Supporting Information

A Complementary DSC-NMR Methodology for Elucidating Isocyanurate Formation Pathways in Polyurethanes

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S1. Materials and methods

p-Tolyl isocyanate (pTI) was procured from Fischer Scientific. pTI was distilled under vacuum to obtain a colorless liquid and stored under Ar prior to use. 2-Ethoxyethanol was purchased from TCI Chemicals and stored over 4Å molecular sieves. Catalysts, potassium acetate (KOAc) and potassium-2-ethylhexanoate (K-2-EH) were purchased from Merck and TCI Chemicals, respectively, and used as received. Deuterated $CDCl_3$ was obtained from Merck and dried over 4Å molecular sieves.

Differential scanning calorimetry (DSC) analysis: DSC was performed on a TA Q2000 (TA Instruments).

NMR Spectroscopy: ^{1}H NMR and ^{13}C NMR spectroscopy were performed using a Bruker UltraShield 400 MHz instrument (operating at 400 MHz for ^{1}H, 101 MHz for ^{13}C) at room temperature. ^{1}H NMR spectra were taken using 32 scans and a relaxation time of 2 s. ^{13}C NMR spectra were taken using 1024 scans, and a relaxation time of 4 s per scan.

Thermogravimetric Analysis: Thermogravimetric measurements were performed using a TGA550 (TA Instruments). 5-15 mg of the compound was put on a platinum pan for measurement. The samples were first equilibrated at 100 °C for 10 min, followed by heating from 100 to 800 °C at a rate of 10 °C·min^{-1} under a nitrogen atmosphere.

Fourier Transformation Infrared Spectroscopy (FT-IR): FT-IR spectra was recorded in attenuated total reflection (ATR) mode on a Thermo-Scientific NICOLET iS20 FTIR Spectrometer. 8 scans were performed over the wavenumber range of 4000 to 450 cm^{-1}.

S2. General Procedure (GP) and analysis

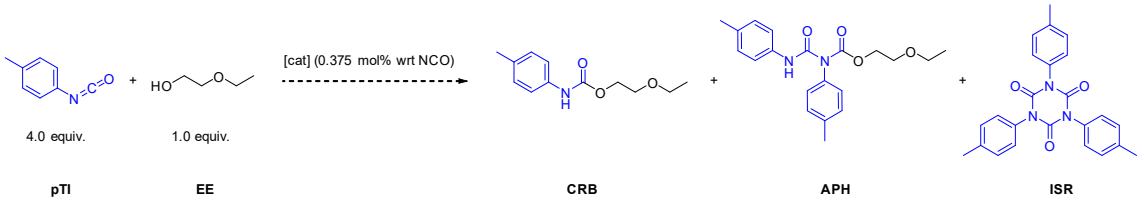
A stock solution of catalyst in 2-ethoxyethanol (EE) was prepared (KOAc: 8.8 mg in 582 µL EE; K-2-EH: 16.4 mg in 582 µL EE). To a vial containing 24.2 µL of this catalyst solution in EE, 125 µL pTI was added and thoroughly mixed. 7–8 mg (~ 8 µL) of the reaction mixture was transferred to a tared DSC pan using a micropipette. The pan was hermetically sealed with a lid and placed in the DSC instrument for analysis. It is important to note that the time between sample preparation and the start of DSC measurement could be limited to approximately 5 minutes, minimizing reaction during the initial stage. The scan was run from 25 to 120 °C at 10 °C·min^{-1} under an argon atmosphere.

Upon completion of the reaction, the DSC pan was carefully pierced with a needle and placed in a vial containing 500 µL solution of the quenching agent thionyl chloride in $CDCl_3$ (approximately 10 µL $SOCl_2$ in 25 mL $CDCl_3$, thionyl chloride about 10 times the amount of catalyst). A ^{1}H NMR spectrum of the resulting solution was recorded. Note: It is recommended to record NMR immediately after sample preparation, as samples with unreacted isocyanate can gradually form urea over time, potentially affecting the isocyanate balance.

Data point measurements: Based on insights from the complete DSC exotherm for a reaction with a given catalyst, the composition of the reaction mixture was analyzed at several representative points of interest along the DSC curve. This was performed by stopping the run at the desired temperature or position on the exotherm. Subsequently, the DSC pan was pierced and immediately quenched (as explained above) for ^{1}H NMR analysis.

S3. General reaction scheme, methods of analysis and calculations

S3.1. General reaction scheme showing reactants and products



Scheme S1. Catalytic reaction scheme illustrating the reaction of p-tolyl isocyanate (pTI) with 2-ethoxyethanol (EE) in a ratio 4:1 pTI:EE and, carbamate (CRB), allophanate (APH) and isocyanurate (ISR) as the expected products.

Method of analysis: ^{1}H NMR in $CDCl_3$

S3.2. Calculations

Characteristic reference peaks of molecules on NMR spectrum used for calculations

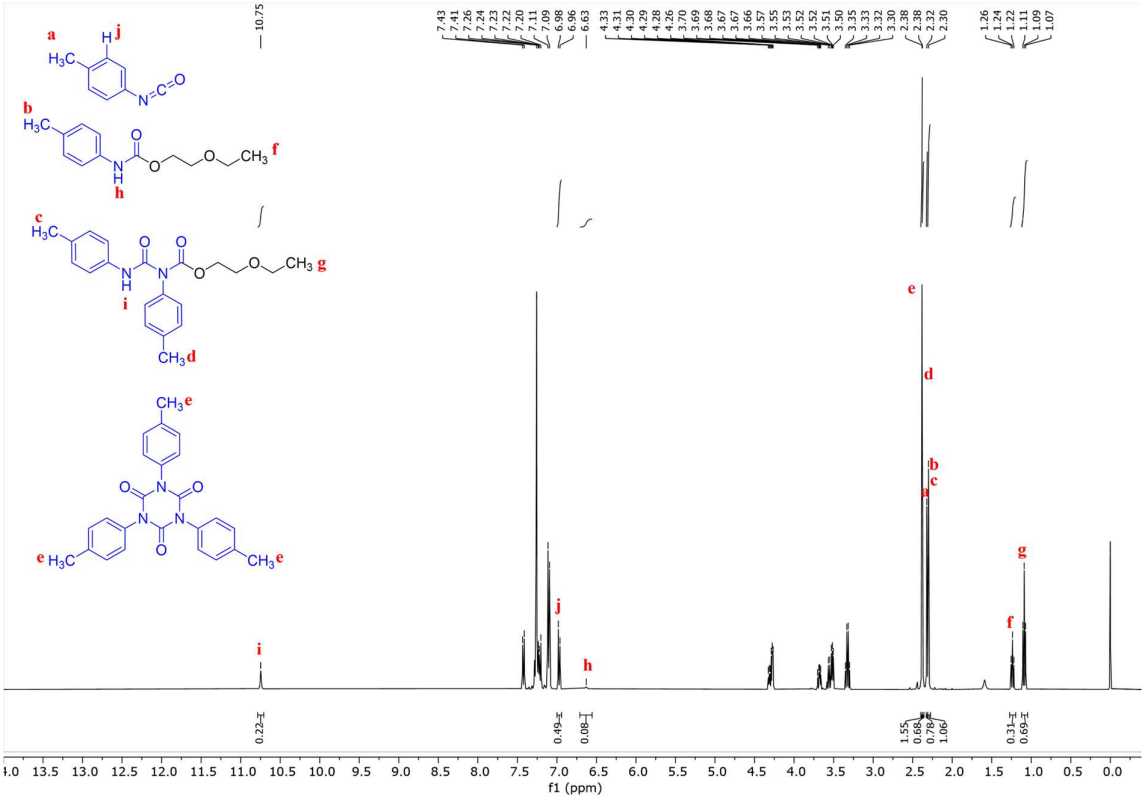


Figure S1. Typical ^{1}H NMR spectrum of the catalytic reaction mixture highlighting the characteristic signals corresponding to the reactant and products.

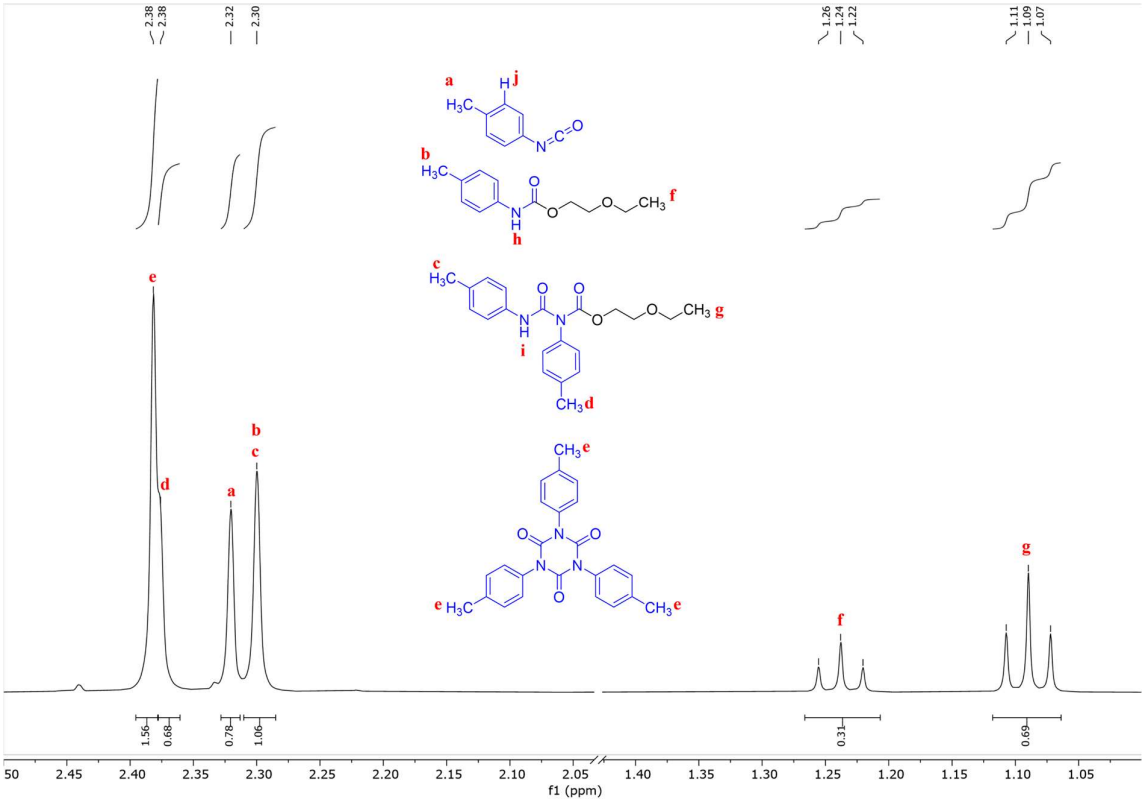


Figure S2. ^{1}H NMR spectrum of the catalytic reaction mixture in the region of 1.0 – 2.50 ppm highlighting the characteristic signals corresponding to the reactant and products.

A. Molar equivalent (mol equiv.) of a molecule

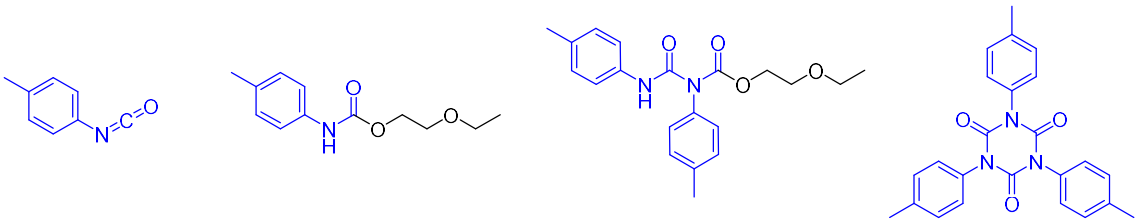
The molar equivalents of a molecule was calculated from the integration of a characteristic single -CH_3 (tolyl or ethoxyethanol moiety) present in the molecule

- mol equiv. of pTI = Integration at 2.32 ppm (**a**)
- mol equiv. of CRB = Integration at 1.24 ppm (**f**)
- mol equiv. of APH = Integration at 1.09 ppm (**g**)
- mol equiv. of ISR = Integration at 2.38 ppm (**e**) ÷ 3

B. Other important NMR information

- Sum of integrals at 1.09 and 1.24 ppm i.e. **g** + **f** ~ 1.0; This also indicates the equivalents of ethoxyethanol (EE) moiety present in the molecules
- Sum of integrals at 1.09 and 1.24 ppm i.e. **g** + **f** = Sum of integral at 2.30 ppm (**b** + **c**),
- Sum of integrals at 2.30, 2.32, 2.37, 2.38 ppm i.e. **a** + **b** + **c** + **d** + **e** ~ 4.0; This also indicates the equivalents of p-tolyl isocyanate (pTI) moiety present in the molecules
- mol equivalent < 0.05 is considered as 'trace' amount.
- Error considered in calculation of molar equivalents is ±0.05 mol equiv.. The values have been rounded to 1 decimal place.

C. Molar equivalent (mol equiv.) of NCO present in a molecule



pTI	CRB	APH	ISR
1 NCO unit	1 NCO unit	2 NCO units	3 NCO units

Molar equivalent (mol equiv.) of NCO present in a molecule = "No. of tolyl -CH_3" present in a molecule

- mol equiv. of NCO in pTI = **a**
- mol equiv. of NCO in CRB = **f** = **b**
- mol equiv. of NCO in APH = **g** × 2 = **c** + **d**
- mol equiv. of NCO in ISR = **e**
- Error considered in calculation of molar equivalents of NCO is ±0.05 mol equiv. NCO. The values have been rounded to 1 decimal place.

D. %NCO of a molecule

$$\%\mathrm{NCO} = \frac{\mathbf{a}\text{ or }\mathbf{b}\text{ or }\mathbf{c}\text{ or }\mathbf{d}\text{ or }\mathbf{e}}{\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d}+\mathbf{e}} \times 100$$

- Error considered in calculation of %NCO is ±5%. The values have been rounded to 1 decimal place.

E. Isocyanate Balance (I.B.)

$$I.B. = \frac{Sum\ of\ integration\ of\ tolyl - CH3}{total\ initial\ NCO} \times 100$$

$$I.B. = \frac{\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d}+\mathbf{e}}{4} \times 100$$

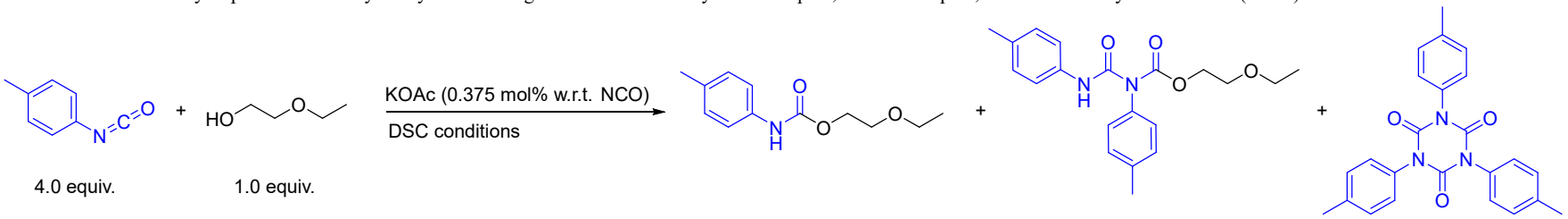
- The isocyanate balance is essentially used to check the calculations. Theoretically, it should amount to 100%. An error margin of ±10% is acceptable for the isocyanate balance calculation.

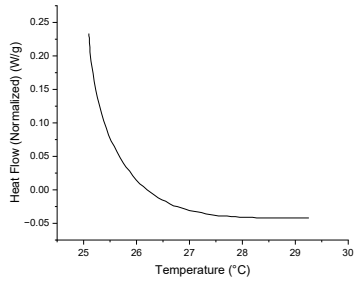
F. Catalyst concentrations mentioned in mol% are always given with respect to initial NCO unless otherwise stated.

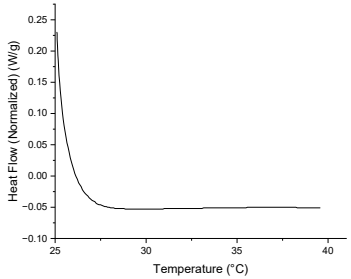
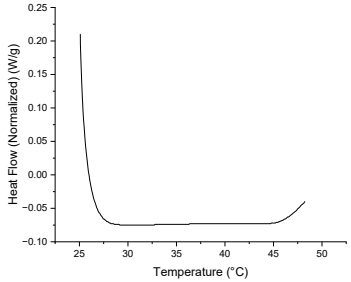
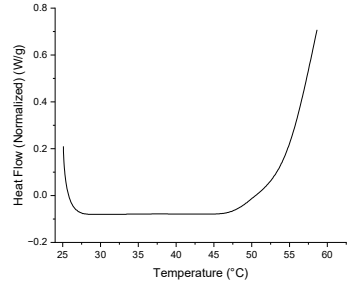
S4. Results

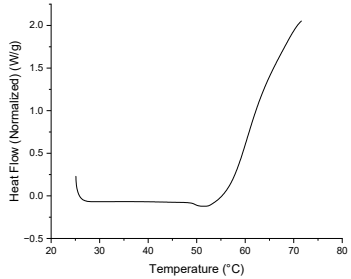
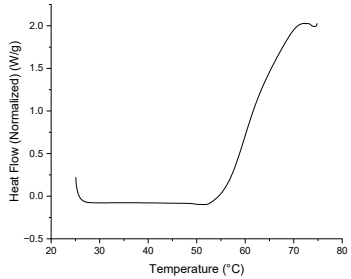
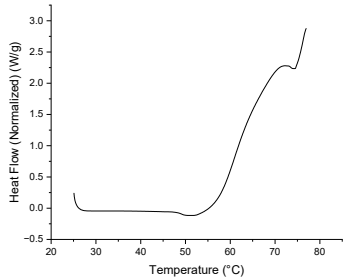
S4.1. Reaction pathway study using DSC and NMR – with KOAc as catalyst

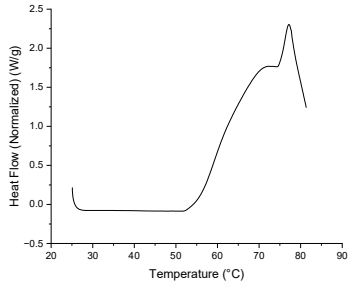
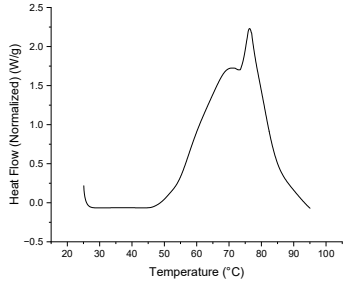
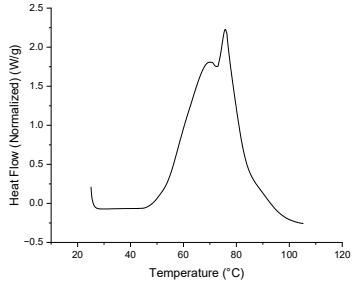
Table S1. Reaction study of pTI:EE 4:1 catalyzed by KOAc using DSC and NMR analyses: mol equiv., NCO mol equiv., %NCO and isocyanate balance (%I.B.).

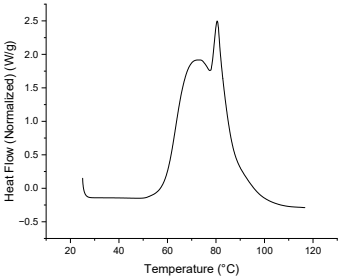


Run No.	DSC Exotherm	T (°C)	mol equiv.				NCO mol equiv.				%NCO pTI:CRB:APH:ISR	I.B. (%)
			pTI	CRB	APH	ISR	pTI	CRB	APH	ISR		
t_0[a]		25	3.1	0.9	0.0	0.0	3.1	0.9	0.0	0.0	77 : 23 : - : -	100
1		29	3.0	1.0	0.0	0.0	3.0	1.0	0.0	0.0	75 : 25 : - : -	100

2		40	3.0	1.0	0.0	0.0	3.0	1.0	0.0	0.0	75 : 25 : - : -	99
3		49	2.8	0.9	0.1	0.0 (trace)	2.8	0.9	0.2	0.1	70 : 22 : 6 : 2	99
4		59	2.0	0.5	0.5	0.1	2.0	0.5	1.0	0.4	52 : 13 : 24 : 11	99

5		72	0.8	0.3	0.7	0.5	0.8	0.3	1.4	1.5	19 : 8 : 35 : 38	99
6		75	0.4	0.4	0.6	0.6	0.4	0.4	1.3	1.9	10 : 9 : 32 : 49	99
7		77	0.2	0.4	0.6	0.7	0.2	0.4	1.1	2.1	4 : 11 : 30 : 54	95

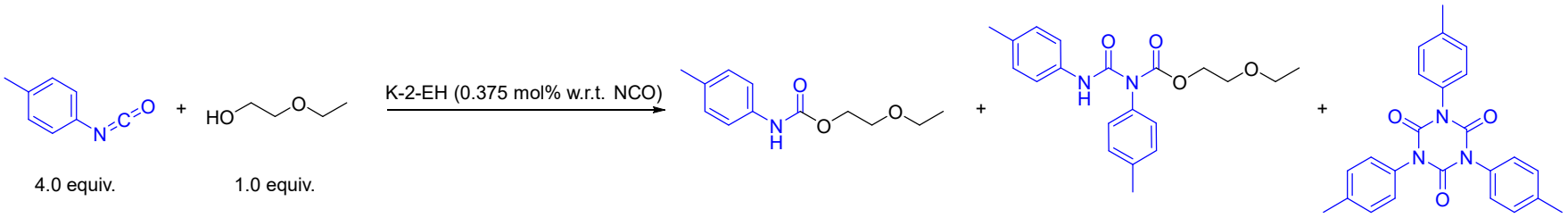
8		81	0.1	0.6	0.4	0.8	0.1	0.6	0.8	2.4	2 : 15 : 21 : 62	98
9		95	0.0	1.0	0.0	1.0	0.0	1.0	0.0	3.1	- : 24 : - : 76	102
10		105	0.0	1.0	0.0	1.0	0.0	1.0	0.0	3.1	- : 25 : - : 75	102

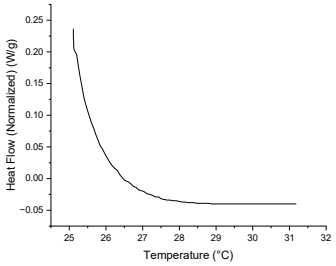
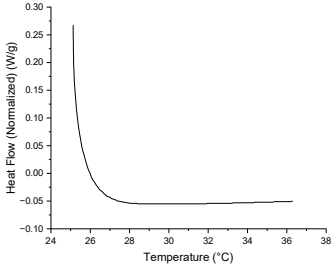
11		120	0.0	1.0	0.0	1.0	0.0	1.0	0.0	3.0	- : 25 : - : 75	100

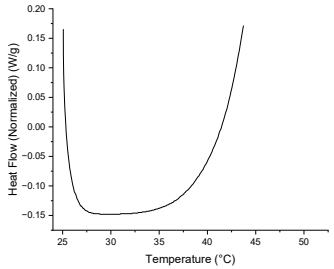
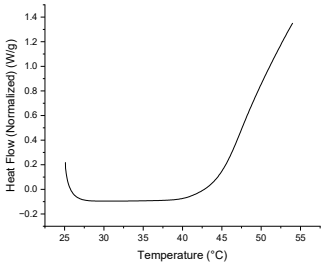
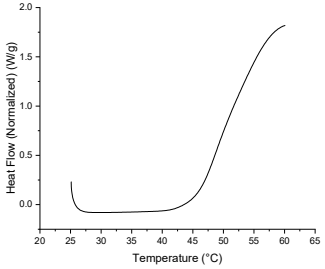
Reaction conditions: pTI (4.0 equiv.), EE (1.0 equiv.), KOAc (0.375 mol% w.r.t. total NCO), DSC conditions. mol equiv., NCO mol equiv., %NCO and isocyanate balance (%I.B.) determined by ^{1}H NMR. DSC conditions: temperature ramp from 25 – 120 °C at a rate of 10 °C·min^{-1}. [a] 0.08 mol equivalent EE present along with 0.92 mol equivalent CRB.

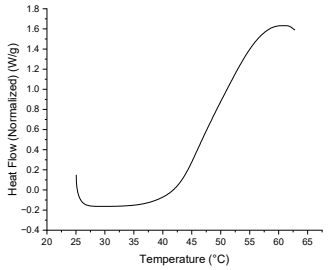
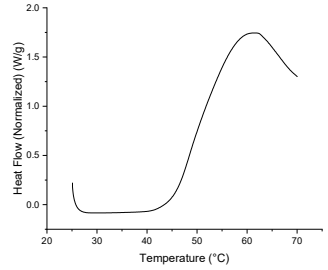
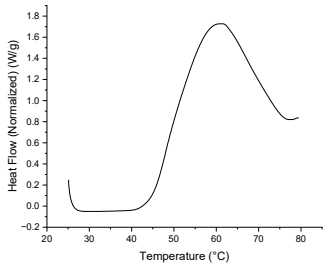
S4.2. Reaction pathway study using DSC and NMR – with K-2-EH as catalyst

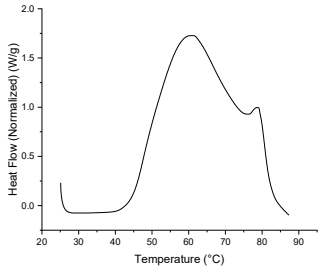
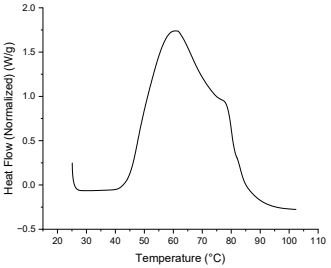
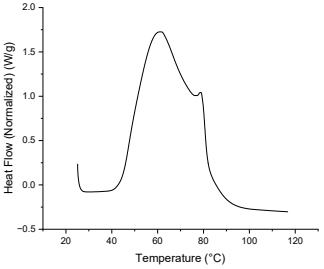
Table S2. Reaction study of pTI:EE 4:1 catalyzed by K-2-EH using DSC and NMR analyses: mol equiv., NCO mol equiv., %NCO and isocyanate balance (%I.B.).



Run No.	DSC Exotherm	T (°C)	mol equiv.				NCO mol equiv.				%NCO pTI:CRB:APH:ISR	I.B. (%)
			pTI	CRB	APH	ISR	pTI	CRB	APH	ISR		
t_0[a]		25	3.1	1.0	0.0	0.0	3.1	1.0	0.0	0.0	76 : 24 : - : -	100
1		31	3.0	1.0	0.0 (trace)	0.0 (trace)	3.0	1.0	0.1	0.0	74 : 24 : 1 : 1	101
2		37	3.0	1.0	0.0 (trace)	0.0 (trace)	3.0	1.0	0.1	0.0	73 : 24 : 2 : 1	101

3		44	2.6	0.8	0.2	0.1	2.6	0.8	0.5	0.3	63 : 19 : 11 : 7	101
4		54	1.7	0.5	0.5	0.3	1.7	0.5	1.1	0.9	41 : 11 : 27 : 21	102
5		60	1.0	0.3	0.7	0.4	1.0	0.3	1.3	1.3	25 : 8 : 33 : 33	101

6		63	0.8	0.3	0.7	0.5	0.8	0.3	1.4	1.6	18 : 7 : 34 : 40	102
7		70	0.3	0.4	0.6	0.7	0.3	0.4	1.2	2.1	7 : 10 : 30 : 53	99
8		79	0.0	0.8	0.2	0.9	0.0	0.8	0.4	2.7	- : 21 : 9 : 70	98

9		87	0.0	1.0	0.1	1.0	0.0	1.0	0.1	3.0	- : 23 : 2 : 74	101
10		102	0.0	1.0	0.0	1.0	0.0	1.0	0.0	3.0	- : 25 : - : 75	101
11		120	0.0	1.0	0.0	1.0	0.0	1.0	0.0	3.0	- : 25 : - : 75	100

Reaction conditions: pTI (4.0 equiv.), EE (1.0 equiv.), K-2-EH (0.375 mol% w.r.t. total NCO), DSC conditions. mol equiv., NCO mol equiv., %NCO and isocyanate balance (%I.B.) determined by ^{1}H NMR. DSC conditions: temperature ramp from 25 – 120 °C at a rate of 10 °C·min^{-1}. [a] 0.04 mol equivalent EE present along with 0.96 mol equivalent CRB.

S4.3. TGA analysis of APH

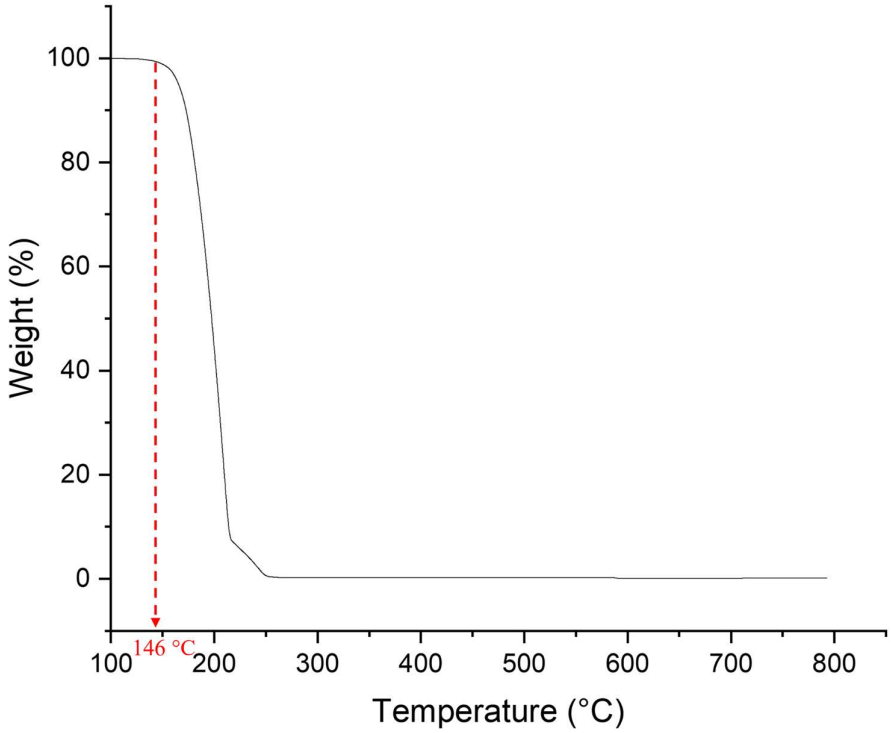


Figure S3. TGA analysis of APH indicates the onset of degradation at 146 °C, with a 5% weight loss ($T_{d5\%}$) observed at 165 °C.

S4.4. APH self-degradation studies

A. General Procedure (GP) and analysis

A catalyst solution of K-2-EH (3.8 mg in 1000 µL diglyme) in diglyme was prepared. APH (20 mg, 56.1 µmol) was taken in a vial. 20 µL catalyst solution was added to the vial and mixed thoroughly to produce a clear viscous oil. Approximately 10 mg of the reaction mixture was transferred to a tared DSC pan, along with a hermetic lid, using a micropipette. The pan was hermetically sealed with the lid and placed in the DSC instrument for analysis. The experiments were carried out from 25 to 120 °C at a rate of 10 °C·min^{-1} under an argon atmosphere. After the run, the DSC pan was pierced with a needle and placed in a vial containing 500 µL solution of the quenching agent thionyl chloride in $CDCl_3$ (10 µL $SOCl_2$ in 25 mL $CDCl_3$).

Deviation from GP for the study of APH degradation in the absence of a catalyst

20 µL Diglyme used instead of 20 µL K-2-EH/diglyme (3.8 mg in 1000 µL diglyme)

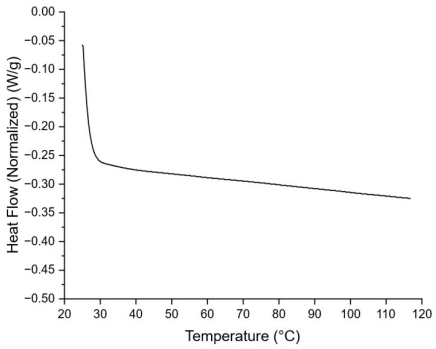
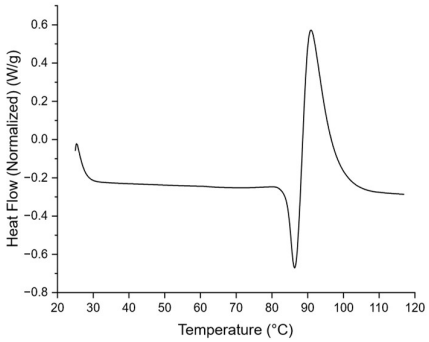
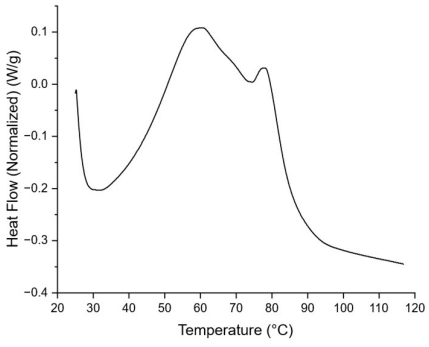
Deviation from GP for the study of 1:1 APH:pTI

Instead of 20 µL K-2-EH/diglyme (3.8 mg in 1000 µL diglyme), the following stock solutions were prepared and used:

Stock Solution	Volume used in reaction
pTI (74.7 mg in 1000 µL diglyme)	10 µL
K-2-EH in diglyme (11.3 mg in 1000 µL diglyme)	10 µL

B. Results

Table S3. APH self-decomposition studies using DSC.

Reaction condition	DSC exotherm	Reaction composition at the end of the run %NCO pTI:CRB:APH:ISR
No catalyst (only diglyme)		- : - : >99 : -
Presence of catalyst		- : 50 : - : 47
1:1 APH:pTI ; presence of catalyst		- : 33 : - : 66

Reaction conditions: APH (20 mg, 56.1 µmol), K-2-EH (0.750 mol% relative to APH, 0.4 µmol, 76.7 µg), diglyme (20 µL). Modified conditions: Absence of catalyst conditions - No K-2-EH was used; presence of catalyst and equivalent of pTI - K-2-EH (1.125 mol% relative to APH or 0.375 mol% relative to NCO/NCO derived molecules, 0.6 µmol, 112.5 µg), pTI (7.5 mg). DSC conditions: Temperature range 25 – 120 °C, heating ramp: 10 °C·min^{-1}. %NCO determined by ^{1}H NMR analysis.

C. NMR spectra of selected experiments

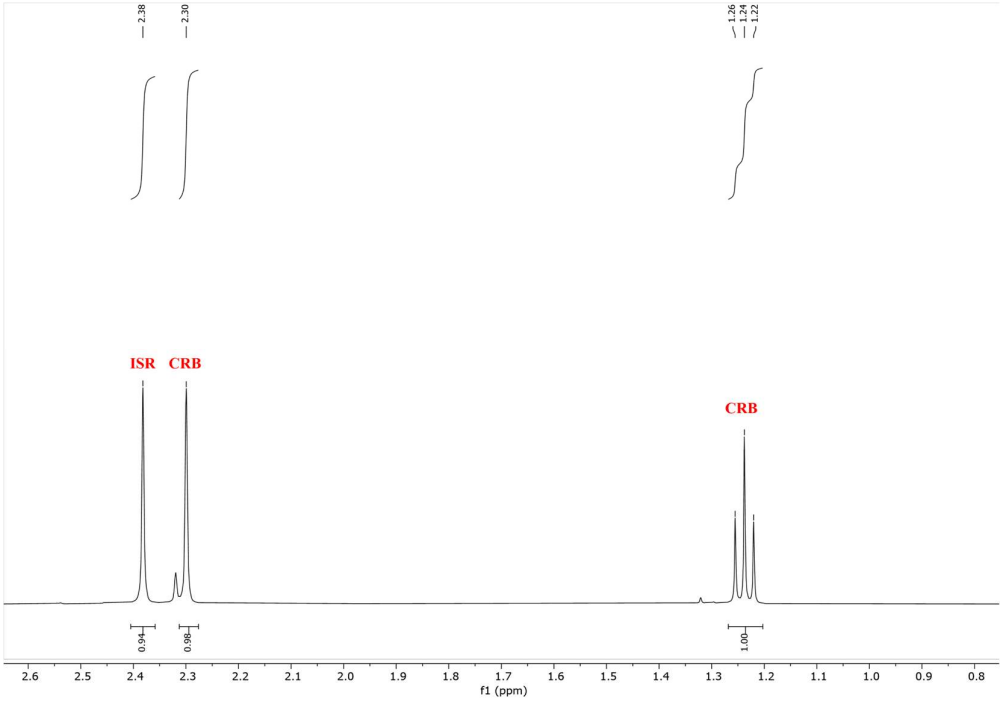


Figure S4. [1]H NMR spectra of the reaction mixture after complete catalytic degradation of APH, showing the formation of ISR and CRB.

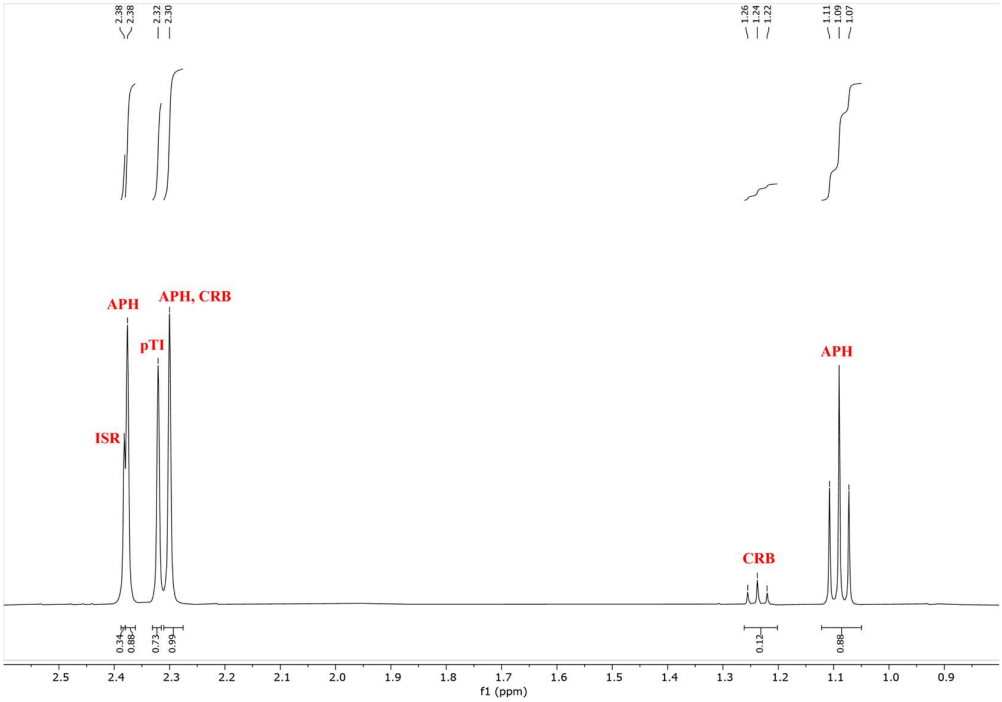


Figure S5. [1]H NMR spectra of the catalytic reaction mixture at 25 °C after addition of 1 mol equiv. pTI to APH, in the presence of K-2-EH, showing unreacted pTI and APH, and increased formation of ISR (0.34 NCO mol equiv.) compared to CRB (0.12 NCO mol equiv.). The spectrum was recorded 5 min. after mixing the components.

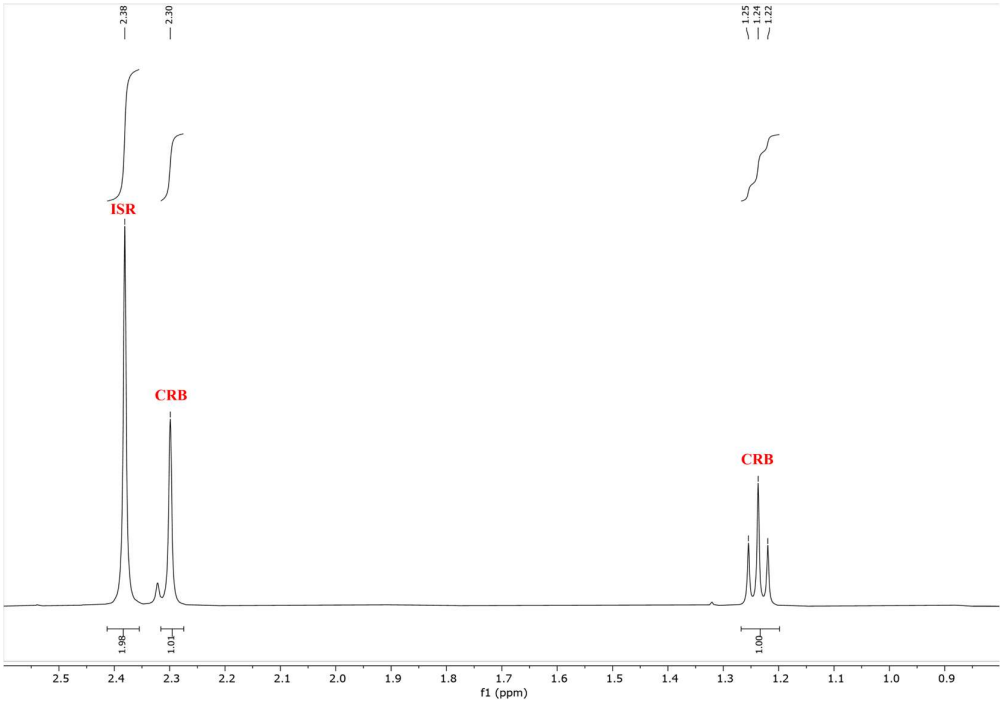


Figure S6. ^{1}H NMR spectra of the completed reaction after the addition of 1 mol equiv. pTI and catalytic amounts of K-2-EH to APH, showing the formation of ISR and CRB.

S4.5. Influence of NMR solvent on catalytic degradation of APH

A. General Procedure

A catalyst solution of K-2-EH (3.8 mg in 1000 µL diglyme) in diglyme was prepared. APH (20 mg, 56.1 µmol) was taken in a vial. 20 µL catalyst solution was added to the vial and mixed thoroughly to produce a clear viscous oil. NMR solvent ($CDCl_3$ or DMSO-d_6, 0.6 mL) was added to the reaction mixture and the sample was immediately subjected to NMR analysis. The time between sample preparation and data acquisition was limited to 5 min.

B. Results

i) $CDCl_3$ as NMR solvent: APH remains largely unreacted; 3% CRB formation observed.

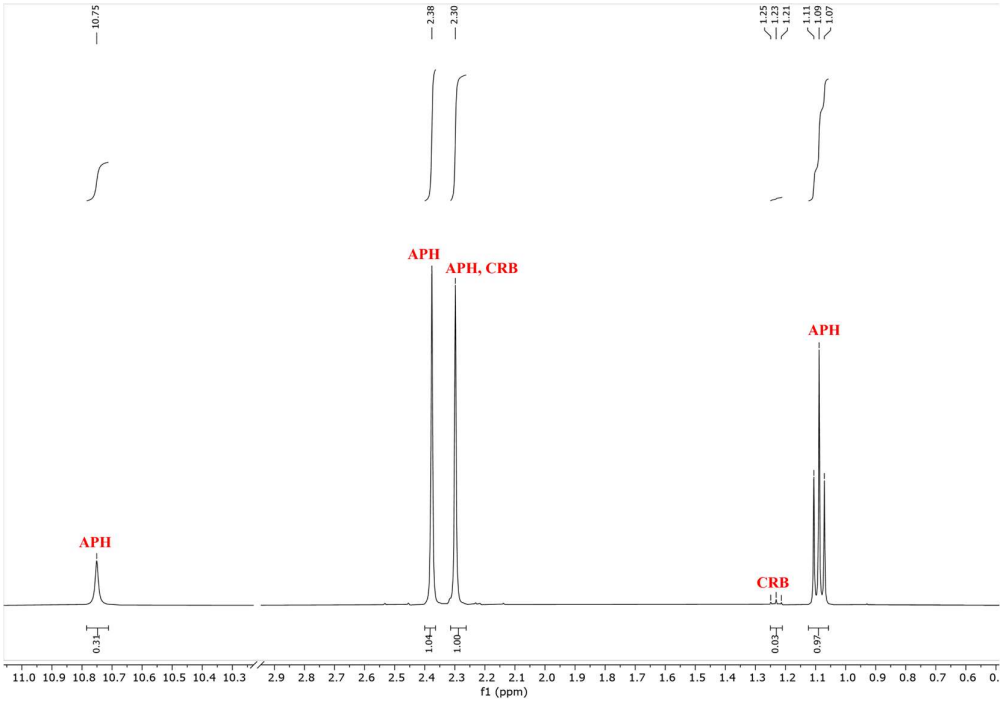


Figure S7. ^{1}H NMR spectra of the catalytic degradation of APH recorded in $CDCl_3$ at room temperature after 5 mins of sample preparation, showing that APH remains largely unreacted, with only ~3% CRB is observed.

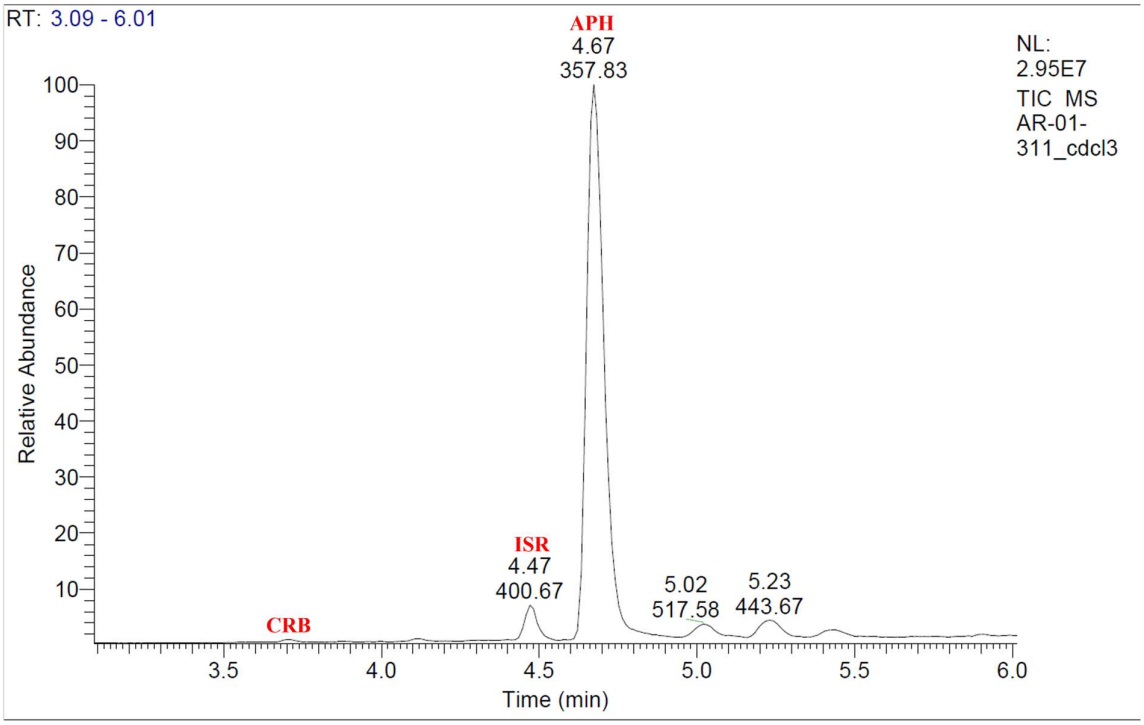


Figure S8. LC-MS spectra confirming unreacted APH and small formation of ISR and CRB in the presence of $CDCl_3$ as the NMR solvent.

ii) DSMSO-d_6 as NMR solvent: Almost complete conversion of APH to CRB and ISR observed; 5% APH remains unreacted.

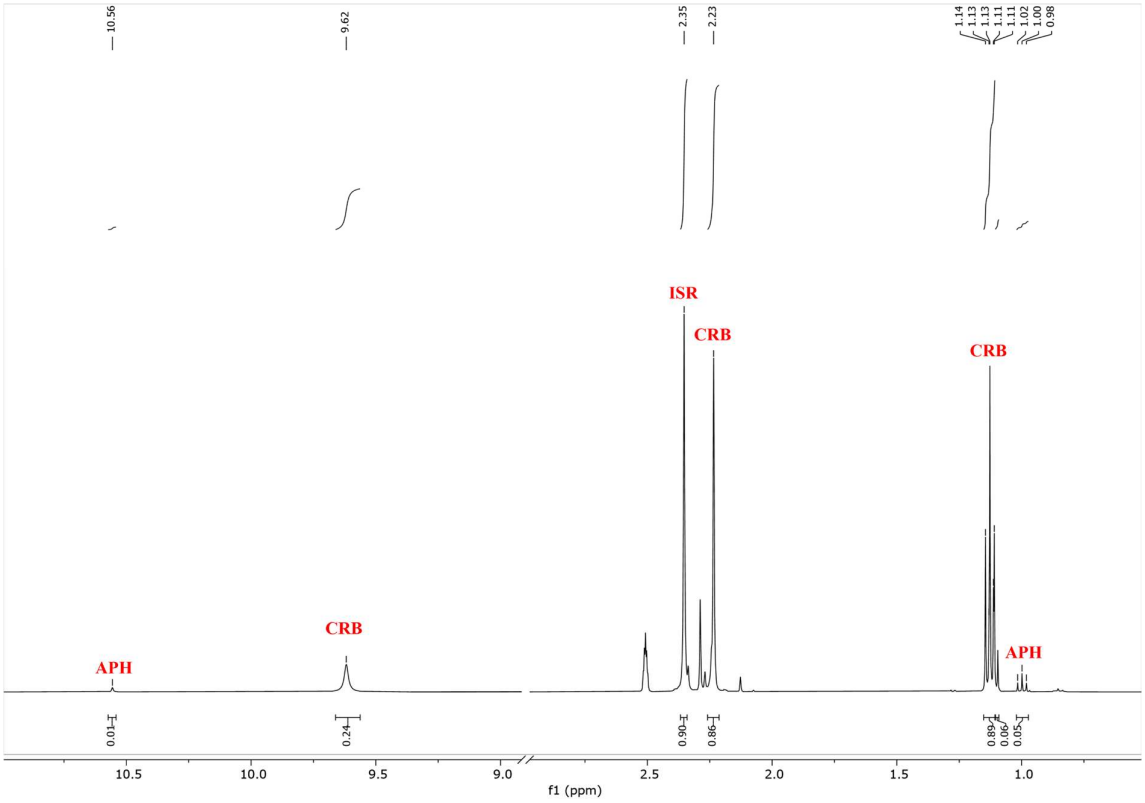


Figure S9. ^{1}H NMR spectra of the catalytic degradation of APH recorded in DMSO-d_6 at room temperature after 5 mins of sample preparation, showing near-complete catalytic conversion of APH to CRB and ISR, with approximately 5% APH remaining unreacted.

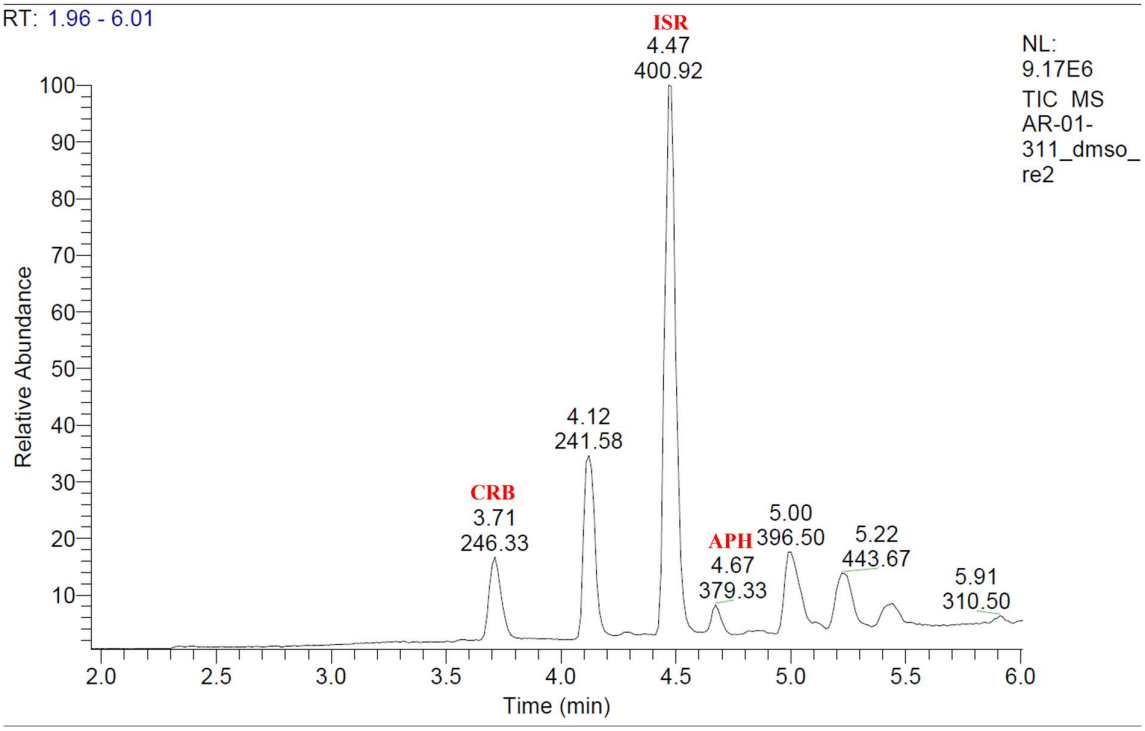
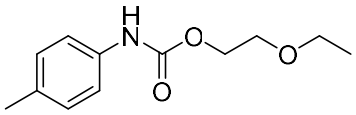


Figure S10. LC-MS spectra confirming formation of CRB and ISR from APH in the presence of DMSO-d_6 as the NMR solvent.

S4.6. Synthesis of reference molecules



2-Ethoxyethyl p-tolylcarbamate (CRB)

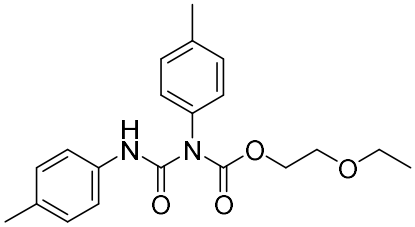
The compound was synthesized according to a modified literature procedure reported by Al Nabulsi et al.[1]

Ethoxyethanol (EE, 27.1 g, 300.4 mmol) was added to *p*-tolyl isocyanate (pTI, 10.0 g, 75.1 mmol) in a 100 mL three-necked round-bottom flask equipped with a reflux condenser and maintained under an argon atmosphere. The reaction mixture was stirred and heated at 120 °C for 2 h. Completion of the reaction was confirmed by the disappearance of the isocyanate stretching band at 2272 cm^{-1} in the IR spectrum. The mixture was then allowed to cool to room temperature (r.t.), diluted with chloroform (50 mL) and transferred to a separatory funnel. The organic phase was washed successively with 1 M NaOH (3 × 20 mL), water (1 × 20 mL), and brine (1 × 20 mL). The organic layer was dried over anhydrous $MgSO_4$, filtered and the solvent was removed *in vacuo* to yield a yellow-brown viscous oil. The oil was purified by passage through a short silica filter column, yielding a light-yellow, viscous oil (16.1 g, 96% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 6.5 Hz, 2H), 7.10 (d, *J* = 6.4 Hz, 2H), 6.69 (s, 1H), 4.35 – 4.24 (m, 2H), 3.68 (m, 2H), 3.56 (q, *J* = 6.0, 5.0 Hz, 2H), 2.30 (s, 3H), 1.24 (t, *J* = 6.1 Hz, 3H)

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.48, 135.24, 133.04, 129.55, 118.79, 68.69, 66.65, 64.29, 20.74, 15.12.

The NMR spectra are in agreement with literature.



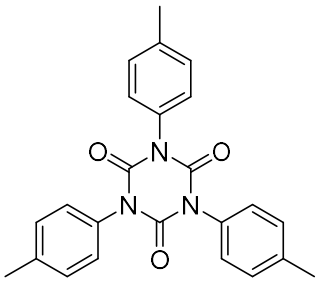
2-Ethoxyethyl p-tolyl(p-tolylcarbamoyl)carbamate (APH)

The compound was synthesized according to a modified literature procedure reported by Kogon et al.[2]

To a solution of *p*-tolyl isocyanate (pTI, 1.9 g, 14.1 mmol) and 2-ethoxyethyl p-tolylcarbamate (CRB, 3.0 g, 13.4 mmol) in a Schlenk flask under argon atmosphere, cobalt-2-ethylhexanoate 65% wt. in mineral spirits, (35.7 mg, 0.5 mol% w.r.t. CRB) was added and stirred overnight at 50 °C. The reaction mixture was checked for consumption of CRB by TLC in 20% ethyl acetate/hexane. On consumption of CRB, the reaction was allowed to cool and excess pTI was removed *in vacuo* to yield a blue viscous oil. The viscous oil was subjected to column chromatography using dichloromethane (DCM) as eluent. The collected fractions corresponding to the product were pooled and the solvent was removed *in vacuo* to yield a colorless viscous oil, which solidified to form a waxy solid on refrigeration (4.0 g, 84% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.75 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.13-7.07 (m, 4H), 4.28 (m, 2H), 3.51 (m, 2H), 3.32 (q, *J* = 7.0 Hz, 2H), 2.38 (s, 3H), 2.30 (s, 3H), 1.09 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 156.03, 151.51, 138.05, 135.26, 134.47, 133.45, 129.58, 129.45, 128.46, 119.88, 67.72, 66.66, 66.40, 21.18, 20.80, 15.06.



1,3,5-tri-p-tolyl-1,3,5-triazinane-2,4,6-trione (ISR)

To a solution of p-tolyl isocyanate (pTI, 3.0 g, 22.5 mmol) in dry THF (6 mL) taken in a Schlenk flask under argon atmosphere, a catalyst solution of potassium 2-ethylhexanoate in THF (10 mol% w.r.t. NCO, 411 mg in 3 mL THF) was added. The solution was stirred at 40 °C until the disappearance of NCO stretching vibration at 2270 cm^{-1} as observed by IR measurement. The warm solution was then added to a cooled pentane (50 mL). The precipitate was filtered and dried in a vacuum oven at 60 °C overnight, yielding a white, powdery solid (2.9 g, 97% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, J = 2.8 Hz, 12H), 2.38 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.90, 139.29, 131.09, 129.99, 128.09, 21.25.

The NMR spectra are in agreement with literature.[3]

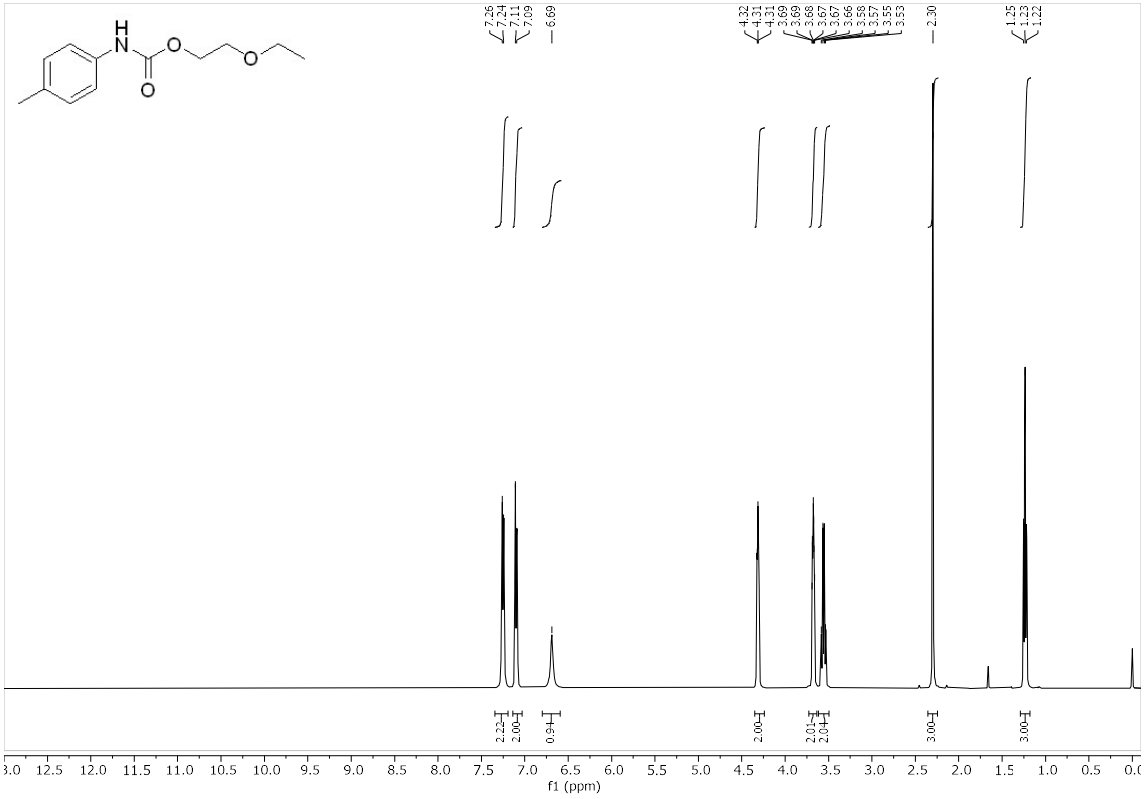
S5. References

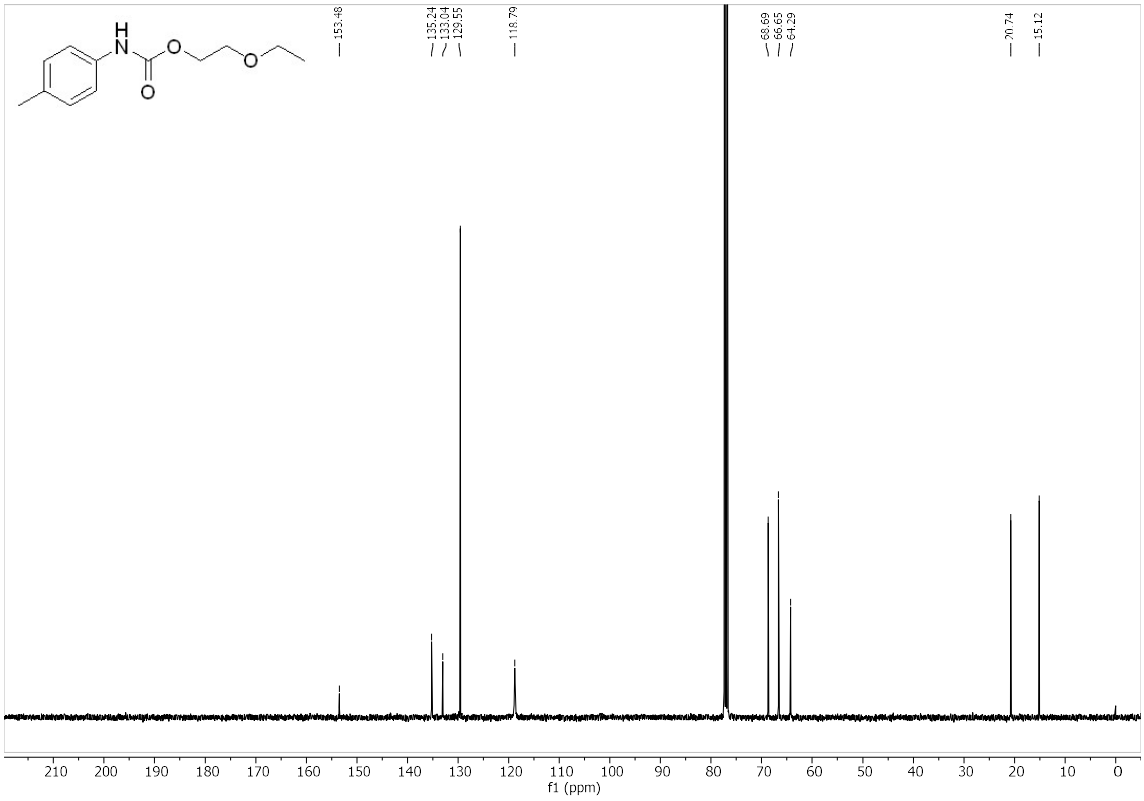
[1] A. Al Nabulsi, D. Cozzula, T. Hagen, W. Leitner and T. E. Müller, *Polym. Chem.*, 2018, **9**, 4891–4899.

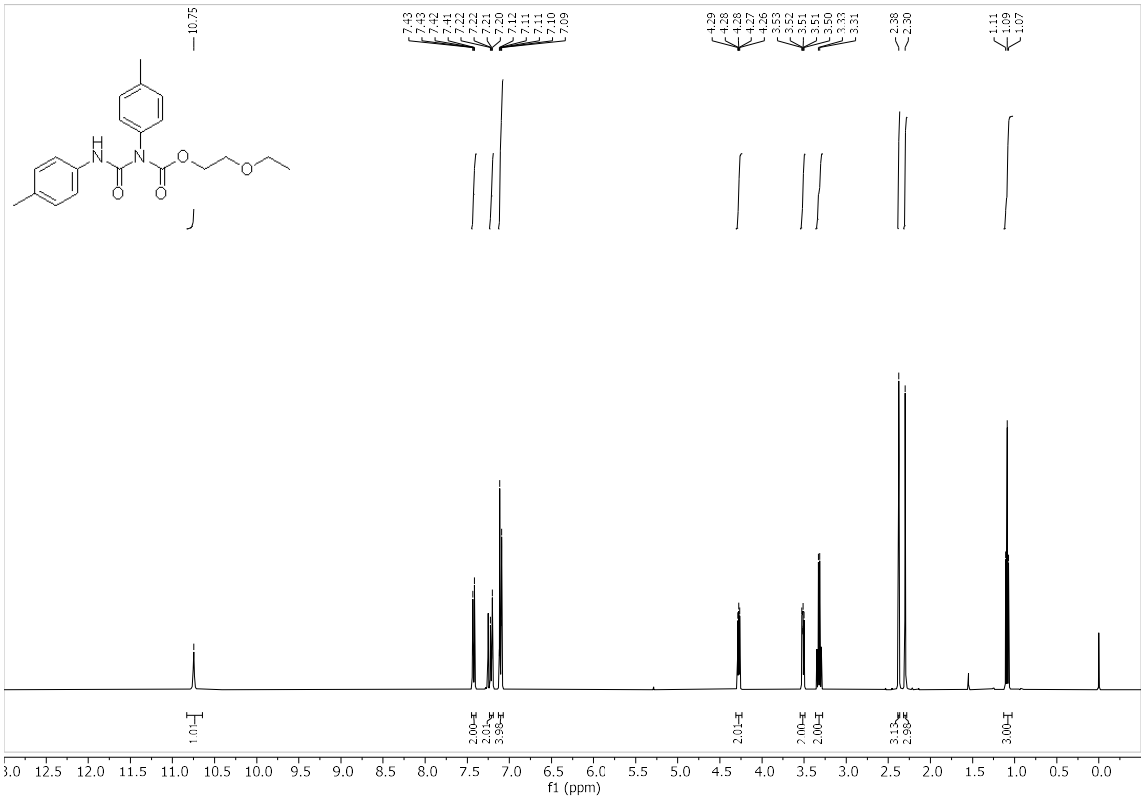
[2] I. C. Kogon, *J. Org. Chem.*, 1961, **26**, 3004–3005.

[3] Y. Guo, M. Muuronen, P. Deglmann, F. Lucas, R. P. Sijbesma and Ž. Tomović, *J. Org. Chem.*, 2021, **86**, 5651–5659.

S6. NMR spectra of synthesized reference molecules



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7.42
7.41
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7.21
7.20
7.12
7.11
7.11
7.10
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4.29
4.28
4.28
4.27
4.26
3.53
3.52
3.51
3.51
3.50
3.33
3.31
2.38
2.30
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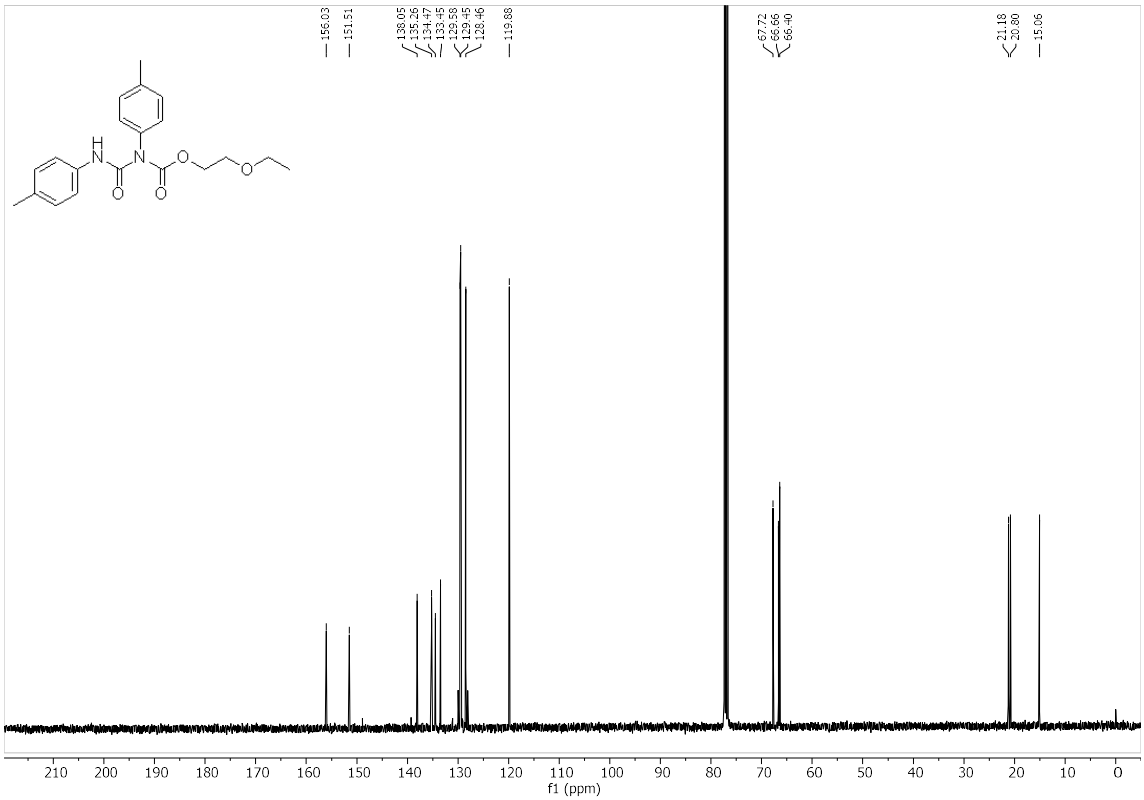
2.00
3.13
2.98
3.00
f1 (ppm)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135.26
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67.72
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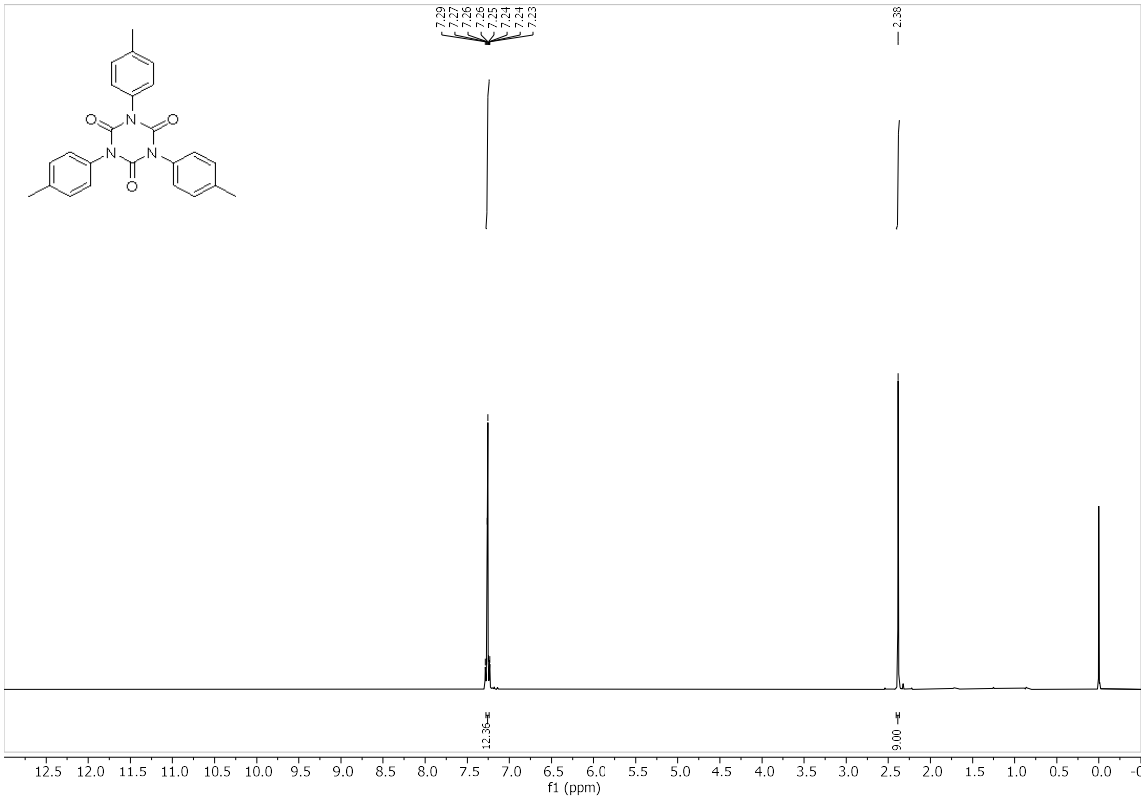
15.06
f1 (ppm)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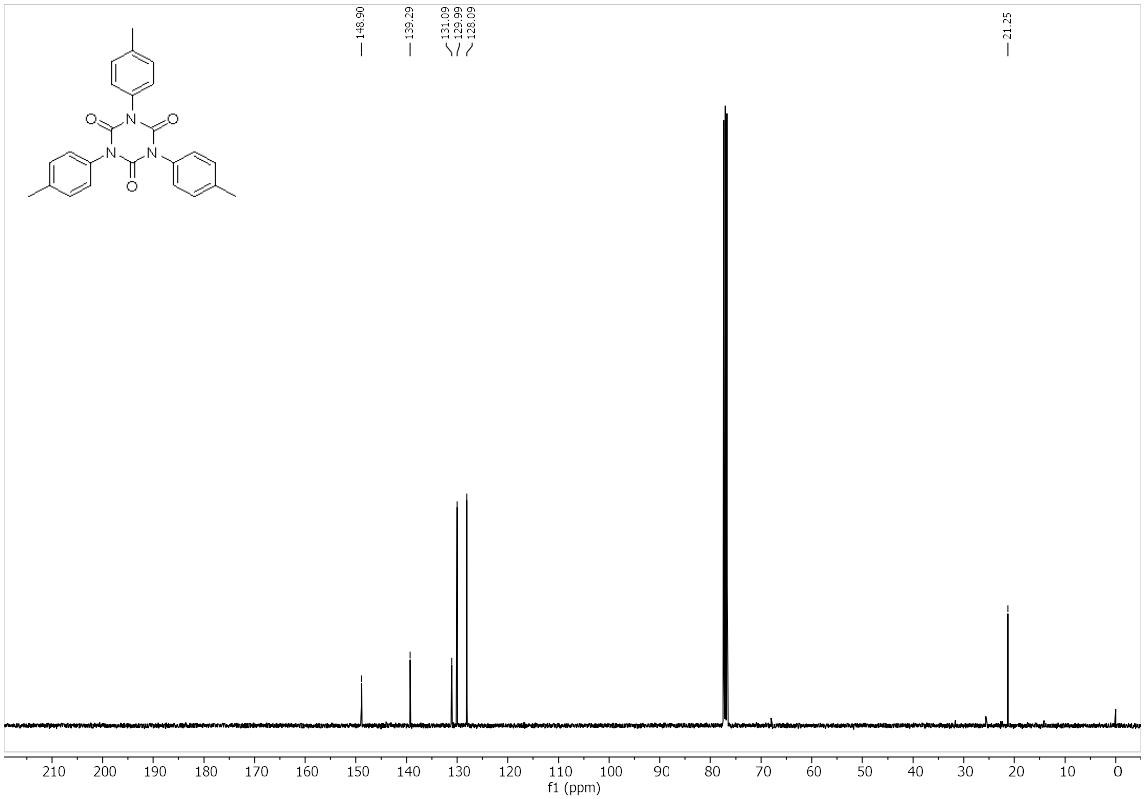
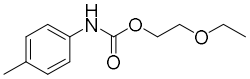
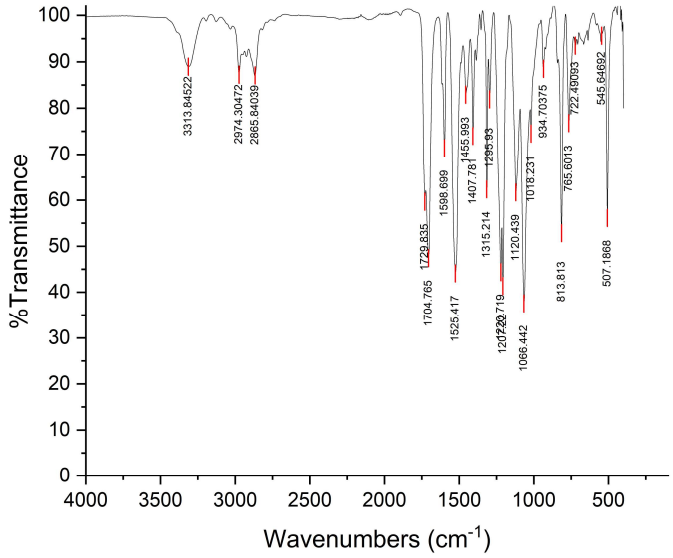
9.00
f1 (ppm)

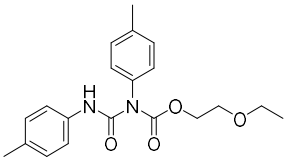

148.90
139.29
131.09
129.99
128.09
21.35
f1 (ppm)

S7. FT-IR spectra of synthesized reference molecules

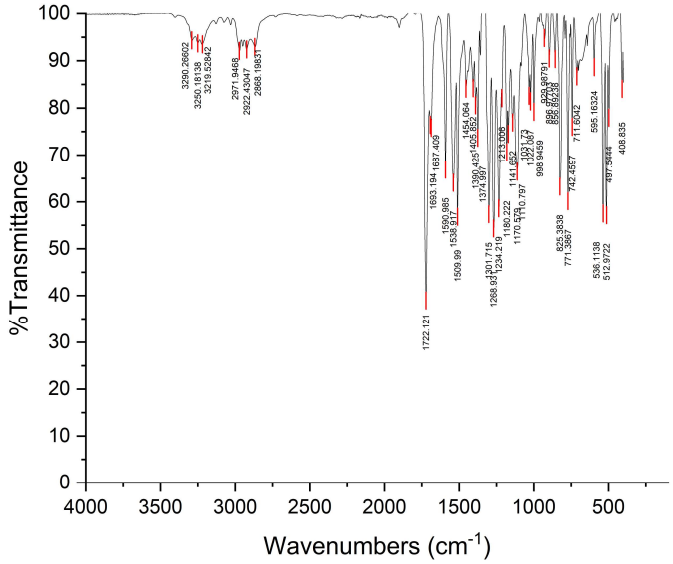


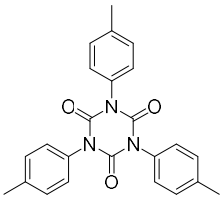
2-Ethoxyethyl p-tolylcarbamate (CRB)





2-Ethoxyethyl p-tolyl(p-tolylcarbamoyl)carbamate (APH)





1,3,5-tri-p-tolyl-1,3,5-triazinane-2,4,6-trione (ISR)