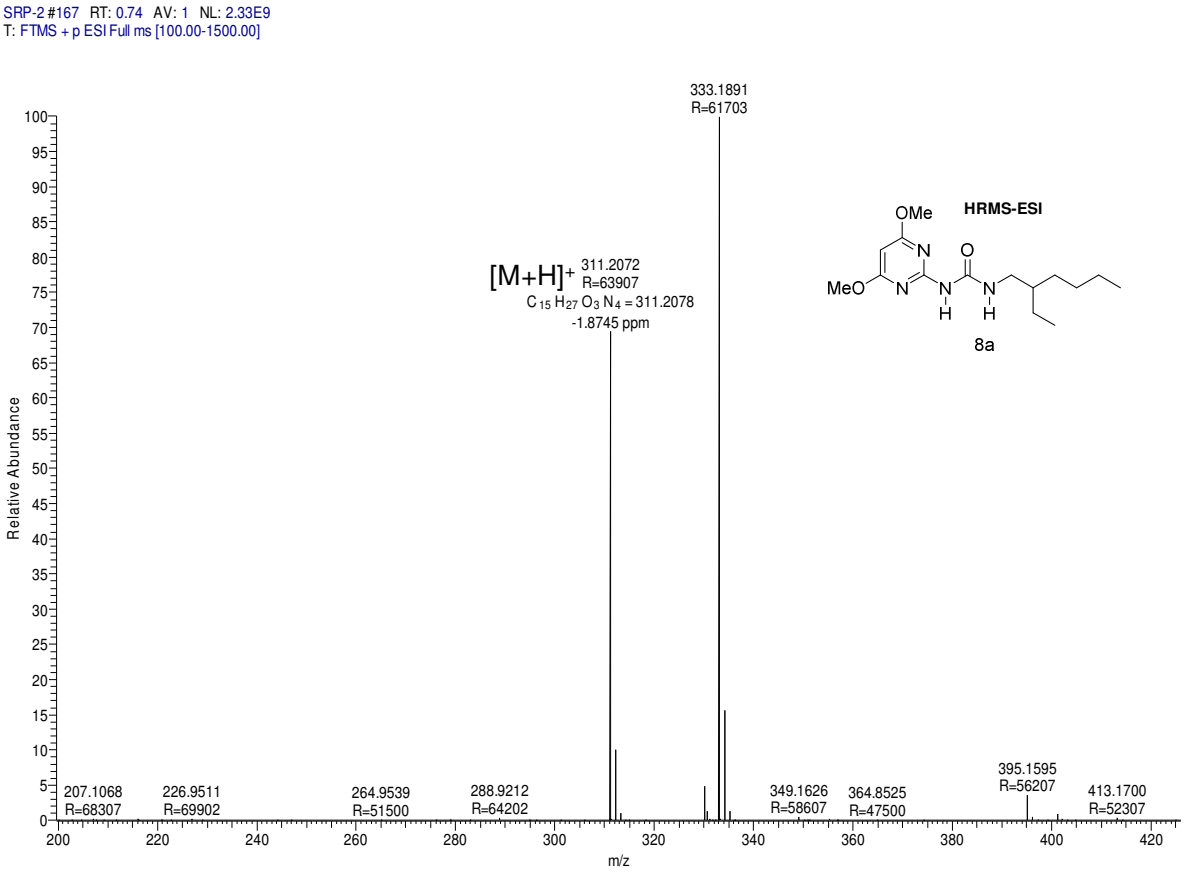
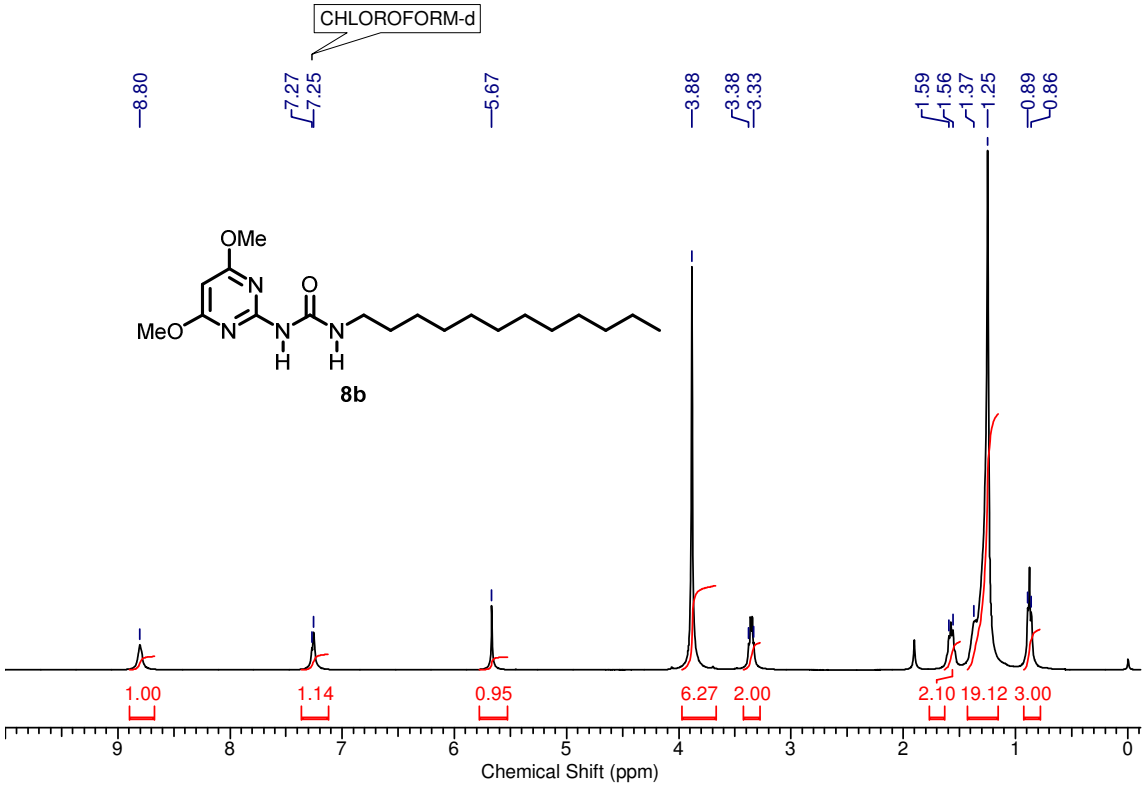


DEPT-135 NMR spectrum of compound **8a** ($CDCl_3$, 100 MHz, 298 K)





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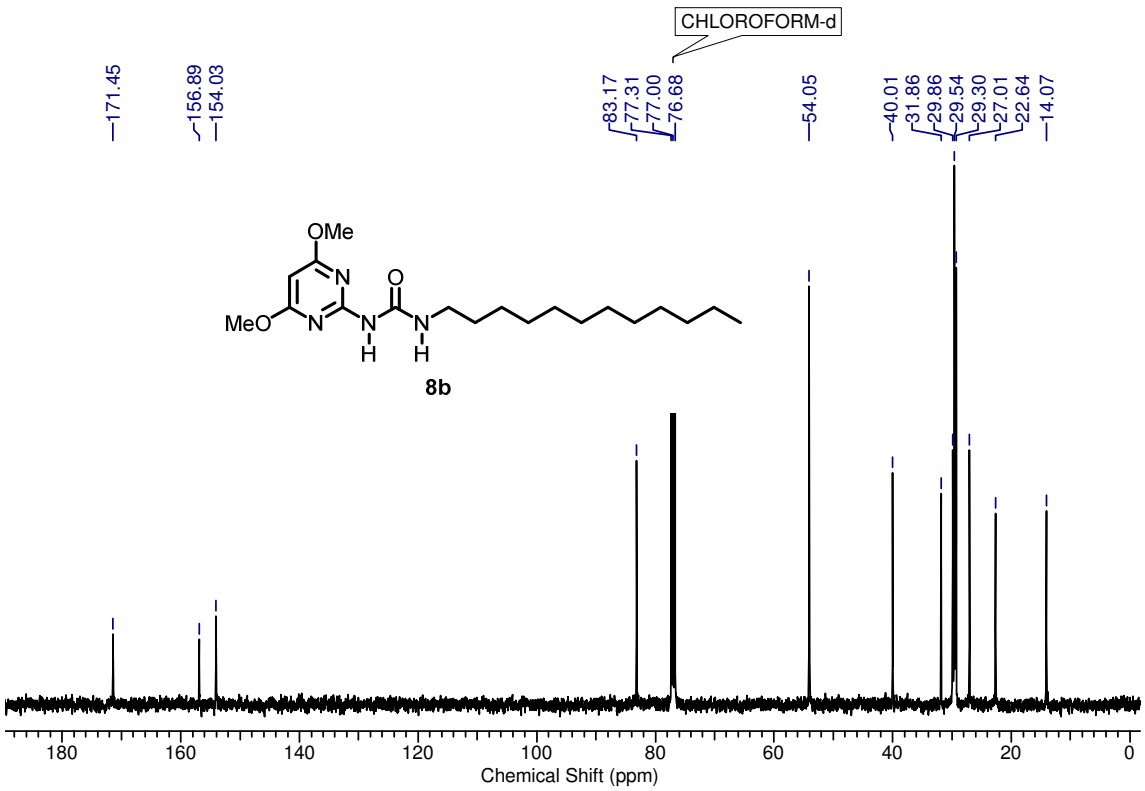

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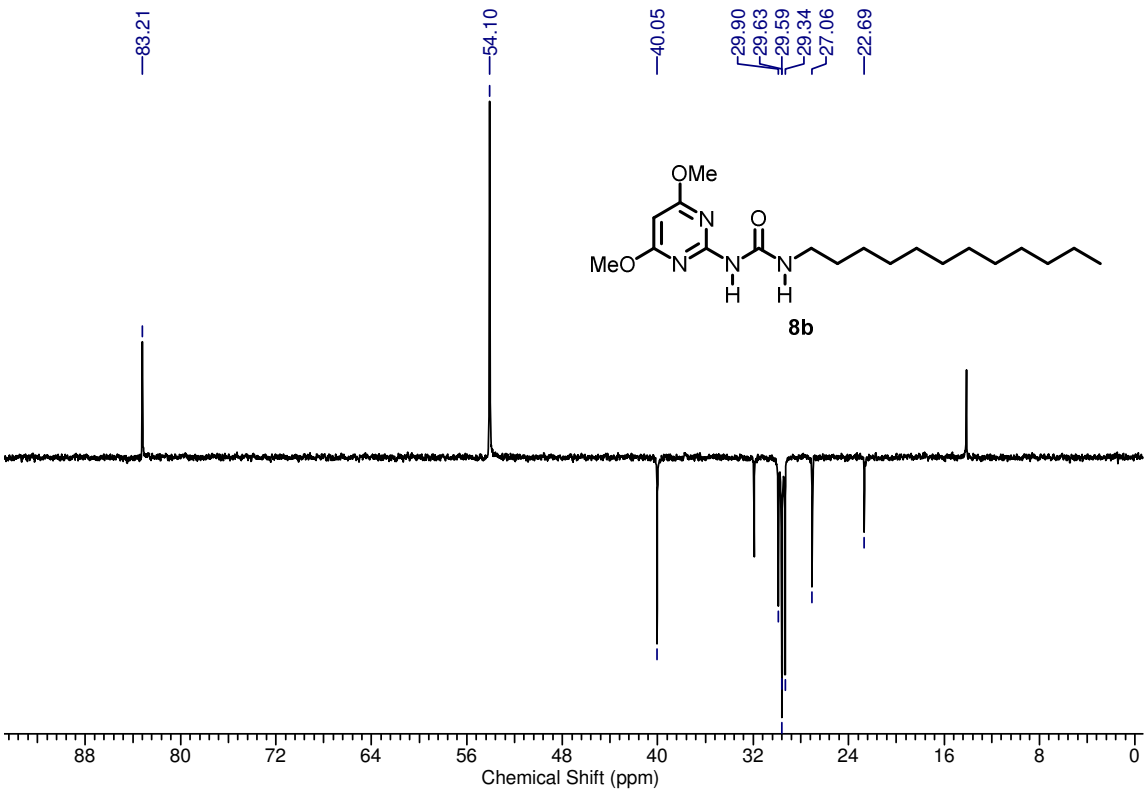

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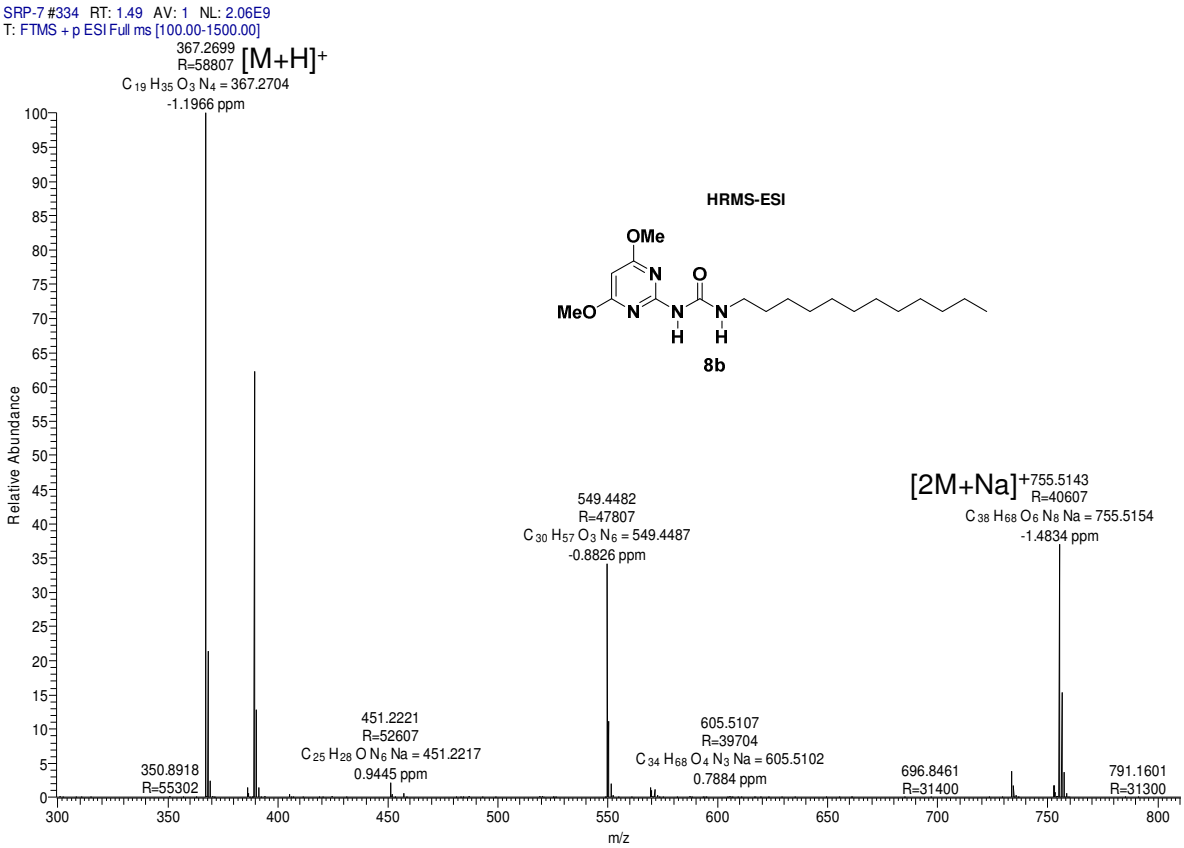
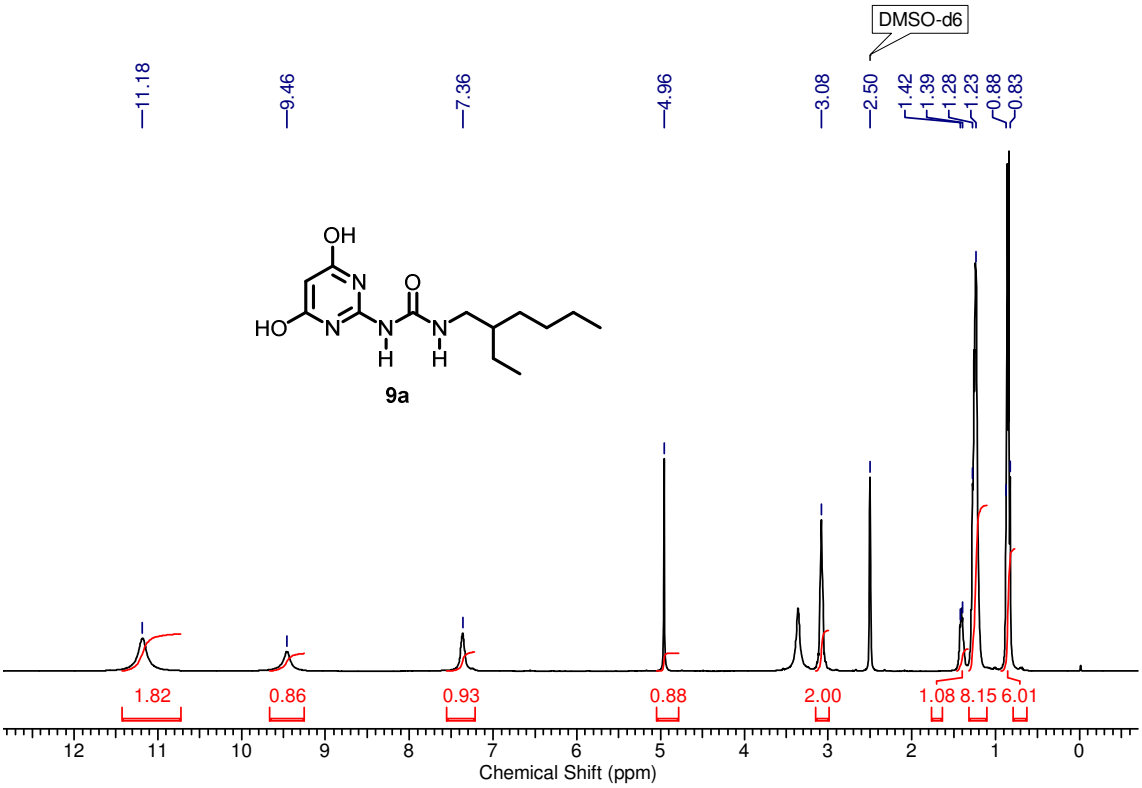
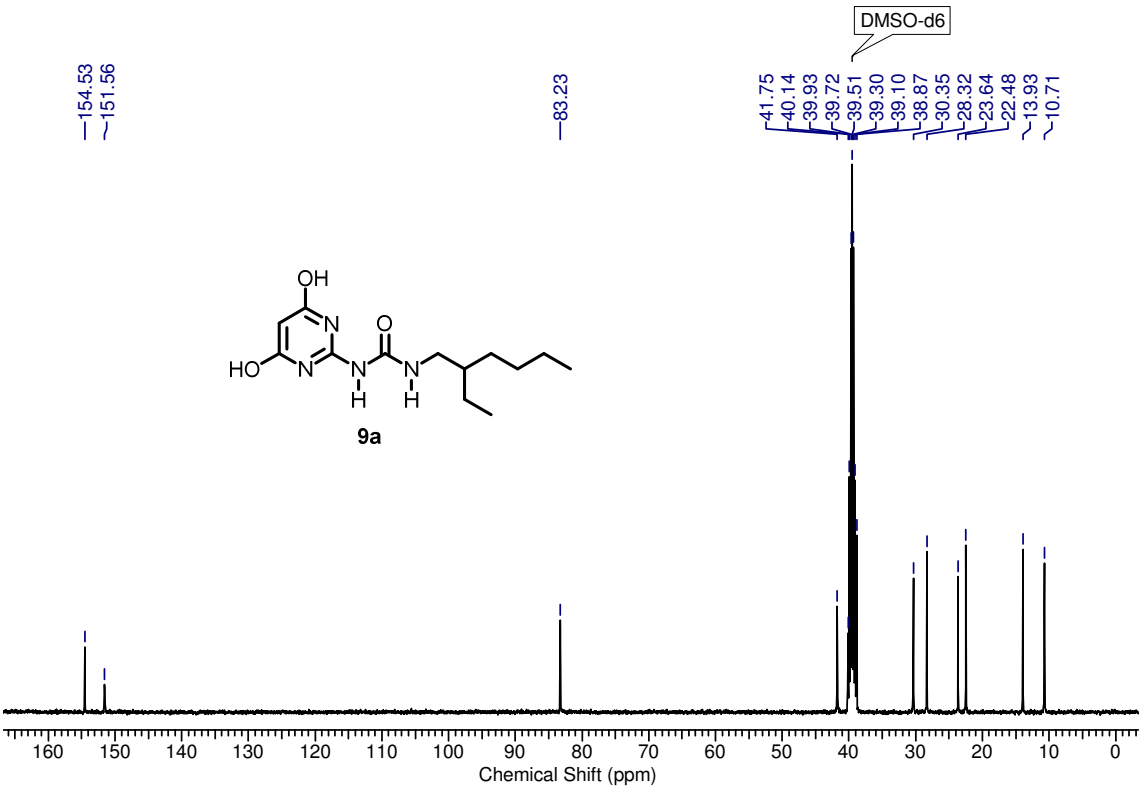
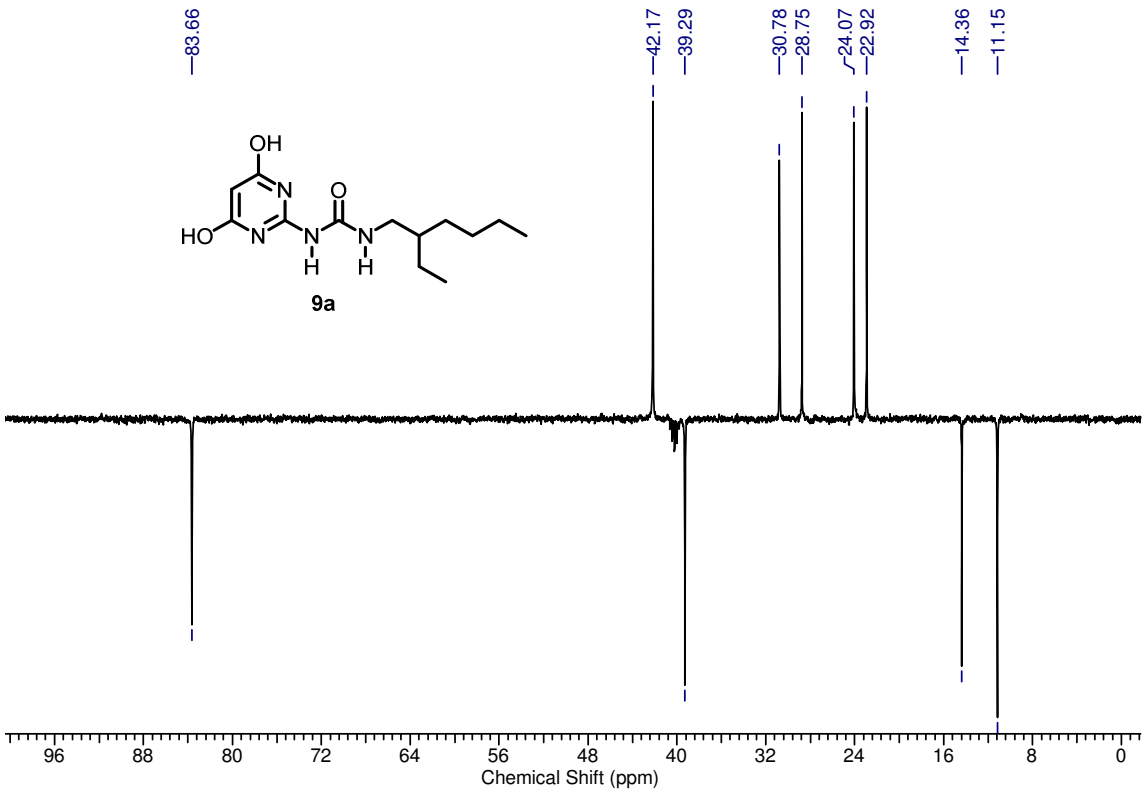




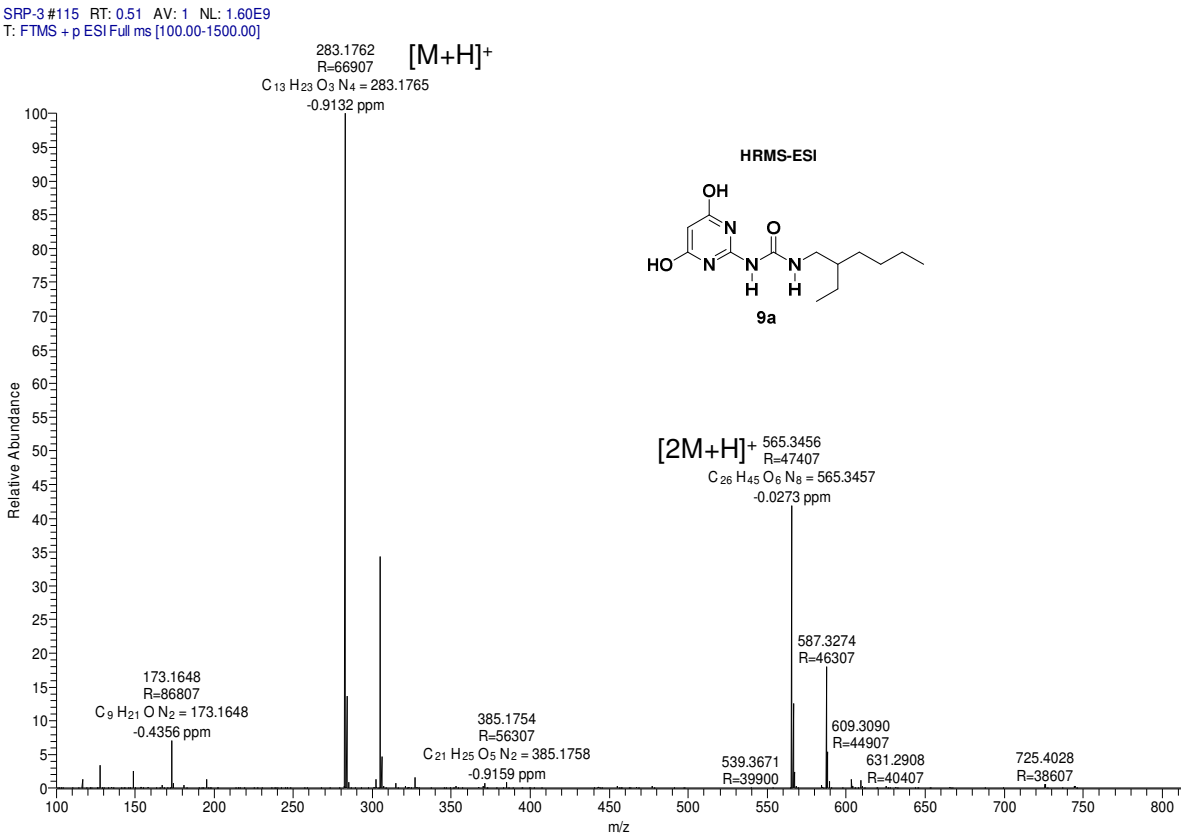
^{1}H NMR spectrum of compound **9a** (DMSO-d_6, 400 MHz, 298 K)

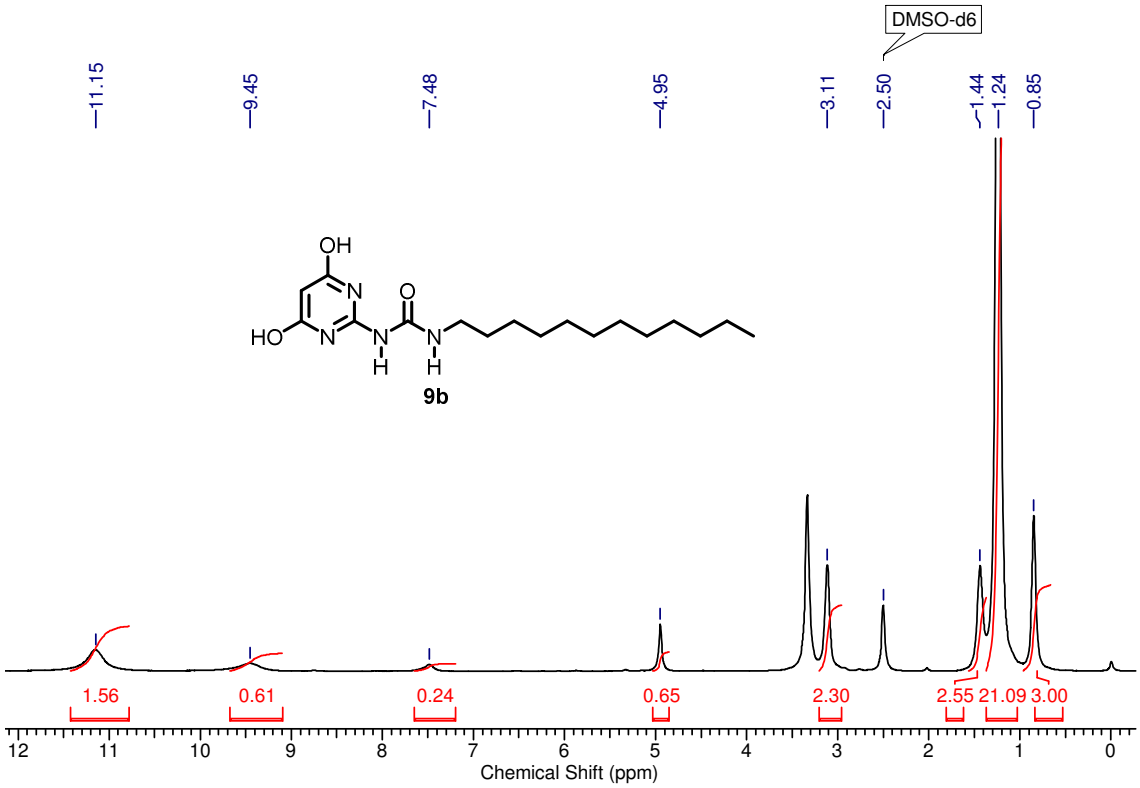


^{13}C NMR spectrum of compound **9a** (DMSO-d_6, 100 MHz, 298 K)

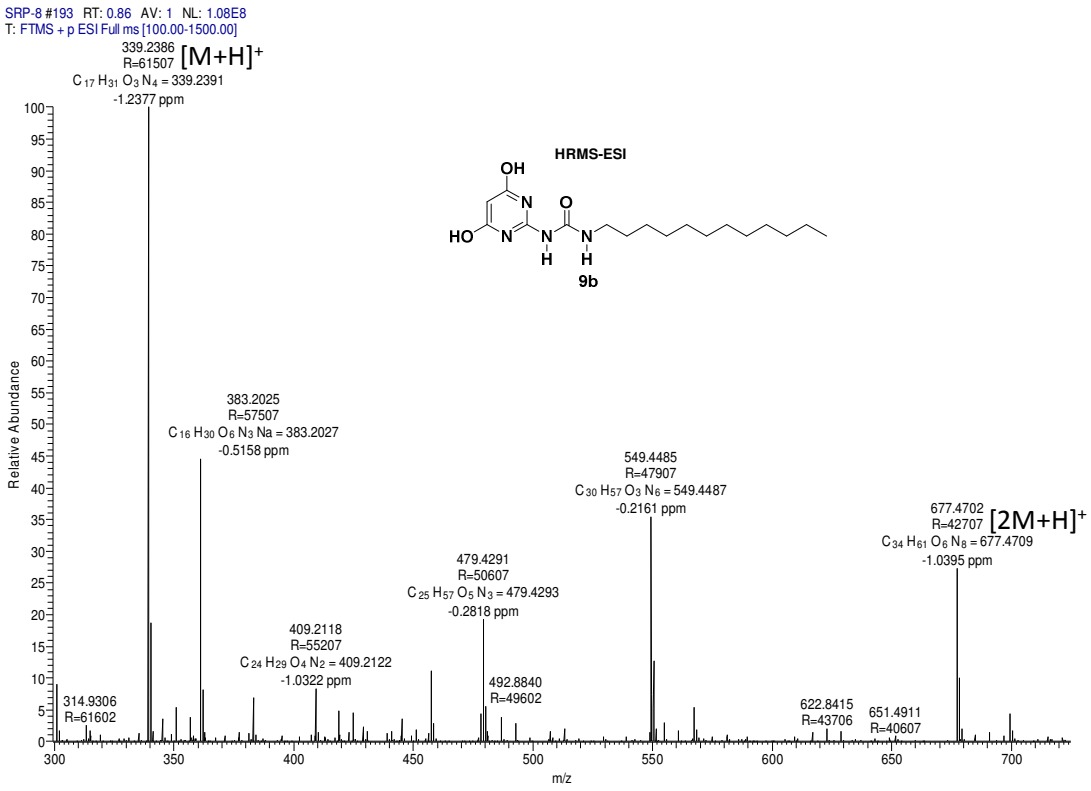


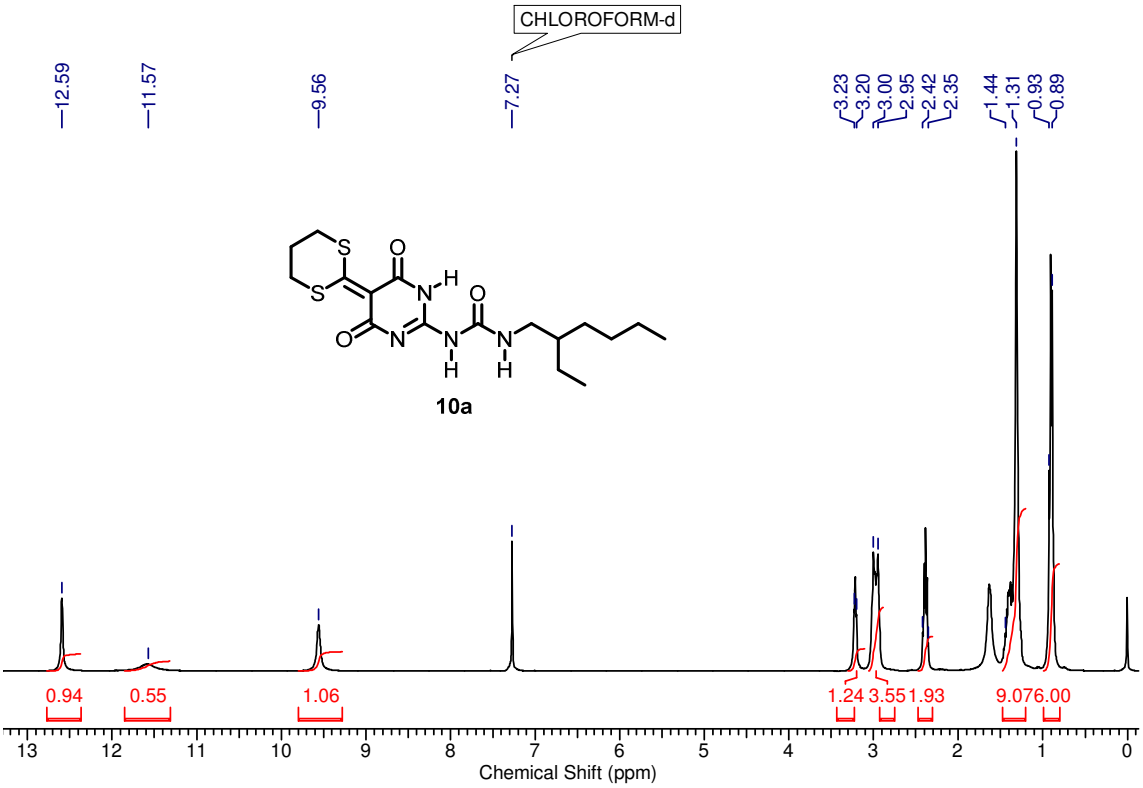
DEPT-135 NMR spectrum of compound **9a** (DMSO-d_6, 100 MHz, 298 K)





^{1}H NMR spectrum of compound **9b** (DMSO-d_6, 400 MHz, 298 K)





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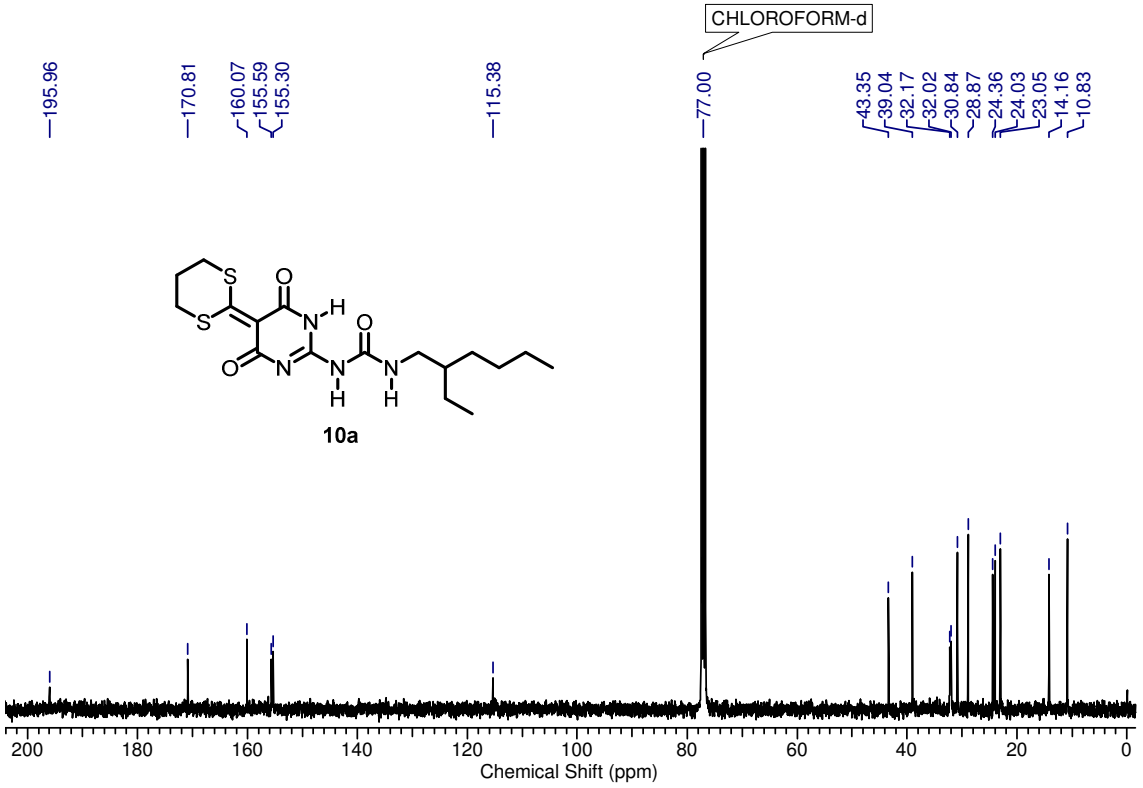

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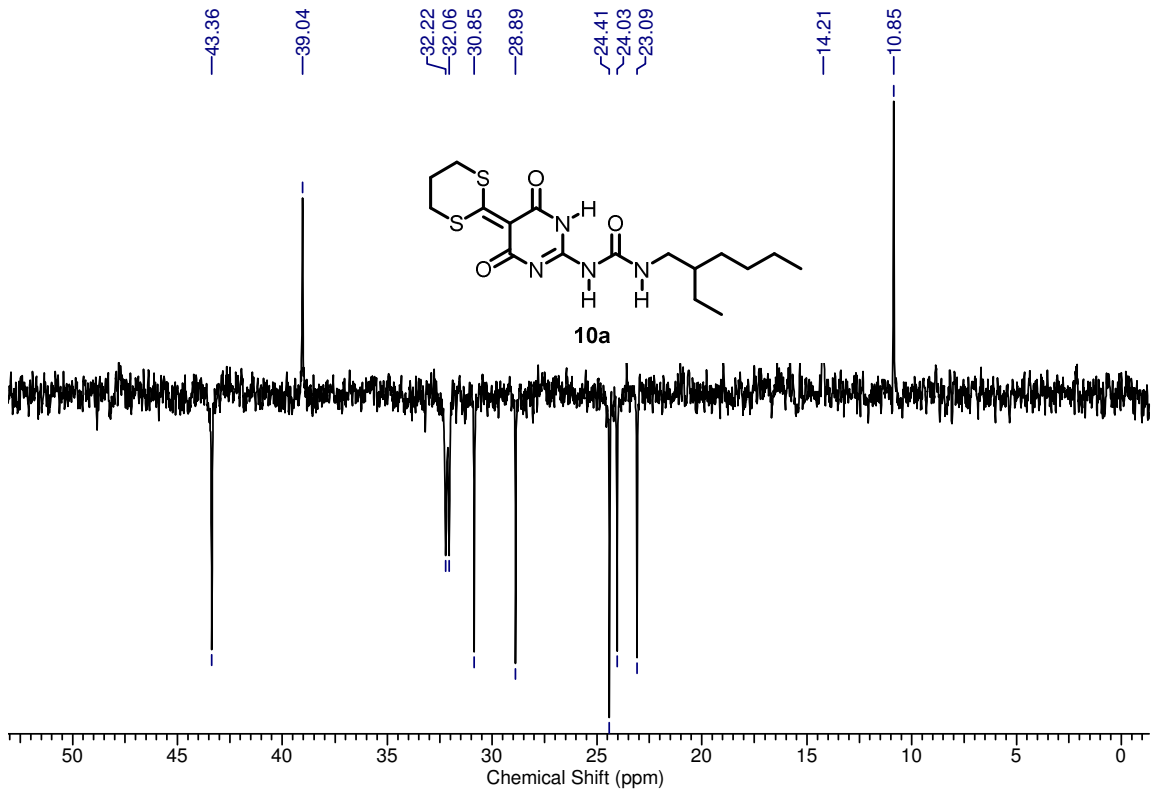
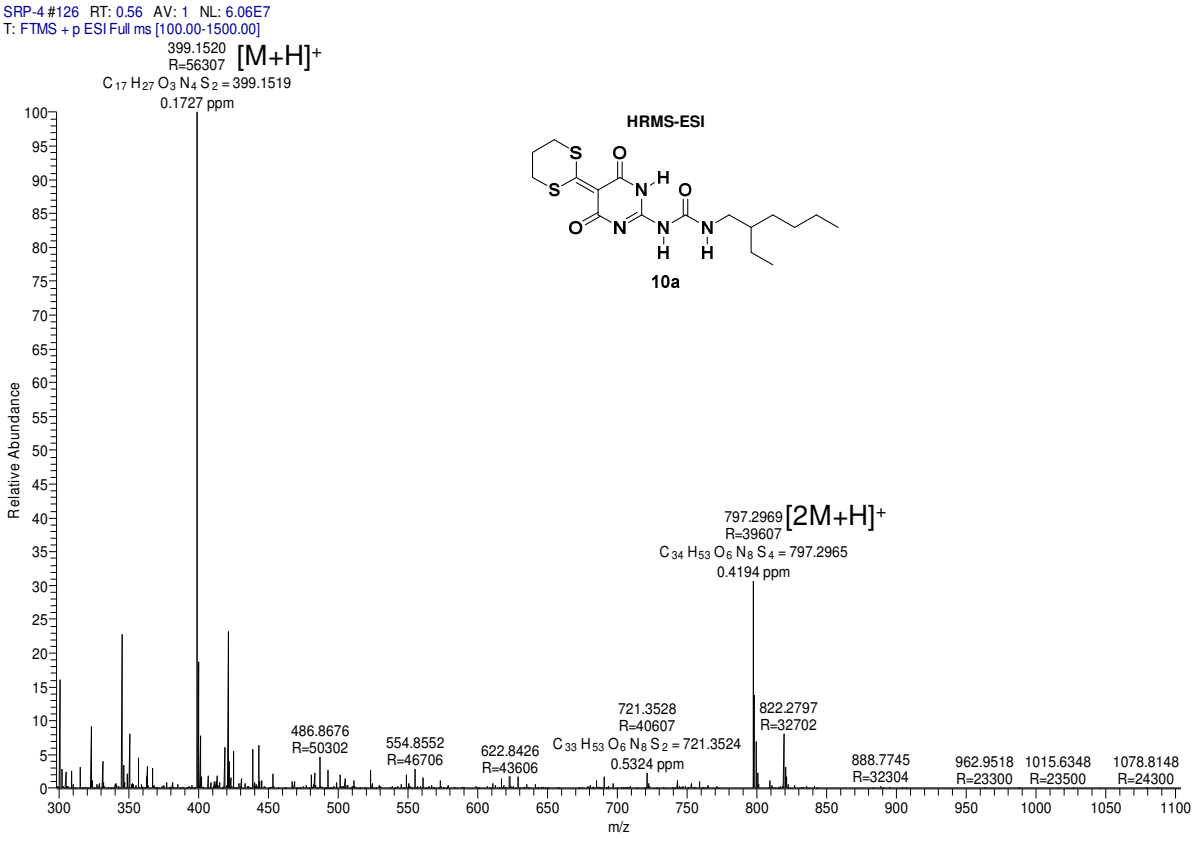
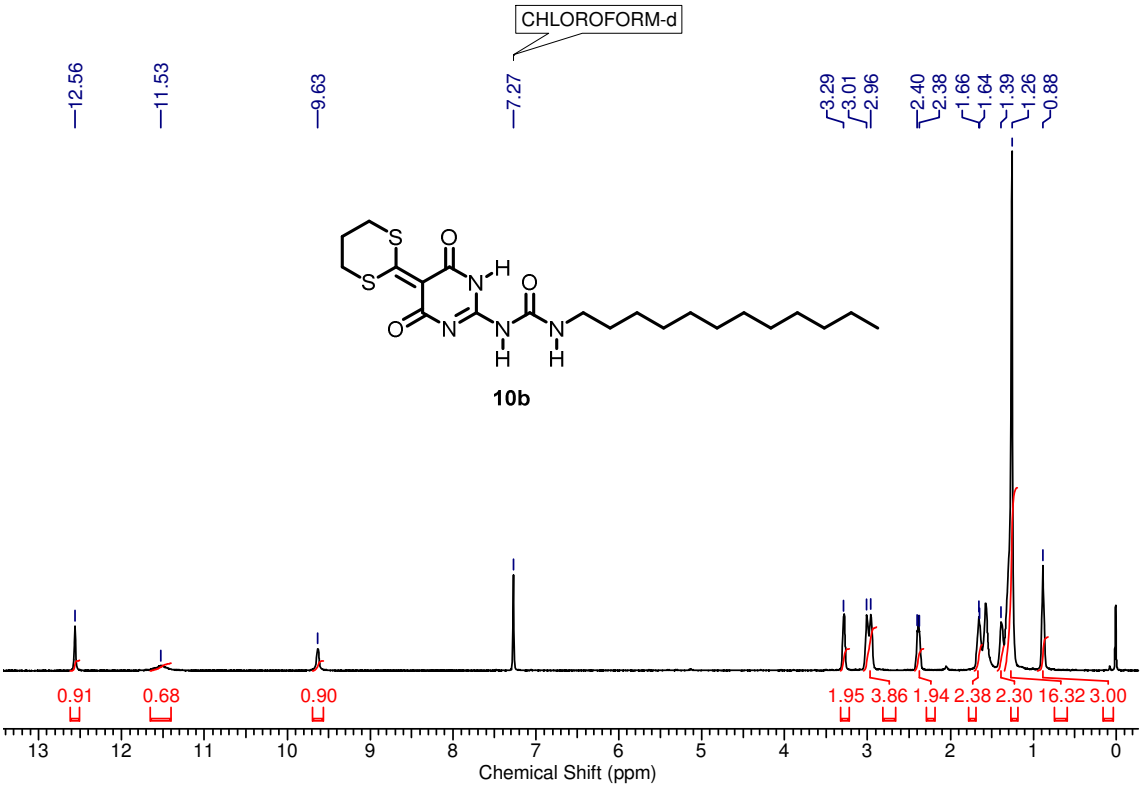
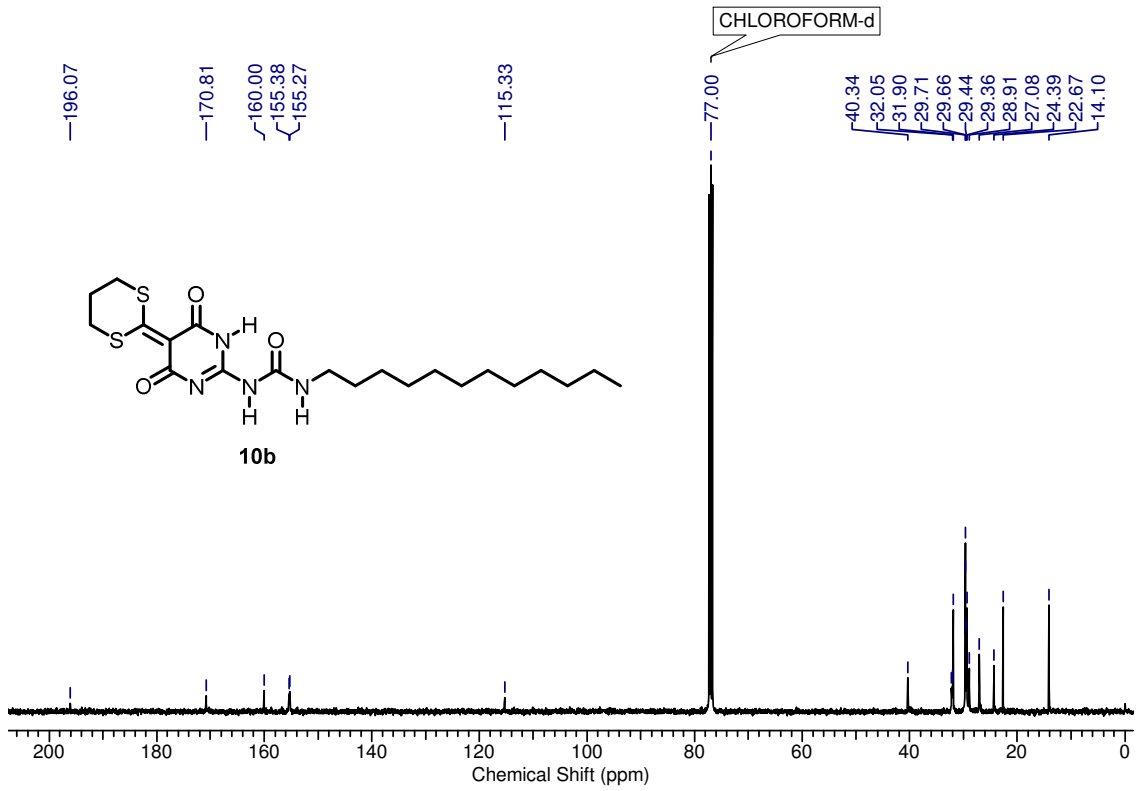


DEPT-135 NMR spectrum of compound **10a** ($CDCl_3$, 100 MHz, 298 K)

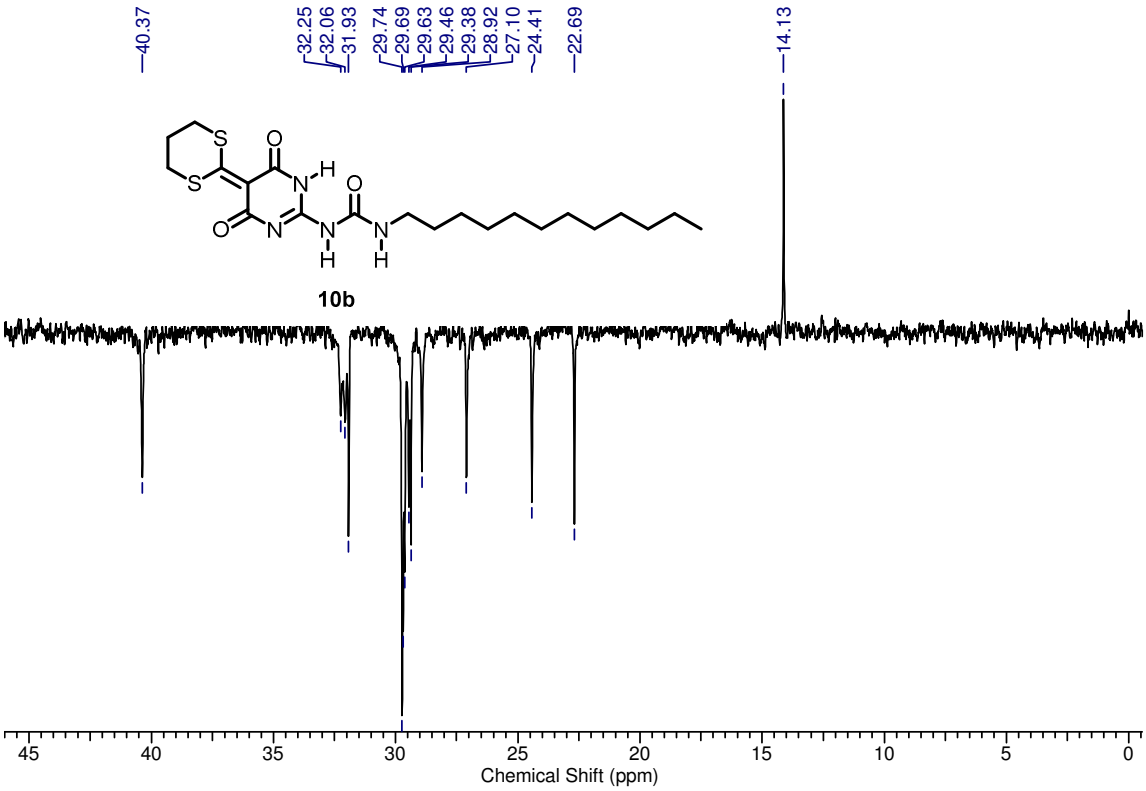




^{1}H NMR spectrum of compound **10b** ($CDCl_3$, 500 MHz, 298 K)



^{13}C NMR spectrum of compound **10b** ($CDCl_3$, 125 MHz, 298 K)



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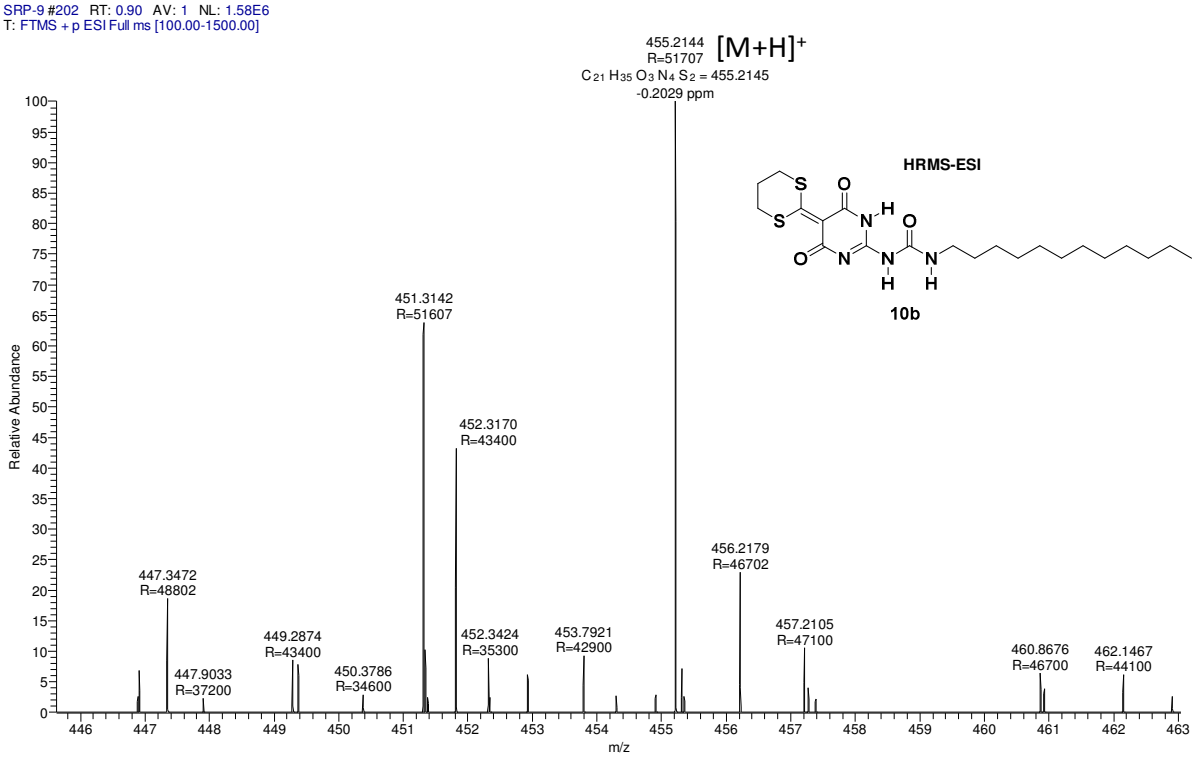
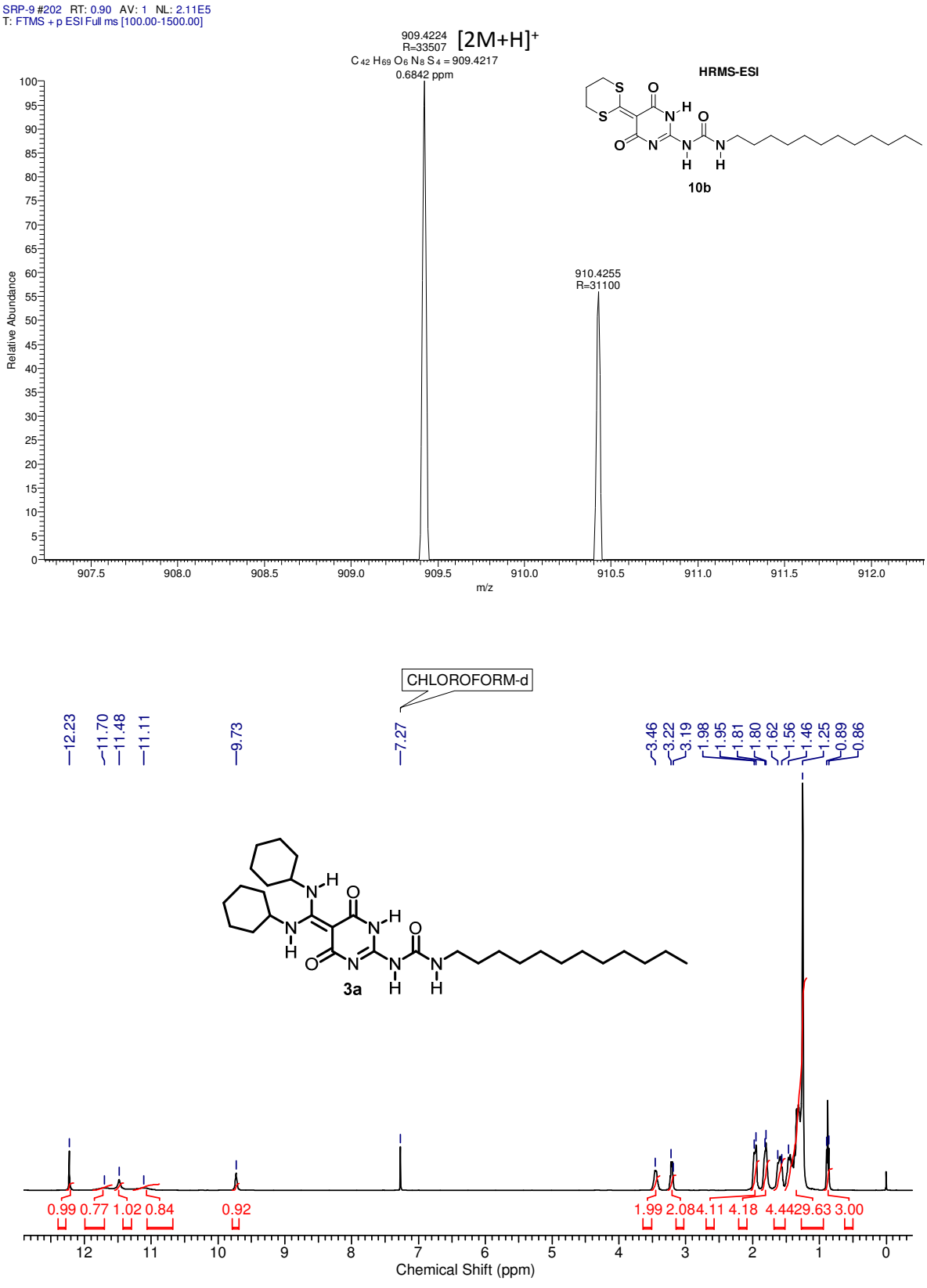
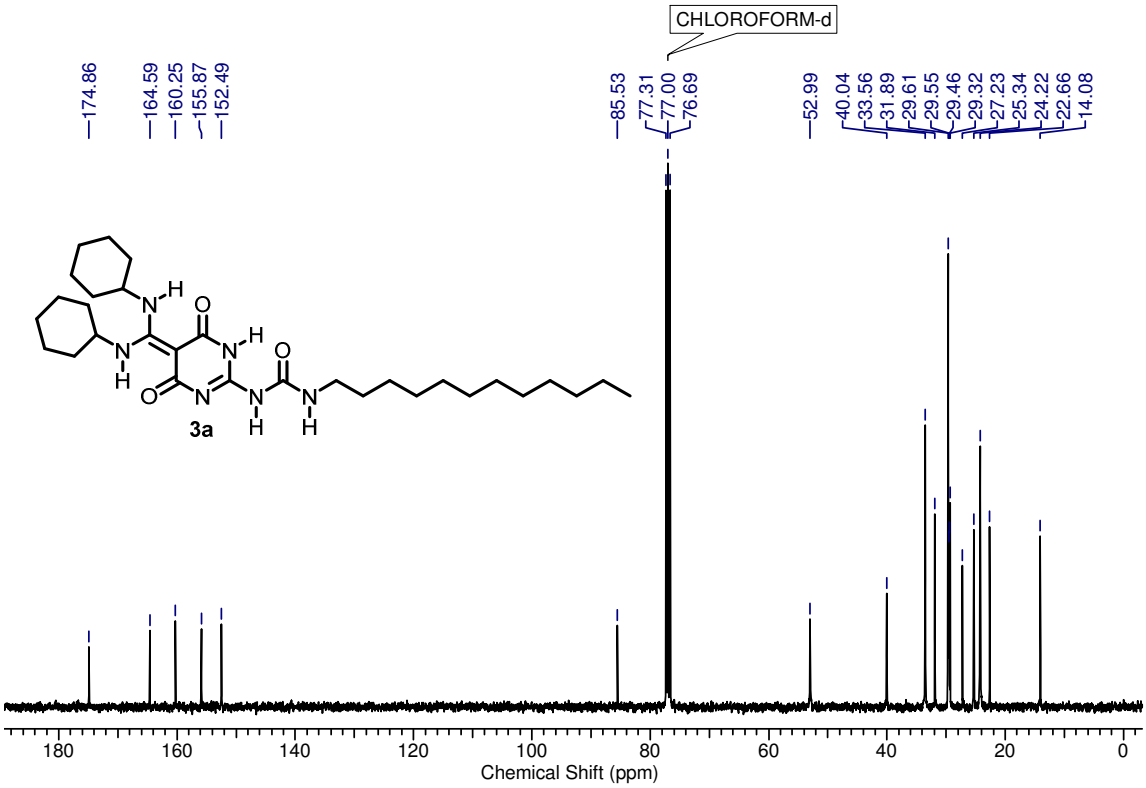
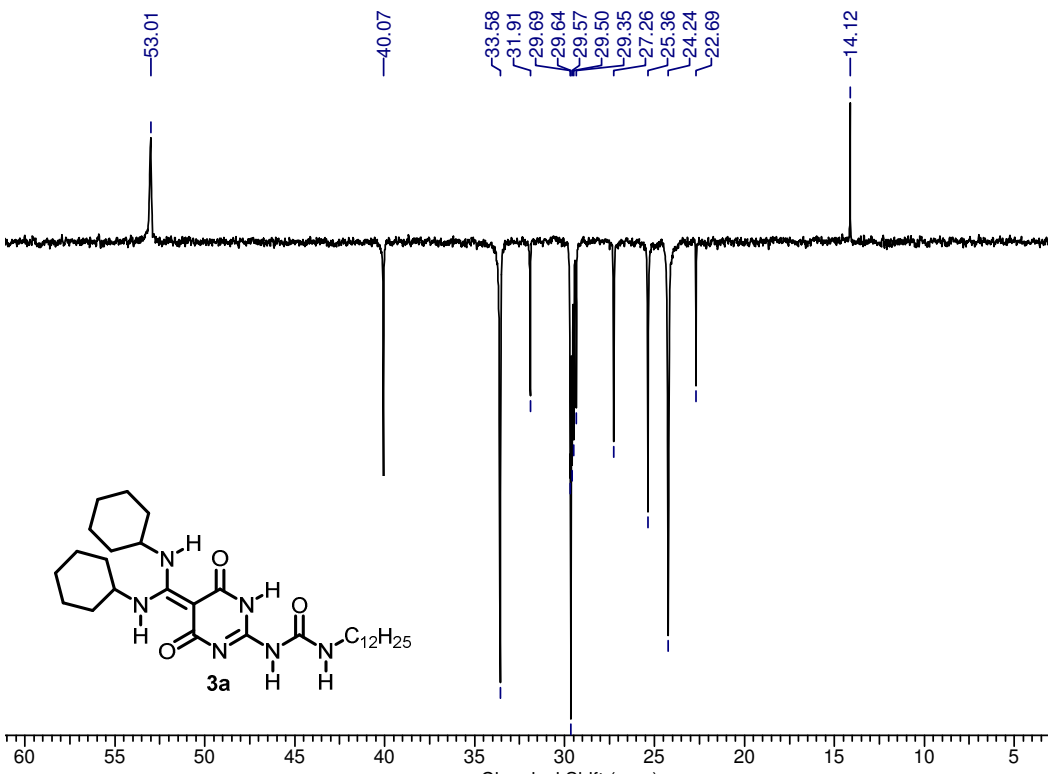




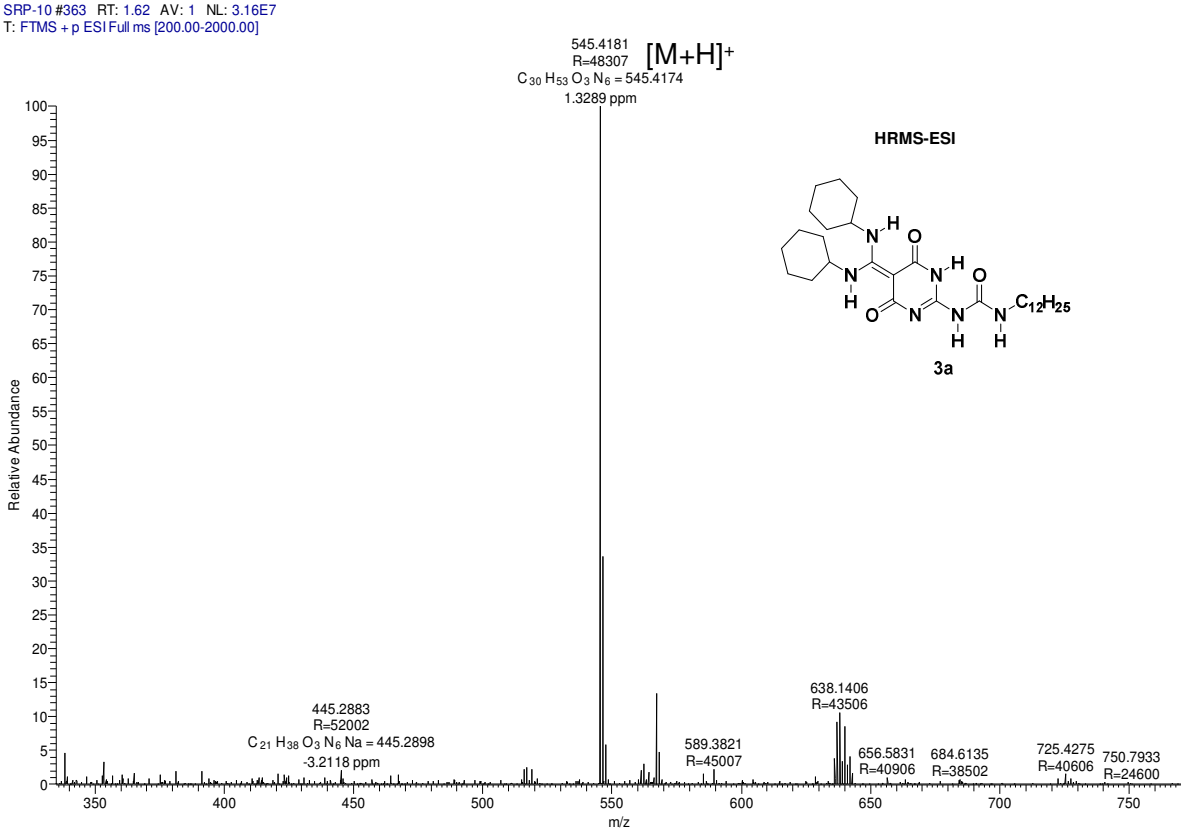
^{1}H NMR spectrum of compound **3a** ($CDCl_3$, 400 MHz, 298 K)



^{13}C NMR spectrum of compound **3a** ($CDCl_3$, 100 MHz, 298 K)



DEPT-135 NMR spectrum of compound **3a** ($CDCl_3$, 100 MHz, 298 K)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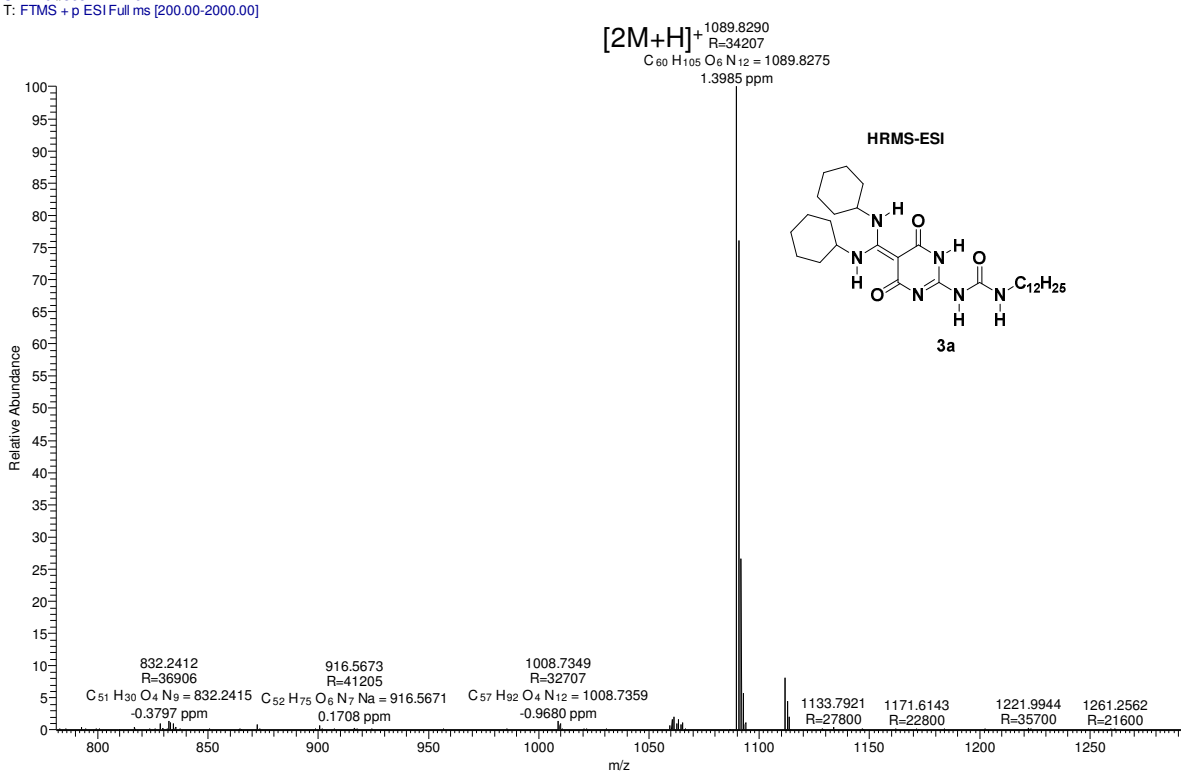
R=48307
[M+H]+
C30 H53 O3 N6 = 545.4174
1.3289 ppm
HRMS-ESI
3a
Relative Abundance
m/z
445.2883
R=52002
C21 H38 O3 N6 Na = 445.2898
-3.2118 ppm
589.3821
R=45007
638.1406
R=43506
656.5831
R=40906
684.6135
R=38502
725.4275
R=40606
750.7933
R=24600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T: FTMS + p ESI Full ms [200.00-2000.00]
[2M+H]+
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R=34207
C60 H105 O6 N12 = 1089.8275
1.3985 ppm
HRMS-ESI
3a
Relative Abundance
m/z
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R=36906
C51 H30 O4 N9 = 832.2415
-0.3797 ppm
916.5673
R=41205
C52 H75 O6 N7 Na = 916.5671
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C57 H92 O4 N12 = 1008.7359
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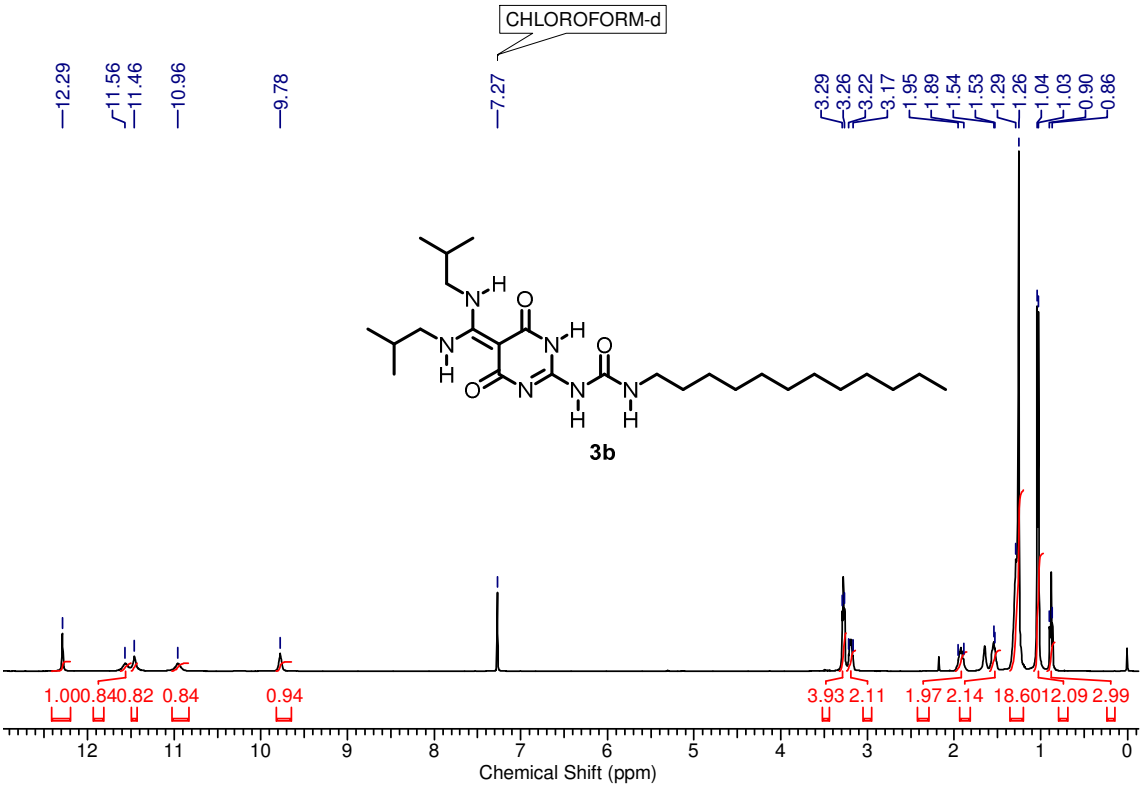
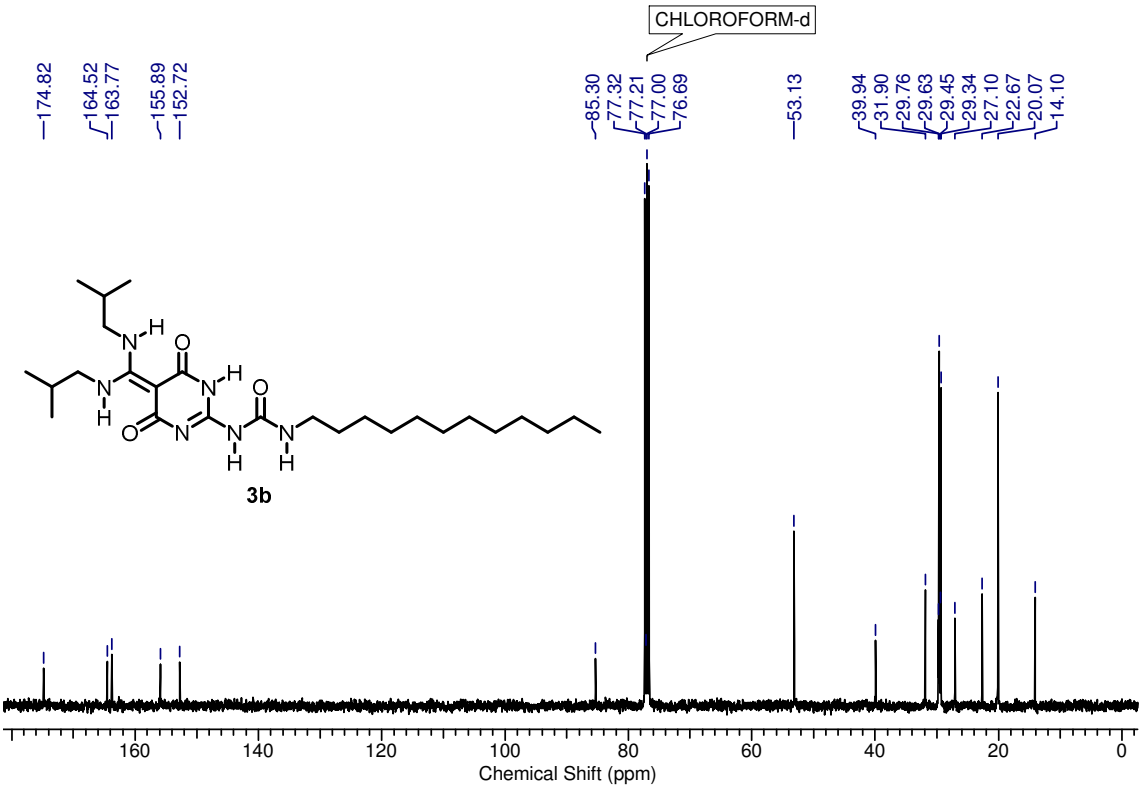
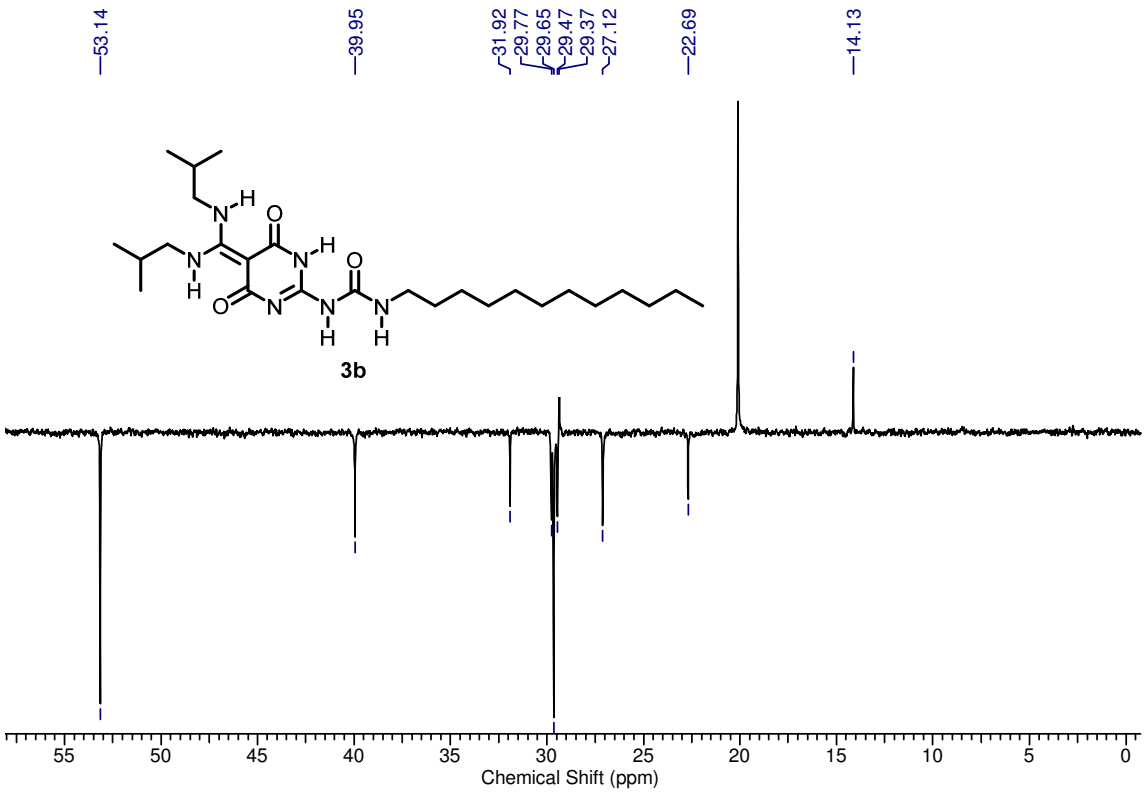


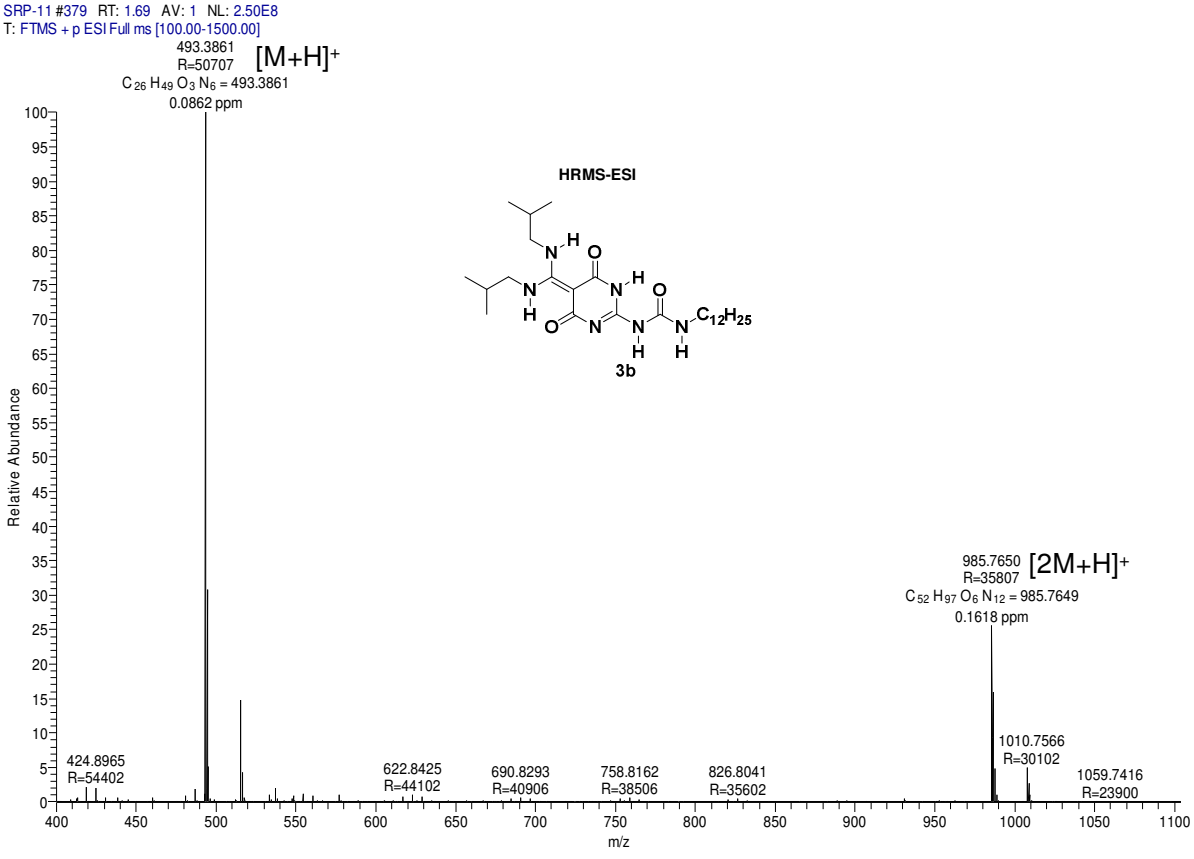
^{1}H NMR spectrum of compound **3b** ($CDCl_3$, 400 MHz, 298 K)

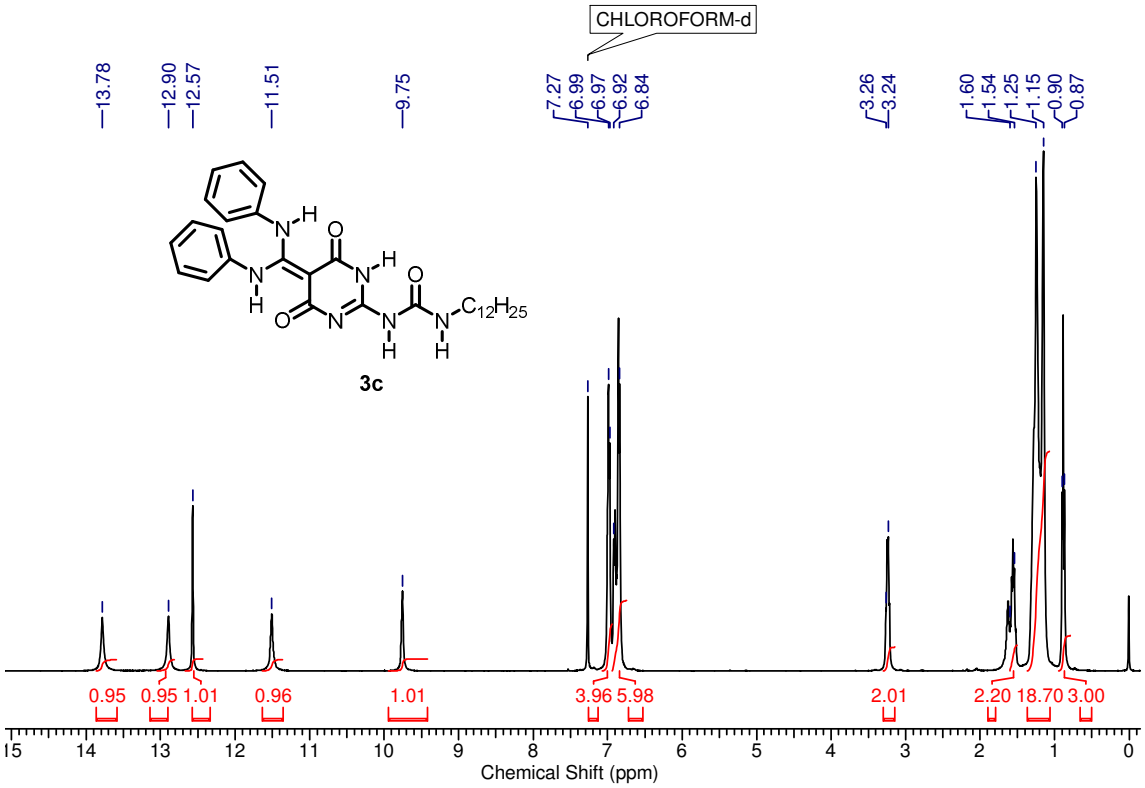


^{13}C NMR spectrum of compound **3b** ($CDCl_3$, 100 MHz, 298 K)



DEPT-135 NMR spectrum of compound **3b** ($CDCl_3$, 100 MHz, 298 K)





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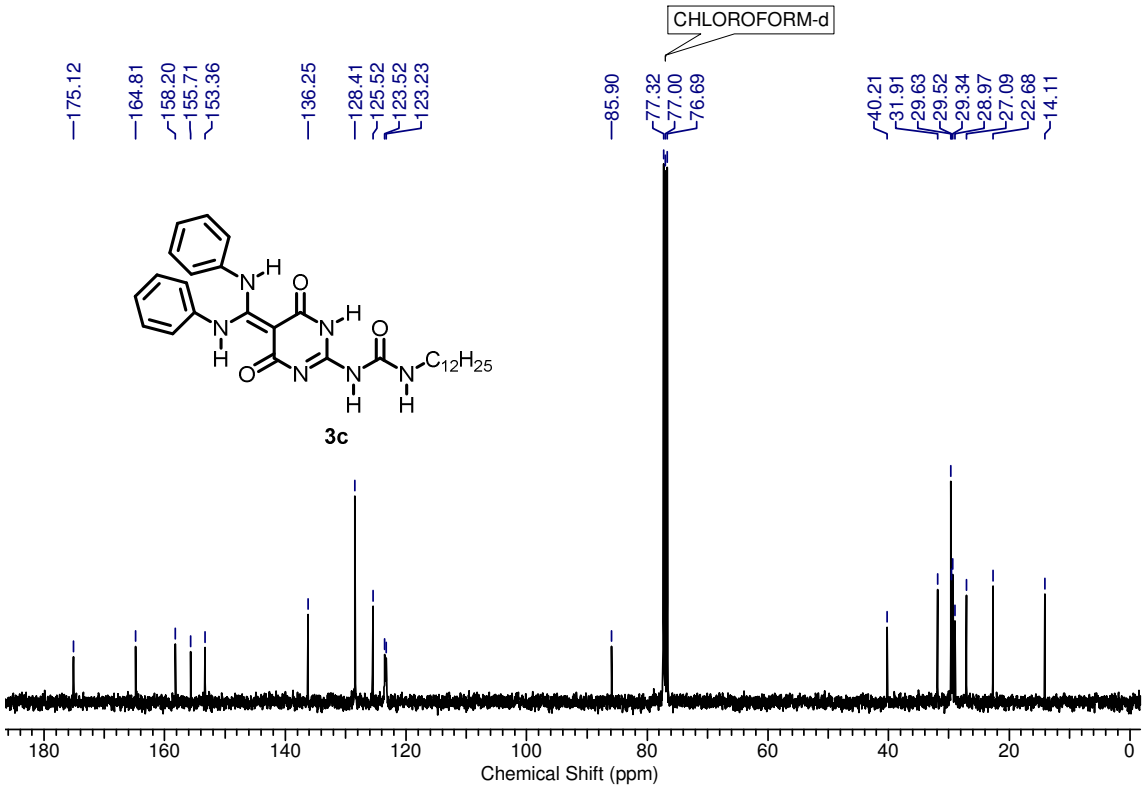
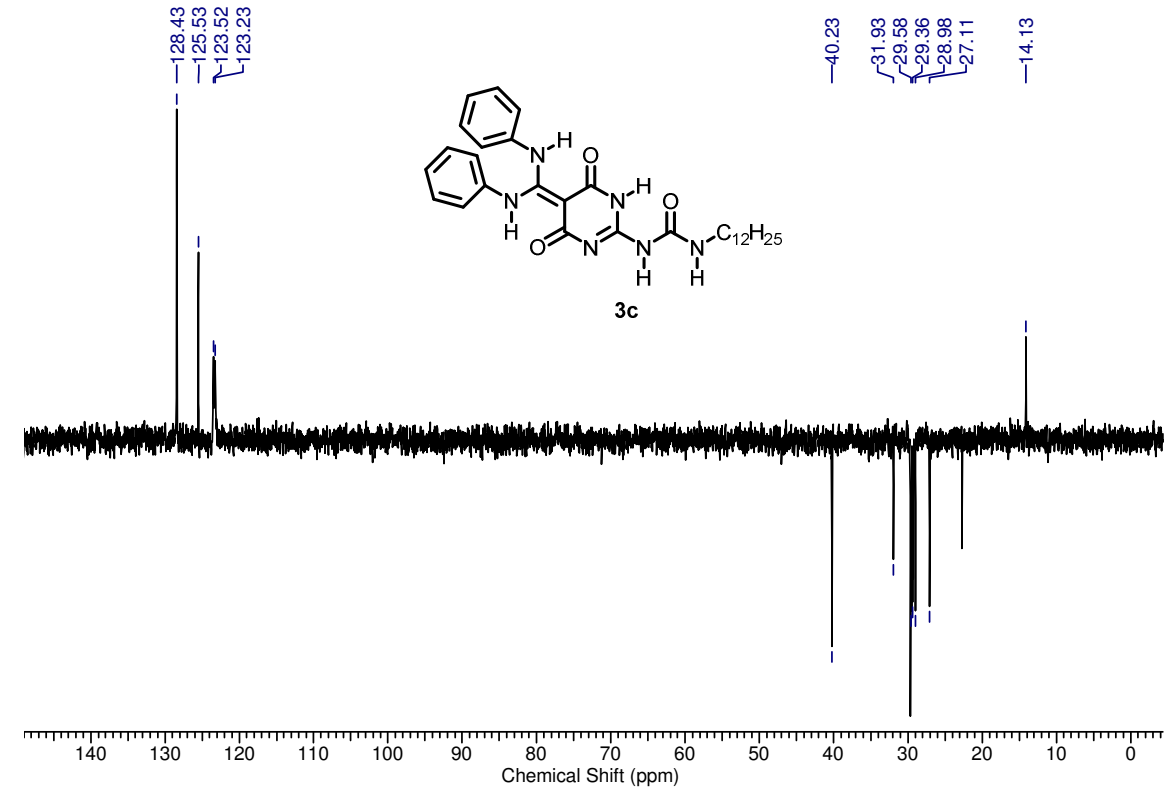
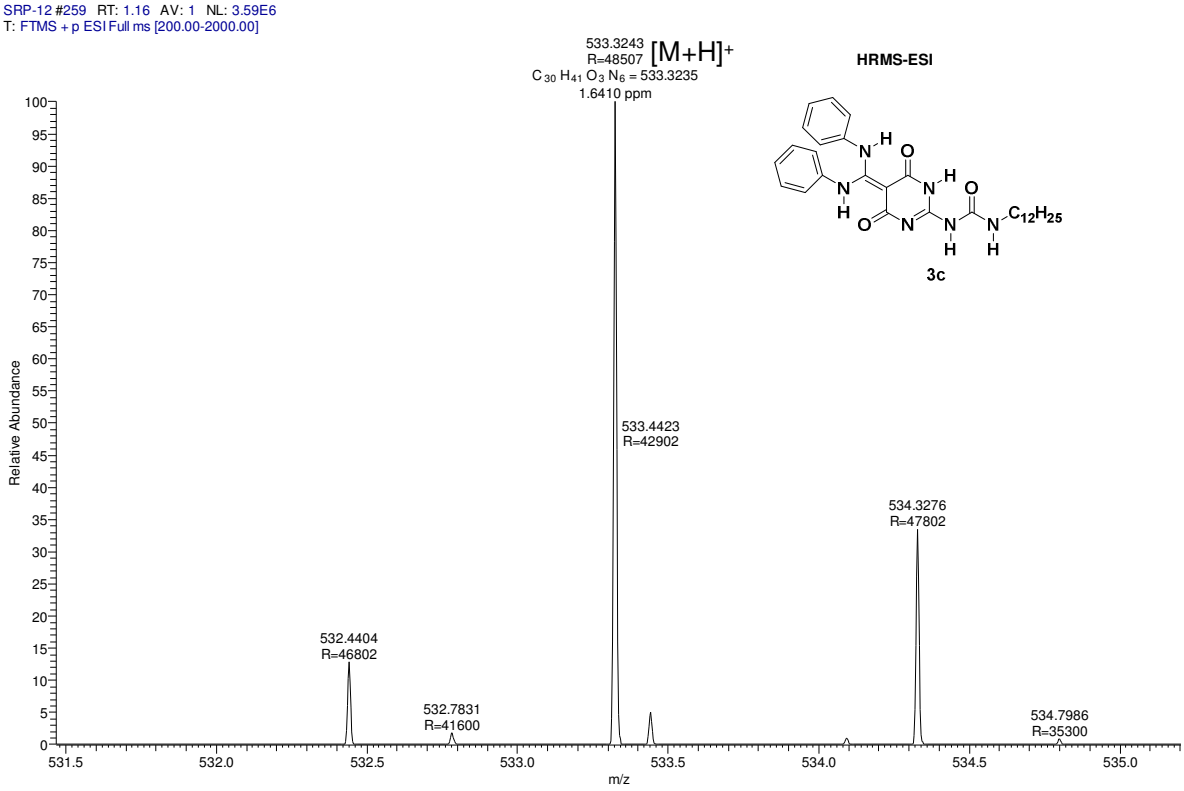
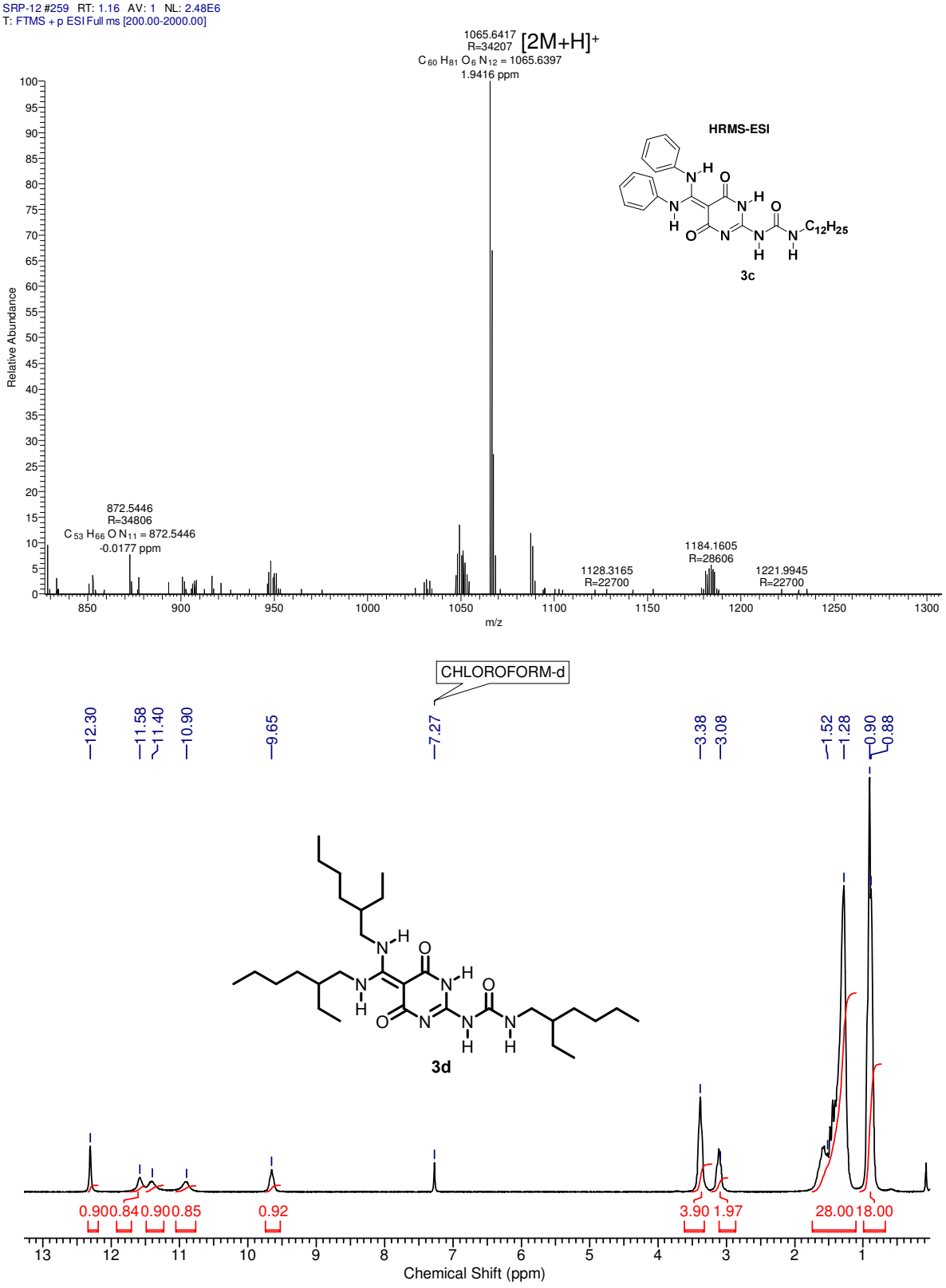


^{13}C NMR spectrum of compound **3c** ($CDCl_3$, 100 MHz, 298 K)



DEPT-135 NMR spectrum of compound **3c** ($CDCl_3$, 100 MHz, 298 K)





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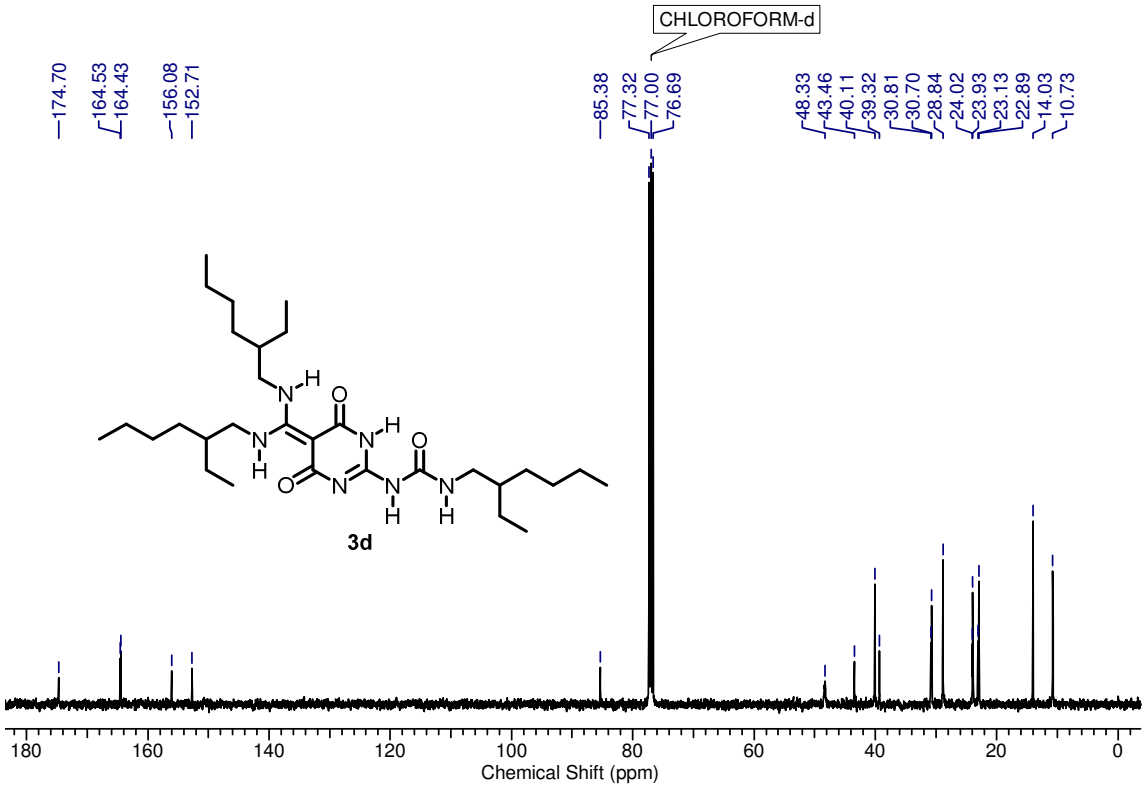
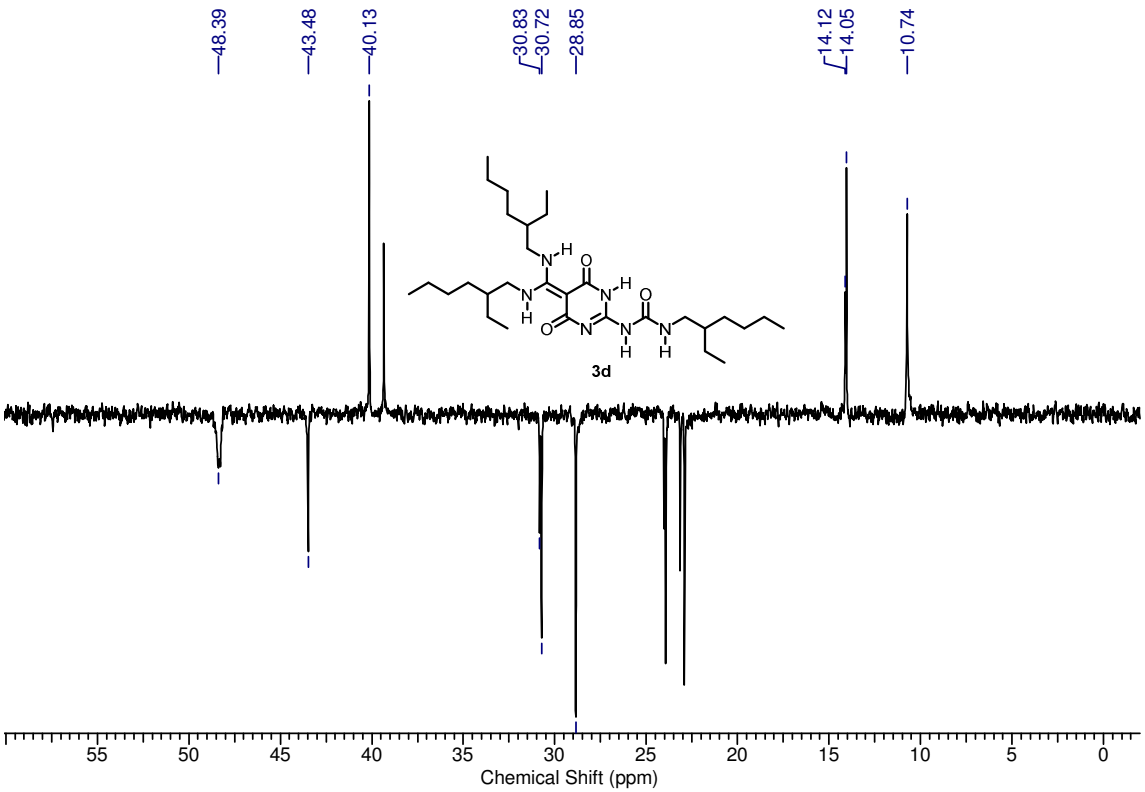
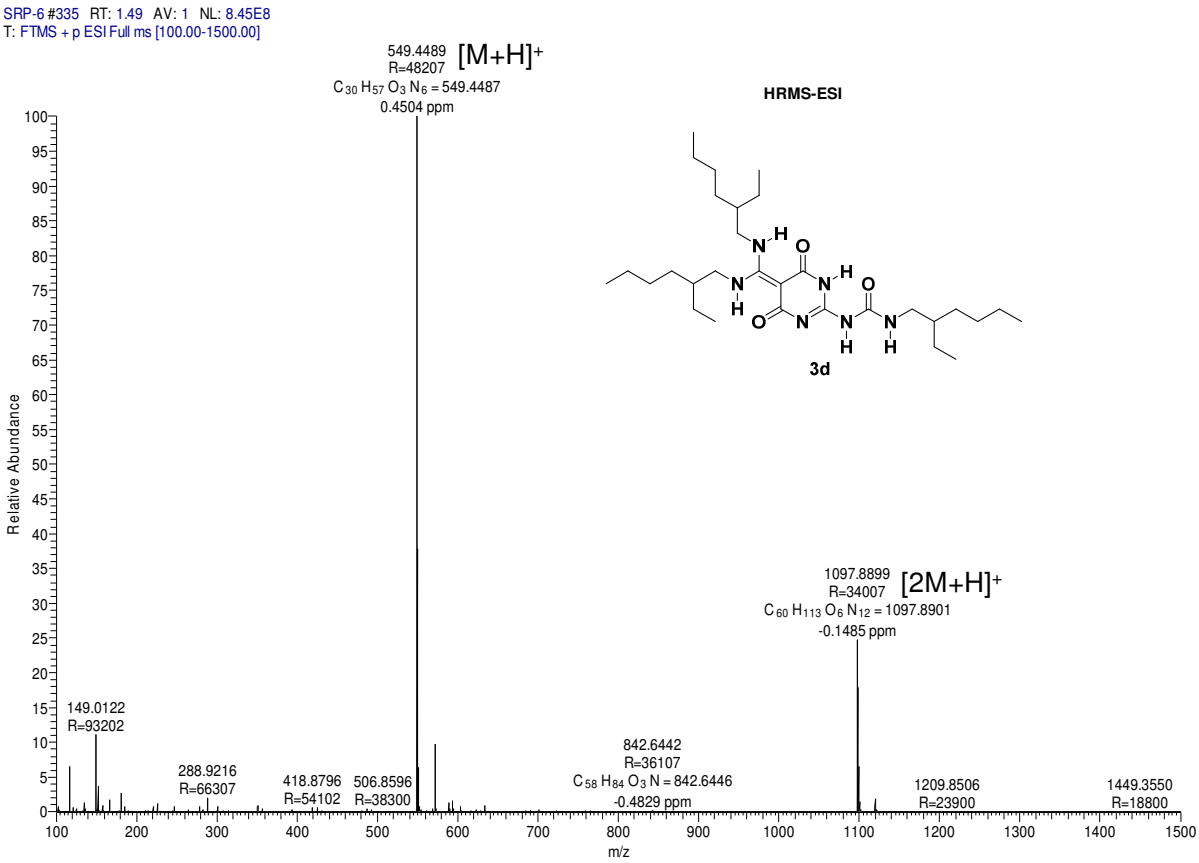
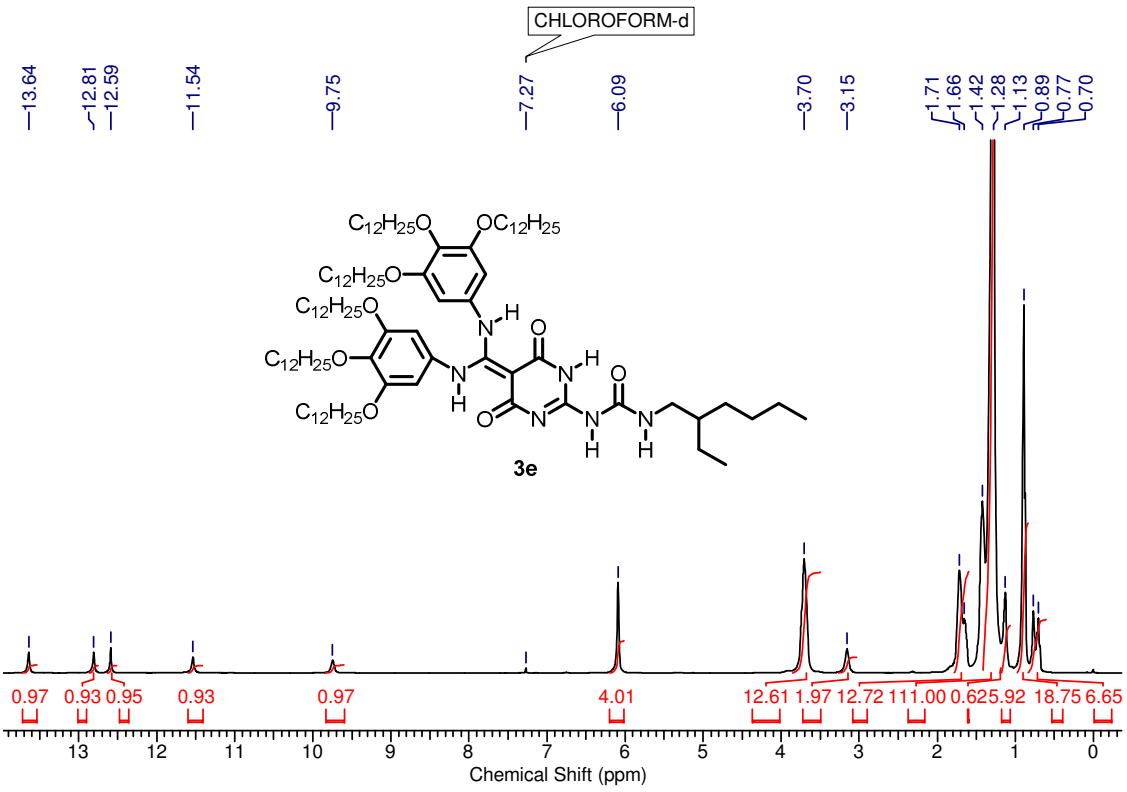


^{13}C NMR spectrum of compound **3d** ($CDCl_3$, 100 MHz, 298 K)

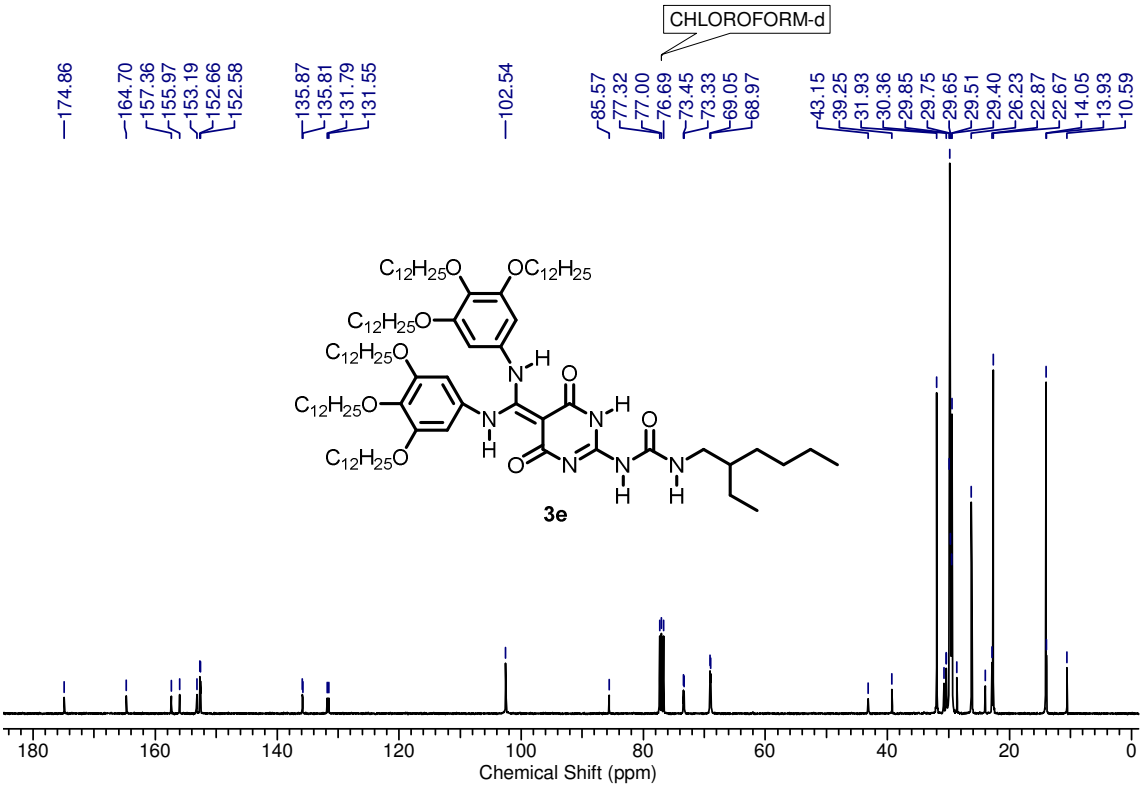


DEPT-135 NMR spectrum of compound **3d** ($CDCl_3$, 100 MHz, 298 K)

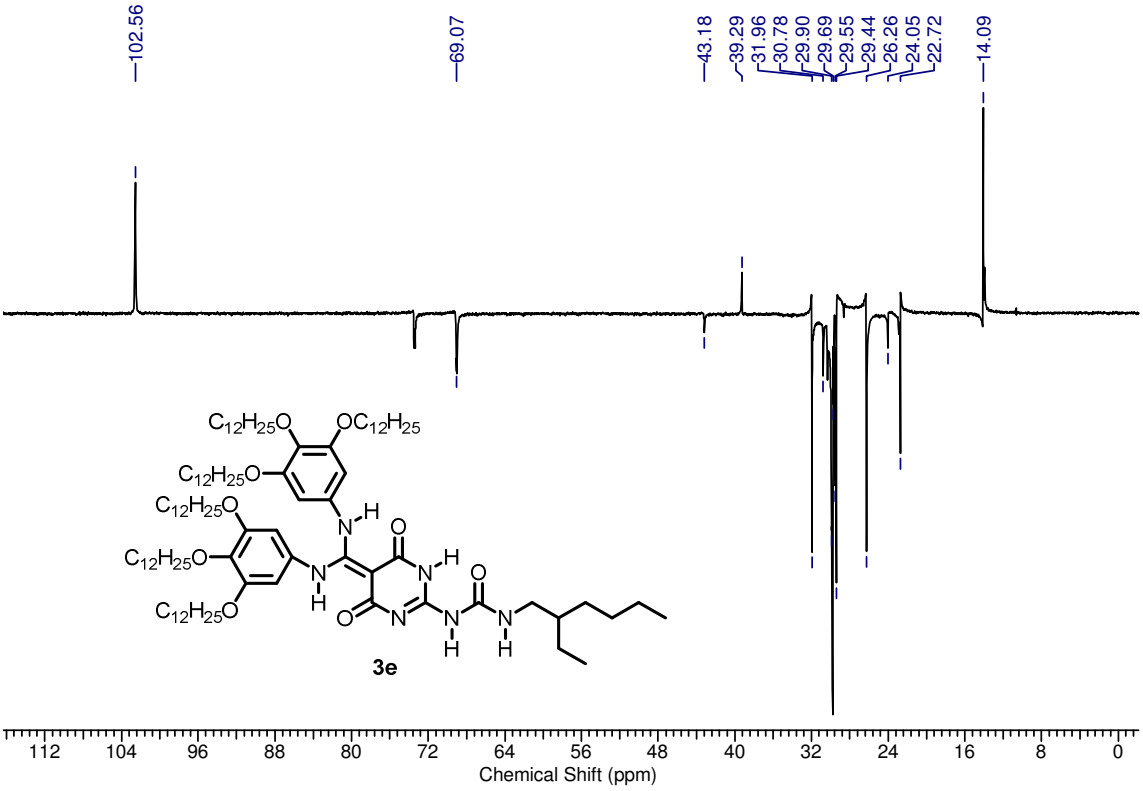




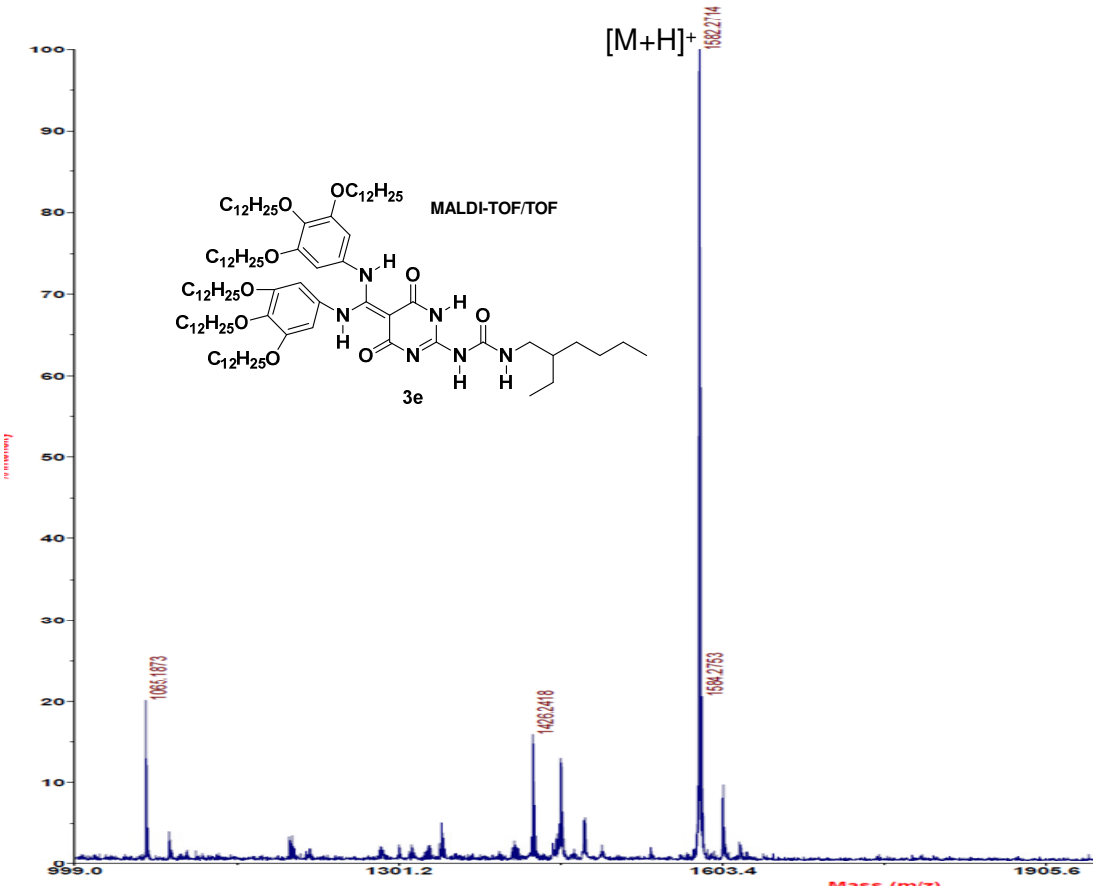
^{1}H NMR spectrum of compound **3e** ($CDCl_3$, 400 MHz, 298 K)

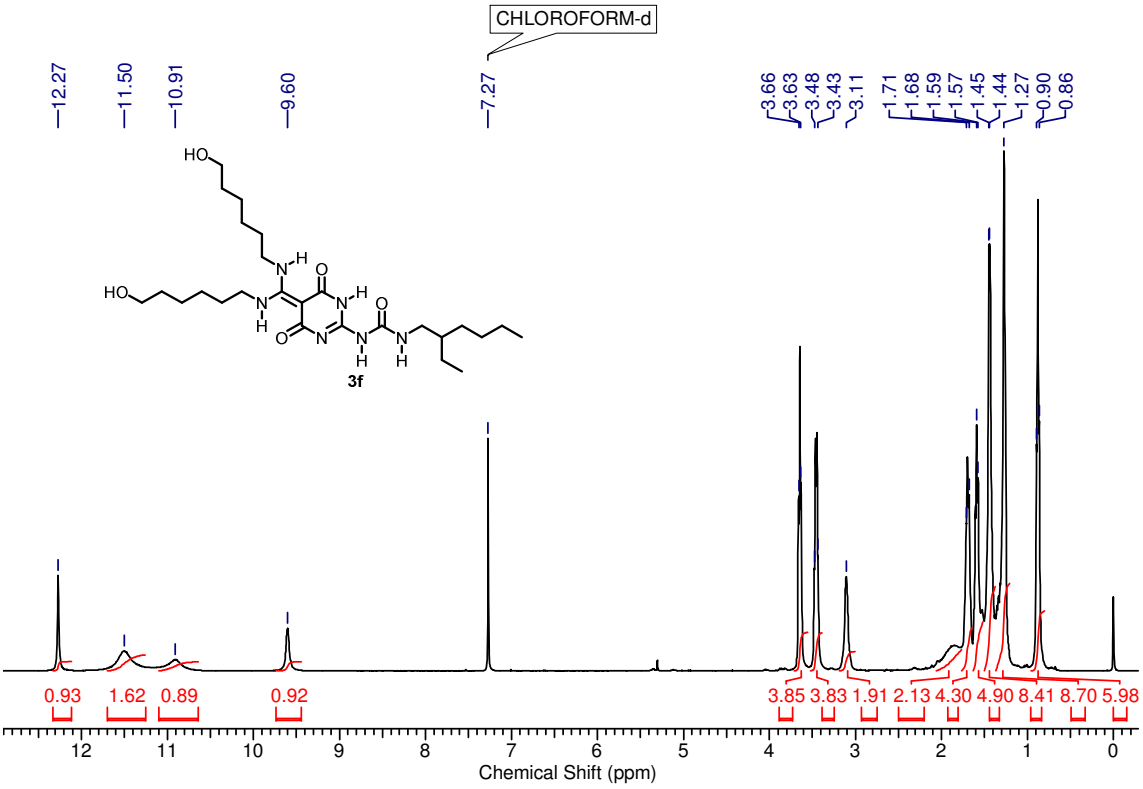


^{13}C NMR spectrum of compound **3e** ($CDCl_3$, 100 MHz, 298 K)

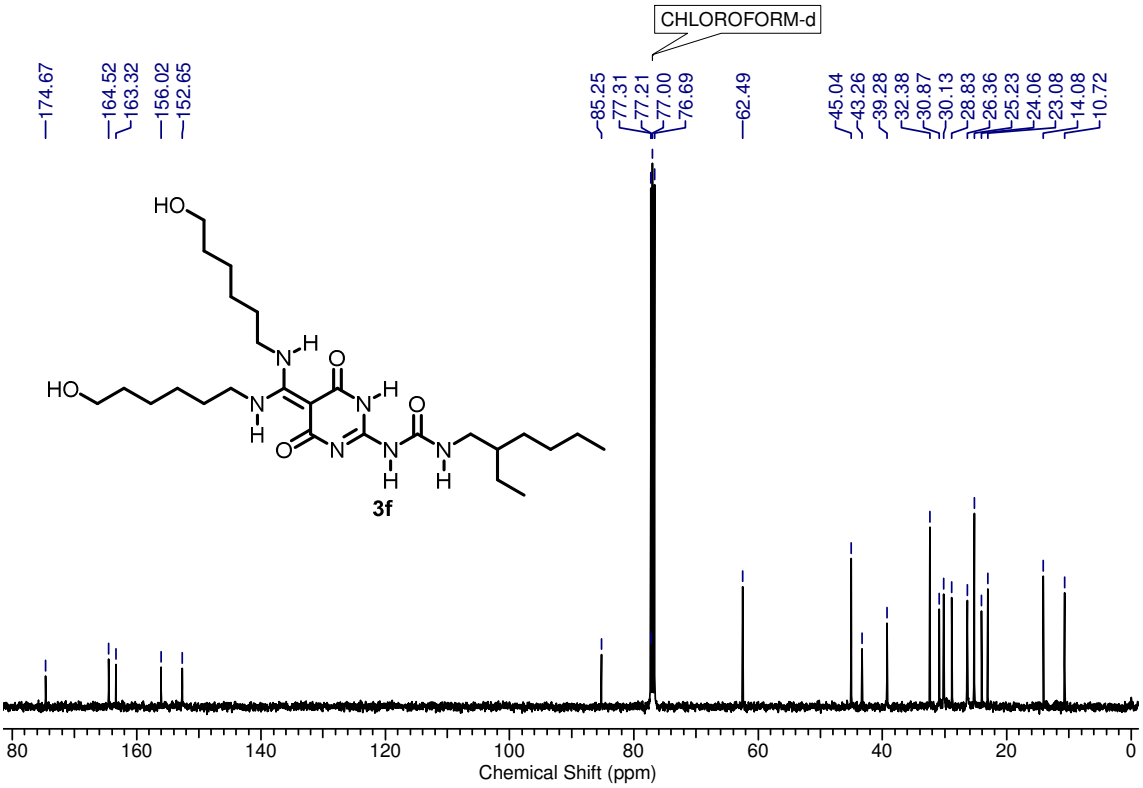


DEPT-135 NMR spectrum of compound **3e** ($CDCl_3$, 100 MHz, 298 K)

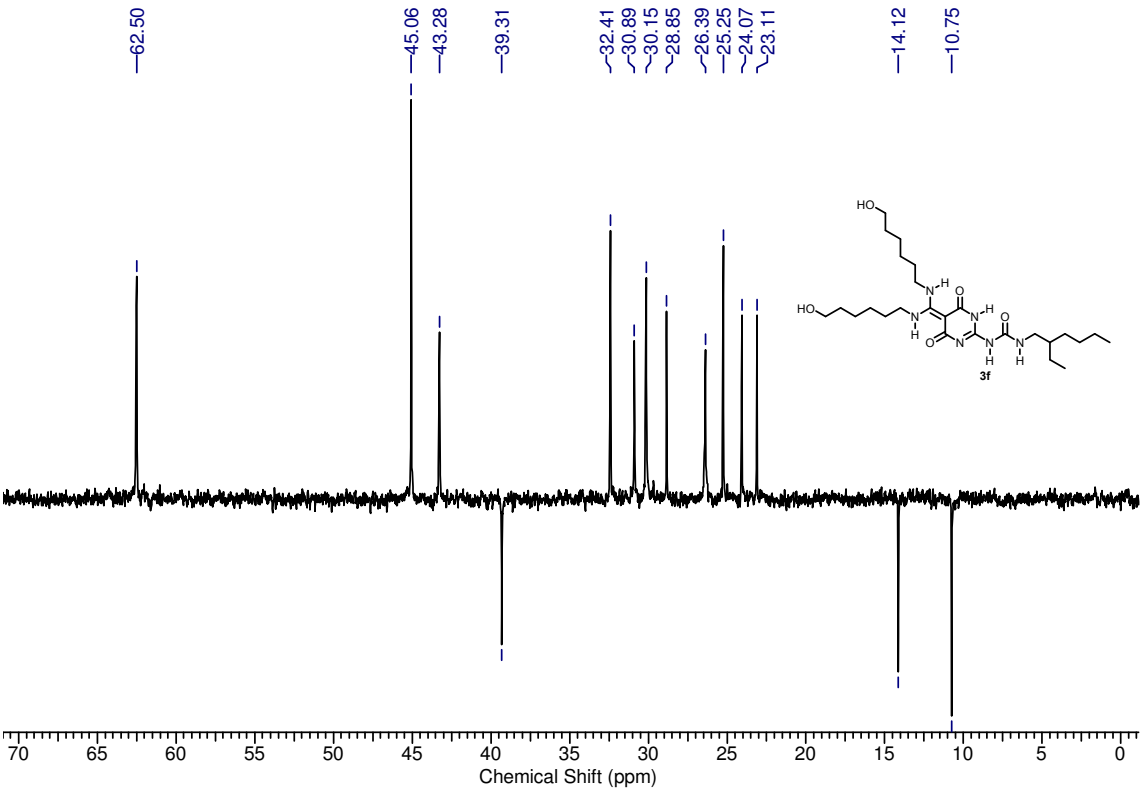




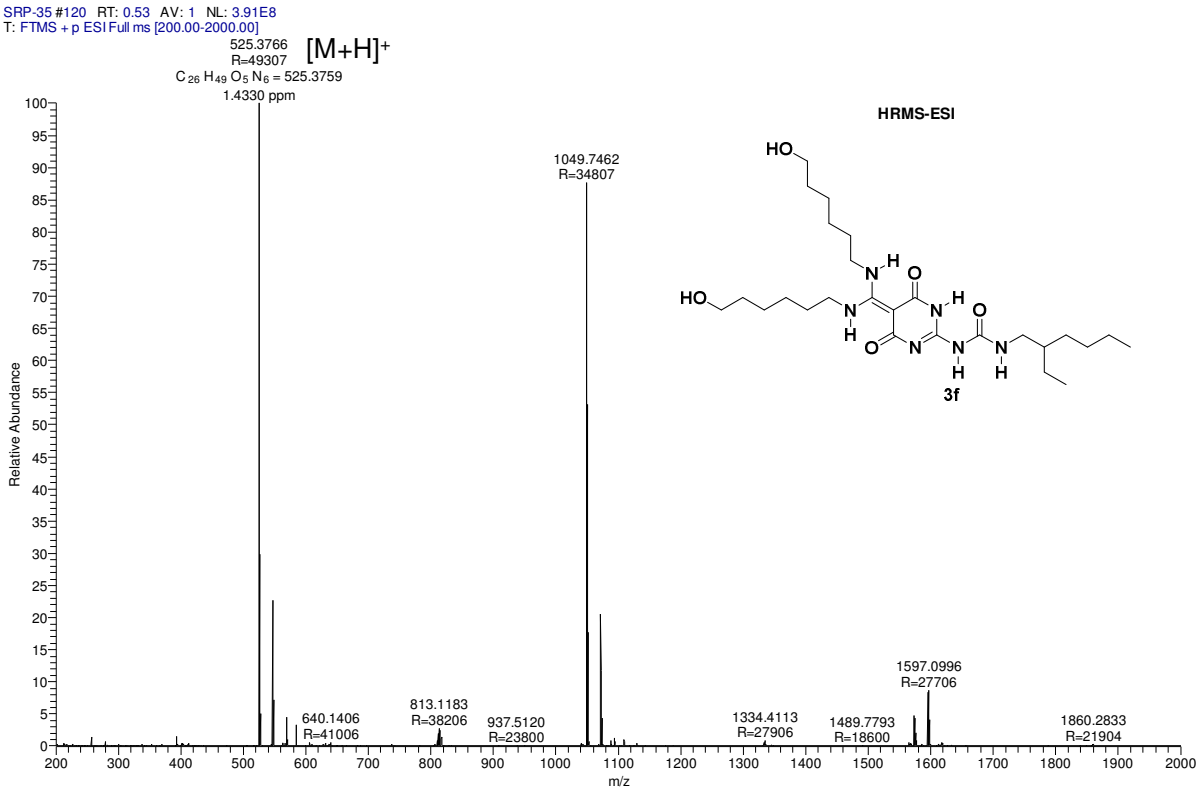
^{1}H NMR spectrum of compound **3f** ($CDCl_3$, 400 MHz, 298 K)

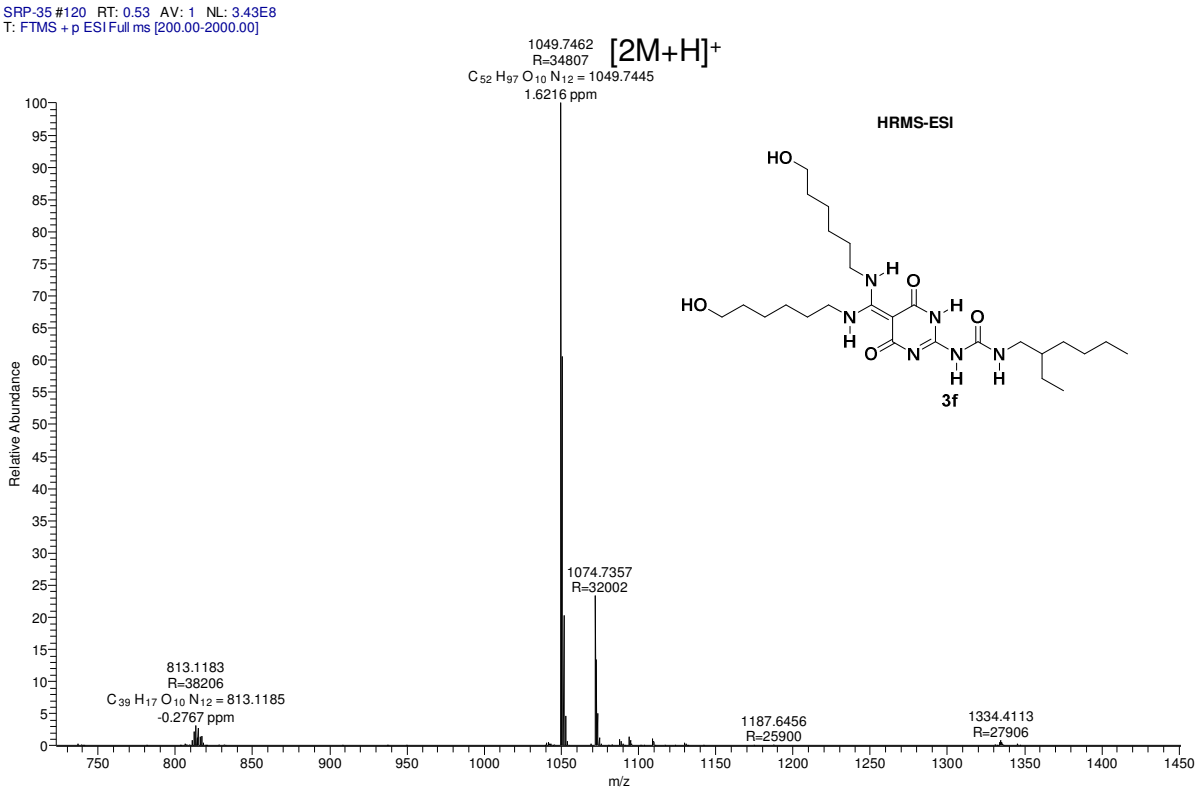


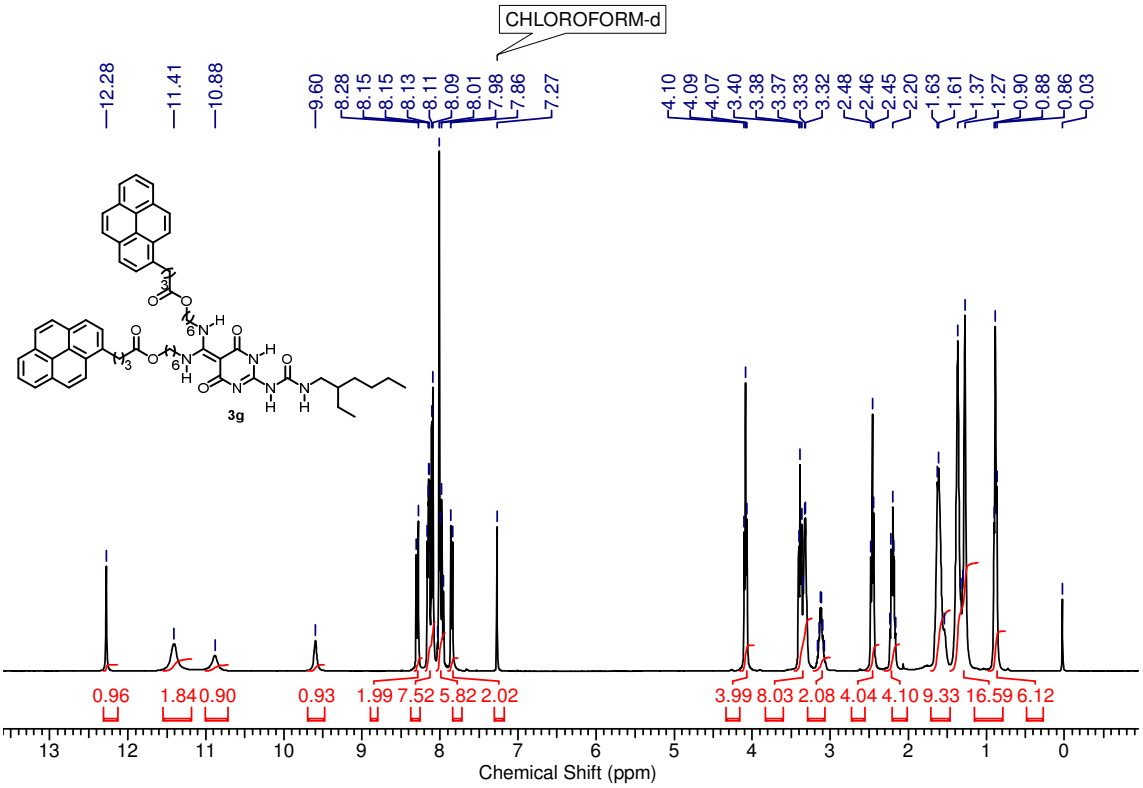
^{13}C NMR spectrum of compound **3f** ($CDCl_3$, 100 MHz, 298 K)



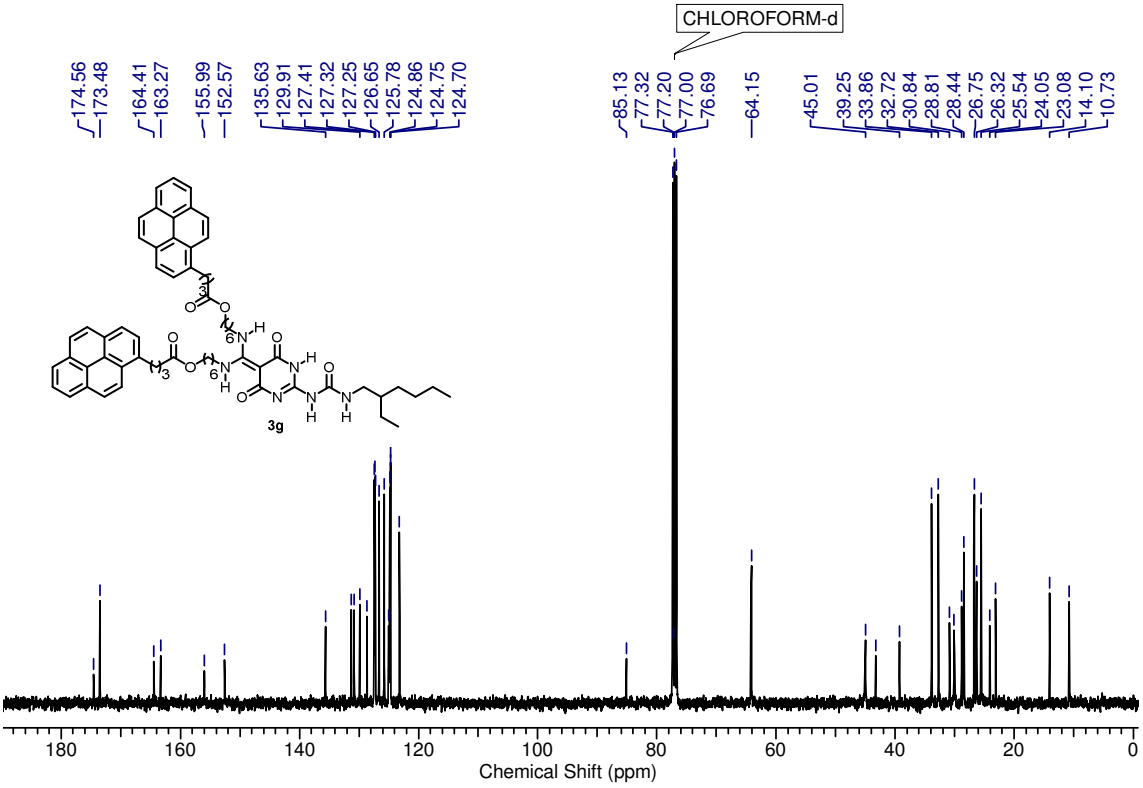
DEPT-135 NMR spectrum of compound **3f** ($CDCl_3$, 100 MHz, 298 K)


SRP-35 #120 RT: 0.53 AV: 1 NL: 3.91E8
T: FTMS + p ESI Full ms [200.00-2000.00]
525.3766
R=49307
[M+H]+
C26 H49 O5 N6 = 525.3759
1.4330 ppm
HRMS-ESI
1049.7462
R=34807
640.1406
R=41006
813.1183
R=38206
937.5120
R=23800
1334.4113
R=27906
1489.7793
R=18600
1597.0996
R=27706
1860.2833
R=21904
Relative Abundance
m/z
3f

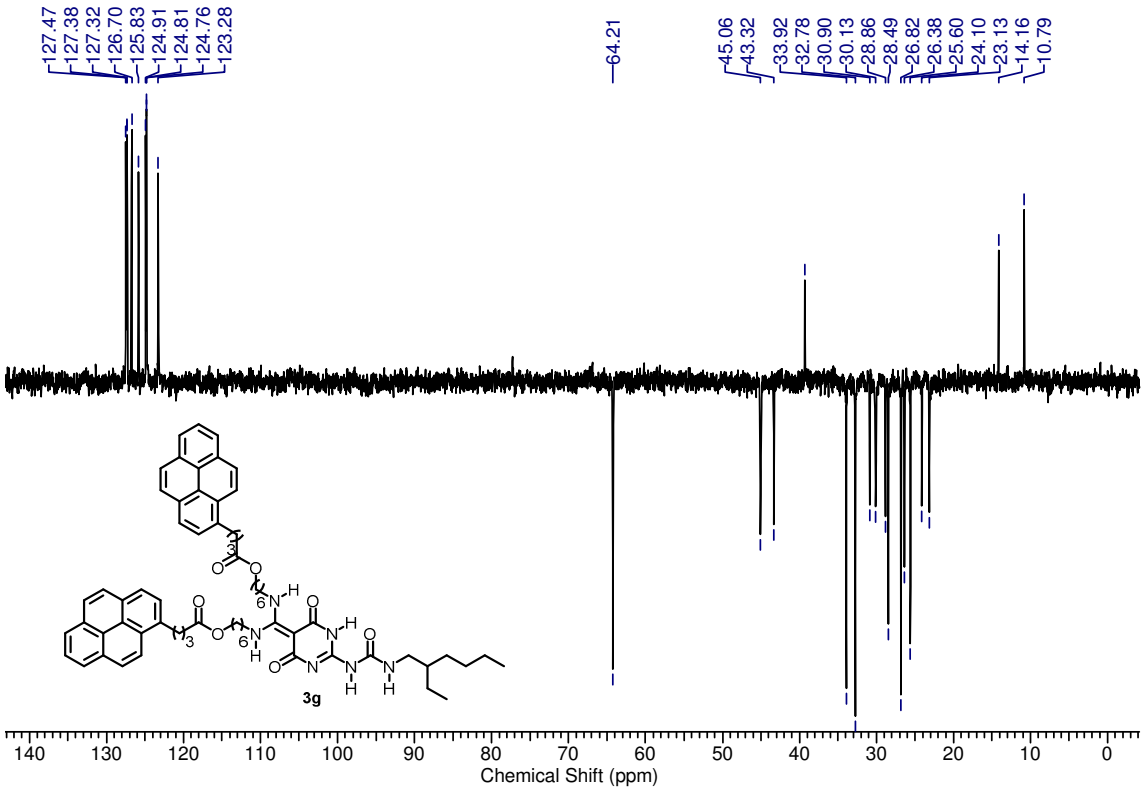

SRP-35 #120 RT: 0.53 AV: 1 NL: 3.43E8
T: FTMS + p ESI Full ms [200.00-2000.00]
1049.7462
R=34807
[2M+H]+
C52 H97 O10 N12 = 1049.7445
1.6216 ppm
HRMS-ESI
1074.7357
R=32002
813.1183
R=38206
C39 H17 O10 N12 = 813.1185
-0.2767 ppm
1187.6456
R=25900
1334.4113
R=27906
Relative Abundance
m/z
3f



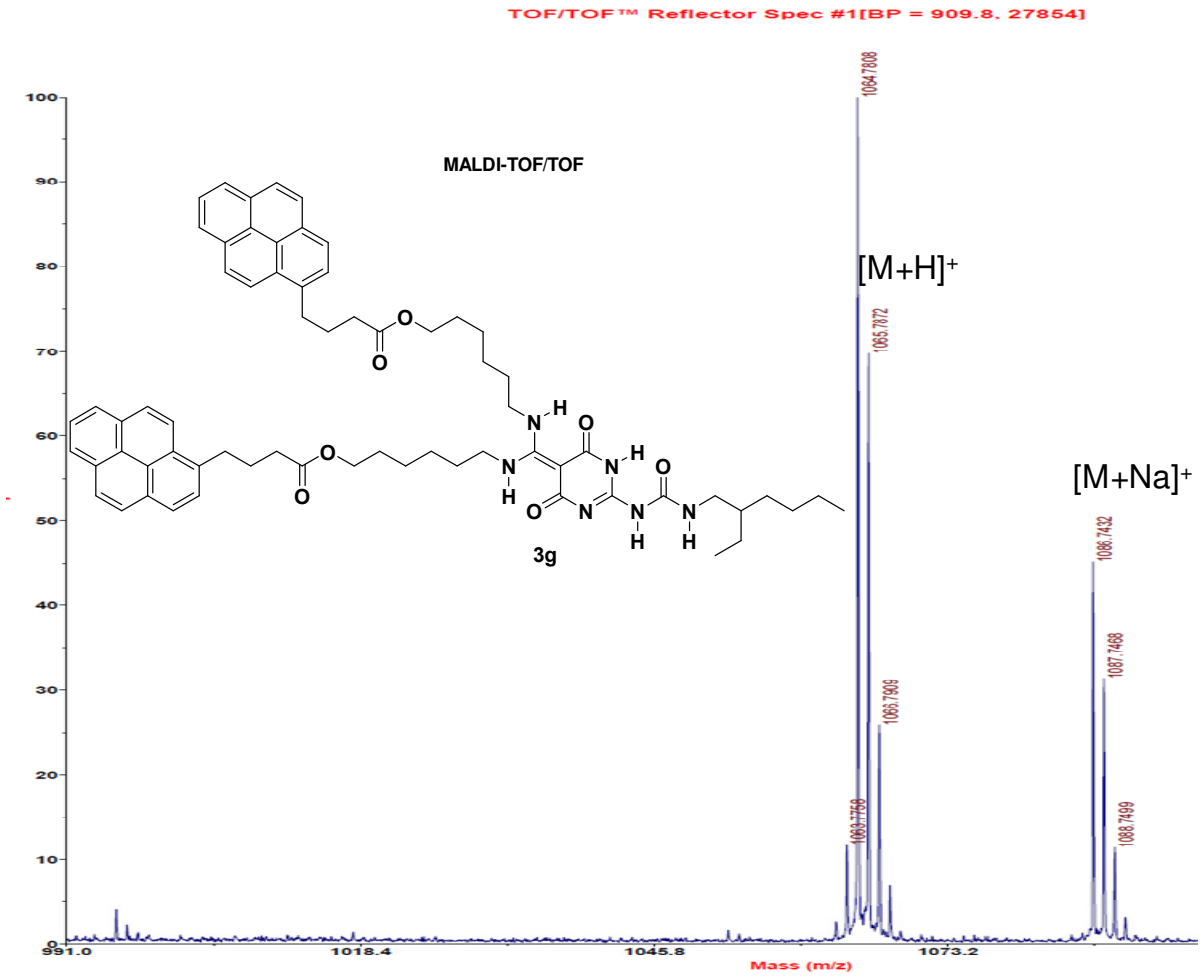
^{1}H NMR spectrum of compound **3g** ($CDCl_3$, 400 MHz, 298 K)

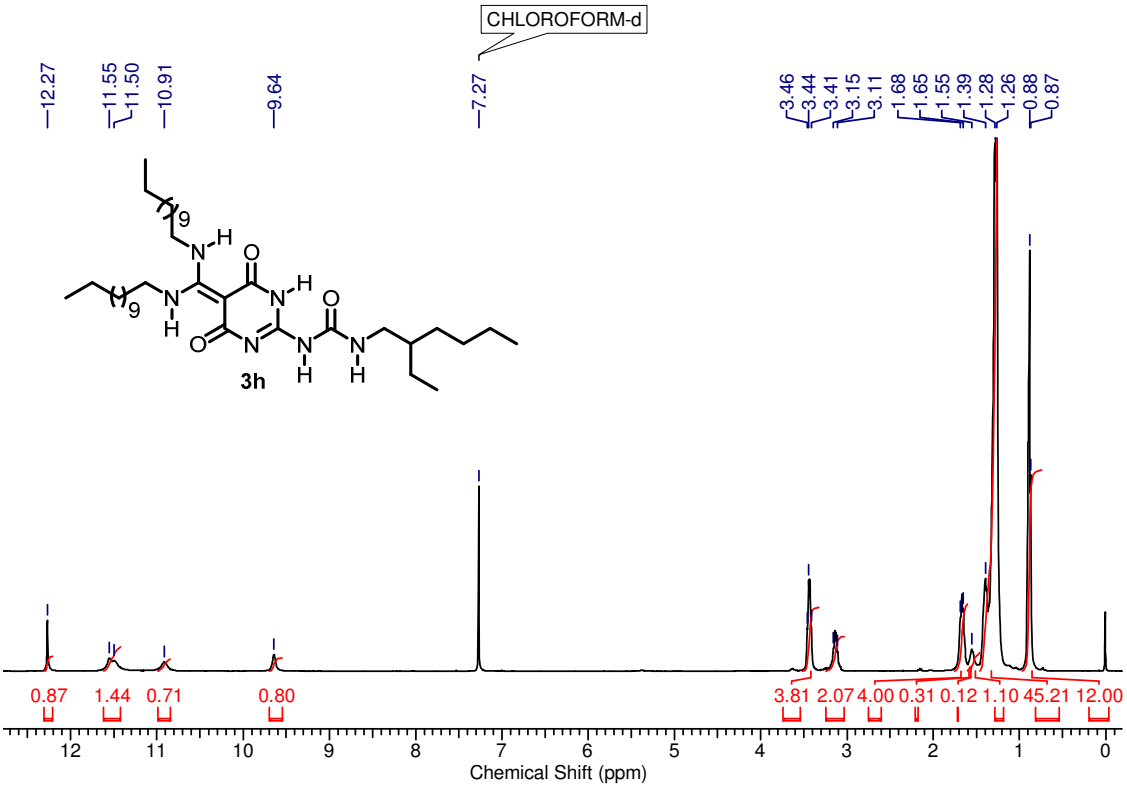


^{13}C NMR spectrum of compound **3g** ($CDCl_3$, 100 MHz, 298 K)

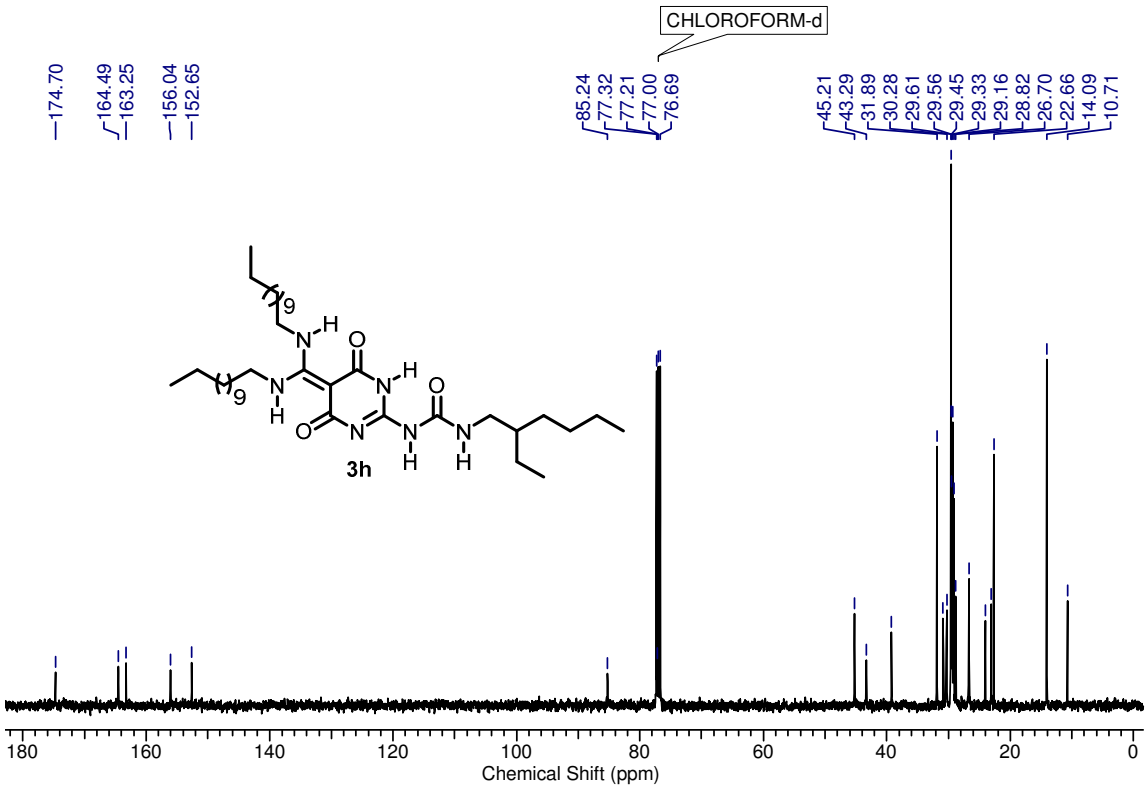


DEPT-135 NMR spectrum of compound **3g** ($CDCl_3$, 100 MHz, 298 K)

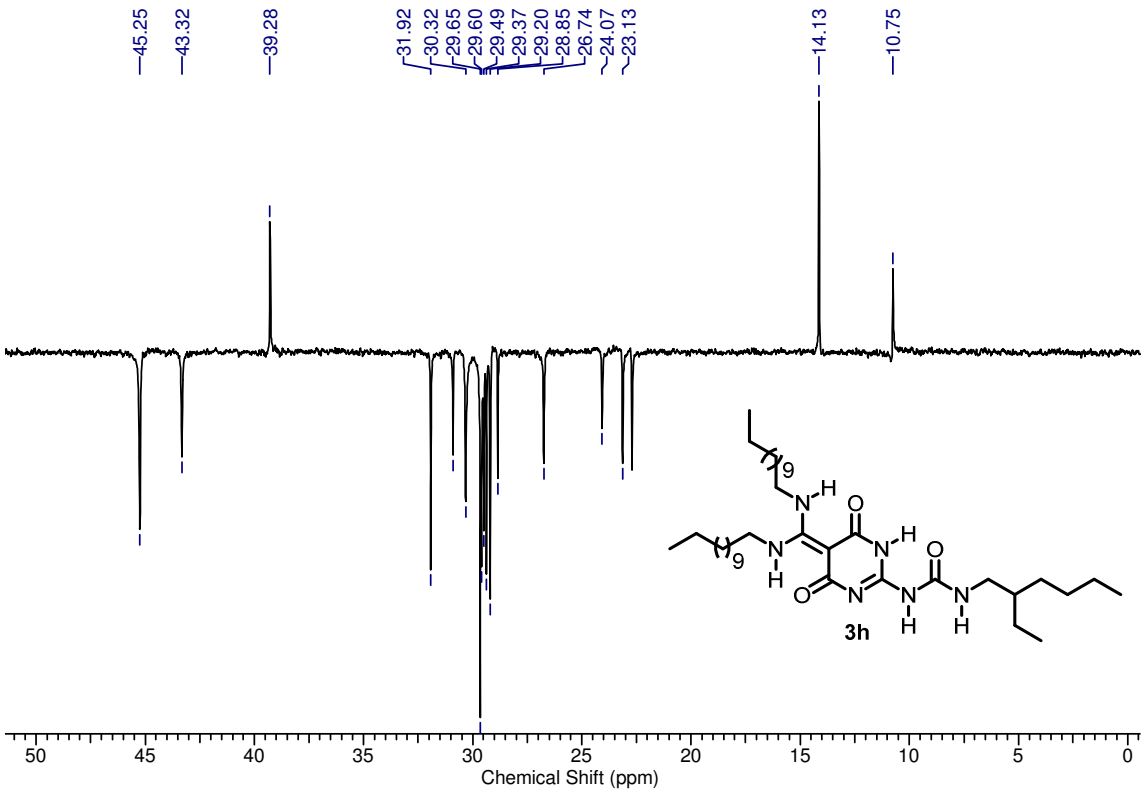




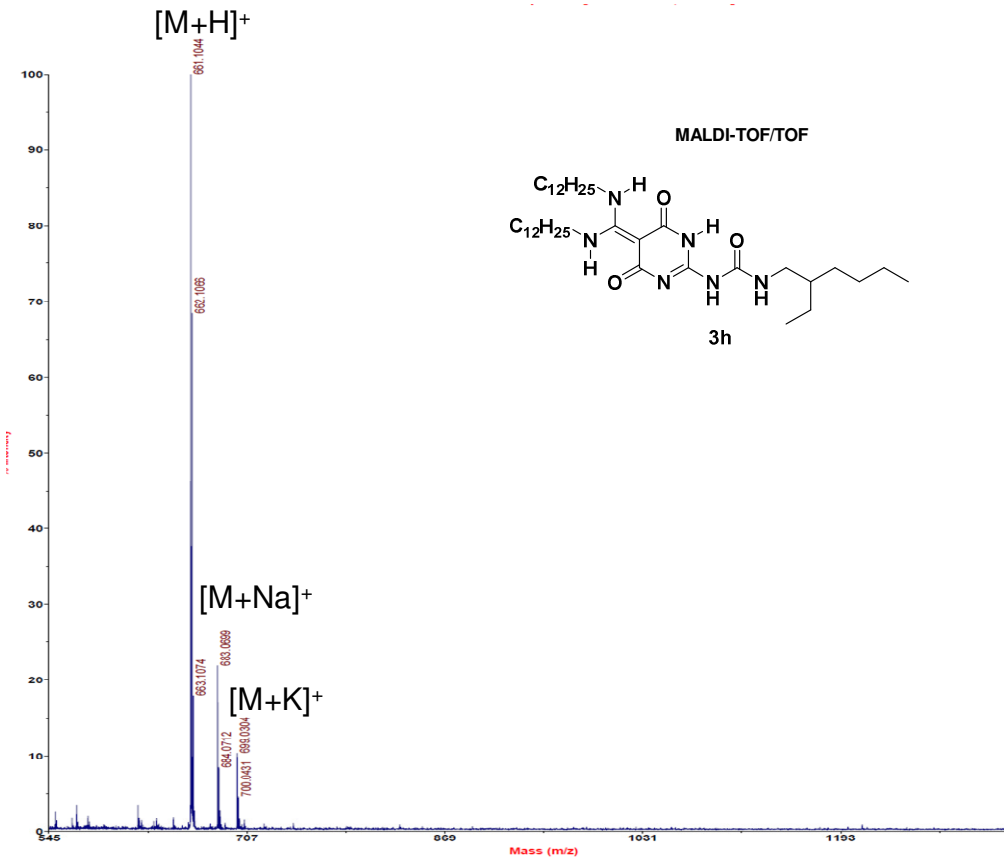
^{1}H NMR spectrum of compound **3h** ($CDCl_3$, 400 MHz, 298 K)



^{13}C NMR spectrum of compound **3h** ($CDCl_3$, 100 MHz, 298 K)



DEPT-135 NMR spectrum of compound **3h** ($CDCl_3$, 100 MHz, 298 K)



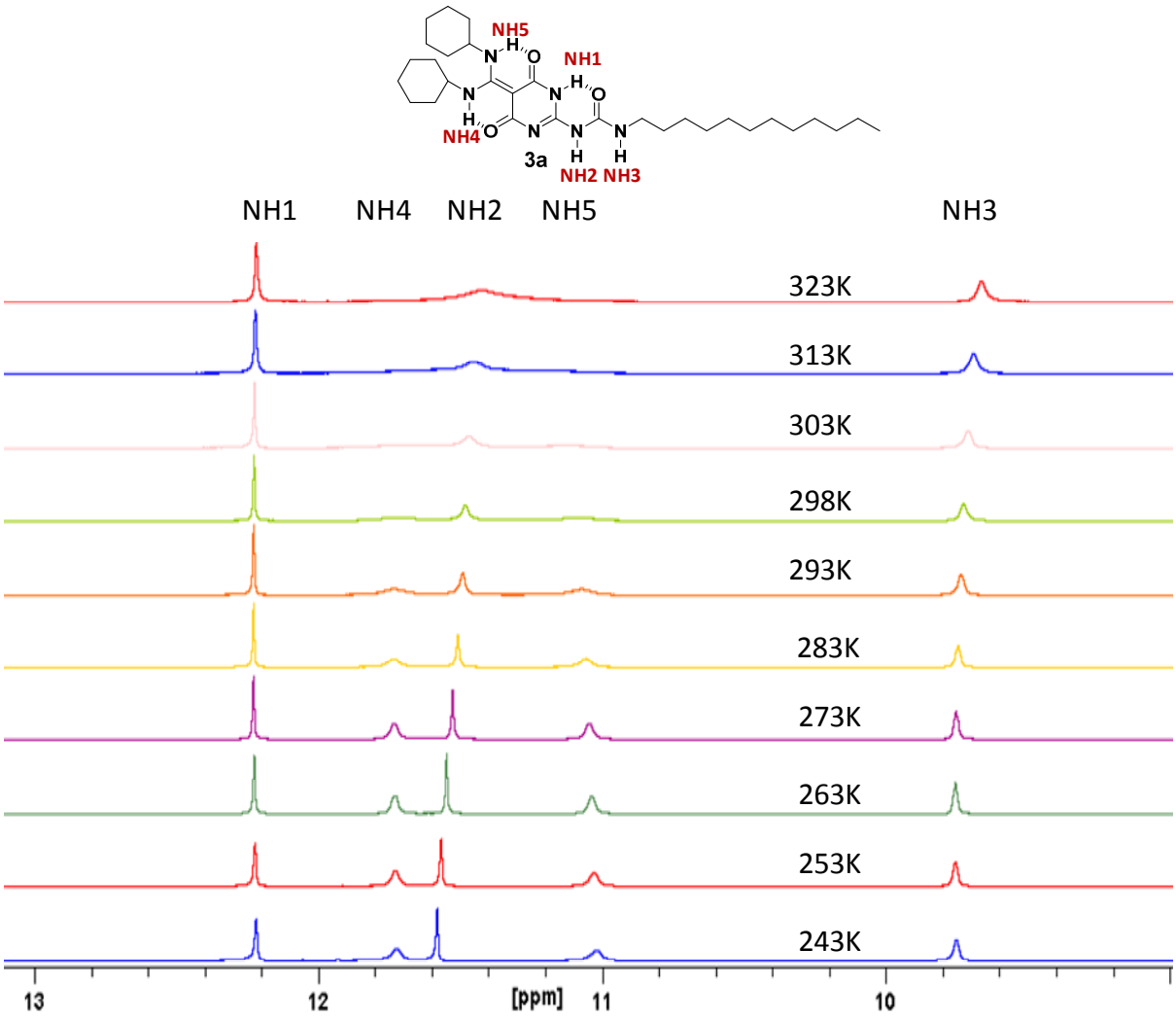


Figure S1. Stacked partial ^{1}H NMR spectra (700 MHz) of **3a** at different temperatures, (10 mM in $CDCl_3$), showing the temperature-dependent changes of NH1, NH2, NH3, NH4 and NH5.

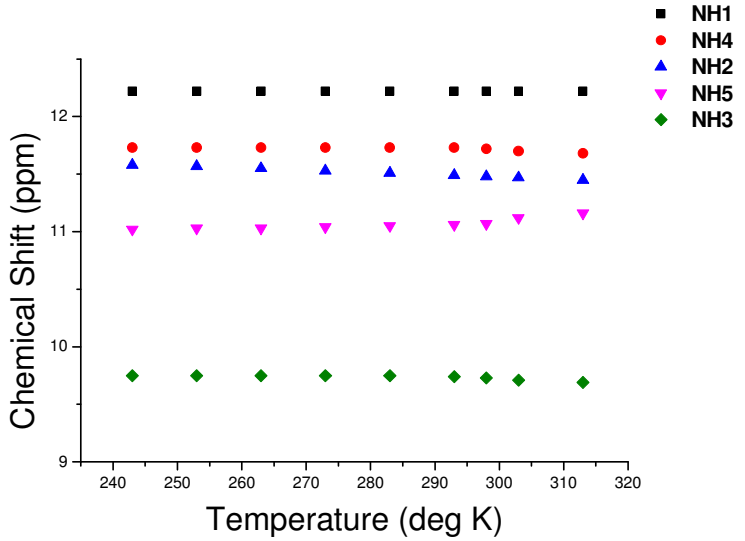


Figure S2. Plot of the chemical shifts of NH1, NH2, NH3, NH4 and NH5 of **3a** at different temperatures (10 mM in $CDCl_3$, 700 MHz).

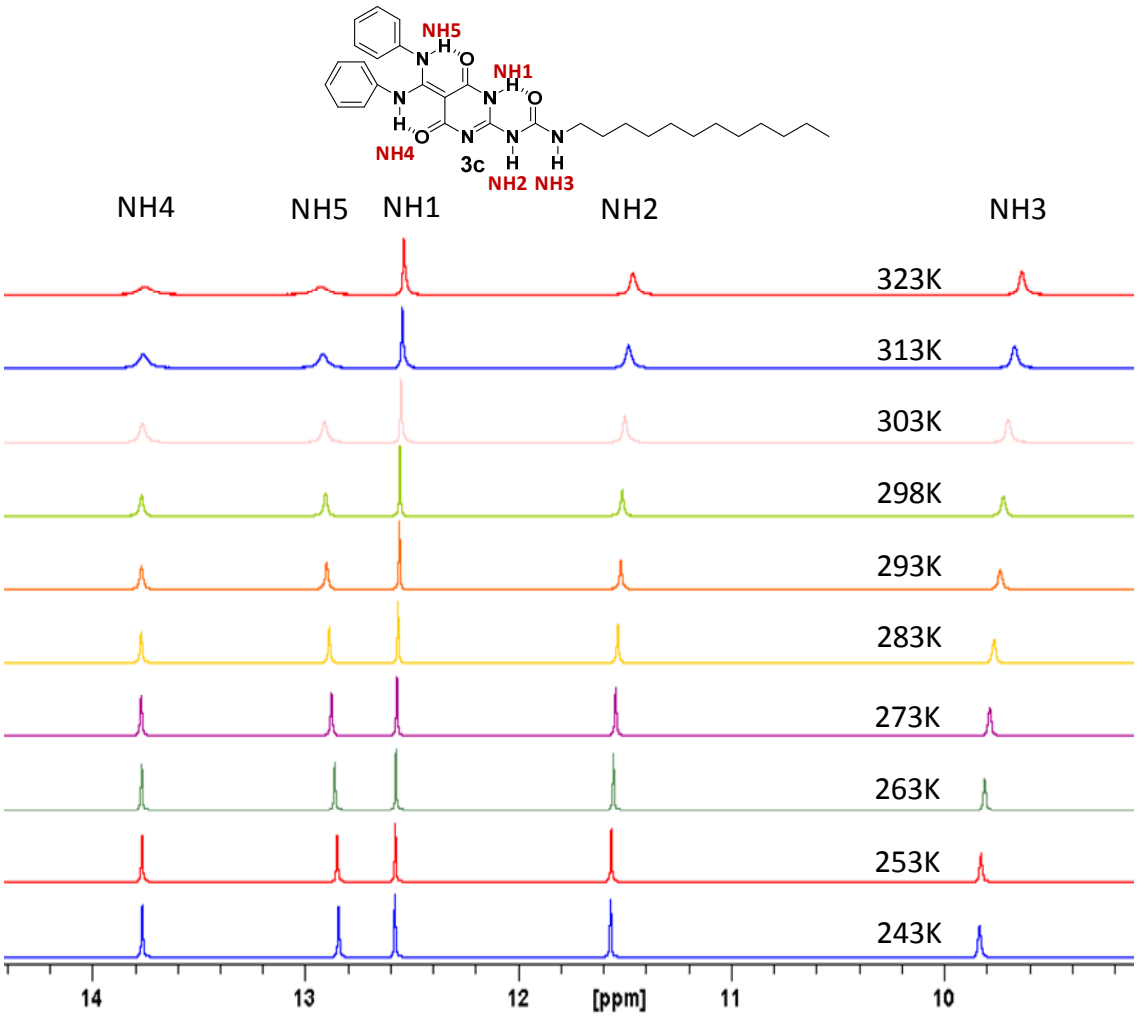


Figure S3. Stacked partial ^{1}H NMR spectra (700 MHz) of **3c** at different temperatures, (10 mM in $CDCl_3$), showing the temperature-dependent changes of NH1, NH2, NH3, NH4 and NH5.

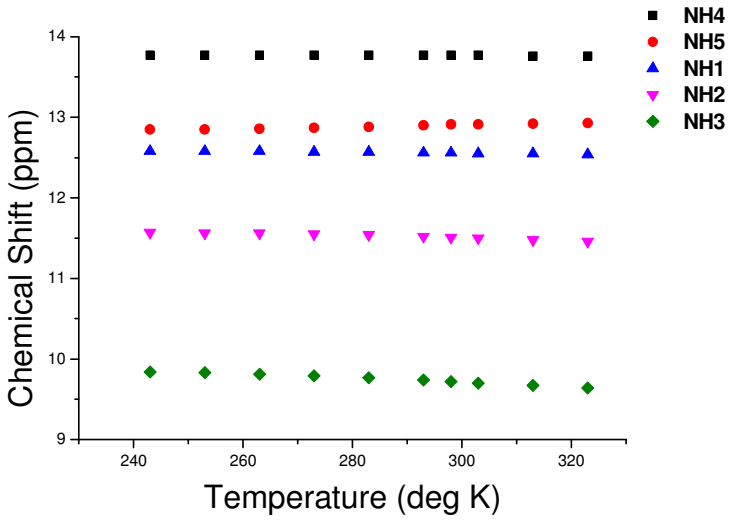


Figure S4. Plot of the chemical shifts of NH1, NH2, NH3, NH4 and NH5 of **3c** at different temperatures (10 mM in $CDCl_3$, 700 MHz).

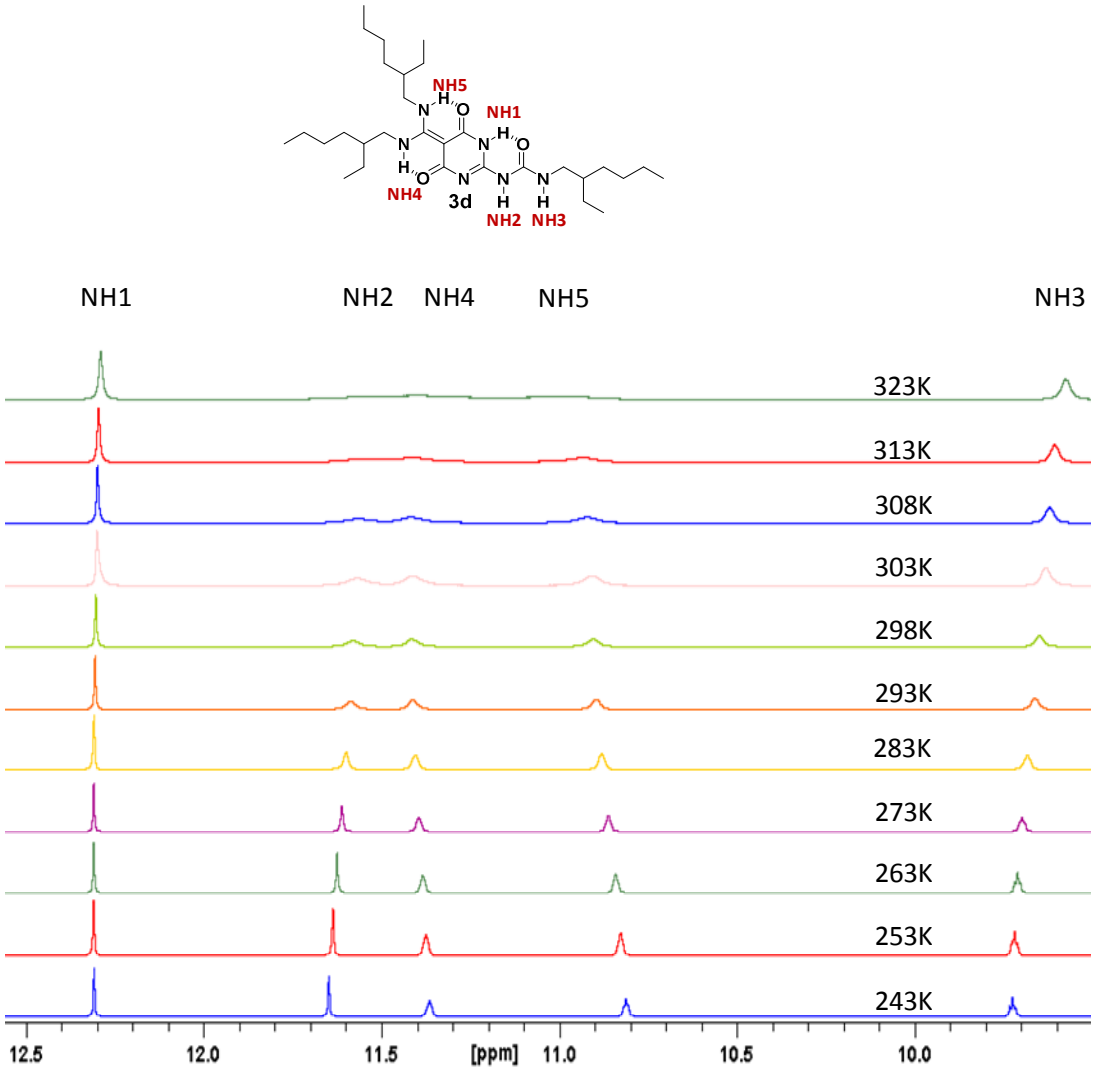


Figure S5. Stacked partial ^{1}H NMR spectra (700 MHz) of **3d** at different temperatures, (10 mM in $CDCl_3$), showing the temperature-dependent changes of NH1, NH2, NH3, NH4 and NH5.

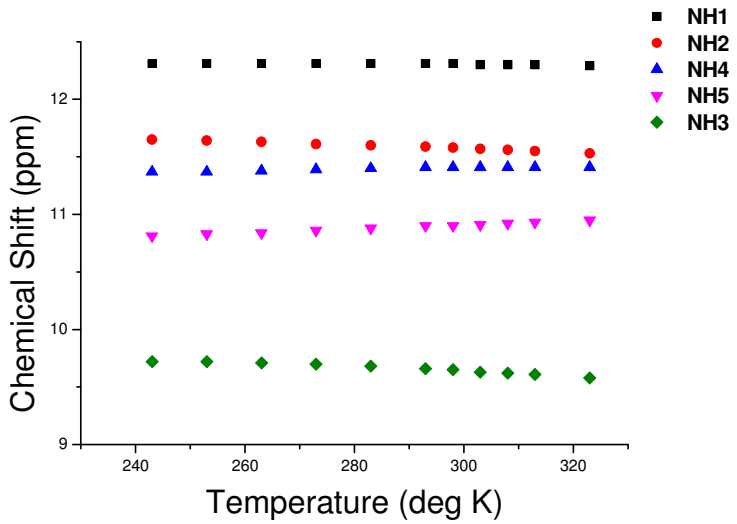


Figure S6. Plot of the chemical shifts of NH1, NH2, NH3, NH4 and NH5 of **3d** at different temperatures (10 mM in $CDCl_3$, 700 MHz).

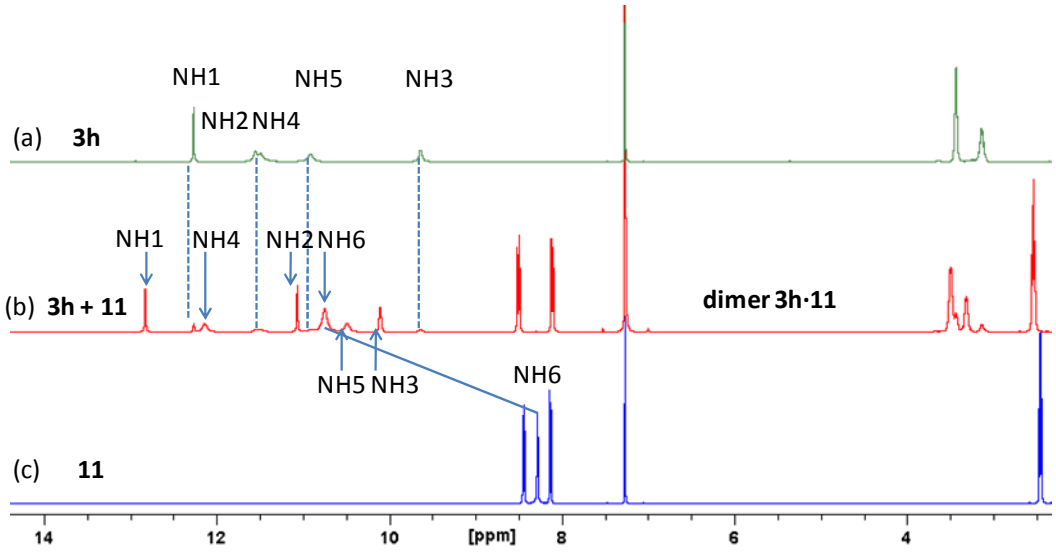


Figure S7. Partial ^{1}H NMR (500 MHz, 10 mM) of (a) **3h**, (b) **3h+11** (1:1), and (c) **11** in $CDCl_3$ at 298 K.

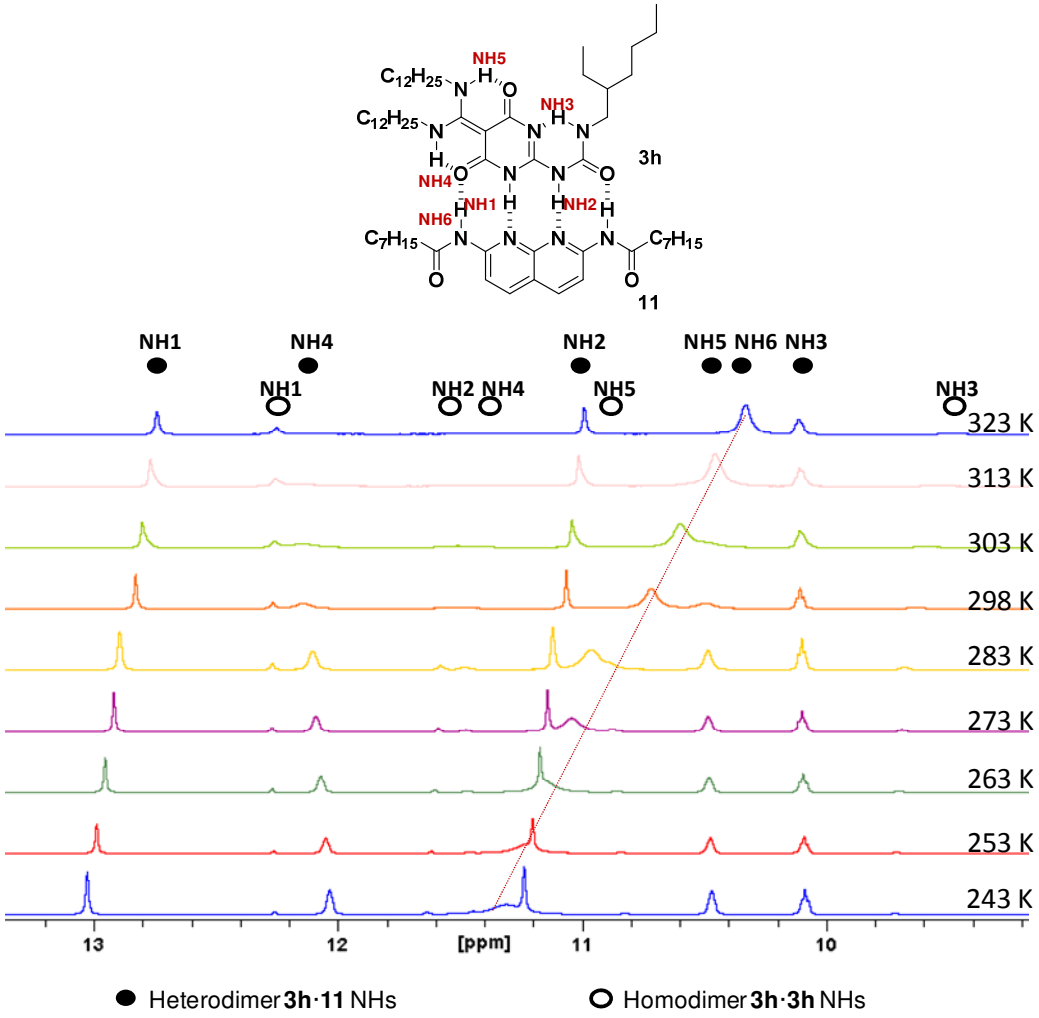


Figure S8. Stacked partial ^{1}H NMR spectra (400 MHz) of heterodimer **3h·11** at different temperatures, (10 mM in $CDCl_3$), showing the temperature-dependent changes of NH1, NH2, NH3, NH4, NH5 and NH6.

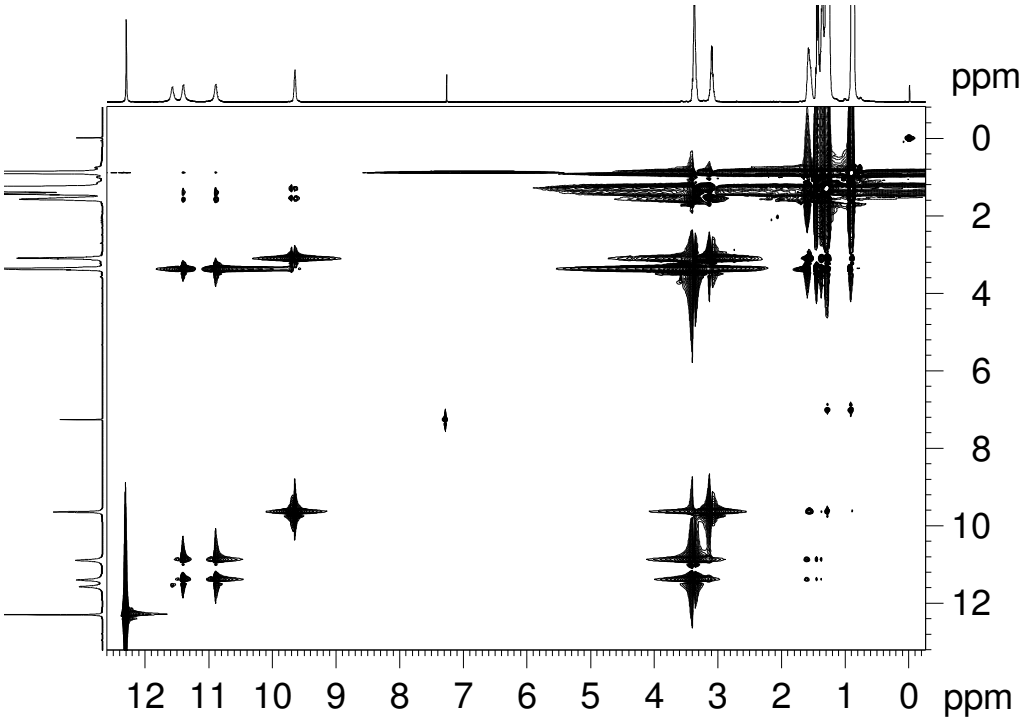


Figure S9. 2D TOCSY spectra of **3d** (500 MHz, $CDCl_3$).

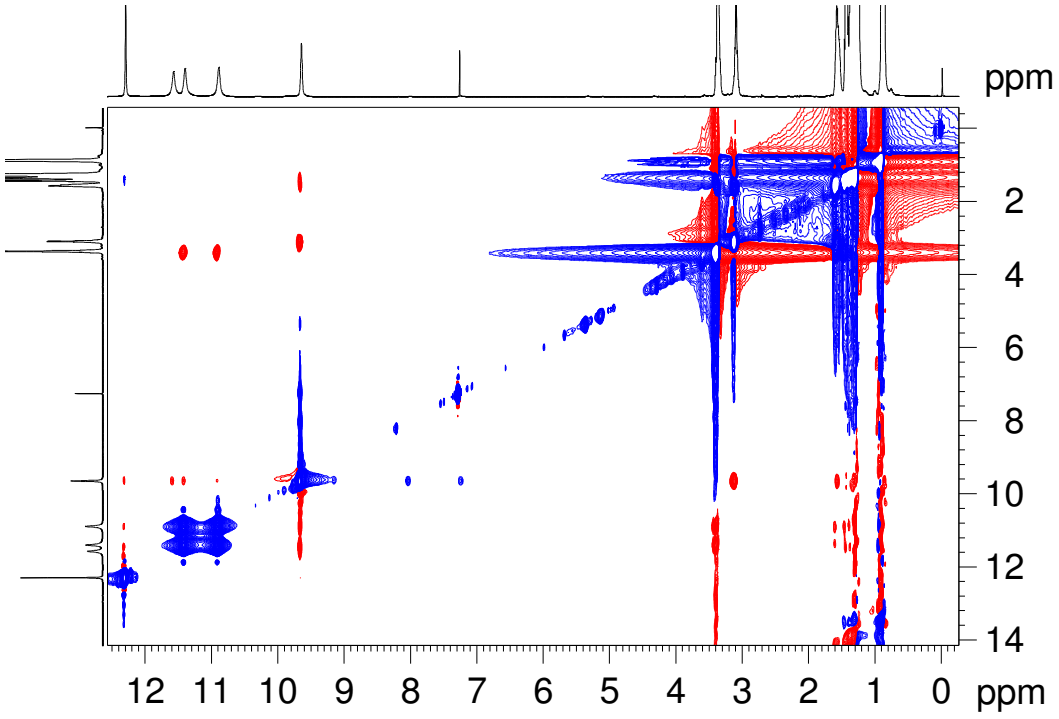


Figure S10. 2D ROESY spectra of **3d** (500 MHz, $CDCl_3$).

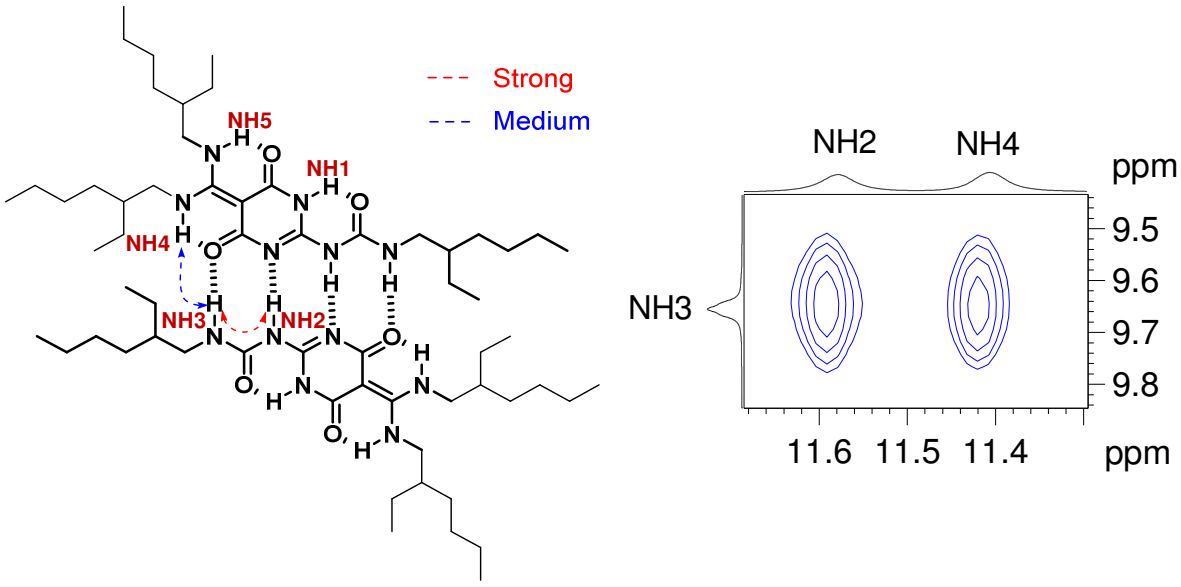


Figure S11. 2D extract of **3d** (500 MHz, $CDCl_3$).

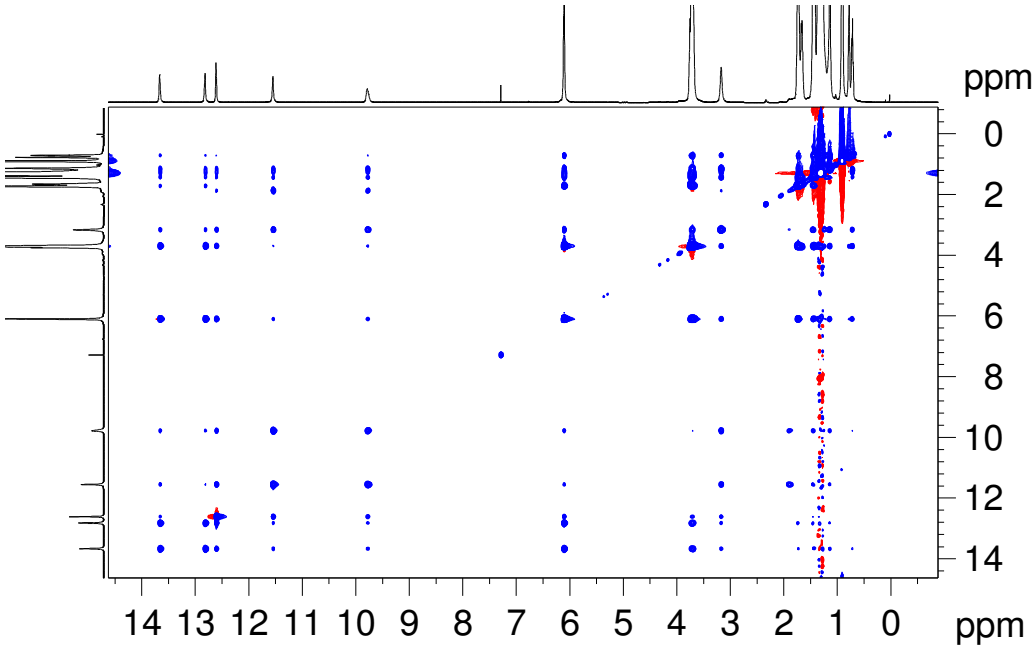


Figure S12. 2D NOESY spectra of **3e** (500 MHZ, $CDCl_3$).

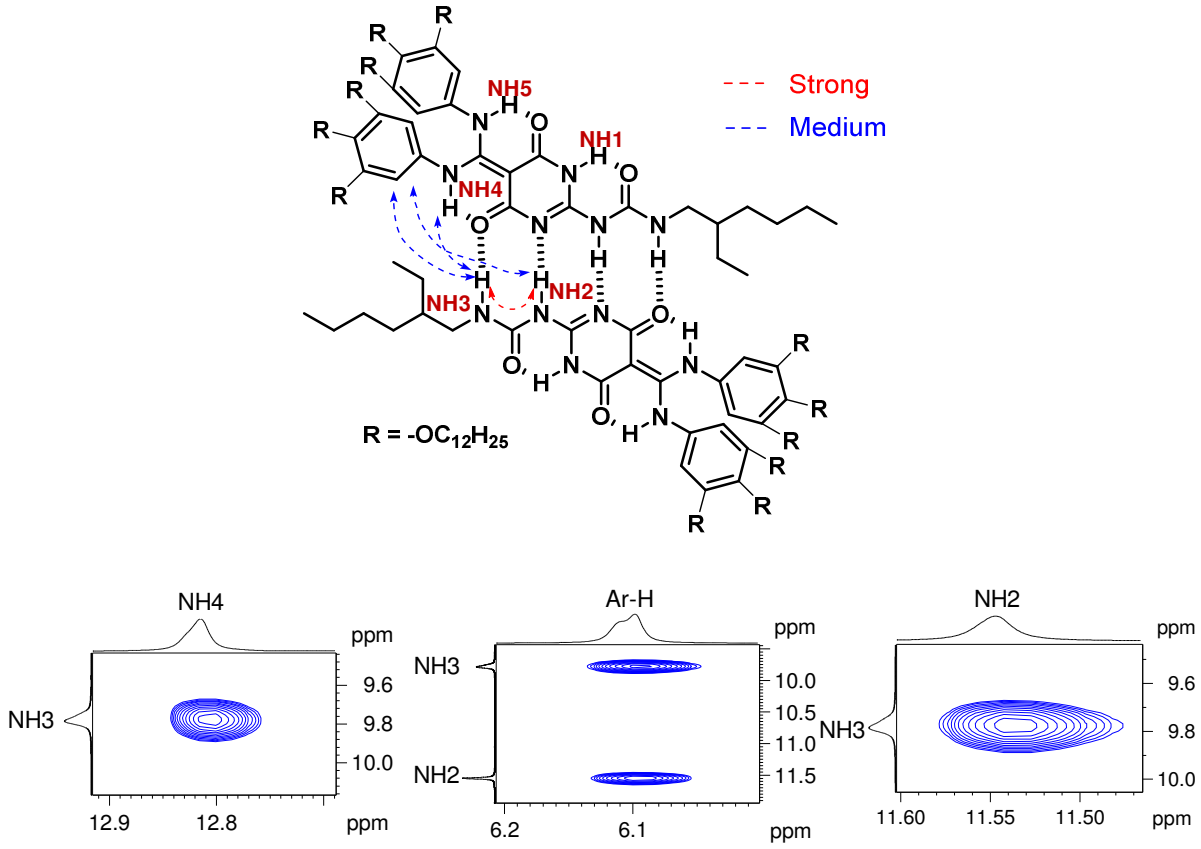


Figure S13. 2D extracts of **3e** (500 MHz, $CDCl_3$).

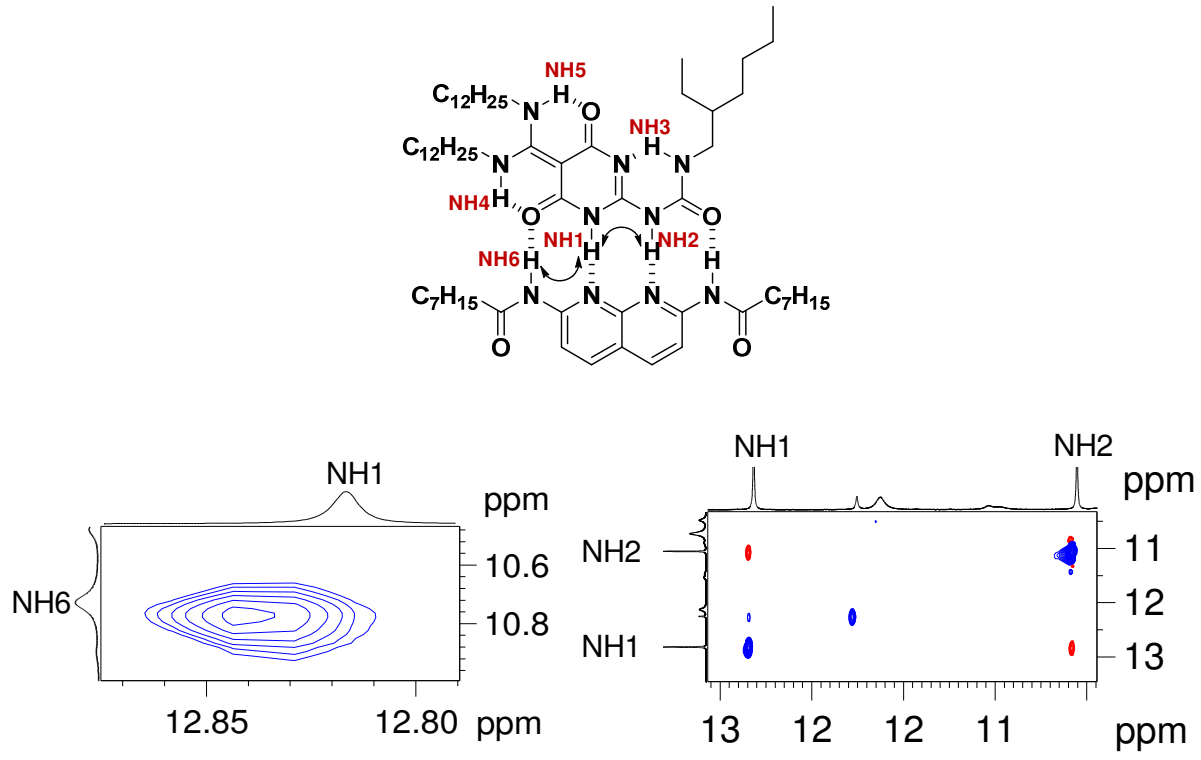
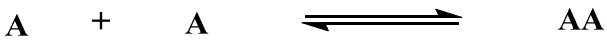


Figure S14. 2D extract of the heterodimer **3h·11** (500 MHz, $CDCl_3$).

Nonlinear regression analysis is based on the following equation[1]:



$$K_{\mathrm{d}} = \frac{[AA]}{[A]\Lambda 2}$$

$$[\mathrm{A}] = [\mathrm{A}]_0 - 2[\mathrm{AA}]$$

$$[AA] = \frac{4K_{\mathrm{d}}[\mathrm{A}]_0 + 1 - \sqrt{8[\mathrm{A}]_0 + 1}}{8K_d}$$

$$\delta_{\mathrm{obs}} = \frac{2[AA]}{[A]_0}\delta_{\mathrm{d}} + \frac{[A]}{[A]_0}\delta_{\mathrm{f}}$$

$$= \delta_{\mathrm{f}} + (\delta_{\mathrm{d}} - \delta_{\mathrm{f}})\,\frac{4K_{\mathrm{d}}[\mathrm{A}]_0 + 1 - \sqrt{8K_{\mathrm{d}}[\mathrm{A}]_0 + 1}}{4K_{\mathrm{d}}[\mathrm{A}]_0}$$

[A] : the concentration of unbound free species

$[\mathrm{A}]_0$: the total concentration

[AA] : the concentration of dimer

K_{d} : the dimerization constant

δ_{d} : the limiting bound chemical shift of the dimer

δ_{f}: the free chemical shift

δ_{obs} : chemical shift measured by experiment

Methodological description for the NMR dilution studies of **3d**:

Solutions (0.6 mL volume each) of different concentration of **3d** (from 100 mM to 0.4 mM) in dry $CDCl_3$ were prepared from 100 mM (2.5 mL) stock solution of compound **3d** in dry $CDCl_3$.

100 μM and 10 μM solutions (0.6 mL volume each) of compound **3d** in dry $CDCl_3$ were prepared from 10 mM and 1 mM stock solutions of compound **3d** in dry $CDCl_3$, respectively.

^{1}H NMR spectra of compound **3d** were recorded in different concentrations of dry $CDCl_3$ (from 100 mM to 10 μM) on AV 500 MHz Bruker NMR spectrometer at ambient temperature (298 K). We observed no significant change in chemical shift of urea protons (Fig. S15).

Further, to study the strong duplex formation of the compound **3d**, dilution studies were carried out in various DMSO-d_6/$CDCl_3$ mixtures.

5% DMSO-d_6/$CDCl_3$ Solutions

Initially, solutions (0.5 mL volume each) of different concentration of **3d** (from 60 mM to 0.4 mM) in dry $CDCl_3$ were prepared from 100 mM stock solution of compound **3d** in dry $CDCl_3$. Further, 5% DMSO-d_6 was added to these solutions (by assuming 0.5 ml of $CDCl_3$ as 95%).

10% DMSO-d_6/$CDCl_3$, 20% DMSO-d_6/$CDCl_3$ and 30% DMSO-d_6/$CDCl_3$ solutions were prepared following the same procedure used for the preparation of 5% DMSO-d_6/$CDCl_3$ solutions.

The ^{1}H NMR spectra of compound **3d** were recorded in different concentration of 5% DMSO-d_6/$CDCl_3$ solution (from 60 mM to 0.4 mM), 10% DMSO-d_6/$CDCl_3$ solution (from 100 mM to 0.4 mM) and 20% DMSO-d_6/$CDCl_3$ solution (80 mM to 2mM) on 500 MHz Bruker NMR spectrometer at ambient temperature (298 K). We observed no significant change in chemical shift of urea protons (Figs. S16, S17 and S18, respectively).

Origin software was used to derive the dimerization constant from the non-linear regression analysis. Nonlinear regression analysis[1] of chemical shift of NH5 urea proton of **3d** in 30% DMSO-d_6/$CDCl_3$ gave a dimerization constant $K_{dim} = (2.75 \pm 0.12) \times 10\ M^{-1}$ (Fig. S19).

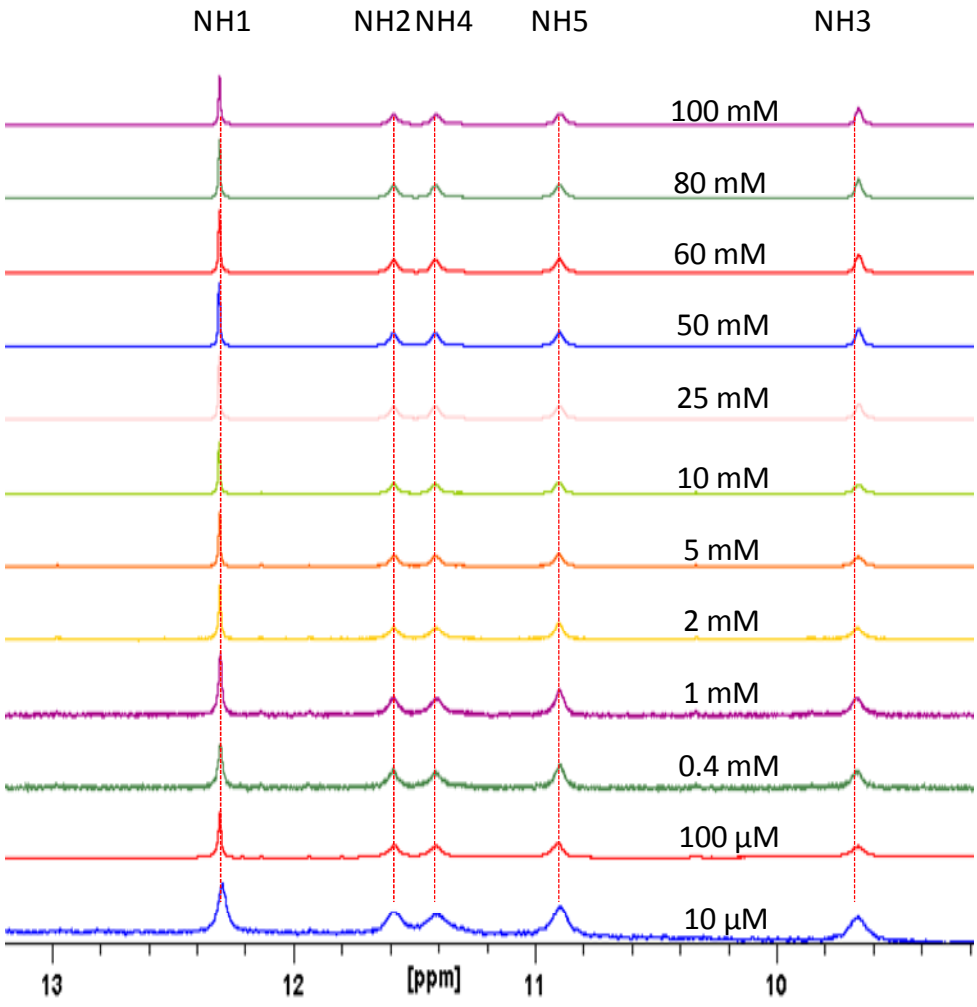


Figure S15. Stacked partial ^{1}H NMR spectra of compound **3d** at different concentration in $CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.

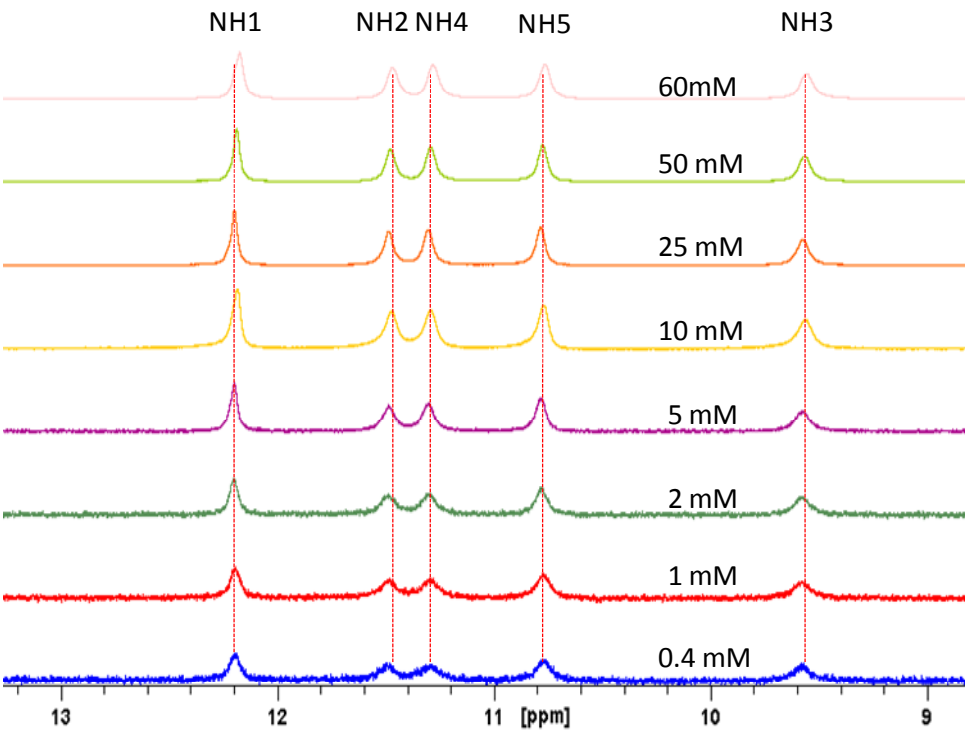


Figure S16. Stacked partial ^{1}H NMR spectra of compound **3d** at different concentration in 5% DMSO-d_6/$CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.

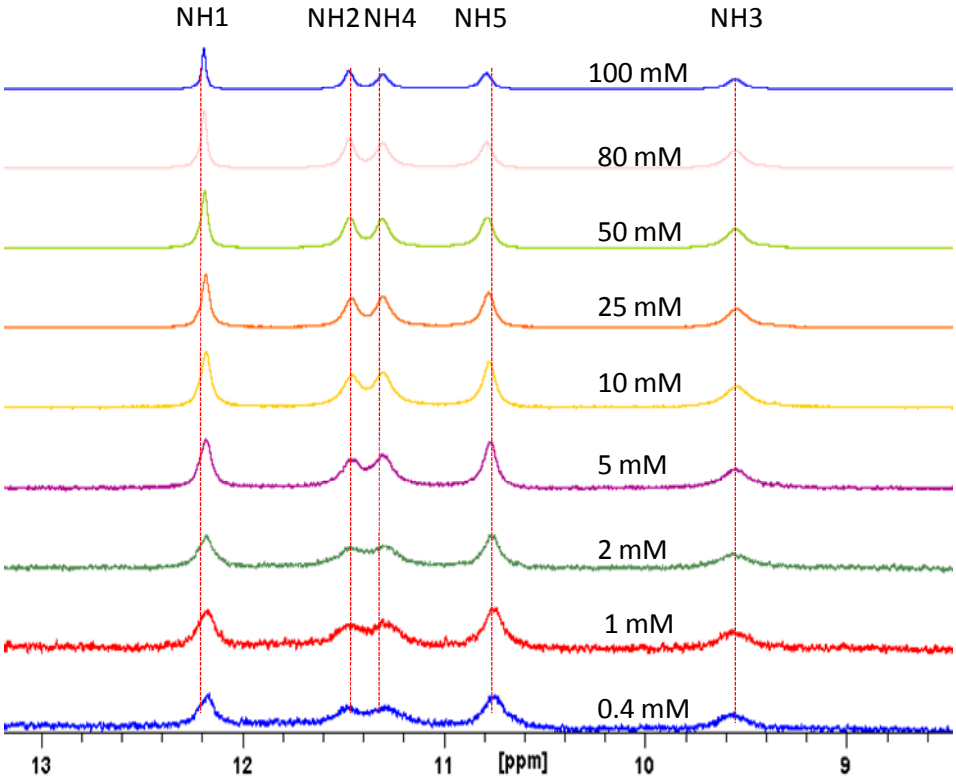


Figure S17. Stacked partial ^{1}H NMR spectra of compound **3d** at different concentration in 10% DMSO-d_6/$CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.

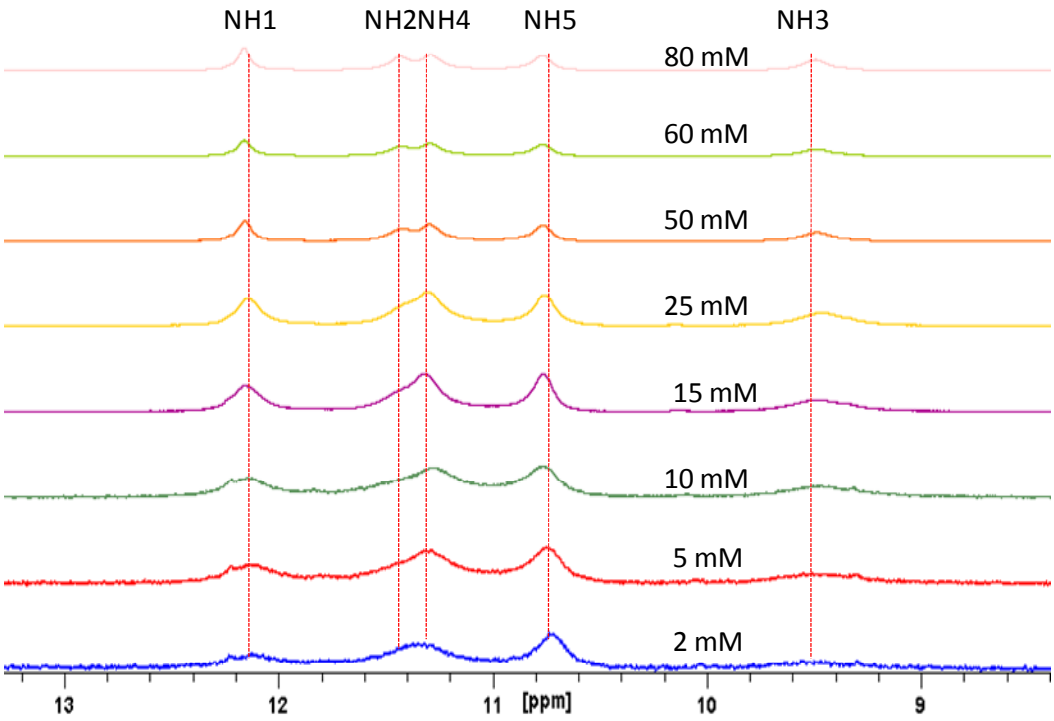
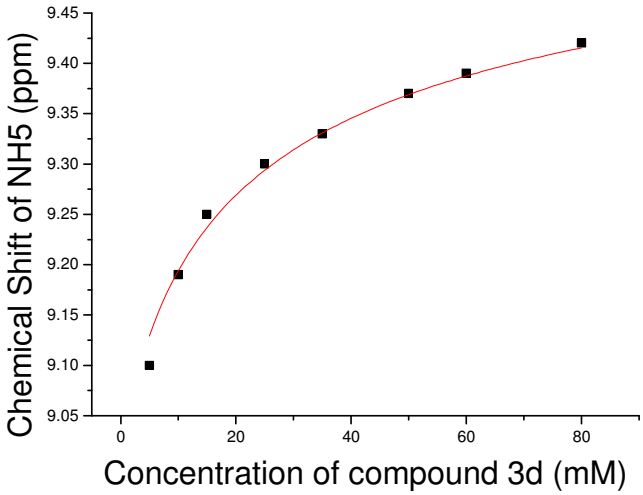


Figure S18. Stacked partial ^{1}H NMR spectra of compound **3d** at different concentration in 20% DMSO-d_6/$CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.



K_{dim} = (2.75 ± 0.12) x 10 M^{-1} R^2 = 0.9866

Figure S19. Determination of the dimerization constant of **3d·3d** in 30% DMSO-d_6/$CDCl_3$ at 298 K. Fitting result based on NH5.

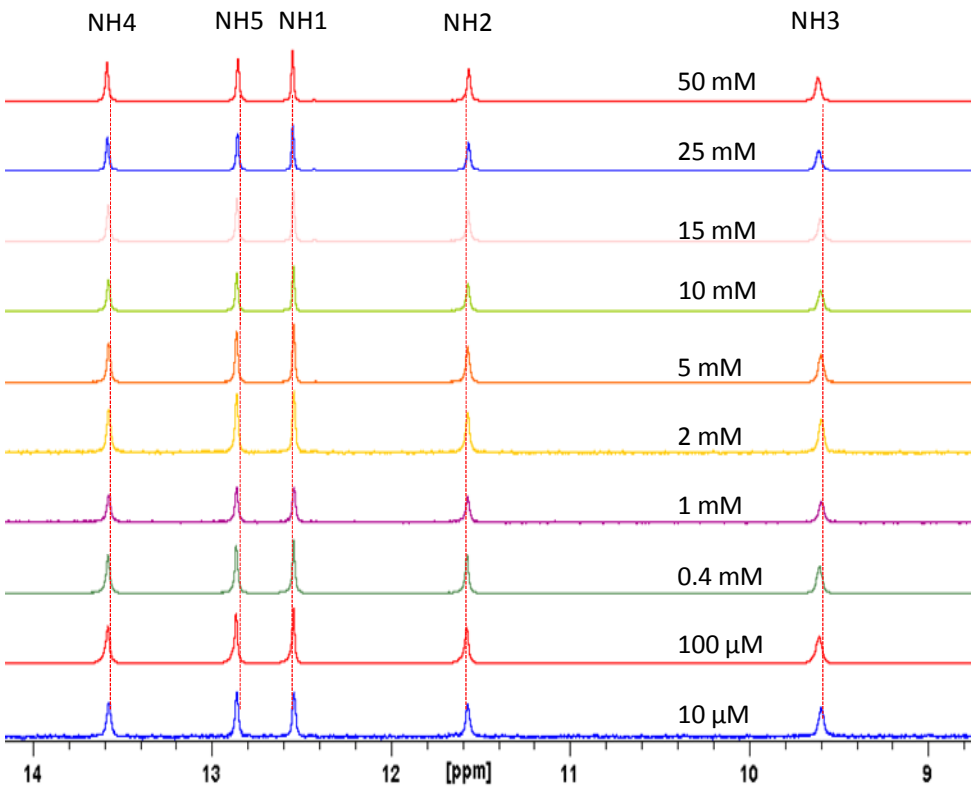


Figure S20. Stacked partial ^{1}H NMR spectra of compound **3e** at different concentration in $CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.

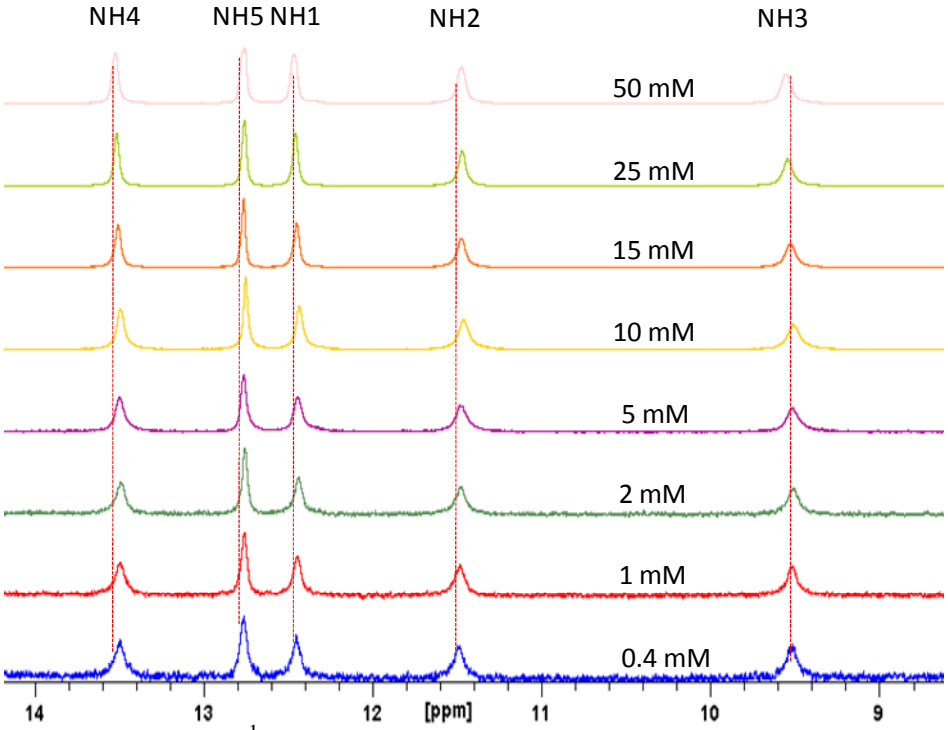


Figure S21. Stacked partial ^{1}H NMR spectra of compound **3e** at different concentration in 5% DMSO-d_6/$CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.

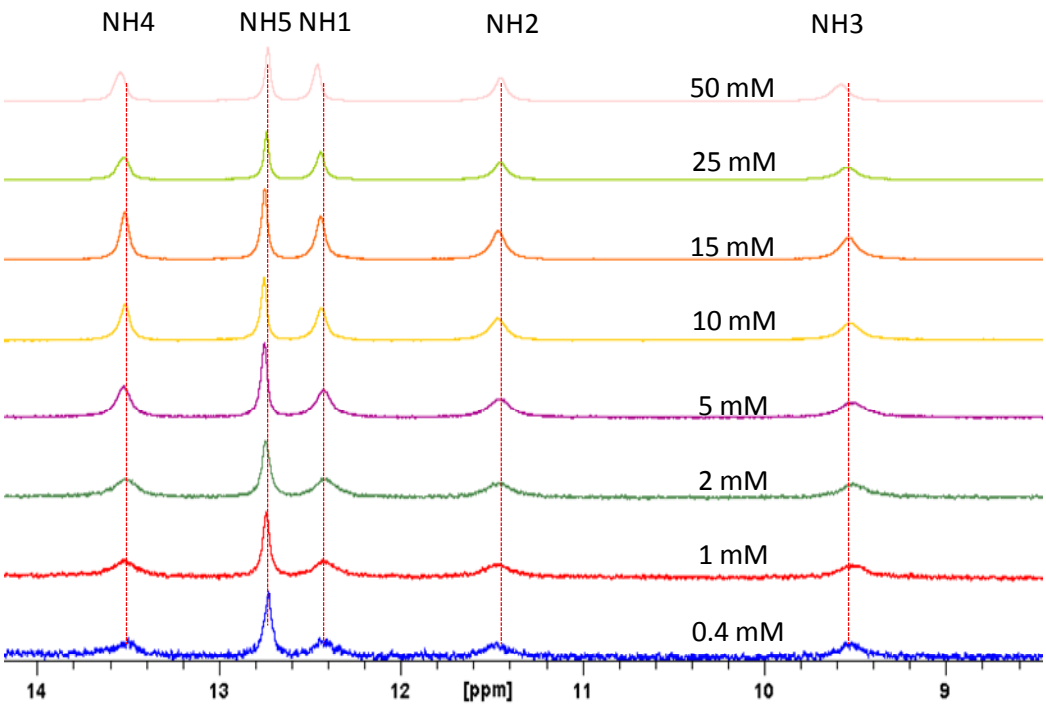
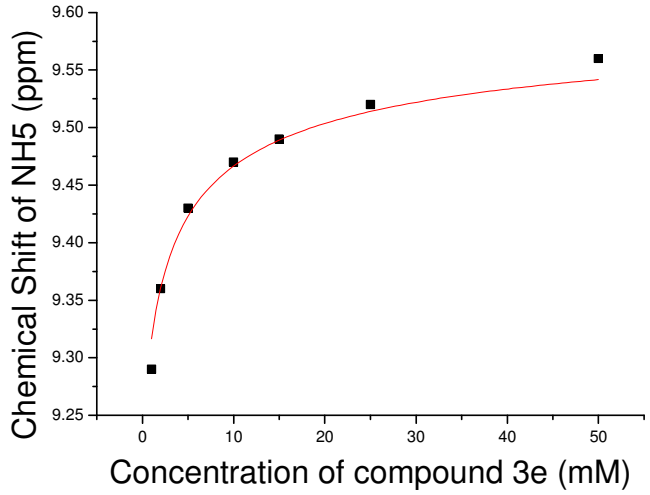
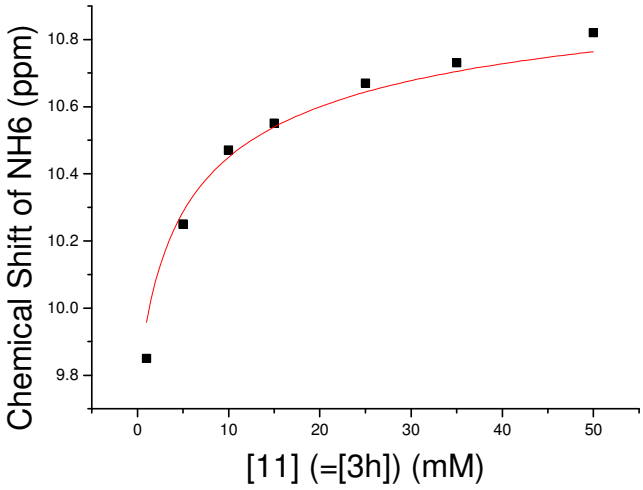


Figure S22. Stacked partial ^{1}H NMR spectra of compound **3e** at different concentration in 10% DMSO-d_6/$CDCl_3$ (500 MHz, 298 K), showing no chemical shift change of protons NH1, NH2, NH3, NH4 and NH5.



K_{dim} = (2.094 ± 0.195) x 10^2 M^{-1} R^2 = 0.9785

Figure S23. Determination of the dimerization constant of **3e·3e** in 20% DMSO-d_6/$CDCl_3$ at 298 K. Fitting result based on NH5.



K_a = (2.0837 ± 0.2233) x 10^2 M^{-1} R^2 = 0.9731

Figure S24. Determination of the association constant of **3h·11** in 10% DMSO-d_6/$CDCl_3$ at 298 K. Fitting result based on NH6.

Fluorescence experiments and emission spectra of 3g at various concentrations

Fluorescence emission spectra were measured with a Perkin-Elmer LS55 luminescence spectrometer set to an excitation wavelength of 346 nm. The chloroform used for fluorescence spectroscopy was of spectrophotometric grade and was used as received. For determination of the K_{dim} of **3g**, fluorescence spectra were measured in the concentration range from 10^{-9} to 10^{-7} M in chloroform. The excimer band (λ_{max} = 490 nm) was integrated from 450 to 600 nm, to exclude as much of the monomer emission bands (λ_{max} = 379-419 nm) as possible. The data was fitted into a dimerization equation described by Wilcox.[1a]

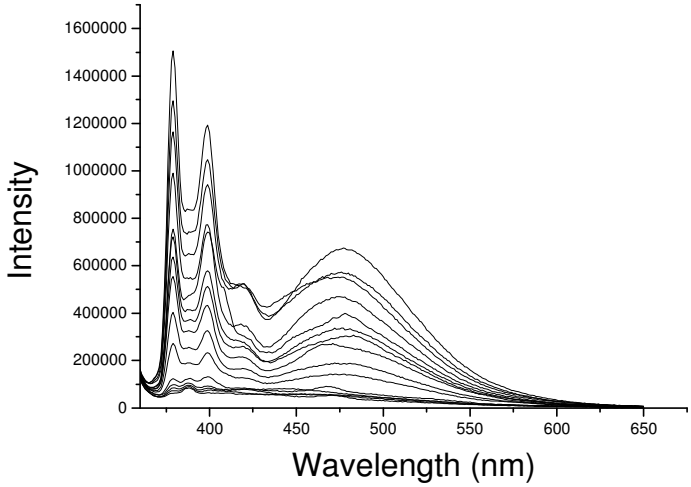
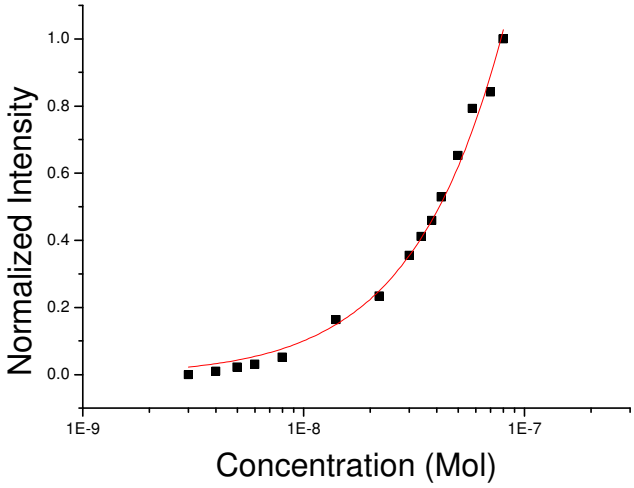


Figure S25. Fluorescence emission spectra (λ_{ex} = 346 nm) of the **3g** dimer in the concentration range of 10^{-9} to 10^{-7} M in chloroform.



$K_{dim} = 3.44 \pm 3.11 \times 10^{8}\ M^{-1}$ $R^2 = 0.9918$

Figure S26. Plot of the normalized intensity of **3g** *vs* concentration, measured in chloroform, curve is derived from the nonlinear curve fit.

X-ray crystal structure analysis of compounds 3a, 3c and 3f

X-ray intensity data measurements of compounds **3c** and **3f** were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (MoK_α = 0.71073Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ with a frame time of 40 secs keeping the sample-to-detector distance fixed at 4 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).[2] All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). ShelX-97 was used for structure solution and full matrix least-squares refinement on F^2.[3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms.

X-ray intensity data measurements of compound **3a** was carried out on a Super Nova source X-ray Diffractometer system (Agilent Technologies) equipped with a CCD area detector and operated at 250 W power (50 kV, 0.8 mA) to generate Mo Kα radiation (λ = 0.71073 Å) at 298 (2) K. Initial scans of each specimen were performed to obtain preliminary unit cell parameters and to assess the mosaicity (breadth of spots between frames) of the crystal to select the required frame width for data collection. CrysAlis^{Pro} program software was used suite to carry out overlapping φ and ω scans at detector (2θ) settings (2θ = 28). Following data collection, reflections were sampled from all regions of the Ewald sphere to redetermine unit cell parameters for data integration. Following exhaustive review of collected frames, the resolution of the data set was judged. Data were integrated using CrysAlis^{Pro} software with a narrow frame algorithm. Data were subsequently corrected for absorption by the program SCALE3 ABSPACK[4] scaling algorithm. ShelX-97 was used for structure solution and full matrix least-squares refinement on F^2.[3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms.

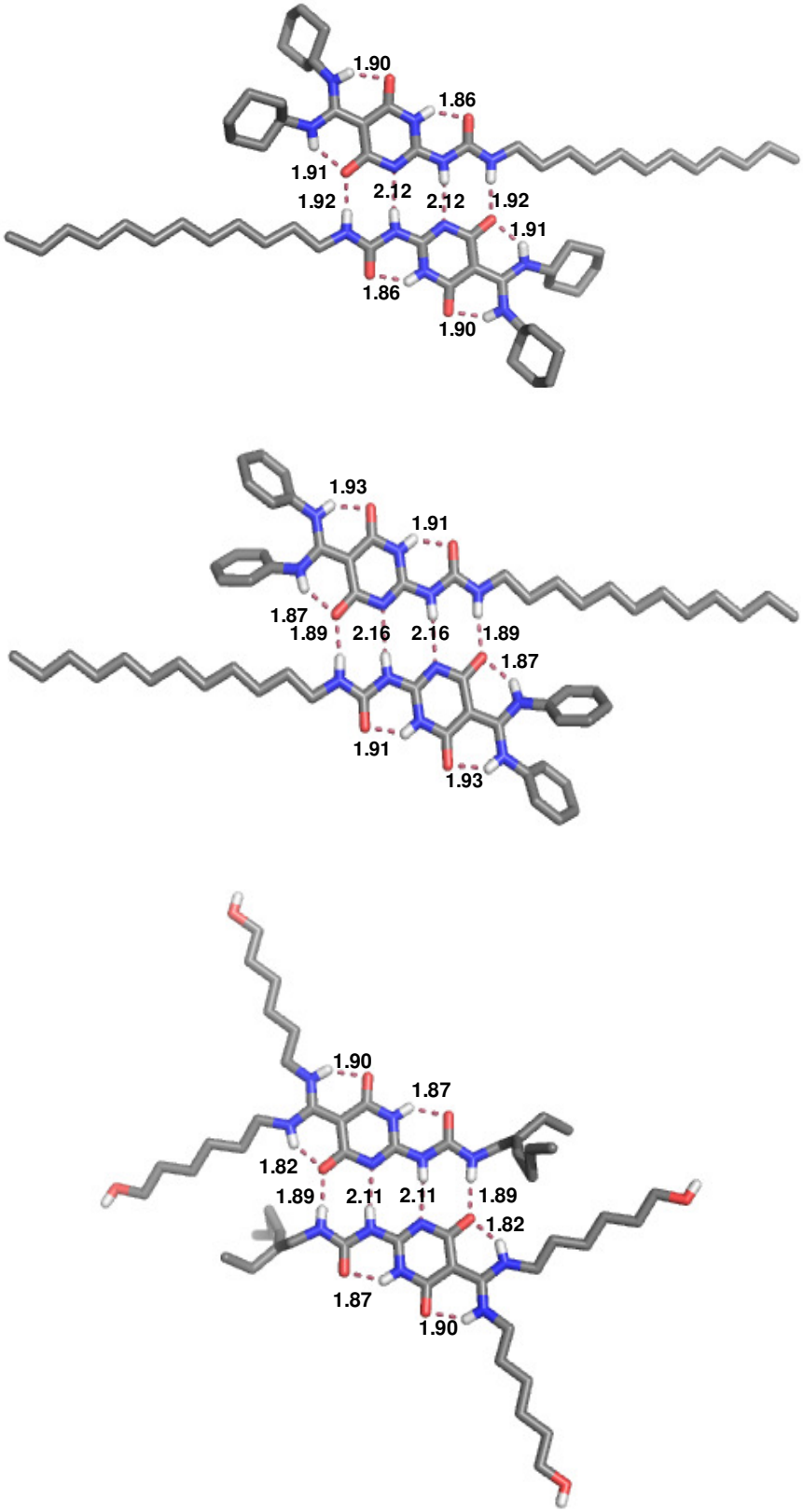


Figure S27. Single-crystal X-ray structure of dimer **3a** (top), dimer **3c** (middle) and dimer **3f** (below). Hydrogen bonding highlighted in dashes (salmon colored), above which hydrogen bond lengths (N-H···O and N-H···N) are displayed in Å. All hydrogens, other than those at the hydrogen-bonding sites, have been removed for clarity.

Table S1. Crystal data and structure refinement for compound **3a**.

Identification code	srpcy533	
Empirical formula	$C_{30}\ H_{52}\ N_6\ O_3$	
Formula weight	544.77	
Temperature	297(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.8629(8) Å	α = 107.076(5)°.
	b = 13.3106(7) Å	β = 91.166(7)°.
	c = 17.3781(11) Å	γ = 91.431(7)°.
Volume	1516.4(2) $Å^3$	
Z	2	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	596	
Crystal size	0.540 x 0.330 x 0.230 mm^3	
Theta range for data collection	3.075 to 25.500°.	
Index ranges	-8<=h<=8, -14<=k<=16, -17<=l<=21	
Reflections collected	10667	
Independent reflections	5559 [R(int) = 0.0691]	
Completeness to theta = 25.242°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.982 and 0.959	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5559 / 192 / 407	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0930, wR2 = 0.2218	
R indices (all data)	R1 = 0.1735, wR2 = 0.2822	
Largest diff. peak and hole	0.274 and -0.425 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement of **3c**.

Identification code	A	
Empirical formula	C_{31} H_{42} Cl_2 N_6 O_3	
Formula weight	617.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.3827(4) Å	α = 73.523(2)°.
	b = 11.1000(6) Å	β = 84.484(2)°.
	c = 16.5626(9) Å	γ = 73.317(2)°.
Volume	1584.30(14) $Å^3$	
Z	2	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.247 mm^{-1}	
F(000)	656	
Crystal size	0.430 x 0.370 x 0.210 mm^3	
Theta range for data collection	2.266 to 25.000°.	
Index ranges	-11<=h<=10, -13<=k<=13, -19<=l<=19	
Reflections collected	70013	
Independent reflections	5570 [R(int) = 0.0777]	
Completeness to theta = 25.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.950 and 0.901	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5570 / 0 / 380	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0674, wR2 = 0.1670	
R indices (all data)	R1 = 0.0866, wR2 = 0.1810	
Largest diff. peak and hole	1.318 and -1.129 e.$Å^{-3}$	

Table S3. Crystal data and structure refinement of **3f**.

Identification code	mo_SRP_aminohexanol_0m	
Empirical formula	$C_{27}\ H_{52}\ N_6\ O_6$	
Formula weight	556.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.5829(13) Å	α = 91.627(4)°.
	b = 9.4082(14) Å	β = 102.132(4)°.
	c = 19.835(3) Å	γ = 101.559(5)°.
Volume	1530.0(4) $Å^3$	
Z	2	
Density (calculated)	1.209 Mg/m^3	
Absorption coefficient	0.086 mm^{-1}	
F(000)	608	
Crystal size	0.180 x 0.120 x 0.080 mm^3	
Theta range for data collection	2.382 to 26.172°.	
Index ranges	-10<=h<=10, -10<=k<=11, -24<=l<=24	
Reflections collected	28642	
Independent reflections	5794 [R(int) = 0.0528]	
Completeness to theta = 25.242°	95.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.993 and 0.985	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5794 / 290 / 444	
Goodness-of-fit on F^2	1.107	
Final R indices [I>2sigma(I)]	R1 = 0.0792, wR2 = 0.1515	
R indices (all data)	R1 = 0.1037, wR2 = 0.1616	
Extinction coefficient	0.0113(17)	
Largest diff. peak and hole	0.455 and -0.374 $e.Å^{-3}$	

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