

Supporting information

Rapid, controlled ring-opening polymerization of salicylic acid O-carboxyanhydride for poly(salicylate) synthesis

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Experimental Section.

General Methods.

All polymerizations were carried out in a dry and oxygen-free nitrogen atmosphere by using Schlenk techniques or under a nitrogen atmosphere in a Vigor glovebox. Tetrahydrofuran (THF) and diethyl ether (EE) were distilled over sodium/benzophenone and stored over 4 Å molecular sieves prior to use. Anhydrous dichloromethane (DCM), anhydrous chloroform (TCM), anhydrous 1,4-dioxane (DOX) were purchased from J&K SCIENTIFIC LTD and used without treatment. Triphosgene and triethylamine purchased from Innochem was used without treatment. 1,8-diazabicycloundec-7-ene (DBU), 1-benzyl alcohol, hexanol and 1,6-hexanediol were purchased from Acros and dried with KOH overnight, following distillation in vacuum three times. CDCl₃ was purchased from Cambridge Isotope Laboratories Inc. 4-Dimethylaminopyridine (DMAP), 1,5-diazabicyclo[4.3.0]non-5-ene (DBN), 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) and 2-tert-butylimino-2-diethylamino-1,3-dimethyl-perhydro-1,3,2-diaza phosphorine (BEMP), were purchased from Innochem and used without treatment.

Characterization.

The ¹H NMR was carried out on a 400 MHz or 500 MHz NMR instrument (Bruker Corporation, Germany) at room temperature using CDCl₃ (δ = 7.26 ppm for ¹H NMR, 77.16 ppm for ¹³C NMR) as solvent. GPC measurements were carried out by Agilent LC 1260 instrument equipped with a differential refractive-index detector. One guard column and two 7.5 x 300 mm PLgel MIXED-C columns were used. The measurements were performed using DMF as eluent (flow rate of 1.0 mL/min at 55 °C, 0.04 M LiBr), and polymethyl methacrylate standards were employed for calibration. Polymer solutions at the concentrations between 4.0 and 6.0 mg/mL were injected at an injection volume of 80 μL.

Matrix-assisted laser desorption/ionization mass spectra (MALDI-TOF MS) were carried out on a Bruker Autoflex III (laser frequency 100 Hz, 355 nm and detector voltage of 1689 V). *In situ* IR study was carried out by using ReactIR 15^m with MCT Detector from METTLER TOLEDO AutoChem. DiComp (Diamond) probe was connected via AgX 6 mm x 2 m Fiber (Silver Halide). Spectra were taken from 2000 cm⁻¹ to 650 cm⁻¹ at 8 wavenumber resolution and the automatic sampling interval was 15 second. In the process of polymerization, the sample was taken from the polymerization system at the determined time, and spotted on the KBr plate for scanning on FT-IR (Nicolet 6700, the accumulation rate was 16 times with 4 wavenumber resolution). The monomer conversion was determined by the intensity ratio between 1738 cm⁻¹ and 1754 cm⁻¹, conversion% = $I_{1738} / (I_{1738} + I_{1754})$.¹

Thermal stability properties were measured by thermogravimetric analysis (TGA) on a TA Q500 analyzer. The test was carried out at a rate of 10 °C min⁻¹ from room temperature to 600 °C under a nitrogen atmosphere. Thermal transition properties were measured by differential scanning calorimetry (DSC) on a TA-Q2000 thermal analyzer. The sample was first heated to 250 °C at a heating rate of 10 °C min⁻¹, was then rapidly cooled to -50 °C and maintained at this temperature for 2 min. Then, it was heated to 250 °C at the heating rate of 10 °C min⁻¹ and maintained at 250 °C for 2 min. Then the sample was cooled down to 0 °C at a rate of 10 °C min⁻¹.

Synthesis of SAOCA monomer.

To a solution of triphosgene (15 mmol) and activated charcoal (~90 mg) in anhydrous diethyl ether (40 mL), salicylic acid (36.0 mmol) was stepwise added. The reaction mixture was stirred for 3 hours at -20°C. Subsequently, a solution of triethylamine (4 mL, 28 mmol) in diethyl ether solution (20 mL) was gradually participated. The reaction mixture was stirred for 3 hours at room temperature, and the mixture was filtered over MgSO₄. The filtrate was concentrated and the resulting residue was recrystallized from THF/ether/hexane (v/v/v = 5/15/3) twice to give white crystal in a yield of 35%. ¹H NMR (400 MHz, CDCl₃), δ (ppm): 8.10 (*d*, *J* = 7.8 Hz, 1H, *ArH*), 7.84 (*t*, *J* = 7.9 Hz, 1H, *ArH*), 7.46 (*t*, *J* = 7.6 Hz, 1H, *ArH*), 7.34 (*d*, *J* = 8.4 Hz, 1H, *ArH*). ¹³C NMR (CDCl₃, 125 MHz), δ (ppm): 155.71 (C=O), 153.81 (*ArC*), 142.15 (OC=OO), 138.67 (*ArC*), 130.08 (*ArC*), 126.78 (*ArC*), 116.82 (*ArC*), 109.83 (*ArC*).

Polymerization procedure.

A typical procedure for polymerization of SAOCA was performed in a 10 mL Schlenk in a Vigor glovebox. The given amount of organobase and initiator was stirred in 1.0 mL anhydrous THF for 10 min, followed by adding 123 mg SAOCA (0.75 mmol). The mixture was kept stirring at 25 °C. After a specific time, a small aliquot of polymer solution was taken out for determining monomer conversion. After stopping stirring, the final polymer was precipitated at the bottom of the flask. The solid was separated for dissolving in DCM and precipitated in the mixture of ethyl acetate/hexane (v/v = 1/1), and washed twice using the same solution. The polymers obtained were dried in vacuum.

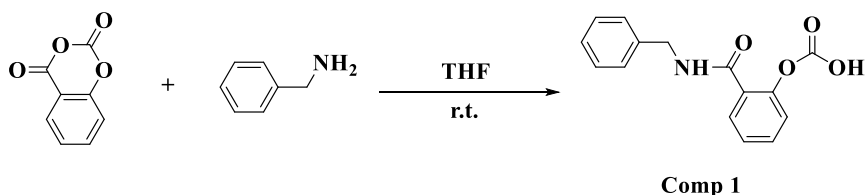
Computational Details

All calculations were performed with the Gaussian 09 program.² Geometry optimizations of all stationary points for the asymmetric reduction reaction of arylimines were performed with the M06-2X functional,³ which has been proven to be suitable to describe the dispersion effects. The 6-31G(d) basis set⁴ was applied for all elements in substrates and the latent catalyst. Frequency calculations at the same level were performed to confirm each stationary point to be either a minimum or a transition structure. Intrinsic reaction coordinate (IRC)⁵ calculations were performed to confirm the connection of each transition state to its corresponding reactant and product. All figures of structures were prepared using CYLView.⁶

References:

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Scheme S1. Synthesis formula of Comp 1.

Table S1. Thermal properties of homopolymer poly(salicylate)s.

| Entry | DBU:BnOH:SAOCA | TGA | | | DSC | |
|-------|----------------|----------------------|-------------------------|---------------------|---------------------|---------------------|
| | | T _{5%} (°C) | T _{d max} (°C) | T _g (°C) | T _m (°C) | T _c (°C) |
| 1 | 1:1:50 | 293.3 | 369.4 | 108.7 | 177.0 | 169.1 |
| 2 | 1:1:100 | 299.8 | 372.7 | 128.3 | 178.7 | 169.0 |

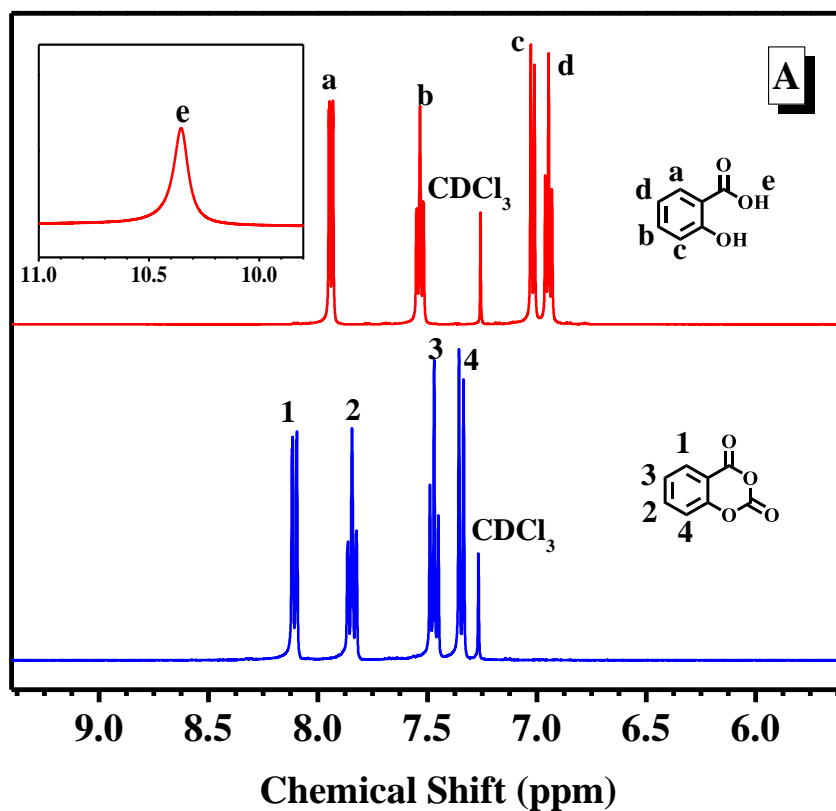


Figure S1. Comparative ^1H NMR spectra of SA and SAOCA.

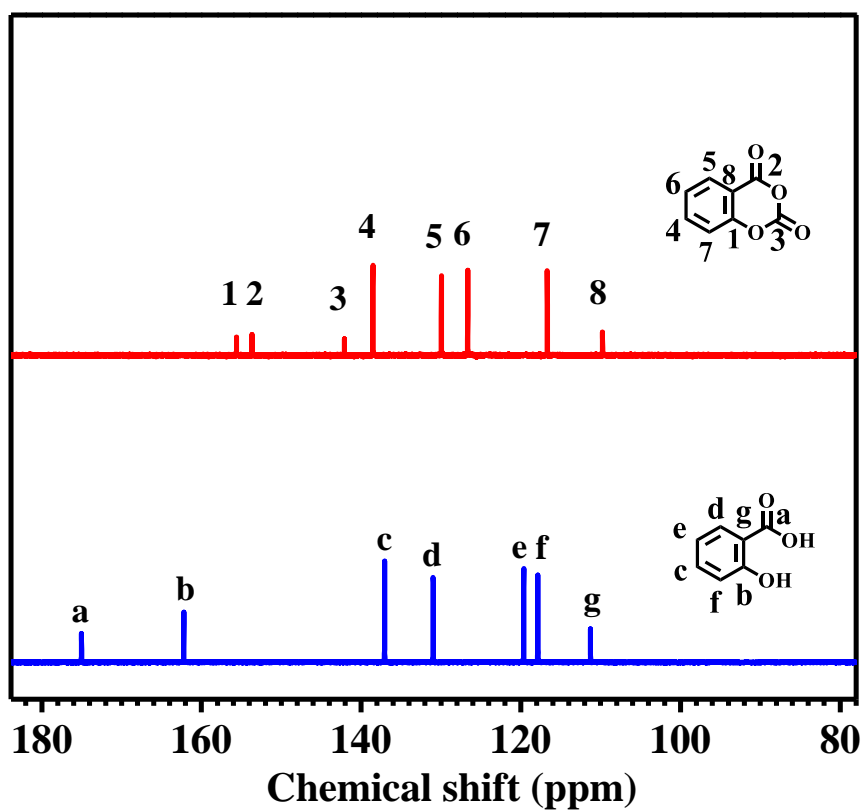


Figure S2. Comparative ^{13}C NMR spectra of SA and SAOCA.

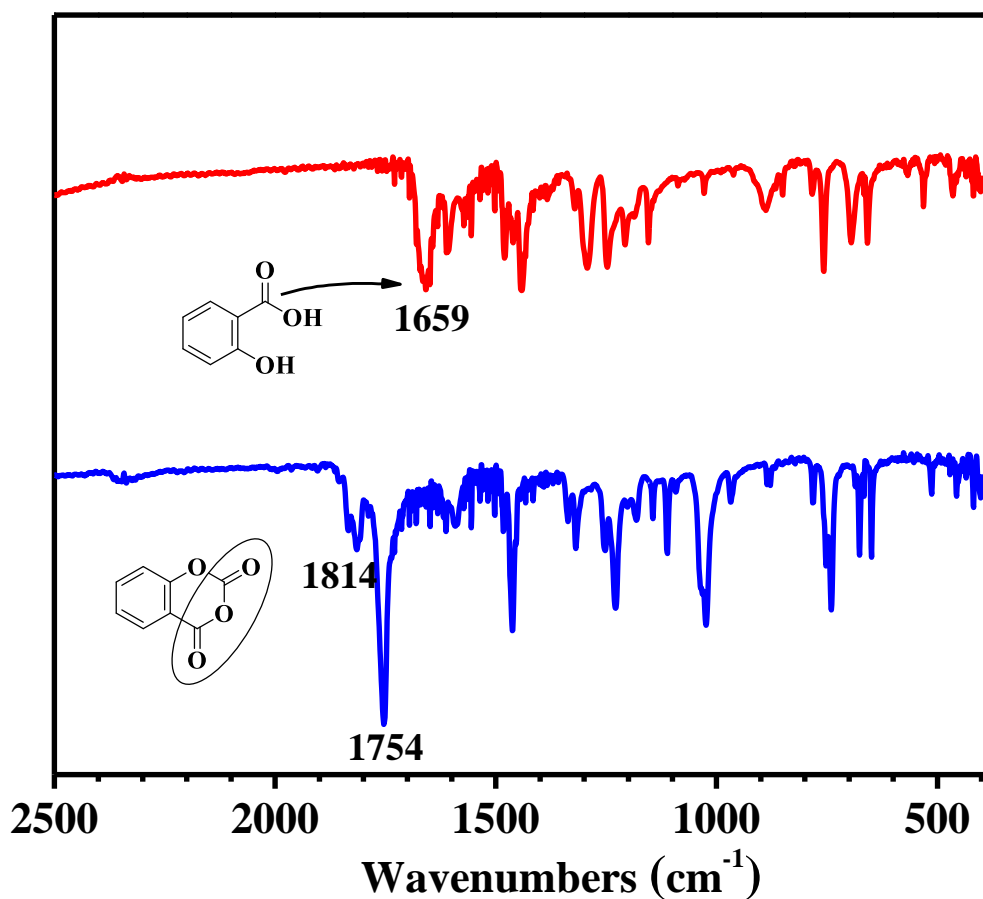


Figure S3. Comparative FTIR spectra of SA and SAOCA.

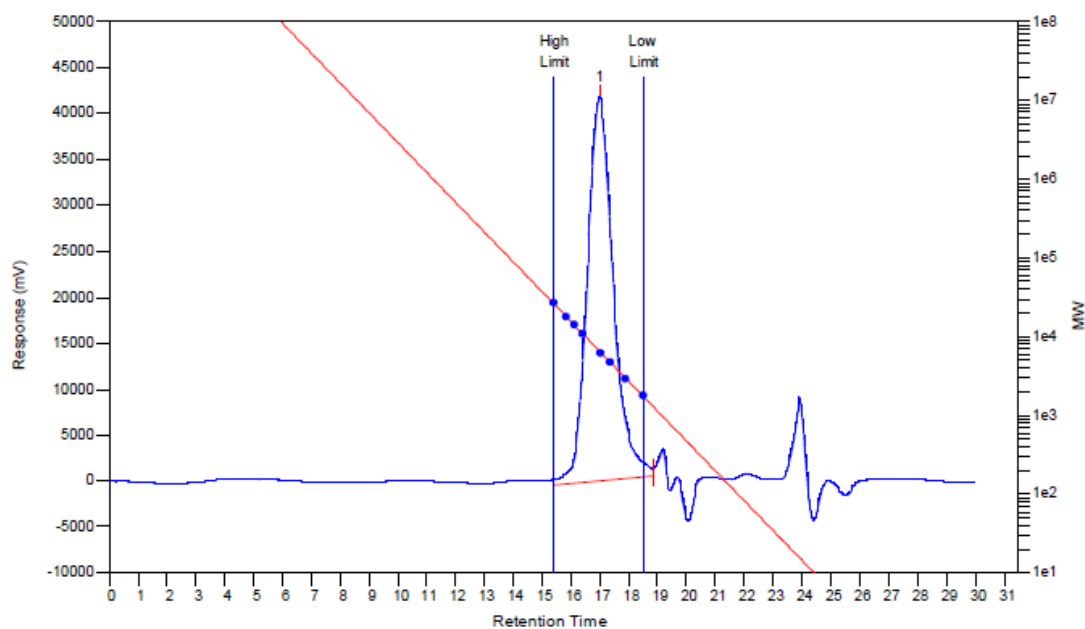


Figure S4. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M. (Table 1, Entry 2).

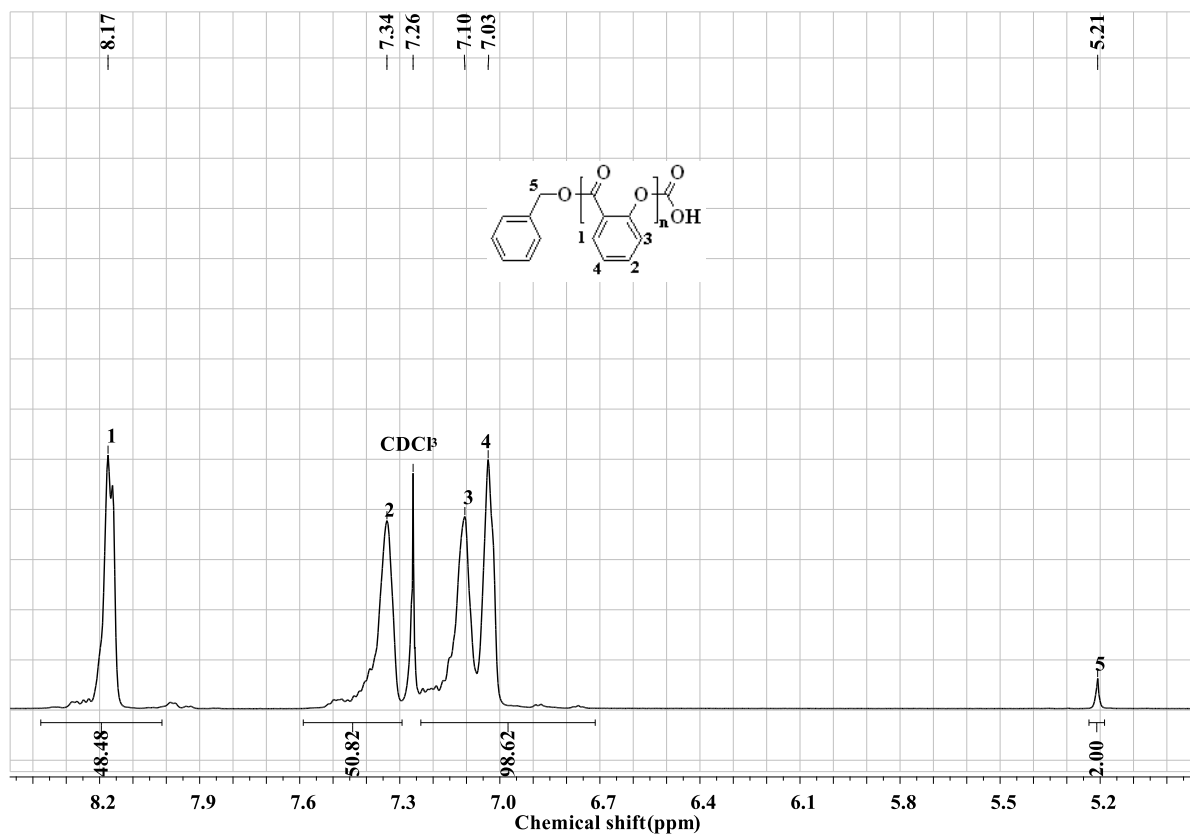


Figure S5. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 1/1/50 in THF at 25 °C, [SAOCA] = 0.75 M.

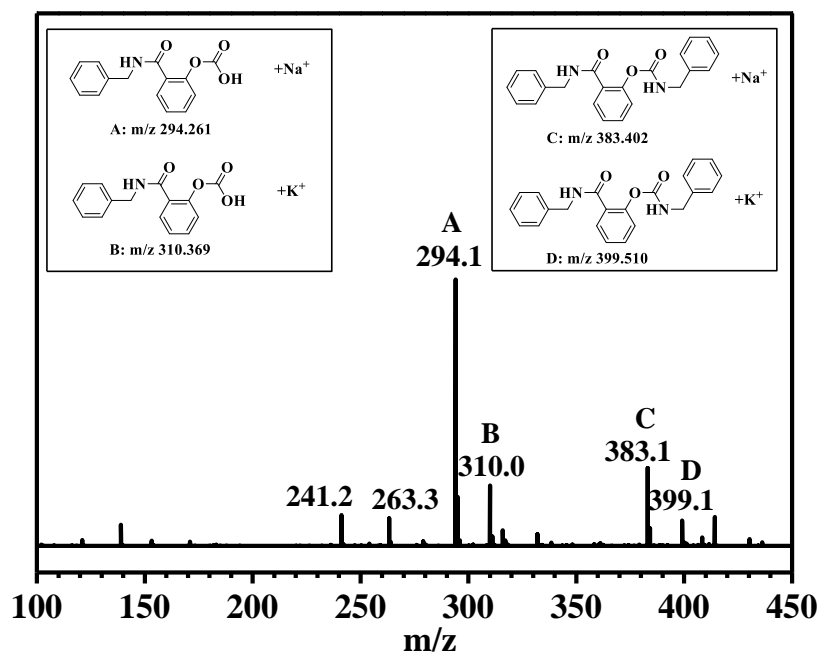


Figure S6. ESI MS spectrum of ring-opening SAOCA initiated by BnNH₂.

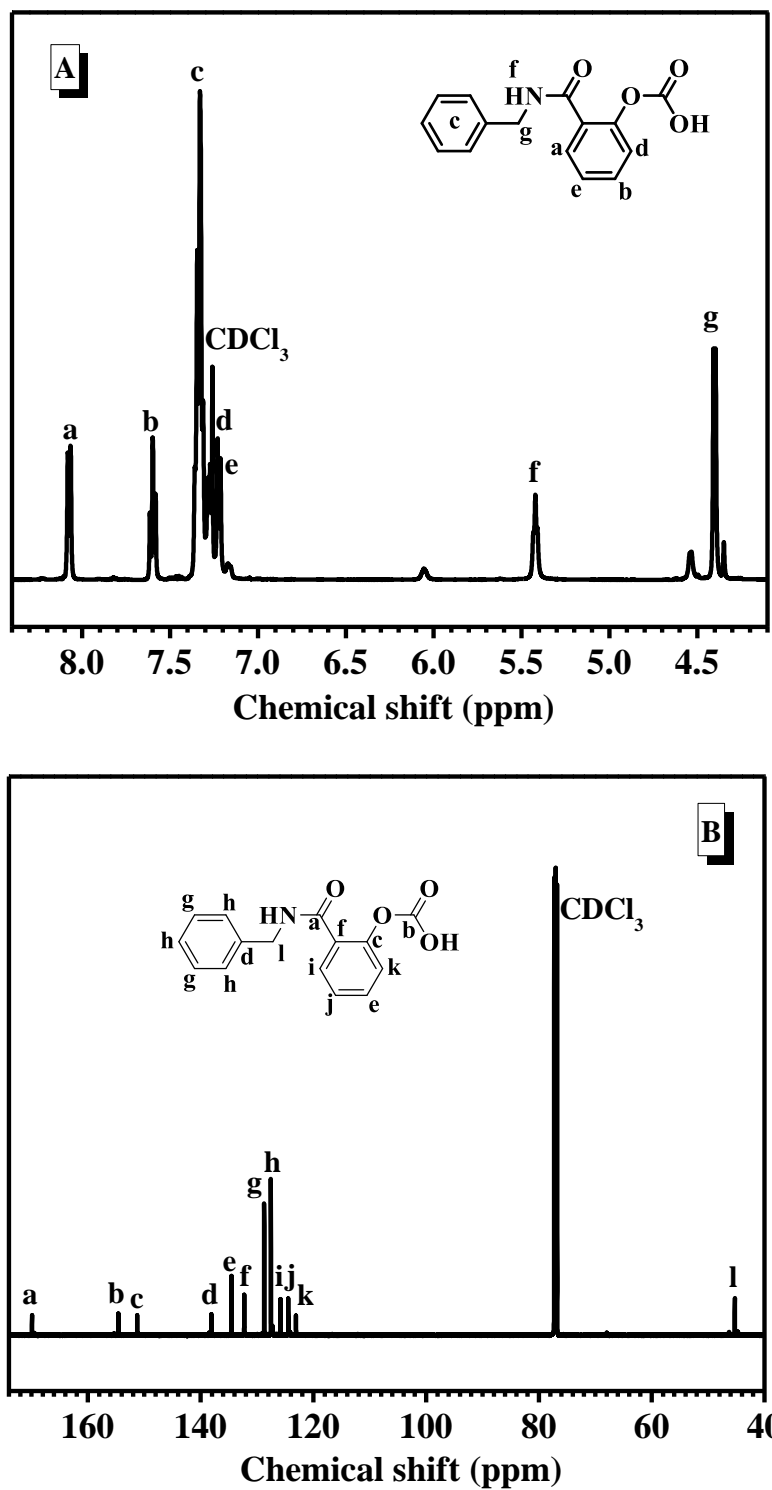


Figure S7. NMR spectra of ring-opening SAOCA initiated by BnNH₂. (A) ¹H NMR; (B) ¹³C NMR.

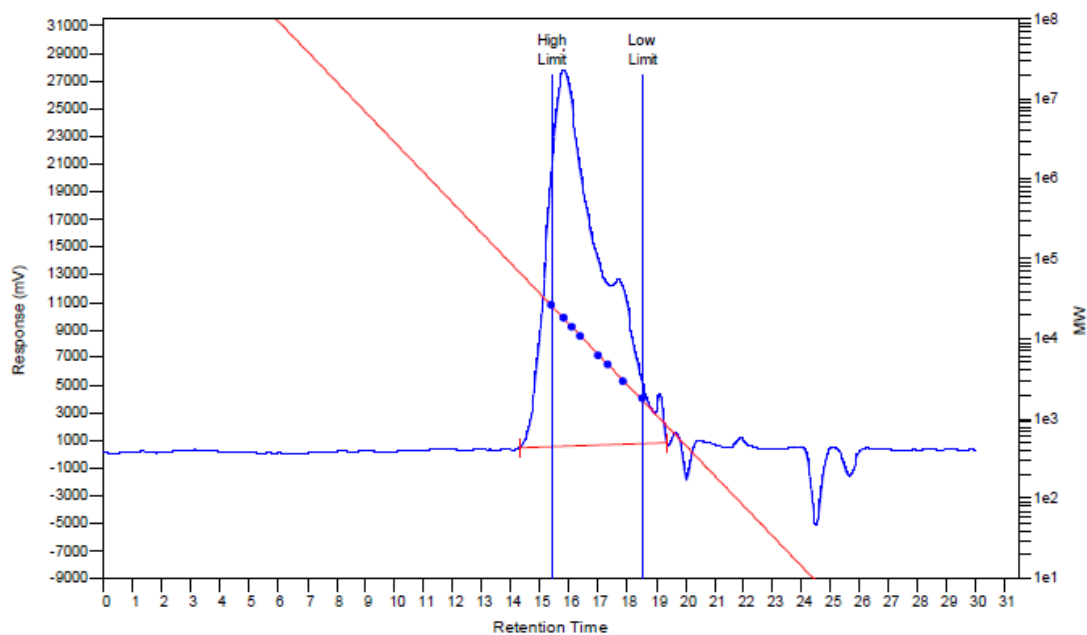
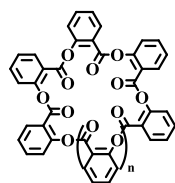
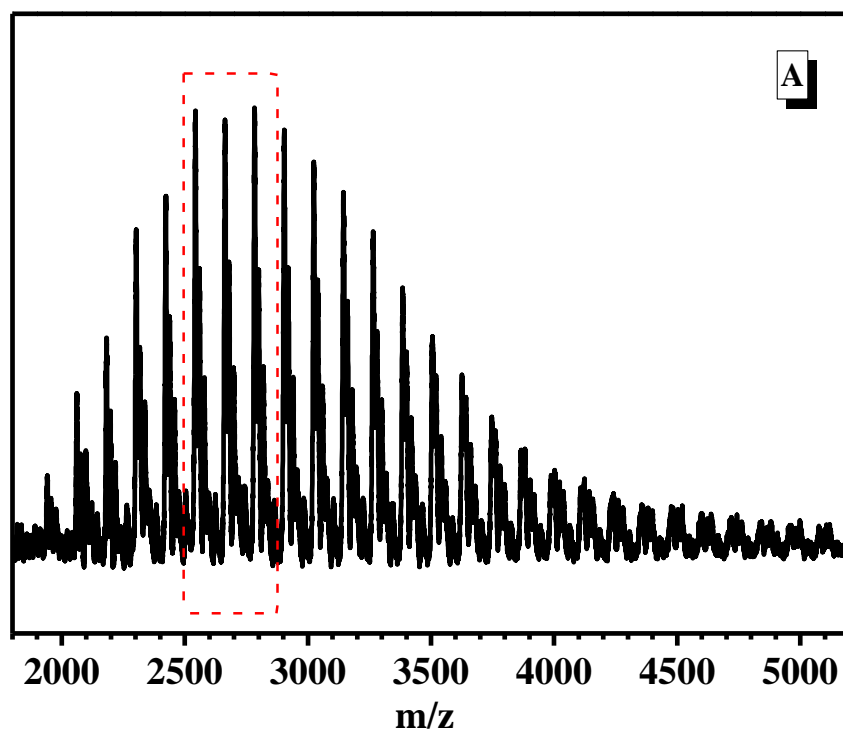
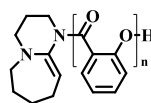


Figure S8. GPC trace of the resulting polymer in the catalysis of DBU only in THF at 25 °C, [SAOCA]/[DBU] = 50:1. (Table 1, Entry 1)



■ $m/z = 120.11 \cdot n + \text{Na}^+$

◆ $m/z = 120.11 \cdot n + \text{K}^+$



● $m/z = 152.24 + 120.11 \cdot n + \text{Na}^+$

○ $m/z = 152.24 + 120.11 \cdot n + \text{K}^+$

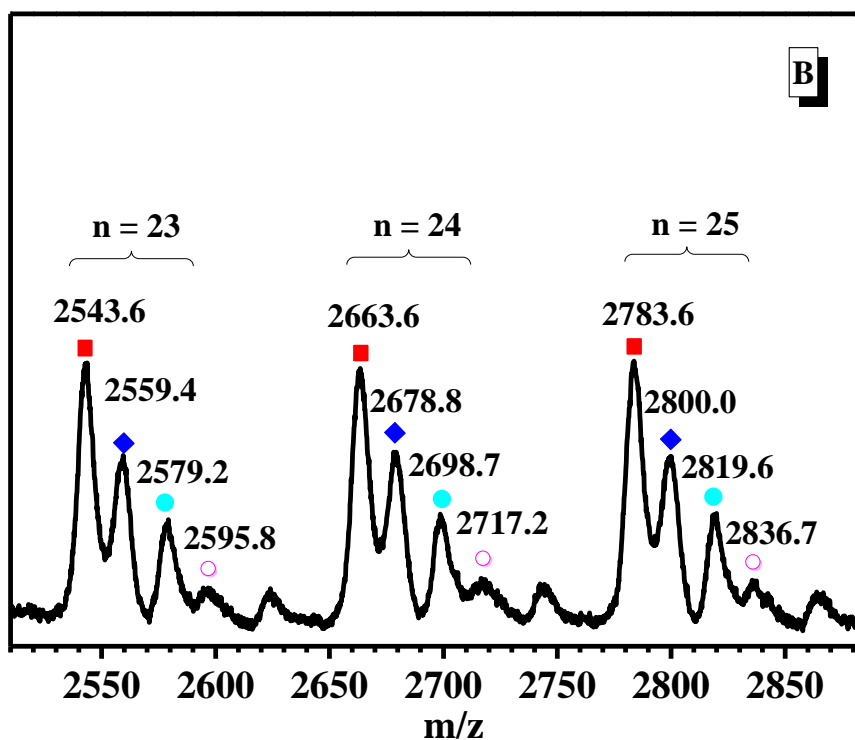


Figure S9. MALDI-TOF of the resulting polymer in the catalysis of DBU only in THF at 25 °C, [SAOCA]/[DBU] = 50:1. (Table 1, Entry 1) (A) full spectrum; (B) Zoomed-in region.

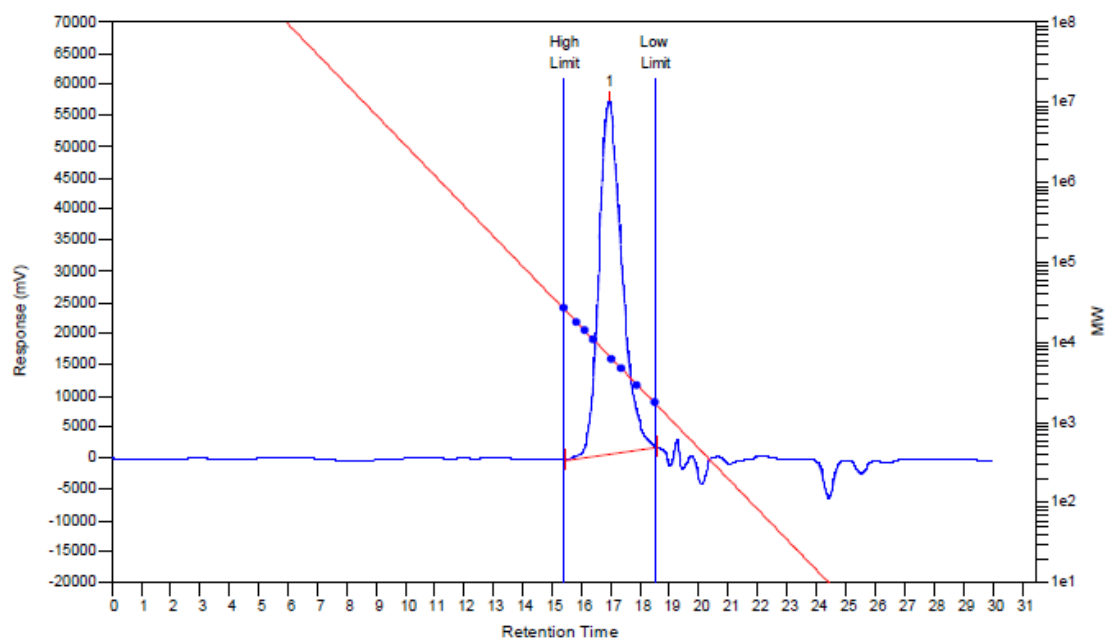


Figure S10. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 0.75:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 3).

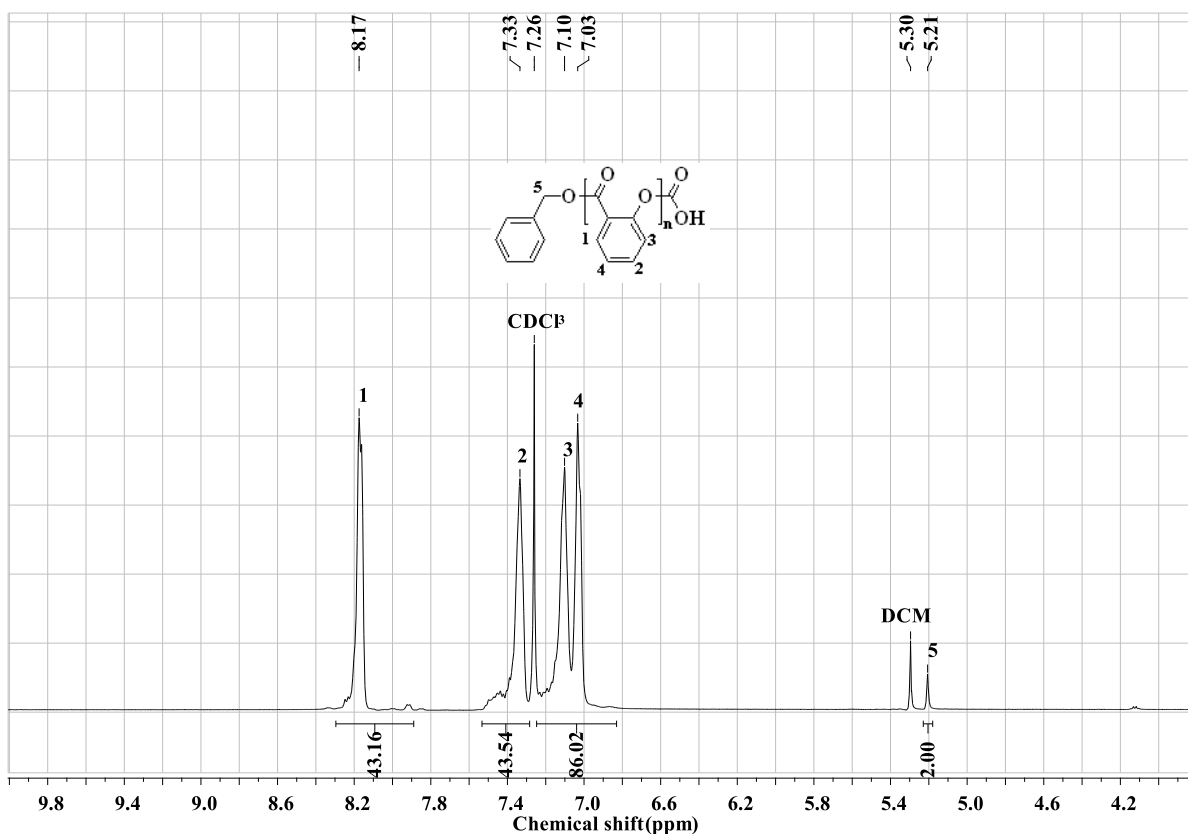


Figure S11. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of $[\text{DBU}]/[\text{BnOH}]/[\text{SAOCA}] = 0.75/1/50$ in THF at 25 °C, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 3).

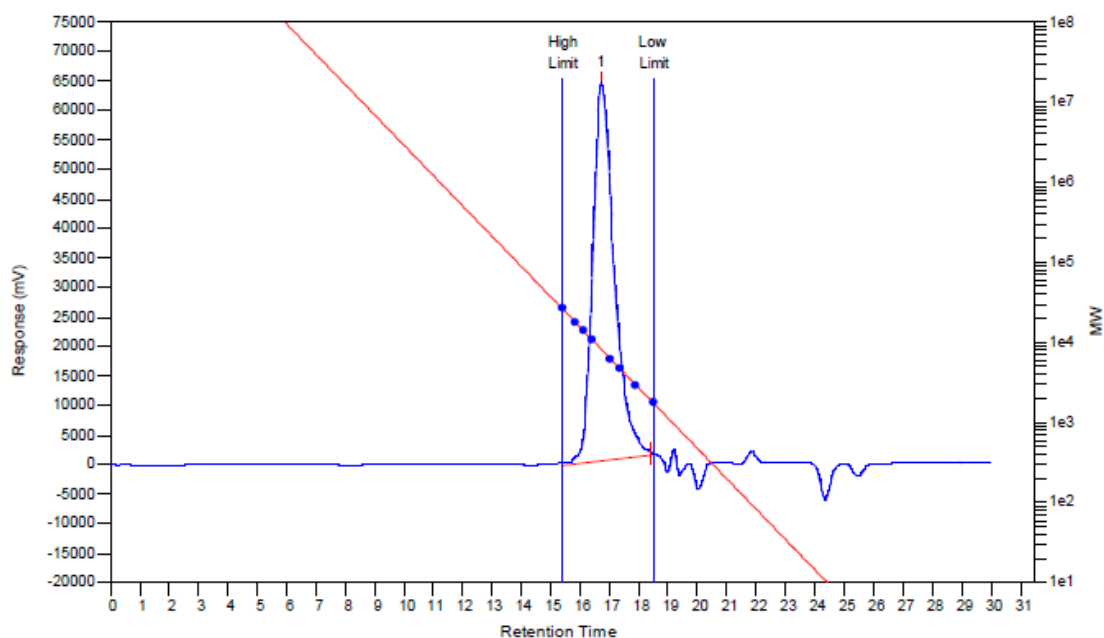


Figure S12. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 0.5:1 in THF at 25 °C, $[\text{SAOCA}]/[\text{BnOH}] = 50:1$, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 4).

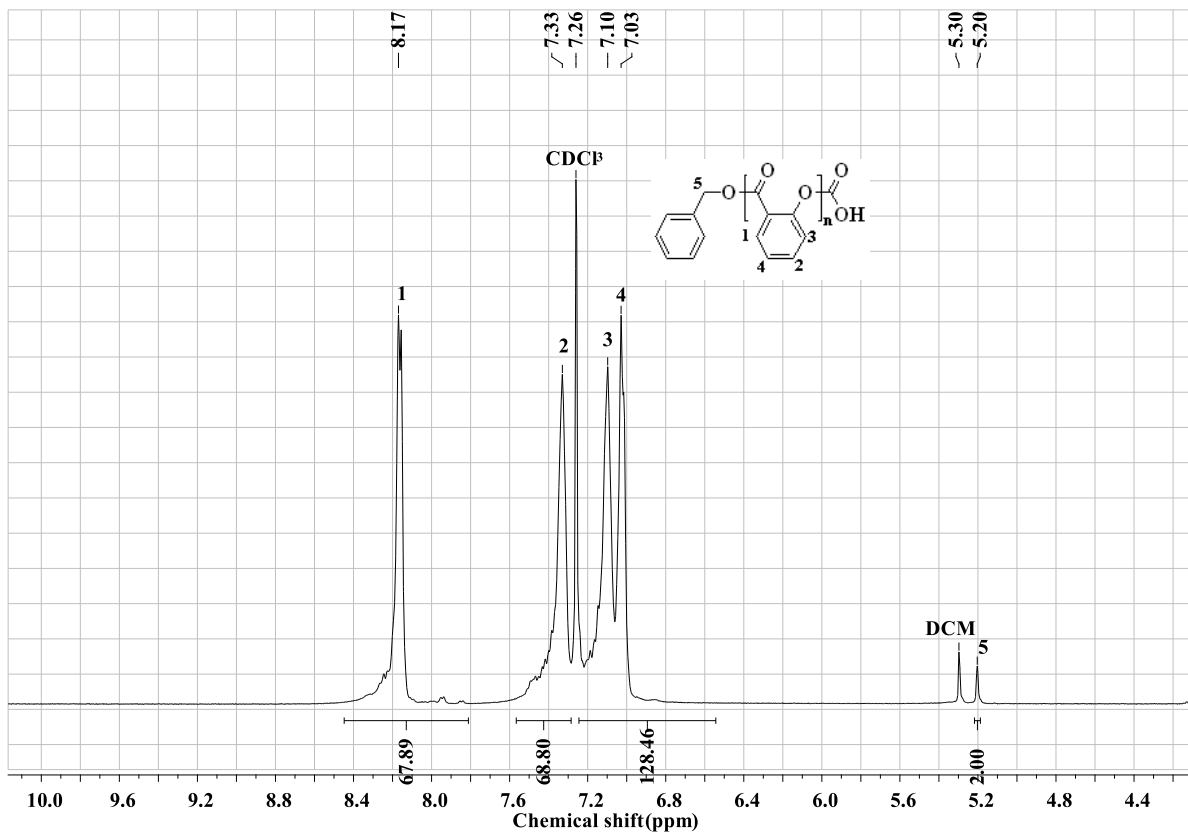
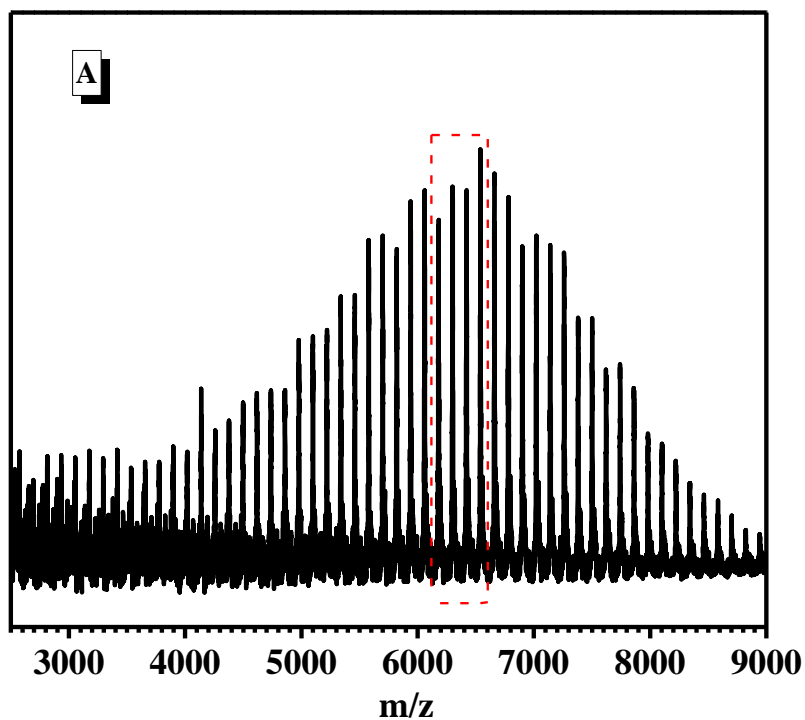


Figure S13. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 0.5/1/50 in THF at 25 °C, [SAOCA] = 0.75 M (Table 1, Entry 4).



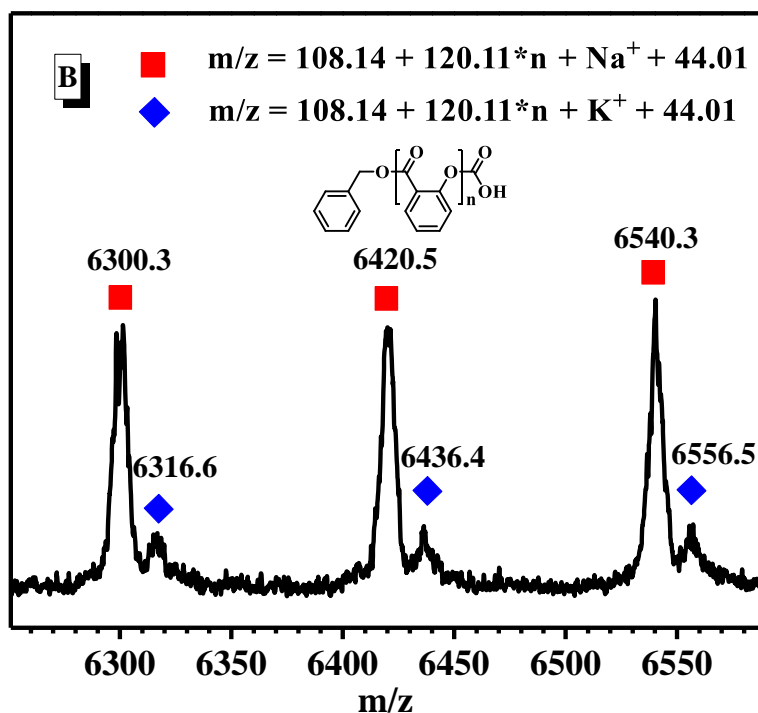


Figure S14. MALDI-TOF of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 0.5:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M. (A) Full spectrum; (B) Zoomed in region.

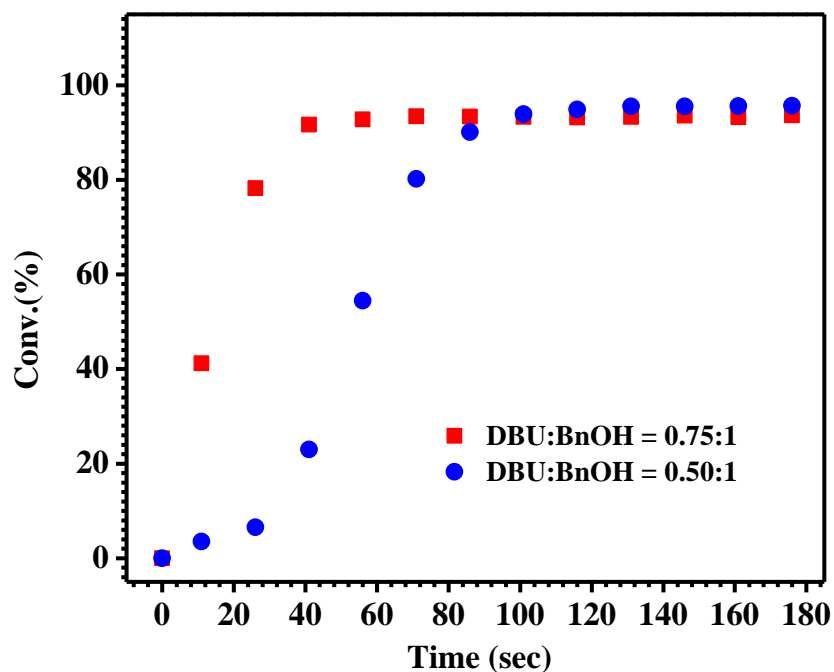


Figure S15. A plot of SAOCA conversion vs. time at various feeding ratios of DBU and BnOH in THF at 25 °C, [SAOCA] = 0.75 M, [BnOH]/[SAOCA] = 1/50.

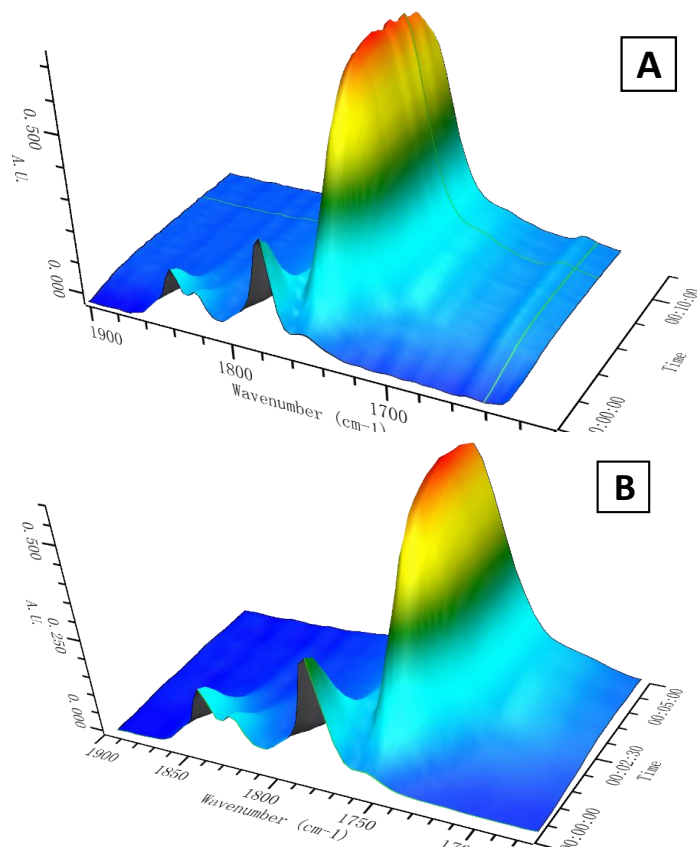


Figure S16. 3D kinetic behavior profile *in situ* IR in THF, 0 °C. (A) [DBU]/[BnOH]/[SAOCA] = 0.5/1/50, [SAOCA] = 0.75; (B) [DBU]/[BnOH]/[SAOCA] = 0.75/1/50.

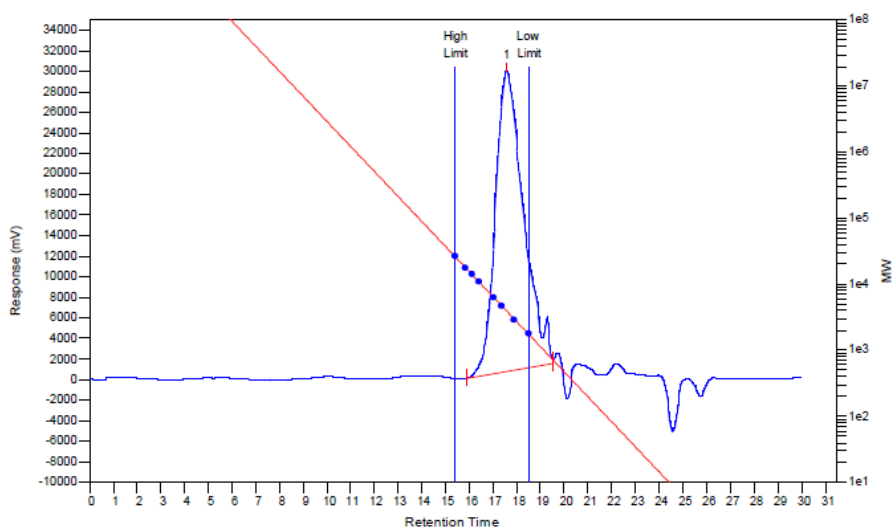


Figure S17. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 2:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 5).

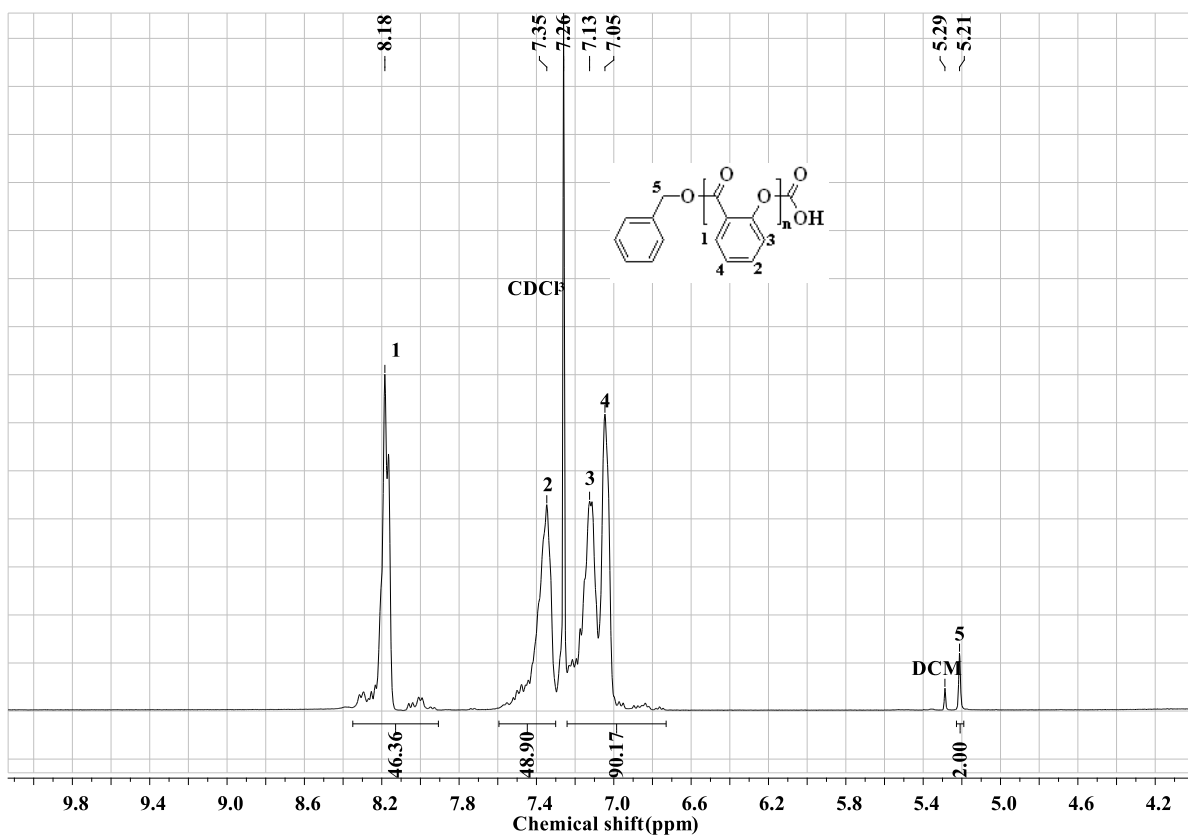
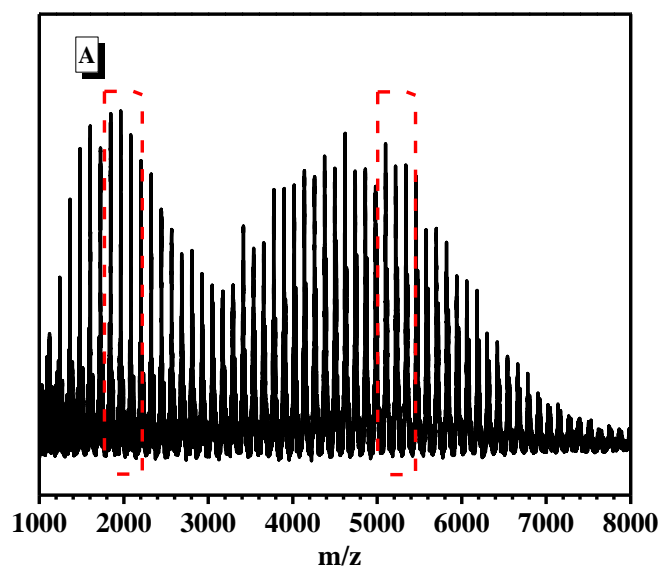


Figure S18. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 2/1/50 in THF at 25 °C, [SAOCA] = 0.75 M (Table 1, Entry 5).



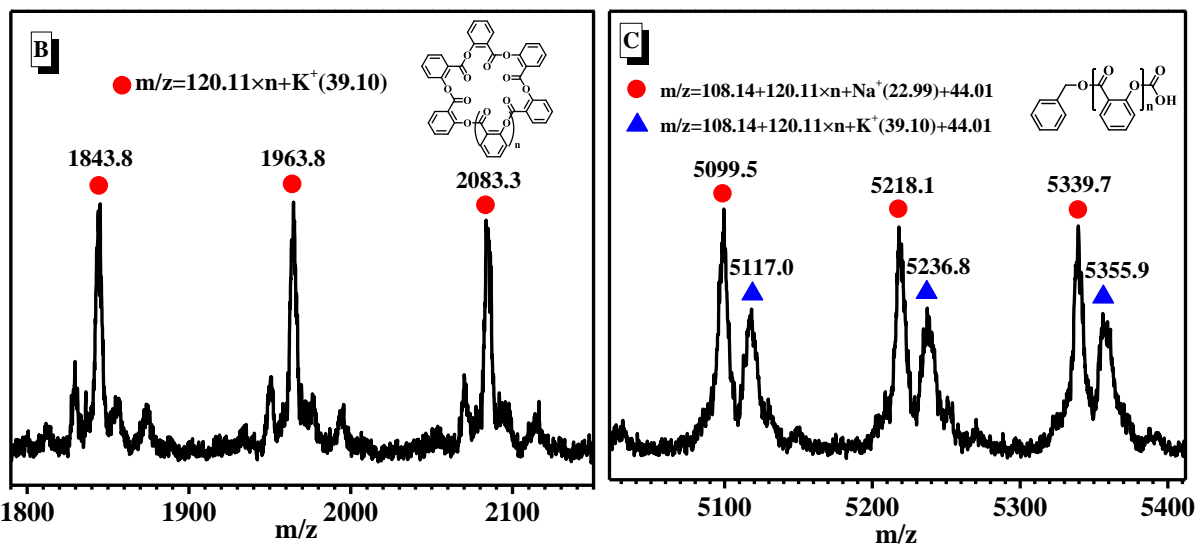


Figure S19. MALDI-TOF of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 2:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M. (A) Full spectrum; (B) and (C) Zoomed region in the different range.

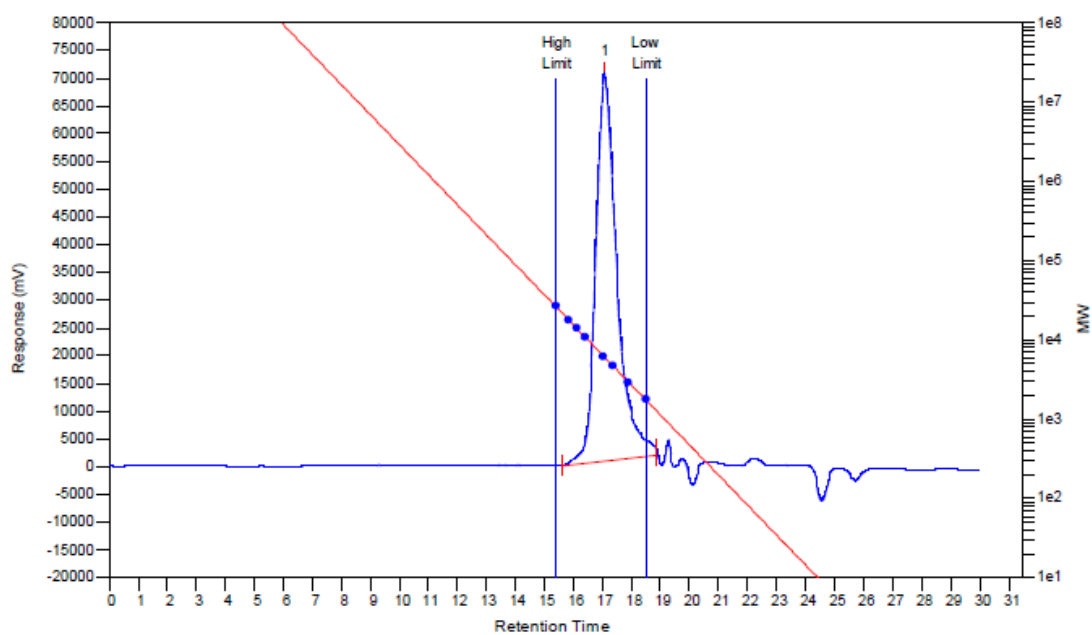


Figure S20. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in DCM at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 6).

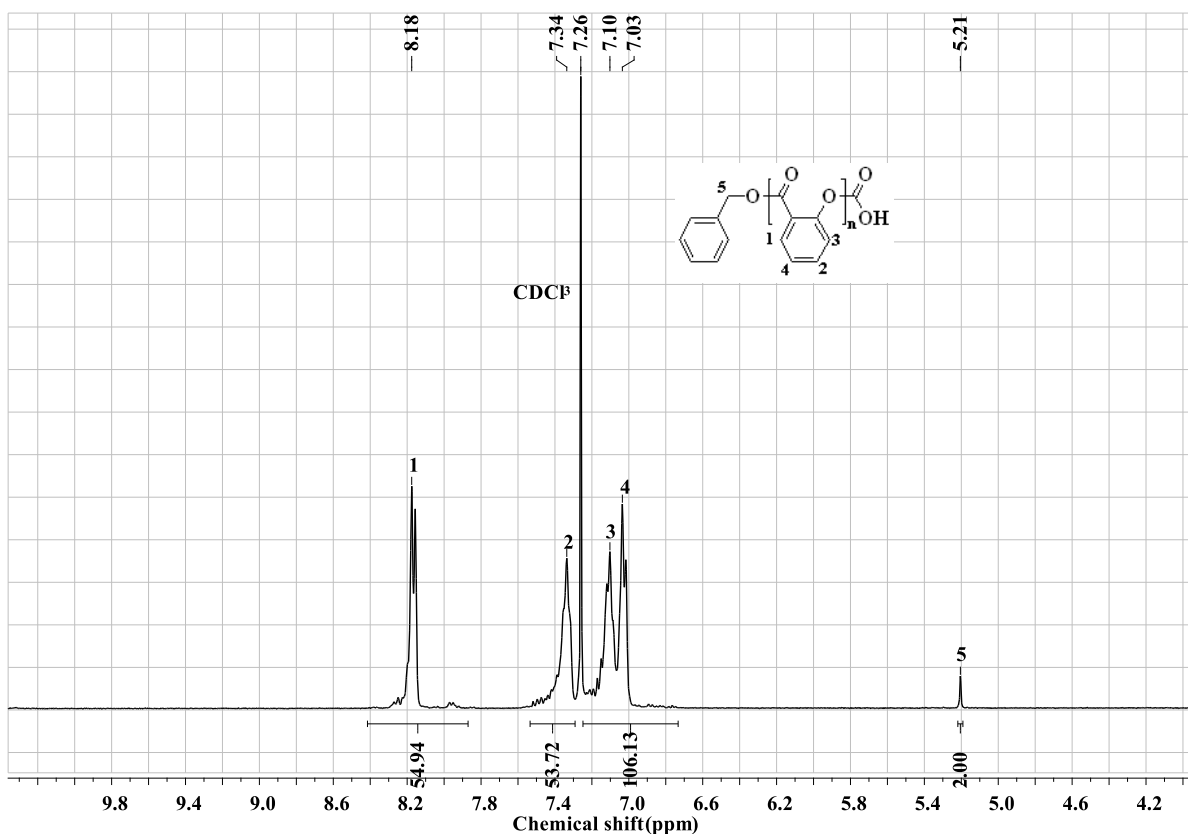


Figure S21. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of $[\text{DBU}]/[\text{BnOH}]/[\text{SAOCA}] = 1/1/50$ in DCM at 25 °C, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 6).

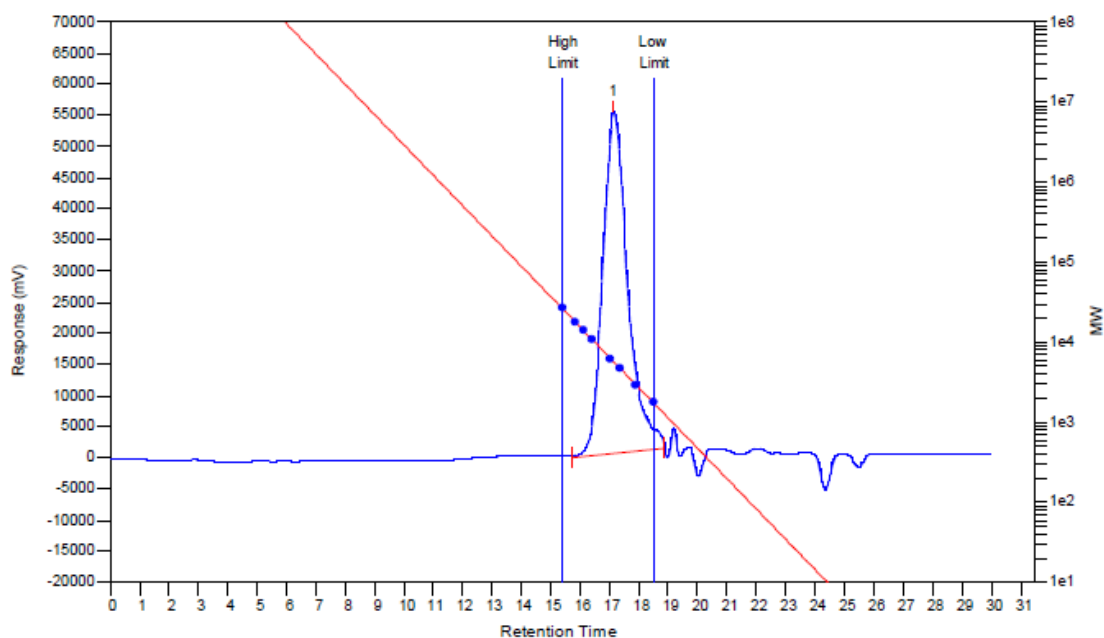


Figure S22. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in dioxane at 25 °C, $[\text{SAOCA}]/[\text{BnOH}] = 50:1$, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 7).

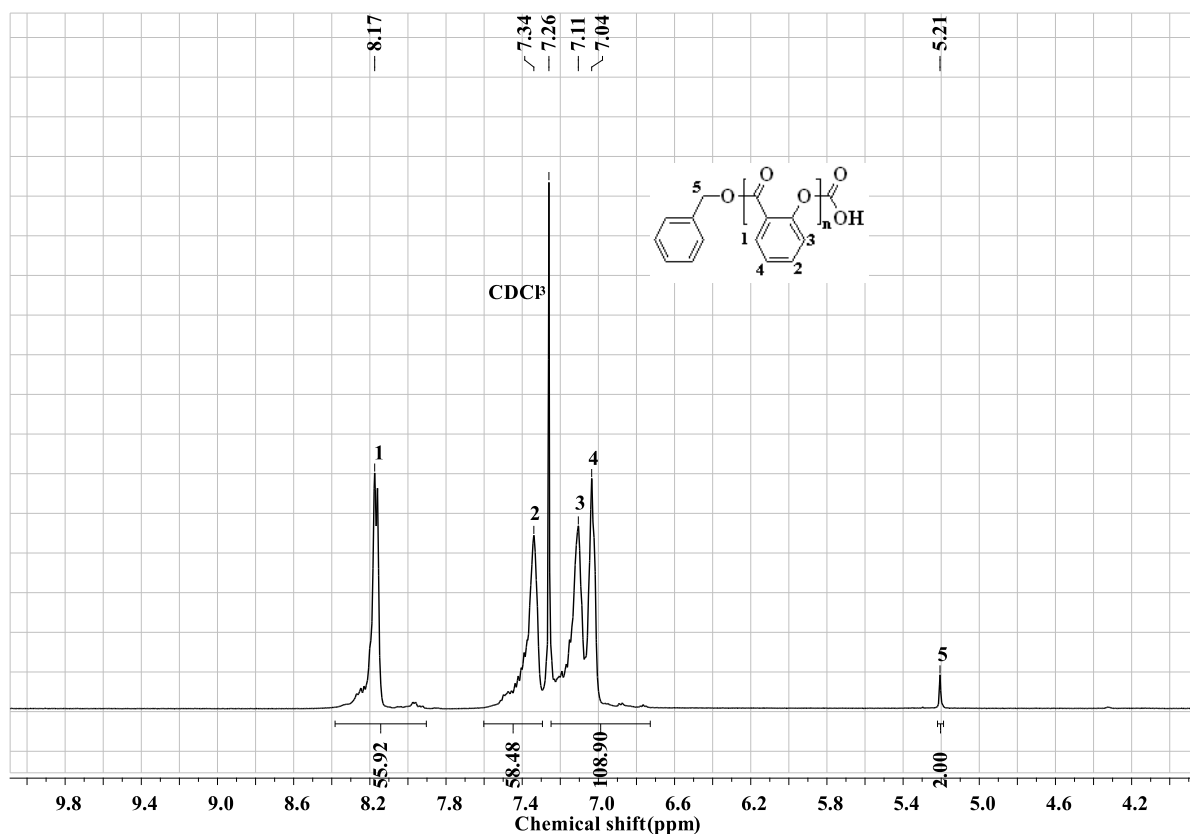


Figure S23. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of $[\text{DBU}]/[\text{BnOH}]/[\text{SAOCA}] = 1/1/50$ in dioxane at 25°C , $[\text{SAOCA}] = 0.75\text{ M}$ (Table 1, Entry 7).

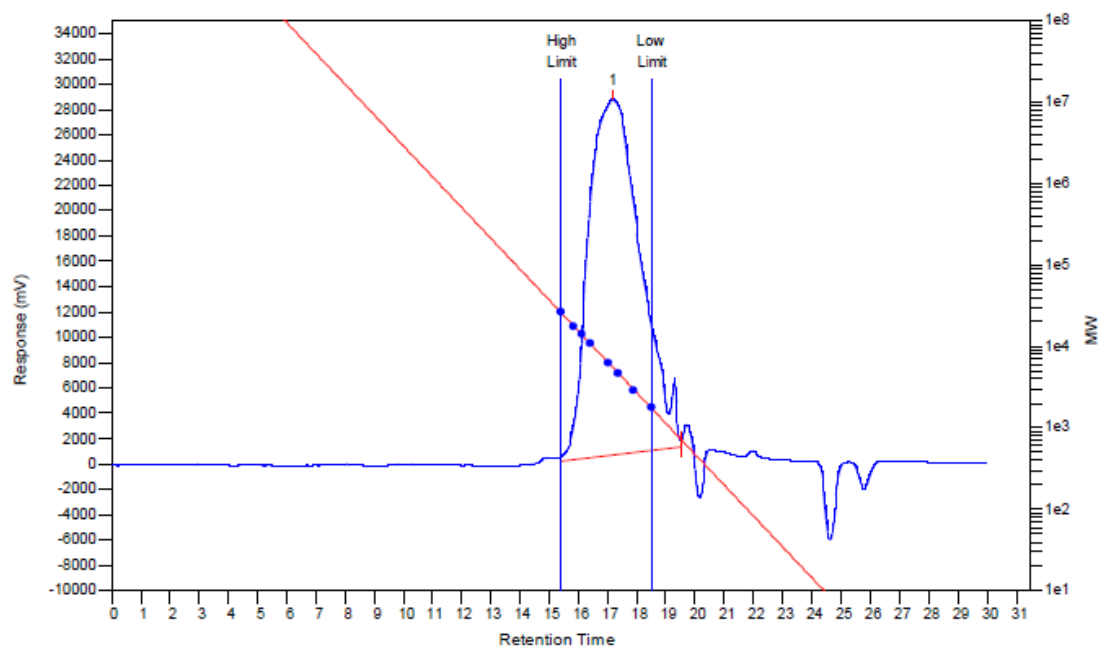


Figure S24. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in TCM at 25°C , $[\text{SAOCA}]/[\text{BnOH}] = 50:1$, $[\text{SAOCA}] = 0.75\text{ M}$ (Table 1, Entry 8).

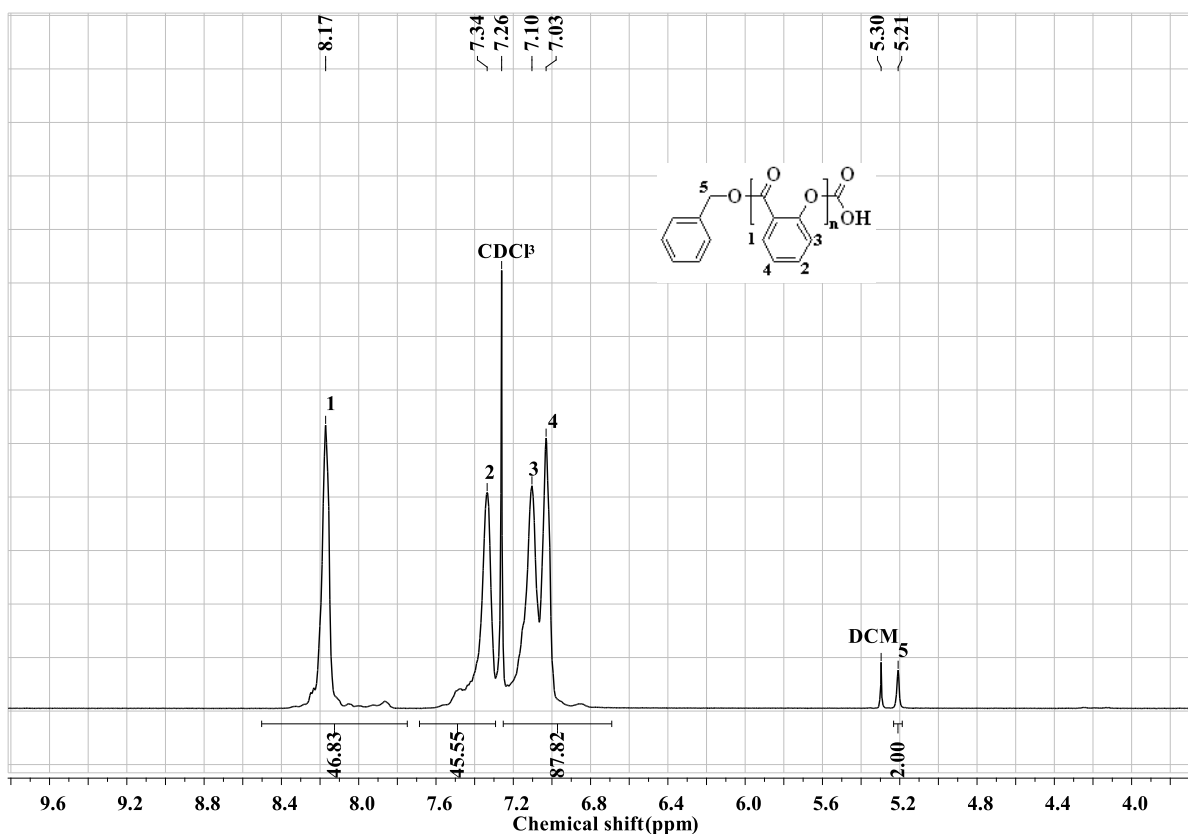


Figure S25. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 1/1/50 in TCM at 25 °C, [SAOCA] = 0.75 M (Table 1, Entry 8).

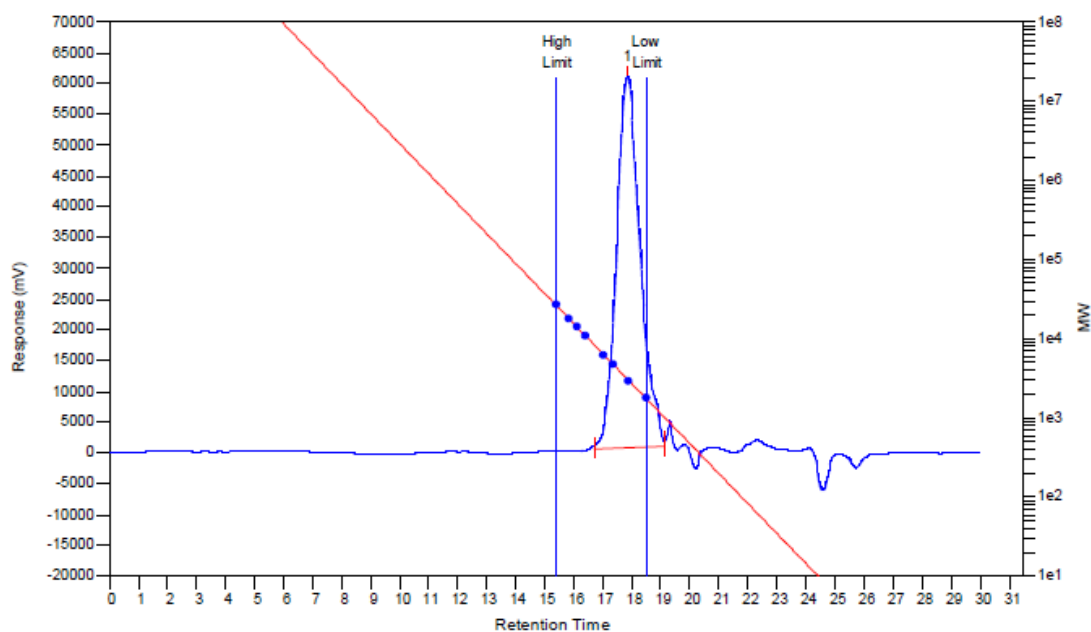


Figure S26. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 30:1, [SAOCA] = 0.75 M (Table 1, Entry 9).

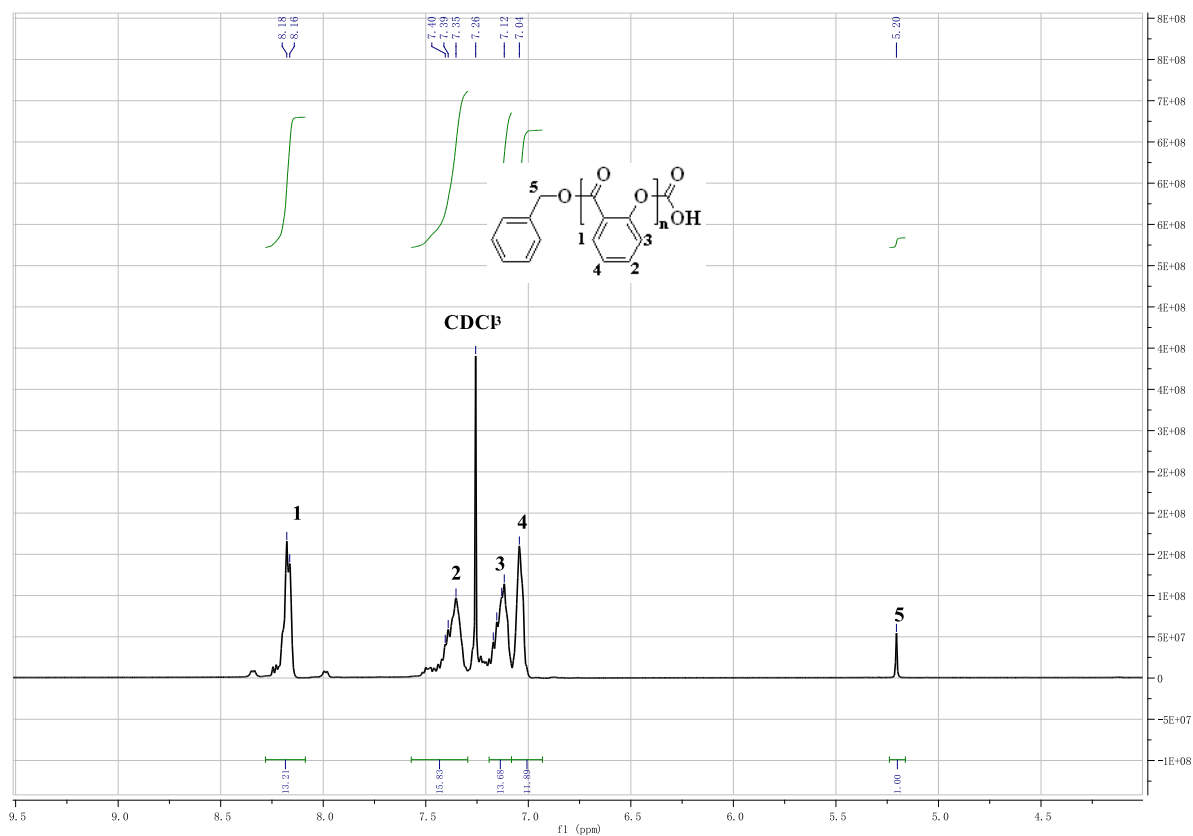
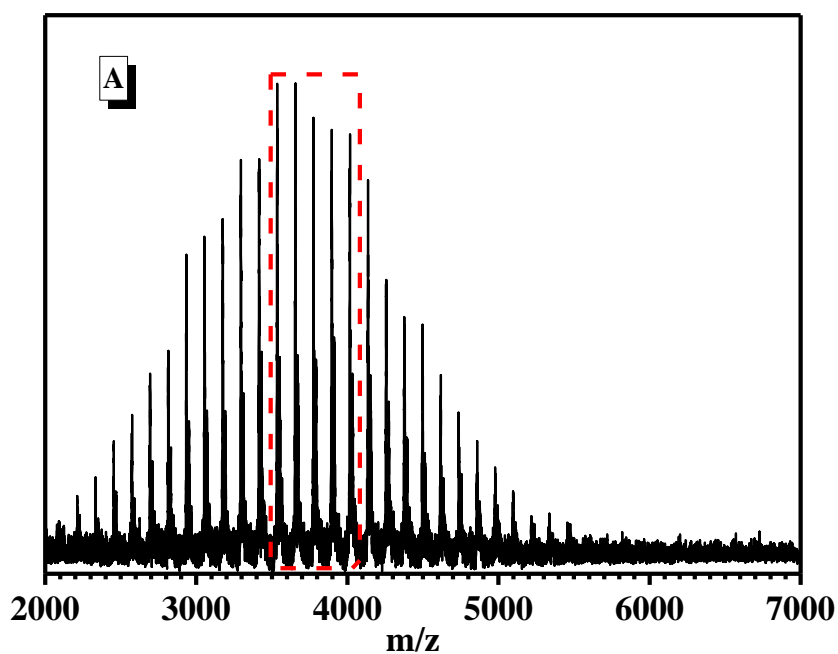


Figure S27. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of $[\text{DBU}]/[\text{BnOH}]/[\text{SAOCA}] = 1/1/30$ in THF at 25 °C, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 9).



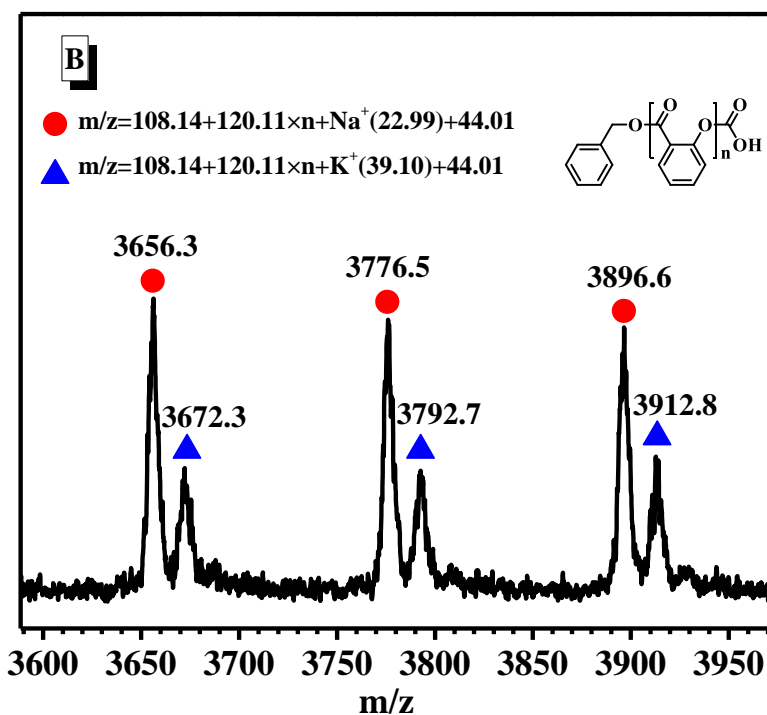


Figure S28. MALDI-TOF of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 30:1, [SAOCA] = 0.75 M. (A) Full spectrum; (B) Zoomed in region.

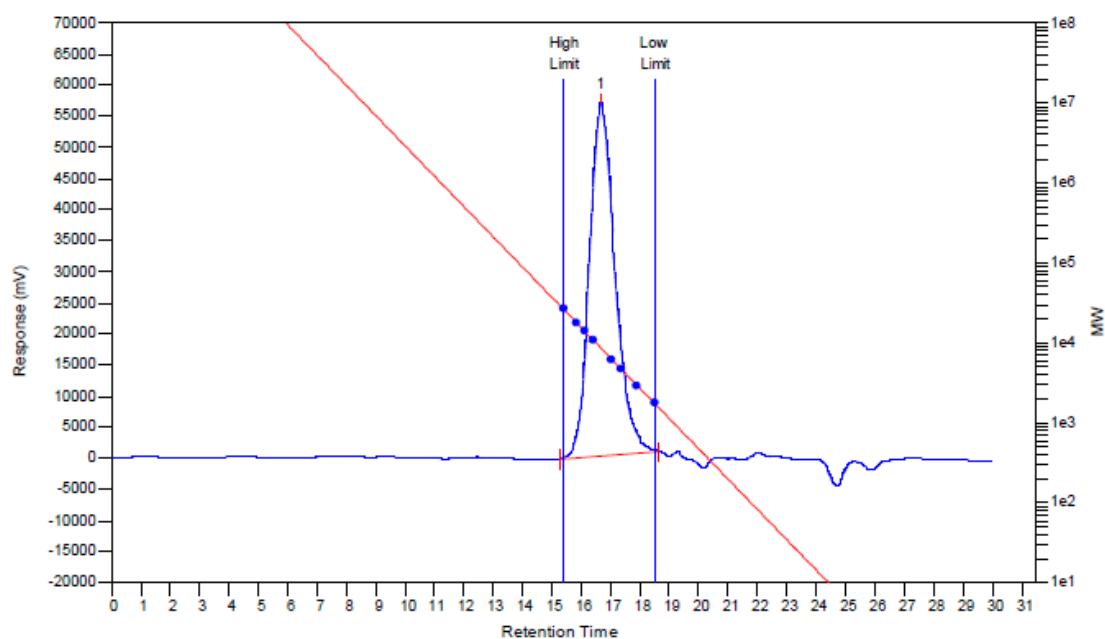


Figure S29. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 75:1, [SAOCA] = 0.75 M (Table 1, Entry 10).

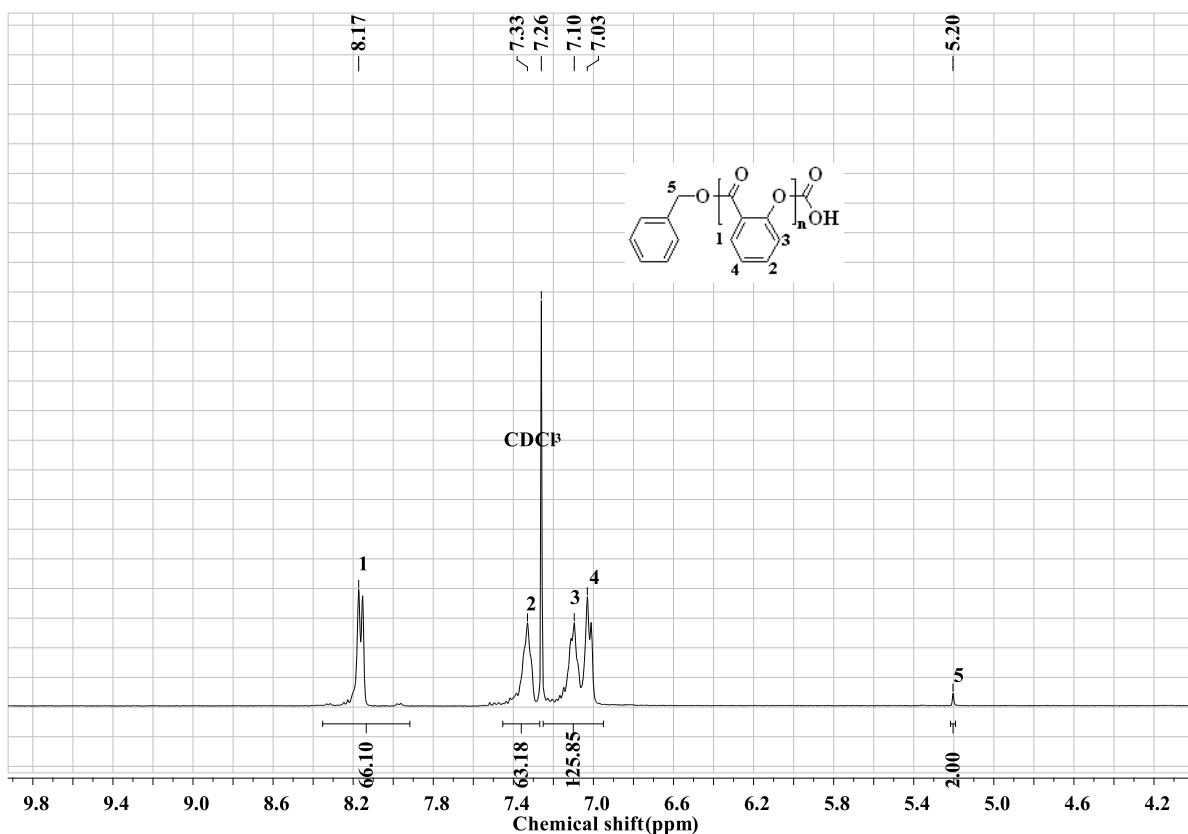


Figure S30. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of $[\text{DBU}]/[\text{BnOH}]/[\text{SAOCA}] = 1/1/75$ in THF at 25 °C, $[\text{SAOCA}] = 0.75$ M (Table 1, Entry 10).

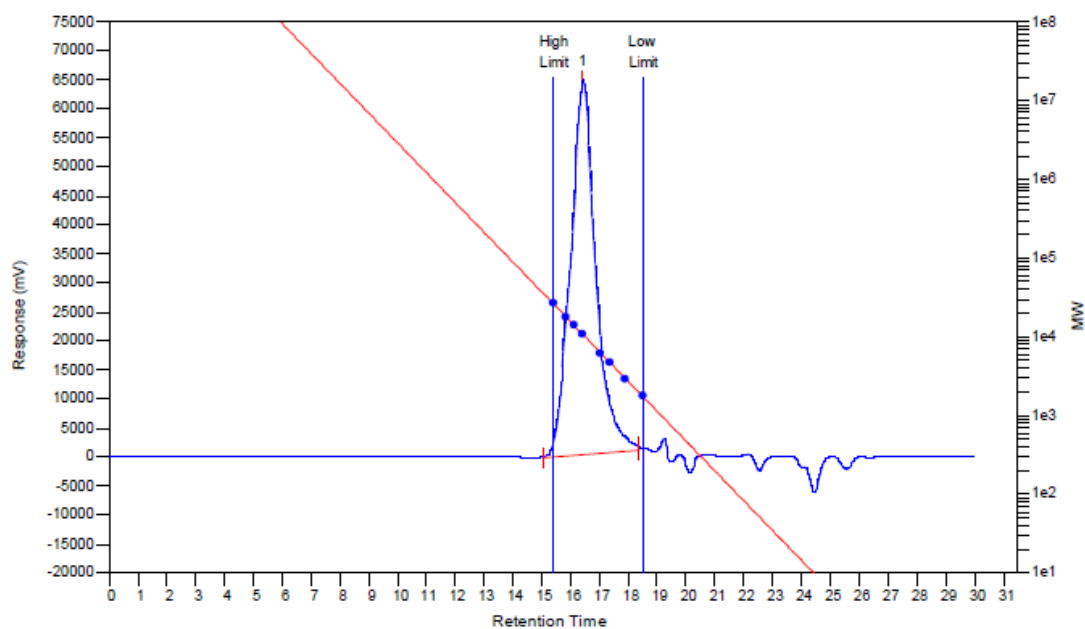


Figure S31. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, $[\text{SAOCA}]/[\text{BnOH}] = 100:1$, $[\text{SAOCA}] = 1.0$ M (Table 1, Entry 11).

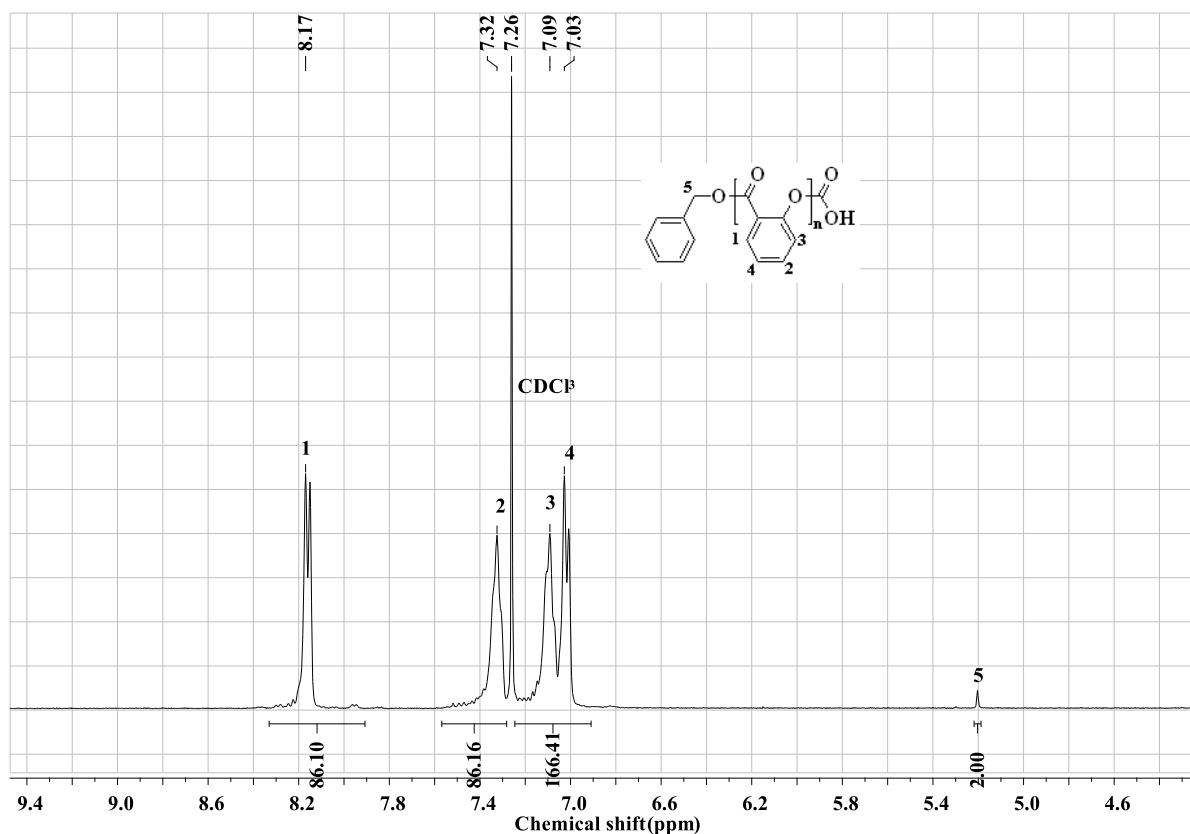


Figure S32. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 1/1/100 in THF at 25 °C, [SAOCA] = 1.0 M (Table 1, Entry 11).

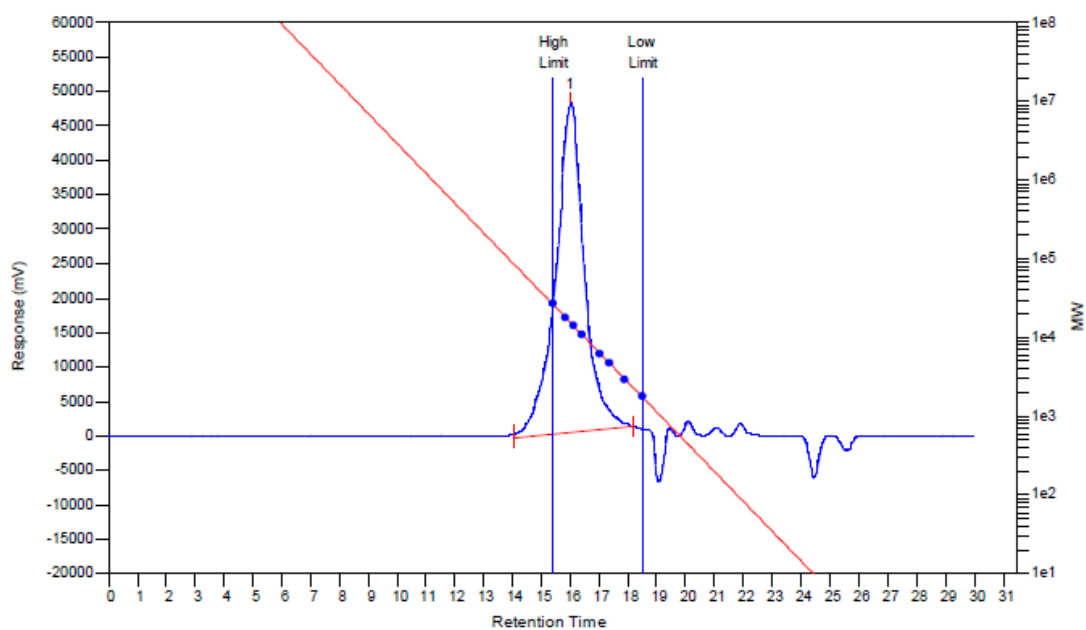


Figure S33. GPC trace of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 150:1, [SAOCA] = 1.5 M (Table 1, Entry 12).

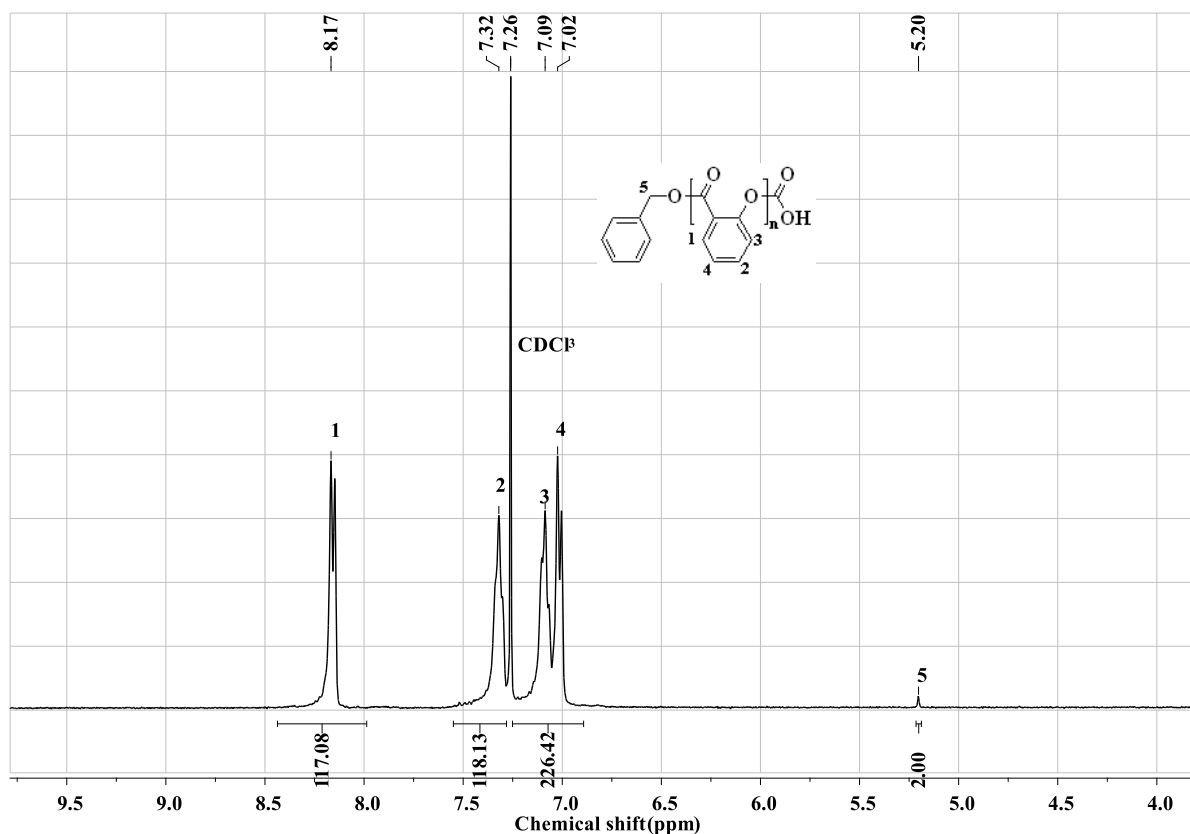


Figure S34. ¹H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[BnOH]/[SAOCA] = 1/1/150 in THF at 25 °C, [SAOCA] = 1.5 M (Table 1, Entry 12).

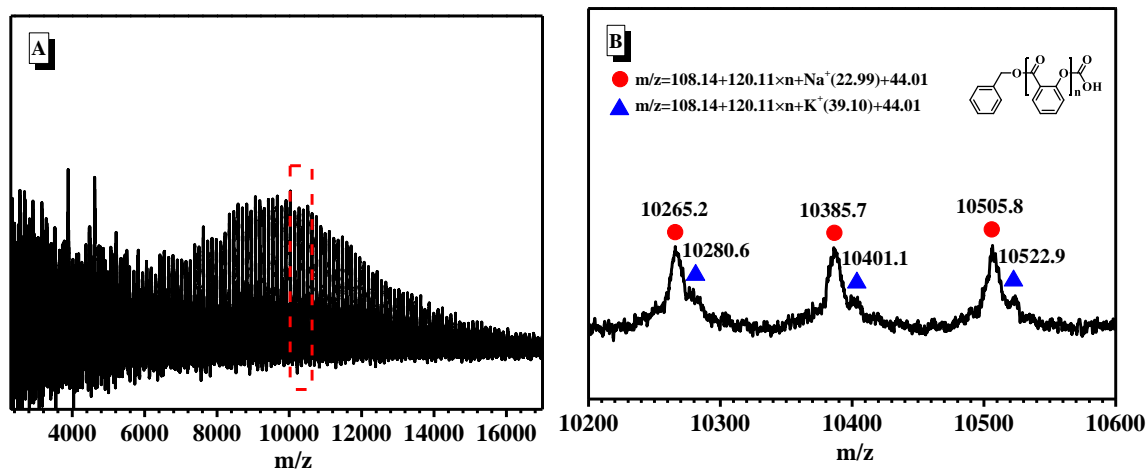


Figure S35. MALDI-TOF of the resulting polymer in the catalysis of DBU and BnOH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[BnOH] = 150:1, [SAOCA] = 1.5 M. (A) Full spectrum; (B) Zoomed in region.

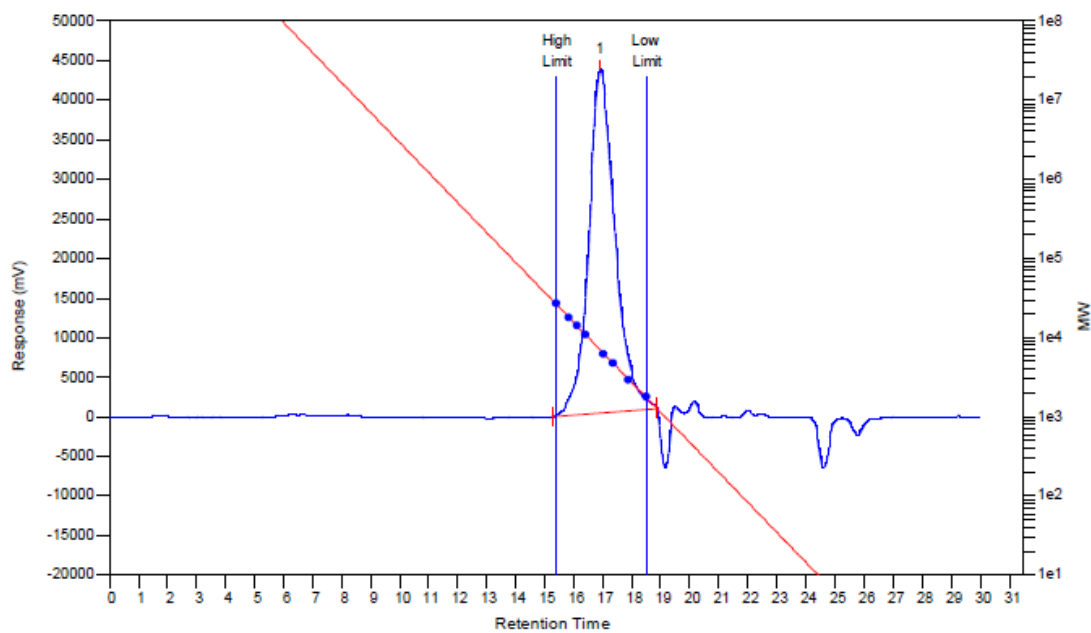


Figure S36. GPC trace of the resulting polymer in the catalysis of DBU and Hex-OH with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[HexOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 14).

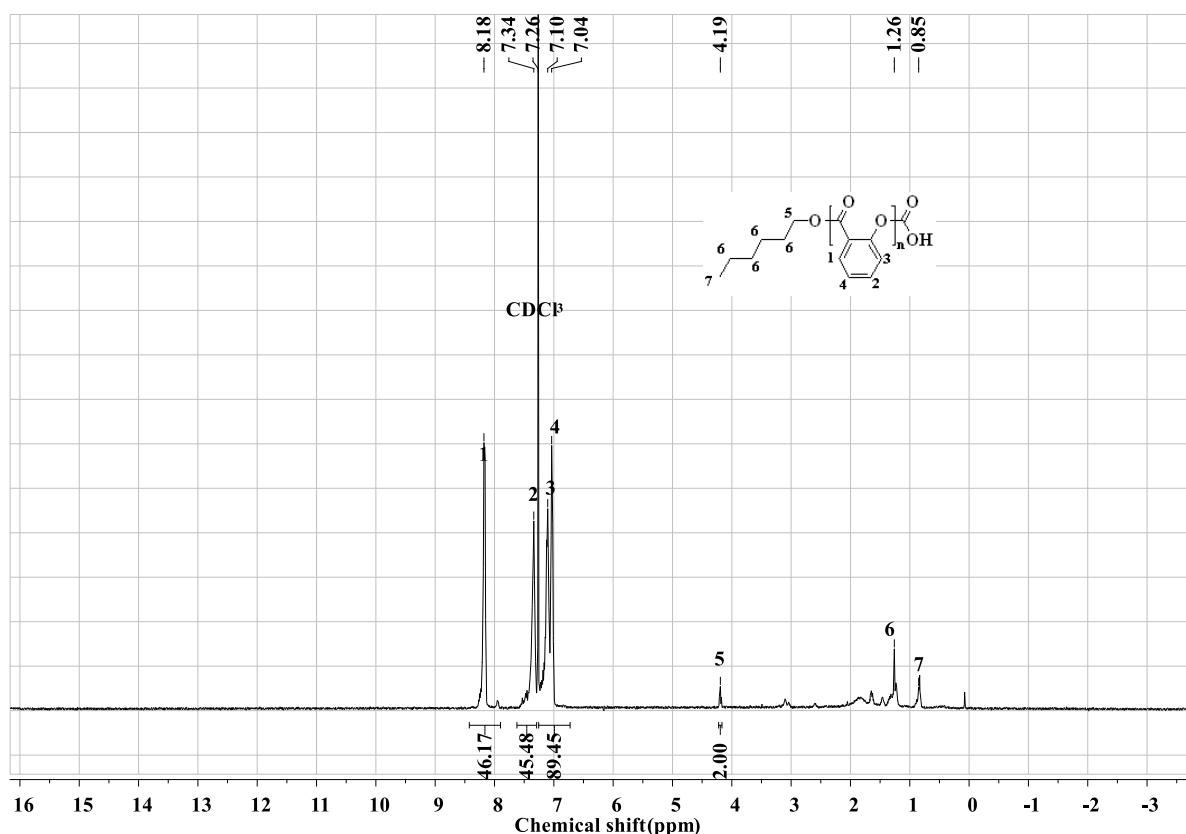


Figure S37. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[HexOH]/[SAOCA] = 1/1/50 in THF at 25 °C, [SAOCA] = 0.75 M (Table 1, Entry 14).

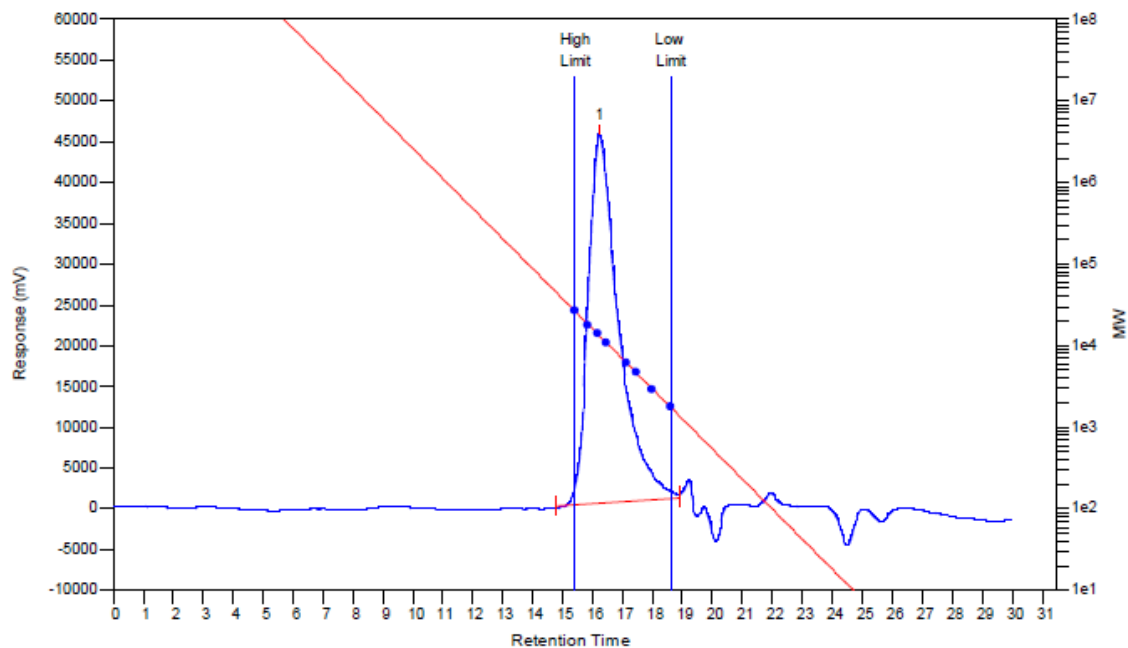


Figure S38. GPC trace of the resulting polymer in the catalysis of DBU and 1,6-HDO with molar ratio of 1:1 in THF at 25 °C, [SAOCA]/[HDO] = 50:1, [SAOCA] = 1.2 M (Table 1, Entry 15).

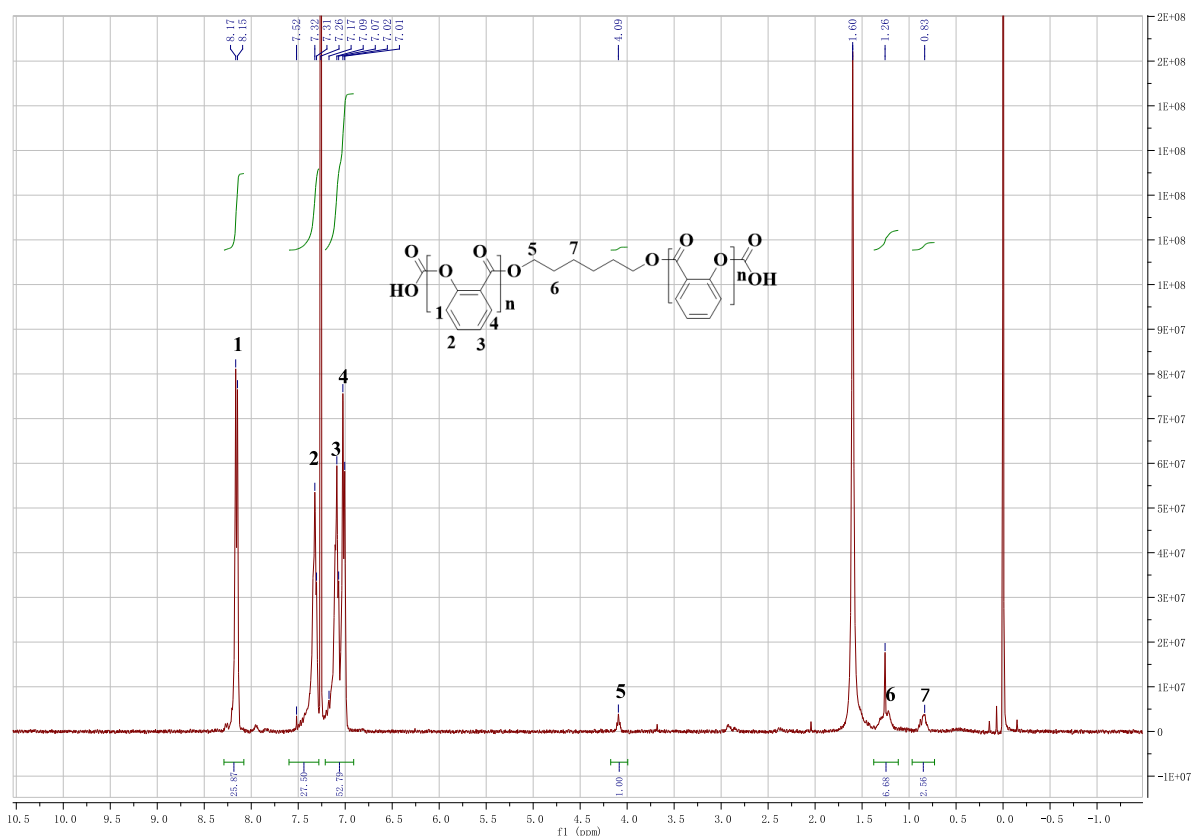


Figure S39. ^1H NMR spectrum of the resulting polymer afforded via ROP of SAOCA in the catalysis of [DBU]/[HDO]/[SAOCA] = 1/1/100 in THF at 25 °C, [SAOCA] = 1.2 M (Table 1, Entry 15).

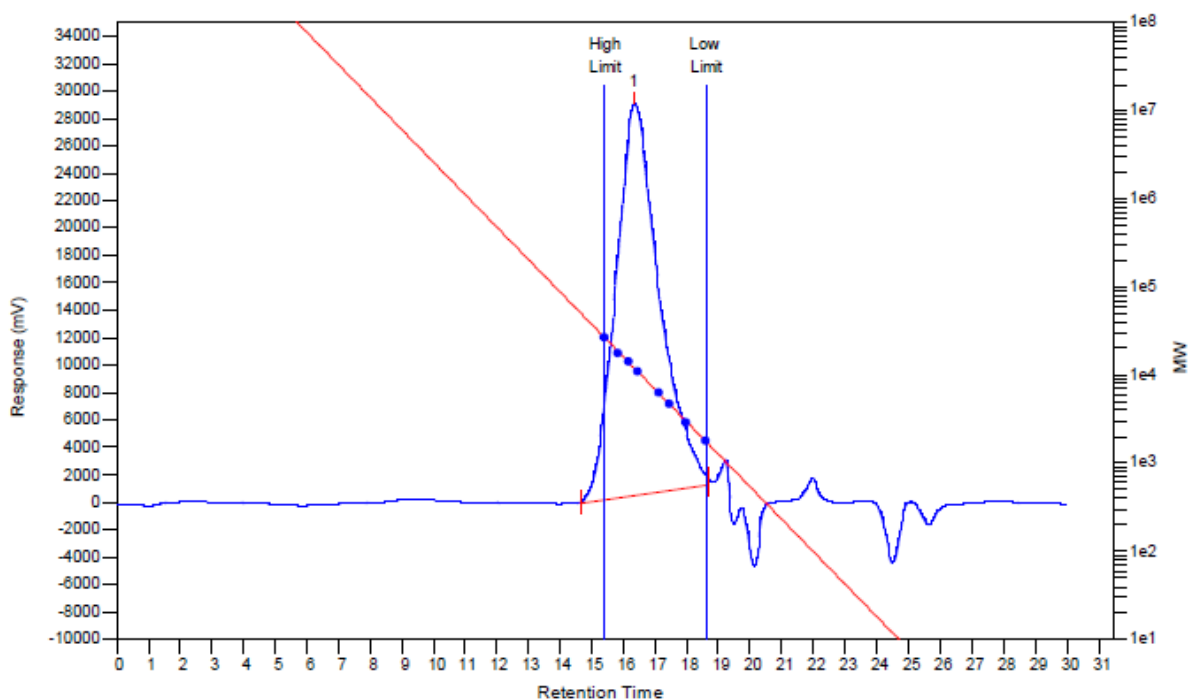


Figure S40. GPC trace of the resulting polymer in the catalysis of DBN and BnOH with molar ratio of 0.5:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 16).

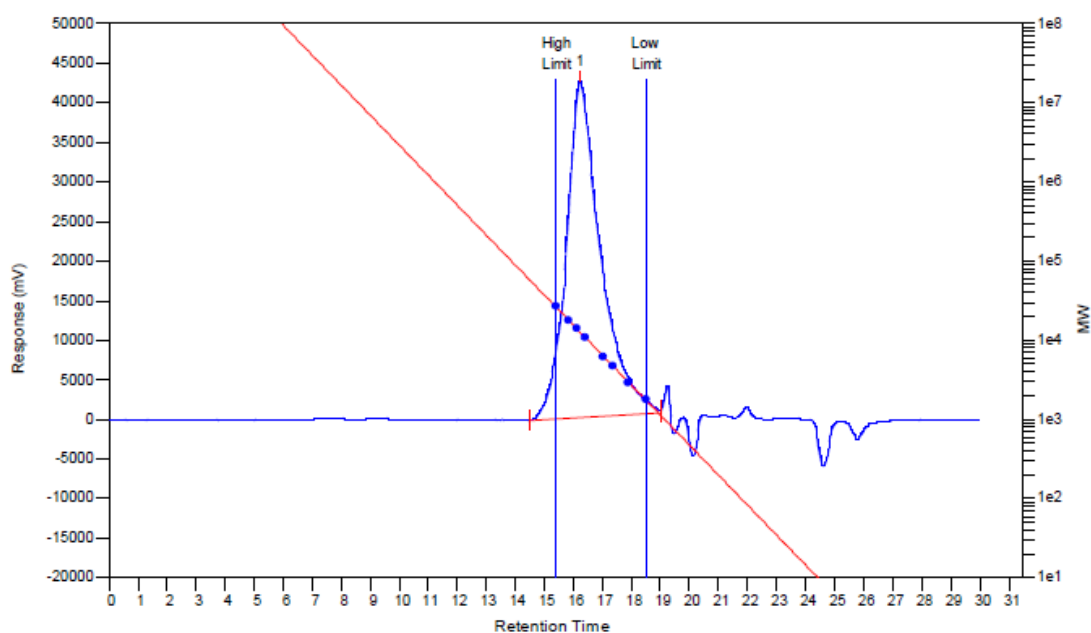


Figure S41. GPC trace of the resulting polymer in the catalysis of TBD and BnOH with molar ratio of 0.5:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 17).

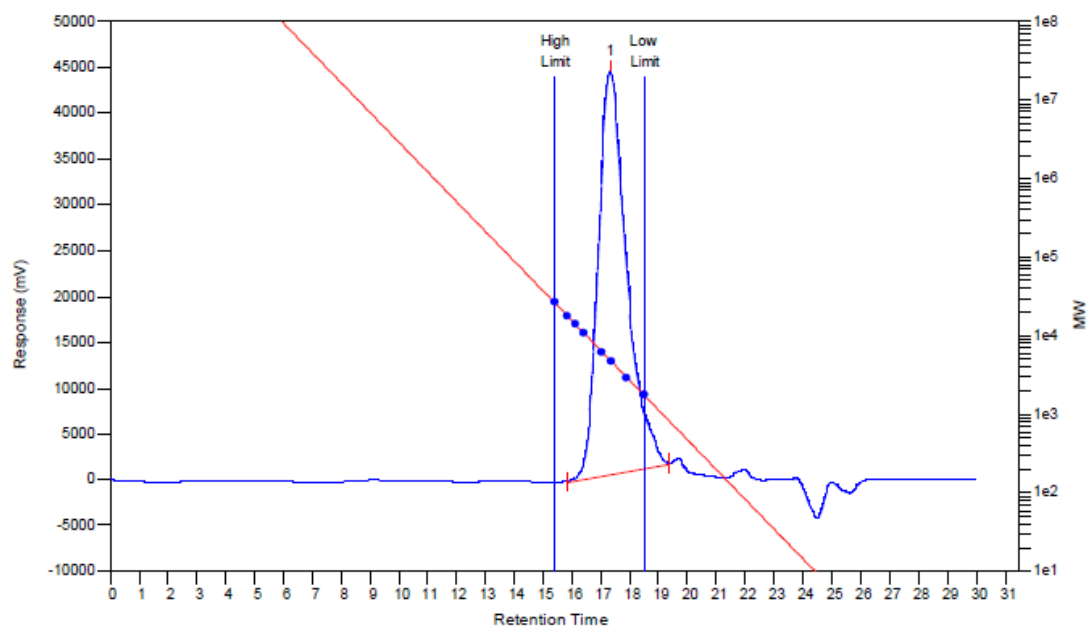


Figure S42. GPC trace of the resulting polymer in the catalysis of BEMP and BnOH with molar ratio of 0.25:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 18).

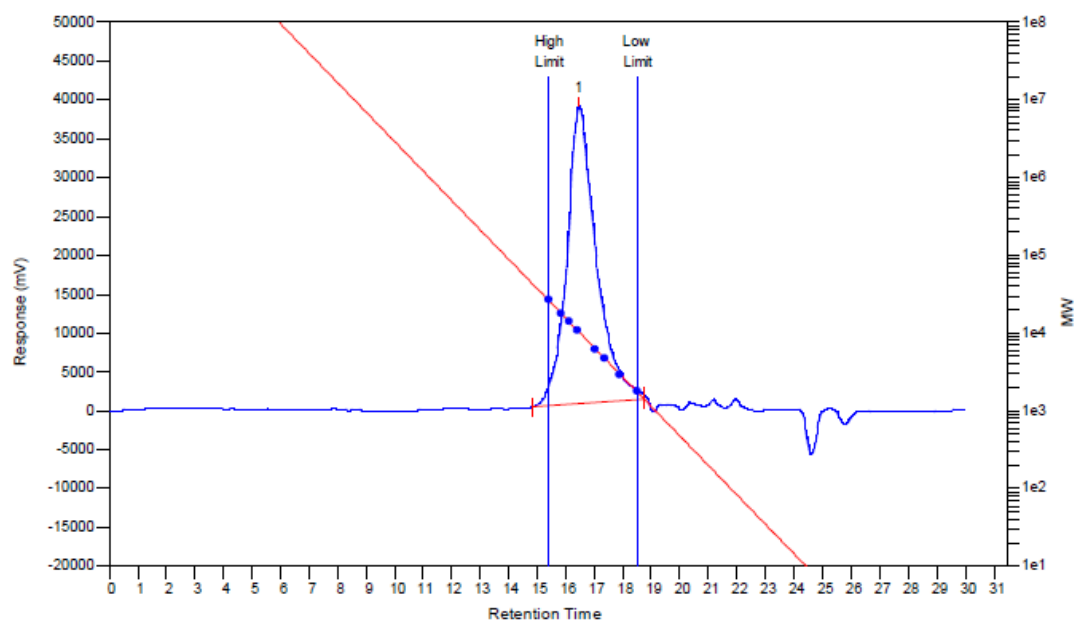


Figure S43. GPC trace of the resulting polymer in the catalysis of DMAP and BnOH with molar ratio of 0.5:1 in THF at 25 °C, [SAOCA]/[BnOH] = 50:1, [SAOCA] = 0.75 M (Table 1, Entry 19).

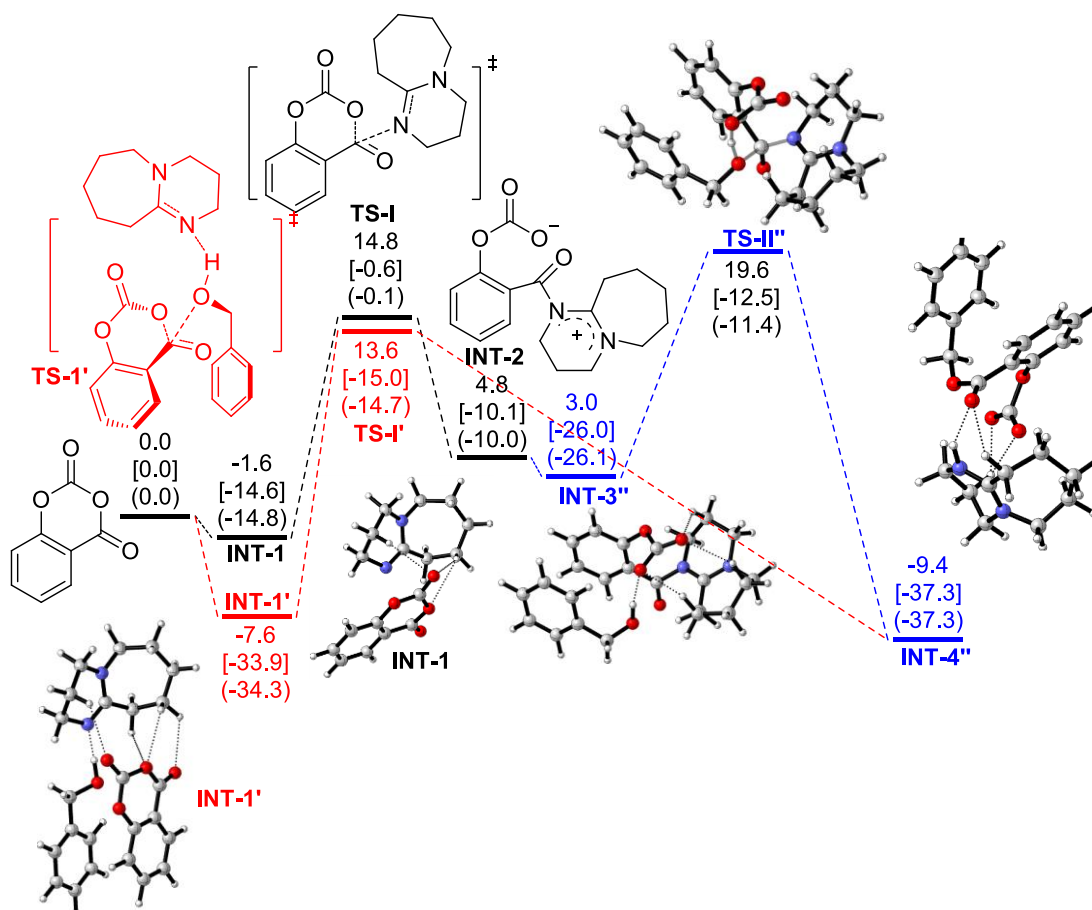


Figure S44. DBU induced nucleophilic attack of benzyl alcohol to SAOCA.

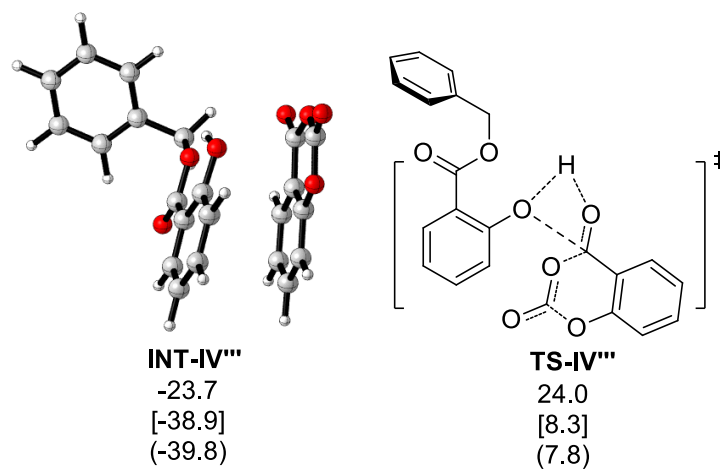
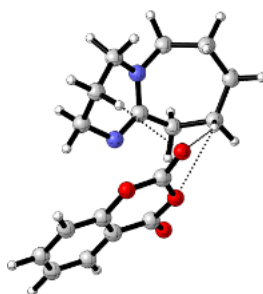


Figure S45. Nucleophilic attack of benzyl 2-hydroxybenzoate to SAOCA without DBU.

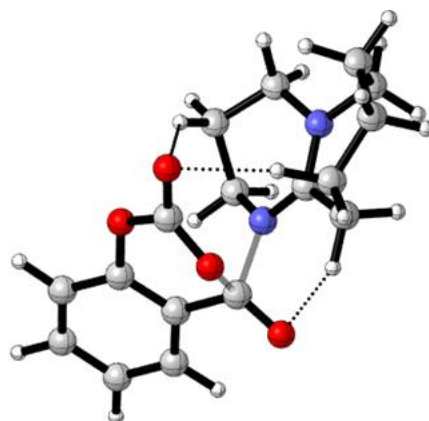
Coordinates of All Stationary Points



INT-1

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| C | -4.41903800 | 0.13163700 | 0.29616700 |
| C | -2.51420200 | 1.85688500 | 0.20322200 |
| C | 0.05987700 | -1.97113800 | -0.77109300 |
| C | -4.02288000 | 1.60682400 | 0.23223700 |
| C | -2.29082400 | -2.43080100 | -0.19931400 |
| C | -0.85471200 | -2.62726700 | 0.26103700 |
| N | -2.48890800 | -1.08936200 | -0.74937100 |
| N | -0.19718500 | -0.54137300 | -0.85480800 |
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| H | -0.85279600 | 1.78003800 | -1.19327100 |
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| H | -2.33901800 | 2.93803800 | 0.19740100 |
| H | -2.05193700 | 1.47220600 | 1.11917700 |
| H | -0.10993700 | -2.43518100 | -1.75536800 |
| H | 1.11402500 | -2.13031100 | -0.52312600 |
| H | -4.45810500 | 2.13317000 | 1.08919400 |

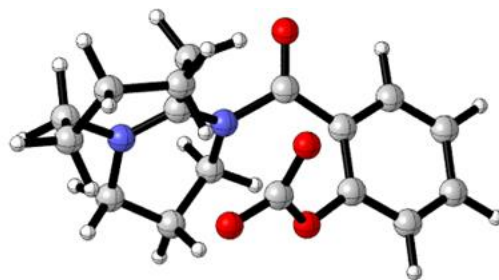
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| H | -0.64614000 | -3.69528400 | 0.37404400 |
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| H | 3.53818600 | -2.12703900 | 1.30366800 |
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TS-I

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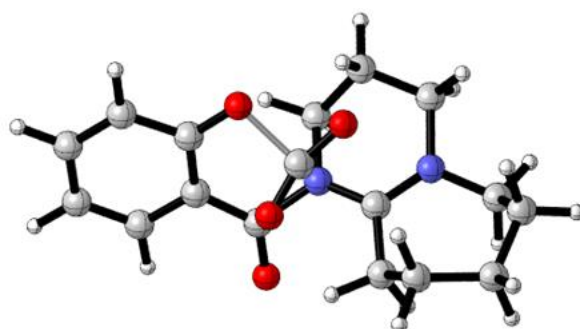
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| O | 0.83584100 | 1.84967300 | -1.65447200 |
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INT-2

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| C | -3.92912400 | 1.56733900 | 0.66853500 |
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| C | 4.74537600 | 0.54947100 | -0.63247600 |
| O | 1.36972400 | -0.74119500 | 1.42248300 |
| O | 0.45475700 | 1.35928400 | 1.37868600 |
| C | 1.04705300 | 0.64422700 | -1.18433900 |
| C | 0.23255000 | 0.18635100 | 1.66706000 |
| O | 0.89035800 | 1.54924400 | -1.96342500 |
| O | -0.75342900 | -0.43528900 | 2.06065700 |
| H | 5.82366000 | -0.28268100 | 1.03709900 |
| H | 3.76454800 | -0.98535900 | 2.25166400 |
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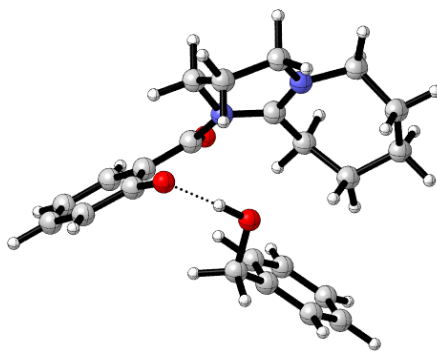


TS-II

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| C | 3.69505400 | 0.39415700 | -0.86958400 |
| C | 4.31735600 | -0.15772500 | 0.41031600 |

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| C | -0.23720800 | 1.72054800 | -1.19409600 |
| C | 3.96023900 | -1.62557400 | 0.61639600 |
| C | 2.08227000 | 2.24105400 | -0.58551700 |
| C | 0.63277500 | 2.57410900 | -0.29481900 |
| N | 2.28583900 | 0.79175700 | -0.74662000 |
| N | 0.03787600 | 0.29968200 | -0.92484200 |
| H | 2.15044800 | -1.92542300 | -1.44959300 |
| H | 0.70026900 | -2.11932500 | -0.50436000 |
| H | 4.22051900 | 1.29511400 | -1.19642300 |
| H | 3.78697400 | -0.33580200 | -1.68136600 |
| H | 3.97585700 | 0.44406400 | 1.26217900 |
| H | 5.40466200 | -0.04295200 | 0.34397800 |
| H | 2.27701000 | -2.91562900 | 0.95237600 |
| H | 2.06281100 | -1.28819800 | 1.55872100 |
| H | -0.01913800 | 1.90281200 | -2.25523400 |
| H | -1.29301700 | 1.89355700 | -1.00922300 |
| H | 4.43870800 | -1.99530100 | 1.52908200 |
| H | 4.37264300 | -2.21379800 | -0.21549000 |
| H | 2.42659900 | 2.73036300 | -1.50496100 |
| H | 2.73421200 | 2.56295100 | 0.23432300 |
| H | 0.36511200 | 2.35389600 | 0.73994200 |
| H | 0.45686800 | 3.63472800 | -0.49113100 |
| C | -4.90800400 | 0.02157700 | 0.49746800 |
| C | -3.83993000 | 0.64673700 | 1.08944500 |
| C | -2.50025200 | 0.48756800 | 0.60586900 |
| C | -2.35120300 | -0.35161500 | -0.55392400 |
| C | -3.47182500 | -1.00350600 | -1.12438300 |
| C | -4.73646600 | -0.82285700 | -0.62347600 |
| O | -1.52423300 | 1.07165900 | 1.19173200 |

| | | | |
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| C | -0.03836700 | -0.18424300 | 1.98224600 |
| O | -0.84627100 | -1.55002600 | -1.95748700 |
| O | 0.74318200 | 0.63696400 | 2.30518700 |
| H | -5.90554600 | 0.17251200 | 0.90287200 |
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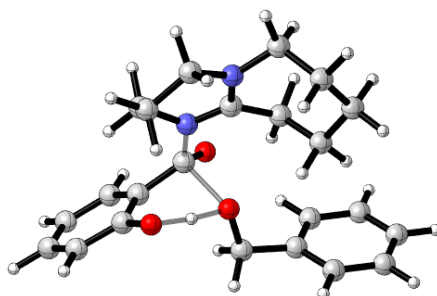


INT-3

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| C | 0.96137100 | 2.88465800 | 0.36050600 |
| C | -4.08808500 | 0.31975300 | -0.02789100 |
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| C | 0.25748800 | 3.49164000 | -0.83595600 |
| N | -1.73027500 | 2.52885800 | 0.25281900 |
| N | 0.33662300 | 1.59018500 | 0.66872300 |
| C | 5.01833100 | -0.41673100 | -0.36819900 |
| C | 4.14386600 | 0.24605300 | -1.18934000 |

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| C | 2.48144800 | 0.27119100 | 0.59329500 |
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| C | 4.65621500 | -0.77513300 | 0.95132300 |
| O | 2.01904100 | 1.17963900 | -1.58401600 |
| C | 1.20185500 | 0.53440600 | 1.23157000 |
| O | 0.81137900 | 0.00709100 | 2.25519500 |
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| H | -0.97083800 | -0.54949400 | 1.23040700 |
| H | -3.42217000 | 3.66823200 | 0.45474800 |
| H | -3.35846200 | 2.30182800 | 1.55592900 |
| H | -3.66859600 | 1.90251700 | -1.45230800 |
| H | -5.06021400 | 2.21230900 | -0.41198500 |
| H | -2.82261000 | -1.39604300 | 0.23611100 |
| H | -2.23151000 | -0.28554700 | -0.97910500 |
| H | 0.86072200 | 3.52587800 | 1.24680400 |
| H | 2.01376100 | 2.71109900 | 0.16111300 |
| H | -4.72803400 | -0.23318700 | -0.72357900 |
| H | -4.55939500 | 0.23847100 | 0.96215800 |
| H | -1.30720000 | 4.57397700 | 0.19741800 |
| H | -1.82280800 | 3.85748900 | -1.33878100 |
| H | 0.37083500 | 2.80042500 | -1.67367200 |
| H | 0.70961200 | 4.44840000 | -1.10825800 |
| H | 6.00649600 | -0.67679300 | -0.74005400 |
| H | 4.40820200 | 0.51024000 | -2.20828900 |
| H | 3.09573600 | -0.68698700 | 2.41367600 |
| H | 5.35484200 | -1.30188800 | 1.59162700 |
| C | -0.83760600 | -3.67634800 | 1.26486900 |
| C | -0.06030900 | -2.83274500 | 0.47711200 |
| C | -0.32715300 | -2.68943600 | -0.88796900 |

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|---|-------------|-------------|-------------|
| C | -1.37275100 | -3.41843100 | -1.45196200 |
| C | -2.14913500 | -4.27211300 | -0.66911900 |
| C | -1.88670800 | -4.39697300 | 0.69251100 |
| C | 0.44808500 | -1.67648900 | -1.69330500 |
| O | -0.03196800 | -0.39305700 | -1.35611000 |
| H | -0.62231400 | -3.77563300 | 2.32448800 |
| H | 0.75672200 | -2.26750100 | 0.92255800 |
| H | -1.58562400 | -3.30775300 | -2.51247900 |
| H | -2.96004200 | -4.83547400 | -1.12120600 |
| H | -2.49114300 | -5.05863900 | 1.30561700 |
| H | 1.52015700 | -1.75755300 | -1.45953600 |
| H | 0.32396600 | -1.88074000 | -2.76753300 |
| H | 0.69239200 | 0.26668300 | -1.54919000 |

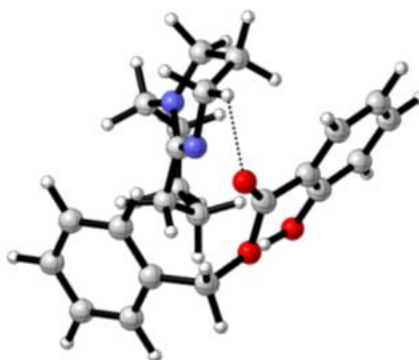


TS-III

| | | | |
|---|-------------|------------|-------------|
| C | -0.31350500 | 1.67444300 | 0.67735500 |
| C | -1.53502200 | 0.87322100 | 1.05303200 |
| C | -1.79436000 | 3.62902500 | 0.45608500 |
| C | -2.82978400 | 3.23150800 | -0.59579300 |
| C | -2.56067200 | 0.73314600 | -0.08718200 |
| C | 2.04109900 | 2.08927700 | 0.49693500 |
| C | -3.51735900 | 1.91119100 | -0.25756500 |
| C | 0.50599400 | 3.75963200 | -0.40084000 |
| C | 1.74290000 | 2.94661200 | -0.72081400 |
| N | -0.49952000 | 2.95147100 | 0.30659000 |

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|---|-------------|-------------|-------------|
| N | 0.91549500 | 1.17586400 | 0.72254100 |
| C | 5.00734800 | -1.61192400 | -0.42257200 |
| C | 4.15734900 | -0.98748500 | -1.32318300 |
| C | 2.87091300 | -0.57627900 | -0.93156300 |
| C | 2.49073300 | -0.77968700 | 0.41873400 |
| C | 3.34851000 | -1.43972300 | 1.30234900 |
| C | 4.60739300 | -1.85801900 | 0.89406300 |
| O | 2.04010100 | -0.01761200 | -1.79755600 |
| C | 1.18963900 | -0.29626300 | 0.97716800 |
| O | 0.66500000 | -0.81078000 | 1.94357400 |
| H | -1.99106000 | 1.36167400 | 1.92607800 |
| H | -1.21052600 | -0.10806900 | 1.37826600 |
| H | -1.57259400 | 4.69786100 | 0.39353000 |
| H | -2.18331100 | 3.44730000 | 1.46297600 |
| H | -2.33431800 | 3.16955800 | -1.57342300 |
| H | -3.57583800 | 4.03113300 | -0.66493400 |
| H | -3.14721600 | -0.16651700 | 0.12840800 |
| H | -2.01480400 | 0.52104900 | -1.01155600 |
| H | 2.15886500 | 2.71380400 | 1.39252700 |
| H | 2.94434900 | 1.49877900 | 0.37052300 |
| H | -4.24599400 | 1.67074500 | -1.03903200 |
| H | -4.09098200 | 2.04680100 | 0.67060200 |
| H | 0.75385400 | 4.61866100 | 0.23485400 |
| H | 0.03144600 | 4.14410800 | -1.31098800 |
| H | 1.59305400 | 2.27943900 | -1.57365000 |
| H | 2.57778800 | 3.61583700 | -0.94294700 |
| H | 5.99360000 | -1.92571200 | -0.75357400 |
| H | 4.44689700 | -0.82036200 | -2.35537700 |
| H | 3.00406400 | -1.60235600 | 2.31928900 |
| H | 5.27098400 | -2.36247100 | 1.58785300 |

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|---|-------------|-------------|-------------|
| C | -3.27679800 | -2.86453700 | 1.19383800 |
| C | -1.94060400 | -2.63318300 | 0.87570400 |
| C | -1.54464400 | -2.46458700 | -0.45366600 |
| C | -2.50895700 | -2.54375000 | -1.45909300 |
| C | -3.84648000 | -2.77760500 | -1.14720100 |
| C | -4.23409800 | -2.93495200 | 0.18206200 |
| C | -0.11258600 | -2.09806500 | -0.77395000 |
| O | 0.05859800 | -0.71160400 | -0.67134100 |
| H | -3.57239900 | -2.99400800 | 2.23095600 |
| H | -1.18775800 | -2.56160900 | 1.65795500 |
| H | -2.20603400 | -2.41216900 | -2.49529900 |
| H | -4.58642400 | -2.83849100 | -1.93995000 |
| H | -5.27568400 | -3.11858600 | 0.42814200 |
| H | 0.55841700 | -2.61782900 | -0.06783000 |
| H | 0.14658800 | -2.44644600 | -1.78595400 |
| H | 1.01154800 | -0.30546900 | -1.39218900 |

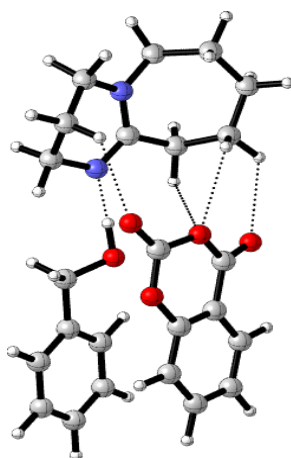


INT-4

| | | | |
|---|-------------|-------------|-------------|
| C | -0.34905600 | -1.31408900 | -0.54898000 |
| C | -1.36484700 | -1.36259600 | 0.56866700 |
| C | -0.53701900 | -3.78795800 | -0.72778200 |
| C | -0.22108300 | -4.31605000 | 0.67508600 |
| C | -0.89061800 | -2.11576800 | 1.82396800 |
| C | 0.98032700 | -0.20660700 | -2.08526000 |

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|---|-------------|-------------|-------------|
| C | -1.05256500 | -3.63543200 | 1.76168300 |
| C | 1.36421400 | -2.61594200 | -1.77141800 |
| C | 2.05611800 | -1.26157400 | -1.84059900 |
| N | 0.09319200 | -2.51881000 | -1.05430600 |
| N | 0.05372800 | -0.16548600 | -0.96442500 |
| C | 4.40316600 | 0.38469900 | 0.93635800 |
| C | 3.25145000 | 0.13672200 | 1.66667500 |
| C | 2.05448600 | 0.79199200 | 1.35172700 |
| C | 2.03526500 | 1.71229600 | 0.28718300 |
| C | 3.20591800 | 1.93445400 | -0.44721700 |
| C | 4.38881000 | 1.28468700 | -0.13285400 |
| O | 0.97912600 | 0.47255800 | 2.09450600 |
| C | 0.82086200 | 2.44625700 | -0.15439900 |
| O | 0.71114900 | 3.00199900 | -1.22090600 |
| H | -2.30550300 | -1.79803900 | 0.20241300 |
| H | -1.58913900 | -0.31918500 | 0.80507200 |
| H | -0.19465500 | -4.50400700 | -1.48284400 |
| H | -1.62342100 | -3.70400500 | -0.85477200 |
| H | 0.85014700 | -4.17313400 | 0.87013400 |
| H | -0.40977200 | -5.39612100 | 0.69963700 |
| H | -1.46660000 | -1.74327200 | 2.67871500 |
| H | 0.15471500 | -1.85325600 | 2.02151700 |
| H | 0.43121500 | -0.45867400 | -3.00728700 |
| H | 1.41173600 | 0.78772900 | -2.22596600 |
| H | -0.79282400 | -4.06443700 | 2.73630200 |
| H | -2.11248200 | -3.87329200 | 1.59006400 |
| H | 1.17177200 | -2.99646800 | -2.78478700 |
| H | 2.00193300 | -3.35373600 | -1.26398200 |
| H | 2.55616300 | -1.03291700 | -0.89209000 |
| H | 2.81513700 | -1.27197900 | -2.62851400 |

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|---|-------------|-------------|-------------|
| H | 5.32118500 | -0.13252800 | 1.19900700 |
| H | 3.24041000 | -0.56747300 | 2.49178700 |
| H | 3.15172500 | 2.63516600 | -1.27461700 |
| H | 5.28856100 | 1.47388500 | -0.70754700 |
| C | -3.39213100 | 0.71965000 | -1.53450800 |
| C | -2.42399900 | 1.65288000 | -1.18023100 |
| C | -2.43726700 | 2.22556200 | 0.09402400 |
| C | -3.42724500 | 1.85453100 | 1.00437700 |
| C | -4.39983100 | 0.92196300 | 0.64961000 |
| C | -4.38131500 | 0.35442000 | -0.62176400 |
| C | -1.35840900 | 3.19449200 | 0.49188700 |
| O | -0.13658700 | 2.49734100 | 0.80700100 |
| H | -3.37251500 | 0.27244400 | -2.52350900 |
| H | -1.63630400 | 1.92741100 | -1.87530900 |
| H | -3.43648400 | 2.29855900 | 1.99705400 |
| H | -5.16874800 | 0.64146400 | 1.36262600 |
| H | -5.13782200 | -0.37236500 | -0.90245200 |
| H | -1.14403300 | 3.91133500 | -0.30185200 |
| H | -1.62412600 | 3.72584100 | 1.40827700 |
| H | 0.21040900 | 0.96441500 | 1.75182100 |

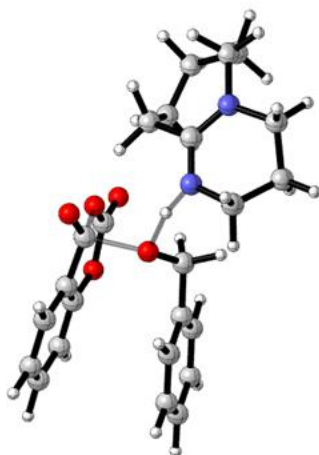


INT-1'

| | | | |
|---|-------------|------------|------------|
| C | -3.04949700 | 0.56796000 | 0.75883400 |
|---|-------------|------------|------------|

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|---|-------------|-------------|-------------|
| C | -2.81473000 | -0.78622000 | 1.38560500 |
| C | -5.48495200 | 0.10148400 | 0.83922700 |
| C | -5.67086000 | -1.20330400 | 0.06142200 |
| C | -3.23989600 | -1.95042000 | 0.47184700 |
| C | -2.24671400 | 2.58199700 | -0.15503200 |
| C | -4.72569100 | -2.30741300 | 0.53376600 |
| C | -4.61756400 | 1.98460200 | -0.51040400 |
| C | -3.34394700 | 2.44016500 | -1.20330100 |
| N | -4.33487500 | 0.88846800 | 0.41328900 |
| N | -2.02654100 | 1.32030800 | 0.53561800 |
| H | -3.33014500 | -0.85895600 | 2.35286500 |
| H | -1.74290600 | -0.85257100 | 1.58626900 |
| H | -6.36052100 | 0.74633000 | 0.71235600 |
| H | -5.41267700 | -0.11029900 | 1.91275300 |
| H | -5.51503200 | -0.99773600 | -1.00590000 |
| H | -6.70812900 | -1.54032200 | 0.17552300 |
| H | -2.65133800 | -2.82636000 | 0.75634200 |
| H | -2.94594700 | -1.71192700 | -0.55780700 |
| H | -2.51523900 | 3.36310900 | 0.57215800 |
| H | -1.30589200 | 2.87815900 | -0.62777600 |
| H | -4.90169700 | -3.21055600 | -0.06145800 |
| H | -4.98337700 | -2.56566100 | 1.57127500 |
| H | -5.08072500 | 2.81793300 | 0.03735300 |
| H | -5.35044500 | 1.63017000 | -1.24673800 |
| H | -3.01851800 | 1.69227600 | -1.93294100 |
| H | -3.52365800 | 3.38199000 | -1.72947000 |
| C | 4.55489600 | -1.49083000 | -0.88532200 |
| C | 3.65673500 | -0.64628000 | -1.52145000 |
| C | 2.29927400 | -0.83036300 | -1.28610100 |
| C | 1.84297800 | -1.83462100 | -0.44592300 |

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|---|-------------|-------------|-------------|
| C | 2.75559400 | -2.67956000 | 0.18987800 |
| C | 4.11192500 | -2.50920000 | -0.03178500 |
| O | 1.42523000 | 0.02617400 | -1.89779700 |
| O | -0.37966400 | -1.16763400 | -1.06168500 |
| C | 0.40079600 | -1.98076900 | -0.25457200 |
| C | 0.09056100 | -0.05993100 | -1.68937300 |
| O | -0.15038800 | -2.75926600 | 0.46854400 |
| O | -0.64641100 | 0.76182600 | -2.13638000 |
| H | 5.61846000 | -1.34574800 | -1.04466300 |
| H | 3.98078500 | 0.16453000 | -2.16306600 |
| H | 2.37124400 | -3.45344600 | 0.84606300 |
| H | 4.83053300 | -3.15665100 | 0.45849800 |
| C | 5.04286300 | 2.17922100 | 0.33126400 |
| C | 3.68244700 | 2.38757500 | 0.11561200 |
| C | 2.73052600 | 1.62004100 | 0.78768100 |
| C | 3.15878800 | 0.63091000 | 1.67494000 |
| C | 4.51737900 | 0.42019200 | 1.89053800 |
| C | 5.46421900 | 1.19354500 | 1.22066900 |
| C | 1.25433400 | 1.85165200 | 0.56488300 |
| O | 0.55030900 | 0.64519800 | 0.72254000 |
| H | 5.77338100 | 2.78299800 | -0.19919500 |
| H | 3.35460900 | 3.14760400 | -0.59013400 |
| H | 2.41232700 | 0.01963100 | 2.17223900 |
| H | 4.83922700 | -0.35739700 | 2.57745900 |
| H | 6.52413600 | 1.02735100 | 1.38889000 |
| H | 0.89105300 | 2.60523400 | 1.28270900 |
| H | 1.10637700 | 2.27114200 | -0.44463600 |
| H | -0.43537200 | 0.86474900 | 0.73949500 |

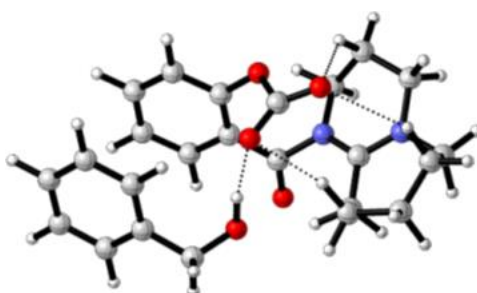


TS-I'

| | | | |
|---|-------------|-------------|-------------|
| C | -3.11836200 | 0.29004200 | 0.76602500 |
| C | -2.79488500 | -1.17385900 | 0.70336600 |
| C | -5.40377200 | -0.23230800 | 0.04831900 |
| C | -5.16145200 | -0.87263700 | -1.32263100 |
| C | -2.77081000 | -1.67873800 | -0.75028300 |
| C | -2.36152900 | 2.55446200 | 1.10047200 |
| C | -4.15587300 | -2.02827800 | -1.29756400 |
| C | -4.64243400 | 2.13607100 | 0.23119600 |
| C | -3.36305200 | 2.93262800 | 0.01751100 |
| N | -4.35144200 | 0.71250500 | 0.43833300 |
| N | -2.15710900 | 1.11507000 | 1.08864200 |
| H | -3.53514800 | -1.73428100 | 1.28707700 |
| H | -1.83078200 | -1.32334600 | 1.19377100 |
| H | -6.33603300 | 0.33845400 | 0.04656000 |
| H | -5.51026400 | -1.00098700 | 0.82039000 |
| H | -4.82842700 | -0.08903800 | -2.01671400 |
| H | -6.12052600 | -1.24353400 | -1.70174200 |
| H | -2.12088000 | -2.55632800 | -0.79619200 |
| H | -2.28481500 | -0.92553000 | -1.38551500 |
| H | -2.72407700 | 2.86719200 | 2.08743500 |

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|---|-------------|-------------|-------------|
| H | -1.38746800 | 3.02364600 | 0.94070100 |
| H | -4.05267600 | -2.42938600 | -2.31115100 |
| H | -4.57736800 | -2.83799300 | -0.68542200 |
| H | -5.20238100 | 2.51964900 | 1.09326600 |
| H | -5.28946400 | 2.21579300 | -0.64832100 |
| H | -2.93806100 | 2.69252600 | -0.96344900 |
| H | -3.58673900 | 4.00191100 | 0.03878100 |
| C | 4.94101400 | -0.64475900 | 1.08297000 |
| C | 4.23351900 | -1.18319800 | 0.01513100 |
| C | 2.85811500 | -1.33665100 | 0.13973200 |
| C | 2.18903200 | -0.95804300 | 1.29185000 |
| C | 2.90912900 | -0.44057100 | 2.36357200 |
| C | 4.28515400 | -0.27982600 | 2.26151500 |
| O | 2.18499400 | -1.85408800 | -0.94585900 |
| O | 0.21882900 | -1.92357900 | 0.25303600 |
| C | 0.70484900 | -1.06410700 | 1.34878400 |
| C | 0.86922400 | -2.18109600 | -0.87862100 |
| O | 0.05959900 | -1.14984700 | 2.37400700 |
| O | 0.33832600 | -2.69539100 | -1.82376100 |
| H | 6.01449800 | -0.51015200 | 0.99515800 |
| H | 4.71602900 | -1.47003300 | -0.91240200 |
| H | 2.35987300 | -0.16524700 | 3.25831400 |
| H | 4.84963900 | 0.12975500 | 3.09268600 |
| C | 3.65735700 | 1.45209500 | -2.58119900 |
| C | 2.36674700 | 1.02187300 | -2.27996100 |
| C | 1.79541300 | 1.31305500 | -1.04214500 |
| C | 2.53503200 | 2.03166100 | -0.10149100 |
| C | 3.82573800 | 2.45655100 | -0.39732800 |
| C | 4.38995400 | 2.17046400 | -1.63999400 |
| C | 0.39535100 | 0.84112700 | -0.70077400 |

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|---|-------------|------------|-------------|
| O | 0.23876700 | 0.52191200 | 0.65160300 |
| H | 4.09548300 | 1.21184400 | -3.54536100 |
| H | 1.80894400 | 0.42733700 | -3.00018600 |
| H | 2.09795800 | 2.21386400 | 0.87573400 |
| H | 4.39919700 | 2.99999800 | 0.34798100 |
| H | 5.40018200 | 2.49637600 | -1.86870400 |
| H | -0.32144800 | 1.64764400 | -0.94875100 |
| H | 0.11917500 | 0.00352000 | -1.36376600 |
| H | -1.07941800 | 0.75551200 | 1.03808000 |

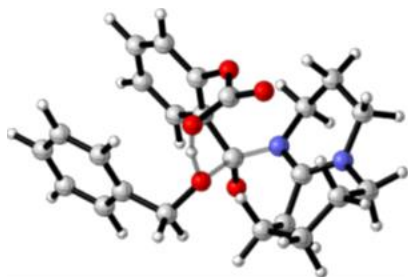


INT-3''

| | | | |
|---|-------------|-------------|-------------|
| C | 2.50856000 | -0.05171600 | -0.83038600 |
| C | 2.13016400 | -1.49390000 | -1.06258100 |
| C | 4.76230700 | -0.80316000 | -0.27177400 |
| C | 4.51169600 | -1.69137900 | 0.94842100 |
| C | 2.17946100 | -2.39130000 | 0.19196400 |
| C | 2.02000600 | 2.33809100 | -0.92183700 |
| C | 3.57140600 | -2.84823900 | 0.61732100 |
| C | 4.17015600 | 1.56398400 | 0.03844600 |
| C | 3.01920100 | 2.53888400 | 0.19985100 |
| N | 3.74403900 | 0.24308600 | -0.45208200 |
| N | 1.61416000 | 0.92546600 | -1.00152500 |
| C | -3.14666600 | 2.32725600 | 0.39825100 |
| C | -1.96208400 | 2.24498000 | 1.11710800 |
| C | -0.81987900 | 1.69295200 | 0.53987100 |
| C | -0.86817700 | 1.24865000 | -0.79745200 |

| | | | |
|---|-------------|-------------|-------------|
| C | -2.08557300 | 1.30289900 | -1.49286500 |
| C | -3.21887500 | 1.83913700 | -0.90746700 |
| O | 0.32265900 | 1.66611700 | 1.27444700 |
| O | -0.01785100 | -0.55806100 | 1.62155100 |
| C | 0.27597500 | 0.69887400 | -1.55941100 |
| C | 0.81173200 | 0.36005600 | 1.70054600 |
| O | 0.18744000 | 0.16714700 | -2.63440900 |
| O | 1.98815500 | 0.39382700 | 2.04920900 |
| H | 2.79856400 | -1.88373600 | -1.84218600 |
| H | 1.12047900 | -1.53880100 | -1.46281900 |
| H | 5.71149000 | -0.26971800 | -0.18237800 |
| H | 4.82292700 | -1.40383600 | -1.18558100 |
| H | 4.08370700 | -1.07747000 | 1.75039900 |
| H | 5.47464100 | -2.08327700 | 1.29363400 |
| H | 1.56554400 | -3.26495100 | -0.04878100 |
| H | 1.68022800 | -1.88191500 | 1.02008900 |
| H | 2.44394000 | 2.61354600 | -1.89648400 |
| H | 1.12061600 | 2.93052700 | -0.75426700 |
| H | 3.47624100 | -3.50070500 | 1.49137800 |
| H | 4.02450600 | -3.45528900 | -0.18063000 |
| H | 4.93060900 | 1.93764400 | -0.65786500 |
| H | 4.64575200 | 1.39296300 | 1.00934600 |
| H | 2.52122300 | 2.35960500 | 1.15125000 |
| H | 3.40373900 | 3.56184000 | 0.16901500 |
| H | -4.03131600 | 2.74611700 | 0.86864700 |
| H | -1.89247000 | 2.58499400 | 2.14460900 |
| H | -2.10842700 | 0.91093900 | -2.50412500 |
| H | -4.15653100 | 1.86258200 | -1.45138400 |
| C | -4.36077000 | -0.36700700 | 1.58157800 |
| C | -3.24576400 | -1.07237100 | 1.14105800 |

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|---|-------------|-------------|-------------|
| C | -3.26717100 | -1.72252300 | -0.09693000 |
| C | -4.40951300 | -1.62504500 | -0.89187500 |
| C | -5.52455800 | -0.91191700 | -0.45497500 |
| C | -5.50461100 | -0.28674200 | 0.78849900 |
| C | -2.07858300 | -2.55291700 | -0.53507900 |
| O | -0.87480100 | -1.82824900 | -0.63141600 |
| H | -4.33323500 | 0.13057300 | 2.54702600 |
| H | -2.34876500 | -1.10722700 | 1.75584000 |
| H | -4.42831500 | -2.11924900 | -1.86037400 |
| H | -6.40847100 | -0.85020900 | -1.08320200 |
| H | -6.37454400 | 0.26185200 | 1.13783400 |
| H | -1.96393700 | -3.39898100 | 0.16102500 |
| H | -2.27119900 | -2.97368700 | -1.52715200 |
| H | -0.66986600 | -1.41553800 | 0.23563500 |

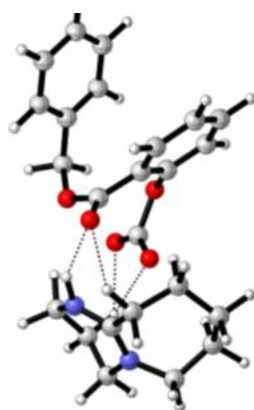


TS-II''

| | | | |
|---|------------|-------------|-------------|
| C | 2.29726000 | -0.25588700 | -0.87993200 |
| C | 2.17339500 | -1.75911100 | -0.89825000 |
| C | 4.67140000 | -0.59889200 | -0.38570700 |
| C | 4.55266300 | -1.27356800 | 0.98559500 |
| C | 2.30659600 | -2.39620600 | 0.49833100 |
| C | 1.51831600 | 1.91705400 | -1.50589200 |
| C | 3.75687400 | -2.57918000 | 0.94308600 |
| C | 3.80888400 | 1.69148900 | -0.55407500 |
| C | 2.57096300 | 2.56926200 | -0.62615300 |
| N | 3.51962900 | 0.25689200 | -0.71175900 |

| | | | |
|---|-------------|-------------|-------------|
| N | 1.25414200 | 0.53807900 | -1.07357200 |
| C | -3.30300100 | 2.51409200 | 0.43767400 |
| C | -2.06597900 | 2.47538100 | 1.07304600 |
| C | -1.01688200 | 1.75282200 | 0.51656300 |
| C | -1.19010400 | 1.05385700 | -0.68794000 |
| C | -2.42877200 | 1.12789100 | -1.32251900 |
| C | -3.48257400 | 1.84747200 | -0.77082800 |
| O | 0.22599400 | 1.90224700 | 1.10972000 |
| O | 0.14766800 | -0.14004700 | 2.11014100 |
| C | -0.19563300 | 0.06634900 | -1.30180000 |
| C | 0.86490600 | 0.89899500 | 1.82296100 |
| O | -0.42075200 | -0.47485800 | -2.37845000 |
| O | 2.02626500 | 1.10231600 | 2.10275900 |
| H | 2.96801000 | -2.13409600 | -1.55476000 |
| H | 1.23126500 | -2.01017400 | -1.37434900 |
| H | 5.54000900 | 0.06244100 | -0.40965500 |
| H | 4.82291700 | -1.33933200 | -1.17831100 |
| H | 4.08219900 | -0.56550200 | 1.68031400 |
| H | 5.56349000 | -1.47997200 | 1.35401300 |
| H | 1.81079400 | -3.37221600 | 0.46855200 |
| H | 1.76586500 | -1.78860800 | 1.23034400 |
| H | 1.84291700 | 1.87780800 | -2.55369100 |
| H | 0.58107300 | 2.47069500 | -1.46310200 |
| H | 3.77178400 | -3.04045700 | 1.93589100 |
| H | 4.26256200 | -3.27970500 | 0.26278200 |
| H | 4.53704600 | 1.95042700 | -1.33164500 |
| H | 4.29030900 | 1.81426100 | 0.42173600 |
| H | 2.16394000 | 2.71119300 | 0.37257000 |
| H | 2.84019000 | 3.54487800 | -1.04010800 |
| H | -4.12026900 | 3.07101700 | 0.88513500 |

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|---|-------------|-------------|-------------|
| H | -1.88332000 | 3.01017700 | 1.99903900 |
| H | -2.54563800 | 0.57105600 | -2.24628400 |
| H | -4.44326600 | 1.87185500 | -1.27435900 |
| C | -4.31501900 | -0.72371100 | 1.43044100 |
| C | -2.99828700 | -1.10156500 | 1.19262600 |
| C | -2.65312900 | -1.73888000 | -0.00265800 |
| C | -3.64645200 | -1.99698100 | -0.94572500 |
| C | -4.96847600 | -1.62800300 | -0.70454200 |
| C | -5.30488400 | -0.98792100 | 0.48431800 |
| C | -1.21832800 | -2.13587200 | -0.27985200 |
| O | -0.28217200 | -1.11612800 | -0.01311100 |
| H | -4.56900100 | -0.21423200 | 2.35522200 |
| H | -2.23045400 | -0.87079500 | 1.92726300 |
| H | -3.37660400 | -2.47090100 | -1.88636100 |
| H | -5.73151700 | -1.83118800 | -1.45001200 |
| H | -6.33222700 | -0.69106900 | 0.67264500 |
| H | -0.93383100 | -3.00139600 | 0.33459900 |
| H | -1.11186700 | -2.41650800 | -1.33528600 |
| H | -0.19121800 | -0.63602300 | 1.13404800 |

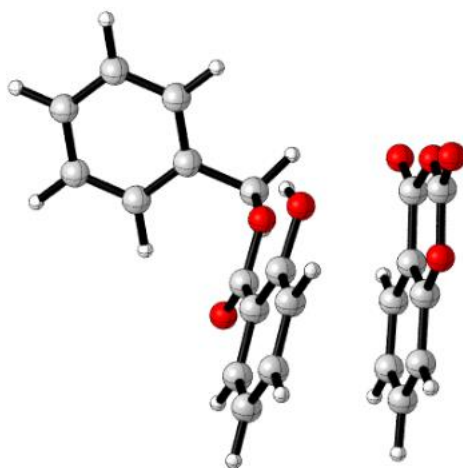


INT-4''

| | | | |
|---|-------------|-------------|------------|
| C | -3.06441100 | 0.37517500 | 1.09510900 |
| C | -2.72782400 | -0.83178600 | 1.93064900 |
| C | -4.88229000 | -0.86578100 | 0.05448000 |

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|---|-------------|-------------|-------------|
| C | -4.03222100 | -1.94421500 | -0.62798800 |
| C | -2.16084900 | -2.01445900 | 1.12521500 |
| C | -2.32336000 | 2.58934200 | 0.28835000 |
| C | -3.22676000 | -2.79386400 | 0.35755200 |
| C | -4.51339900 | 1.60339700 | -0.39210300 |
| C | -3.27033700 | 2.33385300 | -0.87358700 |
| N | -4.14211300 | 0.37481800 | 0.32073000 |
| N | -2.30377300 | 1.44669600 | 1.21061800 |
| H | -3.63542000 | -1.13557400 | 2.46839000 |
| H | -1.99092000 | -0.52012900 | 2.67042100 |
| H | -5.72027300 | -0.57985500 | -0.58327900 |
| H | -5.31411800 | -1.24500400 | 0.98957100 |
| H | -3.35629800 | -1.45632900 | -1.34032500 |
| H | -4.70789200 | -2.59699600 | -1.19191600 |
| H | -1.66469800 | -2.68175000 | 1.83737400 |
| H | -1.40071300 | -1.63753600 | 0.43686100 |
| H | -2.60750700 | 3.48073000 | 0.85790200 |
| H | -1.30797700 | 2.71037200 | -0.09768200 |
| H | -2.74133200 | -3.60853200 | -0.18969200 |
| H | -3.92340800 | -3.26433200 | 1.06774200 |
| H | -5.11226600 | 2.22987500 | 0.28234800 |
| H | -5.14244800 | 1.32004800 | -1.23749900 |
| H | -2.74842500 | 1.73605200 | -1.62068500 |
| H | -3.55468300 | 3.28637300 | -1.32797100 |
| C | 2.51213700 | -3.07060400 | -1.06195900 |
| C | 1.88961200 | -2.10422600 | -1.83891500 |
| C | 1.30108300 | -0.98180500 | -1.24856700 |
| C | 1.33911300 | -0.85099200 | 0.14994400 |
| C | 1.92937800 | -1.85582800 | 0.92318200 |
| C | 2.53227100 | -2.95408500 | 0.32863800 |

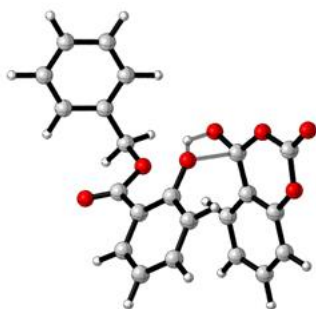
| | | | |
|---|-------------|-------------|-------------|
| O | 0.80350200 | -0.03907600 | -2.07443000 |
| O | -1.23815100 | -0.06019000 | -1.05086100 |
| C | 0.73927100 | 0.28619300 | 0.89944800 |
| C | -0.48094300 | 0.59997700 | -1.78045100 |
| O | 0.10858600 | 0.10439400 | 1.92637800 |
| O | -0.57325300 | 1.69580000 | -2.31727200 |
| H | 2.97536900 | -3.92700900 | -1.54290700 |
| H | 1.84492600 | -2.18360600 | -2.91978300 |
| H | 1.92263600 | -1.73996100 | 2.00239700 |
| H | 3.01054500 | -3.71226500 | 0.93915600 |
| C | 5.27653200 | 0.15050600 | -0.51358800 |
| C | 4.06603700 | 0.72545300 | -0.89125400 |
| C | 3.29469600 | 1.41767300 | 0.04104000 |
| C | 3.74700400 | 1.53121800 | 1.35769900 |
| C | 4.95320200 | 0.95234500 | 1.73804000 |
| C | 5.72016600 | 0.26090500 | 0.80158200 |
| C | 1.96642900 | 2.00654000 | -0.35757700 |
| O | 0.88503000 | 1.55810500 | 0.49519200 |
| H | 5.86529200 | -0.39610500 | -1.24352900 |
| H | 3.69626400 | 0.61467700 | -1.90753500 |
| H | 3.13978200 | 2.06271000 | 2.08666500 |
| H | 5.29657900 | 1.04045500 | 2.76420500 |
| H | 6.66002900 | -0.19396800 | 1.09870700 |
| H | 1.95775400 | 3.08750900 | -0.19732400 |
| H | 1.71799900 | 1.80777200 | -1.39974200 |
| H | -1.43051700 | 1.28989700 | 1.71699800 |



INT-4''

| | | | |
|---|-------------|-------------|-------------|
| C | 2.39070400 | -2.53270900 | 2.07870000 |
| C | 1.98287500 | -1.21595000 | 2.21008700 |
| C | 0.91970200 | -0.72589000 | 1.44240600 |
| C | 0.26467400 | -1.58063400 | 0.53626500 |
| C | 0.69599900 | -2.91018600 | 0.42294000 |
| C | 1.74924900 | -3.39183700 | 1.17985600 |
| O | 0.63035900 | 0.58599400 | 1.60365700 |
| C | -0.84533100 | -1.17165400 | -0.36176700 |
| O | -1.38396800 | -1.90120700 | -1.15912300 |
| C | -5.54029800 | -0.92971400 | 0.09597100 |
| C | -4.32407400 | -0.74860500 | -0.55604600 |
| C | -3.59714700 | 0.42963500 | -0.36933200 |
| C | -4.10043900 | 1.42044400 | 0.47537900 |
| C | -5.31569200 | 1.23914500 | 1.12879600 |
| C | -6.03666500 | 0.06261900 | 0.93868500 |
| C | -2.26895700 | 0.62810500 | -1.04625200 |
| O | -1.18965000 | 0.13198700 | -0.21620900 |
| H | 3.21710100 | -2.89580000 | 2.68221300 |
| H | 2.47313300 | -0.52751900 | 2.89043000 |
| H | 0.17468300 | -3.54373000 | -0.28724000 |

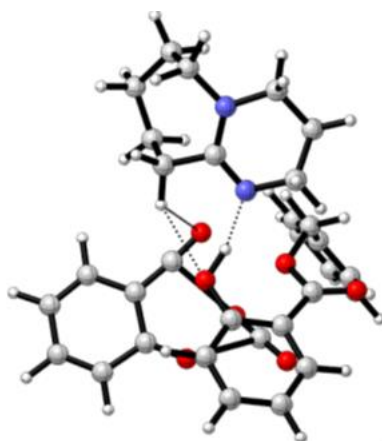
| | | | |
|---|-------------|-------------|-------------|
| H | 2.06922400 | -4.42312300 | 1.08023000 |
| H | -0.19148200 | 0.79247400 | 1.11955600 |
| H | -6.10235400 | -1.84600700 | -0.05463200 |
| H | -3.92434600 | -1.52055000 | -1.20678000 |
| H | -3.53763800 | 2.33996600 | 0.61643300 |
| H | -5.70115700 | 2.01577700 | 1.78166700 |
| H | -6.98628300 | -0.07972000 | 1.44503100 |
| H | -2.22149000 | 0.10776000 | -2.00432600 |
| H | -2.03147000 | 1.68338200 | -1.18331000 |
| C | 2.84172000 | -1.54757700 | -1.93042000 |
| C | 3.39174600 | -0.80352400 | -0.89642600 |
| C | 2.81608300 | 0.42439700 | -0.58832900 |
| C | 1.72845000 | 0.90857200 | -1.30072200 |
| C | 1.18759800 | 0.15374100 | -2.34594700 |
| C | 1.74097800 | -1.07627400 | -2.65860700 |
| O | 3.32685100 | 1.11552100 | 0.47459100 |
| O | 1.78073700 | 2.81775000 | 0.15335800 |
| C | 1.12866300 | 2.17460400 | -0.88044400 |
| C | 2.78089300 | 2.28101900 | 0.90341900 |
| O | 0.15171900 | 2.69073200 | -1.34303600 |
| O | 3.19427500 | 2.83170100 | 1.86838300 |
| H | 3.26704200 | -2.51746900 | -2.16694700 |
| H | 4.22487800 | -1.16239100 | -0.30349800 |
| H | 0.32830400 | 0.54973400 | -2.87864400 |
| H | 1.31490100 | -1.67896500 | -3.45244900 |



TS-IV'''

| | | | |
|---|-------------|-------------|-------------|
| C | 2.08448000 | -2.40586300 | 2.09237600 |
| C | 1.70176200 | -1.09843300 | 1.84368000 |
| C | 0.54058900 | -0.80507000 | 1.10247700 |
| C | -0.22796300 | -1.88742900 | 0.61330300 |
| C | 0.15050300 | -3.20040300 | 0.91804100 |
| C | 1.30439100 | -3.47135800 | 1.63521900 |
| O | 0.23827900 | 0.47536600 | 0.90640400 |
| C | -1.46315700 | -1.73988200 | -0.20029100 |
| O | -2.33414700 | -2.57319900 | -0.28380000 |
| C | -5.72293800 | 0.10218100 | 0.58536400 |
| C | -4.77424100 | -0.47007000 | -0.25821400 |
| C | -3.73002100 | 0.30434000 | -0.76449200 |
| C | -3.63496200 | 1.65211100 | -0.40966200 |
| C | -4.57929700 | 2.22213600 | 0.43786600 |
| C | -5.62661300 | 1.44722200 | 0.93306900 |
| C | -2.68014700 | -0.30495100 | -1.65368600 |
| O | -1.48187000 | -0.58908300 | -0.90653100 |
| H | 2.98823700 | -2.59836100 | 2.66294500 |
| H | 2.27759000 | -0.26170500 | 2.22922300 |
| H | -0.48789400 | -4.00208900 | 0.56053500 |
| H | 1.59134900 | -4.49564700 | 1.84593100 |
| H | -0.45650200 | 0.99977200 | -0.13487500 |
| H | -6.53495600 | -0.50373200 | 0.97485900 |

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|---|-------------|-------------|-------------|
| H | -4.82787800 | -1.52334200 | -0.51731400 |
| H | -2.81474900 | 2.25196400 | -0.79819500 |
| H | -4.50049600 | 3.26989300 | 0.70995200 |
| H | -6.36594400 | 1.89209100 | 1.59185000 |
| H | -3.03175400 | -1.22636800 | -2.12183900 |
| H | -2.35001800 | 0.40258100 | -2.41713400 |
| C | 3.93691600 | -1.27874400 | -1.69857200 |
| C | 4.30788200 | -0.28041700 | -0.80547300 |
| C | 3.35611000 | 0.66666800 | -0.45653500 |
| C | 2.07503000 | 0.64060100 | -0.99204300 |
| C | 1.70482600 | -0.38035500 | -1.87197400 |
| C | 2.64332500 | -1.33501700 | -2.23006300 |
| O | 3.70765700 | 1.62937800 | 0.45739100 |
| O | 1.63115900 | 2.64041100 | 0.22701000 |
| C | 1.12218300 | 1.59673200 | -0.46497700 |
| C | 2.88253200 | 2.64696400 | 0.78645700 |
| O | -0.07065800 | 1.75574500 | -0.90477100 |
| O | 3.21750400 | 3.51965400 | 1.51256700 |
| H | 4.66550700 | -2.03209300 | -1.97942600 |
| H | 5.29997000 | -0.22795000 | -0.37262900 |
| H | 0.68361500 | -0.40450100 | -2.23848800 |
| H | 2.37339500 | -2.13248000 | -2.91276900 |

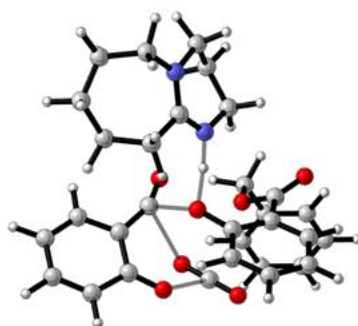


INT-5

| | | | |
|---|-------------|-------------|-------------|
| C | -2.66978900 | 1.76027100 | 3.79719000 |
| C | -1.69653200 | 1.98074500 | 2.83976900 |
| C | -1.10984300 | 0.91171600 | 2.14823600 |
| C | -1.54511900 | -0.39627300 | 2.43365800 |
| C | -2.51503400 | -0.60119100 | 3.42631400 |
| C | -3.08063100 | 0.45965600 | 4.10839700 |
| O | -0.15031100 | 1.22255900 | 1.25399000 |
| C | -1.08552500 | -1.61054600 | 1.71921800 |
| O | -1.19892400 | -2.74100800 | 2.14262000 |
| C | -2.80480500 | -4.03081500 | -1.99094800 |
| C | -1.95826300 | -3.59862600 | -0.97490600 |
| C | -0.77413300 | -2.92424400 | -1.28896100 |
| C | -0.44184900 | -2.70780600 | -2.62495900 |
| C | -1.28229400 | -3.15241400 | -3.64244000 |
| C | -2.46799600 | -3.80843200 | -3.32577200 |
| C | 0.10675500 | -2.40712700 | -0.18358000 |
| O | -0.53014600 | -1.33301100 | 0.52051700 |
| H | -3.10994900 | 2.60717100 | 4.31558800 |
| H | -1.35444800 | 2.98079800 | 2.59449100 |
| H | -2.81802600 | -1.62381900 | 3.62556100 |

| | | | |
|---|-------------|-------------|-------------|
| H | -3.83907500 | 0.28586400 | 4.86377700 |
| H | -3.72803300 | -4.54434200 | -1.74108800 |
| H | -2.21270700 | -3.76259000 | 0.06884000 |
| H | 0.47236300 | -2.17200100 | -2.86758900 |
| H | -1.01817500 | -2.97481800 | -4.68026100 |
| H | -3.13042500 | -4.14623900 | -4.11672000 |
| H | 0.34846100 | -3.19987900 | 0.52962700 |
| H | 1.02726700 | -1.97147300 | -0.58252700 |
| H | 0.55041000 | 0.50731600 | 1.20423900 |
| C | 3.14587100 | 0.26777600 | 0.81040400 |
| C | 2.93194400 | 1.51856600 | -0.01068800 |
| C | 5.57349100 | 0.50722700 | 0.35516800 |
| C | 5.66708000 | 0.47368800 | -1.17354900 |
| C | 3.25436000 | 1.31723700 | -1.50223800 |
| C | 2.34176600 | -1.47827200 | 2.15320800 |
| C | 4.73471100 | 1.47575200 | -1.85533900 |
| C | 4.70135100 | -1.55101800 | 1.41546000 |
| C | 3.41940400 | -2.36043100 | 1.53126600 |
| N | 4.42602700 | -0.21243000 | 0.89469400 |
| N | 2.11370600 | -0.28614900 | 1.35005200 |
| H | 3.53601800 | 2.34250200 | 0.39057800 |
| H | 1.88788500 | 1.80669700 | 0.12818000 |
| H | 6.46057500 | 0.04099700 | 0.79430400 |
| H | 5.56691600 | 1.54474600 | 0.70962100 |
| H | 5.44614800 | -0.54695100 | -1.51287100 |
| H | 6.69977100 | 0.69213800 | -1.46931700 |
| H | 2.68370900 | 2.05405500 | -2.08005300 |
| H | 2.89301400 | 0.32944800 | -1.81614500 |
| H | 2.64790200 | -1.18101000 | 3.16679700 |
| H | 1.40028600 | -2.02486300 | 2.25786600 |

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|---|-------------|-------------|-------------|
| H | 4.85679100 | 1.39880800 | -2.94144900 |
| H | 5.05204100 | 2.49088800 | -1.57796400 |
| H | 5.19310500 | -1.46836300 | 2.39455300 |
| H | 5.40696500 | -2.04506900 | 0.73559300 |
| H | 3.08974300 | -2.67925300 | 0.53585200 |
| H | 3.59949600 | -3.25849500 | 2.12832000 |
| C | -2.15687800 | 5.03855000 | -1.36291300 |
| C | -2.73452000 | 4.03838600 | -0.65395600 |
| C | -2.21810700 | 2.67104500 | -0.67363200 |
| C | -0.99092700 | 2.52324900 | -1.48537400 |
| C | -0.41259200 | 3.61203300 | -2.23678400 |
| C | -0.98547600 | 4.83668500 | -2.17745700 |
| O | -2.75337200 | 1.74137700 | -0.07836000 |
| O | -2.59685700 | -0.37133700 | -1.95192000 |
| C | -0.36663700 | 1.32827100 | -1.48537200 |
| C | -3.05181500 | -0.70110500 | -0.93003600 |
| O | 0.22921900 | 0.34935500 | -1.54438800 |
| O | -3.53095300 | -1.07765300 | 0.05949600 |
| H | -2.58885500 | 6.03498500 | -1.32358300 |
| H | -3.62011400 | 4.19749400 | -0.04799100 |
| H | 0.47355400 | 3.43038000 | -2.83727900 |
| H | -0.56781300 | 5.66734800 | -2.73412400 |

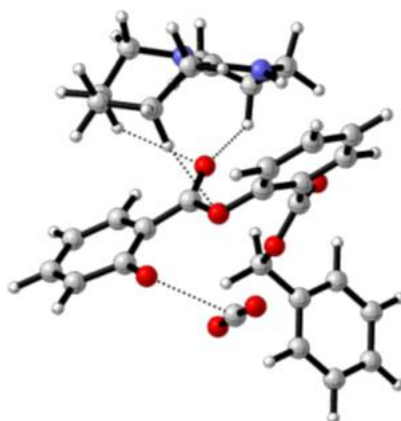


TS-IV

| | | | |
|---|-------------|-------------|-------------|
| C | -0.71732200 | 0.93026100 | 4.23314400 |
| C | -0.05504600 | 1.12632100 | 3.03341900 |
| C | -0.33828500 | 0.32693300 | 1.91193800 |
| C | -1.34537900 | -0.65614700 | 2.04013100 |
| C | -1.98032800 | -0.86605400 | 3.27105500 |
| C | -1.67546300 | -0.08042900 | 4.36881600 |
| O | 0.41571400 | 0.42735200 | 0.81404500 |
| C | -1.85501100 | -1.44933500 | 0.89870200 |
| O | -2.31572200 | -2.56972100 | 0.97756100 |
| C | -6.18290900 | -1.57006200 | -0.83014900 |
| C | -4.82473200 | -1.87114200 | -0.79197100 |
| C | -3.90513700 | -1.05645800 | -1.45832600 |
| C | -4.36390000 | 0.05712200 | -2.16527600 |
| C | -5.72282700 | 0.35837500 | -2.20187500 |
| C | -6.63396900 | -0.45533800 | -1.53379400 |
| C | -2.42943300 | -1.36278500 | -1.40804600 |
| O | -1.80401400 | -0.76408200 | -0.26312800 |
| H | -0.48150100 | 1.56711100 | 5.08117400 |
| H | 0.68946000 | 1.90533100 | 2.91664200 |
| H | -2.73400200 | -1.64530500 | 3.32892100 |
| H | -2.18481200 | -0.23480300 | 5.31394400 |
| H | -6.89118700 | -2.20705000 | -0.30939400 |
| H | -4.46306400 | -2.73097200 | -0.23692700 |

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|---|-------------|-------------|-------------|
| H | -3.65002300 | 0.69283700 | -2.68173400 |
| H | -6.06928600 | 1.22685400 | -2.75335000 |
| H | -7.69390400 | -0.22190500 | -1.56180900 |
| H | -2.25755300 | -2.44262400 | -1.38464900 |
| H | -1.90839300 | -0.91800300 | -2.25828900 |
| H | 0.96121000 | -0.75997200 | 0.51433400 |
| C | 2.86268800 | -1.62536800 | 0.33497800 |
| C | 3.45053100 | -0.31125200 | 0.77997000 |
| C | 5.13891700 | -2.51757600 | 0.08344700 |
| C | 5.76526900 | -1.57579600 | -0.94822000 |
| C | 4.19258300 | 0.38851300 | -0.37513800 |
| C | 0.88480000 | -2.86483600 | -0.30874300 |
| C | 5.62839900 | -0.09596700 | -0.58342200 |
| C | 3.14477200 | -3.84061100 | -0.65339400 |
| C | 1.80037700 | -3.55638400 | -1.30813200 |
| N | 3.68284400 | -2.62538400 | -0.03431900 |
| N | 1.56440700 | -1.71022400 | 0.25895700 |
| H | 4.12511600 | -0.46676400 | 1.63009200 |
| H | 2.61940200 | 0.31119600 | 1.11998100 |
| H | 5.52797000 | -3.53141600 | -0.03918800 |
| H | 5.40393000 | -2.20416000 | 1.09922300 |
| H | 5.30547700 | -1.77534600 | -1.92510400 |
| H | 6.82884100 | -1.82286700 | -1.04053200 |
| H | 4.20115300 | 1.46383200 | -0.17148700 |
| H | 3.61051600 | 0.26193000 | -1.29829000 |
| H | 0.57433800 | -3.54382600 | 0.49393400 |
| H | -0.01994500 | -2.49454600 | -0.79591400 |
| H | 6.10189600 | 0.50893500 | -1.36393200 |
| H | 6.19605900 | 0.08905600 | 0.33915800 |
| H | 3.05148600 | -4.62798900 | 0.10544200 |

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|---|-------------|-------------|-------------|
| H | 3.86915500 | -4.17909900 | -1.40068600 |
| H | 1.94826700 | -2.89817800 | -2.17144400 |
| H | 1.35600100 | -4.48924400 | -1.66297300 |
| C | 2.43825200 | 4.84546300 | -0.71382100 |
| C | 1.47910600 | 4.54766300 | 0.20077200 |
| C | 0.67438200 | 3.33017300 | 0.12588000 |
| C | 1.10481900 | 2.41344500 | -0.93373700 |
| C | 2.08676200 | 2.78892800 | -1.91579100 |
| C | 2.74746200 | 3.97187700 | -1.80890100 |
| O | -0.28582400 | 3.12913400 | 0.87232900 |
| O | -1.98649100 | 1.99471600 | -1.17097200 |
| C | 0.59343500 | 1.15034700 | -1.11275700 |
| C | -2.42233400 | 1.91026500 | -0.08921200 |
| O | 0.40399100 | 0.19044400 | -1.73333100 |
| O | -2.92852300 | 1.81902800 | 0.94992800 |
| H | 2.98531600 | 5.78093100 | -0.62575700 |
| H | 1.23385300 | 5.22476600 | 1.01247500 |
| H | 2.30089100 | 2.09880300 | -2.72808300 |
| H | 3.49665200 | 4.25590000 | -2.53898200 |

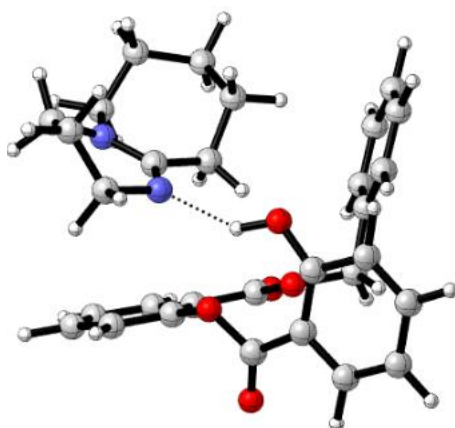


INT-6

| | | | |
|---|-------------|-------------|-------------|
| C | 1.12247800 | -2.28133300 | 3.38486700 |
| C | 1.07474400 | -0.99215800 | 2.86403500 |
| C | 0.27466600 | -0.70685400 | 1.75471700 |
| C | -0.51007900 | -1.72147500 | 1.18802400 |
| C | -0.44706800 | -3.01313200 | 1.71510200 |
| C | 0.36933000 | -3.30542800 | 2.80323900 |
| O | 0.29610500 | 0.58073400 | 1.31911600 |
| C | -1.39095000 | -1.48918200 | 0.00721100 |
| O | -1.58326500 | -2.32512700 | -0.85190900 |
| C | -5.93959700 | -1.61187200 | -1.55902600 |
| C | -4.58165300 | -1.31637600 | -1.64043600 |
| C | -4.08481900 | -0.13827800 | -1.08028300 |
| C | -4.95684000 | 0.73662800 | -0.42967200 |
| C | -6.31417800 | 0.44001300 | -0.34630500 |
| C | -6.80691900 | -0.73350300 | -0.91313000 |
| C | -2.61629800 | 0.18294000 | -1.14174700 |
| O | -1.93847900 | -0.28189300 | 0.04248900 |
| H | 1.74201000 | -2.48618500 | 4.25270800 |
| H | 1.63810800 | -0.17386100 | 3.30120700 |
| H | -1.06070000 | -3.78127100 | 1.25290900 |
| H | 0.39869500 | -4.31005400 | 3.21149400 |

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|---|-------------|-------------|-------------|
| H | -6.32175300 | -2.52772400 | -1.99944500 |
| H | -3.89329900 | -2.00188300 | -2.12642500 |
| H | -4.56090200 | 1.64709000 | 0.01273700 |
| H | -6.98791000 | 1.12547200 | 0.15835000 |
| H | -7.86625100 | -0.96351700 | -0.85125500 |
| H | -2.13662900 | -0.27228800 | -2.01165900 |
| H | -2.43693500 | 1.25950900 | -1.13481000 |
| H | 2.02298000 | -2.83176900 | 0.92329800 |
| C | 3.14110500 | -1.72630900 | -0.32378300 |
| C | 3.89651200 | -1.10272000 | 0.82291200 |
| C | 4.38573900 | -0.33649400 | -1.88872200 |
| C | 3.96712400 | 1.05935700 | -1.42548200 |
| C | 3.67298200 | 0.40310800 | 1.04988900 |
| C | 1.55622000 | -3.44118500 | -1.07302000 |
| C | 4.33464300 | 1.33213600 | 0.03223400 |
| C | 2.57511300 | -1.83332400 | -2.70612400 |
| C | 1.30214100 | -2.54738500 | -2.27700500 |
| N | 3.39252100 | -1.37389500 | -1.57049900 |
| N | 2.28589400 | -2.69781800 | -0.04857900 |
| H | 4.96422400 | -1.30233600 | 0.65849600 |
| H | 3.61173900 | -1.64867600 | 1.72651600 |
| H | 4.50498800 | -0.37024200 | -2.97383700 |
| H | 5.35200900 | -0.62297900 | -1.45660100 |
| H | 2.88864300 | 1.17757000 | -1.57729500 |
| H | 4.46652700 | 1.79907700 | -2.05985800 |
| H | 4.07973000 | 0.63032700 | 2.04138600 |
| H | 2.60502500 | 0.61509400 | 1.10855500 |
| H | 2.14299400 | -4.32738800 | -1.34363900 |
| H | 0.60479100 | -3.75959600 | -0.64431800 |
| H | 4.05393800 | 2.36027700 | 0.28147200 |

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|---|-------------|-------------|-------------|
| H | 5.42713200 | 1.26198800 | 0.13815400 |
| H | 3.21209000 | -2.47074500 | -3.33135600 |
| H | 2.31442200 | -0.93922400 | -3.28073900 |
| H | 0.54258600 | -1.81547700 | -2.01235000 |
| H | 0.93178800 | -3.15303700 | -3.10773900 |
| C | 0.91747800 | 4.91612400 | -1.15538500 |
| C | 0.75421800 | 4.65545000 | 0.17132800 |
| C | 0.54042700 | 3.31101300 | 0.70000400 |
| C | 0.58812700 | 2.25959400 | -0.31725900 |
| C | 0.74914500 | 2.58571500 | -1.69541300 |
| C | 0.90549300 | 3.87218000 | -2.12743600 |
| O | 0.35472200 | 3.13034800 | 1.91758900 |
| O | -2.30970000 | 2.32578900 | 1.21561000 |
| C | 0.55491500 | 0.86558300 | -0.01446100 |
| C | -1.91984800 | 1.87168800 | 2.21653500 |
| O | 0.79706300 | -0.06906200 | -0.78268300 |
| O | -1.64408100 | 1.38405000 | 3.23598700 |
| H | 1.05255800 | 5.94395900 | -1.48606600 |
| H | 0.75070100 | 5.45130500 | 0.91002700 |
| H | 0.73329700 | 1.76157600 | -2.40587600 |
| H | 1.00947600 | 4.10116000 | -3.18252200 |



INT-7

| | | | |
|---|-------------|-------------|-------------|
| C | -1.52481400 | 3.67647200 | 1.35780900 |
| C | -0.38094500 | 3.33795800 | 0.64093400 |
| C | 0.22823500 | 2.10741100 | 0.84706600 |
| C | -0.28782800 | 1.19957300 | 1.78068700 |
| C | -1.42072200 | 1.56816200 | 2.50935100 |
| C | -2.04463100 | 2.79260800 | 2.30012000 |
| O | 1.31633600 | 1.80102800 | 0.05561200 |
| C | 0.25033900 | -0.17334300 | 2.03975500 |
| O | -0.12747800 | -0.86757800 | 2.95426900 |
| C | -0.91577300 | -4.61150000 | 1.04883500 |
| C | -0.03610500 | -3.67440400 | 1.58568800 |
| C | 0.80212100 | -2.93811300 | 0.74727600 |
| C | 0.74485800 | -3.13568600 | -0.63508200 |
| C | -0.14150500 | -4.06558800 | -1.17107600 |
| C | -0.96779600 | -4.80881500 | -0.32956500 |
| C | 1.71959600 | -1.88629900 | 1.31145000 |
| O | 1.16292400 | -0.56659200 | 1.14038300 |
| H | -1.99871700 | 4.63841400 | 1.18850500 |
| H | 0.06060800 | 4.01745800 | -0.08042300 |
| H | -1.80074300 | 0.85924500 | 3.23825600 |
| H | -2.92837100 | 3.05657100 | 2.87148700 |

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|---|-------------|-------------|-------------|
| H | -1.56253100 | -5.18467000 | 1.70599600 |
| H | -0.00758400 | -3.49334000 | 2.65584100 |
| H | 1.37218500 | -2.53304300 | -1.28698200 |
| H | -0.18717300 | -4.21032500 | -2.24588400 |
| H | -1.65564000 | -5.53743200 | -0.74844600 |
| H | 1.91414100 | -2.04882000 | 2.37362700 |
| H | 2.66264100 | -1.84134200 | 0.76185600 |
| C | -1.83788400 | 0.31825000 | -0.88284700 |
| C | -2.09990200 | -0.90575600 | -0.03709500 |
| C | -4.07666000 | 1.13132000 | -0.18866600 |
| C | -5.03787800 | 0.04637900 | -0.68461400 |
| C | -3.22106400 | -1.78862800 | -0.61508600 |
| C | -0.52653000 | 1.49469400 | -2.43843700 |
| C | -4.63643600 | -1.35642000 | -0.22511700 |
| C | -2.82416300 | 2.28413200 | -1.98810000 |
| C | -1.83763900 | 1.92269500 | -3.08715500 |
| N | -2.85489800 | 1.23534200 | -0.97460500 |
| N | -0.71425200 | 0.38614500 | -1.51241800 |
| H | -2.33646600 | -0.63730600 | 1.00074400 |
| H | -1.16430400 | -1.46504200 | -0.02738600 |
| H | -4.55572000 | 2.11486100 | -0.23279900 |
| H | -3.82696200 | 0.96353400 | 0.86550200 |
| H | -5.07980900 | 0.09363800 | -1.78114400 |
| H | -6.04690500 | 0.26683100 | -0.31604800 |
| H | -3.05900000 | -2.81032600 | -0.25667700 |
| H | -3.11813600 | -1.82182000 | -1.70784000 |
| H | -0.08243500 | 2.35280300 | -1.91281900 |
| H | 0.20263100 | 1.17988300 | -3.19160400 |
| H | -5.35698400 | -2.08364700 | -0.61670500 |
| H | -4.71954500 | -1.39706000 | 0.87035600 |

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|---|-------------|-------------|-------------|
| H | -2.55130900 | 3.24363200 | -1.52432100 |
| H | -3.83513300 | 2.39279000 | -2.40038400 |
| H | -2.23749100 | 1.08927800 | -3.67629400 |
| H | -1.69478200 | 2.77414600 | -3.75893300 |
| C | 5.58455500 | -0.27441200 | -1.57096100 |
| C | 4.26963700 | -0.50980900 | -1.92604200 |
| C | 3.20387400 | 0.09013100 | -1.23065400 |
| C | 3.51382200 | 0.94570400 | -0.15250900 |
| C | 4.85651600 | 1.15103100 | 0.20578700 |
| C | 5.89260000 | 0.56151300 | -0.49188400 |
| O | 1.98673500 | -0.26136000 | -1.66549300 |
| C | 2.51950600 | 1.63176100 | 0.69556300 |
| O | 2.71139800 | 2.04312700 | 1.80865200 |
| H | 6.38077000 | -0.75249900 | -2.13373200 |
| H | 4.01454200 | -1.16699200 | -2.75057000 |
| H | 5.04878400 | 1.79632600 | 1.05690800 |
| H | 6.92274200 | 0.74163900 | -0.20611900 |
| H | 1.20710400 | 0.07708500 | -1.16479500 |