

New Journal of Chemistry

Supporting information

Synthesis, bioactivity and 3D-QSAR of Azamacrolide compounds with a carbamate or urea moiety as potential fungicides and inhibitors of quorum sensing

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1. The inhibition rate of target compounds against plant pathogens

Table S1 The inhibition rate of target compounds against plant pathogens (50 mg/L).

Comp.	Inhibitory rate (%) ^a					
	<i>A.s.</i>	<i>B.c.</i>	<i>V.m.</i>	<i>M.k.</i>	<i>G.z.</i>	<i>S.s.</i>
D16	39.30	13.84	20.78	56.92	40.52	65.97
D12	7.37	-1.04	2.92	11.64	18.59	19.47
D16-1	26.99	10.42	6.51	-9.74	3.32	61.95
D16-2	33.33	12.80	10.71	15.41	27.88	76.70
D16-3	30.18	11.76	12.01	12.89	29.00	77.58
D16-4	38.34	15.10	7.19	-13.64	19.19	95.58
D16-5	19.30	0.69	12.34	8.81	26.39	84.66
D16-6	28.00	19.08	2.93	25.13	28.14	84.66
D16-7	18.10	1.82	5.48	-1.30	-5.54	89.97
D16-8	12.88	9.64	4.79	21.75	-12.18	87.61
D16-9	29.14	8.07	11.30	24.35	-25.46	84.37
D16-10	14.39	8.65	10.71	4.09	17.47	90.86
D16-11	18.25	4.50	7.79	4.72	18.22	81.42
D16-12	20.35	1.38	9.74	3.14	28.25	67.26
D16-13	24.54	35.94	15.75	20.13	9.23	51.33
D16-14	47.02	46.02	21.75	41.82	40.89	94.10
D16-15	49.12	37.72	32.14	47.48	42.38	77.86
D16-16	34.05	28.39	9.59	5.84	-2.21	92.63
D16-17	40.18	44.27	24.66	46.43	7.01	97.35
D16-18	48.50	58.88	22.93	72.02	45.02	96.17
D16-19	96.32	41.67	95.89	96.10	95.57	60.47
D16-20	48.42	6.92	18.51	22.96	42.75	84.07
D16-21	13.68	14.88	20.13	22.64	8.55	75.81
D12-1	56.50	41.78	24.39	82.12	58.44	53.99
D12-2	49.82	18.34	49.35	47.48	44.61	66.03
D12-3	21.40	32.53	12.01	26.73	28.25	32.44
D12-4	50.50	43.09	33.66	60.62	37.66	70.29
D12-5	44.56	14.19	27.27	49.37	45.72	59.54
D12-6	38.00	38.49	27.80	51.55	48.05	62.32
D12-7	43.50	35.20	19.51	48.70	47.19	67.75
D12-8	51.50	23.03	21.46	55.96	50.65	53.62
D12-9	61.00	41.78	33.17	91.97	55.41	53.99
D12-10	13.68	95.85	20.13	96.23	8.55	52.78
D12-11	-1.05	-1.73	6.49	14.15	-7.06	33.97
D12-12	33.68	36.68	20.78	93.08	49.44	41.98
D12-13	67.02	56.06	47.40	76.10	64.31	66.67

D12-14	31.36	22.36	16.29	41.84	-8.70	65.97
D12-15	29.27	12.46	22.04	36.39	13.04	79.83
D12-16	47.00	44.08	23.41	69.17	34.63	45.29
D12-17	18.25	-2.77	8.44	66.67	34.57	29.17
D12-18	56.00	43.09	30.24	58.29	52.81	80.43
fludioxonil	100.00	100.00		100.00	100.00	100.00
carbendazim		100.00	100.00	100.00	100.00	

^a A.s., *Alternaria solani*; B.c., *Botrytis cinerea*; V.m., *Valsa mali*; G.z., *Gibberella zeae*; S.s., *Sclerotinia sclerotiorum*. All values are the mean of three replicates.

2. Antibacterial activity of test compounds against *Agrobacterium tumefaciens*

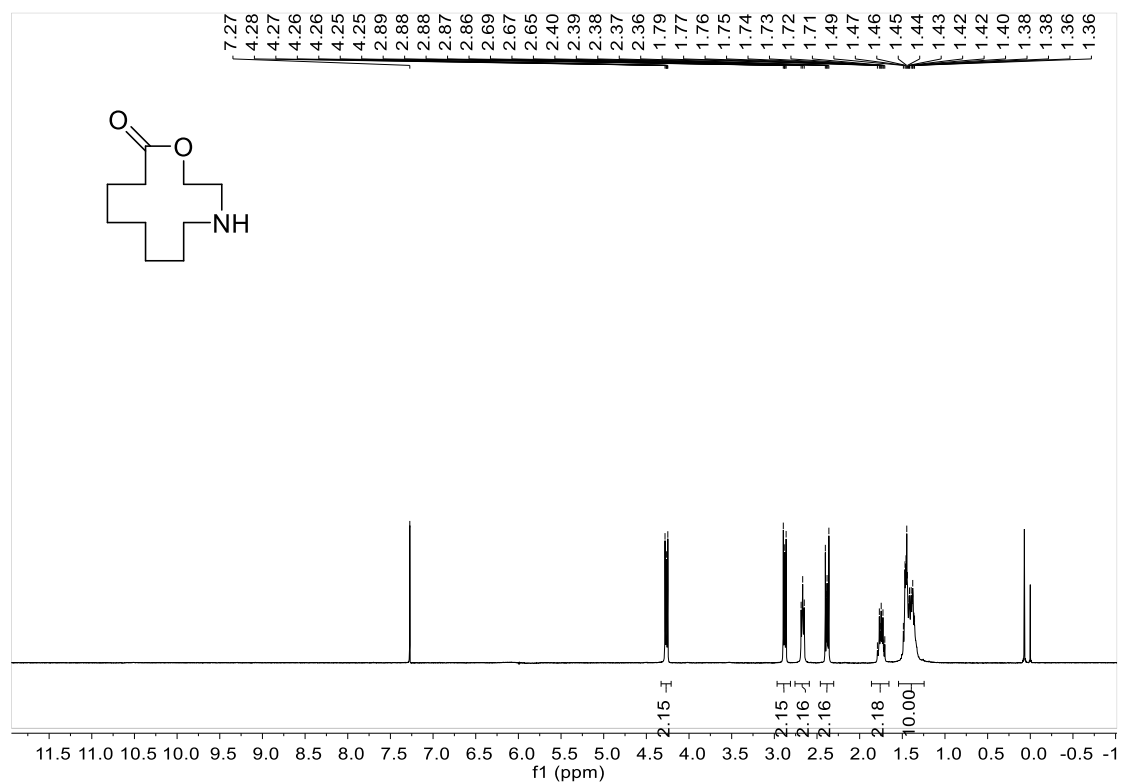
Table S2 Antibacterial activity of test compounds at different concentrations against *Agrobacterium tumefaciens in vitro*

Compound	OD ₆₀₀ value			
	200 mg/L	100 mg/L	50 mg/L	25 mg/L
D16-1	0.373	0.768	0.794	0.809
D16-2	0.334	0.728	0.786	0.830
D16-3	0.356	0.754	0.808	0.822
D16-4	0.355	0.799	0.817	0.833
D16-5	0.387	0.713	0.792	0.797
D16-6	0.379	0.742	0.819	0.802
D16-7	0.410	0.772	0.791	0.789
D16-8	0.422	0.793	0.789	0.811
D16-9	0.398	0.791	0.779	0.816
D16-10	0.349	0.804	0.824	0.822
D16-11	0.375	0.741	0.805	0.814
D16-12	0.421	0.784	0.812	0.799
D16-13	0.376	0.758	0.806	0.823
D16-14	0.386	0.768	0.809	0.822
D16-15	0.398	0.726	0.796	0.818
D16-16	0.457	0.776	0.825	0.826
D16-17	0.379	0.809	0.810	0.827
D16-18	0.418	0.795	0.796	0.816
D16-19	0.465	0.765	0.807	0.814
D16-20	0.490	0.818	0.810	0.827
D16-21	0.348	0.770	0.829	0.810
D12-1	0.403	0.772	0.786	0.829
D12-2	0.384	0.787	0.823	0.815
D12-3	0.377	0.731	0.809	0.821
D12-4	0.423	0.739	0.811	0.828
D12-5	0.394	0.741	0.788	0.819

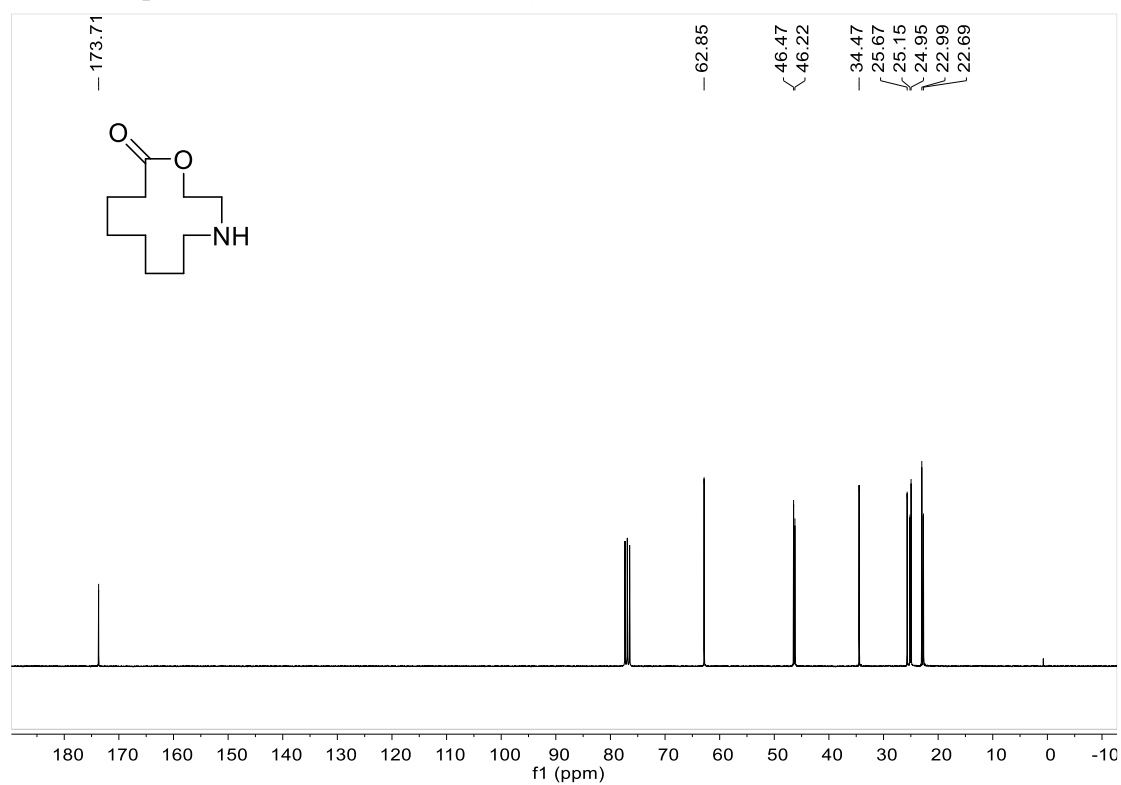
D12-6	0.363	0.743	0.806	0.807
D12-7	0.442	0.766	0.817	0.811
D12-8	0.485	0.715	0.801	0.831
D12-9	0.469	0.736	0.808	0.825
D12-10	0.482	0.745	0.798	0.818
D12-11	0.383	0.747	0.793	0.813
D12-12	0.455	0.702	0.819	0.810
D12-13	0.384	0.746	0.811	0.828
D12-14	0.331	0.793	0.802	0.816
D12-15	0.301	0.768	0.813	0.826
D12-16	0.487	0.768	0.787	0.817
D12-17	0.373	0.776	0.789	0.807
D12-18	0.369	0.719	0.818	0.829
Blank control			0.780	
DMSO			0.765	

^1H NMR spectrum and ^{13}C NMR spectrum

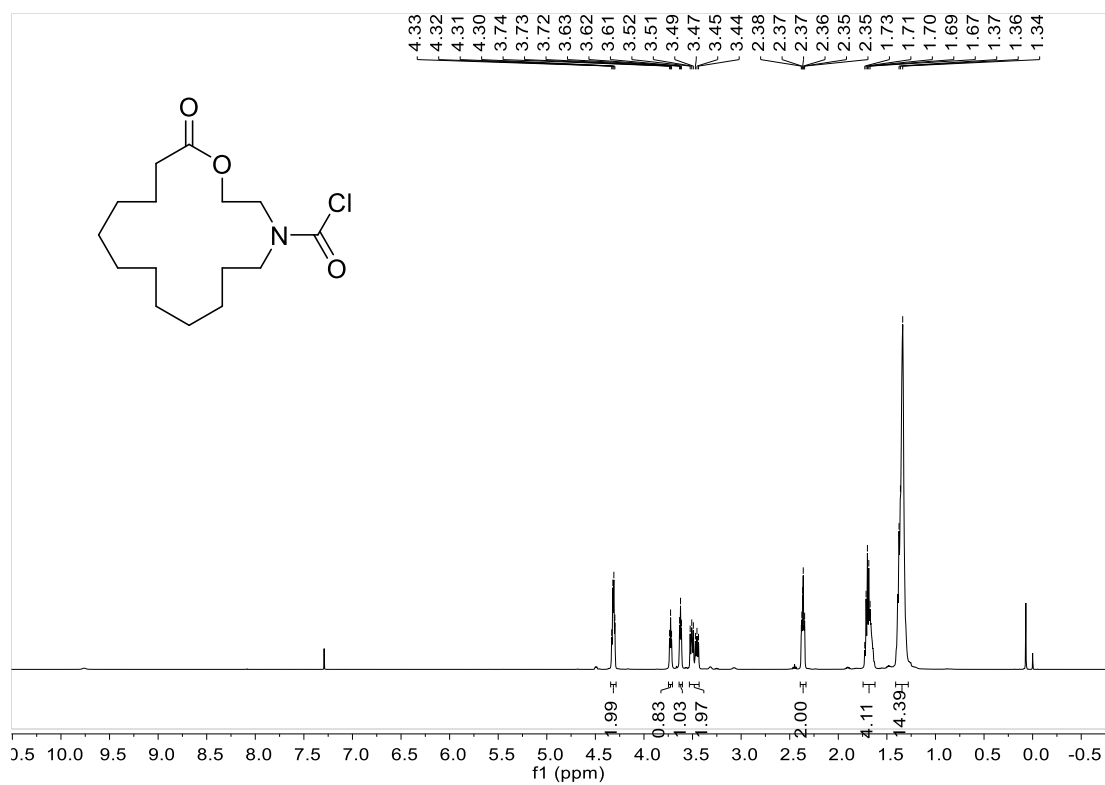
^1H NMR spectrum of D12 (300 MHz, CDCl_3)



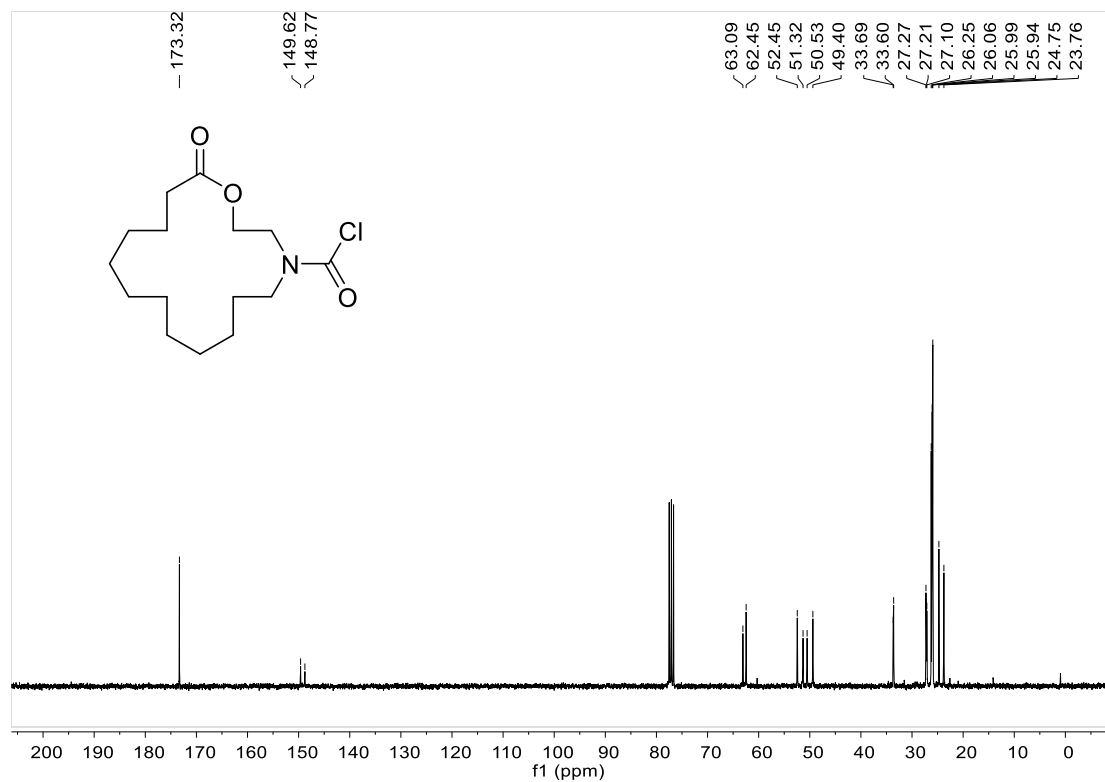
^{13}C NMR spectrum of D12 (75 MHz, CDCl_3)



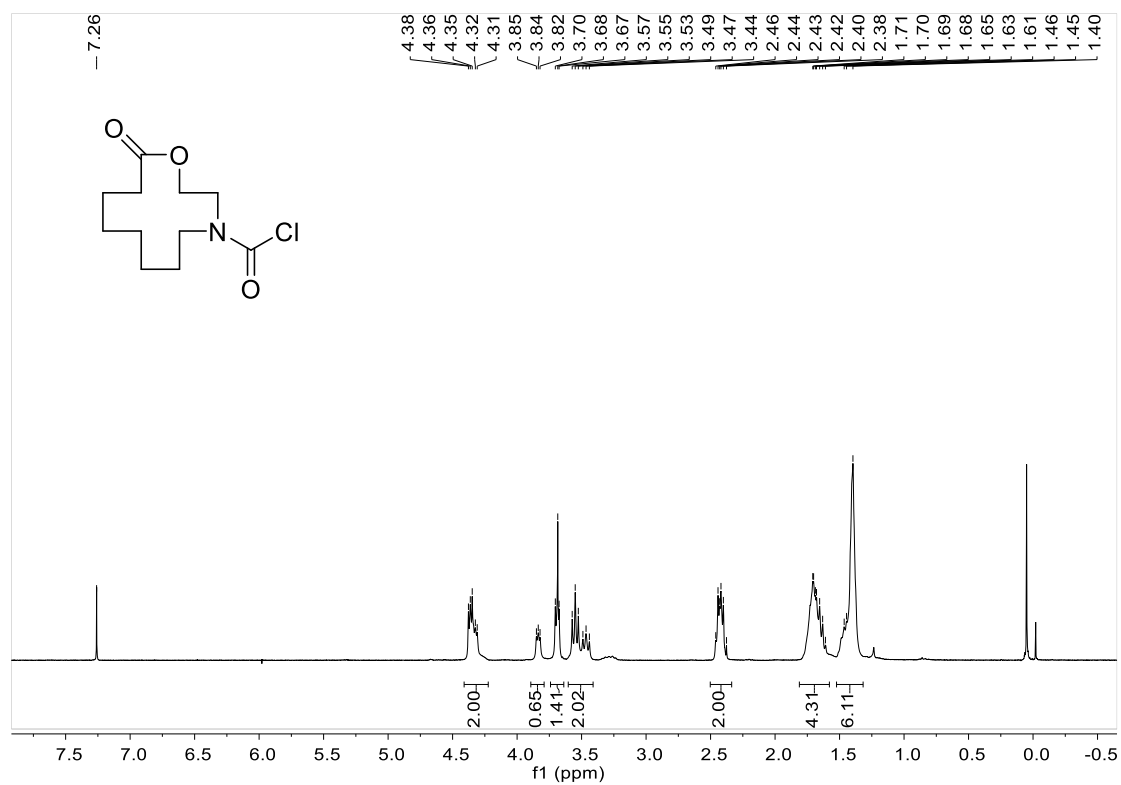
¹H NMR spectrum of D16-XL (300 MHz, CDCl₃)



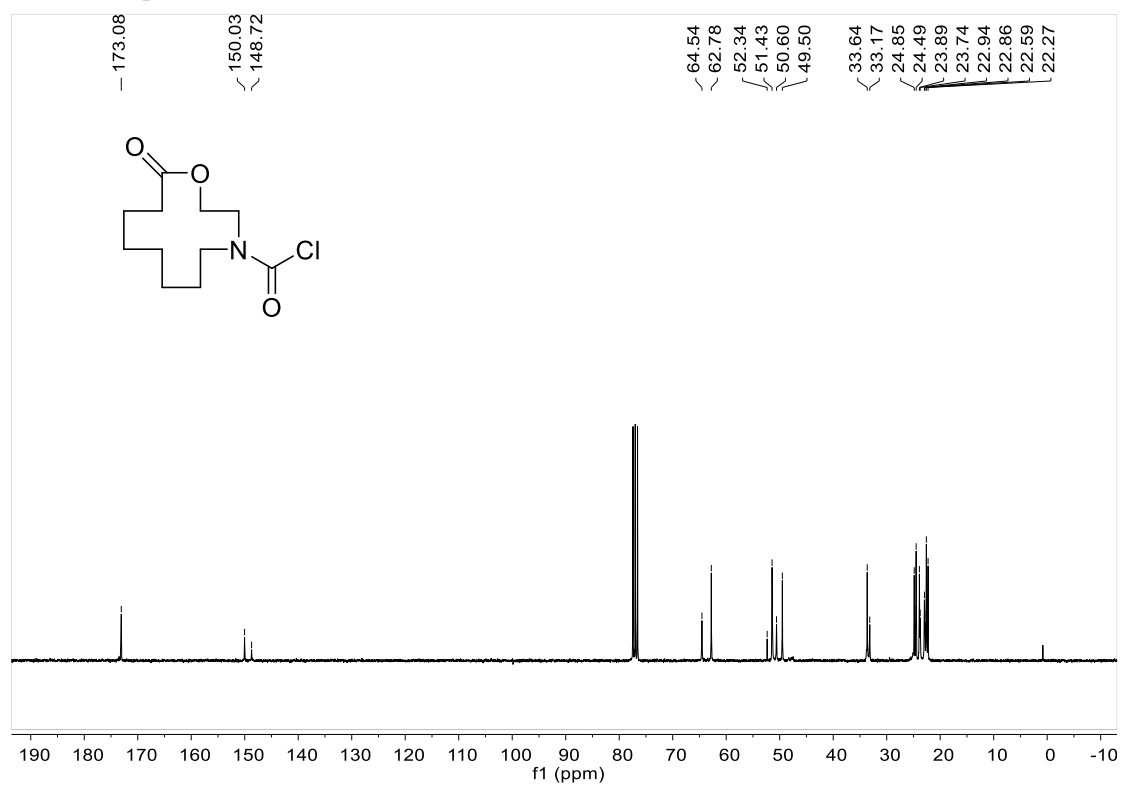
¹³C NMR spectrum of D16-XL (75 MHz, CDCl₃)



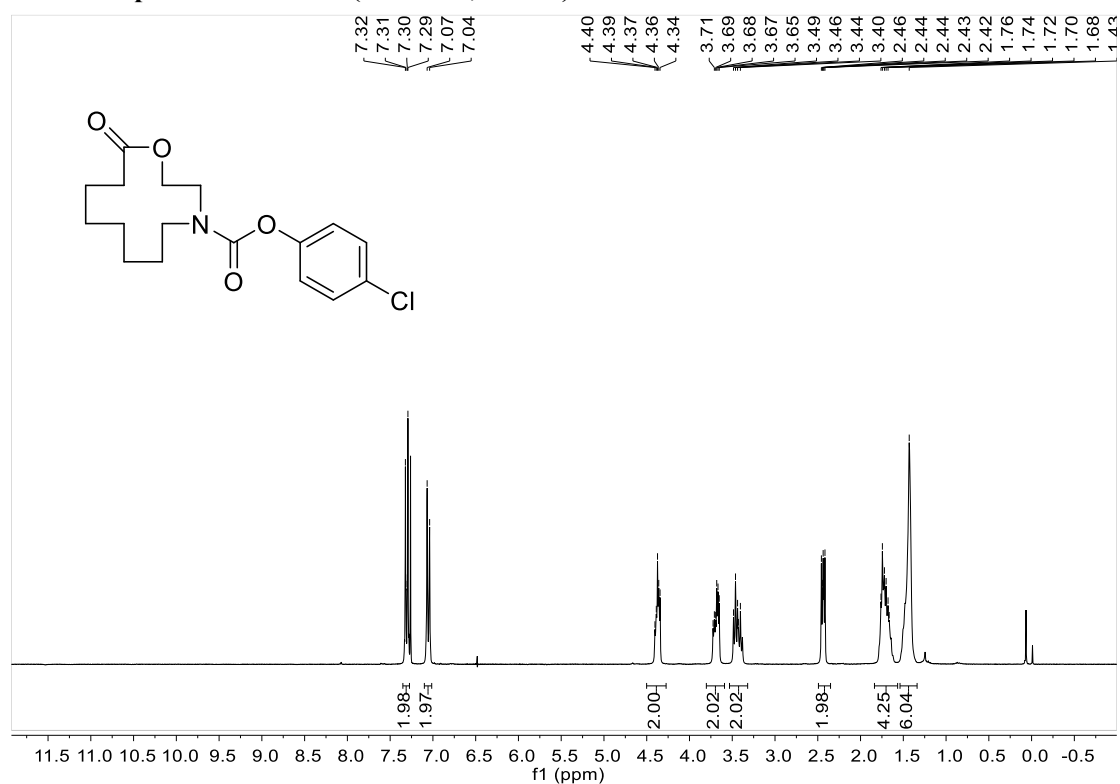
¹H NMR spectrum of D12-XL (300 MHz, CDCl₃)



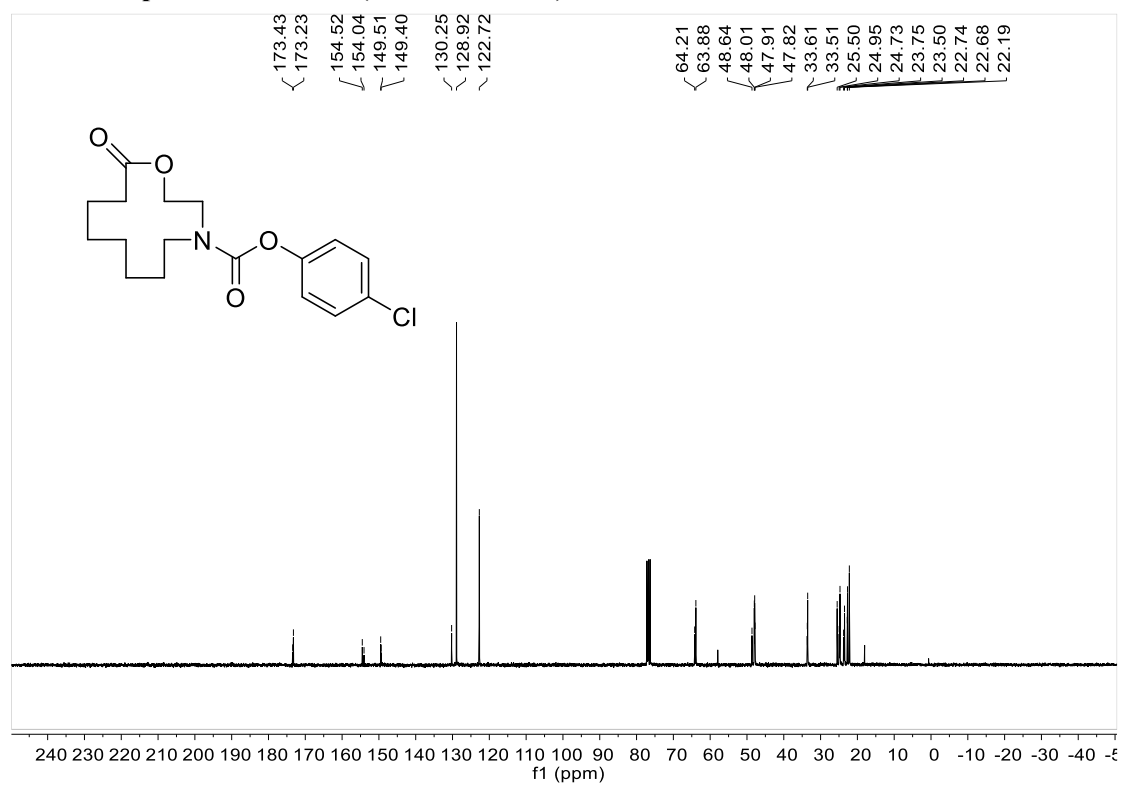
¹³C NMR spectrum of D12-XL (75 MHz, CDCl₃)



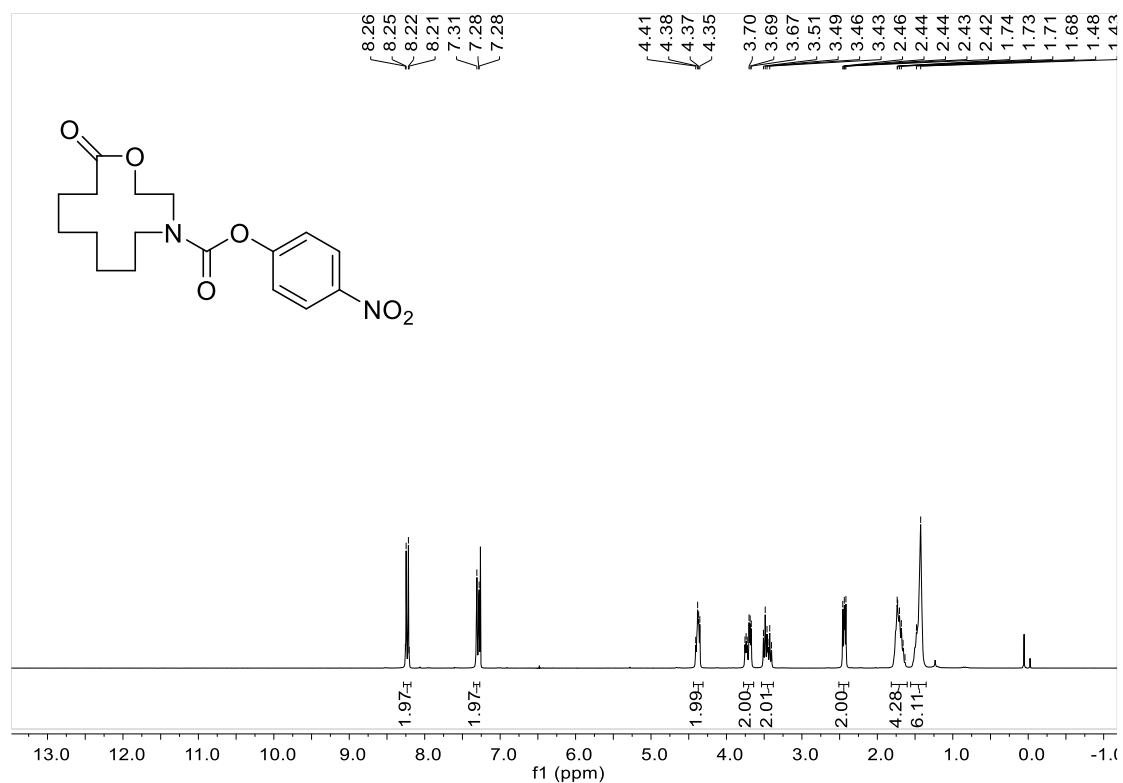
¹H NMR spectrum of D12-1 (300 MHz, CDCl₃)



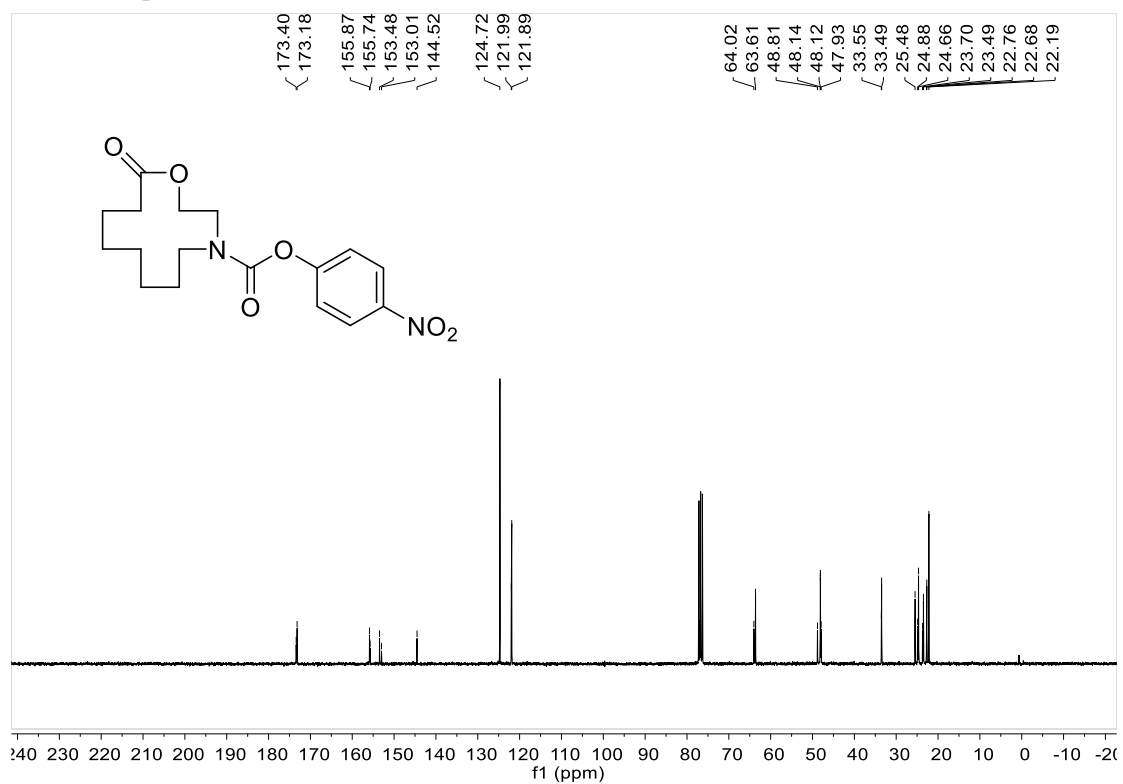
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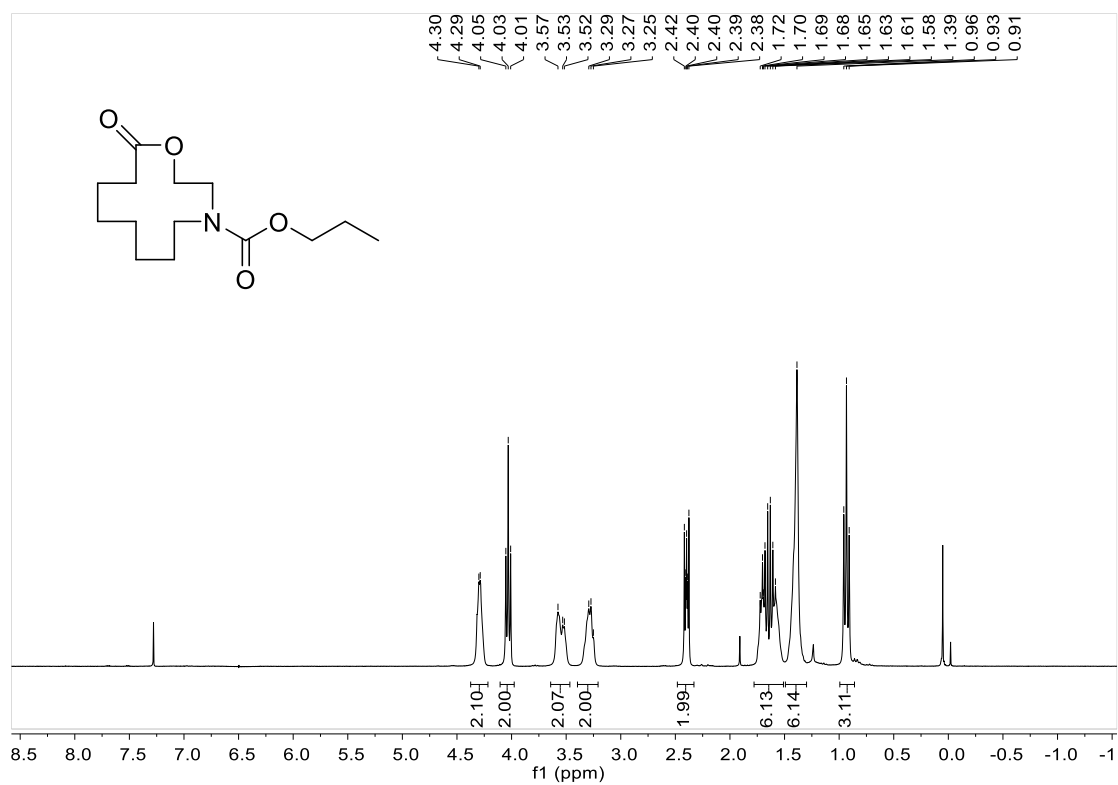
¹H NMR spectrum of D12-2 (300 MHz, CDCl₃)



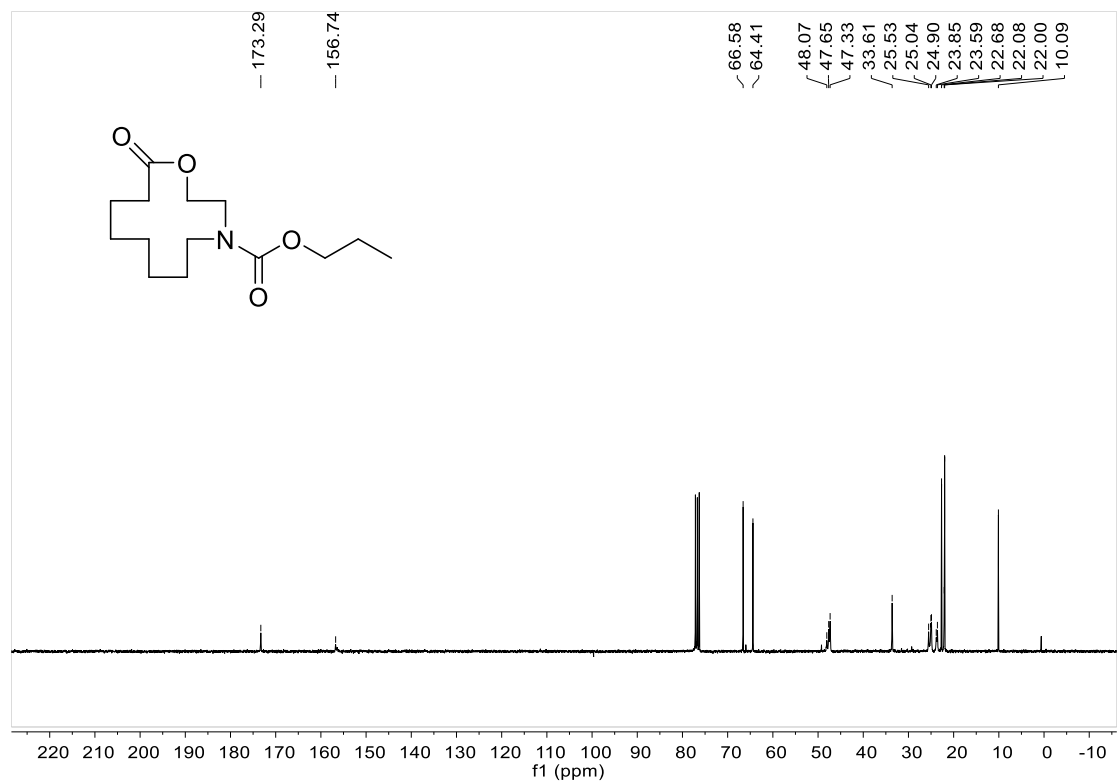
¹³C NMR spectrum of D12-2 (75 MHz, CDCl₃)



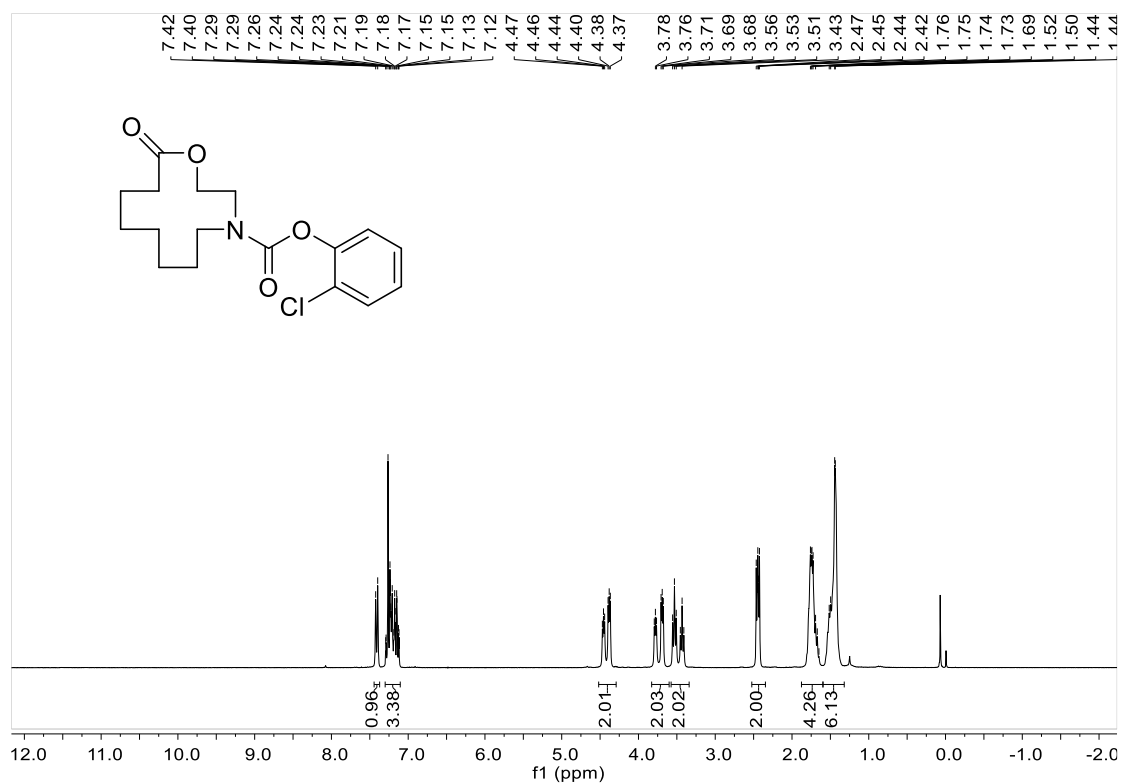
¹H NMR spectrum of D12-3 (300 MHz, CDCl₃)



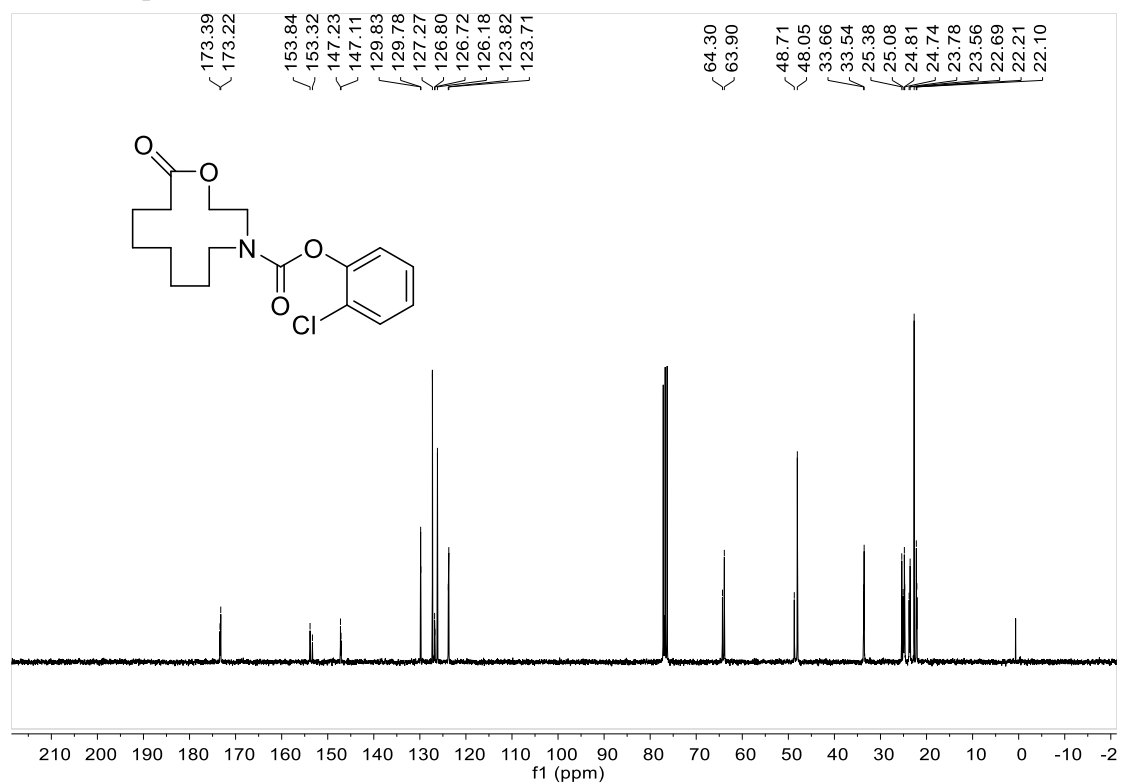
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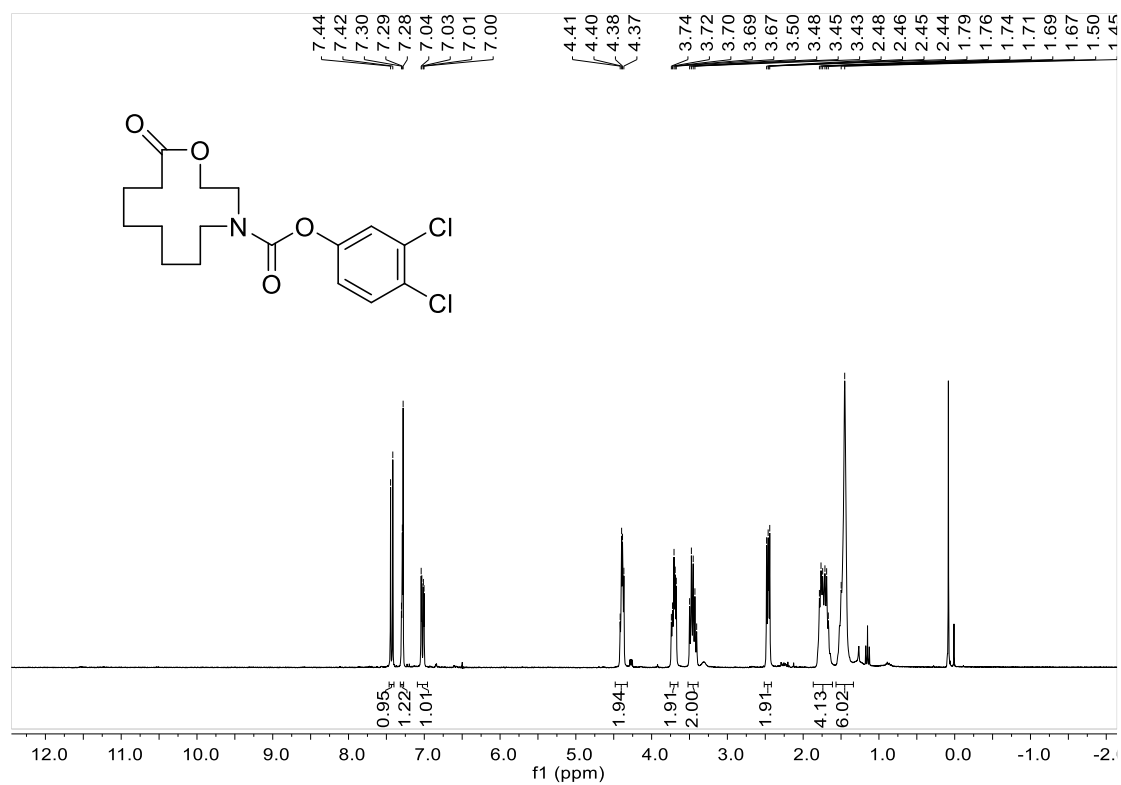
¹H NMR spectrum of D12-4 (300 MHz, CDCl₃)



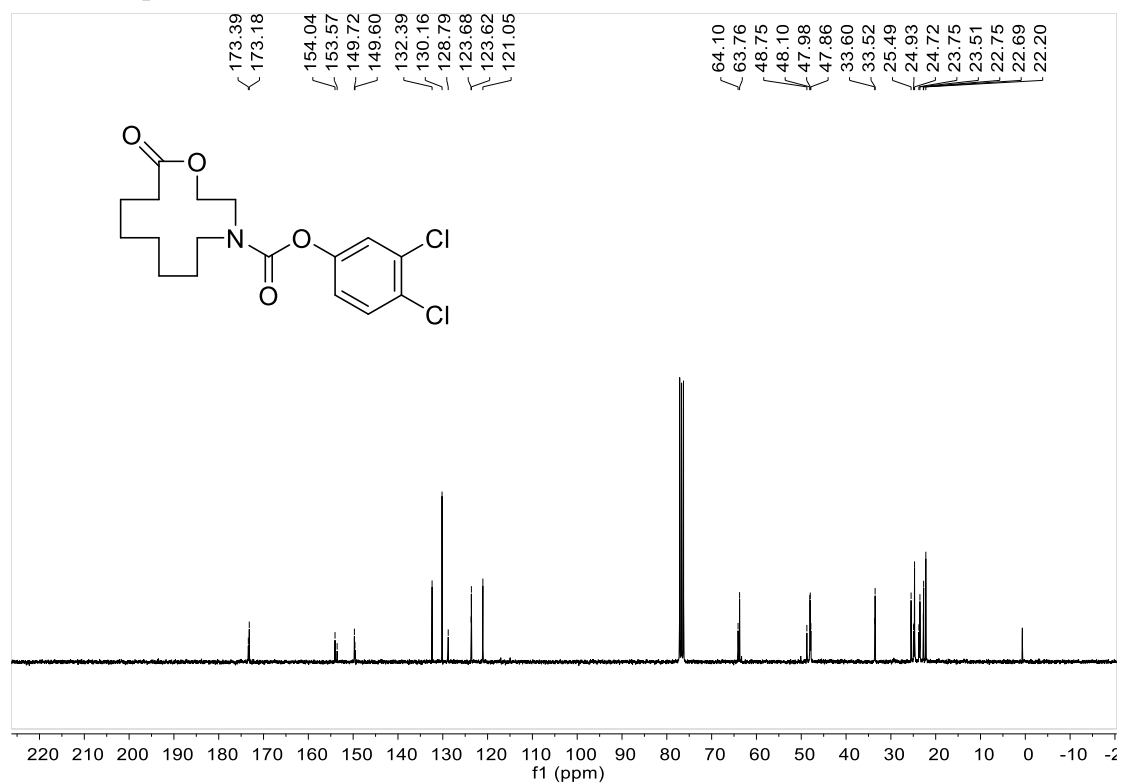
¹³C NMR spectrum of D12-4 (75 MHz, CDCl₃)



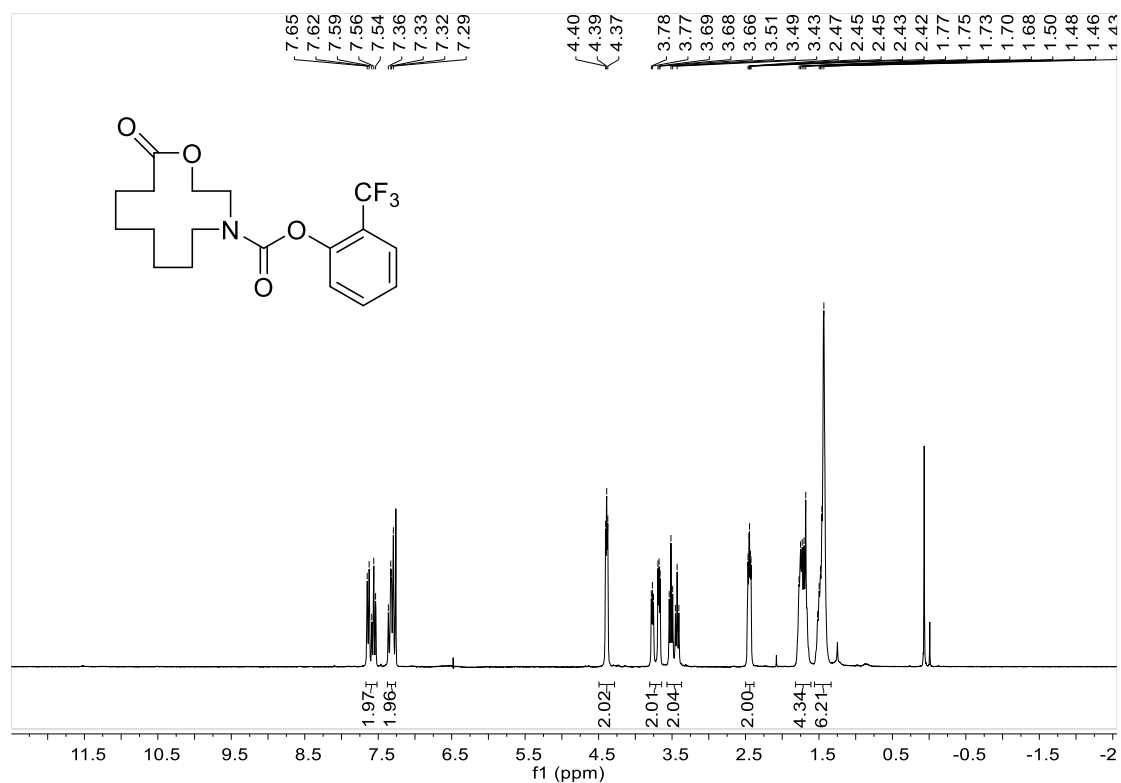
¹H NMR spectrum of D12-5 (300 MHz, CDCl₃)



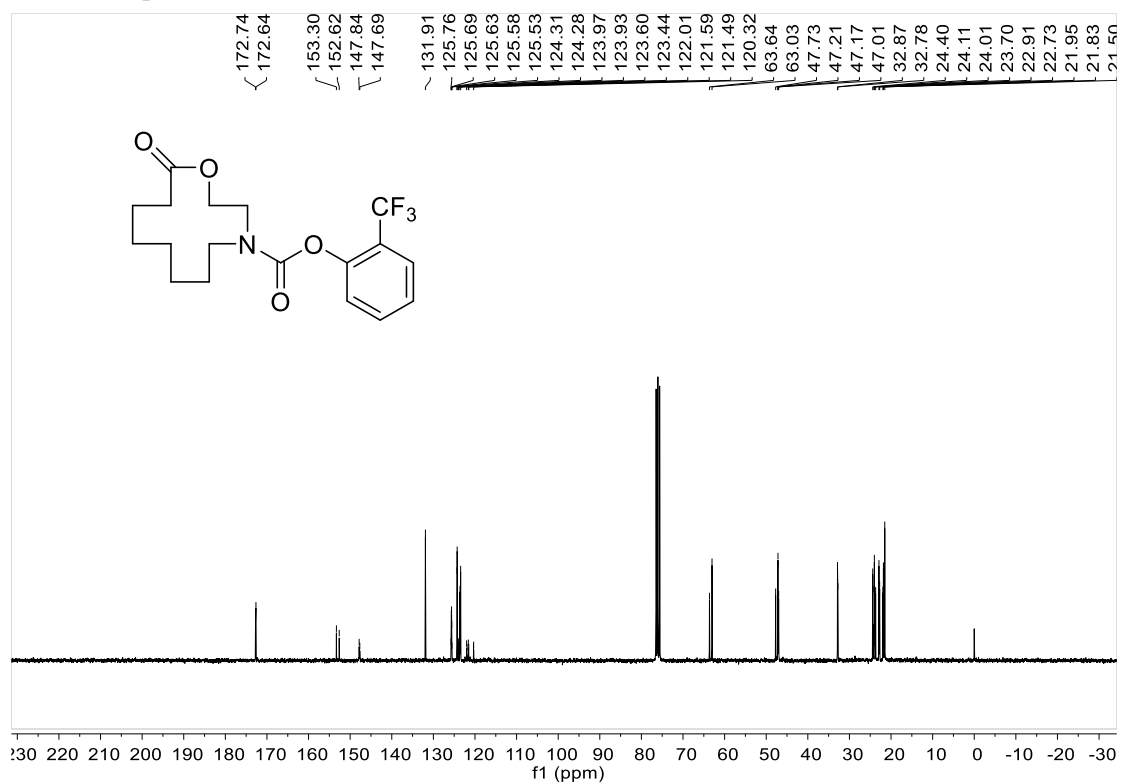
¹³C NMR spectrum of D12-5 (75 MHz, CDCl₃)



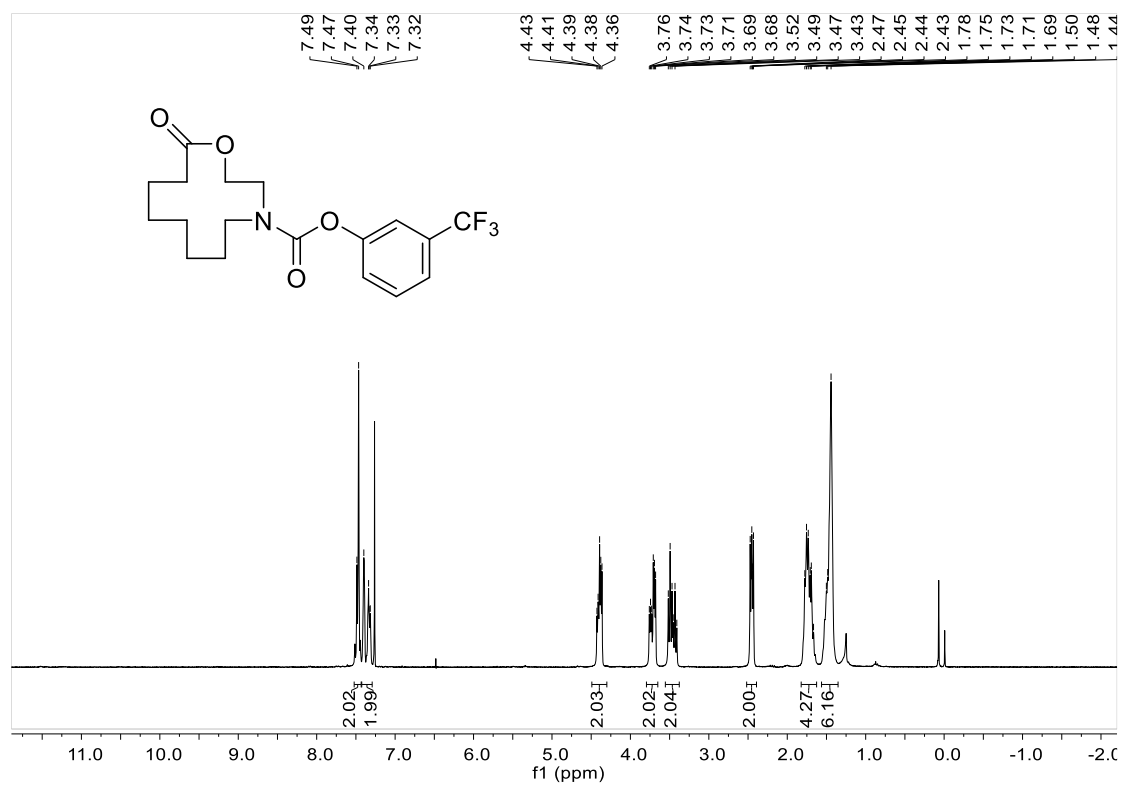
¹H NMR spectrum of D12-6 (300 MHz, CDCl₃)



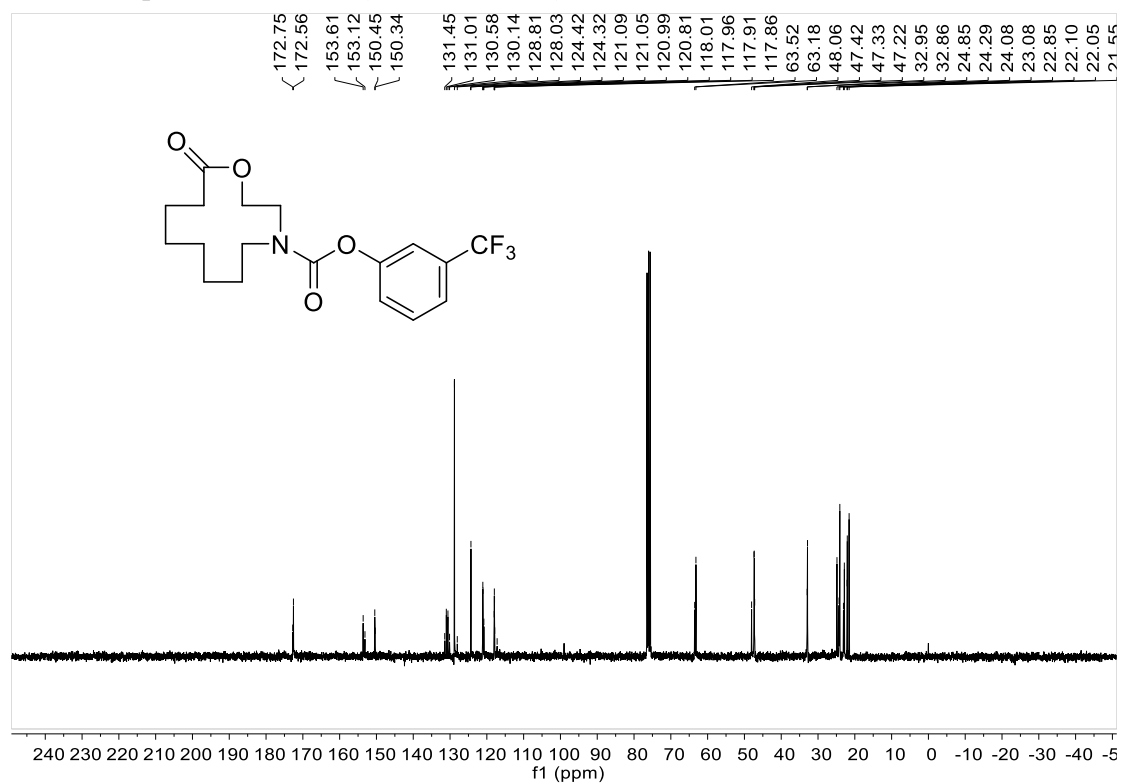
¹³C NMR spectrum of D12-6 (75 MHz, CDCl₃)



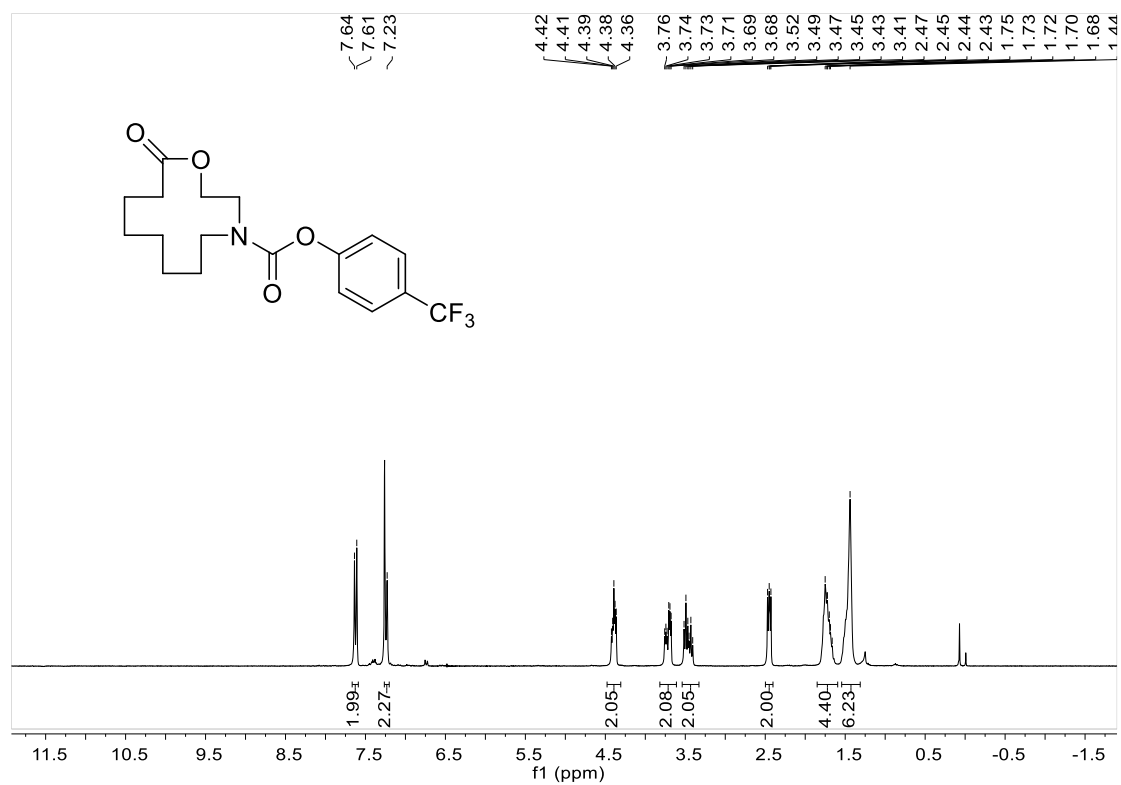
¹H NMR spectrum of D12-7 (300 MHz, CDCl₃)



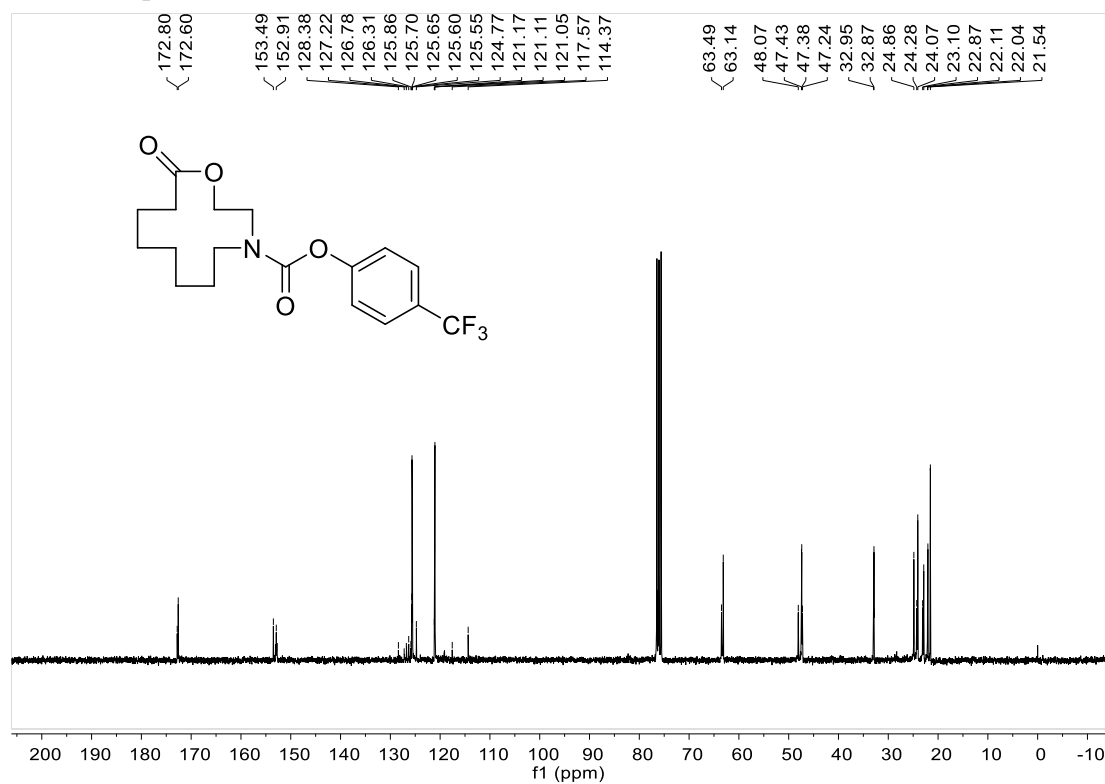
¹³C NMR spectrum of D12-7 (75 MHz, CDCl₃)



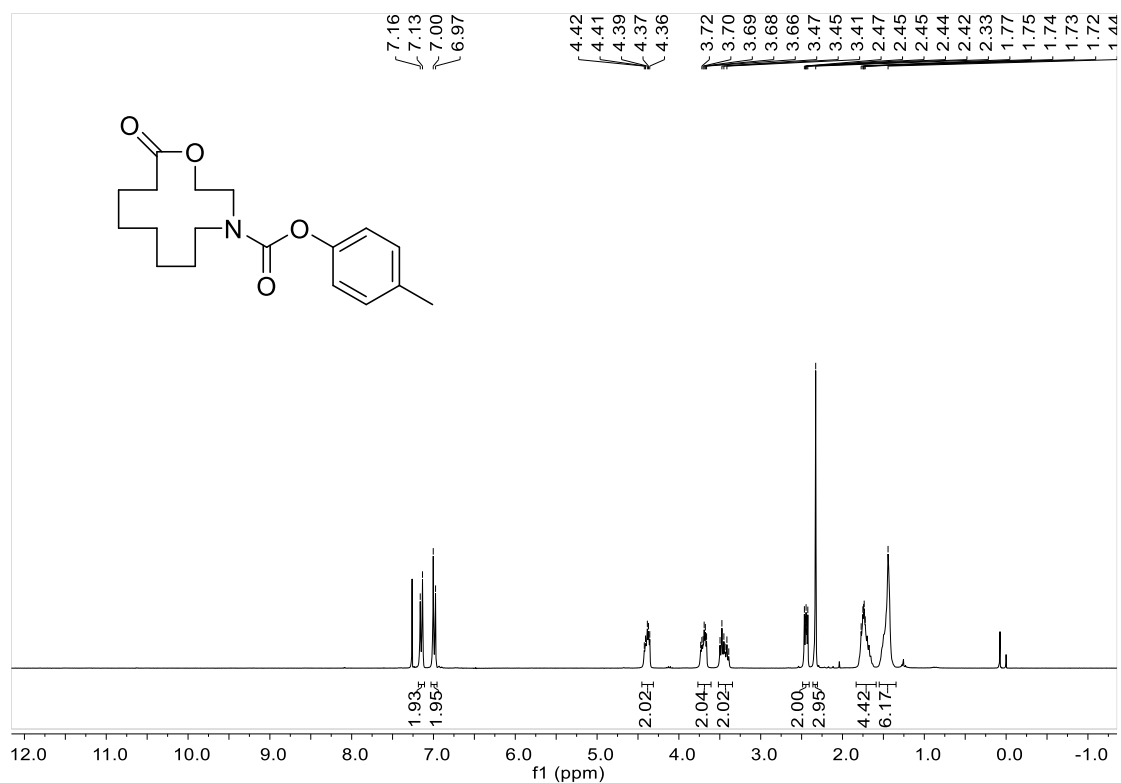
¹H NMR spectrum of D12-8 (300 MHz, CDCl₃)



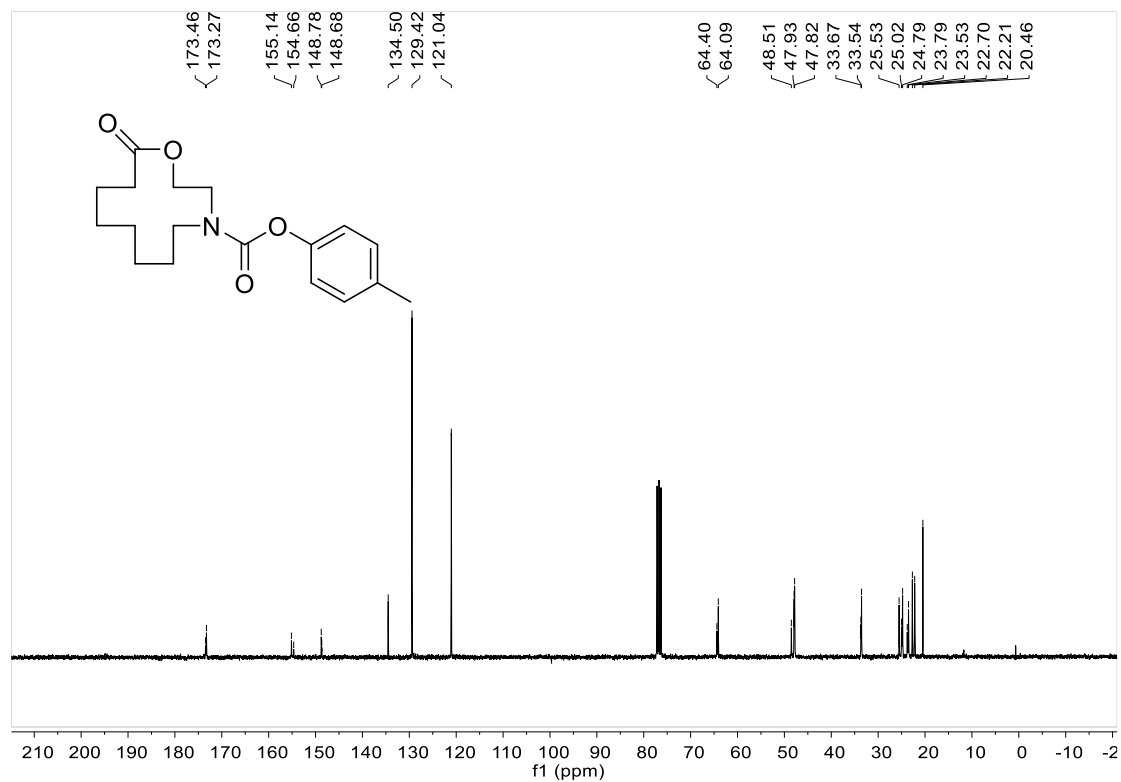
¹³C NMR spectrum of D12-8 (75 MHz, CDCl₃)



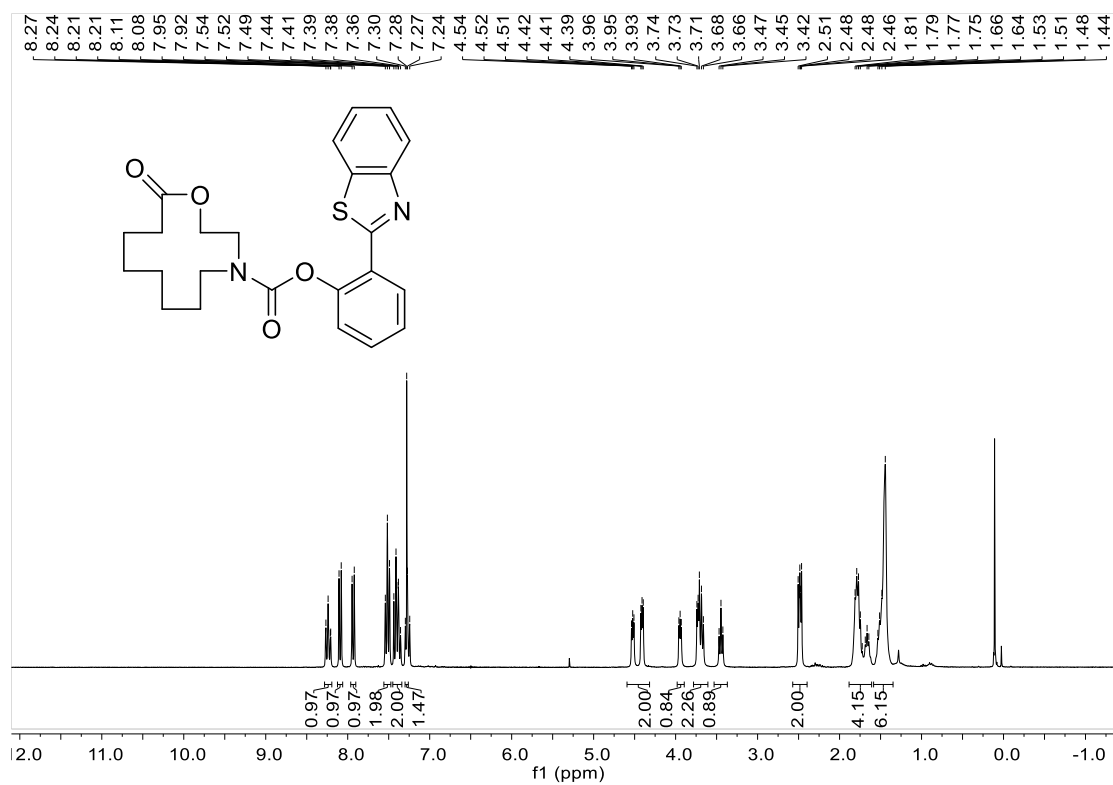
¹H NMR spectrum of D12-9 (300 MHz, CDCl₃)



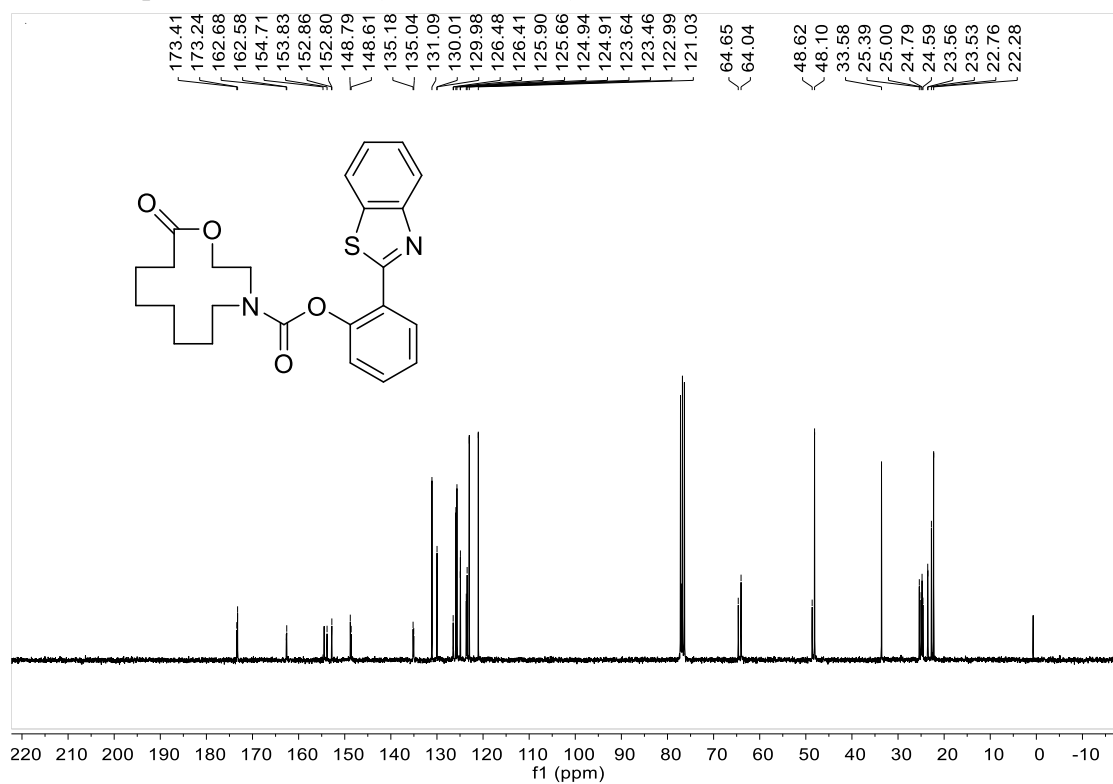
¹³C NMR spectrum of D12-9 (75 MHz, CDCl₃)



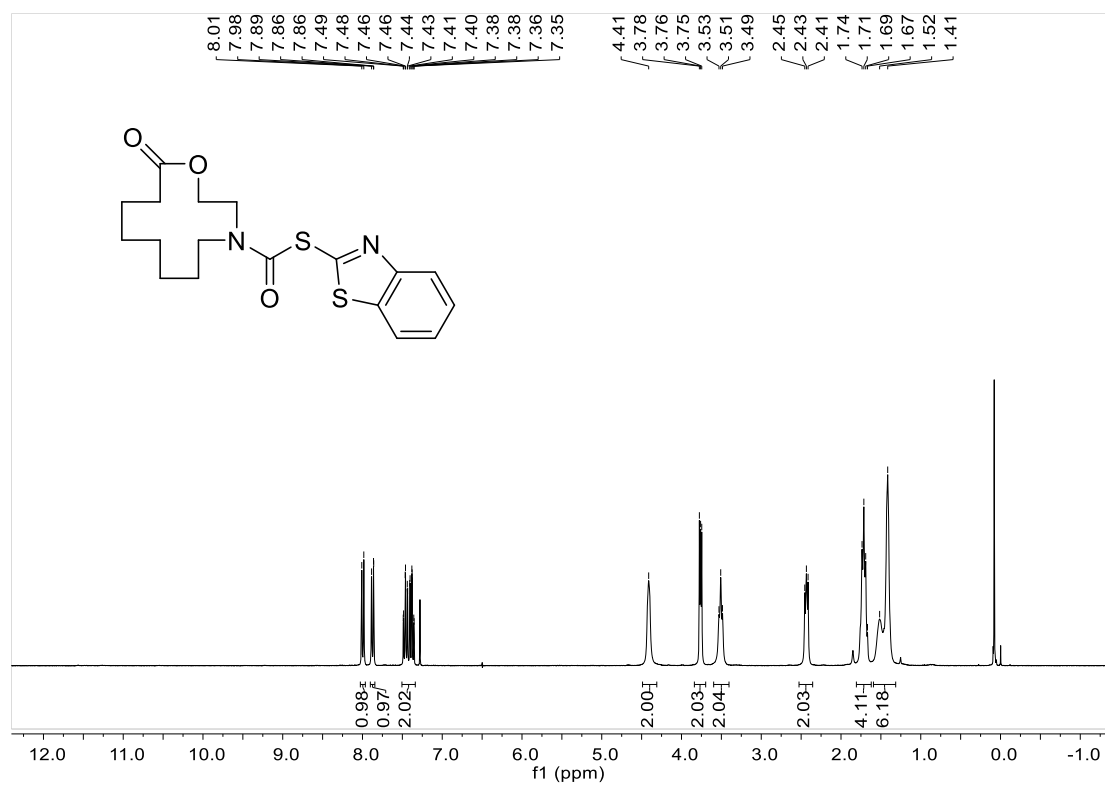
¹H NMR spectrum of D12-10 (300 MHz, CDCl₃)



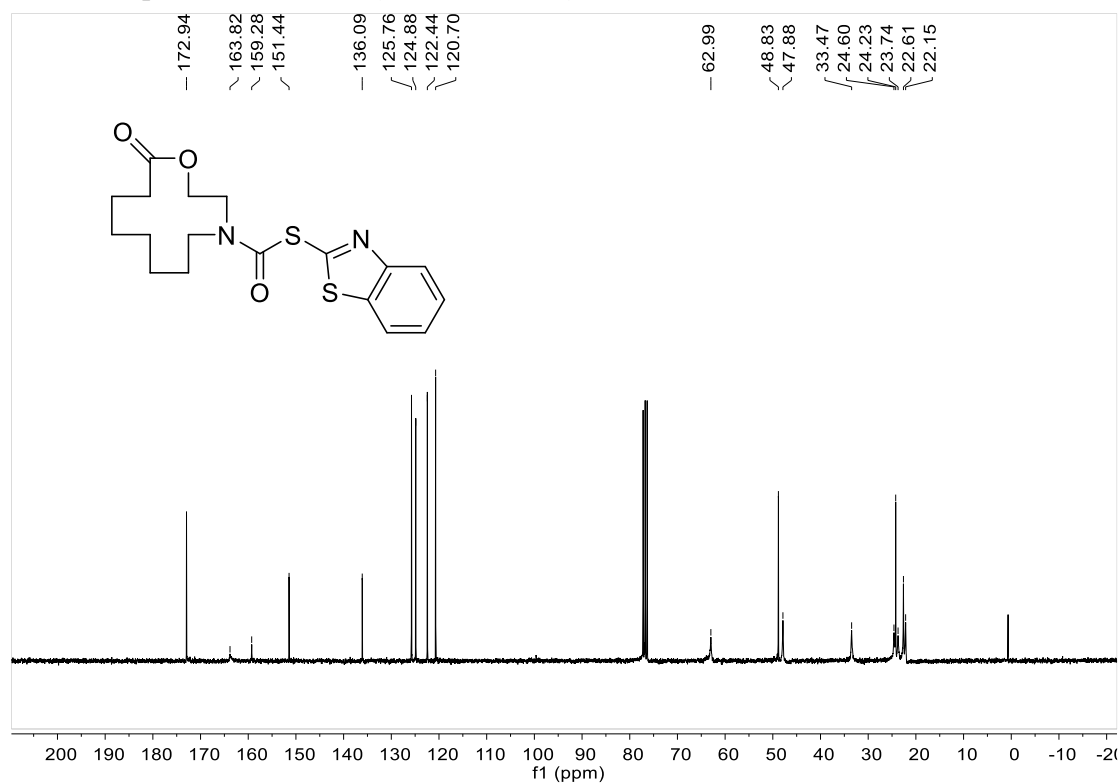
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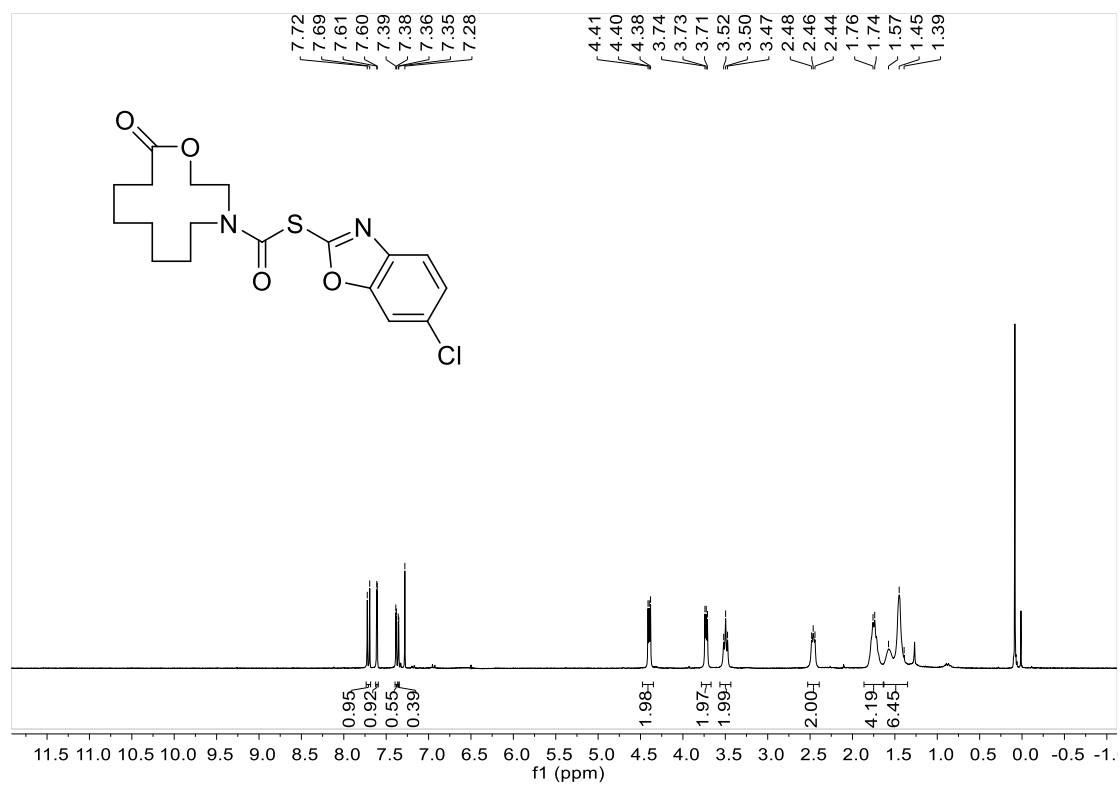
¹H NMR spectrum of D12-11 (300 MHz, CDCl₃)



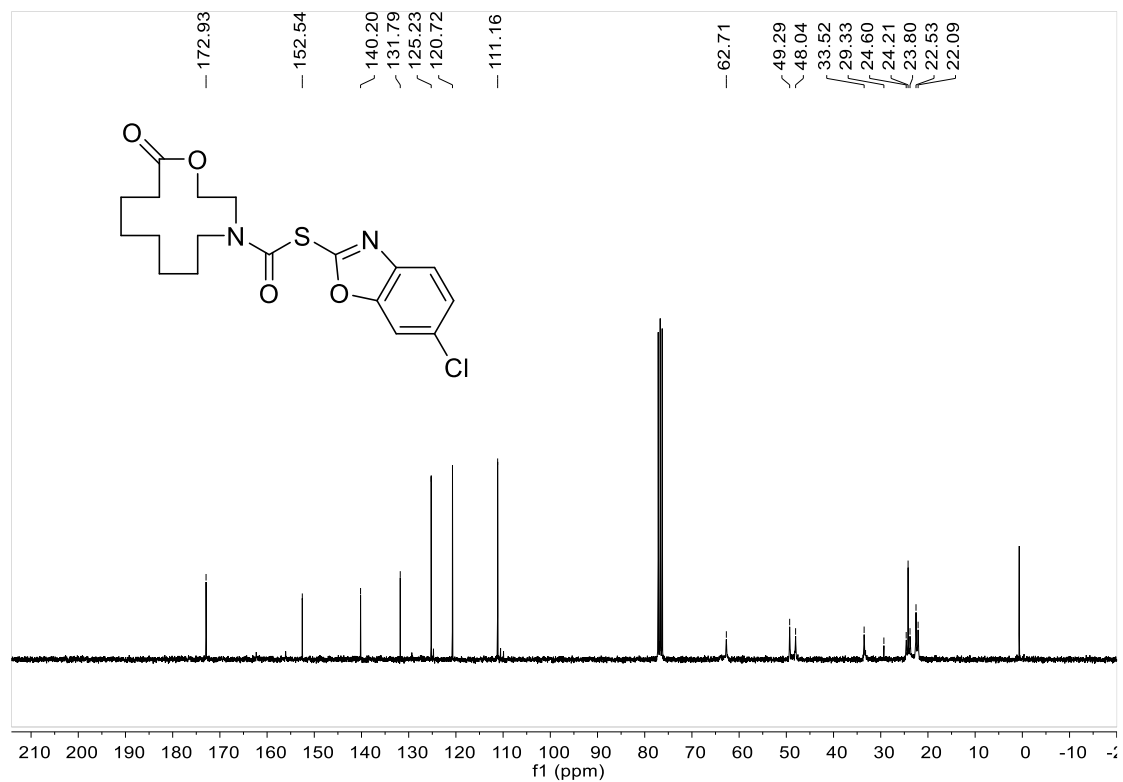
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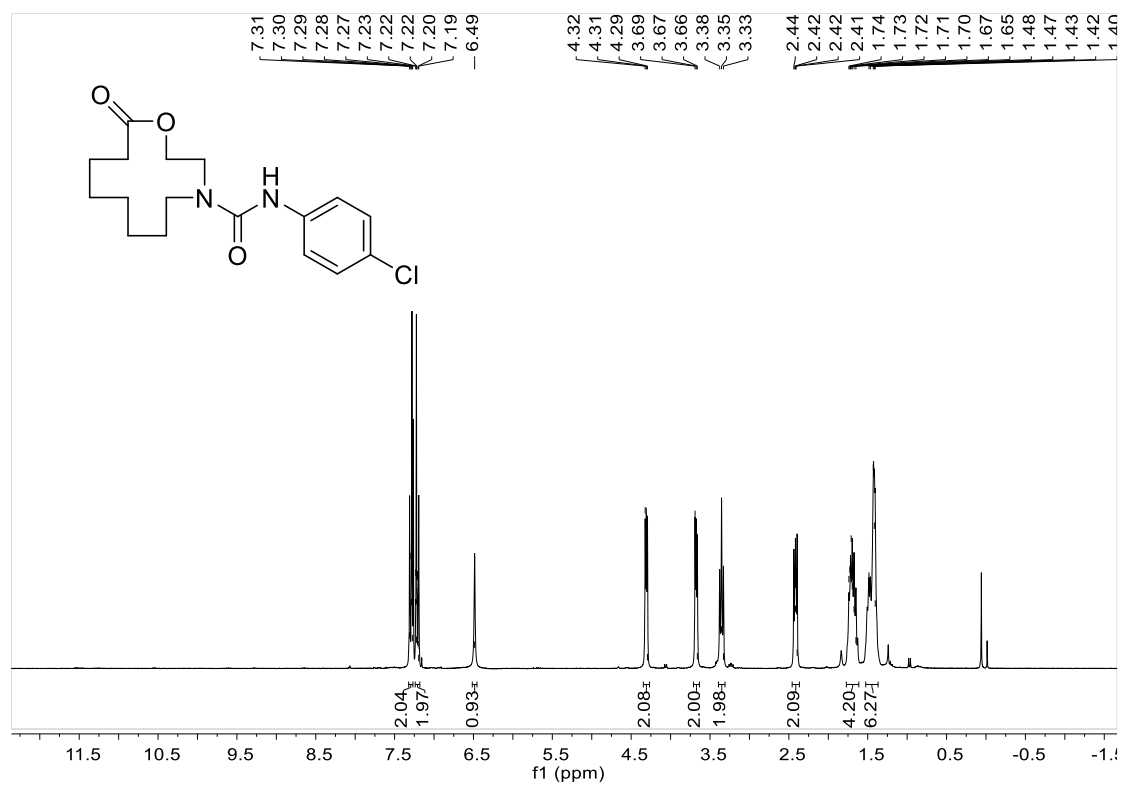
¹H NMR spectrum of D12-12 (300 MHz, CDCl₃)



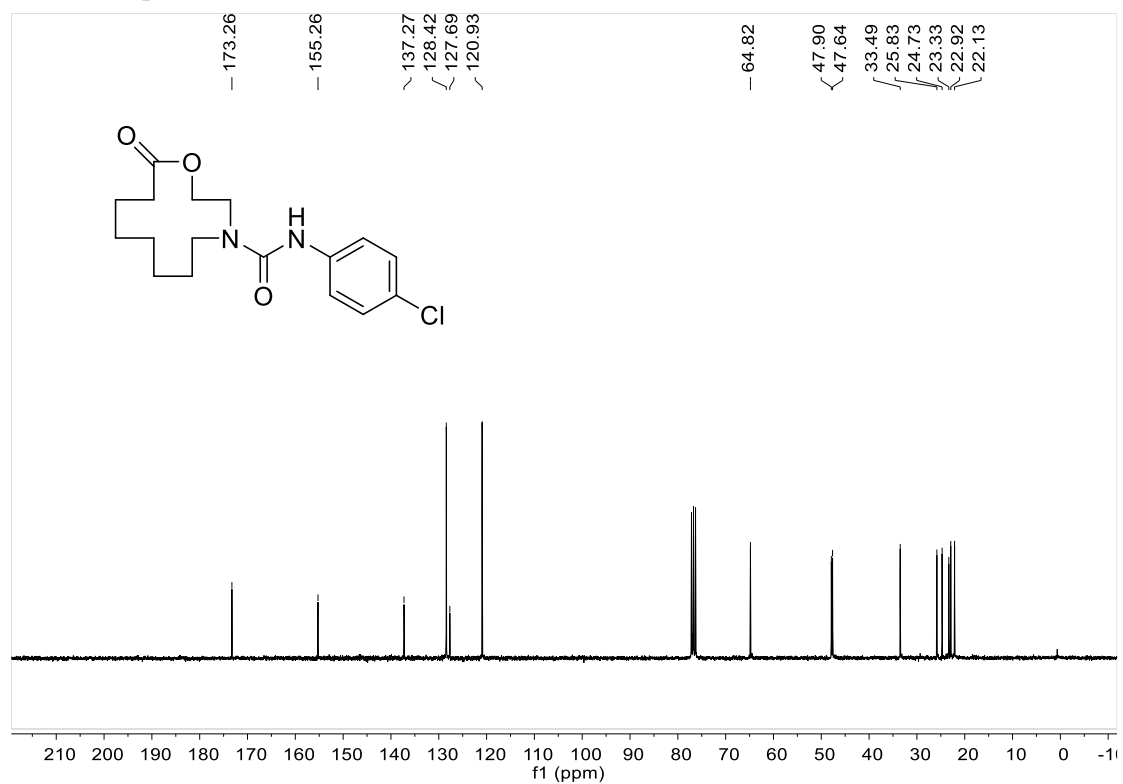
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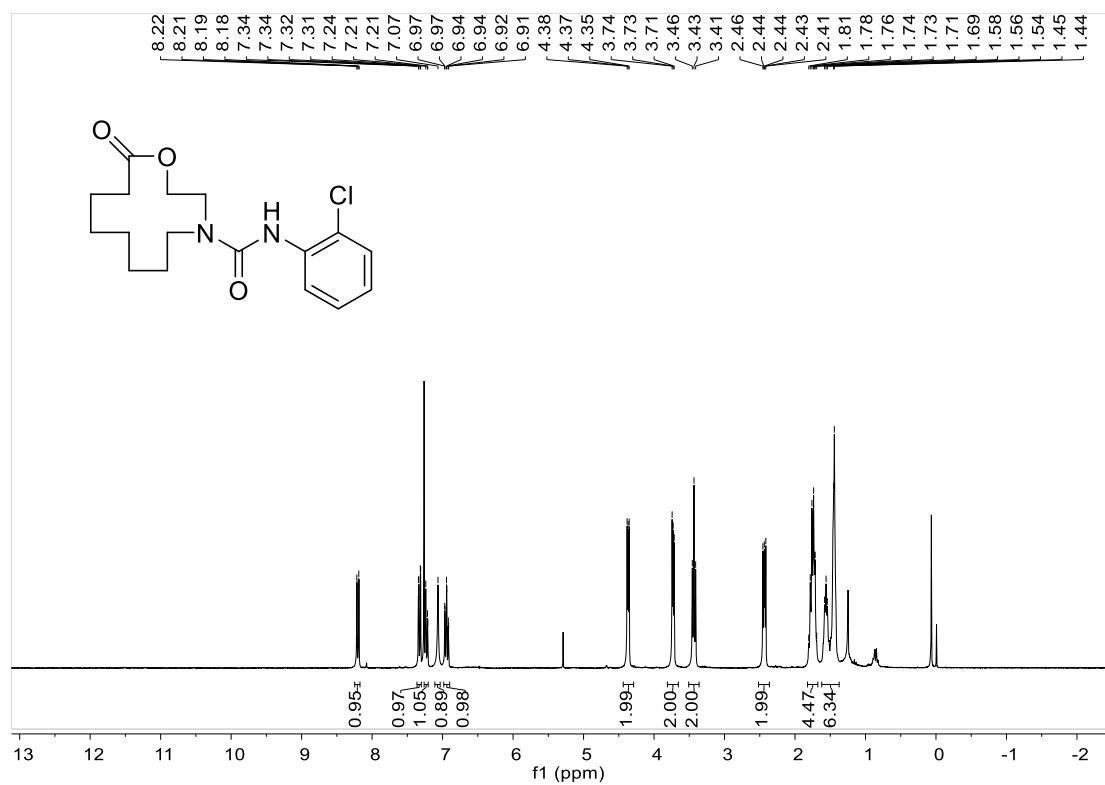
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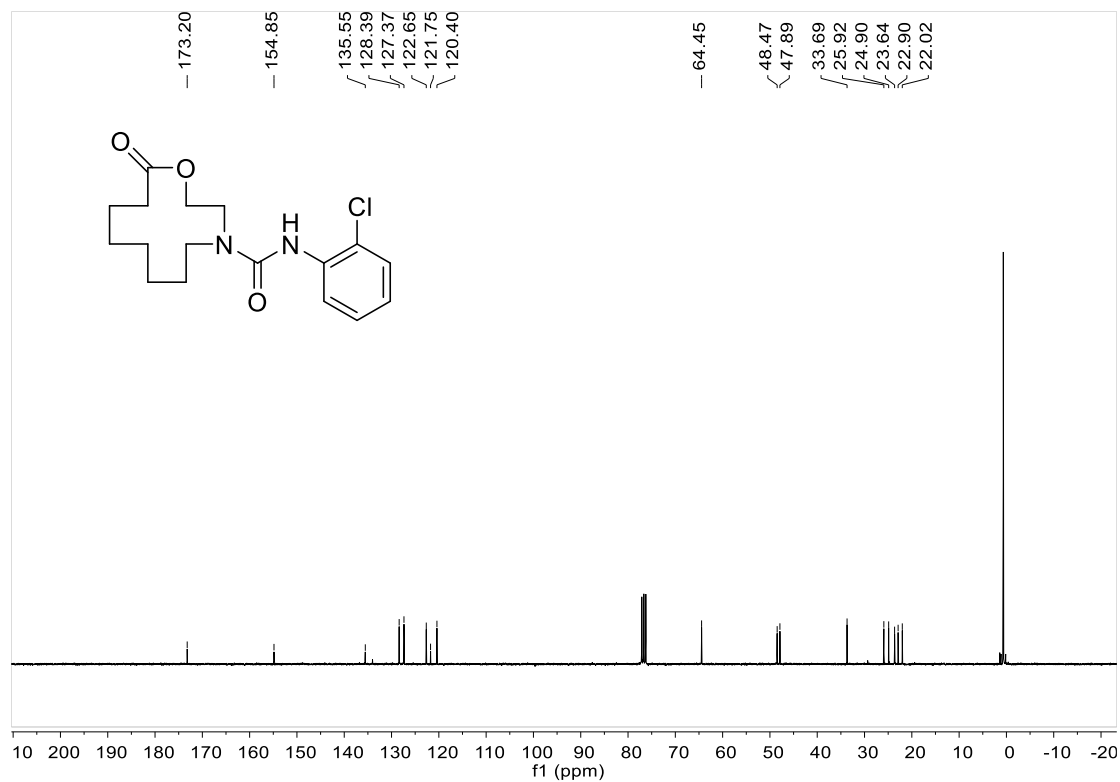
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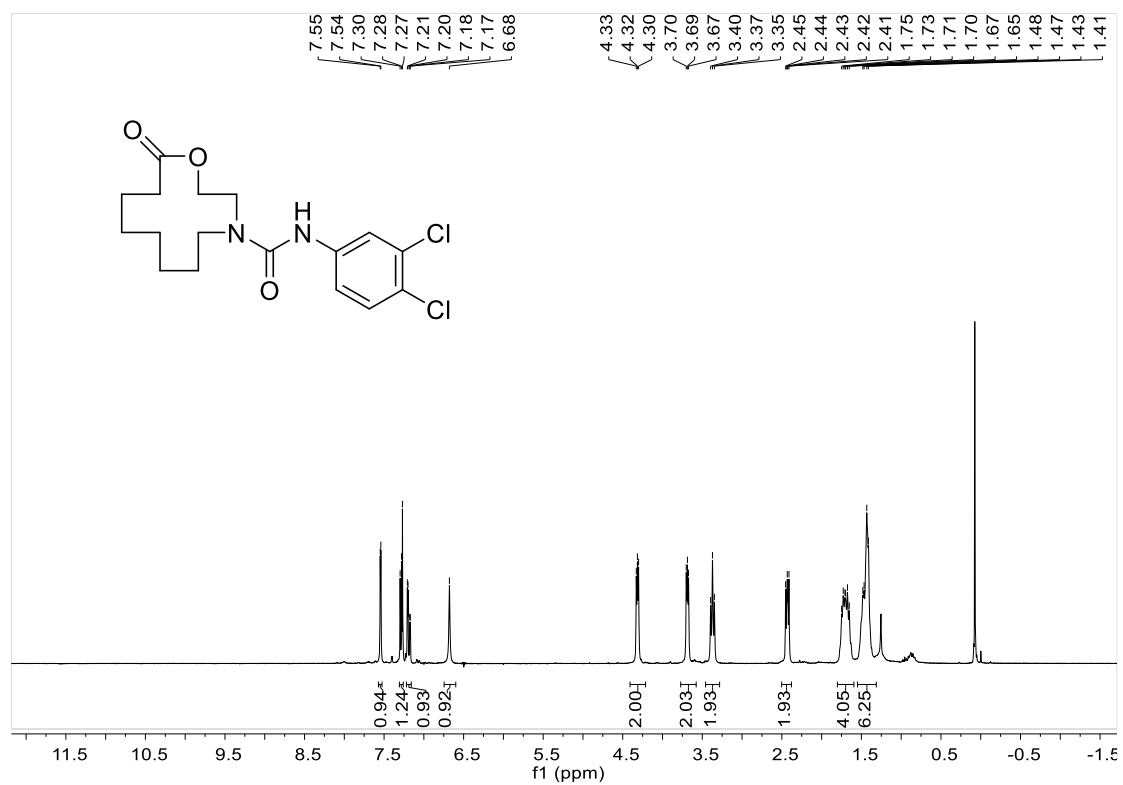
¹H NMR spectrum of D12-14 (300 MHz, CDCl₃)



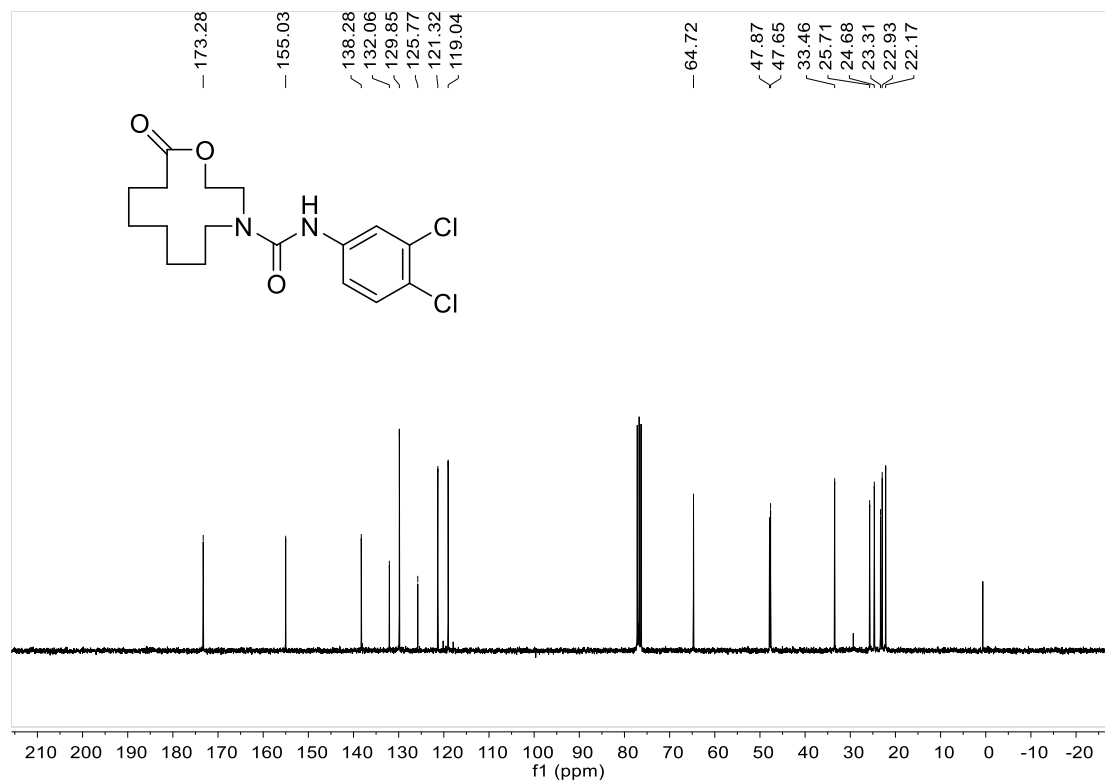
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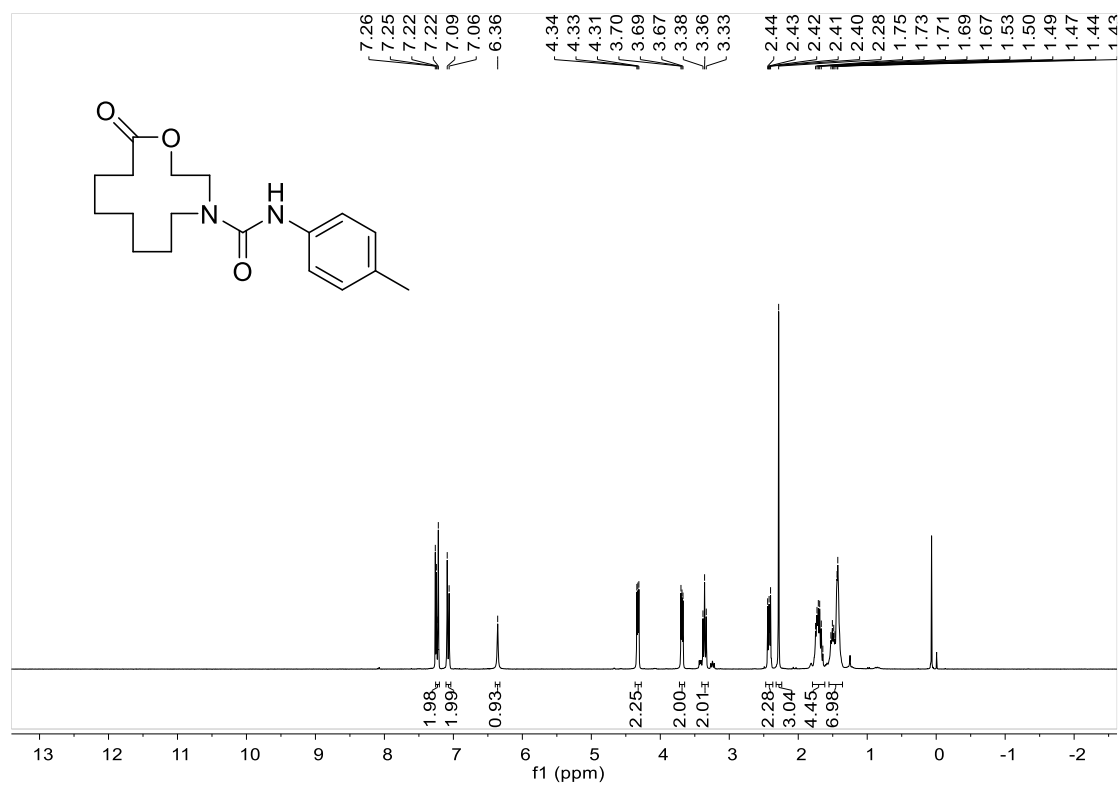
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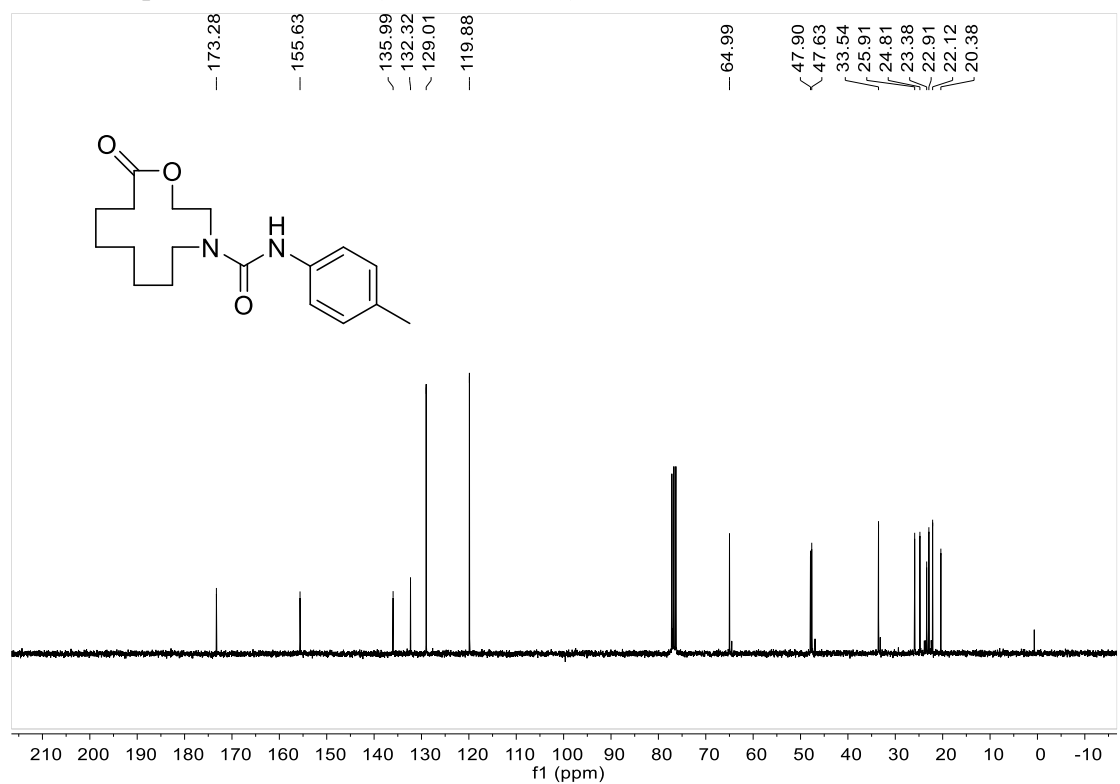
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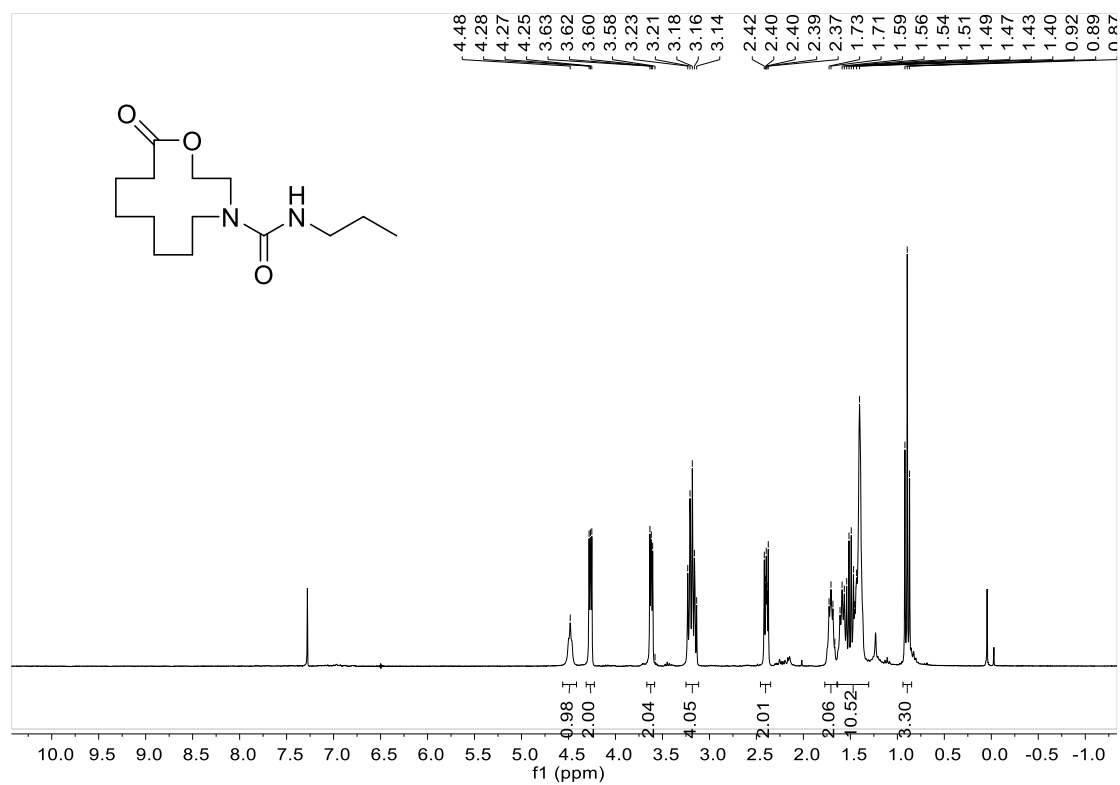
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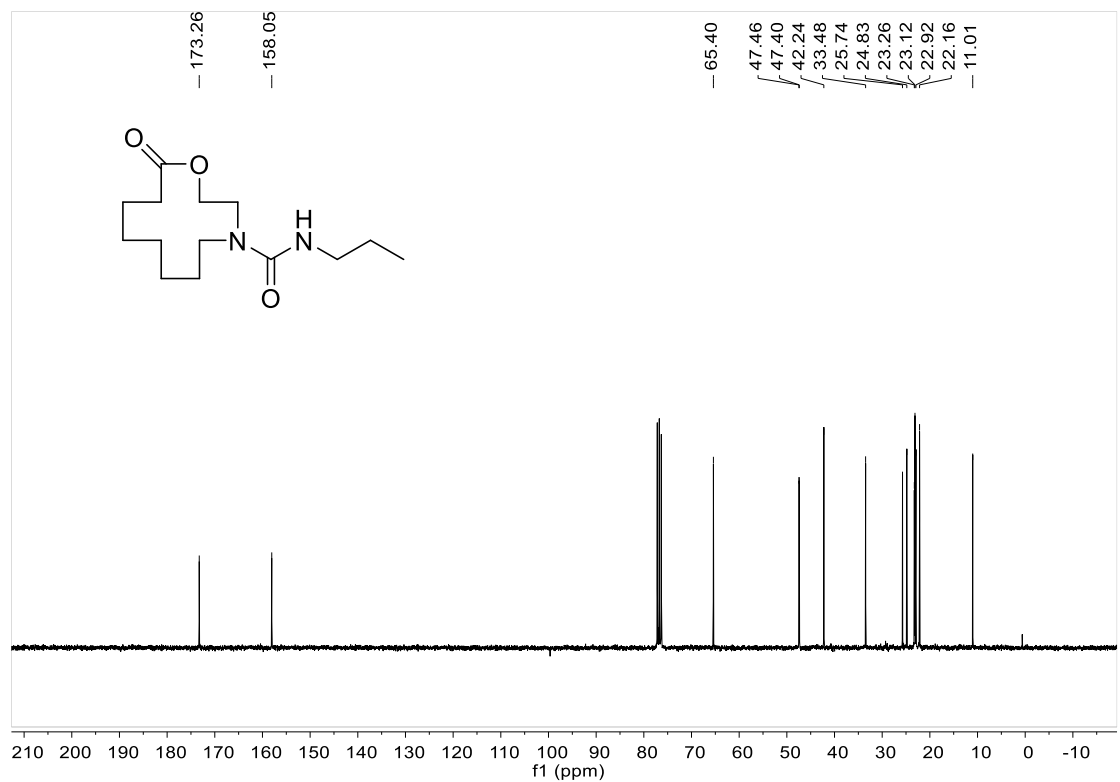
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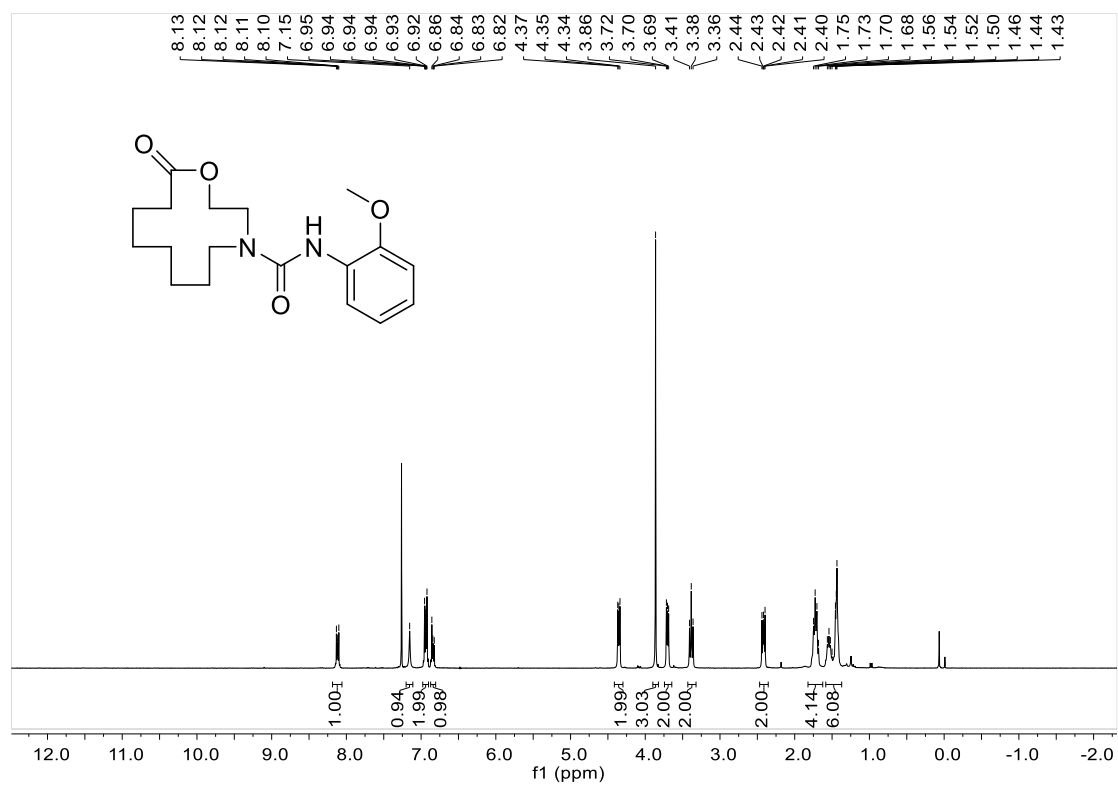
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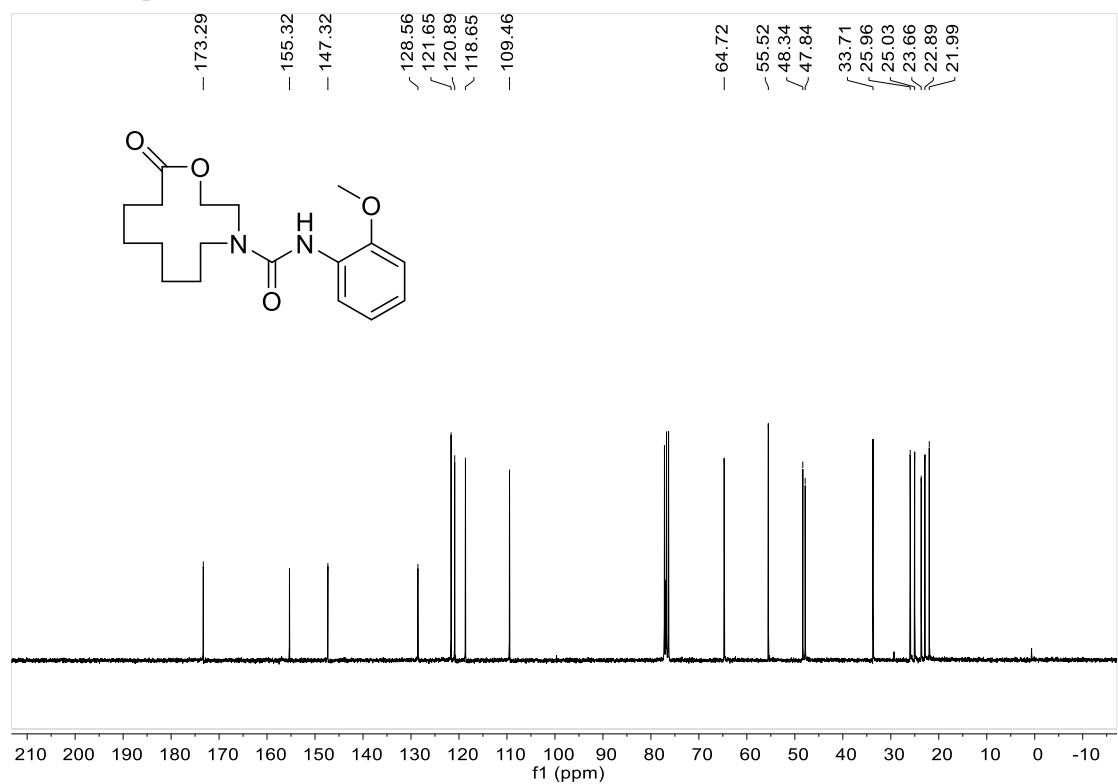
¹³C NMR spectrum of D12-17 (75 MHz, CDCl₃)



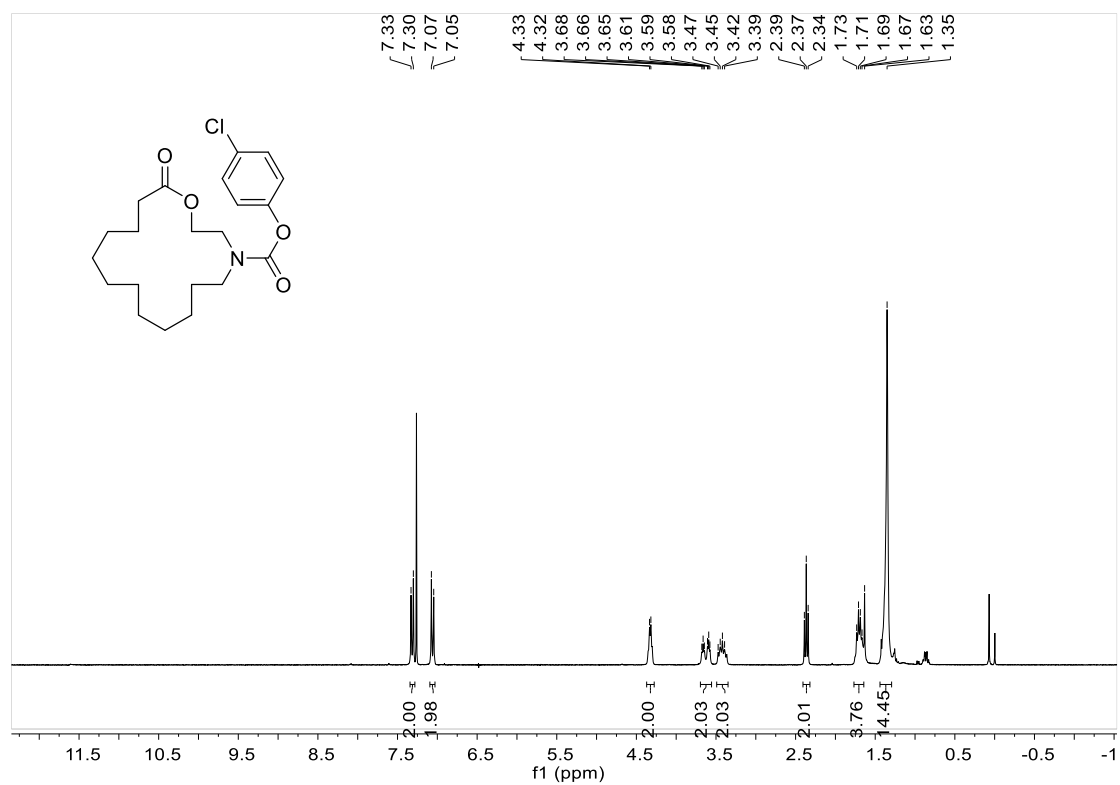
¹H NMR spectrum of D12-18 (300 MHz, CDCl₃)



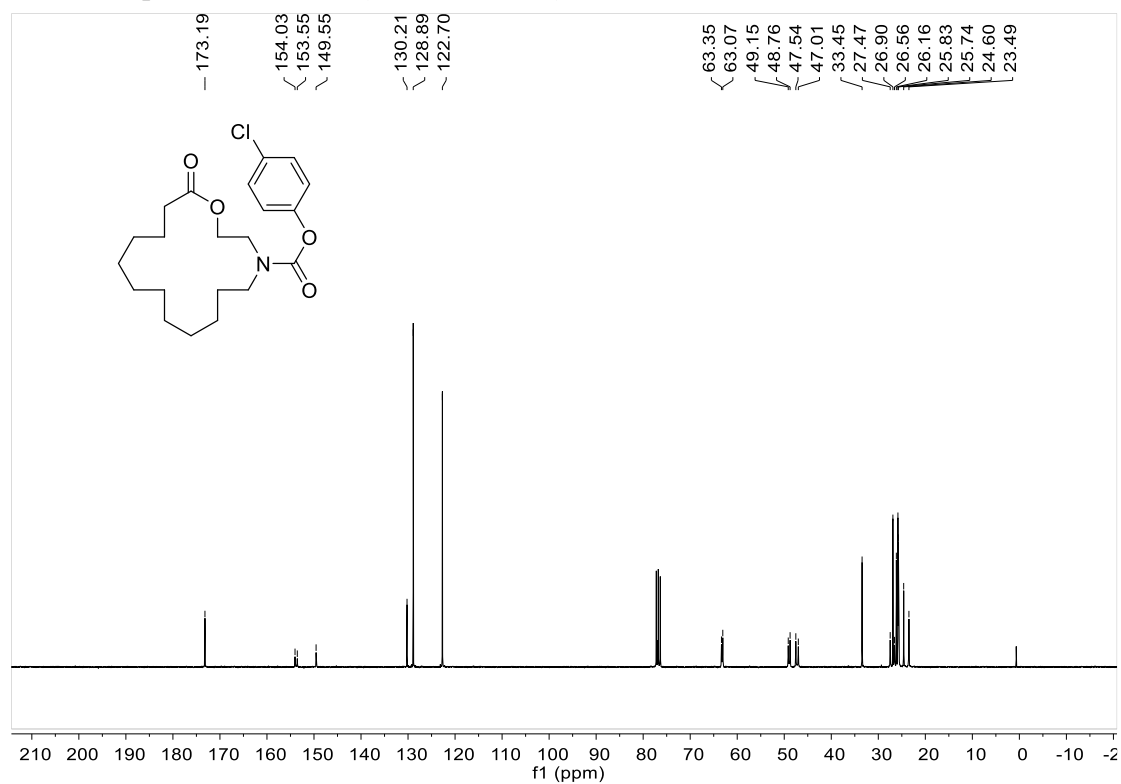
¹³C NMR spectrum of D12-18 (75 MHz, CDCl₃)



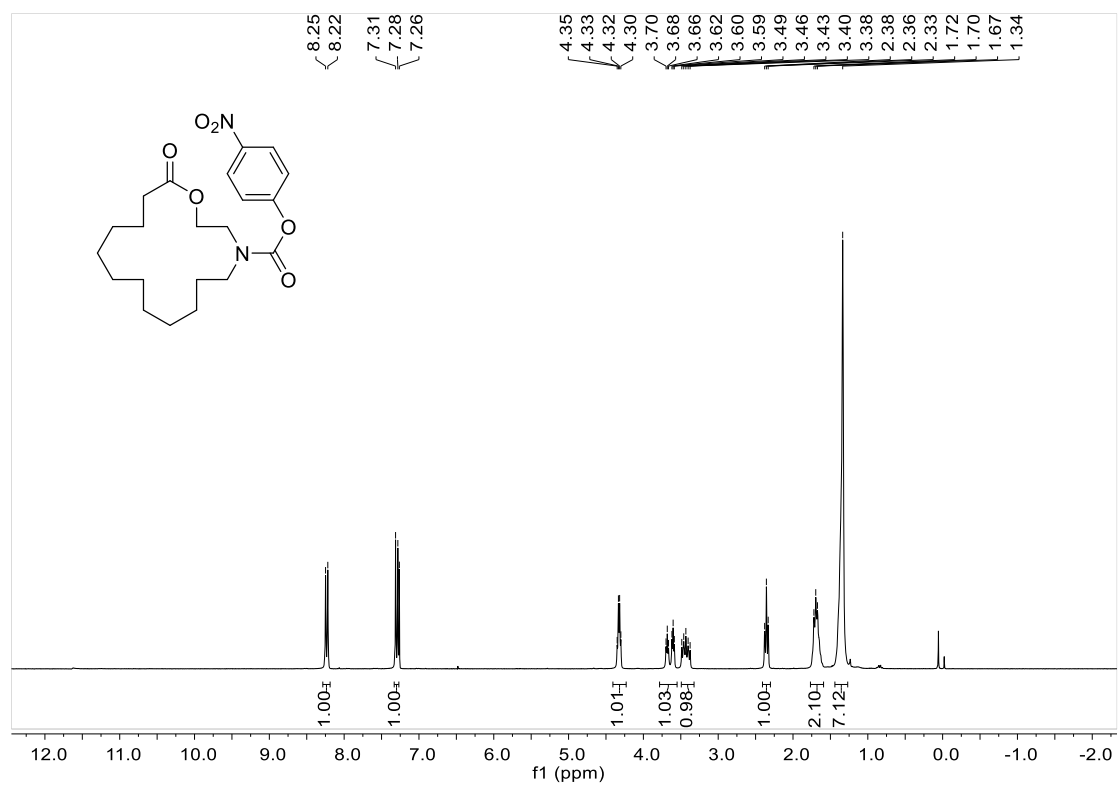
¹H NMR spectrum of D16-1 (300 MHz, CDCl₃)



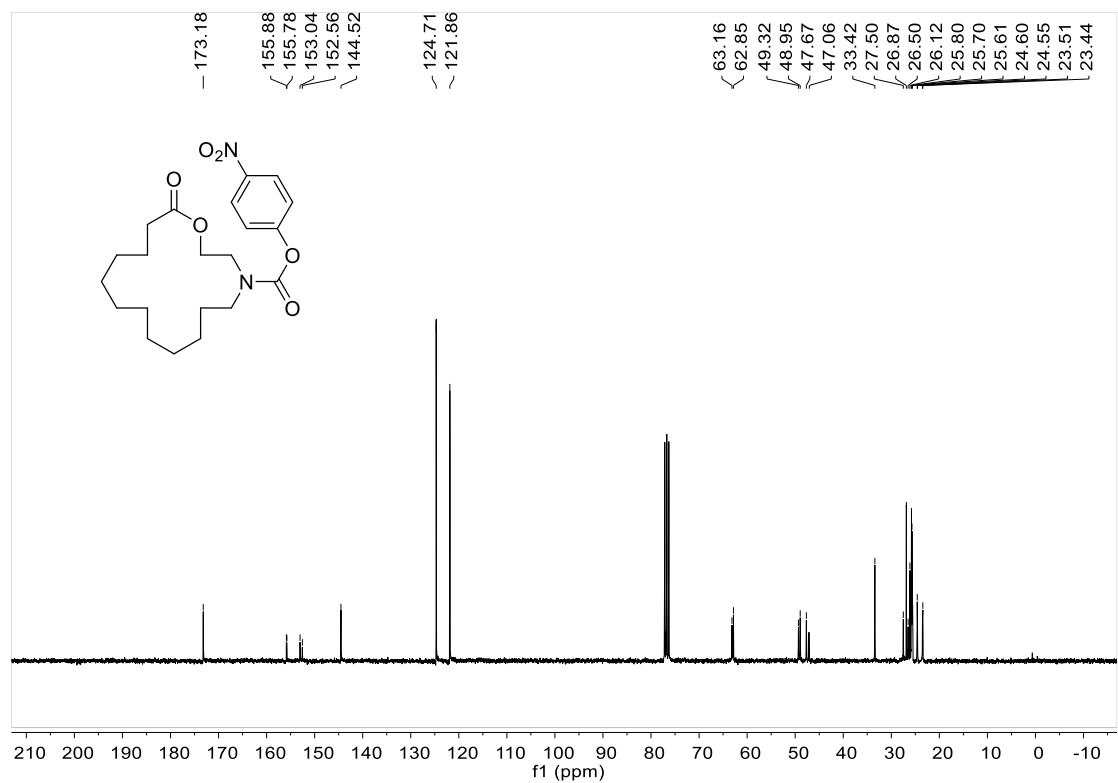
¹³C NMR spectrum of D16-1 (75 MHz, CDCl₃)



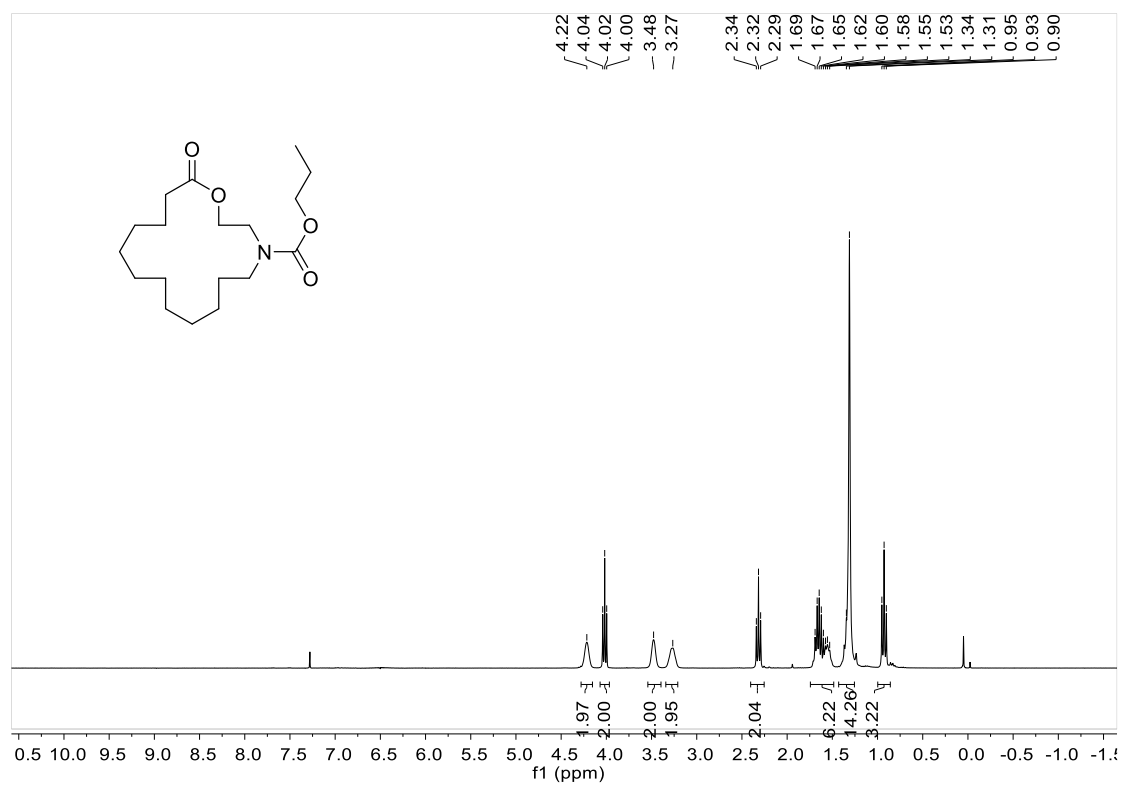
¹H NMR spectrum of D16-2 (300 MHz, CDCl₃)



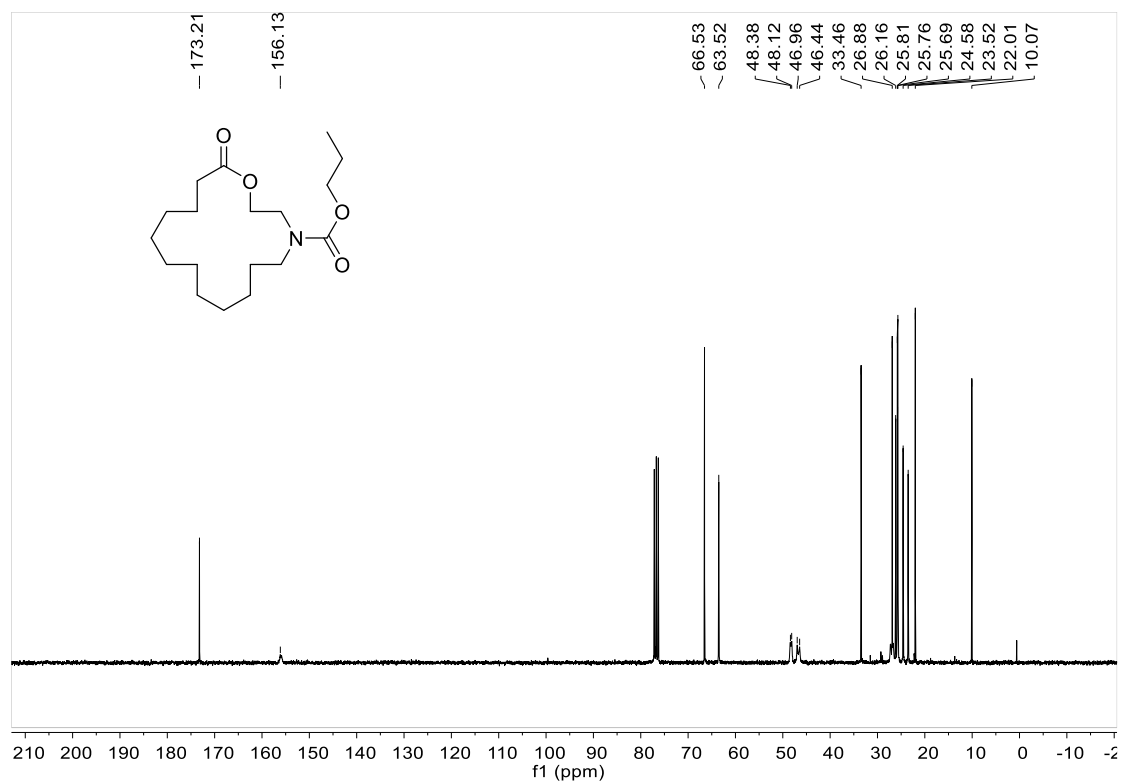
¹³C NMR spectrum of D16-2 (75 MHz, CDCl₃)



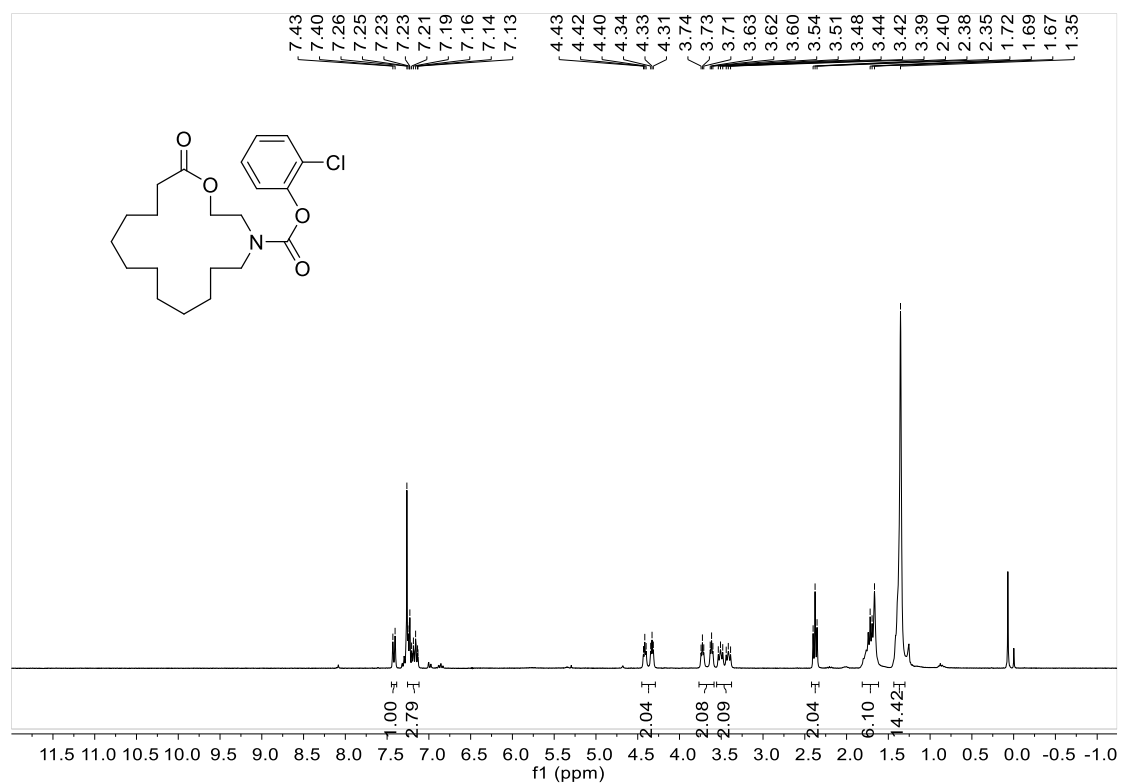
¹H NMR spectrum of D16-3 (300 MHz, CDCl₃)



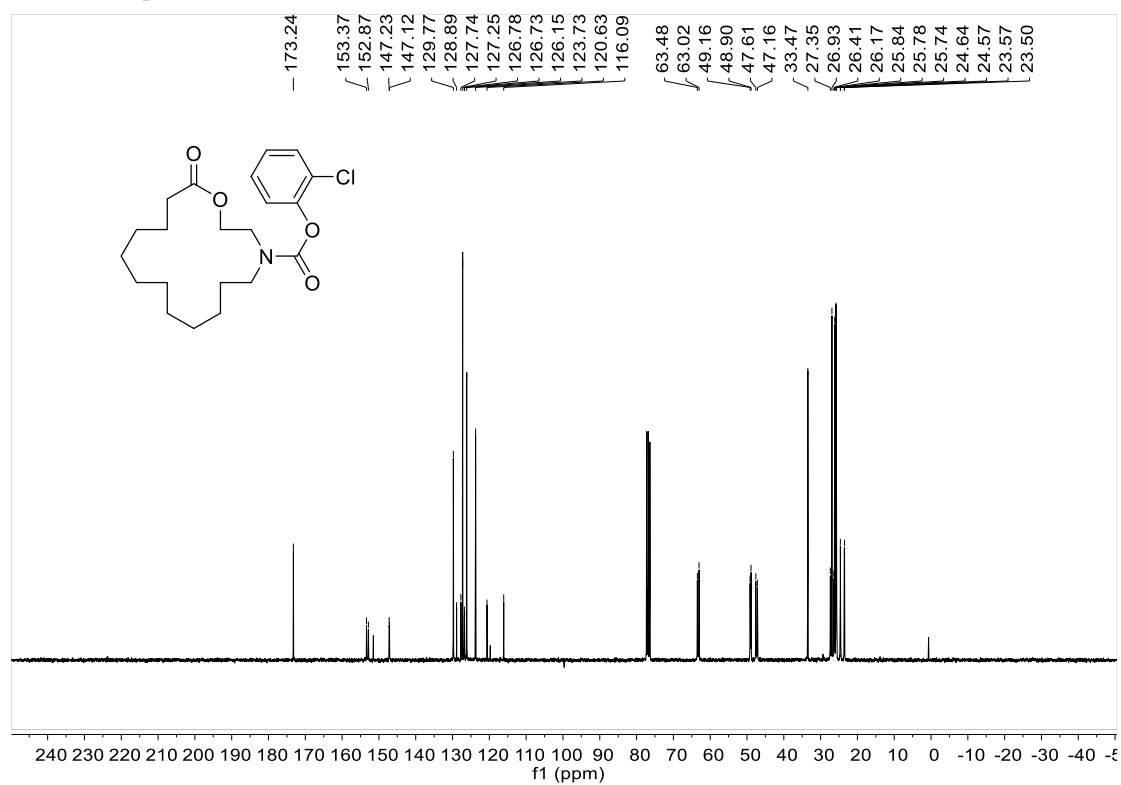
¹³C NMR spectrum of D16-3 (75 MHz, CDCl₃)



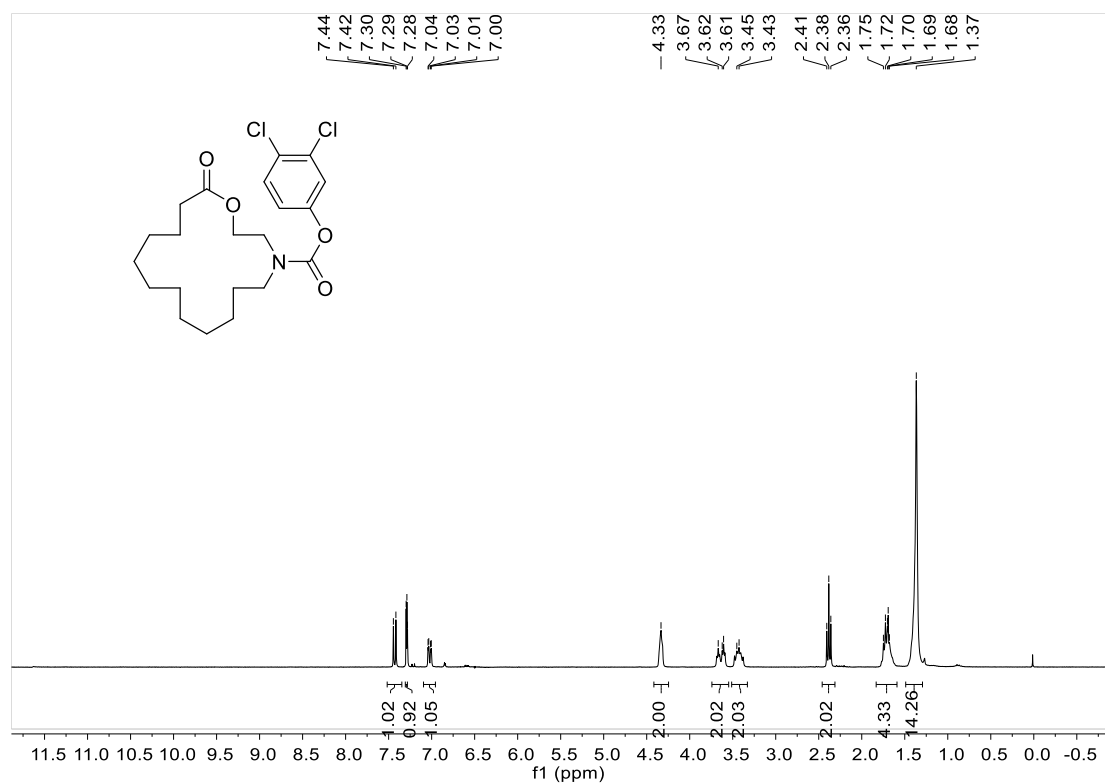
¹H NMR spectrum of D16-4 (300 MHz, CDCl₃)



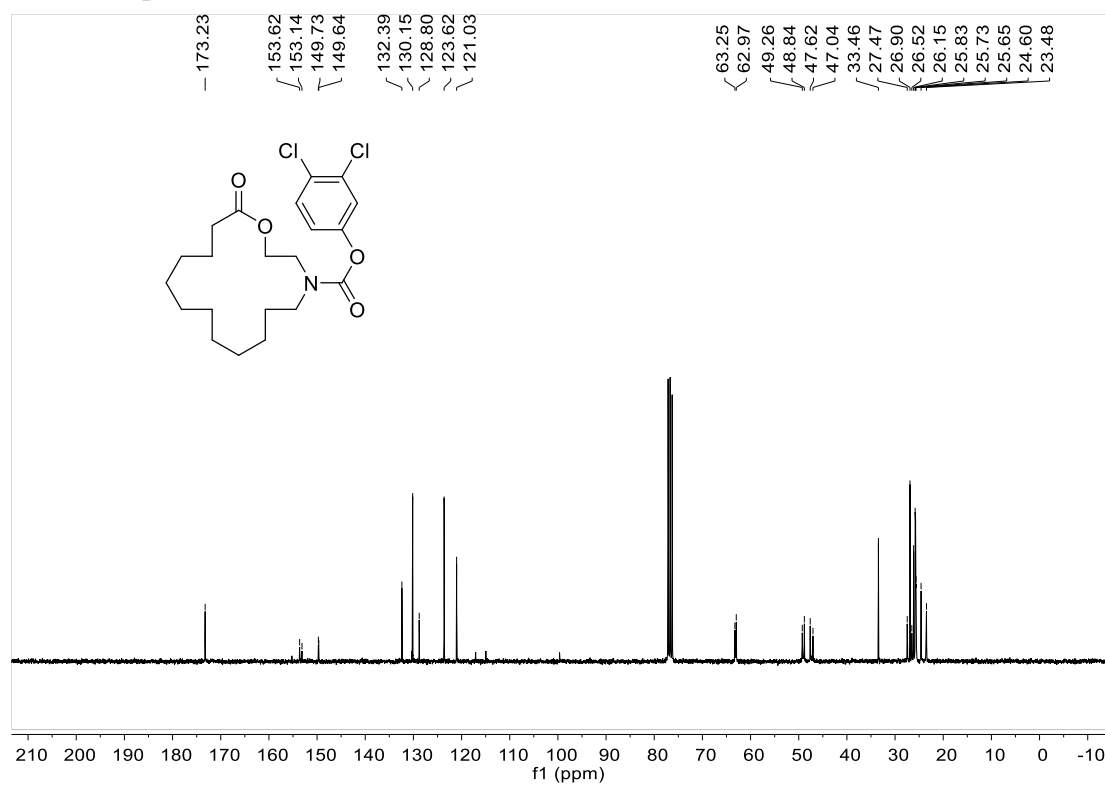
¹³C NMR spectrum of D16-4 (75 MHz, CDCl₃)



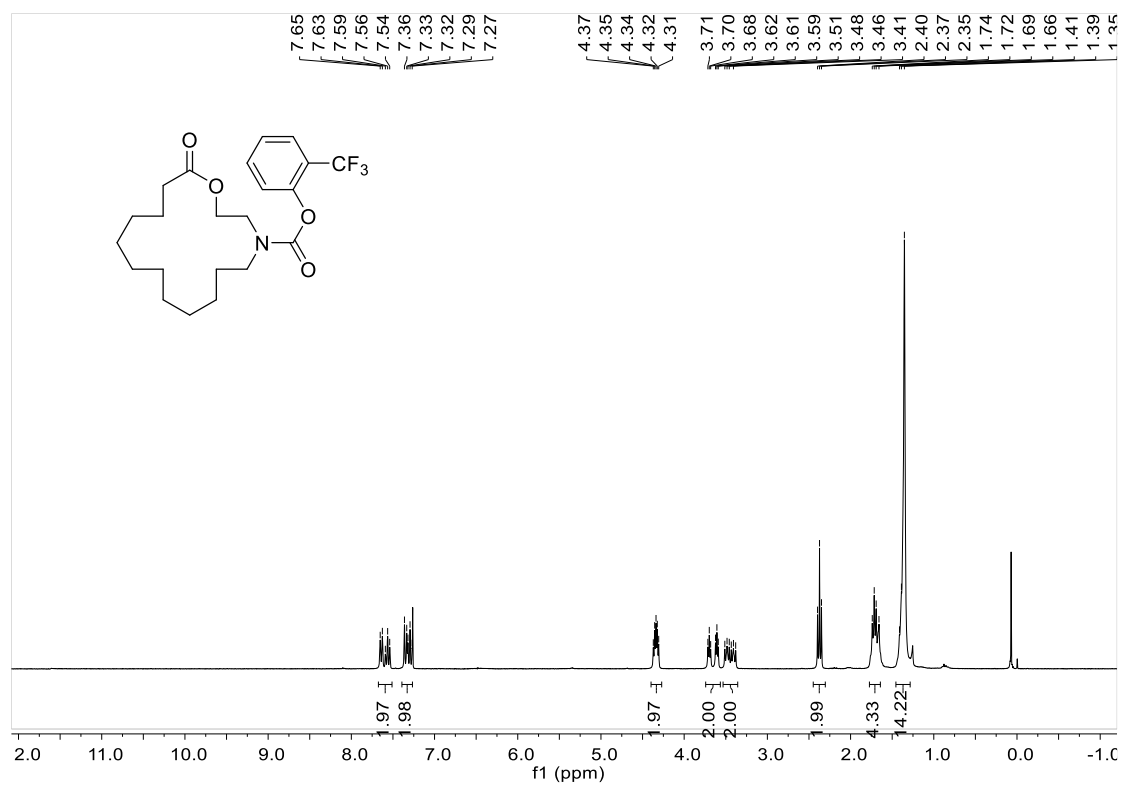
¹H NMR spectrum of D16-5 (300 MHz, CDCl₃)



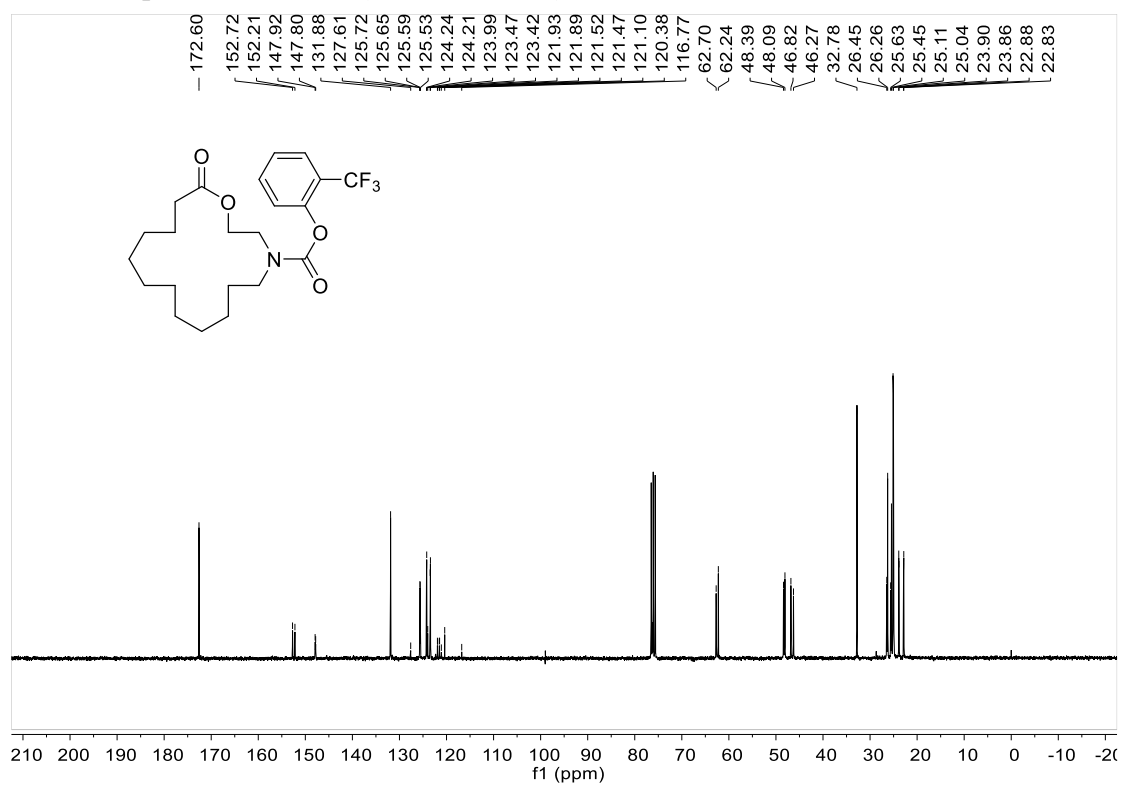
¹³C NMR spectrum of D16-5 (75 MHz, CDCl₃)



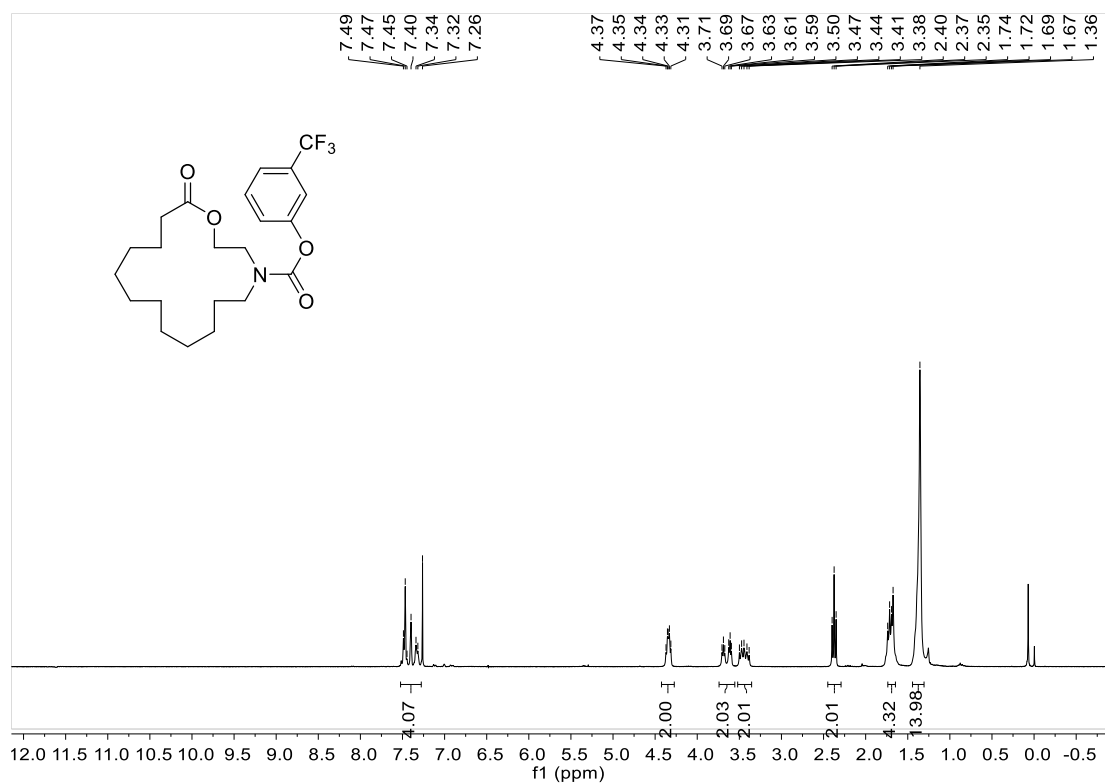
¹H NMR spectrum of D16-6 (300 MHz, CDCl₃)



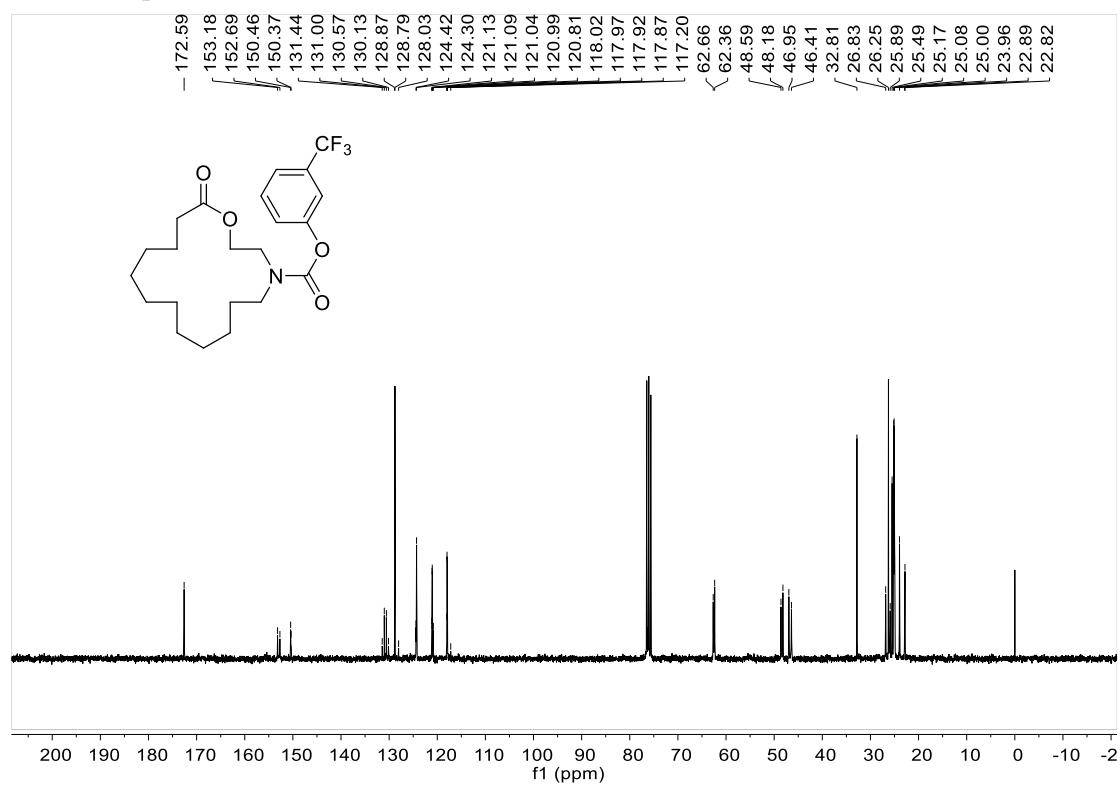
¹³C NMR spectrum of D16-6 (75 MHz, CDCl₃)



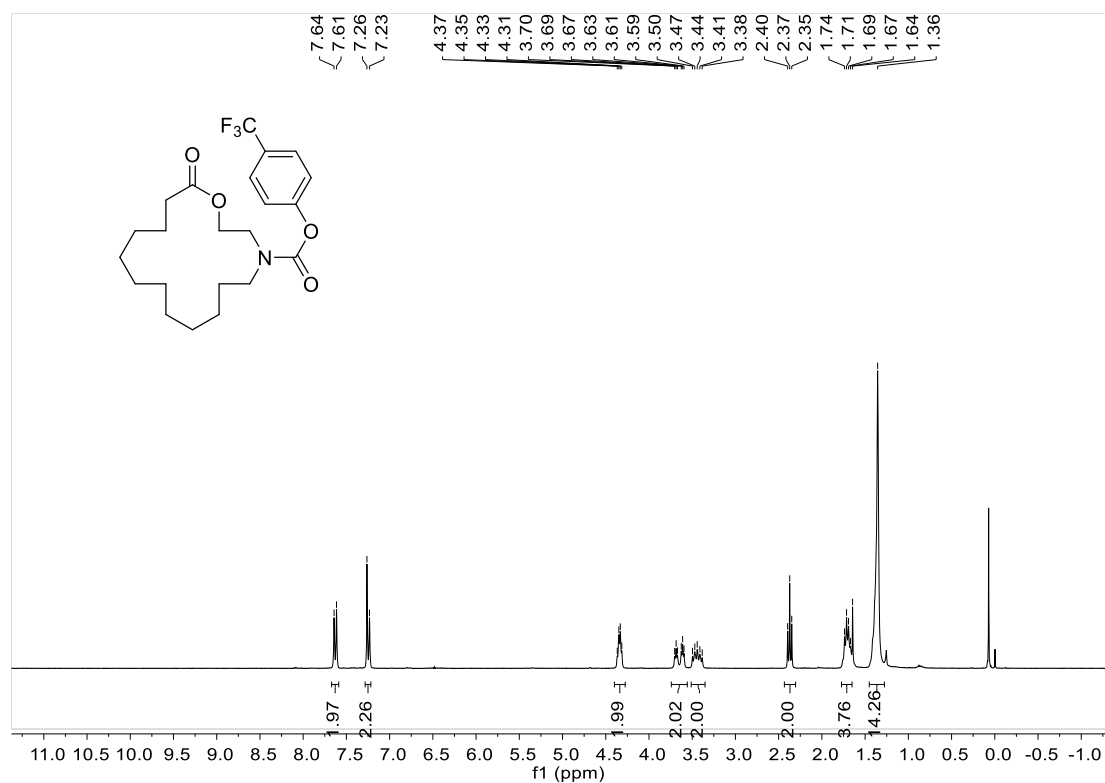
¹H NMR spectrum of D16-7 (300 MHz, CDCl₃)



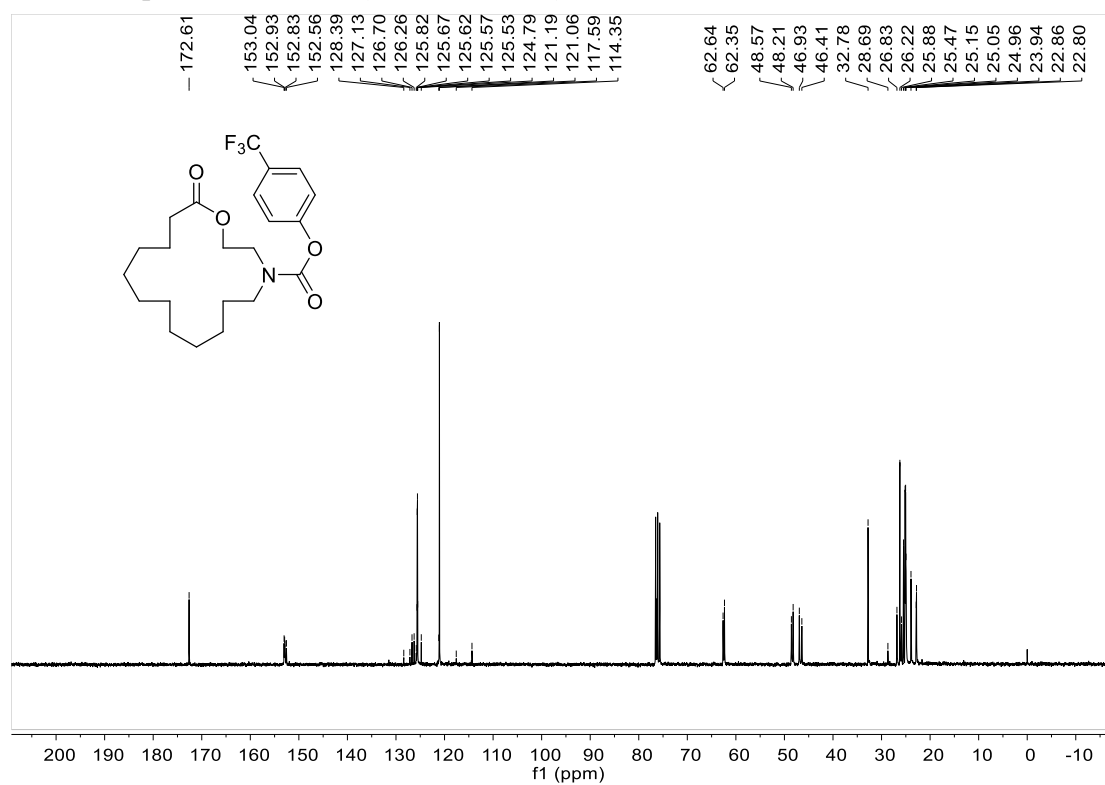
¹³C NMR spectrum of D16-7 (75 MHz, CDCl₃)



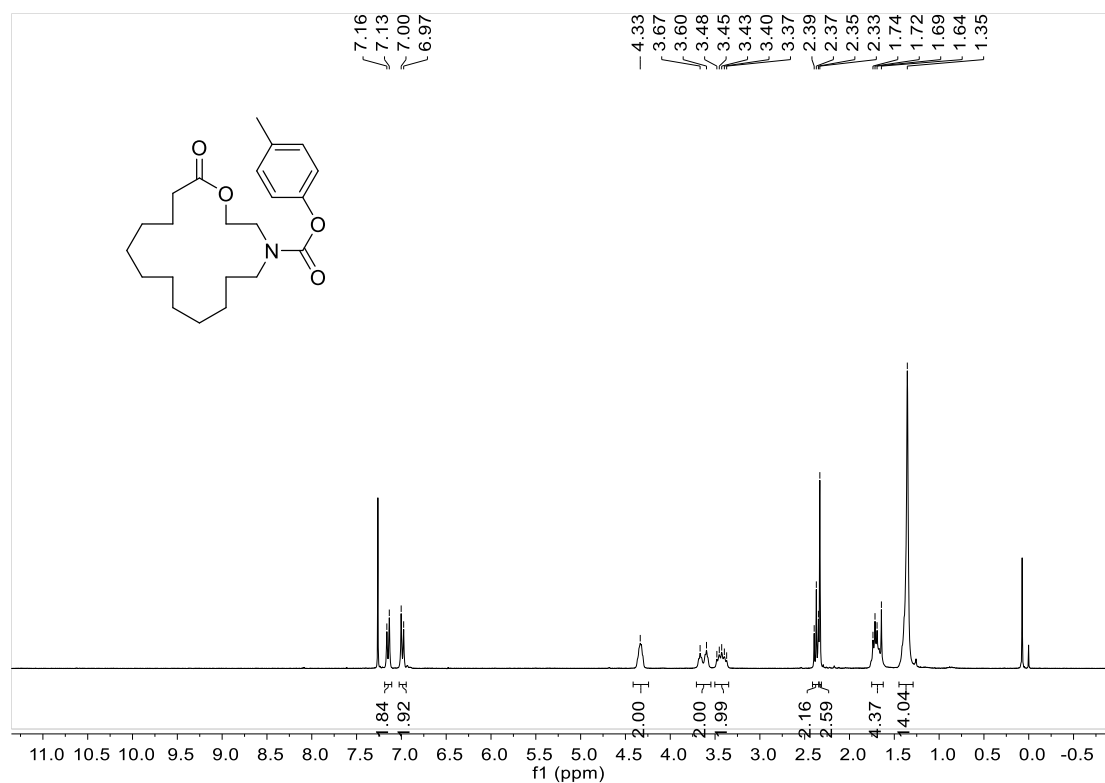
¹H NMR spectrum of D16-8 (300 MHz, CDCl₃)



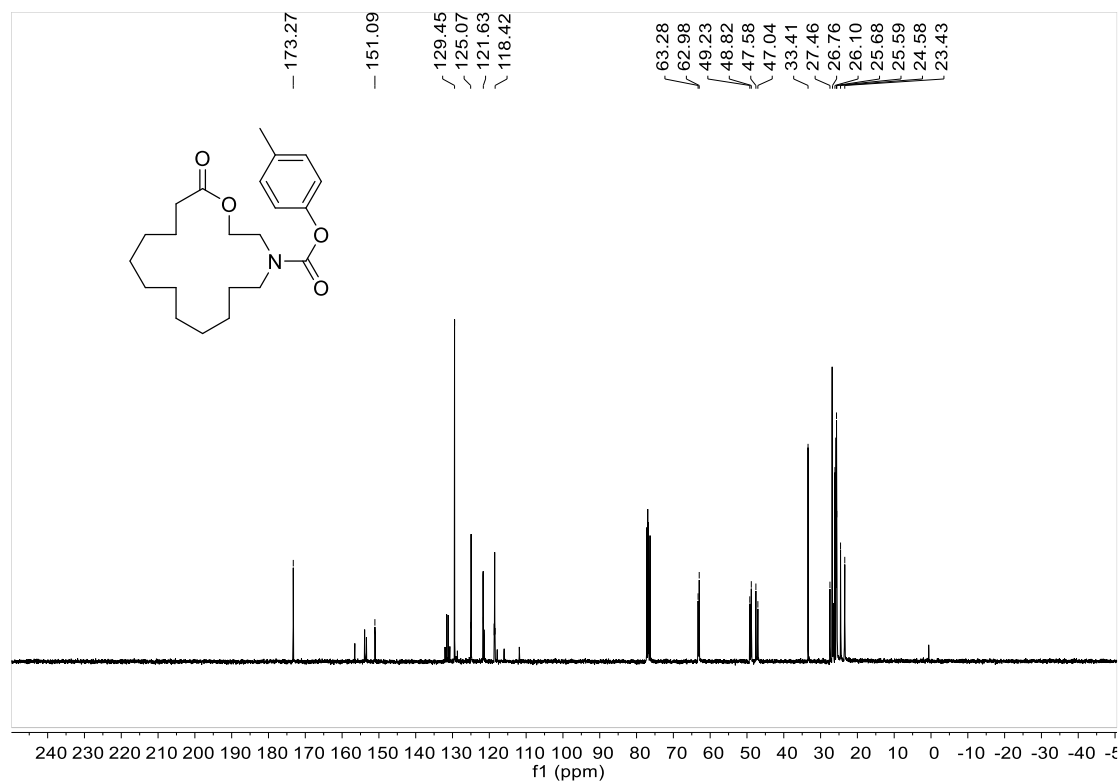
¹³C NMR spectrum of D16-8 (75 MHz, CDCl₃)



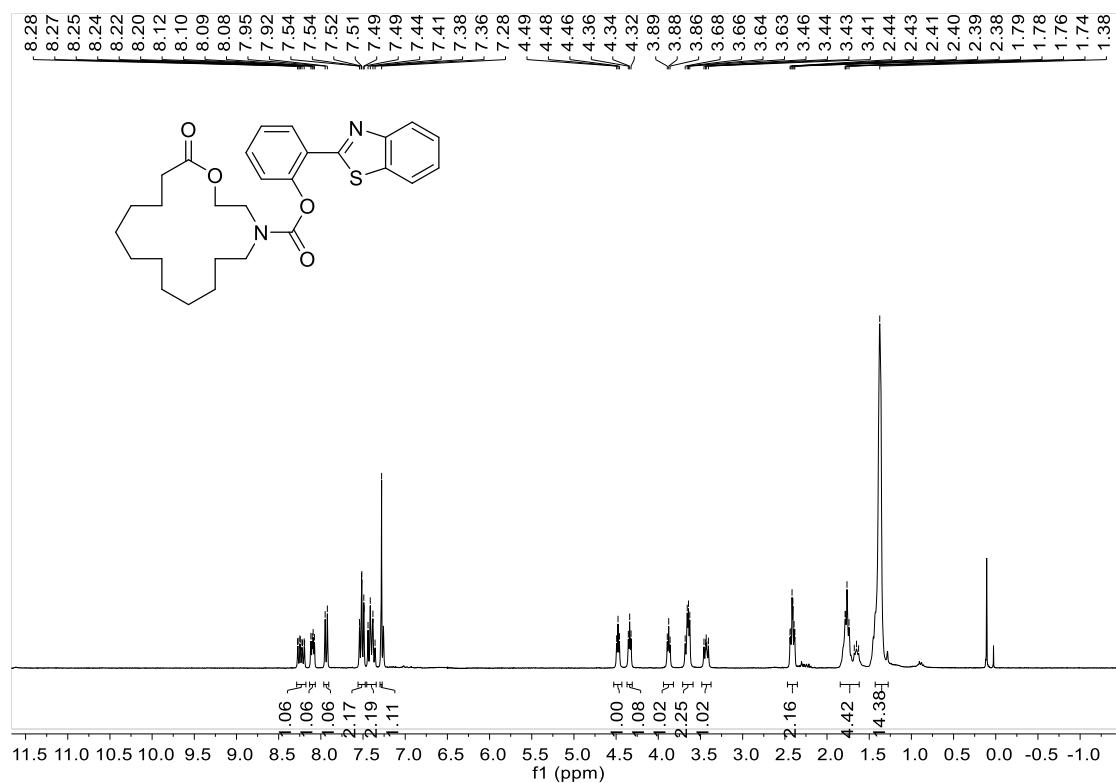
¹H NMR spectrum of D16-9 (300 MHz, CDCl₃)



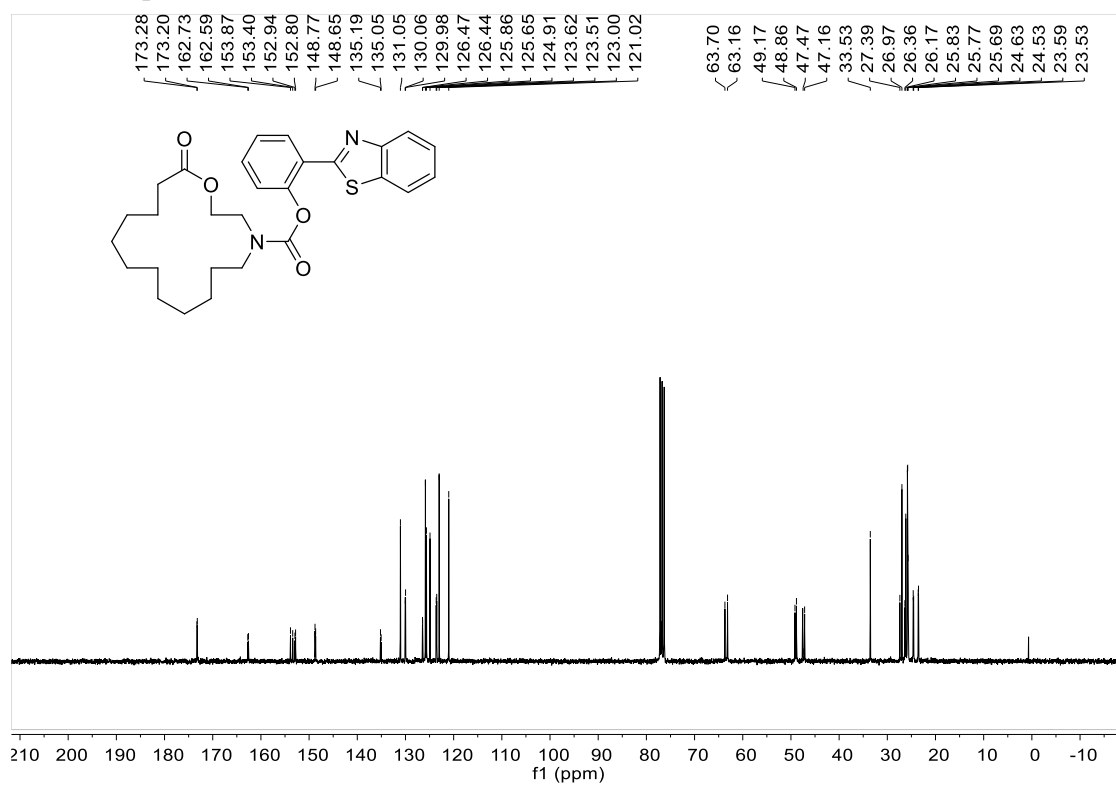
¹³C NMR spectrum of D16-9 (75 MHz, CDCl₃)



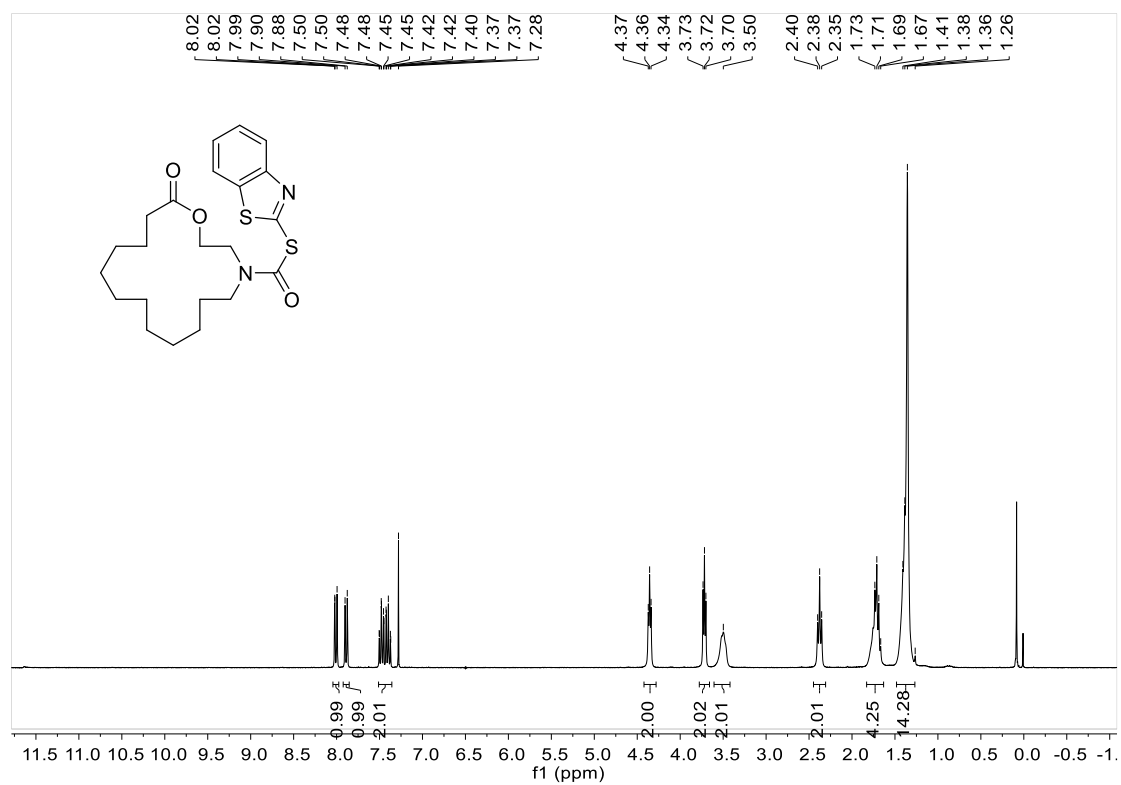
¹H NMR spectrum of D16-10 (300 MHz, CDCl₃)



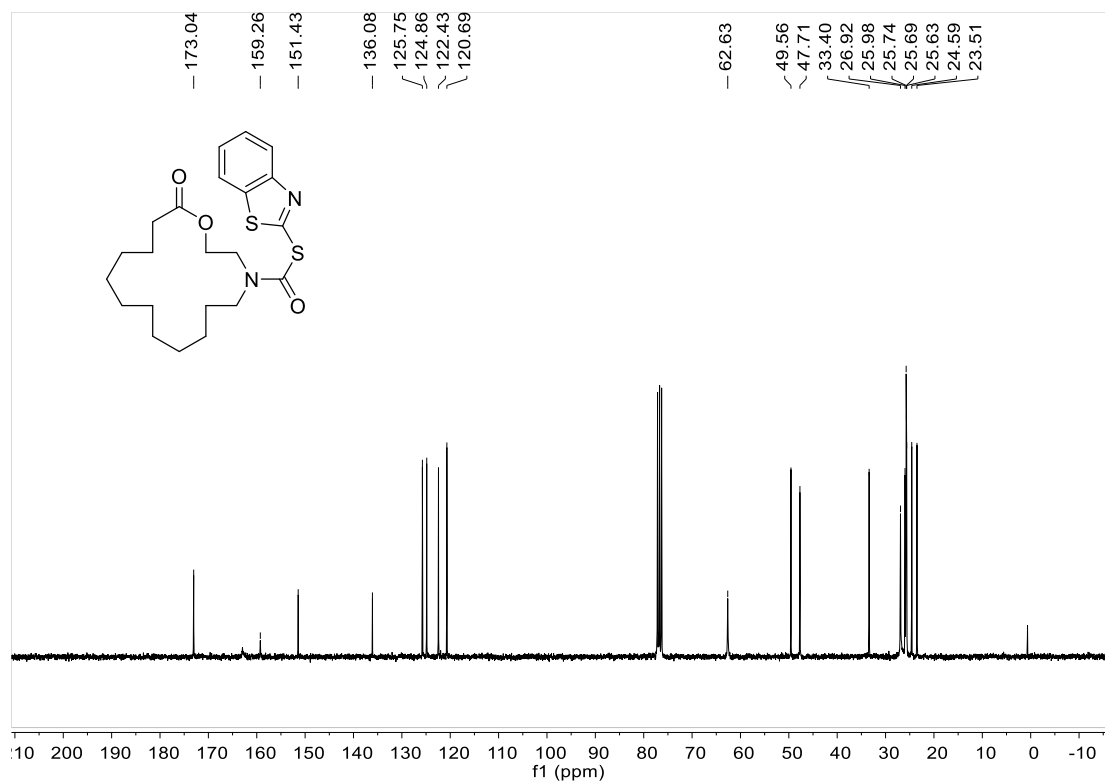
¹³C NMR spectrum of D16-10 (75 MHz, CDCl₃)



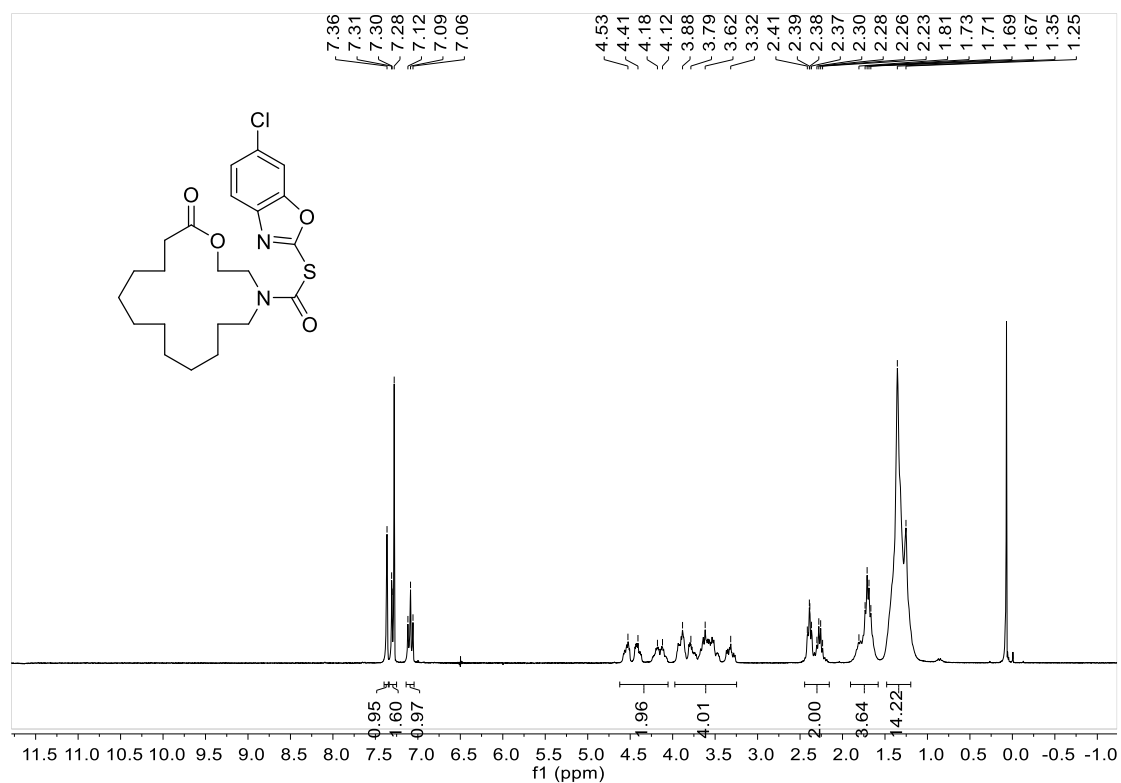
¹H NMR spectrum of D16-11 (300 MHz, CDCl₃)



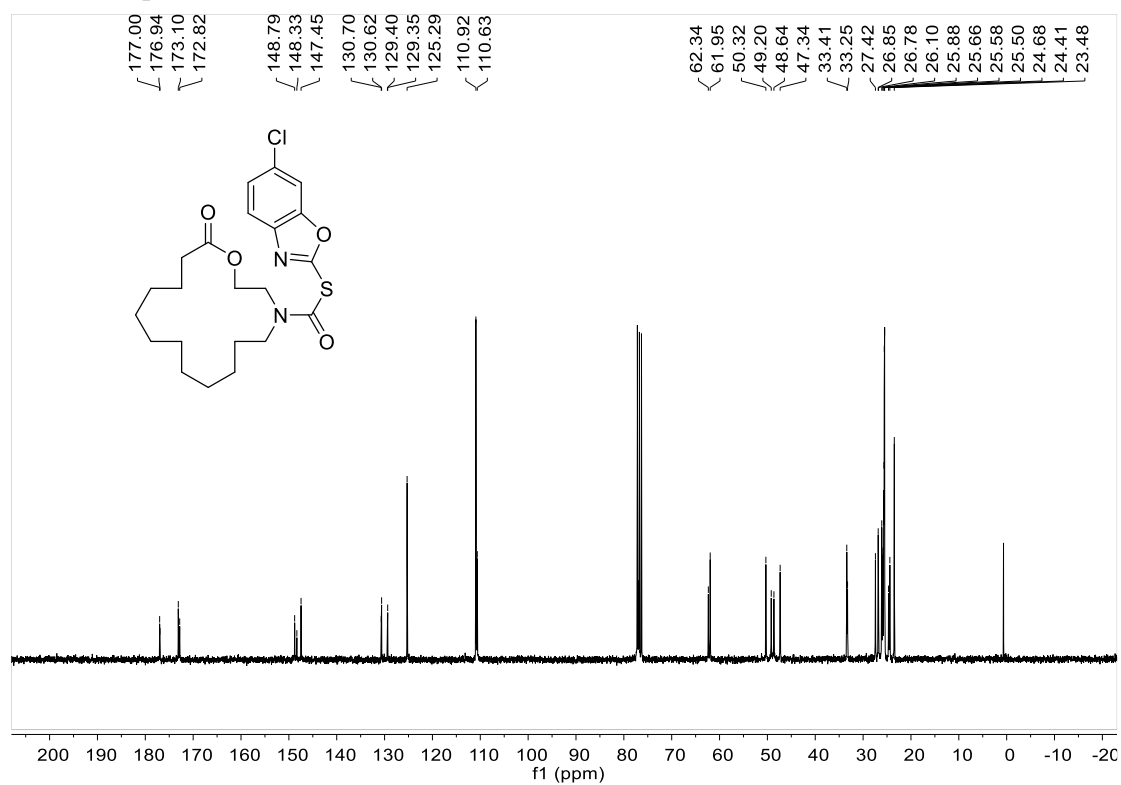
¹³C NMR spectrum of D16-11 (75 MHz, CDCl₃)



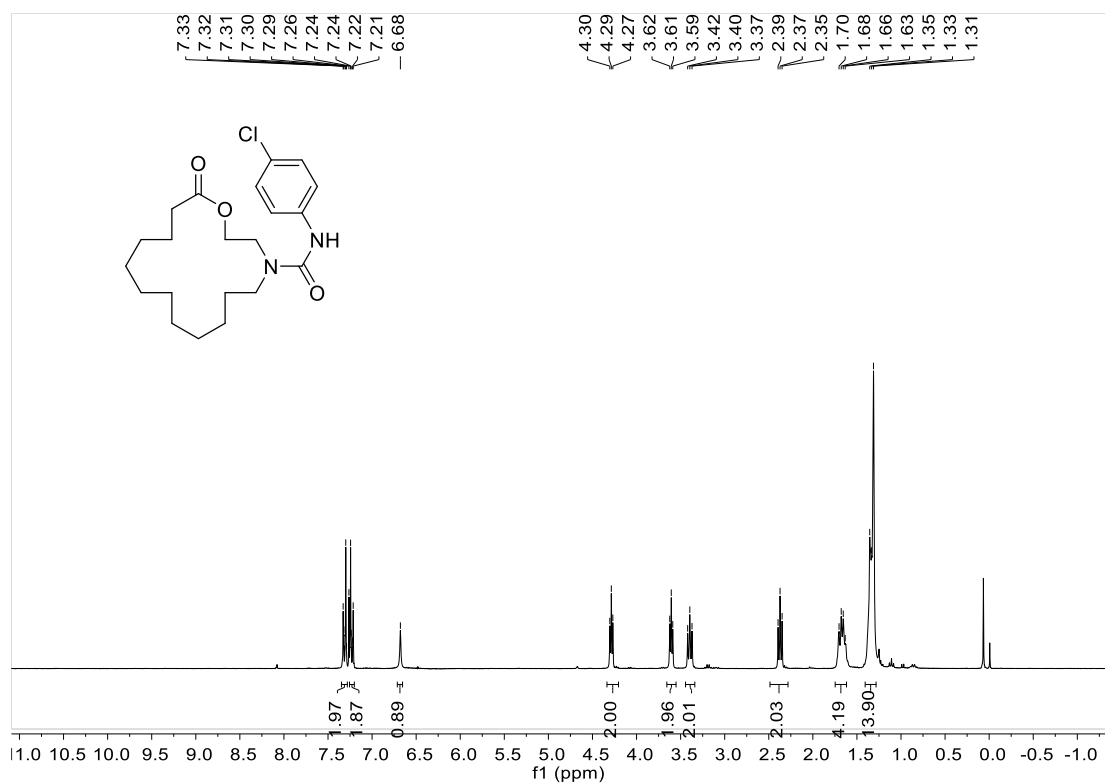
¹H NMR spectrum of D16-12 (300 MHz, CDCl₃)



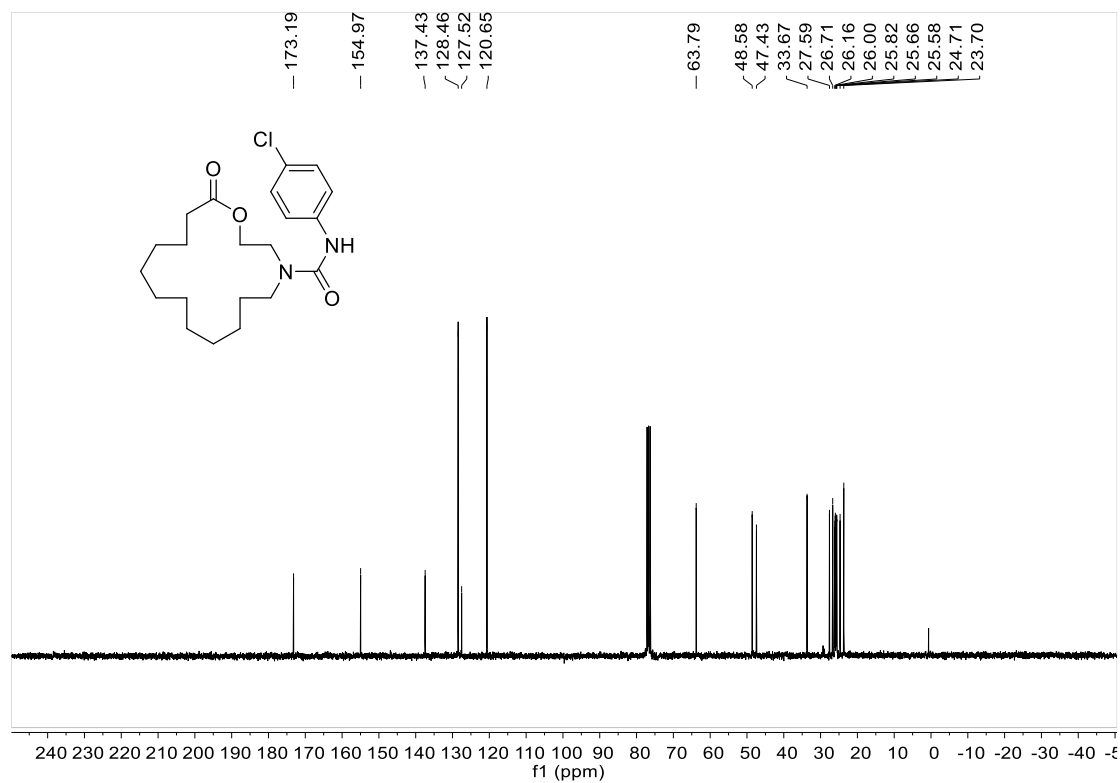
¹³C NMR spectrum of D16-12 (75 MHz, CDCl₃)



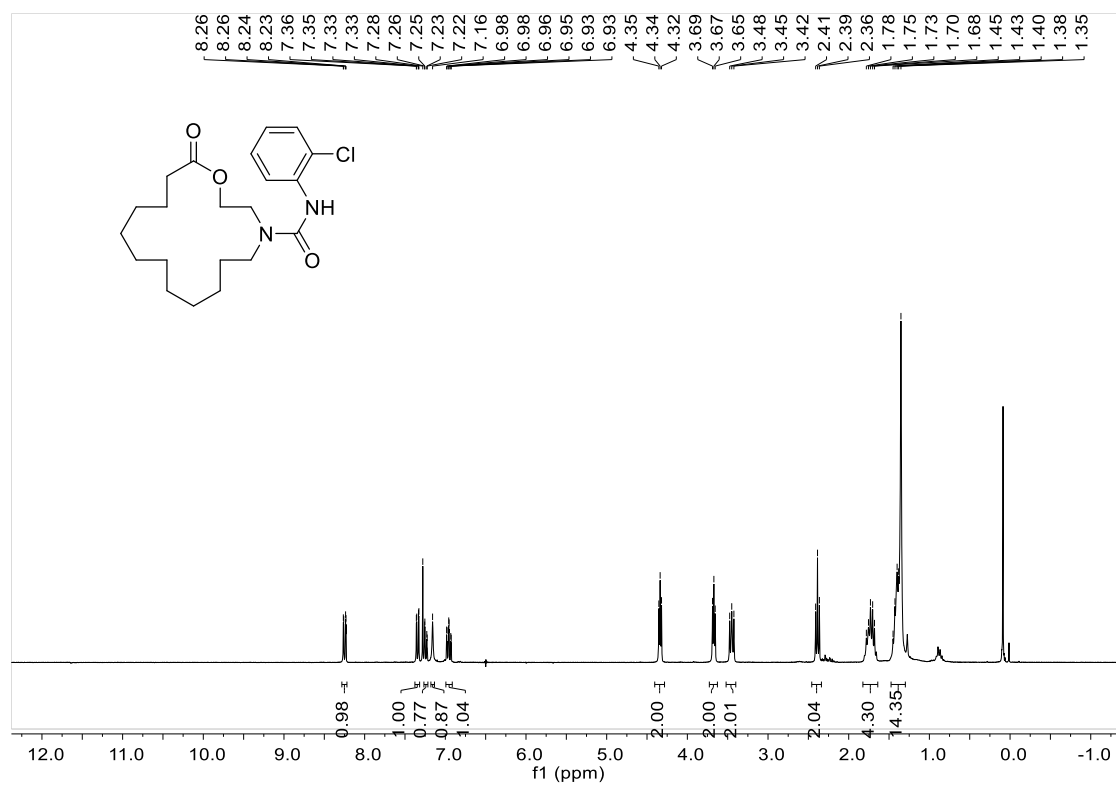
¹H NMR spectrum of D16-13 (300 MHz, CDCl₃)



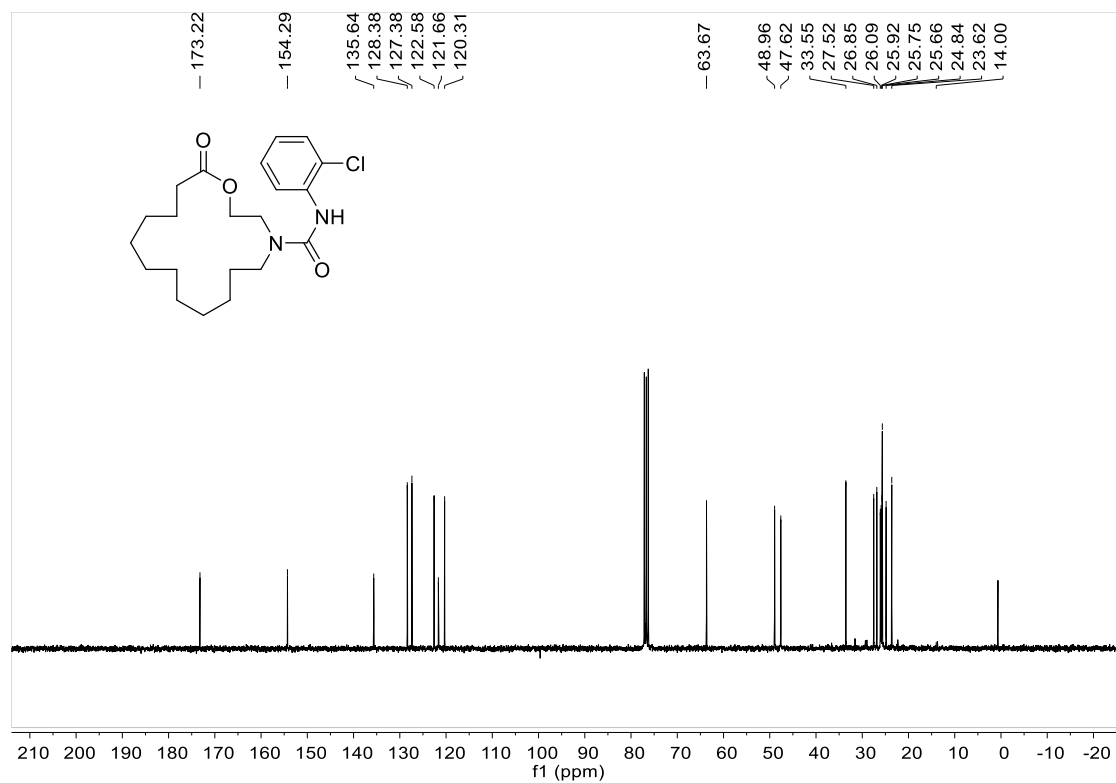
¹³C NMR spectrum of D16-13 (75 MHz, CDCl₃)



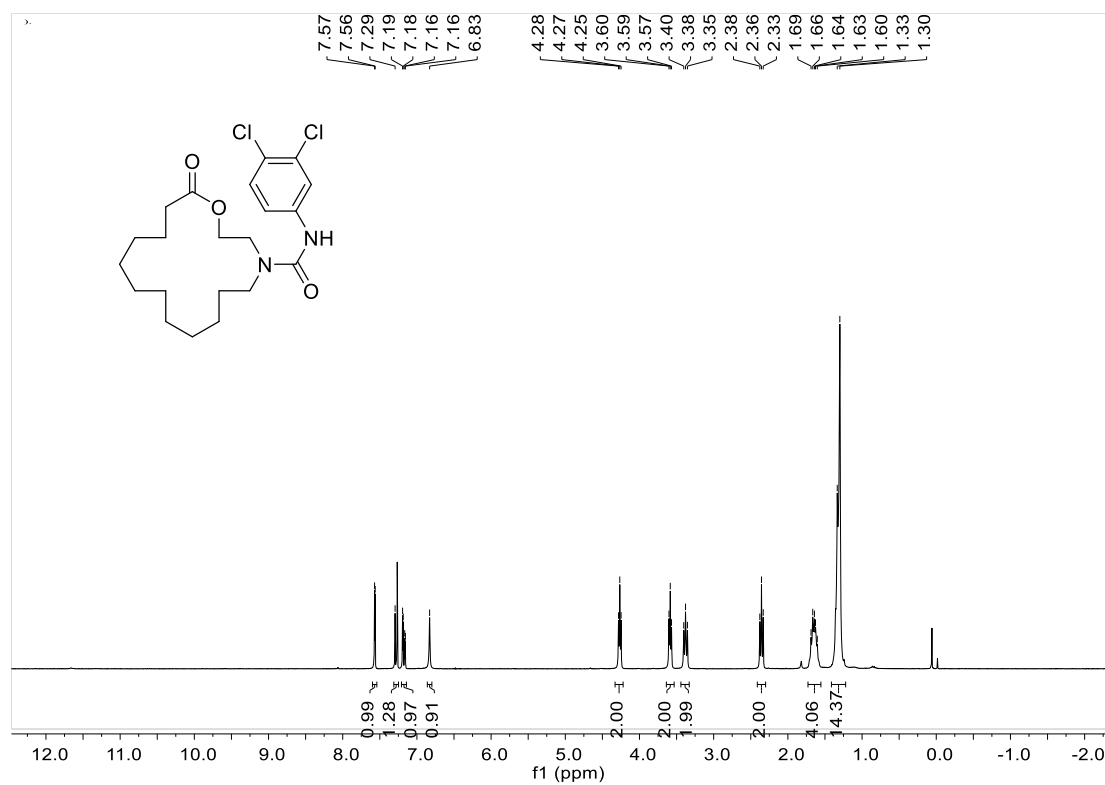
¹H NMR spectrum of D16-14 (300 MHz, CDCl₃)



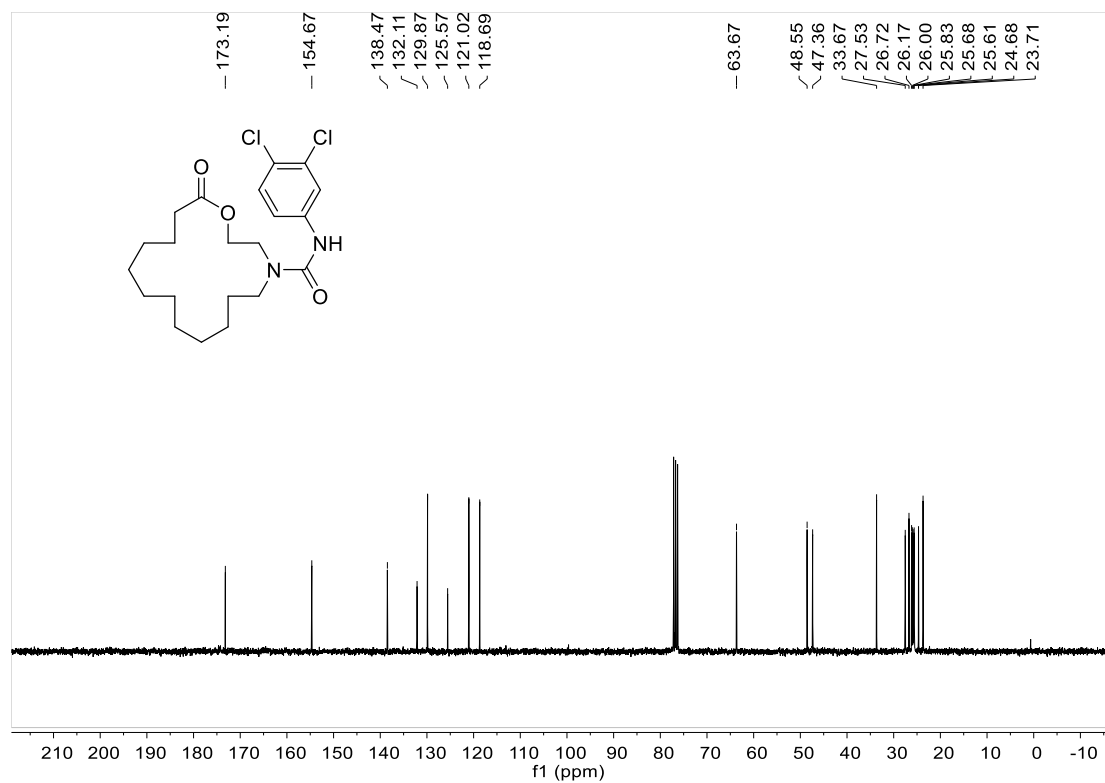
¹³C NMR spectrum of D16-14 (75 MHz, CDCl₃)



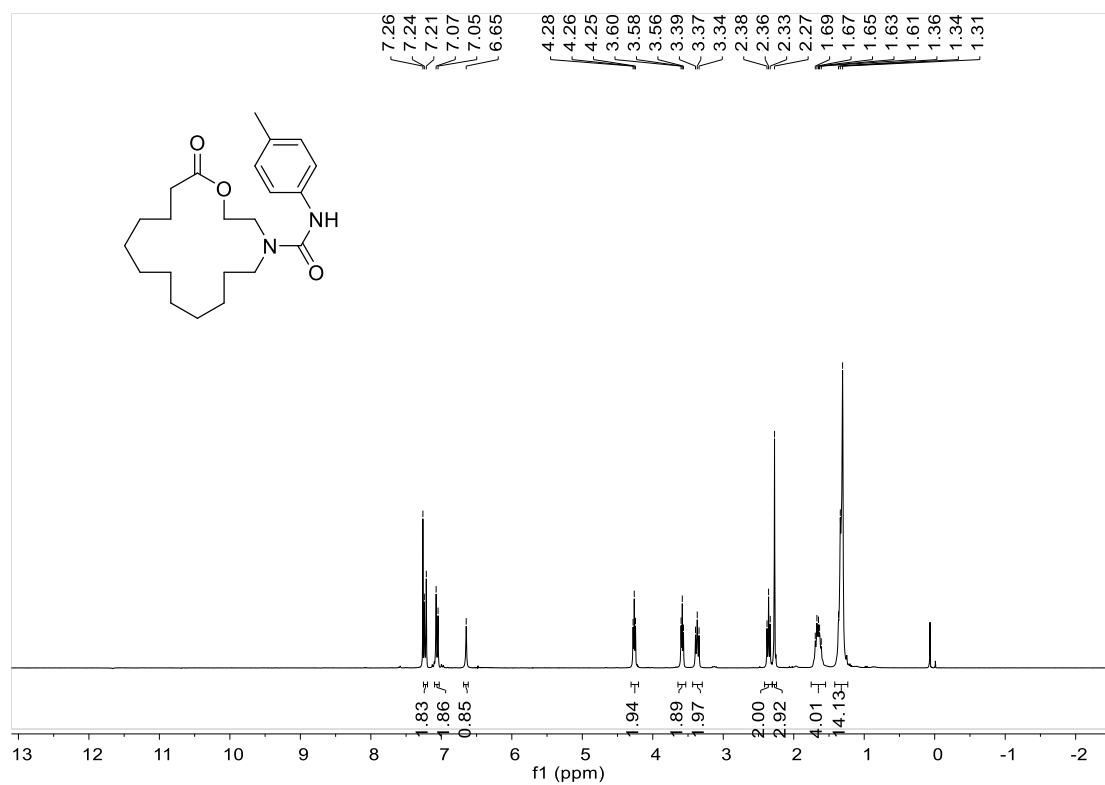
¹H NMR spectrum of D16-15 (300 MHz, CDCl₃)



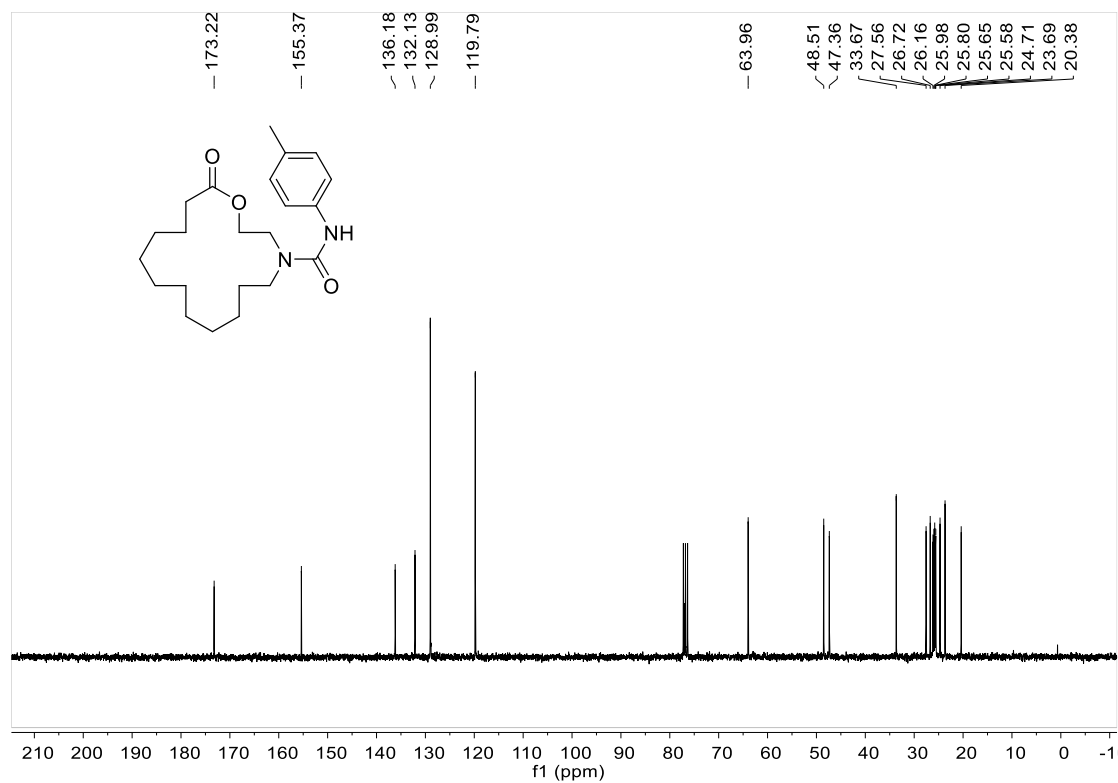
¹³C NMR spectrum of D16-15 (75 MHz, CDCl₃)



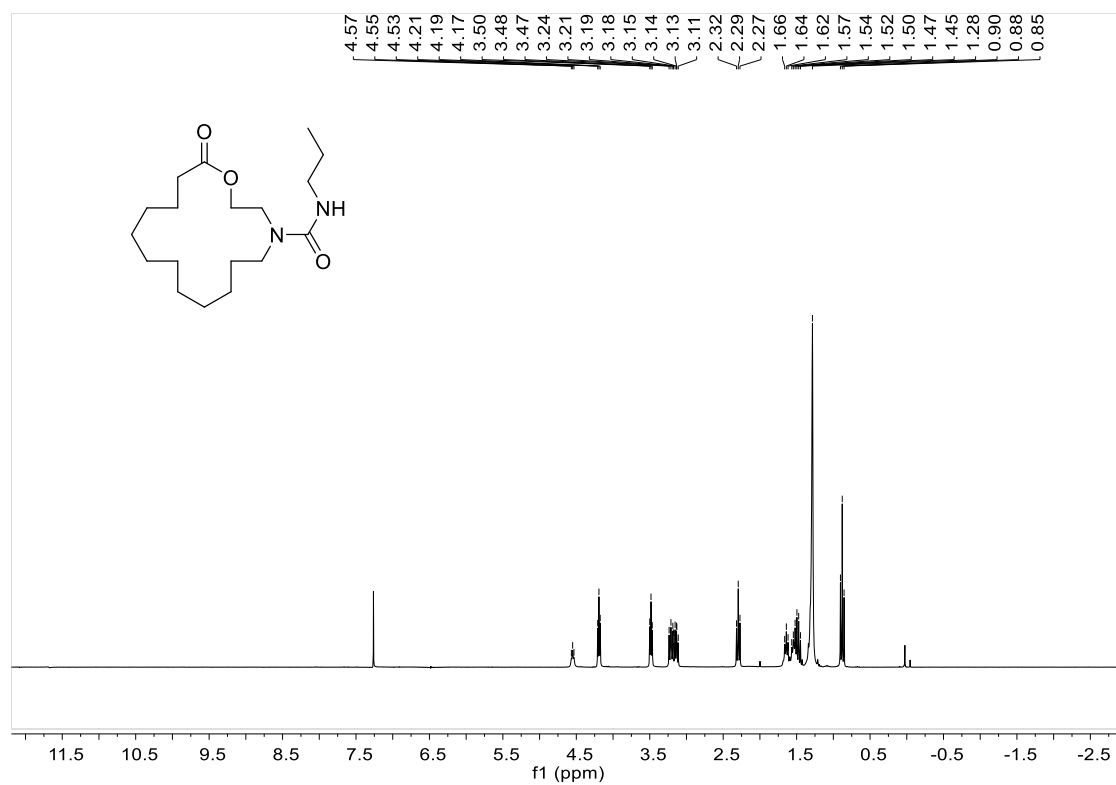
¹H NMR spectrum of D16-16 (300 MHz, CDCl₃)



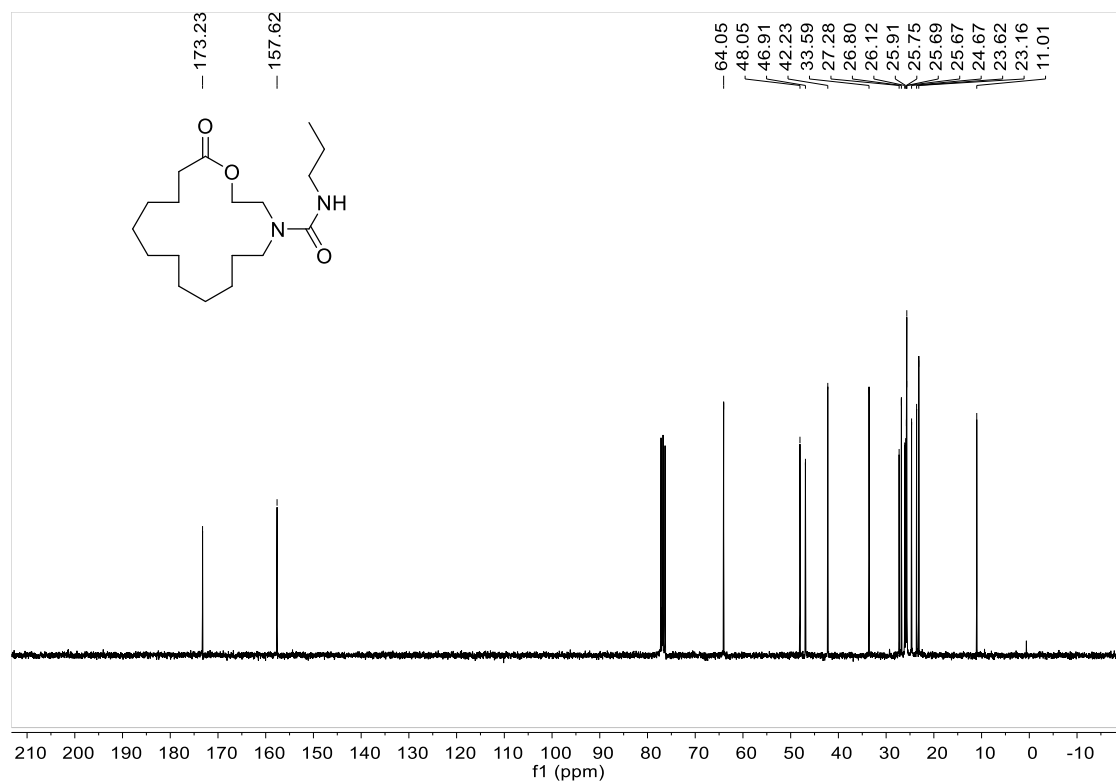
¹³C NMR spectrum of D16-16 (75 MHz, CDCl₃)



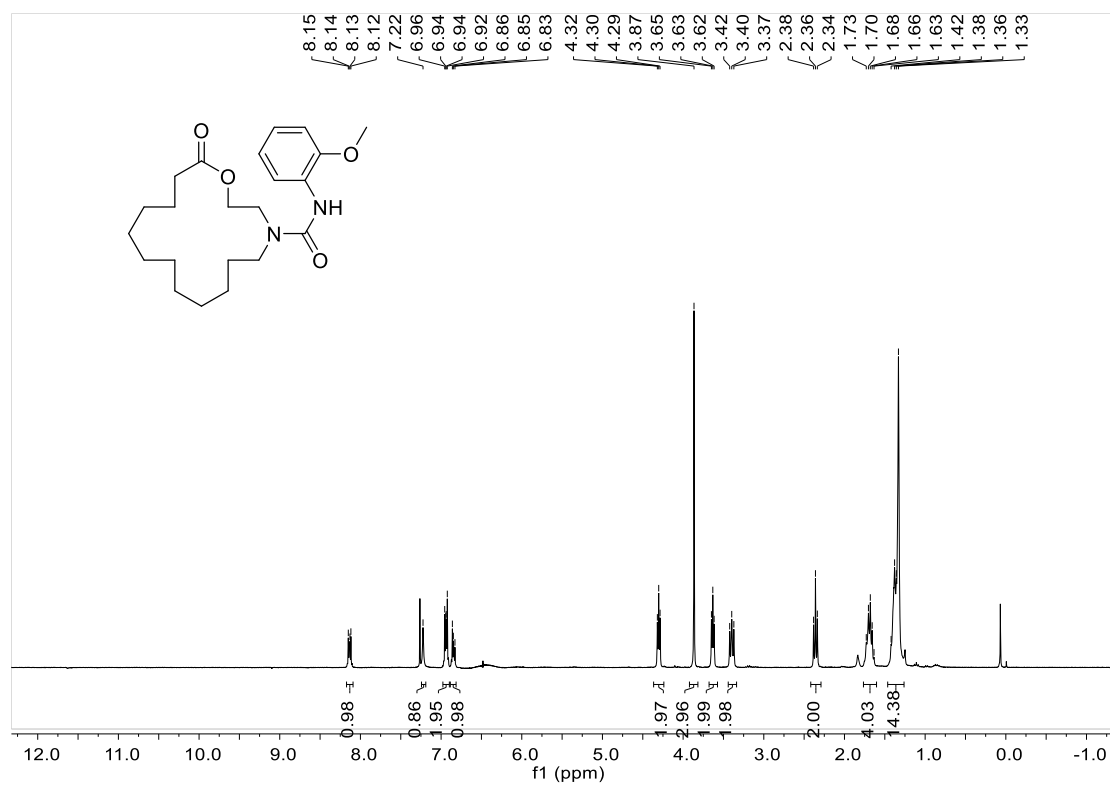
¹H NMR spectrum of D16-17 (300 MHz, CDCl₃)



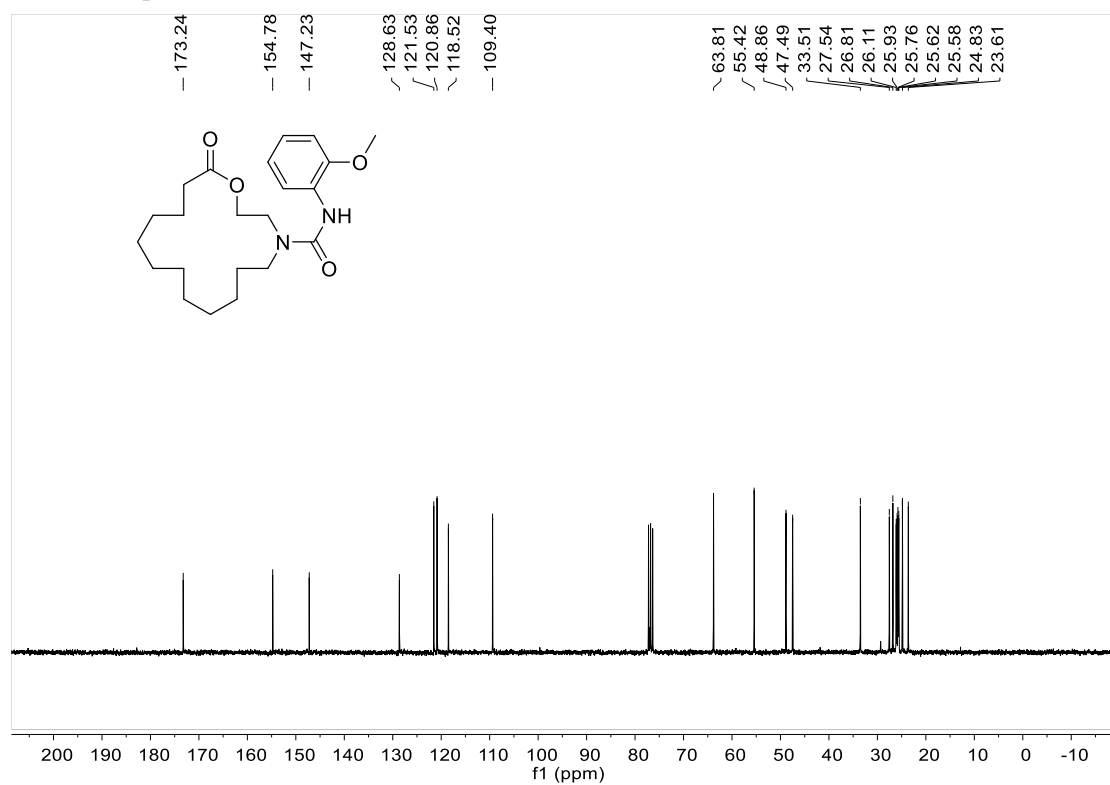
¹³C NMR spectrum of D16-17 (75 MHz, CDCl₃)



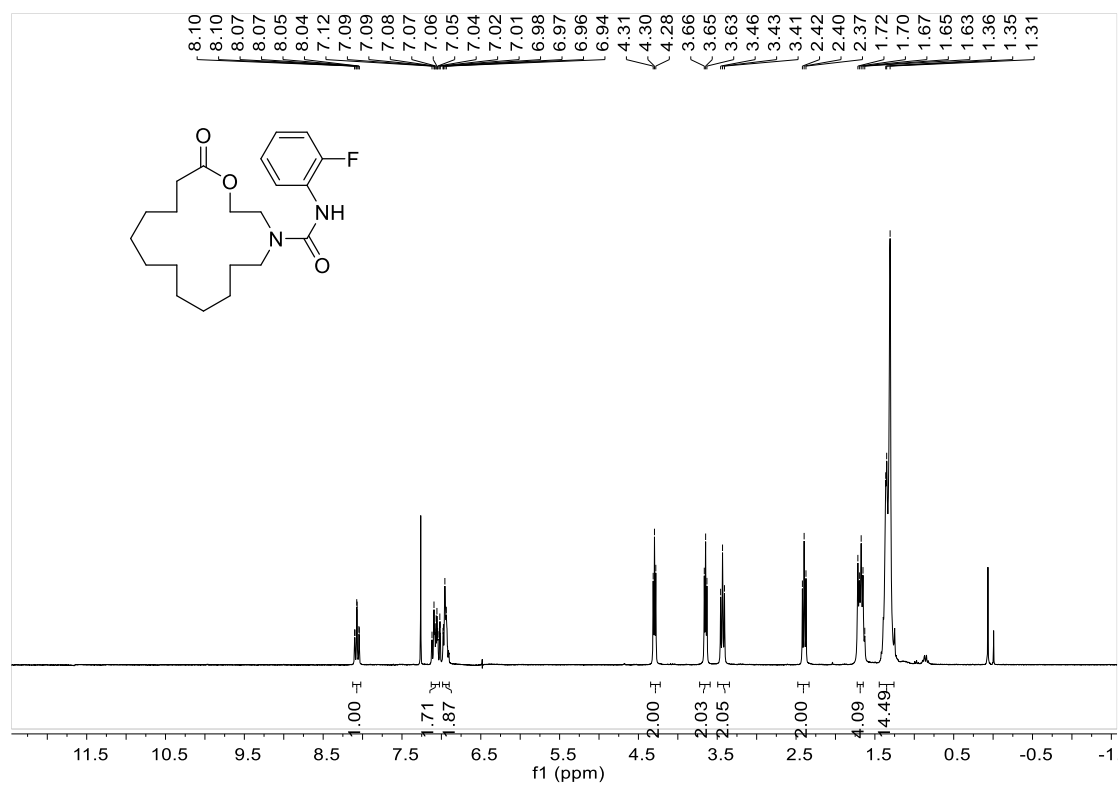
¹H NMR spectrum of D16-18 (300 MHz, CDCl₃)



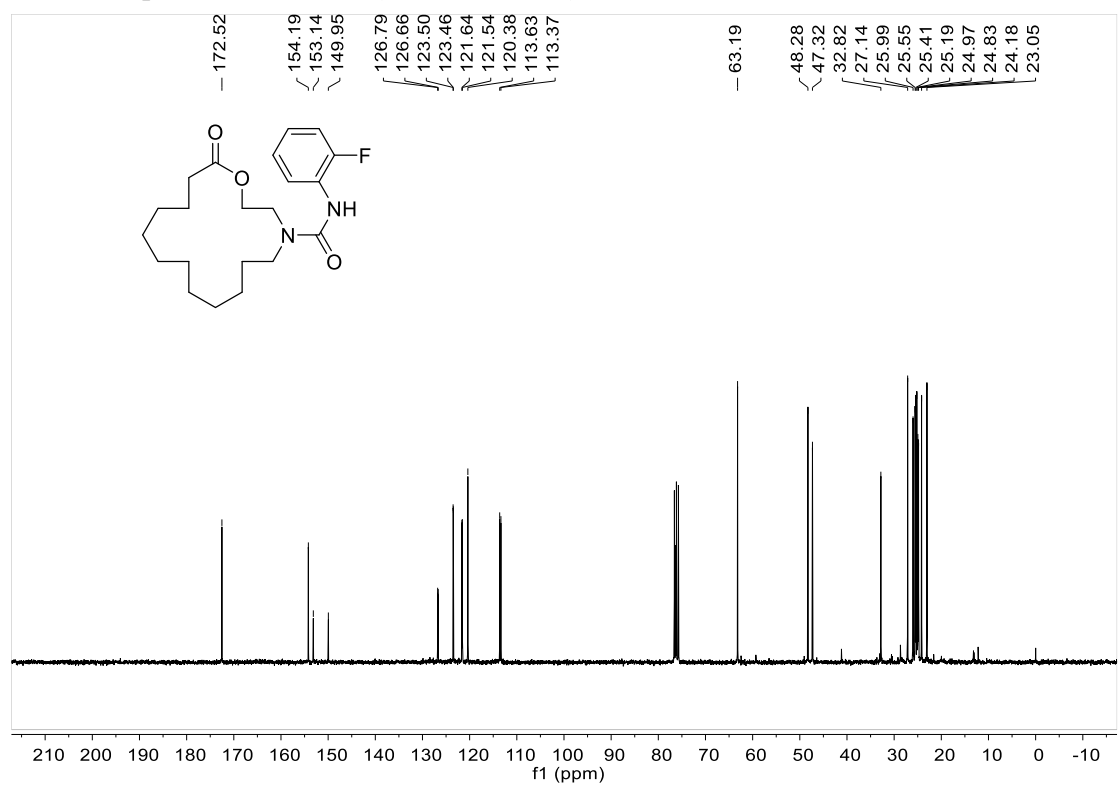
¹³C NMR spectrum of D16-18 (75 MHz, CDCl₃)



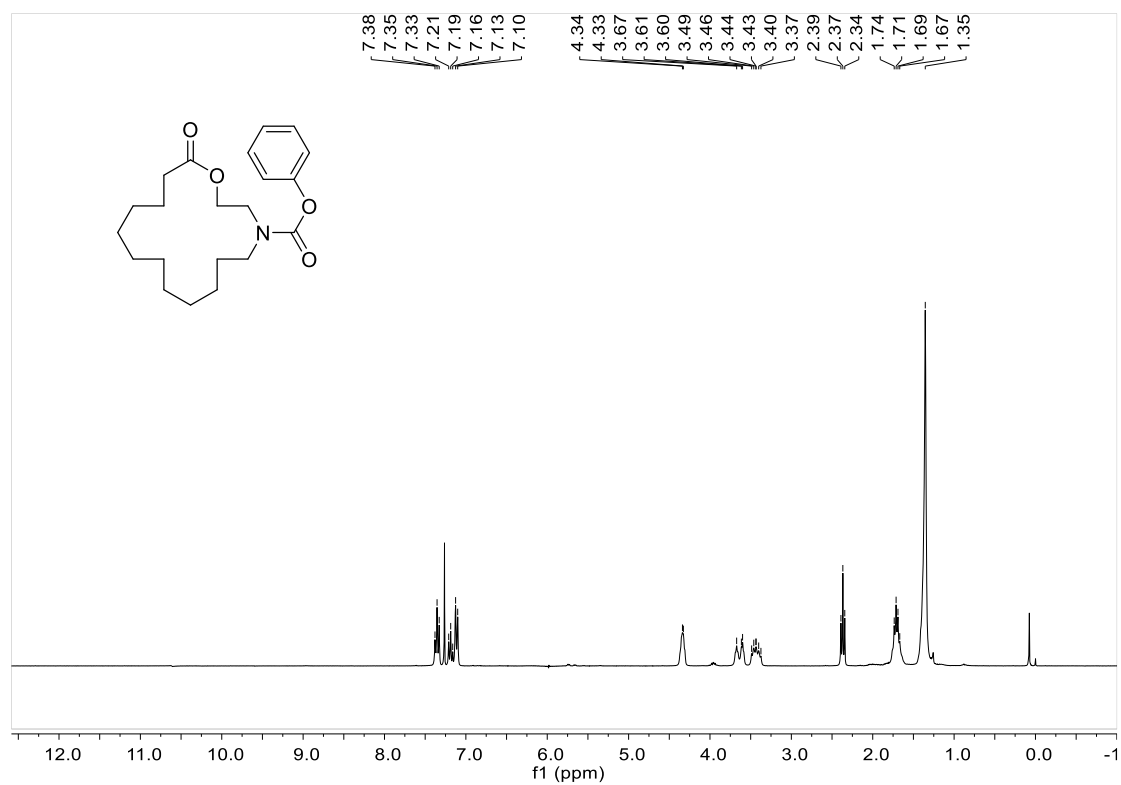
¹H NMR spectrum of D16-19 (300 MHz, CDCl₃)



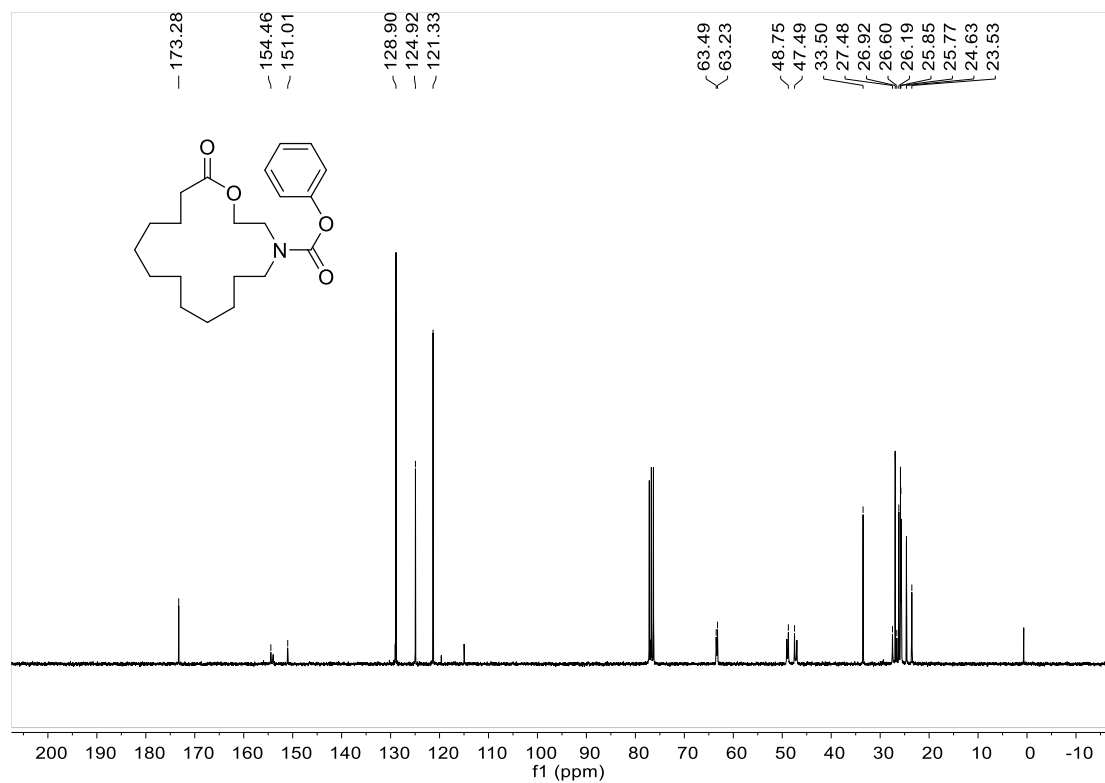
¹³C NMR spectrum of D16-19 (75 MHz, CDCl₃)



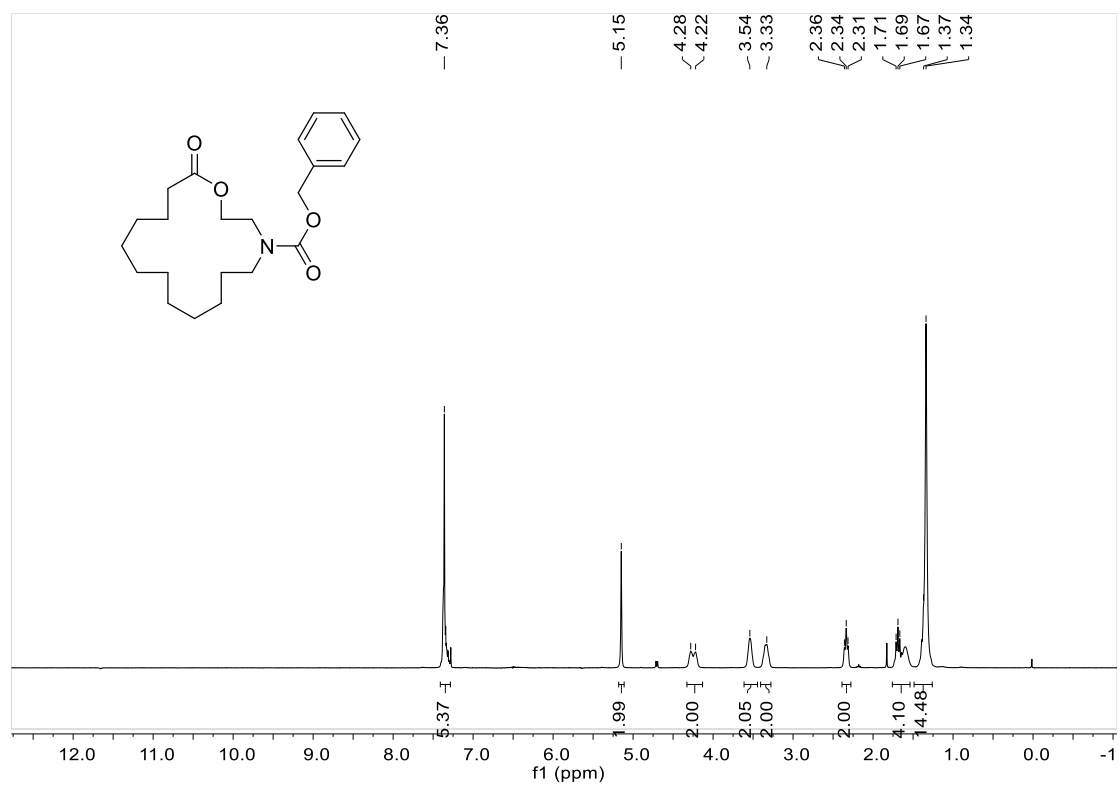
¹H NMR spectrum of D16-20 (300 MHz, CDCl₃)



¹³C NMR spectrum of D16-20 (75 MHz, CDCl₃)



¹H NMR spectrum of D16-21 (300 MHz, CDCl₃)



¹³C NMR spectrum of D16-21 (75 MHz, CDCl₃)

