

Supporting information

An efficient strategy for achieving controlled ring-opening polymerization of *O*-carboxyanhydrides via amine initiation in collaboration with metal-alkoxide catalysis

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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. Anhydrous dichloromethane (DCM), anhydrous dimethylformamide (DMF), anhydrous chloroform (TCM), anhydrous 1,4-dioxane, ZnMe_2 (1.0 M in toluene), sodium nitrite and L-phenylalanine were purchased from J&K SCIENTIFIC LTD and used without treatment. $\text{Zn}(\text{OTf})_2$ and $\text{Zn}(\text{OAc})_2$ were purchased from Alfa Aesar and used without treatment. Triphosgene purchased from Innochem was used without treatment. Toluene, hexane, pentane and tetrahydrofuran (THF) were distilled over sodium/benzophenone and stored over 4Å molecular sieves prior to use. 1-Hexylamine purchased from Acros was directly used without treatment. Aniline, benzylamine, cyclohexylamine were dried with KOH for overnight, following distillation in vacuum three times. CDCl_3 and C_6D_6 were purchased from Cambridge Isotope Laboratories Inc, and THF- d_8 was purchased from J&K SCIENTIFIC LTD. CDCl_3 was distilled over CaH_2 and stored over 4Å molecular sieves. C_6D_6 and THF- d_8 were dried over 4Å molecular sieve prior to use.

Characterization.

The ^1H NMR were carried out on a 400 MHz or 500 MHz NMR instrument (Bruker Corporation, Germany) at room temperature using CDCl_3 ($\delta = 7.26$ ppm for ^1H NMR, 77.16 ppm for ^{13}C NMR), C_6D_6 or THF- d_8 ($\delta = 1.72$ ppm for ^1H NMR, 25.31 ppm for ^{13}C 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 THF as eluent (flow rate of 1.0 mL/min at 35 °C), and polystyrene standards were employed for calibration. Polymer solutions with concentrations between 3.0 and 5.0 mg/mL were injected at an injection volume of 40 μL . Desorption/ionization-time of flight mass spectrometer (MALDI-TOF MS) experiments were carried out on a Bruker Autoflex III (laser frequency 100 Hz, 355 nm and detector voltage of 1689 V). *In situ* IR study of monomer polymerization 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 polymerization solution was taken from the 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 1760 cm^{-1} and

1800 cm⁻¹, conversion% = $I_{1760} / (I_{1760} + I_{1800})$.¹

Synthesis of OCA monomers

As reported², PheOCA and ManOCA were synthesized by the modified procedure. The preparation of Phe-OCA as example was described in detailed.

The preparation of 2-hydroxyl-3-phenylpropanoic acid (HPPA). L-Phenylalanine (33.04 g, 200 mmol) in 1 M sulfuric acid was diazotized with 5 M sodium nitrite (3.0 equiv, 600 mmol) at 0 °C. The mixture was stirred for 1 h at 0 °C and then kept stirring at room temperature overnight. The reaction mixture was extraction with ethyl acetate (3 × 300 mL). The combined extracts were washed with brine (3 × 100 mL), dried over anhydrous MgSO₄, filtered and evaporated to give a white solid. Upon recrystallization from diethyl ether, pure 2-hydroxyl-3-phenylpropanoic acid was afforded in a yield of 81%. ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.24-7.33 (m, 5H, *ArH*), 4.53 (dd, *J* = 7.2 Hz, 2H, -CH), 3.19- 3.24 (dd, *J* = 14.0 Hz, 1H, CH₂), 2.98- 3.03 (dd, *J* = 14.0 Hz, 1H, CH₂). ¹³C NMR (CDCl₃, 100 MHz, δ ppm) : 40.33 (-CH₂), 71.15 (CH), 127.36 (*ArC*), 128.79 (*ArC*), 129.68 (*ArC*), 135.93 (*ArC*), 177.87 (C=O).

Preparation of Phe-OCA. To a solution of HPPA (30.0 mmol) and activated charcoal (~90 mg) in anhydrous THF (30 mL), triphosgene (20 mmol) was added in one portion. The reaction mixture was stirred for 8 hours at room temperature. The mixture was filtered over celite, the filtrate was concentrated and the resulting residue was recrystallized from THF/hexane (v/v = 6/25) four times to give colourless crystal in a yield of 52%. ¹H NMR (CDCl₃, 500 MHz, δ ppm): 7.34-7.35 (m, 3H, *ArH*), 7.21-7.23 (m, 2H, *ArH*), 5.29 (t, *J* = 4.5 Hz, 1H, CH), 3.36-3.40 (dd, *J* = 15.0 Hz, 1H, CH₂), 3.22-3.26 (dd, *J* = 15.0 Hz, 1H, CH₂). ¹³C NMR (CDCl₃, 125 MHz, δ ppm) : 36.57 (-CH₂), 80.03 (CH), 128.56 (*ArC*), 129.31 (*ArC*), 129.80 (*ArC*), 131.64 (*ArC*), 147.92 (OC=OO), 166.44(C=OO).

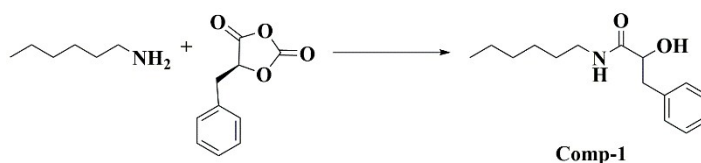
Similar operation was performed to prepare Man-OCA. To a solution of (S)-(+)-Mandelic acid (60.0 mmol) and activated charcoal (~900 mg) in anhydrous THF (60 mL), triphosgene (40 mmol) was added and stirred overnight at room temperature. After filtering over celite, the filtrate was concentrated and the resulting residue was recrystallized from THF/hexane (v/v = 1/5) four times to give colourless crystal in a yield of 20%. ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.42-7.51 (m, 5H, *ArH*), 6.09 (s, 1H, CH). ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 80.56 (CH), 126.27 (*ArC*), 129.39 (*ArC*), 129.69 (*ArC*), 130.94 (*ArC*), 148.12 (OC=OO), 165.44(C=OO).

Synthesis of Zn(C₆F₅)₂

$\text{Zn}(\text{C}_6\text{F}_5)_2$ was synthesized according to the literature.³ A solution of $\text{B}(\text{C}_6\text{F}_5)_3$ (2.0 g, 4.0 mmol) in anhydrous toluene (40 mL) was treated with a solution of ZnMe_2 in toluene (6.0 mmol) at room temperature. The mixture was stirred for 30 min. Removal of volatiles left a white solid, which was recrystallized from toluene/light petroleum at $-20\text{ }^\circ\text{C}$ to give $\text{Zn}(\text{C}_6\text{F}_5)_2$ (1.23 g) as needlelike crystal in a yield of 77%. ^{19}F NMR (C_6D_6 , 376 MHz, δ ppm): 117.98 (m, 4F, *o-F*), 152.53 (t, $J = 18.8$ Hz, 2F, *p-F*), 160.53 (m, 4F, *m-F*).

Polymerization procedure.

A typical procedure for polymerization of Phe-OCA was performed in a 25 mL Schlenk in a Vigor glovebox. The given amount of Lewis acid and 1-hexylamine was stirred in 1.0 mL anhydrous THF before taken out from the glovebox. The reaction mixture was then connected to a vacuum line and stirred for 10 min at $50\text{ }^\circ\text{C}$, followed by adding 144.2 mg PheOCA (0.75 mmol). After a specific time, a small aliquot of polymer solution was taken out for determining monomer conversion. The final reaction solution was precipitated in the mixture of diethyl ether/hexane ($v/v = 1/2$), and washed twice using the same solution. The obtained polymers were dried under vacuum.



Scheme S1. Preparation route of Comp-1.

Preparation of *N*-hexyl-2-hydroxyl-3-phenyl-propanamide (Comp-1). Phe-OCA (288.3 mg, 1.5 mmol) in 2.0 mL dry THF was treated with 1-hexyl- NH_2 (151.8 mg, 1.5 mmol) at $50\text{ }^\circ\text{C}$. After PheOCA was completely consumed by FTIR monitoring, the mixture was concentrated in vacuum and followed by flash chromatography (DCM/methanol $v/v = 99/1$). The obtained crude product was recrystallized in dry THF, and then dried under vacuum to give a white crystal in a yield of 86%.

Computational Details

All calculations were performed with the Gaussian 09 program.⁴ Geometry optimizations of all stationary points for the FLP controlled ring-opening polymerization reaction of *O*-

carboxyanhydrides (OCAs) were performed with the M06-2X functional,⁵ which has been proven to be suitable to describe the dispersion effects. The 6-31G(d) basis set⁶ was applied for all elements in substrates and the latent catalytic species. 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)⁷ 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.⁸

Table S1. ROP of Phe-OCA initiated by Zn(C₆F₅)₂ and 1-hexyl-NH₂

Run	Solvent	Zn(C ₆ F ₅) ₂ : 1-hexyl-NH ₂ :M ^a	Temp. (°C)	Time (h)	Conv. ^b (%)	$M_{n, \text{cald}}^{\text{c}}$ (kg/mol)	$M_{n, \text{NMR}}^{\text{d}}$ (kg/mol)	$M_{n, \text{GPC}}$ (kg/mol)	\bar{D}^{e}
1	CH ₂ Cl ₂	1:1:50	25	24	28	2.2	—	—	—
2	CHCl ₃	1:1:50	25	24	27	2.1	—	—	—
3	dioxane	1:1:50	25	4	>99	7.5	—	1.6	1.36
4	DMF	1:1:50	25	0.5	>99	7.5	—	5.2	1.26
5	THF	1:1:50	25	5	>99	7.5	7.6	7.4	1.08
6	THF	0:1:50	25	24	0	0	—	—	—
7	THF	1:0:50	25	24	38	2.9	—	0.6	2.78
8	THF	1:1:50	40	2.5	>99	7.5	7.6	7.7	1.08
9	THF	1:1:50	50	1.5	>99	7.5	7.6	7.4	1.08
10	THF	1:1:50	60	1.0	>99	7.5	8.6	8.3	1.08

Note: ^a Indicating the molar ratio of Zn(C₆F₅)₂, initiator and monomer. ^b The monomer conversion was determined by the intensity ratio between the peaks at 1760 cm⁻¹ and 1800 cm⁻¹ in FT-IR spectroscopy. Conv.% = $I_{1760} / (I_{1760} + I_{1800})$. ^c Calculated by $[M]_0/[I]_0 \times (M_w \text{ of monomer} - M_w \text{ of CO}_2) \times \text{monomer conversion} + M_w \text{ of initiator}$. ^d Determined from the relative integration of the signals of the backbone methine units and chain ends in ¹H NMR spectra. ^e Measured by GPC in THF against polystyrene standards.

Table S2. ROP of Phe-OCA initiated by Zn(C₆F₅)₂ and 1-hexyl-NH₂ varying molar ratio.

Run	Solvent	Zn(C ₆ F ₅) ₂ : 1-hexyl-NH ₂ :M ^a	Temp. (°C)	Time (h)	Conv. ^b (%)	$M_{n, \text{cald}}^{\text{c}}$ (kg/mol)	$M_{n, \text{NMR}}^{\text{d}}$ (kg/mol)	$M_{n, \text{GPC}}$ (kg/mol) ^e	\bar{D}^{e}
1	THF	0.5:1:50	50	19	>99	7.5	6.0	6.1	1.10
2	THF	1.5:1:50	50	0.6	>99	7.5	7.4	7.3	1.08
3	THF	2.0:1:50	50	0.3	>99	7.5	7.1	7.1	1.08
4	THF	5.0:1:50	50	0.2	>99	7.5	8.3	7.6	1.07
5	THF	10.0:1:50	50	0.2	>99	7.5	7.9	7.4	1.08

Note: ^a Indicating the molar ratio of Zn(C₆F₅)₂, initiator and monomer. ^b The monomer conversion was determined by the intensity ratio between the peaks at 1760 cm⁻¹ and 1800 cm⁻¹ in FT-IR spectroscopy. Conv.% = $I_{1760} / (I_{1760} + I_{1800})$. ^c Calculated by $[M]_0/[I]_0 \times (M_w \text{ of monomer} - M_w \text{ of CO}_2) \times \text{monomer conversion} + M_w \text{ of initiator}$.

CO₂) \times monomer conversion + M_w of initiator. ^d Determined from the relative integration of the signals of the backbone methine units and chain ends in ¹H NMR spectra. ^e Measured by GPC in THF against polystyrene standards.

References.

1. Quan Y F, and Rong T. *J. Am. Chem. Soc.*, **2017**, *139*, 6177.
2. Qian Y, Rong T, Yun X X, Lawrence W. D, Timothy M. F, Jian J C. *Biomacromolecules* **2013**, *14*, 920.
3. (a) Mathias L, Axel S, Alexander V, *Angew. Chem. Int. Ed.*, **2009**, *48*, 7444-7447. (b) Dennis A. W, Timothy J. W, David L. H, Manfred B, *Organometallics*, **2001**, *20*, 3772.
4. Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.
5. (a) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157. (b) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.
6. For the 6-31G(d) basis set, see: (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257. (c) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213. (d) Dill, J. D.; Pople, J. A. *J. Chem. Phys.* **1975**, *62*, 2921. (e) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654. (f) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.
7. (a) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523. (b) Gonzalez, C.; Schlegel, H. B.

J. Chem. Phys. **1989**, *90*, 2154.

8. Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke: Sherbrooke, Québec, Canada, 2009;
<http://www.cylview.org>.

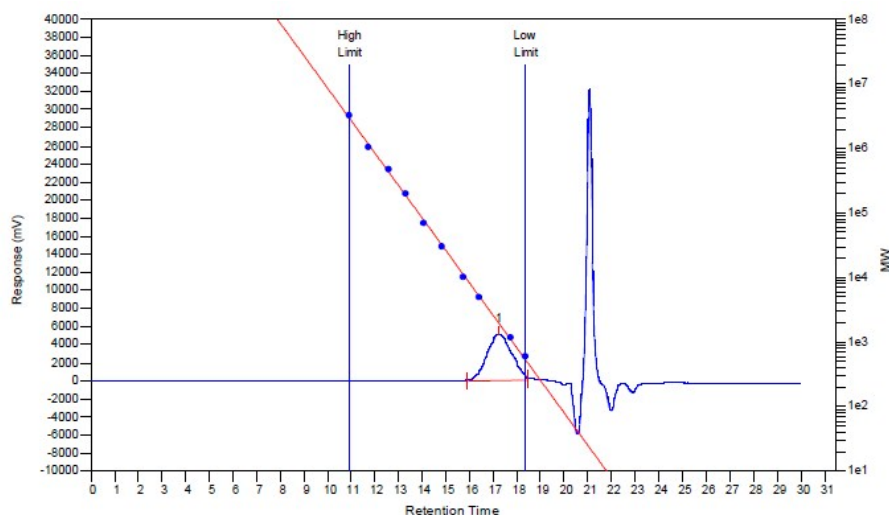


Figure S1. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in dioxane at 25 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

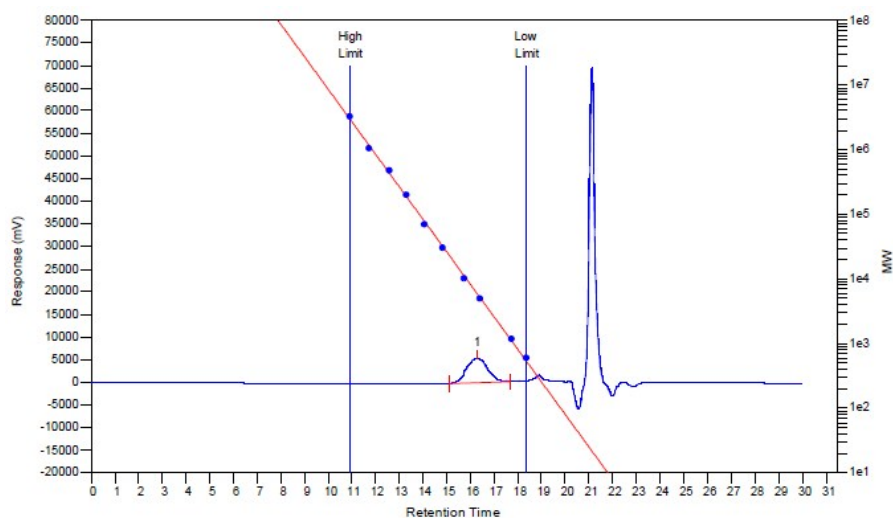


Figure S2. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in DMF at 25 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

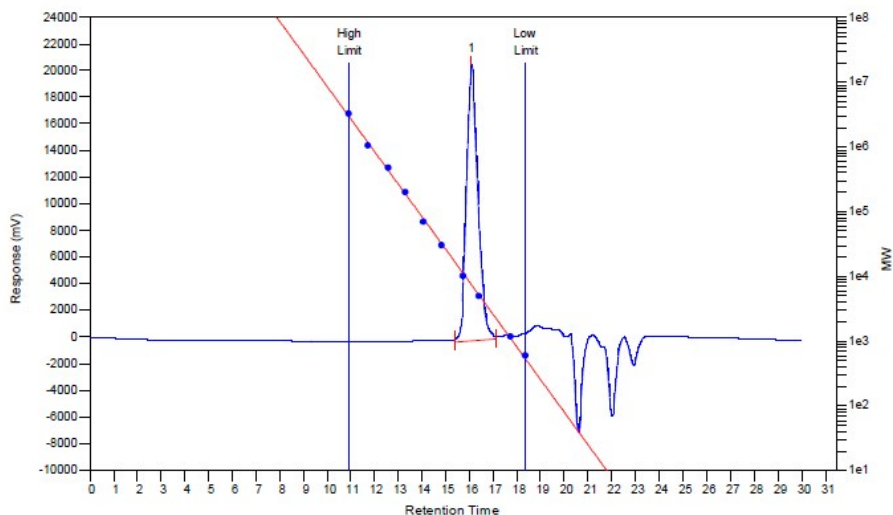


Figure S3. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 25 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

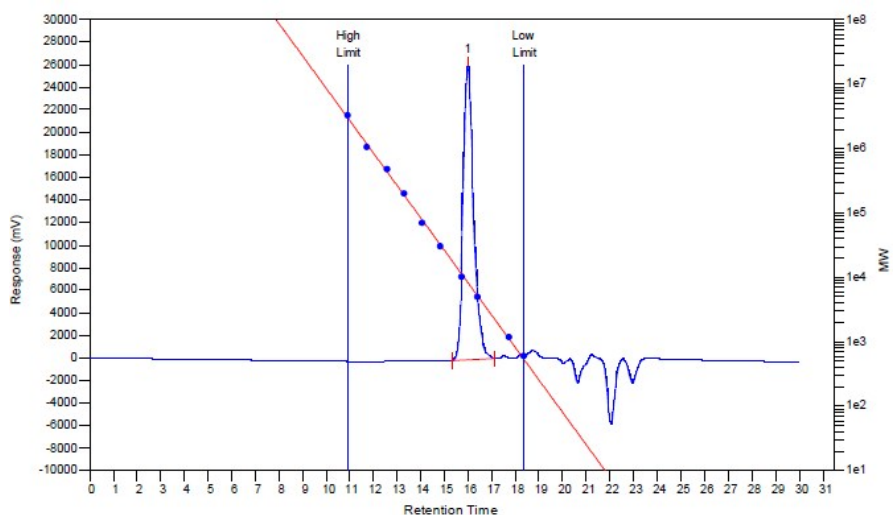


Figure S4. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 40 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

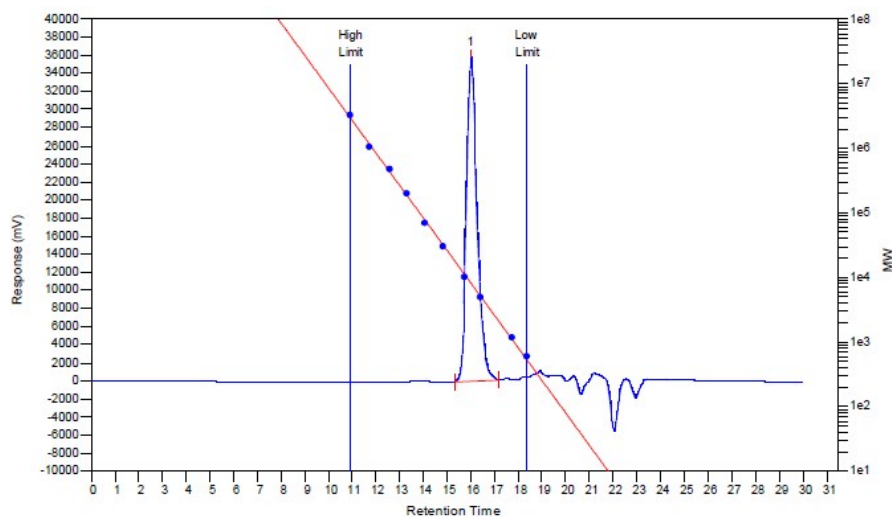


Figure S5. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

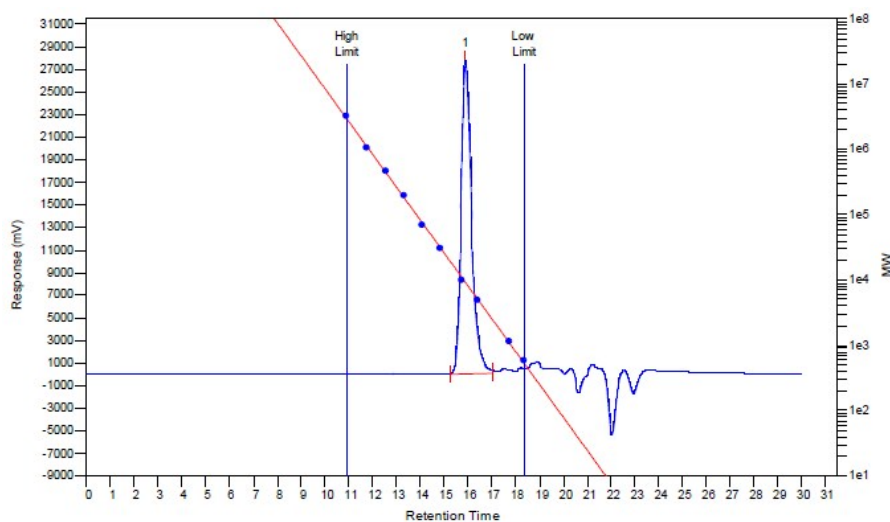


Figure S6. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 60 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1/1$.

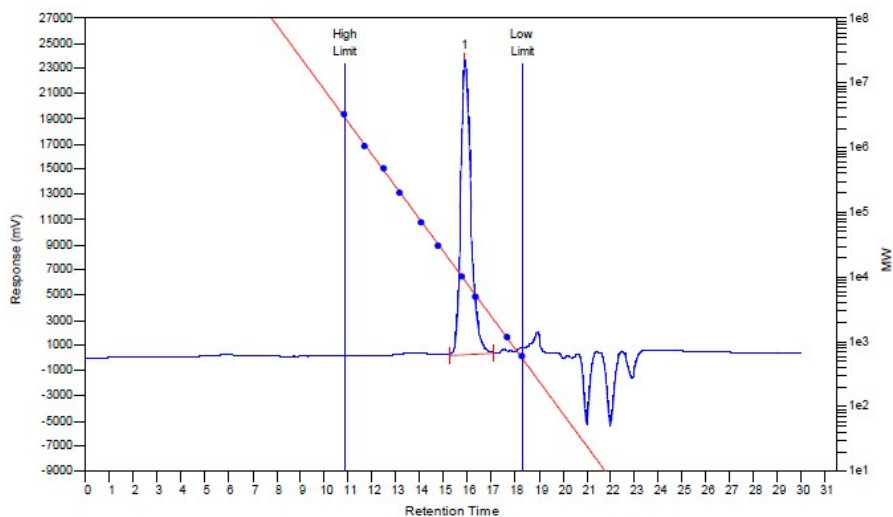


Figure S7. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and cyclohex- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/\text{cyclohex-NH}_2 = 50/1/1$.

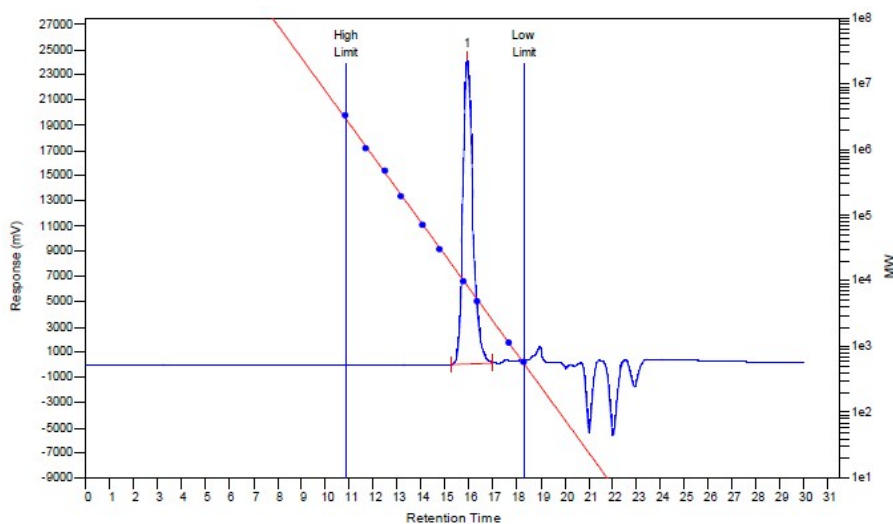


Figure S8. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and benzy- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/\text{benzyl-NH}_2 = 50/1/1$.

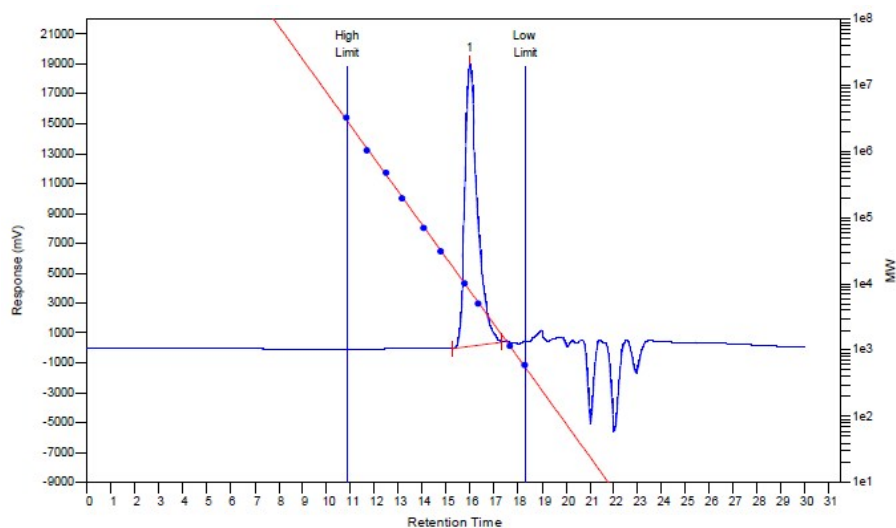


Figure S9. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and phenyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/\text{phenyl-NH}_2 = 50/1/1$.

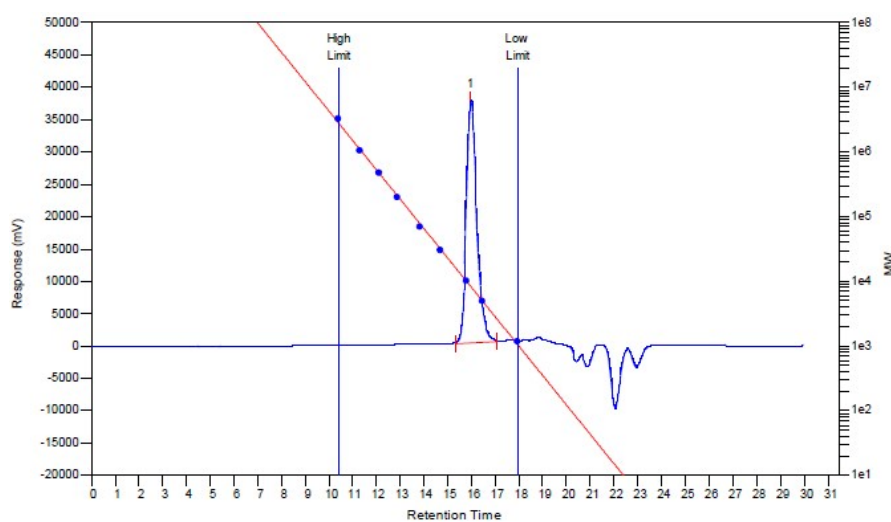


Figure S10. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and diethylamine in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/\text{diethylamine} = 50/1/1$.

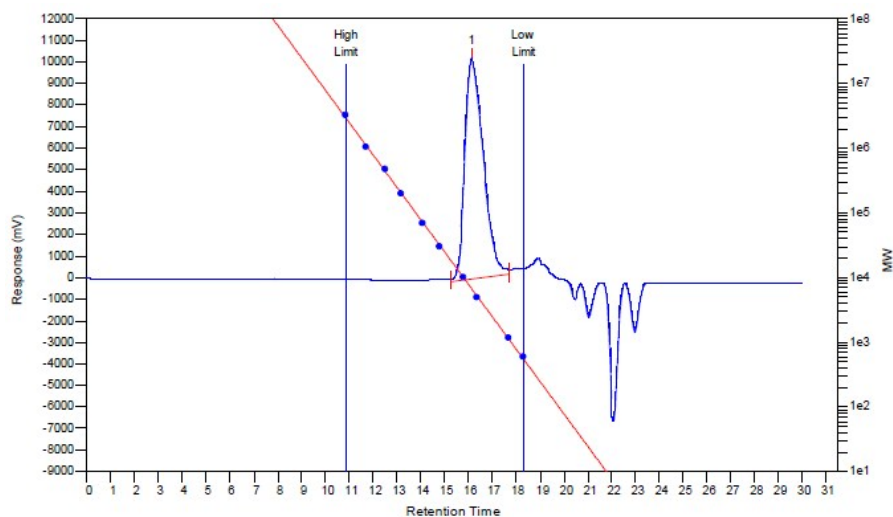


Figure S11. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl-OH in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-OH} = 50/1/1$.

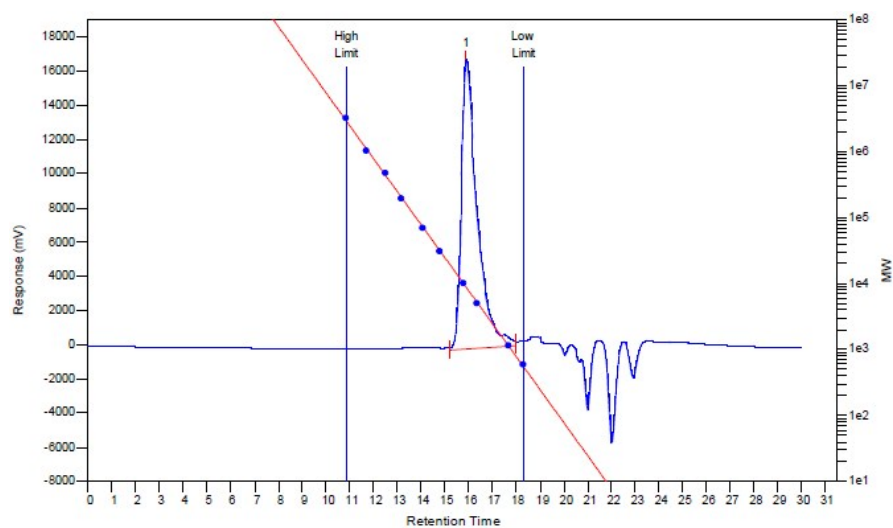


Figure S12. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and benzyl-OH in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/\text{benzyl-OH} = 50/1/1$.

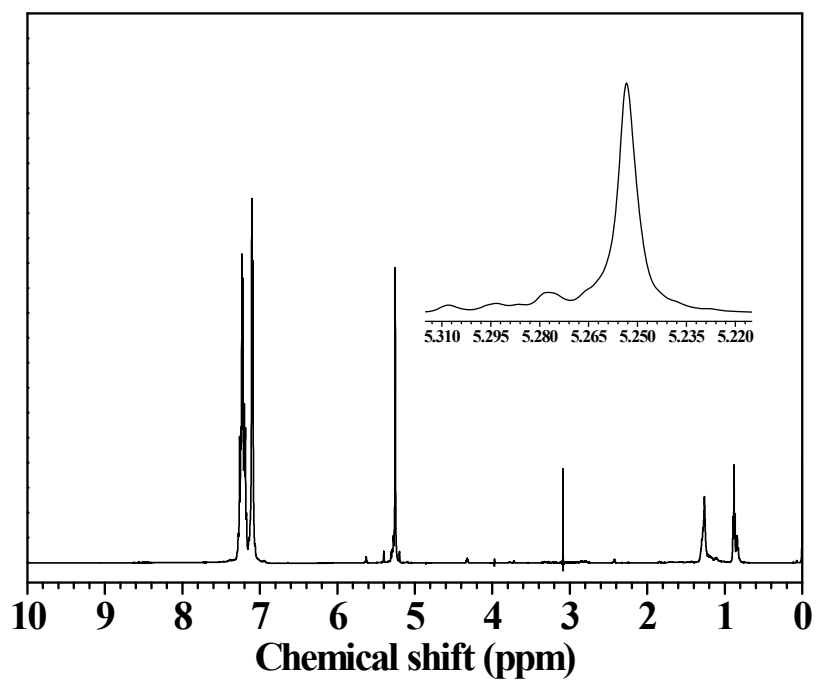


Figure S13. Homonuclear decoupled ¹H NMR spectrum of Poly(1) mediated by Zn(C₆F₅)₂ and 1-hexyl-amine at the feeding ratio of 50/1/1.

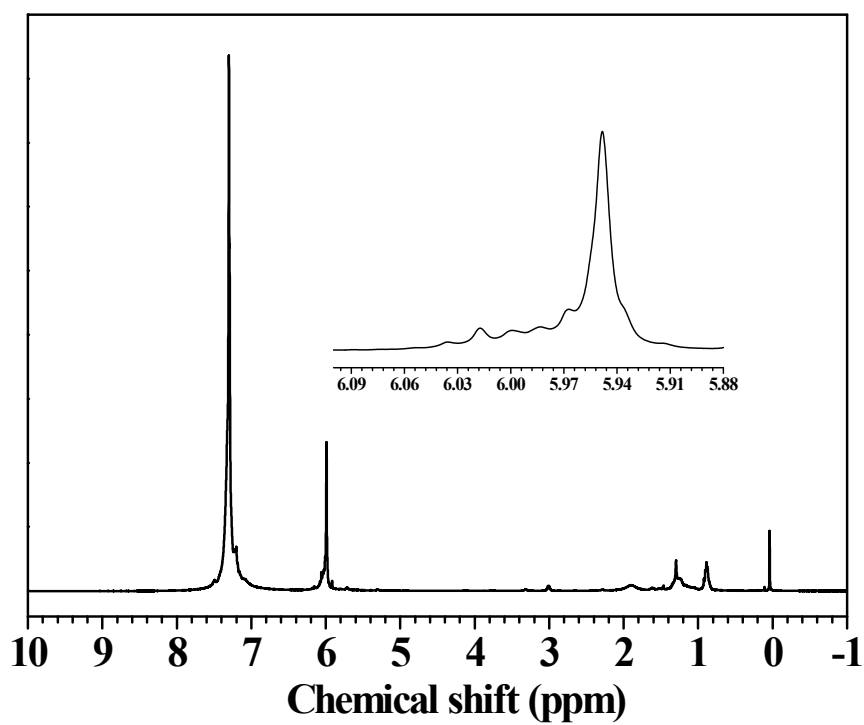


Figure S14. ¹H NMR spectrum of Poly(2) mediated by Zn(C₆F₅)₂ and 1-hexyl-amine at the feeding ratio of 50/1/1.

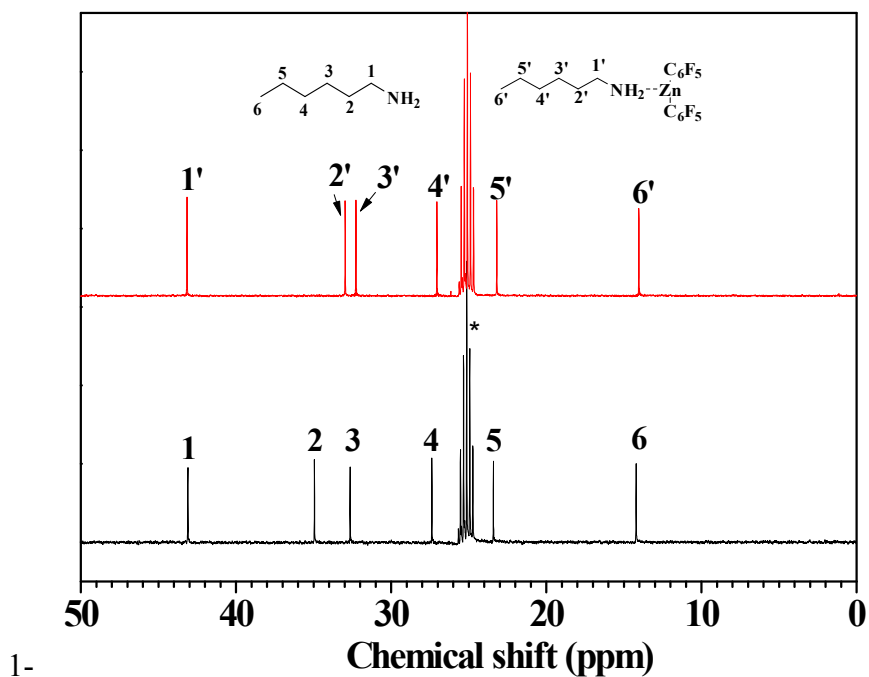


Figure S15. ^{13}C NMR spectra of 1-hexyl- NH_2 before and after the addition of $\text{Zn}(\text{C}_6\text{F}_5)_2$ at 25 °C. The peaks marked as asterisk were deuterated THF.

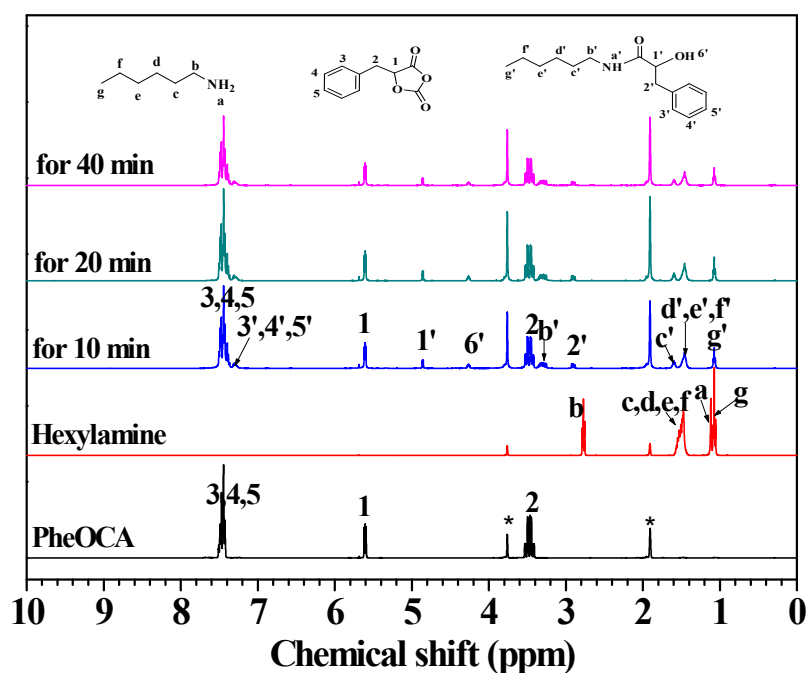


Figure S16. ^1H NMR spectra of the ring-opening of Phe-OCA initiated by 1-hexyl- NH_2 alone at 25 °C. The peaks marked as asterisk were deuterated THF.

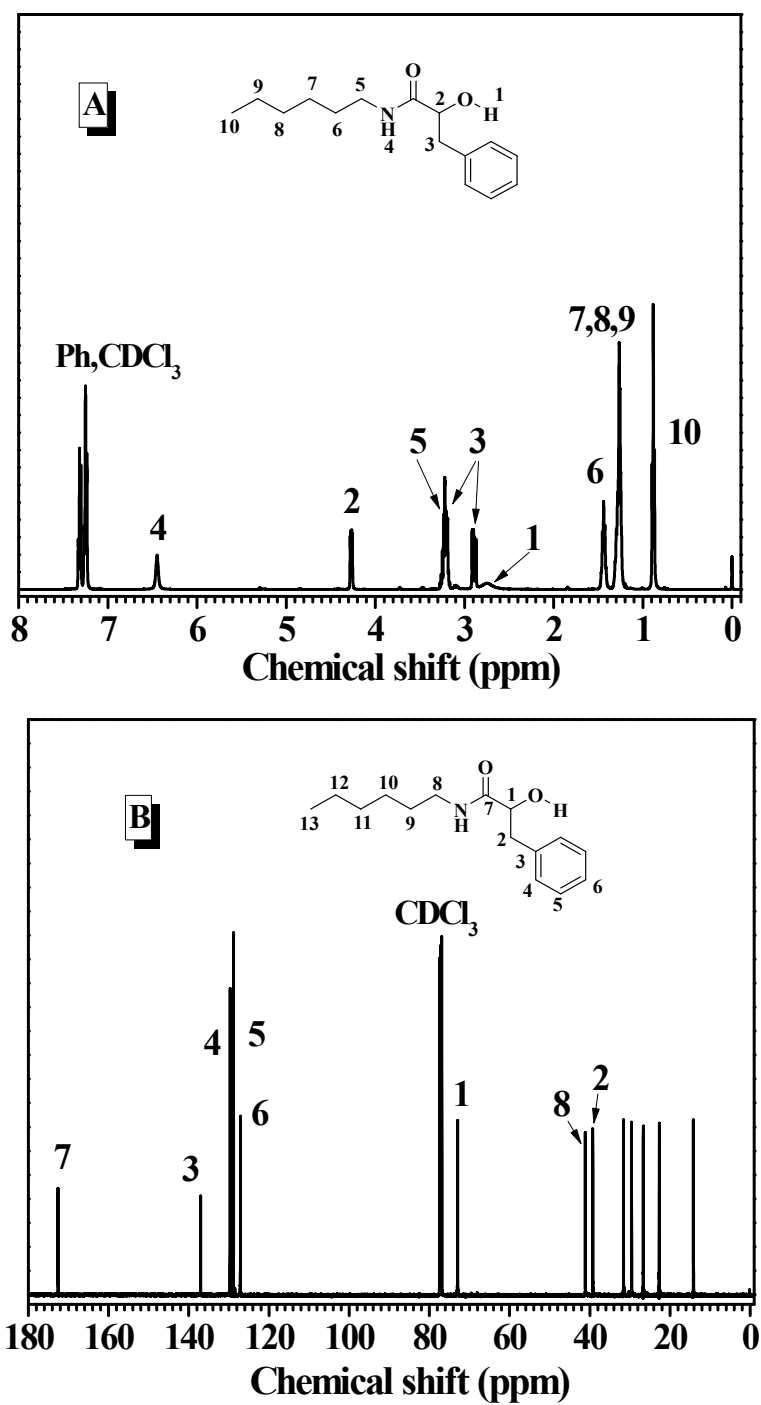


Figure S17. NMR spectra of *N*-hexyl-2-hydroxy-3-phenyl-propanamide (Comp 1). (A) ^1H NMR spectrum; (B) ^{13}C NMR spectrum.

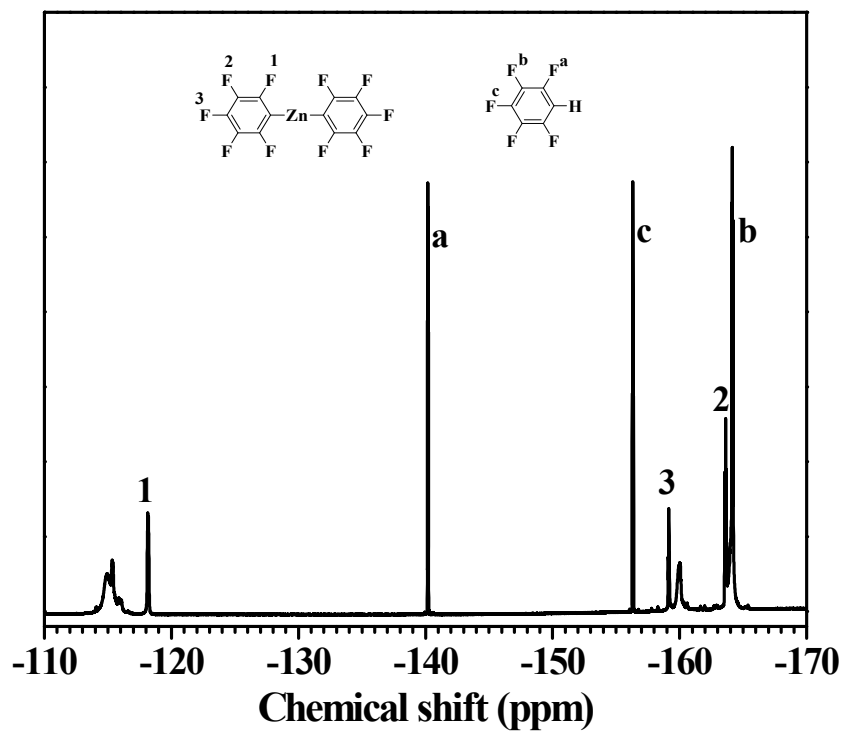


Figure S18. ^{19}F NMR spectrum of $\text{Zn}(\text{C}_6\text{F}_5)_2$ after adding Comp 1 with molar ratio of 1 to 1.

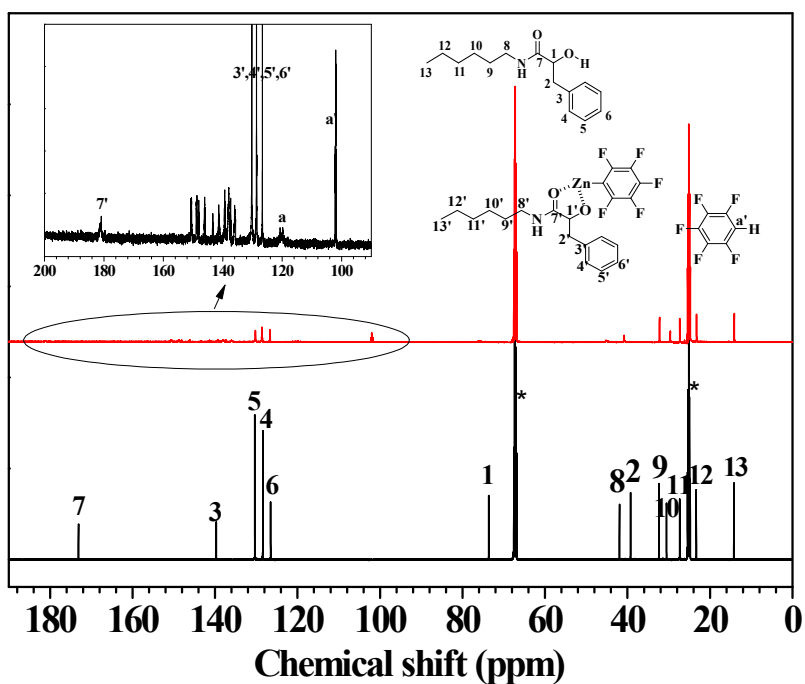


Figure S19. ^{13}C NMR spectra of Comp 1 before and after adding $\text{Zn}(\text{C}_6\text{F}_5)_2$ with molar ratio of 1 to 1. The peaks marked as asterisk were deuterated THF.

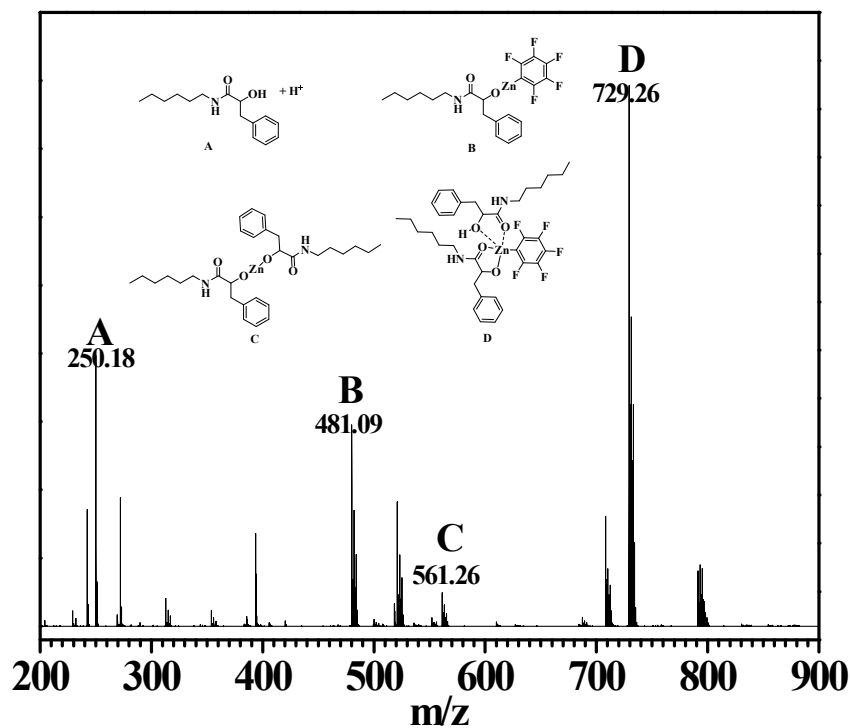


Figure S20. Electrospray ionization mass spectrum (ESI-MS) of Comp-1 complexing with $\text{Zn}(\text{C}_6\text{F}_5)_2$ with molar ratio of 1 to 1.

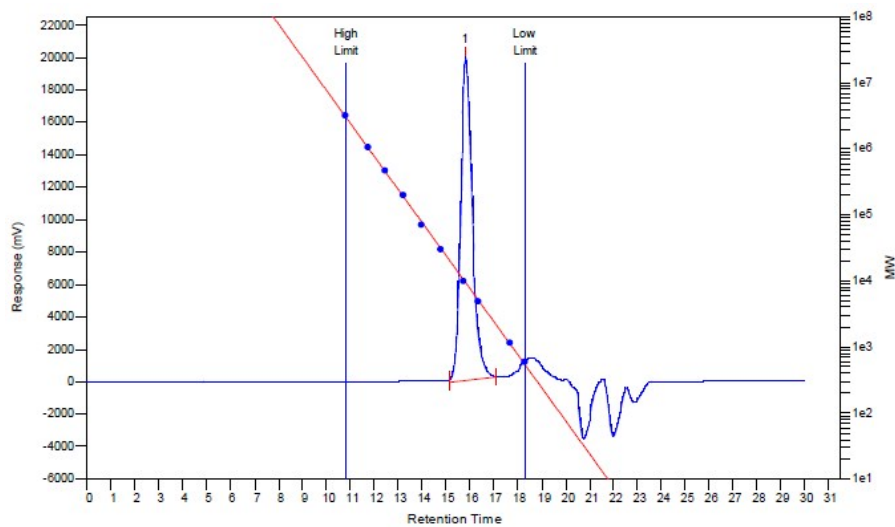


Figure S21. GPC curve of the resulting ROP of Phe-OCA in the presence of Comp-1 and $\text{Zn}(\text{C}_6\text{F}_5)_2$. $[\text{Phe-OCA}]:[\text{Zn}(\text{C}_6\text{F}_5)_2]:[\text{Comp-1}] = 50:1:1$.

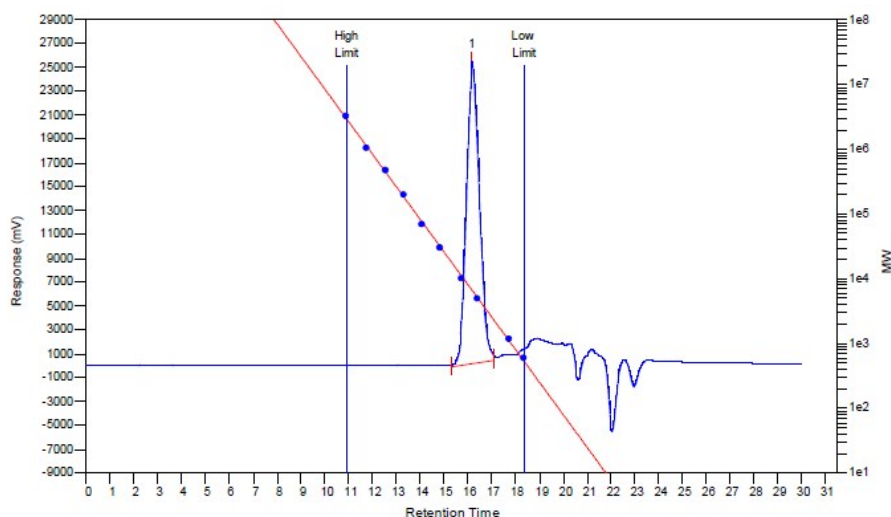


Figure S22. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/0.5/1$.

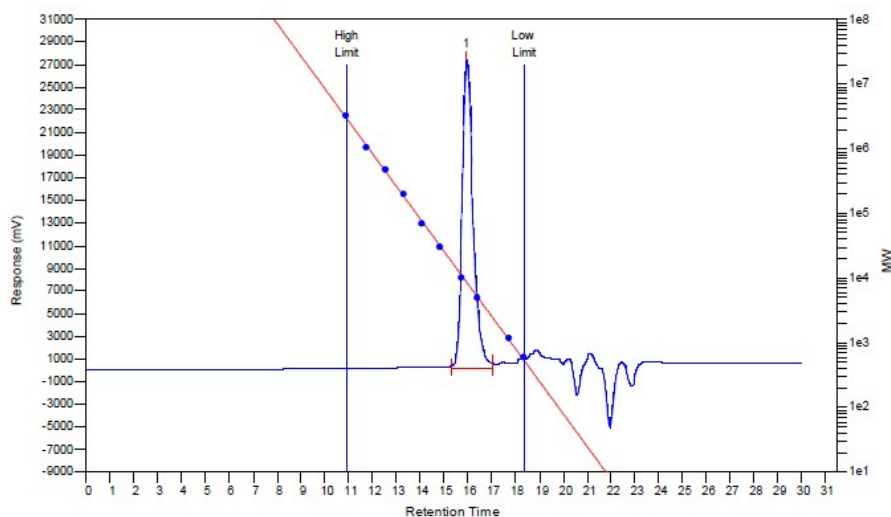


Figure S23. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/1.5/1$.

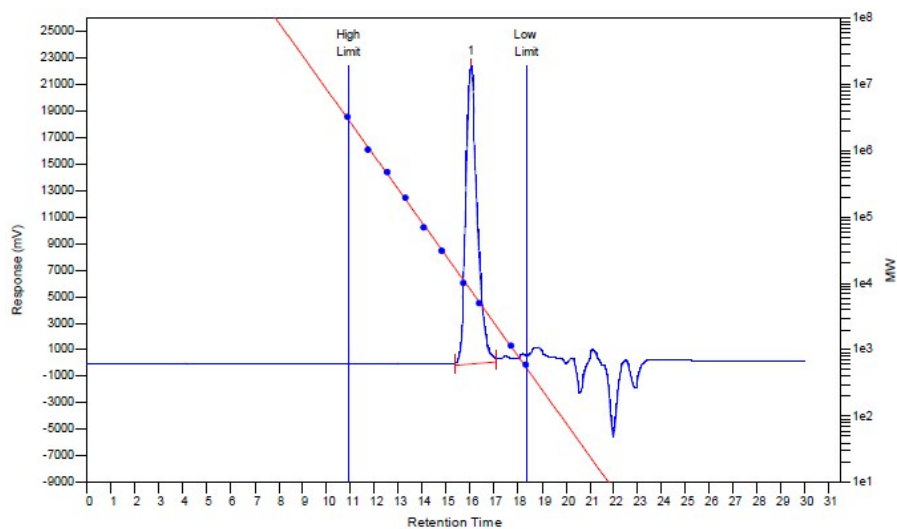


Figure S24. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/2.0/1$.

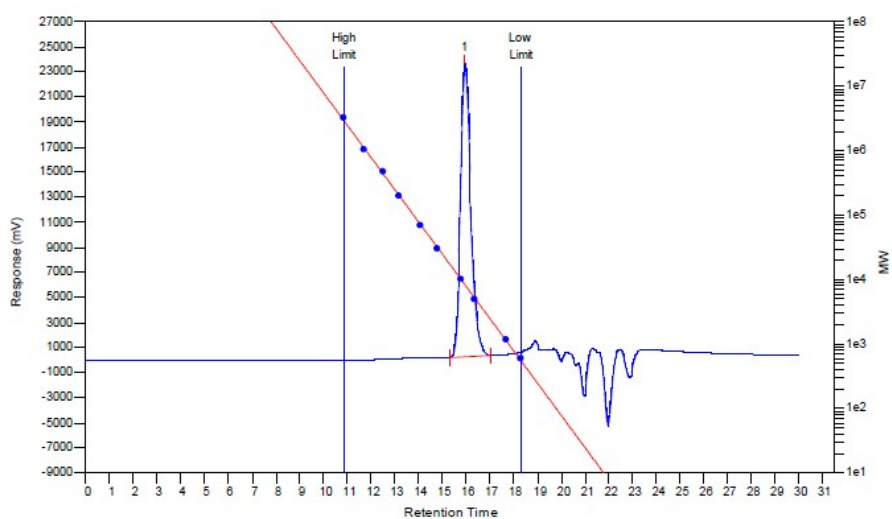


Figure S25. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/5.0/1$.

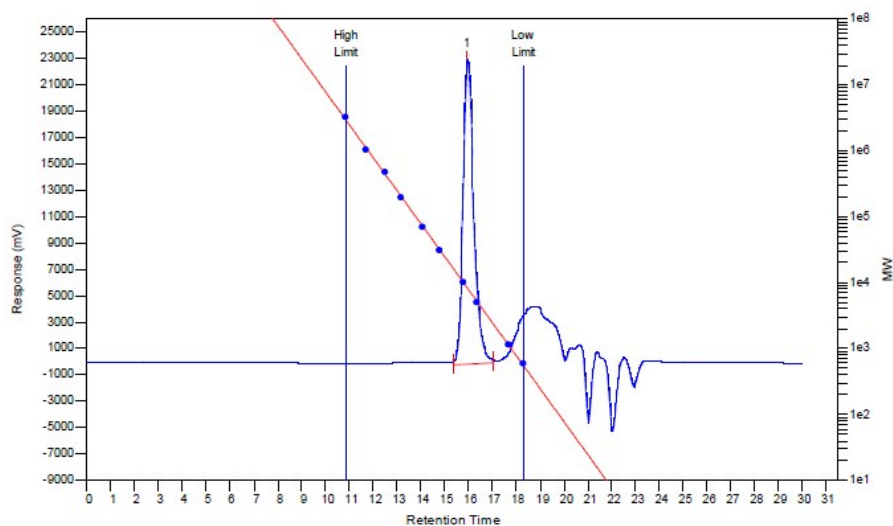


Figure S26. GPC curve of Phe-OCA polymerization in the presence of $\text{Zn}(\text{C}_6\text{F}_5)_2$ and 1-hexyl- NH_2 in THF at 50 °C. $[\text{Phe-OCA}] = 0.75 \text{ M}$ and $\text{Phe-OCA}/\text{Zn}(\text{C}_6\text{F}_5)_2/1\text{-hexyl-NH}_2 = 50/10.0/1$.

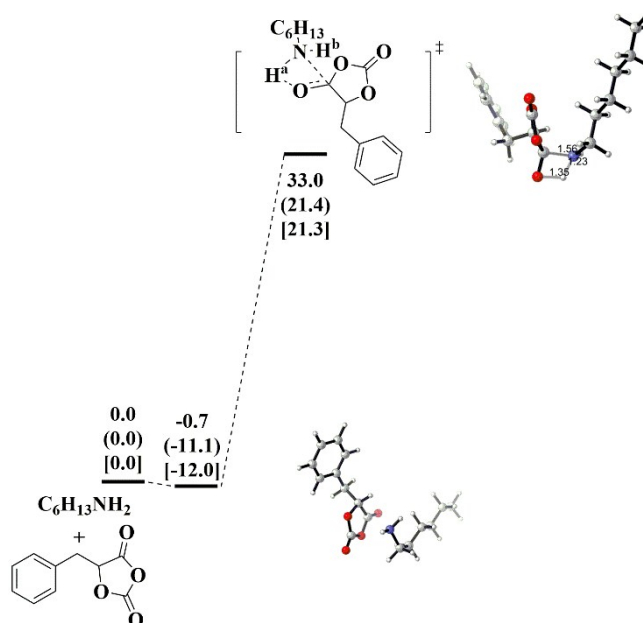


Figure S27. Energy profile of 1-hexyl- NH_2 alone nucleophilically attacking Phe-OCA and the corresponding optimized structures.

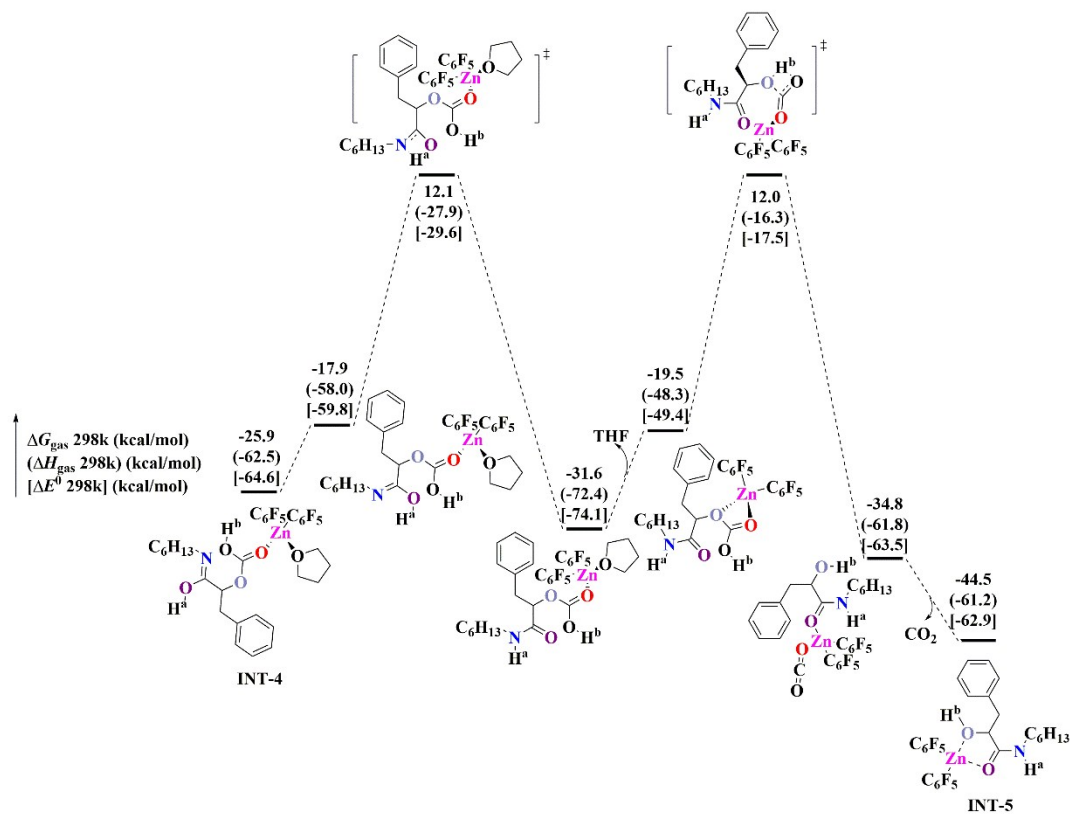
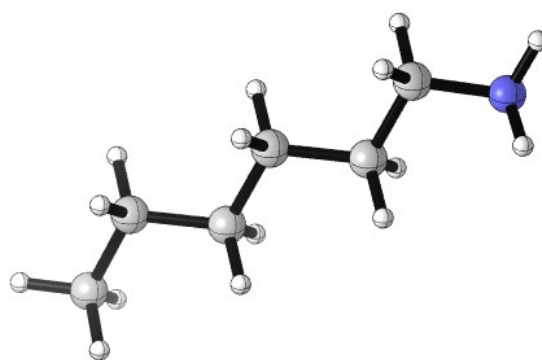


Figure S28. DFT computation of acy-oxygen cleavage and decarboxylation.

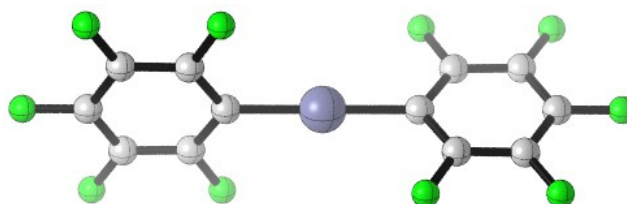
Coordinates of All Stationary Points



1-hexyl-NH₂

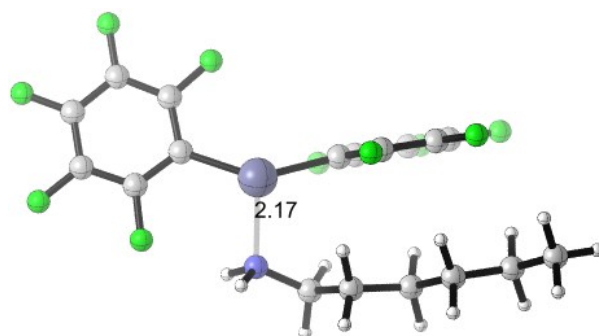
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H	3.80596500	-0.97354900	-0.95966000	H	4.69342900	0.25857500	-0.05696200
C	2.52701000	0.49891700	-0.00700000	H	2.54283300	1.12977400	0.88842300
H	2.50769800	1.18038400	-0.86448900	C	1.25152300	-0.34085600	-0.00507700

H 1.23545800	-0.97540300	-0.89971800	H 1.26814500	-1.02200900	0.85429000
C -0.02240400	0.49935300	0.04178700	H -0.03837900	1.17847700	-0.81931200
H -0.00319300	1.13485200	0.93558100	C -1.29342100	-0.34570800	0.05103600
H -1.31612900	-0.97759400	-0.84604000	H -1.29155400	-1.02308400	0.91074000
C -2.56217000	0.49503000	0.10073400	H -2.56005200	1.19811800	-0.74596800
H -2.55759400	1.09627700	1.01495500	N -3.74395000	-0.36736800	0.13787200
H -4.59290600	0.18018700	0.21672900	H -3.81548000	-0.90415600	-0.72004400



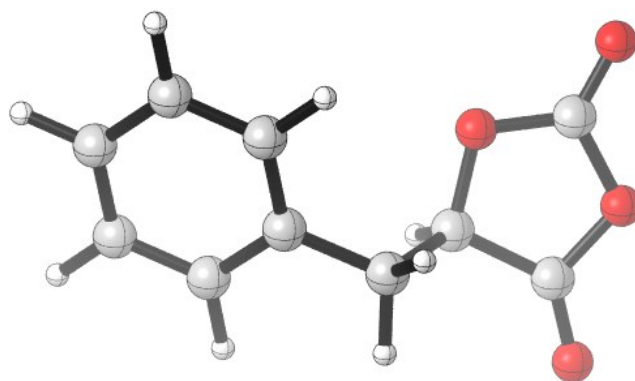
Zn(C₆F₅)₂

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F -4.75168800	-1.66865300	-1.65156000	F -2.05220500	-1.67184400	-1.65554600
F 2.05209200	1.67129100	-1.65632700	F 4.75155500	1.66899400	-1.65160000
F 6.09630700	0.00015400	0.00207300	F 4.74931000	-1.66916100	1.65355600
F 2.04977900	-1.67193700	1.65404600	C -1.96794500	-0.00006300	-0.00061200
C -2.69570700	0.83586000	0.82726100	C -4.08056000	0.85538900	0.84687500
C -4.77285900	0.00058200	0.00088500	C -4.08186200	-0.85456500	-0.84582900
C -2.69699500	-0.83568400	-0.82764700	C 1.96794700	-0.00033100	-0.00122000
C 2.69690600	0.83541800	-0.82820200	C 4.08177500	0.85473300	-0.84599400
C 4.77285600	-0.00006100	0.00099900	C 4.08064600	-0.85505500	0.84687800
C 2.69579500	-0.83597200	0.82687000			



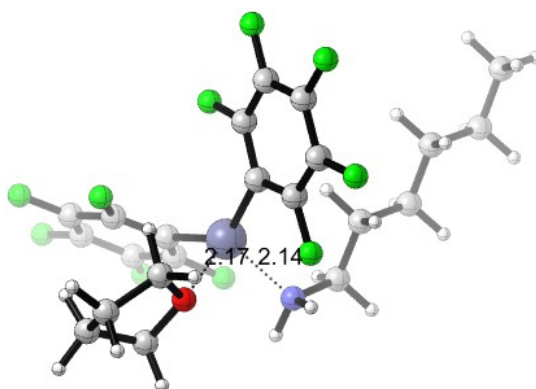
FLP

Zn	-0.79889800	0.40388400	-0.25266100	C	0.97821400	-0.62501000	-0.15604600
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C	3.23243000	-1.26109500	-0.85356100	F	4.20632000	-1.21769600	-1.76226800
C	3.44320600	-1.92085900	0.34703000	F	4.60478800	-2.51870500	0.58559800
C	2.43866500	-1.93984000	1.30313800	F	2.64427600	-2.55615700	2.46400000
C	1.24418800	-1.29220000	1.02531500	F	0.31108600	-1.29582300	2.00109300
C	-2.80266900	0.08806400	-0.08671300	C	-3.37222900	-1.12956600	-0.40559700
F	-2.58173200	-2.17965300	-0.69084100	C	-4.74036800	-1.33728900	-0.48977300
F	-5.24710100	-2.52501800	-0.81452800	C	-5.59635700	-0.27358300	-0.24492500
F	-6.91152300	-0.44350600	-0.32758000	C	-5.07427100	0.96826800	0.08075700
F	-5.89480300	1.99622400	0.29855900	C	-3.69782200	1.10927700	0.15028100
F	-3.23830000	2.35751500	0.43406800	C	6.67087100	1.21967300	-1.24799000
C	5.68207200	1.25639600	-0.08649600	C	4.37694900	1.95807400	-0.45438900
C	3.36622100	1.96663800	0.68939900	C	2.00287200	2.51456000	0.27123000
C	0.95043900	2.34987400	1.36311000	N	-0.40738500	2.27588600	0.77295200
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H	3.23046700	0.94010100	1.05241000	H	2.08656700	3.56963400	-0.01466800
H	1.67252600	1.97314300	-0.62119700	H	1.01851900	3.16332300	2.09176600
H	1.11678900	1.41225600	1.89952500	H	-1.12482600	2.33530000	1.49261900
H	-0.57546800	3.07657600	0.16654900				



Phe-OCA

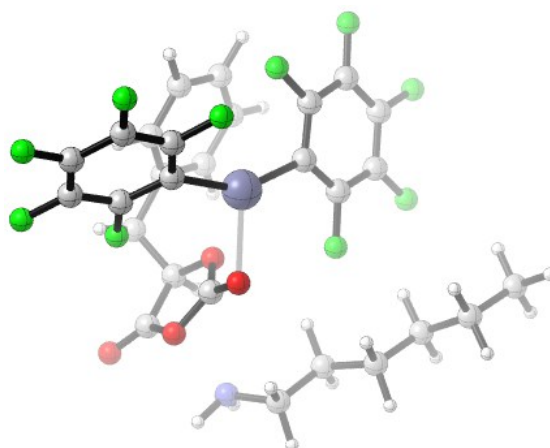
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H	-0.05932700	-1.95267000	0.86002900	C	0.93690300	-0.51374200	-0.33860800
H	0.59080200	-0.85223100	-1.31842100	O	3.16887400	-0.01519000	0.01801900
C	2.47741600	1.15919600	-0.19078000	C	2.31208600	-1.07978100	-0.05086900
O	2.63870000	-2.20428400	0.11205400	O	2.97507700	2.22522800	-0.17788500
O	1.17826900	0.89264400	-0.40147300	C	-1.45950000	-0.38076700	0.40337200
C	-1.82988900	0.94211000	0.64533300	C	-2.37583600	-1.24293700	-0.19788400
C	-3.09678200	1.39327700	0.29349600	H	-1.12035300	1.62115700	1.10564500
C	-3.64357900	-0.79292900	-0.55084500	H	-2.09939500	-2.27630000	-0.38320100
C	-4.00594800	0.52715600	-0.30572700	H	-3.37367000	2.42257700	0.48810300
H	-4.34866900	-1.47461000	-1.01153300	H	-4.99373400	0.87879000	-0.57812400



INT-1

Zn	-0.39543700	-0.14341900	-0.59919000	C	1.23820700	-1.08333200	0.21392300
C	2.17300500	-1.69031800	-0.59913500	F	2.00636900	-1.65276500	-1.94889200

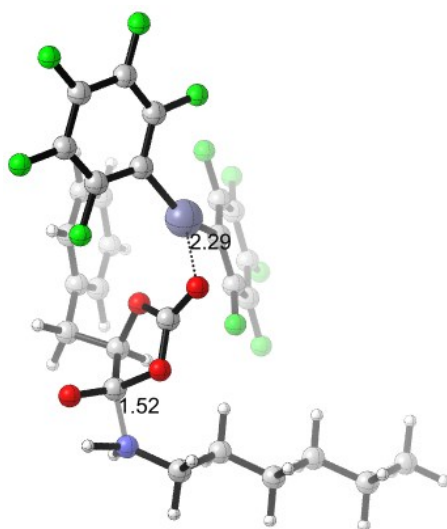
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C 3.51363300	-2.40514300	1.23375400	F 4.58337700	-3.02941600	1.71538500
C 2.60794800	-1.80770100	2.09726000	F 2.82084200	-1.86579700	3.41015300
C 1.49744700	-1.16434200	1.56853400	F 0.65425000	-0.59492000	2.44697000
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F -2.47065900	-1.34507600	1.35539800	C -4.08664600	0.32149800	1.57126800
F -4.79483700	-0.45461200	2.38945400	C -4.55891100	1.58354600	1.24206900
F -5.70919200	2.01642200	1.74646500	C -3.82995100	2.38870800	0.38044000
F -4.29183600	3.59582000	0.05833800	C -2.63357800	1.90625900	-0.12941800
F -1.96901400	2.72148500	-0.98323300	C -1.04009500	-3.10908600	-1.19048500
O -1.26770600	-1.77991900	-1.72889100	C -2.60551400	-1.68392400	-2.25956800
C -3.36303200	-2.83281200	-1.61377600	C -2.27986000	-3.91431200	-1.56522000
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H -2.99693100	-0.69671800	-2.00927400	H -2.55353500	-1.79742400	-3.34717600
H -3.66894700	-2.55488600	-0.60243600	H -4.24353600	-3.12464400	-2.18560800
H -2.48595200	-4.69928200	-0.83851100	H -2.15854200	-4.37389800	-2.54926600
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C 4.05282900	3.14054900	-0.08266300	C 2.94665700	3.25794900	-1.12901200
C 2.09569300	1.99439700	-1.22114600	C 0.96378500	2.13418600	-2.22831700
N 0.23218000	0.85177000	-2.38833400	H 5.59254600	4.09398100	2.05314900
H 6.67658700	3.40906600	0.83998800	H 6.64379700	5.15439800	1.10947300
H 4.29680600	5.25449300	0.23751100	H 5.37802900	4.58412700	-0.97134600
H 4.68187600	2.27303600	-0.31634500	H 3.60416900	2.94041100	0.89770500
H 3.39322400	3.47089800	-2.10771000	H 2.30560800	4.11359900	-0.88579700
H 2.72871900	1.14118000	-1.49537700	H 1.67879900	1.76391300	-0.23377200
H 1.35872000	2.47020000	-3.19303900	H 0.24357800	2.87753000	-1.88253800
H -0.56975200	0.99133300	-2.99813000	H 0.83244200	0.16774600	-2.84749200



INT-2

Zn	0.71130900	0.50289400	-0.85609100	C	-0.90340800	1.56261300	-0.47173800
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C	-3.26997400	1.80039300	0.07199100	F	-4.49602200	1.27499700	0.15610000
C	-3.06946400	3.12246100	0.44759500	F	-4.08876600	3.84953200	0.89473900
C	-1.79986700	3.67588100	0.36469900	F	-1.59322200	4.93134400	0.76580600
C	-0.75575900	2.88653700	-0.09693500	F	0.45949000	3.45978700	-0.13114100
C	2.68636900	0.34209600	-0.92360400	C	3.45055700	1.19583900	-1.69956900
F	2.85110100	2.17073200	-2.40294500	C	4.83385000	1.10693300	-1.80202300
F	5.52783800	1.95256900	-2.55981500	C	5.49645000	0.10933700	-1.09836200
F	6.81836400	0.00129700	-1.17966200	C	4.77443300	-0.77809300	-0.30942600
F	5.40585700	-1.73432700	0.36956000	C	3.39639000	-0.63426100	-0.25321900
F	2.72903800	-1.52708300	0.53096100	C	0.90905700	-1.58901000	2.93391800
C	0.02631200	-2.28947900	1.89320800	O	0.69705400	-3.35689800	-0.07960900
C	0.28283400	-2.11923300	-0.35540700	C	0.62679400	-3.55380400	1.30988400
O	1.05900900	-4.51849800	1.83908400	O	0.31269300	-1.59023300	-1.44184600
O	-0.13424200	-1.47103100	0.72605300	C	0.62535200	-0.10357900	2.95199900
C	1.59055700	0.79174600	2.48667400	C	-0.61705200	0.39018900	3.35685300
C	1.32753400	2.15973400	2.44071400	C	-0.88589300	1.75463500	3.30288200
C	0.08701600	2.64300100	2.84679200	H	1.96175800	-1.76319400	2.70268300
H	0.70221000	-2.05531700	3.90255700	H	-0.97349900	-2.51398600	2.26976500
H	2.55852600	0.41514100	2.16793000	H	-1.38062500	-0.29581800	3.71776600

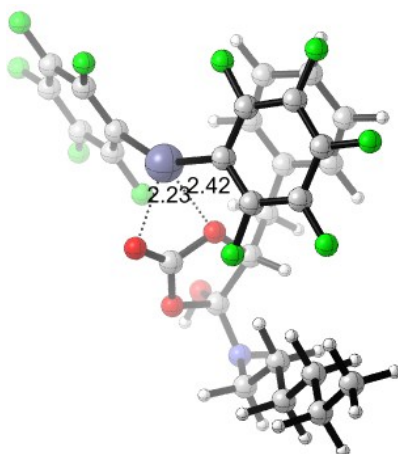
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C -5.48342800	-0.73383100	-2.63356400	C -5.14646100	-1.58816100	-1.41437200
C -4.01398900	-2.58067100	-1.67079700	C -3.46254200	-3.17317600	-0.37749000
C -2.40884200	-4.24448000	-0.61443800	N -1.75671100	-4.60283900	0.65243600
H -7.54634900	-0.31005700	-2.09695600	H -6.38601700	0.90385200	-1.53997200
H -6.85803800	0.84578900	-3.24632300	H -5.72746100	-1.38388300	-3.48412400
H -4.58672600	-0.16930700	-2.92191400	H -4.86158600	-0.92586200	-0.58933600
H -6.04280600	-2.13210500	-1.08448200	H -3.19663800	-2.07267600	-2.19907200
H -4.36477900	-3.38320700	-2.33440500	H -3.02042600	-2.36786500	0.22326200
H -4.28404600	-3.59882300	0.21775500	H -1.63724500	-3.86021400	-1.29449300
H -2.86892100	-5.10706200	-1.12010500	H -2.46932100	-4.90963600	1.31397100
H -1.14682200	-5.40796800	0.51340600			



TS-1

Zn 1.15129500	0.22359800	-0.92971600	C -0.24919200	1.63960500	-0.66188600
C -1.59632600	1.37610900	-0.49300500	F -2.08426300	0.13342400	-0.75007500
C -2.52580600	2.31047500	-0.05896600	F -3.81362300	1.98406500	0.10462300
C -2.09456900	3.60177700	0.21439400	F -2.95872300	4.52022700	0.64469100
C -0.75501300	3.92607000	0.04726800	F -0.33393100	5.15768900	0.34274400
C 0.12917200	2.94306500	-0.38151200	F 1.42170700	3.29852500	-0.49123800
C 3.07467300	-0.31834300	-0.93384600	C 4.04991200	0.42496400	-1.57850500

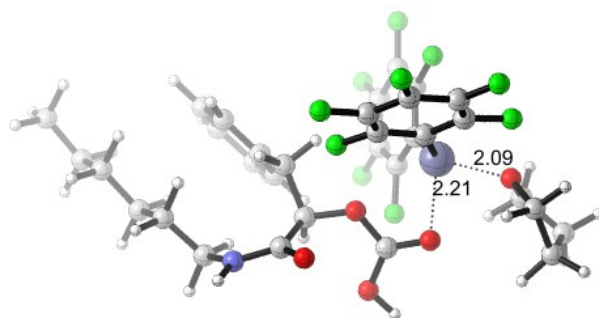
F 3.70535600	1.54805400	-2.23684800	C 5.39424200	0.07310200	-1.59590200
F 6.30016500	0.81716400	-2.23276800	C 5.79378100	-1.08052100	-0.93271700
F 7.07572900	-1.43991600	-0.93279400	C 4.85270700	-1.85952700	-0.27031600
F 5.23911900	-2.96603200	0.36782100	C 3.52275200	-1.45926600	-0.28888800
F 2.64207700	-2.24181500	0.37304500	C -0.32163600	-1.25012300	2.96136700
C -1.02801900	-1.51442800	1.64608400	O -1.19034200	-2.97864200	-0.16851800
C -0.37384100	-1.99350700	-0.47382300	C -1.37178400	-2.98536500	1.32282800
O -0.73827800	-3.94506600	1.93811600	O 0.12392500	-1.73040700	-1.54745200
O -0.11609000	-1.21163700	0.58294800	C 0.24567700	0.15281100	2.92454900
C 1.56414100	0.35872400	2.50630800	C -0.55973800	1.26150700	3.19549600
C 2.07072800	1.65049200	2.36955400	C -0.05278300	2.55460200	3.06817200
C 1.26385700	2.75135700	2.65502700	H 0.46167800	-2.00308100	3.08584600
H -1.03921600	-1.36918200	3.78104100	H -1.90287200	-0.86198300	1.51410000
H 2.19012000	-0.50046600	2.27577400	H -1.58995200	1.11597700	3.51598100
H 3.09257300	1.79635000	2.03189100	H -0.68685200	3.40856300	3.28935200
H 1.65464600	3.75771900	2.53992100	C -7.40859500	0.44130700	-3.00060900
C -6.91676300	-0.94017400	-2.57459400	C -5.86768100	-0.87115300	-1.46678900
C -5.36873500	-2.24809400	-1.03197500	C -4.31313500	-2.16355400	0.06937800
C -3.80341200	-3.53749800	0.47929600	N -2.79097600	-3.46759400	1.55962500
H -7.86097000	0.97213500	-2.15655500	H -6.58000800	1.05306900	-3.37169900
H -8.15748200	0.37240500	-3.79421100	H -7.76607600	-1.54562100	-2.23201800
H -6.49214200	-1.46471100	-3.44020100	H -5.01475700	-0.26823200	-1.80623000
H -6.28851600	-0.34398400	-0.59904500	H -4.94333200	-2.77095400	-1.89910100
H -6.21756800	-2.85420100	-0.68579500	H -3.47531300	-1.55326100	-0.28241200
H -4.73887900	-1.65184100	0.94532900	H -3.34130500	-4.05696900	-0.36230500
H -4.61659900	-4.16294300	0.86070700	H -3.17172400	-2.98952800	2.37968700
H -2.02135500	-4.35695400	1.94216000			



INT-3

Zn	0.97352700	0.53920400	-0.98266400	C	-0.56965600	1.74922900	-0.72372600
C	-1.89080500	1.34330300	-0.79376200	F	-2.19395400	0.11114100	-1.26158600
C	-2.96119900	2.13543500	-0.40040500	F	-4.22300900	1.70310400	-0.49062200
C	-2.70586000	3.40572000	0.10074300	F	-3.71249500	4.17846600	0.50108000
C	-1.39774800	3.85993900	0.18884300	F	-1.14364300	5.06267200	0.70730600
C	-0.36965300	3.02757500	-0.23386900	F	0.87919900	3.51057600	-0.11181300
C	2.90536700	0.10885600	-0.84127500	C	3.88875100	0.92960300	-1.36449400
F	3.54572700	2.07402100	-1.97921700	C	5.24726900	0.64416800	-1.28940300
F	6.16006600	1.46774200	-1.80199100	C	5.65214400	-0.52936200	-0.66775500
F	6.94549200	-0.82566500	-0.57801400	C	4.70328100	-1.39299000	-0.13455800
F	5.09005000	-2.51961900	0.46408400	C	3.36314300	-1.05077500	-0.24158300
F	2.47699400	-1.92202700	0.30481500	C	0.27435500	-1.60964900	2.60849300
C	-0.59615900	-1.96136000	1.40828600	O	-0.29328900	-3.19159400	-0.57841500
C	-0.01994900	-1.92048500	-0.80152600	C	-0.50412000	-3.41664700	0.84697300
O	0.59387500	-4.01789100	1.39917900	O	0.33982100	-1.41901700	-1.84228500
O	-0.17396800	-1.16920700	0.28766300	C	0.33602300	-0.10392600	2.74108100
C	1.49842900	0.57281500	2.36549700	C	-0.78265700	0.63768100	3.12654500
C	1.54497100	1.96495700	2.37262600	C	-0.74038000	2.02962900	3.13229700
C	0.42254800	2.69662500	2.75267200	H	1.27285300	-2.02507900	2.46384600
H	-0.16189500	-2.07951100	3.49749800	H	-1.63893500	-1.69893600	1.59955200
H	2.37181200	0.00041200	2.06477000	H	-1.69668300	0.12494500	3.42044500

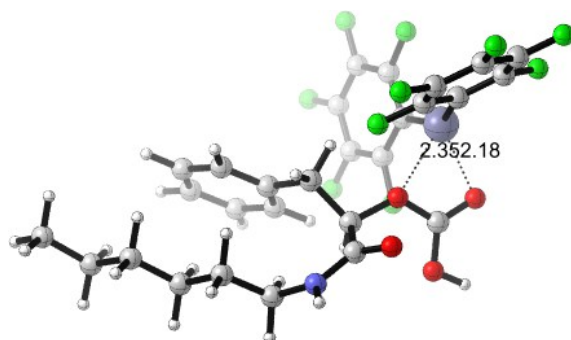
H 2.44967800	2.47693900	2.05978300	H -1.61965300	2.59594800	3.42482000
H 0.44423400	3.78207000	2.72488200	C -7.21488200	0.13546100	-1.76766900
C -6.60480200	-1.26377200	-1.74294300	C -5.37601900	-1.33450200	-0.84051400
C -4.73156500	-2.71740800	-0.79299600	C -3.49649800	-2.74254700	0.10596000
C -2.78721000	-4.09560400	0.06264800	N -1.63276900	-4.28609200	0.94788500
H -7.54701600	0.43260800	-0.76720300	H -6.47762900	0.87320400	-2.10099500
H -8.07742600	0.18840200	-2.43812700	H -7.35319200	-1.99152100	-1.40260400
H -6.32232800	-1.56357200	-2.76038700	H -4.63137500	-0.60740600	-1.18388900
H -5.65572700	-1.02582700	0.17718000	H -4.44351500	-3.01897300	-1.80956900
H -5.46019800	-3.46143300	-0.44211800	H -2.81971500	-1.94265000	-0.22153100
H -3.79198200	-2.50864700	1.13951000	H -2.45340500	-4.30133100	-0.95829200
H -3.49568200	-4.88863000	0.32454900	H -1.89929900	-4.37490000	1.92464600
H 0.55661000	-4.95340500	1.13533500			



INT-4

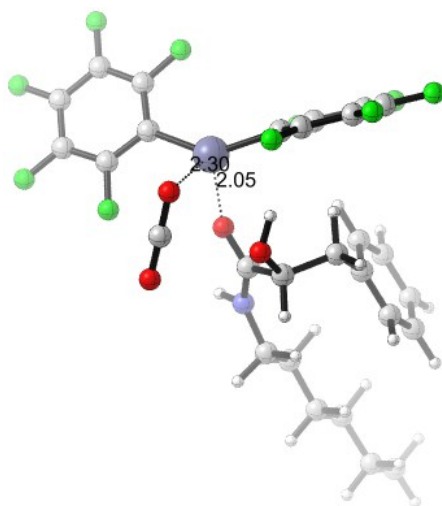
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C 0.00620500	2.57053700	-0.23192500	F -0.03897400	2.36670700	-1.57885400
C -0.96292300	3.43316500	0.26231700	F -1.86563300	4.00001200	-0.54699000
C -1.00929900	3.67481500	1.62710500	F -1.94195200	4.47884800	2.13193300
C -0.07467300	3.07211600	2.45831900	F -0.11204300	3.30585500	3.77002900
C 0.87721100	2.22884000	1.89548200	F 1.75564600	1.66679400	2.74712800
C 2.88827200	-1.26096700	0.65000400	C 4.19334900	-1.49135300	1.05023000
F 5.10602700	-0.49848400	0.96396000	C 4.65537300	-2.69928800	1.55748300
F 5.92920000	-2.86118700	1.92227400	C 3.76003400	-3.75132400	1.68778600
F 4.16690300	-4.92213800	2.17524000	C 2.43514300	-3.57413600	1.31469700

F 1.56943900	-4.58048800	1.45270800	C 2.03663200	-2.34168300	0.81210500
F 0.72852400	-2.23662700	0.49750700	C 4.95336100	0.94805300	-1.49423500
O 3.96842200	1.63354900	-0.68629700	C 3.64359900	2.91422600	-1.26626300
C 4.74050200	3.17029100	-2.29108300	C 5.03320900	1.75096400	-2.78536900
H 5.89588200	0.94802900	-0.94086800	H 4.61926000	-0.08315400	-1.63186300
H 2.65737900	2.83982200	-1.73977900	H 3.59901400	3.64364700	-0.45515400
H 4.41654600	3.84998900	-3.08204800	H 5.62495500	3.59610200	-1.80649800
H 4.25085700	1.42224800	-3.47627000	H 6.00405900	1.65167700	-3.27533300
C -1.71924800	-0.75375700	-0.02554000	C -1.18804000	-0.70422500	-1.47047300
O 0.25790000	0.03718100	-3.55295000	C 0.89695800	0.01837100	-2.39694900
C -1.23269900	-2.05739600	-2.20634500	O -0.20484300	-2.64891000	-2.47350000
O 2.06526000	0.34982400	-2.24557200	O 0.18789600	-0.33379100	-1.35774400
C -2.94755300	0.07780100	0.27627700	C -3.19687600	1.30171900	-0.34951300
C -3.81970500	-0.34517100	1.28357100	C -4.29465800	2.07905500	0.01597800
C -4.91762400	0.42706800	1.65162900	C -5.16171100	1.64165800	1.01361200
H -0.89667000	-0.39800100	0.60561500	H -1.88873100	-1.79440500	0.26994300
H -1.68933200	0.06447800	-2.06536200	H -2.51798100	1.68104400	-1.10951200
H -3.63092600	-1.29027600	1.78824300	H -4.45620000	3.03481000	-0.47188200
H -5.58507900	0.07762600	2.43462100	H -6.01673700	2.24640900	1.29891800
C -8.76489900	-1.67827600	1.56398600	C -7.95701100	-1.22263200	0.35229400
C -6.75431100	-2.12237500	0.07772700	C -5.90596400	-1.63582100	-1.09322700
C -4.64430600	-2.47108600	-1.29845200	C -3.75280900	-1.86770000	-2.37918400
N -2.46488500	-2.52807500	-2.52411100	H -9.14358200	-2.69613200	1.42265500
H -8.14426600	-1.67949400	2.46697000	H -9.62185700	-1.02379100	1.74730600
H -8.60063600	-1.19477000	-0.53642000	H -7.59935800	-0.19580700	0.50701700
H -6.12519800	-2.16597900	0.97830200	H -7.09592600	-3.15021900	-0.10947300
H -5.61587700	-0.59018800	-0.91273500	H -6.50900400	-1.63931400	-2.01217500
H -4.07848600	-2.52046100	-0.36012800	H -4.90434600	-3.50446500	-1.56309400
H -3.58483700	-0.81203400	-2.14829700	H -4.26816200	-1.89149900	-3.34731200
H -2.43988300	-3.43336800	-2.97786500	H 0.89090100	0.31307400	-4.23661600



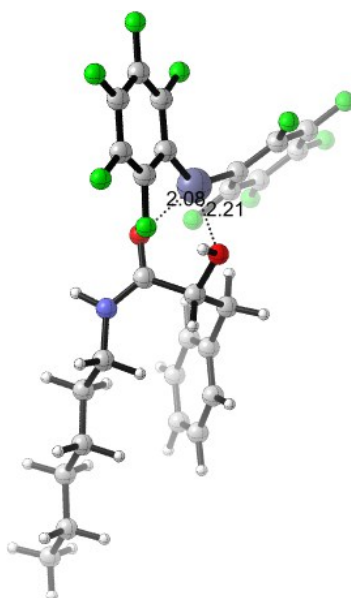
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C	1.04810200	3.63188100	0.70719100	F	2.11596000	3.78064900	1.49651400
C	0.91954100	4.39457000	-0.44454100	F	1.84725700	5.29281000	-0.75824000
C	-0.18606200	4.21342100	-1.26547200	F	-0.31323300	4.94363800	-2.37118400
C	-1.13174500	3.25607100	-0.91733500	F	-2.16558900	3.09895000	-1.76047000
C	-3.45454800	-0.45173300	-0.35899600	C	-4.83622200	-0.40197300	-0.35052900
F	-5.45855000	0.66698800	0.18093900	C	-5.64214300	-1.41164600	-0.85916000
F	-6.97196000	-1.32434800	-0.82864200	C	-5.03684000	-2.53520200	-1.40739600
F	-5.78424100	-3.51892700	-1.90158900	C	-3.65187800	-2.63195700	-1.43954100
F	-3.07462400	-3.70967200	-1.97216500	C	-2.89900700	-1.58975100	-0.91607200
F	-1.55698600	-1.72210900	-0.97983800	C	1.11867300	-0.75276100	-0.16606800
C	0.66980800	-0.98925900	1.28812400	O	-0.52664800	-0.57223600	3.61929800
C	-1.20123800	-0.16734000	2.56469400	C	0.52106000	-2.47575500	1.66349600
O	-0.58195500	-2.95986600	1.82652600	O	-2.26016300	0.43895300	2.58667300
O	-0.63831900	-0.40781000	1.39708400	C	2.45719300	-0.07092400	-0.36215400
C	2.92047200	0.93452600	0.49105800	C	3.21657800	-0.38848800	-1.49206900
C	4.11873900	1.59560000	0.22745700	C	4.41329700	0.27026700	-1.75932100
C	4.87180900	1.26255400	-0.89552200	H	0.34528300	-0.12790100	-0.62817600
H	1.09686900	-1.69941500	-0.71583300	H	1.31327300	-0.47077500	2.00348800
H	2.34090200	1.23570900	1.35976700	H	2.86124100	-1.15845100	-2.17346600
H	4.44940800	2.38314700	0.89693100	H	4.98964400	0.00500200	-2.64127900
H	5.80460000	1.77804600	-1.10131900	C	7.88853100	-2.34162800	-2.42445000
C	7.20820200	-2.06625400	-1.08658800	C	5.87887000	-2.80363800	-0.94328900

C	5.16137800	-2.48601900	0.36507200	C	3.79018100	-3.15111000	0.46233900
C	3.04362000	-2.70011800	1.71366700	N	1.67220600	-3.18048500	1.78773200
H	8.08503300	-3.41159800	-2.55093300	H	7.25251600	-2.02273900	-3.25783700
H	8.84220400	-1.81298500	-2.50894700	H	7.87400600	-2.35488300	-0.26303400
H	7.02795700	-0.98863000	-0.97402400	H	5.22377900	-2.53100000	-1.78321400
H	6.04649800	-3.88691100	-1.02332200	H	5.03608200	-1.39644400	0.44826200
H	5.78674200	-2.79545800	1.21423200	H	3.19169800	-2.89143700	-0.41936300
H	3.89189000	-4.24436500	0.46252500	H	3.03863600	-1.60671600	1.74726600
H	3.57888200	-3.03171400	2.61166000	H	1.51891500	-4.15900600	2.00070900
H	-1.03126000	-0.32073100	4.41237900				



Zn	-1.95059400	0.24777500	0.28750900	C	-3.34720200	-1.03201200	-0.32418800
C	-3.45765100	-2.28977000	0.23964300	F	-2.60356500	-2.66291700	1.22318400
C	-4.40633900	-3.22941200	-0.13942900	F	-4.46886200	-4.43165700	0.43579300
C	-5.30336500	-2.89552600	-1.14574200	F	-6.22793100	-3.77167500	-1.53167800
C	-5.23643100	-1.64528200	-1.74643100	F	-6.10138100	-1.33061300	-2.71093300
C	-4.26243200	-0.74881500	-1.32270900	F	-4.23812400	0.44824100	-1.93344200
C	-1.30553300	2.13402000	0.05125500	C	-0.70721500	2.40752200	-1.16638800
F	-0.64589600	1.43701900	-2.10509300	C	-0.09428100	3.61239800	-1.48011000
F	0.49609900	3.80988500	-2.65710600	C	-0.09170000	4.62336200	-0.52572100
F	0.48778500	5.78907600	-0.79331600	C	-0.68048700	4.40577500	0.71386500
F	-0.65669900	5.36607400	1.63558500	C	-1.27011400	3.17127800	0.96343600

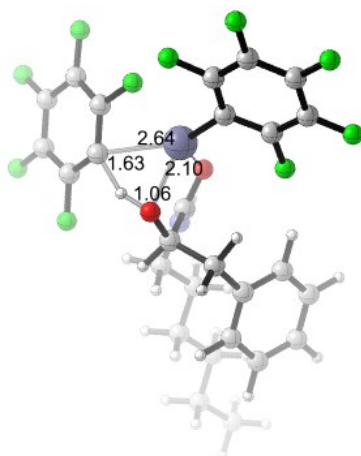
F	-1.75533300	2.97527600	2.20999600	C	2.00797700	1.48718900	1.10771200
C	1.41522500	0.32604400	1.93270200	O	-2.30791600	-0.13067100	2.52790700
C	-1.61764700	-0.95181700	3.00213900	C	0.92798800	-0.82188400	1.04059200
O	-0.22879400	-0.81845600	0.57306700	O	-0.96143600	-1.76780500	3.48991100
O	0.35630700	0.77738500	2.73845300	C	3.05786300	1.12289500	0.08653600
C	4.40688400	1.02529600	0.43986400	C	2.69363700	0.91588700	-1.24759600
C	5.37500300	0.73637500	-0.51930800	C	3.66054200	0.63376100	-2.21018700
C	5.00339600	0.54701600	-1.84935600	H	2.40619300	2.20463700	1.83293600
H	1.17381300	1.97522400	0.59403400	H	2.16660500	-0.05979900	2.62630100
H	4.70353000	1.20312500	1.47208600	H	1.64945000	1.00056000	-1.54249100
H	6.42093200	0.67620200	-0.23164800	H	3.36351100	0.49390100	-3.24472900
H	5.75884600	0.34173800	-2.60167400	C	8.74445600	-3.32757000	-1.54256200
C	7.83461400	-3.02989800	-0.35382700	C	6.36415700	-2.92901900	-0.75258900
C	5.44286300	-2.64410300	0.43024300	C	3.98611800	-2.47223900	0.00971800
C	3.09984300	-2.11347100	1.19641900	N	1.73072900	-1.84712700	0.76658100
H	8.47606900	-4.28055900	-2.01049700	H	8.65655500	-2.54720500	-2.30604100
H	9.79395700	-3.38532900	-1.24087300	H	7.95147600	-3.81162200	0.40761000
H	8.14248300	-2.08913500	0.12193700	H	6.24202600	-2.13128200	-1.49891800
H	6.05287200	-3.86129300	-1.24418200	H	5.77682400	-1.72530900	0.93298800
H	5.52841300	-3.45328700	1.16878300	H	3.90508900	-1.67494000	-0.73776100
H	3.62065000	-3.39663900	-0.45854800	H	3.50004000	-1.22118300	1.67757700
H	3.09086300	-2.92201100	1.93774600	H	1.29625300	-2.54463100	0.16846300
H	-0.15489200	1.45547500	2.26607200				



INT-5

C	1.43059800	0.96989500	1.38304600	C	0.98564800	-0.49115700	1.24461800
C	1.02064200	-0.90983400	-0.22993000	O	0.06245600	-0.58872800	-0.95165600
O	-0.36676600	-0.53272300	1.68410700	C	2.85415500	1.24199600	0.95981300
C	3.92865500	0.84381600	1.76247400	C	3.11567800	1.93525000	-0.22450600
C	5.23873200	1.13683100	1.39261800	C	4.42590700	2.23843000	-0.59158000
C	5.48918200	1.84239200	0.21609700	C	9.59481800	-1.31718500	-0.72992900
C	8.34007900	-1.83772100	-0.03444400	C	7.06187800	-1.48746200	-0.79281700
C	5.80088400	-2.00895000	-0.10948700	C	4.52533900	-1.57032900	-0.82294900
C	3.27982800	-2.04215000	-0.08336900	N	2.06307400	-1.56747100	-0.73477500
Zn	-1.69304000	-0.00009900	-0.00256400	C	-1.92286600	1.98613600	-0.07948300
C	-1.07649000	2.85160400	-0.74760800	C	-2.99897600	2.58881600	0.55027000
C	-1.25653700	4.22710300	-0.80489800	C	-3.24062500	3.95700300	0.52346900
C	-2.35768800	4.77922500	-0.16413100	F	0.01786300	2.36439900	-1.38067700
F	-0.40050300	5.01641100	-1.45754500	F	-2.56238000	6.09393400	-0.20492800
F	-4.29358600	4.49169000	1.14216600	F	-3.87443600	1.83651100	1.24017900
H	1.27703800	1.24147900	2.43270200	H	0.73946200	1.57065400	0.78309900
H	1.59220100	-1.15073500	1.87153600	H	3.73568600	0.32290200	2.69906500
H	2.28315600	2.26065900	-0.84232400	H	6.06361600	0.83245300	2.03052500
H	4.61365500	2.79281200	-1.50571900	H	6.50914200	2.08934000	-0.06257100

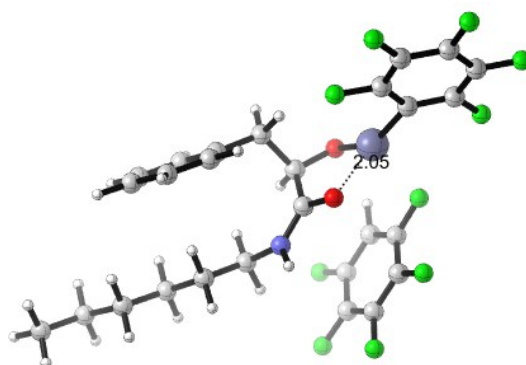
H 9.69168900	-1.74605500	-1.73280000	H 9.55799000	-0.22780900	-0.83761700
H 10.49897100	-1.56888500	-0.16881600	H 8.40571600	-2.92708800	0.08335300
H 8.27889700	-1.42183000	0.98017400	H 6.98563500	-0.39577400	-0.89476200
H 7.11943300	-1.88928900	-1.81399200	H 5.77284400	-1.63882500	0.92512400
H 5.84021500	-3.10549500	-0.04823300	H 4.49407700	-0.47720300	-0.89515900
H 4.51676500	-1.96459600	-1.84866600	H 3.30862000	-1.65644700	0.93648100
H 3.25072100	-3.13740600	-0.02814700	H 1.97456600	-1.75215100	-1.72986300
C -2.80062500	-1.69018300	-0.02694300	C -4.08319800	-1.71386400	-0.55036500
C -2.32769600	-2.92193900	0.37829800	C -4.85133300	-2.86773100	-0.65869900
C -3.03647500	-4.11161300	0.30345200	C -4.31891800	-4.07545600	-0.22654600
F -1.06275400	-3.02831700	0.90426900	F -2.51476100	-5.26737100	0.71828200
F -5.03301200	-5.19400400	-0.32020600	F -6.07831400	-2.84023800	-1.17646400
F -4.64451600	-0.57934200	-0.99712100	H -0.63192200	-1.46441900	1.79688900



TS-2

C -0.84073200	-1.80757700	1.46904400	C -0.77594100	-0.27728600	1.34532500
C -0.89700200	0.11946500	-0.13414600	O 0.11735700	0.00470500	-0.86925900
O 0.49067200	0.13041000	1.82507300	C -2.04994800	-2.43990000	0.82382000
C -3.27667600	-2.51248400	1.49024900	C -1.94910000	-2.97311000	-0.46474400
C -4.37679300	-3.12065300	0.88849600	C -3.04515800	-3.58689700	-1.06663600
C -4.26015900	-3.66647200	-0.38918900	C -9.24622000	-1.61036100	-0.80324000

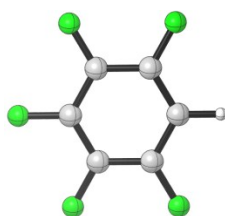
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C -5.76645700	-0.00099700	-0.05157500	C -4.43411600	0.00019400	-0.79551200
C -3.34204200	0.70083300	0.00263800	N -2.04244200	0.53531700	-0.64577400
Zn 1.80082600	0.21705600	0.18294500	C 3.33632400	-1.02277300	0.01580600
C 3.07817600	-2.33744600	-0.32893000	C 4.66865600	-0.70646000	0.21571600
C 4.06272200	-3.30345100	-0.48157300	C 5.69797400	-1.62996200	0.07573000
C 5.38654700	-2.93681800	-0.27685200	F 1.80113000	-2.73465300	-0.53579700
F 3.76393700	-4.55837100	-0.81837000	F 6.35537100	-3.83746000	-0.41683700
F 6.96964600	-1.28449200	0.27143800	F 5.01908700	0.54132300	0.56290000
H -0.79481300	-2.03998500	2.53741200	H 0.07279500	-2.19947400	1.00824900
H -1.55501400	0.20719000	1.93902100	H -3.36406600	-2.10969500	2.49767100
H -0.99377000	-2.92486900	-0.98324500	H -5.32137300	-3.18086700	1.42203100
H -2.94585100	-4.01310600	-2.05998800	H -5.11210300	-4.15515700	-0.85204300
H -9.44806300	-1.14846000	-1.77540700	H -8.92421600	-2.64113800	-0.98655100
H -10.18679100	-1.64636700	-0.24668400	H -8.52684200	0.18773000	0.15428100
H -8.00517700	-1.29573800	0.93686400	H -6.49081100	-1.79084700	-0.99520200
H -7.01333600	-0.30944100	-1.78648500	H -5.61900700	-0.46090400	0.93596500
H -6.09970300	1.03026300	0.12922600	H -4.11608500	-1.03211700	-0.98265800
H -4.55220200	0.48695600	-1.77352400	H -3.29177900	0.25973400	0.99806700
H -3.54345300	1.77149800	0.12092400	H -1.99273800	0.75008900	-1.63805600
C 0.67058800	2.53189000	0.76268400	C 1.64534200	3.00344900	-0.07587300
C -0.42057500	3.36545000	0.89445300	C 1.64260300	4.22879800	-0.72087200
C -0.51268600	4.61216400	0.28681200	C 0.53702000	5.04734600	-0.51610900
F -1.49281100	2.95827300	1.61781600	F -1.58520900	5.39058000	0.43916100
F 0.47001200	6.23552500	-1.11180500	F 2.62728000	4.62303800	-1.52573200
F 2.69986300	2.14257000	-0.34953800	H 0.53210600	1.18167400	1.67247500



INT-6

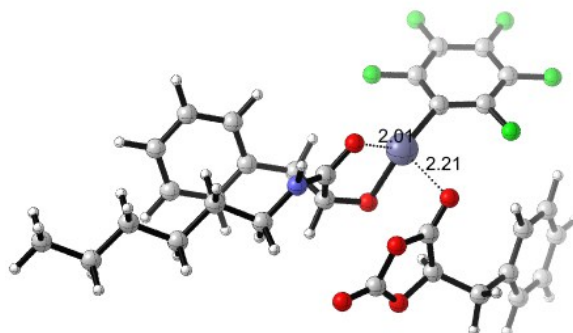
C	-0.58492600	-1.74033600	1.71086900	C	-0.53845700	-0.19396600	1.56601900
C	-0.61290800	0.13888800	0.06324600	O	0.46481700	0.12349600	-0.58312600
O	0.64432900	0.28620100	2.08406500	C	-1.73893000	-2.46096300	1.06197300
C	-2.98519300	-2.56053600	1.68921900	C	-1.56781600	-3.07039400	-0.18564300
C	-4.02863800	-3.26737300	1.09431200	C	-2.60484100	-3.78536200	-0.77990200
C	-3.83713800	-3.89066300	-0.13814300	C	-8.80374000	-2.15181600	-1.10173300
C	-7.82122800	-1.29874600	-0.30377000	C	-6.45863100	-1.18617800	-0.98350400
C	-5.46909600	-0.32537400	-0.20296500	C	-4.08401300	-0.30433000	-0.84263800
C	-3.10164300	0.52693300	-0.02794000	N	-1.74835800	0.42793300	-0.56682500
Zn	1.99331600	0.18247800	0.77782200	C	3.74783500	-0.50323000	0.22954800
C	3.73839800	-1.79379800	-0.26854700	C	4.97496300	0.13267200	0.23692800
C	4.86859100	-2.44298600	-0.74286500	C	6.14122900	-0.46737800	-0.22290000
C	6.08034300	-1.76457500	-0.71614700	F	2.57372900	-2.47858700	-0.30499800
F	4.81481900	-3.68657300	-1.22057500	F	7.18288700	-2.35777900	-1.16604700
F	7.30846800	0.17598600	-0.20200900	F	5.07944300	1.38953700	0.69963400
H	-0.55011200	-1.93815500	2.78668800	H	0.35794500	-2.10853100	1.28716800
H	-1.40121300	0.25027800	2.08564600	H	-3.12887100	-2.10101500	2.66540300
H	-0.59985000	-3.00072700	-0.67829600	H	-4.98736400	-3.34604800	1.59967600
H	-2.44745600	-4.26747400	-1.73980500	H	-4.64368100	-4.45749700	-0.59341200
H	-8.97626500	-1.72179600	-2.09397300	H	-8.41370500	-3.16547700	-1.24328100
H	-9.77076300	-2.23138600	-0.59725900	H	-8.23774800	-0.29416900	-0.15539800
H	-7.68732000	-1.72738800	0.69827200	H	-6.03118000	-2.19052800	-1.11208600

H -6.58603300	-0.77334500	-1.99394000	H -5.37847200	-0.71818200	0.81946300
H -5.85974100	0.69777300	-0.11246500	H -3.69530500	-1.32577700	-0.91911900
H -4.15040900	0.09739200	-1.86352200	H -3.09104200	0.16843900	1.00184500
H -3.40631600	1.58227400	-0.01093500	H -1.63856600	0.57531600	-1.56661200
C -0.19895100	2.99682800	1.37904000	C 0.72263000	2.92722500	0.34988200
C -1.48096600	3.41859800	1.06550900	C 0.40811400	3.25813500	-0.95822700
C -1.83040500	3.76614700	-0.23329400	C -0.88333300	3.68377200	-1.24604000
F -2.42974200	3.45307400	2.00017800	F -3.07956200	4.12294700	-0.52192800
F -1.22070800	3.98693100	-2.49341000	F 1.30603700	3.13794500	-1.92588200
F 1.96697900	2.45122000	0.58351900	H 0.06067800	2.64908100	2.37147000



C₆F₅H

C 0.00008500	1.12408500	-0.00011900	C -1.20814400	0.42648000	-0.00057200
C -1.20832500	-0.96823200	0.00002800	C 0.00013100	-1.66597900	-0.00011900
C 1.20803100	-0.96847400	-0.00014500	C 1.20803900	0.42666400	0.00025100
H -0.00026200	-2.76565900	0.00029500	F 2.37735100	-1.64315200	-0.00029700
F 2.37727100	1.10149400	0.00046900	F -0.00000900	2.47408500	-0.00014700
F -2.37706600	1.10184700	0.00002400	F -2.37739600	-1.64334200	0.00036800

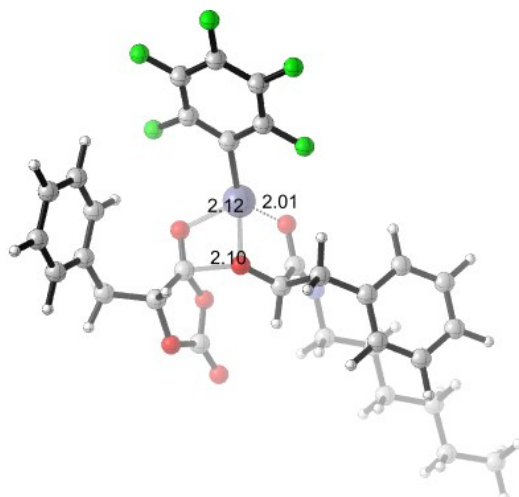


INT-7'

C 1.59316300	1.02933300	1.37065700	C 1.27549100	-0.23061200	0.52622200
C 1.60361000	0.07866500	-0.94678100	O 0.71813100	0.66727400	-1.62393000

O	-0.06515700	-0.53965200	0.62496000	C	3.01647300	1.52449000	1.33257400
C	4.02203000	0.87691600	2.05922400	C	3.35663300	2.65696100	0.58684900
C	5.32853100	1.35929600	2.05634100	C	4.66002600	3.14953100	0.58855300
C	5.64845500	2.50502000	1.32845900	C	10.13753600	-0.01375900	0.04537300
C	8.83408400	-0.79946200	0.15986200	C	7.67706100	-0.12874000	-0.57741900
C	6.36652600	-0.90120500	-0.45860800	C	5.20053500	-0.19586300	-1.14640400
C	3.89745300	-0.95749500	-0.94447500	N	2.76129500	-0.23421400	-1.51132200
Zn	-1.05645000	0.49891000	-0.68597000	C	-2.65285500	1.66164100	-0.59017300
C	-2.51854800	2.88798600	0.03572100	C	-3.94252900	1.32551600	-0.96066500
C	-3.57820900	3.74709900	0.29308200	C	-5.04514300	2.13231700	-0.71175100
C	-4.85711100	3.35514200	-0.08182600	F	-1.29511800	3.29624000	0.43476400
F	-3.39495500	4.92158800	0.89672100	F	-5.89662000	4.14946300	0.16125700
F	-6.27433700	1.73952600	-1.05579300	F	-4.19384100	0.16213900	-1.59037000
H	1.29756600	0.77498100	2.39355400	H	0.90958900	1.81750200	1.03042400
H	1.89920900	-1.06652300	0.87715500	H	3.76952400	-0.00054700	2.65172800
H	2.58271900	3.16952300	0.02006400	H	6.09565500	0.85072000	2.63371700
H	4.90129000	4.04110900	0.01807800	H	6.66240900	2.89326200	1.34174900
H	10.43777400	0.09403500	-1.00231600	H	10.02431700	0.99254100	0.46274000
H	10.95393200	-0.50855900	0.57896800	H	8.97622200	-1.81350800	-0.23539000
H	8.56476600	-0.91730000	1.21800900	H	7.52916500	0.88490900	-0.17921700
H	7.93921200	-0.00837300	-1.63798300	H	6.12198100	-1.03085600	0.60515500
H	6.49245000	-1.91043200	-0.87464300	H	5.08398200	0.81432300	-0.73836800
H	5.40909100	-0.09062000	-2.22049100	H	3.72232900	-1.09313500	0.12278200
H	3.94065600	-1.95436100	-1.39744400	H	2.82621800	0.03159100	-2.48983000
C	-2.44597200	-4.08515000	0.14360700	C	-1.28862100	-3.09273400	0.32242600
O	0.24582000	-2.52399500	-1.31900000	C	0.86218800	-3.34841200	-0.39079400
C	-1.00172900	-2.23661200	-0.88804700	O	-1.71826500	-1.45880100	-1.47062300
O	2.01698200	-3.61667100	-0.43363600	O	-0.03378300	-3.76691200	0.50264200
C	-3.75345400	-3.50923900	0.64442500	C	-4.34285600	-4.02678800	1.79824000
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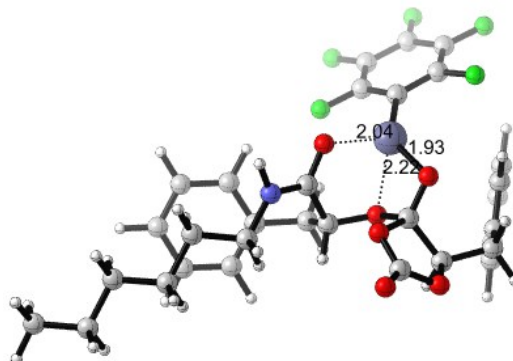
C	-5.52305100	-1.86066500	0.51189300	C	-6.10619800	-2.38578200	1.66321000
H	-2.18177200	-4.97314800	0.72584000	H	-2.51795700	-4.39489500	-0.90549000
H	-1.44414800	-2.43341100	1.17917000	H	-3.87950300	-4.86827800	2.30726300
H	-3.91456700	-2.00812100	-0.89598300	H	-5.96630600	-3.88842200	3.19922200
H	-5.96694200	-1.00914500	0.00403400	H	-7.01695300	-1.94934600	2.06104600



INT-7''

C	-1.50281000	-0.97248600	1.34756400	C	-1.23360900	0.24394600	0.43036500
C	-1.56818000	-0.14774500	-1.01915300	O	-0.68078400	-0.75668900	-1.67411400
O	0.10840200	0.57802400	0.50142700	C	-2.91612800	-1.49855600	1.34385100
C	-3.93084300	-0.83802500	2.04535100	C	-3.23465900	-2.67045400	0.65240200
C	-5.22724500	-1.34630100	2.07029200	C	-4.52796600	-3.18795200	0.68212600
C	-5.52633200	-2.52992600	1.39640500	C	-10.08351500	-0.10781900	0.10117900
C	-8.79091300	0.70208800	0.15520000	C	-7.63737800	0.01520000	-0.57252700
C	-6.33540000	0.80891200	-0.51131400	C	-5.17405400	0.08612100	-1.18853100
C	-3.87190700	0.86083900	-1.03720500	N	-2.74145300	0.10752800	-1.57708200
Zn	1.12463200	-0.49278700	-0.83354500	C	2.71426300	-1.64722800	-0.63401300
C	2.57677700	-2.84695100	0.04005800	C	4.00932100	-1.30226400	-0.97597600
C	3.64158700	-3.67472800	0.36913700	C	5.11624000	-2.07758200	-0.65560500
C	4.92570400	-3.27548400	0.02014400	F	1.34716400	-3.25801000	0.41704300
F	3.45786900	-4.82613400	1.01526200	F	5.96901200	-4.03978400	0.33259300
F	6.34976600	-1.67944100	-0.97462000	F	4.25709800	-0.15930700	-1.64347200
H	-1.20689600	-0.65597000	2.35271300	H	-0.80379300	-1.76124800	1.04285100

H -1.86495000	1.08569100	0.74830800	H -3.69451700	0.07059700	2.59615000
H -2.45239300	-3.19223500	0.10589400	H -6.00233700	-0.82739500	2.62732800
H -4.75287200	-4.10935400	0.15400400	H -6.53224300	-2.93721500	1.43183700
H-10.40105000	-0.26760400	-0.93474100	H -9.94648100	-1.09248300	0.56092500
H-10.89782500	0.39802900	0.62742300	H -8.95611500	1.69467900	-0.28305700
H -8.50424900	0.87249900	1.20156400	H -7.46847300	-0.97804000	-0.13305200
H -7.91616300	-0.15568600	-1.62184400	H -6.07395200	0.98818200	0.54120400
H -6.48117700	1.79730000	-0.96842300	H -5.04374500	-0.90628400	-0.74218700
H -5.39768300	-0.06418200	-2.25409300	H -3.68845100	1.05217700	0.01987800
H -3.91816100	1.83412100	-1.53881000	H -2.81788100	-0.21208100	-2.53854100
C 2.24882300	4.04661800	0.13331100	C 1.12256000	3.04915800	0.44163900
O -0.44597500	2.50744900	-1.18351300	C -1.02862600	3.35535200	-0.26784800
C 0.78995500	2.13862600	-0.72343600	O 1.55286500	1.49641300	-1.43153300
O -2.16716300	3.69254400	-0.32263100	O -0.13269300	3.71522600	0.65458200
C 3.59008800	3.52303600	0.60212400	C 4.19630400	4.08043700	1.72885700
C 4.20990400	2.44536000	-0.03746000	C 5.40092200	3.57342200	2.21011500
C 5.40843600	1.92962000	0.44904700	C 6.00692300	2.49380100	1.57352700
H 2.00197300	4.96976100	0.66675700	H 2.26092700	4.27910500	-0.93773600
H 1.34696400	2.45696300	1.32817500	H 3.72212000	4.91818100	2.23428500
H 3.75288900	1.99871400	-0.91305800	H 5.86276000	4.02102200	3.08473000
H 5.86750300	1.08547800	-0.05724200	H 6.94262100	2.09430800	1.95193300



TS3

C -1.05547400	-0.53025200	1.30091200	C -1.08282100	0.66429400	0.33666900
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C -1.36160200	0.18419500	-1.09336800	O -0.40918800	-0.29440600	-1.74951400
O 0.22521000	1.20912600	0.36131600	C -2.31818400	-1.35911700	1.29165600
C -3.44301200	-0.97775000	2.02937800	C -2.36773900	-2.54036500	0.54629400
C -4.59048200	-1.76874300	2.03434700	C -3.51078900	-3.33670800	0.55527100
C -4.62275900	-2.95513300	1.30324300	C -9.67065300	-1.31605800	0.38227100
C -8.53692300	-0.29498400	0.41587000	C -7.32910200	-0.73256400	-0.40967100
C -6.18733700	0.27955900	-0.38051100	C -4.95502600	-0.20600600	-1.13844900
C -3.80249500	0.78474400	-1.03115800	N -2.58046300	0.23150200	-1.60787100
Zn 1.47798300	0.20736900	-1.17566800	C 2.74298400	-1.28028200	-0.88622600
C 2.32759500	-2.50029100	-0.38375300	C 4.10783200	-1.14990400	-1.06859600
C 3.19212700	-3.53795100	-0.06187600	C 5.02362800	-2.14413600	-0.75285800
C 4.55561300	-3.34994200	-0.24669400	F 1.01199700	-2.72695400	-0.16821200
F 2.74207700	-4.69450100	0.42456800	F 5.40957700	-4.32067200	0.06370500
F 6.33317800	-1.95296100	-0.91260000	F 4.61451700	-0.00355600	-1.56078500
H -0.85302400	-0.13058200	2.29959400	H -0.20262700	-1.15544300	1.01728000
H -1.80495400	1.41813900	0.65457000	H -3.41220500	-0.06599000	2.62324100
H -1.49277000	-2.84478100	-0.02291200	H -5.45423800	-1.46642500	2.61978300
H -3.52814900	-4.25985200	-0.01536800	H -5.51051200	-3.57992700	1.31937200
H -10.02375400	-1.47406800	-0.64221200	H -9.33535000	-2.28389600	0.77029600
H -10.52350800	-0.99036600	0.98424600	H -8.89812500	0.67279700	0.04524700
H -8.22002400	-0.12724200	1.45398400	H -6.95871700	-1.69623300	-0.03196800
H -7.63949200	-0.90788200	-1.44917900	H -5.90528100	0.47121100	0.66478900
H -6.53110800	1.23860000	-0.79180700	H -4.62295900	-1.16604400	-0.72633600
H -5.20571200	-0.37413100	-2.19488500	H -3.62415500	1.00126600	0.02227100
H -4.03227900	1.73313800	-1.53118800	H -2.63584300	-0.11737000	-2.56024700
C 2.22870000	4.01824700	0.60967200	C 0.77042300	3.60737900	0.53974300
O -0.74445300	2.81762100	-1.02947400	C -0.96248600	4.14197400	-0.83856500
C 0.50746600	2.42619700	-0.41957600	O 1.43926900	2.13793700	-1.28813200
O -1.86085800	4.75056200	-1.32952700	O -0.03266600	4.65615400	-0.01244200
C 3.04724800	2.96893600	1.32976400	C 2.96449800	2.84989600	2.71965800

C 3.88426600	2.09720600	0.62889900	C 3.70183600	1.88386600	3.39759800
C 4.63495300	1.13801700	1.30645900	C 4.54247300	1.02665400	2.69130200
H 2.28514700	4.97627800	1.13772300	H 2.59290300	4.16238700	-0.41037000
H 0.37945900	3.36772600	1.53573800	H 2.32549100	3.53123400	3.27834100
H 3.95125300	2.17749100	-0.45198800	H 3.62848400	1.80736500	4.47826500
H 5.29990600	0.48798400	0.74608500	H 5.12672900	0.27900600	3.21865700