Deceleration of thermal ring closure in a glass-forming mexylaminotriazine-substituted merocyanine (MC) linked to intramolecular hydrogen bonding

Supporting Information

Konrad Piskorz,[a] Julian M. Dust,[b] Erwin Buncel,[a] Olivier Lebel,[c,*] and Jean-Michel Nunzi[a,d,*]

[a] Department of Chemistry, Queens University, Kingston, ON, K7L 3N6 Canada

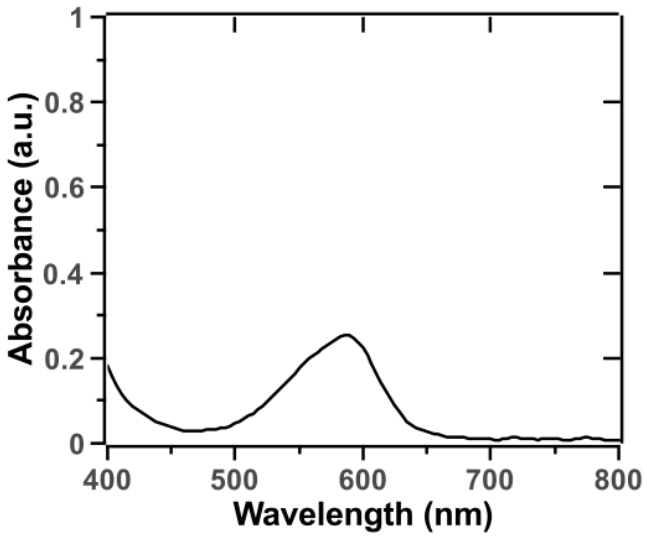
[b] Department of Chemistry and Environmental Science, Grenfell Campus, Memorial University of Newfoundland, Corner Brook, NL, A2H 5G4, Canada

[c] Department of Chemistry and Chemical Engineering, Royal Military College, Kingston, ON, K7K 7B4, Canada

[d] Department of Physics, Engineering Physics and Astronomy, Queens University, Kingston, ON, K7L 3N6 Canada

Corresponding author email: nunzijm@queensu.ca, Olivier.Lebel@rmc.ca

a)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0.8
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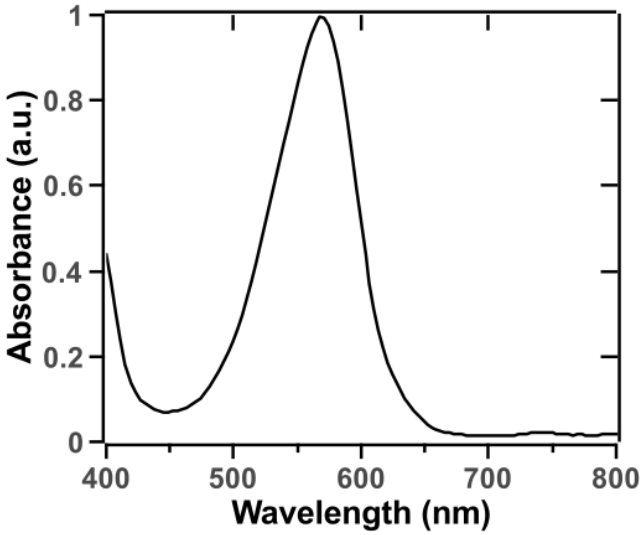
600
700
800
Wavelength (nm)

b)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Wavelength (nm)

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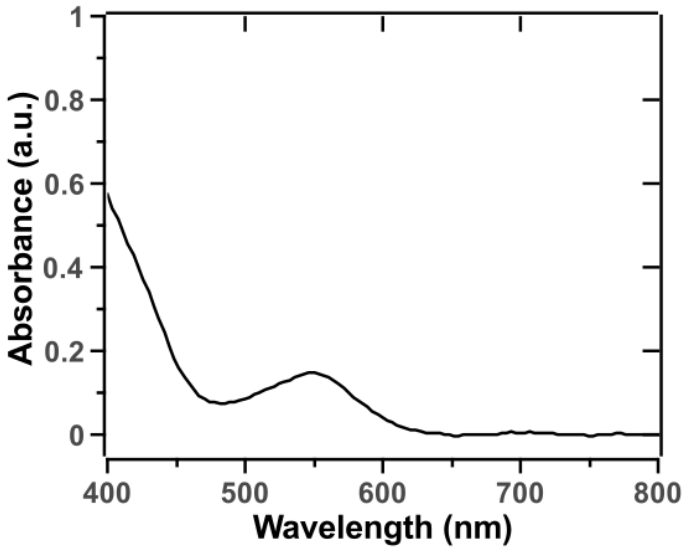


Figure S1. Visible spectra of merocyanine **5a** in various solvents (4 x 10^{-5}M), recorded after 90s irradiation. a) Toluene, 30 °C; b) THF, -20 °C; c) 1-Propanol, 20 °C.

Table S1. Arrhenius data for the ring closure reaction of MC **5a** in toluene.

T (°C)	T (K)	1/T (K^{-1})	ln k_{5a}	k_{5a}
10.0	283.2	0.003521	-5.708	3.32 x 10^{-3}
20.0	293.2	0.003411	-4.500	1.11 x 10^{-2}
30.0	303.2	0.003298	-3.583	2.78 x 10^{-2}
40.0	313.2	0.003193	-2.500	8.21 x 10^{-2}
50.0	323.2	0.003095	-1.583	2.01 x 10^{-1}

Table S2. Arrhenius data for the ring closure reaction of MC **5a** in THF.

T (°C)	K	1/T (K^{-1})	ln k_{5a}	k_{5a}
0.0	273.2	0.003661	-7.587	5.07 x 10^{-4}
10.0	283.2	0.003531	-5.973	2.55 x 10^{-3}
20.0	293.2	0.003411	-4.643	9.63 x 10^{-3}

30.0	303.2	0.003298	-3.601	2.73×10^{-2}
40.0	313.2	0.003193	-2.191	1.12×10^{-1}
50.0	323.2	0.003095	-1.242	2.89×10^{-1}

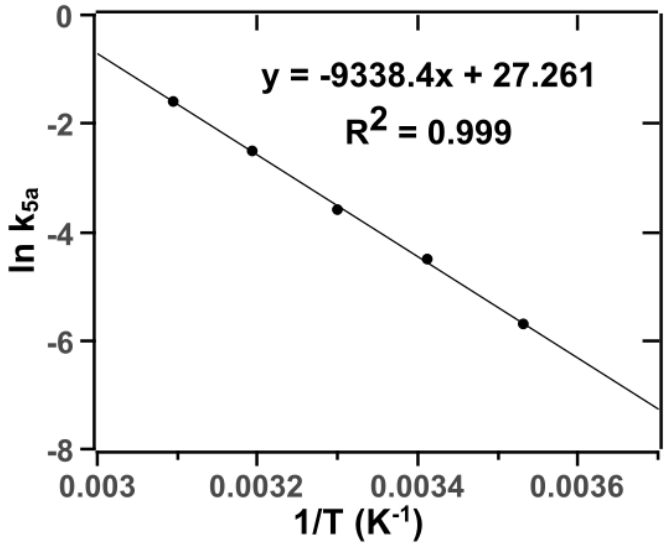
Table S3. Arrhenius data for the ring closure reaction of MC **5a** in DMF.

T (ºC)	K	1/T (K^{-1})	ln k_{5a}	k_{5a}
-15.0	258.2	0.003874	-11.55	9.64×10^{-6}
0.0	273.2	0.003661	-9.369	8.53×10^{-5}
10.0	283.2	0.003531	-7.126	8.04×10^{-4}
25.0	298.2	0.003540	-5.830	2.94×10^{-3}
30.0	303.2	0.003298	-5.056	6.37×10^{-3}
40.0	313.2	0.003193	-4.211	1.48×10^{-2}
50.0	323.2	0.003095	-2.634	7.18×10^{-2}

Table S4. Arrhenius data for the ring closure reaction of MC **5a** in 1-propanol.

T (ºC)	K	1/T (K^{-1})	ln k_{5a}	k_{5a}
20.0	293.2	0.003411	-6.870	1.04×10^{-3}
25.0	298.2	0.003540	-6.174	2.08×10^{-3}
40.0	313.2	0.003193	-4.522	1.09×10^{-2}
50.0	323.2	0.003095	-3.391	3.37×10^{-2}

a)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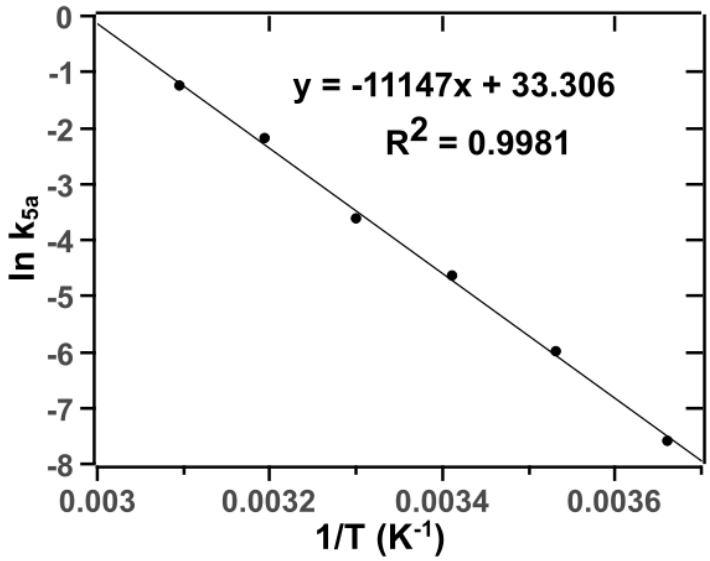
0.0034
0.0036

b)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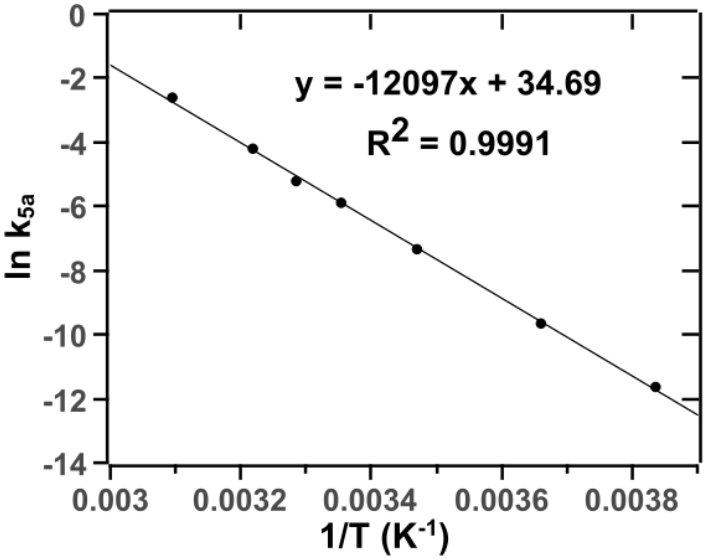
0.0034
0.0036

c)



d)

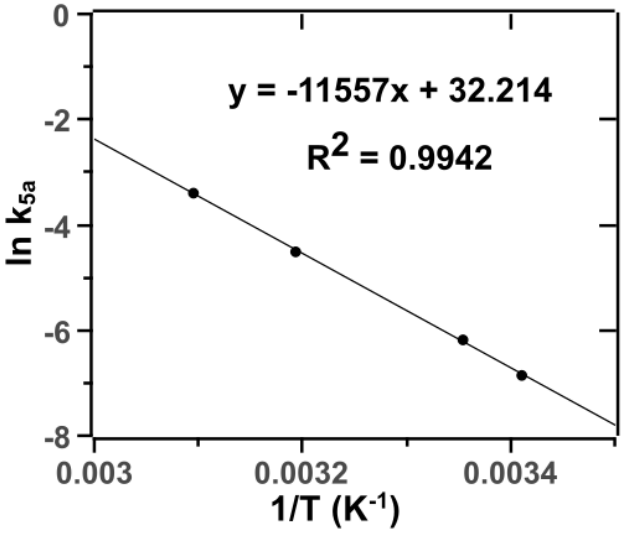
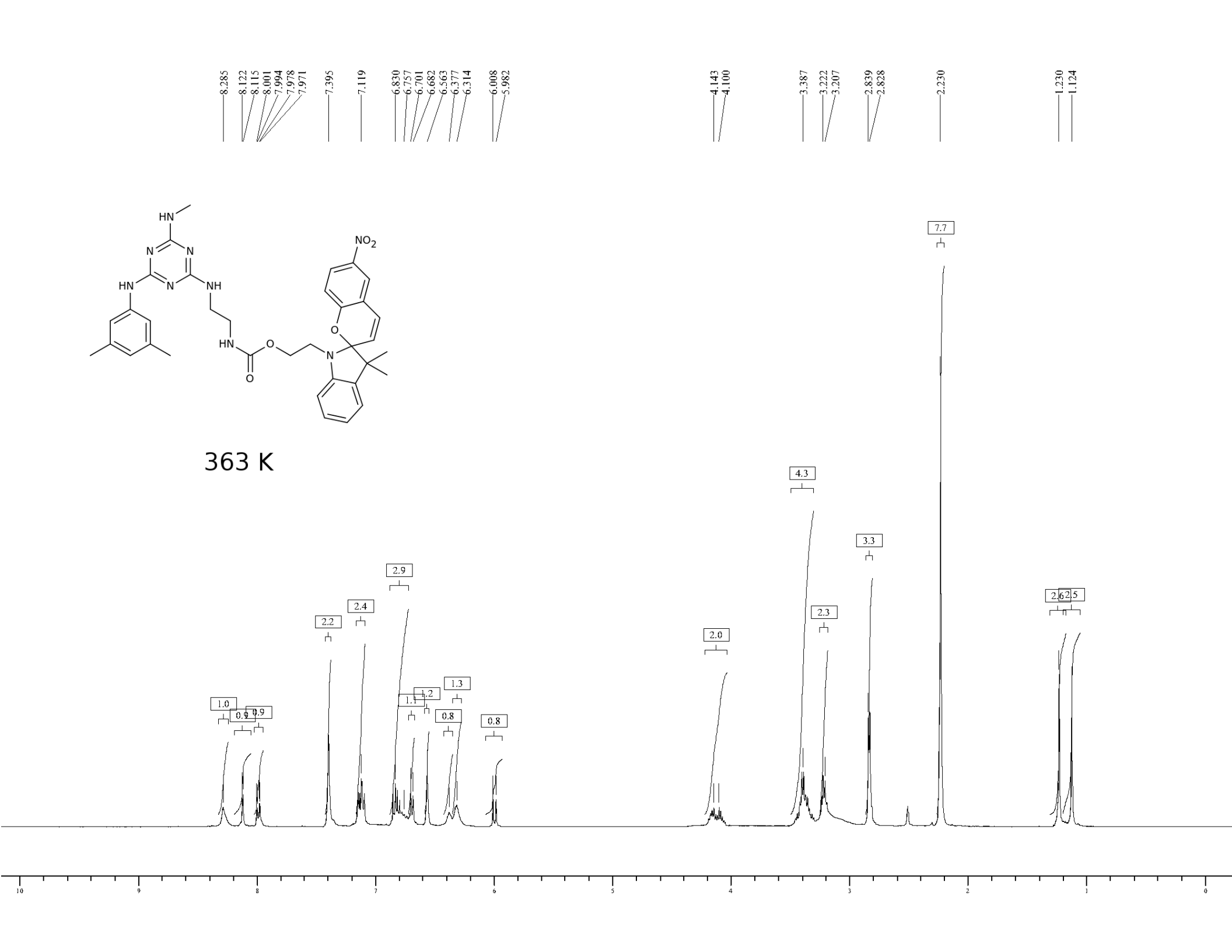


Figure S2. Arrhenius plots for the ring closure reaction of MC **5a**. a) Toluene; b) THF; c) DMF; d) 1-propanol.

Figure S3. NMR spectra of SP **5**. a) ^{1}H spectrum; b) ^{13}C spectrum; c) HSQC spectrum.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6.377
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3.207
2.839
2.828
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1.124
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N
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HN
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NH
HN
O
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N
O
NO2
363 K
7.7
4.3
3.3
2.9
2.4
2.3
2.2
2.0
2.6
2.5
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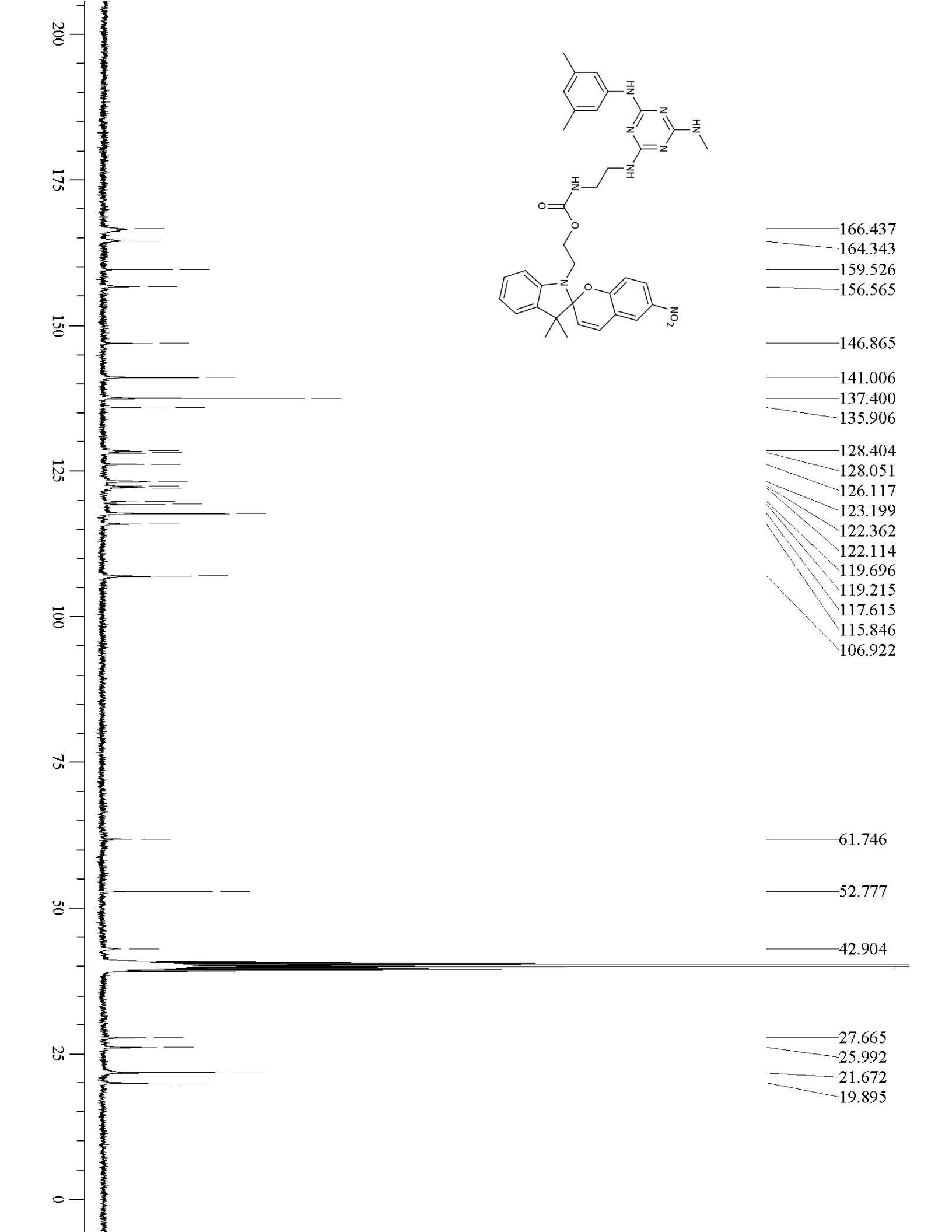
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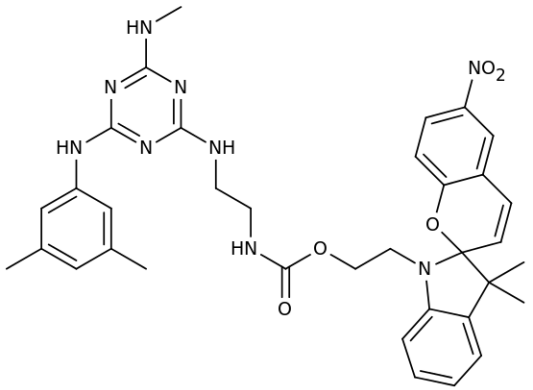
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HN
O
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O
NO2

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30
40
50
60
70
80
90
100
110
120
130
140
150
f1 (ppm)
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5