Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Interplay between Chalcogen Bonds and Dynamic Covalent Bonds

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1. General Methods

General. ^{1}H NMR and ^{13}C NMR spectra were recorded on a 400 MHz Bruker Biospin Avance III spectrometer or a 400 MHz JEOL JNM-ECZ400S spectrometer. The chemical shifts (δ) for ^{1}H NMR spectra, given in ppm, are referenced to the residual proton signal of the deuterated solvent. Mass spectral analysis (ESI-HRMS) were performed on ThermoScientificLCQ Fleet mass spectrometer and a Bruker IMPACT-II spectrometer Infrared. (IR) spectra were recorded with a KBr pellet, and wavenumbers are given in cm^{-1}. Crystallographic data was collected on a Mercury single crystal diffractometer. The structures were solved with direct methods by using SHELXS-97 and refined with the full-matrix least-squares technique based on F2. Deuterium solvents were purchased from Aldrich. All other reagents were obtained from commercial sources and were used without further purification, unless indicated otherwise.

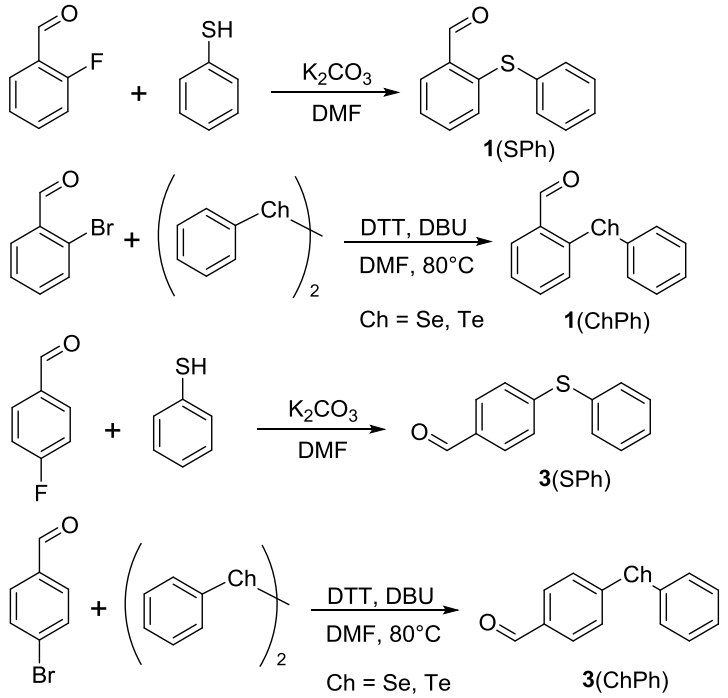
DCRs in Acetonitrile. Dynamic Covalent Reactions (DCRs) were performed *in situ* in CD_3CN without isolation and purification. To a stirred solution of **1** (15 mM, 1.0 equiv.) in CD_3CN (0.60 mL), were added 1-butylamine (15 mM, 1.2 equiv.) and activated 3 Å molecular sieves (MS, 4-8 mesh). The mixture was stirred at room temperature overnight and characterized by ^{1}H NMR and ESI-MS. For competition experiments, both aldehydes (15 mM each, 1.0 equiv.) were mixed with 1-butylamine (15 mM, 1.0 equiv.) in CD_3CN (0.60 mL). The mixture was tracked by ^{1}H NMR until the equilibrium was reached. All competition experiments were performed twice to ensure reproducibility. To explore the thermodynamic and kinetic selectivity, $Zn(OTf)_2$ (1.5 mM, 0.1 equiv.) was added to the competition experiments. Furthermore, aldehydes **1**(SPh) and **5** (15 mM each, 1.0 equiv.) were mixed with 1-butylamine (15 mM, 1.0 equiv.) and different Lewis acid (1.5 mM, 0.1 equiv.) in CD_3CN (0.6 mL), and the mixture was stirred overnight and characterized by ^{1}H NMR to determine the extent of acceleration.

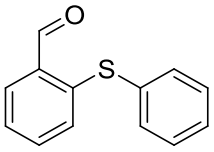
DFT Calculations. Geometry optimization and frequencies calculations were performed by using Gaussian 09 packages,[S1] with the DFT method and basis set of

M06-2X-D3/def2-TZVP. The default settings of def2-TZVP for Te in G09 was made up of relativistic effective core potential and the Stuttgart-Dresden effective core potential frozen core basis set MWB28. We also included the PCM of acetonitrile and the ultrafine integration grid during the optimization and frequency analysis. All the geometries were determined without imaginary frequencies by frequency analysis. The torsion scans of open and closed conformations of **1**(SePh)/**1**(SeMe) along the C-SePh/C-SeMe bond were conducted, and the resulting conformers 1, 2, and 3 were found to account for the major population (Figures S22 and S23). Therefore, these conformers were set as initial structures of **1**(ChR)/**2**(ChR) for optimization and the subsequent analysis. For the simplicity methylamine was used for **2**(ChR). Generalized Kohn-Sham energy decomposition analysis (GKS-EDA) was employed to calculate the total interaction energy of **1**/**2** and dissect the contributing factors to chalcogen bonding by the modified GAMESS (version: 2020-R2) from XMVB team.[S2] The same levels of M06-2X-D3/def2-TZVP was also used for GKS-EDA calculation. Unlike G09, the mixed basis set for Te was manually specified in GAMESS. The NBO analysis[S3] was implemented by NBO 3.1 module in G09. The electronic density cubes for Atoms in Molecules (AIM) and Noncovalent Interaction (NCI)[S4] were generated by Multiwfn 3.80[S5] and presented by VMD 1.90.[S6] See more details in associated Figures and Tables if necessary.

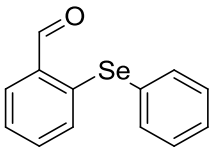
2. Synthesis and Characterization

Scheme S1. General synthetic routes of **1**(ChPh) and **3**(ChPh).

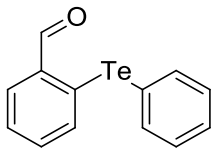




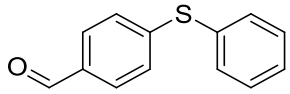
2-(phenylthio)benzaldehyde: The reported procedure[S7] was used to afford the title compound as a yellow solid (yield: 88%). ^{1}H NMR ($CDCl_3$): δ 10.19 (s, 1H), 7.74 (dd, J=7.6, 1.6 Hz, 2H), 7.47 (ddd, J=8.1, 7.3, 1.6 Hz, 1H), 7.29-7.25 (m, 1H), 7.21 (ddd, J=7.5, 7.5, 1.1 Hz, 1H), 2.43 (s, 3H).



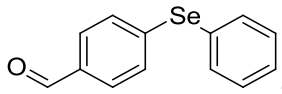
2-(phenylselenyl)benzaldehyde: The reported procedure[S8] was used to afford the title compound as a yellow solid (yield: 78%). ^{1}H NMR (CD_3CN): δ 10.16 (s, 1H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.72-7.67 (m, 2H), 7.57-7.46 (m, 3H), 7.44-7.34 (m, 2H), 6.99 (d, *J* = 7.2 Hz, 1H).



2-(phenyltellanyl)benzaldehyde: Diphenyl ditelluride[S9] (246 mg, 0.6 mmol) was added to a solution of DTT (dithiothreitol) (154 mg, 1.0 mmol) in anhydrous DMF (2 mL) under N_2 atmosphere. After stirring at 80 ℃ for 30 min, *o*-bromobenzaldehyde (185 mg, 1.0 mmol) was added to the reaction mixture, and the mixture was stirred for 15 min. 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU, 0.375 mL, 2.5 mmol) was added, and the mixture was stirred for further 15 min. The solvent was removed under reduced pressure, and the residue was extracted with ethyl acetate. The combined organic layer was dried over anhydrous $MgSO_4$. The crude product was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 20:1) to afford the title compound as a yellow solid (210 mg, 68%). MP: 55.5-55.9 ^oC. ^1H NMR (CD_3CN): δ 10.19 (s, 1H), 8.01 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.98-7.94 (m, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.46-7.40 (m, 3H), 7.3 (td, *J* = 7.2, 1.2 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (CD_3CN): δ 195.0, 142.3, 138.1, 136.9, 134.9, 133.9, 130.8, 130.1, 127.1, 126.1, 117.2. ESI-HRMS m/z: $[M + H]^+$ calcd for $C_{13}H_{11}OTe$ 312.9867; found: 312.9862.

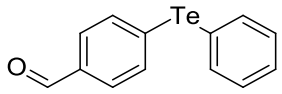


4-(phenylsulfanyl)benzaldehyde: The reported procedure[S10] was used to afford the title compound as a white liquid (yield: 91%). ^1H NMR ($CDCl_3$): δ 9.91 (s, 1H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.37-7.60 (m, 5H), 7.24 (d, *J* = 8.4 Hz, 2H).



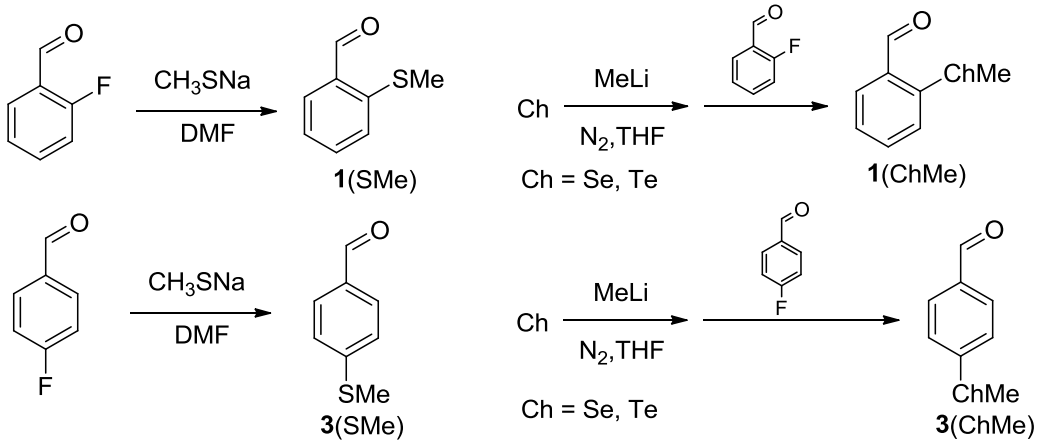
4-(phenylselenyl)benzaldehyde: Diphenyl diselenide[S11] (187 mg, 0.6 mmol) was added to a solution of DTT (dithiothreitol) (154 mg, 1.0 mmol) in anhydrous DMF (2 mL) under N_2 atmosphere. After stirring at 80 ℃ for 30 min, *p*-bromobenzaldehyde (185 mg, 1.0 mmol) was added to the reaction mixture, and the mixture was stirred for 15 min. 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU, 0.375 mL, 2.5 mmol) was added, and the mixture was stirred for further 15 min. The solvent was removed under reduced pressure, and the residue was extracted with ethyl acetate. The combined organic layer was dried over anhydrous $MgSO_4$. The crude product was

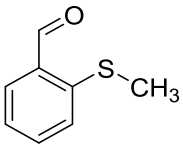
purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 30:1) to afford the title compound as a yellow liquid (195 mg, 74%). ^{1}H NMR ($CDCl_3$): δ 9.92 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.65-7.59 (m, 2H), 7.45-7.35 (m, 5H). ^{13}C NMR ($CDCl_3$): δ 191.4, 142.8, 135.6, 134.4, 130.1, 130.1, 129.9, 128.9, 127.9. ESI-HRMS m/z: $[M + H]^+$ calcd for $C_{13}H_{11}OSe$ 262.9970; found: 262.9968.



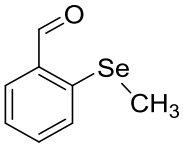
4-(phenyltellanyl)benzaldehyde: Diphenyl ditelluride (246 mg, 0.6 mmol) was added to a solution of DTT (dithiothreitol) (154 mg, 1.0 mmol) in anhydrous DMF (2 mL) under N_2 atmosphere. After stirring at 80 ℃ for 30 min, *p*-bromobenzaldehyde (185 mg, 1.0 mmol) was added to the reaction mixture, and the mixture was stirred for 15 min. 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU, 0.375 mL, 2.5 mmol) was added, and the mixture was stirred for further 15 min. The solvent was removed under reduced pressure, and the residue was extracted with ethyl acetate. The combined organic layer was dried over anhydrous $MgSO_4$. The crude product was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 30:1) to give the title compound as a yellow solid (195 mg, 63%). MP: 46.7-47.1 ^{o}C. ^{1}H NMR ($CDCl_3$): δ 9.92 (s, 1H), 7.85 (d, *J* = 6.8 Hz, 2H), 7.67-7.60 (m, 4H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR ($CDCl_3$): δ 191.7, 140.0, 135.7, 135.2, 130.0, 130.0, 129.0, 126.8, 113.0. ESI-HRMS m/z: $[M + H]^+$ calcd for $C_{13}H_{11}OTe$ 312.9867; found: 312.9862.

Scheme S2. General synthetic routes of **1**(ChMe) and **3**(ChMe).

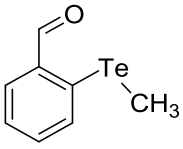




2-(methylthio)benzaldehyde: The reported procedure[S12] was used to afford the title compound as a yellow oil (yield: 85%). ^{1}H NMR ($CDCl_3$): δ 10.26 (s, 1H), 7.82 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.54 (td, *J* = 8.0, 1.6 Hz, 1H), 7.35 (d, 8.0 Hz, 1H), 7.21 (td, *J* = 7.2, 1.2 Hz, 1H), 2.50 (s, 3H).

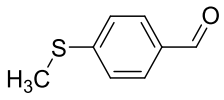


2-(methylselenyl)benzaldehyde: Selenium (0.50 g, 6.3 mmol) was suspended in degassed anhydrous THF (40 mL) under argon atmosphere. The suspension was cooled to -10 ℃, and MeLi (5.3 mL, 7.0 mmol, 1.1 eq.) was added dropwise. The resulting white suspension was stirred for 40 min. 2-Fluorobenzaldehyde (0.94 g, 7.6 mmol, 1.2 eq.) was added dropwise to give a clear orange solution, which was stirred overnight at room temperature, quenched with water, and extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude mixture was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 20:1) to afford the title compound as a yellow oil (0.86 g, 68%).^{1}H NMR ($CDCl_3$): δ 10.14 (s, 1H), 7.82 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.52-7.42 (m, 2H), 7.34 (td, *J* = 7.6, 1.2 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 192.6, 138.8, 135.6, 134.3, 133.9, 127.9, 124.9, 5.92. ESI-HRMS m/z: $[M + Na]^+$ calcd for C_8H_9NaOSe 222.9633; found: 222.9630.

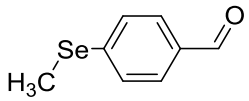


2-(methyltellanyl)benzaldehyde: Tellurium (0.80 g, 6.3 mmol) was suspended in degassed anhydrous THF (40 mL) under argon atmosphere. The suspension was cooled to -10 ℃, and MeLi (5.3 mL, 7.0 mmol, 1.1 eq.) was added dropwise. The resulting suspension was stirred for 40 min. 2-Fluorobenzaldehyde (0.94 g, 7.6 mmol, 1.2 eq.) was added dropwise to give a clear orange solution, which was stirred overnight at

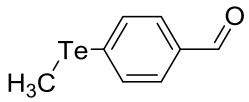
room temperature, quenched with water, and extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude mixture was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 20:1) to afford the title compound as a yellow oil (0.66 g, 42%). ^{1}H NMR ($CDCl_3$): δ 10.17 (s, 1H), 7.82 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.44 (td, *J* = 7.2, 1.6 Hz, 1H), 7.38 (td, *J* = 7.2, 1.2 Hz, 1H), 2.02 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 193.0, 137.2, 136.6, 133.7, 132.4, 125.6, 123.5, -16.1. ESI-HRMS m/z: $[M + H]^+$ calcd for C_8H_9OTe 250.9716; found: 250.9720.



4-(methylthio)benzaldehyde: The reported procedure[S6] was used to afford the title compound as a yellow oil (yield: 80%). ^{1}H NMR ($CDCl_3$): δ 9.92 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 2.54 (s, 3H).



4-(methylselenyl)benzaldehyde: Selenium (0.50 g, 6.3 mmol) was suspended in degassed anhydrous THF (40 mL) under argon atmosphere. The suspension was cooled to -10 ℃, and MeLi (5.3 mL, 7.0 mmol, 1.1 eq.) was added dropwise. The resulting white suspension was stirred for 40 min. 4-Fluorobenzaldehyde (0.94 g, 7.6 mmol, 1.2 eq.) was added dropwise to give a clear orange solution, which was stirred overnight at room temperature, quenched with water, and extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude mixture was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 30:1) to afford the title compound as a yellow oil (0.73 g, 58%). ^{1}H NMR ($CDCl_3$): δ 9.93 (s, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 191.6, 142.6, 134.0, 130.1, 129.0, 6.56. ESI-HRMS m/z: $[M + Na]^+$ calcd for C_8H_9NaOSe 222.9633; found: 222.9631.



4-(methyltellanyl)benzaldehyde: Tellurium (0.80 g, 6.3 mmol) was suspended in degassed anhydrous THF (40 mL) under argon atmosphere. The suspension was cooled to -10 ℃, and MeLi (5.3 mL, 7.0 mmol, 1.1 eq.) was added dropwise. The resulting suspension was stirred for 40 min. 4-Fluorobenzaldehyde (0.94 g, 7.6 mmol, 1.2 eq.) was added dropwise to give a clear orange solution, which was stirred overnight at room temperature, quenched with water, and extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The crude mixture was purified by column chromatography (SiO_2, petroleum ether: ethyl acetate = 20:1) to afford the title compound as a yellow oil (0.47 g, 30%). ^{1}H NMR ($CDCl_3$): δ 9.94 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.65 (d, *J* = 8.4 Hz, 2H), 2.28 (s, 3H). ^{13}C NMR ($CDCl_3$): δ 191.2, 135.3, 135.1, 129.9, 124.2, -16.1. ESI-HRMS m/z: $[M + H]^+$ calcd for C_8H_9OTe 250.9716; found: 250.9719.

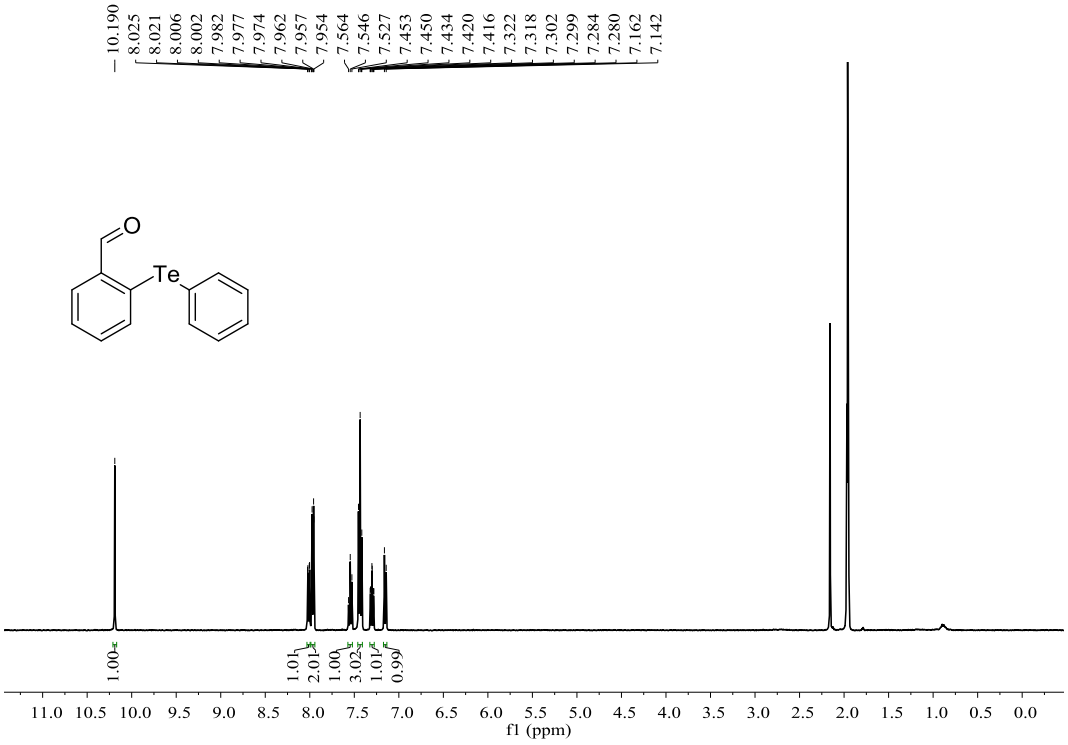


Figure S1. ^{1}H NMR spectrum of **1**(TePh) in CD_3CN.

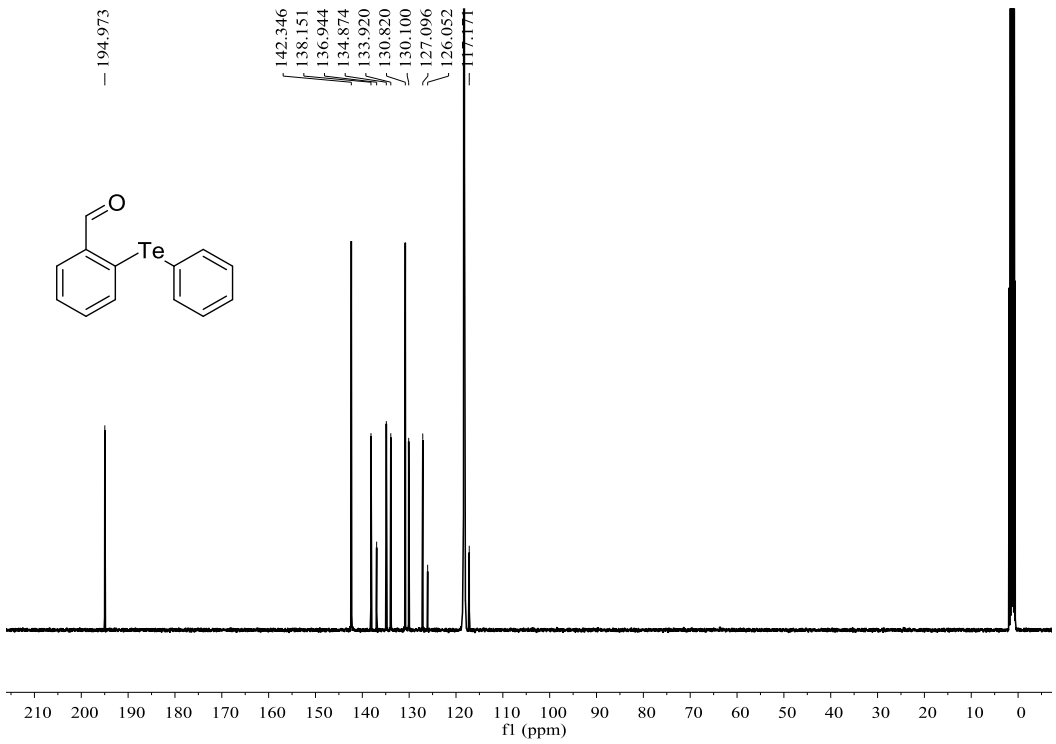


Figure S2. ^{13}C NMR spectrum of **1**(TePh) in CD_3CN.

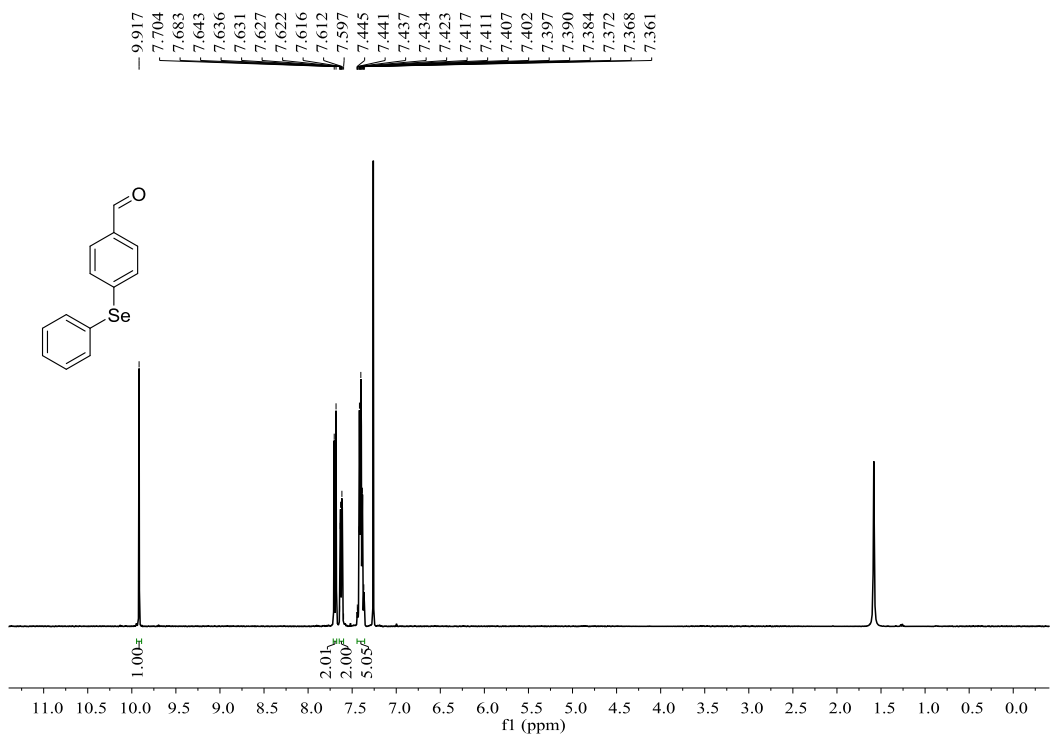


Figure S3. ^{1}H NMR spectrum of **3**(SePh) in $CDCl_3$.

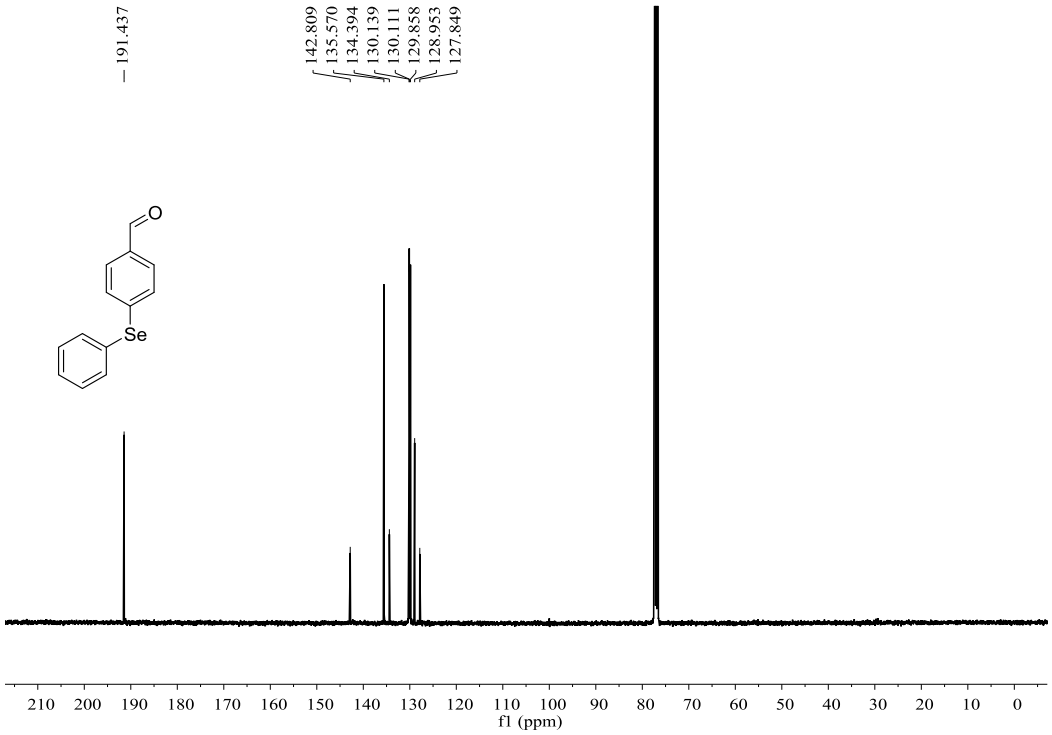


Figure S4. ^{13}C NMR spectrum of **3**(SePh) in $CDCl_3$.

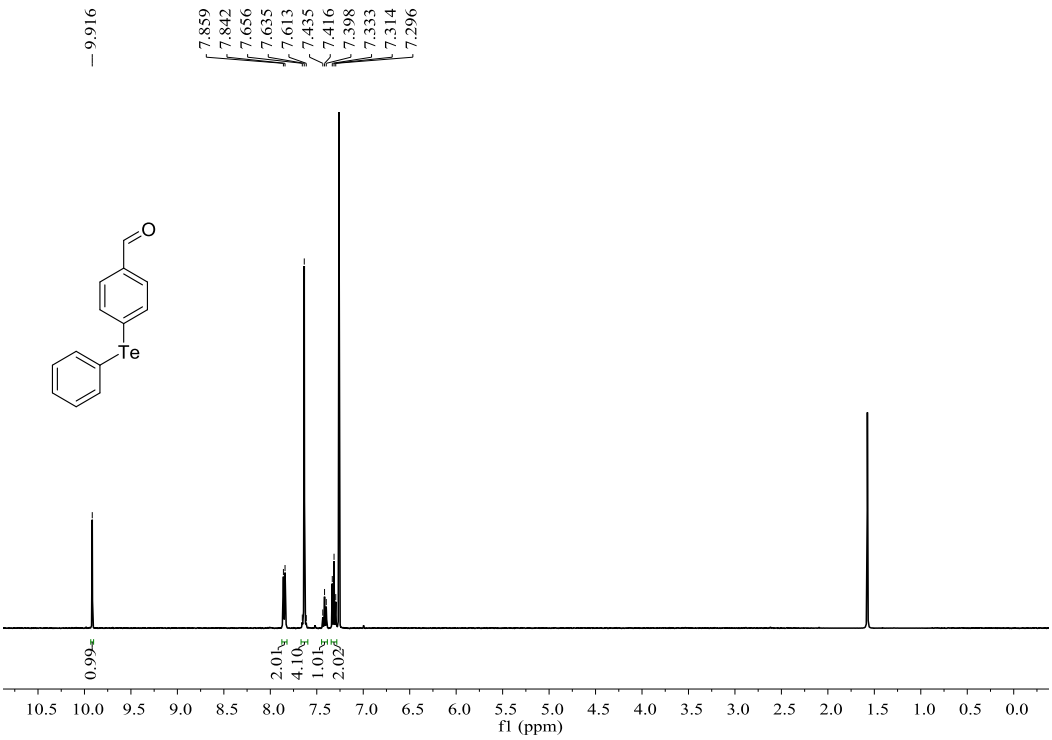


Figure S5. ^{1}H NMR spectrum of **3**(TePh) in $CDCl_3$.

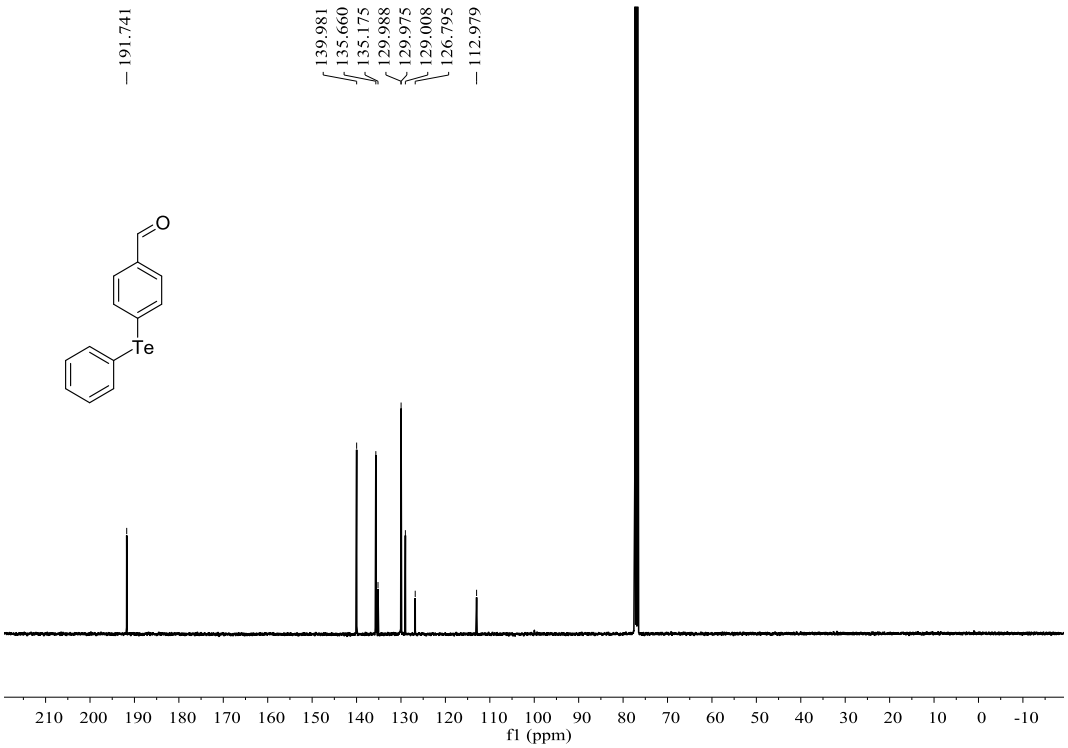


Figure S6. ^{13}C NMR spectrum of **3**(TePh) in $CDCl_3$.

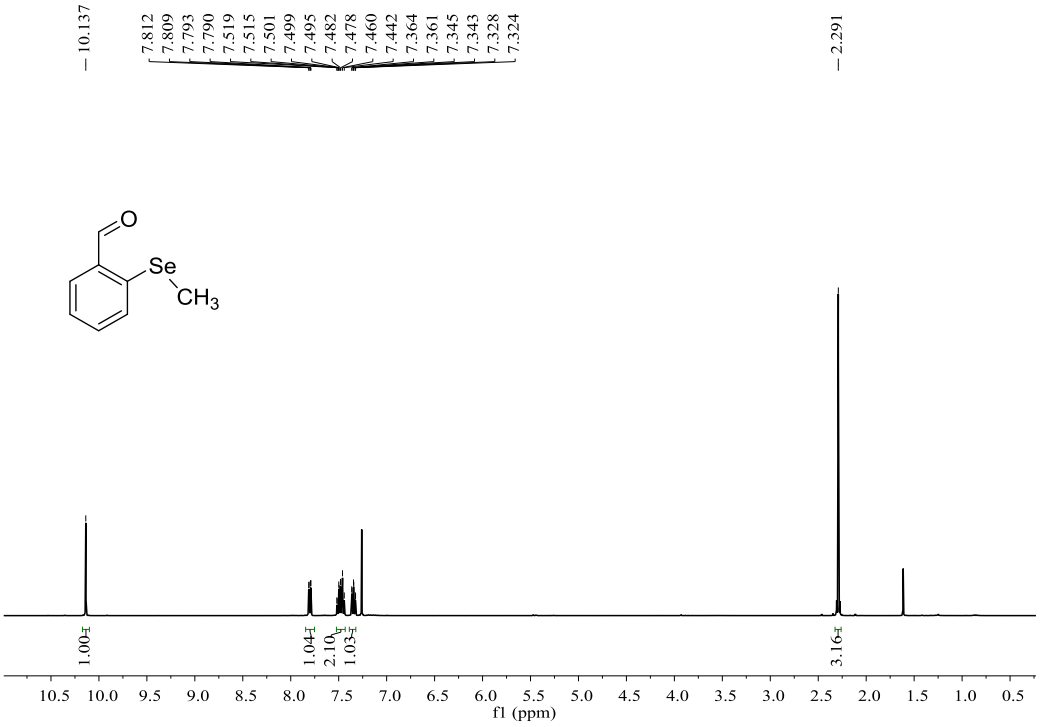


Figure S7. ^{1}H NMR spectrum of **1**(SeMe) in $CDCl_3$.

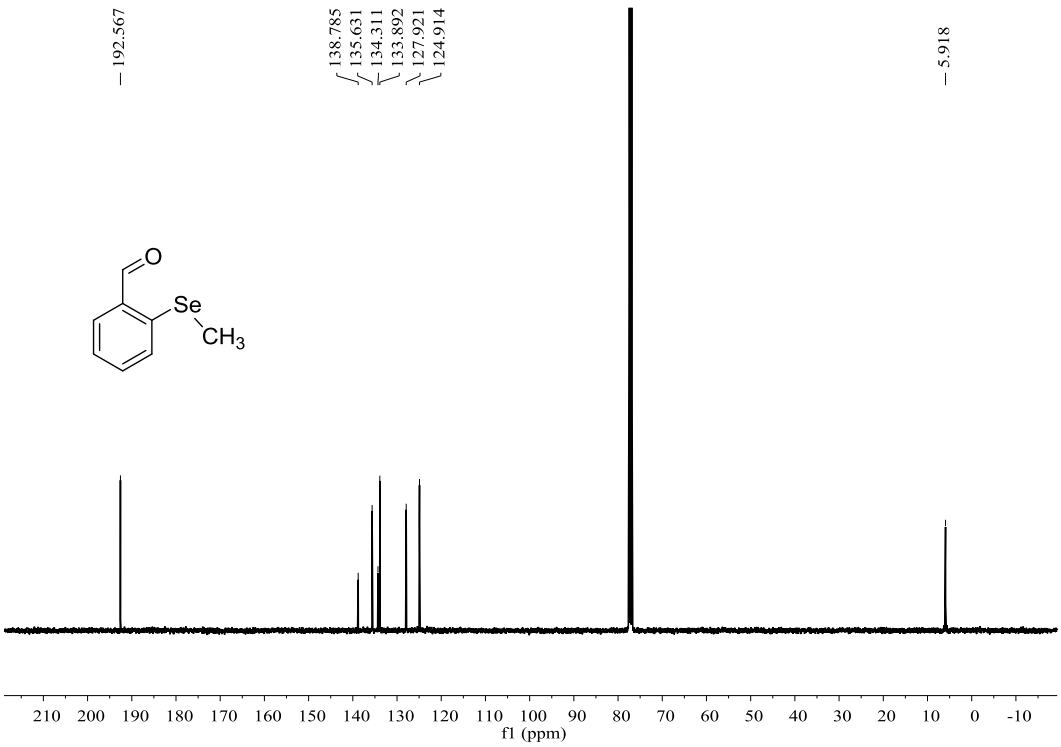


Figure S8. ^{13}C NMR spectrum of **1**(SeMe) in $CDCl_3$.

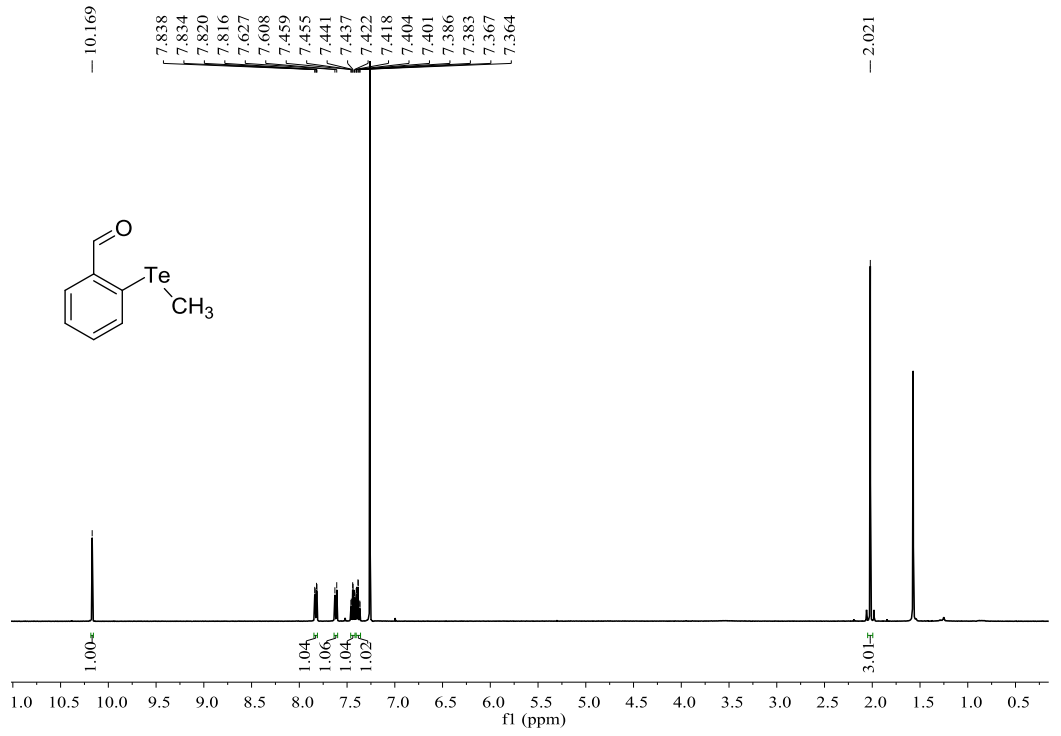


Figure S9. ^{1}H NMR spectrum of **1**(TeMe) in $CDCl_3$.

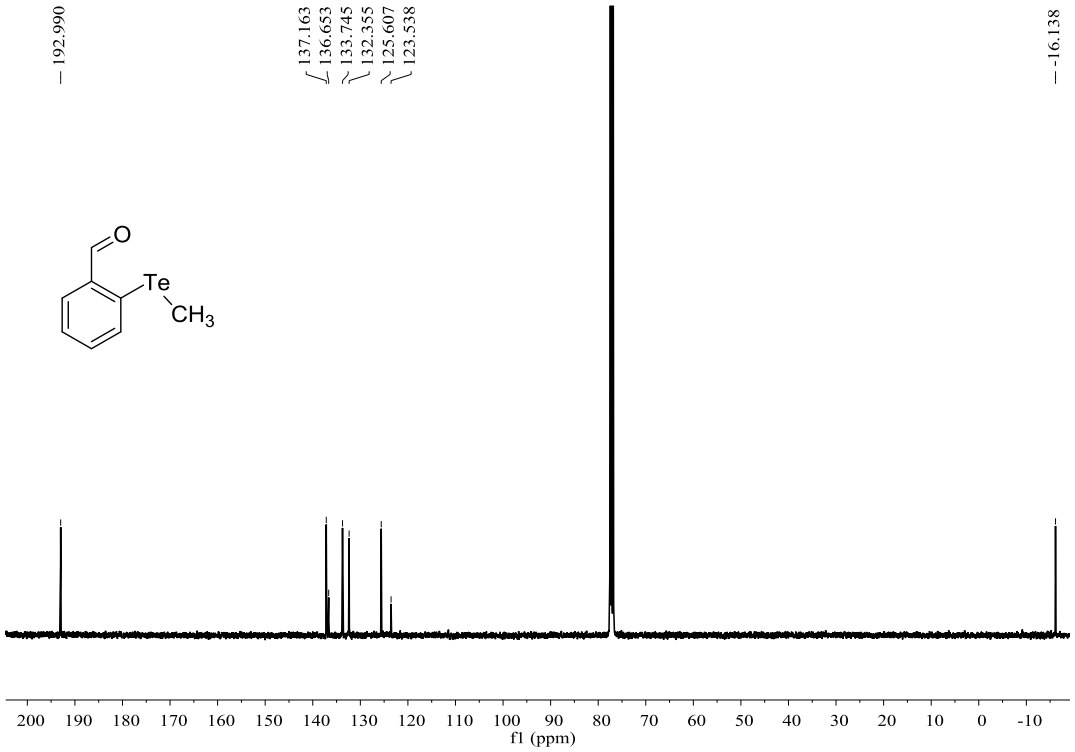


Figure S10. ^{13}C NMR spectrum of **1**(TeMe) in $CDCl_3$.

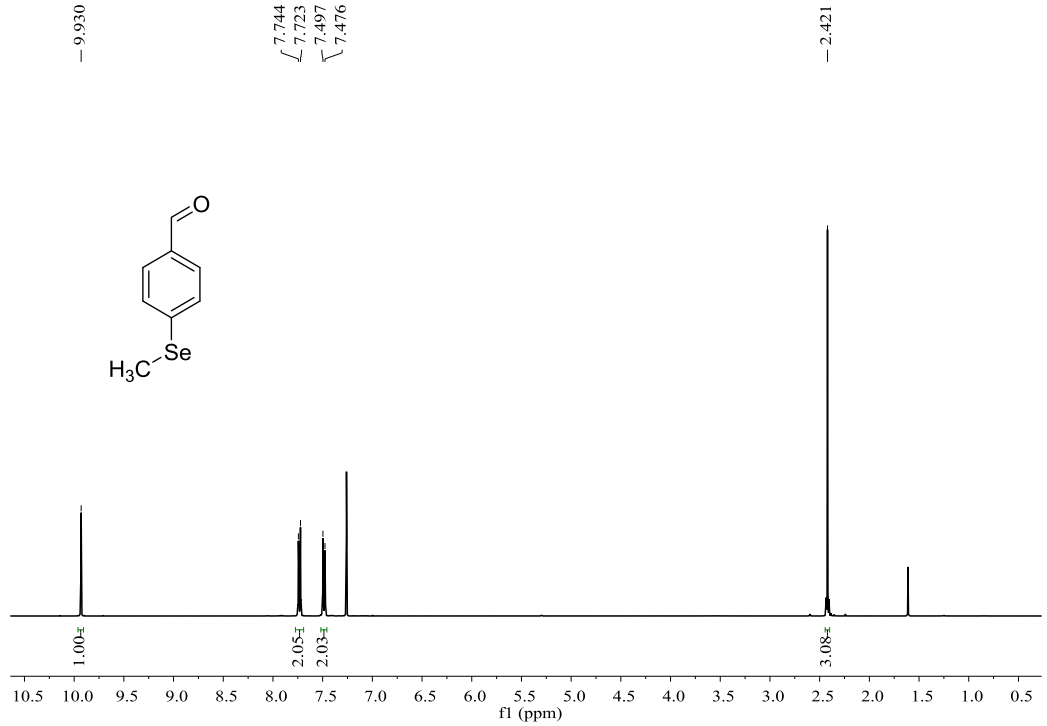


Figure S11. ^{1}H NMR spectrum of **2**(SeMe) in $CDCl_3$.

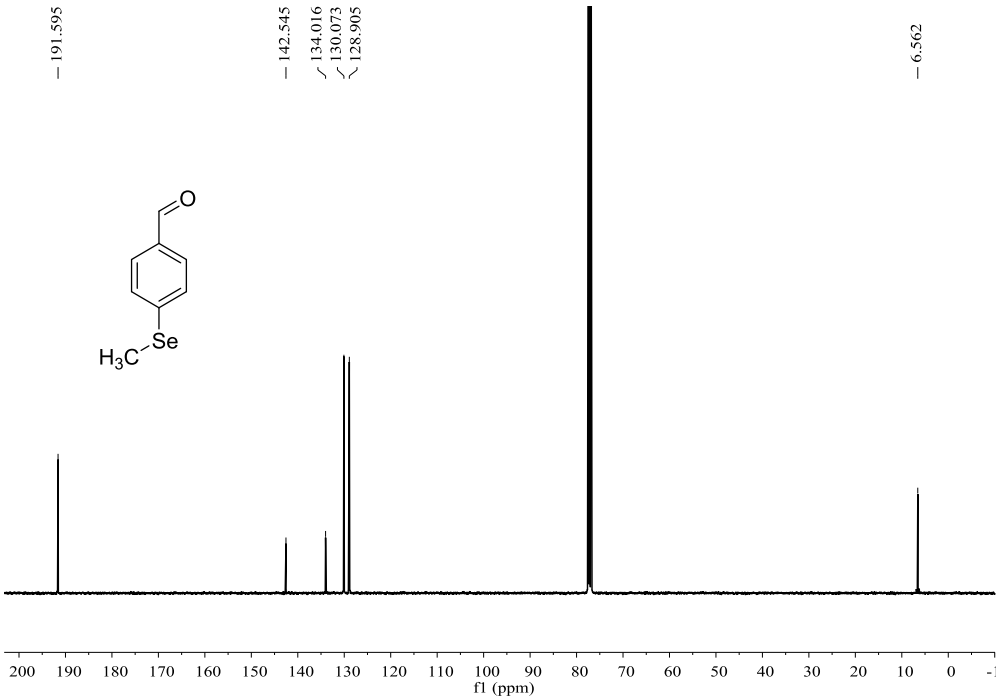


Figure S12. ^{13}C NMR spectrum of **2**(SeMe) in $CDCl_3$.

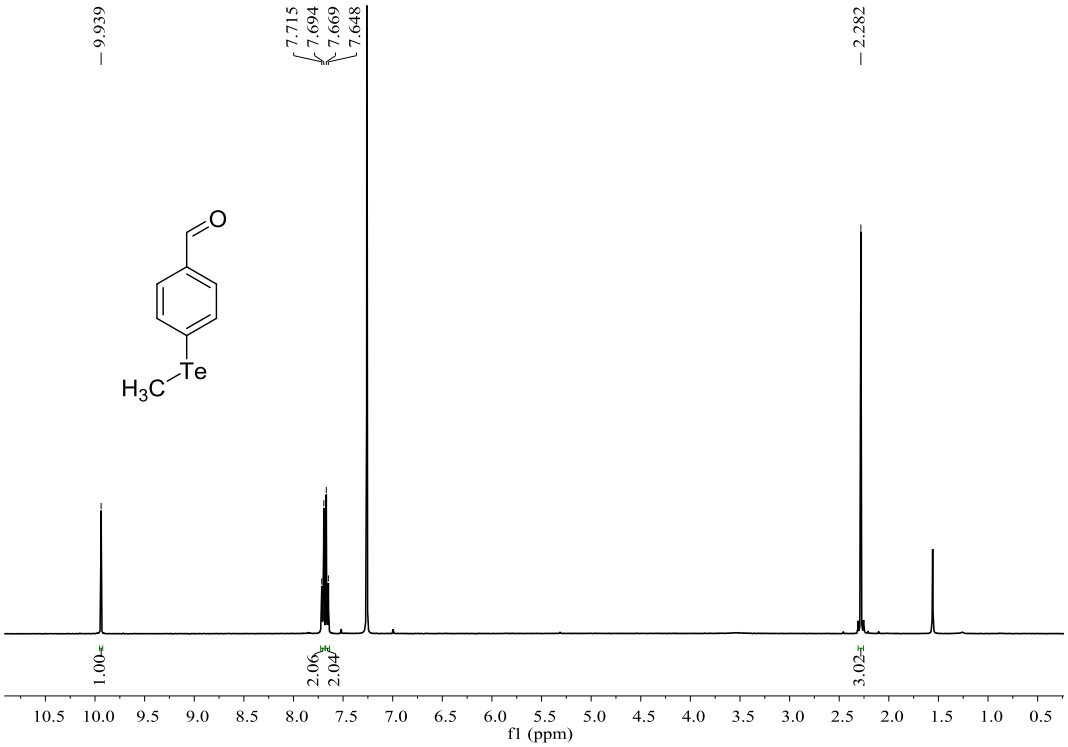


Figure S13. ^{1}H NMR spectrum of **2**(TeMe) in $CDCl_3$.

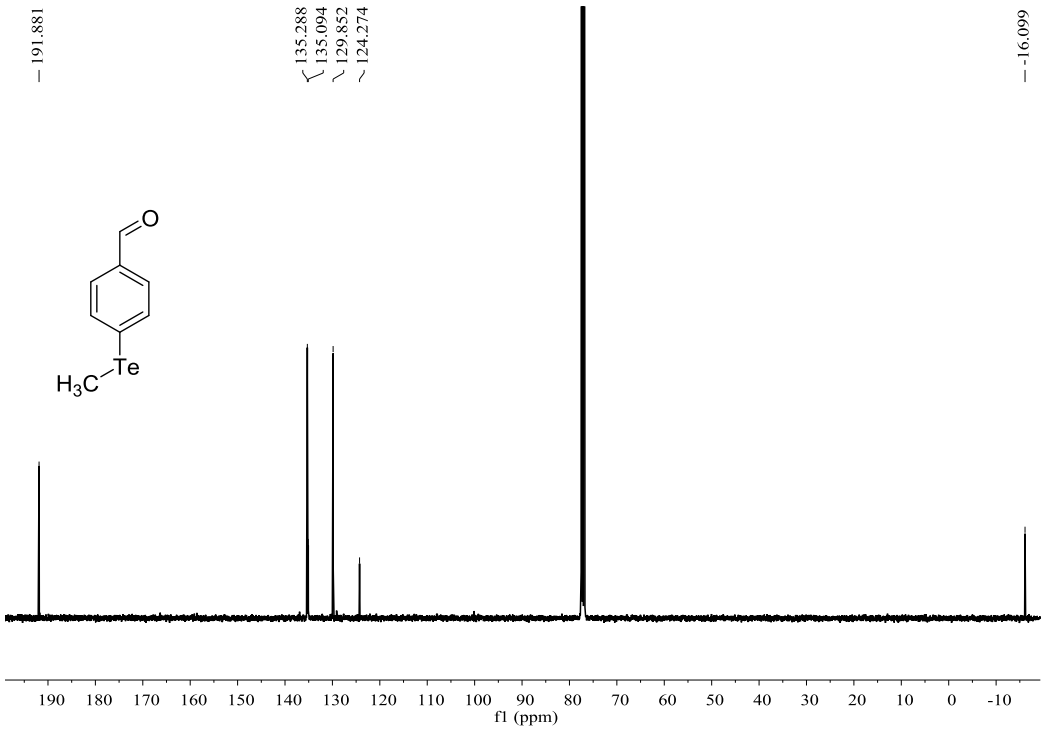


Figure S14. ^{13}C NMR spectrum of **2**(TeMe) in $CDCl_3$.

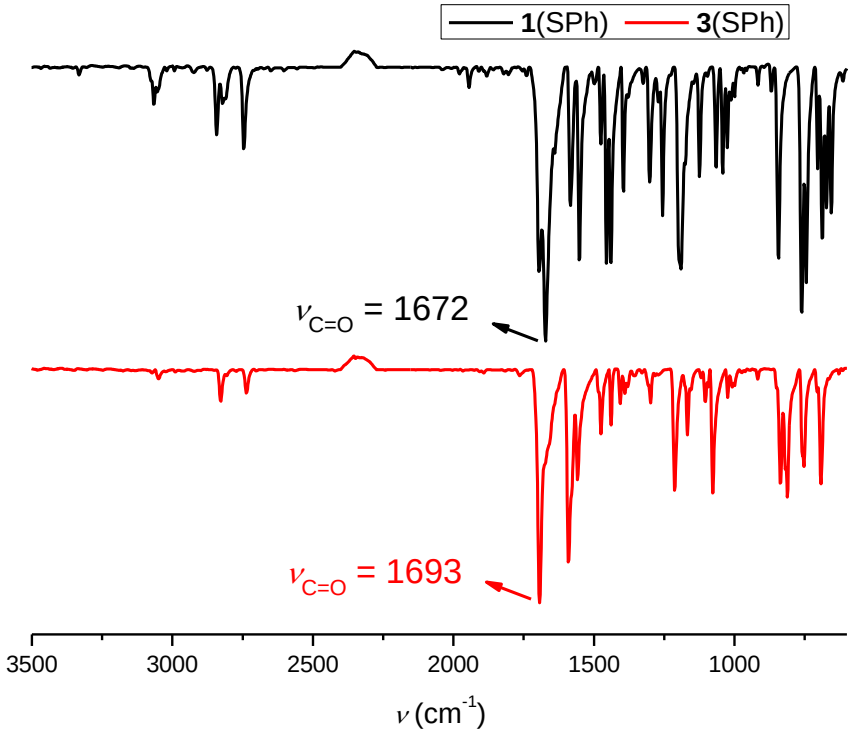


Figure S15. IR spectra of **1**(SPh) and **3**(SPh).

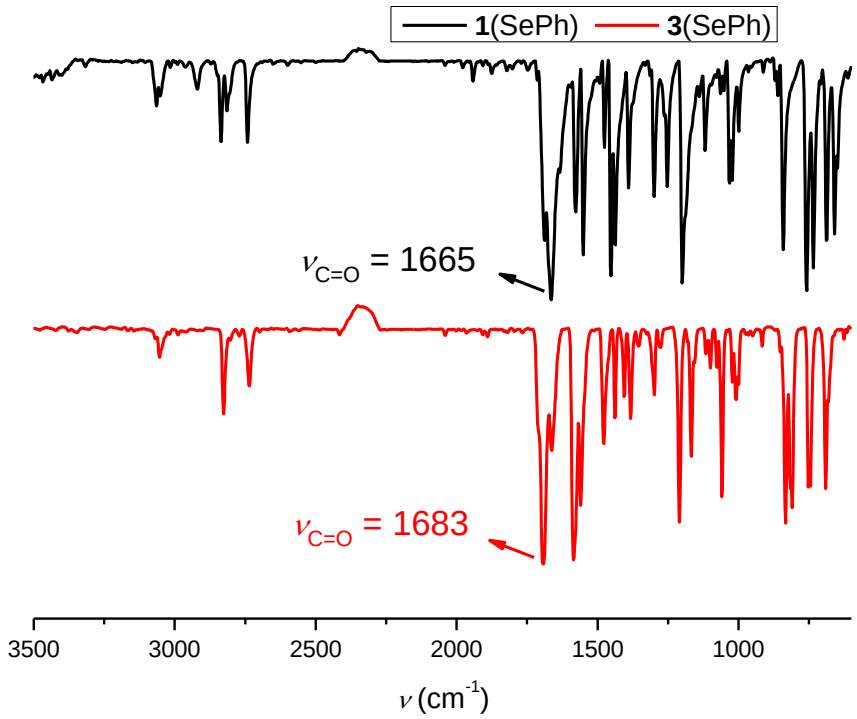


Figure S16. IR spectra of **1**(SePh) and **3**(SePh).

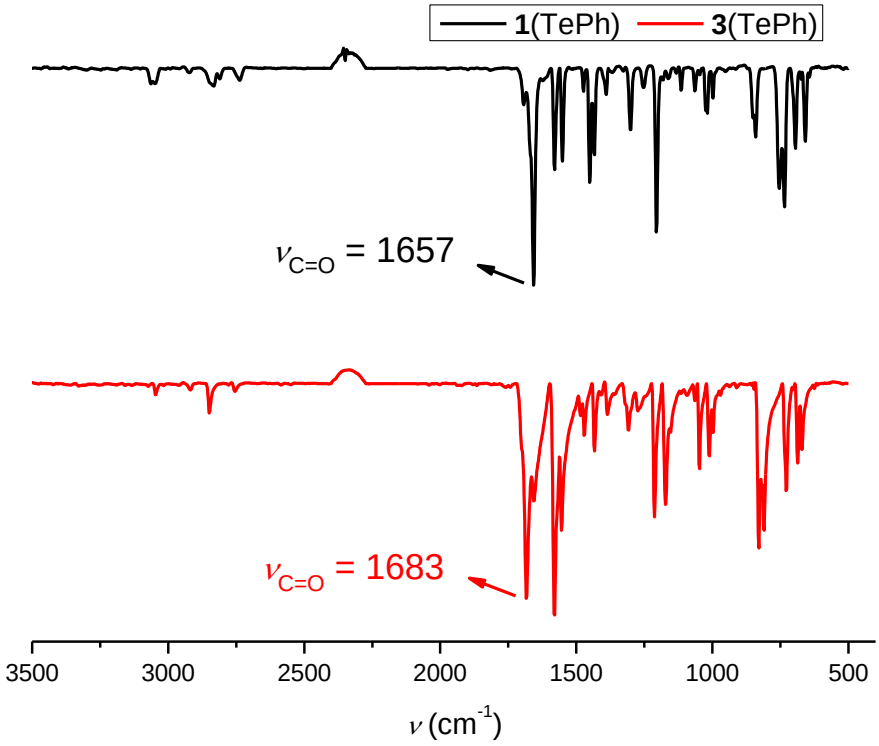


Figure S17. IR spectra of **1**(TePh) and **3**(TePh).

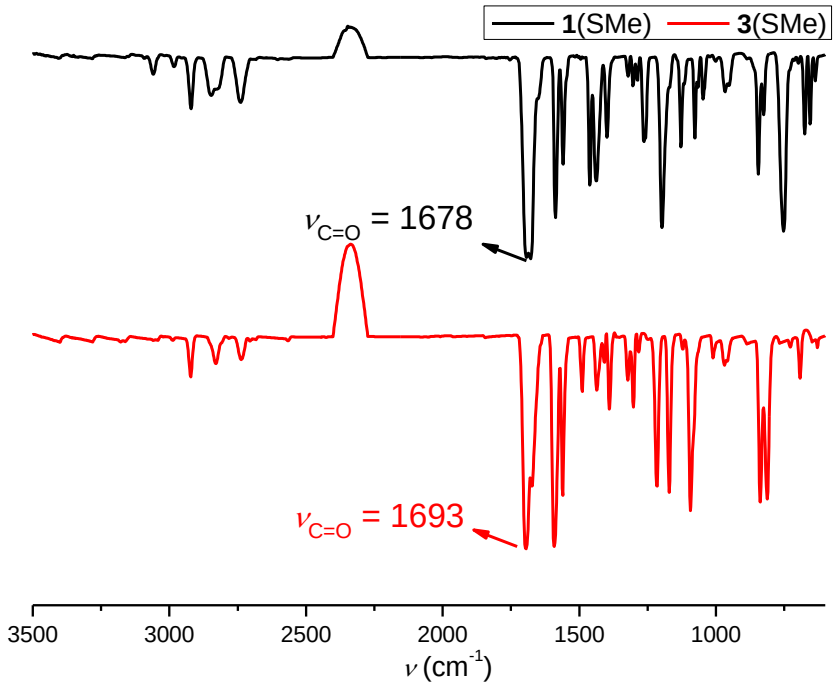


Figure S18. IR spectra of **1**(SMe) and **3**(SMe).

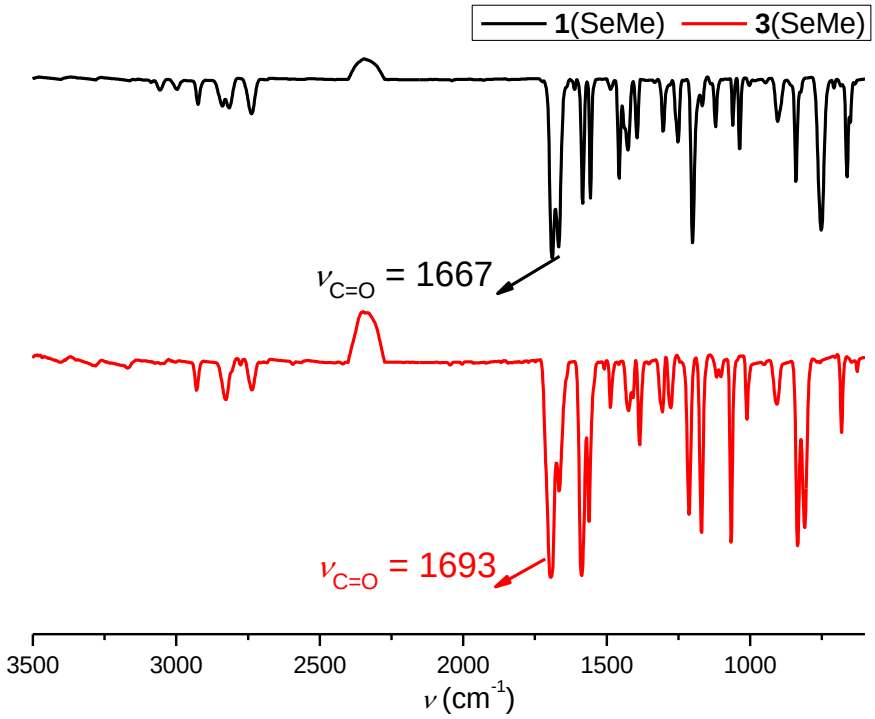


Figure S19. IR spectra of **1**(SeMe) and **3**(SeMe).

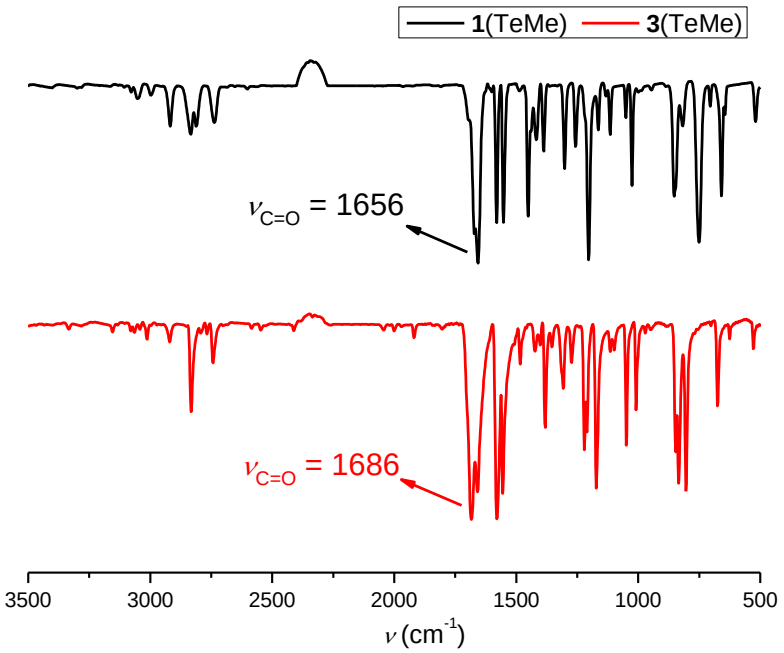


Figure S20. IR spectra of **1**(TeMe) and **3**(TeMe).

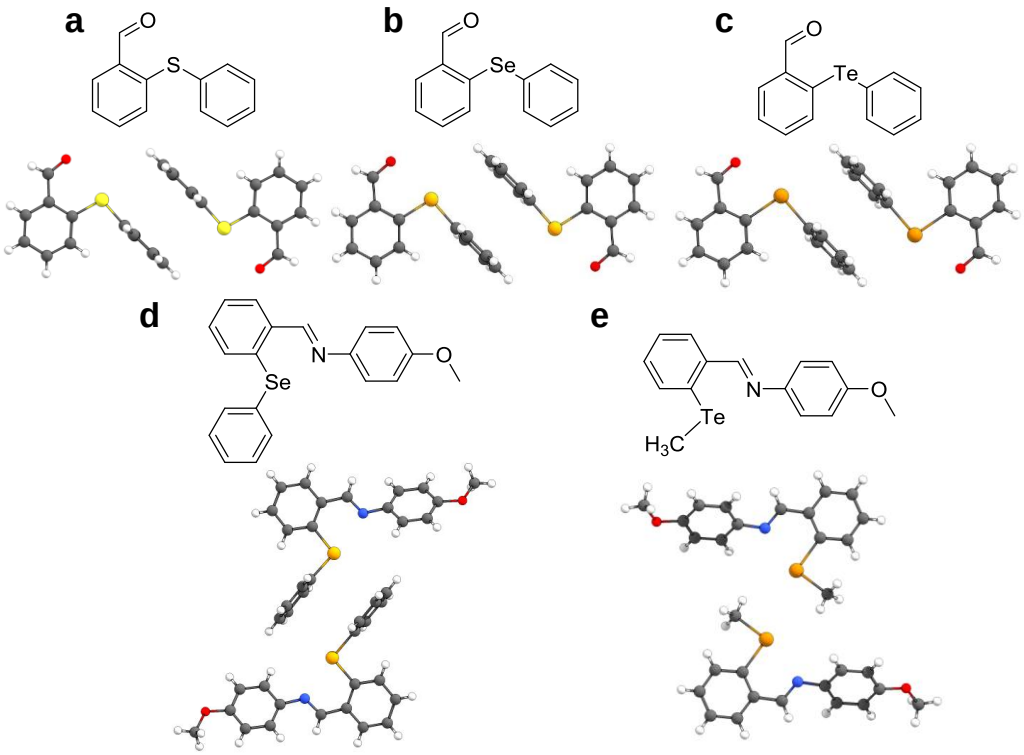


Figure S21. Crystal structures of **1**(SPh) (a), **1**(SePh) (b), **1**(TePh) (c), **2**(SePh) (d), and **2**(TeMe) (e).

Table S1. Summary of crystallographic data for **1**(ChPh), **2**(SePh).and **2**(TeMe).

	1(SPh)	**1**(SePh)	**1**(TePh)	**2**(SePh)	**2**(TeMe)
Formula	$C_{13}H_{10}OS$	$C_{13}H_{10}OSe$	$C_{52}H_{40}O_4Te_4$	$C_{40}H_{34}N_2O_2Se_2$	$C_{15}H_{15}NOTe$
Formula weight	214.29	261.18	1239.24	732.61	354.89
T / K	293	173	293	293	293
Crystallization solvent	Cyclohexane	CH_3CN	Cyclohexane	CH_3CN	CH_3CN
Color	Yellow	Yellow	Yellow	Yellow	Yellow
Crystal system	monoclinic	monoclinic	Triclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	P-1	$P2_1$	$P2_1/n$
a / Å	8.015(4)	7.970(3)	10.316(10)	11.837(4)	11.210(3)
b / Å	17.042(8)	17.025(8)	14.674(2)	9.820(4)	8.764(3)
c / Å	8.046(4)	8.191(4)	15.854(10)	15.814(5)	14.297(4)
α / °	90.00	90.00	86.359(10)	90.00	90.00
β / °	95.110(8)	96.584(4)	85.562(10)	110.667(4)	95.914(3)
γ / °	90.00	90.00	77.915(10)	90.00	90.00
V / Å^3	1094.6(9)	1104.0(9)	2336.8(4)	1719.7(11)	1397.2(7)
Z	4	4	2	2	4
D_x / g cm^{-3}	1.300	1.571	1.761	1.415	1.687
μ / mm^{-1}	0.263	2.982	13.420	2.031	11.428
F(000)	448	520	1184	744	692
θ range / °	2.39 to 27.44	4.52 to 48.87	2.43 to 60.572	2.61 to 59.82	5.14 to 60.32
GOF on F^2	0.980	1.060	0.986	0.983	1.087
R_1 [$I > 2\sigma(I)$]	0.0421	0.0289	0.0439	0.0470	0.0317
wR_2 (all data)	0.1216	0.0782	0.1217	0.1293	0.932

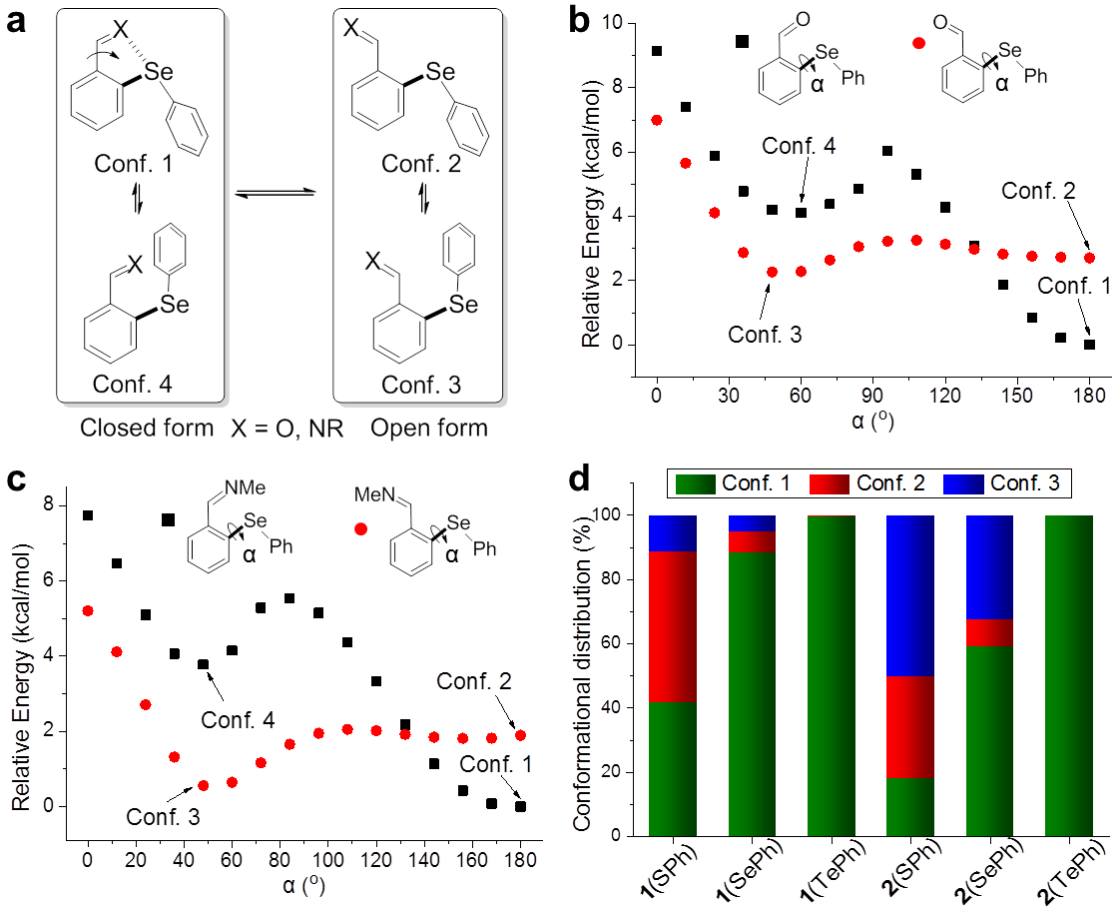


Figure S22. (a) The open and closed conformations of **1**(SePh) and **2**(SePh). (b) The plot of energies of open and closed conformers of **1**(SePh) versus α. (c) The plot of energies of open and closed conformers of **2**(SePh) versus α. (d) Comparison of conformer distribution of **1**(ChPh) and **2**(ChPh).

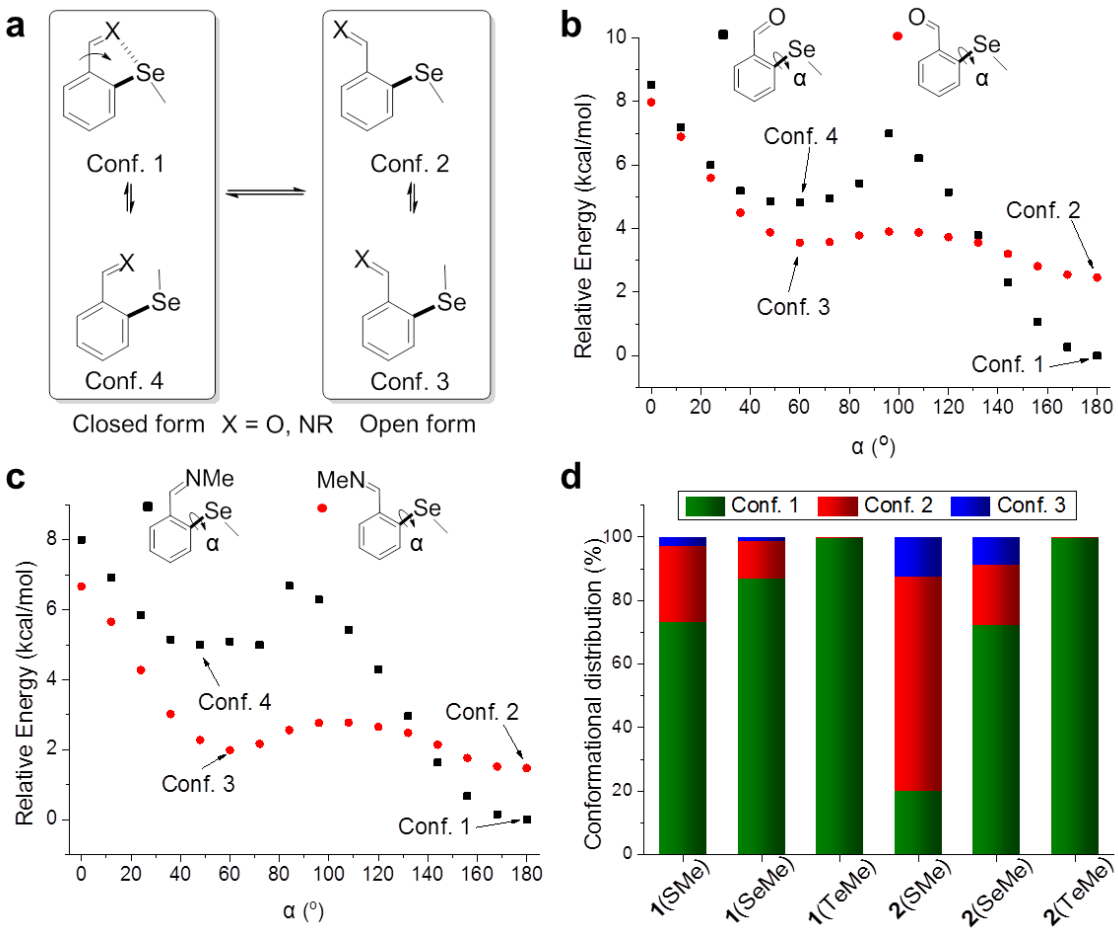


Figure S23. (a) The open and closed conformations of **1**(SeMe) and **2**(SeMe). (b) The plot of electronic energies of open and closed conformers of **1**(SeMe) versus α. (c) The plot of electronic energies of open and closed conformers of **2**(SeMe) versus α. α is defined with the rotation about C-SeMe bond (bold). (d) Comparison of conformer distribution of **1**(ChMe) and **2**(ChMe).

3. Dynamic Covalent Reactions

(1) Imine formation

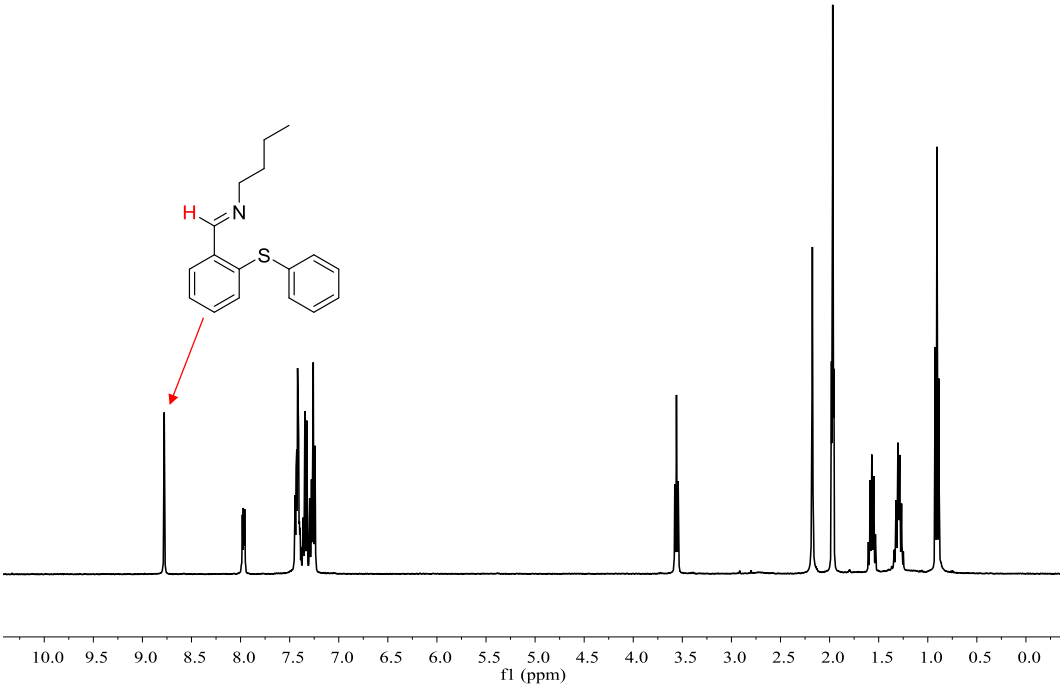


Figure S24. ^{1}H NMR spectrum of the reaction of **1**(SPh) and 1-butylamine in CD_3CN.

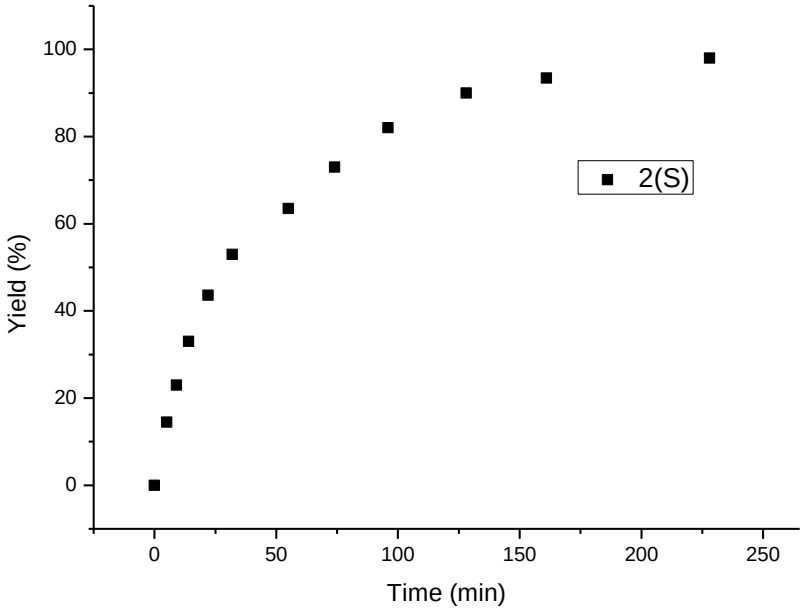


Figure S25. Kinetic profile of the reaction of **1**(SPh) and 1-butylamine in CD_3CN.

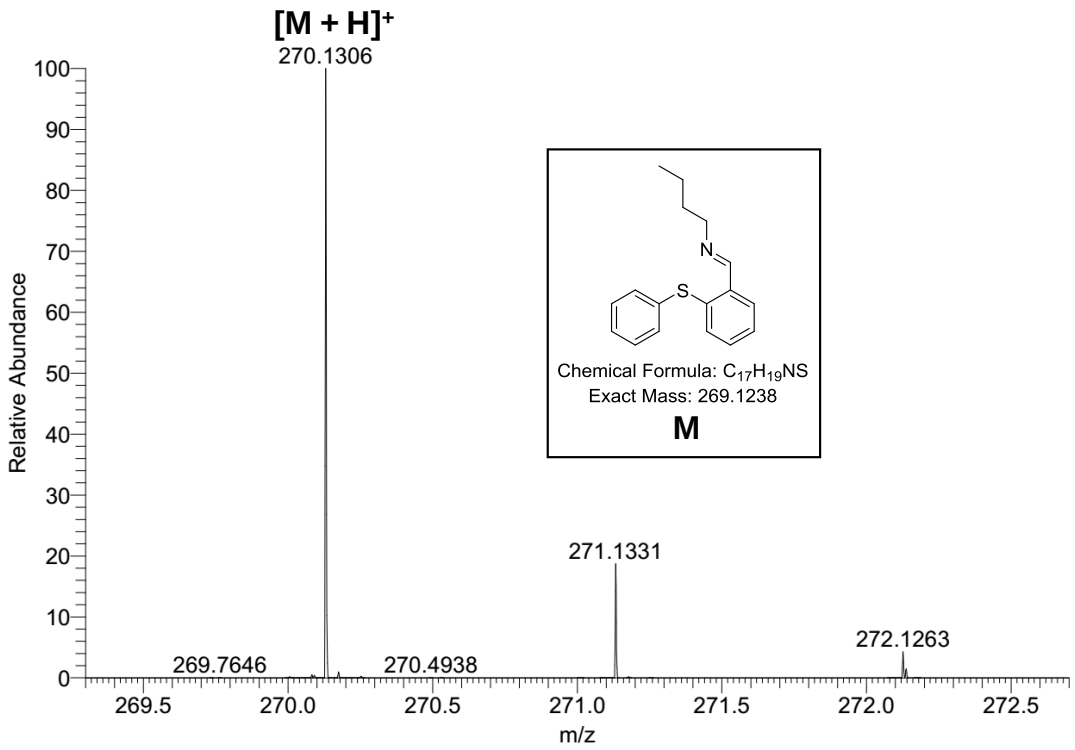


Figure S26. ESI-MS spectrum of the reaction of **1**(SPh) and 1-butylamine in CD_3CN.

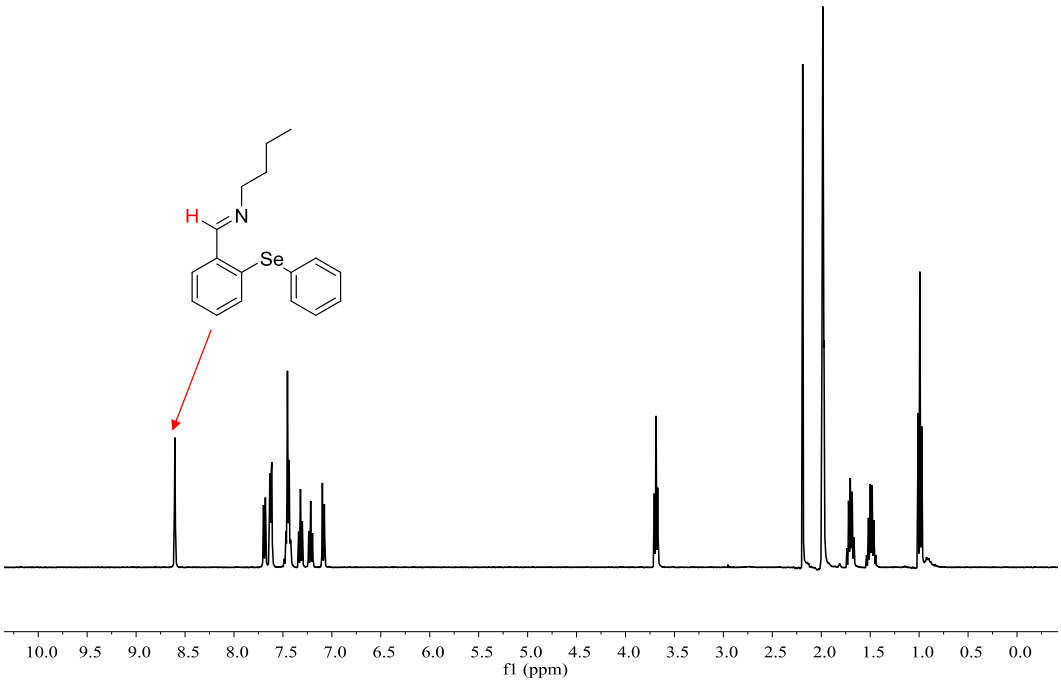


Figure S27. ^1H NMR spectrum of the reaction of **1**(SePh) and 1-butylamine in CD_3CN.

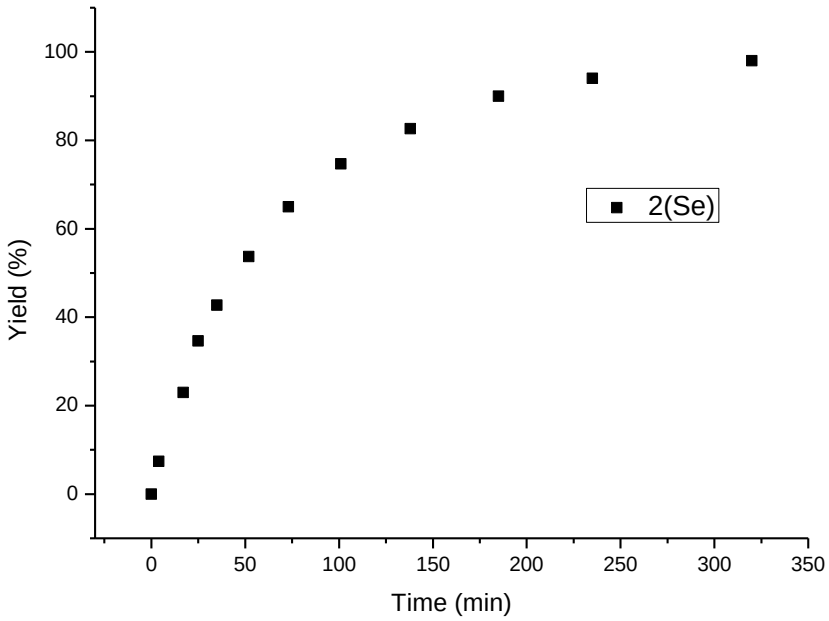


Figure S28. Kinetic profile of the reaction of **1**(SePh) and 1-butylamine in CD_3CN.

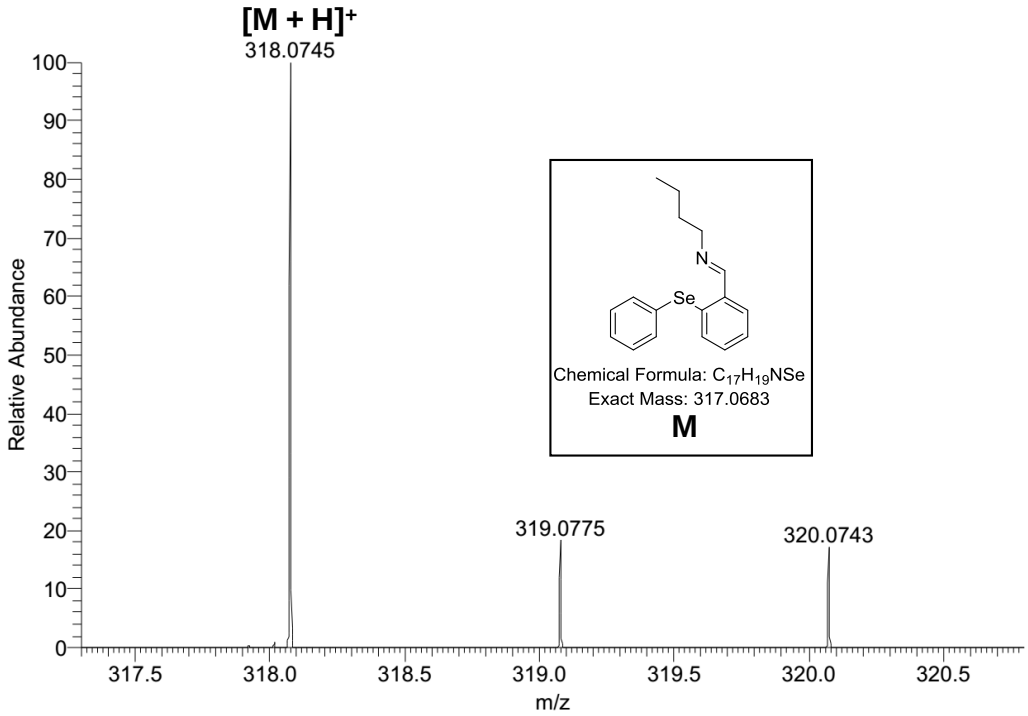


Figure S29. ESI-MS spectrum of the reaction of **1**(SePh) and 1-butylamine in CD_3CN.

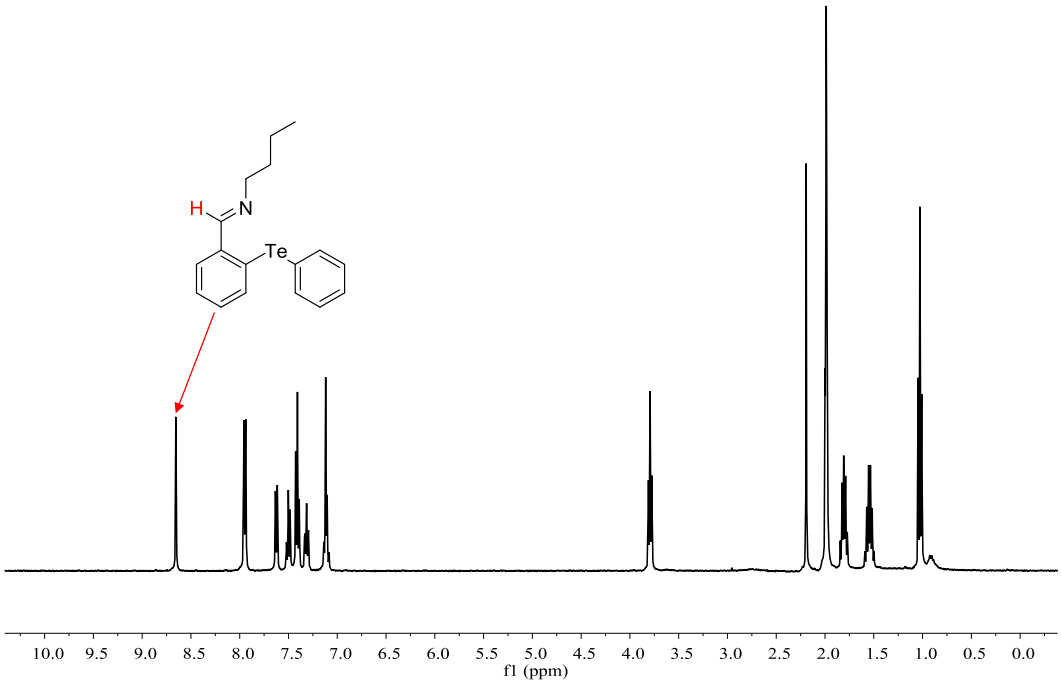


Figure S30. ^{1}H NMR spectrum of the reaction of **1**(TePh) and 1-butylamine in CD_3CN.

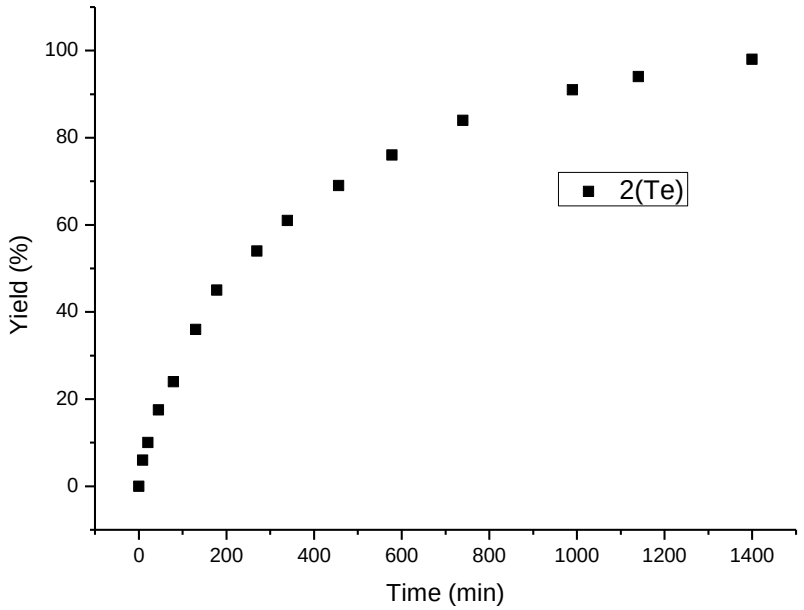


Figure S31. Kinetic profile of the reaction of **1**(TePh) and 1-butylamine in CD_3CN.

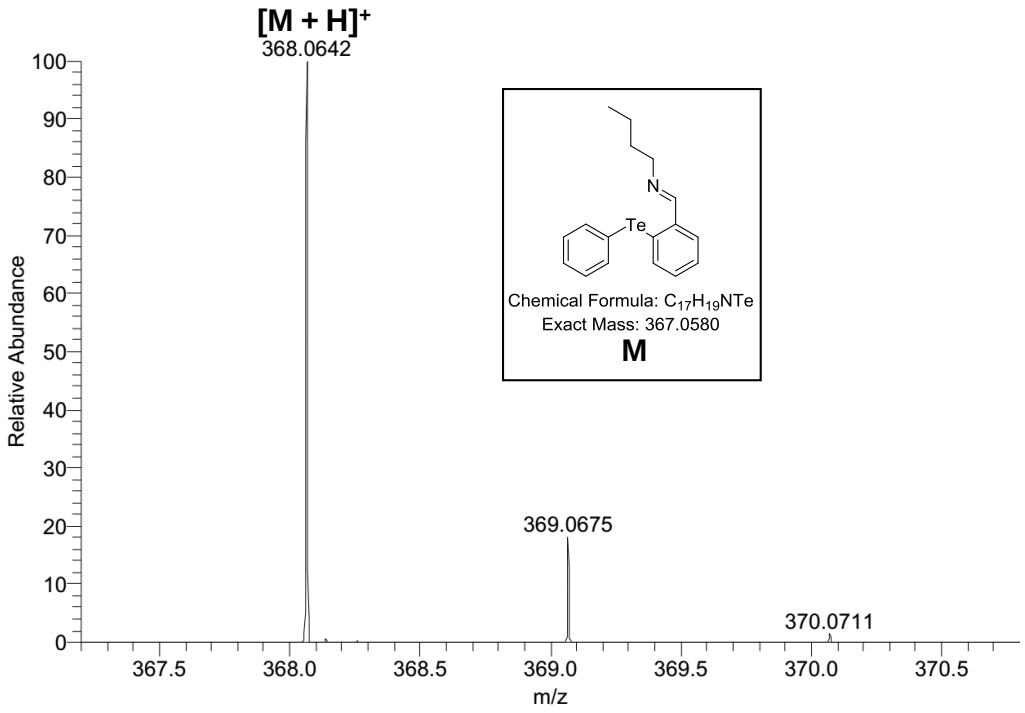


Figure S32. ESI-MS spectrum of the reaction of **1**(TePh) and 1-butylamine in CD_3CN.

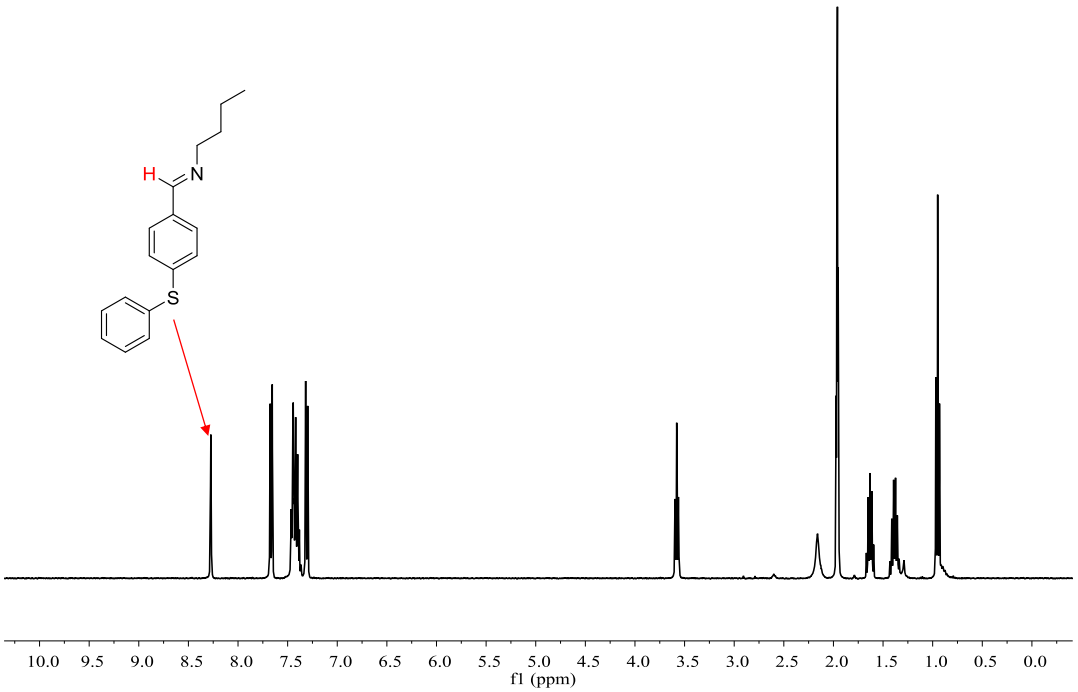


Figure S33. ^1H NMR spectrum of the reaction of **3**(SPh) and 1-butylamine in CD_3CN.

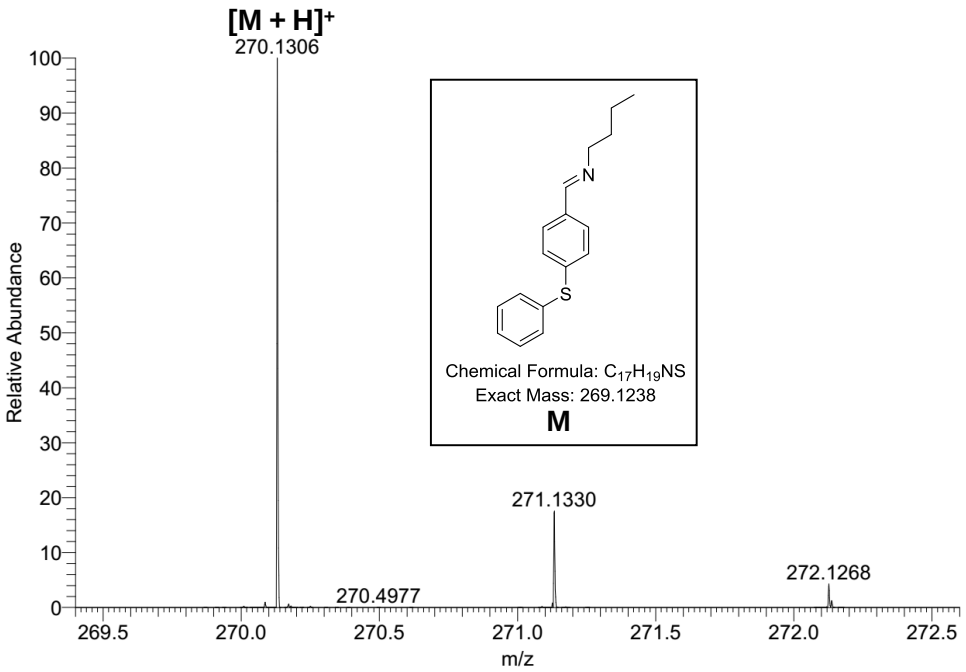


Figure S34. ESI-MS spectrum of the reaction of **3**(SPh) and 1-butylamine in CD_3CN.

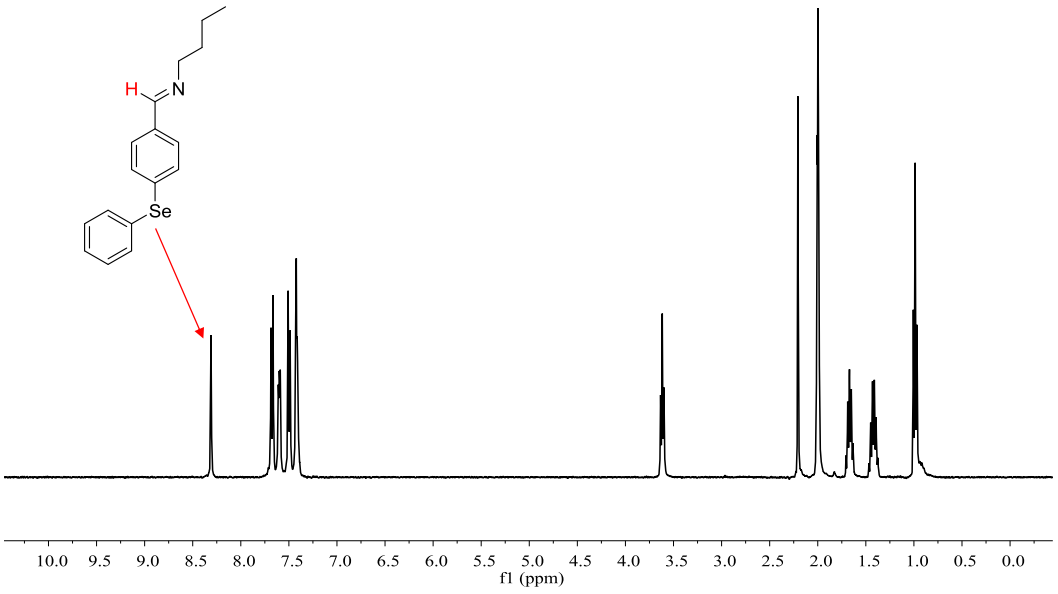


Figure S35. ^1H NMR spectrum of the reaction of **3**(SePh) and 1-butylamine in CD_3CN.

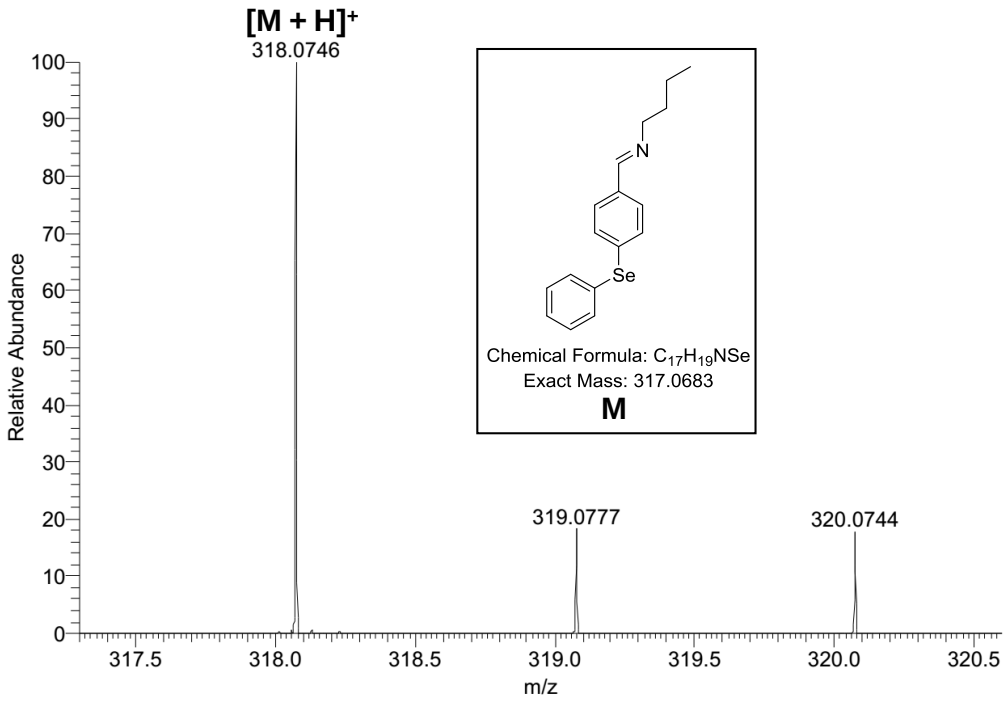


Figure S36. ESI-MS spectrum of the reaction of **3**(SePh) and 1-butylamine in CD_3CN.

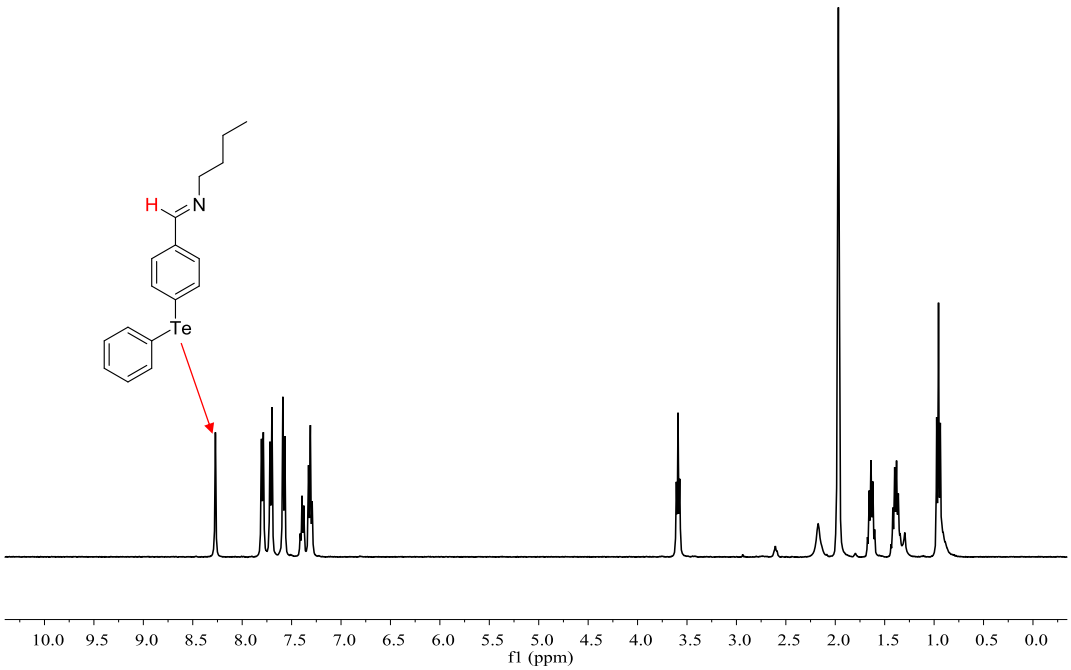


Figure S37. ^1H NMR spectrum of the reaction of **3**(TePh) and 1-butylamine in CD_3CN.

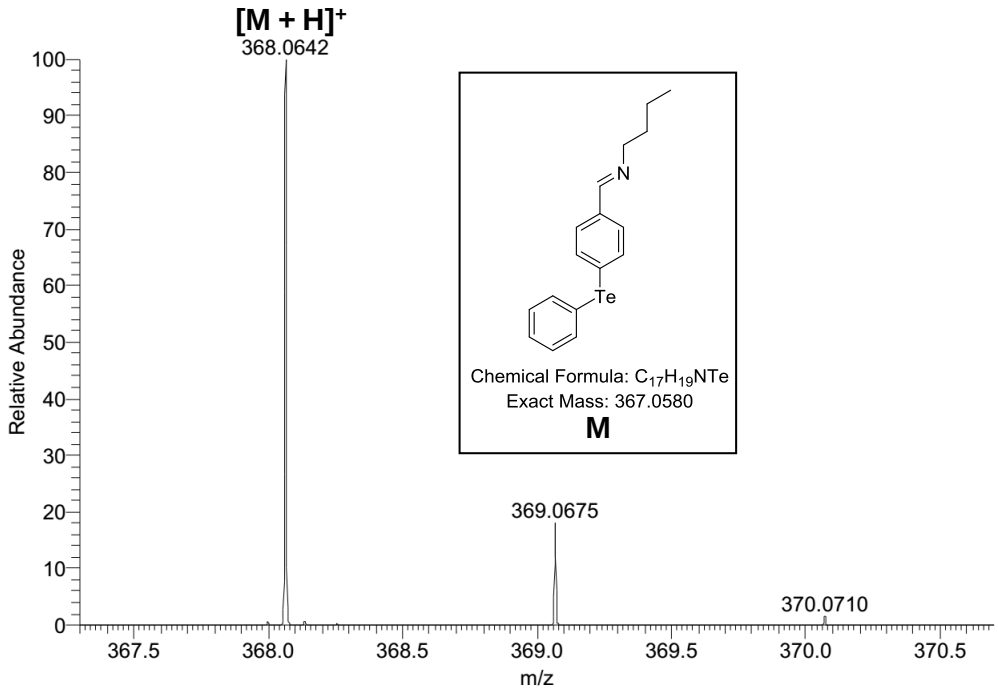


Figure S38. ESI-MS spectrum of the reaction of **3**(TePh) and 1-butylamine in CD_3CN.

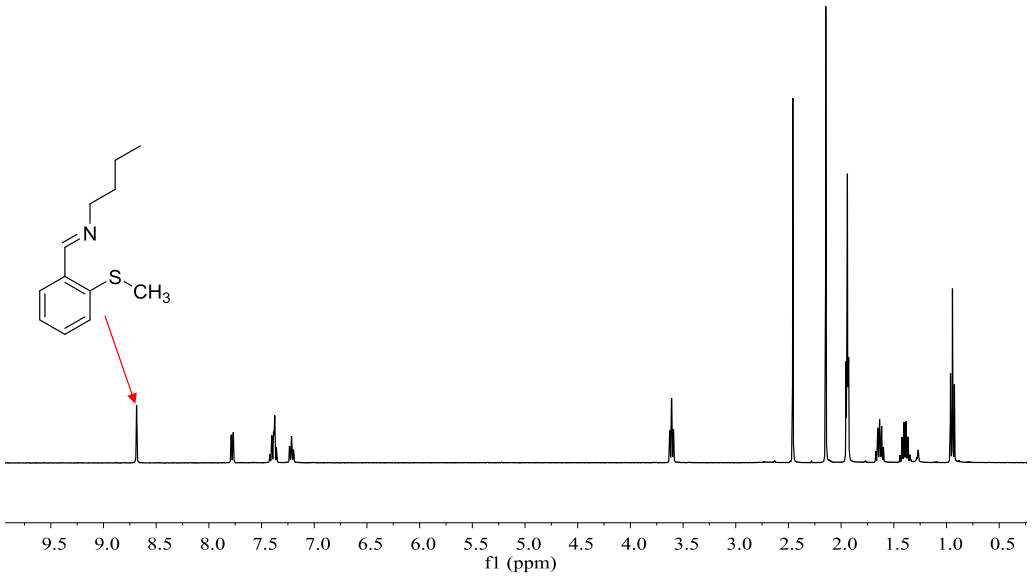


Figure S39. ^1H NMR spectrum of the reaction of **1**(SMe) and 1-butylamine in CD_3CN.

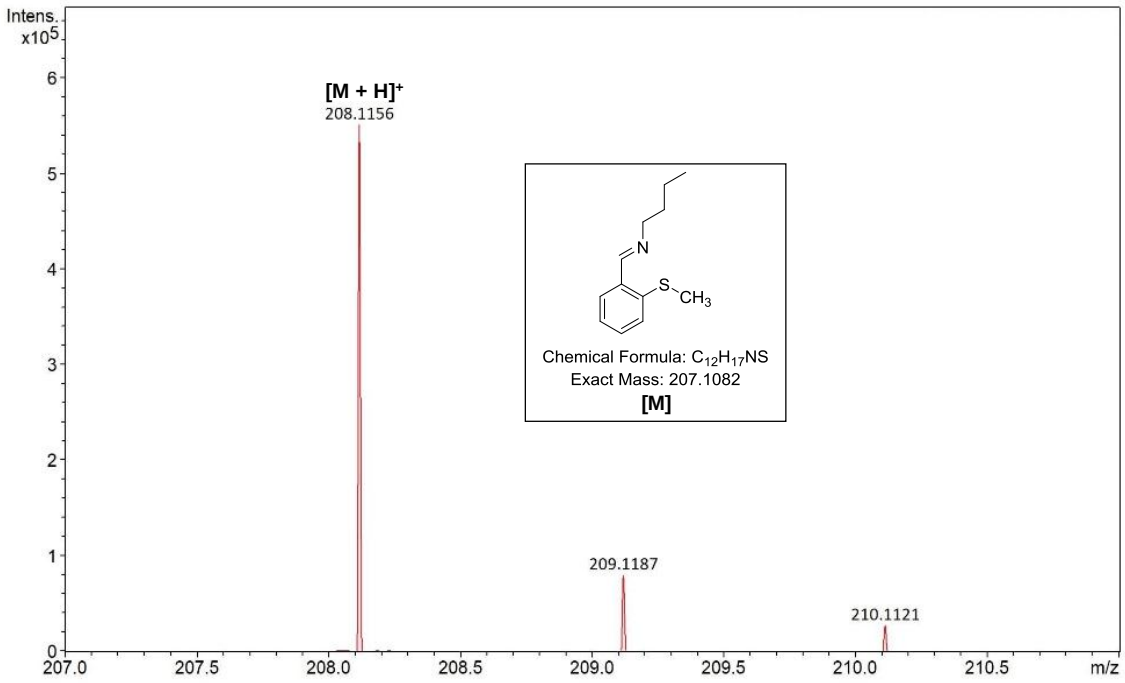


Figure S40. ESI-MS spectrum of the reaction of **1**(SMe) and 1-butylamine in CD_3CN.

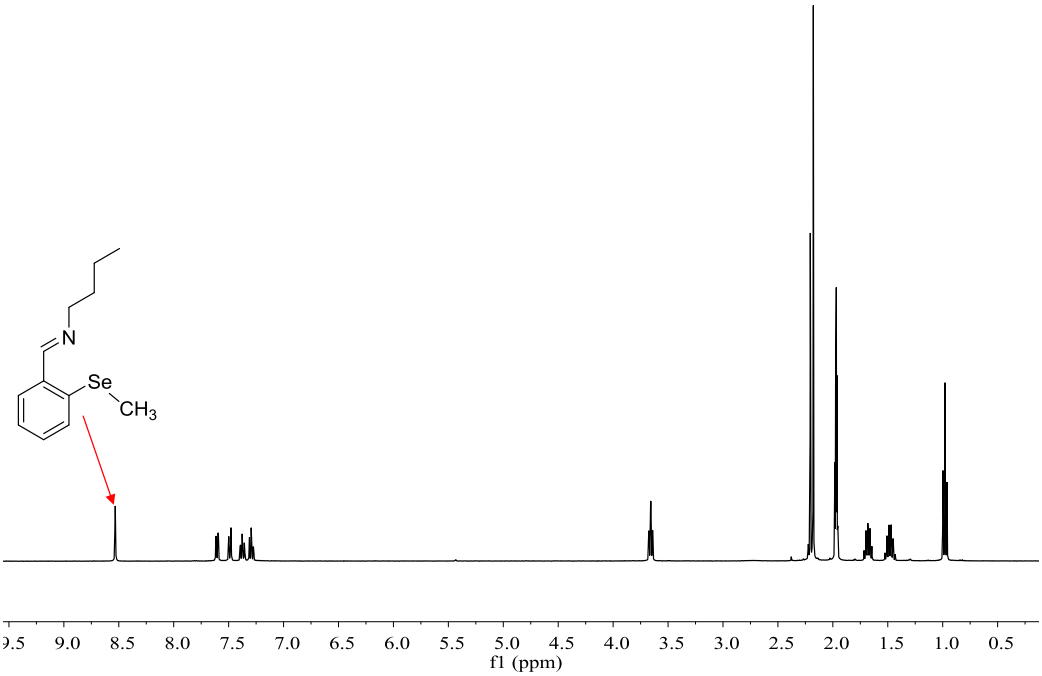


Figure S41. ^1H NMR spectrum of the reaction of **1**(SeMe) and 1-butylamine in CD_3CN.

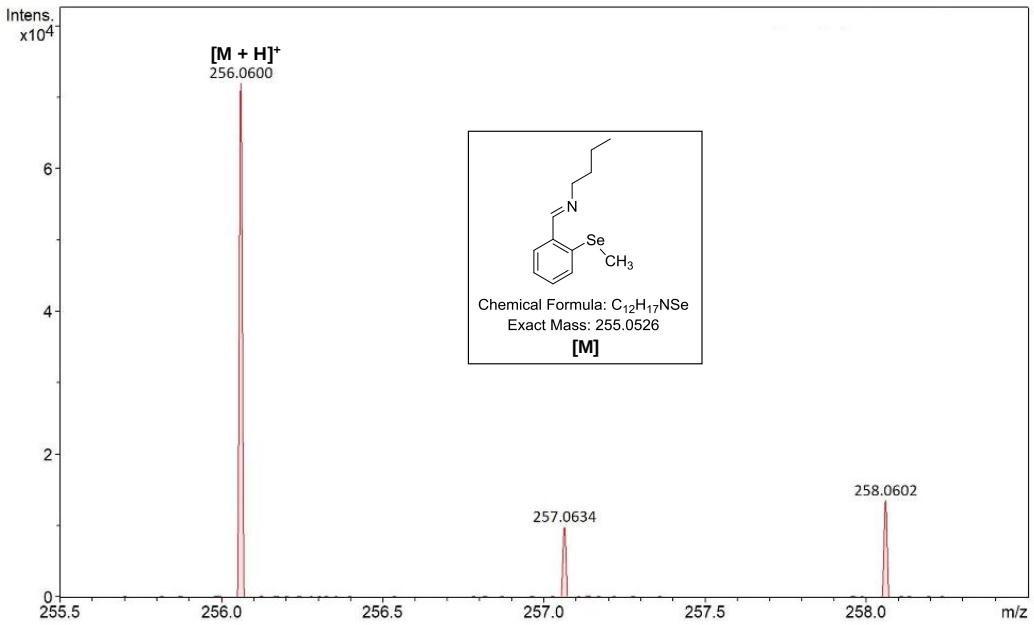


Figure S42. ESI-MS spectrum of the reaction of **1**(SeMe) and 1-butylamine in CD_3CN.

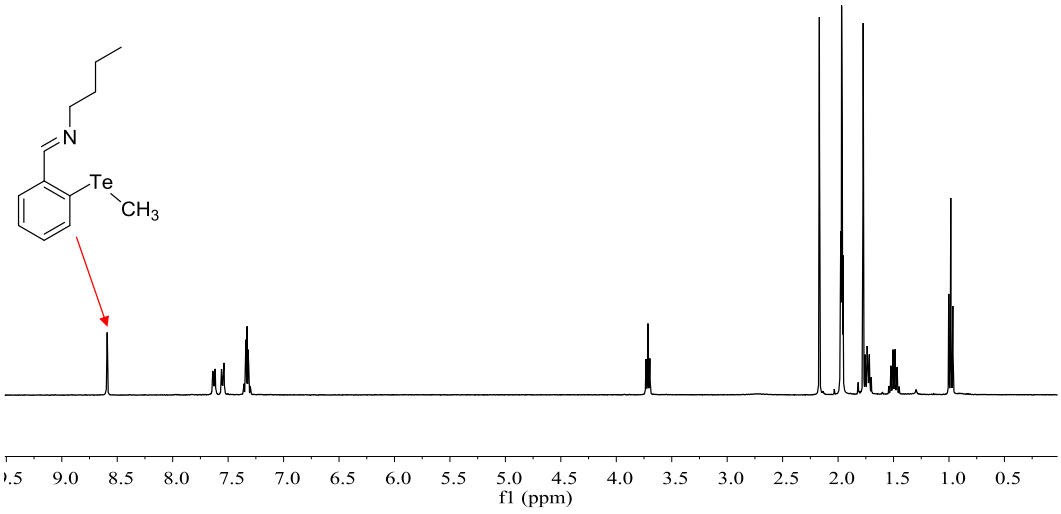


Figure S43. ^1H NMR spectrum of the reaction of **1**(TeMe) and 1-butylamine in CD_3CN.

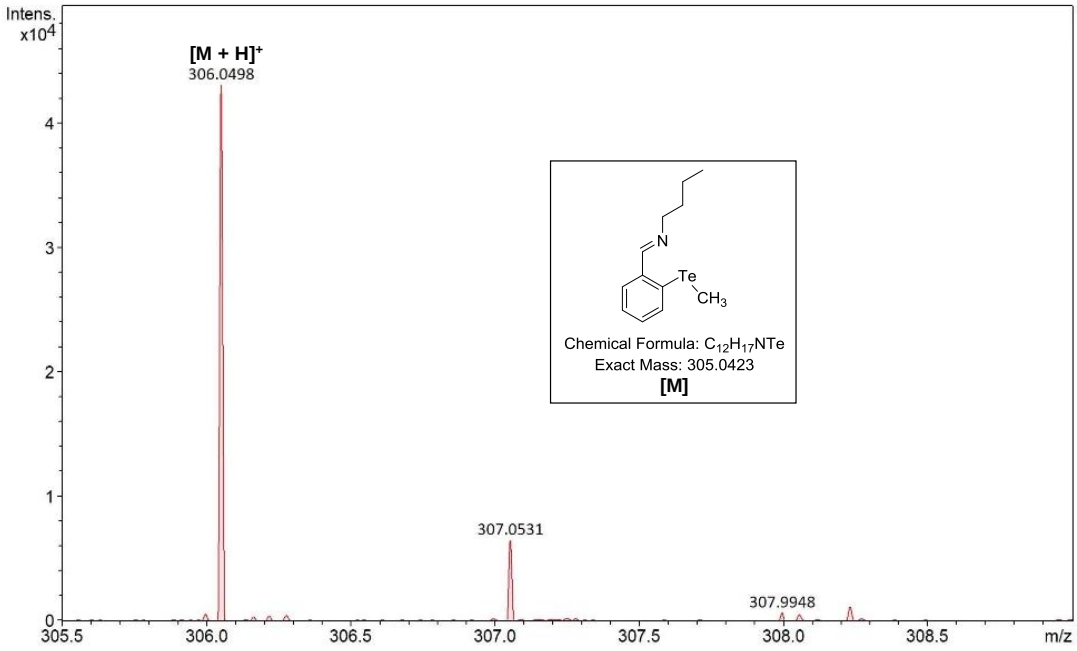


Figure S44. ESI-MS spectrum of the reaction of **1**(TeMe) and 1-butylamine in CD_3CN.

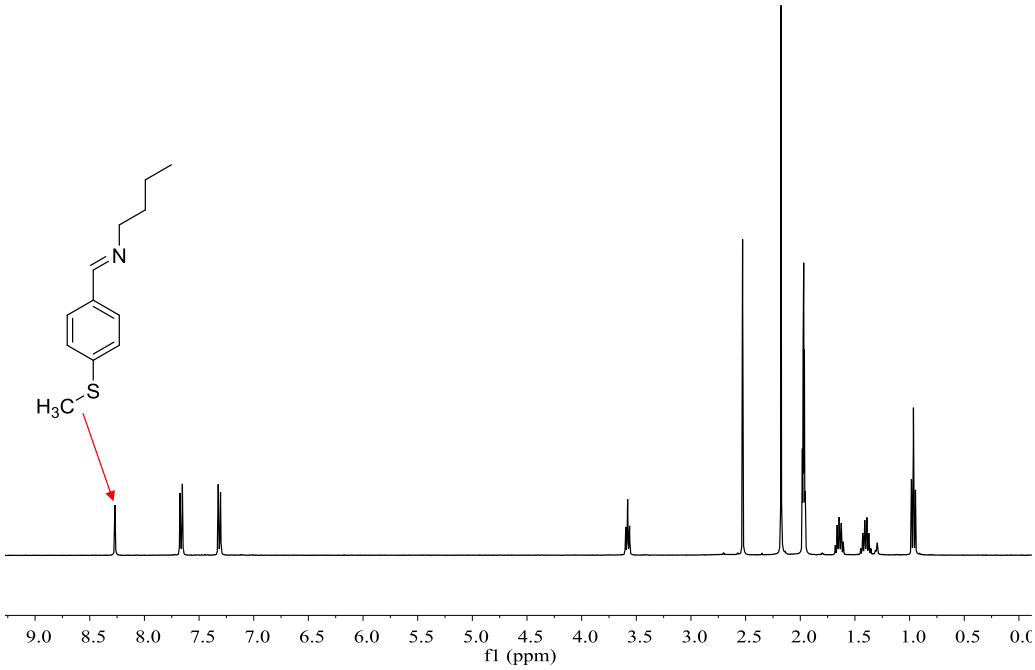


Figure S45. ^1H NMR spectrum of the reaction of **3**(SMe) and 1-butylamine in CD_3CN.

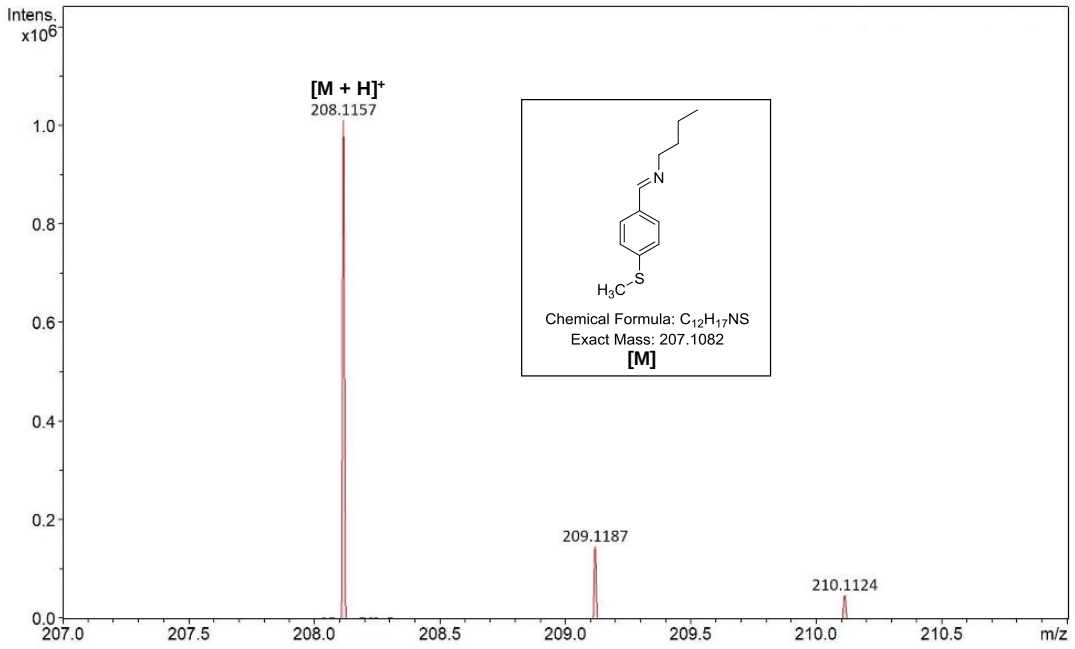


Figure S46. ESI-MS spectrum of the reaction of **3**(SMe) and 1-butylamine in CD_3CN.

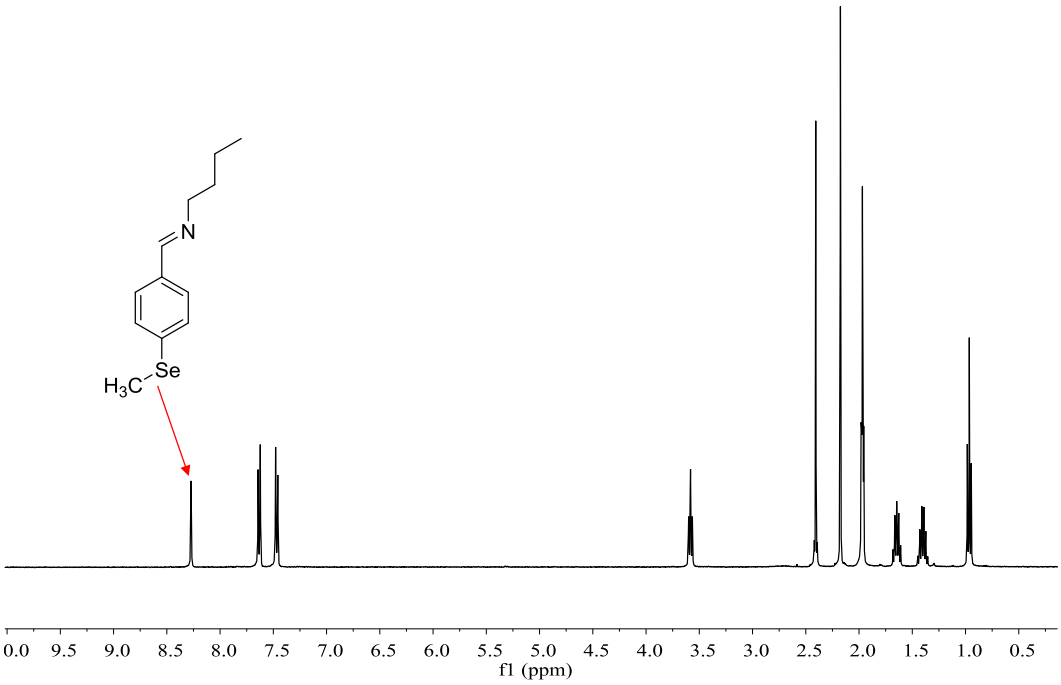


Figure S47. ^1H NMR spectrum of the reaction of **3**(SeMe) and 1-butylamine in CD_3CN.

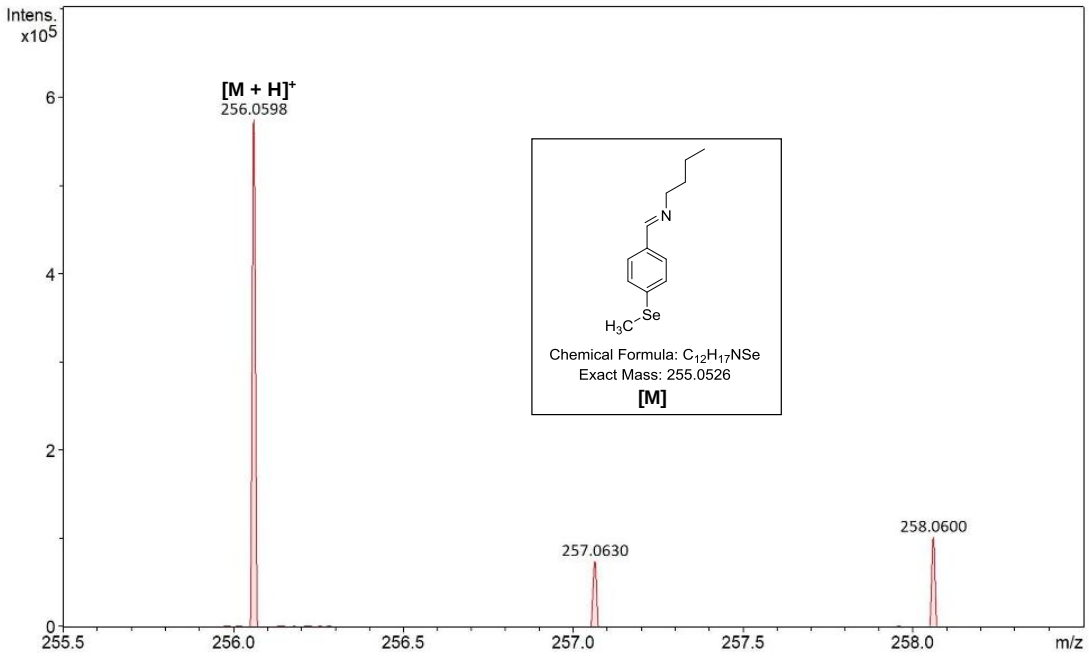


Figure S48. ESI-MS spectrum of the reaction of **3**(SeMe) and 1-butylamine in CD_3CN.

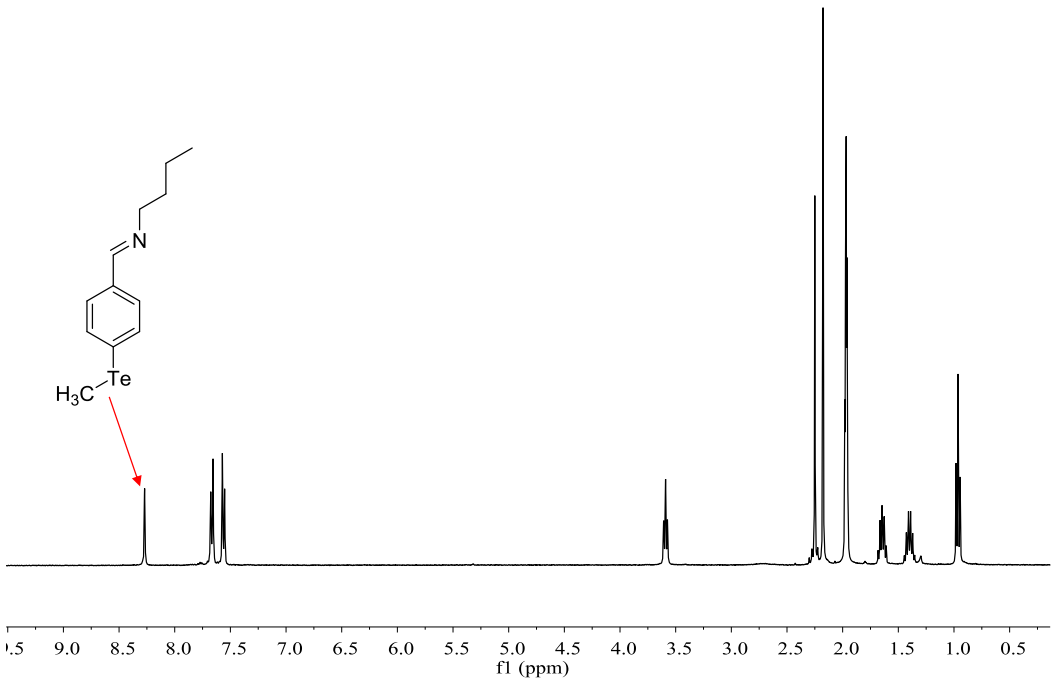


Figure S49. ^1H NMR spectrum of the reaction of **3**(TeMe) and 1-butylamine in CD_3CN.

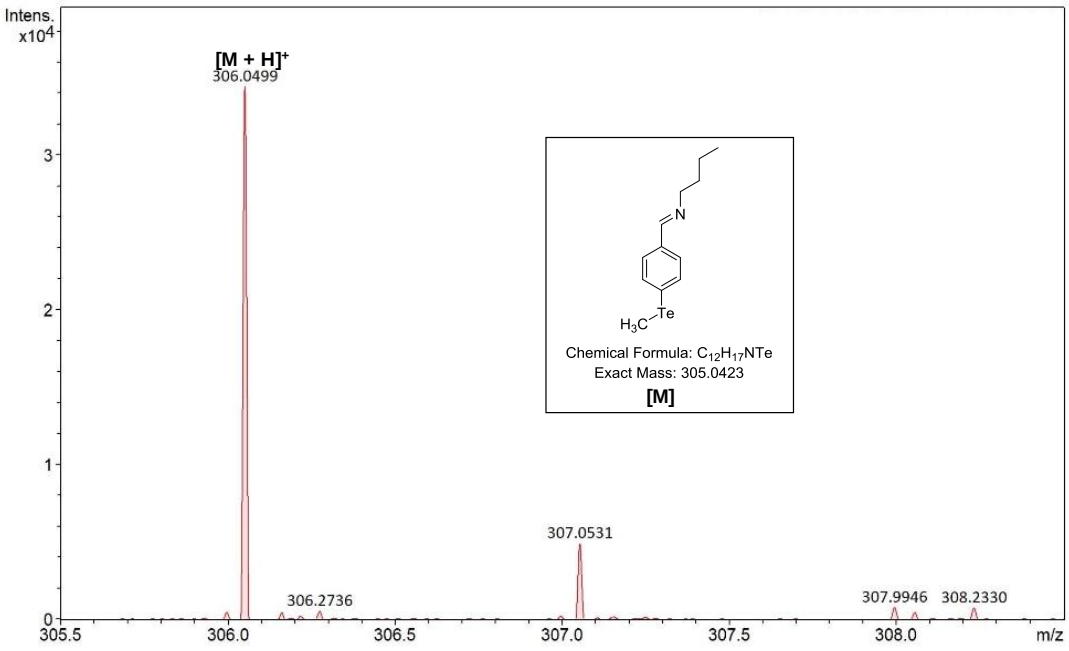


Figure S50. ESI-MS spectrum of the reaction of **3**(TeMe) and 1-butylamine in CD_3CN.

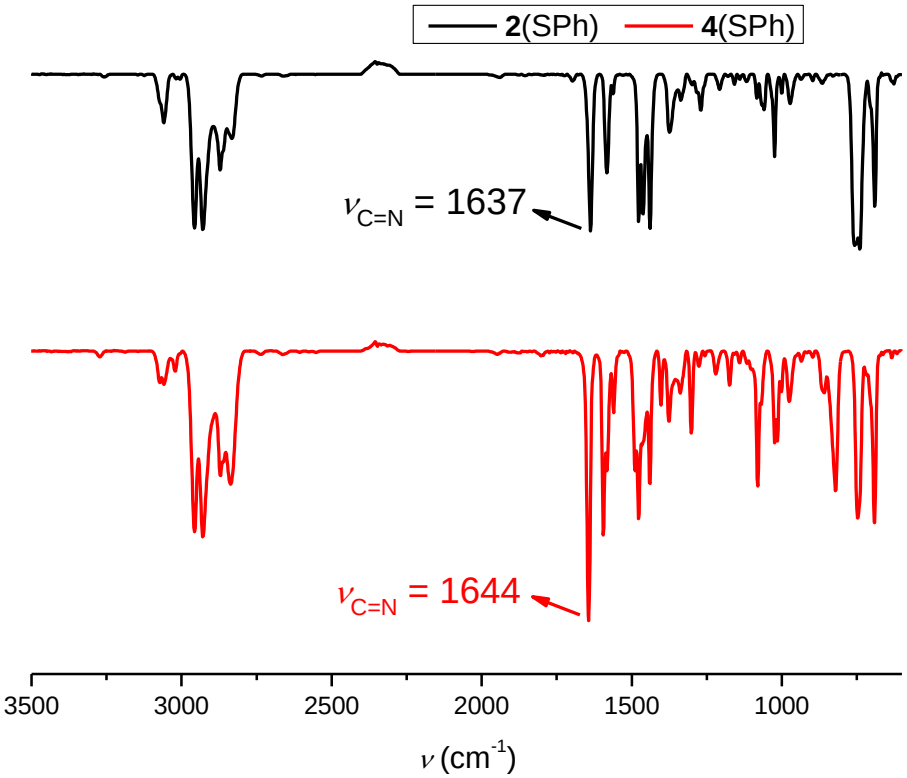


Figure S51. IR spectra of **2**(SPh) and **4**(SPh).

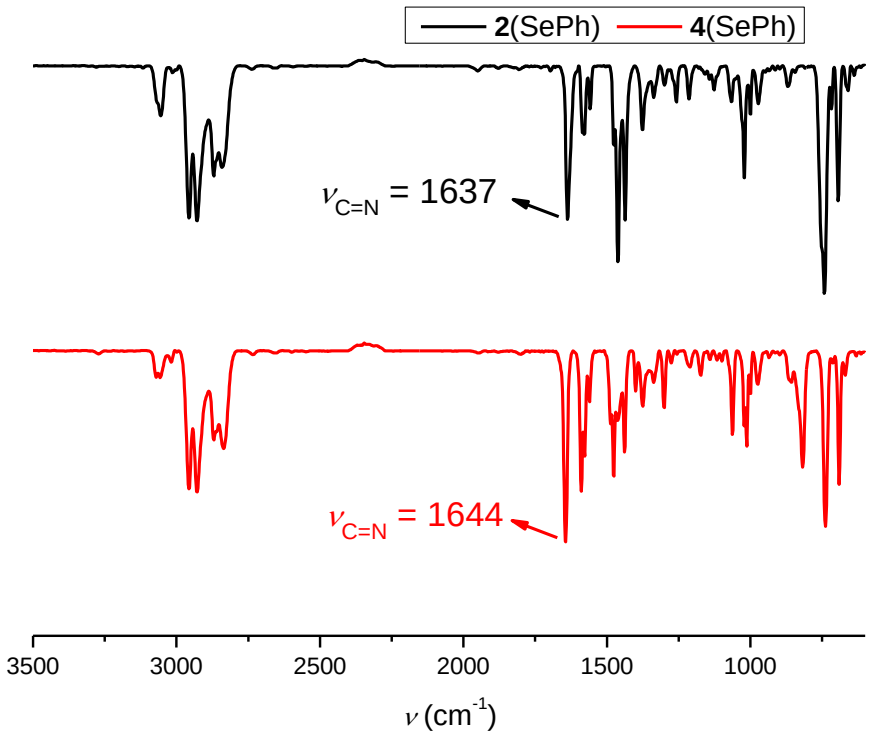


Figure S52. IR spectra of **2**(SePh) and **4**(SePh).

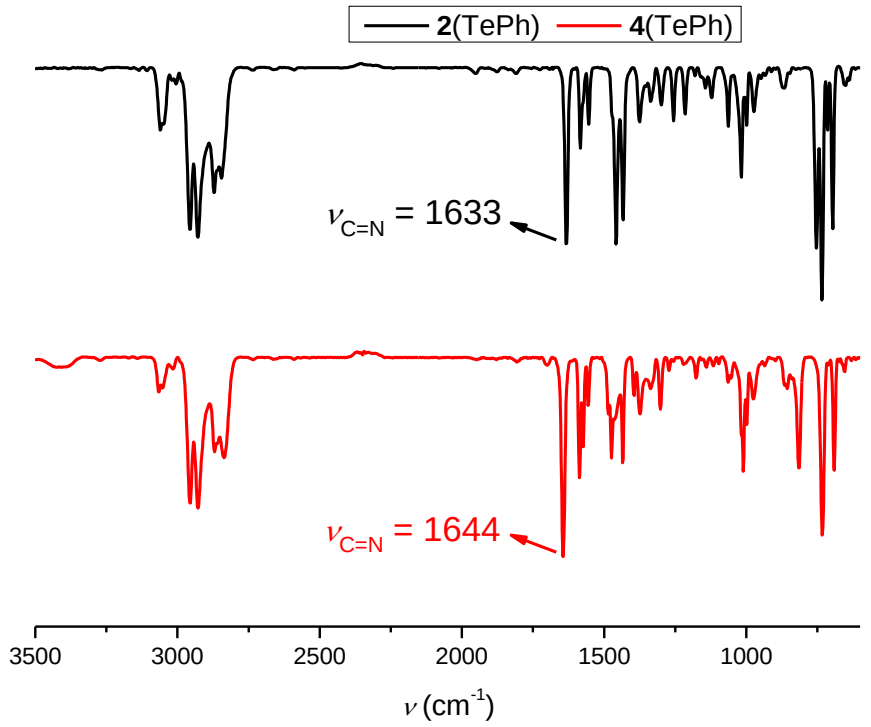
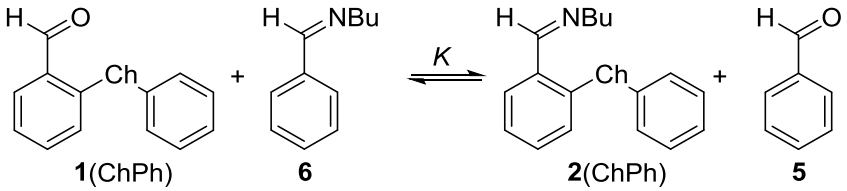


Figure S53. IR spectra of **2**(TePh) and **4**(TePh).

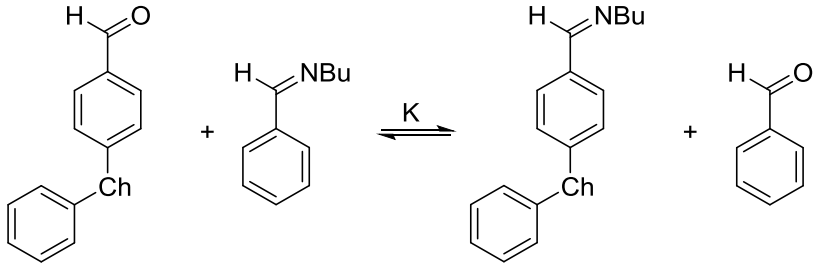
(2) Imine exchange

Table S2. The equilibrium constant and equilibrating time of the different imine exchange reactions in CD_3CN.



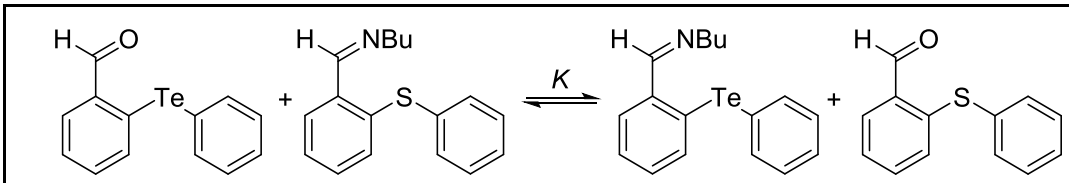
1(ChPh) **6** **2**(ChPh) **5**

Panel	Ch	Sequence of adding reagents	Solvent	*K*	Equilibrating time
a	S	**1**(ChPh) and **5** simultaneously reacted with 1-butylamine	CD_3CN	2.0	55 days
b	Se		CD_3CN	1.7	140 days
c	Te		CD_3CN	8.2	340 days



3(ChPh) **6** **4**(ChPh) **5**

Panel	Ch	Sequence of adding reagents	Solvent	*K*	Equilibrating time
d	S	**3**(ChPh) and **5** simultaneously reacted with 1-butylamine	CD_3CN	0.94	1 day
e	Se		CD_3CN	0.97	1 day
f	Te		CD_3CN	1.1	1 day



Panel	Sequence of adding reagents	Solvent	*Q*	Time
g	**1**(SPh) and **1**(TePh) simultaneously reacted with 1-butylamine	CD_3CN	0.23	375 days

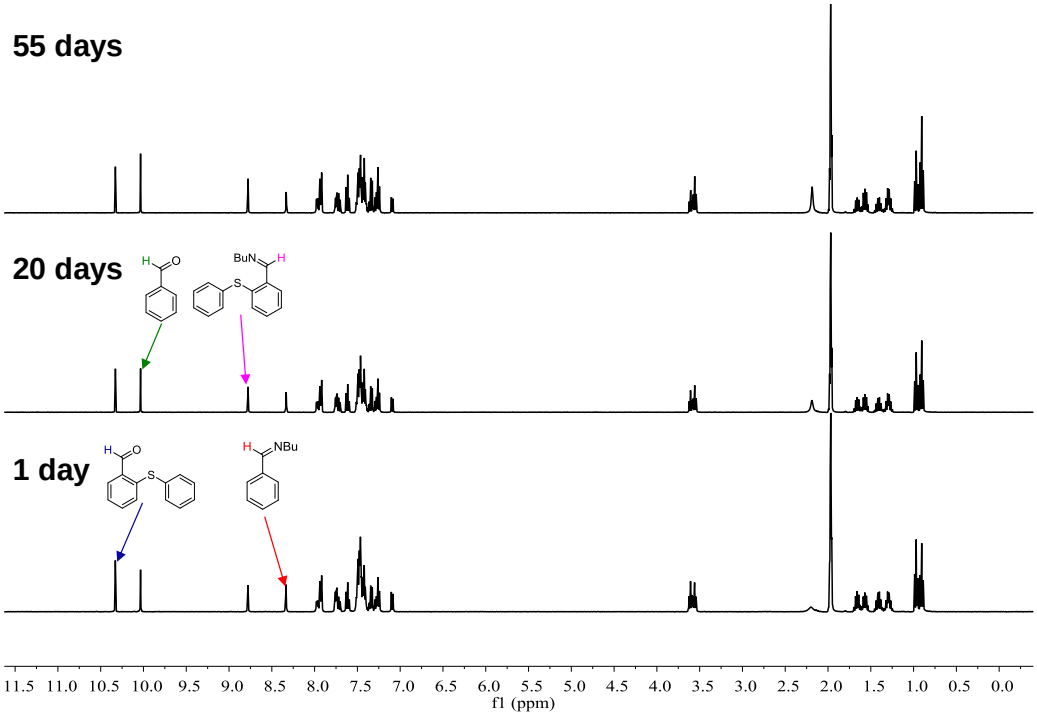


Figure S54. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** for the reaction with 1-butylamine in CD_3CN at varied time (the corresponding spectra of panel a in Table S2).

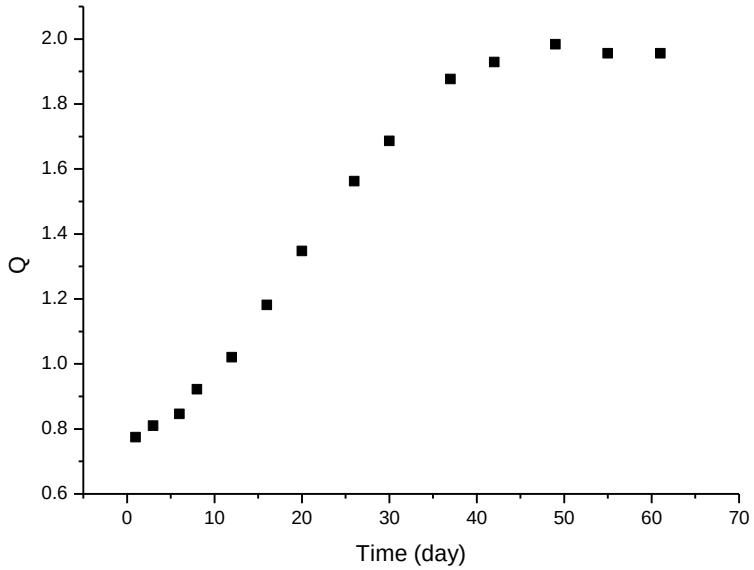


Figure S55. Kinetic profile of the competition between **1**(SPh) and **5** for the reaction with 1-butylamine in CD_3CN.

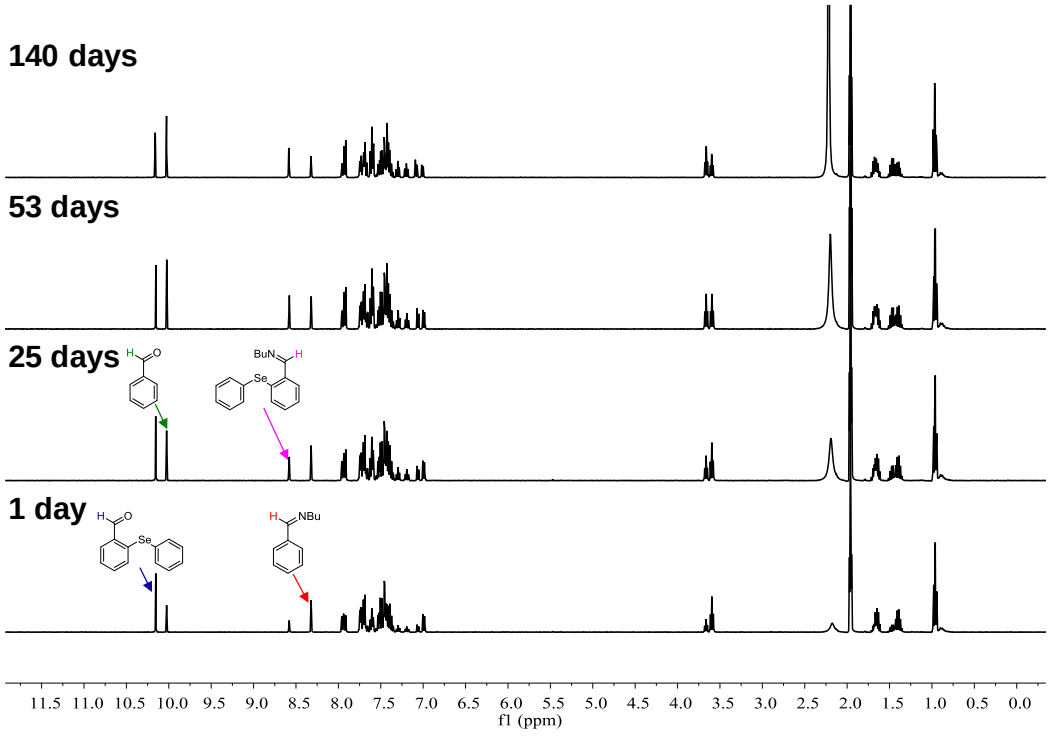


Figure S56. ^1H NMR spectra of the competition between **1**(SePh) and **5** for the reaction with 1-butylamine in CD_3CN at varied time (the corresponding spectra of panel b in Table S2).

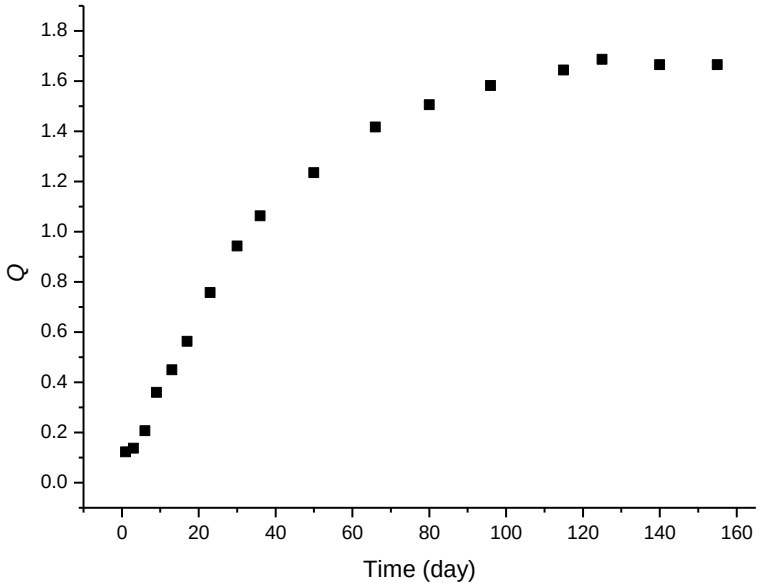


Figure S57. Kinetic profile of the competition between **1**(SePh) and **5** for the reaction with 1-butylamine in CD_3CN.

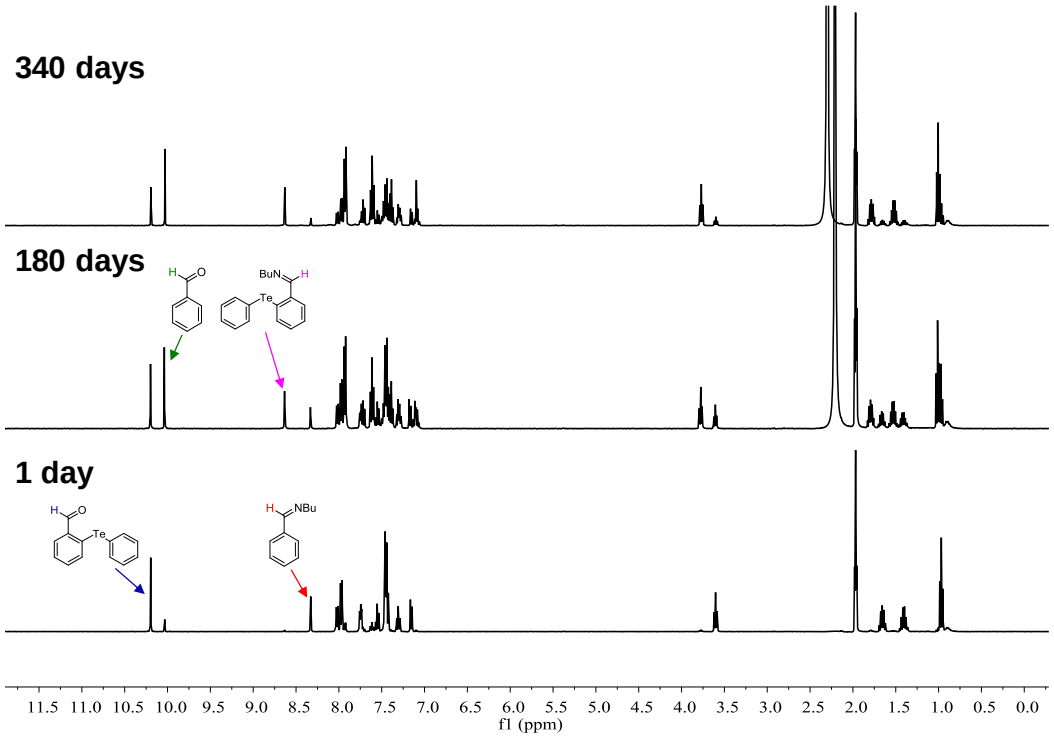


Figure S58. ^1H NMR spectra of the competition between **1**(TePh) and **5** for the reaction with 1-butylamine in CD_3CN at varied time (the corresponding spectra of panel c in Table S2).

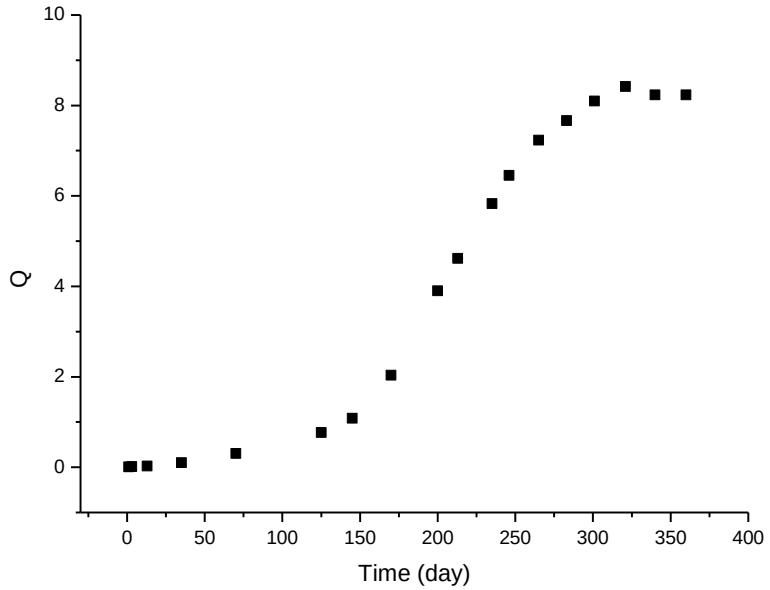


Figure S59. Kinetic profile of the competition between **1**(TePh) and **5** for the reaction with 1-butylamine in CD_3CN.

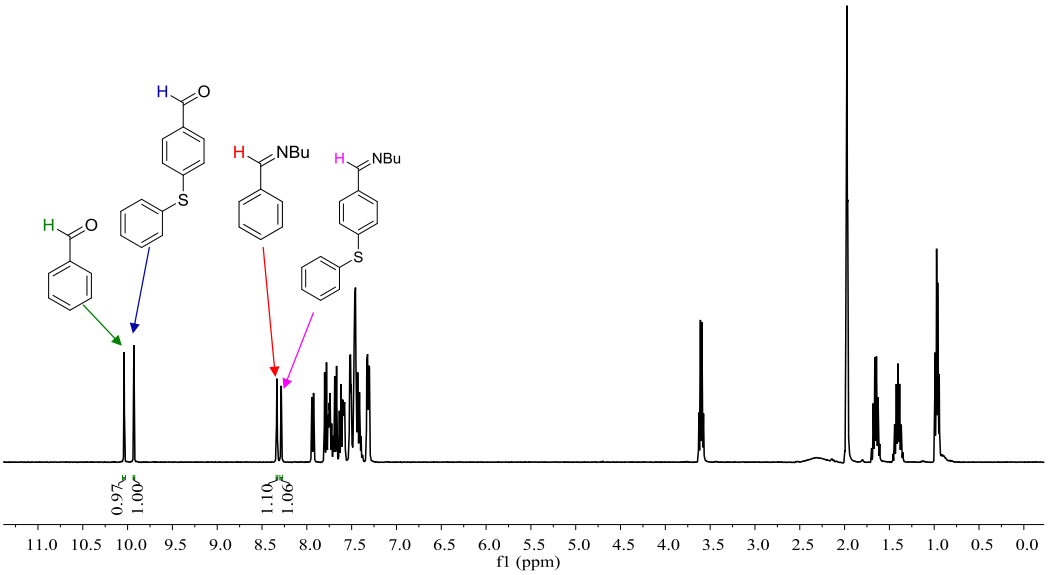


Figure S60. ^1H NMR spectrum of the competition between **3**(SPh) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel d in Table S2).

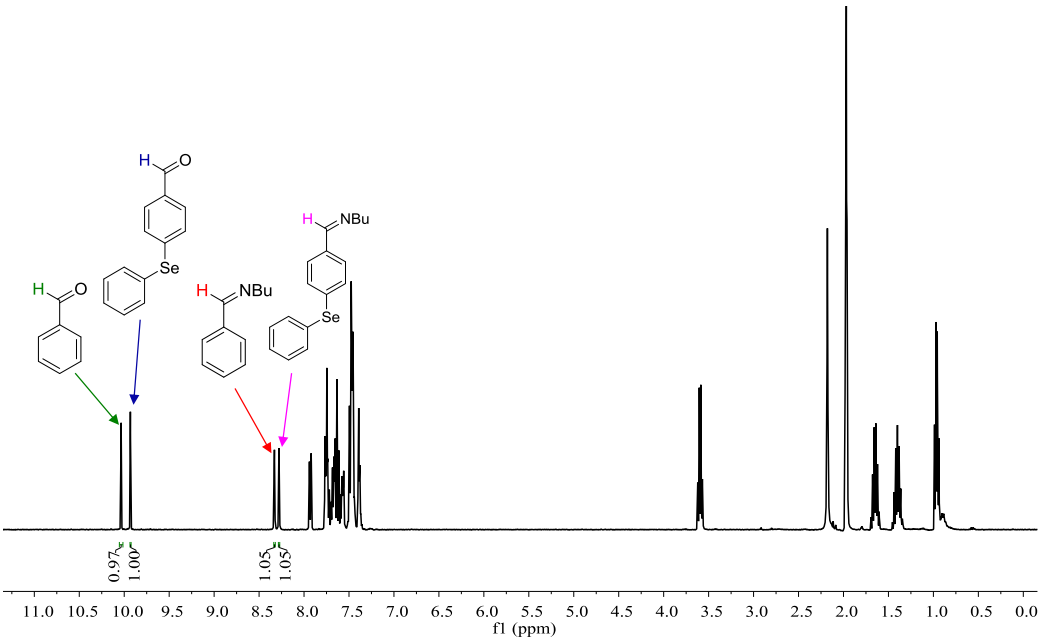


Figure S61. ^{1}H NMR spectrum of the competition between **3**(SePh) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel e in Table S2).

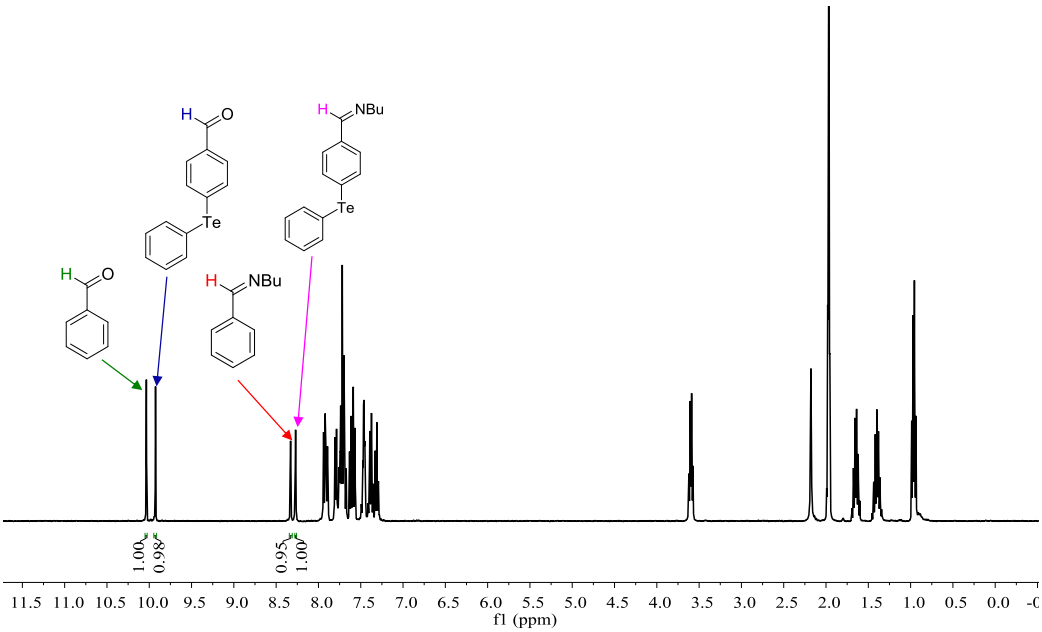


Figure S62. ^{1}H NMR spectrum of the competition between **3**(TePh) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel f in Table S2).

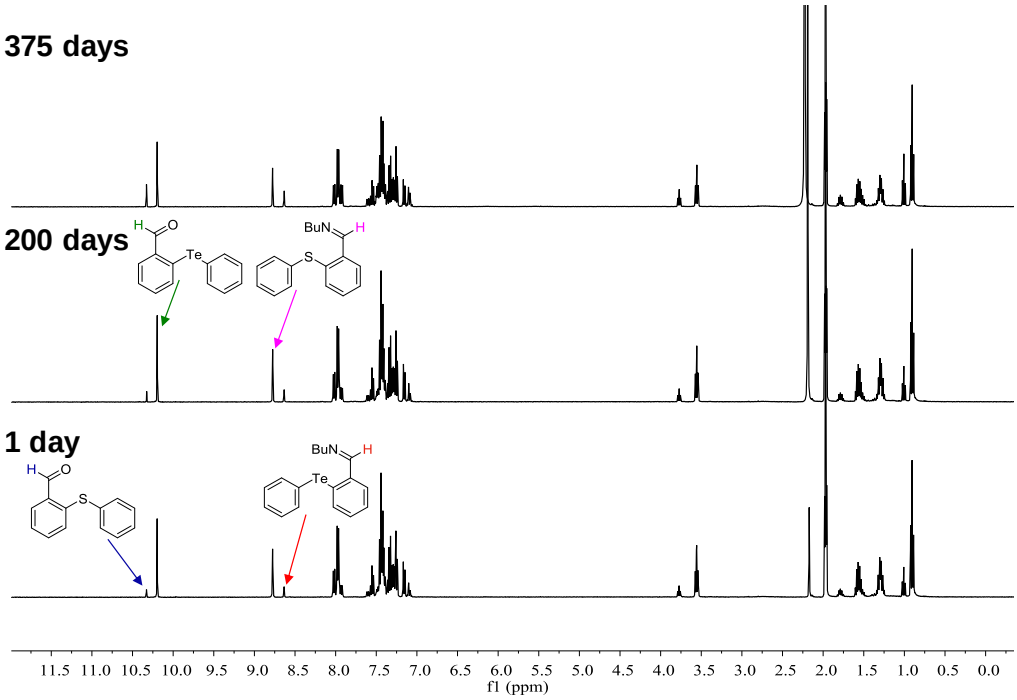


Figure S63. ^{1}H NMR spectra of the competition between **1**(SPh) and **1**(TePh) for the reaction with 1-butylamine in CD_3CN at varied time (the corresponding spectra of panel g in Table S2).

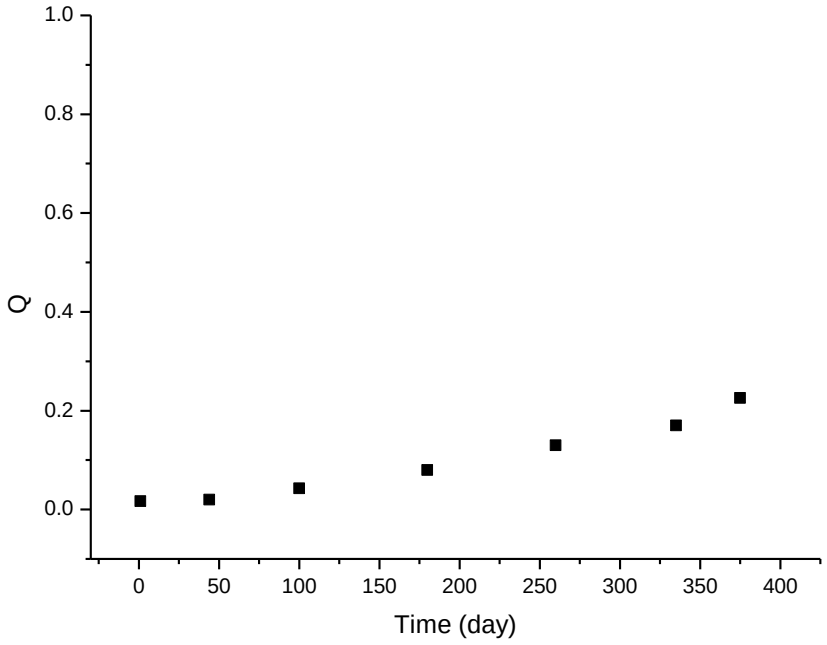
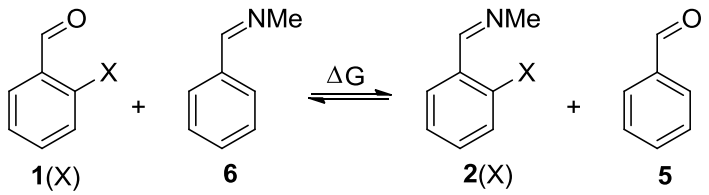


Figure S64. Kinetic profile of the competition between **1**(SPh) and **1**(TePh) for the reaction with 1-butylamine in CD_3CN.

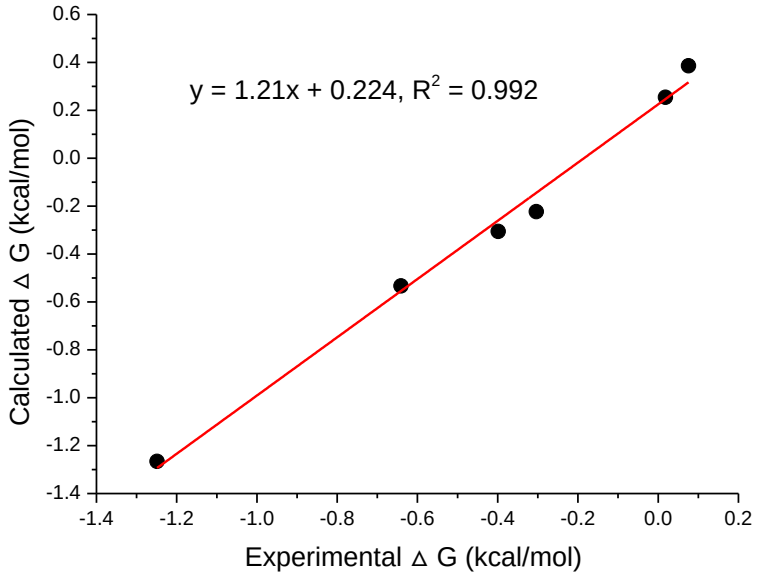
Table S3. The experimental and calculated ΔG of aldehyde exchange, with calculated G of each component listed. A linear correlation of calculated and experimental ΔG is shown (R^2 = 0.992), which indicates the accuracy of the M06-2X-D3/def2-TZVP.



1(X) **6** **2**(X) **5**

X	**1**(X)	**6**	**2**(X)	**5**	ΔG_{cacld}	ΔG_{exp}
SPh	-974.63585	-364.86119	-994.01640	-345.48113	-0.31	-0.40
SePh	-2978.0259	-364.86119	-2997.4063	-345.48113	-0.22	-0.30
TePh	-844.38940	-364.86119	-863.77149	-345.48113	-1.27	-1.25
SMe	-782.95258	-364.86119	-802.33224	-345.48113	0.25	0.02
SeMe	-2786.3443	-364.86119	-2805.7237	-345.48113	0.39	0.08
TeMe	-652.70890	-364.86119	-672.08982	-345.48113	-0.53	-0.64

* *n*-Bu group of imines was replaced with Me group for simplicity of the calculation.



4. DFT Calculations

Table S4. GKS-EDA results of the conformer 1 of **1**/**2** (kcal/mol).

Conf.1	ΔE^{ele}	$\Delta E^{ex\text{-}rep}$	ΔE^{pol}	ΔE^{disp}	ΔE^{corr}	ΔE^{TOT}
1(SPh)	-3.82	9.89	-4.05	-0.80	-1.20	0.01
1(SePh)	-5.45	12.56	-5.82	-0.80	-1.24	-0.74
1(TePh)	-9.41	20.45	-12.13	-0.70	-1.27	-3.06
1(SMe)	-3.43	8.03	-2.56	-0.75	-1.33	-0.05
1(SeMe)	-4.70	10.21	-4.01	-0.76	-1.47	-0.73
1(TeMe)	-7.58	15.94	-8.91	-0.68	-1.55	-2.79
2(SPh)	-4.99	11.14	-3.37	-1.24	-1.22	0.31
2(SePh)	-7.80	15.40	-5.73	-1.37	-1.31	-0.81
2(TePh)	-16.18	31.86	-16.43	-1.55	-1.80	-4.09
2(SMe)	-3.97	9.28	-2.50	-1.16	-1.35	0.30
2(SeMe)	-6.21	12.53	-4.30	-1.29	-1.49	-0.76
2(TeMe)	-12.38	23.88	-11.74	-1.45	-1.95	-3.64

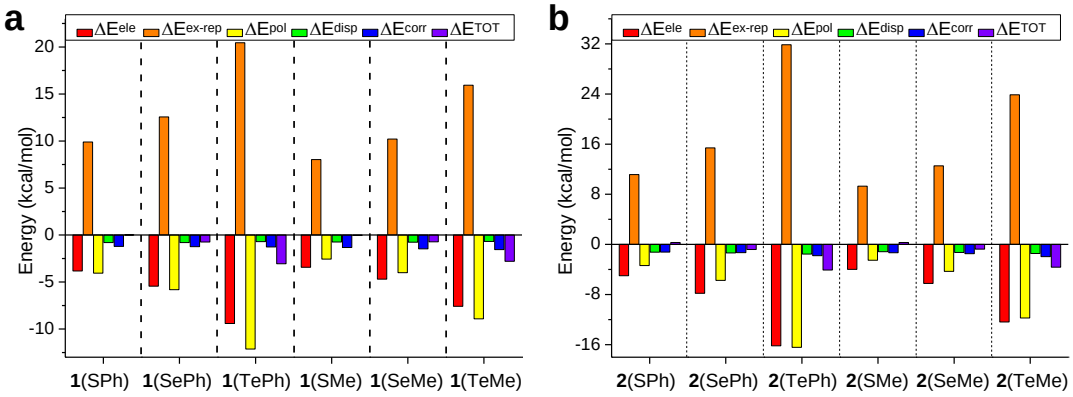
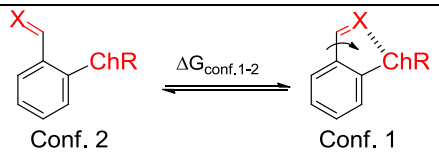


Table S5. The difference ($\Delta\Delta E^{TOT}_{conf.1\text{-}2}$, kcal/mol) between interaction energies of conformers 1 and 2 of **1**/**2** (kcal/mol).

Conf.1-2	$\Delta\Delta E^{ele}$	$\Delta\Delta E^{ex\text{-}rep}$	$\Delta\Delta E^{pol}$	$\Delta\Delta E^{disp}$	$\Delta\Delta E^{corr}$	$\Delta\Delta E^{TOT}$
1(SPh)	-1.90	3.04	-1.85	0.08	-1.75	-2.37
1(SePh)	-3.55	4.15	-2.58	0.03	-1.68	-3.63
1(TePh)	-7.53	10.86	-8.02	0.12	-1.72	-6.29
1(SMe)	-0.77	2.04	-1.84	0.00	-1.80	-2.37
1(SeMe)	-2.22	3.88	-3.26	0.03	-1.90	-3.47
1(TeMe)	-5.53	8.99	-7.51	0.11	-1.97	-5.91
2(SPh)	-3.07	4.29	-1.16	-0.36	-1.77	-2.07
2(SePh)	-5.50	8.46	-3.97	-0.29	-1.91	-3.20
2(TePh)	-13.73	22.65	-13.23	-0.51	-2.36	-7.18

2(SMe)	-1.13	3.44	-1.96	-0.28	-1.85	-1.78
2(SeMe)	-3.32	6.25	-3.75	-0.33	-2.00	-3.17
2(TeMe)	-9.73	16.87	-10.75	-0.47	-2.47	-6.55

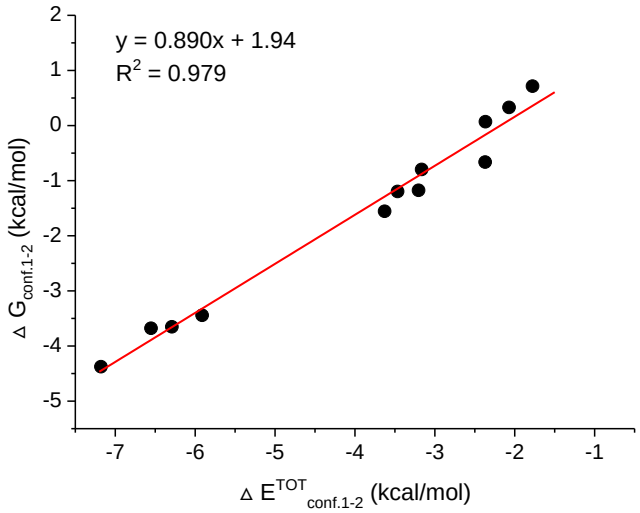
Table S6. Calculated conformational energy difference $\Delta G_{conf.1\text{-}2}$ (kcal/mol), the difference ($\Delta\Delta E^{TOT}{}_{conf.1\text{-}2}$, kcal/mol) between interaction energies of conformers 1 and 2. Structural fragments for GKS-EDA were highlighted in red.



Conf. 2 Conf. 1

X = O, NMe
Ch = S, Se, Te
R = Me, Ph

	$\Delta G_{conf.\ 1\text{-}2}$	$\Delta\Delta E^{TOT}{}_{conf.1\text{-}2}$
1(SPh)	0.07	-2.37
1(SePh)	-1.55	-3.63
1(TePh)	-3.65	-6.29
1(SMe)	-0.66	-2.37
1(SeMe)	-1.20	-3.47
1(TeMe)	-3.44	-5.91
2(SPh)	0.33	-2.07
2(SePh)	-1.17	-3.20
2(TePh)	-4.38	-7.18
2(SMe)	0.72	-1.78
2(SeMe)	-0.80	-3.17
2(TeMe)	-3.68	-6.55



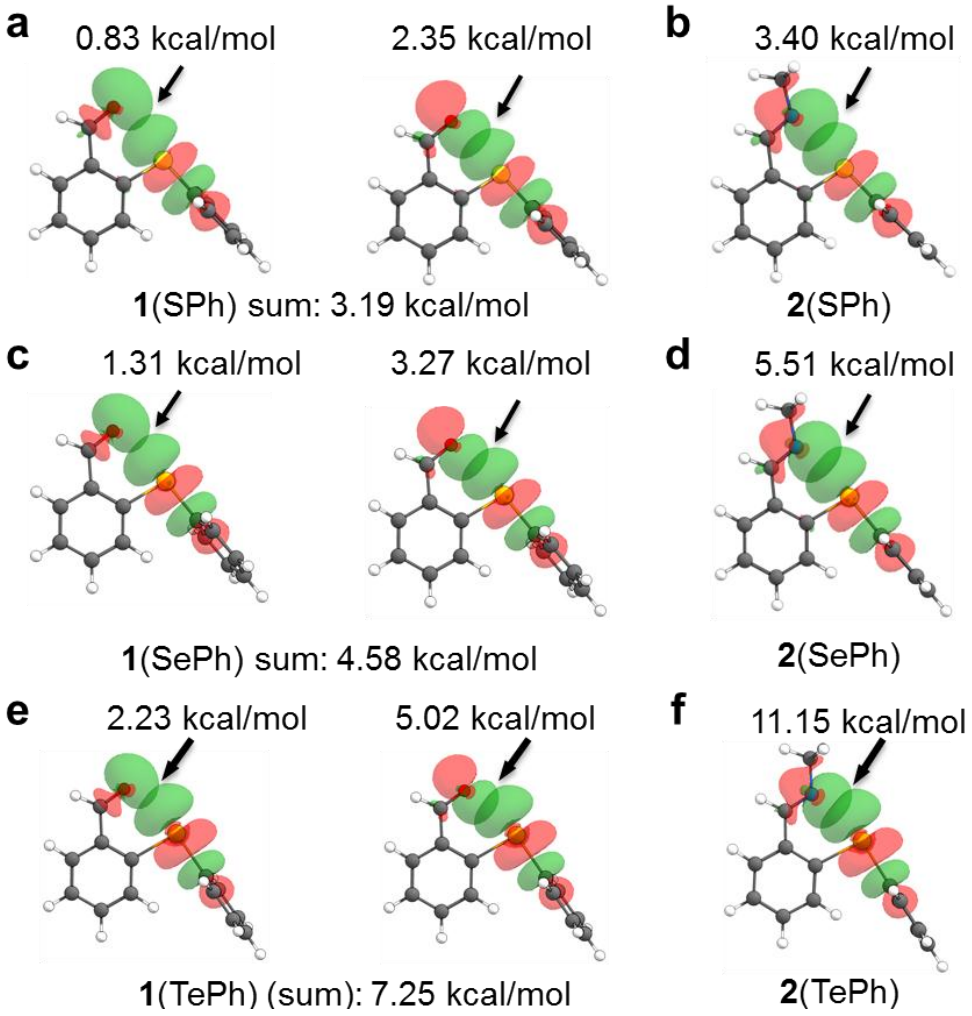


Figure S65. NBO orbitals and stabilization energies of n→σ* interactions in **1**(SPh) (a), **2**(SPh) (b), **1**(SePh) (c), **2**(SePh) (d), **1**(TePh) (e), and **2**(TePh) (f), respectively.

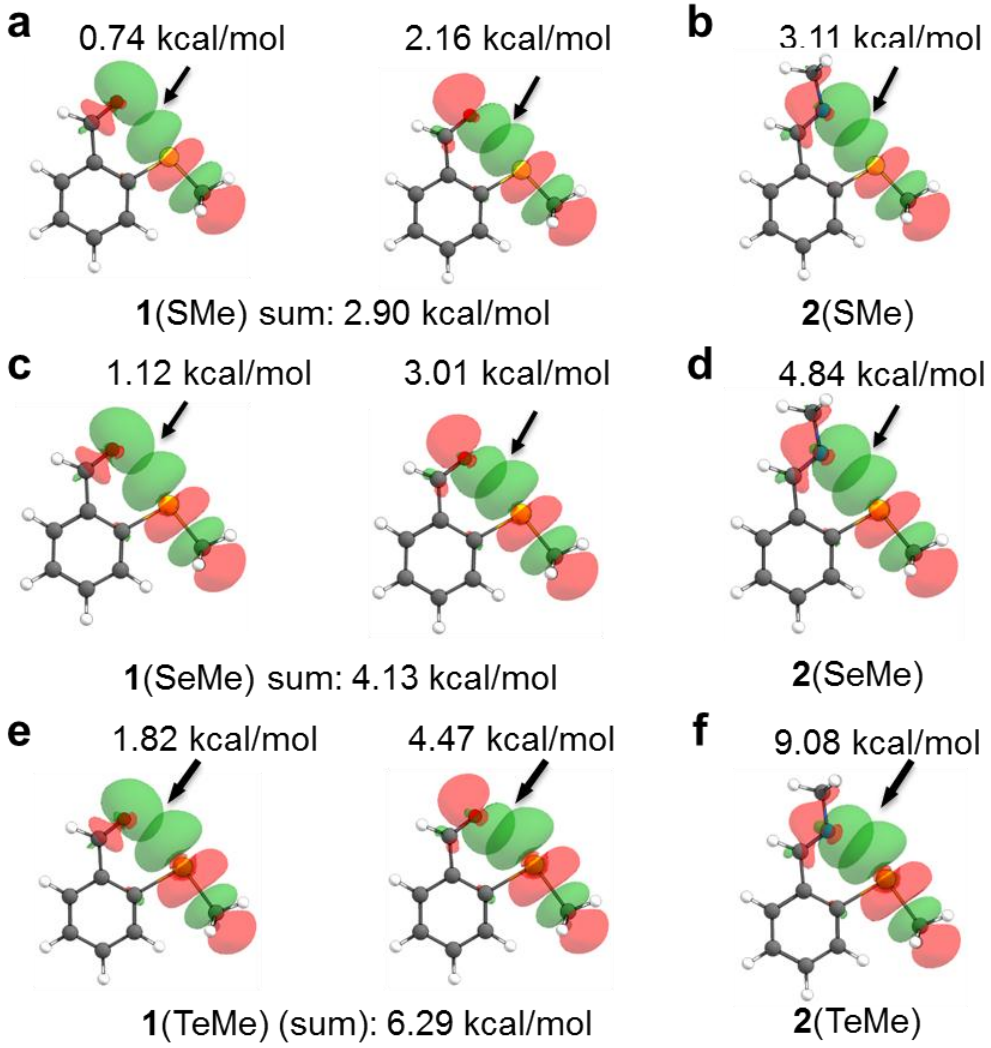


Figure S66. NBO orbitals and stabilization energies of n→σ* interactions in **1**(SMe) (a), **2**(SMe) (b), **1**(SeMe) (c), **2**(SeMe) (d), **1**(TeMe) (e), and **2**(TeMe) (f), respectively.

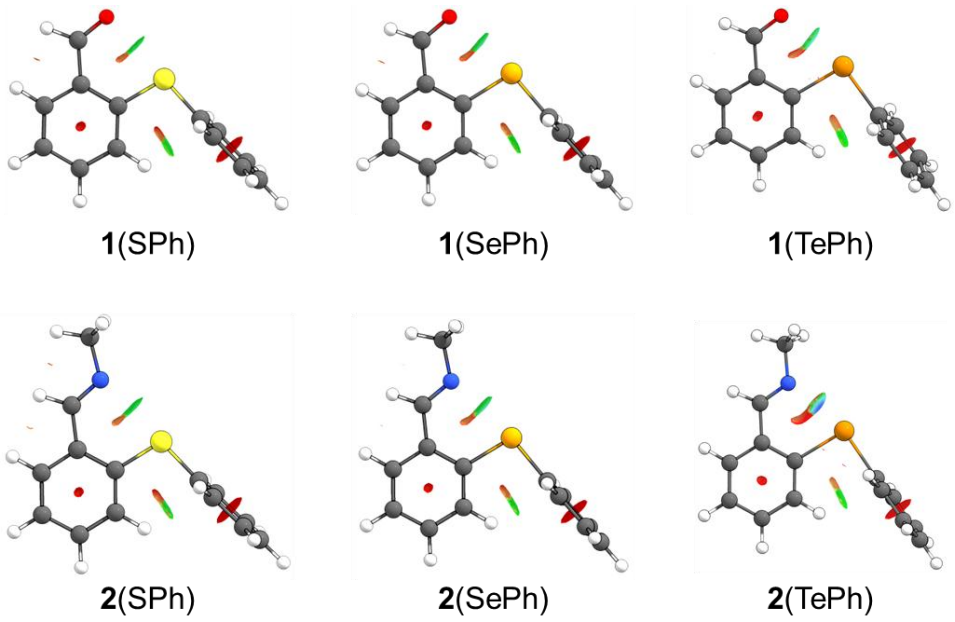


Figure S67. NCI plots of conformer 1 for **1**(ChPh) and **2**(ChPh).

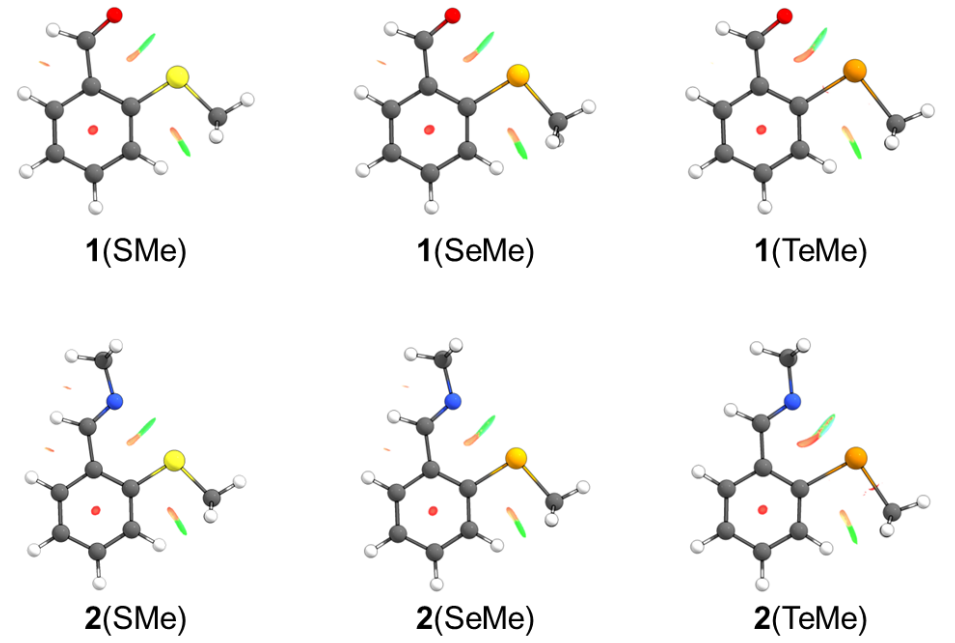


Figure S68. NCI plots of conformer 1 for **1**(ChMe) and **2**(ChMe).

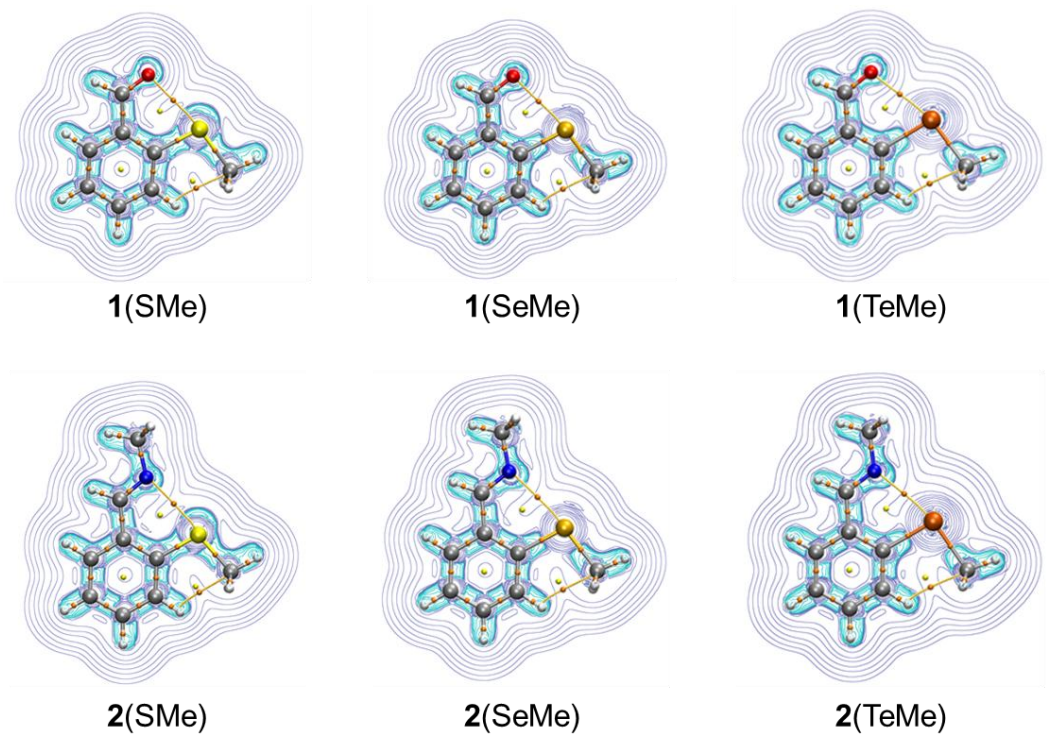


Figure S69. Contour line diagram of the Laplacian distribution $\nabla^2\rho(r)$ and bond paths of conformer 1 for **1**(ChMe) and **2**(ChMe).

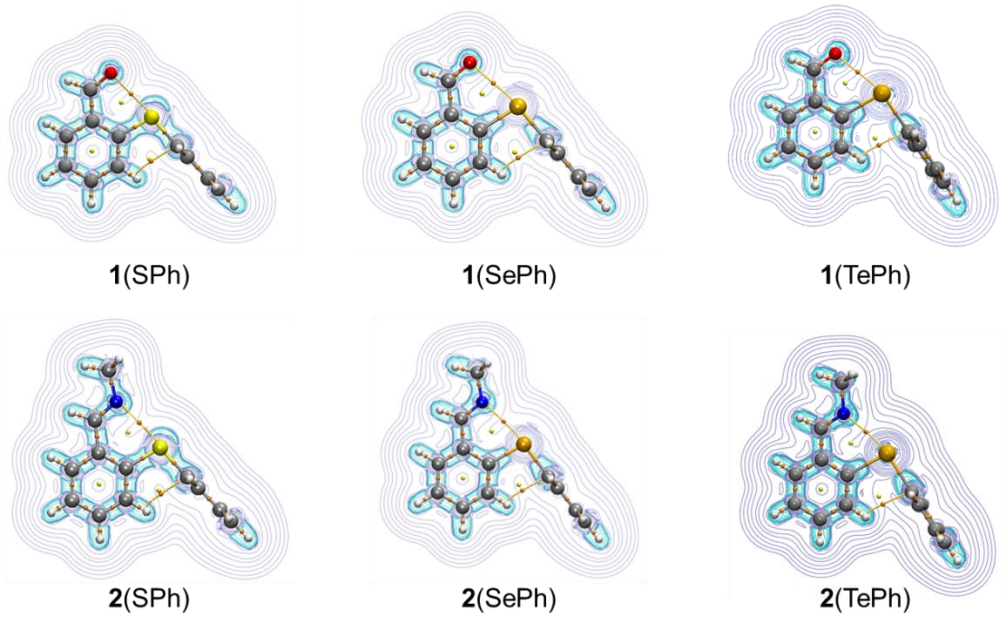


Figure S70. Contour line diagram of the Laplacian distribution $\nabla^2\rho(\mathbf{r})$ and bond paths of conformer 1 for **1**(ChPh) and **2**(ChPh).

Table S7. The calculated parameters of BCP for chalcogen bonding (Ch···O/Ch···N), including density of all electrons ρ(**r**) (in au), Laplacian of electron density $\nabla^2\rho(\mathbf{r})$ (in au), total energy density H(**r**) (in hartree), potential energy density V(**r**) (in hartree), Lagrangian kinetic energy G(**r**) (in hartree), Wiberg bond index (W), and the eigenvalues of hessian for the conformer 1 of **1**(ChPh), **2**(ChPh), **1**(ChMe), and **2**(ChMe).

	ρ(**r**)	$\nabla^2\rho(\mathbf{r})$	H(**r**)	V(**r**)	G(**r**)	W	$\lambda_1, \lambda_2, \lambda_3$
1(SPh)	0.018	0.070	0.0017	-0.0141	0.0158	0.028	-0.014, -0.013, +0.098
2(SPh)	0.018	0.061	0.0012	-0.0130	0.0141	0.035	-0.014, -0.012, +0.087
1(SePh)	0.020	0.071	0.0015	-0.0148	0.0163	0.036	-0.015, -0.014, +0.100
2(SePh)	0.021	0.064	0.0007	-0.0145	0.0152	0.049	-0.016, -0.013, +0.093
1(TePh)	0.023	0.073	0.0004	-0.0175	0.0180	0.058	-0.017, -0.015, +0.105
2(TePh)	0.029	0.070	-0.0018	-0.0211	0.0193	0.102	-0.023, -0.018, +0.111
1(SMe)	0.0177	0.0690	0.0018	-0.0137	0.0155	0.027	-0.014, -0.013, +0.096
2(SMe)	0.0177	0.0600	0.0012	-0.0126	0.0138	0.035	-0.014, -0.011, +0.085
1(SeMe)	0.0189	0.0693	0.0015	-0.0143	0.0158	0.034	-0.014, -0.013, +0.097
2(SeMe)	0.0196	0.0613	0.0008	-0.0136	0.0145	0.046	-0.015, -0.012, +0.088
1(TeMe)	0.0215	0.0705	0.0006	-0.0164	0.0170	0.053	-0.016, -0.014, +0.100
2(TeMe)	0.0257	0.0661	-0.0010	-0.0185	0.0175	0.085	-0.019, -0.016, +0.101

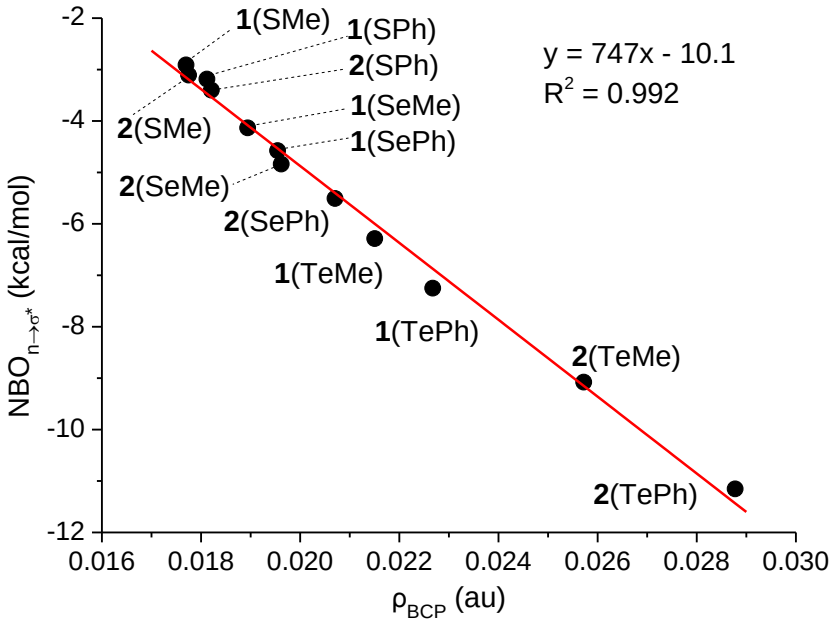
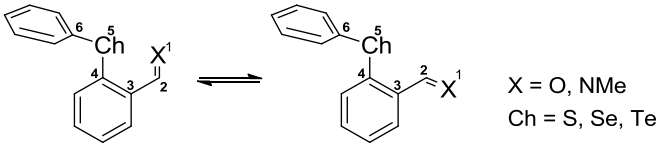


Table S8. Calculated bond length (D), Wiberg bond index (W), and their difference between closed and open conformers for **1**(ChPh) and **2**(ChPh).

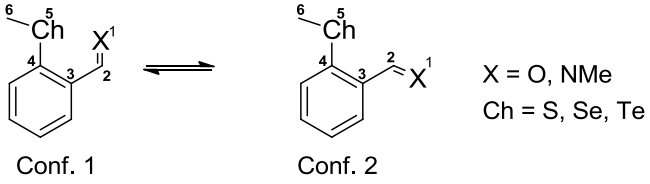


Conf. 1 Conf. 2

1(SPh)-Conf. 1	D (Å)	W	**1**(SPh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.210	1.781	O1-C2	1.209	1.806	0.001	-0.025
C2-C3	1.469	1.064	C2-C3	1.480	1.039	-0.011	0.025
C3-C4	1.410	1.310	C3-C4	1.403	1.350	0.007	-0.039
C4-S5	1.770	1.085	C4-S5	1.776	1.058	-0.006	0.027
S5-C6	1.777	1.010	S5-C6	1.774	1.025	0.003	-0.015
1(SePh)-Conf. 1	D (Å)	W	**1**(SePh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.210	1.774	O1-C2	1.208	1.809	0.003	-0.035
C2-C3	1.468	1.063	C2-C3	1.478	1.039	-0.011	0.024
C3-C4	1.406	1.325	C3-C4	1.403	1.352	0.004	-0.028
C4-Se5	1.922	1.046	C4-Se5	1.931	1.025	-0.009	0.021
Se5-C6	1.925	0.977	Se5-C6	1.919	0.994	0.007	-0.017
1(TePh)-Conf. 1	D (Å)	W	**1**(TePh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.213	1.751	O1-C2	1.207	1.811	0.007	-0.060
C2-C3	1.464	1.070	C2-C3	1.478	1.038	-0.014	0.031
C3-C4	1.404	1.335	C3-C4	1.402	1.364	0.003	-0.030
C4-Te5	2.118	0.980	C4-Te5	2.133	0.962	-0.015	0.017
Te5-C6	2.125	0.904	Te5-C6	2.111	0.944	0.014	-0.040
2(SPh)-Conf. 1	D (Å)	W	**1**(SPh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.263	1.852	N1-C2	1.263	1.875	0.000	-0.023
C2-C3	1.470	1.072	C2-C3	1.478	1.049	-0.008	0.022
C3-C4	1.411	1.321	C3-C4	1.400	1.370	0.011	-0.049
C4-S5	1.777	1.072	C4-S5	1.778	1.043	-0.001	0.029
S5-C6	1.779	1.006	S5-C6	1.774	1.034	0.005	-0.028
2(SePh)-Conf. 1	D (Å)	W	**2**(SePh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.263	1.848	N1-C2	1.263	1.877	0.000	-0.029
C2-C3	1.468	1.070	C2-C3	1.477	1.049	-0.009	0.021
C3-C4	1.408	1.334	C3-C4	1.401	1.371	0.007	-0.037
C4-Se5	1.929	1.034	C4-Se5	1.930	1.016	-0.002	0.018
Se5-C6	1.930	0.965	Se5-C6	1.920	0.999	0.010	-0.035

2(TePh)-Conf. 1	D (Å)	W	**2**(TePh)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.264	1.827	N1-C2	1.262	1.879	0.002	-0.052
C2-C3	1.465	1.073	C2-C3	1.477	1.049	-0.013	0.025
C3-C4	1.405	1.343	C3-C4	1.401	1.376	0.004	-0.033
C4-Te5	2.123	0.969	C4-Te5	2.132	0.960	-0.009	0.009
Te5-C6	2.139	0.869	Te5-C6	2.112	0.944	0.027	-0.075

Table S9. Calculated bond length (D), Wiberg bond index (W), and the difference between closed and open conformers for **1**(ChMe) and **2**(ChMe).

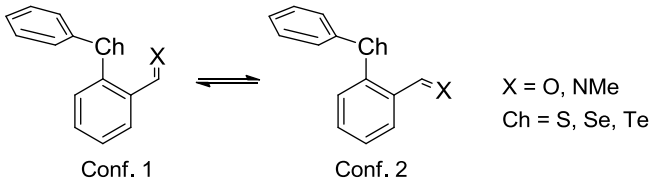


Conf. 1 Conf. 2

1(SMe)-Conf. 1	D (Å)	W	**1**(SMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.210	1.780	O1-C2	1.209	1.804	0.001	-0.024
C2-C3	1.469	1.067	C2-C3	1.478	1.044	-0.009	0.023
C3-C4	1.413	1.303	C3-C4	1.409	1.330	0.004	-0.027
C4-S5	1.757	1.113	C4-S5	1.764	1.090	-0.007	0.023
S5-C6	1.800	1.018	S5-C6	1.797	1.026	0.003	-0.008
1(SeMe)-Conf. 1	D (Å)	W	**1**(SeMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.210	1.775	O1-C2	1.208	1.808	0.002	-0.033
C2-C3	1.468	1.065	C2-C3	1.478	1.040	-0.010	0.025
C3-C4	1.408	1.319	C3-C4	1.405	1.346	0.004	-0.027
C4-Se5	1.911	1.067	C4-Se5	1.920	1.046	-0.009	0.021
Se5-C6	1.946	0.996	Se5-C6	1.942	1.011	0.005	-0.014
1(TeMe)-Conf. 1	D (Å)	W	**1**(TeMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
O1-C2	1.213	1.755	O1-C2	1.207	1.810	0.006	-0.055
C2-C3	1.465	1.070	C2-C3	1.478	1.040	-0.013	0.030
C3-C4	1.405	1.331	C3-C4	1.403	1.360	0.003	-0.029
C4-Te5	2.110	0.995	C4-Te5	2.125	0.977	-0.015	0.018
Te5-C6	2.140	0.947	Te5-C6	2.130	0.982	0.010	-0.034
2(SMe)-Conf. 1	D (Å)	W	**1**(SMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.263	1.853	N1-C2	1.263	1.876	0.000	-0.023
C2-C3	1.469	1.073	C2-C3	1.477	1.051	-0.008	0.022
C3-C4	1.414	1.313	C3-C4	1.408	1.341	0.006	-0.028

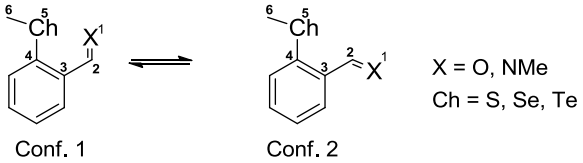
C4-S5	1.764	1.099	C4-S5	1.768	1.076	-0.004	0.022
S5-C6	1.801	1.014	S5-C6	1.797	1.027	0.004	-0.013
2(SeMe)-Conf. 1	D (Å)	W	**2**(SeMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.263	1.849	N1-C2	1.263	1.878	0.000	-0.029
C2-C3	1.469	1.071	C2-C3	1.477	1.049	-0.009	0.022
C3-C4	1.409	1.328	C3-C4	1.404	1.357	0.005	-0.029
C4-Se5	1.918	1.055	C4-Se5	1.922	1.037	-0.004	0.018
Se5-C6	1.950	0.987	Se5-C6	1.942	1.011	0.008	-0.025
2(TeMe)-Conf. 1	D (Å)	W	**2**(TeMe)-Conf. 2	D (Å)	W	ΔD (Å)	ΔW
N1-C2	1.263	1.833	N1-C2	1.262	1.879	0.002	-0.046
C2-C3	1.465	1.073	C2-C3	1.477	1.049	-0.012	0.024
C3-C4	1.406	1.339	C3-C4	1.402	1.371	0.004	-0.032
C4-Te5	2.115	0.982	C4-Te5	2.124	0.974	-0.009	0.008
Te5-C6	2.151	0.919	Te5-C6	2.131	0.981	0.020	-0.063

Table S10. NPA charge (in e) of the atoms involved with chalcogen bond in conformer 1 or conformer 2 for **1**(ChPh) and **2**(ChPh).



NPA Charge	O	Ch	NPA Charge	N	Ch
1(SPh)-Conf. 1	-0.562	0.341	**2**(SPh)-Conf. 1	-0.421	0.332
1(SPh)-Conf. 2	-0.560	0.293	**2**(SPh)-Conf. 2	-0.416	0.287
1(SePh)-Conf. 1	-0.565	0.425	**2**(SePh)-Conf. 1	-0.426	0.417
1(SePh)-Conf. 2	-0.556	0.361	**2**(SePh)-Conf. 2	-0.413	0.355
1(TePh)-Conf. 1	-0.577	0.624	**2**(TePh)-Conf. 1	-0.442	0.618
1(TePh)-Conf. 2	-0.554	0.537	**2**(TePh)-Conf. 2	-0.410	0.527

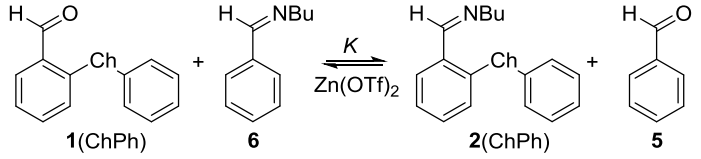
Table S11. NPA charge (in e) of the atoms involved with chalcogen bond in conformer 1 or conformer 2 for **1**(ChMe) and **2**(ChMe).



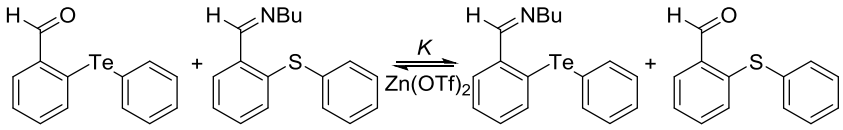
NPA Charge	O	Ch	NPA Charge	N	Ch
1(SMe)-Conf. 1	-0.562	0.326	**2**(SMe)-Conf. 1	-0.424	0.316
1(SMe)-Conf. 2	-0.560	0.270	**2**(SMe)-Conf. 2	-0.416	0.258
1(SeMe)-Conf. 1	-0.565	0.400	**2**(SeMe)-Conf. 1	-0.427	0.391
1(SeMe)-Conf. 2	-0.556	0.331	**2**(SeMe)-Conf. 2	-0.411	0.319
1(TeMe)-Conf. 1	-0.576	0.584	**2**(TeMe)-Conf. 1	-0.440	0.580
1(TeMe)-Conf. 2	-0.553	0.494	**2**(TeMe)-Conf. 2	-0.409	0.481

5. Control over Thermodynamic and Kinetic Selectivity

Table S12. The equilibrium constant and equilibrating time of the different imine exchange reactions in CD_3CN.



Panel	Ch	Sequence of adding reagents	Solvent	*K*	Equilibrating time
a	S	**1**(ChPh) and **5** simultaneously reacted with 1-butylamine	CD_3CN	2.0	2 days
b	Se		CD_3CN	1.7	8 days
c	Te		CD_3CN	8.2	44 days



Panel	Sequence of adding reagents	Solvent	*K*	Equilibrating time
d	**1**(SPh) and **1**(TePh) simultaneously reacted with 1-butylamine	CD_3CN	4.2	31 days

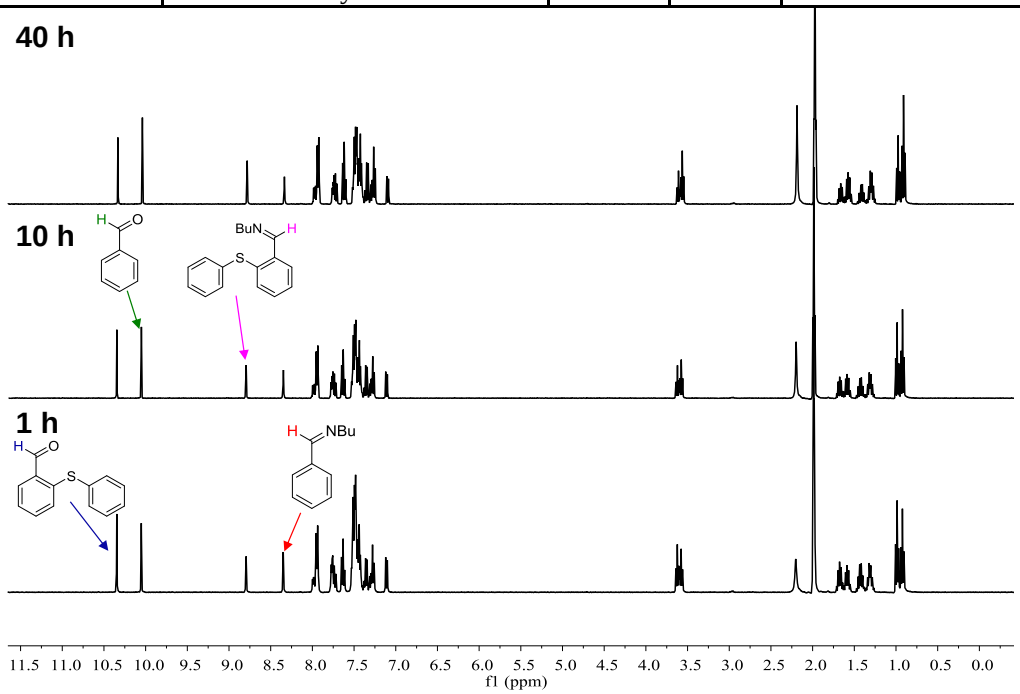


Figure S71. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel a in Table S12).

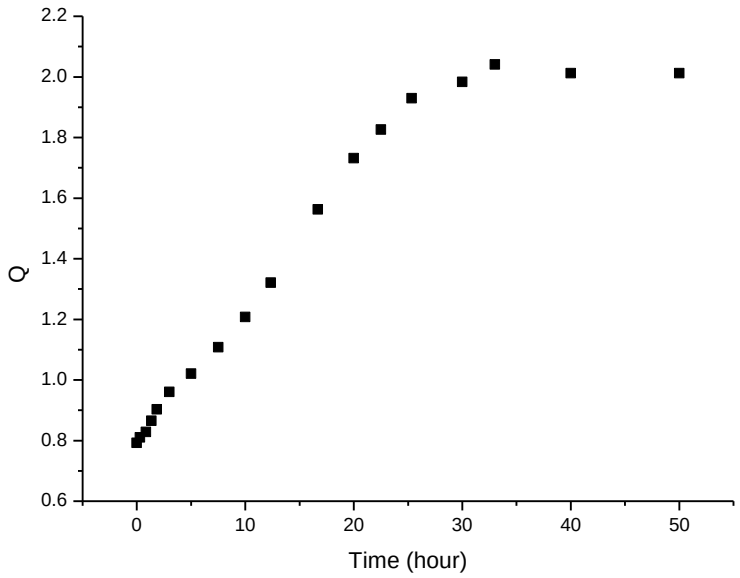


Figure S72. Kinetic profile of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

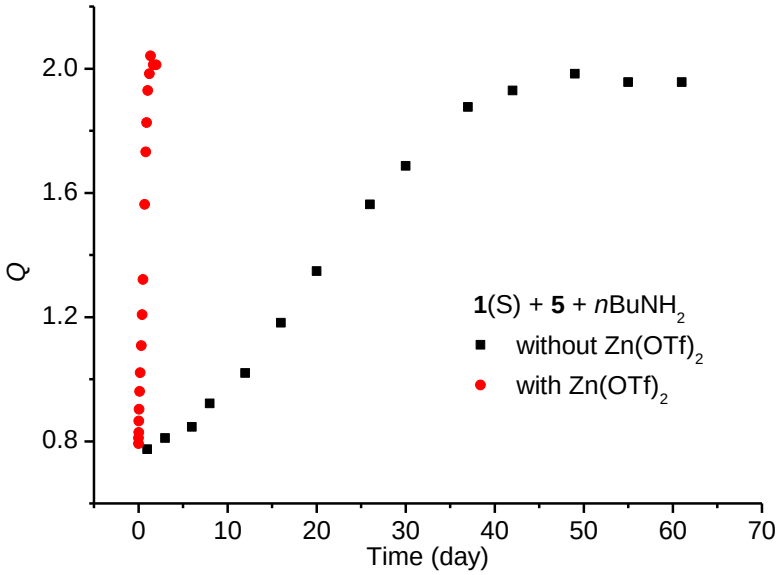


Figure S73. The effect of $Zn(OTf)_2$ (0.1 equiv.) on the kinetics of the reaction of **1**(SPh), **5** (1.0 equiv.), and 1-butylamine (1.0 equiv.).

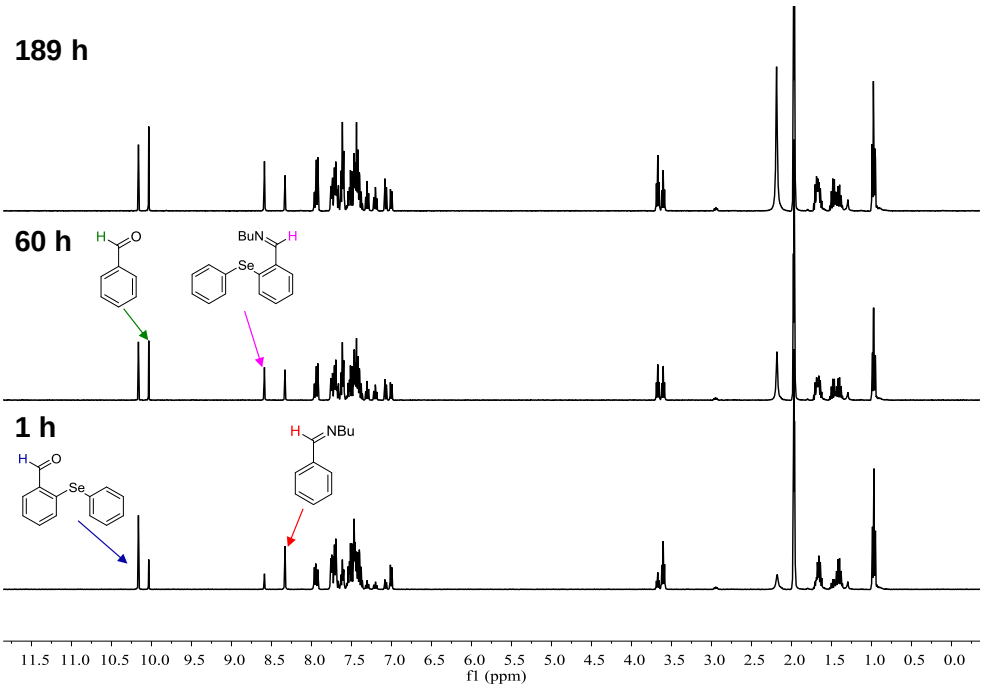


Figure S74. ^{1}H NMR spectra of the competition between **1**(SePh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel b in Table S12).

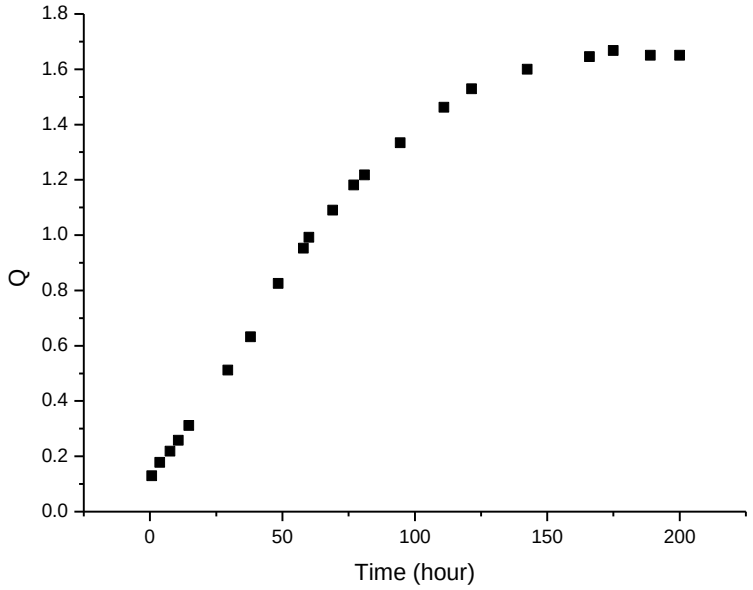


Figure S75. Kinetic profile of the competition between **1**(SePh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

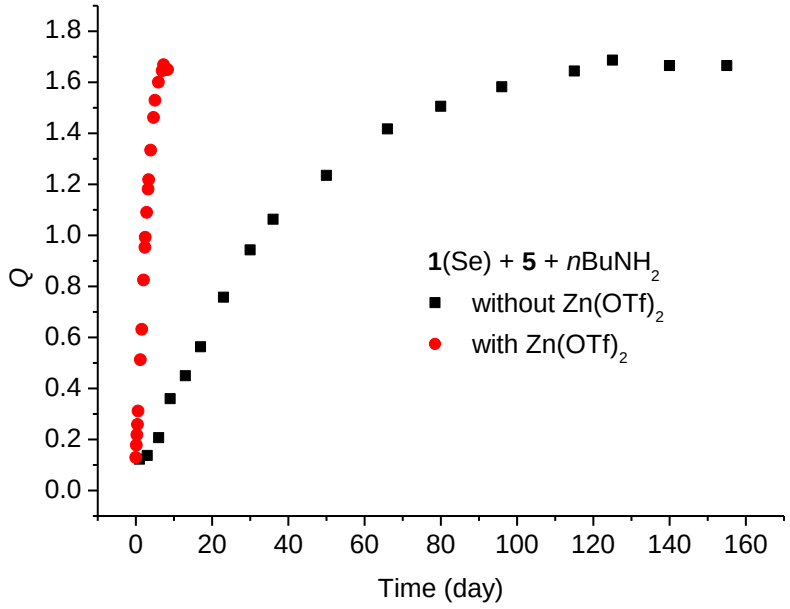


Figure S76. The effect of $Zn(OTf)_2$ (0.1 equiv.) on the kinetics of the reaction of **1**(SePh), **5** (1.0 equiv.), and 1-butylamine (1.0 equiv.).

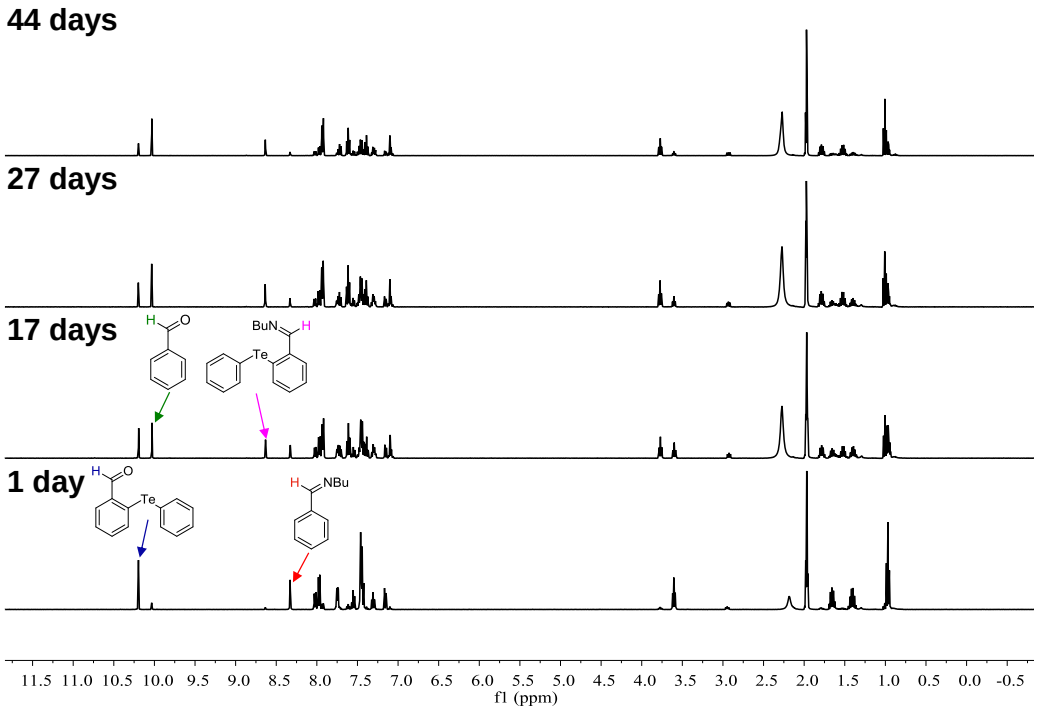


Figure S77. ^{1}H NMR spectra of the competition between **1**(TePh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel c in Table S12).

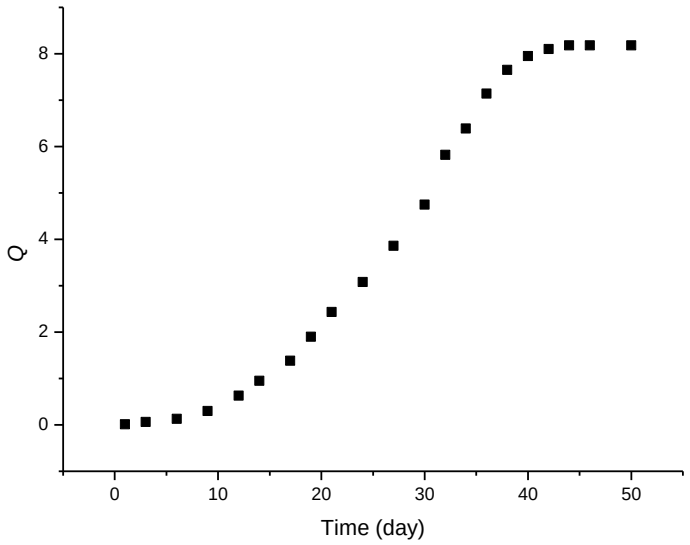


Figure S78. Kinetic profile of the competition between **1**(TePh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

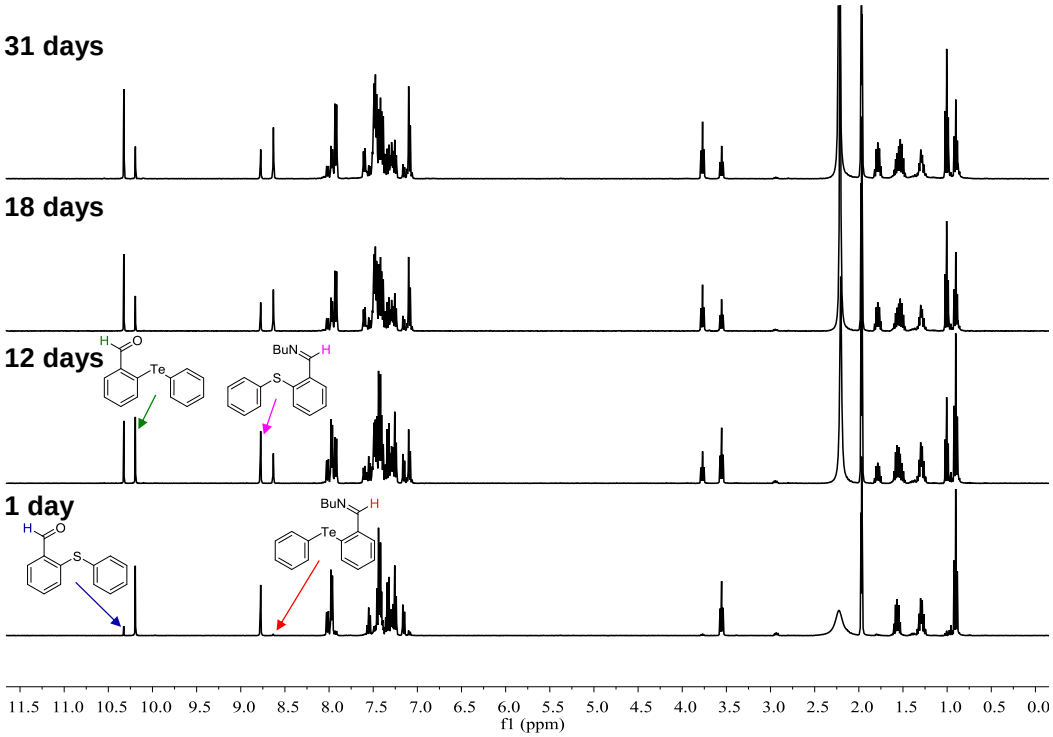


Figure S79. ^1H NMR spectra of the competition between **1**(SPh) and **1**(TePh) (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel d in Table S12).

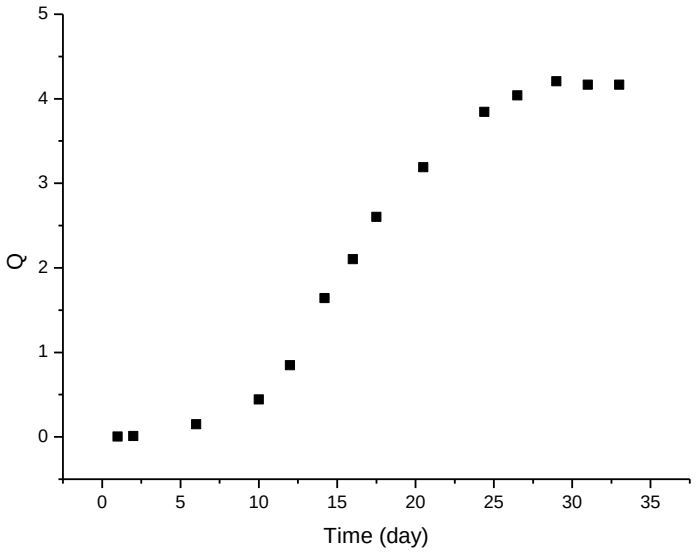


Figure S80. Kinetic profile of the competition between **1**(SPh) and **1**(TePh) (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

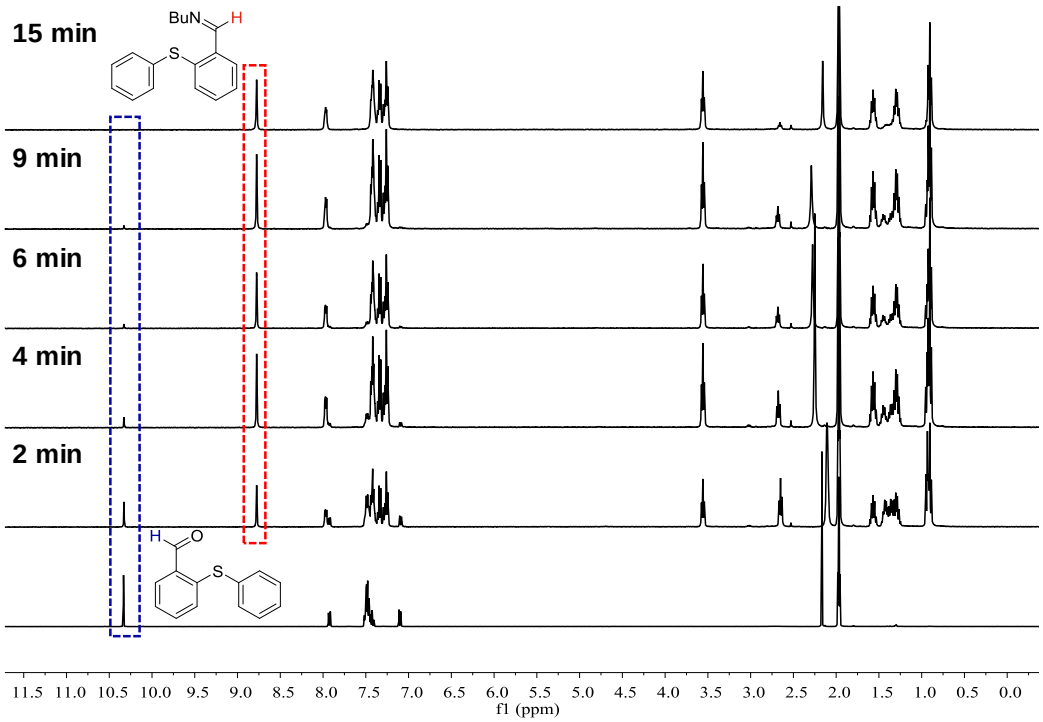


Figure S81. ^1H NMR spectra of the reaction of **1**(SPh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

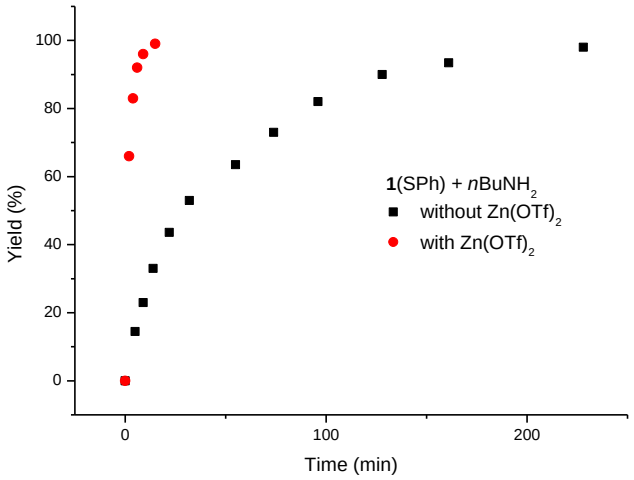


Figure S82. Kinetic profiles of the reactions of **1**(SPh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) and in the absence of $Zn(OTf)_2$ in CD_3CN.

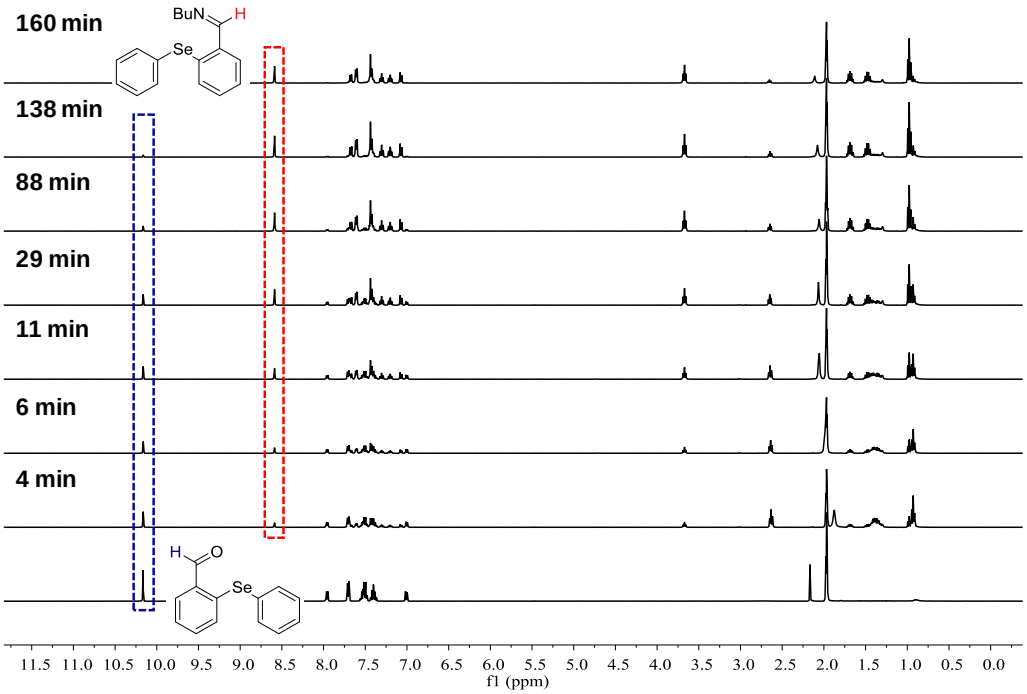


Figure S83. ^1H NMR spectra of the reaction of **1**(SePh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

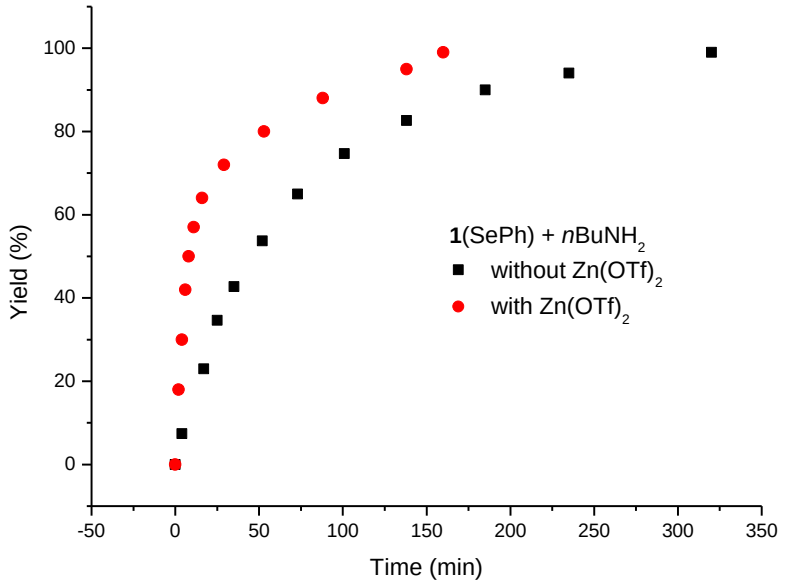


Figure S84. Kinetic profiles of the reactions of **1**(SePh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) and in the absence of $Zn(OTf)_2$ in CD_3CN.

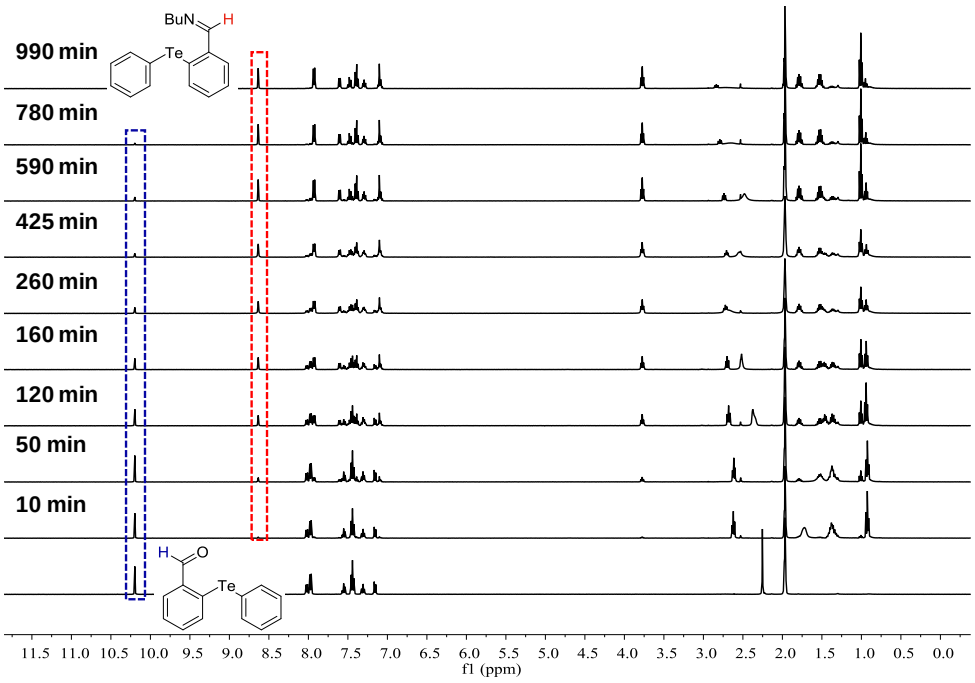


Figure S85. ^1H NMR spectra of the reaction of **1**(TePh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

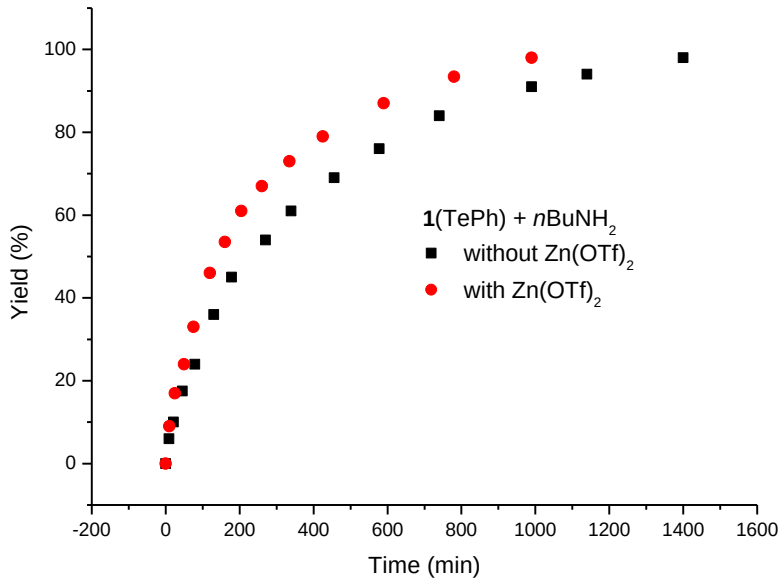
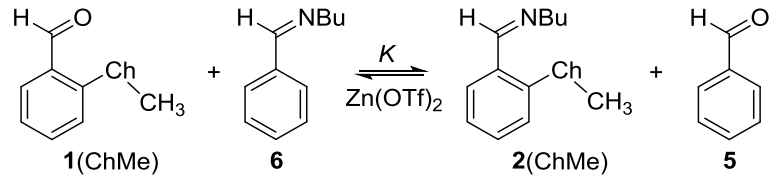


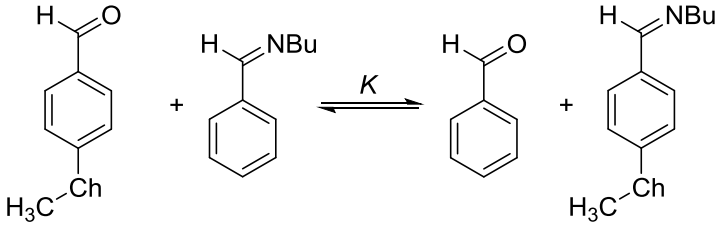
Figure S86. Kinetic profiles of the reactions of **1**(TePh) (15 mM, 1.0 equiv.) and 1-butylamine (1.2 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) and in the absence of $Zn(OTf)_2$ in CD_3CN.

Table S13. The equilibrium constant and equilibrating time of the different imine exchange reactions in CD_3CN.



1(ChMe) **6** **2**(ChMe) **5**

Panel	Ch	Sequence of adding reagents	Solvent	*K*	Equilibrating time
a	S	**1**(ChMe) and **5** simultaneously reacted with 1-butylamine	CD_3CN	0.97	3 days
b	Se		CD_3CN	0.88	12 days
c	Te		CD_3CN	2.9	21 days



3(ChMe) **6** **5** **4**(ChMe)

Panel		Sequence of adding reagents	Solvent	*K*	Equilibrating time
d	S	**3**(ChMe) and **5** simultaneously reacted with 1-butylamine	CD_3CN	0.57	1 day
e	Se		CD_3CN	0.66	1 day
f	Te		CD_3CN	0.87	1 day

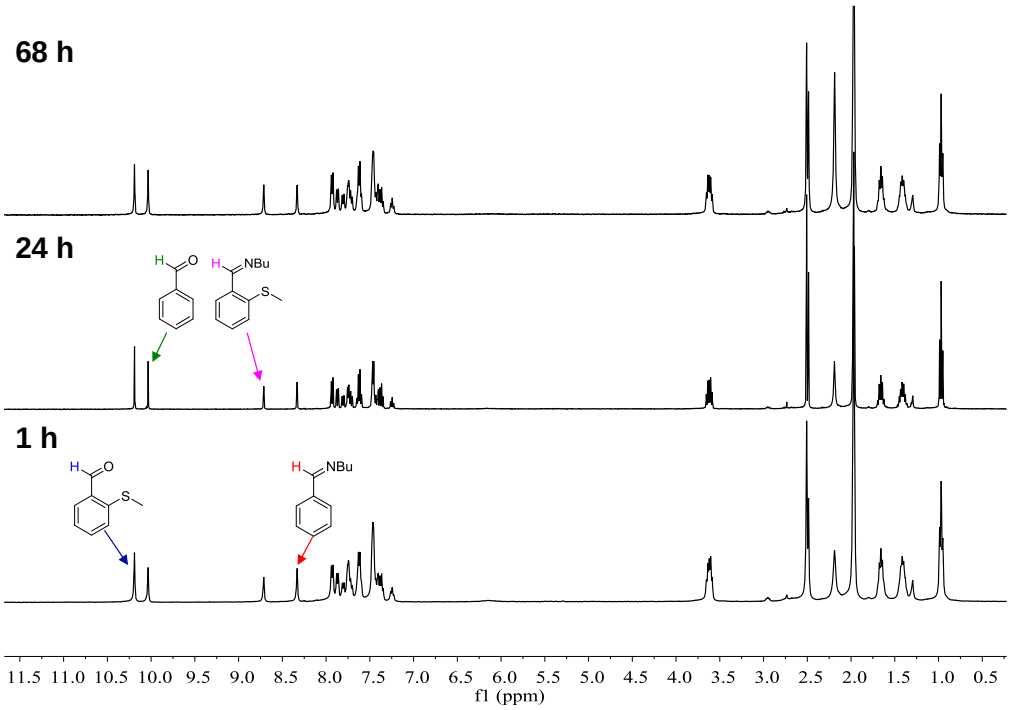


Figure S87. ^{1}H NMR spectra of the competition between **1**(SMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel a in Table S13).

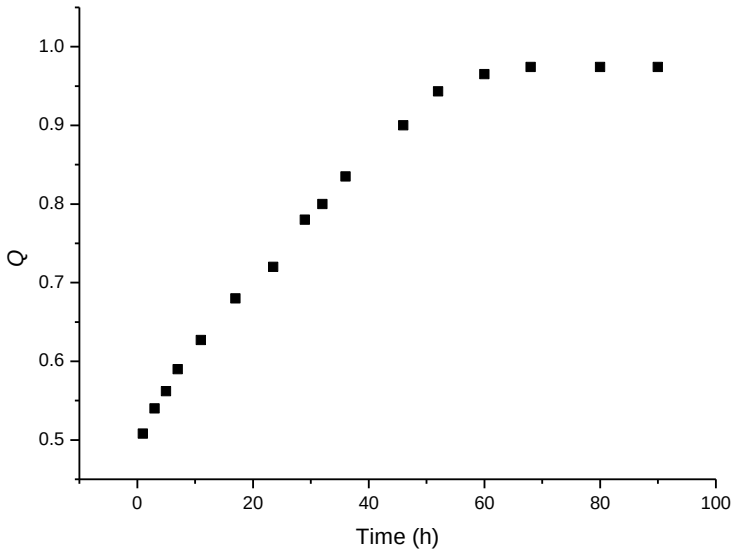


Figure S88. Kinetic profile of the competition between **1**(SMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

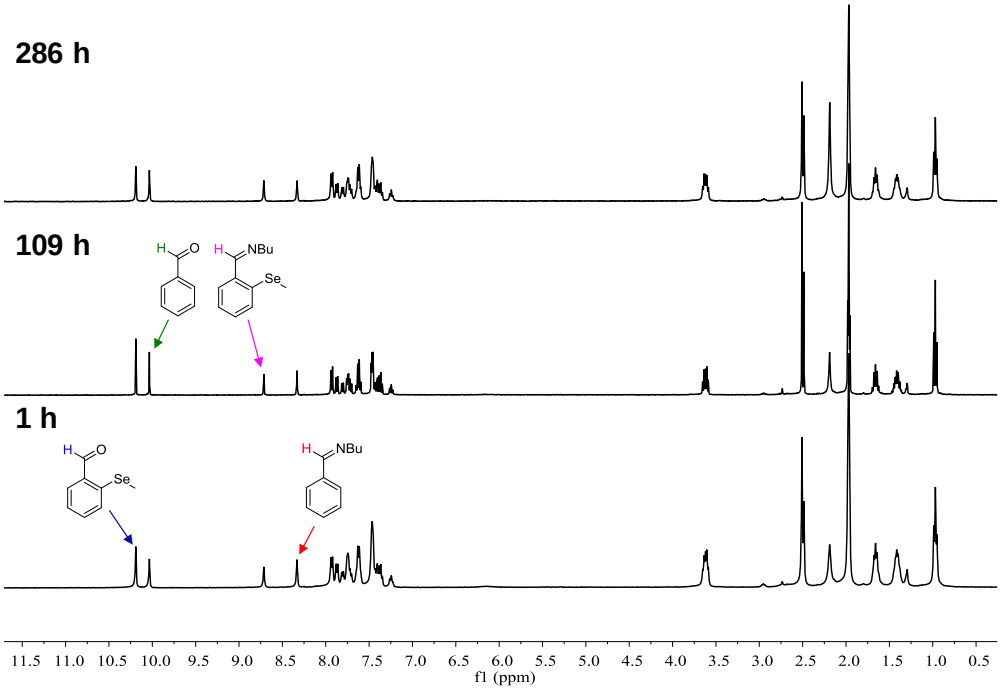


Figure S89. ^1H NMR spectra of the competition between **1**(SeMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel b in Table S13).

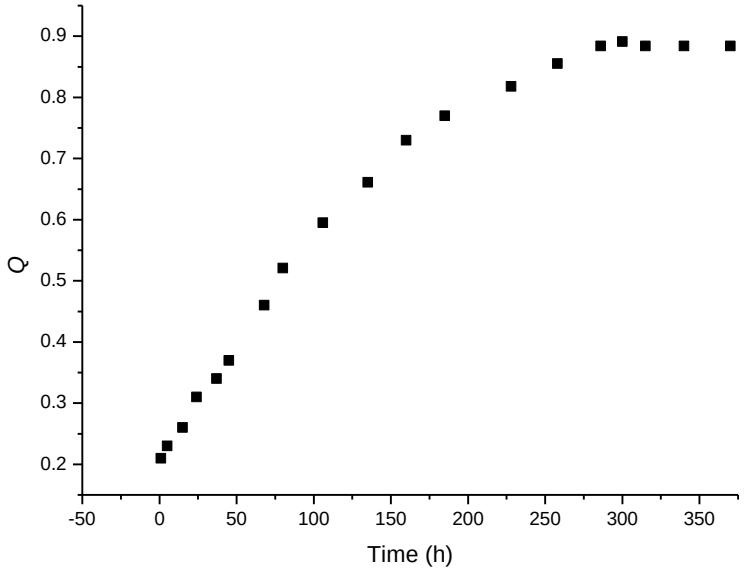


Figure S90. Kinetic profile of the competition between **1**(SeMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

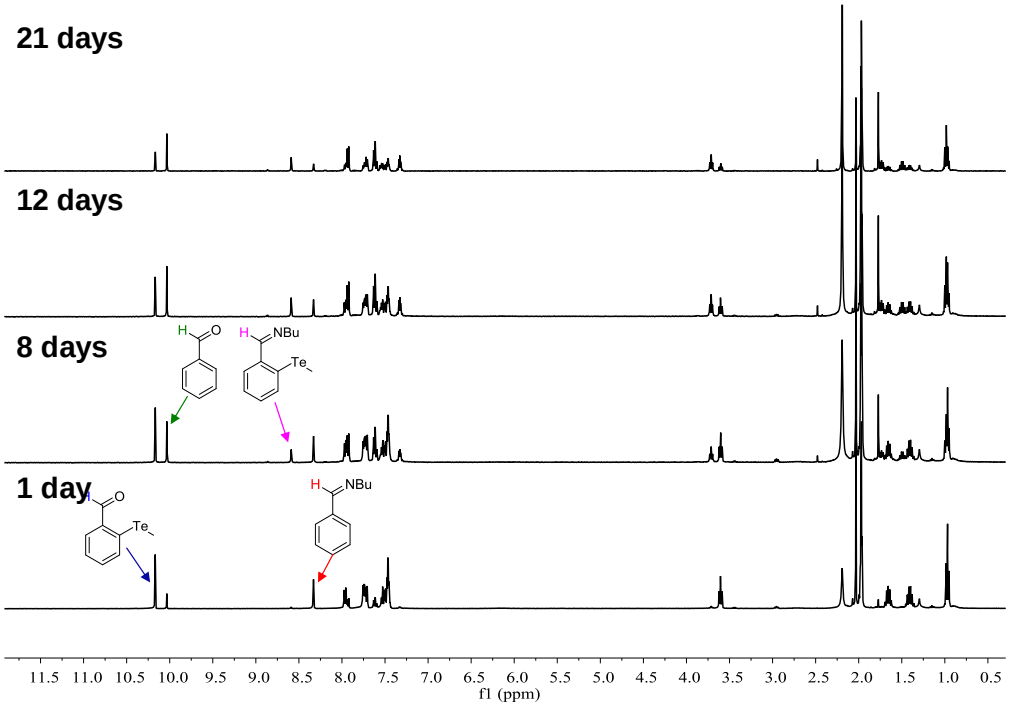


Figure S91. ^1H NMR spectra of the competition between **1**(TeMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time (the corresponding spectra of panel c in Table S13).

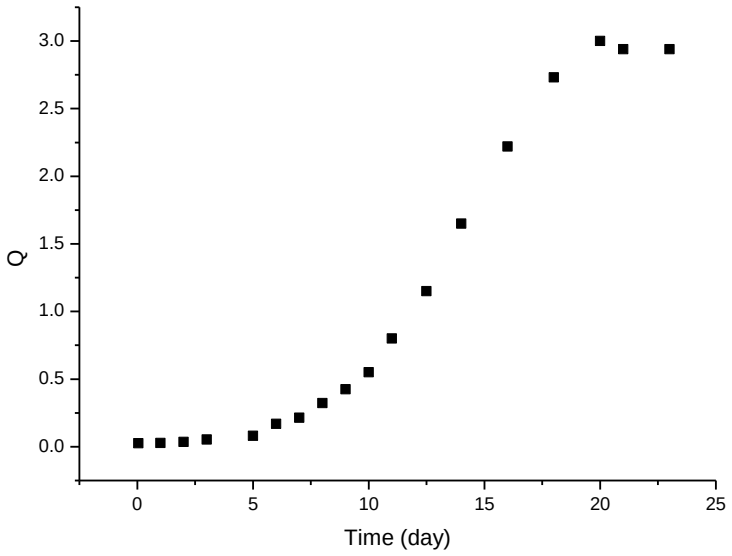


Figure S92. Kinetic profile of the competition between **1**(TeMe) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in the presence of $Zn(OTf)_2$ (0.1 equiv.) in CD_3CN at varied time.

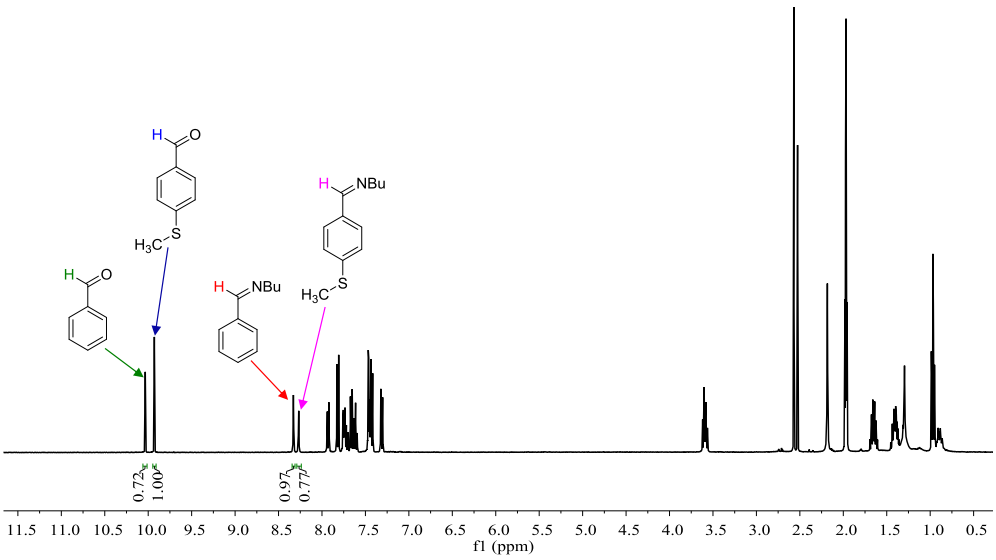


Figure S93. ^1H NMR spectrum of the competition between **3**(SMe) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel d in Table S13).

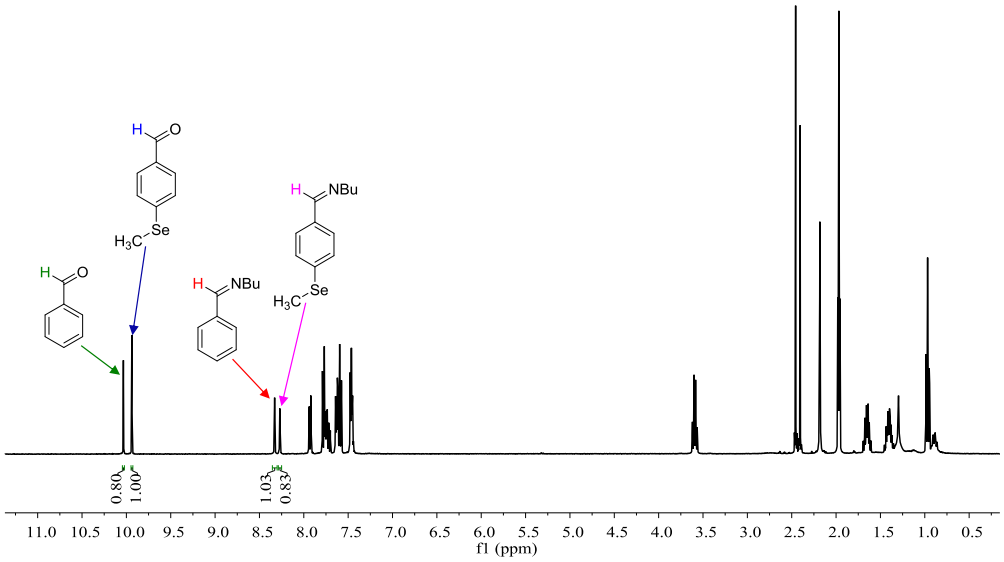


Figure S94. ^{1}H NMR spectrum of the competition between **3**(SeMe) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel e in Table S13).

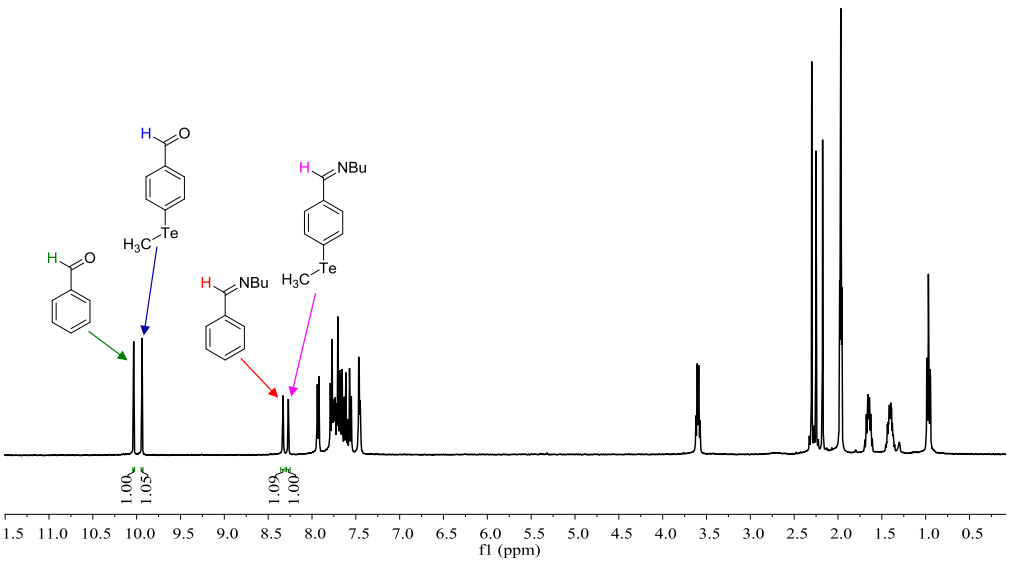
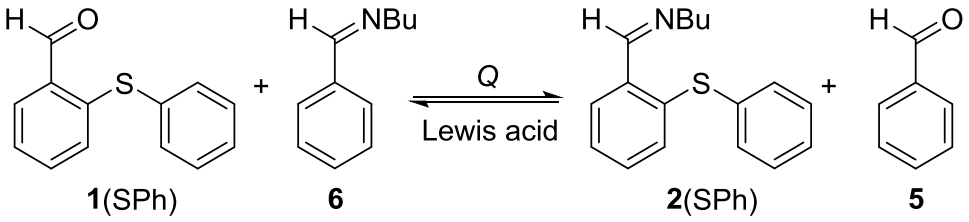


Figure S95. ^{1}H NMR spectrum of the competition between **3**(TeMe) and **5** for the reaction with 1-butylamine in CD_3CN (the corresponding spectra of panel f in Table S13).

Scheme S3. The effect of Lewis acid on imine exchange in CD_3CN.



Lewis acid = CH_3SO_3H, $Zn(OTf)_2$, $Cd(NO_3)_2$, $Mg(OTf)_2$, $In(OTf)_3$, $Fe(OTf)_3$, $Eu(OTf)_3$, $Sm(OTf)_3$

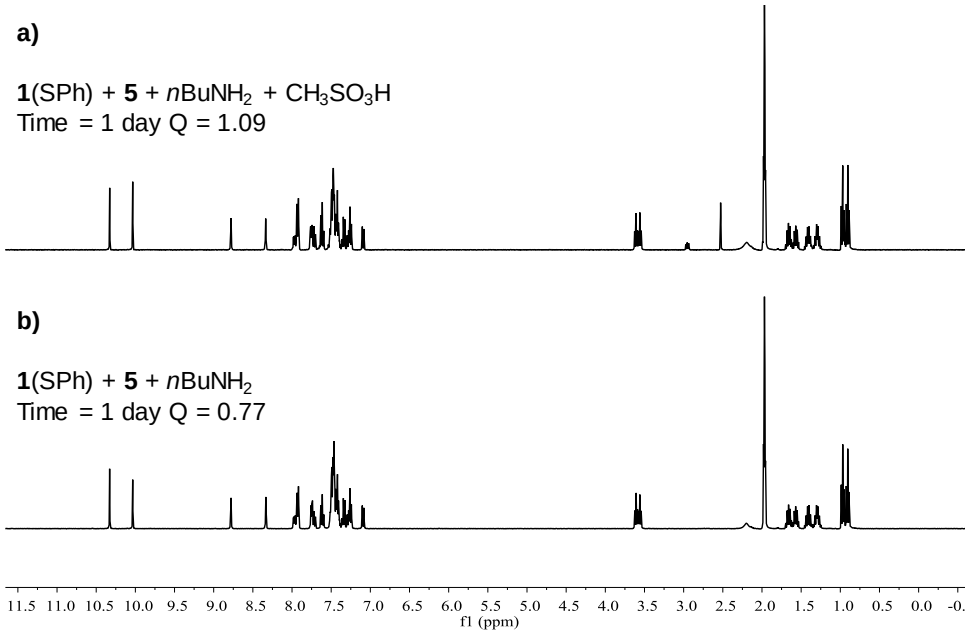


Figure S96. ^1H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of CH_3SO_3H (0.1 equiv.), (b) In the absence of CH_3SO_3H.

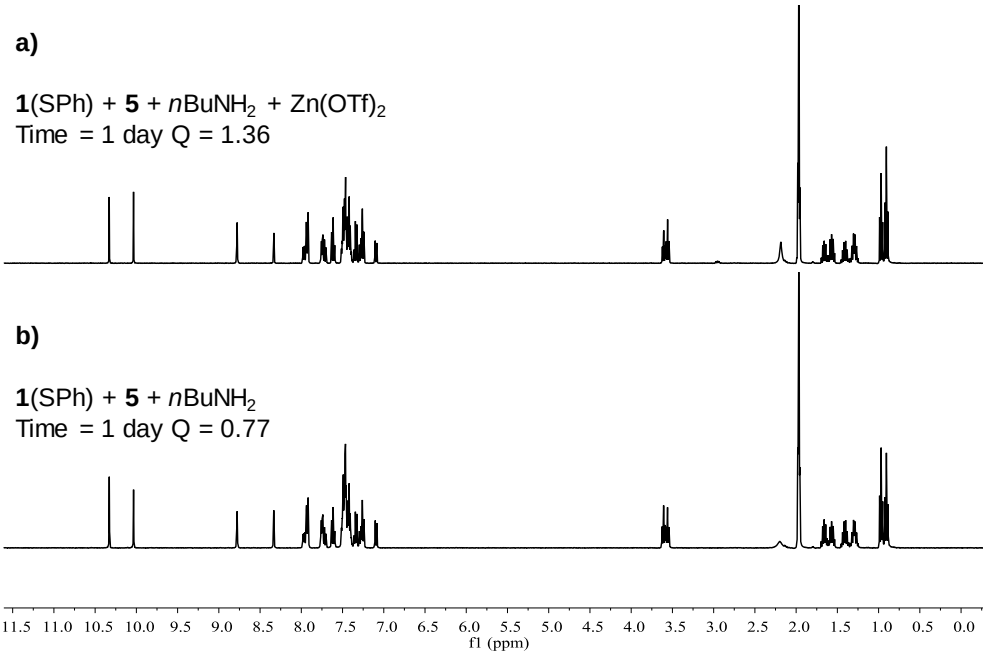


Figure S97. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Zn(OTf)_2$ (0.1 equiv.) (b) In the absence of $Zn(OTf)_2$.

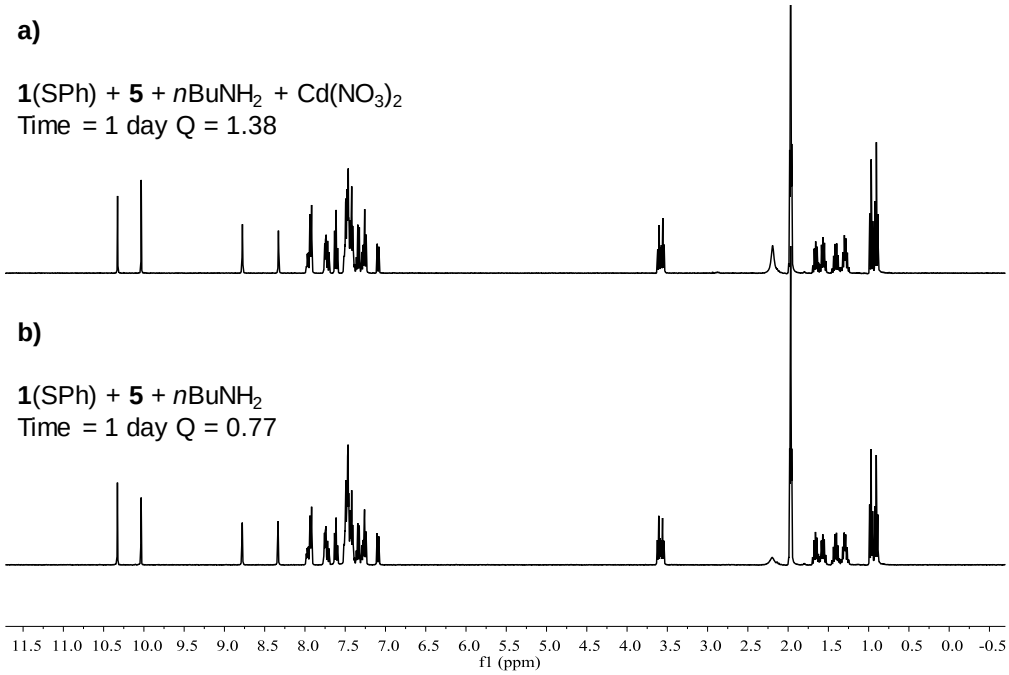


Figure S98. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Cd(NO_3)_2$ (0.1 equiv.) (b) In the absence of $Cd(NO_3)_2$.

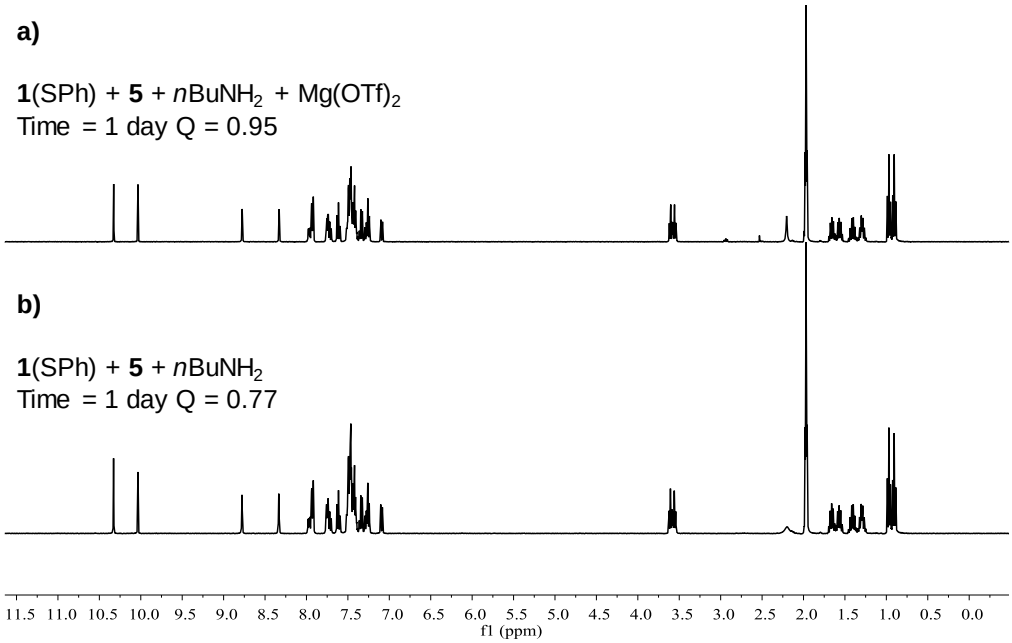


Figure S99. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Mg(OTf)_2$ (0.1 equiv.) (b) In the absence of $Mg(OTf)_2$.

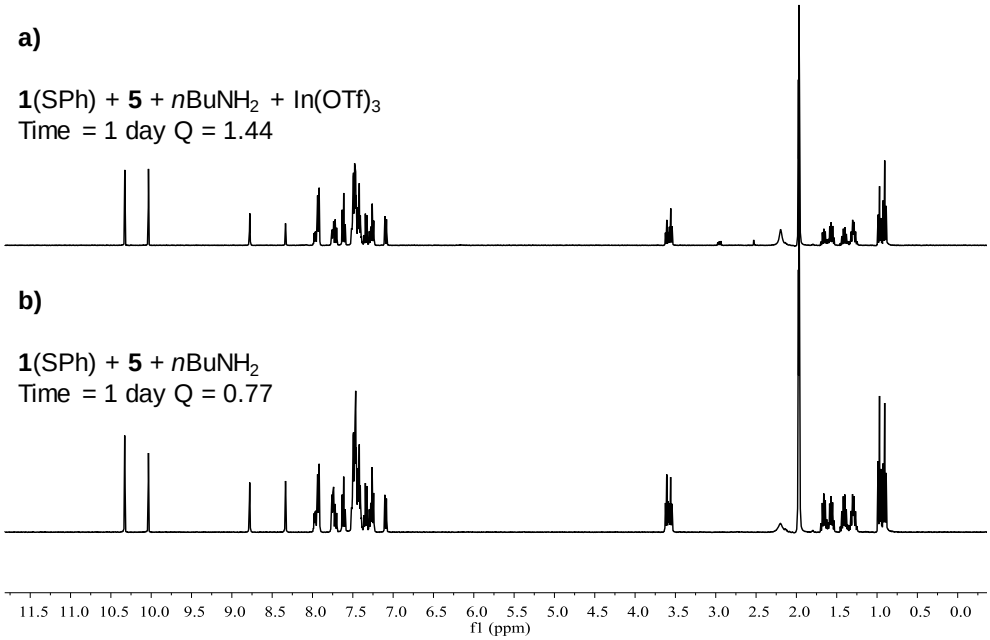


Figure S100. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $In(OTf)_3$ (0.1 equiv.) (b) In the absence of $In(OTf)_3$.

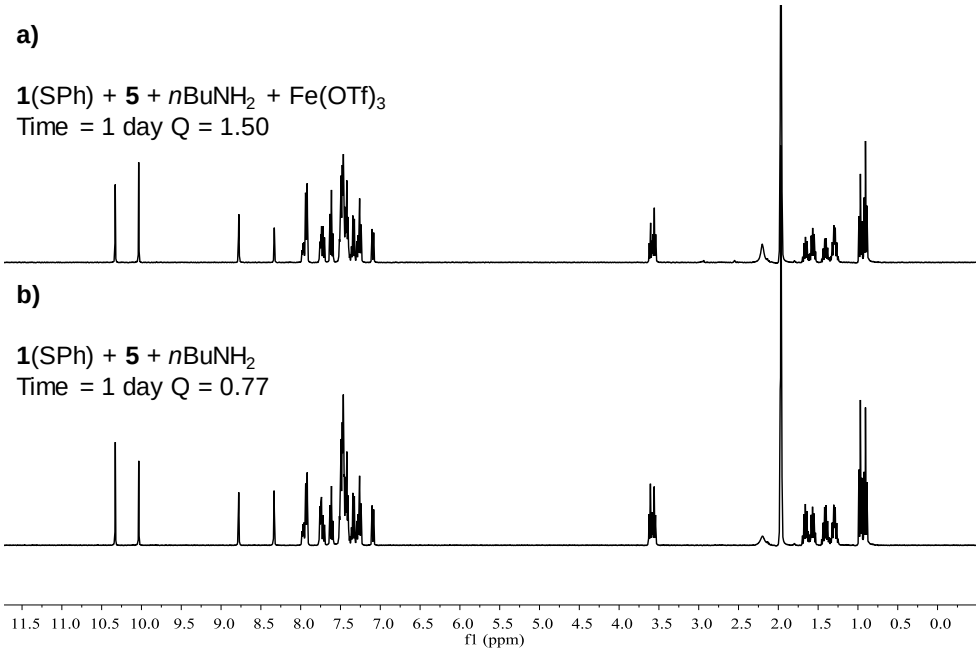


Figure S101. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Fe(OTf)_3$ (0.1 equiv.) (b) In the absence of $Fe(OTf)_3$.

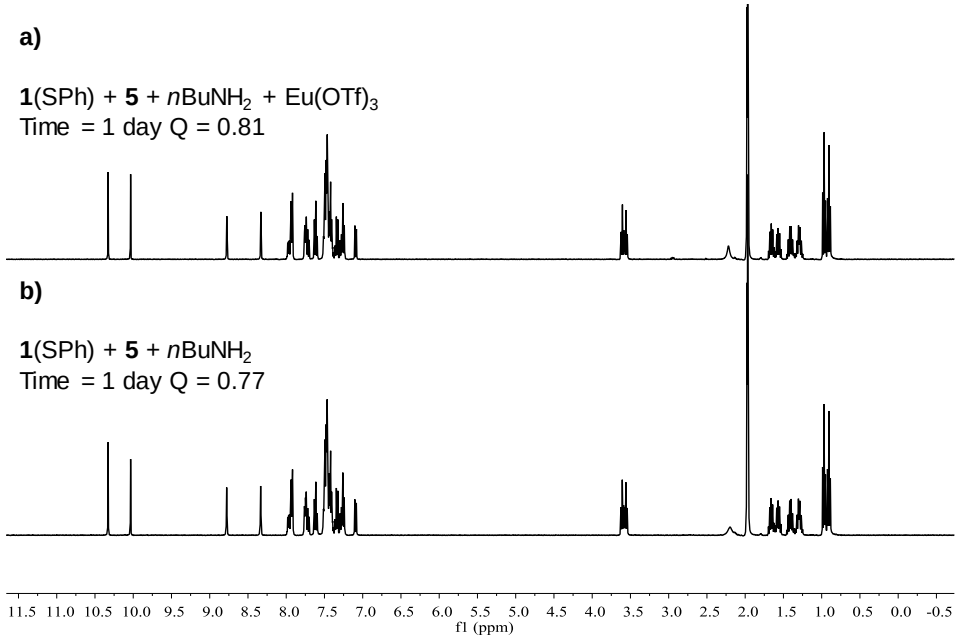


Figure S102. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Eu(OTf)_3$ (0.1 equiv.) (b) In the absence of $Eu(OTf)_3$.

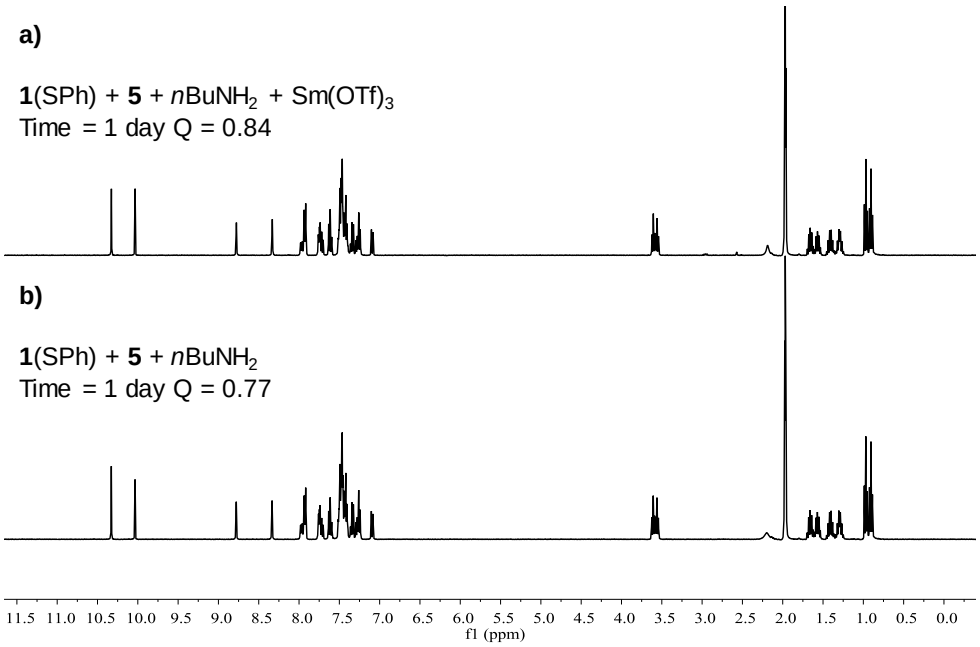


Figure S103. ^{1}H NMR spectra of the competition between **1**(SPh) and **5** (1.0 equiv.) for the reaction with 1-butylamine (1.0 equiv.) in CD_3CN. (a) In the presence of $Sm(OTf)_3$ (0.1 equiv.) (b) In the absence of $Sm(OTf)_3$.

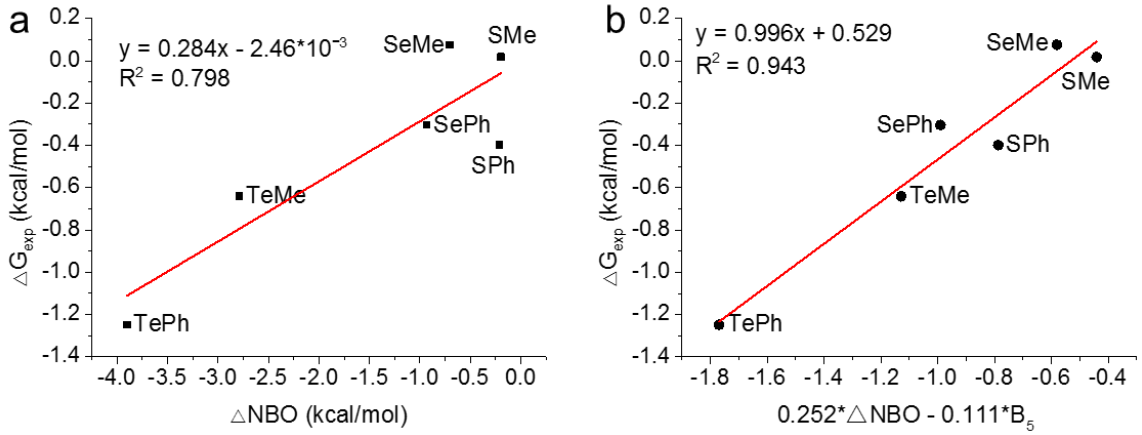


Figure S104. (a) Correlation between ΔG values of imine exchange 1 and ΔNBO of conformers 1 of **1**/**2**, (b) Multivariate correlation of ΔG values of imine exchange 1 with ΔNBO of conformers 1 of **1**/**2** and sterimol parameter (B_5) of ChalR.

6. Molecular Coordinates

1(SPh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -974.635937 hartree

C	-2.80895800	-2.28176700	-0.00002500
C	-3.30537900	-0.99257400	0.00001500
C	-2.45461500	0.11436500	-0.00000300
C	-1.05649100	-0.07056300	0.00000500
C	-0.56686800	-1.37675700	-0.00006000
C	-1.43153800	-2.46130200	-0.00006400
H	-3.47740800	-3.13128100	-0.00004400
H	-4.37522500	-0.81887900	0.00002500
H	0.49808800	-1.55722600	-0.00013600
H	-1.01544300	-3.46068800	-0.00008500
C	-3.10220700	1.43280100	0.00002200
H	-4.20566400	1.39532900	-0.00009400
C	1.62071100	0.57805300	-0.00009400
C	2.25954200	0.30389800	-1.20573700
C	2.25932100	0.30380700	1.20570300
C	3.53069100	-0.25447100	-1.20342900
H	1.75806600	0.52443400	-2.13947200
C	3.53044000	-0.25454700	1.20361400
H	1.75762000	0.52429800	2.13932500
C	4.16533200	-0.53508100	0.00013100
H	4.02487800	-0.46870400	-2.14194900
H	4.02448400	-0.46886000	2.14219200
H	5.15652600	-0.96937700	0.00023200
S	0.01459300	1.33871500	-0.00011400
O	-2.52741200	2.49704300	0.00017000

1(SPh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -974.636049 hartree

C	-2.77434000	2.18060700	0.08121400
C	-3.20165100	0.88538400	-0.12733400
C	-2.31034200	-0.18750800	-0.04693800
C	-0.96308600	0.04912400	0.26568500
C	-0.53934300	1.36057800	0.48260500
C	-1.43442500	2.41157400	0.38336900
H	-3.46936800	3.00594300	0.01005200
H	-4.23386300	0.66980700	-0.37135800
H	0.49337800	1.55782400	0.73604800
H	-1.08344400	3.42129700	0.55349200
C	-2.82770300	-1.54395100	-0.33257800
H	-2.07644000	-2.34237200	-0.43462900
C	1.72394400	-0.58673200	0.09707800
C	2.71437800	-0.58205700	1.07197100
C	1.98637600	-0.07450500	-1.17200400
C	3.97115300	-0.06629400	0.77608000
H	2.50060700	-0.97574000	2.05710100
C	3.23512600	0.45544200	-1.45433000
H	1.21199600	-0.08953900	-1.92868000
C	4.23064700	0.45662300	-0.48220400
H	4.74166400	-0.06607300	1.53578700
H	3.43571900	0.85898800	-2.43817000
H	5.20689800	0.86471800	-0.70855600
S	0.15129100	-1.31817500	0.46965000
O	-4.00152500	-1.79547200	-0.47264500

1(SPh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -974.634701 hartree

C	-3.61370900	0.37154800	0.79783500
C	-2.67431400	1.18941400	0.19158000
C	-1.51877400	0.65243300	-0.36908900
C	-1.28838600	-0.72816600	-0.28883800
C	-2.23062100	-1.54415500	0.32669800
C	-3.39338200	-0.99821900	0.85536300
H	-4.51313600	0.79767800	1.22120800
H	-2.82743100	2.25886100	0.12477500
H	-2.04434400	-2.60736600	0.40039100
H	-4.11969500	-1.64700200	1.32705000
C	-0.58378700	1.57080700	-1.06744700
H	0.16449000	1.09826000	-1.72169400
C	1.48601300	-0.66326600	-0.15649000
C	2.70456600	-0.59916700	-0.82853400
C	1.36551800	-0.11679300	1.11823000
C	3.79758000	0.00416800	-0.22283400
H	2.79308000	-1.01369600	-1.82507500
C	2.46006000	0.50063100	1.70795100
H	0.42436000	-0.17232200	1.65003500
C	3.67848400	0.56111300	1.04381800
H	4.74100000	0.04975000	-0.75115400
H	2.35815800	0.92897500	2.69663700
S	0.15381600	-1.50726100	-0.97254900
O	-0.63771000	2.77244300	-0.96504900
H	4.52865300	1.04139400	1.50954100

1(SePh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -2978.026234 hartree

C	2.78908300	2.54660100	-0.00012300
C	3.33552700	1.27768100	-0.00003600
C	2.52308900	0.14188400	-0.00000500
C	1.12299800	0.27570000	-0.00006800

C	0.58152100	1.55881500	-0.00015700
C	1.40563300	2.67580600	-0.00018500
H	3.42483500	3.42097500	-0.00013800
H	4.41120100	1.14403400	0.00002100
H	-0.48996500	1.69906400	-0.00019300
H	0.95396200	3.65966700	-0.00024900
C	3.20649300	-1.15724100	0.00010200
H	4.30832200	-1.09869000	0.00017000
C	-1.71151200	-0.41256300	0.00002800
C	-2.33954300	-0.11395700	-1.20524300
C	-2.33927400	-0.11343500	1.20532100
C	-3.58938700	0.49220700	-1.20313400
H	-1.84998700	-0.35028100	-2.14142300
C	-3.58910000	0.49273700	1.20323200
H	-1.84949100	-0.34935800	2.14148500
C	-4.21342400	0.79655700	0.00004900
H	-4.07463000	0.72559600	-2.14190300
H	-4.07413300	0.72655400	2.14200300
H	-5.18737300	1.26836800	0.00006700
O	2.65038400	-2.23225400	0.00012900
Se	0.00387000	-1.28684300	0.00001300

1(SePh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -2978.023755 hartree

C	2.71804200	2.49094900	0.00001700
C	3.25816500	1.22008400	0.00001200
C	2.43649900	0.09153600	0.00008600
C	1.04163700	0.24175300	0.00011800
C	0.50234800	1.52535600	0.00002200
C	1.33470200	2.63497400	-0.00000600
H	3.36017100	3.36094300	-0.00000400
H	4.32988400	1.06789600	-0.00002200
H	-0.56892200	1.66921200	-0.00004500
H	0.89274000	3.62321100	-0.00008900
C	3.08207300	-1.23846500	0.00001600
H	2.40990200	-2.11289100	0.00060200
C	-1.81144100	-0.46372800	0.00003800
C	-2.43552000	-0.16610300	-1.20698000
C	-2.43564400	-0.16581000	1.20689100
C	-3.68511600	0.44006100	-1.20370700
H	-1.94474200	-0.40269600	-2.14199700
C	-3.68521700	0.44042500	1.20334100
H	-1.94499800	-0.40216700	2.14204100
C	-4.30874100	0.74391400	-0.00025300
H	-4.17009600	0.67381700	-2.14237700
H	-4.17021700	0.67450800	2.14191800
H	-5.28255200	1.21586700	-0.00039900
O	4.27772700	-1.40755200	-0.00059700
Se	-0.09422700	-1.31991000	0.00022300

1(SePh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -2978.023569 hartree

C	-3.66111600	0.93099000	0.69410900
C	-2.67721300	1.50759600	-0.09097800
C	-1.54970300	0.78113300	-0.46880800
C	-1.39564700	-0.53602900	-0.01961200
C	-2.38104600	-1.10912300	0.77567900
C	-3.51479100	-0.38330600	1.11858900
H	-4.53752200	1.50015800	0.97308900
H	-2.77140400	2.52703100	-0.44263300
H	-2.25553000	-2.12047600	1.13906200
H	-4.27629900	-0.84446800	1.73385700
C	-0.56922200	1.43615500	-1.37218500
H	0.14070300	0.76860900	-1.88410000
C	1.53822300	-0.44354200	0.13056400
C	2.75550700	-0.49843500	-0.54077200
C	1.37131100	0.42104700	1.20743300
C	3.80711400	0.30944500	-0.12814700
H	2.88113700	-1.16152500	-1.38761100
C	2.42228300	1.23890400	1.60046000
H	0.42849700	0.45988600	1.73843500
C	3.64217600	1.18356700	0.93803800
H	4.75260700	0.26257800	-0.65272100
H	2.28636200	1.91561000	2.43415900
Se	0.13411500	-1.62247400	-0.45169400
O	-0.54935500	2.62573300	-1.57630800
H	4.45910800	1.82042300	1.25028800

1(TePh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -844.389425 hartree

C	2.77390600	2.81980300	-0.00007000
C	3.37495700	1.57579100	-0.00000400
C	2.60247200	0.41211300	0.00001600
C	1.20023300	0.48322800	-0.00005000
C	0.60648400	1.74306700	-0.00009700
C	1.38510000	2.89310500	-0.00010900
H	3.37212300	3.72044500	-0.00006300
H	4.45528200	1.48561100	0.00001700
H	-0.47076600	1.84027900	-0.00012900
H	0.89606300	3.85910100	-0.00014200
C	3.30853300	-0.87042200	0.00011300
H	4.40889300	-0.81184800	0.00024300
C	-1.83171000	-0.25755200	-0.00003200
C	-2.45300100	0.07447200	-1.20286000
C	-2.45277000	0.07466200	1.20286900
C	-3.67481100	0.73670300	-1.20233800
H	-1.98137100	-0.17928700	-2.14427400

C	-3.67458100	0.73690000	1.20247500
H	-1.98097500	-0.17894900	2.14423800
C	-4.28561200	1.06898100	0.00010200
H	-4.14849500	0.99245600	-2.14149400
H	-4.14809800	0.99278300	2.14168100
H	-5.23722100	1.58466000	0.00014800
O	2.75142500	-1.94847100	0.00006400
Te	0.02976900	-1.28197300	-0.00001600

1(TePh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -844.383606 hartree

C	2.73965200	2.73895800	-0.00838200
C	3.32754300	1.48960800	0.00315000
C	2.54520800	0.33251900	0.00420000
C	1.14685600	0.42576300	-0.00667300
C	0.56259200	1.69041400	-0.01842700
C	1.35170600	2.83189700	-0.01905100
H	3.34907000	3.63233800	-0.00919100
H	4.40430500	1.37788000	0.01171800
H	-0.51377400	1.79723100	-0.02740400
H	0.87392200	3.80341700	-0.02832000
C	3.23960400	-0.97198300	0.01739000
H	2.59689700	-1.87093200	0.02053300
C	-1.92910800	-0.28370600	0.00260600
C	-2.55180700	0.04555800	-1.19919700
C	-2.52951700	0.05998500	1.21175700
C	-3.76575100	0.72137400	-1.18934400
H	-2.09022300	-0.22001500	-2.14155000
C	-3.74318900	0.73614300	1.21632700
H	-2.05079300	-0.19490800	2.14851300
C	-4.36068900	1.06712500	0.01704100
H	-4.24509000	0.97687000	-2.12545100
H	-4.20508800	1.00299800	2.15801800
H	-5.30638300	1.59331600	0.02270700
O	4.43886400	-1.10488400	0.02503500
Te	-0.08696800	-1.31463600	-0.00804300

1(TePh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -844.383184 hartree

C	-3.73362800	1.34285400	0.56035500
C	-2.69149700	1.80466300	-0.22424000
C	-1.59309100	0.99096100	-0.50196500
C	-1.52344400	-0.29592500	0.04589700
C	-2.57044300	-0.74856700	0.84435000
C	-3.67480100	0.05841400	1.08639600
H	-4.58687800	1.97672000	0.76096100
H	-2.71542400	2.79823300	-0.65347000
H	-2.52155800	-1.73206300	1.29379500
H	-4.48254200	-0.31466500	1.70275100
C	-0.55285500	1.52860300	-1.41572400
H	0.12307900	0.78714200	-1.87025300
C	1.62499100	-0.20449400	0.23213400
C	2.83897500	-0.25976100	-0.44682900
C	1.42128400	0.76602500	1.20963000
C	3.84600100	0.64837400	-0.14290300
H	3.00174200	-1.00066100	-1.21999700
C	2.42440400	1.68361400	1.49404800
H	0.48305200	0.81294800	1.74935500
C	3.63916900	1.62471200	0.82234500
H	4.78815900	0.59854000	-0.67345600
H	2.25677000	2.44071200	2.24931500
Te	0.11725100	-1.61418200	-0.23540600
O	-0.44925900	2.69943000	-1.69102900
H	4.42022700	2.33830500	1.04936800

2(SPh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -994.015758 hartree

C	-1.97828500	-3.02386200	0.00003900
C	-2.73495300	-1.86654900	0.00020500
C	-2.14995600	-0.59776300	0.00010800
C	-0.74262800	-0.49321800	-0.00012600
C	0.01199100	-1.66728000	-0.00029900
C	-0.59555300	-2.91370800	-0.00022600
H	-2.45739400	-3.99329700	0.00011700
H	-3.81675500	-1.93013000	0.00040600
H	1.09082900	-1.61612000	-0.00049400
H	0.02433000	-3.80107700	-0.00036600
C	-3.08277300	0.53800700	0.00023900
H	-4.14270900	0.25201400	0.00063200
C	1.75910300	0.67503900	-0.00002500
C	2.44264600	0.53741400	-1.20482800
C	2.44243300	0.53733600	1.20488500
C	3.80157600	0.25247200	-1.20311800
H	1.90682600	0.65010700	-2.13887300
C	3.80136600	0.25238200	1.20340300
H	1.90645200	0.64996200	2.13884500
C	4.48101800	0.10879800	0.00020000
H	4.32929000	0.14489000	-2.14178400
H	4.32889300	0.14474500	2.14216700
H	5.54054300	-0.11152300	0.00026800
N	-2.73693800	1.75261600	-0.00015700
C	-3.78283000	2.75367100	0.00000400
H	-3.66757800	3.39120500	-0.87781900
H	-4.78934200	2.32163700	0.00047400
H	-3.66694400	3.39162600	0.87744600
S	0.03332500	1.10507500	-0.00016800

2(SPh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -994.016283 hartree

C	-2.10686100	2.76960700	-0.07467700
C	-2.68076200	1.52250400	-0.22026800
C	-1.94827400	0.35474600	0.01733900
C	-0.61251100	0.46754700	0.42246800
C	-0.03918900	1.73080700	0.57975000
C	-0.77580800	2.87209500	0.32389600
H	-2.68667900	3.66121700	-0.27277700
H	-3.70979800	1.41948800	-0.53797100
H	0.98914000	1.81182000	0.90751600
H	-0.31516800	3.84389800	0.44482100
C	-2.59314100	-0.95855000	-0.19135700
H	-1.92446200	-1.81523500	-0.32377900
C	1.92994600	-0.60660500	0.20375700
C	3.03706100	-0.87681200	1.00069800
C	2.10445800	-0.11389600	-1.08820500
C	4.31704800	-0.66015500	0.50362900
H	2.89688300	-1.24946200	2.00730800
C	3.38284300	0.11928200	-1.56920700
H	1.24089100	0.08905300	-1.70915800
C	4.49285000	-0.15735600	-0.77716400
H	5.17503700	-0.87383600	1.12761300
H	3.51375900	0.50826600	-2.57066100
H	5.48934300	0.02045200	-1.15934100
N	-3.84861300	-1.09134300	-0.23236600
C	-4.37727200	-2.41599700	-0.48273800
H	-4.99291000	-2.38871800	-1.38329200
H	-3.59782000	-3.17542100	-0.60361800
H	-5.03107900	-2.70101200	0.34287800
S	0.31942600	-0.98715000	0.84184400

2(SPh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -994.016716 hartree

C	-3.67535700	0.22088800	0.85481200
C	-2.65014800	1.06805100	0.46596300
C	-1.51865900	0.57735100	-0.18247500
C	-1.41801000	-0.80208100	-0.41428800
C	-2.44660800	-1.65127500	-0.01654900
C	-3.57769100	-1.14169500	0.60462700
H	-4.55077700	0.62273300	1.34755400
H	-2.71572300	2.13354700	0.64308800
H	-2.34965400	-2.71542700	-0.18736800
H	-4.37308300	-1.81151200	0.90371900
C	-0.46356800	1.51442000	-0.62401900
H	0.16482300	1.18181300	-1.45720400
C	1.34853900	-0.99550000	-0.25154600
C	2.57778800	-0.84647800	-0.88935600
C	1.24315300	-0.75867500	1.11614700
C	3.69597900	-0.46838400	-0.15903200
H	2.65519900	-1.01719500	-1.95601400
C	2.36254300	-0.36335200	1.83484100
H	0.29054400	-0.87584800	1.61696700
C	3.59182200	-0.21966100	1.20327100
H	4.64745000	-0.35503300	-0.66225200
H	2.27180500	-0.17308300	2.89648100
S	-0.02512700	-1.53190200	-1.23944800
H	4.46155900	0.08700000	1.76887600
N	-0.29833000	2.64103600	-0.07921400
C	0.75097100	3.49134300	-0.60262600
H	1.45301800	3.72255000	0.19996900
H	1.29573300	3.03739900	-1.43712900
H	0.31491600	4.43652200	-0.92964100

2(SePh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -2997.406695 hartree

C	-1.96230200	-3.21930000	-0.00006000
C	-2.75719800	-2.08770500	0.00002300
C	-2.20792100	-0.80292400	0.00002800
C	-0.80816900	-0.65540200	-0.00004500
C	-0.01446800	-1.80084300	-0.00012900
C	-0.58311600	-3.06654700	-0.00013900
H	-2.40979100	-4.20384200	-0.00007300
H	-3.83660100	-2.18463700	0.00008700
H	1.06262100	-1.71560500	-0.00018500
H	0.06303800	-3.93501900	-0.00020200
C	-3.15972600	0.31512100	0.00010800
H	-4.21777000	0.02416800	0.00027700
C	1.84982900	0.56060500	0.00002100
C	2.52668900	0.39047700	-1.20414100
C	2.52654900	0.39018400	1.20421200
C	3.87141800	0.04148200	-1.20278500
H	2.00082500	0.52580200	-2.14091500
C	3.87127800	0.04118400	1.20293100
H	2.00058300	0.52528700	2.14096200
C	4.54369100	-0.13440600	0.00008900
H	4.39299400	-0.09187200	-2.14173900
H	4.39274200	-0.09240300	2.14191300
H	5.59137200	-0.40578100	0.00011900
N	-2.81271300	1.52906500	-0.00001200
C	-3.84879600	2.53965100	0.00007700
H	-3.72769700	3.17582600	-0.87780700
H	-4.85819000	2.11529800	0.00024200
H	-3.72744100	3.17592600	0.87785200
Se	-0.00365400	1.09746900	-0.00004600

2(SePh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -2997.404824 hartree

C	2.03906100	2.98137300	-0.11015600
C	2.72180800	1.79733200	0.09106300
C	2.06675800	0.56394200	0.03328300
C	0.69303700	0.54043000	-0.23840100
C	0.00814400	1.73517600	-0.45199700
C	0.67468400	2.94697700	-0.38084700
H	2.56134100	3.92710500	-0.05397000
H	3.78154600	1.79830400	0.30946000
H	-1.04971200	1.71958800	-0.67823300
H	0.12663300	3.86611000	-0.54324800
C	2.83590100	-0.67355700	0.27821900
H	2.25733700	-1.56787800	0.53666600
C	-2.01349700	-0.56248300	0.00018000
C	-3.00229000	-0.66496200	-0.97078100
C	-2.32253000	-0.07520300	1.26743200
C	-4.30519500	-0.28148600	-0.67143000
H	-2.75639500	-1.03610700	-1.95712300
C	-3.61987800	0.32243300	1.55392600
H	-1.55000100	-0.00356100	2.02264100
C	-4.61352400	0.21589600	0.58641900
H	-5.07443400	-0.36420300	-1.42812400
H	-3.85734500	0.70726100	2.53718000
H	-5.62627600	0.52061300	0.81542800
N	4.09645100	-0.71014700	0.21270500
C	4.75132100	-1.96811300	0.50476100
H	5.43559300	-1.82633700	1.34282800
H	4.04998200	-2.77352600	0.74616000
H	5.35501600	-2.26346100	-0.35463000
Se	-0.22974200	-1.14704100	-0.40394100

2(SePh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -2997.406131 hartree

C	-3.64586400	0.90570400	0.92091900
C	-2.55371300	1.55496000	0.36941700
C	-1.49008900	0.83758400	-0.17754200
C	-1.52970800	-0.56185100	-0.13567200
C	-2.62420300	-1.21276600	0.42529200
C	-3.68596600	-0.48260600	0.94023800
H	-4.46616900	1.48017300	1.33052600
H	-2.51138500	2.63579200	0.33557100
H	-2.63755100	-2.29392000	0.47023800
H	-4.53472300	-0.99973700	1.36821900
C	-0.36691900	1.56949700	-0.80239700
H	0.18360400	1.03752500	-1.58603900
C	1.37621600	-0.86034200	0.09229900
C	2.58748800	-0.73734400	-0.57972400
C	1.25978600	-0.42730400	1.40899300
C	3.68459600	-0.18570500	0.07063100
H	2.67262200	-1.05919900	-1.61017200
C	2.35477200	0.14055100	2.04522400
H	0.31720200	-0.52423900	1.93340300
C	3.56976500	0.25969700	1.38043600
H	4.62555700	-0.09204200	-0.45594600
H	2.25823200	0.48476400	3.06687400
Se	-0.10946700	-1.65830800	-0.83310700
H	4.42159200	0.70048600	1.88121300
N	-0.06274200	2.74647600	-0.46298300
C	1.03943600	3.38057000	-1.15691700
H	1.79670600	3.67280500	-0.42781200
H	1.49895800	2.73569600	-1.91349000
H	0.68284500	4.29516400	-1.63327400

2(TePh)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -863.771498 hartree

C	3.21458500	-0.084131000	0.000157000
H	4.28041800	0.170504000	0.000393000
N	2.81629900	-1.283271000	0.000017000
C	3.78590500	-2.356782000	0.000183000
H	3.62648200	-2.983000000	-0.878427000
H	4.81702100	-1.991433000	0.000451000
H	3.62614200	-2.983086000	0.878677000
Te	0.06442700	-1.120859000	-0.000018000
C	-1.96432900	-0.44234500	0.000088000
C	-2.64125700	-0.23299200	-1.200746000
C	-2.64094200	-0.23203300	1.200935000
C	-3.96657100	0.18658000	-1.201808000
H	-2.13119200	-0.39259200	-2.143290000
C	-3.96624800	0.18752600	1.202012000
H	-2.13060900	-0.39088900	2.143462000
C	-4.62997000	0.39829100	0.000102000
H	-4.47995800	0.34770500	-2.141320000
H	-4.47940100	0.34939300	2.141523000
H	-5.66188100	0.72507800	0.000122000
C	2.27037900	1.03553600	0.000004000
C	2.79110900	2.33124800	-0.000057000
C	0.87959800	0.83894800	-0.000094000
C	1.95812200	3.43560400	-0.000218000
H	3.86747600	2.45925800	0.000024000
C	0.05027200	1.95847300	-0.000232000
C	0.58264000	3.24109900	-0.000298000
H	2.37294900	4.43451900	-0.000274000
H	-1.02475200	1.83995800	-0.000295000
H	-0.08677500	4.09198900	-0.000406000

2(TePh)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -863.764526 hartree

C	2.04696800	3.19496700	-0.06702100
C	2.79771900	2.03911400	0.03742300
C	2.18932800	0.78132200	0.04240000
C	0.79464100	0.69486700	-0.05868100
C	0.04283400	1.86297100	-0.16949600
C	0.66346500	3.10316400	-0.17017900
H	2.53259500	4.16174200	-0.06540800
H	3.87557600	2.08343200	0.12308400
H	-1.03453200	1.81338800	-0.25738400
H	0.06157900	3.99920500	-0.25254800
C	3.03197800	-0.42610700	0.16211500
H	2.51823600	-1.36598000	0.40464200
C	-2.14911200	-0.44658500	0.02631100
C	-2.91133800	-0.29167400	-1.12892100
C	-2.69232400	-0.10836200	1.26407600
C	-4.20820400	0.20149700	-1.04541800
H	-2.49421300	-0.54952000	-2.09383300
C	-3.98648700	0.38972500	1.34226800
H	-2.10611900	-0.22947900	2.16609300
C	-4.74492700	0.54383300	0.18841400
H	-4.79588200	0.32014600	-1.94652200
H	-4.40237000	0.65406300	2.30591900
H	-5.75410100	0.92966000	0.25159600
N	4.28481000	-0.40522900	0.01299800
C	5.00887400	-1.64819600	0.17575000
H	5.74369300	-1.52941600	0.97351900
H	4.35909200	-2.49800400	0.40943000
H	5.56218900	-1.86060500	-0.74012800
Te	-0.17999800	-1.20067800	-0.09545600

2(TePh)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -863.764721 hartree

C	-3.55708600	1.65170600	0.79998600
C	-2.39340600	2.06611000	0.17459600
C	-1.43119300	1.14405800	-0.24050300
C	-1.64309000	-0.21839200	0.00853900
C	-2.81192500	-0.62863300	0.64667200
C	-3.77179000	0.29832700	1.02817300
H	-4.29669600	2.38025600	1.10510400
H	-2.21415600	3.11542700	-0.02090200
H	-2.96925400	-1.67807700	0.86124500
H	-4.67786400	-0.03720600	1.51584600
C	-0.22970700	1.63375800	-0.95192000
H	0.22898800	0.93859100	-1.66460300
C	1.43883200	-0.70583300	0.31481300
C	2.61403300	-0.59738700	-0.42267500
C	1.35820000	-0.12619900	1.57805100
C	3.70573900	0.08244100	0.10562400
H	2.67906400	-1.02837100	-1.41426100
C	2.44382800	0.57003300	2.09231200
H	0.44674400	-0.20637000	2.15822700
C	3.62038200	0.67239400	1.35926600
H	4.61726400	0.16241800	-0.47278400
H	2.37146900	1.02770200	3.07061200
Te	-0.23069500	-1.71854900	-0.50275900
H	4.46634600	1.21244100	1.76392700
N	0.24114000	2.78955000	-0.76397400
C	1.40858900	3.17012800	-1.53304400
H	2.21278700	3.44074900	-0.84708500
H	1.75967300	2.37646500	-2.20138300
H	1.17533900	4.05861900	-2.12198000

1(SMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -782.952923 hartree

C	2.63265800	-0.88127800	0.00011900
C	2.20810100	0.43379300	0.00008500
C	0.85162800	0.76109000	-0.00005700
C	-0.12437900	-0.26034900	-0.00008500
C	0.31951700	-1.58429400	-0.00011700
C	1.67382100	-1.88546200	-0.00001200
H	3.68642700	-1.12212400	0.00026100
H	2.93190300	1.24063600	0.00016600
H	-0.38630800	-2.40012600	-0.00029500
H	1.97737300	-2.92459700	0.00000300
C	0.53063500	2.19411800	-0.00021900
H	1.41510700	2.85526900	-0.00051500
S	-1.83236200	0.15280900	-0.00012500
O	-0.58309800	2.66639300	0.00028100
C	-2.62435300	-1.46319300	0.00016800
H	-2.37862000	-2.03184000	0.89480500
H	-3.69092800	-1.24732400	-0.00013000
H	-2.37814300	-2.03254500	-0.89383300

1(SMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -782.951868 hartree

C	-1.81195500	1.92106000	0.00016700
C	-2.01668500	0.55481100	0.00022200
C	-0.94271400	-0.33403800	0.00005000
C	0.37850000	0.15443800	-0.00016000
C	0.57438700	1.53606200	-0.00028300
C	-0.50812800	2.40291700	-0.00010500
H	-2.65048500	2.60360300	0.00036700
H	-3.01658900	0.14027100	0.00032400
H	1.57063000	1.95121100	-0.00058100

H	-0.32471200	3.46979200	-0.00024500
C	-1.23860600	-1.78202600	-0.00003200
H	-0.37241000	-2.46277000	-0.00003800
S	1.72433200	-0.98647400	0.00000200
O	-2.35757100	-2.23948200	-0.00011900
C	3.17032500	0.08057500	0.00018500
H	3.20719500	0.69750100	0.89532800
H	4.01897700	-0.60012500	0.00063800
H	3.20790600	0.69716100	-0.89513800

1(SMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -782.949845 hartree

C	2.63207700	-0.42282000	0.25489200
C	1.86449800	0.72334200	0.14618300
C	0.49665000	0.64215700	-0.10939500
C	-0.11593400	-0.61335200	-0.23154400
C	0.66370800	-1.76083500	-0.12185100
C	2.02889800	-1.66659000	0.11130100
H	3.69437400	-0.35064600	0.44542200
H	2.31184100	1.70453100	0.24035400
H	0.19129500	-2.73000000	-0.21160700
H	2.62024700	-2.56949900	0.19089300
C	-0.25927600	1.90577600	-0.28837000
H	-1.27863000	1.80469400	-0.69202700
S	-1.85897400	-0.80816600	-0.53385100
O	0.19770700	2.99580300	-0.03976200
C	-2.53094700	-0.22909400	1.04435700
H	-2.32213600	0.82732800	1.20144000
H	-3.60792600	-0.37542100	0.98858400
H	-2.12518600	-0.81826500	1.86320600

1(SeMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -2786.344590 hartree

C	3.03986800	-0.86580200	-0.00008300
C	2.60446000	0.44571300	-0.00006800
C	1.24335100	0.75583100	-0.00001100
C	0.28210400	-0.27345900	0.00001400
C	0.73373400	-1.59204800	0.00009800
C	2.09160000	-1.88067300	0.00003200
H	4.09594400	-1.09682700	-0.00017700
H	3.32002500	1.25994000	-0.00006800
H	0.03428200	-2.41408800	0.00025400
H	2.40668700	-2.91639300	0.00011500
C	0.89526400	2.18179900	0.00010100
H	1.76095300	2.86637100	0.00027400
Se	-1.58429300	0.13754800	-0.00006000
O	-0.23225800	2.62179300	0.00005800
C	-2.30539900	-1.67033900	0.00004700
H	-2.00936400	-2.21006900	0.89565200
H	-3.38478600	-1.53585400	0.00032300
H	-2.00962000	-2.21016900	-0.89556300

1(SeMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -2786.342685 hartree

C	-2.55963600	1.64977400	-0.00002700
C	-2.49607400	0.26980700	-0.00003200
C	-1.26807000	-0.39216200	-0.00000800
C	-0.07192300	0.34433300	0.00001500
C	-0.14476000	1.73570400	0.00003800
C	-1.37502400	2.37714000	0.00001800
H	-3.51504700	2.15609800	-0.00005500
H	-3.39651100	-0.33094400	-0.00005200
H	0.75222500	2.33670300	0.00007400
H	-1.40300900	3.45934800	0.00004100
C	-1.27640900	-1.87044500	0.00002700
H	-0.29269700	-2.36890300	0.00006900
Se	1.62176900	-0.56085600	-0.00001100
O	-2.28231000	-2.53916000	0.00001700
C	2.82281400	0.96491300	-0.00000100
H	2.68387400	1.56170400	0.89680900
H	3.82019100	0.53223100	-0.00005200
H	2.68379600	1.56176200	-0.89675900

1(SeMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -2786.340790 hartree

C	2.94531300	-0.82534000	0.22085900
C	2.39716400	0.43790900	0.09090700
C	1.02503300	0.60350600	-0.09847800
C	0.18757500	-0.51882400	-0.12868300
C	0.74555500	-1.78630700	0.00418300
C	2.11583700	-1.93923700	0.16779900
H	4.01147500	-0.94495300	0.35873300
H	3.02146000	1.32191800	0.11632300
H	0.10222600	-2.65597500	-0.01005900
H	2.53343700	-2.93293100	0.26545000
C	0.51392900	1.98045200	-0.30701400
H	-0.52050500	2.05946800	-0.67662600
Se	-1.72606500	-0.39929000	-0.34277500
O	1.17576200	2.97271700	-0.11811700
C	-2.13042500	0.52802700	1.32869200
H	-1.73130300	1.53860800	1.31515600
H	-3.21478900	0.56392900	1.39974200
H	-1.72177000	-0.03703200	2.16096100

1(TeMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -652.708930 hartree

C	3.39682700	-0.84121000	-0.00004200
C	2.95089500	0.46669600	0.00006900
C	1.58449900	0.75481000	0.00000800
C	0.63302600	-0.27942000	0.00025100
C	1.09763800	-1.59334800	0.00018100
C	2.45910900	-1.86766400	0.00008600
H	4.45508900	-1.06275000	-0.00028100
H	3.65757700	1.28884200	-0.00004100
H	0.40519600	-2.42291300	0.00019400
H	2.78790300	-2.89923600	0.00002600
C	1.19415000	2.16648300	-0.00039200
H	2.02576200	2.89009800	-0.00117600
Te	-1.43538500	0.13698400	0.00013800
O	0.04449000	2.55336500	-0.00007400
C	-2.06043800	-1.91008900	-0.00063200
H	-1.71712200	-2.42238700	0.89414800
H	-3.14836300	-1.87763900	-0.00116100
H	-1.71619700	-2.42162700	-0.89548700

1(TeMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -652.703443 hartree

C	3.03867500	-1.52287800	0.00011000
C	2.87456700	-0.15147000	0.00019900
C	1.59859900	0.41529000	0.00003100
C	0.45951200	-0.40320200	-0.00016200
C	0.63718700	-1.78571400	-0.00032600
C	1.91100000	-2.33674600	-0.00017800
H	4.02888100	-1.95758400	0.00024800
H	3.72888600	0.51345300	0.00033200
H	-0.21344700	-2.45223400	-0.00062200
H	2.01992600	-3.41391300	-0.00032800
C	1.49713500	1.88968400	0.00001400
H	0.47610500	2.31179100	-0.00024200
Te	-1.50466400	0.40793600	-0.00010600
O	2.44465900	2.63729800	0.00021000
C	-2.54142800	-1.45289400	0.00066500
H	-2.30451200	-2.01717700	0.89758600
H	-3.59689100	-1.19017400	0.00090700
H	-2.30517700	-2.01764500	-0.89614100

1(TeMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -652.702860 hartree

C	3.28987000	-0.90707400	0.21743400
C	2.78767500	0.36986200	0.04769400
C	1.41722700	0.58059900	-0.11514400
C	0.53098400	-0.50334100	-0.07437300
C	1.04765200	-1.78525000	0.10325800
C	2.41508300	-1.98728600	0.23450000
H	4.35394800	-1.06391000	0.33263000
H	3.44613200	1.22879700	0.01971400
H	0.37748100	-2.63364800	0.15218900
H	2.79554200	-2.99230700	0.36450600
C	0.96211200	1.96749900	-0.37632200
H	-0.06425500	2.07094300	-0.76490100
Te	-1.58265800	-0.31609400	-0.23386900
O	1.65521000	2.94303100	-0.21529900
C	-1.82075900	1.02696200	1.41544800
H	-1.47951600	2.02440800	1.15531300
H	-2.88359100	1.04953900	1.64421000
H	-1.26827800	0.63698800	2.26494800

2(SMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -802.331534 hartree

C	-1.97789500	-2.24372100	0.00017000
C	-0.59546300	-2.19195600	0.00053000
C	0.10224900	-0.98253000	0.00023900
C	-0.62300700	0.23091300	-0.00021400
C	-2.01843300	0.16444900	-0.00065100
C	-2.68567900	-1.05166400	-0.00047700
H	-2.49223600	-3.19489800	0.00035700
H	-0.02288500	-3.11207900	0.00106500
H	-2.60844600	1.06743400	-0.00120400
H	-3.76815100	-1.05757200	-0.00085200
C	1.56763800	-1.09143000	0.00034500
H	1.94246300	-2.12346800	0.00157600
S	0.22156000	1.77925900	-0.00020700
C	-1.13566900	2.96342700	0.00084500
H	-1.75057500	2.87637900	0.89456000
H	-0.64876000	3.93690800	0.00165400
H	-1.75054800	2.87799400	-0.89308500
N	2.36519100	-0.11180000	-0.00071600
C	3.78427600	-0.39847400	-0.00013100
H	4.24192900	0.06119700	0.87725200
H	4.00532000	-1.47137800	0.00095800
H	4.24247900	0.05985000	-0.87788900

2(SMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -802.332674 hartree

C	0.30307200	2.76549200	-0.00611400
C	-0.74527800	1.86315800	-0.04062100
C	-0.51923200	0.48789400	-0.04190700
C	0.80353700	0.00789400	-0.00685900
C	1.85599300	0.92310900	0.02698200
C	1.60634100	2.28727900	0.02592900
H	0.10840400	3.82945500	-0.00953400

H	-1.77060300	2.20724900	-0.07350600
H	2.88010900	0.58275300	0.05756800
H	2.44053700	2.97665500	0.04986700
C	-1.66943100	-0.43796100	-0.09391200
H	-1.45252300	-1.48367500	-0.33881200
S	1.07413200	-1.73903300	0.01988900
C	2.86537100	-1.88040400	-0.00827700
H	3.31269700	-1.44794100	0.88408500
H	3.06381700	-2.94995600	-0.02328500
H	3.28345600	-1.42700700	-0.90456700
N	-2.85564000	-0.05895700	0.11827800
C	-3.90882200	-1.04700500	0.01616400
H	-3.53944100	-2.04695800	-0.23430500
H	-4.44926700	-1.09136100	0.96294000
H	-4.62312500	-0.72872800	-0.74492400

2(SMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -802.331100 hartree

C	1.71201700	-2.26952700	0.23522600
C	0.37220900	-1.93770500	0.13070000
C	-0.02685000	-0.62320300	-0.11224900
C	0.95253400	0.37432700	-0.22711900
C	2.29932900	0.03290500	-0.12233100
C	2.68027800	-1.28189800	0.09905400
H	2.00268600	-3.29625800	0.41467600
H	-0.39441400	-2.69635100	0.21835700
H	3.04683500	0.81083000	-0.20654600
H	3.73054900	-1.53181300	0.17384100
C	-1.46382100	-0.31791600	-0.27847900
H	-1.70169500	0.61307900	-0.80481700
S	0.54545700	2.08154200	-0.51606700
C	-0.29588400	2.49223100	1.03291400
H	0.36515100	2.31175700	1.87732800
H	-0.53661600	3.55228600	0.97899200
H	-1.21568900	1.92173400	1.14704000
N	-2.36946300	-1.09012700	0.14370300
C	-3.74525400	-0.71192600	-0.10373200
H	-3.84084000	0.23785400	-0.64017800
H	-4.23243100	-1.49969000	-0.68056000
H	-4.27195500	-0.64093400	0.84910300

2(SeMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -2805.724178 hartree

C	2.68495700	1.91765000	-0.00009400
C	1.34756700	2.27086600	-0.00026700
C	0.33207300	1.31192400	-0.00012900
C	0.67570300	-0.05484600	0.00012300
C	2.02700100	-0.39962600	0.00036800
C	3.01860200	0.57130300	0.00026100
H	3.45352600	2.67844700	-0.00022100
H	1.06562800	3.31738000	-0.00051400
H	2.32827000	-1.43591100	0.00065100
H	4.05685600	0.26504900	0.00045900
C	-1.04401200	1.82469400	-0.00023400
H	-1.12776800	2.91900400	-0.00064400
Se	-0.67425100	-1.41692200	0.00003100
C	0.47059800	-2.99525500	-0.00037500
H	1.08586900	-3.03878900	0.89466600
H	-0.22245300	-3.83399700	-0.00061100
H	1.08589300	-3.03818500	-0.89542600
N	-2.07141600	1.09035200	0.00017400
C	-3.36893300	1.73192600	0.00013800
H	-3.92882100	1.40697600	0.87829100
H	-3.30451100	2.82513400	-0.00041400
H	-3.92937200	1.40596400	-0.87725000

2(SeMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -2805.722910 hartree

C	-0.77255100	3.01109000	-0.00604100
C	-1.53217900	1.85584500	-0.04778700
C	-0.93394800	0.59562000	-0.04889800
C	0.46632900	0.50248500	-0.00853700
C	1.22750300	1.66859100	0.03501900
C	0.61241400	2.91194700	0.03433500
H	-1.25290100	3.98030900	-0.00985400
H	-2.61248600	1.90408000	-0.08696000
H	2.30594100	1.62262900	0.07284500
H	1.22343800	3.80491800	0.06501800
C	-1.78560400	-0.61033100	-0.10482100
H	-1.29155000	-1.55339200	-0.36743400
Se	1.29818600	-1.23010300	0.01993000
C	3.16944100	-0.71335000	-0.03835600
H	3.44471500	-0.16127100	0.85569900
H	3.71857900	-1.65102700	-0.07137900
H	3.37697200	-0.13659000	-0.93534600
N	-3.02730100	-0.57669200	0.12167800
C	-3.76856200	-1.81560800	0.01407700
H	-3.14053700	-2.67218900	-0.25207100
H	-4.26594300	-2.01686300	0.96400300
H	-4.55052200	-1.69798400	-0.73783400

2(SeMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -2805.722202 hartree

C	0.03620400	3.14956000	0.19583100
C	0.99006100	2.15388500	0.07670600
C	0.62041700	0.81903600	-0.09780500

C	-0.74132300	0.49123100	-0.12678600
C	-1.69729000	1.49687200	-0.00513600
C	-1.31317300	2.82109400	0.14560500
H	0.34210400	4.17994700	0.32073100
H	2.04528100	2.39292400	0.09903500
H	-2.74740200	1.23611100	-0.01771200
H	-2.06751500	3.59210400	0.23371800
C	1.67308800	-0.20315600	-0.28140500
H	1.36904700	-1.12182700	-0.79591900
Se	-1.37097600	-1.31935400	-0.32675900
C	-0.59083100	-2.07216700	1.29824200
H	-0.92121200	-1.49443700	2.15630900
H	-0.96313100	-3.09121200	1.37017800
H	0.49393900	-2.08111800	1.23460700
N	2.85935300	-0.02704900	0.11346800
C	3.81898900	-1.07953600	-0.14918600
H	3.38298000	-1.94047200	-0.66661500
H	4.63447800	-0.67537900	-0.75110100
H	4.25230400	-1.41017200	0.79588700

2(TeMe)-conformer 1 (acetonitrile)

Imaginary frequency: 0

G = -672.089842 hartree

C	3.56551900	-0.48711000	0.00007400
C	2.89337700	0.72217400	0.00028000
C	1.49813600	0.77470400	0.00013900
C	0.75140400	-0.41646700	-0.00014200
C	1.44098000	-1.62801100	-0.00038100
C	2.82930900	-1.66443500	-0.00028800
H	4.64682600	-0.51310600	0.00018200
H	3.44822000	1.65344700	0.00055800
H	0.90309200	-2.56505200	-0.00066800
H	3.33388200	-2.62229500	-0.00048100
C	0.87006100	2.09866900	0.00030500
H	1.54969700	2.95880000	0.00088000
Te	-1.36365700	-0.39306200	-0.00006800
C	-1.58057400	-2.53280700	0.00056600
H	-1.14738100	-2.97506700	0.89432200
H	-2.65539100	-2.70859500	0.00096200
H	-1.14800200	-2.97554200	-0.89325800
N	-0.38484800	2.24546500	-0.00022000
C	-0.93769600	3.58247000	-0.00008800
H	-1.57257500	3.70736100	0.87798700
H	-0.16565200	4.35800500	0.00050400
H	-1.57172700	3.70789600	-0.87870500

2(TeMe)-conformer 2 (acetonitrile)

Imaginary frequency: 0

G = -672.083981 hartree

C	-1.77412100	2.91622100	-0.00301400
C	-2.24094000	1.61519700	-0.04241700
C	-1.35993500	0.53187800	-0.04585600
C	0.02184900	0.76837400	-0.01048800
C	0.48483800	2.08251900	0.03298400
C	-0.40428700	3.14743300	0.03440400
H	-2.46958100	3.74494000	-0.00477400
H	-3.30257800	1.40824400	-0.07620300
H	1.54470400	2.29271400	0.06795700
H	-0.02174700	4.15970300	0.06417200
C	-1.90498000	-0.84048500	-0.09346600
H	-1.19562600	-1.64710400	-0.32133600
Te	1.40746800	-0.84156500	0.01306300
C	3.17746400	0.34417400	-0.04191000
H	3.25627400	0.95141200	0.85475800
H	3.99964100	-0.36708900	-0.07604500
H	3.18875500	0.95980200	-0.93658200
N	-3.12408100	-1.10164700	0.10182300
C	-3.54582700	-2.48357600	0.01231300
H	-2.72446300	-3.17130900	-0.21448300
H	-4.00871000	-2.77637000	0.95581800
H	-4.31080600	-2.57244400	-0.76064000

2(TeMe)-conformer 3 (acetonitrile)

Imaginary frequency: 0

G = -672.083727 hartree

C	2.49429700	2.38740800	0.18568000
C	2.53244900	1.01168500	0.04287600
C	1.35774200	0.27035000	-0.10333900
C	0.12323500	0.93218600	-0.07750700
C	0.09377700	2.31843500	0.07180900
C	1.26986600	3.04481700	0.18991700
H	3.41461200	2.94744800	0.28746200
H	3.47677500	0.48318700	0.02438600
H	-0.85705000	2.83466800	0.10969500
H	1.22754900	4.12098400	0.29766900
C	1.45605700	-1.18988800	-0.31444500
H	0.62319900	-1.65552700	-0.85530800
Te	-1.74221600	-0.07382800	-0.22123300
C	-1.40032300	-1.45663800	1.37646600
H	-0.99151400	-0.91390000	2.22370700
H	-2.36972900	-1.87419000	1.63779000
H	-0.72675500	-2.24911800	1.06431700
N	2.44474500	-1.86701900	0.08250200
C	2.44997700	-3.28553300	-0.21047900
H	1.55489300	-3.61729800	-0.74730700
H	3.33291000	-3.52326000	-0.80592000
H	2.53469800	-3.84176600	0.72423900

5 (acetonitrile)

Imaginary frequency: 0

G = -345.481128 hartree

C	0.52882200	0.20448400	-0.00005500
C	0.03960800	-1.10161300	-0.00007100
C	-1.32613300	-1.32205000	-0.00003700
C	-2.20465800	-0.24043300	0.00002900
C	-1.72022500	1.06097600	0.00006400
C	-0.35031100	1.28324500	0.00001400
H	-1.71357000	-2.33224600	-0.00003500
H	-3.27262500	-0.41661900	0.00002900
H	-2.40695300	1.89679100	0.00020200
C	1.98230900	0.46543000	-0.00011000
O	2.83106200	-0.39352400	0.00018700
H	2.26533300	1.53311400	-0.00060100
H	0.74043600	-1.92664100	-0.00010300
H	0.04240700	2.29356400	-0.00000200

6 (acetonitrile)

Imaginary frequency: 0

G = -364.861195 hartree

C	0.03684100	0.20378700	0.00003400
C	0.53592600	-1.09969400	0.00000900
C	1.90239200	-1.32135800	-0.00002500
C	2.78642800	-0.24508500	-0.00004400
C	2.29711800	1.05351800	0.00000700
C	0.92599100	1.27557500	-0.00001100
H	2.28492000	-2.33389300	-0.00003300
H	3.85421100	-0.42202500	-0.00007800
H	2.98076000	1.89238200	0.00000500
C	-1.41267200	0.47719800	0.00003800
H	-1.69239200	1.53879200	-0.00003300
H	-0.16112200	-1.92730500	-0.00001500
N	-2.28690400	-0.43350800	0.00020100
C	-3.67868100	-0.03421800	-0.00009700
H	-4.17102300	-0.45534300	-0.87812200
H	-4.17199800	-0.45706600	0.87652500
H	-3.81445900	1.05247600	0.00083500
H	0.53937500	2.28820400	0.00003900

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