Electronic Supplementary Material (ESI) for Energy & Environmental Science

Electronic Supplementary Information

CO_2 capture and activation by superbase/polyethylene glycol and its subsequent conversion

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1. General experimental methods:

Caution

Experiments using compressed gases CO_2 are potentially hazardous and must only be carried out by using the appropriate equipment and under rigorous safety precautions.

Materials

Superbases and PEG used in this work were purchased from Alfa Aesar-A Johnson Matthey Company and dried under vacuum at 70 ^oC for one week before use. CO_2 with a purity of 99.999% was commercially available. Amines was refluxed for 10 h with CaH_2 and distilled prior to use. $NH_2PEG150NH_2$[1] and aziridines[2] was synthesized according to the reported method.

Experimental methods

^1H NMR spectra was recorded at Bruck 400 spectrometer in $CDCl_3$ and $CDCl_3$ (7.26 ppm) was used as internal reference, ^{13}C NMR was recorded at 100.6 MHz in $CDCl_3$ and $CDCl_3$ (77.0 ppm) was used as internal reference. GC analyses were performed on Shimadzu GC-2014, equipped with a capillary column (RTX-17, 30 m × 0.25 μm) using a flame ionization detector. *In situ* FTIR was collected on a Mettler Toledo React IR ic10, Diamond ATR probe, using ic IR analysis system. The probe is placed in the middle of the absorption mixture, which is constantly stirred by magnetic whisk, and the spectra are collected *in situ* during CO_2 absorption. Infrared (IR) spectra were recorded on a Bruker Tensor27 FT-IR spectrophotometer with KBr pellets.

General procedure for CO_2 absorption

In a typical procedure, CO_2 capture was carried out in a 10 mL Schlenk flask. The absorbents were charged into the reactor at room temperature. Then, the air in the flask was replaced by CO_2 and a needle was used for CO_2 bubbling, which was inserted in the bottom of the flask. The absorption reaction was conducted at 40 ^oC with a CO_2 bubbling rate of 0.1 L/min. The amount of CO_2 absorbed was determined by an Analytical Balance within an accuracy of $\pm$0.0001 g every five minutes. Absorption/desorption was determined by several cycles of repeated experiments.

General procedure for synthesis of value-added chemicals using captured CO_2

Taking the systhesis of 1,3-dibutylurea as an example: Firstly, DBU (3 mmol, 0.4567 g) and PEG_{150} (3 mmol, 0.45 g) were charged into a glass tube, in which CO_2 was bubbled through a needle. Then, 1-butylamine was added after CO_2 absorption reached equilibrium. The tube was placed into a 25 mL stainless steel autoclave and then the mixture was stirred at predetermined temperature for 5 min to reach the equilibration. When the reaction finished, the reactor was cooled in ice-water and CO_2 was ejected slowly. An aliquot of sample was taken from the resultant mixture and dissolved in dry CH_2Cl_2 for GC analysis.

2. Characterization of the absorption system, amidinium/guanidinium alkylcarbonate salts, aziridines, ureas and oxazolidinones

DBU (1,8-diazabicyclo[5.4.0]undec-7-ene):

^1H NMR (400 MHz, $CDCl_3$) δ 3.23 (t, ^3J = 5.6 Hz, 2 H), 3.13-3.18 (m, 4 H), 2.33-2.35 (m, 2 H), 1.72-1.77 (m, 2 H), 1.60 (s, 4 H), 1.52 (s, 2 H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 161.6, 52.8, 48.3, 44.0, 37.2, 29.7, 28.4, 25.9, 22.3. IR 3420, 2924, 2851, 1616, 1486, 1441, 1366, 1312, 1260, 1233, 1183, 1115, 1060, 991, 955 cm^{-1}.

PEG_{150} (triethylene glycol, MW = 150 Da):

^1H NMR (400 MHz, $CDCl_3$) δ 3.71 (t, ^3J = 4.8 Hz, 4 H), 3.65 (s, 4 H), 3.59 (t, ^3J = 4.8 Hz, 4 H), 3.40 (s, 2 H); ^{13}C NMR (100.6 MHz, CDCl3) δ 72.6, 70.3, 61.5. IR 3446, 2865, 2360, 2341, 2136, 1954, 1653, 1457, 1351, 1082, 937, 889, 830, 571, 525 cm^{-1}.

DBU/PEG_{150} + CO_2:

^1H NMR (400 MHz, $CDCl_3$) δ 3.56-3.70 (m, 12 H), 3.29-3.34 (m, 6 H), 2.61 (s, 2 H), 1.85-1.90 (m, 2 H), 1.66-1.67 (m, 4 H), 1.59 (s, 2 H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 164.1, 158.5, 72.6, 70.3, 64.1, 61.3, 53.5, 48.4, 40.6, 34.1, 29.3, 27.6, 24.8, 20.8.

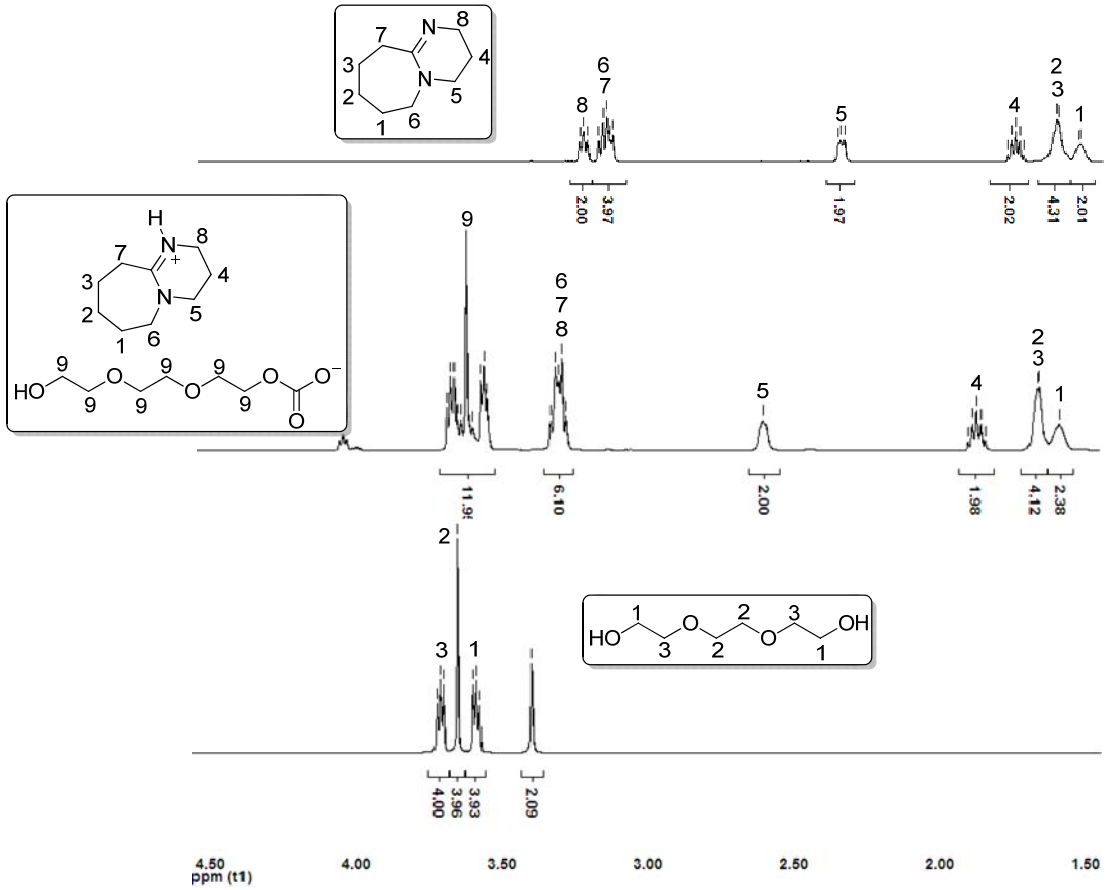


Fig. S1 The ^{1}H NMR of DBU, PEG_{150} and DBU/PEG_{150} + CO_2 ($CDCl_3$, 400 MHz).

Table S1 The comparison of ^{1}H and ^{13}C NMR chemical shifts of DBU, PEG_{150} and DBU/PEG_{150} + CO_2

	DBU	DBU$PEG_{150}CO_2$	PEG_{150}
^{1}H NMR /ppm	1.52 (2H)	1.59 (2H)	
	1.60 (4H)	1.60-1.67 (4H)	
	1.72-1.77 (2H)	1.85-1.90 (2H)	
	2.33-2.35 (2H)	2.61 (2H)	
	3.13-3.18 (4H)		
	3.23 (2H)	3.29-3.34 (6H)	
		3.56-3.70 (12H)	3.59-3.71 (12H)
^{13}C NMR /ppm	22.3	20.8	
	25.9	24.8	
	28.4	27.6	
	29.7	29.3	
	37.2	34.1	
	44.0	40.6	
	48.3	48.4	
	52.8	53.5	
		61.3	61.5
		64.1	
		70.3	70.3
		72.6	72.6
		158.5	
	161.6	164.1	

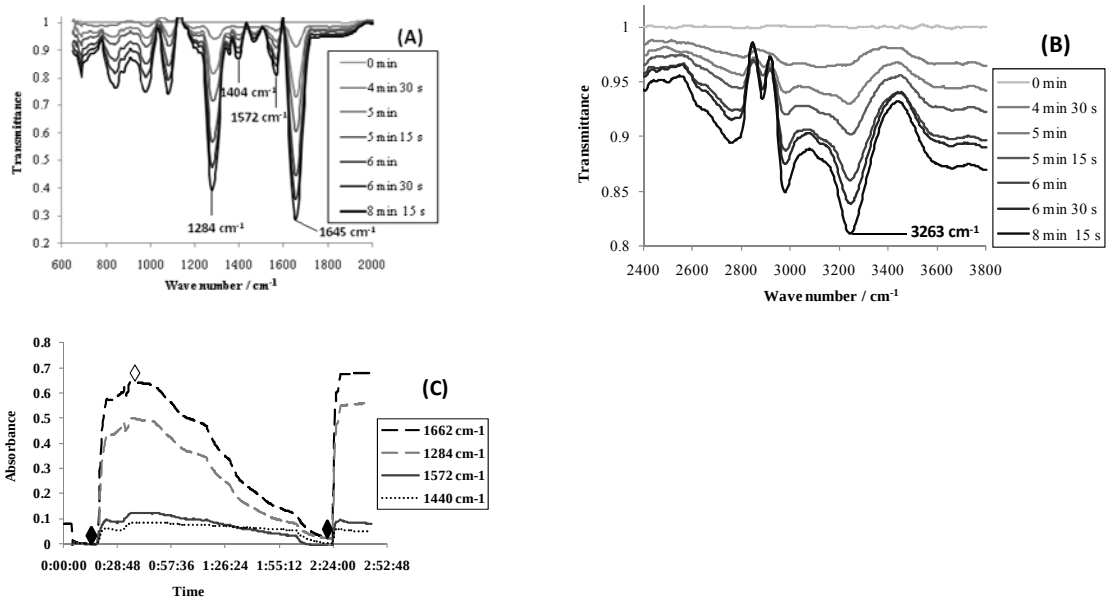


Figure S2. Results of *in situ* FT-IR spectroscopy monitoring CO_2 capture by DBU/PEG_{150} system at various times starting from CO_2 bubbling; The spectrum of DBU and PEG_{150} was subtracted; ◆: CO_2 began to be bubbled at 40 °C; ◇: Temperature was gradually increased form 40 °C to 120 °C.

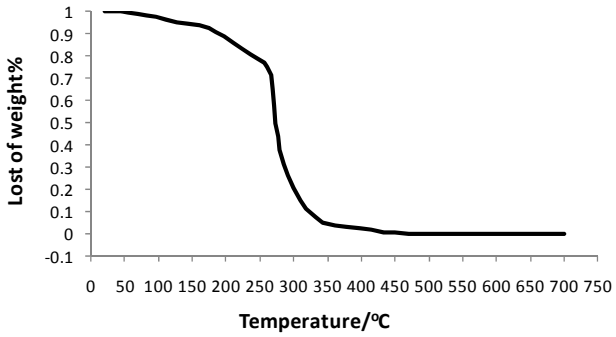


Figure S3. The scanning thermogravimetric analysis (TGA) results for DBU/PEG_{600}+CO_2 with a 10 °C min^{-1} temperature ramping rate to 700 °C.

PEG_{600} (polyethylene glycol, MW = 600 Da):

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.57-3.69 (m, 44H), 2.75 (s, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ72.4, 70.4, 70.2, 61.6. IR 3375, 2870, 1636, 1457, 1350, 1297, 1249, 1107, 951, 845, 735, 559 cm^{-1}.

DBU/PEG_{600} + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.59-3.70 (m, 53H), 3.29 (t, ^3J = 5.6 Hz, 2H), 3.20-3.24 (m, 4H), 2.46 (s, 2H), 1.78-1.84 (m, 2H), 1.65 (s, 4H), 1.57 (s, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 164.6, 157.7, 77.2, 72.0, 69.8, 69.6, 63.5, 60.6, 53.3, 47.9, 38.4, 32.1, 28.5, 26.5, 23.8, 19.4. IR 3350, 2867, 2361, 2343, 1647, 1613, 1456, 1351, 1315, 1291, 1250, 1110, 993, 953, 885, 837, 731, 694, 546, 526 cm^{-1}.

TBD (1,5,7-triazabicyclo[4.4.0]dec-5-ene):

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.29 (t, ^3J = 5.6 Hz, 4H), 3.24 (t, ^3J = 6 Hz, 4H), 1.96 (m, 4H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 151.2, 46.6, 38.0, 20.7. IR 3477, 3418, 3234, 3157, 2967, 2943, 2875, 2797, 2749, 2361, 2343, 1662, 1573, 1477, 1445, 1421, 1378, 1321, 1295, 1202, 1069, 884, 711, 671, 590 cm^{-1}.

TBD/PEG_{600} + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56-3.68 (m, 62H), 3.21-3.27 (m, 8H), 1.91-1.97 (m, 4H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 158.8, 150.7, 77.2, 72.0, 69.9, 69.7, 64.0, 60.7, 46.2, 37.0, 20.3. IR 3308, 3160, 2869, 2362, 1943, 1667, 1574, 1456, 1377, 1350, 1323, 1291, 1252, 1203, 1107, 951, 844, 745, 730, 714 cm^{-1}.

DBN (1,5-diazabicyclo[4.3.0]non-5-ene):

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.28 (t, ^3J = 4.8 Hz, 2H), 3.21 (t, ^3J = 6.8 Hz, 2H), 3.13 (t, ^3J = 6 Hz, 2H), 2.38 (t, ^3J = 7.6 Hz, 2H), 1.83-1.91 (m, 2H), 1.70-1.76 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ160.5, 51.2, 43.8, 42.8, 31.3, 20.6, 19.4. IR 3409, 2929, 2845, 1651, 1496, 1422, 1363, 1288, 1232, 1195, 1133, 1051, 961, 903, 737, 677, 574 cm^{-1}.

DBN/PEG_{600} + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.58-3.72 (m, 58H), 3.31 (t, ^3J = 5.6 Hz, 2H), 3.26 (t, ^3J = 6.4 Hz, 2H), 3.17 (t, ^3J = 6 Hz, 2H), 2.45 (t, ^3J = 8 Hz, 2H), 1.88-1.95 (m, 2H), 1.74-1.80 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ162.8, 157.6, 77.2, 72.0, 69.8, 69.5, 63.4, 60.4, 52.0, 41.9, 38.6, 29.4, 18.5, 18.3. IR 3394, 2870, 2361, 2342, 1681, 1651, 1457, 1350, 1291, 1251, 1107, 952, 837, 747, 730, 698 cm^{-1}.

TMG(tetramethylguanidine):

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.01 (s, 1H), 2.70 (s, 12H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 167.9, 39.3. IR 3420, 3334, 3000, 2942, 2845, 2789, 2360, 2341, 1599, 1494, 1458, 1425, 1409, 1382, 1255, 1198, 1145, 1058, 1010, 892, 779, 734, 562, 544 cm^{-1}.

TMG/PEG_{600} + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.55-3.69 (m, 60H), 2.71 (s, 12H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 163.6, 157.4, 77.2, 72.1, 69.9, 69.7, 63.4, 60.6, 38.9. IR 3393, 2870, 2361, 2343, 1647, 1472, 1457, 1351, 1277, 1251, 1108, 952, 838, 749 cm^{-1}.

DMICH(N-(1,3-dimethylimidazolidin-2-ylidene)cyclohexanamine):

^{1}H NMR (400 MHz, $CDCl_3$) δ3.38–3.43 (m, 1H), 3.11 (s, 4H), 2.76 (s, 6H), 1.15–1.72 (m, 10H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 155.4, 54.0, 44.9, 36.5, 31.3, 25.8, 25.2.

DMICH/PEG_{600} + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.56-3.69 (m, 56H), 3.34-3.39 (m, 1H), 3.17 (s, 4H), 2.79 (s, 6H), 1.54-1.73 (m, 5H), 1.13-1.41 (m, 5H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 157.5, 157.3, 124.4, 77.2, 72.3, 70.2, 70.0, 63.6, 61.1, 54.1, 59.2, 44.7, 36.1, 35.0, 34.9, 25.1, 18.0. IR 3393, 2922, 2867, 2361, 2342, 1653, 1635, 1472, 1456, 1350, 1279, 1256, 1109, 1035, 952, 890, 847, 763, 729, 698 cm^{-1}.

$NH_2PEG_{150}NH_2$:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.47 (s, 4 H), 3.35 (t, ^3J = 5.2 Hz, 4 H), 2.71 (t, ^3J = 5.2 Hz, 4 H), 1.17 (s, 1 H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 73.2, 70.0, 41.5. IR 3393, 2869, 1576, 1473, 1375, 1352, 1307, 1114, 817 cm^{-1}.

$NH_2PEG_{150}NH_2$/PEG_{150}(molar ratio: 1: 2) + CO_2:

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (t, ^3J = 4 Hz, 12H), 3.66 (s, 8H), 3.59-3.62 (m, 12H), 3.54 (t, ^3J = 4.8 Hz, 2H), 3.26 (s, 1H), 2.89 (s, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 162.8, 72.3, 69.8, 68.2, 60.7, 40.9, 39.3. IR 3365, 2870, 2361, 2342, 1576, 1558, 1473, 1457, 1350, 1311, 1117, 1078, 936, 888, 821, 748 cm^{-1}.

1,3-Dipropyl urea:

^{1}H NMR (300 MHz, $CDCl_3$) δ 4.90 (bd, N-H), 3.08 (t, ^3J = 6.45 Hz, 4H), 1.41-1.54 (m, 4H), 0.89 (t, ^3J = 7.5 Hz, 6H); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 158.8, 42.1, 23.4, 11.3.

1,3-Diisopropyl urea:

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.80-3.87 (m, 2H), 1.14 (d, ^3J = 6.4 Hz, 12H); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 157.0, 42.2, 23.5.

1,3-Dibutyl urea:

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (s, 2 H), 3.12-3.13 (m, 4H), 1.42-1.49 (m, 4H), 1.28-1.37 (m, 4H), 0.91 (t, ^3J = 7.2 Hz, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 158.7, 40.2, 32.3, 20.0, 13.7.

1,1,3,3-Tetrabutyl urea:

^{1}H NMR (300 MHz, $CDCl_3$) δ 2.56 (t, ^3J = 7.2 Hz, 8H), 1.36-1.49 (m, 8H), 1.24-1.33 (m, 8H), 0.87 (t, ^3J = 7.2 Hz, 12H); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ 164.3, 49.7, 32.2, 20.5, 13.9.

Octahydro-benzoimidazol-2-one:

^{1}H NMR (300 MHz, D_2O) δ 3.12-3.32 (m, 2H), 1.53-1.60 (m, 4H), 1.15-1.35 (m, 4H); ^{13}C NMR (75.5 MHz, D_2O) δ 164.1, 53.3, 32.2, 24.2.

1-Ethyl-2-phenylaziridine:

^{1}H NMR (400 MHz, $CDCl_3$) δ7.18-7.31 (m, 5H), 2.44 (q, ^3J = 9.6 Hz, 2H), 2.30 (dd, ^3J = 4.4 Hz, ^3J = 4.8 Hz, 1H), 1.89 (d, ^2J = 4.4 Hz, 1H), 1.65 (d, ^2J = 8.8 Hz, 1H), 1.17 (t, ^3J = 9.6 Hz, 3H); ESI-MS calcd for $C_{10}H_{13}N$ 147.10, found 148.31 $[M + H]^+$.

1-Propyl-2-phenylaziridine:

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.95 (t, ^3J = 10.0 Hz, 3H), 1.60-1.67 (m, 3H), 1.89 (d, ^2J = 4.0 Hz, 1H), 2.24-2.33 (m, 2H), 2.43-2.51 (m, 1H), 7.18-7.31 (m, 5H); ESI-MS calcd for $C_{11}H_{15}N$ 161.12, found 162.28 $[M + H]^+$.

2-(4-Chlorophenyl)-1-ethylaziridine:

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.18 (t, ^3J = 6.9 Hz, 3H), 1.65 (d, ^2J = 6.6 Hz, 1H), 1.83 (d, ^2J = 3.3 Hz, 1H), 2.25-2.46 (m, 3H), 7.15-7.23 (m, 4H); ESI-MS calcd for $C_{10}H_{12}NCl$ 181.66, found 182.13 $[M + H]^+$.

2-(4-Methylphenyl)-1-ethylaziridine:

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.19 (t, ^3J = 7.2 Hz, 3H), 1.62 (d, ^2J = 6.4 Hz, 1H), 1.86 (d, ^2J = 3.2 Hz, 1H), 2.26 (dd, ^3J = 3.6 Hz, ^3J = 3.2 Hz, 1H), 2.31 (s, 3H), 2.37-2.48 (m, 2H), 7.09-7.15 (m, 4H); ESI-MS calcd for $C_{11}H_{15}N$ 161.24, found 162.20 $[M + H]^+$.

3-Ethyl-5-phenyloxazolidin-2-one:

Colorless liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.17 (t, ^3J = 7.2 Hz, 3H), 3.29-3.45 (m, 3H), 3.92 (t, ^3J = 8.7 Hz, 1H), 5.48 (t, ^3J = 7.8 Hz, 1H), 7.34-7.42 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 12.4, 38.8, 51.5, 74.2, 125.4, 128.6, 128.8, 138.8, 157.5; ESI-MS calcd for $C_{11}H_{13}NO_2$ 191.09, found 192.29 $(M + H)^+$, 214.38 $(M + Na)^+$, 405.01 $(2 M + Na)^+$.

3-Ethyl-4-phenyloxazolidin-2-one:

Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.05 (t, ^3J = 7.2 Hz, 3H), 2.79-2.88 (m, 1H), 3.48-3.57 (m, 1H), 4.10 (t, ^3J = 8.0 Hz, 1H), 4.62 (t, ^3J = 8.8 Hz, 1H), 4.81 (t, ^3J = 7.2 Hz, 1H), 7.30 7.44 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 12.1, 36.8, 59.3, 69.7, 126.9, 129.0, 129.2, 137.8, 158.1; ESI-MS calcd for $C_{11}H_{13}NO_2$ 191.09, found 192.29 $(M + H)^+$, 214.38 $(M + Na)^+$, 405.01 $(2M + Na)^+$.

3-Propyl-5-phenyloxazolidin-2-one:

Colorless liquid; ^{1}H NMR (300 MHz, $CDCl_3$) δ 0.91 (t, ^3J=7.2 Hz, 3H), 1.52-1.61 (m, 2H), 3.18-3.31 (m, 2H) 3.40 (t, ^3J=8.0 Hz, 1H), 3.90 (t, ^3J=8.8 Hz, 1H), 5.46 (t, ^3J=8.0 Hz, 1H), 7.31-7.37 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 10.7, 20.3, 45.5, 51.8, 74.0, 125.2, 128.4, 128.5, 138.7, 157.6; ESI-MS calcd for $C_{12}H_{15}NO_2$ 205.11, found 206.30 $(M + H)^+$, 228.30 $(M + Na)^+$, 433.04 $(2M + Na)^+$.

3-Ethyl-5-(4-chlorophenyl)oxazolidin-2-one:

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.17 (t, ^3J=7.3 Hz, 3H), 3.30-3.43 (m, 2H), 3.69-3.76 (m, 1H), 3.92 (t, ^3J=8.7 Hz, 1H), 5.44 (t, ^3J=8.0 Hz, 1H), 7.27-7.38 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.6, 38.9, 51.5, 73.6, 126.9, 129.1, 134.7, 137.4, 157.4; ESI-MS calcd for $C_{11}H_{12}ClNO_2$ 225.67, found 451.64 $(2M + H)^+$.

3-Ethyl-5-p-tolyloxazolidin-2-one:

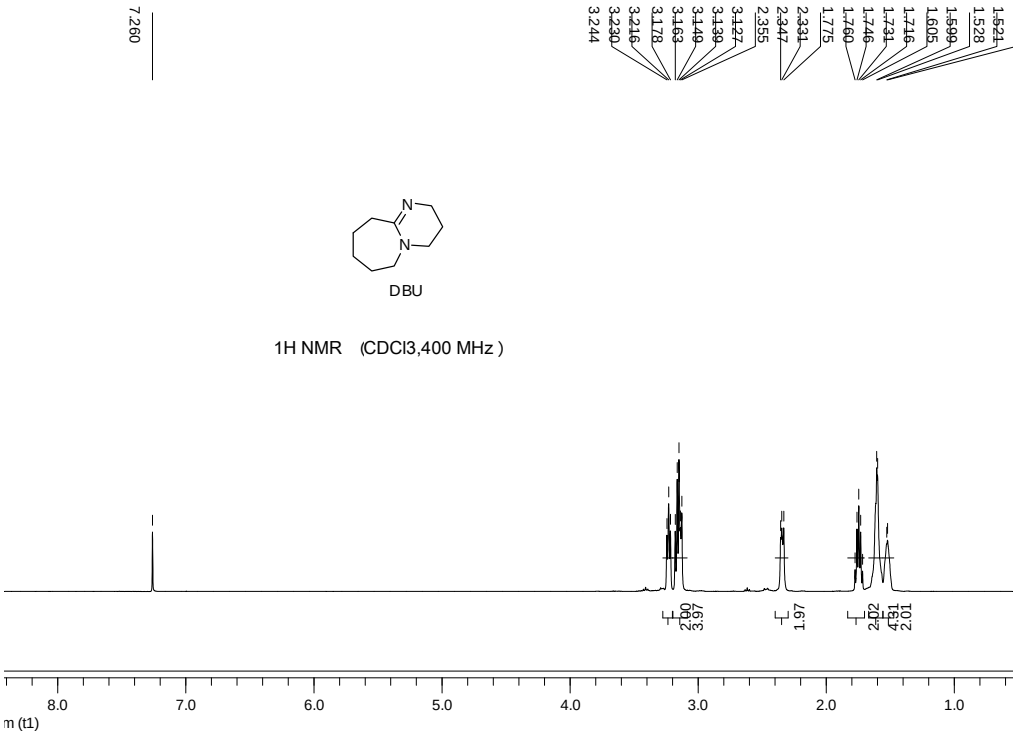
White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.18 (t, ^3J=7.3 Hz, 3H), 1.62 (d, ^3J=6.4 Hz, 1H),1.87 (d, ^3J=3.2 Hz, 1H), 2.27 (dd, ^3J=6.6 Hz, ^2J=3.2 Hz, 1H), 2.31 (s, 3H), 2.36-2.48 (m, 2H), 7.09- 7.15 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 12.6, 21.2, 38.9, 51.6, 74.3, 125.6, 129.5, 135.8, 138.7, 157.7; ESI-MS calcd for $C_{12}H_{15}NO_2$ 205.25, found 206.45 $(M + H)^+$, 411.15 $(2M + H)^+$.

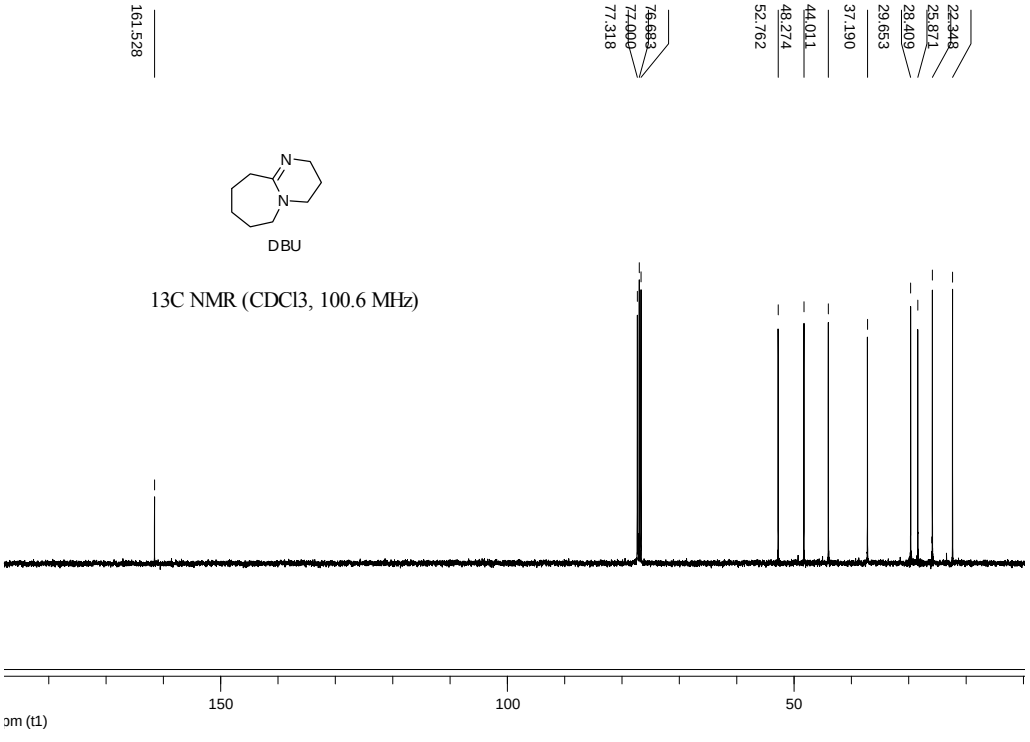
3. Reference

(1) Gansow, O. A.; Kausar, A. R.; Triplett, K. B. *J. Heterocyclic Chem.* **1981**, *18*, 297.

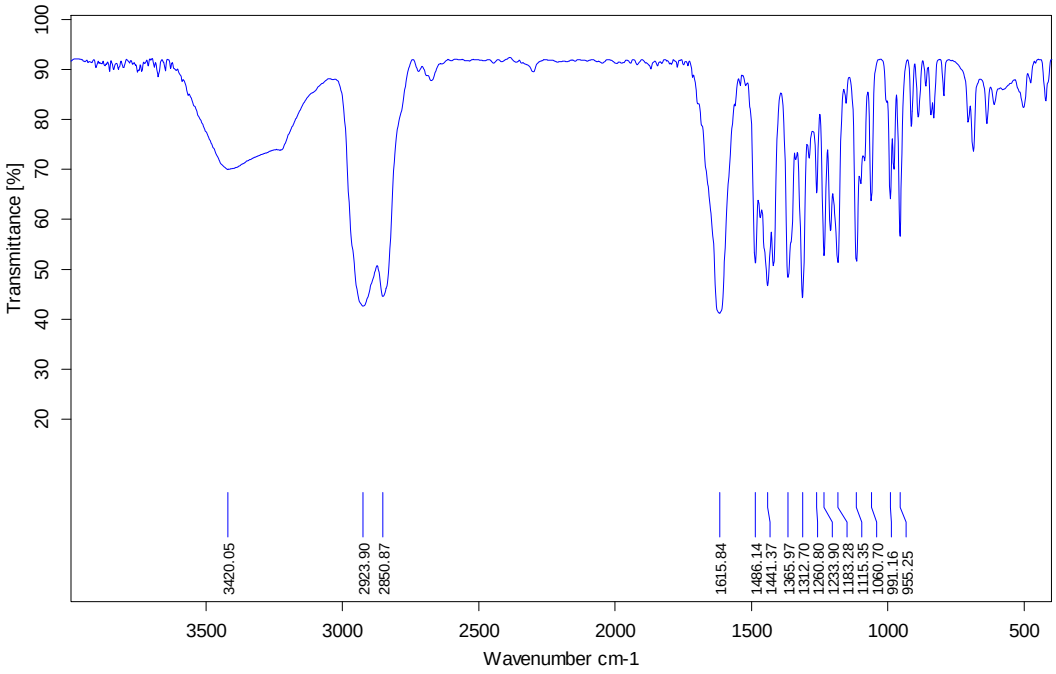
(2) Du, Y.; Wu, Y.; Liu, A.-H. and He, L.-N. *J. Org. Chem.* **2008**, *73*, 4709.

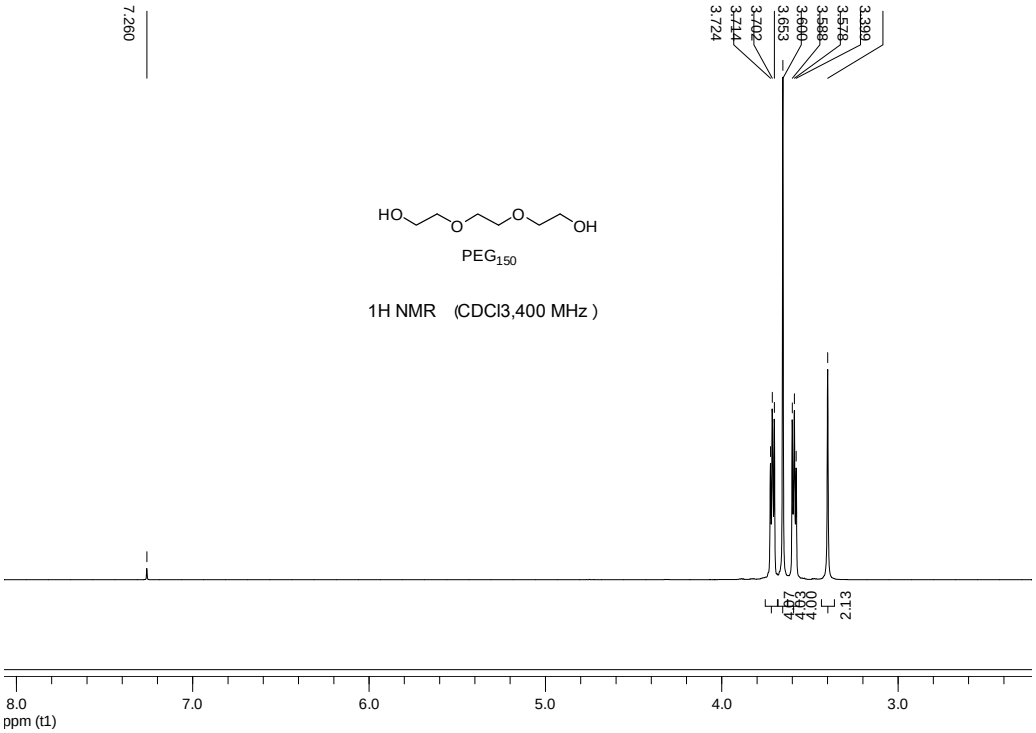
4. The ^{1}H NMR and ^{13}C NMR Charts, IR spectra for the absorption system, amidinium/guanidinium alkylcarbonate salts, urea and oxazolidinones

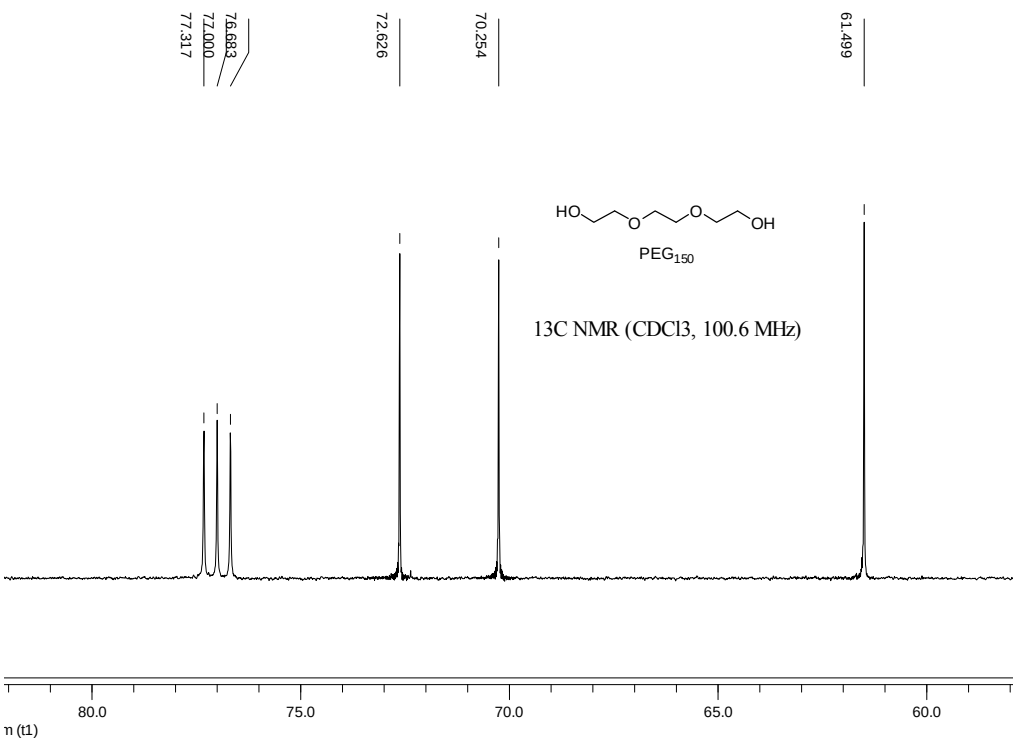




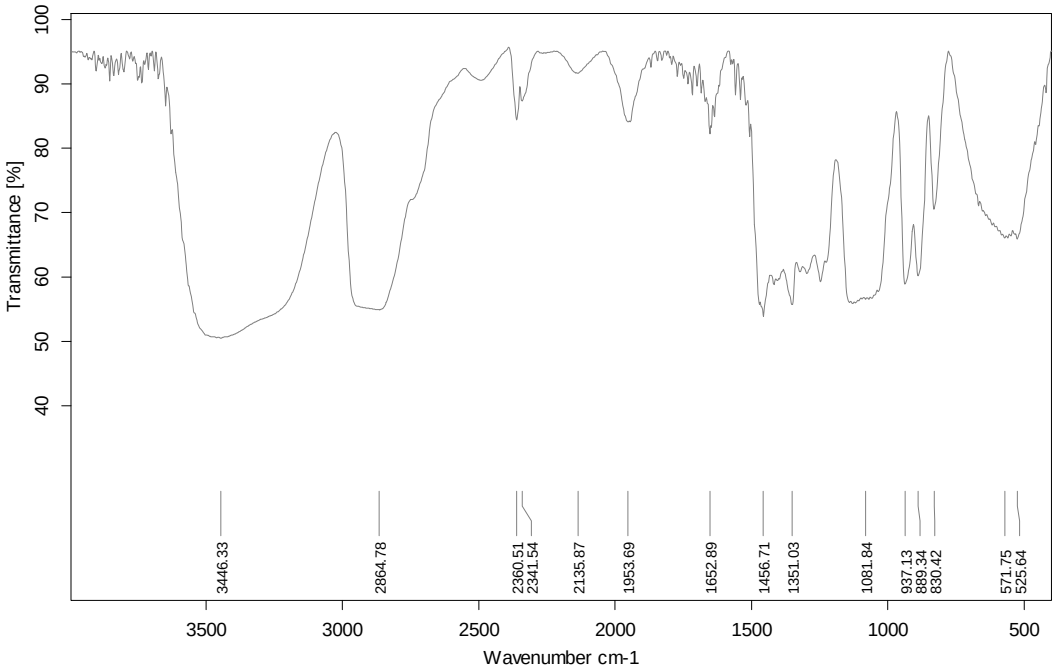
IR spectrum of DBU:

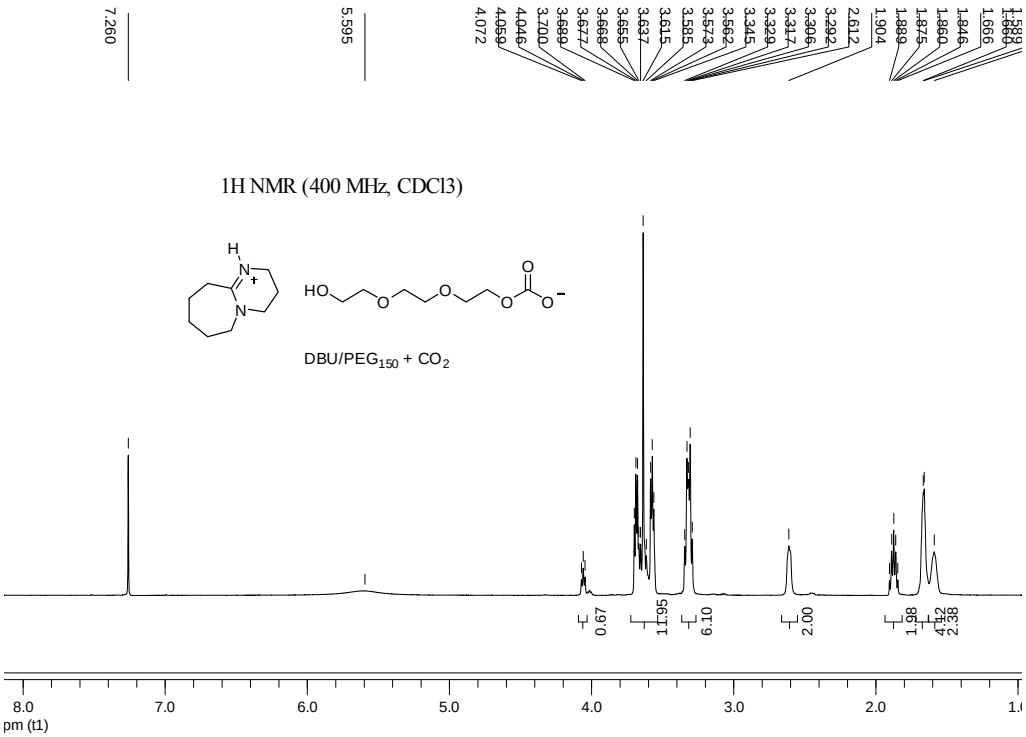






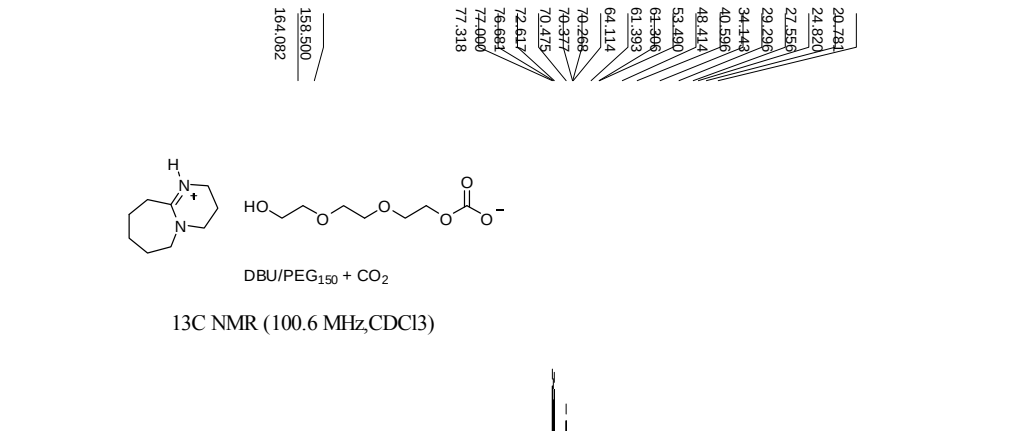
IR spectrum of PEG_{150}:





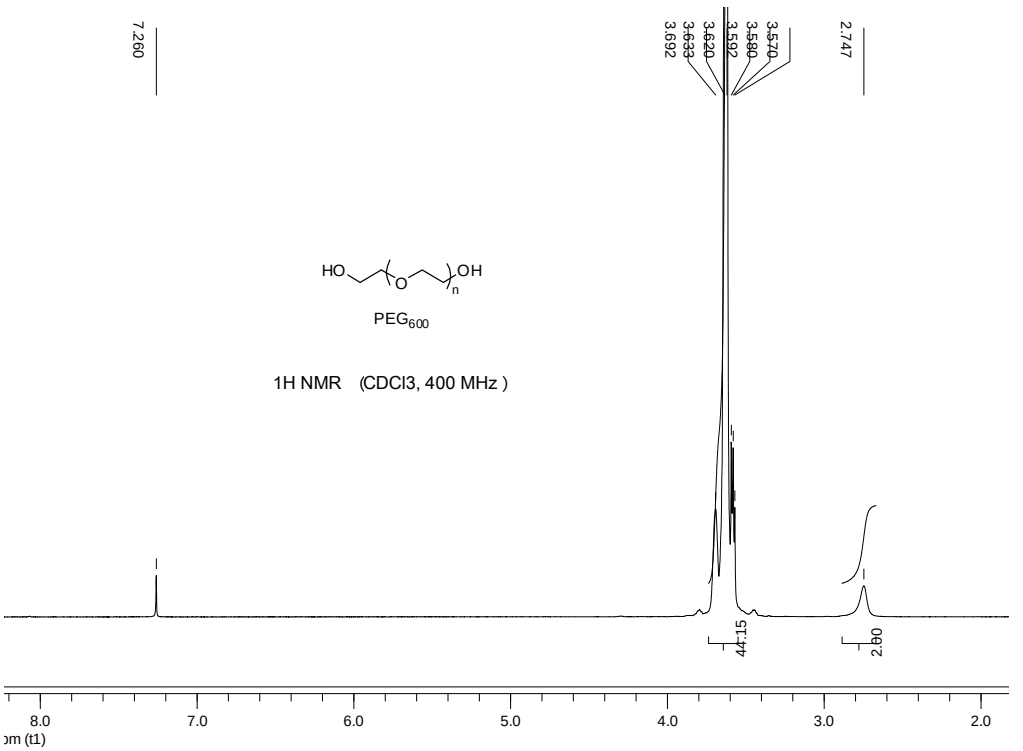
1H NMR (400 MHz, CDCl3)

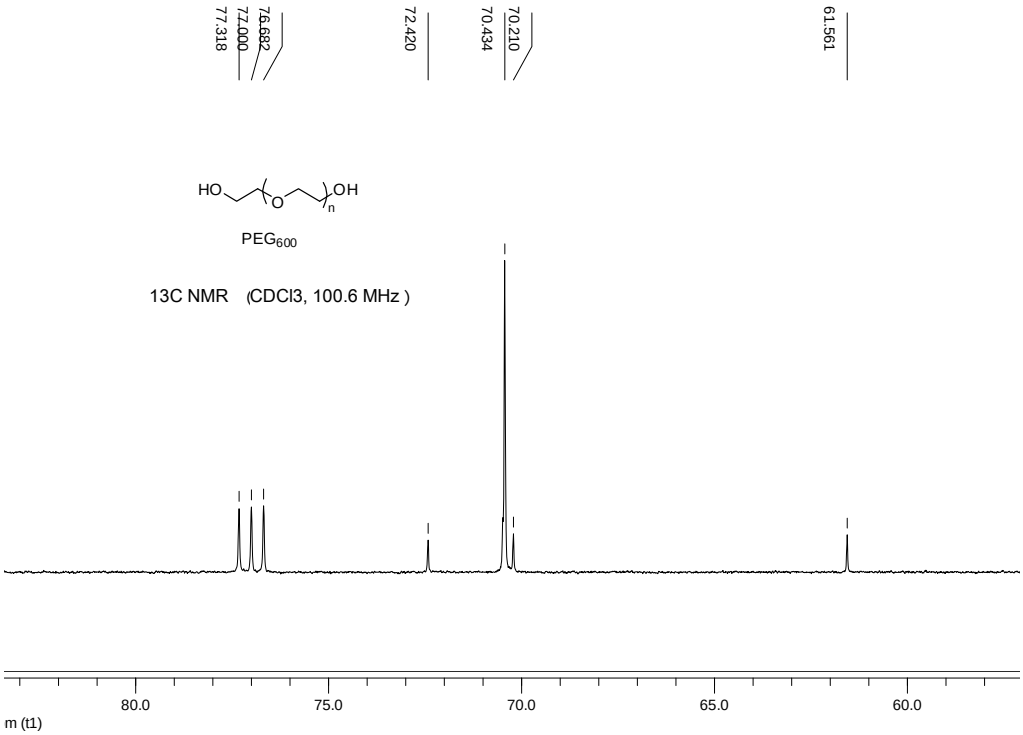
DBU/PEG$_{150}$ + CO_2



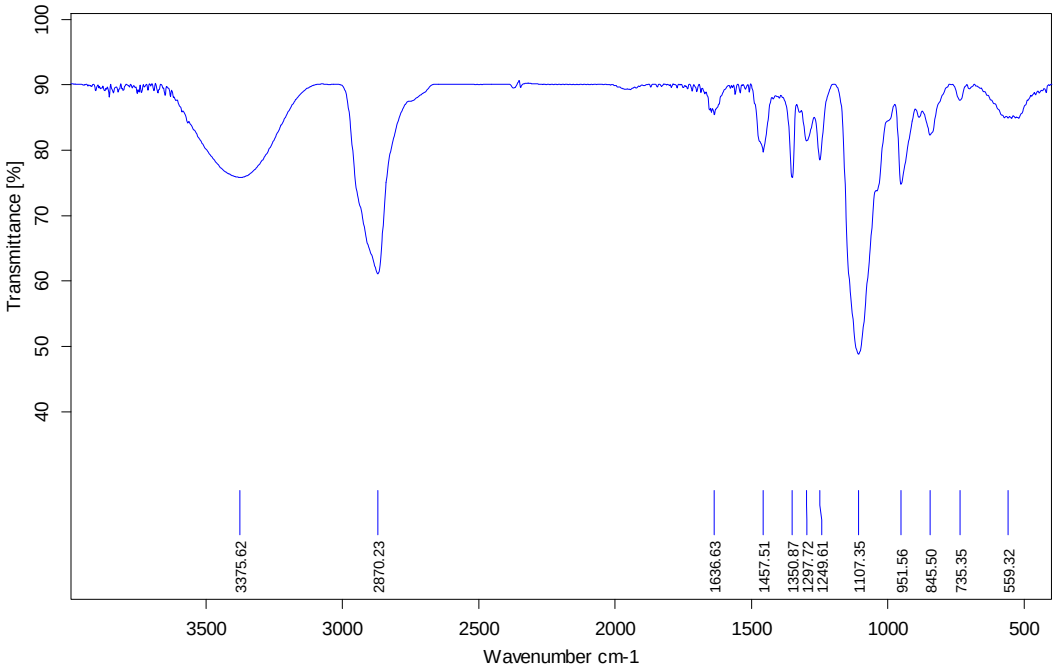
DBU/PEG$_{150}$ + CO_2

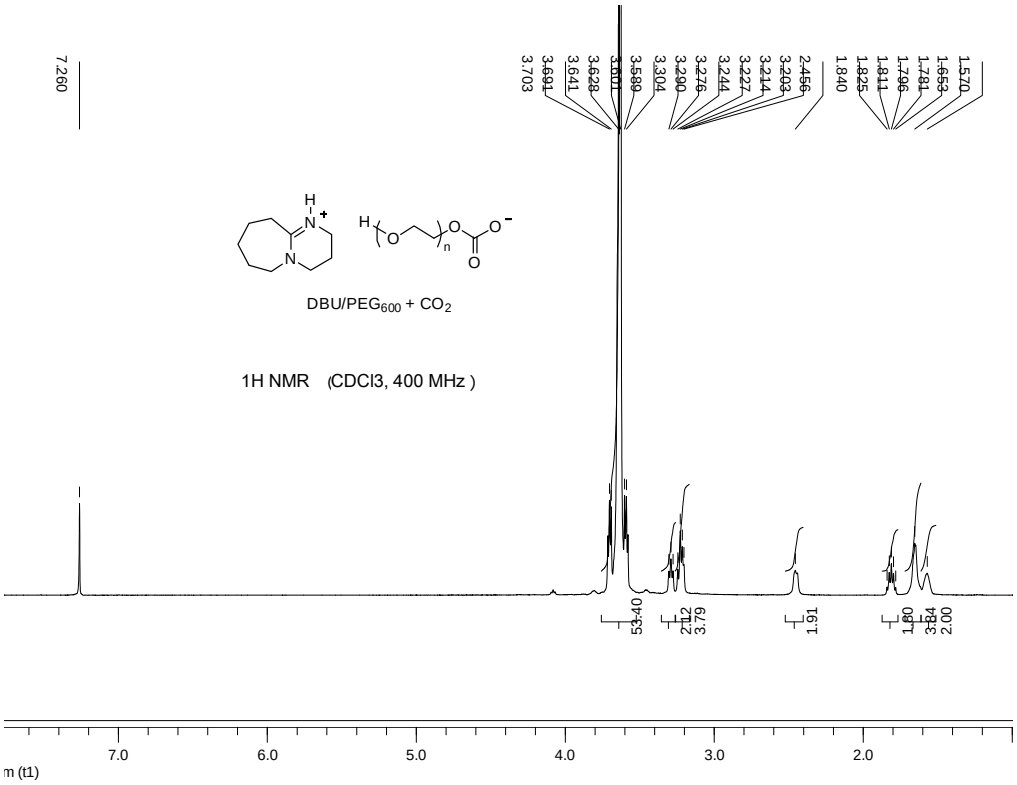
13C NMR (100.6 MHz,CDCl3)

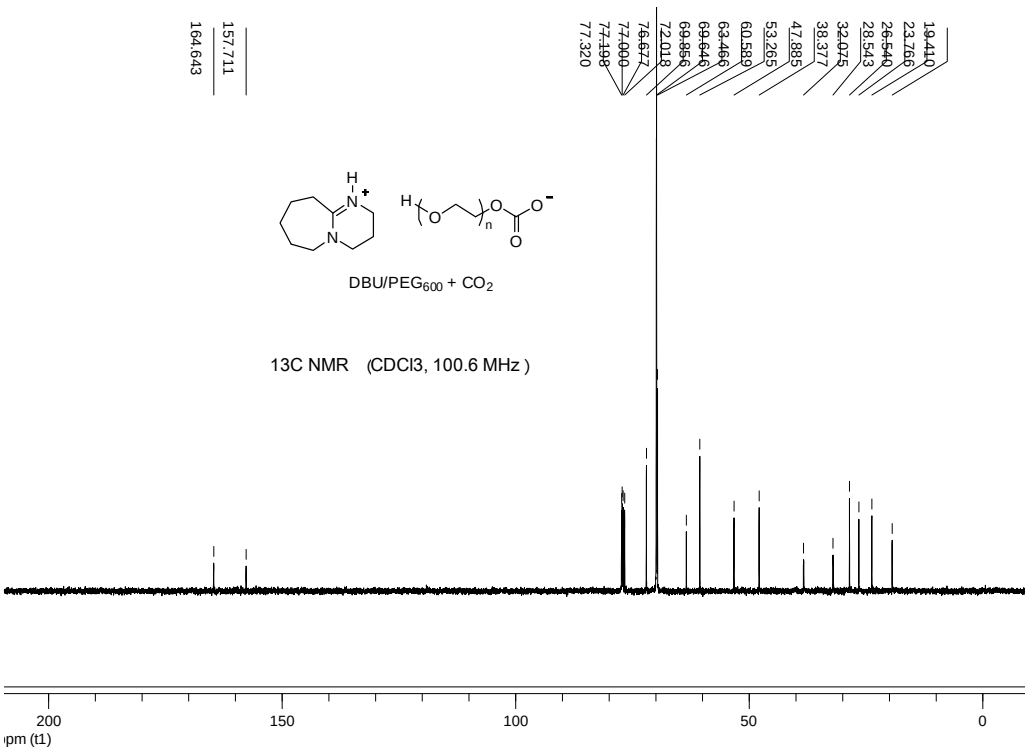




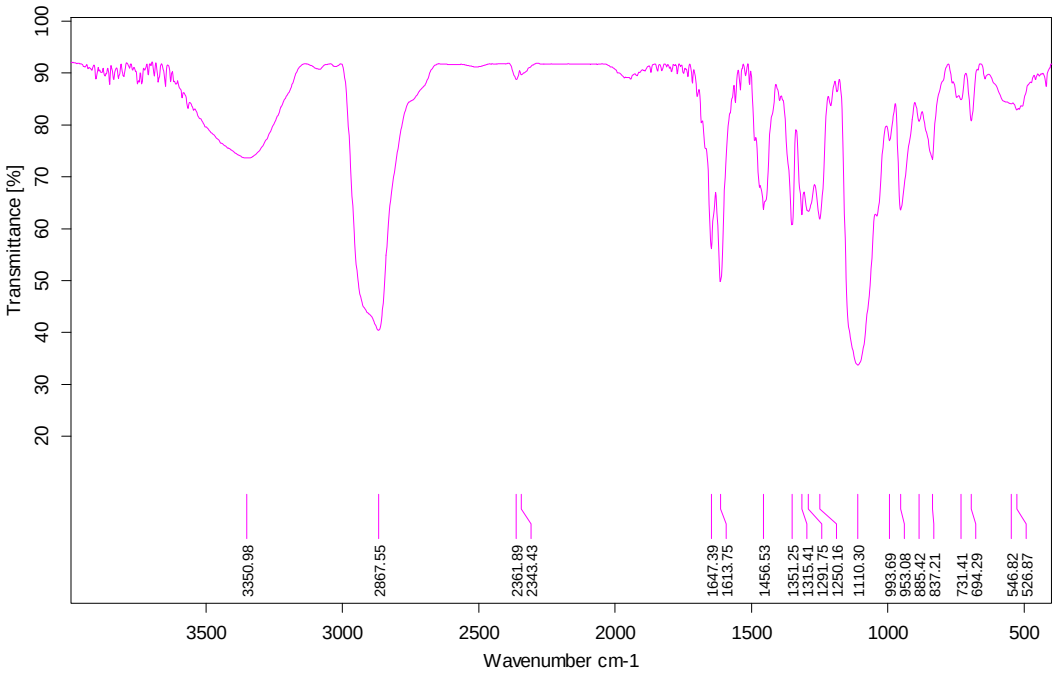
IR spectrum of PEG_{600}:

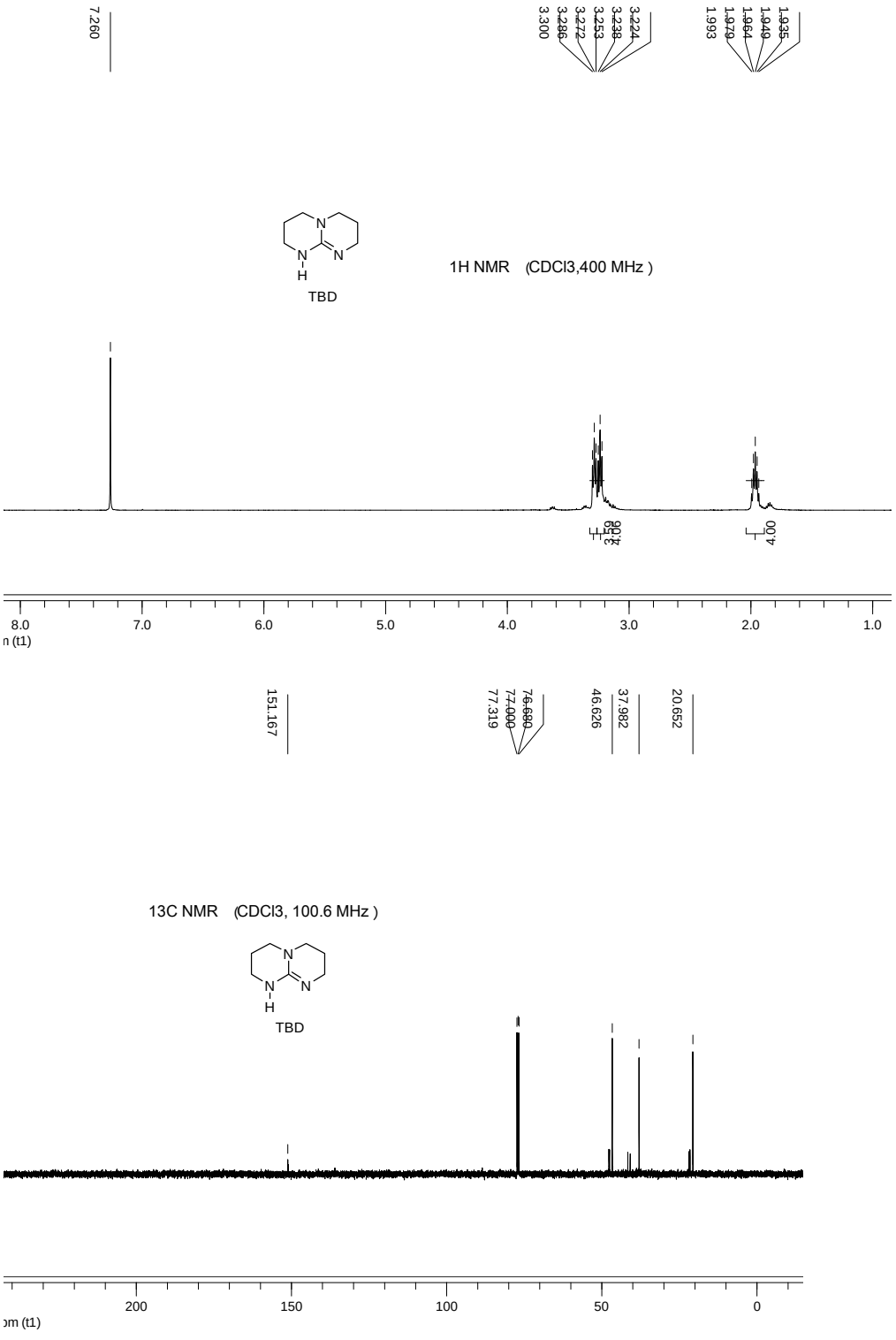

Transmittance [%]
100
90
80
70
60
50
40
3375.62
2870.23
1636.63
1457.51
1350.87
1297.72
1249.61
1107.35
951.56
845.50
735.35
559.32
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


7.260
3.703
3.691
3.641
3.628
3.601
3.589
3.304
3.290
3.276
3.244
3.227
3.214
3.203
2.496
1.840
1.825
1.811
1.796
1.781
1.653
1.570
DBU/PEG600 + CO2
1H NMR (CDCl3, 400 MHz)
5.40
2.12
3.79
1.91
1.80
3.84
2.00
7.0
6.0
5.0
4.0
3.0
2.0
m (t1)

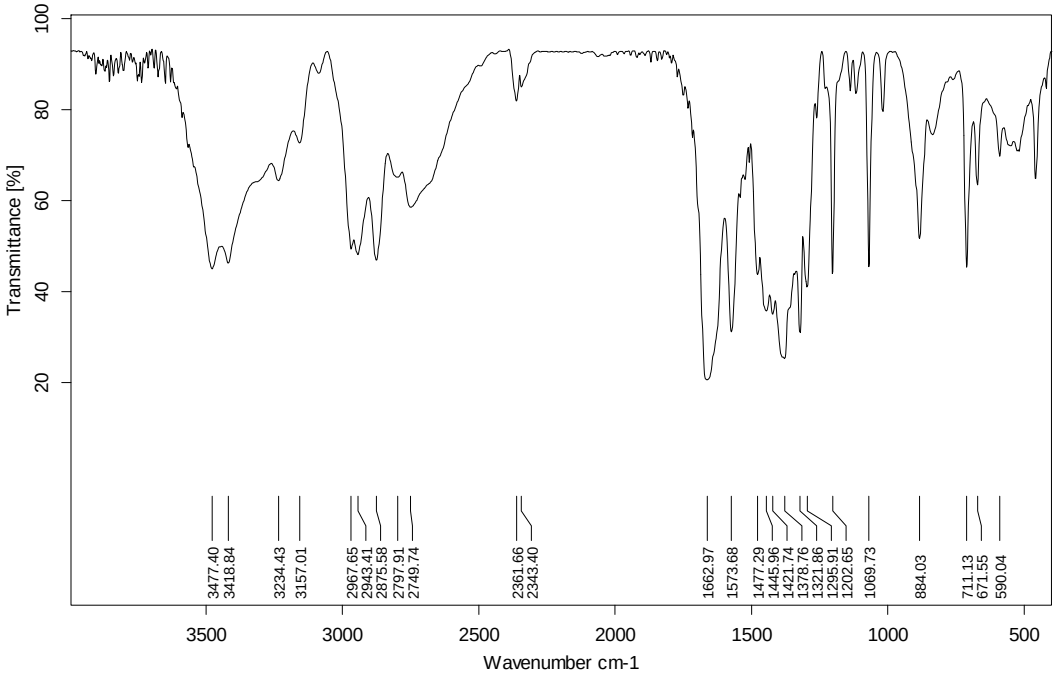


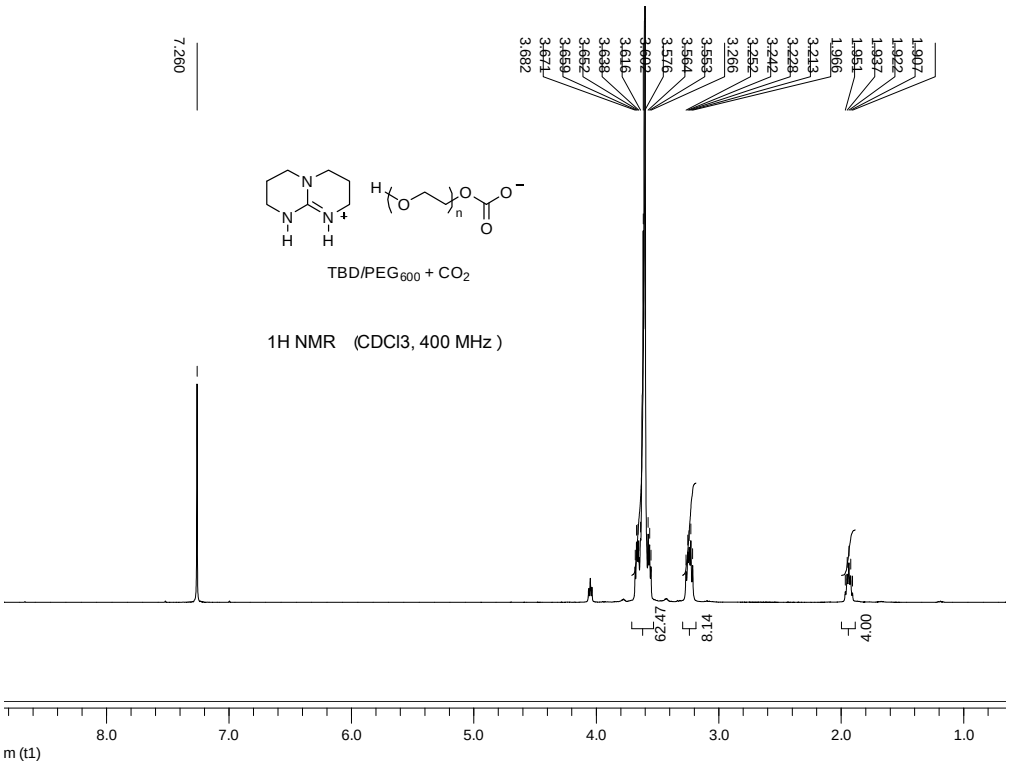
IR spectrum of DBU/PEG$_{600}$ + CO$_2$:

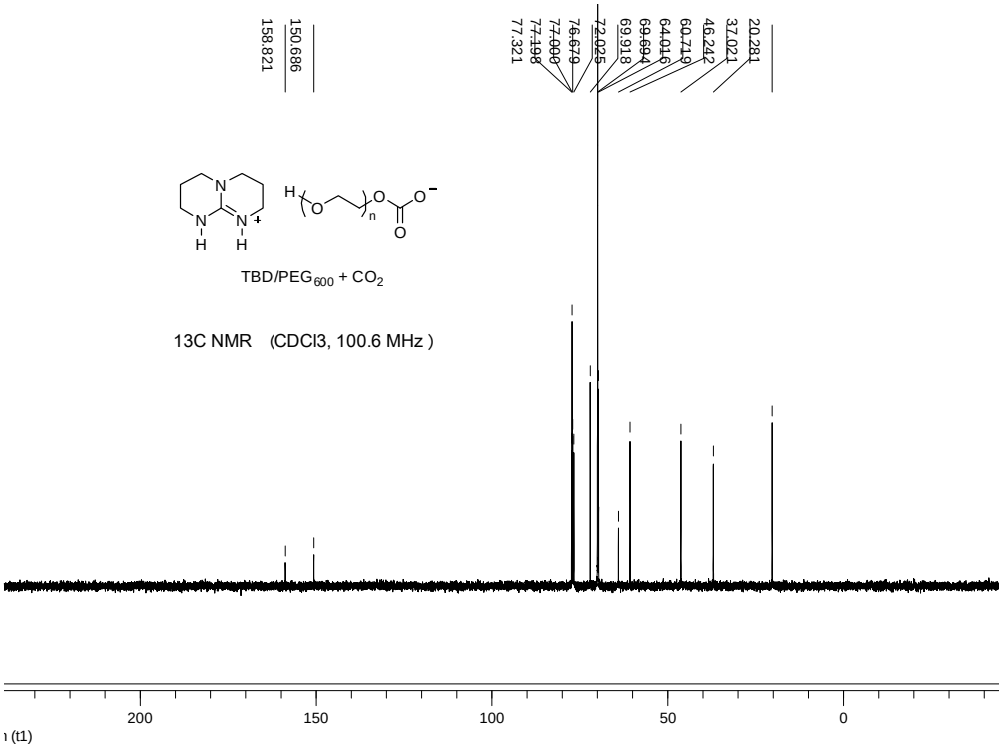




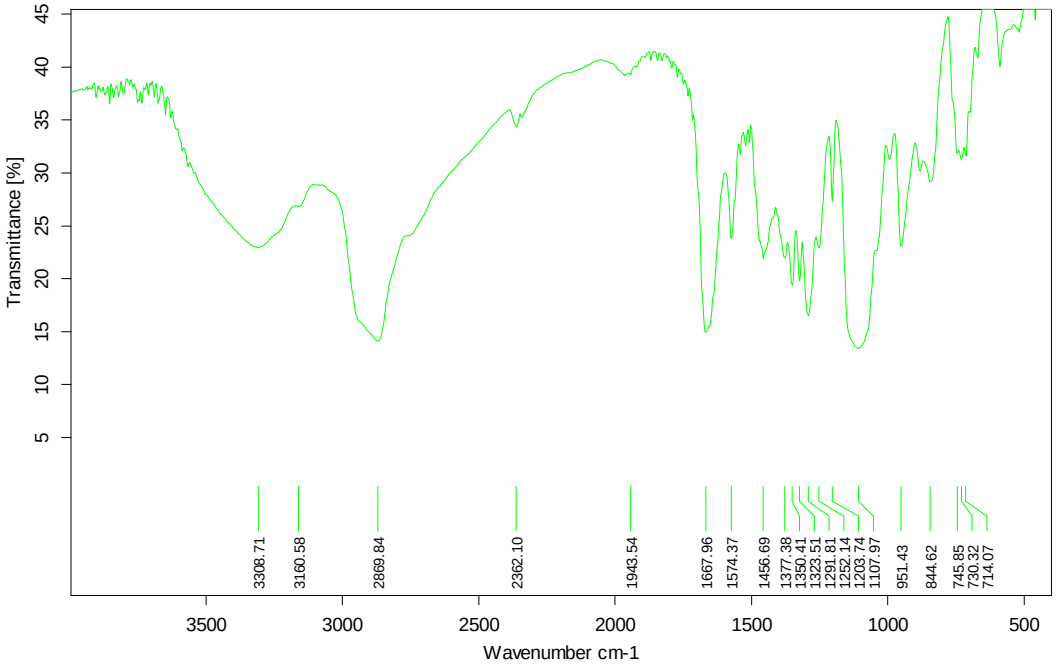
IR spectrum of TBD:

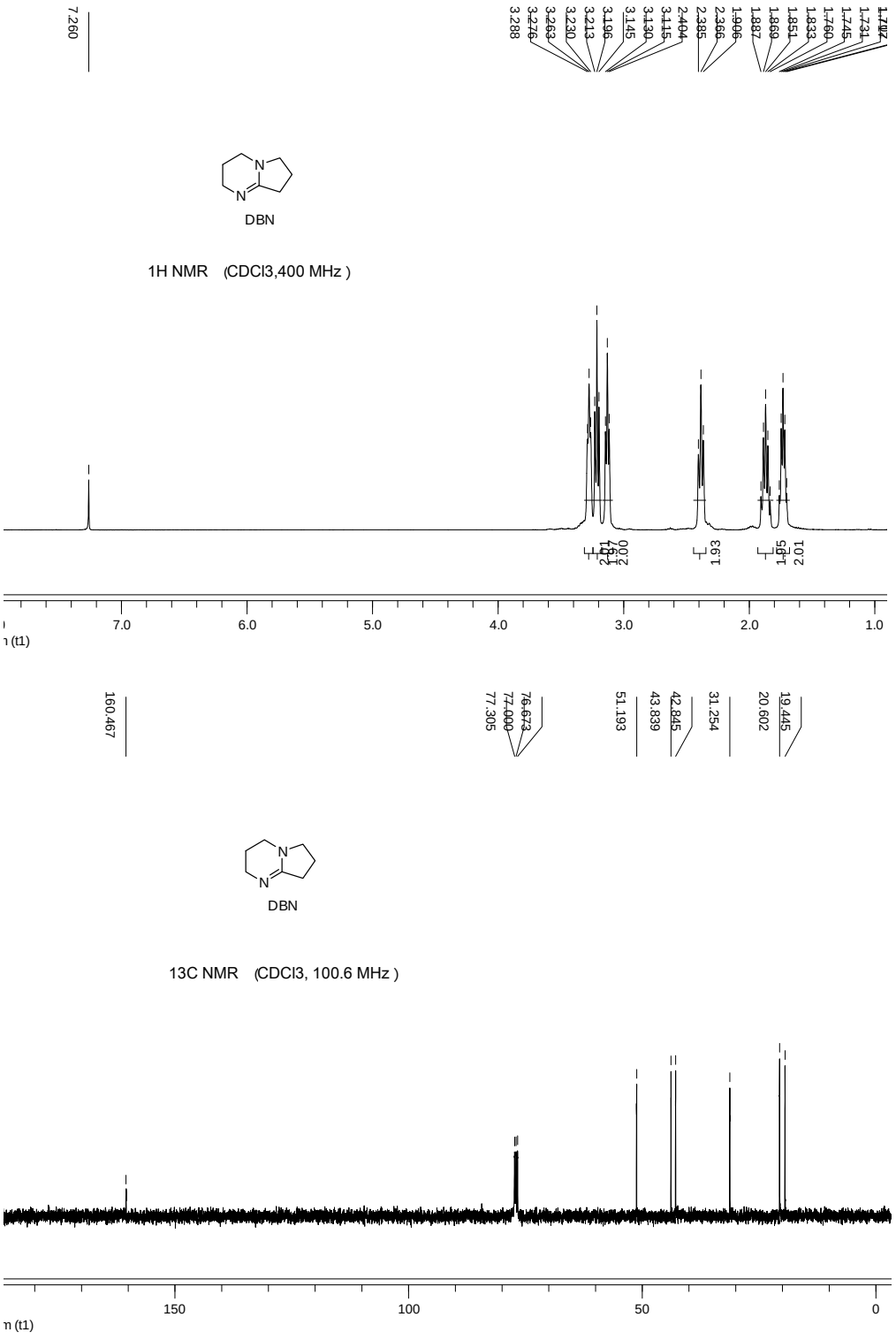

Transmittance [%]
100
80
60
40
20
3477.40
3418.84
3234.43
3157.01
2967.65
2943.41
2875.58
2797.91
2749.74
2361.66
2343.40
1662.97
1573.68
1477.29
1445.96
1421.74
1378.76
1321.86
1295.91
1202.65
1069.73
884.03
711.13
671.55
590.04
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1


7.260
3.689
3.671
3.659
3.650
3.638
3.616
3.602
3.576
3.564
3.553
3.226
3.252
3.242
3.228
3.213
1.690
1.651
1.637
1.622
1.607
TBD/PEG600 + CO2
1H NMR (CDCl3, 400 MHz)
62.47
8.14
4.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
m (t1)

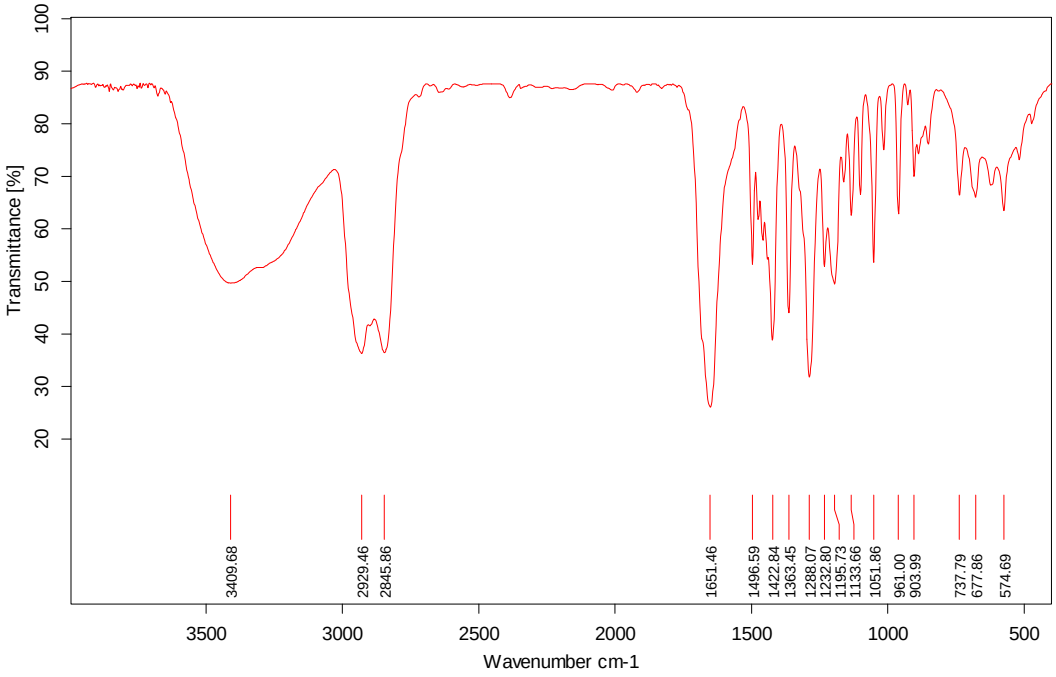


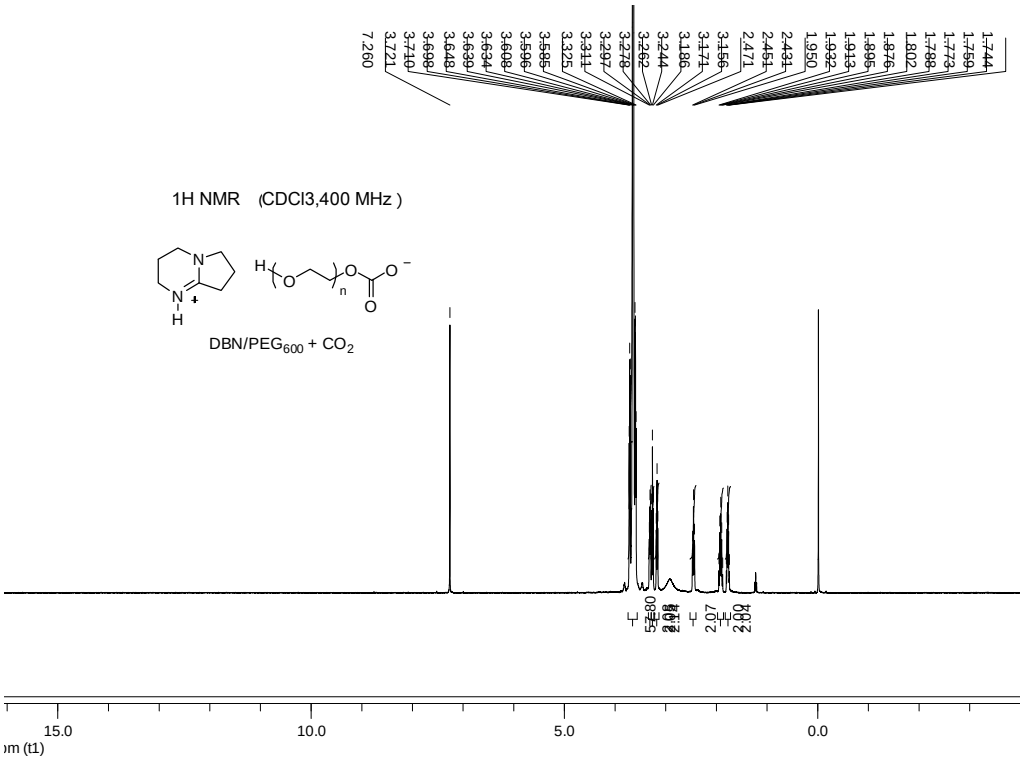
IR spectrum of TBD/PEG$_{600}$ + CO$_2$:

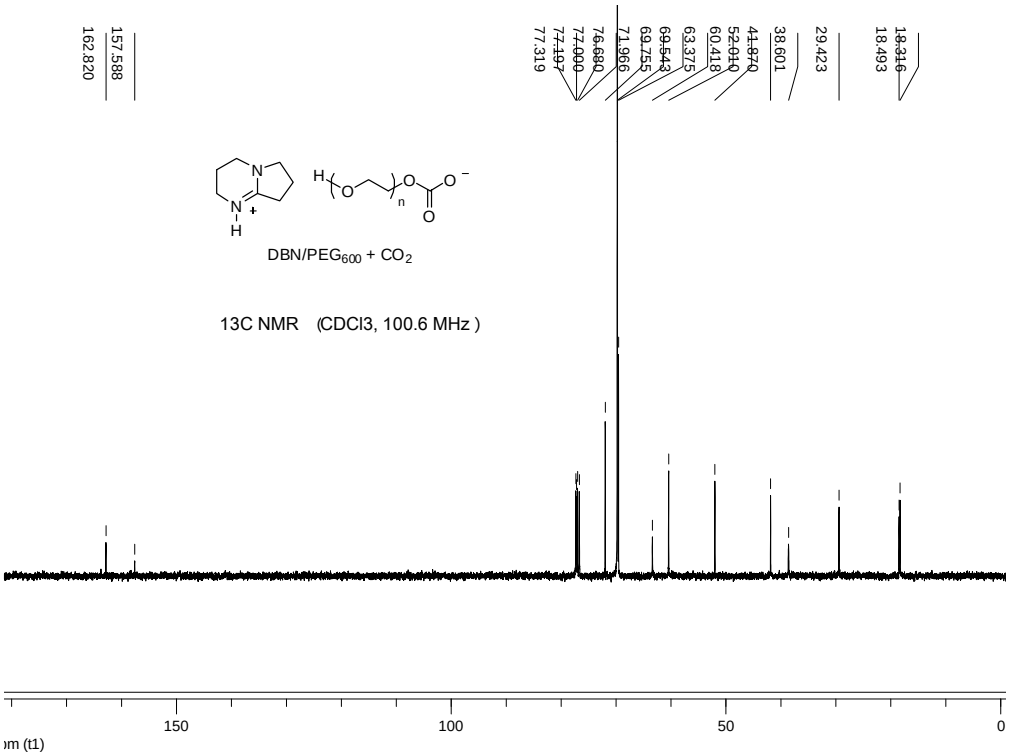




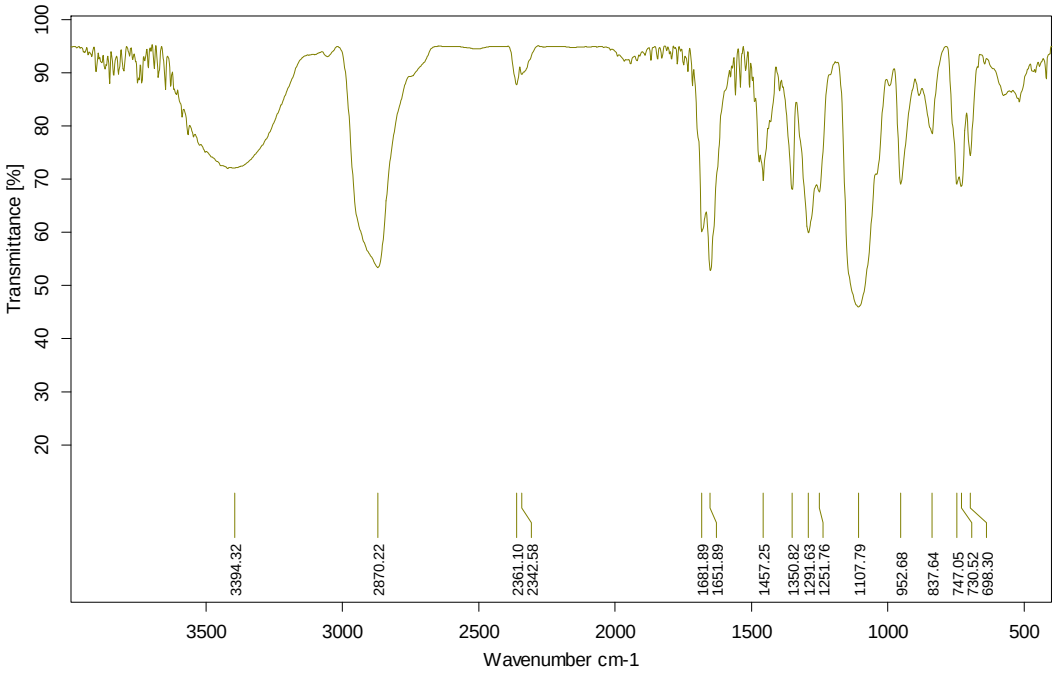
IR spectrum of DBN:

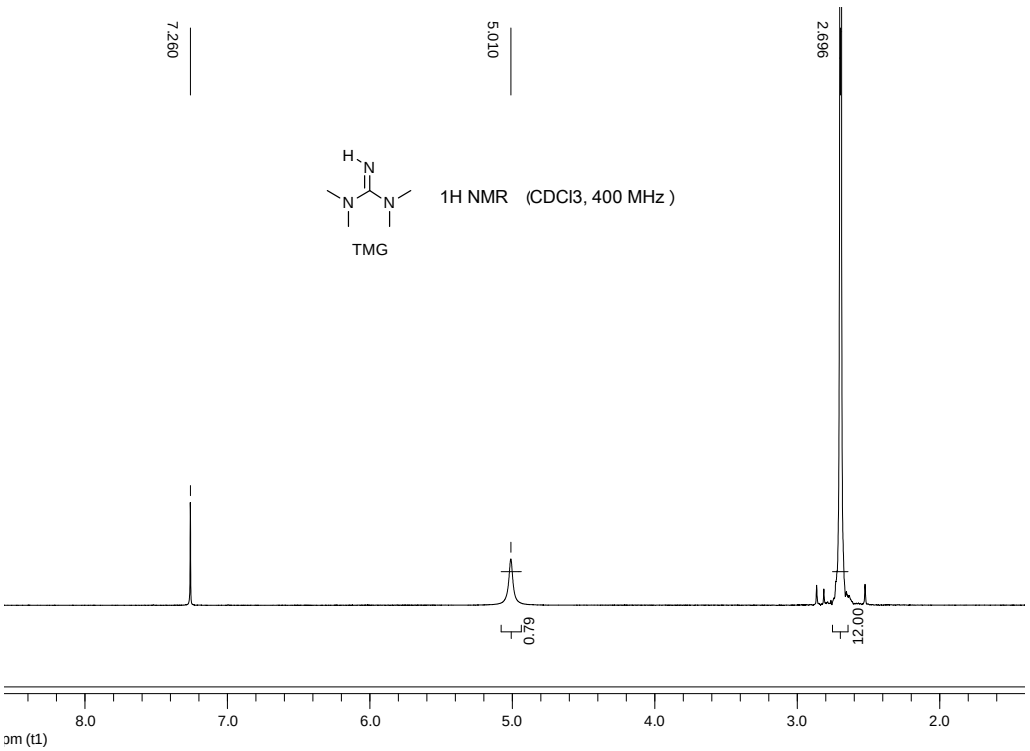

Transmittance [%]
100
90
80
70
60
50
40
30
20
3409.68
2929.46
2845.86
1651.46
1496.59
1422.84
1363.45
1288.07
1232.80
1195.73
1133.66
1051.86
961.00
903.99
737.79
677.86
574.69
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

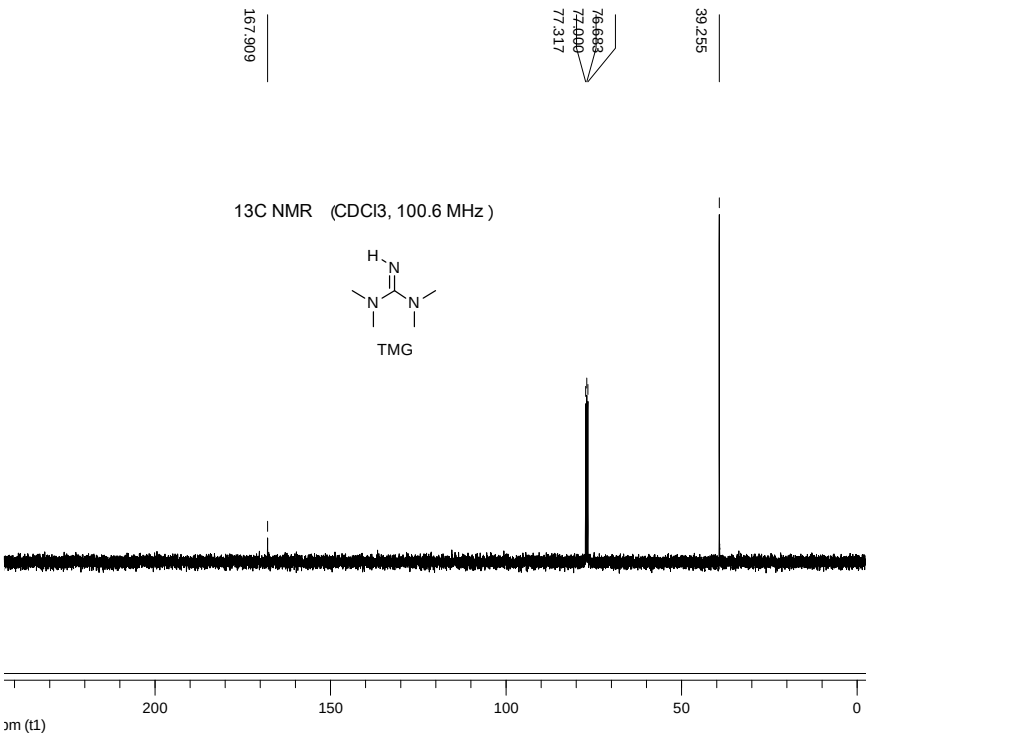

1H NMR (CDCl3,400 MHz)
DBN/PEG600 + CO2
15.0
10.0
5.0
0.0



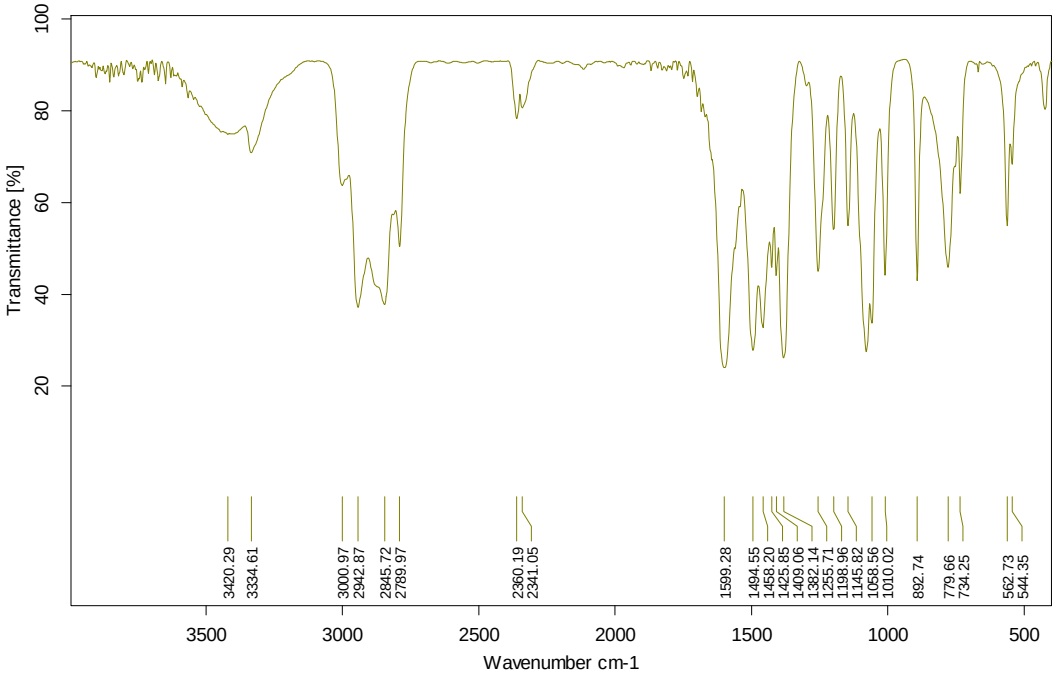
IR spectrum of DBN/PEG$_{600}$ + CO$_2$:

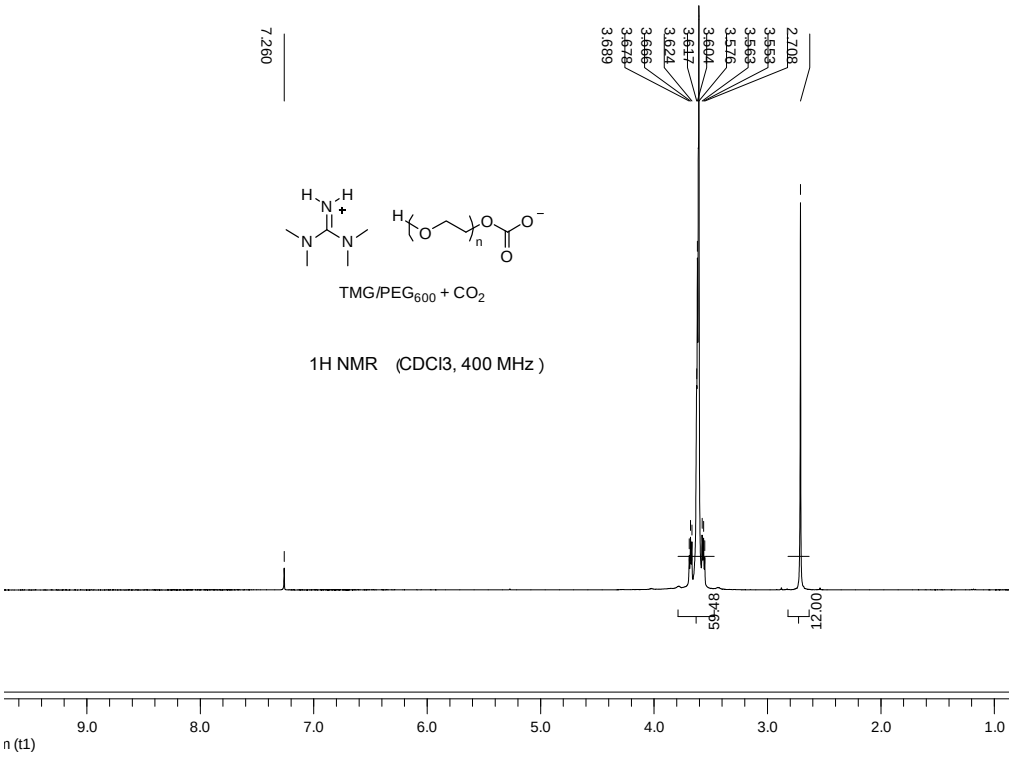


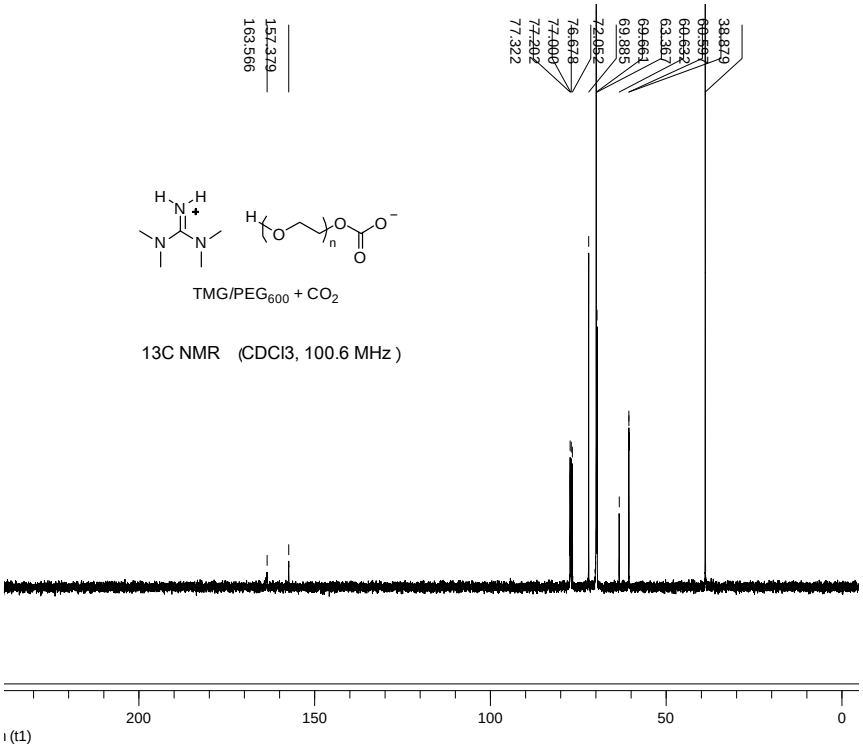




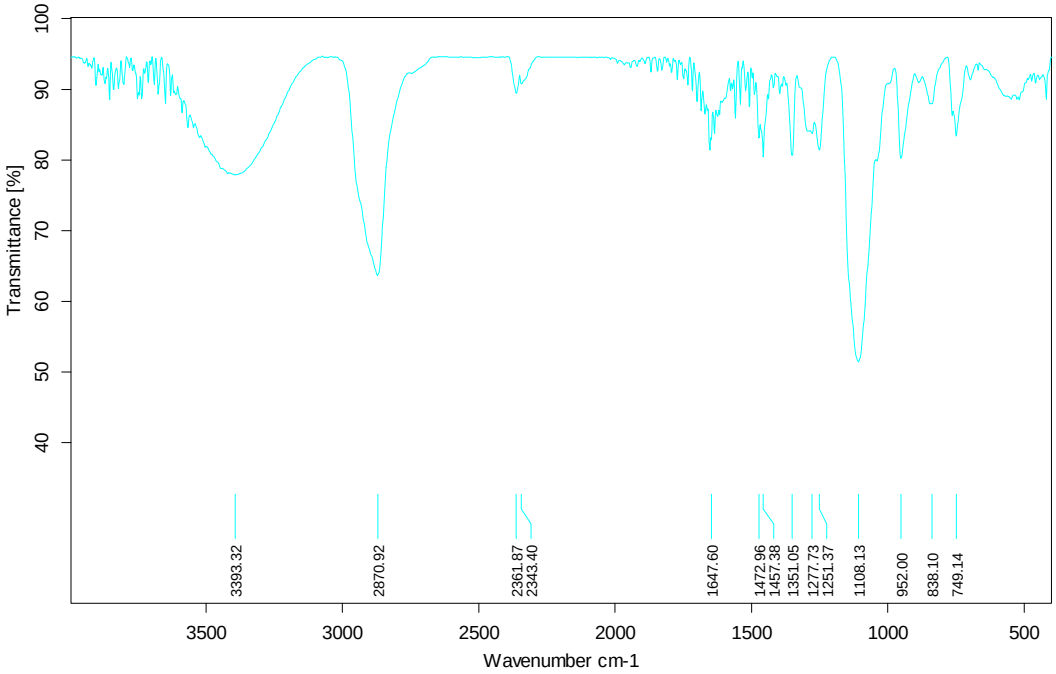
IR spectrum of TMG:

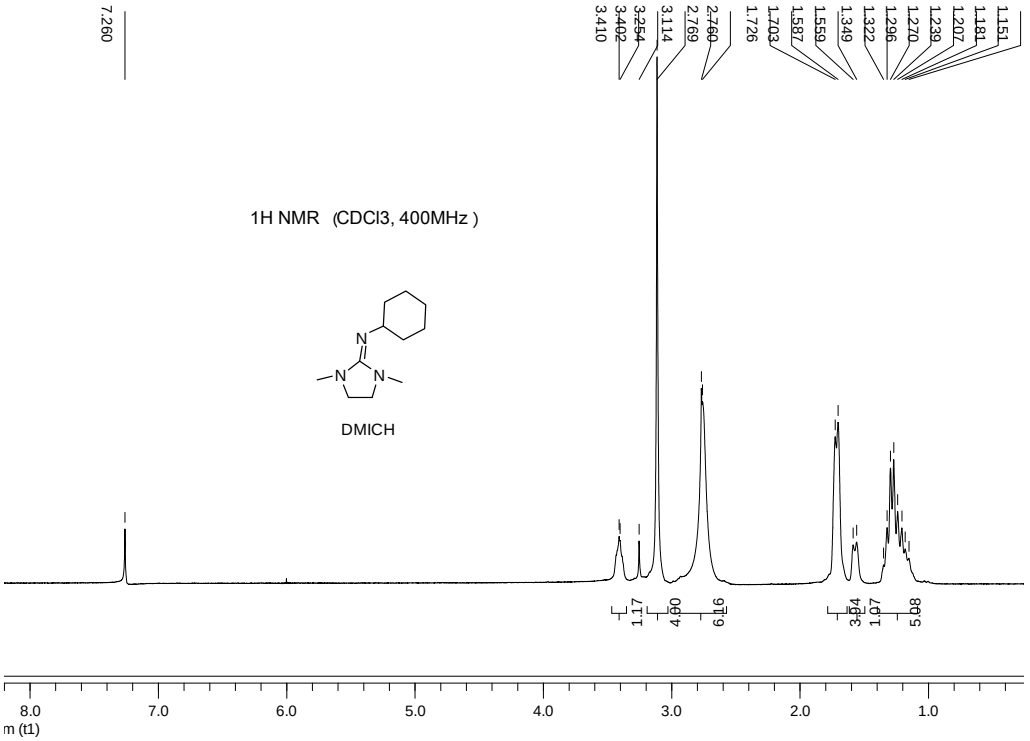

Transmittance [%]
100
80
60
40
20
3420.29
3334.61
3000.97
2942.87
2845.72
2789.97
2360.19
2341.05
1599.28
1494.55
1458.20
1425.85
1409.06
1382.14
1255.71
1198.96
1145.82
1058.56
1010.02
892.74
779.66
734.25
562.73
544.35
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

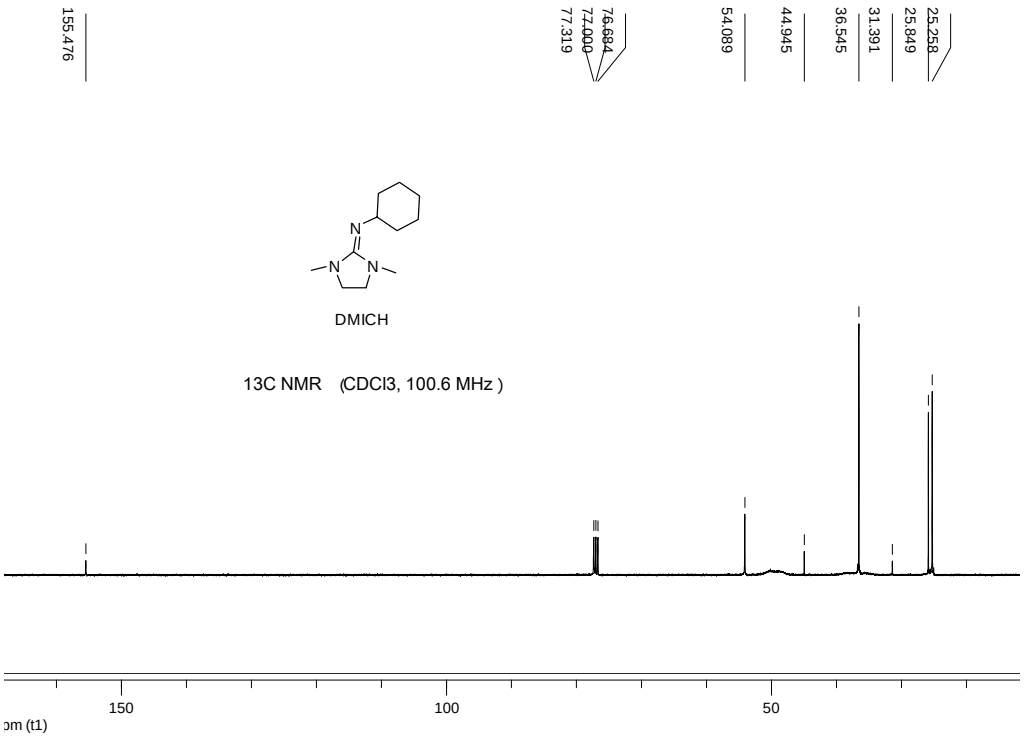

7.260
3.689
3.678
3.666
3.624
3.617
3.604
3.576
3.553
3.542
2.708
TMG/PEG600 + CO2
1H NMR (CDCl3, 400 MHz)
59.48
12.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
n (t1)

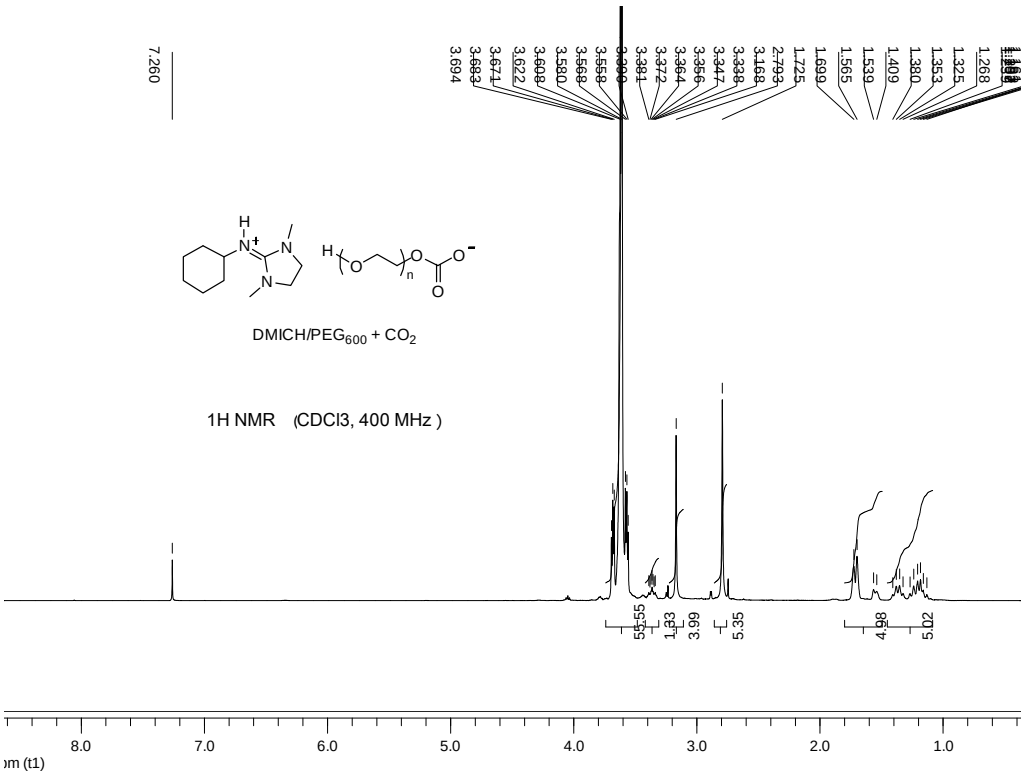


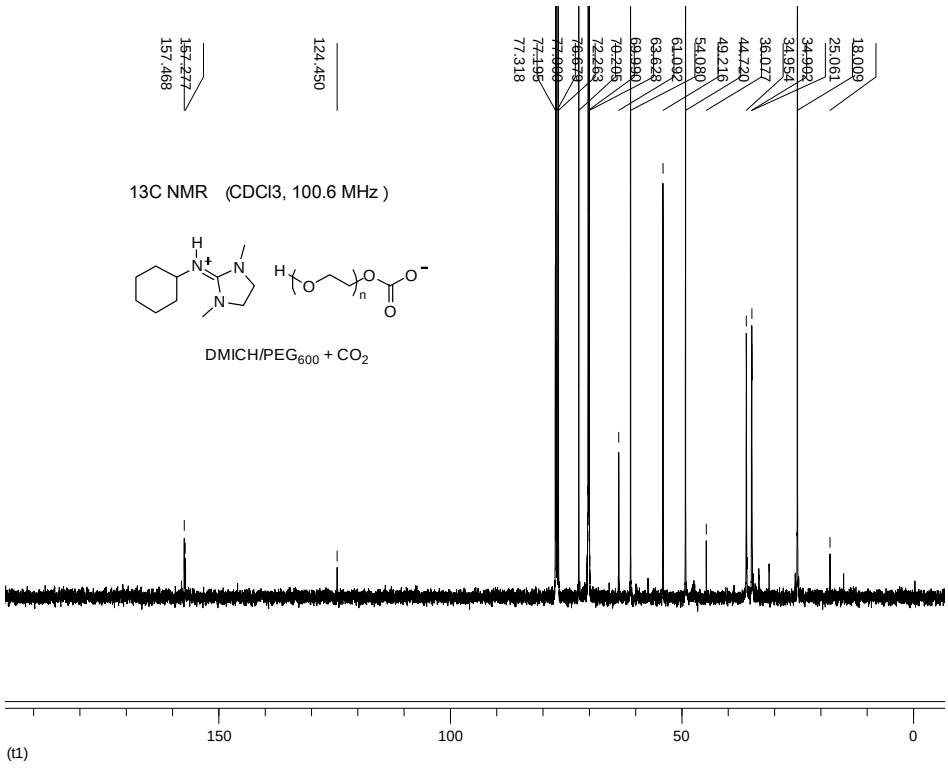
IR spectrum of TMG/PEG$_{600}$ + CO$_2$:



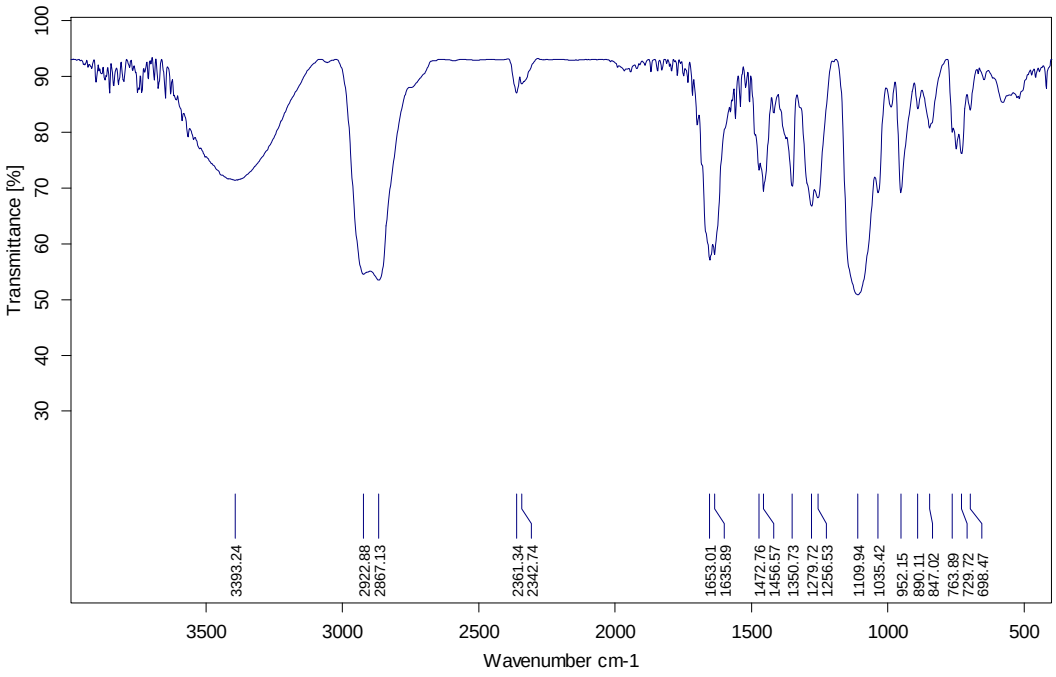

7.260
3.410
3.402
3.254
3.114
2.769
2.760
1.726
1.703
1.587
1.559
1.349
1.322
1.296
1.270
1.239
1.207
1.181
1.151
1H NMR (CDCl3, 400MHz)
DMICH
1.17
4.50
6.16
3.44
1.07
5.68
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
m (t1)

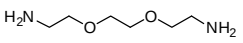

155.476
77.319
77.000
76.684
54.089
44.945
36.545
31.391
25.849
25.258
DMICH
13C NMR (CDCl3, 100.6 MHz)
150
100
50
pm (t1)



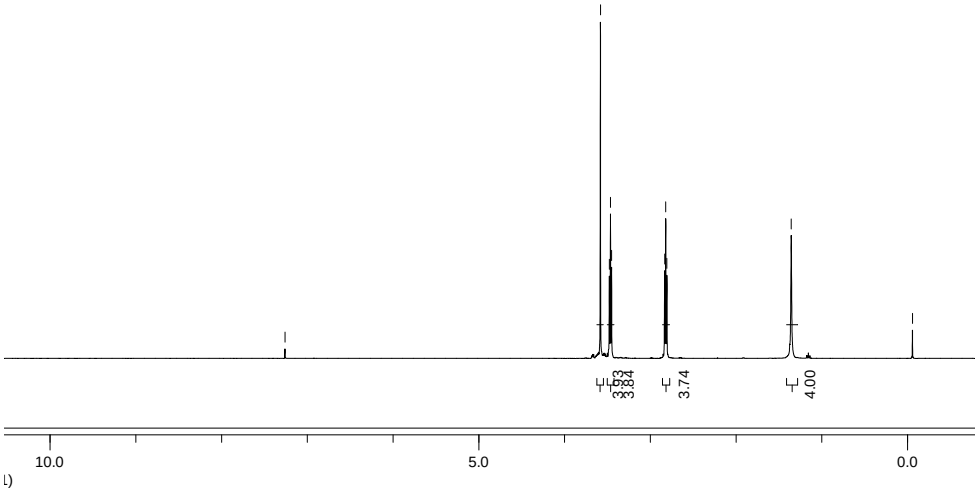


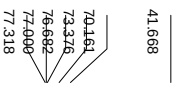
IR spectrum of DMICH/PEG$_{600}$ + CO$_2$:

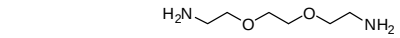




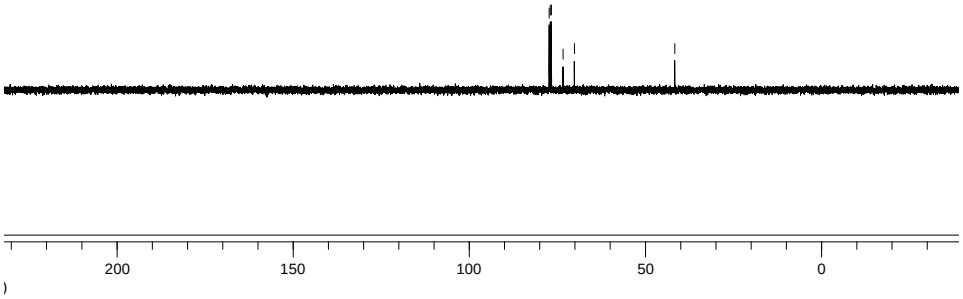
1H NMR (400 MHz,CDCl3)



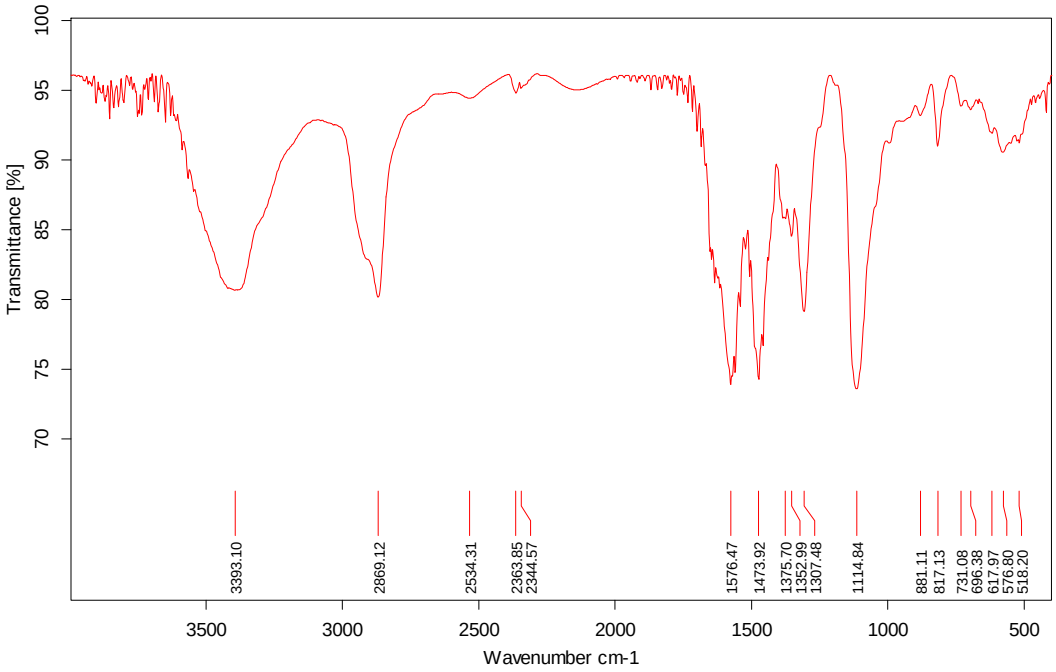


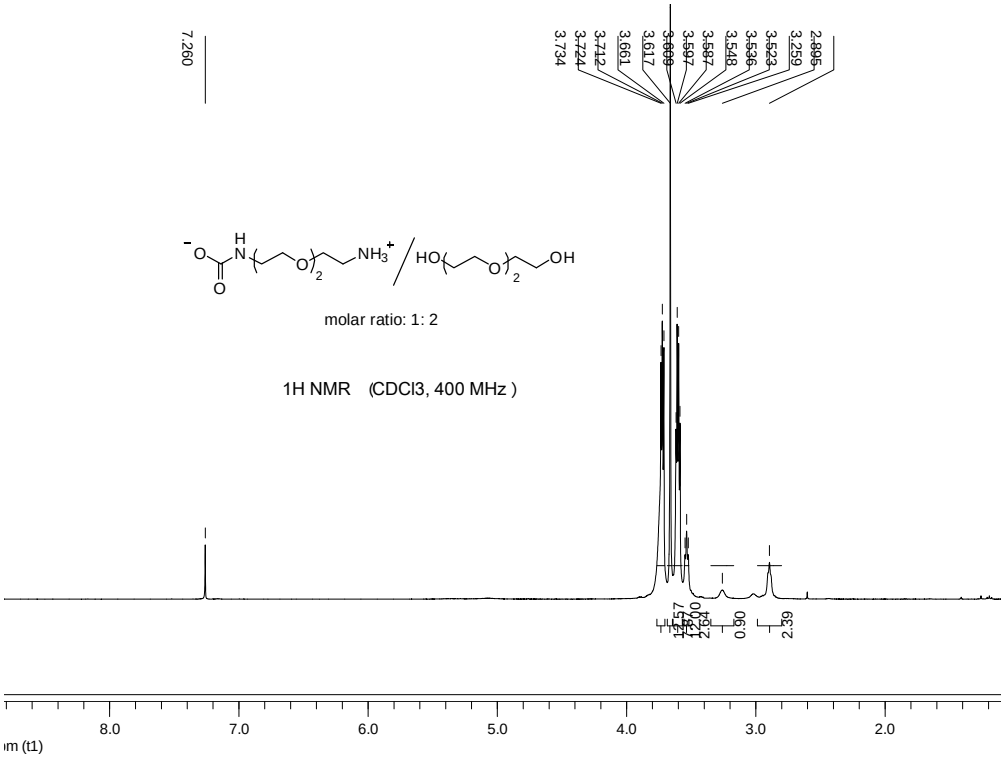


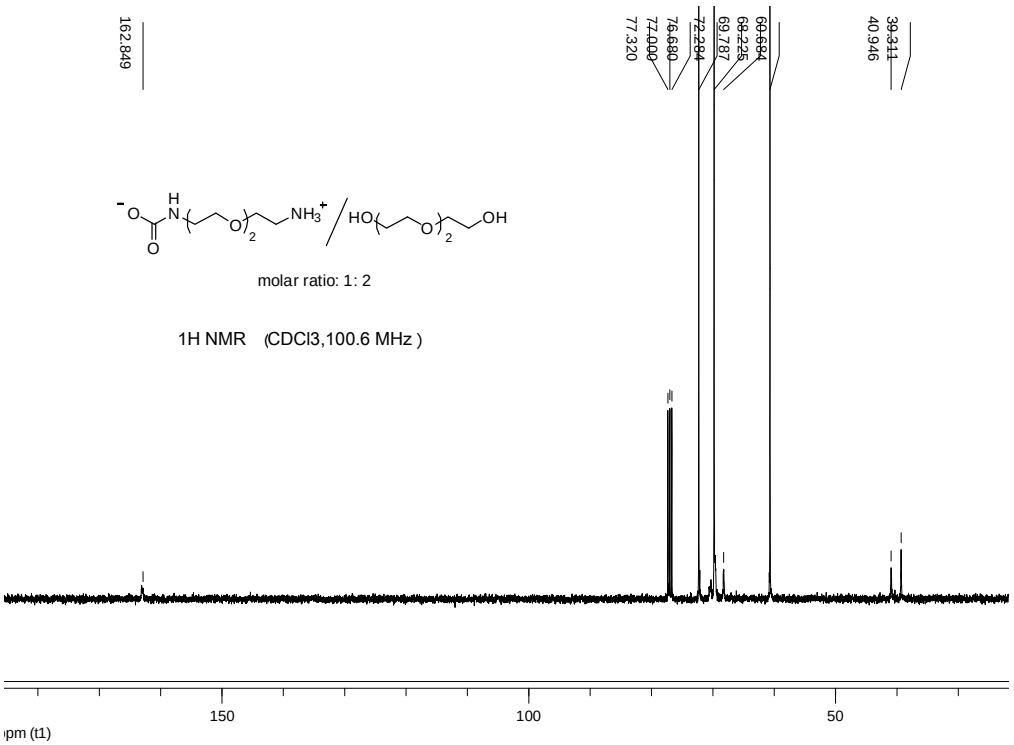
13C NMR (CDCl3,100.6 MHz)



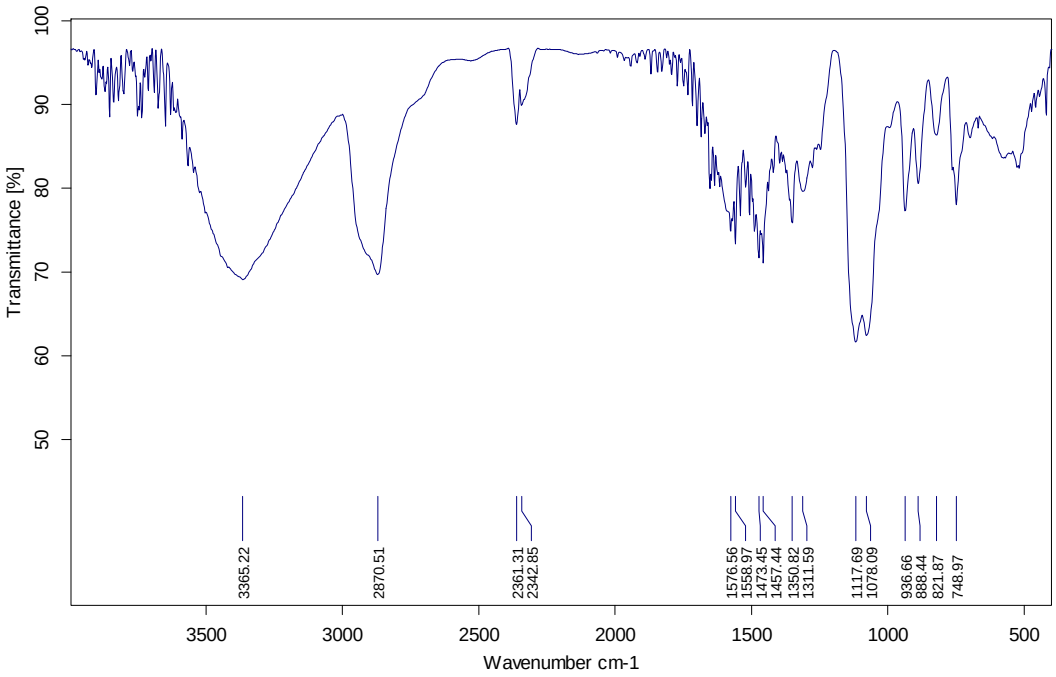
IR spectrum of $NH_2PEG_{150}NH_2$:



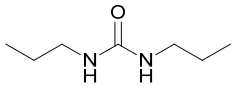




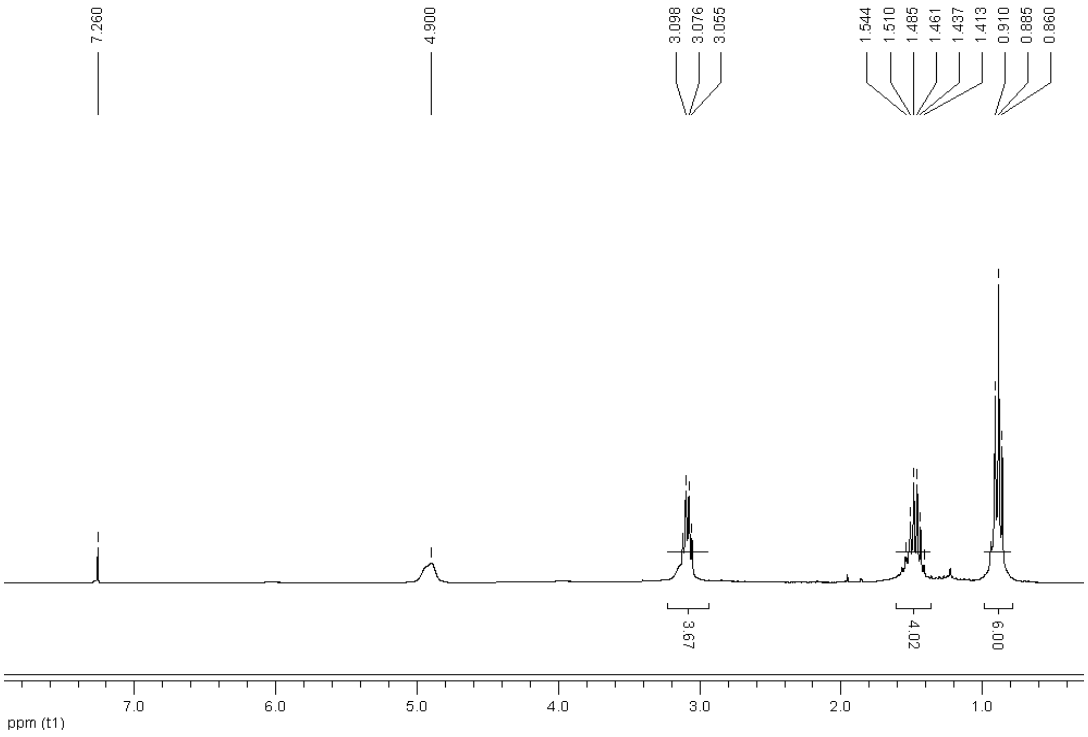
IR spectrum of $NH_2PEG_{150}NH_2/PEG_{150}$ (molar ratio: 1: 2) + CO_2:



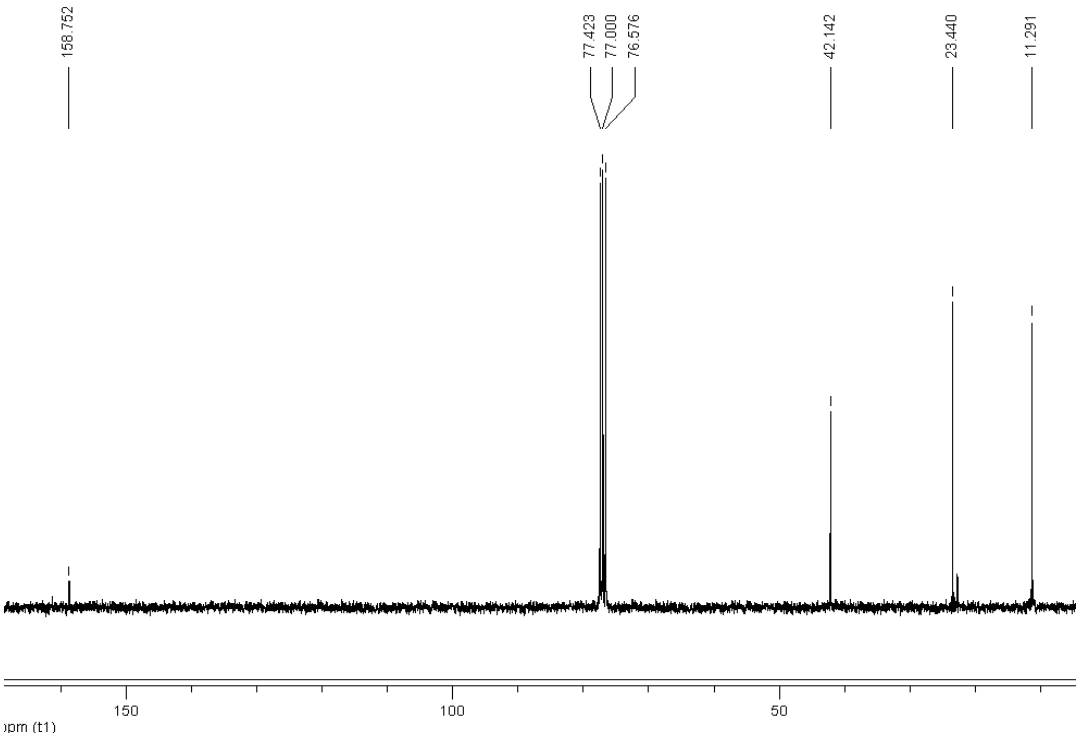
1,3-Dipropyl urea:



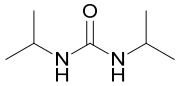
^{1}H NMR ($CDCl_3$, 300 MHz)



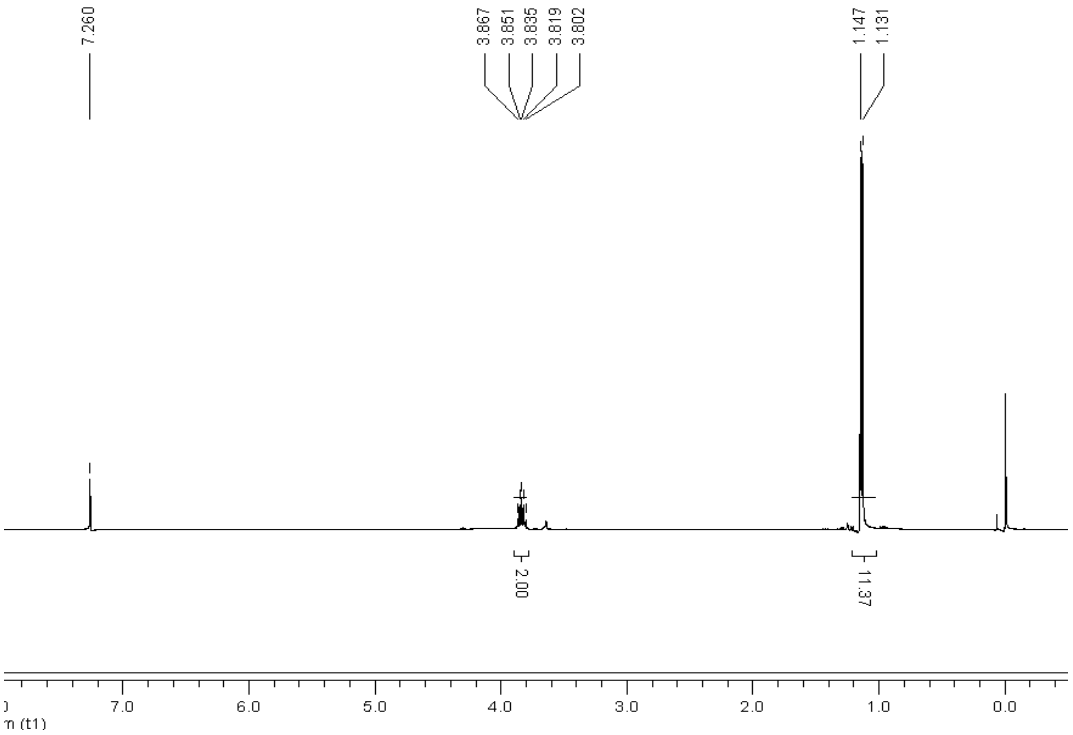
^{13}C NMR ($CDCl_3$, 75.5 MHz)



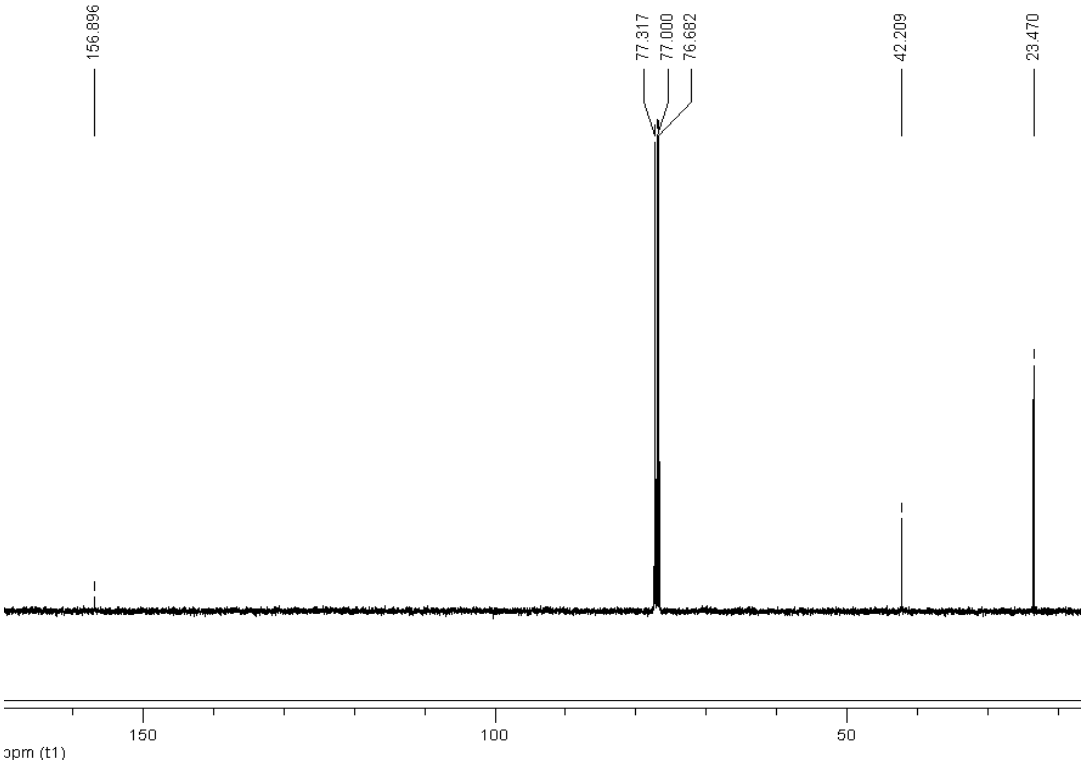
1,3-Diisopropyl-urea:

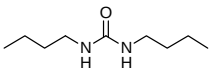


^{1}H NMR ($CDCl_3$, 300 MHz)

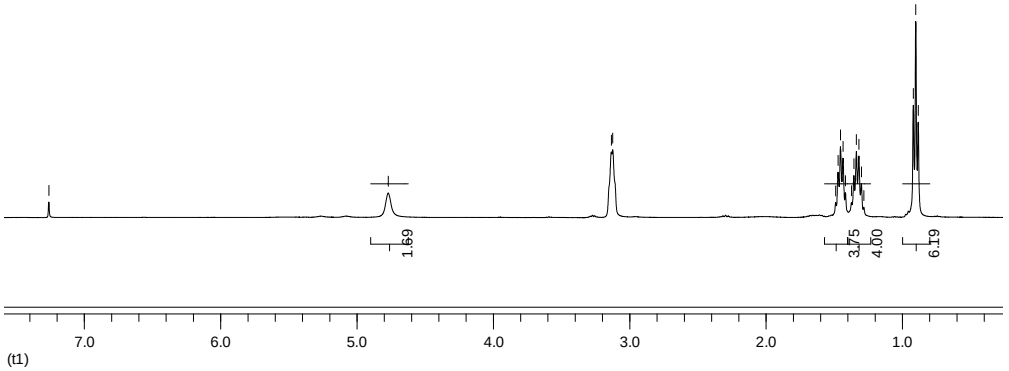


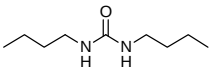
^{13}C NMR ($CDCl_3$, 75.5 MHz)



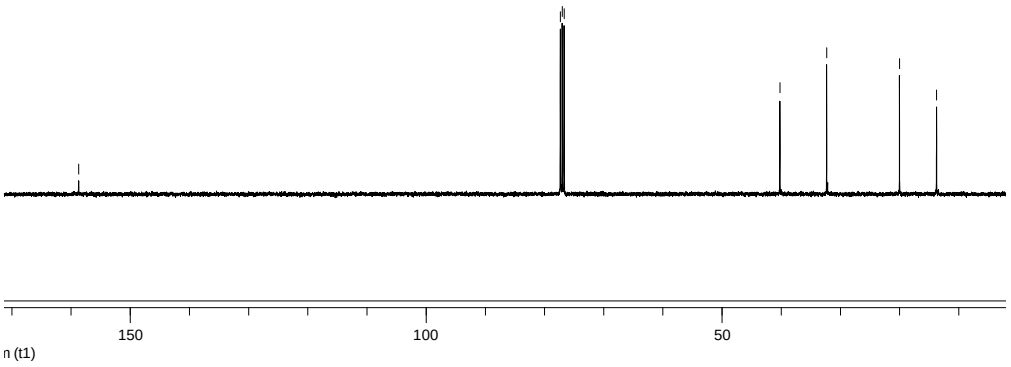


1H NMR (CDCl3,400 MHz)

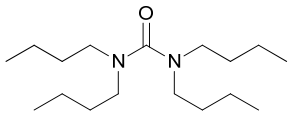




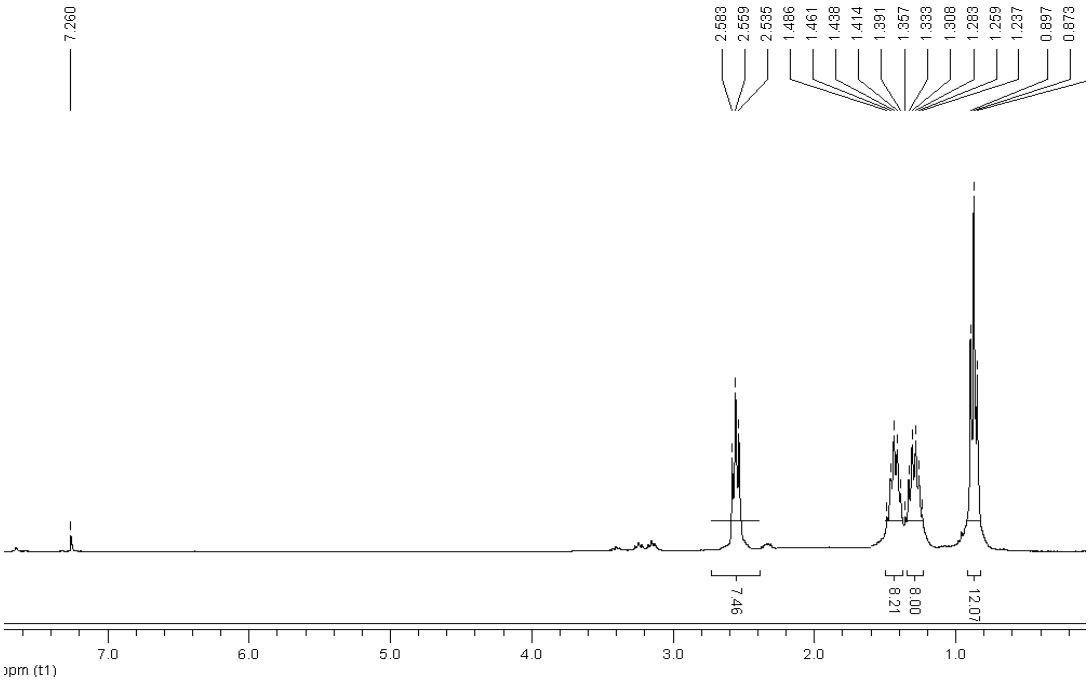
13C NMR (100.6 MHz,CDCl3)



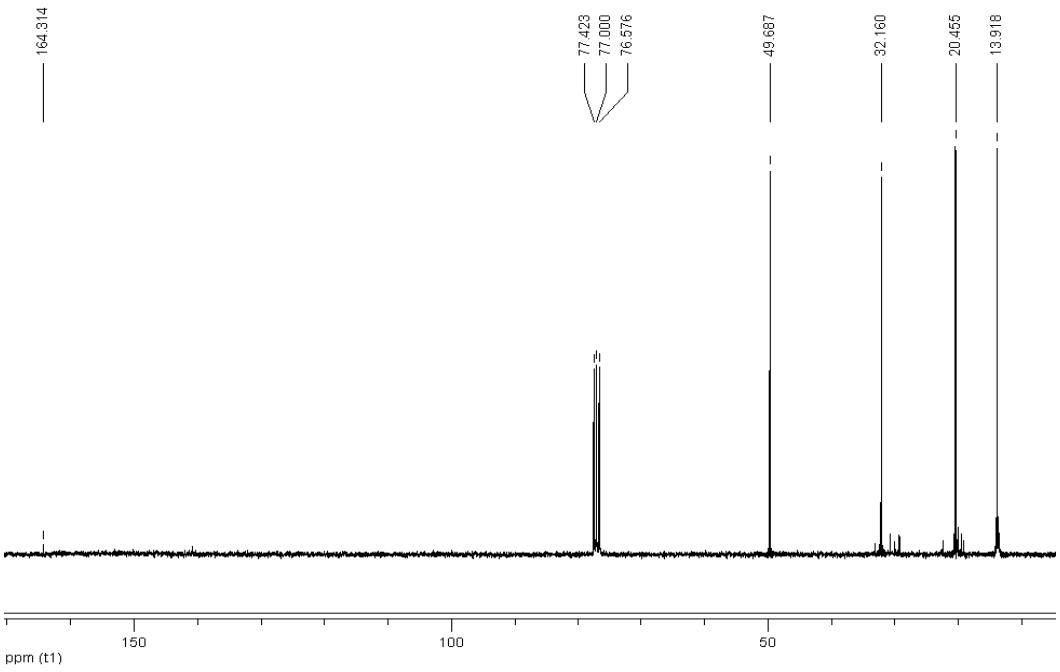
1,1,3,3-Tetrabutyl urea:



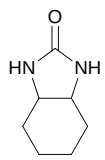
^{1}H NMR ($CDCl_3$, 300 MHz)



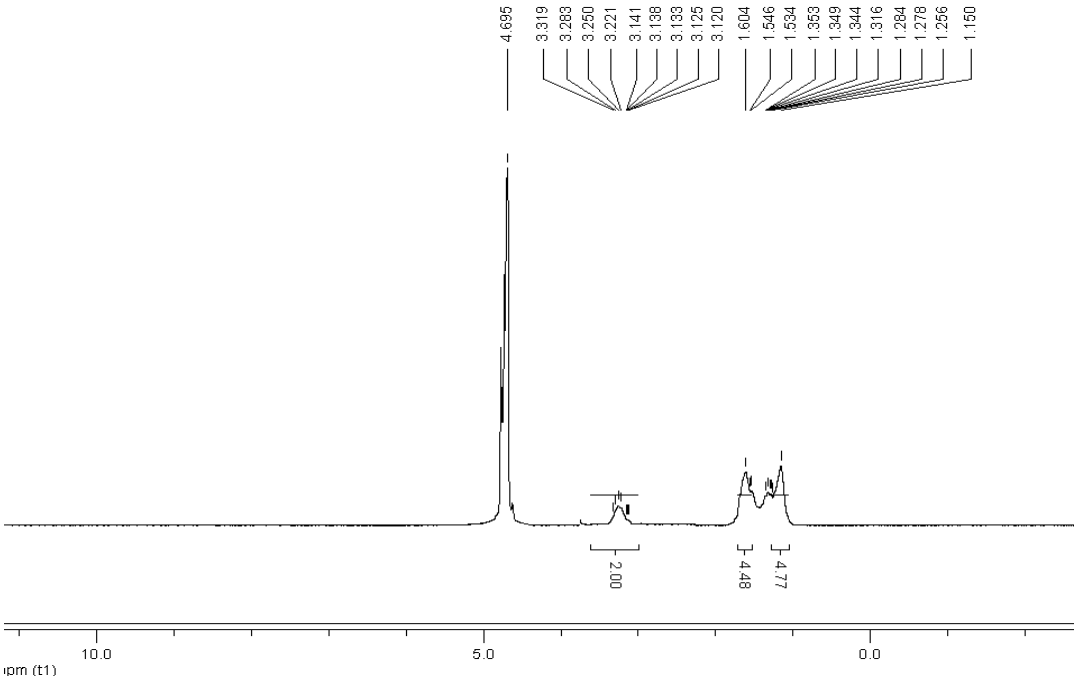
^{13}C NMR ($CDCl_3$, 75.5 MHz)



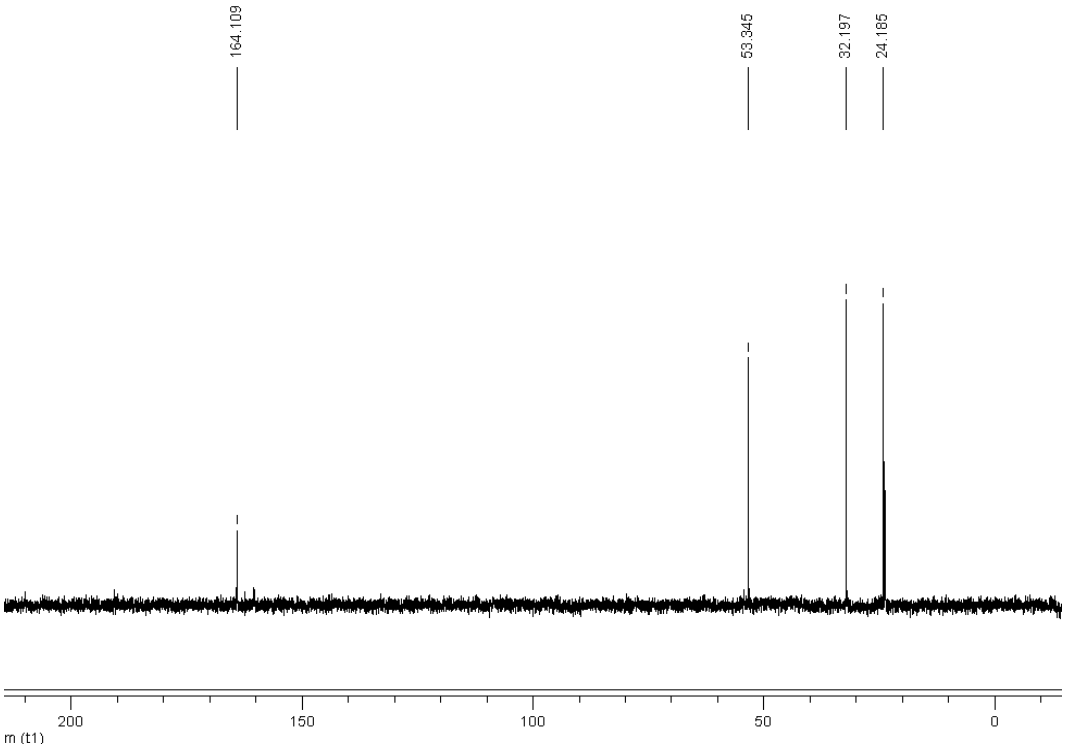
Octahydro-benzoimidazol-2-one:

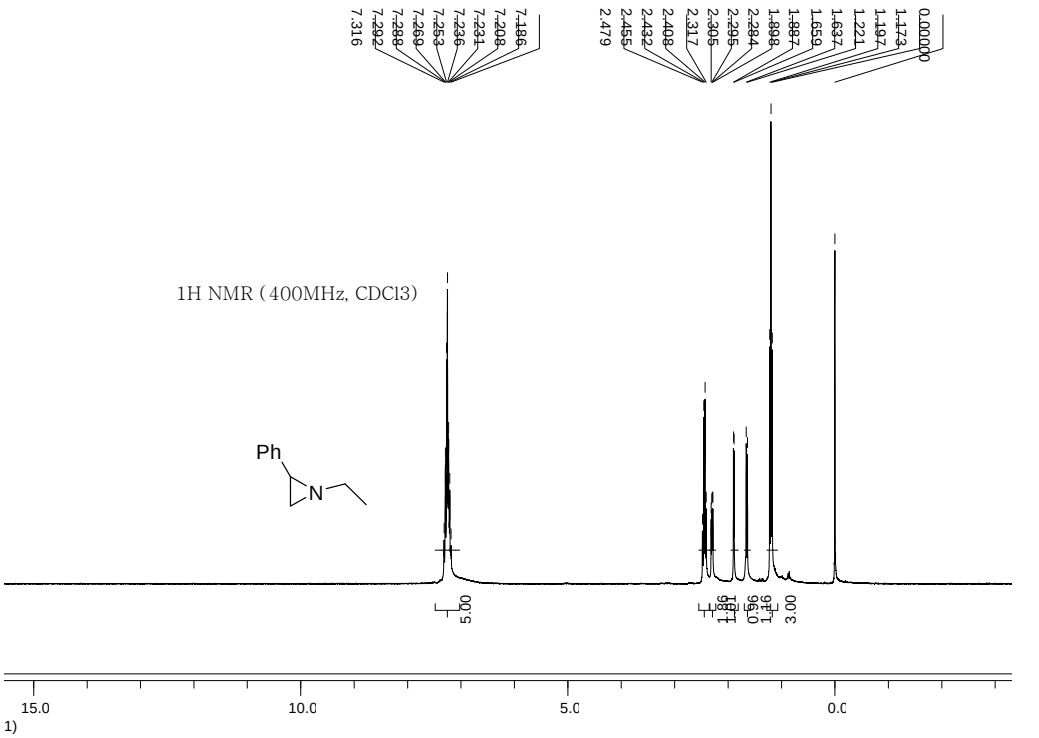


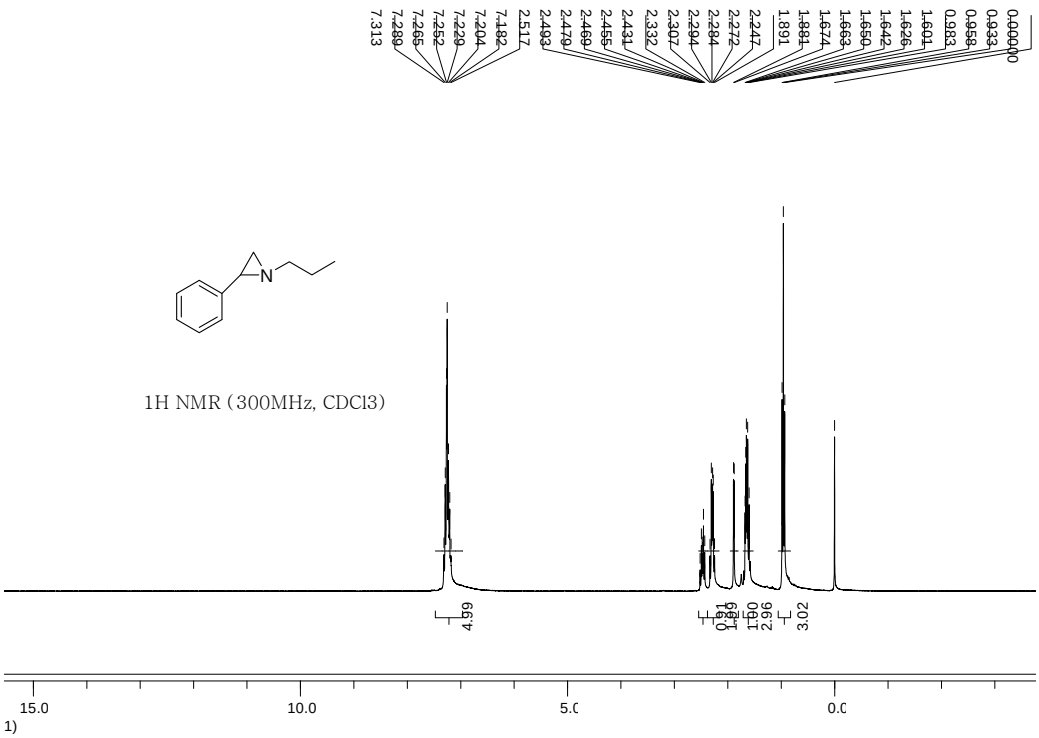
^{1}H NMR (D_2O, 300 MHz)

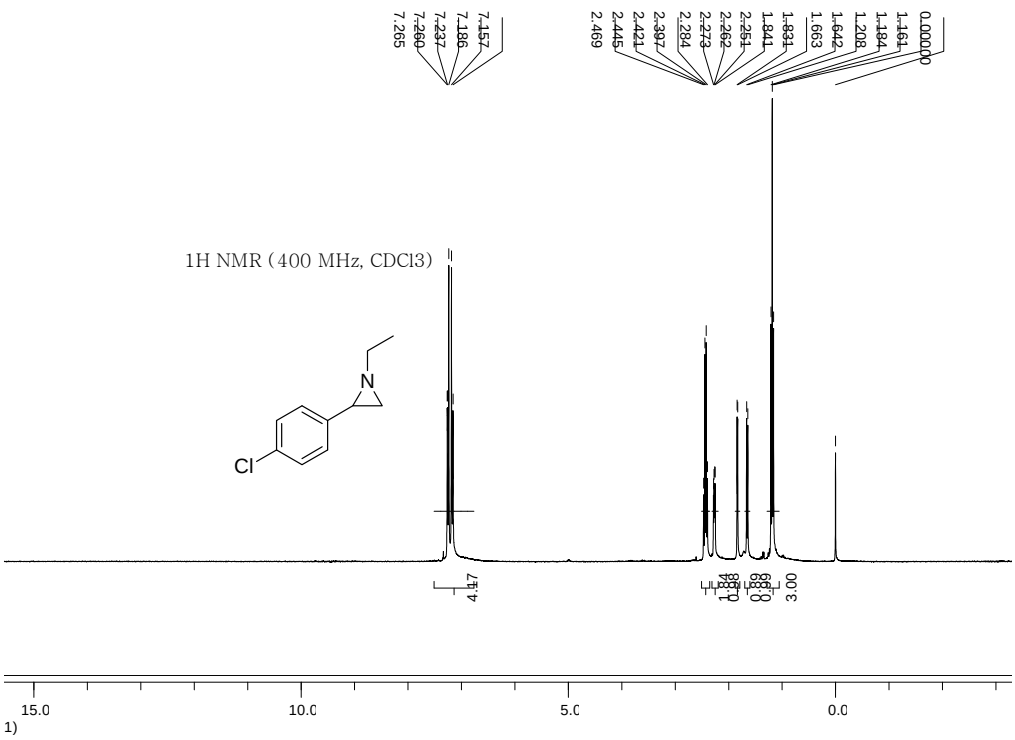


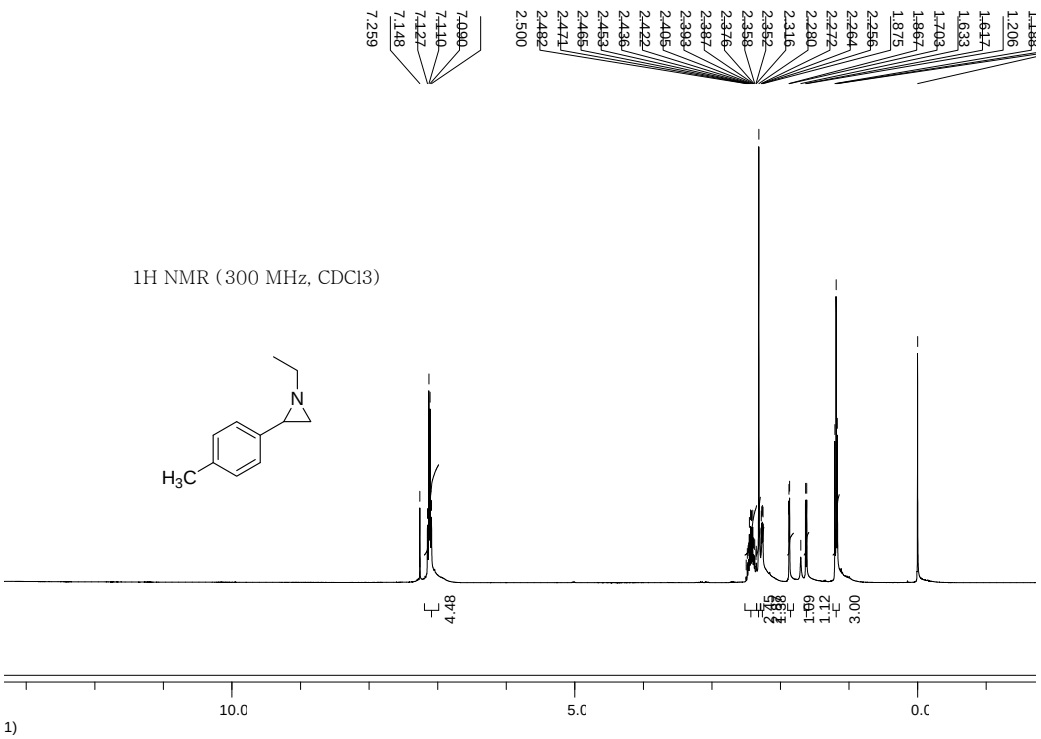
^{13}C NMR (D_2O, 75.5 MHz)

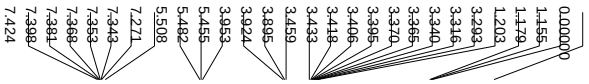


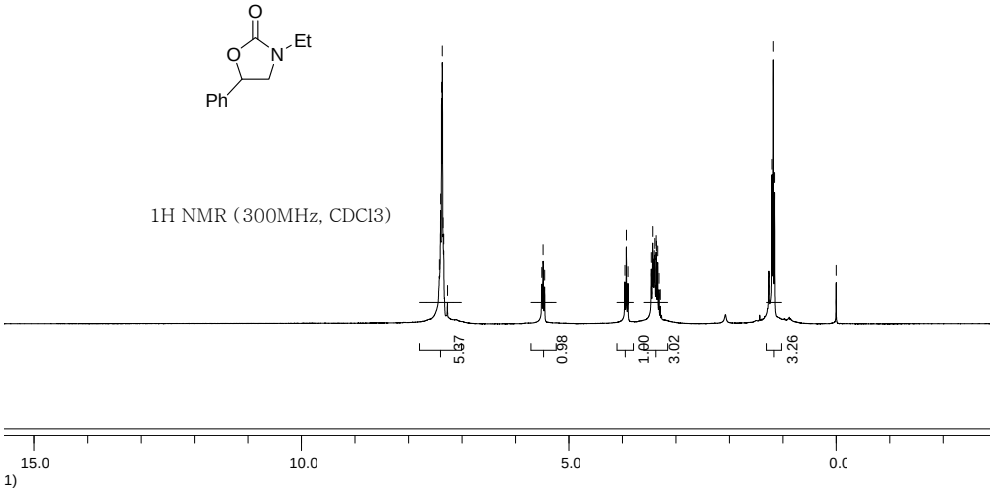

1H NMR (400MHz, CDCl3)
Ph
N
15.0
10.0
5.0
0.0

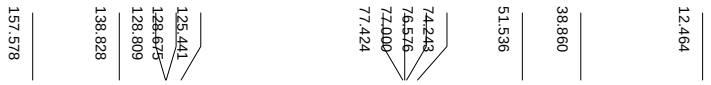

1H NMR (300MHz, CDCl3)
N
15.0
10.0
5.0
0.0

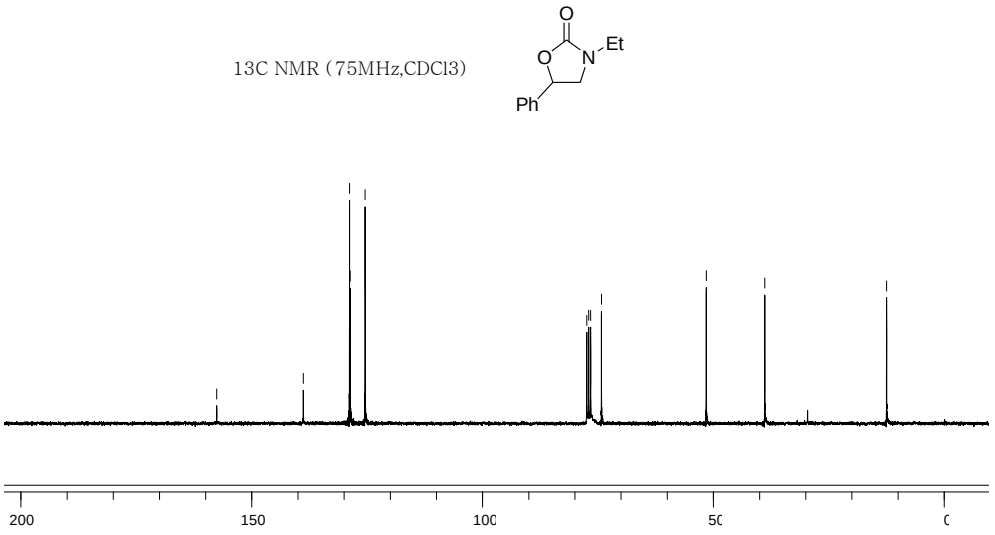

1H NMR (400 MHz, CDCl3)
N
Cl
7.265
7.260
7.237
7.186
7.157
2.469
2.445
2.421
2.397
2.284
2.273
2.262
2.251
1.841
1.831
1.663
1.642
1.208
1.184
1.161
0.00000
4.47
3.00
15.0
10.0
5.0
0.0
1)

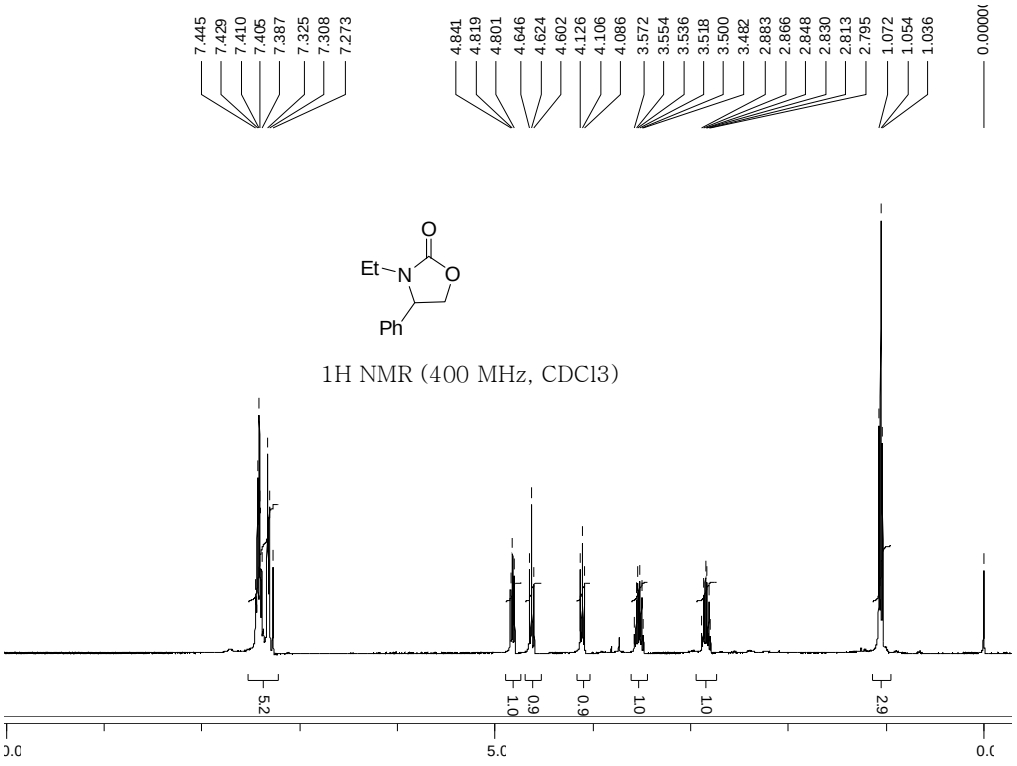

1H NMR (300 MHz, CDCl3)
N
H3C
7.259
7.148
7.127
7.110
7.090
2.500
2.482
2.471
2.465
2.453
2.436
2.422
2.405
2.392
2.387
2.376
2.358
2.352
2.316
2.280
2.272
2.264
2.256
1.875
1.867
1.703
1.633
1.617
1.206
4.48
3.00
10.0
5.0
0.0
1)

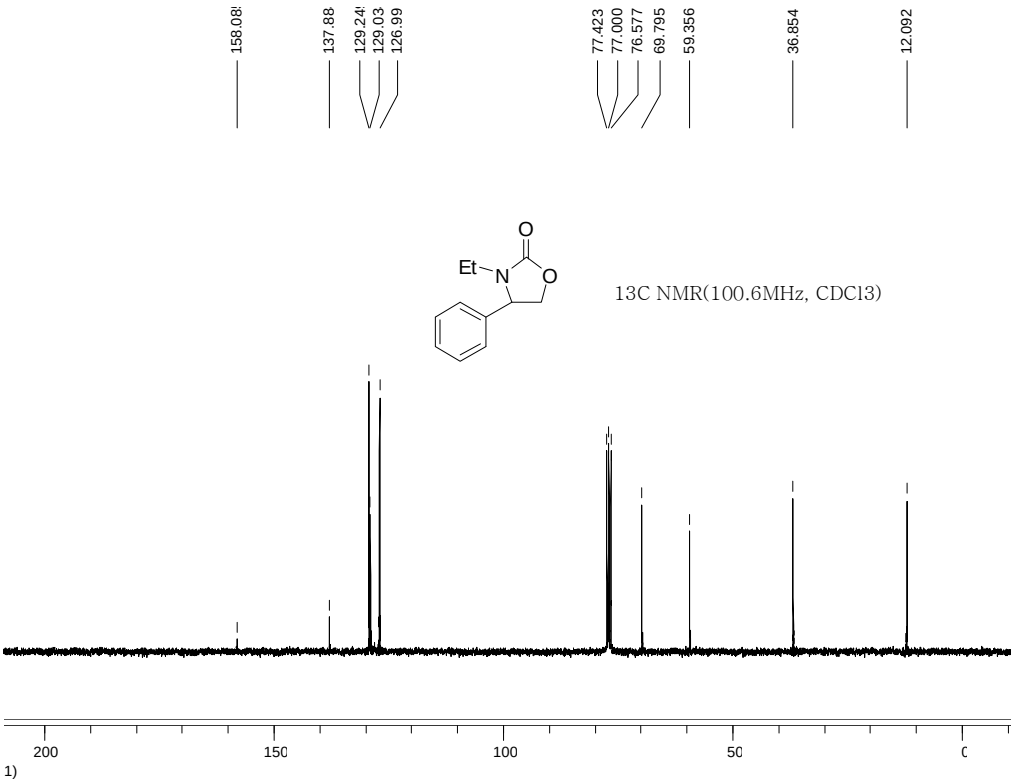

7.424
7.398
7.381
7.368
7.353
7.343
7.271
5.508
5.482
5.455
3.953
3.924
3.895
3.459
3.433
3.418
3.406
3.396
3.370
3.365
3.340
3.316
3.293
1.203
1.179
1.155
0.00000

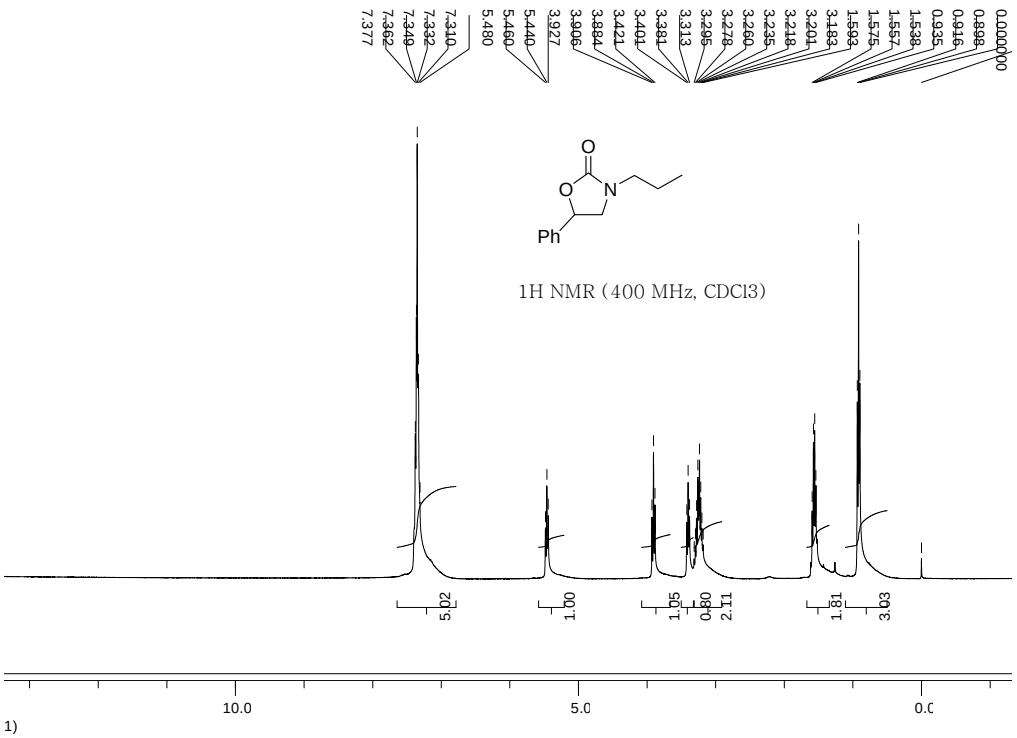

O
O
N
Et
Ph
1H NMR (300MHz, CDCl3)
4.57
0.98
1.00
3.02
3.26
15.0
10.0
5.0
0.0
1)

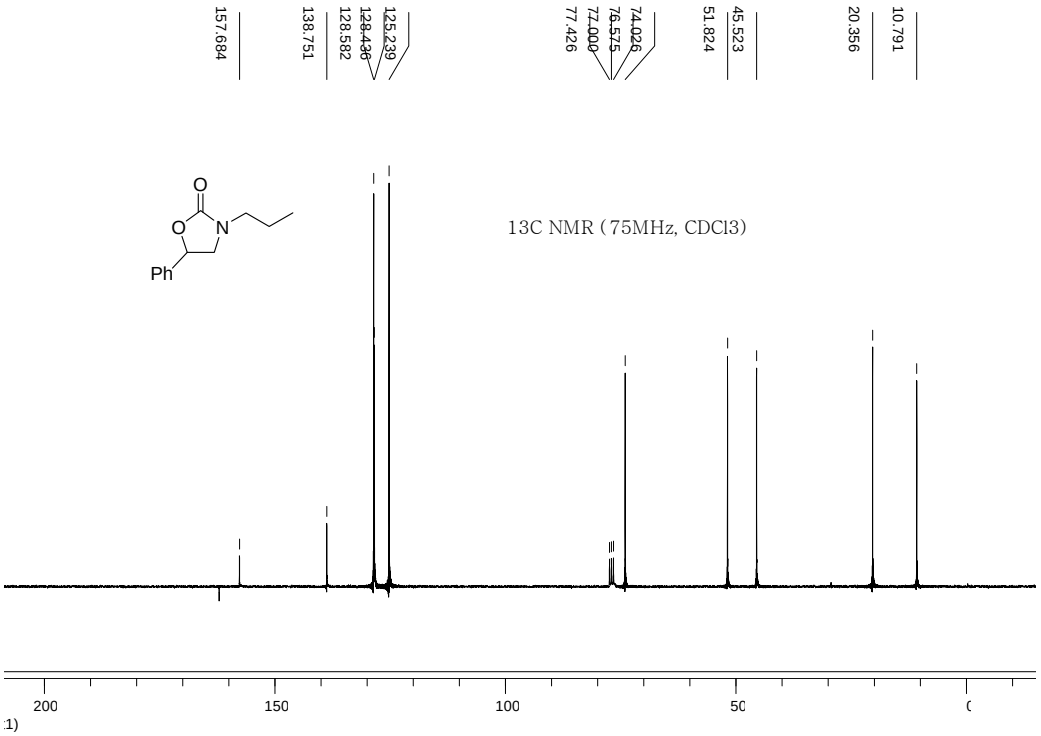

157.578
138.828
128.809
128.675
125.441
77.424
77.000
76.576
74.243
51.536
38.860
12.464

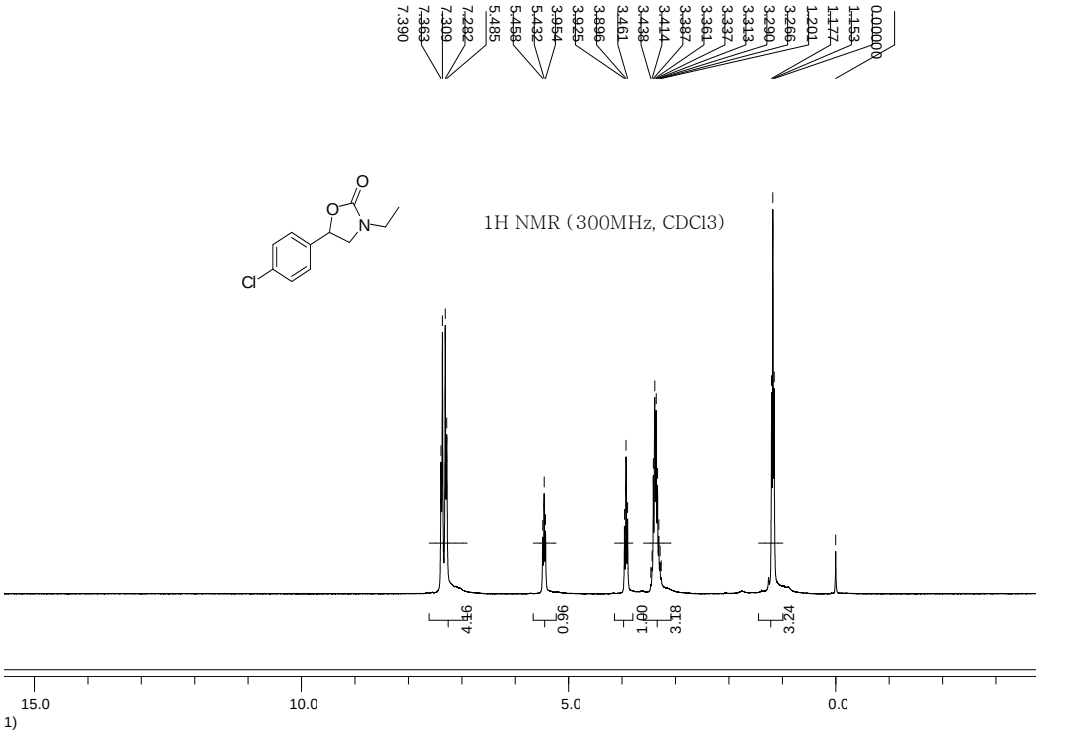

13C NMR (75MHz,CDCl3)
O
O
N
Et
Ph
200
150
100
50
0

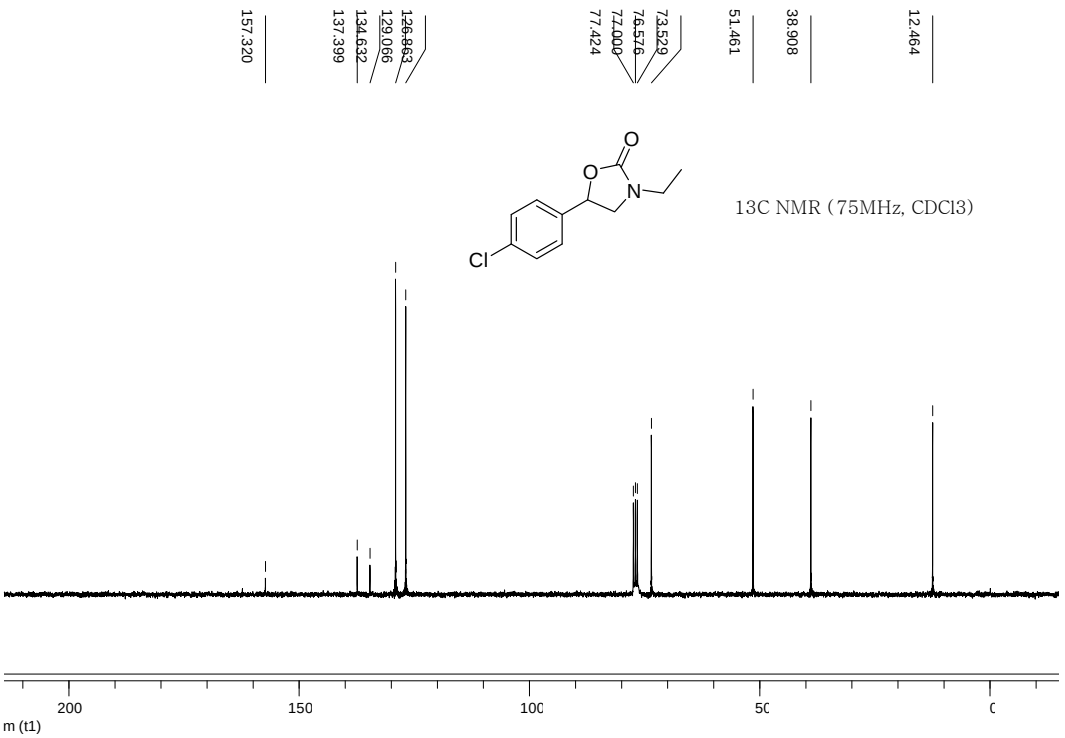

7.445
7.429
7.410
7.405
7.387
7.325
7.308
7.273
4.841
4.819
4.801
4.646
4.624
4.602
4.126
4.106
4.086
3.572
3.554
3.536
3.518
3.500
3.482
2.883
2.866
2.848
2.830
2.813
2.795
1.072
1.054
1.036
0.0000
Et
N
O
O
Ph
1H NMR (400 MHz, CDCl3)
5.2
1.0
0.9
0.9
1.0
1.0
2.9

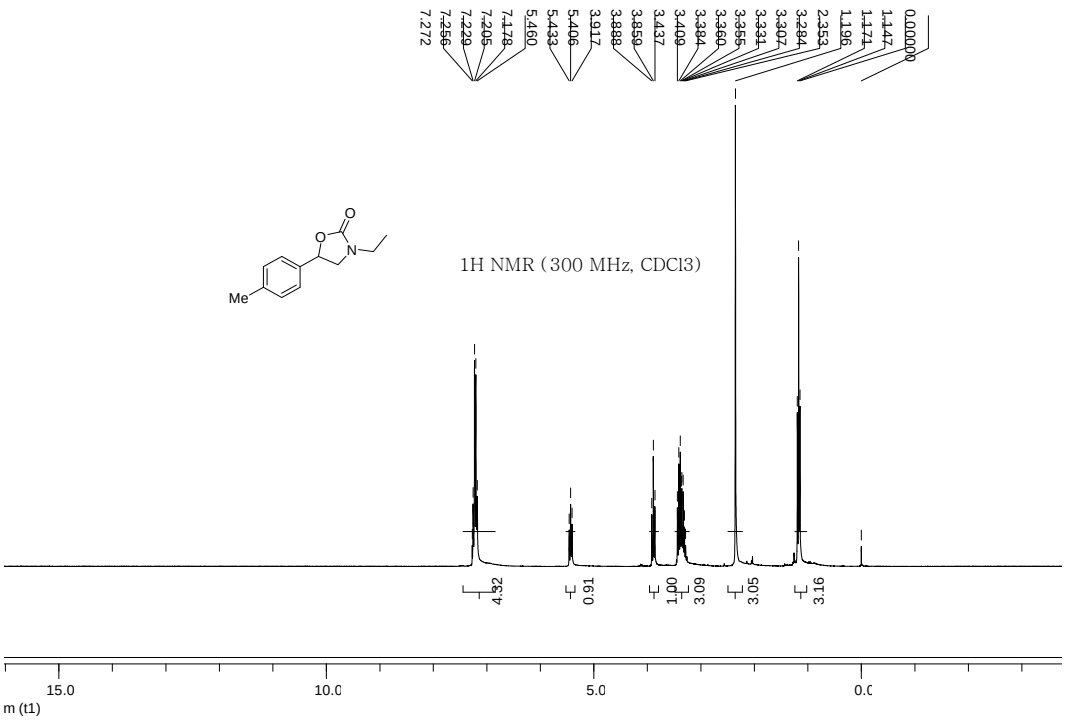

158.08
137.88
129.24
129.03
126.99
77.423
77.000
76.577
69.795
59.356
36.854
12.092
Et
N
O
O
13C NMR(100.6MHz, CDCl3)
200
150
100
50

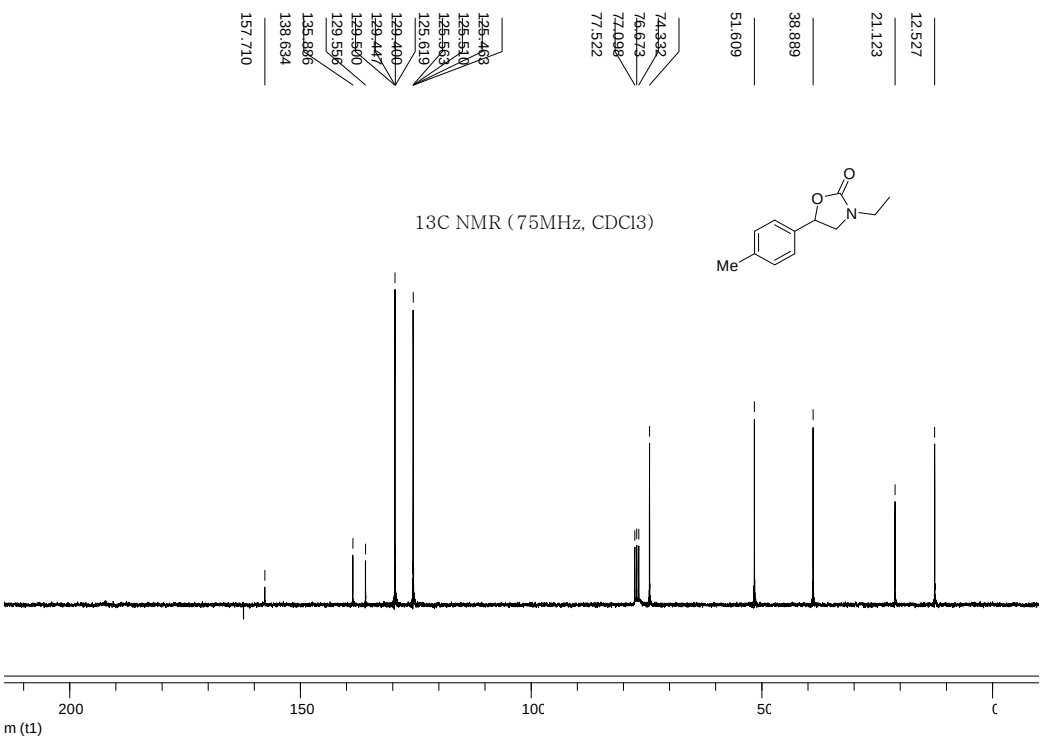

7.377
7.362
7.349
7.332
7.310
5.480
5.460
5.440
3.927
3.906
3.884
3.421
3.401
3.381
3.313
3.295
3.278
3.260
3.235
3.218
3.201
3.183
1.593
1.575
1.557
1.538
0.935
0.916
0.898
0.000000
O
O
N
Ph
1H NMR (400 MHz, CDCl3)
5.02
1.00
1.05
0.80
2.11
1.18
3.03
10.0
5.0
1)


157.684
138.751
128.582
128.436
125.239
77.426
77.000
76.575
74.026
51.824
45.523
20.356
10.791
O
O
N
Ph
13C NMR (75MHz, CDCl3)
200
150
100
50
1)


7.390
7.363
7.309
7.282
5.485
5.458
5.432
3.954
3.925
3.896
3.461
3.438
3.414
3.387
3.361
3.337
3.313
3.290
3.266
1.201
1.177
1.153
0.00000
1H NMR (300MHz, CDCl3)
O
O
N
Cl
4.16
0.96
1.00
3.18
3.24
15.0
10.0
5.0
0.0
1)


157.320
137.399
134.632
129.066
126.863
77.424
77.000
76.576
73.529
51.461
38.908
12.464
13C NMR (75MHz, CDCl3)
O
O
N
Cl
200
150
100
50
0
m (t1)


7.272
7.256
7.229
7.205
7.178
5.460
5.433
5.406
3.917
3.888
3.859
3.437
3.409
3.384
3.360
3.356
3.331
3.307
3.284
2.353
1.196
1.171
1.147
0.00000
1H NMR (300 MHz, CDCl3)
Me
4.32
0.91
1.00
3.09
3.05
3.13
15.0
10.0
5.0
0.0
m (t1)


157.710
138.634
135.886
129.556
129.500
129.447
129.409
125.619
125.563
125.510
125.468
77.522
77.098
76.673
74.332
51.609
38.889
21.123
12.527
13C NMR (75MHz, CDCl3)
Me
200
150
100
50
0
m (t1)