

Electronic Supporting Information (ESI)

**Quantifying the enamine-type nucleophilic reactivity of
 α -aryl vinyl azides**

Prabaharan Thiruvengadam, Jan Brossette, Christoph Gross, Hendrik Zipse* and Armin R. Ofial*

Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5-13,
81377 München (Germany)

Table of contents

1. Supplementary Tables and Figures	S2
1.1 Determination of the Nucleophilicity Parameters N (and s_N) for Vinyl Azides 1	S2
1.2 Correlation of VA Nucleophilicities N with Hammett Substituent Parameters σ_p	S8
2. General	S9
3. Synthesis of Vinyl Azides	S10
4. Amides from Reactions of Benzhydrylium Ions with Vinyl Azides	S14
5. Kinetics of the Reactions of Benzhydrylium Ions with Vinyl Azides	S17
6. Copies of NMR (^1H , ^{13}C , and ^{19}F) and IR Spectra	S35
7. Quantum-Chemical Calculations	S62
7.1 Methods	S62
7.2 FMO Plots	S63
7.3 Molecular Structures	S64
7.4 Regioselectivity of VAs	S65
7.5 Computed Reaction Barriers	S65
7.6 Methyl Cation Affinities (MCA)	S66
7.7 Computed Properties	S69
7.8 XYZ Coordinates	S72
8. References	S90

1. Supplementary Tables and Figures

1.1 Determination of the Nucleophilicity Parameters N (and s_N) for Vinyl Azides **1**

Table S1. Second-order rate constants k_2 (CH_2Cl_2 , 20 °C) for the reactions of the VA **1** with the benzhydrylium ions **2** and nucleophilicity parameters N (and s_N) for **1**.

Vinyl azides	Electrophiles	Electrophilicity E^a	k_2 ($\text{M}^{-1} \text{s}^{-1}$)	$\lg k_2$	N (s_N)
1a	2d	-3.14	9.92×10^2	3.00	6.08 (0.99)
1a	2e	-3.85	1.00×10^2	2.00	
1a	2f	-4.72	3.68×10^1	1.57	
1a	2g	-5.53	2.90	0.46	
1b	2c	-1.36	4.32×10^3	3.64	5.47 (0.87)
1b	2d	-3.14	1.02×10^2	2.01	
1b	2e	-3.85	1.39×10^1	1.14	
1b	2f	-4.72	7.02	0.85	
1c	2c	-1.36	2.31×10^3	3.36	5.17 (0.86)
1c	2d	-3.14	5.90×10^1	1.77	
1c	2e	-3.85	5.22	0.72	
1c	2f	-4.72	4.75	0.68	
1d	2c	-1.36	1.14×10^3	3.06	4.57 (0.94)
1d	2d	-3.14	2.34×10^1	1.37	
1d	2e	-3.85	2.65	0.42	
1d	2f	-4.72	1.33	0.12	
1d	2g	-5.53	1.05×10^{-1}	-0.98	
1e	2c	-1.36	4.36×10^2	2.64	4.13 (0.96)
1e	2d	-3.14	9.91	1.00	
1e	2e	-3.85	1.73	0.24	
1f	2a	+0.61	7.04×10^2	2.85	3.10 (0.77)
1f	2b	0.00	2.46×10^2	2.39	
1f	2c	-1.36	2.17×10^1	1.34	
1h	2c	-1.36	4.42×10^3	3.65	5.39 (0.89)
1h	2d	-3.14	7.31×10^1	1.86	
1h	2f	-4.72	4.64	0.67	
1i	2b	0.00	5.74×10^2	2.76	3.17 (0.88)
1i	2c	-1.36	4.74×10^1	1.68	
1i	2d	-3.14	9.85×10^{-1}	-0.01	

^a From ref. 11b, main text.

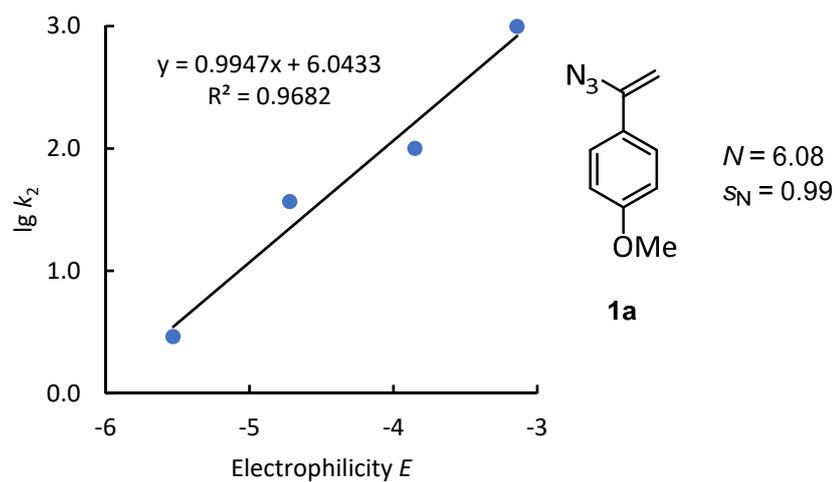


Figure S1: Linear relationship of $\log k_2(\mathbf{1a}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

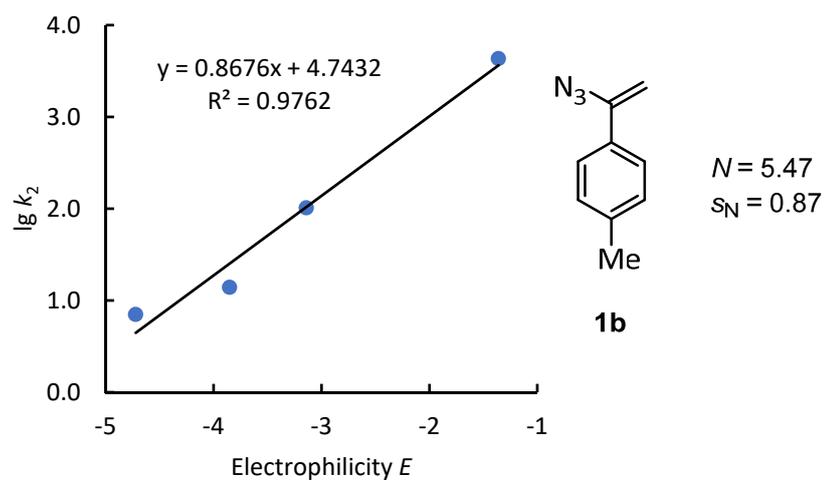


Figure S2: Linear relationship of $\log k_2(\mathbf{1b}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

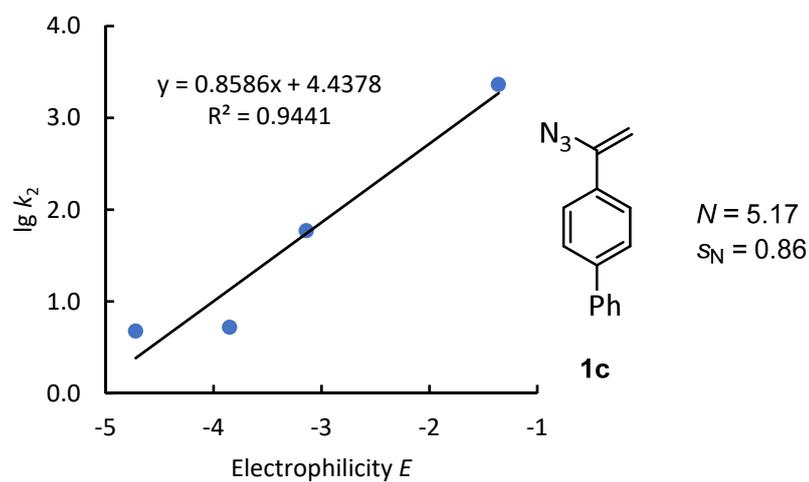


Figure S3: Linear relationship of $\log k_2(\mathbf{1c}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

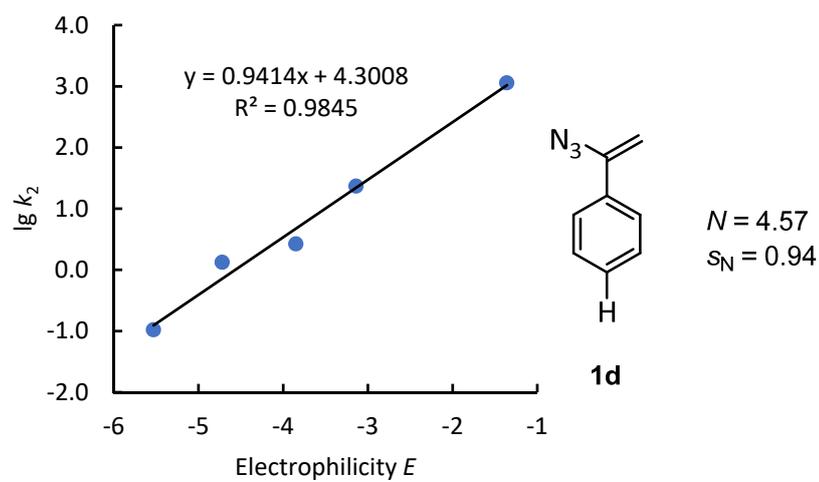


Figure S4: Linear relationship of $\log k_2(\mathbf{1d}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

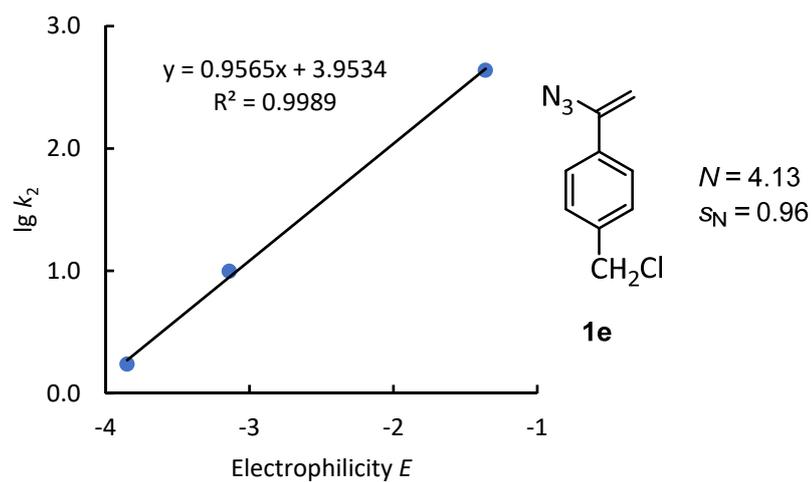


Figure S5: Linear relationship of $\log k_2(\mathbf{1e}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

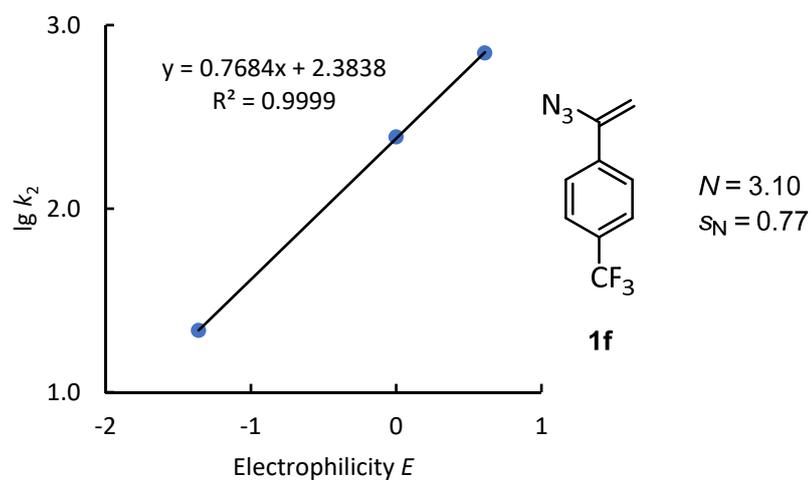


Figure S6: Linear relationship of $\log k_2(\mathbf{1f}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

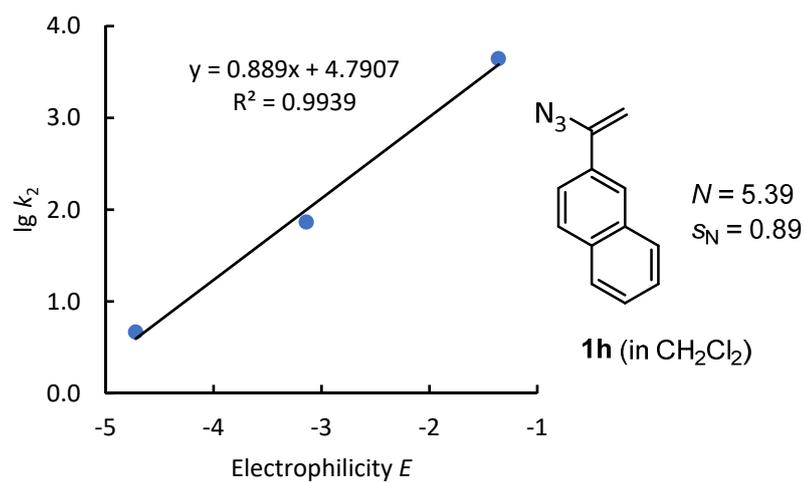


Figure S7: Linear relationship of $\log k_2(\mathbf{1h}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

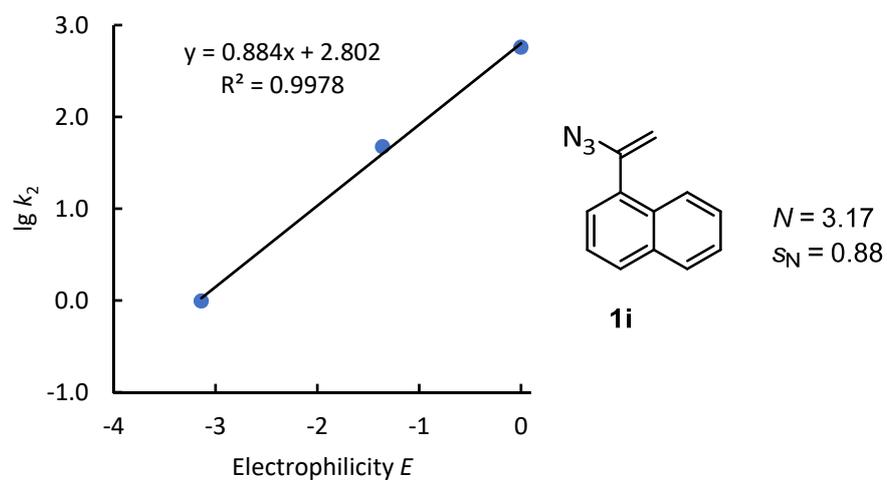


Figure S8: Linear relationship of $\log k_2(\mathbf{1i}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (CH_2Cl_2 , 20 °C); with data from Table S1.

Table S2. Second-order rate constants k_2 (Cyrene, 20 °C) for the reactions of the VA **1h** with the benzhydrylium ions **2** and nucleophilicity parameters N (and s_N) for **1h** in Cyrene.^a

Vinyl azide	Electrophiles	Electrophilicity E^b	k_2 ($M^{-1} s^{-1}$)	$\lg k_2$	N (s_N)
1h	2d	-3.14	5.83×10^2	2.77	6.00 (0.90)
1h	2e	-3.85	2.83×10^1	1.45	
1h	2f	-4.72	4.26×10^1	1.63	
1h	2g	-5.53	1.81	0.26	

^a Cyrene = dihydrolevoglucosenon. ^b From ref. 11b, main text.

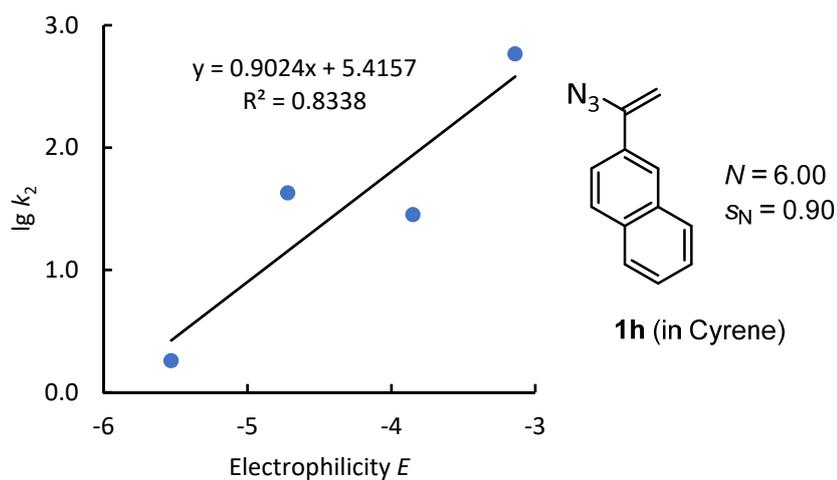


Figure S9: Linear relationship of $\lg k_2(\mathbf{1h}+\mathbf{2})$ with the electrophilicity E of the benzhydrylium ions **2** (Cyrene, 20 °C) ; with data from Table S2.

1.2 Correlation of VA Nucleophilicities N with Hammett Substituent Parameters σ_p

Vinyl azides	4-X groups	Hammett σ_p	N
1a	4-OMe	-0.27	6.08
1b	4-Me	-0.17	5.47
1c	4-Ph	-0.01	5.17
1d	H	± 0.00	4.57
1e	4-CH ₂ Cl	+0.12	4.13
1f	4-CF ₃	+0.54	3.01

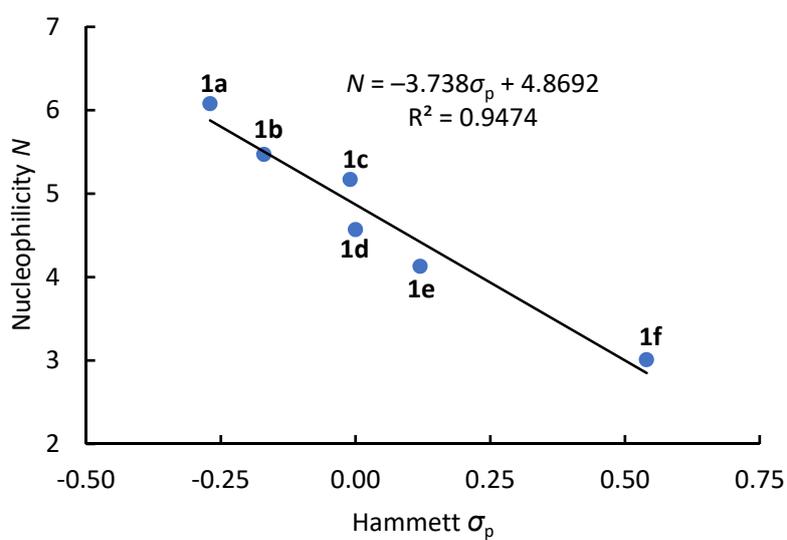


Figure S10: Linear correlation of nucleophilicity parameters N of vinyl azides **1** with the Hammett substituent constants σ_p for substituents at the 4-position of the aromatic ring in α -aryl vinyl azides (σ_p from ref. 15, main text).

2. General

Commercial reagents and dry solvents (stored over molecular sieves) were used without further purification as purchased from Sigma-Aldrich or Acros Organics. Dichloromethane was dried over CaH_2 , diethyl ether was dried over sodium and distilled. For thin-layer chromatography, silica gel plates with F-254 fluorescence indicator (Merck) were used. Purification by flash column chromatography was performed using Merck silica gel 60 (0.040–0.063 mm) with freshly distilled solvents.

Melting points were acquired using Büchi Melting Point B-560 devices and are not corrected.

Nuclear magnetic resonance (NMR) spectra were recorded on 400 and 600 MHz spectrometers. Residual solvent signals were used as internal reference (δ_{H} 7.26 ppm, δ_{C} 77.16 ppm for CDCl_3 ; δ_{H} 5.32 ppm, δ_{C} 53.84 ppm for CD_2Cl_2).⁵¹ NMR signals were assigned based on information from additional 2D NMR experiments (COSY, gHSQC, gHMBC).

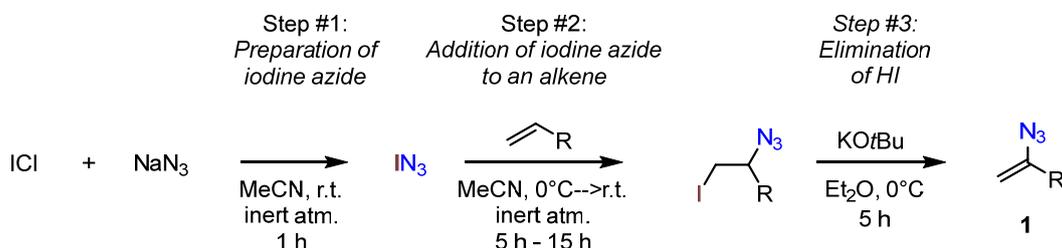
Infrared (IR) spectra were recorded on a Perkin Elmer Spectrum BX-59343 instrument with a Smiths Detection DuraSAMPLIR II Diamond ATR sensor or a Bruker Tensor 27 FT-IR instrument with a "Platinum" Diamond ATR sensor for detection in the range 4500–600 cm^{-1} as a film for liquids or neat for solids.

High resolution (HRMS) mass spectra were recorded on a Thermo Exploris 120, a Thermo Finnigan LTQ FT Ultra, or a Thermo Finnigan LTQ Orbitrap XL instrument. For ionization of the samples, electrospray ionization (ESI) was applied.

3. Synthesis of Vinyl Azides

General Procedure (GP):

Vinyl azides **1** were synthesized in a one-pot three-step procedure in analogy to the procedure reported in ref.^{S2}

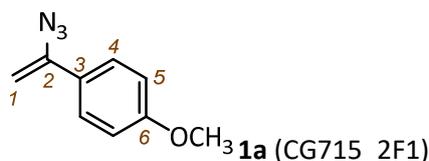


Step #1: Iodine monochloride (1.1 equiv.) was added to a flame-dried Schlenk flask and dissolved in MeCN (8 mL) under nitrogen atmosphere. Sodium azide (2.0 equiv.) was added to the orange-brown acetonitrile solution under room temperature, and the resulting suspension was stirred for 1 h at room temperature.

Step #2: To the reaction mixture from Step #1, a solution of the alkene (1.0 equiv., dissolved in 8 mL CH₂Cl₂) was added slowly at 0°C. Then, the mixture was allowed to warm up to room temperature while it was stirred overnight. The reaction mixture was quenched with aq. sat. Na₂S₂O₃ solution, and the organic materials were extracted three times with diethyl ether (3 × 20 mL). The combined organic phases were washed with brine and dried over MgSO₄. After evaporation of volatiles, the resulting crude materials were used immediately and without further purification for Step #3.

Step #3: The crude material from Step #2 was dissolved in diethyl ether (16 mL) under argon atmosphere. Then, KOtBu was added in portions at 0°C. The suspension was stirred for 5 h at 0 °C (ice cooling). Subsequently, the reaction mixture was filtered through Celite, and the solvent was removed under reduced pressure. The resulting crude product was purified by flash column chromatography (silica gel, *n*-pentane or *n*-pentane/EtOAc mixtures) to give the vinyl azides **1**.

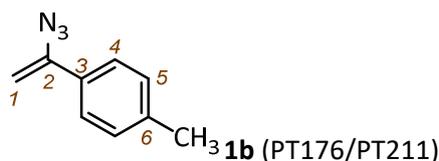
1-(1-Azidovinyl)-4-methoxybenzene (1a) was synthesized according to GP from iodine monochloride (0.23 mL, 0.72 g, 4.4 mmol), sodium azide (0.52 g, 8.0 mmol), 1-methoxy-4-vinylbenzene (0.54 g, 4.0 mmol), and KOtBu (0.70 g, 6.2 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane:EtOAc 98:2) and recrystallized (*n*-pentane, -24°C) to give **1a** (0.280 g, 40%) as a light-yellow solid.



NMR spectroscopic data agree with those reported in ref. S3.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.50 (d, $J = 8.9$ Hz, 2 H, 4-H), 6.88 (d, $J = 9.0$ Hz, 2 H, 5-H), 5.32 (d, $J = 2.3$ Hz, 1 H, 1- H^b), 4.86 (d, $J = 2.3$ Hz, 1 H, 1- H^a), 3.82 ppm (s, 3 H, 6- OCH_3).

1-(1-Azidovinyl)-4-methylbenzene (1b) was synthesized according to *GP* from iodine monochloride (1.14 g, 7.0 mmol), sodium azide (0.82 g, 13 mmol), 1-methyl-4-vinylbenzene (0.59 g, 5.0 mmol), and KOtBu (0.67 g, 6.0 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane/ $\text{EtOAc} = 98:2$) to afford **1b** (0.36 g, 45%) as a light-yellow solid.

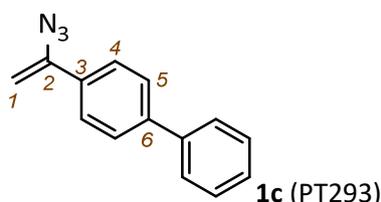


The NMR spectroscopic data agree with those reported in ref. S4.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.46 (d, $J = 8.3$ Hz, 2 H, 4-H), 7.17 (d, $J = 7.9$ Hz, 2 H, 5-H), 5.39 (d, $J = 2.3$ Hz, 1 H, 1- H^b), 4.91 (d, $J = 2.3$ Hz, 1 H, 1- H^a), 2.37 ppm (s, 3 H, 6- CH_3).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 145.1, 139.3, 131.6, 129.3, 125.6, 97.3, 21.4 ppm.

4-(1-Azidovinyl)-1,1'-biphenyl (1c) was synthesized according to *GP* from iodine monochloride (0.45 g, 2.8 mmol), sodium azide (0.41 g, 6.3 mmol), 4-vinyl-1,1'-biphenyl (0.45 g, 2.5 mmol), and KOtBu (0.42 g, 3.7 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane) to afford **1c** (0.30 g, 54%) as a light-yellow solid.

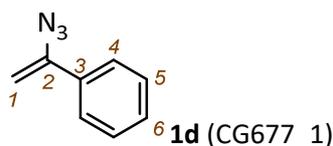


The NMR spectroscopic data agree with those reported in ref. S4.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.66–7.62 (m, 2 H), 7.62–7.57 (m, 4 H), 7.47–7.42 (m, 2 H), 7.39–7.34 (m, 1 H), 5.49 (d, $J = 2.5$ Hz, 1 H, 1- H^b), 4.99 (d, $J = 2.5$ Hz, 1 H, 1- H^a) ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 144.8, 142.0, 140.5, 133.3, 129.0, 127.8, 127.3, 127.2, 126.1, 98.0 ppm.

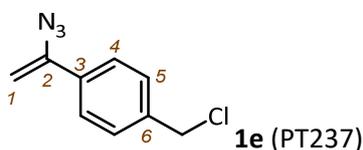
(1-Azidovinyl)benzene (1d) was synthesized according to *GP* from iodine monochloride (0.23 mL, 0.72 g, 4.4 mmol), sodium azide (0.52 g, 8.0 mmol), styrene (0.42 g, 4.0 mmol), and KOtBu (0.70 g, 6.2 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane) to give **1d** (0.32 g, 55%) as a light-yellow oil.



NMR spectroscopic data agree with those reported in ref. S4.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.58–7.54 (m, 2 H, 4-H), 7.39–7.35 (m, 3 H, 5-H and 6-H), 5.44 (d, $J = 2.3$ Hz, 1 H, 1- H^a), 4.96 ppm (d, $J = 2.4$ Hz, 1 H, 1- H^b).

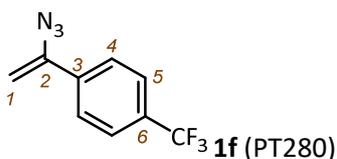
1-(1-Azidovinyl)-4-(chloromethyl)benzene (1e) was synthesized according to *GP* from iodine monochloride (1.85 g, 11.4 mmol), sodium azide (1.62 g, 25 mmol), 1-(chloromethyl)-4-vinylbenzene (1.38 g, 9.0 mmol), and KOtBu (1.35 g, 12 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane/ $\text{EtOAc} = 98:2$) to afford **1e** (0.98 g, 56%) as a brown liquid.



$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.56 (d, $J = 8.4$ Hz, 2 H, 4-H), 7.38 (d, $J = 8.5$ Hz, 2 H, 5-H), 5.46 (d, $J = 2.5$ Hz, 1 H, 1- H^b), 4.98 (d, $J = 2.6$ Hz, 1 H, 1- H^a), 4.59 ppm (s, 2 H, 6- CH_2Cl).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 144.6, 138.4, 134.5, 128.8, 126.0, 98.5, 45.8 ppm.

1-(1-Azidovinyl)-4-(trifluoromethyl)benzene (1f) was synthesized according to *GP* from iodine monochloride (0.59 g, 3.6 mmol), sodium azide (0.49 g, 7.5 mmol), 1-(trifluoromethyl)-4-vinylbenzene (0.52 g, 3.0 mmol), and KOtBu (0.50 g, 4.5 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane) to give **1f** (0.35 g, 55%) as a light brown liquid.



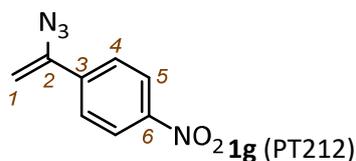
NMR spectroscopic data agree with those reported in ref. S5.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.68 (d, $J = 8.3$ Hz, 2 H, 4-H), 7.61 (d, $J = 8.4$ Hz, 2 H, 5-H), 5.55 (d, $J = 2.8$ Hz, 1 H, 1- H^b), 5.07 (d, $J = 2.8$ Hz, 1 H, 1- H^a) ppm.

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 144.1, 137.7 (br), 131.1 (q, $^2J_{\text{C,F}} = 32.6$ Hz), 126.0, 125.6 (q, $^3J_{\text{C,F}} = 3.9$ Hz), 124.1 (q, $^1J_{\text{C,F}} = 272.2$ Hz), 99.7 ppm.

1-(1-Azidovinyl)-4-nitrobenzene (1g) was synthesized according to *GP* from iodine monochloride (0.92 g, 5.7 mmol), sodium azide (0.81 g, 13 mmol), 1-nitro-4-vinylbenzene (0.74 g, 5.0 mmol), and KOtBu (0.67 g, 6.0 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-

pentane) and recrystallized (*n*-pentane/Et₂O mixture, -24°C) to give **1g** (0.44 g, 46%) as a light yellow solid.

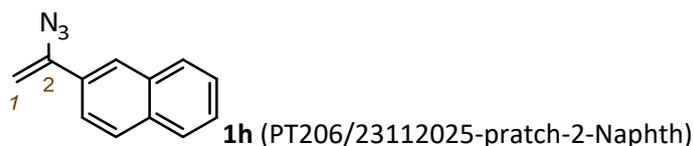


The NMR spectroscopic data agree with those reported in ref. S4.

¹H NMR (400 MHz, CDCl₃): δ 8.22 (d, *J* = 8.9 Hz, 2 H, 4-H), 7.74 (d, *J* = 8.9 Hz, 2 H, 5-H), 5.64 (d, *J* = 3.0 Hz, 1 H, 1-H^b), 5.16 ppm (d, *J* = 3.0 Hz, 1 H, 1-H^a).

¹³C{¹H} NMR (101 MHz, CDCl₃): δ 148.2, 143.5, 140.3, 126.5, 123.9, 101.2 ppm.

2-(1-Azidovinyl)naphthalene (1h) was synthesized according to *GP* from iodine monochloride (2.27 g, 14 mmol), sodium azide (1.62 g, 25 mmol), 2-vinylnaphthalene (1.54 g, 10 mmol), and KOtBu (1.35 g, 12 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane) to give **1h** (1.09 g, 56%) as a light yellow solid.

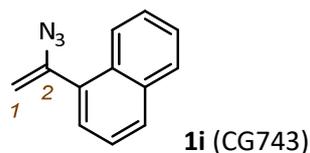


NMR spectroscopic data agree with those reported in ref. S3.

¹H NMR (400 MHz, CDCl₃): δ 8.06 (d, *J* = 1.9 Hz, 1 H), 7.88–7.81 (m, 3 H), 7.67 (dd, *J* = 8.7 Hz, 1.9 Hz, 1 H), 7.53–7.48 (m, 2 H), 5.60 (d, *J* = 2.6 Hz, 1 H), 5.07 ppm (d, *J* = 2.5 Hz, 1 H).

¹³C{¹H} NMR (101 MHz, CDCl₃): δ 145.1, 133.6, 133.2, 131.6, 128.7, 128.3, 127.7, 126.8, 126.6, 125.1, 123.2, 98.4 ppm.

1-(1-Azidovinyl)naphthalene (1i) was synthesized according to *GP* from iodine monochloride (0.19 mL, 0.58 g, 3.6 mmol), sodium azide (0.42 g, 6.5 mmol), 1-vinylnaphthalene (0.50 g, 3.2 mmol), and KOtBu (0.56 g, 5.0 mmol). The crude product was purified by flash column chromatography (silica gel, *n*-pentane) to give **1i** (0.210 g, 34%) as a light-yellow oil.



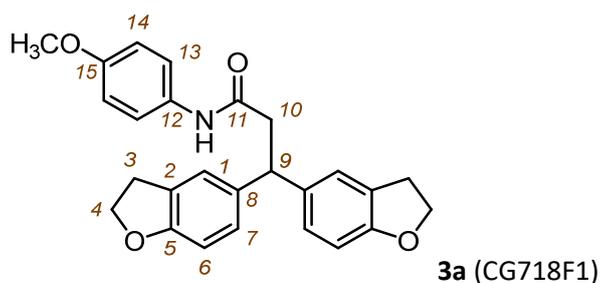
NMR spectroscopic data agree with those reported in refs. S4, S6.

¹H NMR (400 MHz, CDCl₃): δ 8.14 (d, *J* = 8.2 Hz, 1 H), 7.90–7.88 (m, 2 H), 7.59–7.46 (m, 4 H), 5.25 (d, *J* = 1.1 Hz, 1 H, 1-H^a), 4.94 ppm (d, *J* = 1.0 Hz, 1 H, 1-H^b).

$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3): δ 144.6, 133.7, 133.1, 130.9, 129.8, 128.6, 127.1, 127.0, 126.4, 125.3, 125.1, 104.1 ppm.

4. Amides from Reactions of Benzhydrylium Ions with Vinyl Azides

3,3-Bis(2,3-dihydrobenzofuran-5-yl)-N-(4-methoxyphenyl)propanamide (3a) was prepared by mixing a solution of **2c** [preformed at -20°C in 8 mL CH_2Cl_2 from $\text{Ar}_2\text{CH-OH}$ (30.0 mg, 0.11 mmol) by addition of $\text{HBF}_4\cdot\text{Et}_2\text{O}$ (16.7 μl , 0.12 mmol)] with the vinyl azide **1a** (21.5 mg, 0.12 mmol, dissolved in 2 mL CH_2Cl_2) under nitrogen atmosphere at -20°C . After 30 min the reaction was quenched by addition of aqueous hydrochloric acid. The reaction mixture was extracted with dichloromethane (3×10 mL), and the combined organic phases were washed with brine (10 mL) and dried (over MgSO_4). Then, volatiles were removed under reduced pressure. The crude product was purified by column chromatography (basic Al_2O_3 , eluent: *n*-pentane:EtOAc: NEt_3 50:49:1) to give **3a** as a colorless oil (26.0 mg, 57%).



R_f (*n*-pentane/EtOAc/ NEt_3 50:49:1, basic Al_2O_3 , UV) = 0.6

^1H NMR (600 MHz, CDCl_3): δ 7.18 (d, $J = 9.1$ Hz, 2 H, 13-H), 7.06 (s, 2 H, 1-H), 7.01 (s, 1 H, NH), 7.00 (d, $J = 8.2$ Hz, 2 H, 7-H), 6.78 (d, $J = 8.9$ Hz, 2 H, 14-H), 6.70 (d, $J = 8.2$ Hz, 2 H, 6-H), 4.52 (t, $J = 8.7$ Hz, 4 H, 4-H), 4.48 (t, $J = 7.8$ Hz, 1 H, 9-H), 3.75 (s, 3 H, 15-OCH₃), 3.12 (t, $J = 8.7$ Hz, 4 H, 3-H), 2.96 ppm (d, $J = 7.8$ Hz, 2 H, 10-H).

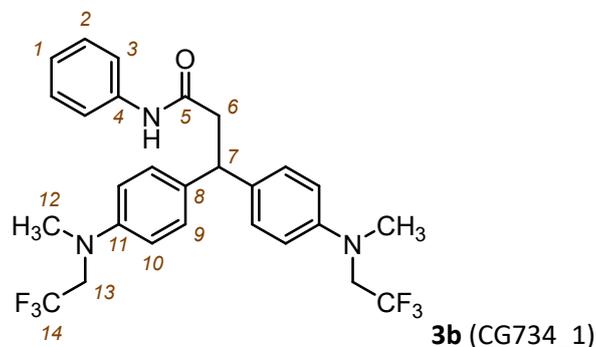
$^{13}\text{C}\{^1\text{H}\}$ NMR (151 MHz, CDCl_3): δ 169.8 (C_q, C-11), 158.8 (C_q, C-5), 156.5 (C_q, C-15), 136.3 (C_q, C-8), 130.8 (C_q, C-12), 127.6 (C_q, C-2), 127.0 (CH, C-7), 124.5 (CH, C-1), 122.1 (CH, C-13), 114.1 (CH, C-14), 109.3 (CH, C-6), 71.4 (CH₂, C-4), 55.6 (CH₃, 15-OCH₃), 46.6 (CH, C-9), 44.9 (CH₂, C-10), 29.9 ppm (CH₂, C-3).

HRMS (pos. ESI): m/z calcd for $\text{C}_{26}\text{H}_{26}\text{NO}_4^+$ [$\text{M} + \text{H}^+$]: 416.1856; found: 416.1854.

IR (film, ATR): $\tilde{\nu}$ 3294, 2957, 2896, 1651, 1603, 1541, 1510, 1490, 1239, 1102, 1033, 982, 943, 828, 730 cm^{-1} .

3,3-Bis(4-(methyl(2,2,2-trifluoroethyl)amino)phenyl)-N-phenylpropanamide (3b) was prepared by mixing a solution **2e** [preformed in 8 mL CH_2Cl_2 from $\text{Ar}_2\text{CH-OH}$ (33.0 mg, 0.081 mmol) by addition of $\text{HBF}_4\cdot\text{Et}_2\text{O}$ (12 μl , 0.089 mmol) at -20°C] with the vinyl azide **1d** (13.0 mg, 0.089 mmol, dissolved in 2 mL CH_2Cl_2) under nitrogen atmosphere at -20°C . After 60 min the reaction was quenched by addition

of aqueous hydrochloric acid. The reaction mixture was extracted with dichloromethane (3 × 10 mL), and the combined organic phases were washed with brine (10 mL) and dried (over MgSO₄). Then, volatiles were removed under reduced pressure. The crude product was purified by column chromatography (basic Al₂O₃, eluent: *n*-pentane:EtOAc:NEt₃ 70:28:2 and silica/*n*-pentane:EtOAc:NEt₃ 70:28:2) to give **3b** as a white solid (18.0 mg, 42%); m.p. 138°C.



R_f (*n*-pentane/EtOAc/NEt₃ 70:28:2, basic Al₂O₃, UV) = 0.45

¹H NMR (400 MHz, CD₂Cl₂): δ 7.31 (d, *J* = 7.1 Hz, 2 H, 3-H), 7.27–7.23 (m, 2 H, 2-H), 7.15 (d, *J* = 8.8 Hz, 4 H, 9-H), 7.07–7.04 (m, 2 H, 1-H, 4-NH), 6.74 (d, *J* = 8.9 Hz, 4 H, 10-H), 4.44 (t, *J* = 7.8 Hz, 1 H, 7-H), 3.84 (q, *J*_{H,F} = 9.1 Hz, 4 H, 13-H), 3.00–2.99 ppm (m, 8 H, 6-H and 12-H).

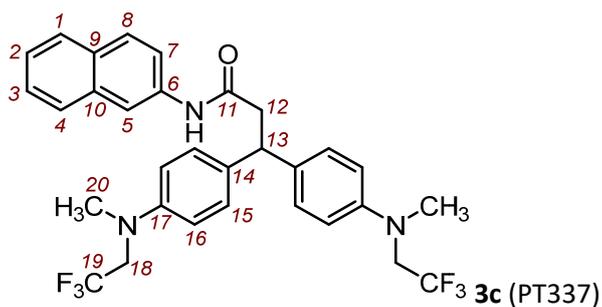
¹³C{¹H} NMR (101 MHz, CD₂Cl₂): δ 169.9 (C_q, C-5), 147.7 (C_q, C-11), 138.4 (C_q, C-4), 134.3 (C_q, C-8), 129.2 (CH, C-2), 128.6 (CH, C-9), 126.2 (C_q, q, ¹*J*_{C,F} = 282.9 Hz, C-14), 124.4 (CH, C-1), 120.2 (CH, C-3), 113.3 (CH, q, ⁵*J*_{C,F} = 0.9 Hz, C-10), 54.6 (CH₂, q, ²*J*_{C,F} = 32.3 Hz, C-13), 45.9 (CH, C-7), 44.7 (CH₂, C-6), 39.5 ppm (CH₃, q, ⁴*J*_{C,F} = 1.0 Hz, C-12).

¹⁹F NMR (376 MHz, CD₂Cl₂): δ -70.96 ppm (t, *J*_{F,H} = 9.1 Hz, CF₃).

HRMS (pos. ESI): *m/z* calcd for C₂₇H₂₇F₆N₃NaO⁺ [M + Na⁺]: 541.1951; found: 541.1963.

IR (neat, ATR): $\tilde{\nu}$ 3257, 2917, 1658, 1602, 1552, 1517, 1371, 1264, 1159, 1139, 1093, 987, 821, 807, 759, 694, 657 cm⁻¹.

3,3-Bis(4-(methyl(2,2,2-trifluoroethyl)amino)phenyl)-N-(naphthalen-2-yl)propanamide (3c) was obtained by dissolving preformed **2e** (20 mg, 0.042 mmol in 5.0 mL) in dichloromethane (5.0 mL) at -40 °C. After 10 min of stirring, a dichloromethane solution of the vinyl azide **1h** (9.0 mg, 0.046 mmol in 2.0 mL) and water (2 mg, 0.084 mmol) were added. The reaction mixture was stirred for 4 h at -40 °C under a nitrogen atmosphere (the reaction progress was monitored by thin layer chromatography). Upon completion, aqueous ammonia (2 M) was added. The phases were separated, and the aqueous phase was extracted with dichloromethane (3 × 10 mL). The combined organic layers were washed with brine (10 mL), dried over MgSO₄, and concentrated under reduced pressure. The crude product was purified by column chromatography (silica gel, eluent: *n*-pentane/EtOAc 70:30) to afford **3c** as a white solid (13.0 mg, 55%); m.p. 146°C.



R_f (*n*-pentane/EtOAc 70:30, SiO₂, UV) = 0.40

¹H NMR (400 MHz, CDCl₃): δ 7.99 (d, J = 2.2 Hz, 1 H), 7.75–7.69 (m, 3 H), 7.45–7.35 (m, 2 H), 7.18–7.16 (m, 5 H), 7.03 (s, 1 H, NH), 6.74 (d, J = 8.8 Hz, 4 H, 16-H), 4.49 (t, J = 7.7 Hz, 1 H, 13-H), 3.81 (q, $J_{H,F}$ = 8.9 Hz, 4 H, 18-H), 3.07 (d, J = 7.8 Hz, 2 H, 12-H), 3.01 ppm (s, 6 H, 20-H).

¹³C{¹H} NMR (101 MHz, CDCl₃): δ 170.1 (C_q, C-11), 147.4 (C_q), 135.2 (C_q), 133.9 (C_q), 133.7 (C_q), 130.7 (C_q), 128.7 (CH), 128.6 (CH), 127.7 (CH), 127.6 (CH), 126.6 (CH), 125.4 (C_q, q, $^1J_{C,F}$ = 282 Hz, CF₃, C-19), 125.1 (CH), 120.0 (CH), 116.8 (CH), 113.1 (CH), 54.5 (CH₂, q, $^2J_{C,F}$ = 32.5 Hz, 18-H), 45.8 (CH, C-13), 45.1 (CH₂, C-12), 39.3 ppm (CH₃, C-20).

¹⁹F NMR (376 MHz, CDCl₃): δ –70.50 ppm (t, $J_{F,H}$ = 8.9 Hz, CF₃).

HRMS (pos. ESI): m/z calcd for C₃₁H₂₉F₆N₃NaO⁺ [M + Na⁺]: 596.2107; found: 596.2106.

IR (film, ATR): $\tilde{\nu}$ 3294, 2923, 1655, 1611, 1551, 1518, 1371, 1264, 1160, 1146, 1094, 987, 815, 658 cm⁻¹.

5. Kinetics of the Reactions of Benzhydrylium Ions with Vinyl Azides

Solutions for kinetic measurements were prepared by using dry dichloromethane (Sigma-Aldrich, for HPLC, $\geq 99.8\%$), which was stirred for two weeks over sulfuric acid (96%), separated, washed, and distilled over CaH_2 and then kept under an atmosphere of dry nitrogen. CyreneTM was purchased (Sigma-Aldrich, $\geq 98.5\%$ by GC) and used without further purification.

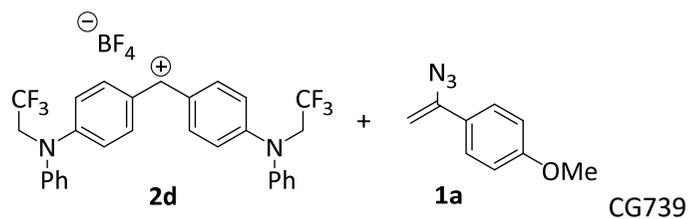
The kinetics of the reactions of the vinyl azides **1** with benzhydrylium ions **2** were followed photometrically at the absorbance maxima of the colored benzhydrylium ions by using UV-Vis spectroscopy. For fast reactions, AppliedPhotophysics SX.20 stopped-flow instruments were used. The kinetics of slower reactions were followed by using a conventional J&M TIDAS diode array spectrophotometer, controlled by TIDASDAQ3 (v3) software and connected to a Hellma 661.502-QX quartz Suprasil immersion probe (light path $d = 5$ mm) via fiber optic cables and standard SMA connectors. The temperature (20.0 ± 0.2 °C) in all kinetic experiments was maintained constant by using circulating bath cryostats. The vinyl azides **1** were used in at least 2.5-fold excess over the benzhydrylium ions **2** (that is, $[\mathbf{2}]_0 \ll [\mathbf{1}]_0$) to ensure pseudo-first order reaction conditions. Least squares-fitting of the mono-exponential decay function

$$A_t = A_0 \exp(-k_{\text{obs}}t) + C$$

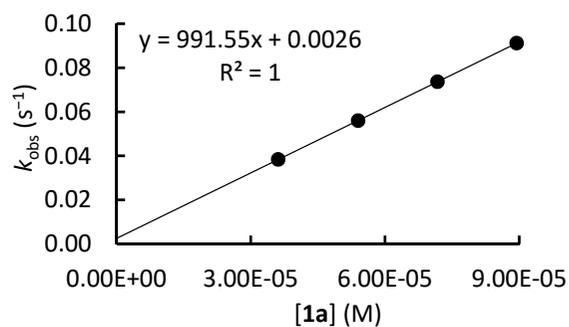
to the time-dependent experimental absorbances A_t was used to calculate the first-order rate constants k_{obs} (s^{-1}) at four to five different nucleophile concentrations (k_{obs} at only three [**1c**] and [**1f**] were determined for the reactions of **2c** with **1c** and **1f**, respectively). Subsequently, the second-order rate constants k_2^{exp} ($\text{M}^{-1} \text{s}^{-1}$) of the bimolecular reactions were calculated as the slopes of the linear correlations of k_{obs} vs $[\mathbf{1}]_0$, the initial concentrations of the vinyl azides.

Raw and evaluated data of kinetic measurements are available at Open Data LMU, DOI: 10.5282/ubm/data.761.

1a + 2d in CH₂Cl₂ (conventional photometry, detection at λ = 601 nm)

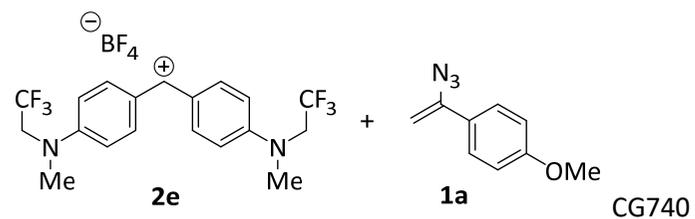


[2d] ₀ (M)	[1a] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
8.24 × 10 ⁻⁶	3.61 × 10 ⁻⁵	3.84 × 10 ⁻²
7.86 × 10 ⁻⁶	5.40 × 10 ⁻⁵	5.60 × 10 ⁻²
7.99 × 10 ⁻⁶	7.17 × 10 ⁻⁵	7.37 × 10 ⁻²
8.21 × 10 ⁻⁶	8.94 × 10 ⁻⁵	9.12 × 10 ⁻²

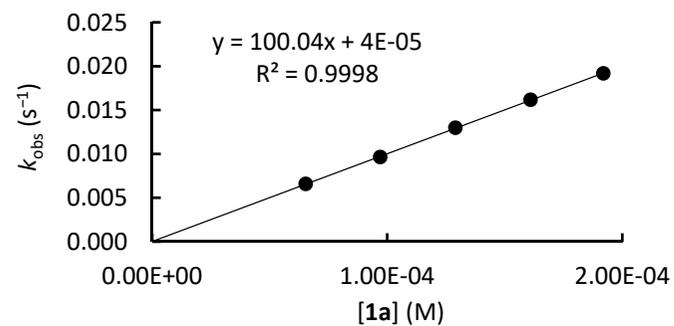


$$k_2 = (9.92 \pm 0.02) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1a + 2e in CH₂Cl₂ (conventional photometry, detection at λ = 593 nm)

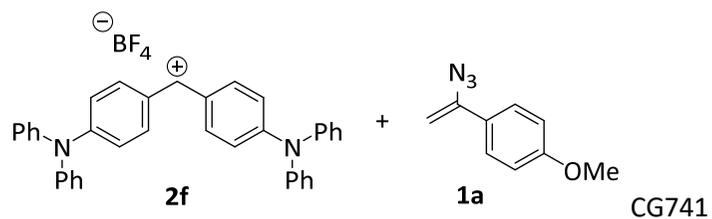


[2e] ₀ (M)	[1a] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
7.55 × 10 ⁻⁶	6.53 × 10 ⁻⁵	6.60 × 10 ⁻³
8.52 × 10 ⁻⁶	9.70 × 10 ⁻⁵	9.65 × 10 ⁻³
8.36 × 10 ⁻⁶	1.29 × 10 ⁻⁴	1.30 × 10 ⁻²
8.33 × 10 ⁻⁶	1.61 × 10 ⁻⁴	1.62 × 10 ⁻²
8.55 × 10 ⁻⁶	1.92 × 10 ⁻⁴	1.92 × 10 ⁻²

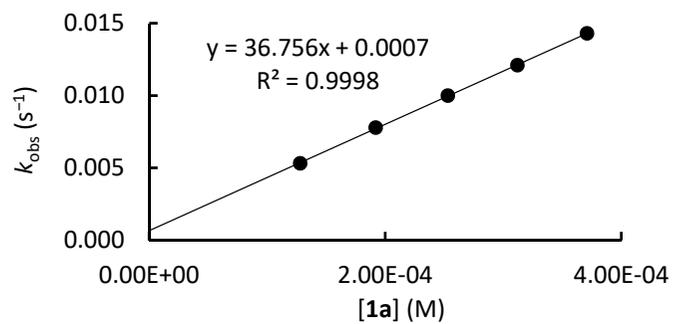


$$k_2 = (1.00 \pm 0.01) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1a + 2f in CH₂Cl₂ (conventional photometry, detection at λ = 674 nm)

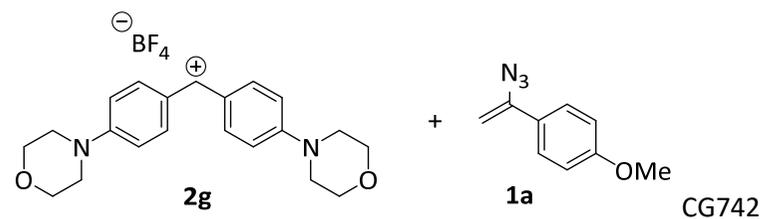


[2f] ₀ (M)	[1a] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.05 × 10 ⁻⁵	1.28 × 10 ⁻⁴	5.32 × 10 ⁻³
1.04 × 10 ⁻⁵	1.92 × 10 ⁻⁴	7.79 × 10 ⁻³
1.02 × 10 ⁻⁵	2.53 × 10 ⁻⁴	1.00 × 10 ⁻²
1.01 × 10 ⁻⁵	3.12 × 10 ⁻⁴	1.21 × 10 ⁻²
9.88 × 10 ⁻⁶	3.71 × 10 ⁻⁴	1.43 × 10 ⁻²

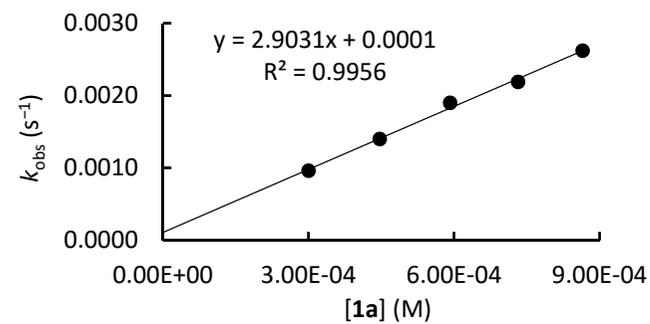


$$k_2 = (3.68 \pm 0.03) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

1a + 2g in CH₂Cl₂ (conventional photometry, detection at λ = 620 nm)

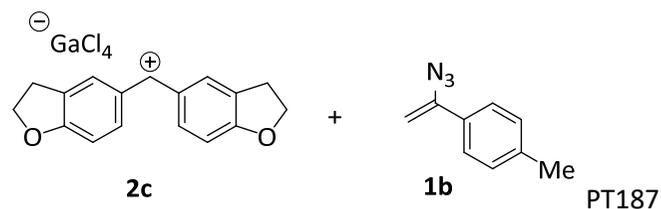


[2g] ₀ (M)	[1a] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
7.65 × 10 ⁻⁶	3.00 × 10 ⁻⁴	9.62 × 10 ⁻⁴
7.72 × 10 ⁻⁶	4.47 × 10 ⁻⁴	1.40 × 10 ⁻³
7.62 × 10 ⁻⁶	5.92 × 10 ⁻⁴	1.90 × 10 ⁻³
7.33 × 10 ⁻⁶	7.32 × 10 ⁻⁴	2.19 × 10 ⁻³
7.10 × 10 ⁻⁶	8.65 × 10 ⁻⁴	2.62 × 10 ⁻³

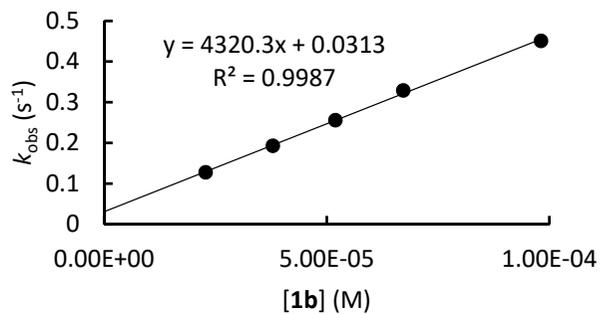


$$k_2 = (2.90 \pm 0.11) \text{ M}^{-1} \text{ s}^{-1}$$

1b + **2c** in CH₂Cl₂ (conventional photometry, detection at λ = 535 nm)

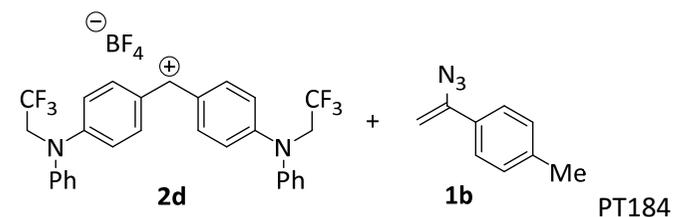


[2c] ₀ (M)	[1b] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
7.60 × 10 ⁻⁶	2.28 × 10 ⁻⁵	0.128
7.58 × 10 ⁻⁶	3.79 × 10 ⁻⁵	0.193
7.42 × 10 ⁻⁶	5.19 × 10 ⁻⁵	0.256
7.46 × 10 ⁻⁶	6.72 × 10 ⁻⁵	0.329
7.55 × 10 ⁻⁶	9.81 × 10 ⁻⁵	0.451

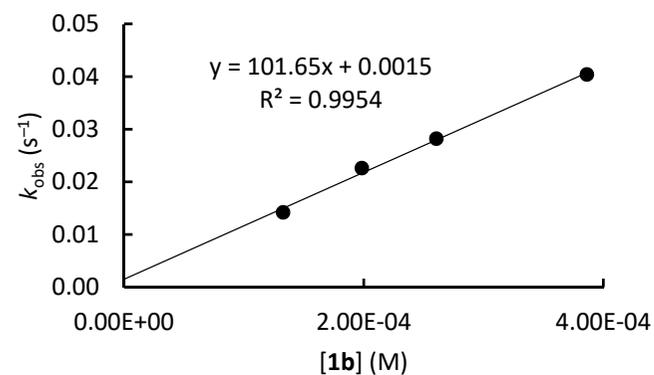


$$k_2 = (4.32 \pm 0.09) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$$

1b + **2d** in CH₂Cl₂ (conventional photometry, detection at λ = 601 nm)

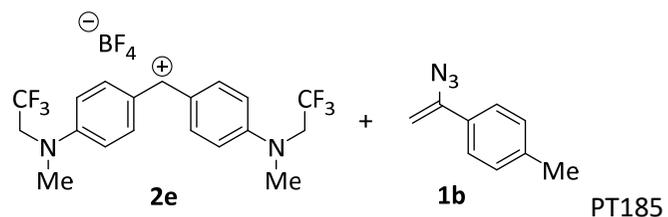


[2d] ₀ (M)	[1b] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.33 × 10 ⁻⁵	1.33 × 10 ⁻⁴	1.42 × 10 ⁻²
1.32 × 10 ⁻⁵	1.98 × 10 ⁻⁴	2.26 × 10 ⁻²
1.30 × 10 ⁻⁵	2.61 × 10 ⁻⁴	2.82 × 10 ⁻²
1.29 × 10 ⁻⁵	3.86 × 10 ⁻⁴	4.04 × 10 ⁻²

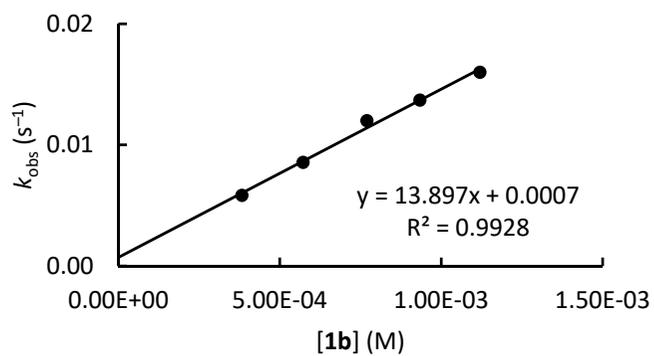


$$k_2 = (1.02 \pm 0.05) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1b + **2e** in CH₂Cl₂ (conventional photometry, detection at λ = 593 nm)

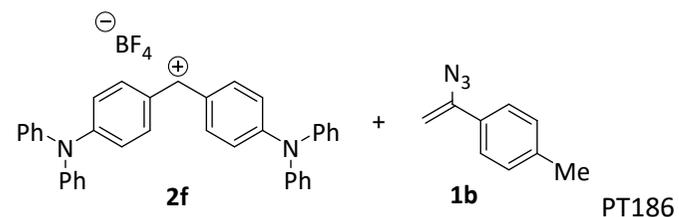


[2e] ₀ (M)	[1b] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
9.58 × 10 ⁻⁶	3.83 × 10 ⁻⁴	5.84 × 10 ⁻³
9.53 × 10 ⁻⁶	5.72 × 10 ⁻⁴	8.56 × 10 ⁻³
9.62 × 10 ⁻⁶	7.70 × 10 ⁻⁴	1.20 × 10 ⁻²
9.34 × 10 ⁻⁶	9.34 × 10 ⁻⁴	1.37 × 10 ⁻²
9.30 × 10 ⁻⁶	1.12 × 10 ⁻³	1.60 × 10 ⁻²

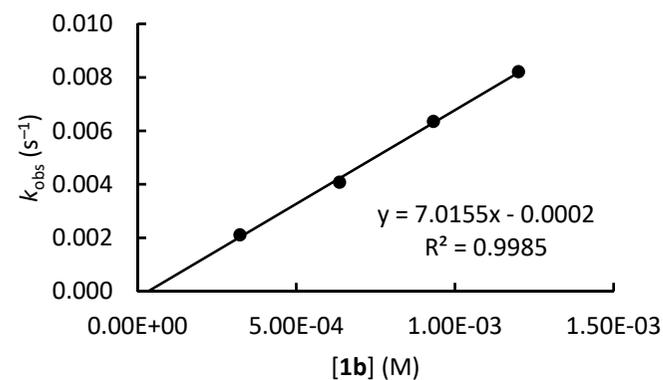


$$k_2 = (1.39 \pm 0.07) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

1b + **2f** in CH₂Cl₂ (conventional photometry, detection at λ = 672 nm)

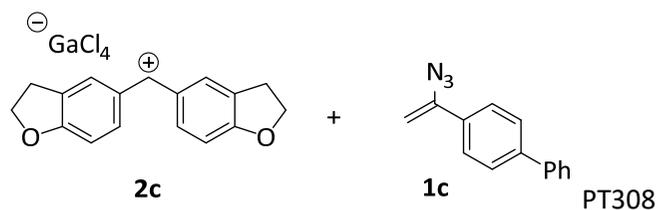


[2f] ₀ (M)	[1b] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.29 × 10 ⁻⁵	3.22 × 10 ⁻⁴	2.11 × 10 ⁻³
1.27 × 10 ⁻⁵	6.36 × 10 ⁻⁴	4.08 × 10 ⁻³
1.24 × 10 ⁻⁵	9.32 × 10 ⁻⁴	6.35 × 10 ⁻³
1.20 × 10 ⁻⁵	1.20 × 10 ⁻³	8.21 × 10 ⁻³

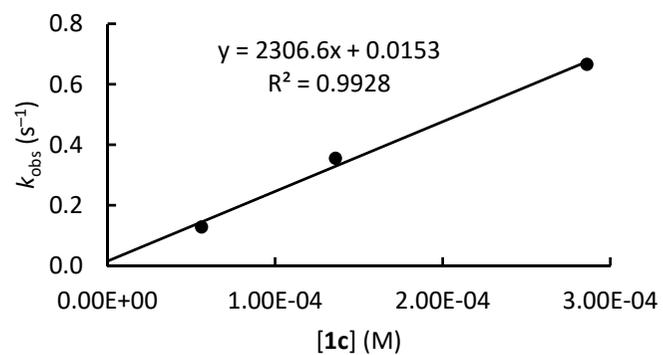


$$k_2 = (7.02 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$$

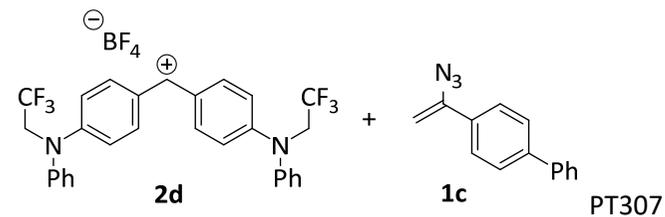
1c + 2c (generated in solution from $\text{Ar}_2\text{CH-Cl} + 3 \text{ equiv. GaCl}_3$) in CH_2Cl_2
(conventional photometry, detection at $\lambda = 535 \text{ nm}$)



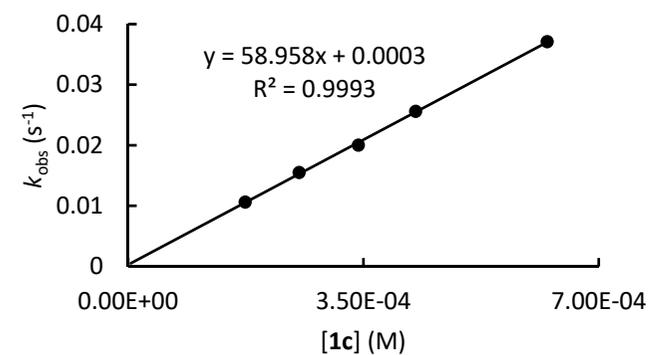
$[\mathbf{2c}]_0 \text{ (M)}$	$[\mathbf{1c}]_0 \text{ (M)}$	$k_{\text{obs}} \text{ (s}^{-1}\text{)}$
1.87×10^{-5}	5.62×10^{-5}	1.28×10^{-1}
1.94×10^{-5}	1.36×10^{-4}	3.55×10^{-1}
1.91×10^{-5}	2.86×10^{-4}	6.66×10^{-1}



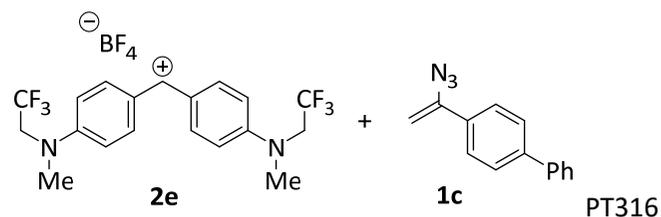
1c + 2d in CH_2Cl_2 (conventional photometry, detection at $\lambda = 601 \text{ nm}$)



$[\mathbf{2d}]_0 \text{ (M)}$	$[\mathbf{1c}]_0 \text{ (M)}$	$k_{\text{obs}} \text{ (s}^{-1}\text{)}$
8.71×10^{-6}	1.74×10^{-4}	1.06×10^{-2}
8.48×10^{-6}	2.55×10^{-4}	1.55×10^{-2}
8.56×10^{-6}	3.43×10^{-4}	2.00×10^{-2}
8.56×10^{-6}	4.28×10^{-4}	2.56×10^{-2}
8.56×10^{-6}	6.23×10^{-4}	3.71×10^{-2}

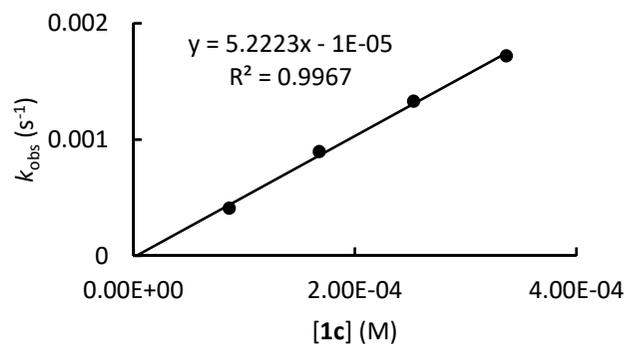


1c + 2e in CH₂Cl₂ (conventional photometry, detection at λ = 593 nm)



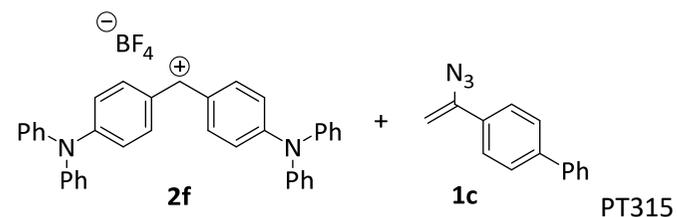
[2e] ₀ (M)	[1c] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
5.77 × 10 ⁻⁶	8.65 × 10 ⁻⁵	4.09 × 10 ⁻⁴
5.59 × 10 ⁻⁶	1.68 × 10 ⁻⁴	8.97 × 10 ⁻⁴
5.62 × 10 ⁻⁶	2.53 × 10 ⁻⁴	1.33 × 10 ⁻³
5.61 × 10 ⁻⁶	3.37 × 10 ⁻⁴	1.72 × 10 ⁻³

Only data from the first 35% of conversion were used to determine *k*_{obs}.



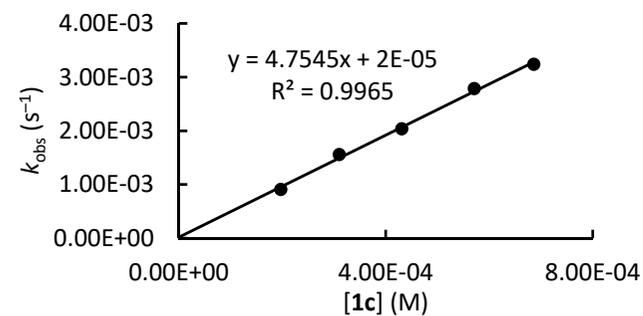
$$k_2 = (5.22 \pm 0.22) \text{ M}^{-1} \text{ s}^{-1}$$

1c + 2f in CH₂Cl₂ (conventional photometry, detection at λ = 672 nm)



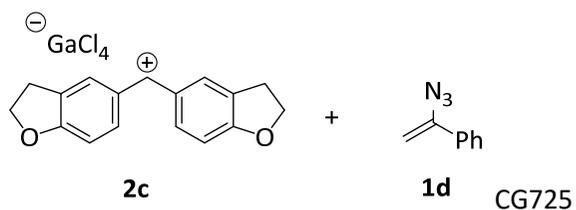
[2f] ₀ (M)	[1c] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
9.84 × 10 ⁻⁶	1.97 × 10 ⁻⁴	9.10 × 10 ⁻⁴
9.70 × 10 ⁻⁶	3.10 × 10 ⁻⁴	1.56 × 10 ⁻³
9.57 × 10 ⁻⁶	4.31 × 10 ⁻⁴	2.04 × 10 ⁻³
9.51 × 10 ⁻⁶	5.71 × 10 ⁻⁴	2.79 × 10 ⁻³
9.52 × 10 ⁻⁶	6.86 × 10 ⁻⁴	3.24 × 10 ⁻³

Only data from the first half-life time were used to determine *k*_{obs}.

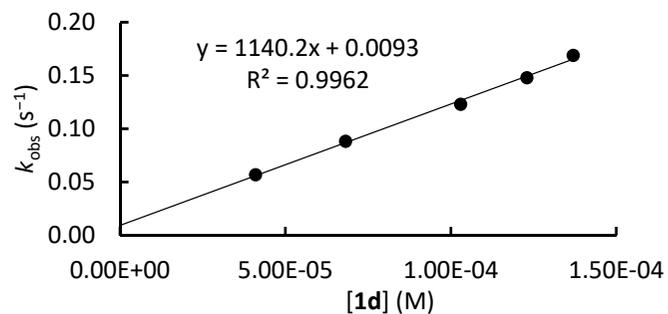


$$k_2 = (4.75 \pm 0.16) \text{ M}^{-1} \text{ s}^{-1}$$

1d + 2c (generated in CH₂Cl₂ solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in dichloromethane (conventional photometry, detection at λ = 535 nm)

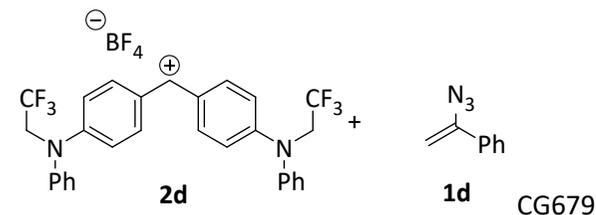


[2c] ₀ (M)	[1d] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.37 × 10 ⁻⁵	4.10 × 10 ⁻⁵	5.68 × 10 ⁻²
1.36 × 10 ⁻⁵	6.82 × 10 ⁻⁵	8.83 × 10 ⁻²
1.37 × 10 ⁻⁵	1.03 × 10 ⁻⁴	1.23 × 10 ⁻¹
1.37 × 10 ⁻⁵	1.23 × 10 ⁻⁴	1.48 × 10 ⁻¹
1.37 × 10 ⁻⁵	1.37 × 10 ⁻⁴	1.69 × 10 ⁻¹

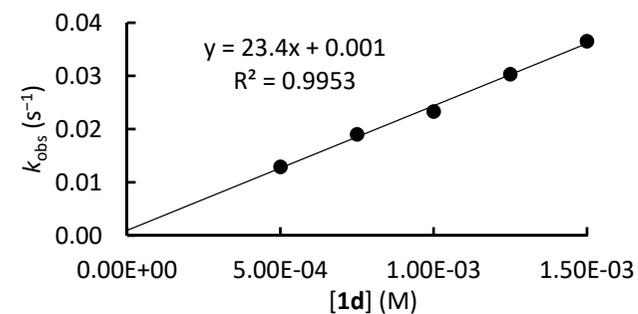


$$k_2 = (1.14 \pm 0.04) \times 10^3 \text{ M}^{-1} \text{ s}^{-1}$$

1d + 2d in CH₂Cl₂ (stopped-flow method, detection at λ = 601 nm)

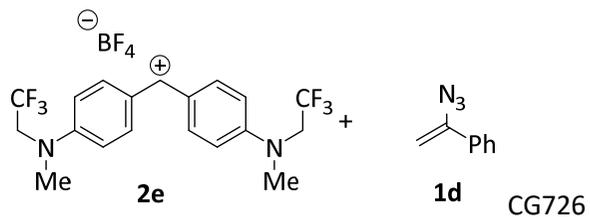


[2d] ₀ (M)	[1d] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
3.73 × 10 ⁻⁶	5.00 × 10 ⁻⁴	1.29 × 10 ⁻²
3.10 × 10 ⁻⁶	7.50 × 10 ⁻⁴	1.90 × 10 ⁻²
3.10 × 10 ⁻⁶	1.00 × 10 ⁻³	2.33 × 10 ⁻²
3.02 × 10 ⁻⁶	1.25 × 10 ⁻³	3.03 × 10 ⁻²
2.86 × 10 ⁻⁶	1.50 × 10 ⁻³	3.65 × 10 ⁻²

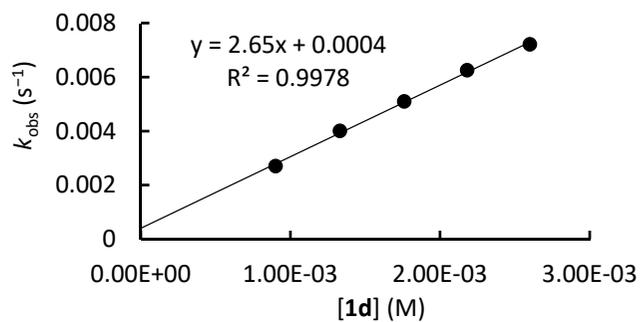


$$k_2 = (2.34 \pm 0.09) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

1d + 2e in CH₂Cl₂ (conventional photometry, detection at λ = 593 nm)

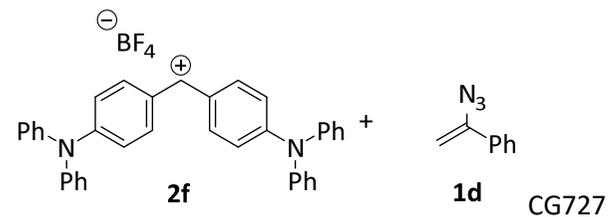


[2e] ₀ (M)	[1d] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.19 × 10 ⁻⁵	9.00 × 10 ⁻⁴	2.70 × 10 ⁻³
1.24 × 10 ⁻⁵	1.33 × 10 ⁻³	4.01 × 10 ⁻³
1.27 × 10 ⁻⁵	1.76 × 10 ⁻³	5.10 × 10 ⁻³
1.27 × 10 ⁻⁵	2.18 × 10 ⁻³	6.25 × 10 ⁻³
1.26 × 10 ⁻⁵	2.60 × 10 ⁻³	7.21 × 10 ⁻³

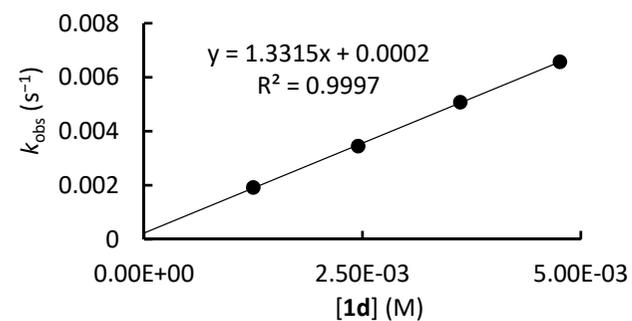


$$k_2 = (2.65 \pm 0.07) \text{ M}^{-1} \text{ s}^{-1}$$

1d + 2f in CH₂Cl₂ (conventional photometry, detection at λ = 674 nm)

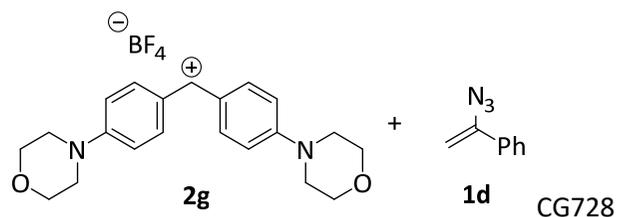


[2f] ₀ (M)	[1d] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.08 × 10 ⁻⁵	1.25 × 10 ⁻³	1.92 × 10 ⁻³
1.08 × 10 ⁻⁵	2.45 × 10 ⁻³	3.45 × 10 ⁻³
1.11 × 10 ⁻⁵	3.62 × 10 ⁻³	5.08 × 10 ⁻³
1.03 × 10 ⁻⁵	4.76 × 10 ⁻³	6.57 × 10 ⁻³

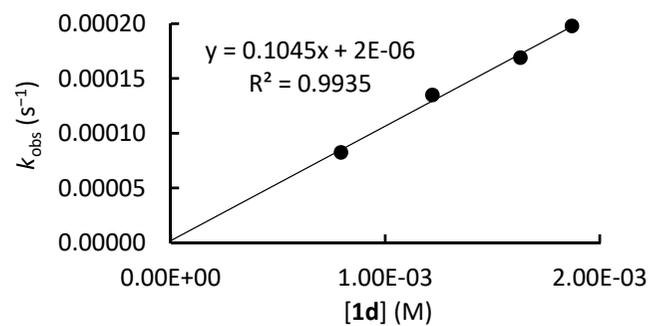


$$k_2 = (1.33 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$$

1d + 2g in CH₂Cl₂ (conventional photometry, detection at λ = 620 nm)

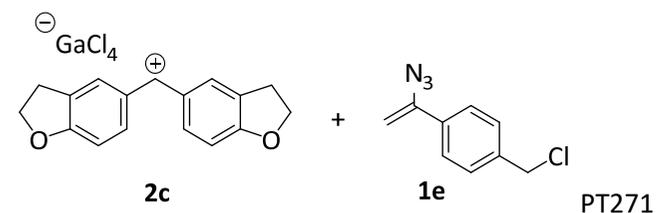


[2g] ₀ (M)	[1d] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
8.47 × 10 ⁻⁶	7.94 × 10 ⁻⁴	8.25 × 10 ⁻⁵
7.71 × 10 ⁻⁶	1.22 × 10 ⁻³	1.35 × 10 ⁻⁴
8.11 × 10 ⁻⁶	1.63 × 10 ⁻³	1.69 × 10 ⁻⁴
8.22 × 10 ⁻⁶	1.87 × 10 ⁻³	1.98 × 10 ⁻⁴

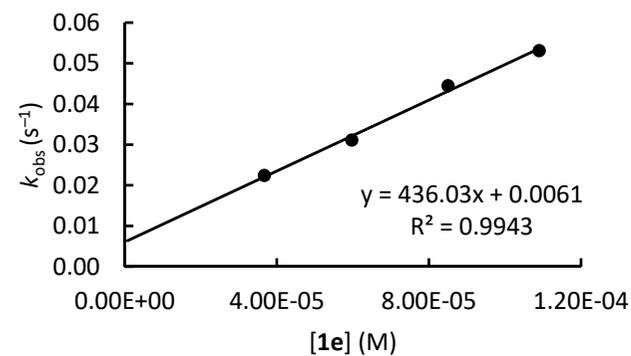


$$k_2 = (1.05 \pm 0.06) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

1e + 2c (generated in solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 535 nm)

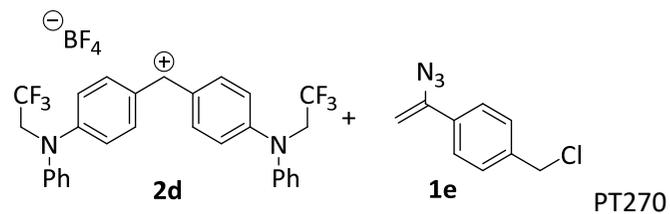


[2c] ₀ (M)	[1e] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.22 × 10 ⁻⁵	3.67 × 10 ⁻⁵	2.24 × 10 ⁻²
1.19 × 10 ⁻⁵	5.97 × 10 ⁻⁵	3.11 × 10 ⁻²
1.21 × 10 ⁻⁵	8.50 × 10 ⁻⁵	4.45 × 10 ⁻²
1.21 × 10 ⁻⁵	1.09 × 10 ⁻⁴	5.31 × 10 ⁻²

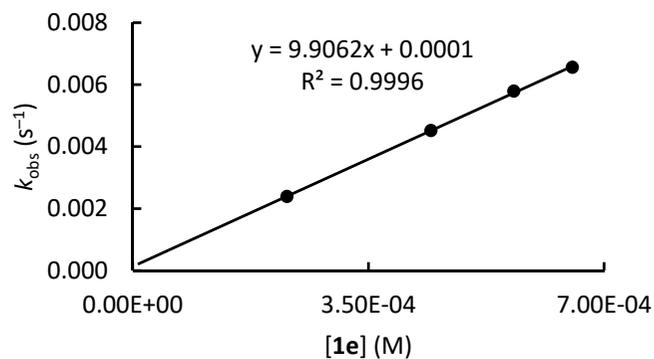


$$k_2 = (4.36 \pm 0.23) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1e + 2d in CH₂Cl₂ (conventional photometry, detection at λ = 601 nm)

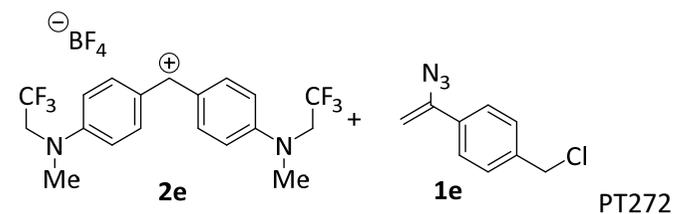


[2d] ₀ (M)	[1e] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
2.29 × 10 ⁻⁵	2.29 × 10 ⁻⁴	2.39 × 10 ⁻³
2.22 × 10 ⁻⁵	4.43 × 10 ⁻⁴	4.52 × 10 ⁻³
2.26 × 10 ⁻⁵	5.66 × 10 ⁻⁴	5.79 × 10 ⁻³
2.18 × 10 ⁻⁵	6.53 × 10 ⁻⁴	6.56 × 10 ⁻³



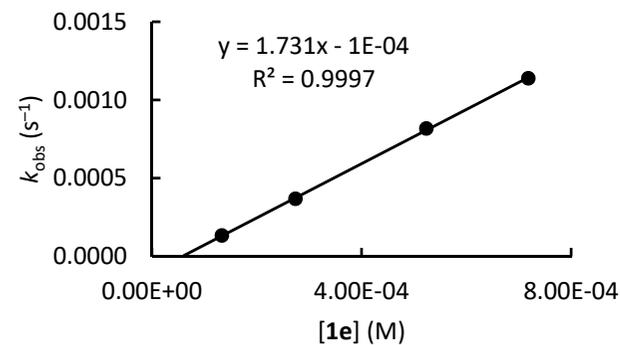
$$k_2 = (9.91 \pm 0.15) \text{ M}^{-1} \text{ s}^{-1}$$

1e + 2e in CH₂Cl₂ (conventional photometry, detection at λ = 593 nm)



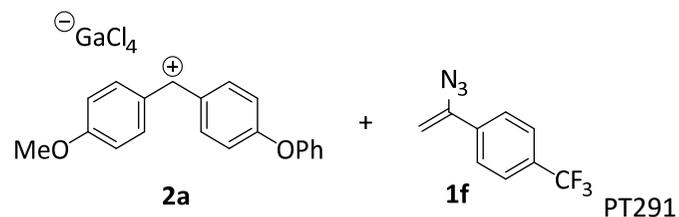
[2e] ₀ (M)	[1e] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
8.89 × 10 ⁻⁶	1.33 × 10 ⁻⁴	1.34 × 10 ⁻⁴
9.13 × 10 ⁻⁶	2.74 × 10 ⁻⁴	3.68 × 10 ⁻⁴
8.73 × 10 ⁻⁶	5.24 × 10 ⁻⁴	8.18 × 10 ⁻⁴
8.65 × 10 ⁻⁶	7.18 × 10 ⁻⁴	1.14 × 10 ⁻³

Only data from the first half-life time were used to determine *k*_{obs}.

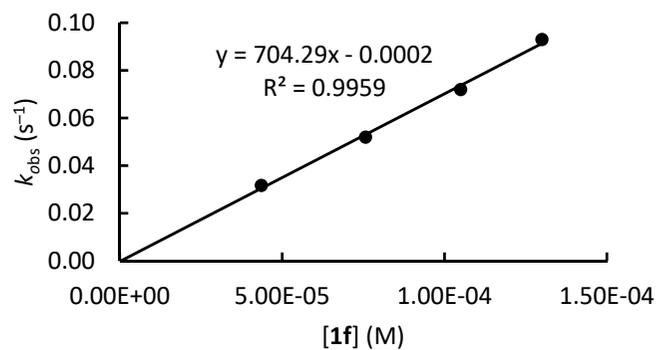


$$k_2 = (1.73 \pm 0.02) \text{ M}^{-1} \text{ s}^{-1}$$

1f + 2a (generated in solution from Ar₂CH–Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 516 nm)

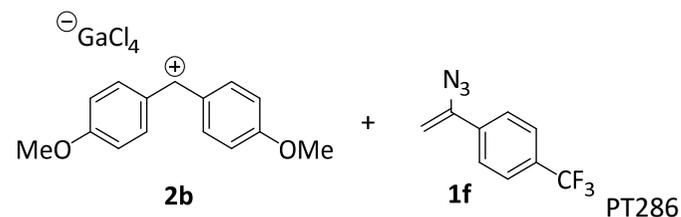


[2a] ₀ (M)	[1f] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.45 × 10 ⁻⁵	4.36 × 10 ⁻⁵	3.17 × 10 ⁻²
1.48 × 10 ⁻⁵	7.57 × 10 ⁻⁵	5.20 × 10 ⁻²
1.50 × 10 ⁻⁵	1.05 × 10 ⁻⁴	7.20 × 10 ⁻²
1.44 × 10 ⁻⁵	1.30 × 10 ⁻⁴	9.30 × 10 ⁻²

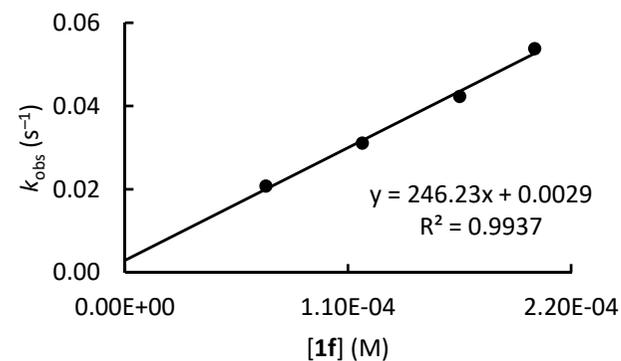


$$k_2 = (7.04 \pm 0.32) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1f + 2b (generated in solution from Ar₂CH–Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 512 nm)

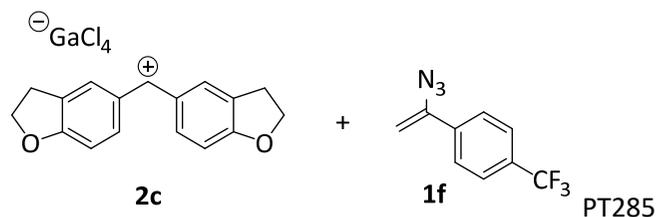


[2b] ₀ (M)	[1f] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
2.32 × 10 ⁻⁵	6.95 × 10 ⁻⁵	2.08 × 10 ⁻²
2.29 × 10 ⁻⁵	1.17 × 10 ⁻⁴	3.11 × 10 ⁻²
2.30 × 10 ⁻⁵	1.65 × 10 ⁻⁴	4.23 × 10 ⁻²
2.27 × 10 ⁻⁵	2.02 × 10 ⁻⁴	5.38 × 10 ⁻²

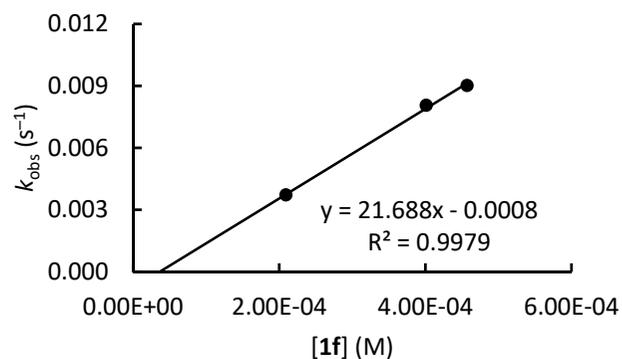


$$k_2 = (2.46 \pm 0.14) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

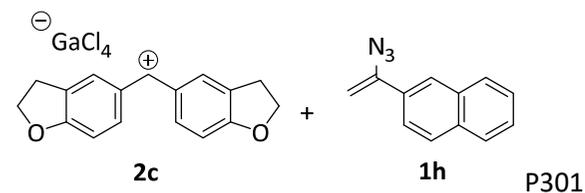
1f + 2c (generated in solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 535 nm)



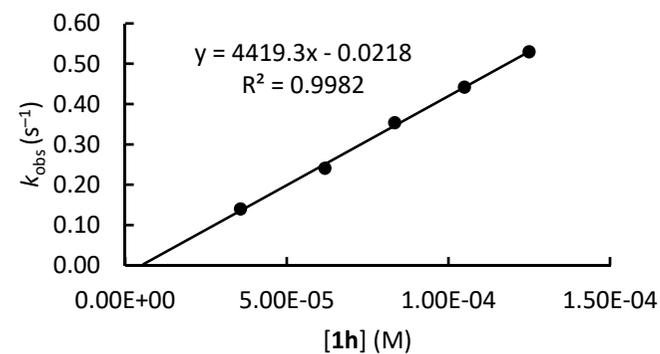
[2c] ₀ (M)	[1f] ₀ (M)	k _{obs} (s ⁻¹)
1.04 × 10 ⁻⁵	2.09 × 10 ⁻⁴	3.72 × 10 ⁻³
1.00 × 10 ⁻⁵	4.01 × 10 ⁻⁴	8.06 × 10 ⁻³
9.93 × 10 ⁻⁶	4.57 × 10 ⁻⁴	9.02 × 10 ⁻³



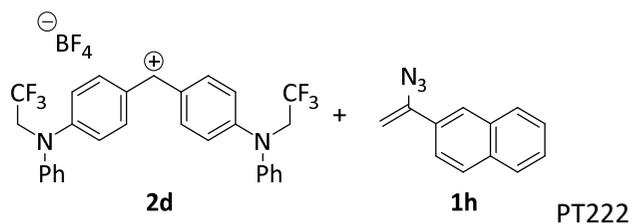
1h + 2c (generated in solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 535 nm)



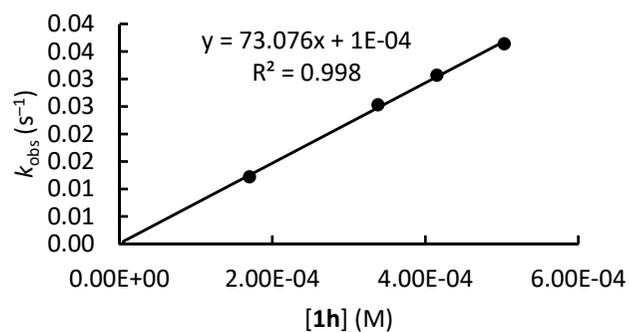
[2c] ₀ (M)	[1h] ₀ (M)	k _{obs} (s ⁻¹)
1.43 × 10 ⁻⁵	3.57 × 10 ⁻⁵	1.40 × 10 ⁻¹
1.55 × 10 ⁻⁵	6.18 × 10 ⁻⁵	2.41 × 10 ⁻¹
1.52 × 10 ⁻⁵	8.34 × 10 ⁻⁵	3.54 × 10 ⁻¹
1.50 × 10 ⁻⁵	1.05 × 10 ⁻⁴	4.42 × 10 ⁻¹
1.47 × 10 ⁻⁵	1.25 × 10 ⁻⁴	5.29 × 10 ⁻¹



1h + 2d in CH₂Cl₂ (conventional photometry, detection at λ = 601 nm)

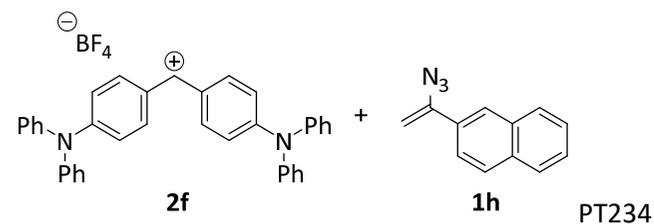


[2d] ₀ (M)	[1h] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.70 × 10 ⁻⁵	1.70 × 10 ⁻⁴	1.22 × 10 ⁻²
1.69 × 10 ⁻⁵	3.38 × 10 ⁻⁴	2.53 × 10 ⁻²
1.66 × 10 ⁻⁵	4.15 × 10 ⁻⁴	3.07 × 10 ⁻²
1.68 × 10 ⁻⁵	5.03 × 10 ⁻⁴	3.64 × 10 ⁻²

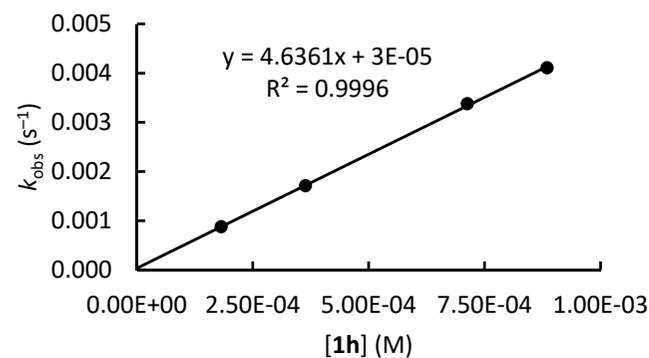


$$k_2 = (7.31 \pm 0.23) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

1h + 2f in CH₂Cl₂ (conventional photometry, detection at λ = 672 nm)

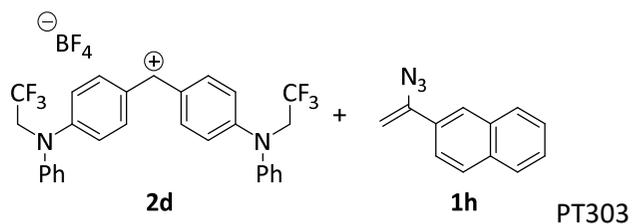


[2f] ₀ (M)	[1h] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
1.82 × 10 ⁻⁵	1.82 × 10 ⁻⁴	8.77 × 10 ⁻⁴
1.82 × 10 ⁻⁵	3.64 × 10 ⁻⁴	1.71 × 10 ⁻³
1.78 × 10 ⁻⁵	7.13 × 10 ⁻⁴	3.38 × 10 ⁻³
1.77 × 10 ⁻⁵	8.85 × 10 ⁻⁴	4.11 × 10 ⁻³

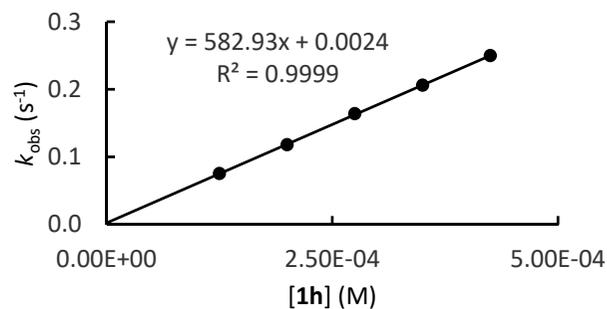


$$k_2 = (4.64 \pm 0.06) \text{ M}^{-1} \text{ s}^{-1}$$

1h + 2d in Cyrene (stopped-flow, detection at $\lambda = 601$ nm)

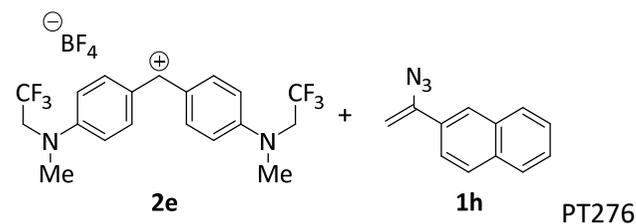


$[2d]_0$ (M)	$[1h]_0$ (M)	k_{obs} (s^{-1})
5.0×10^{-5}	1.25×10^{-4}	7.54×10^{-2}
5.0×10^{-5}	2.00×10^{-4}	1.18×10^{-1}
5.0×10^{-5}	2.75×10^{-4}	1.64×10^{-1}
5.0×10^{-5}	3.50×10^{-4}	2.06×10^{-1}
5.0×10^{-5}	4.25×10^{-4}	2.50×10^{-1}



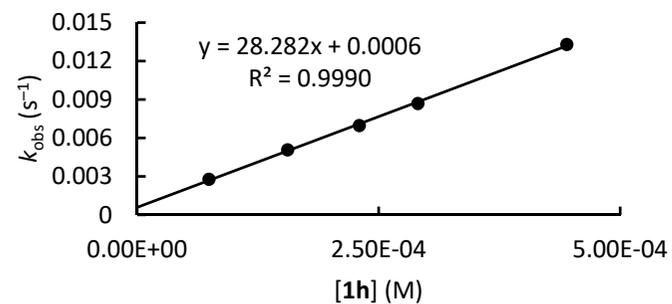
$$k_2 = (5.83 \pm 0.04) \times 10^2 \text{ M}^{-1} \text{ s}^{-1}$$

1h + 2e in Cyrene (conventional photometry, detection at $\lambda = 593$ nm)



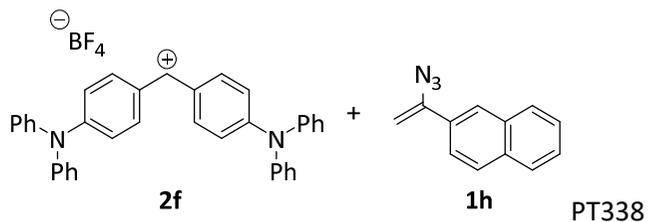
$[2e]_0$ (M)	$[1h]_0$ (M)	k_{obs} (s^{-1})
1.56×10^{-5}	7.43×10^{-5}	2.78×10^{-3}
1.53×10^{-5}	1.56×10^{-4}	5.08×10^{-3}
1.45×10^{-5}	2.30×10^{-4}	6.97×10^{-3}
1.48×10^{-5}	2.91×10^{-4}	8.69×10^{-3}
1.49×10^{-5}	4.45×10^{-4}	1.33×10^{-2}

Only data from the first half-life time were used to determine k_{obs} .

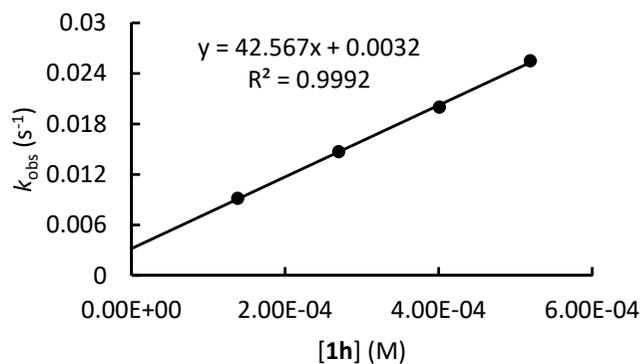


$$k_2 = (2.83 \pm 0.05) \times 10^1 \text{ M}^{-1} \text{ s}^{-1}$$

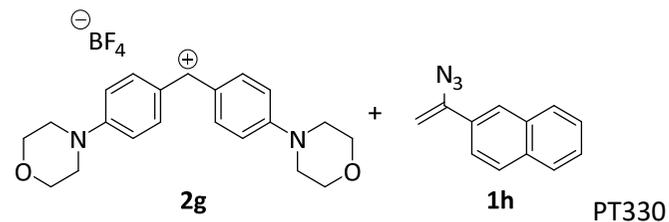
1h + 2f in Cyrene (conventional photometry, detection at $\lambda = 672$ nm)



$[2f]_0$ (M)	$[1h]_0$ (M)	k_{obs} (s^{-1})
2.76×10^{-5}	1.38×10^{-4}	9.17×10^{-3}
2.70×10^{-5}	2.70×10^{-4}	1.47×10^{-2}
2.67×10^{-5}	4.01×10^{-4}	2.00×10^{-2}
2.60×10^{-5}	5.19×10^{-4}	2.55×10^{-2}

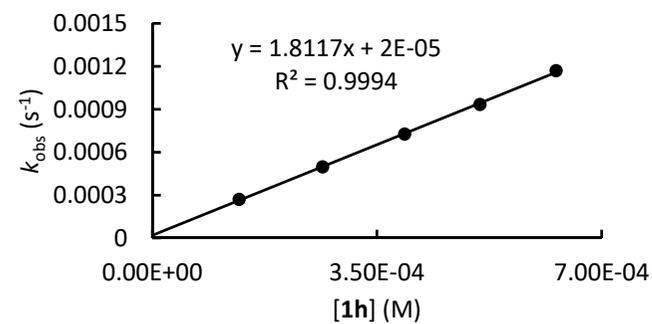


1h + 2g in Cyrene (conventional photometry, detection at 620 nm)

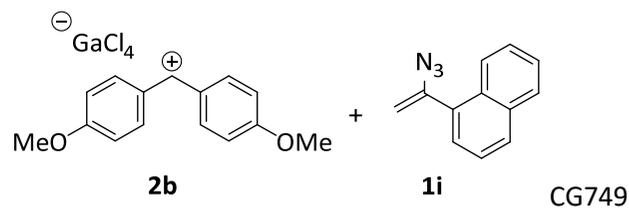


$[2g]_0$ (M)	$[1h]_0$ (M)	k_{obs} (s^{-1})
9.02×10^{-6}	1.35×10^{-4}	2.71×10^{-4}
8.84×10^{-6}	2.65×10^{-4}	4.98×10^{-4}
8.73×10^{-6}	3.93×10^{-4}	7.27×10^{-4}
8.51×10^{-6}	5.10×10^{-4}	9.34×10^{-4}
8.50×10^{-6}	6.29×10^{-4}	1.17×10^{-3}

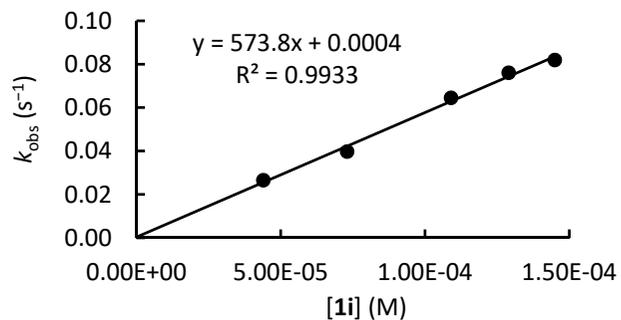
Only data from the first half-life time were used to determine k_{obs} .



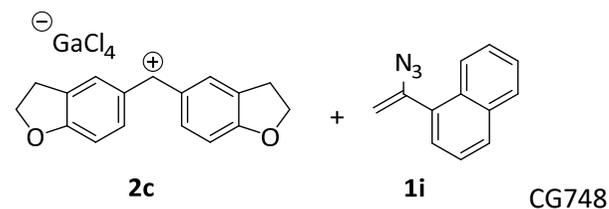
1i + 2b (generated in solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 512 nm)



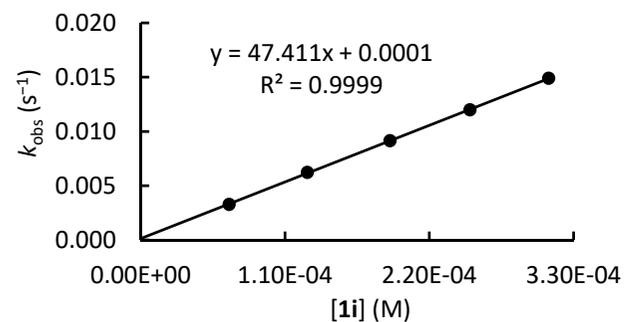
[2b] ₀ (M)	[1i] ₀ (M)	k _{obs} (s ⁻¹)
1.47 × 10 ⁻⁵	4.40 × 10 ⁻⁵	2.66 × 10 ⁻²
1.46 × 10 ⁻⁵	7.30 × 10 ⁻⁵	3.98 × 10 ⁻²
1.45 × 10 ⁻⁵	1.09 × 10 ⁻⁴	6.45 × 10 ⁻²
1.44 × 10 ⁻⁵	1.29 × 10 ⁻⁴	7.61 × 10 ⁻²
1.45 × 10 ⁻⁵	1.45 × 10 ⁻⁴	8.19 × 10 ⁻²



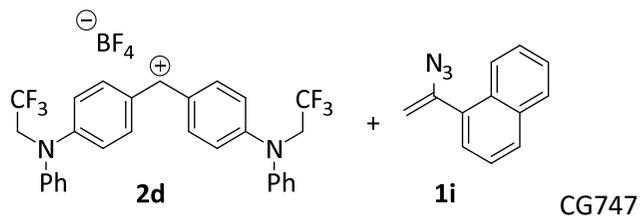
1i + 2c (generated in solution from Ar₂CH-Cl + 3 equiv. GaCl₃) in CH₂Cl₂
(conventional photometry, detection at λ = 535 nm)



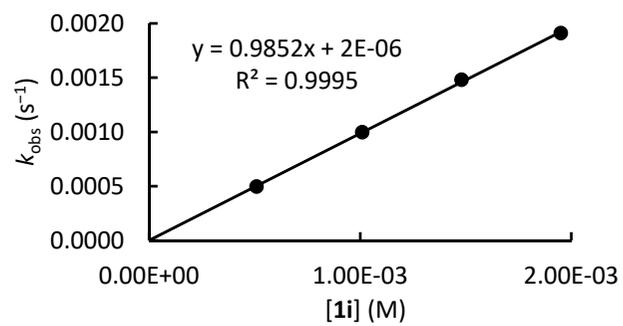
[2c] ₀ (M)	[1i] ₀ (M)	k _{obs} (s ⁻¹)
1.35 × 10 ⁻⁵	6.74 × 10 ⁻⁵	3.29 × 10 ⁻³
1.27 × 10 ⁻⁵	1.27 × 10 ⁻⁴	6.24 × 10 ⁻³
1.27 × 10 ⁻⁵	1.90 × 10 ⁻⁴	9.15 × 10 ⁻³
1.26 × 10 ⁻⁵	2.51 × 10 ⁻⁴	1.20 × 10 ⁻²
1.24 × 10 ⁻⁵	3.11 × 10 ⁻⁴	1.49 × 10 ⁻²



1i + **2d** in CH₂Cl₂ (conventional photometry, detection at $\lambda = 601$ nm)



[2d] ₀ (M)	[1i] ₀ (M)	<i>k</i> _{obs} (s ⁻¹)
9.26×10^{-6}	5.09×10^{-4}	4.97×10^{-4}
9.82×10^{-6}	1.01×10^{-3}	9.98×10^{-4}
9.96×10^{-6}	1.48×10^{-3}	1.48×10^{-3}
9.18×10^{-6}	1.95×10^{-3}	1.91×10^{-3}



$$k_2 = (9.85 \pm 0.16) \times 10^{-1} \text{ M}^{-1} \text{ s}^{-1}$$

6. Copies of NMR (^1H , ^{13}C , and ^{19}F) and IR Spectra

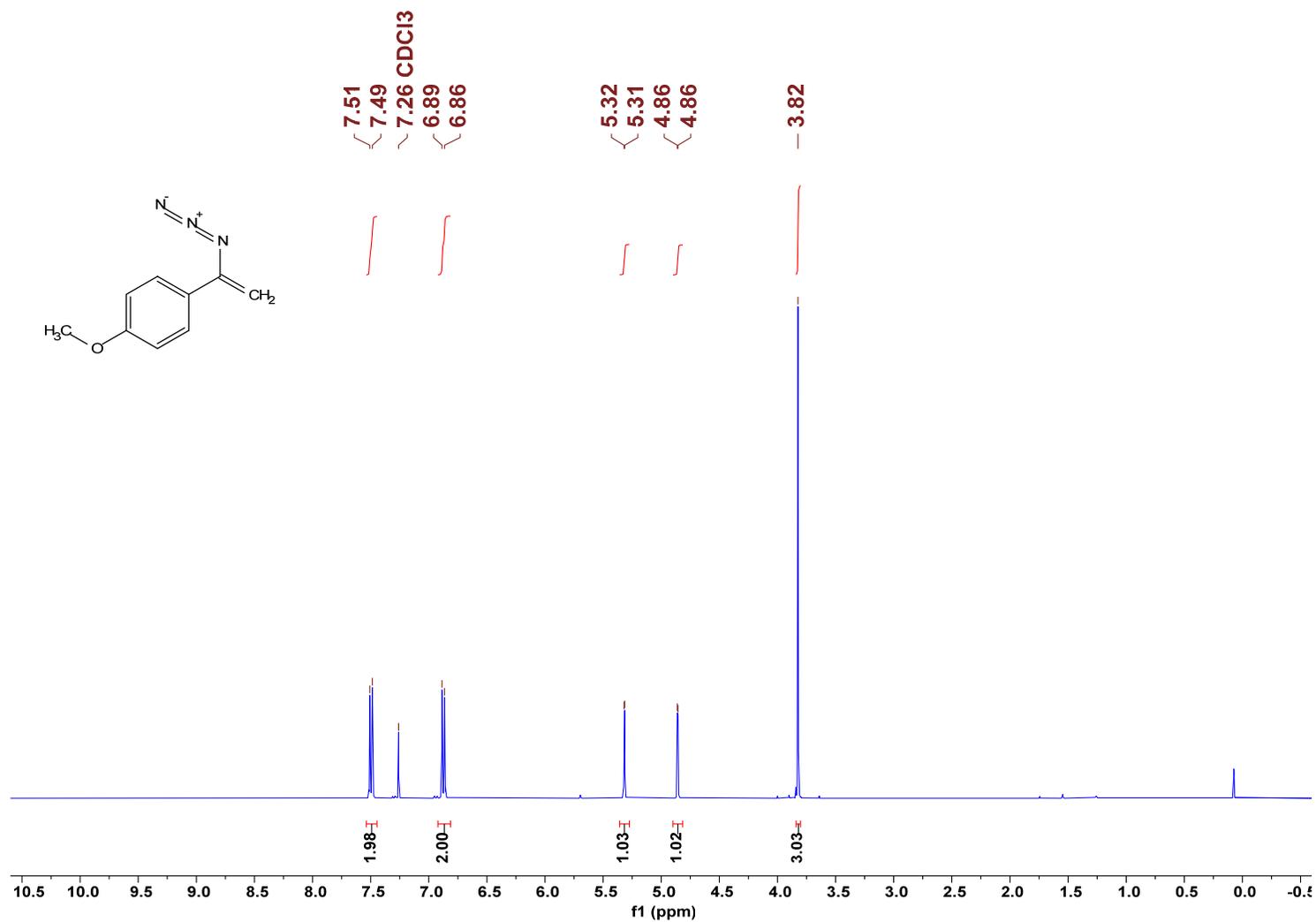


Figure S11: ^1H NMR spectrum of **1a** in CDCl_3 (400 MHz) CG715_2F1

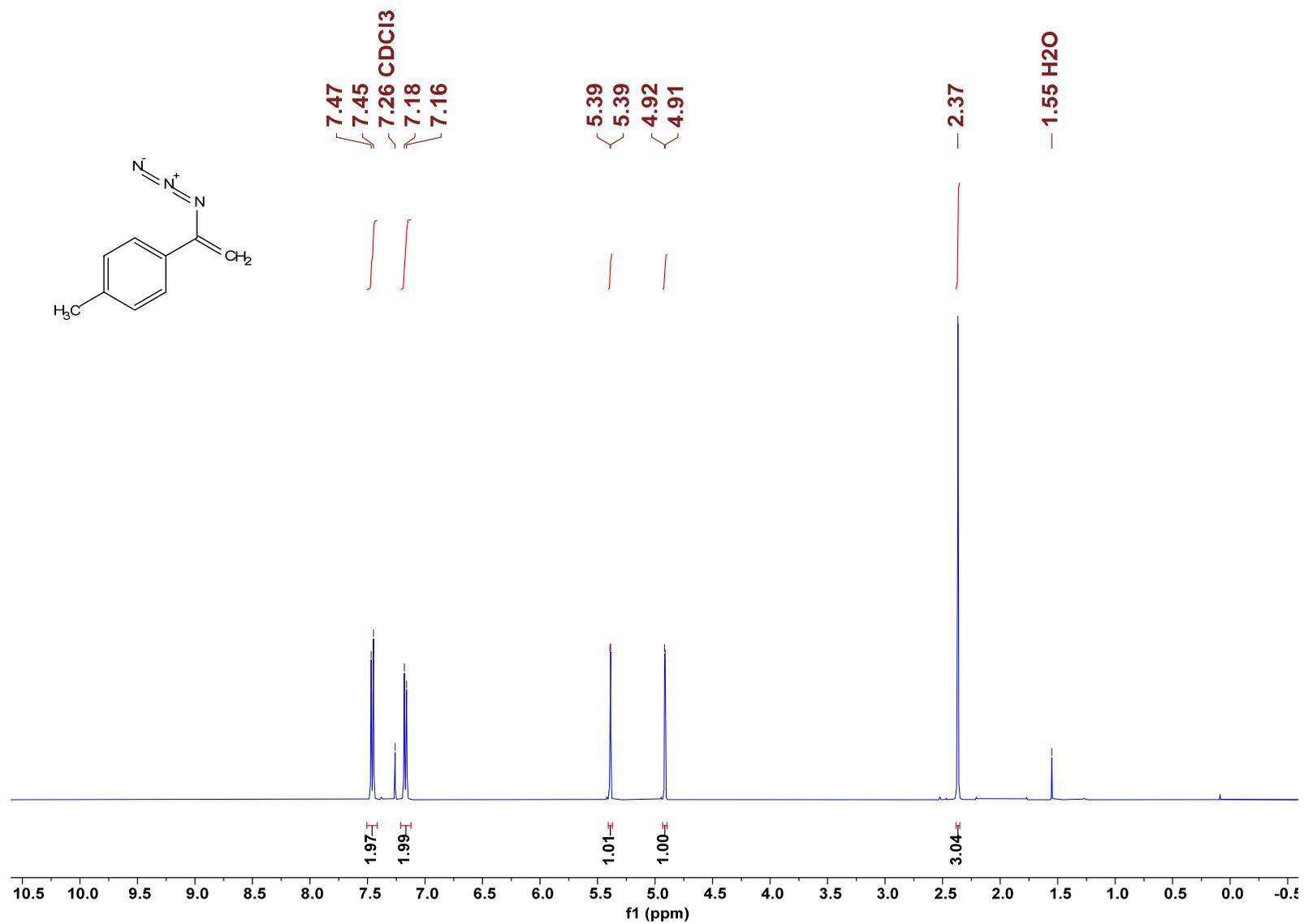


Figure S12: ¹H NMR spectrum of **1b** in CDCl₃ (400 MHz) PT176

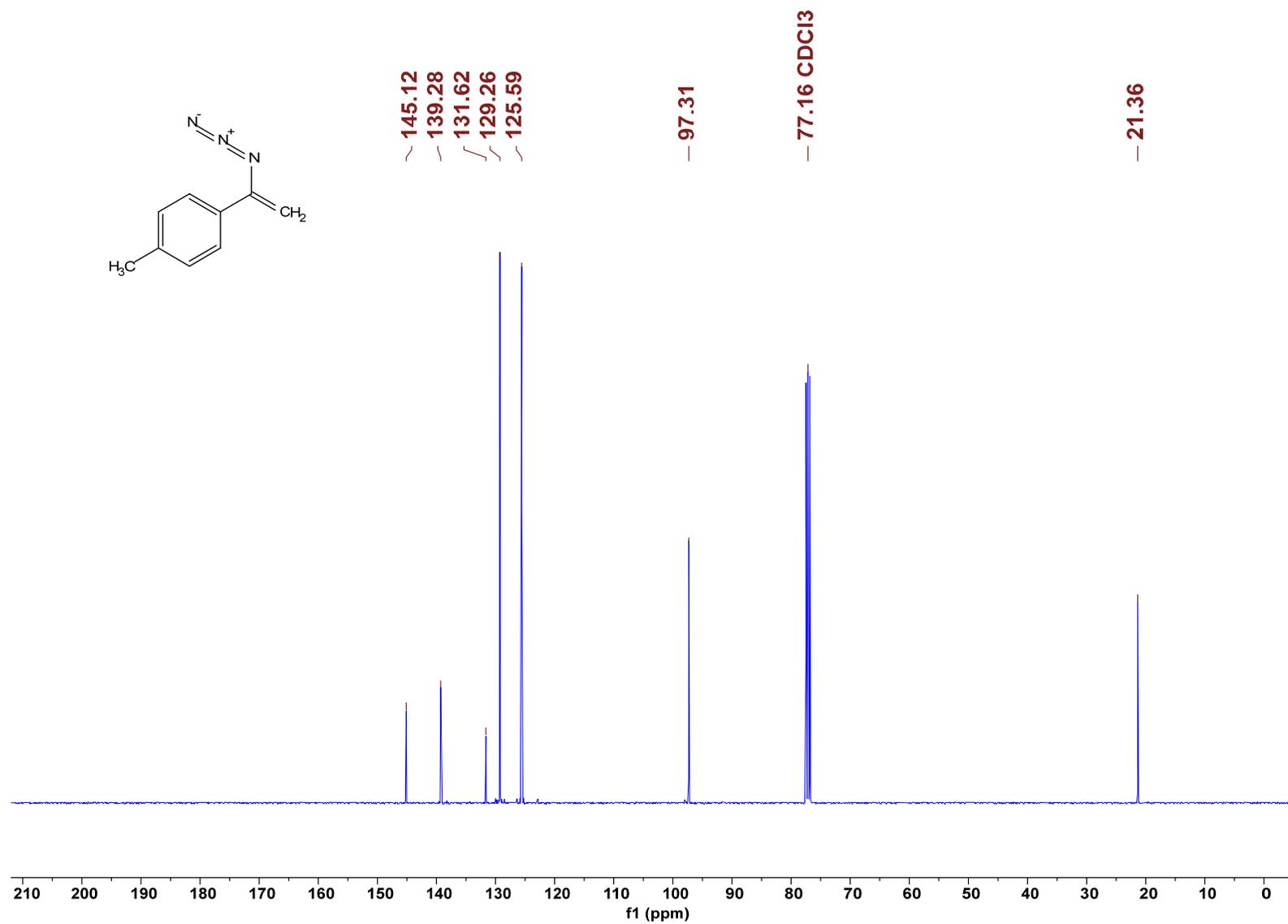


Figure S13: ¹³C NMR spectrum of **1b** in CDCl₃ (101 MHz) PT176

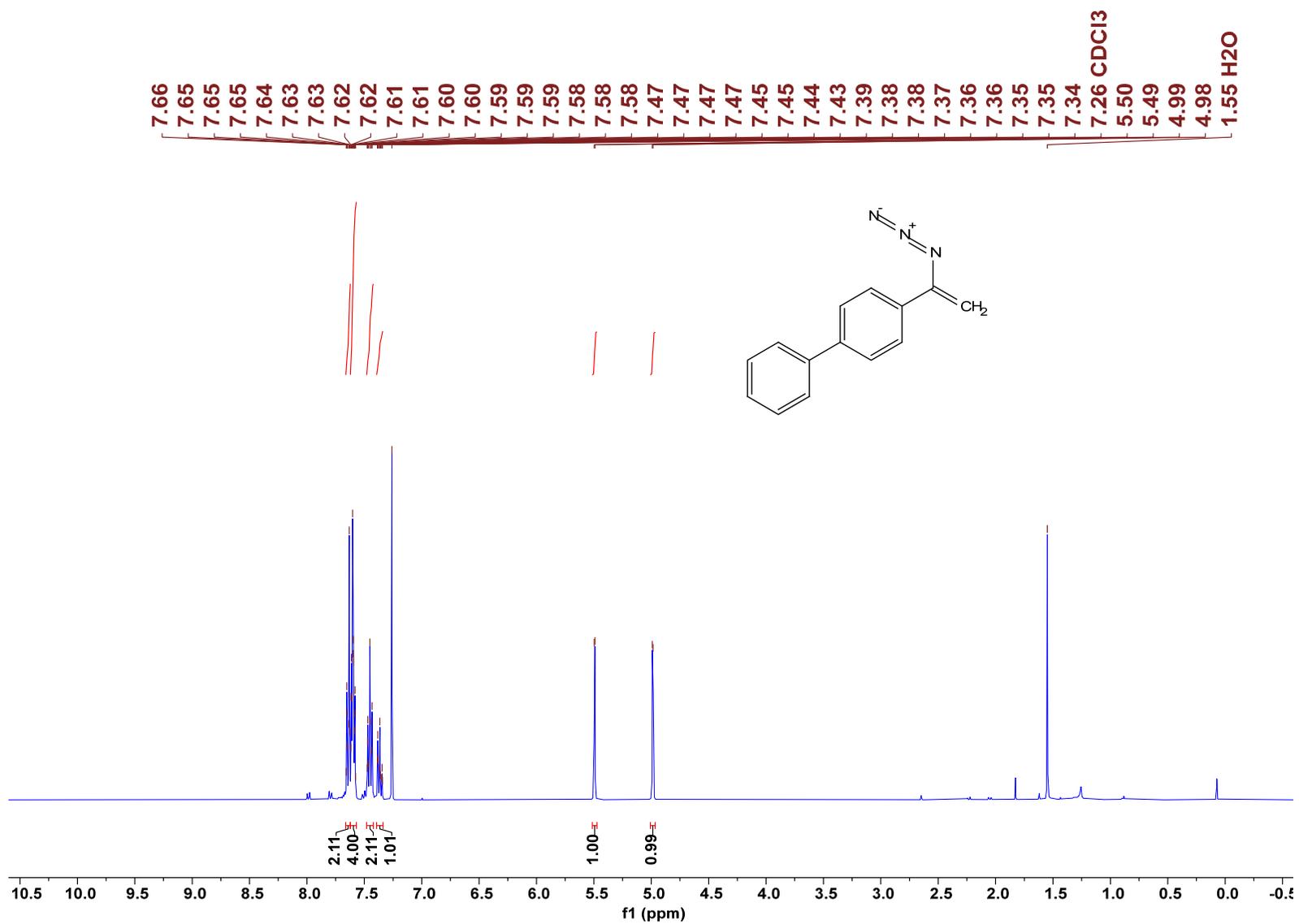


Figure S14: ^1H NMR spectrum of **1c** in CDCl_3 (400 MHz) PT293

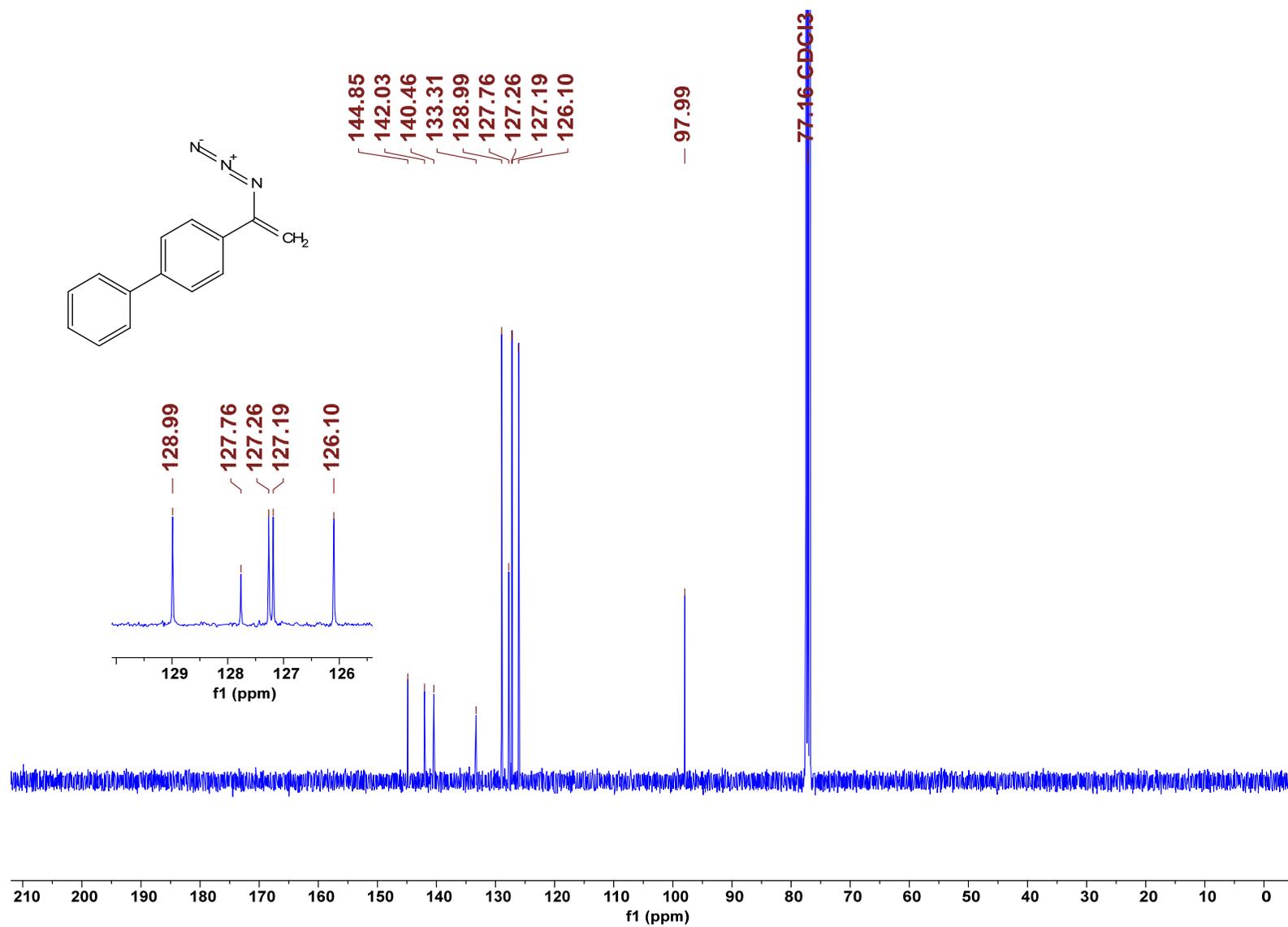


Figure S15: ^{13}C NMR spectrum of **1c** in CDCl_3 (101 MHz) PT293

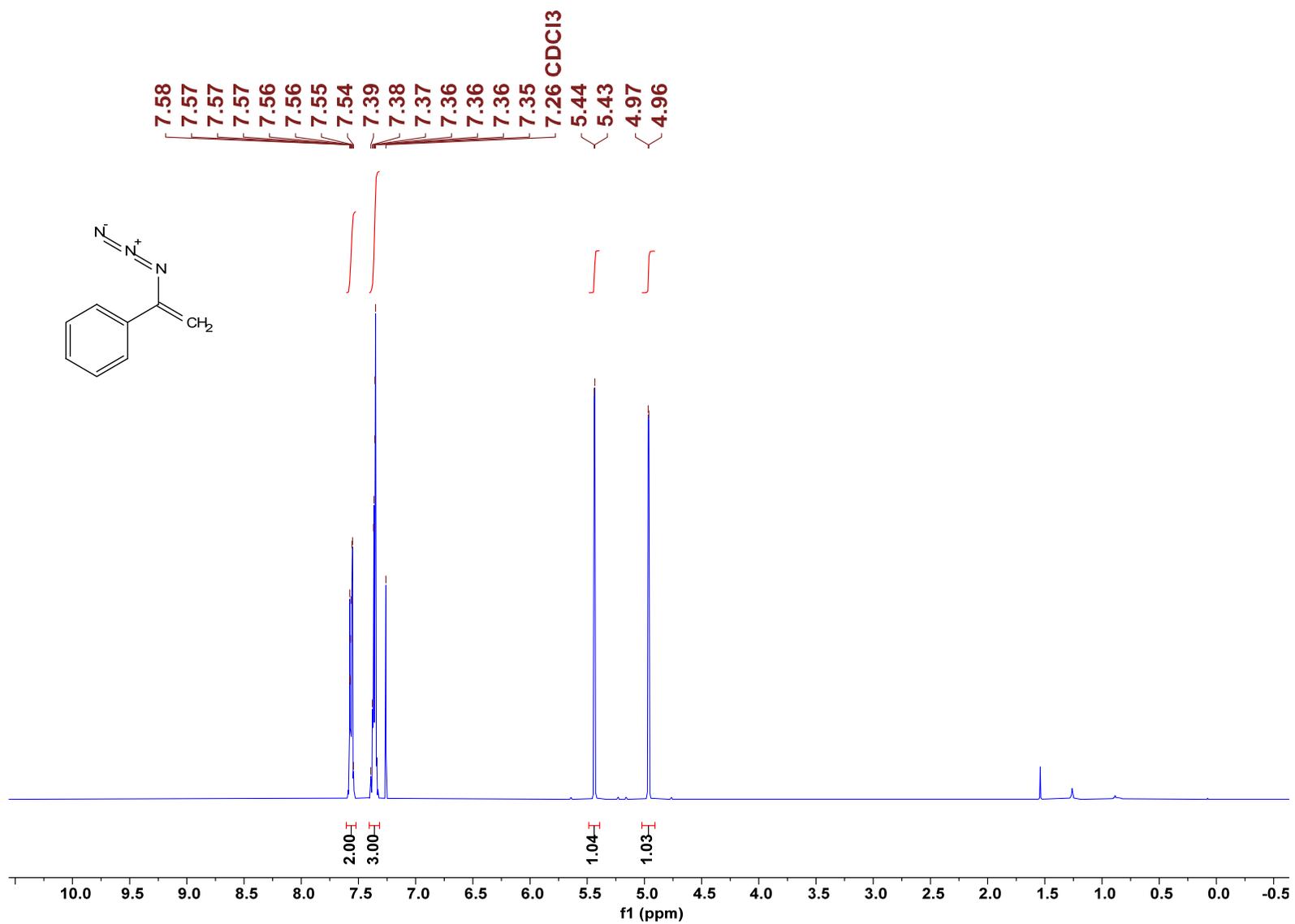


Figure S16: ¹H NMR spectrum of **1d** in CDCl₃ (400 MHz) CG677_1

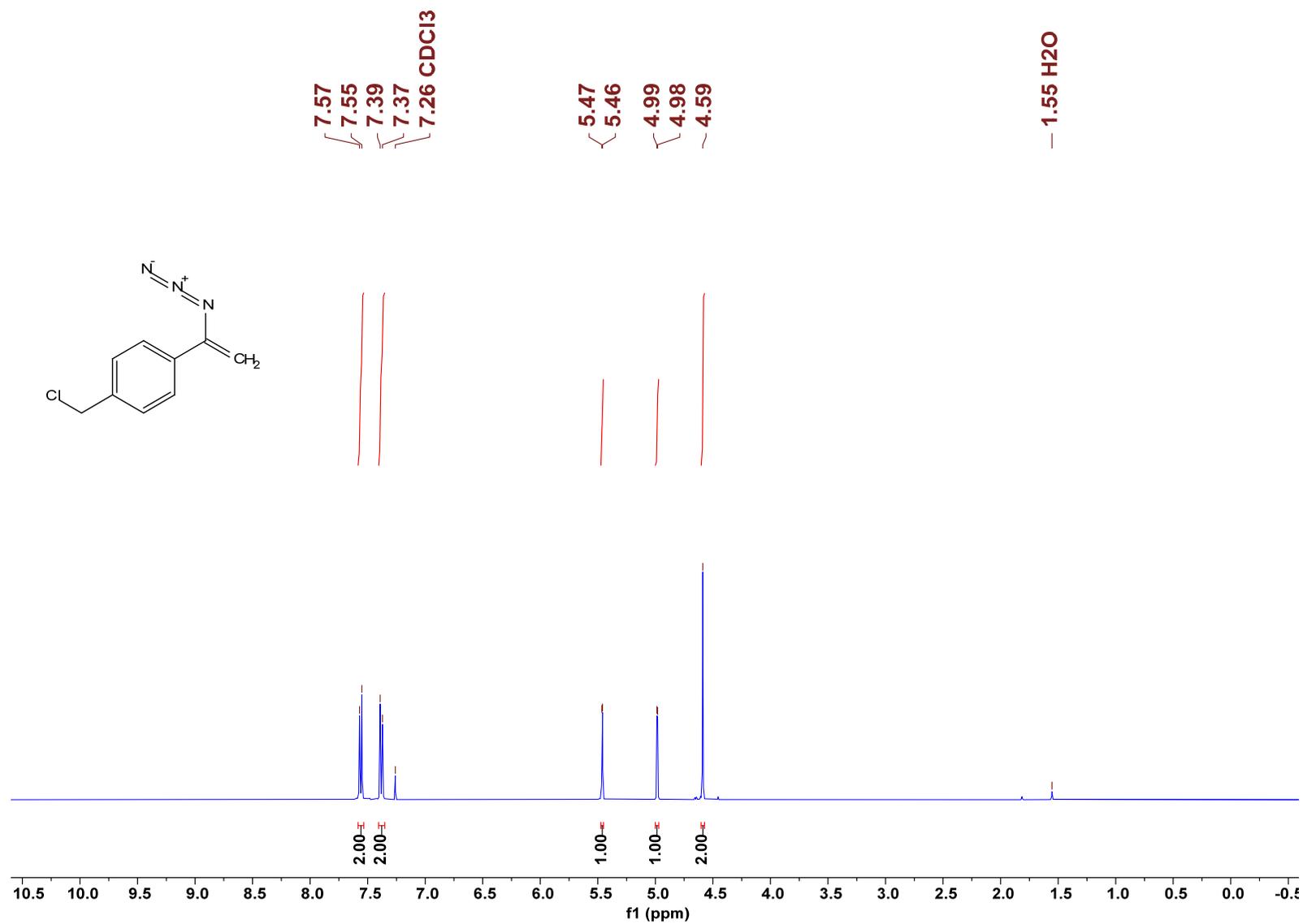


Figure S17: ^1H NMR spectrum of **1e** in CDCl_3 (400 MHz) PT237

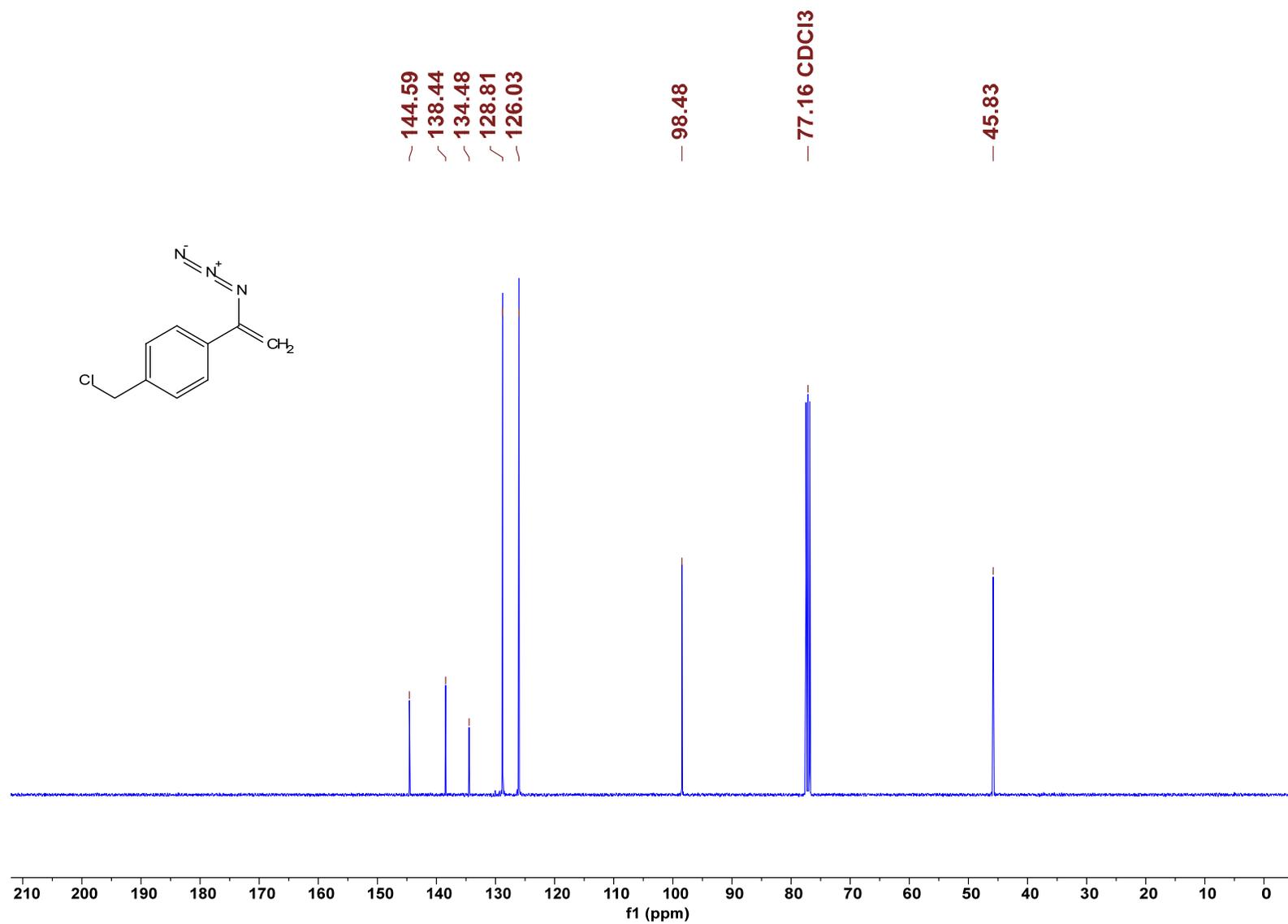


Figure S18: ¹³C NMR spectrum of **1e** in CDCl₃ (101 MHz) PT237

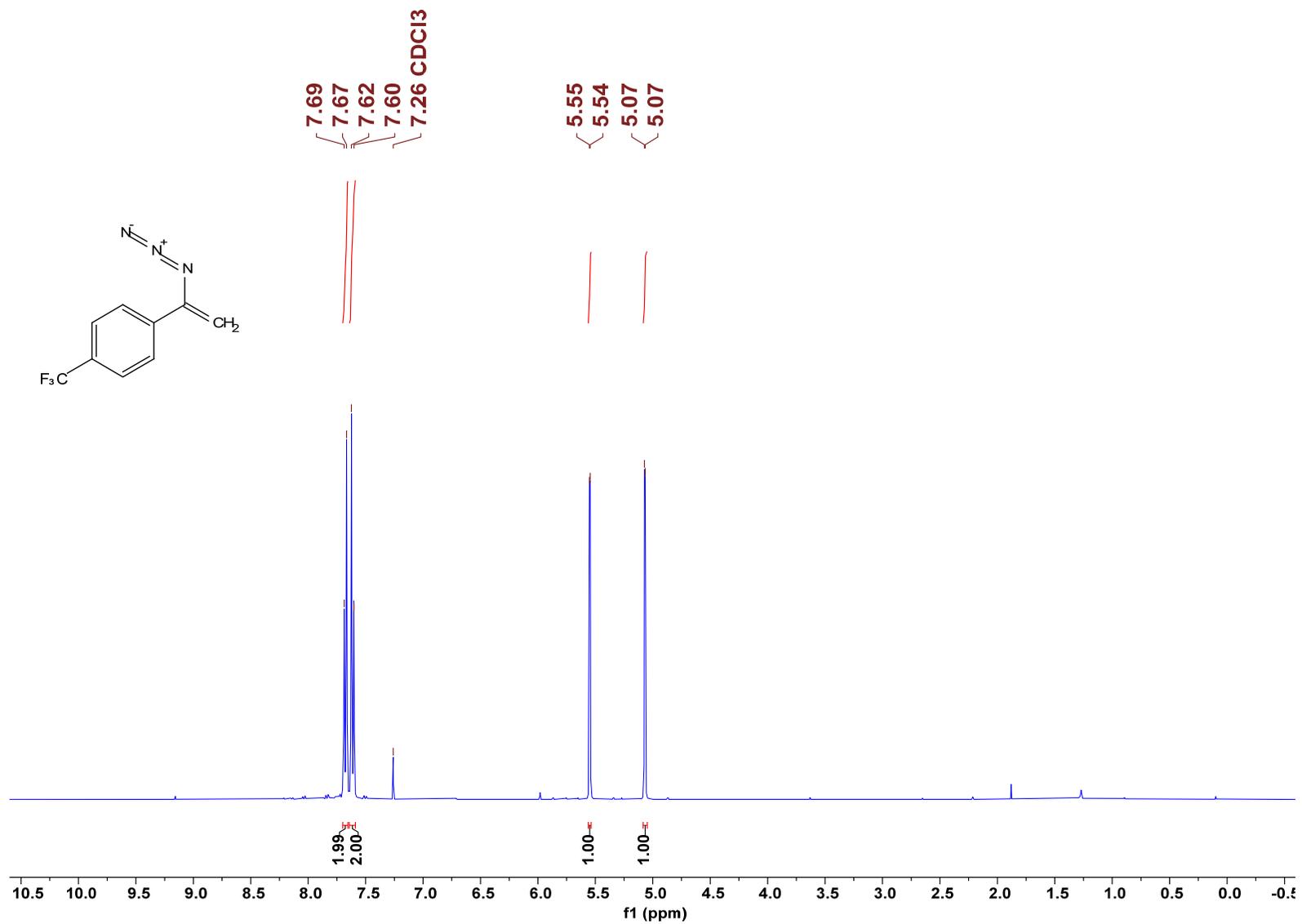


Figure S19: ¹H NMR spectrum of **1f** in CDCl₃ (400 MHz) PT280

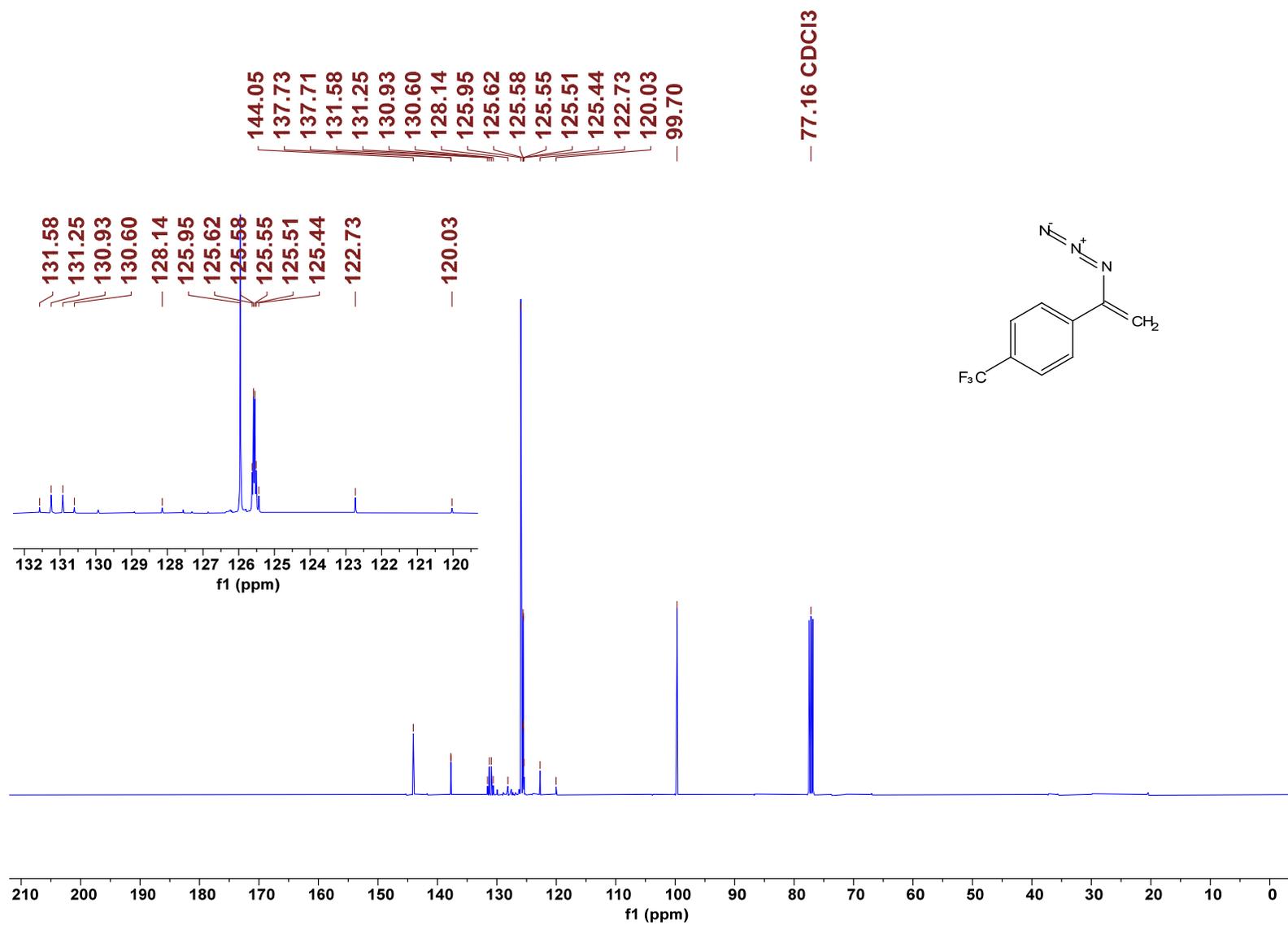


Figure S20: ¹³C NMR spectrum of **1f** in CDCl₃ (101 MHz) PT280

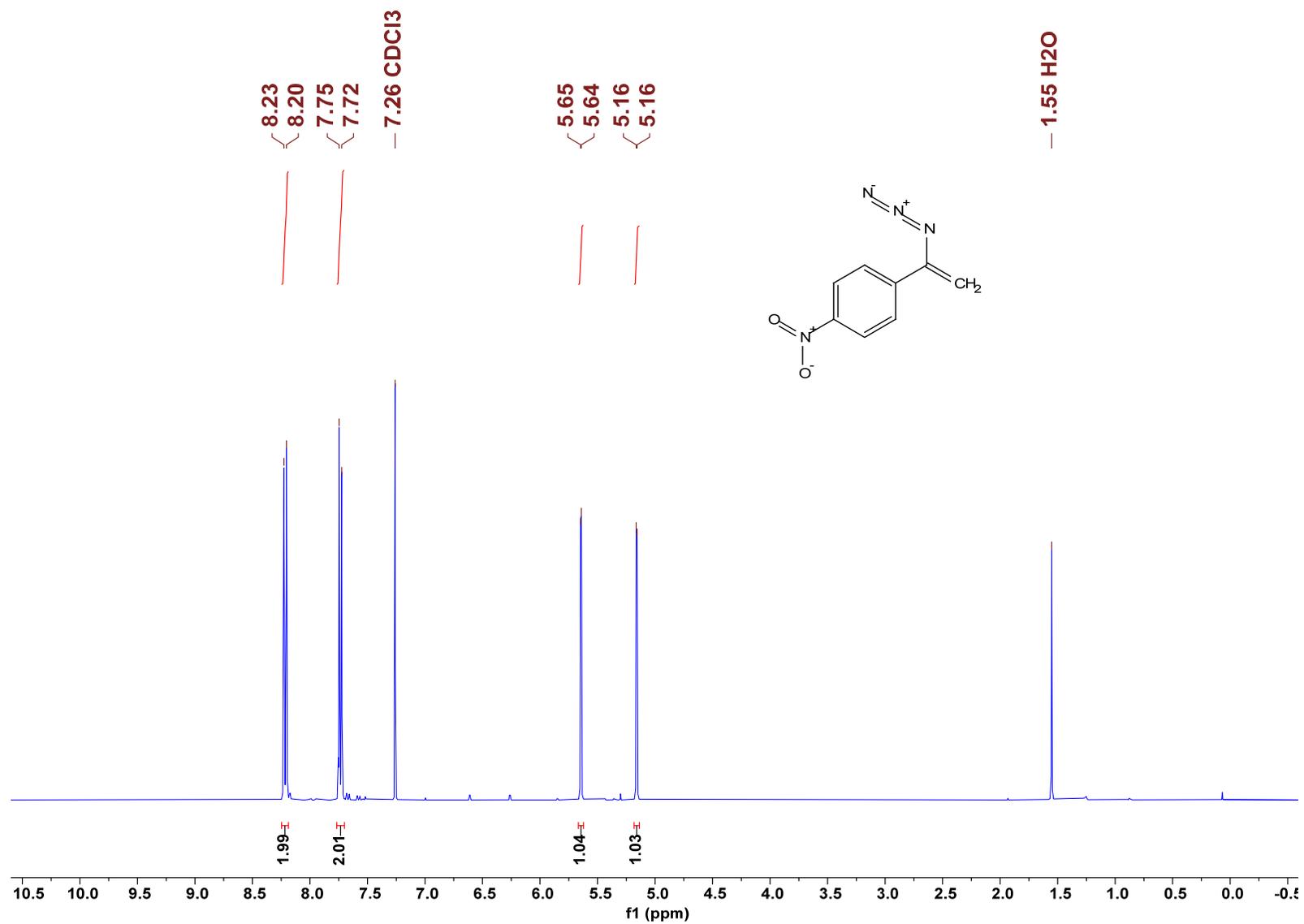


Figure S21: ^1H NMR spectrum of **1g** in CDCl_3 (400 MHz) PT212

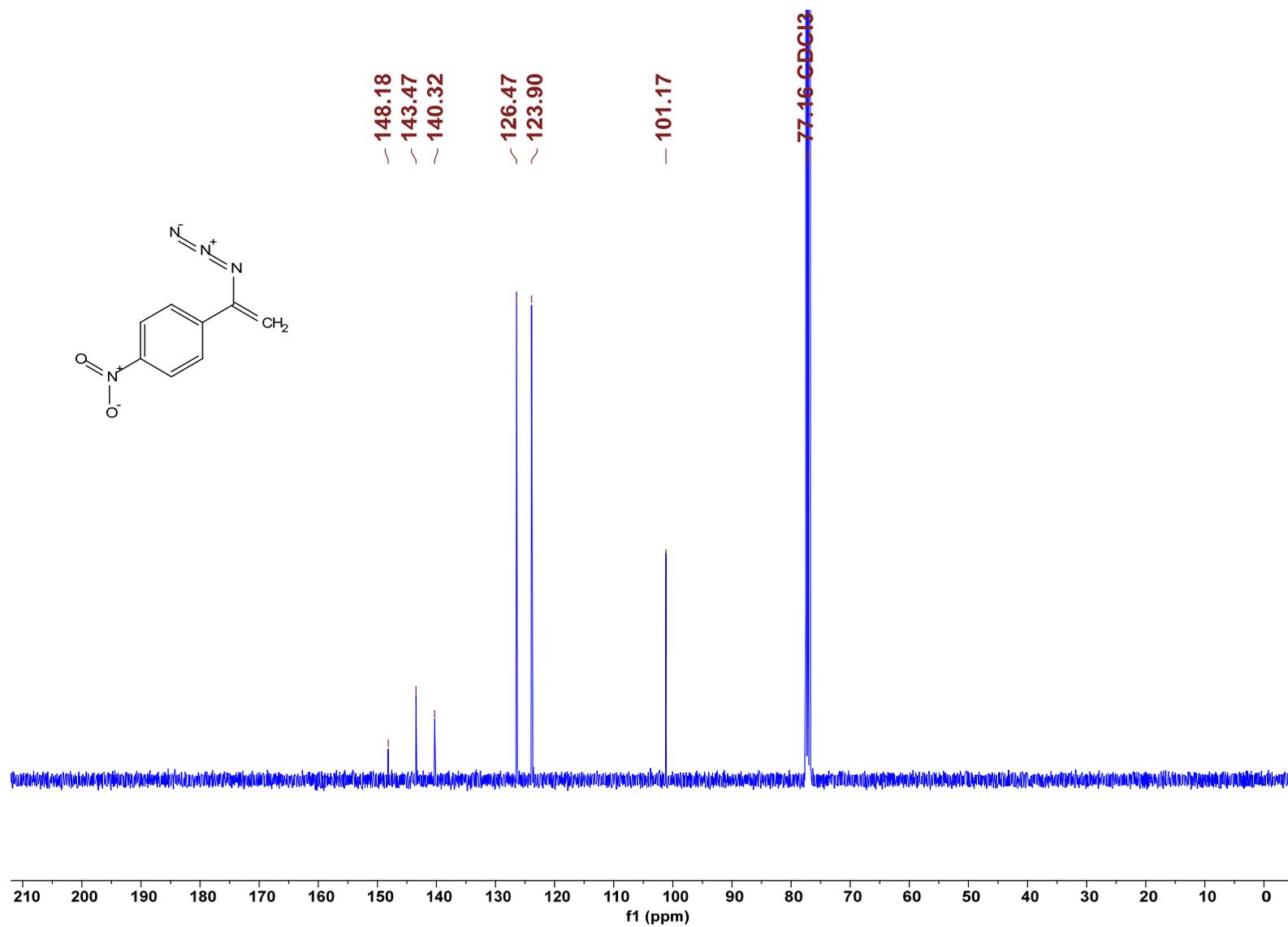


Figure S22: ^{13}C NMR spectrum of **1g** in CDCl_3 (101 MHz) PT212

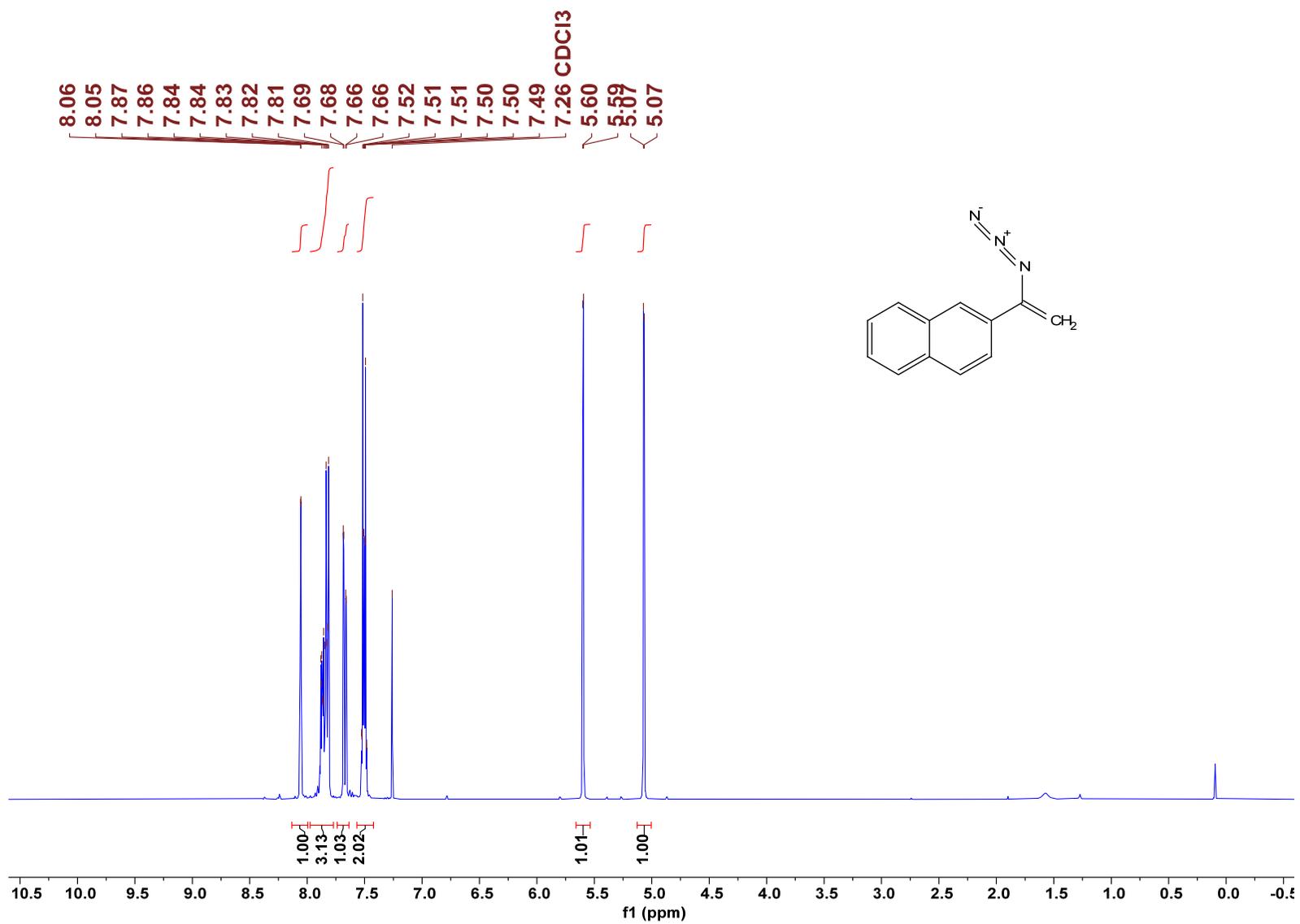


Figure S23: ¹H NMR spectrum of **1h** in CDCl₃ (400 MHz) PT206

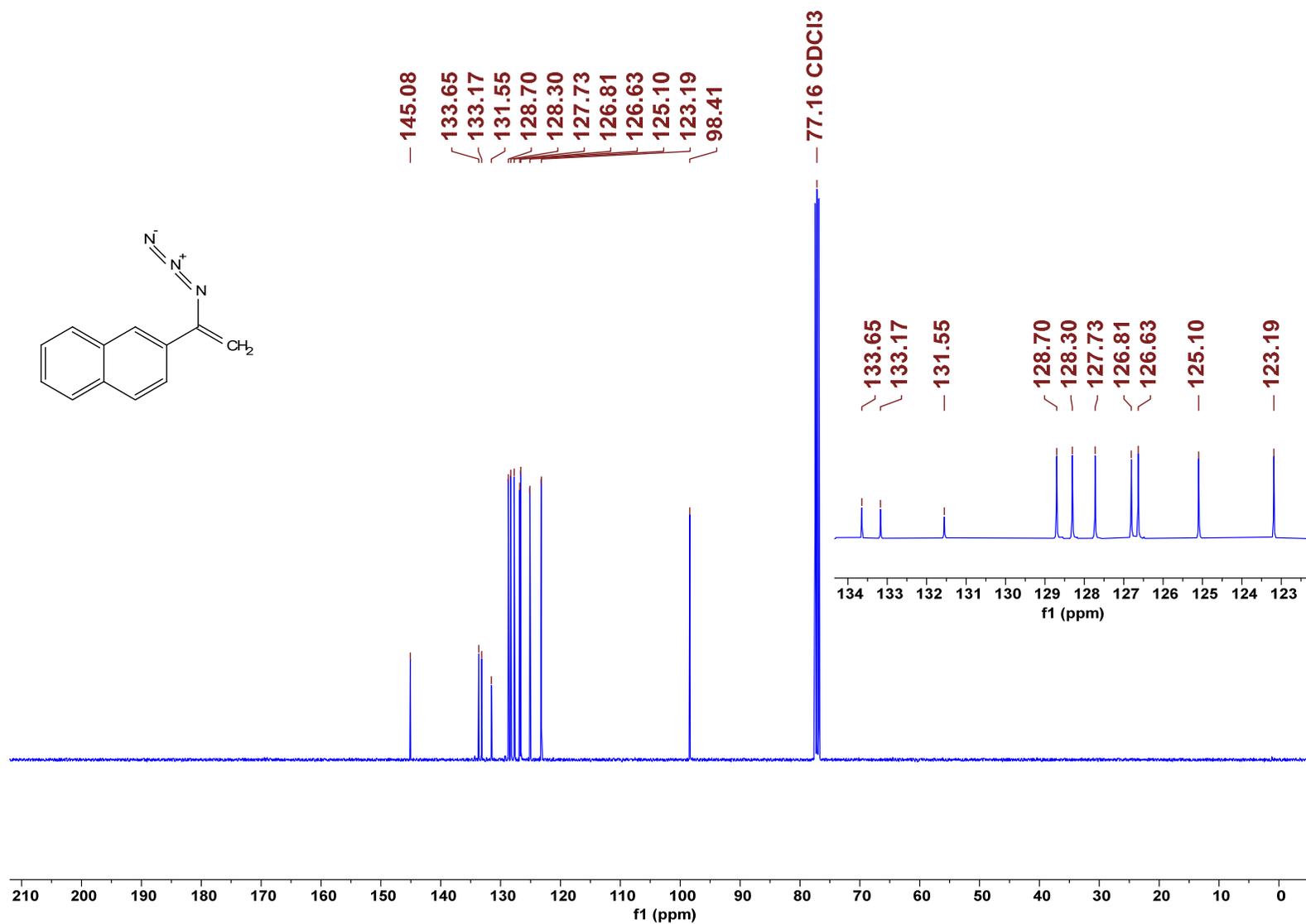


Figure S24: ¹³C NMR spectrum of **1h** in CDCl₃ (101 MHz) PT206

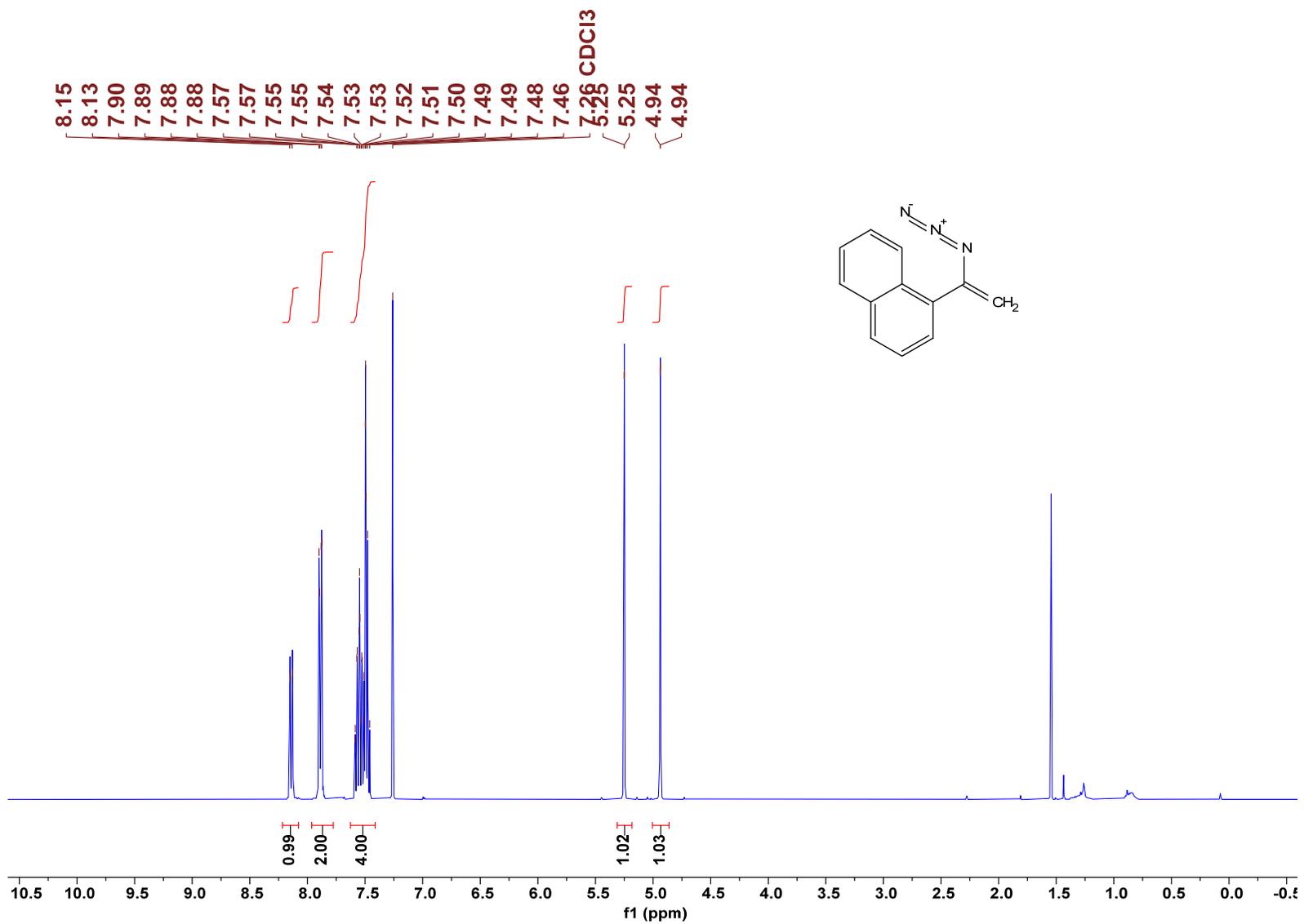


Figure S25: ¹H NMR spectrum of **1i** in CDCl₃ (400 MHz) CG743

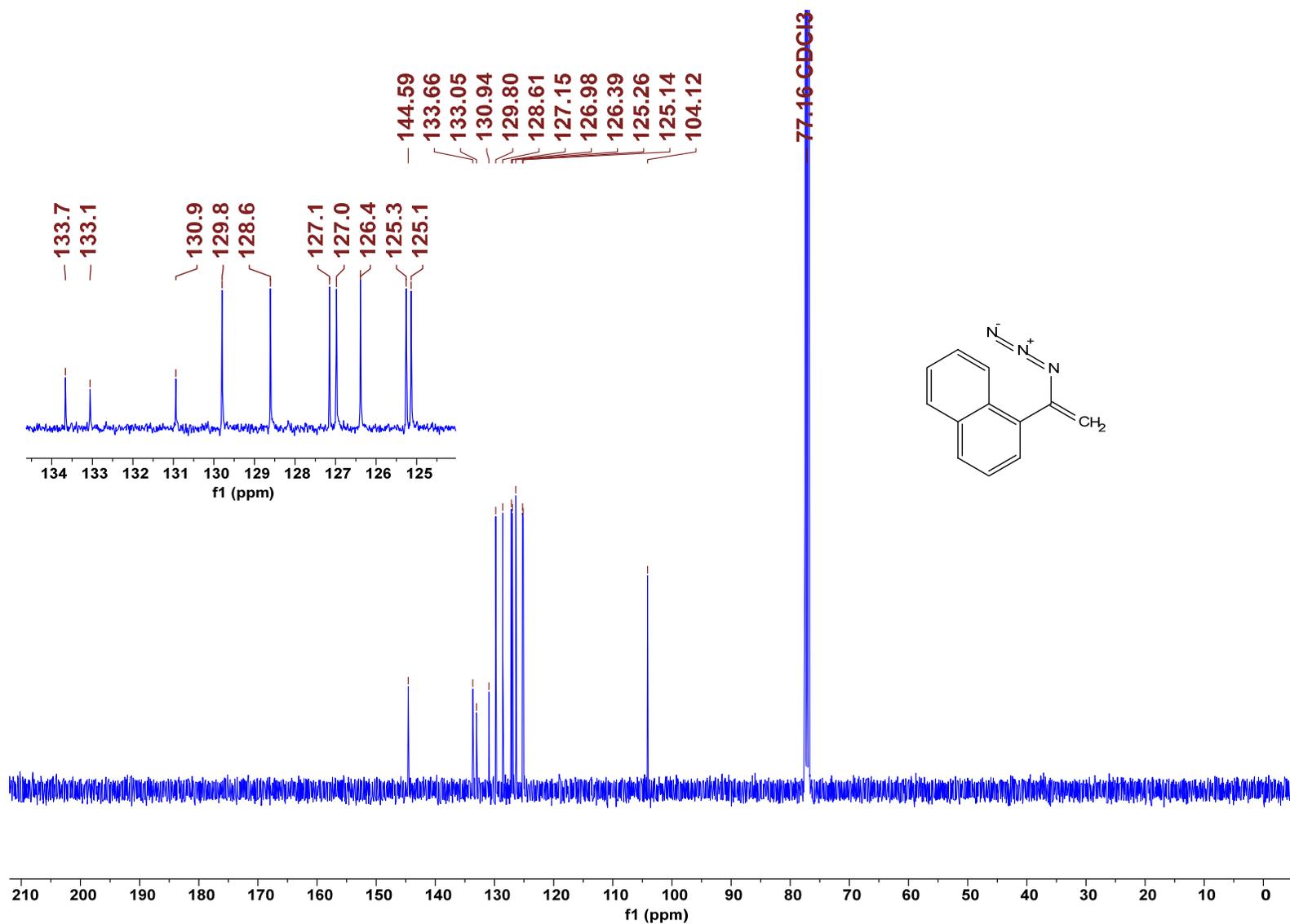


Figure S26: ^{13}C NMR spectrum of **1i** in CDCl_3 (101 MHz) CG743

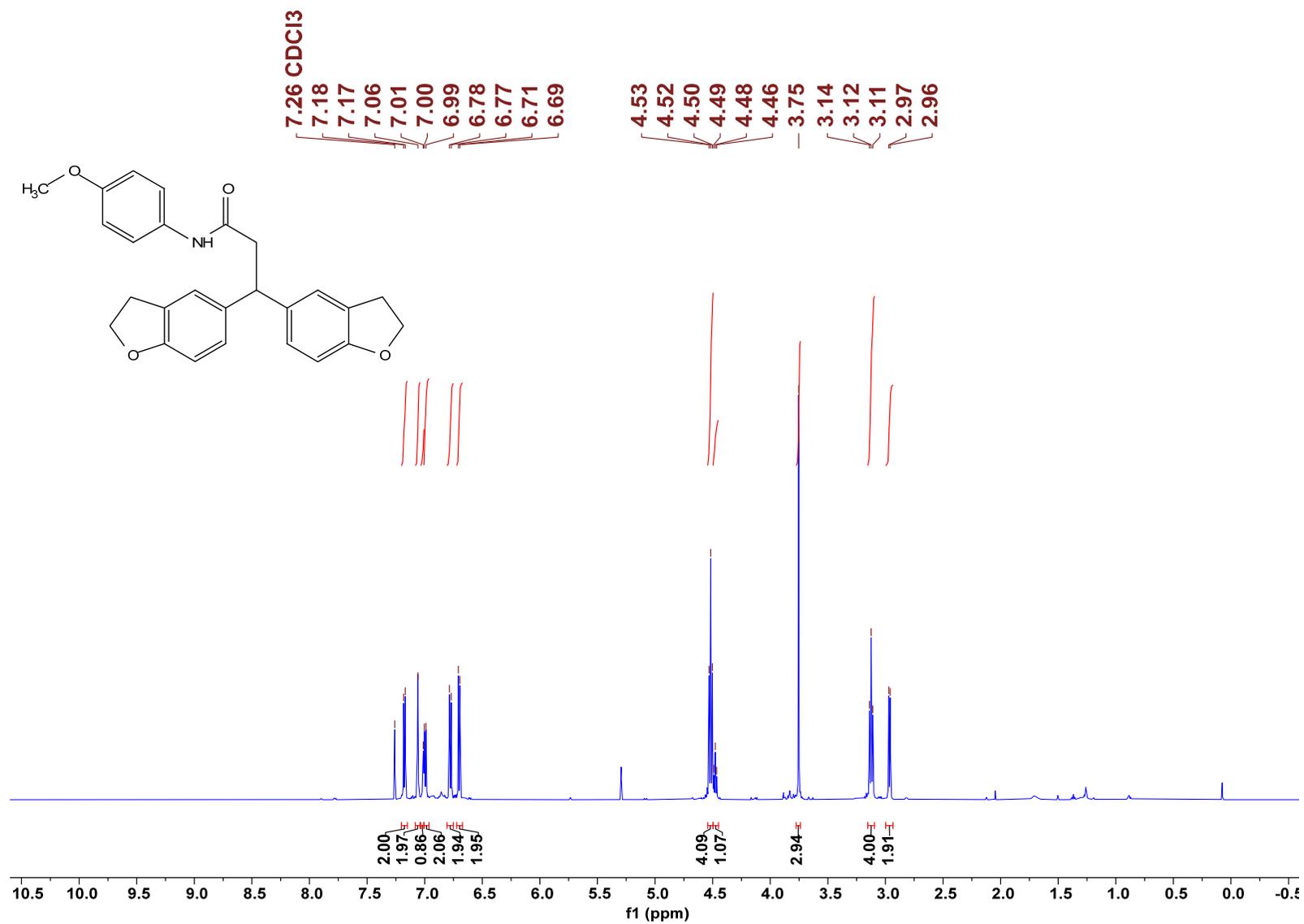


Figure S27: ^1H NMR spectrum of **3a** in CDCl_3 (600 MHz) CG718F1

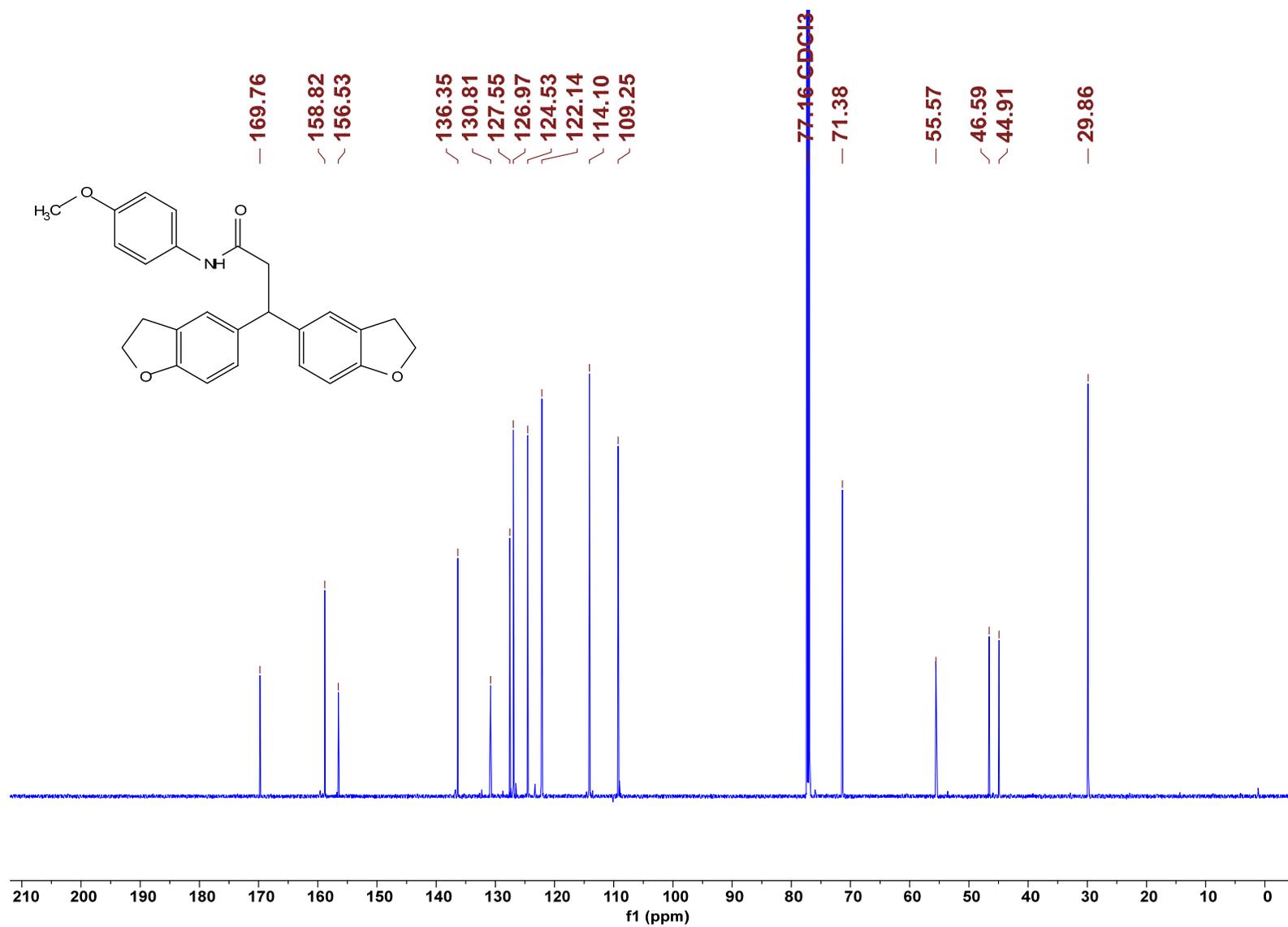


Figure S28: ¹³C NMR spectrum of **3a** in CDCl₃ (151 MHz) CG718F1

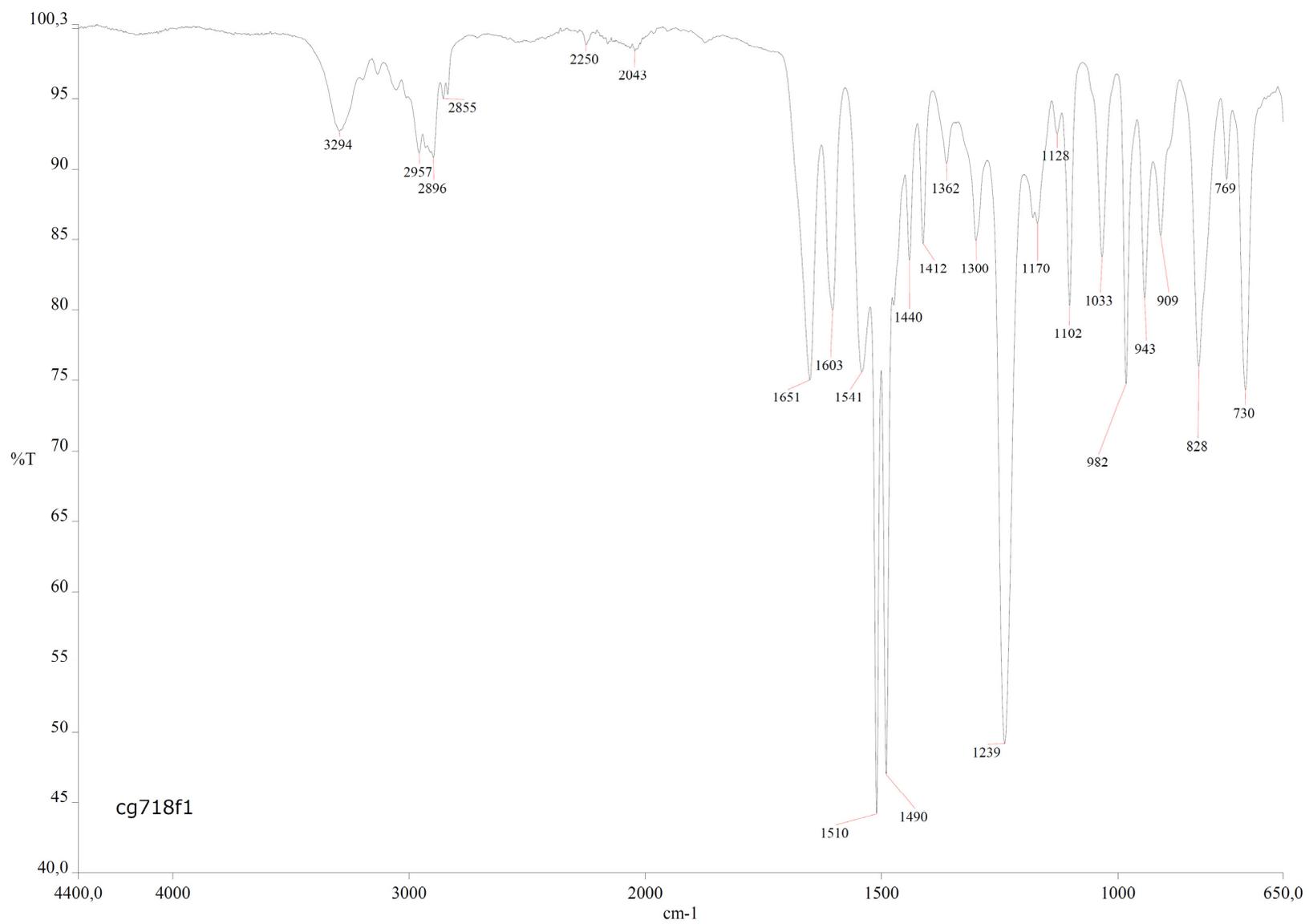


Figure S29: IR spectrum of 3a (neat, ATR probe) CG718F1

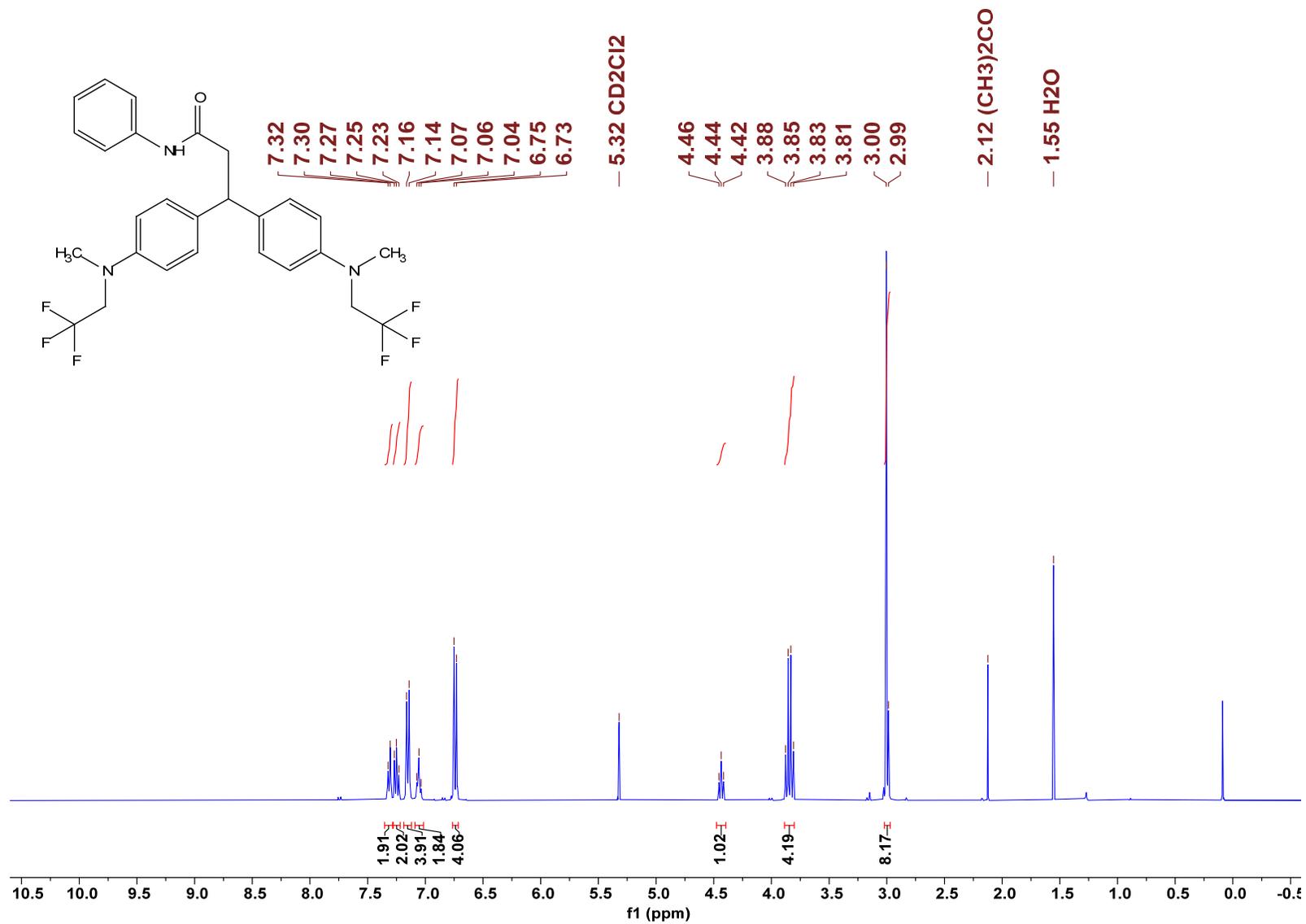


Figure S30: ^1H NMR spectrum of **3b** in CD_2Cl_2 (400 MHz) CG734_1

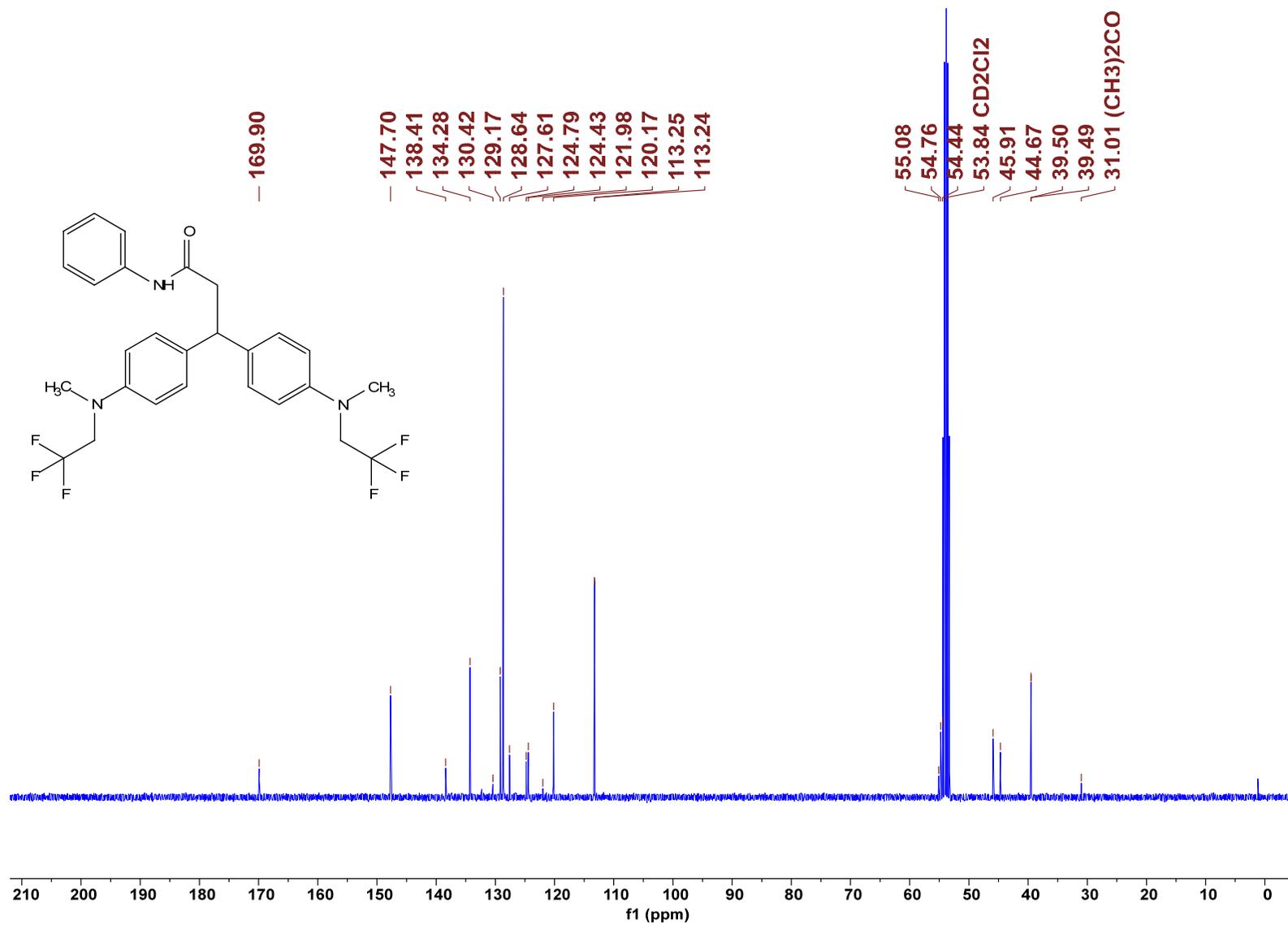


Figure S31: ^{13}C NMR spectrum of **3b** in CD_2Cl_2 (101 MHz) CG734_1

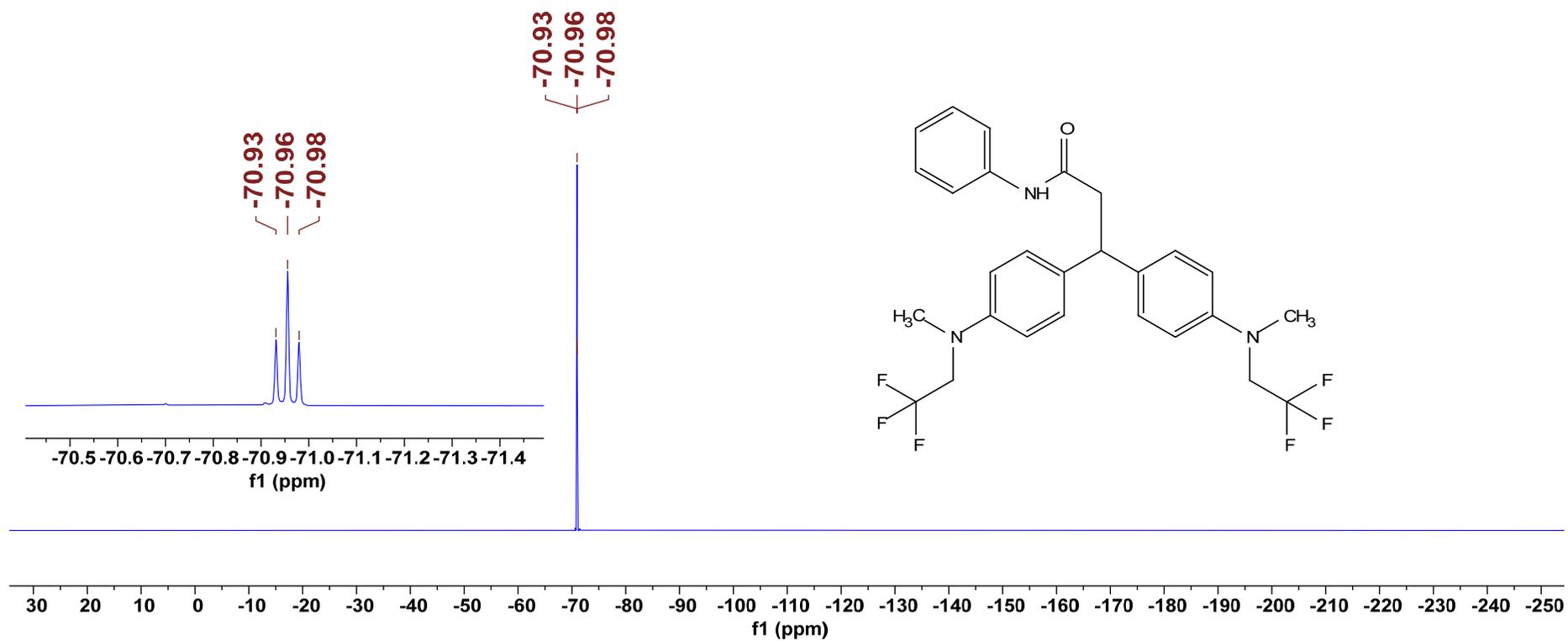


Figure S32: ^{19}F NMR spectrum of **3b** in CD_2Cl_2 (376 MHz) CG734_1

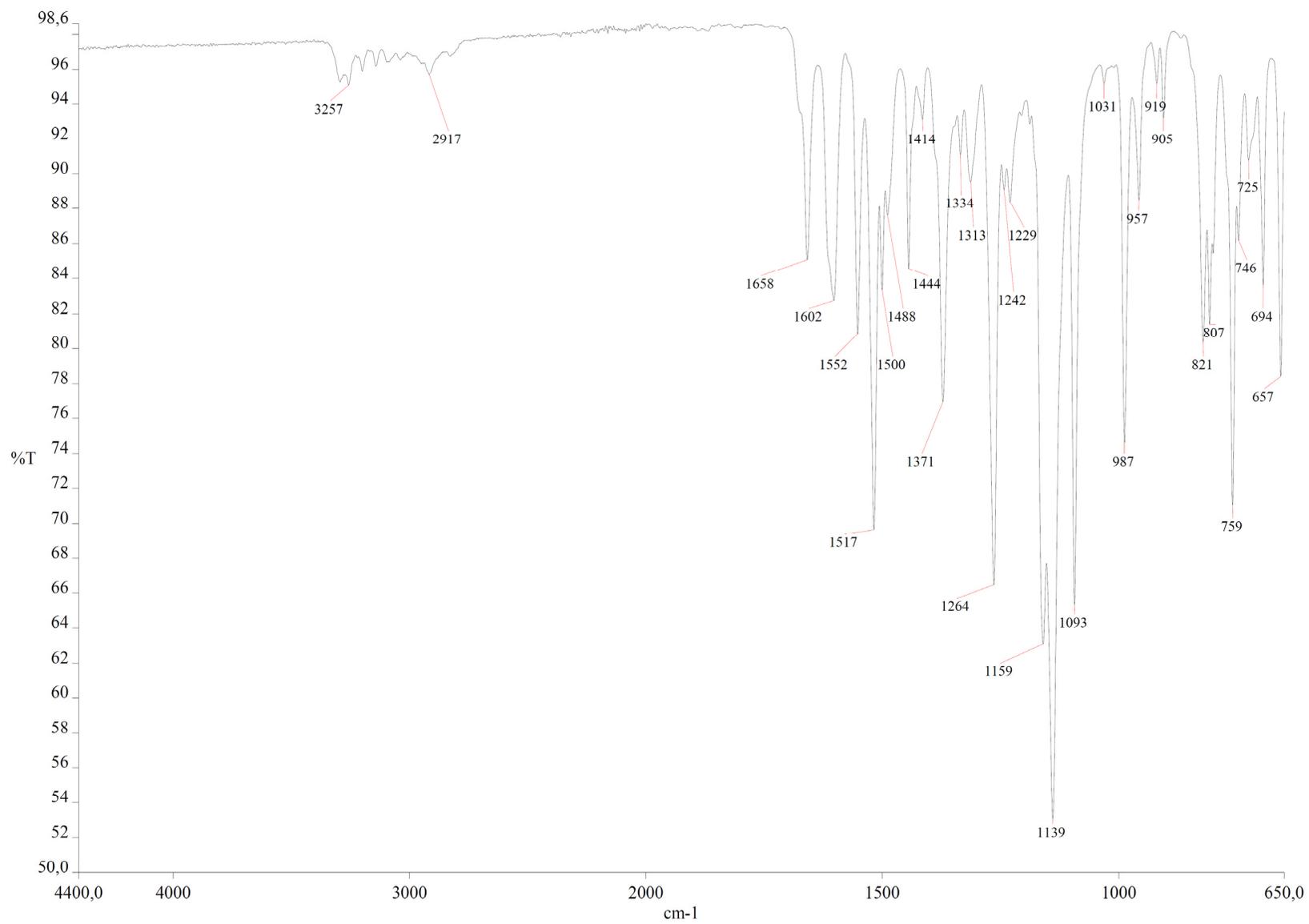


Figure S33: IR spectrum of **3b** (neat, ATR probe) CG734_1

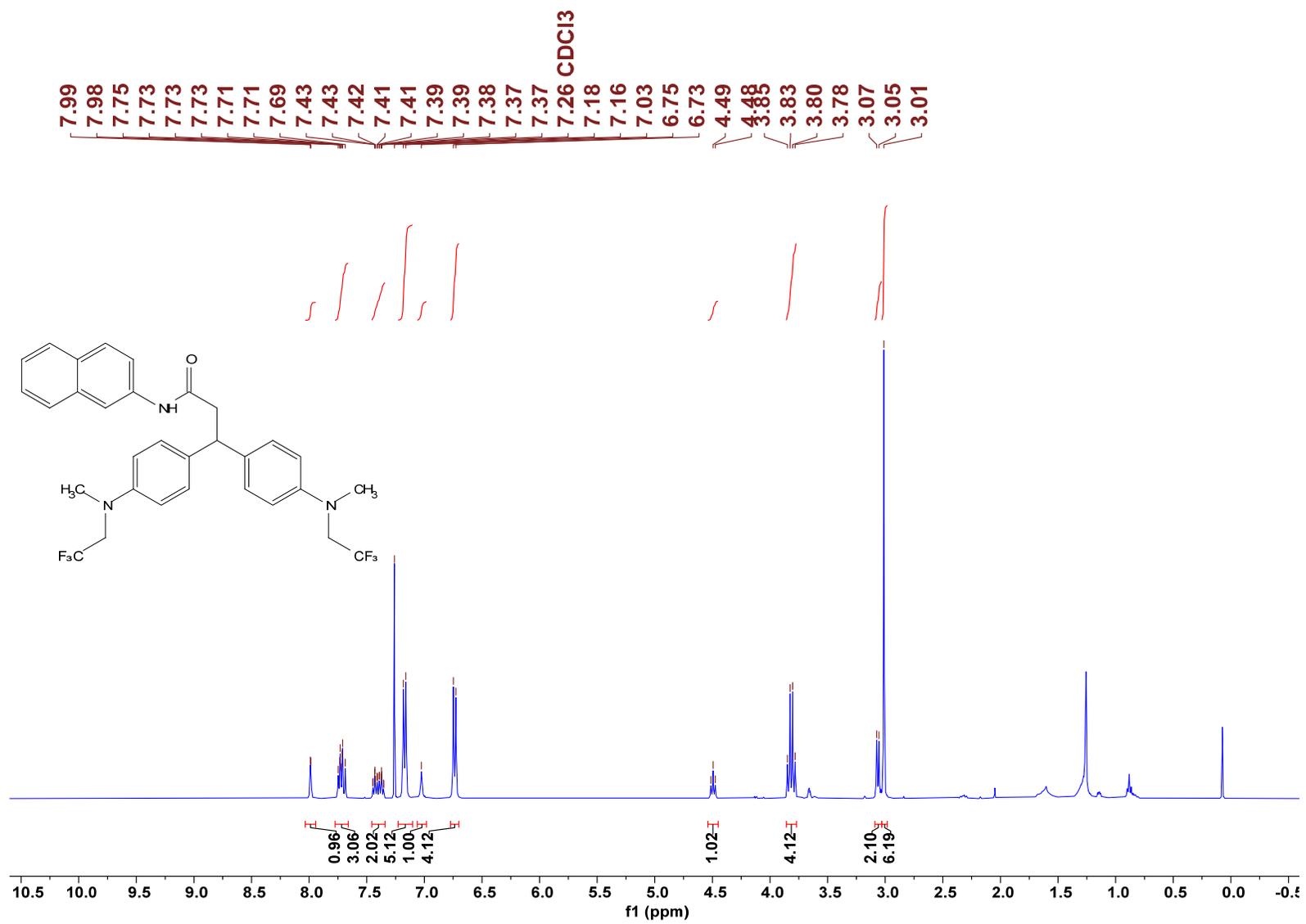


Figure S34: ¹H NMR spectrum of **3c** in CDCl₃ (400 MHz) PT-337

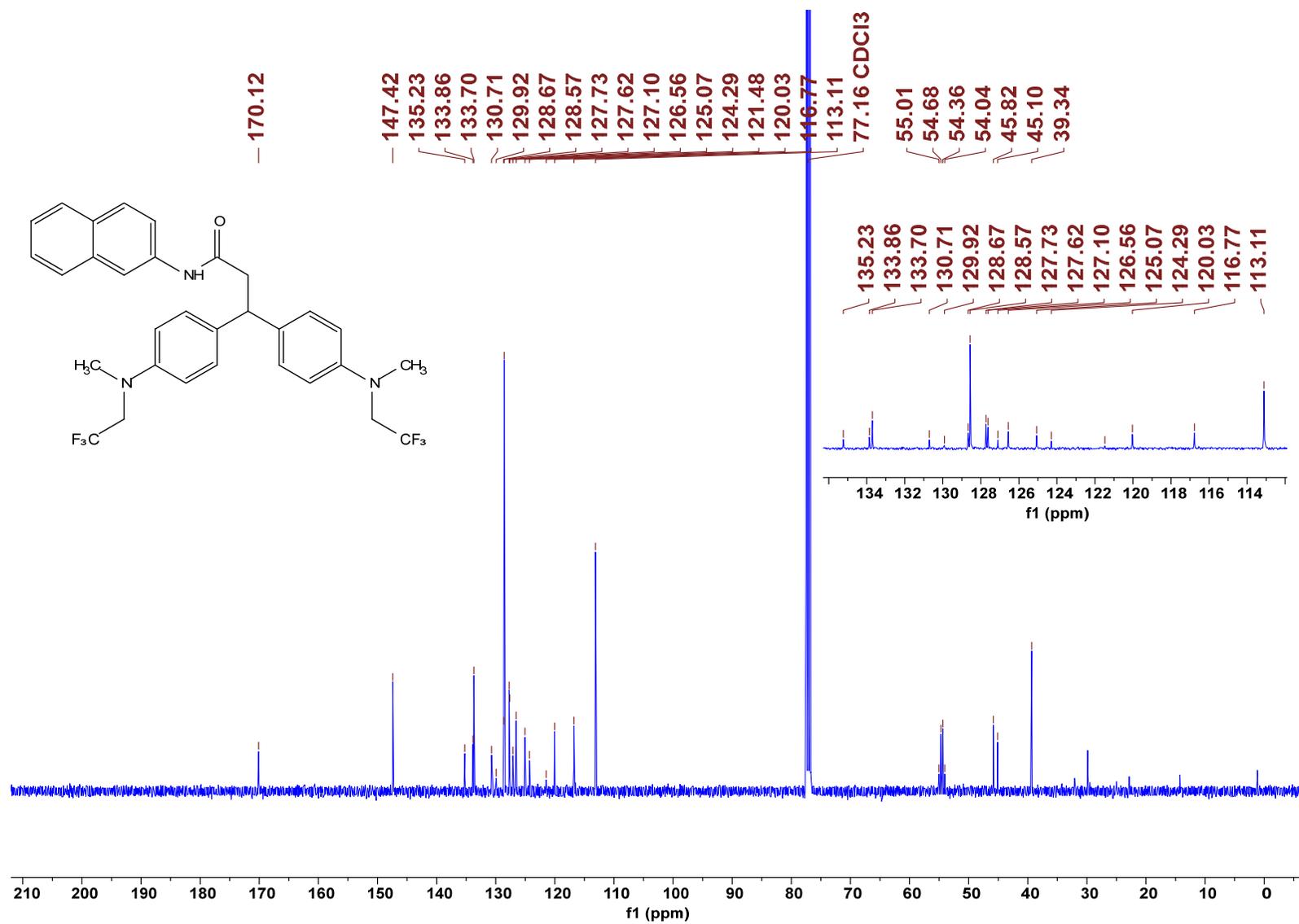


Figure S35: ¹³C NMR spectrum of **3c** in CDCl₃ (101 MHz) PT337

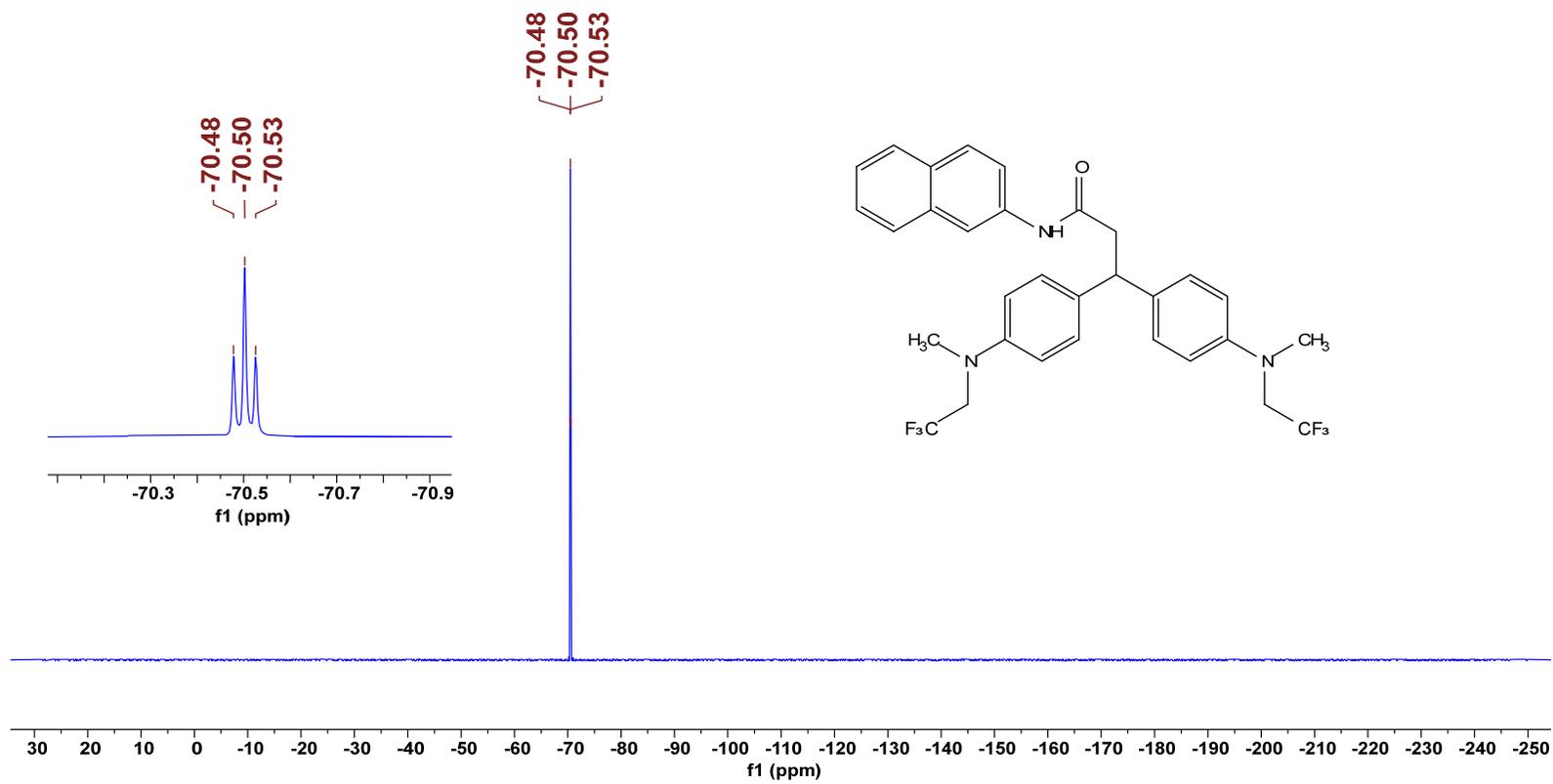


Figure S36: ^{19}F NMR spectrum of **3c** in CD_2Cl_2 (376 MHz) PT337

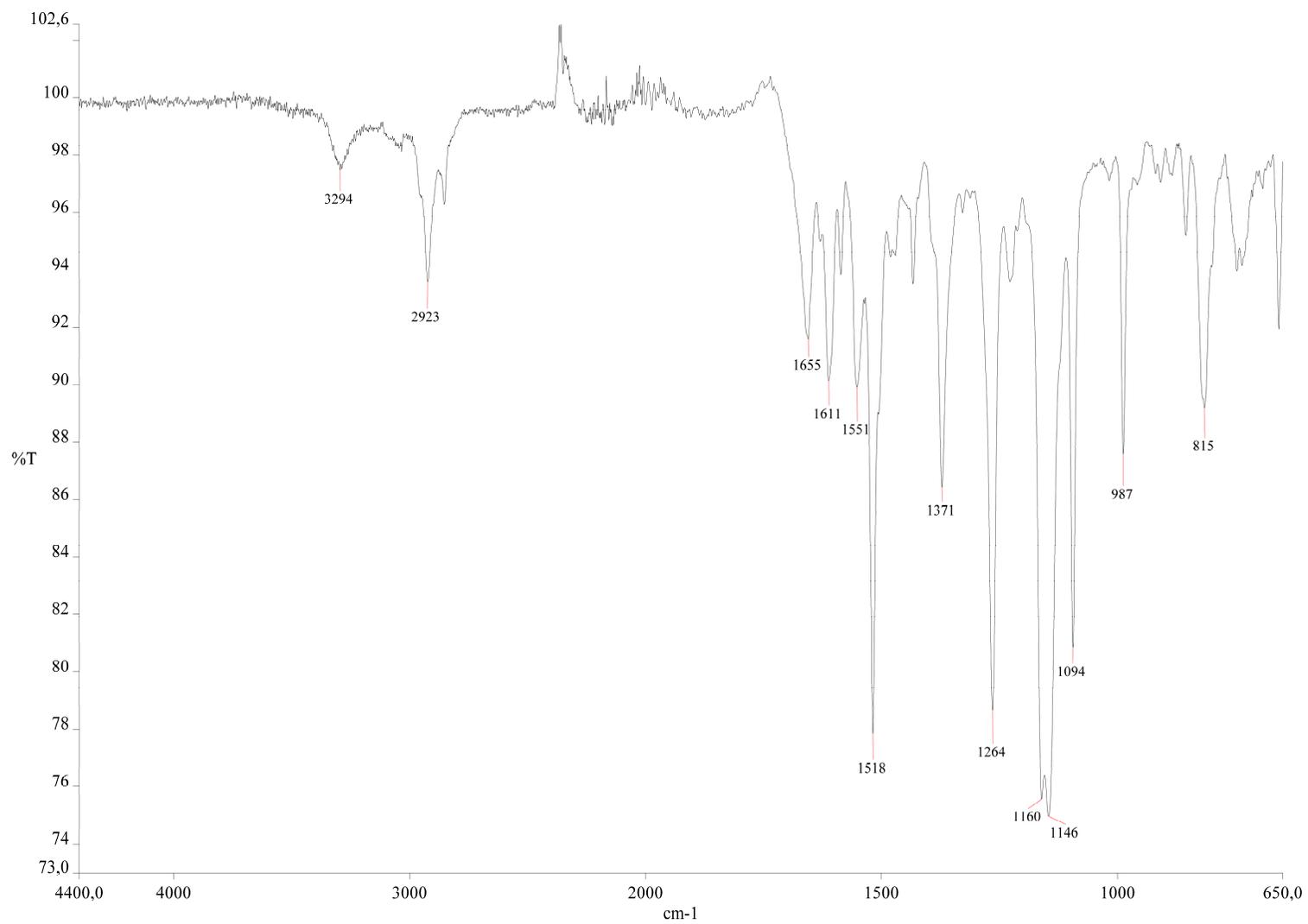


Figure S37: IR spectrum of **3c** (neat, ATR probe) PT337

7. Quantum-Chemical Calculations

7.1 Methods

Quantum chemical calculations were performed using the ORCA 6.0.1 program package.⁵⁷ For all calculations very tight SCF convergence settings (keyword "VERYTIGHTSCF") were used and the integration grid was adjusted with the keyword "DEFGRID3." All other settings were kept to default. Solvation effects were considered by applying the implicit solvation model SMD.⁵⁸ Geometries were optimized using the meta-generalized-gradient approximation r²SCAN-3c.⁵⁹ The nature of the stationary points was verified via frequency calculations. Conformational space was explored using the GOAT algorithm⁵¹⁰ utilizing GFN2-xTB.⁵¹¹ Molecular structures and molecular orbitals were visualized using ChimeraX 1.9.⁵¹²

7.2 FMO Plots

HOMO (-1, -2) and LUMO (+1, +2) of VA **1d** and styrene (**N9**) are shown in Table S3. The higher HOMO energy of **1d** compared to **N9** indicates a higher reactivity of VAs toward electrophiles. However, the lower LUMO energy of **1d** relative to **N9** also suggests a higher reactivity of VAs toward nucleophiles

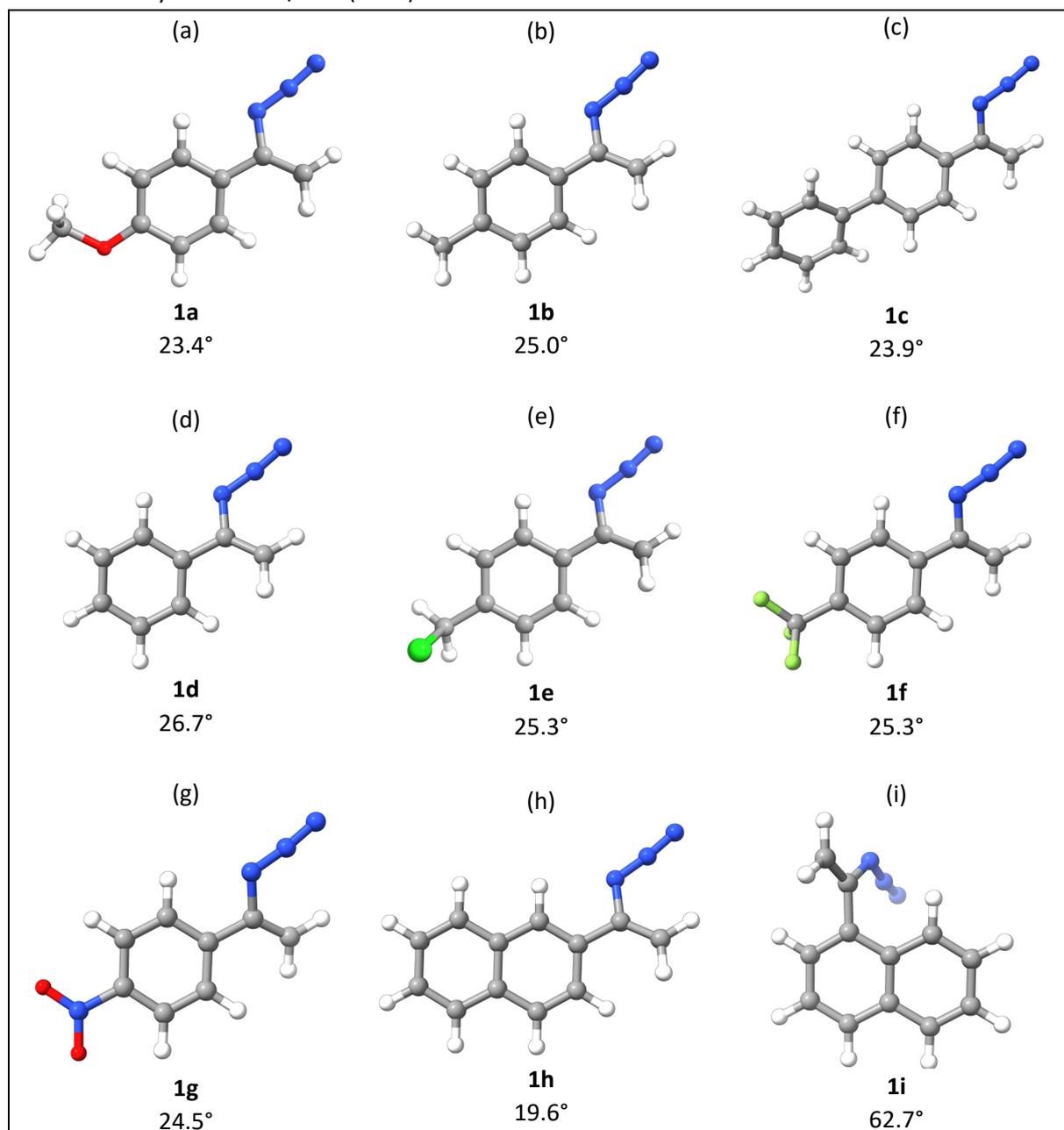
Table S3: HOMO (-1, -2) and LUMO (+1, +2) and orbital energies for (1-azidovinyl)benzene (**1d**) and styrene (**N9**). Level of Theory: r²SCAN-3c/SMD(DCM).

Orbital	Visualized Orbital of 1d	Orbital Energy (eV)	Visualized Orbital of N9	Orbital Energy (eV)
LUMO+2		-1.0515		0.5812
LUMO+1		-1.8793		-0.9663
LUMO		-2.0922		-1.8218
HOMO		-5.7745		-5.8166
HOMO-1		-6.6307		-6.5580
HOMO-2		-6.7666		-7.7676

7.3 Molecular Structures

Table S4 gathers the computed molecular structures of the considered VAs. The naphth-1-yl VA **1i** shows a twist of the vinylic π -system out of the plane of the aromatic system, while for the other VAs the vinylic π -system lies in the plane of the aromatic system, which is also reflected in the dihedral angles. This geometrical property of **1i** indicates unfavorable *peri*-interactions.

Table S4: Computed molecular structures of the considered VAs: (a) **1a**, (b) **1b**, (c) **1c**, (d) **1d**, (e) **1e**, (f) **1f**, (g) **1g**, (h) **1h** and (i) **1i** together with the dihedral angle of the aryl and the vinyl group (C-C-C-C). Level of Theory: r²SCAN-3c/SMD(DCM).



7.4 Regioselectivity of VAs

To investigate whether different regioselectivities are also of importance, we computed different regioisomeric adducts of the reaction of **1d** with the benzhydrylium ion **2c** (Table S5). N_3 could not be optimized as a stationary point, as the optimization led to the corresponding reaction complex. Differences in Gibbs free reaction energies ($\Delta\Delta G_{\text{add}}$) between the different positions clearly show a strong preference for nucleophilic attack at the vinyl group rather than at the azide moiety.

Table S5: Regioisomers of **1d** + **2c** adducts and their difference in reaction energy ($\Delta\Delta G_{\text{add}}$).

$E =$ **2c**

Structure			
Token	C_1	N_1	N_3
$\Delta\Delta G_{\text{add}}$ (kJ mol ⁻¹)	0.0	+87.6	–

7.5 Computed Reaction Barriers

Figure S38a shows the reaction of **1d** with benzhydrylium ions **2c-2g** and Fig. S38b shows the corresponding linear correlation between computed ($\Delta G_{\text{calc}}^{\ddagger}$) and experimentally observed ($\Delta G_{\text{exp}}^{\ddagger}$) reaction barriers. $\Delta G_{\text{calc}}^{\ddagger}$ and $\Delta G_{\text{exp}}^{\ddagger}$ correlate strongly, indicating that the determined second-order rate constants k_2 reflect the C–C bond-formation process. Computed $\Delta G_{\text{calc}}^{\ddagger}$ and $\Delta G_{\text{exp}}^{\ddagger}$ values are given in Table S6.

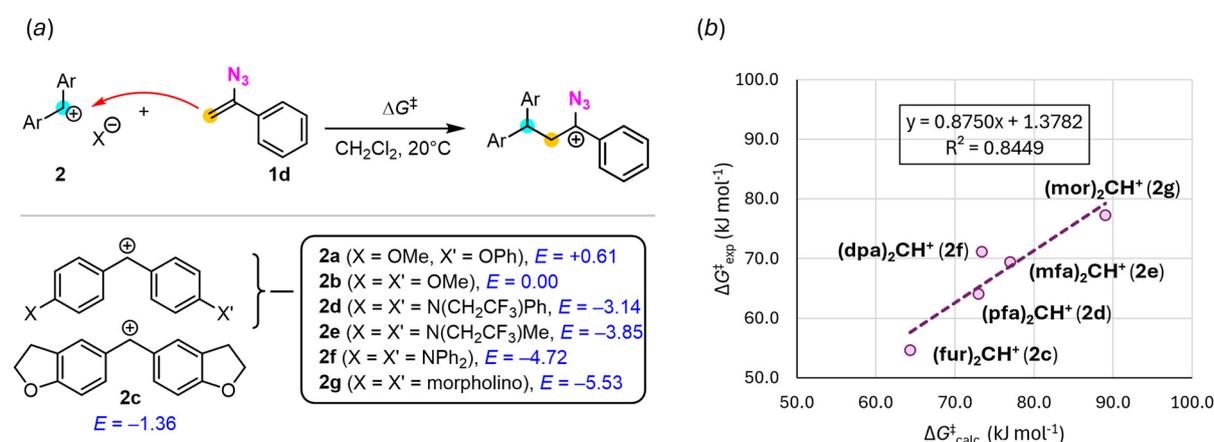


Figure S38: (a) Reaction of **1d** with benzhydrylium ions **2c-2g** and nomenclature of **2**. (b) Linear correlation of DFT-calculated ($\Delta G_{\text{calc}}^{\ddagger}$) and experimentally observed ($\Delta G_{\text{exp}}^{\ddagger}$) reaction barriers. Level of Theory: r²SCAN-3c/SMD(DCM).

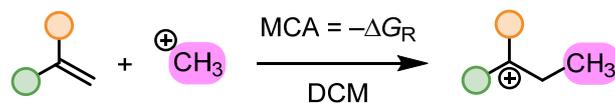
Table S6: DFT calculated ($\Delta G_{\text{calc}}^{\ddagger}$) and experimentally observed ($\Delta G_{\text{exp}}^{\ddagger}$) Gibbs activation barriers for **1d** reacting with benzhydrylium ions **2**. Level of Theory: r²SCAN-3c/SMD(DCM).

Electrophile	$\Delta G_{\text{calc}}^{\ddagger}$ (kJ mol ⁻¹) ^a	$\Delta G_{\text{exp}}^{\ddagger}$ (kJ mol ⁻¹) ^b
2c	+64.3	+54.6
2d	+73.0	+64.1
2e	+77.0	+69.4
2f	+73.4	+71.1
2g	+89.0	+77.3

^a Calculated at 298 K. ^b Calculated from k_2 (20 °C) by using the Eyring equation.

7.6 Methyl Cation Affinities (MCA)

Methyl cation affinities (MCA) for VAs and other α -activated styrene-type π -nucleophiles were computed using the negative Gibbs free energies (ΔG_{R}) of the addition of a methyl cation to the considered double bond as shown in Scheme S1.



Scheme S1. Reaction scheme for the calculation of methyl cation affinities (MCA) in dichloromethane.

Table S7 summarizes the computed MCA values of the considered vinyl azides. Table S8 contains the results of MCA calculations for the π -systems **N1-N15** and their reported nucleophilicity parameters N (and s_{N}).

Table S7: Computed MCA values of vinyl azides **1a-1i**. Level of theory: r²SCAN-3c/SMD(DCM).

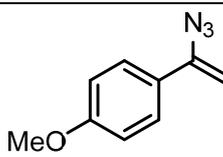
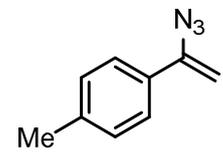
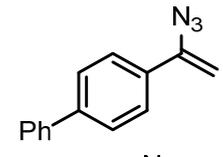
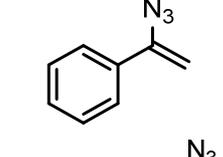
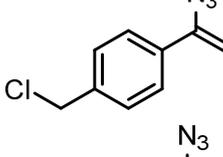
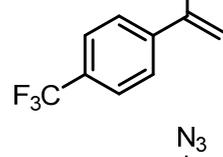
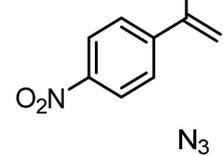
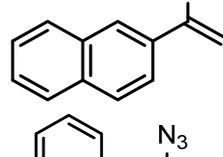
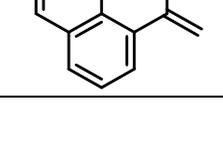
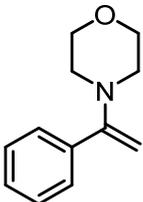
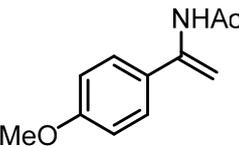
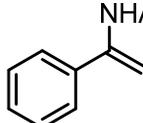
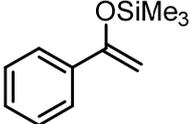
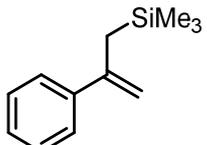
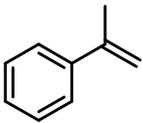
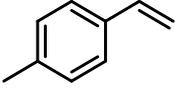
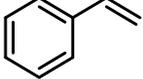
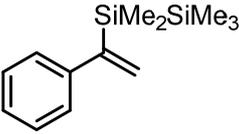
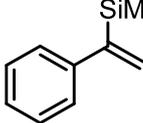
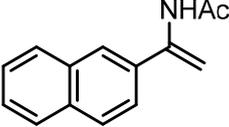
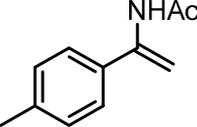
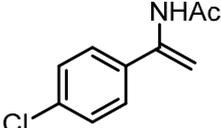
Vinyl azides	MCA (kJ mol ⁻¹)
1a 	365.6
1b 	348.2
1c 	346.3
1d 	336.4
1e 	332.5
1f 	318.2
1g 	308.8
1h 	343.3
1i 	331.9

Table S8: Computed MCA values (this work) and reported, experimentally determined N and s_N parameters (from ref. 12, main text) of α -substituted styrenes **N1-N15**. Level of theory: r^2 SCAN-3c/SMD(DCM).

Nucleophiles		MCA (kJ mol ⁻¹)	N	s_N
	N1	420.3	9.96	0.79
	N2	376.2	7.06	0.85
	N4	354.8	5.73	0.97
	N3	367.8	6.22	0.96
	N5	354.2	5.38	0.89
	N6	406.9	4.80	0.86
	N7	315.0	2.35	1.00
	N8	309.3	1.70	1.06
	N9	291.5	0.78	0.95
	N10	310.9	0.61	1.01
	N11	302.5	-0.65	1.59
	N12	285.9	-1.13	1.46

	N13	360.5	6.28	0.95
	N14	364.1	6.57	0.91
	N15	351.4	5.60	1.00

7.7 Computed Properties

Table S9: Computed energies of benzhydrylium ions **2c-2g**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_h . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
2c	-806.956726274622	-806.66328694	0.23526669	-806.72145958
2d	-1827.12814648430	-1826.63754796	0.39985187	-1826.72829462
2e	-1443.71917607140	-1443.33891583	0.30243130	-1443.41674477
2f	-1536.43239327891	-1535.84768131	0.49557812	-1535.93681516
2g	-1074.82682841192	-1074.37737221	0.37970984	-1074.44711857

Table S10: Computed energies of transition states (TS) for the benzhydrylium ions **2c-2g** with **1d**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_h . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
TS_1d_2c	-1280.102064705639	-1279.66134989	0.36396446	-1279.73810025
TS_1d_2d	-1916.858695332760	-1916.33123768	0.43027332	-1916.42842202
TS_1d_2e	-1916.858695332760	-1916.33123768	0.43027332	-1916.42842202
TS_1d_2f	-2009.572023653569	-2008.84037257	0.62204162	-2008.94998203
TS_1d_2g	-1547.962398585037	-1547.36534214	0.50807821	-1547.45432037

Table S11: Computed energies of H_3C^+ . E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_{h} . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
H_3C^+	-39.574658666589	-39.53942581	0.01235094	-39.56230773

Table S12: Computed energies of vinyl azides **1a-1i**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_{h} . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
1a	-587.650874641607	-587.47009640	0.13094500	-587.51992964
1b	-512.448278665314	-512.27345796	0.12662630	-512.32165236
1c	-704.154143290213	-703.92292519	0.17660291	-703.97754038
1d	-473.142792090684	-472.99679636	0.10167646	-473.04111563
1e	-972.031437781395	-971.86384010	0.11678973	-971.91464805
1f	-810.198944363616	-810.04509558	0.10091613	-810.09802824
1g	-677.642691518212	-677.49180105	0.10063225	-677.54205927
1h	-626.758946100206	-626.56399532	0.14469936	-626.61424674
1i	-626.755946242750	-626.56087566	0.14518332	-626.61076292

Table S13: Computed energies of methylated vinyl azides **1a-1i**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_{h} . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
1a_H₃C⁺	-627.391719612699	-627.16810016	0.17024554	-627.22147408
1b_H₃C⁺	-552.182164793747	-551.96492558	0.16557331	-552.01659149
1c_H₃C⁺	-743.887629312960	-743.61373934	0.21587018	-743.67175913
1d_H₃C⁺	-512.872074447022	-512.68354816	0.14053809	-512.73153635
1e_H₃C⁺	-1011.75945086348	-1011.54926774	0.15584612	-1011.60360474
1f_H₃C⁺	-849.921622807817	-849.72523699	0.14009967	-849.78152314
1g_H₃C⁺	-717.360876046275	-717.16768223	0.13919218	-717.22168387
1h_H₃C⁺	-666.491149736670	-666.25363832	0.18383260	-666.30731714
1i_H₃C⁺	-666.484032792809	-666.24622611	0.18455550	-666.29947729

Table S14: Computed energies of α -substituted styrenes **N1-N15**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_{h} . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
N1	-596.121888031803	-595.86203710	0.21005796	-595.91183007
N2	-632.077546443080	-631.84344881	0.17993534	-631.89761111
N3	-793.456452768669	-793.20302214	0.19587136	-793.26058141

N4	-517.570100723934	-517.37054573	0.15099383	-517.41910690
N5	-757.500648805408	-757.22365454	0.21955796	-757.28109085
N6	-1332.57245329095	-1332.18969524	0.30596708	-1332.26648621
N7	-348.878449634311	-348.70902506	0.12820337	-348.75024626
N8	-348.879818110207	-348.71064096	0.12683053	-348.75298758
N9	-309.574591811819	-309.43425195	0.10178327	-309.47280854
N10	-1087.49708781275	-1087.16854665	0.26099526	-1087.23609255
N11	-757.497746742625	-757.22082579	0.21820370	-757.27954305
N12	-718.192823337655	-717.94468395	0.19347266	-717.99935068
N13	-671.185937282524	-670.93736328	0.19432313	-670.99161415
N14	-556.875429957053	-556.64698473	0.17612131	-556.69930864
N15	-977.153702373803	-976.96258555	0.13944038	-977.01426199

Table S15: Computed energies of methylated **N1-N15**. E_{tot} refers to the total energy, H to the sum of electronic and thermal enthalpies, G_{corr} to thermal correction to Gibbs free energy and G to sum of electronic and thermal free energies. All energies are given in E_h . Level of theory: $r^2\text{SCAN-3c/SMD(DCM)}$.

Name	E_{tot}	H	G_{corr}	G
N1_H₃C⁺	-635.884668586966	-635.58086283	0.25046246	-635.63420613
N2_H₃C⁺	-671.822847366410	-671.54593086	0.21963076	-671.60321661
N3_H₃C⁺	-833.199156899839	-832.90264103	0.23619109	-832.96296581
N4_H₃C⁺	-557.306965938885	-557.06484531	0.19041546	-557.11655048
N5_H₃C⁺	-797.237089842045	-796.91735872	0.25876983	-796.97832001
N6_H₃C⁺	-1372.33170890852	-1371.90482421	0.34793597	-1371.98377294
N7_H₃C⁺	-388.598303236470	-388.38711275	0.16575540	-388.43254784
N8_H₃C⁺	-388.597488404622	-388.38667983	0.16440268	-388.43308573
N9_H₃C⁺	-1127.217488843060	-1126.84643756	0.30068858	-1126.91680026
N10_H₃C⁺	-718.192823337655	-717.94468395	0.19347266	-717.99935068
N11_H₃C⁺	-797.214166516374	-796.89491278	0.25708291	-796.95708360
N12_H₃C⁺	-757.902675187250	-757.61221728	0.23213723	-757.67053796
N13_H₃C⁺	-710.924591953560	-710.63366764	0.23337834	-710.69121362
N14_H₃C⁺	-596.615497677048	-596.34458399	0.21519737	-596.40030030
N15_H₃C⁺	-1016.889088086540	-1016.65549708	0.17866937	-1016.71041872

7.8 XYZ Coordinates

Vinyl Azides

1a	C	1.65488853146125	-1.64795919014219	-4.43985868322553	H	3.48487969719507	-1.54834320063055	-4.28983888196741
	C	0.63349651430909	-0.88476073506579	-5.02423255032728	C	0.40299270397099	0.77693340466844	-4.23841938517589
	C	2.74888466520270	-1.02648813433412	-3.86962794587646	C	2.72045863044913	0.36932627559118	-3.65181053171638
	H	3.51240317778098	-1.63920449955849	-3.39957336166569	H	-0.455191073350762	1.44313502055119	-4.22788683157223
	C	0.72543803368314	0.50954651839264	-5.01838361220643	H	1.58080351286656	1.18380624069791	-3.62719810412621
	C	2.86816400334322	0.37408865869100	-3.86734618343827	H	1.62070289928186	2.15457405143808	-3.14310092488475
	H	-0.04903104152806	1.12760131183347	-5.45799625208065	H	1.41218637012178	-2.25811419752764	-5.36851688612937
	C	1.83425135480405	1.12135867897206	-4.44061542154405	C	3.98083892155946	0.81025407551306	-3.02507577442574
	H	1.89453066856099	2.20530099142847	-4.45192741560650	C	5.20491631114610	0.37328485449490	-3.35851491343644
	H	1.56386665509676	-2.73032078239210	-4.42973694289484	H	5.33248144272398	-0.33783226779392	-4.16571005060331
	C	4.05234473364940	1.03101364953006	-3.28780399909041	H	6.10024769901806	0.72013968303304	-2.85081695486600
	C	5.26064329887957	0.46622803435945	-3.13322587982473	N	3.75100366176980	1.78656968186538	-2.00629783630985
	H	5.44274964343200	-0.54357166675407	-3.48054084336951	N	4.72478086804112	2.29326232474259	-1.46298029929641
	H	6.09152715677726	0.99384942712625	-2.67437843345444	N	5.53992475366465	2.82973847462640	-0.88708716275060
	N	3.77158805713545	2.38050779489861	-2.90117384076963	C	-0.93988018240992	-0.89353361105335	-5.53832256351192
	N	4.69595210575425	3.06608292701802	-2.48328233472279	C	-0.91623289078654	-1.63190926781089	-6.73074047004708
	N	5.46380260943579	3.79539491960797	-2.07938356189524	C	-2.18420189322252	-0.57601891974789	-4.97395837681152
	O	-0.39718104207617	-1.58869552418814	-5.55572079565828	C	-2.09942725950092	-2.03843486958307	-7.33827316373196
	C	-1.46974869569847	-0.85189763555630	-6.15833420215126	C	-3.36579640118485	-0.98557567631303	-5.58243122022961
	H	-1.11239960037527	-0.25446913658157	-7.00613038586964	C	-3.32936999401183	-1.71791738286945	-6.76728306482263
	H	-2.17831304914834	-1.60129000296244	-6.51556753290405	H	0.03539130085056	-1.86904699097240	-7.19894491998719
	H	-1.96445233559993	-0.20191585807945	-5.42610003919286	H	-2.22620213099057	-0.02509342939439	-4.03819652951783
					H	-2.066038150317212	-2.60160709360726	-8.26690347445286
					H	-4.31964596887082	-0.73800596702289	-5.12424198636804
					H	-4.25305543994542	-2.03684700449325	-7.24231792646920
					1d			
					C	0.35645545019085	0.03627597857644	-3.97525248760211
					C	-0.81414088145828	-0.46106864781737	-3.40415686260171
					C	1.40040550557489	0.47273511590176	-3.16925966011578
					H	-1.63104119143590	-0.79685489019207	-4.03693039635448
					H	2.29488901493646	0.88482581121626	-3.62702712208571
					C	-0.93327677563224	-0.51389624646242	-2.01803687009297
					C	1.29400292589670	0.41071154587661	-1.77273411944915
					H	-1.84240393466916	-0.89707970654833	-1.56279841290783
					C	0.10937970374417	-0.07836920218318	-1.20634609890860
					H	0.00893127852734	-0.13028530907067	-0.12659867031711
					H	0.45206479092395	0.09768005018445	-5.05582820845474
					C	2.41557988823034	0.84545311113217	-0.91520347717706
					C	3.70777205457530	0.83334695189469	-1.27417364664078
					H	4.00139598215829	0.45740120671225	-2.24683073144053
					H	4.49656618273761	1.17802173378232	-0.61183584383229
					N	1.96229477265399	1.27599409625831	0.37024723625197
					N	2.80353832973780	1.59075405125488	1.20334906015873
					N	3.48076774242918	1.90886435104808	2.05422593571924
					1e			
					C	1.35709445727798	-0.15244909659731	-5.66188581871940
					C	0.29094024556454	-0.44412674263613	-4.80893832847726
					C	2.56930122805124	0.29451096579397	-5.15251536431165
					H	3.38675651496917	0.51440486131103	-5.83175542792833
					C	0.46326242374541	-0.27733474349591	-3.43085976462894
					C	2.74791830229386	0.45019393704492	-3.77141118256354
					H	-0.36430959281953	-0.48528465872250	-2.75692030735872
					C	1.67120020210059	0.16846378233539	-2.91786142207919
					H	1.76998249260101	0.32212198783027	-1.84765602357881
					H	1.23643003799796	-0.27545030117832	-6.73548472238718
1c	C	1.45722603728777	-1.27647277130560	-4.90507665551862				
	C	0.31631194991284	-0.45910272180768	-4.89216638133965				
	C	2.63380822541913	-0.87395216197497	-4.29384883826594				

C	4.04374860845699	0.89995351369750	-3.22482302541969
C	4.49165232488346	0.63474203554701	-1.98866107203524
H	3.90531858424054	0.02592100564620	-1.31124863160551
H	5.450331539315969	0.99875000646521	-1.63097291466849
N	4.78991604396874	1.65143674944272	-4.18420897673568
N	5.91803770857858	2.01817183054056	-3.87781645537790
N	6.96635192748836	2.41482913468351	-3.71290150335888
C	-1.00789402093392	-0.92264810616772	-5.35613835720928
H	-1.17002153129028	-0.60359853820778	-6.38659857166589
H	-1.85522322305861	-0.63966896101102	-4.72990027139845
Cl	-1.04874075327580	-2.78304117032159	-5.41143980249194

1f			
C	1.40821121040892	-0.19983634839608	-5.66319262405608
C	0.32976446552120	-0.46169240487944	-4.82231459739809
C	2.59686472567313	0.27988759138660	-5.12917481106601
H	3.43320419966956	0.48038940206640	-5.79044669035236
C	0.44089220059706	-0.24759220288491	-3.44789008234346
C	2.72689240981557	0.49353426685000	-3.75123602687033
H	-0.40243900689605	-0.43831818320139	-2.79146050989880
C	1.62867206417415	0.23276968837883	-2.91994084158185
H	1.69169930369802	0.42779244119596	-1.85427840522062
C	1.32675556487635	-0.36550353142904	-6.73266412771555
H	3.99997431310600	0.98323662402097	-3.18353869204005
C	4.40698212104212	0.77380759314967	-1.92323134619219
C	3.80265244872627	0.18891482444118	-1.24062698671758
H	5.35062138352246	1.16039575981166	-1.54951656261054
N	4.76696801729611	1.70033588990703	-4.15068093405672
N	5.88043859432217	2.09557008231137	-3.82506676254019
N	6.91763541893412	2.51366658975147	-3.64573086279175
C	-0.94420044018599	-1.01709940609671	-5.38382100002484
F	-0.97034630051598	-2.37917489084231	-5.33168906204608
F	-1.12986552859675	-0.68109965684671	-6.68158071769832
F	-2.03574833681486	-0.59075798840043	-4.70362209094300

1g			
C	-0.84649670912050	0.42527554002688	-5.05760508233141
C	-1.74901478534074	-0.38442359336949	-4.37800995544541
C	0.25979847170056	0.90824627234580	-4.37672400770301
H	0.97252301303274	1.53484220444140	-4.90175125174206
C	-1.57408650586254	-0.71582025793883	-3.03718507011428
C	0.47169416603773	0.58252771602510	-3.02890968023452
H	-2.30168854321167	-1.33488271515738	-2.52583498340928
C	-0.46658321881680	-0.22560261168786	-2.36828167284785
H	-0.34407516280567	-0.45701013936497	-1.31553733665490
C	-1.00548947407734	0.67003891759097	-6.10118844839070
H	1.66474060028042	1.08131904832485	-2.31782861461082
C	2.21230668267537	0.49307870795420	-1.24369303147060
H	1.79656111673688	-0.42471990670884	-0.84626334096177
H	3.09307902418266	0.89572811615917	-0.75201012379363
N	2.18653312167234	2.26134060046139	-2.92535786673001
N	3.22343538722517	2.73280302743387	-2.47180015346556
N	4.16805794584348	3.26447576518090	-2.14482087619392
N	-2.92271746354203	-0.89832953309037	-5.09079660558949
O	-3.06313690399450	-0.58801427769900	-6.27094963244501
O	-3.70528375426515	-1.61497288216842	-4.47194827189589

1h			
C	1.30139269532186	-0.00365258558914	-5.62538898028775
C	0.22423422944607	-0.41466741519947	-4.79999784148177
C	2.48992183864931	0.40994563428127	-5.08440305244684
H	3.28514936147556	0.74412900449077	-5.74298039275341
C	0.40225590145347	-0.38068858916187	-3.38187956768154
C	2.68138333283739	0.43412223308636	-3.67447812411910
C	1.63991953655550	0.04997862983269	-2.85012628166532
H	1.76154899500915	0.06240415775412	-1.77089081544573
H	1.16680406021668	-0.00829721181794	-6.70435434795062
C	3.97607731217395	0.85816965221740	-3.10850873548544
C	5.14273064099157	0.88631681512846	-3.77171842067791
H	5.20278860788454	0.55980589153764	-4.80235361923398
H	6.06391595096657	1.21638315924829	-3.30052496371952
N	3.85640861082282	1.23521918338414	-1.73483152141450
N	4.87685825967992	1.53531782065175	-1.12806672428699
N	5.74362589271976	1.83781107046307	-0.4638603999067
C	-1.01545719960354	-0.84517921391827	-5.32881740148060
H	-1.14698899841213	-0.86686320292981	-6.40810248238351
C	-0.66871255570062	-0.78392529152461	-2.54561405101009
H	-0.53059709716504	-0.75801129901326	-1.46730726626372
C	-1.86109981265855	-1.20026770328001	-3.08935010770705
H	-2.67691952115355	-1.50776463368105	-2.44047054125232
C	-2.03618836406341	-1.23113452967924	-4.49069930442682
H	-2.98450221953031	-1.56210674320126	-4.90521278732360

1i			
C	2.30218821737542	-0.89365710572459	-2.27887013496508
C	1.59462884528539	-1.78283831975933	-1.50455188603746
C	3.33585026648059	-0.10342160475308	-1.71486628815511
H	0.80702872683303	-2.38119065579266	-1.95410269933035
C	1.88705286661883	-1.93178413928089	-0.13208666354698
C	3.64847853268196	-0.27396202611586	-0.32744770708188
H	1.31720145012749	-2.63702867401924	0.46644136676768
C	2.89638962408041	-1.19682805744736	0.44086759724901
H	3.13917669287085	-1.31599710051010	1.49408527071308
H	2.07464124066455	-0.80544766548429	-3.33784908872266
C	4.10106186458704	0.83292806953805	-2.47701357701929
C	5.13395548908306	1.52824588815897	-1.88108124068688
C	4.71047384292505	0.46845141496680	0.24508297950723
C	5.44357524575641	1.34257082030220	-0.51841321366693
H	5.70298704498117	2.24106730577992	-2.47147238874879
H	6.25913538290825	1.90736015092422	-0.07593094034517
C	4.93563733771826	0.32973662707732	1.29980552369875
C	3.78780572516075	1.09148933409145	-3.90410687399820
C	4.63406206959738	0.85607605858529	-4.91167990516515
H	5.60180567498720	0.41174576174971	-4.70950227294078
H	4.36710847172239	1.09482625093900	-5.93668792922175
N	2.51023108618432	1.63917757587090	-4.22839100087145
N	1.78038024905161	2.01564863845512	-3.31682699057658
N	1.00519104947258	2.39941843504710	-2.58319496695457

Benzhydrylium Ions

2c			
C	-7.71840229853383	2.40443103410730	2.70556147481590

H	-8.39013328648359	2.48859558626959	3.56054366295113	C	-6.44001306585400	-2.65875718523243	8.93102184385249
C	-6.55646987109128	1.64306747593127	2.93755090177663	C	-1.53873295657828	-3.40376723297567	10.53269605016130
C	-6.20148045078306	1.38310517283180	4.29786275062656	C	-1.15359847205126	-2.06553211243084	10.49956475124273
C	-5.75673059724515	1.08099174883405	1.89933096668387	C	-2.56197285186696	-3.85901774074615	9.70619840494357
C	-5.06126137369058	0.68445204800907	4.57983557204590	H	-0.35411724525235	-1.71444224546086	11.14566835986902
C	-4.62492228684571	0.35069310638555	2.17629390912917	H	-2.86185920656790	-4.90351772536664	9.71725117260091
C	-4.27986472945664	0.18193865443398	3.52358295733870	C	-1.79523745173851	-1.17651629983016	9.63931380718945
H	-6.82948600193304	1.77608555999592	5.09353678249191	C	-3.19810269374264	-2.96152122652816	8.85250088925333
H	-6.08128578479733	1.16718039071366	0.86861108300636	C	-1.50169438028497	-0.13100056463847	9.61563379764104
H	-4.03415548265866	-0.10725601565398	1.38981755328388	C	-2.82350055984362	-1.62003951579228	8.81447611461161
C	-8.15095479663365	3.07298829794867	1.54381408281657	H	-3.33774918584779	-0.93549345114467	8.14535733072626
C	-7.28852720569818	3.42604708115267	0.46452392493984	H	-1.03742128369676	-4.10027819437784	11.19853229125795
C	-9.52646138663091	3.45774806786313	1.48072496669012	F	-6.76396023905713	-2.00273933993233	7.79236247668715
C	-7.76101229371015	4.06967356764357	-0.552506821014469	F	-7.58948646951698	-3.10086078850693	9.48740303844846
C	-10.00880583894830	4.06976188860237	0.35780502458986	F	-5.90994063084153	-1.74127591063433	9.77188572441104
C	-9.13011360775572	4.36323485067024	-0.70076707906067	N	-6.78610157867246	-3.39659926328166	-2.12139321740477
H	-6.22262051043798	3.249442522726672	0.5525006464639	H	-4.21320607590561	-4.04537893062330	-2.02196118071575
H	-10.18038251910554	3.22614119263738	2.31772206103944	C	-8.12387143800632	-2.82354893719318	-2.15612190421361
C	-7.10104361661450	4.37001469219542	-1.46223549389249	H	-8.24571756657129	-2.03356976375690	-1.41131184938845
H	-4.41425711480351	0.28663230111712	5.87716217468451	H	-8.30496196780314	-2.38536297596456	-3.14265126385862
C	-3.18896898648988	-0.51932598703117	5.40628379101962	C	-9.21112426558144	-3.86563255366584	-1.93081969043364
O	-3.21297338620206	-0.49924079521257	3.92624855816644	F	-9.05776753170025	-4.53311892288810	-0.76339821454994
H	-5.08542102431802	-0.32077188336337	6.49177078163486	F	-10.42456959519493	-3.27142530205893	-1.90397912864700
H	-2.23466762489552	-0.07999752358575	5.70463270441860	F	-9.23758339511617	-4.79706638357144	-2.91138285524732
C	-11.38091692230508	4.55545179636449	-0.01848993085722	C	-6.10142829720160	-5.31650059208216	-3.47554600755564
C	-11.147732677545296	5.16891867134348	-1.41211423758994	C	-6.29126756747919	-3.94110212755952	-3.35845105982979
O	-9.171295407750480	4.97931760966143	-1.72318571545694	C	-5.63351498446114	-5.83961830325606	-4.67626990422382
H	-11.75379715698153	5.29865171884986	0.69273474785916	H	-5.48713277449666	-6.91153585677779	-4.77340203735965
H	-11.70409392786366	4.67015858645609	-2.20865750681878	C	-6.02466850520227	-3.08792582658295	-4.42615590943632
H	-12.10106462537850	3.73227497483762	-0.05637387139671	C	-5.36600195080039	-4.99512359620713	-5.75211513826319
H	-11.33079914898427	6.24505428029209	-1.45013416611149	H	-6.17086774041363	-2.01679720054264	-4.31504127090477
H	-3.22103709408140	-1.57106726291273	5.69975826693606	H	-5.00521611058228	-5.40797847676883	-6.6897937205116
H	-4.11915329568488	1.16269558534495	6.46296920591941	C	-5.56340671903090	-3.62203116547284	-5.62589970999658
				H	-5.35115750766545	-2.96038015648211	-6.46073171495662
				H	-6.32260284703600	-5.96492776705553	-2.63209899190971

2e

2d

C	-3.52380127243864	-3.54792888665744	2.44664458977616	C	-4.94595053595784	-3.97176545582558	2.00622120751359
H	-2.46691278289114	-3.61210000670917	2.18495421908155	H	-4.51016617390825	-4.81366385637241	1.46685638376949
C	-3.78289142443051	-3.54948578660751	3.82987415729781	C	-4.75619468641266	-4.00898632484792	3.39973895197566
C	-2.68699099960283	-3.32650042446847	4.71109052738130	C	-4.31867650807346	-5.23310658369719	3.98098497484929
C	-5.04481340887492	-3.80905363593158	4.43204186967514	C	-4.91757417986903	-2.90587599485931	4.28319115076439
C	-2.84634645276831	-3.26526953156948	6.06809571175537	C	-4.14144456502619	-5.38159375598819	5.32909952840368
C	-5.21386680353529	-3.77733159840643	5.79062580244027	C	-4.71443222884866	-3.03058840747691	5.63080808575195
C	-4.12524525649579	-3.47156911583881	6.65385225608499	C	-4.34029184898433	-4.27987436955348	6.20897597267854
H	-1.69672297662282	-3.18111576679359	4.28704059104514	C	-4.15626739589001	-6.08906051868185	3.33103888272196
H	-5.89322929677986	-4.09297950892889	3.82026134471536	H	-5.14157452174650	-1.92116370024186	3.88922589101883
H	-6.19699076644580	-3.99405325874414	6.18915243908126	H	-4.81465396850863	-2.15095049431777	6.25408958732292
C	-4.39565219476141	-3.47582052034890	1.34444164986796	C	-5.60231691748296	-3.03131879017532	1.19125685743537
C	-5.75383721360276	-3.05785620788122	1.39587420013715	C	-6.52424973196123	-2.04795999648675	1.64734201971244
C	-3.871604057511254	-3.79141277204336	0.05864671115174	C	-5.37027926859391	-3.05884654152399	-0.21159392819729
C	-6.53975281220594	-3.02447193456974	0.27494368996473	C	-7.11409072240477	-1.16064129524378	0.78935568928114
C	-4.65125122664872	-3.78735831552932	-1.06501633024139	C	-5.93185871746538	-2.18853401617439	-1.07906760838072
C	-6.02191224260390	-3.41674805086652	-0.99053037315101	C	-6.82280341676859	-1.18282721809817	-0.60660161840070
H	-6.17966486739506	-2.70273093233930	2.32694361738232	H	-6.82301534940081	-2.02552115196487	2.68898505661037
H	-2.82227817214760	-4.06209793432186	-0.02611456596310	H	-4.69988143709274	-3.84794414894329	-0.60075664627592
H	-7.56359152311408	-2.68836648526471	0.37807881581300	H	-7.81830791760894	-0.44836315708423	1.20028231395878
H	-1.98634892937086	-3.08058857232771	6.70098940505410	H	-3.85548874418749	-6.35482423805889	5.70655315240251
N	-4.27053696280719	-3.42217938101701	8.01009204590634	N	-4.15401907917540	-4.37563911313338	7.54949159353604
C	-5.49496330421292	-3.82727909711446	8.68489244473174	C	-3.71244232365337	-5.60167901711727	8.18851591565155
H	-6.03352600273801	-4.59336671733962	8.12225331501708	C	-3.07854111044645	-6.20389942656995	7.53369629537412
H	-5.24567193356722	-4.24577492668649	9.66493160055168	H	-3.12654187814141	-5.35848389002783	9.08014718638007
				C	-4.88099994580895	-6.46522583789632	8.64210412647022
				F	-5.68540326047768	-5.81529458410384	9.51653033576550
				F	-5.66565540450963	-6.85672632575705	7.61105517311983
				F	-4.43069836556383	-7.58081846764048	9.25701682384488

N	-7.38695263491434	-0.31086597639976	-1.48038508227592	C	-6.08344682014789	-1.27620514131220	10.80626396655347
H	-5.69670899751053	-2.26160867484109	-2.13316350273640	C	-6.34585763384917	-3.00365450401705	12.47355167765314
C	-8.33567433189952	0.70639497643375	-1.06706873624004	H	-5.72708255703422	-0.29369940706299	10.50979695562735
H	-9.03301072532530	0.91002244585843	-1.88512033197515	H	-6.19341348847776	-3.36136869354540	13.48771399139315
H	-8.92923517448419	0.39310393813615	-0.20523781633390	C	-6.73834223885572	-2.08688540761568	9.87824392001100
C	-7.65413464089708	2.02150062763687	-0.71854798151930	C	-7.00336705941090	-3.80485150367830	11.54181444366860
F	-6.78644869427476	1.89712543772237	0.31278625029549	H	-7.37342439396970	-4.78498154035508	11.82891020501548
F	-6.94881321813826	2.52057732568073	-1.76133374669442	C	-7.20787497031337	-3.34948428426561	10.24433539865355
F	-8.57199798291901	2.94888709392505	-0.36784034445505	C	-7.37302965290907	-3.96153204688636	9.51926923581779
C	-4.40781434856026	-3.22565705461174	8.42715116087067	H	-5.37646369796919	-1.11131625751421	12.82438838178888
H	-3.73630929434123	-2.39420411169701	8.18300800601002	C	-8.26165530879792	-2.86129389664922	-1.54915837876816
H	-5.44653397350023	-2.88819779989966	8.34250120869765	C	-6.96990019200698	-3.04106823663972	-2.04864111278260
H	-4.22426664893726	-3.52263225441930	9.45934648795582	C	-9.08373185573040	-1.89156015044277	-2.11131204897809
C	-7.04240033427587	-0.35398024766728	-2.90755597319836	H	-10.09045141882832	-1.75603245462415	-1.72631719565510
H	-5.96961977242756	-0.18896438005267	-3.05758296484493	C	-6.50919279317285	-2.26873319170097	-3.11636379307829
H	-7.58823947867405	0.43371826969885	-3.42620781432773	C	-8.62929773564709	-1.11290309671956	-3.17412632745332
H	-7.32370657491322	-1.31838392820377	-3.34614637163235	H	-5.50449699581793	-2.42087592041822	-3.50034336373269
				H	-9.27754740314047	-0.36093660937237	-3.61457988406326
				C	-7.34339739645559	-1.30734711319412	-3.67523699183735
				H	-6.98300289606940	-0.70294404448670	-4.50276765769210
				H	-8.61904623444360	-3.48609183295575	-0.73547176121782
2f				2g			
C	-5.44418220806400	-4.59274059197103	4.05358568126589	C	-8.31584277910347	-1.21625755419349	2.67310884194807
H	-4.88500831760515	-5.49032566534960	4.31922053966236	H	-9.10824969375095	-0.48450097373991	2.51083865107543
C	-5.88580067699265	-3.82668582842983	5.14842239349310	C	-8.12268232732199	-1.58237777408214	4.01713583765569
C	-5.31770831988975	-4.09664422904839	6.42699207987550	C	-7.39668729179355	-2.72169520711611	4.46631546404960
C	-6.89493128153385	-2.82310483947974	5.09162341649228	C	-8.74004411718157	-0.79129543435976	5.028776043353161
C	-5.65583118821966	-3.37466271033999	7.53984540167949	C	-7.24357688950216	-3.00301280073912	5.7959547709853
C	-7.24606671965748	-2.100496141376627	6.19923332818427	C	-8.58593991088729	-1.05129751411276	6.36217886417417
C	-6.61801974708811	-2.33696006872256	7.45085659352420	C	-7.80515098459809	-2.16127559683030	6.80563186161699
H	-4.55856510464483	-4.87044576478475	6.506985619293241	H	-7.01490544223490	-3.43779358361923	3.74746761875368
H	-7.45890128238316	-2.67340681491719	4.17778090584694	H	-9.32454488856798	0.07444305585619	4.72694380818863
H	-8.04821563726632	-1.373136357868750	6.134675748878501	H	-9.04420578902096	-0.37689807866970	7.07450225205666
C	-5.60767631473759	-4.38588715911248	2.67111236491361	C	-7.66003548701044	-1.63804669159606	1.50282957706136
C	-5.32684859995341	-5.47314772470740	1.79413426870120	C	-6.41135427558443	-2.32162472654973	1.45290685985071
C	-5.99157178410322	-3.15465708089195	2.06653128094612	C	-8.25522995746945	-1.32469092840255	0.24729558055520
C	-5.49543284996040	-5.37701151777070	0.43903899246354	C	-5.85661051709144	-2.72494967127090	0.27055198572509
C	-6.15685122542478	-3.04551240712004	0.71256650984077	C	-7.72148553368655	-1.73486750579054	-0.94320946309550
C	-5.93943001545825	-4.16093842139420	-0.13913952113063	C	-6.69668070230279	-2.48254855475445	-0.98000420904865
H	-5.01262511071144	-6.42082203745663	2.22366052047104	H	-6.95596208379222	-3.76142042714884	-4.20809639591303
H	-6.08020252324466	-2.25865417244896	2.67048977116744	O	-8.25824166705575	-3.95137185289651	10.42897915571816
H	-5.31166000570422	-6.24019246749921	-0.19101122489201	C	-5.46248484318931	-5.12359335241209	-3.02025041360289
H	-5.16985187749114	-3.58174519212929	8.48686856587438	C	-8.42228405124339	-1.84110924185917	9.2007308572442
N	-6.96299582767376	-1.59823021822472	8.55326980105834	H	-5.59433226654049	-2.10597781660694	-4.02756163979866
C	-9.26800678763260	1.26162790757502	9.074124262550935	H	-7.22175521800750	-1.76554625479267	3.42172783239520
C	-8.70684651633819	2.21999392259601	8.23207468247181	H	-8.13478595499599	-5.04738086841751	8.65977791895445
C	-8.70096074521191	-0.00356291343016	9.17527532120172	H	-6.79248846689129	-5.23086037056332	9.82938929302216
H	-9.15338569796945	3.20720716341340	8.15661676310277	H	-9.88146745535502	-3.43615955426297	9.23121141453829
C	-9.13725971791272	-0.75570726756158	9.82642211651100	H	-9.70125016223555	-2.56098337785379	10.78138127281370
C	-7.56649496672453	1.91047473388056	7.49304426170786	H	-4.04939059462179	-3.50172151943862	-2.76644253486114
C	-7.56208269417153	-0.30763361405753	8.42738417212167	H	-4.59789220682434	-4.27186718637958	-1.25784800649912
C	-7.11488866447185	2.65797668037961	6.84703203800969	N	-7.61688699171305	-2.41666237035269	8.11914065754477
C	-6.98581893102552	0.65139178584126	7.59160755440407	C	-6.44521555889051	-2.52716949713583	-3.47370094938789
H	-6.08403238353420	0.41269293362750	7.03475161181837	C	-7.48200935611748	-4.51488704959650	9.37162872571298
H	-10.15714007183970	1.49655916110300	9.65223992090990	O	-5.92781960526178	-4.74578591119088	-4.3134692528927
N	-6.12366435425230	-4.04909520693017	-1.49345441533049	C	-9.15960884670402	-2.96963176888485	9.92256004142800
H	-6.40679337281759	-2.08374254553298	0.27762216637255	C	-4.91528697473692	-3.92690698270871	-2.24114478018741
C	-4.10067511248186	-5.13447064244418	-2.33968455242731	C	-6.03017049061789	-2.92850029576776	9.36089845561715
C	-5.48120634430090	-4.93963066594144	-2.40942483340532				
C	-3.48363849278593	-5.98570756203558	-3.24924119771168				
C	-2.08403212313314	-6.13343731977710	-3.19866125786137				
C	-6.23931291767729	-5.57714727730018	-3.39240177621430				
C	-4.23408707918014	-6.63024453060034	-4.23094561485680				
H	-7.31219530831053	-5.41336586202949	-3.439377312024083				
H	-3.74691628695224	-7.29001125034950	-4.94302470599401				
C	-5.61013549296888	-6.42079514525887	-4.30090418446742				
H	-6.20048969542415	-6.92151279473319	-5.06292807972796				
H	-3.51810885634311	-4.61395855953349	-1.58471509118084				
C	-5.89064903265133	-1.73969835762579	12.10281048185370				

H	-6.07897452633004	-3.86099556474205	7.85825433041221
H	-7.83087292414738	-4.17692502293426	-3.68058771138984
H	-7.24683785200177	-3.49347402497579	-5.22843590024404
H	-6.27793609719773	-5.59281390910930	-2.44452565661162
H	-4.66363567668481	-5.85666706925318	-3.17000360196447
H	-7.75565550415284	-1.32064644291209	9.90140397051567
H	-9.15730923876804	-1.13239038831493	8.82211717263679

Transition States

TS_1d_2c

C	-5.95930411999726	1.99883777313169	3.82159303621401
H	-7.03443297490023	2.16889695043832	3.78377385498620
C	-5.57580772349999	1.07959730194599	4.87820625123383
C	-6.42848667226335	0.99109908434595	6.01017135042057
C	-4.45156472905993	0.22863383200999	4.81202093797291
C	-6.12590837852475	0.12950190709038	7.03353301438847
C	-4.14326568450209	-0.65668848813681	5.83383937988381
C	-4.98079445624387	-0.67615976490120	6.94557111970486
H	-7.31911206574645	1.61393863395111	6.05839095865016
H	-3.83200721169257	0.21693767396787	3.92390228662159
H	-3.28981661887217	-1.32344339946544	5.7633928429771
C	-5.31020191740438	2.13906944465862	2.53553007322314
C	-3.90741786171640	2.15685264127654	2.36658784705465
C	-6.13603766749979	2.34374900851590	1.40308802355758
C	-3.32325463997350	2.30823915963264	1.11997700332264
C	-5.56653328489787	2.49126292658901	0.15969390126017
C	-4.17358013984484	2.47306194584952	0.02850427416784
H	-3.26191244403963	2.10952076251582	3.23770852643886
H	-7.21660234141968	2.36053956980012	1.52451228846409
H	-2.24502219397569	2.34366921891165	1.00101307096712
C	-6.84427001276759	-0.21648237570519	8.30914971673278
C	-5.81707454116133	-1.11411300488791	9.02072715910761
O	-4.80871215112741	-1.47897734396946	8.00748863521743
H	-7.77239982559590	-0.75860006291490	8.09403062389751
H	-5.28402905118175	-0.58684494773745	9.81830019896329
C	-6.16433639712089	2.66307526897132	-1.20968981093103
C	-4.92572552712601	3.01701312559578	-2.05027243352872
O	-3.75197309916581	2.65267011148030	-1.23659072785560
H	-6.62988953576475	1.73037405861072	-1.54961909329903
H	-4.84845917949063	2.46526917891613	-2.98868158990744
C	-4.29952807856810	5.89469673114913	1.14331100137866
C	-5.28394725450604	6.27278168956023	0.23108095857444
H	-4.65293455759668	5.43179569205927	2.40092709745565
C	-5.00205478319806	6.63541926529881	-0.75344442787678
C	-3.87251157016014	5.16359580063574	3.10444821893078
C	-6.63019768983438	6.20356488846813	0.59054295809721
C	-6.00785711676609	5.33441743559884	2.76633672284056
H	-7.39891343668361	6.50287512380376	-0.11586258457579
C	-6.99320831039162	5.74286425307072	1.84585208794826
H	-8.04302316175964	5.67027219468637	2.11035704828062
H	-3.25010313353904	5.96465935806297	0.87229717706298
C	-6.38807703561525	4.75805708296278	4.04641575750767
C	-5.58828359267178	3.89447331838342	4.77489029555579
H	-4.52383836392697	3.87070198927334	4.58254849641997
H	-5.88728602323672	3.62227781493224	7.78200426554599
N	-7.71769478041415	5.01023888385519	4.39360050636461
N	-8.1697459866826	4.52259768479665	5.43285005367606
N	-8.71789976293168	4.15427550574432	6.34829883632798
H	-4.85262678404607	4.09239695118726	-2.24568286876932
H	-6.92010778579165	3.45293915265418	-1.24779665540111
H	-7.09728464664688	0.66309127290395	8.90763446134567
H	-6.23155369847044	-2.04671327961695	9.40726824209652

TS_1d_2d

C	-7.41096118269823	-1.87057593370978	3.07573601209085
H	-8.49412101553644	-1.88647431338403	3.19553587528788
C	-6.71421519468958	-2.25162553832563	4.29338710416222
C	-7.36462536757901	-2.03993059263519	5.527861232741
C	-5.44874882816287	-2.86841963846892	4.34188886292618
C	-6.79927943620416	-2.39355770003190	6.73156737162593
C	-4.86817405830743	-3.23465522490094	5.53746857310879
C	-5.51869668647971	-2.99663724162989	6.77045613387051
H	-8.35351518116265	-1.58690241301501	5.53216146834907
H	-4.91798466123113	-3.11033920732140	3.42921422614990
H	-3.89827172852351	-3.71811914762874	5.52268916382919
C	-6.98455002707860	-2.19459977416978	1.72883855519338
C	-5.65778465043783	-2.08493082140269	1.26184766915983
C	-7.96061292842834	-2.57387947815332	0.78855518295159
C	-5.32039528909831	-2.40062915200232	-0.03471771363665
C	-7.63934567440516	-2.90650890757872	-0.51226163223016
C	-6.30187153757968	-2.83337774404251	-0.95846139460092
H	-4.88356056503272	-1.68434617608385	1.90883828053143
H	-8.99950424669703	-2.63871655870360	1.10283664936571
H	-4.29468810027373	-2.26983835499838	-0.36097941239608
C	-7.00166221954251	0.76240004083656	-1.13771122454629
C	-8.17846371053656	0.66551104342861	-1.87934392626546
C	-7.04919542170335	0.78920909778460	0.24694783085500
H	-8.13660983249322	0.64074857963069	-2.96479645234443
H	-6.12478624958147	0.88448242132246	0.80537716200400
C	-9.41050085988722	0.61535116286301	-1.22691491348118
H	-8.28394739492707	0.71529887561399	0.91764803078002
C	-10.32897037934493	0.54507142746496	-1.80218719315918
C	-9.46795936679891	0.64353297662026	0.15707735468893
H	-10.42861296377845	0.58102518463824	0.65751241946649
H	-6.04168558183707	0.81794670748470	-1.64299458166078
C	-8.33300543462544	0.64695387294527	2.36855242024136
C	-7.27727503021665	0.22096649951010	3.16434169590411
H	-6.27014457093550	0.27220013634056	2.77077292794519
H	-7.35584912538913	0.34764984191606	4.239697661033455
N	-9.60961489981459	0.86152526995914	2.88922340489255
N	-9.78729498172899	0.77458386367806	4.10716760961417
N	-10.10375694830094	0.73855506895872	5.19025707754501
H	-7.36780087741600	-2.2215929947056	7.63734080270000
N	-4.90829662860549	-3.34327743500012	7.95612024036549
C	-5.42786496472538	-2.92738197765248	9.24582124668754
H	-4.59891198155293	-2.75722523018459	9.94046909213334
H	-5.99541549445250	-1.99593277749120	9.17098660893561
C	-6.32368831896556	-3.97867483839659	9.88731683023040
C	-1.34497743237147	-4.29939017129988	8.42635286910464
C	-1.36861456322472	-5.63189959828718	8.02171197086426
C	-2.50934658024489	-3.53675268611169	8.39503282756707
H	-0.45799745155777	-6.22368482132002	8.04535124559308
H	-2.49614978261635	-2.49309545188005	8.69829421868349
C	-2.56263088252773	-6.20592090026358	7.58843217569603
C	-3.70033315499159	-4.11948153003228	7.96645514777579
H	-2.58701387792352	-7.24687698085697	7.27861799571141
C	-3.73264150107231	-5.45431890585836	7.56468615968855
H	-4.67129312637020	-5.89473152695882	7.23905474494044
H	-0.41579878462735	-3.84639064669058	8.76038721151536
F	-7.36901887743132	-4.32703883849843	9.10066233950163
F	-5.65225736367689	-5.12027803367906	10.16766999514251
F	-6.83097031401369	-3.51408995201609	11.05262643678258
N	-5.94536173632431	-3.11061551712250	-2.26310143501735
H	-8.43581255661161	-3.22916669875449	-1.17142233849317
C	-6.93241609610155	-3.27011922714109	-3.31357968767947
H	-7.85620543767427	-2.73161712032745	-3.08394673381550
H	-6.54186204692885	-2.87277114631182	-4.25638386996554
C	-7.28446429744727	-4.72905103891070	-3.57052125755409
F	-7.72708412773073	-5.36484146608904	-2.46029630706450
F	-8.25881938641391	-4.82054610150913	-4.50544764415024

F -6.22343178090327 -5.43699044072569 -4.02527721508507
C -4.01481953706338 -2.28313874458882 -3.51866266180365
C -4.56643888202050 -3.21575942122753 -2.64176798156356
C -2.68041093655741 -2.401509612538943 -3.897570161538943
H -2.25033248380168 -1.67480592754082 -4.58104131264671
C -3.78926526228799 -4.25897516731937 -2.13839774704991
C -1.89761784626174 -3.43785133647842 -3.39423808949538
H -4.23590707275933 -4.98171036178983 -1.46067679070739
H -0.85617585935514 -3.52618054471902 -3.69012670566596
C -2.45376132096276 -4.36296260512321 -2.51222890242555
H -1.84930100613931 -5.17737321044888 -2.12282151763147
H -4.62629903732014 -1.46797217915348 -3.89706526082931

C -6.46717587096870 -4.57441832686314 -3.45128177555780
F -6.79027265307699 -5.25464039002000 -2.32579725084001
F -7.30890723151650 -4.98599994875604 -4.42749231744315
F -5.21969024336508 -4.97469861591232 -3.79960581459390
H -3.54213093852558 -2.75184669343566 -2.09132476268102
H -4.17157846298051 -2.47483189544471 -3.722374238361979
H -4.12618035404628 -1.13231828888157 -2.56425147305955
C -4.29884933023842 -2.21146815631819 -2.67209561752536
C -3.09939416415848 -3.10626485644670 7.89989996142548
H -2.73153379073237 -3.19838963758844 8.92228334540821
H -2.95132121473661 -4.06813963194188 7.39273838179701
H -2.50437743003520 -2.34066421400794 7.38828213105103

TS_1d_2e

C -7.31560572622702 -1.70675643437577 3.10243001156311
H -8.36891084569842 -1.95875902059289 3.22778945309566
C -6.54388025325089 -1.95538597819342 4.31106146746194
C -7.20692723200403 -1.88917719095579 5.55641928746453
C -5.18635455877125 -2.32489583789910 4.33910759093828
C -6.57053445385693 -2.14272518450606 6.74787857474501
C -4.52999650129022 -2.58960618007619 5.52383982957368
C -5.19356273380368 -2.48710404896209 6.77164604747236
H -8.26380631633273 -1.63269025371487 5.57788438829386
H -4.63691911577130 -2.46831627021088 3.41634084867241
C -3.49555202863287 -2.90651810001943 5.47783003827474
H -6.83822961076095 -1.93042078255564 1.75026599427887
C -5.56845070535453 -1.54205465571534 1.27858427839507
C -7.71333046697753 -2.51149224216066 0.81205895606353
C -5.17610244558963 -1.76965616131474 -0.02305221808797
C -7.33685671748023 -2.75793745681558 -0.49107099176005
C -6.05036965256744 -2.38804084934197 -0.95306983681820
H -4.88805680067803 -1.00149488263964 1.92973629835591
H -8.71114619488738 -2.80292659569119 1.13124431814171
C -4.19600349077194 -1.42922576756658 -0.33388263884569
H -7.55840770021068 0.93480074293735 -1.09527578475601
C -8.69927168334740 0.57312808400469 -1.81082248644376
C -7.58229294363140 0.96209968268424 0.28994528609703
H -8.67437052948188 0.54639585111661 -2.89672242611925
H -6.69060035728206 1.26329406094615 0.82831114898108
C -9.87723553426208 0.26126716904464 -1.13161485695254
C -8.75650437963646 0.62393907562251 0.98749413960424
H -10.76898259672867 -0.01525785128161 -1.68647475579607
C -9.91173570691158 0.28953286395227 0.25310267154013
H -10.82452136919390 0.02148273722494 0.77493525840304
H -6.64502243882760 1.19666769491873 -1.62161147387733
C -8.75743492357021 0.54907817682693 2.43834275874900
C -7.61635379517467 0.34249836072247 3.20727153114528
H -6.65380306973691 0.61334576833573 2.79217330817601
H -7.69573644631728 0.45656773155321 4.28427000713739
N -10.03798586002493 0.49521234957746 2.98803038858694
N -10.16744372541926 0.36722731881484 4.20844713069358
N -10.44564083615187 0.26148946982477 5.29756994357867
H -7.15282517565491 -2.09007100502373 7.65921915019411
N -4.51347457500508 -2.72631164413964 7.93579361862589
C -5.16184831510372 -2.71033195564295 9.22899445314325
H -4.44155767714614 -2.42001963253697 10.00036201184150
H -5.98752950277746 -1.99518577574543 9.26836127431716
C -5.70923841916443 -4.07433351933084 9.62538763299918
F -6.64468980929868 -4.53177590894174 8.75978345776609
F -4.73679222770614 -5.01676641544474 9.67761058002856
F -6.28383856149176 -4.01970569658662 10.84893277816706
N -5.65175411850538 -2.57802043396422 -2.25073701913869
H -8.04834776832295 -3.24671813802566 -1.14474056801864
C -6.55379122765035 -3.06604702074377 -3.26946155802642
H -7.59629893021076 -2.81474287314033 -3.05280891489587
H -6.30441626021361 -2.61485971863484 -4.23596885338779

TS_1d_2f

C -8.94492456567270 -2.44296955723184 2.87904694459107
H -9.89870090130242 -2.94988480191560 2.73515769141450
C -6.56164216469626 -2.37959482431310 4.27656587174489
C -9.58520714100227 -2.48937863479848 5.24643633567997
C -7.24021607860109 -2.253407443329979 4.75144533872355
C -9.32176026794042 -2.45168696893434 6.59463869344183
C -6.95942845450085 -2.225083350592322 6.10141648321462
C -7.99369662690615 -2.31028326366285 7.05658581963607
H -10.61259289167278 -2.62208896321513 4.91512899732224
H -6.40786262406946 -2.20545897014605 4.06027953237103
H -5.92909698458790 -2.13311098885145 6.42765914929619
C -8.03607419092900 -2.61754563366119 1.76368491233760
C -6.81727441496351 -1.92444426766174 1.60697913931785
C -8.39992854884476 -3.51868171322627 0.74279314888165
C -5.97437398983893 -2.18429565122826 0.54890702446907
C -7.55980938844781 -3.79812145372280 -0.31565497919637
C -6.31201312823406 -3.15270849517137 -0.42137749802326
H -6.55235840510317 -1.12692909343440 2.29406091522512
H -9.34868676743793 -4.04467071143363 0.81567581952060
H -5.05430754316515 -1.61847676445774 0.44520659001574
C -8.64887237894175 0.08202602336083 -1.57101169474993
C -9.43451804834712 -0.52862104581531 -2.54806019255888
C -9.03567330391016 0.04625488974841 -0.24022159726622
H -9.12964938182324 -0.49515905454531 -3.59041554073196
H -8.42481082315474 0.54868182880605 0.50157884683450
C -10.61489376109972 -1.17667542807028 -2.18635544597104
H -10.22561822519794 -0.60309678639134 0.13733274720590
C -11.22691947121415 -1.65695447380460 -2.94418627244469
C -11.01286362595431 -1.21208131834103 -0.85885364273751
H -11.92805516562968 -1.72642907798634 -0.58472353131170
H -7.73266112504991 0.59431918341191 -1.85006116460269
C -10.62488129957275 -0.66000621295979 1.53544694245262
C -9.75806804953287 -0.50470052229253 2.60580052473677
H -8.80350604121617 -0.02031743476155 2.44349782421555
H -10.17526662774480 -0.38228553124353 3.60030917019613
N -11.95370034270107 -1.05269464428271 1.71210382677727
N -12.0130954384702 -1.17417441381053 2.85481751257781
N -12.95301602865209 -1.31972519117264 3.82953509436825
H -10.13392699687432 -2.55844290422706 7.30588258591872
N -7.71607336045691 -2.27760576284417 8.41326585416629
C -4.55997965072563 -2.25882710559879 10.36508431565366
C -3.97769195739461 -3.45712682837803 9.95627151421353
C -5.78769110552344 -1.86073056744812 9.84778007362573
H -3.01784016481680 -3.76383255639733 10.36163533702611
H -6.24139217268773 -0.92440074088751 10.16036947776203
C -4.63618088557984 -4.26329930982763 9.02908574036679
C -6.44234658962554 -2.67204128445249 8.91818677690367
H -4.19604266151894 -5.20597025173842 8.71593921795611
C -5.88059359578808 -3.88059359578808 8.51385071708817
H -6.39304781377205 -4.51723098324414 7.80635447457203
H -4.05268087602581 -1.62359904097941 11.08577584308693
N -5.44016765341007 -3.43876918876554 -1.46428504487643

H	-7.85669520556187	-4.53319757164332	-1.05605109469888	H	-7.71682552873307	0.80361841878361	-1.60666103034933
C	-7.00227630102069	-3.34612520349544	-3.34278610887810	C	-10.75639875230766	-0.68776464819274	1.53821977075107
C	-5.91551163486100	-3.95001980687618	-2.70579273654204	C	-9.87878618088287	-0.77657784842232	2.61919043409516
C	-7.45232140947782	-3.84081923722532	-4.56098293836942	H	-8.915326247049712	-0.28829358554330	2.53841912565082
H	-8.29612747127680	-3.36347034864181	-5.05207337074049	H	-10.30587862368740	-0.75943652315593	3.61772692366000
C	-5.27399046932265	-5.03961837458882	-3.30051851159305	N	-12.10331614010065	-1.02746861018435	1.65623101286813
C	-6.81579033124147	-4.92745460474920	-5.15896512399345	N	-12.56517836801033	-1.30635356634300	2.76551093961749
H	-4.42750264987766	-5.50548887525202	-2.80393200002624	N	-13.13147843809609	-1.57643383418707	3.70501809938868
H	-7.16586821357829	-5.30850519563493	-6.11391677052266	H	-10.21822616240868	-3.29622888432813	7.00669858022640
C	-5.72458560510787	-5.51959524846308	-4.52553713414224	H	-8.36723847115309	-4.19501335635864	-1.65926837125284
H	-5.22404353358383	-6.36881995615622	-4.98232900723832	N	-5.83098846559642	-3.27895573150083	-1.96289882804631
H	-7.48703670354157	-2.49048858770570	-2.88259204711972	C	-6.41481478648762	-3.07976211377065	8.58158085245676
C	-10.35239839883040	-0.25693726330501	10.07805152177103	C	-6.73231626322098	-3.11313670606440	-4.23288060882794
C	-9.40873495829329	-0.66889791618035	9.14422033141393	O	-7.56839098964061	-1.97275576913516	10.43154148928239
C	-10.58202986499990	-1.00972541094527	11.22852073635440	C	-5.26914364831114	-1.43228057486859	-3.45883285079792
H	-9.21376412888753	-0.07252669641933	8.25734004109777	C	-8.68925284508706	-3.65813264188214	9.09014506731294
H	-11.31355523826077	-0.68032905729782	11.95885759150792	H	-7.00287651967838	-4.79326745284895	-2.88454568032531
C	-8.69773554688974	-1.85340868388042	9.35528042027419	H	-5.36010913019310	-4.59477598827916	-3.50026036079134
C	-9.86146871344493	-2.18378559884529	11.43977089791841	H	-5.65642331595909	-1.53576488180494	9.89287496457642
H	-10.03604337746908	-2.77796158345873	12.33237891320621	H	-6.89602514755184	-0.97640184473978	8.72974854744852
C	-8.92313615284853	-2.61121120789033	10.50713658215454	H	-9.50648052644630	-2.51456338620360	10.73612912037207
H	-8.36564892521999	-3.52988257681847	10.66638960830603	H	-9.23308970687937	-1.56657335155613	9.24291961687888
H	-10.89922537226315	0.66719676258611	9.91264027007243	H	-4.43336789333044	-1.73930825366108	-1.49693850322422
C	-3.32089027501553	-2.59674902730137	-2.33110767328838	H	-3.90714744580283	-2.92651177583451	-2.69883785785570
C	-4.03711668326561	-3.24130930964700	-1.31912242631889	N	-7.70912093941903	-3.47604171094164	8.01816714485880
C	-1.94678064128419	-2.42695413840234	-2.20316337755556	C	-6.24337995883237	-4.05230834785973	-3.13703298348038
H	-1.39529110993364	-1.92290067109557	-2.99194186807101	C	-6.59708541971577	-1.80097594248603	9.39936199146250
C	-3.37238167997105	-3.71546250997582	-0.18455514339527	O	-5.70393910953502	-2.18539043573006	-4.59265491343200
C	-1.28137427237099	-2.88741888804319	-1.06849836923733	C	-8.83057686451943	-2.36603328714925	9.88796646306227
H	-3.93000143332830	-4.23331824470531	0.59066030817896	C	-4.76573114029359	-2.34313449312370	-2.34107546457147
C	-2.00825099231775	-2.75084197247316	-0.97133595899991	H	-5.66988183810037	-2.90580963328452	7.80550448596638
C	-3.00029460665532	-3.52938864211661	-0.06140867339260	H	-6.65485743178004	-3.88778827945180	9.2320215554753
H	-1.48782831836483	-3.90419304018649	0.82031347509450	H	-6.97935901136521	-3.67477569930140	-5.13960934091564
H	-3.84187783424625	-2.23207177594982	-3.21192758485423	H	-7.63039377826090	-2.56996242503412	-3.89192336185289
				H	-4.46215249229000	-0.77905192378331	-3.80680156260531
				H	-6.09683521898747	-0.80789904910361	-3.08012794412392
				H	-9.65428719473531	-3.98596295319357	8.70321591001098
				H	-8.30993127136289	-4.44697295538143	9.75400325254720

TS_ld_2g

C	-9.18975997186994	-2.68414339890403	2.58591132047341
H	-10.16174618473953	-3.14516639650913	2.40522683318913
C	-8.74973106426217	-2.87136854347841	3.96200529819535
C	-9.72882011624860	-3.02415259104177	4.96715360038120
C	-7.40601236615901	-2.94678636460602	4.38029440220607
C	-9.40959616515301	-3.20810735608541	6.29198349260037
C	-7.06468802215000	-3.13800361434803	5.70091971910489
C	-8.05306464837414	-3.26024659919789	6.71392450757060
H	-10.78005805057190	-2.98019108589846	4.68957373859786
H	-6.60389872382235	-2.91619308074027	3.65223065854274
H	-6.01452608181512	-3.24523313560709	5.94401613925407
C	-8.31238519430169	-2.76548091722032	1.42729834182906
C	-7.05759286744552	-2.13111191571633	1.32599620987637
C	-8.75034367424384	-3.47528749709214	0.29473045558538
C	-6.25951504757054	-2.26820343280500	0.21117897474906
C	-7.96161227564455	-3.63327917932166	-0.82712647685011
H	-6.66631225528229	-3.05944246011082	-0.89615979866283
H	-6.71005981725849	-1.48304810741701	2.12509420330762
H	-9.73889088160845	-3.92922998175775	0.30544627715808
H	-5.30400916725866	-1.75831889893481	0.20486320583814
C	-8.67495169419944	0.33074986180715	-1.41201253243210
C	-9.47684349814933	-0.08972199740571	-2.47254060309531
C	-9.09813222398380	0.15643526737029	-0.10399586072499
H	-9.140950409572942	0.04776172185197	-3.49663471069358
H	-8.46921077727430	0.50962526973617	0.70532001787188
C	-10.71687550032523	-0.67522691289245	-2.21657384575221
C	-10.34054167141375	-0.44619055612104	0.16830047860600
H	-11.34485153499512	-1.00188379654126	-3.04029388834684
C	-11.15069813279950	-0.84919746935742	-0.91209552412605
H	-12.10894380609001	-1.32127178574914	-0.72182795157230

Substituted Styrenes

N1

C	1.57708918199011	-1.74015369985872	-4.55535401597872
C	1.92943417808673	-2.10673851691184	-3.25851188314725
C	1.95263302946775	-0.49808471696115	-5.05929242042354
H	1.69265712503587	-0.22302940440131	-6.07807177765507
C	2.66175488055659	-1.22187424489207	-2.46822427205284
C	2.68164145076657	0.39948150888207	-4.27106975471399
C	3.03852623492531	0.01890036483162	-2.97028321143611
H	3.60315833412372	0.71013815494500	-3.3500938822017
H	1.01566304118566	-2.42778876579141	-5.18227226900206
C	3.04376432809259	1.74636254074446	-4.79074619995181
C	2.13142986681166	2.48532500102743	-5.45748269022722
H	1.11543847338353	2.11964411934395	-5.55818516484739
H	2.35414262799117	3.46250737742221	-5.87019950826051
H	1.63893137737978	-3.07768304055922	-2.86646052828713
H	2.93738070395695	-1.49835506707317	-1.45391455483676
C	5.44364948943213	1.29155574697195	-4.77425457967187
C	4.66229970934512	3.57723653400794	-4.78956090696004

C	6.70832117455230	1.76136210662014	-4.08166013603620	H	5.78724266589792	0.35661149610387	-2.12194878519698
C	5.95885016474787	3.97432027419910	-4.10192795467691	H	-0.27992623036832	0.06955008239068	-2.69298348091035
H	5.60985398261019	1.26949205560469	-5.86695550853819	H	-0.84212572587280	-0.36140227227738	-5.07580587621129
H	4.76475234089597	3.70901061320889	-5.88286490978401	O	5.04221768126239	0.83430363114045	-4.65437594060946
H	6.58530527495432	1.69330643154786	-2.98683462073703	Si	6.72548171934390	0.85106412566096	-4.83134901462659
H	6.25225183552853	4.98147935502339	-4.41523874043227	C	7.41714988166687	-0.84265475875536	-4.44596520066285
H	3.86314534138153	4.24165029907439	-4.44034918464732	H	8.45867186093577	-0.90058332705528	-4.78740767330734
H	5.81602420326623	3.97073775212197	-3.00756824577534	H	7.40644432457486	-1.07574941601557	-3.37625081930979
H	7.55447389523169	1.13495066827601	-4.38210532242808	H	6.85322056027062	-1.62320083523485	-4.97133579065115
H	5.20963218940094	0.27462633080661	-4.44570548920310	C	6.93435430123486	1.27203704443968	-6.63581758727658
O	7.03665821048610	3.10325097407637	-4.44936471444484	H	7.99727481218754	1.33512078061499	-6.89869588479663
N	4.32447681474958	2.19544865972985	-4.44895726624123	H	6.47367724756612	0.51166502667779	-7.27770773082925
				H	6.47347290747293	2.23884951954309	-6.87121905879544
				C	7.47790816143786	2.18045212846124	-3.75273809203090
				H	8.53023506266046	2.32871270052884	-4.02723256087105
				H	6.96130765753428	3.13758025242513	-3.89498192737115
				H	7.44678046073732	1.93273411812024	-2.68636976087418
N2				N4			
C	0.55698508191974	-0.05727414646215	-4.88148666636091	C	0.81773107983565	-1.22405658430105	-4.95268064688464
C	0.25678397038904	-1.26327368942648	-4.24204382983741	C	-0.16884183006638	-0.52417608642825	-4.26050355574628
C	1.68144219183802	0.66508954753996	-4.48976701413049	C	2.15140710926151	-0.84547057951042	-4.84753124569633
H	1.88319957465591	1.61288823767831	-4.98309871064427	C	2.91258659897509	-1.37902186358966	-5.40985011933454
C	1.09118673219115	-1.72990196184274	-3.21724903597278	H	0.18936194168142	0.55824430206980	-3.46072400795473
C	2.52082156485711	0.21638326462592	-3.46469881402706	C	2.52280031899359	0.23700118564204	-4.03957309828553
C	2.20450997519094	-1.00098409112385	-2.84065725580501	C	1.52324250025894	0.93941913575976	-3.35175782904606
H	2.85492484609719	-1.38896662591193	-2.06166303978029	H	1.78899095825742	1.77161409800016	-2.70447385905412
H	-0.07358964565789	0.33348008244538	-5.67193960837988	C	0.54626396582731	-2.06201903858720	-5.58901288492206
C	3.69962605209758	1.00364837504996	-3.03124086408135	C	3.95245912424372	0.61886738727643	-3.90815866999758
C	4.06707486114939	1.09625609770141	-1.74169954629317	H	4.92721284802309	-0.30124761647575	-3.81912794225365
H	3.45389546070156	0.61590632066135	-0.98706161094787	C	4.65460490900739	-1.35086116301816	-3.80815792538245
H	4.94100961065057	1.65049474371774	-1.43006858482332	H	5.96991529418256	-0.03024391025735	-3.73405818700672
H	0.85837860043478	-2.67661236357623	-2.73800720855690	H	-0.57169545351762	1.10633401026838	-2.91197637905040
N	4.37005969535329	1.63644735332984	-4.09685468716312	N	4.15545940498661	2.01084491931608	-3.87181166571307
O	-0.80654490754711	-2.05242096616278	-4.54337657732852	C	5.27359658661728	2.70197114416321	-3.47281243523749
C	-1.67822953727297	-1.62365368800387	-5.59737746506693	O	6.29910620032990	2.16025749158951	-3.07379056110662
H	-2.15041840608104	-0.66318473348642	-5.35616824426268	C	5.15286026297457	4.20382654190235	-3.57306348218511
H	-1.13981071947333	-1.54506000112986	-6.55010389143345	H	5.50201507708638	4.64600413138536	-2.63564017906811
H	-2.44646327830318	-2.39481506811302	-5.67776972702201	H	5.82012639312007	4.55203078436497	-4.36942931340025
C	5.25982671576406	2.68126778294496	-4.04847471115501	H	4.13900670686491	4.55339018556262	-3.78449210595429
O	5.62115367016430	3.21943455177764	-3.00700529754192	H	-1.21117396455954	-0.81811612241388	-4.34790851990258
C	5.76897152052553	3.13710615394079	-5.39539882281280	H	3.37229696250507	2.57333770315953	-4.17471315687922
H	5.53128867602897	4.19910387267721	-5.51419348674614				
H	6.85961332465141	3.04279379675672	-5.40576806402462				
H	5.35342676237601	2.58031221642030	-6.23914300202856				
H	4.15134340317192	1.28419064543984	-5.01835356357484				
N3				N5			
C	1.20700314617233	-0.22115837449615	-5.72968762775837	C	1.24512923803293	0.27707080277155	-4.68970482503934
C	0.19073156590653	-0.20223047518098	-4.77825811096465	C	1.02847278788803	-0.83751800320168	-3.88302388742073
C	2.52915082280888	-0.01065843900459	-5.34994611284414	C	2.36969355673252	1.07472218200402	-4.50040992966679
H	3.31681057428758	-0.02705250041632	-6.09622470236971	H	2.51634091931295	1.94151155693197	-5.13829226426459
C	0.50759460825813	0.03474787939107	-3.44103402987732	C	1.94595271744005	-1.144370823357415	-2.87988963590308
C	2.85916955891037	0.212111952369082	-4.00628936325348	C	3.29556479530179	0.78408557812180	-3.4884008031505
C	1.82664268120656	0.24441891765638	-3.05789482371292	C	3.06614427296168	-0.34361239738623	-2.68552166674718
H	2.05141327057803	0.45531443412370	-2.01659232595822	H	3.79021965226002	-0.60737322709435	-1.91930123874950
H	0.97090488676890	-0.39972933176546	-6.77538603454999	H	0.5355346073833	0.52779731786910	-5.47389252802456
C	4.27567060095520	0.41144132092085	-3.61521478032313	C	4.49952615240088	1.63031077799746	-3.27668347431724
C	4.74811180444980	0.18452557609619	-2.37805493840857	C	4.93889732591480	1.88939550322376	-2.03431825961748
H	4.09787460866347	-0.19370323456802	-1.59881688576862	H	4.41506082363227	1.52581790768123	-1.15458381913506
				H	5.83081316212103	2.48950823119215	-1.87163143651800

H	1.79534902908860	-2.01939360047992	-2.25298284306593	H	6.88869175929980	0.32925772662795	-0.71430439706005
H	0.15563497137208	-1.46571953149704	-4.03861764836850	C	4.82684742302680	-1.21712429601122	-2.77684982651295
Si	6.28490135302768	0.75815946929962	-5.32979811120825	H	4.91183173037110	-1.83166441288692	-1.87143730457940
C	5.19874050697874	-0.55925686346616	-6.11678554859879	H	3.97723340447946	-0.53827467961314	-2.64103693568424
H	4.61016998828406	-1.10225850744900	-5.36813757284026	H	4.60069364132880	-1.88563678672557	-3.61541932722902
H	4.50115346795021	-0.12653671506784	-6.84423407132522	O	6.28512894728970	0.63944394184059	-4.51048517733294
H	5.81895217615876	-1.29285141084685	-6.64810833575972	O	4.16358884959591	1.08686762521126	-5.29788018418162
C	7.31982387516324	1.59827979868308	-6.65588983524621				
H	6.68474661688522	2.10020819894282	-7.39643530990582	N7			
H	7.98702490809023	2.35285866771960	-6.22156111666518	C	1.32625244485047	-0.35586362073624	-5.71915396858859
H	7.94237461812439	0.87037162780284	-7.19077317550954	C	0.38090140361961	-0.67504436787664	-4.74501927795107
C	7.39899358643468	-0.03100113068090	-4.038943068855063	C	2.55419055033095	0.18354061405825	-5.35648466054287
H	7.99909077998182	0.72223479892990	-3.51335688468811	H	3.28933453697621	0.39713405954115	-6.12723094000459
H	6.81700104955942	-0.57800787291319	-3.28735964498214	C	0.68298267375775	-0.45450422342009	-3.40434339364184
H	8.09117779466950	-0.74278668846798	-4.50605039349428	C	2.86854210222559	0.42750817675242	-4.00925184133562
C	5.23714148024419	2.11471543785184	-4.49123571792512	H	1.91432102539967	0.08313207616009	-3.03944048160391
H	4.55440562831658	2.52119508180625	-5.24846136899775	H	2.12498565450194	0.24857906445936	-1.98727204912280
H	5.92409289420099	2.92446778258173	-4.21298462872166	H	1.11061741450412	-0.54141829006775	-6.76815702938207
				C	4.17326146659744	1.01622700990599	-3.61687335433675
N6				C	4.86183717320631	1.81913276401162	-4.44132950227956
C	3.47442889586709	5.80634216285164	-5.78974262789295	H	4.48586816425776	2.10782023914163	-5.41869466800782
C	2.34910083303783	5.66480448062127	-4.98167829486751	H	5.82292134218918	2.22830099009336	-4.14137880505439
C	4.51660998033505	4.88768785406543	-5.70692528146096	H	-0.04223670456646	-0.70383018559194	-2.63419138784605
H	5.38353792149682	4.99056928931219	-6.35394334670401	H	-0.57730098737455	-1.10129617269715	-5.02931132478805
C	2.27325816187347	4.59669976953952	-4.08858577189335	C	4.69629451817882	0.69536923004152	-2.24199680522704
C	4.45049026075395	3.81656389285201	-4.80831573006259	H	4.07809651185352	1.15650473912884	-1.46204074399743
C	3.31173275428132	3.67701526518455	-4.00305888238281	H	4.69052262382955	-0.38511881457984	-2.05575094705417
H	3.24870055765388	2.84965605677318	-3.30256735586671	H	5.71663761327025	1.06820185592481	-2.12119127632772
H	3.53876379241208	6.62943331680957	-6.49635435921999				
C	5.58308725887157	2.86927075955919	-4.70652120501743	N8			
C	6.86654918320065	3.25262213361651	-4.72997824586247	C	1.52017114586756	-0.75045070248449	-5.58894046170353
H	7.10806638026483	4.30801571228887	-4.79569857882867	C	0.33073143717831	-0.57033725195748	-4.87889261399551
H	7.67730261666448	2.53907022994984	-4.65498646668411	C	2.74586740072808	-0.40227327042594	-5.03152354924230
H	1.39964191227319	4.48046585689298	-3.45268619577066	H	3.65838235211370	-0.55010590462156	-5.60520544045559
H	1.53362269792220	6.37977619475693	-5.04932174310998	C	0.41311344677093	-0.02276288017676	-3.59091613486246
Si	4.49994115029461	0.50275818818643	-6.86769161887853	C	2.83055143846682	0.14204122827075	-3.74191824946657
C	2.81897031232229	0.69487143361331	-7.66231942498662	C	1.63304791378913	0.32578005956860	-3.03087023403646
H	2.04820798942856	0.15845375564900	-7.096017616504473	H	1.65212057610806	0.74911733712454	-2.03042602164800
H	2.52625274377486	1.75022505490422	-7.71809665181155	H	1.48674580542002	-1.16761050496060	-6.59307505138392
C	2.82495462895061	0.29057155751268	-8.68222522010368	C	4.14933717156880	0.49280248191409	-3.20452468176813
H	5.79237218930370	1.51904998197584	-7.75760219911486	C	4.42160061677760	1.01700171820108	-2.00384398939265
H	5.85314252238110	1.17464829179878	-8.79897745112816	H	3.65110917725734	1.24731107870046	-1.27225611034529
H	5.53541683143278	2.58406374332569	-7.77497452731367	H	5.44774320233808	1.23231648465256	-1.72039688550921
H	6.78585068080666	1.40912582401391	-7.31132070428812	H	-0.50001646531255	0.13276160769529	-3.02000803285521
C	4.98376721336782	-1.30369242527978	-6.82762945192956	H	4.98143472004224	0.29166139255681	-3.88038571567684
H	5.96682296916366	-1.45521377188431	-6.37007791839641	C	-0.99331015451050	-0.9756775668959	-5.46122801040444
H	4.24832509109618	-1.89865227222271	-6.27328051377905	H	-0.96989931469515	-0.95761050039998	-6.55500809352335
H	5.02311299650227	-1.69991149826701	-7.85095160814975	H	-1.25624787952905	-1.99685217166786	-5.15572706571037
N	5.18547280491510	1.52909307419270	-4.40902332159788	H	-1.79793895637944	-0.31783295738994	-5.11783669119113
Si	6.41016533469271	-0.27229972675034	-3.06700581156057				
C	7.85128362282992	-1.39765031531058	-3.43699200258186	N9			
H	8.75155186336742	-0.82239500692530	-3.68392196211634	C	1.68543205623439	-0.81231728067936	-5.40014522099379
H	8.08291174213192	-2.02149874139030	-2.56491491594349	C	0.38746253004415	-0.51958225455766	-4.9722932484777
H	7.63286582864594	-2.06699112161485	-4.27728038480413	C	2.77983003620743	-0.40653001494217	-4.64833248076283
C	6.77546631071233	0.89000843079133	-1.65083469317351	H	3.78067719491615	-0.64357114130218	-4.99798001889716
H	7.70360430870443	1.44827359058533	-1.82058206869638	C	0.192532467459624	0.18514838454722	-3.79217839304980
H	5.96295656646177	1.61219280760669	-1.50788327037917	C	2.60170553794827	0.30469701278869	-3.44983878037060

C	1.29141458401014	0.59238626764615	-3.03769607815595	C	2.87658760339979	-0.20890927038967	-3.98395945347903
H	1.13670700649669	1.14315467389587	-2.11246124015391	H	3.85876186883315	-0.48421572736082	-3.60915188009423
H	1.84302257708225	-1.36142025560042	-6.32477797759857	H	-0.63789781415834	0.71005733893100	-5.28590682459601
C	3.71879970217203	0.75967885784313	-2.61306911214632	C	3.59548329825958	2.20112956377243	-4.04261877090938
C	5.02376808019060	0.56741335410033	-2.83395748941307	C	3.23234429213263	3.38181268261677	-3.51447644168358
H	5.40325836915462	0.02726797113750	-3.69770931653598	H	2.21307963062919	3.57350545674521	-3.17564711081670
H	5.76055378621612	0.95585867379197	-2.13681946057133	H	3.94144218308602	4.19642598588205	-3.38594538999312
H	-0.81026277196925	0.41898388571195	-3.45285434559892	H	2.17086100183326	-2.23485287479679	-3.93030895038587
H	-0.46536396749129	-0.83967000824776	-5.56953835400452	Si	5.39473137072870	1.93483417178351	-4.60377221443578
H	3.42075458782703	1.31097875923562	-1.72058727471186	C	6.37841003171501	0.93479486321135	-3.34621064248754
				H	7.44323277311118	0.95794589294131	-3.61294559625684
N10				H	6.27928037990065	1.35966089361598	-2.33994606270306
C	1.09585524032631	0.02933774150910	-2.50521529262453	C	6.07563109316556	-0.11684874704852	-3.29970609672046
C	0.36529726893353	-0.19478334963630	-3.67052918811377	H	5.38090173438840	1.05297246375495	-6.26355755123182
C	2.46031012189146	0.29452741919991	-2.57288535788371	H	4.95249935016920	0.04684397331909	-6.18683812989202
H	3.02173453181970	0.48823110963481	-1.66216576648751	H	4.79335495952213	1.61070778284557	-7.00330928116733
C	1.01268772025649	-0.15287356366081	-4.90370963393657	H	6.40127853344031	0.95164206139879	-6.654170889504377
C	3.12389260905438	0.34343054006911	-3.80831751306619	C	6.22535567818590	3.61061689448113	-4.78688650739170
C	2.37542405867974	0.12155457720533	-4.97316980944465	H	7.23834267932411	3.47240253114262	-5.18615648110503
H	2.86951092967593	0.14138643235195	-5.94003278859896	H	5.68257511532486	4.26613923604388	-5.47792666029361
H	0.59979426241349	0.00490927121801	-1.53828136657213	H	6.32205053219158	4.13251607979949	-3.82763747339391
C	4.57383637761218	0.65540810159398	-3.87117908062759	C	-0.38840431178612	-1.97080143569172	-4.85931575887428
C	5.43409209556708	-0.00395436753519	-3.07896932744999	H	-0.12682007570836	-2.89107867378474	-4.32890460572291
H	5.10358510509629	-0.80897555643435	-2.42043438467040	H	-1.38166879320509	-1.64937330192253	-4.52835862511163
H	6.49750659227528	0.22314467015802	-3.06793869107547	H	-0.46735729889005	-2.21373535331783	-5.92670279468806
H	0.45394497759894	-0.33369492972630	-5.81835292025125				
H	-0.70074745522647	-0.39851554203285	-3.61810765744312	N12			
Si	5.15999978866961	2.12105563558132	-4.934054125956596	C	1.36708406066620	-0.28518005826035	-5.65743863260419
C	7.01592314845910	2.344958622416287	-4.67601115885312	C	0.32539999645129	-0.21538057416082	-4.73466489719164
H	7.37023905705963	3.19390585999018	-5.27355460035226	C	2.66060268707960	0.066380798165224005	-5.28361284224005
H	7.27260898637358	2.54675362879103	-3.63018365225702	H	3.46371836206826	-0.00240769920382	-6.01212392709001
C	7.57567645321814	1.45847645677707	-5.00023730796447	C	0.59059122689318	0.20718379649218	-3.43341115972143
H	4.87668781139717	1.83363049985882	-6.78323235334361	C	2.94621576768296	0.47767864358338	-3.97304059395360
H	5.42105283439409	2.60253167250054	-7.34640637335156	C	1.88512473455375	0.55103367745850	-3.05677422269081
H	5.26147639044510	0.85649361066019	-7.10046958674644	H	2.07976810806623	0.89928880359444	-2.04552892724854
H	3.82355941450365	1.89953696872831	-7.07453203824304	H	1.17258584520405	-0.61431188724565	-6.67490202238544
Si	3.98912754124330	4.04529328221034	-4.21744848485545	C	4.32561582076426	0.84228990232131	-3.56727812510510
C	4.56261138656083	5.53129808838096	-5.23499805056340	C	4.80856401744713	0.42584890988032	-2.38569052767894
H	4.04455566001056	6.44260243220124	-4.90805591349419	H	4.23312007277052	-0.22333550789330	-1.723946450239421
H	5.64017920898477	5.70408244962599	-5.12780549068551	H	5.80190853937121	0.70392544074902	-2.04084424326189
H	4.35050669610560	5.39304203074114	-6.30214035123835	H	-0.21675039975079	0.27784998956951	-2.70893483283426
C	2.12325751436644	3.85165667805450	-4.43964795480389	H	-0.68618622146802	-0.48128490103523	-5.02909729048436
H	1.61360184371378	4.78542837213231	-4.16643191938006	H	5.37735957290332	1.97615037073837	-4.67655838503404
H	1.85788138503332	3.62000100776127	-3.80414677033213	C	6.77537695233593	2.69601800379603	-3.64814837640811
H	1.72162739585007	3.05364744331914	-2.393870345142229	H	6.40522631845513	3.22818020164240	-2.76409516051249
C	4.35450277336080	4.37375024615277	-1.76332612768188	H	7.48056734899176	1.92659924856281	-3.31249799157657
H	4.04187130247433	3.53247907092888	-2.22141484841952	H	7.34074000114893	3.41377555780986	-4.25625804327569
H	5.42477425116891	4.53941044895303	-2.04738677227997	C	6.13748081770647	1.03864702691940	-6.12295228821242
H	3.81854561436917	5.26716545228433		H	6.89471423211747	1.66980576224694	-6.60640143104148
N11				H	6.63531010455521	0.12100432358489	-5.78720671654036
C	0.34793349434168	0.44415256983443	-4.90898953029472	H	5.40310684592930	0.76512950545961	-6.88833112766983
C	0.63743039730851	-0.89633490521604	-4.62886393191546	H	4.27928411768942	3.35860819658643	-5.32060451757221
C	1.29910418081940	1.43970503482340	-4.72476999432383	H	3.47913353023227	2.97175225415429	-5.96271851455141
H	1.05181130535772	2.46992357079221	-4.96879825691454				
C	1.91788825694581	-1.20209987339509	-4.16066973029671				
C	2.58457408231017	1.13617121827150	-4.24775116750756				

H	3.81013350798638	3.91085029008769	-4.49701830962019
H	4.86554183624851	4.07280743239655	-5.91231740910061
N13			
C	0.90030500632107	-0.03499108299270	-5.65434834822533
C	-0.07378920283109	-0.32325011657690	-4.64761639225742
C	2.22019844400249	0.29297781710668	-5.26479813689456
C	0.32161937978987	-0.26569378536984	-3.28786190800175
C	2.58655161960531	0.33507241339906	-3.93202015447529
C	1.60805200412445	0.05497147889708	-2.93944384600440
H	1.88407964272058	0.12011030675618	-1.89115898010661
C	3.97838254833532	0.65336567083550	-3.52670857730671
C	4.56301810059274	0.06857617343309	-2.46735103933480
C	4.01383342591210	-0.68269577216376	-1.91093260012461
H	5.57510017734030	0.30192339371927	-2.16892456987043
H	-0.41854757525508	-0.46688780999305	-2.51705390428213
H	2.95205982311289	0.48046159646929	-6.04764565079255
N	4.60442135390480	1.59602343491753	-4.36296623530894
H	3.98523289332766	2.13048285423601	-4.95626464269072
C	5.94371932249060	1.87476880558150	-4.48626643695062
O	6.81854862761138	1.30598713662829	-2.16892456987043
C	6.27140226974585	2.95138215751332	-5.49304954672647
H	6.98519873970104	2.54502954795481	-6.21637676282510
H	5.40011889608738	3.34035297110789	-6.02575549777626
H	6.76802247545497	3.77550497331076	-4.97034909542455
C	0.51598721968937	-0.09367448301965	-7.01757974792386
H	1.25879386082461	0.12216845293773	-7.78196750492340
C	-1.39422684955883	-0.64955967872748	-5.03996726853403
H	-2.13207270214319	-0.86482646086022	-4.27059835102689
C	-0.77380166951805	-0.41706086681754	-7.36693271061989
H	-1.05875384505035	-0.45910172556333	-8.41464497288491
C	-1.73664200136982	-0.69640983141622	-6.37127352283145
H	-2.75197597475795	-0.95001227503592	-6.66349283402245

N14			
C	0.89929504041522	-0.33171199203728	-3.34108961625218
C	-0.03202008700996	-0.41822263658724	-4.37827005744600
C	2.08167769941580	0.38672740426027	-3.49181625815002
C	0.25980634113132	0.24259289278075	-5.57787361274589
C	2.36660989110780	1.05160125169153	-4.69090381006591
C	1.43694542014193	0.96030366734104	-5.73584291304950
H	1.64954366799035	1.44398909501877	-6.68533421818274
C	3.60743124984324	1.85002150000728	-4.85272672754790
C	3.62341196610726	3.01697458117288	-5.51889449428660
H	2.69178096389128	3.40325052908693	-5.91753848919571
H	4.52828719020860	3.59287819997634	-5.65088566213936
H	-0.44346483227468	0.18166635953823	-6.40586048252917
H	2.76943439934192	0.45375593828152	-2.65214743071564
N	4.72774810012887	1.26729818112842	-4.23139575797460
C	4.62293291491266	0.29761308687256	-3.96722728339658
H	5.93601675020186	1.84447998884698	-3.92655300302858
O	6.21405263917326	3.01204563790381	-4.17995181627142
C	6.92113987190838	0.92133298233819	-3.24941710604919
H	7.29871461900030	1.41518327504498	-2.34916962017035
H	6.50366153679214	-0.05235753600145	-2.98011090635925
H	7.77242544510034	0.76919636768569	-3.92179777105117
C	-1.29893214566139	-1.21217133398598	-4.22858211250260

H	-1.25457068297668	-2.13356926177513	-4.82258804005844
H	0.69405957521425	-0.82673088267060	-2.39465195342568
H	-1.47124735547625	-1.49399685195683	-3.18604054221462
H	-2.16600346562461	-0.64398984515396	-4.58259732940900
N15			
C	0.74186965295699	-1.21851829166057	-4.93578602535559
C	-0.10051415206610	-0.28927879737857	-4.33671497316006
C	2.11446005356503	-1.01171903870858	-4.88355515998704
C	0.39901061196018	0.83471566031214	-3.69111451939730
C	2.65251349255343	0.10574490916254	-4.23392543666947
C	1.77521007798505	1.02657435179506	-3.64624928537843
H	2.16326555739281	1.89471918703279	-3.12010536029347
C	4.12264059738549	0.29718602295823	-4.16081390952302
C	4.96135818122915	-0.73160284851858	-3.95546122082672
H	4.54718036070460	-1.72223940484428	-3.80294479600862
H	6.03327159418188	-0.60101300462442	-3.91208614408969
H	-0.27101605473054	1.54782447673683	-3.22191941358186
H	2.77537370399308	-1.72162427076550	-5.37201733388592
N	4.51721999277472	1.63963244790188	-4.30772221290450
H	3.82208022851106	2.25962556798105	-4.70003878975989
C	5.72110287376498	2.21495891094253	-3.97855748175551
O	6.65751656541479	1.59281993655922	-3.48900748196138
C	5.81350926921440	3.69255704467077	-4.27332317142262
H	4.86942669517243	4.14097063130709	-4.59257690485938
H	6.17414519927854	4.20507050976507	-3.37666636878124
H	6.56142425942988	3.84211186486082	-5.05970720877007
H	0.33559460577790	-2.08397997608479	-5.44908361707882
Cl	-1.84213682057683	-0.53773284756598	-4.40650528187081

Methyl Cation

⁺CH₃			
C	4.79802215739245	1.67812592124582	-3.98326233614709
H	5.17511112048160	0.68650951687248	-4.23497022779640
H	5.36889611442256	2.56503652561028	-4.26067903761868
H	3.85081961270338	1.78335986927141	-3.45338389343782

Methylated Vinyl Azides

1a-CH₃⁺			
C	1.35208658242759	0.32062636128678	-5.57540241286209
C	0.72440808519685	-0.87332625424000	-5.15507404726361
C	2.26436064147589	0.92395190998202	-4.74976504735440
H	2.74325960267889	1.84090170794825	-5.07696431324745
C	1.03519420231701	-1.43876366191573	-3.89768759265924
C	2.58640416946322	0.37796521912224	-3.47609618894731
H	0.54166198571880	-2.35923316893393	-3.60272026786060
C	1.93954012191664	-0.82579369546052	-3.07642585557161
H	2.16297112487617	-1.28028297882078	-2.11822688230066
H	1.12175912548194	0.76410058295334	-6.53665756089611
C	3.53733100846277	1.00073037074267	-2.63907896955418
C	3.93687850226325	0.49942813697184	-1.29430293629324

H	3.10921318989294	-0.03977235434924	-0.83243836013587	H	4.25315757239990	1.65148242657137	-0.72673319683054
H	4.16610522610271	1.35238012300346	-0.64449528736607	N	4.84460899811701	-0.19014617460013	-2.50776928744980
N	4.15144126417059	2.09832742585566	-3.16407654947925	N	5.82891804387373	0.14972375442613	-1.81594151021145
N	5.00652173418780	2.70375034486953	-2.48741849576368	N	6.80357212405786	0.29217188907205	-1.27969606060009
N	5.79277372300928	3.36736698312781	-2.03769184633083	C	4.18422948744694	2.99486504824319	-2.43490801871717
O	-0.172614566315026	-1.53716990042417	-5.87105085409679	H	3.56803971216415	3.17420118093270	-3.32007472763621
C	-0.55912999750372	-1.03305264342749	-7.17288154027507	H	4.14856346574942	3.87993631470432	-1.79415664991804
H	0.30589960774857	-1.00675480048820	-7.84263862229395	H	5.21971959767966	2.84001304683249	-2.753144544474984
H	-1.29752836260491	-1.74307813428670	-7.54461628926893	C	-0.51573064962714	-1.24894872969542	-5.85082516290192
H	-1.00850629048381	-0.03979012795289	-7.07815282776216	C	-1.37513868357237	-0.32447109618460	-6.47153455237863
H	5.17089125663166	-0.42057139349497	-1.40113393974431	C	-0.71554550103153	-2.62117309838719	-6.08654843840368
H	5.45051261367394	-0.75016978054489	-0.39685696044352	C	-2.39301786821236	-0.76080152474490	-7.30733900554949
H	4.94580029786714	-1.30024017557423	-2.01050761246450	C	-1.74694616551411	-3.05126272607682	-6.90897153012219
H	6.02622114689956	0.10038391486376	-1.84256473448251	C	-2.58580799102593	-2.12422226290601	-7.52585960351819
1b_CH3⁺				H	-1.22252609252604	0.74095950125012	-6.32862741478916
C	0.41018604217240	0.10003362482399	-3.82555417224060	H	-0.08467359484118	-3.35555251904225	-5.59507788906756
C	0.58163788074442	-0.51840068056233	-5.07574250322979	H	-3.03709444320419	-0.03465495937551	-7.79480734839743
C	1.49475269766853	0.45896703923786	-3.05651831983534	H	-1.90060498311191	-4.11482329652242	-7.06709378832845
H	1.32384835647589	0.93782157528588	-2.09915251837103	H	-3.38794529157164	-2.46348989253336	-8.17523250574670
C	1.88908337487618	-0.75571044208064	-5.54110163560596	1d_CH3⁺			
C	2.81100327482746	0.22230320570307	-3.52388819949845	C	-0.60260084392257	-0.00852346512504	-3.31614852335796
H	2.03103869479400	-1.23031459742017	-6.50799187278537	C	-0.62253456775396	-1.24101415115250	-2.65662229257422
C	2.98244585464069	-0.39438630534728	-4.79123151579992	C	0.36321515188830	0.92519052549173	-3.00367588659672
H	3.98138678003716	-0.58474604354457	-5.16945108512598	H	-1.38586256006622	-1.97251292661792	-2.90641794198284
C	-0.59450768695037	0.29515795318232	-3.46159718093115	H	0.37750735892769	1.88123265063398	-3.51594987714526
H	3.93559984782267	0.62184264131474	-2.75010295826685	C	0.32739735355499	-1.53952436871992	-1.67845348403015
C	3.85130544571750	1.27354301322711	-1.41565992465191	C	1.33033793716135	0.63966270546088	-2.00771044233655
C	2.95066334852292	0.94779070203095	-0.89413919347474	H	0.30541375121334	-2.49964503388302	-1.17315897587305
H	4.70888178537671	0.96548930597382	-0.80616344067493	C	1.29511990025546	-0.61065326703047	-1.34677158220996
N	5.13996721939898	0.43008564283132	-3.34136044801002	H	2.02648688392217	-0.85690529467782	-0.58566068202622
N	6.18122957368562	0.76046461068343	-2.73021138537747	H	-1.34669921077725	0.21466654283942	-4.07402130827620
N	7.21168653251149	0.98986956554055	-2.35385988836944	C	1.59615136315556	1.68443143500476	-1.68443143500476
C	-0.59606305055040	-0.94509578247634	-5.88166319354622	C	3.39026193948535	1.38750896779522	-0.64970480318345
H	-1.47930516186757	-0.34249083188986	-5.65416209475792	H	2.99859421440045	0.76626236073512	0.15687640525483
H	-0.38300680125051	-0.90323190585699	-6.95358547189782	H	3.67181395543185	2.35169106439456	-0.21147642956848
H	-0.84115684082303	-1.98983204738055	-5.64229875850810	N	2.33618940838943	2.71258918466895	-2.44366798167323
C	3.84576115946053	2.81088877958809	-1.56814836717603	N	3.19009349725917	3.60678412445274	-2.23065186730697
H	3.80814646129540	3.25748677833917	-0.57108940060658	N	3.85745336852279	4.50505874461538	-2.20294769095537
H	4.74850615102423	3.16781347157165	-2.07335659064124	C	4.63599845155209	0.71790082616362	-1.27471465215107
H	2.97197936033677	3.14028562196942	-2.13675989165265	H	5.06153241137362	1.33326951981127	-2.07300339441892
1c_CH3⁺				H	5.38839948347628	0.59645441093522	-0.4911437821437
C	0.43806683310132	0.39809980330276	-4.22812769764888	H	4.38621461073245	-0.26525347863242	-1.68194437966001
C	0.56677578362218	-0.79102506636308	-4.97657091558692	1e_CH3⁺			
C	1.44578372028662	0.82695425134355	-3.39723220573346	C	1.33975118134275	0.17593620657571	-5.63670903130389
H	1.30206431811920	1.73934540330109	-2.82963810366243	C	0.37853329123689	-0.41541224163333	-4.80316467793724
C	1.76554570206148	-1.53014261887847	-4.86087477763559	C	2.54719384000776	0.59000545946001	-5.12157932428036
C	2.65080452904792	0.08948655234112	-3.28747999702210	H	3.27964032789873	1.05206224531945	-5.77459858691706
H	1.90169394916622	-2.43312746261906	-5.44657851476269	C	0.65226245910356	-0.59139515617571	-3.44079371324705
C	2.78422702440528	-1.10239563095680	-4.04711350886870	C	2.833131456663425	0.41442520696063	-3.74468263143287
H	3.70069329103331	-1.68014025593358	-3.99083231581495	H	-0.09396429741666	-1.04852106105750	-2.79739490819436
H	-0.48181594762178	0.97080217230724	-4.27881389432337	C	1.86121085239833	-0.18856966956520	-2.91270166598473
C	3.70828064810702	0.54951353651181	-2.45759380105459	H	2.04400561757949	-0.33026731164442	-1.85380761123195
C	3.65171664850895	1.78679989774204	-1.63312030502282	H	1.12520476219433	0.30892369136060	-6.69329762890051
H	2.62586803225873	1.97534322604742	-1.31397973989613	C	4.07481334078607	0.86716592863777	-3.19705786952080
				C	4.44874064780863	0.75165314814989	-1.74604348379264

H	5.12637405462332	-2.18993904421479	0.26485183466987	C	2.68171518680824	0.06894938092013	-4.08821654096740
C	3.16015180552692	0.81000416586030	-3.64347066454081	C	2.01980244249122	-0.63891994000396	-3.04840299122775
C	3.99901139649397	1.27094210235925	-4.79086505323674	H	2.46042026132217	-0.73545981325139	-2.05984211068568
H	5.01914457512373	1.46385295168737	-4.45806553272298	H	0.44280730651007	-0.50763027418399	-6.59748825184564
H	3.59581423834155	2.23303161482748	-5.13419696558884	C	3.89850516045062	0.79365638456515	-3.87293943536142
N	1.81211148364280	0.92251070210790	-3.72438432848753	C	4.76850413359128	1.21170904029594	-5.00754708836720
N	1.29471643782124	1.47858013355605	-4.71875826249568	H	5.81232101490509	1.05296969603178	-4.72662265888721
C	0.64232857419363	1.93171120677477	-5.51114651228682	H	4.55396395884489	0.58307712123472	-5.87211431604458
N	3.99157122994932	0.26736849011715	-5.96091417882060	H	0.34821935800378	-1.85774486790731	-2.49707933902598
H	4.42710646605606	-0.68799090404838	-5.65552352774701	N	4.21647955933029	1.12884573579111	-2.61696125178373
H	2.98170812471332	0.08142382610963	-6.33895231625129	C	4.56040175559698	2.69759807034598	-5.36094801581649
H	4.58852587046946	0.68060793106393	-6.77831477973155	H	3.52970225577818	2.88129951804089	-5.67882051129150

Methylated Substituted Styrenes

N1_CH3+

C	0.90116800387432	-0.68101676598880	-4.40268584211690
C	1.16969688430701	-1.02800696952704	-5.72484596023962
C	1.85397885725002	-0.00524019402280	-3.65006017162411
H	1.64466592888407	0.25976617723441	-2.61756158150361
C	2.39114412609409	-0.68698930242406	-6.30242502250582
C	3.06940160321968	0.36489609233876	-4.23787489025019
C	3.33666804581995	0.01829052051657	-5.56948499120341
H	4.29193973858493	0.27922963071125	-6.01725990347910
H	-0.05070285999734	-0.94509091520516	-3.95153303438971
C	4.10645083163051	1.03675026203840	-3.43295755706158
C	4.57156847189256	0.33330474570290	-2.19863597151933
H	4.91672563969979	1.03592651686499	-1.43666112227996
H	3.71176128473744	-0.20538537724721	-1.78973447447463
H	0.42855744636252	-1.57074725155634	-6.30460582071799
H	2.60956124194298	-0.97147362270494	-7.32749651751945
C	5.81303221585828	2.79800429468135	-3.20495267697939
C	4.11701830600757	2.98399472885280	-4.94305789554405
C	5.41838035377834	4.18797142385613	-2.71841388138833
C	3.79067225564512	4.36750959077488	-4.38199047378003
H	6.58412952384211	2.87913005657204	-3.98076946739736
H	4.88623587908060	3.05251135216833	-5.72029957992480
H	4.66041431454124	4.10590143140498	-1.92247968390713
H	3.46169099733875	5.00796784406900	-5.20543291942377
H	3.21386911681187	2.53525039047201	-5.35544569078552
H	2.97481055475124	4.28308768417470	-3.64553034092996
H	6.30368930664138	4.68955122048297	-2.31761066594059
H	6.20067532533710	2.19544509239643	-2.38575326827729
O	4.92918053875549	4.98413293277574	-3.79267912058611
N	4.64779359270242	2.14768878272520	-3.84224408017451
C	5.67399168892915	-0.68530327813091	-2.54464963100358
H	5.31482194571939	-1.41462212182566	-3.27699402937660
H	6.55833159516618	-0.18768832857666	-2.95438857042529
H	5.96441127976971	-1.22063321925105	-1.63671957299709

N2_CH3+

C	0.88134891843024	-0.55574769412201	-5.60804920469592
C	0.24522202796828	-1.24665690619658	-4.56221851906415
C	2.08460334222399	0.071143786667272	-5.37001989632062
H	2.54875859950116	0.61026517652232	-6.18782309669036
C	0.83740169680073	-1.28941249535004	-3.28189013490904

N3_CH3+

C	0.42525505779051	1.10932073648609	-4.06514310561702
C	0.12642044642502	-0.10633601570387	-3.45039573754697
C	1.74242517422785	1.45357085930135	-4.31665509991450
H	1.95886162289127	2.39879564927598	-4.80175877237078
C	1.14795401917574	-0.98554456343037	-3.08395938048215
C	2.78175273064597	0.57466114011138	-3.94967613225879
C	2.46684415689392	-0.65350138036708	-3.32966174123271
H	3.26226660457188	-1.33218771577566	-3.04157037166949
H	-0.37363473386623	1.78626435118442	-4.35083699665928
H	4.16373886513689	0.91866890721700	-4.19594937230723
C	4.58488493647325	2.24657433942636	-4.71067460061114
H	5.58759622603447	2.17061956585621	-5.13736384574600
H	3.90842273327977	2.57047421445422	-5.50623597896942
H	0.90721172773242	-1.92951743177000	-2.60492722956324
H	-0.90896989337929	-0.37232554575408	-3.25657218393281
C	4.57910042026263	3.28790064518928	-3.56760726374170
H	4.97136341302229	4.23078174411331	-3.95785224682804
H	3.56681671549291	3.45649273628982	-3.19195732468795
H	5.21177238018271	2.96465204966271	-2.73667735177286
O	5.03506581640267	0.03313895101608	-3.88919690913730
Si	6.78804540802461	-0.14939589288749	-4.07092473817994
C	7.03358718039232	-1.76725271822200	-3.20307401856399
H	8.09157606116237	-2.05459733279506	-3.23363974964406
H	6.73433315367934	-1.70243824827553	-2.15041707150254
H	6.45339254721748	-2.56622333997336	-3.67880306277891
C	7.08575477116149	-0.24172604101559	-5.90114530667996
H	6.93636007963764	0.71715228122973	-6.40797256918200
H	8.12354388253235	-0.55308993282465	-6.07691864837351
H	6.43215846597085	-0.98838922014719	-6.36694844727219

C	7.62438545944122	1.26547050836286	-3.20792434694422	H	4.44915554712730	-1.63825733432847	-6.57250306617180
H	7.50498763415326	2.22281203559162	-3.72475246556867	H	4.12329081984408	0.10743193067960	-6.69505746135991
H	7.27062559941985	1.37113465168093	-2.17622003762135	C	6.75042819111225	1.39557371090765	-5.19203278958634
H	8.69960773083063	1.04556206125742	-3.163411139634437	H	5.96842742277314	2.15818204412421	-5.27372181045980
N4_CH3+				H	7.34637180808598	1.60150629440295	-4.29575630482601
C	1.79925041241804	-1.77957972146136	-1.94688420845935	H	7.41190530347025	1.50610040960584	-6.06160782861040
C	1.37868865342643	-2.47474304998442	-3.07932324378144	C	5.06096175668726	-0.57374559592537	-3.44996893821211
C	2.66562851662538	-0.70608479758904	-2.07118131703077	H	5.85132923230364	-0.29055234701482	-2.75131085392341
H	2.97779643576301	-0.16935513607238	-1.18208538633065	H	4.84088837056131	-1.64470416359723	-3.45425123272196
C	1.82026011163716	-2.08989607425815	-4.34576331440562	C	1.69151754374820	-0.57733769920547	-2.88420065166655
C	3.09136319222499	-0.28772993611868	-3.34752690286580	H	0.79585748920864	-1.07457031737538	-3.2670890622796
C	2.66071336676736	-0.99976552959736	-4.48664641879642	H	2.14643660550036	-1.21954721419028	-2.12393652805792
H	3.02903097644302	-0.74633257133047	-5.47691673036441	H	1.39639486062675	0.36575956393390	-2.41618214450501
H	1.45428518811239	-2.08032489100674	-0.96258496567092	N6_CH3+			
C	3.95738679231079	0.87074032818261	-3.46407511230790	C	1.35863833855873	2.83162117476465	-6.00104299750032
C	4.84228804269239	1.28178702850158	-2.34426710329398	C	0.27802568585676	2.07673675720198	-5.54901775495399
H	4.97000458151506	0.43557875525567	-1.66830019216854	C	2.60595133643013	2.69918319605400	-5.40741691971937
H	5.82156112011644	1.55017918104372	-2.74950207934930	H	3.43390760016174	3.29901720698490	-5.76507732655954
H	1.51559869299252	-2.65137437934558	-5.22345388994623	C	0.43998644433201	1.20728284754088	-4.42799366402008
N	3.89720824593552	1.56552779945494	-4.59166194492344	C	2.77812108832949	1.81731856305401	-4.32802620199682
C	4.72571946492110	2.66187966374451	-5.05112325918436	C	1.67491453163767	1.09044027784829	-3.85081109993750
O	5.60232789292889	3.12696861940927	-4.36890086973606	H	1.78618069654315	0.41322906792873	-3.01024884529276
C	4.34846283389778	3.10475414841572	-6.42371308248886	H	1.23049458987240	3.52971625939319	-6.82303341258872
H	4.995477792988665	3.92625973926643	-6.72951208334343	C	4.05752471899988	1.65429363015495	-3.63499574794763
H	4.44077515796399	2.27055662007308	-7.12962690221698	C	4.12485162564174	1.43176037078583	-2.15437319700776
H	3.30027871693024	3.42841186538527	-6.43521517286901	H	4.89850279574294	2.08527260074317	-1.73780326701715
C	0.71325486514419	-3.32697275200320	-2.97530679619168	H	3.16897700417551	1.74044596825146	-1.72658907777592
H	4.26278004549026	2.49336443367834	-1.58262217963970	H	-0.40001356518352	0.62210451547123	-4.11089653632636
H	3.28925243638643	2.25071485087683	-1.14734402817580	H	-0.69198363298425	2.17455954011483	-6.02815102414324
H	4.95172257791330	2.75400156118621	-0.77481094663253	Si	5.43105268910511	0.35945726523045	-6.63208535762101
H	4.15037903529536	3.36165076366975	-2.23576919759019	C	7.133515262101379	-0.35457515732731	-6.41834636371697
H	3.18939872750674	1.28144656753517	-5.26528257025547	H	7.33868656557345	-0.63035150422805	-5.37812654950273
N5_CH3+				H	7.21257459716866	-1.26731516299900	-7.02368429275102
C	4.98101716485608	3.46229987540339	-1.88033247523267	H	7.90968442684341	0.33841333858066	-6.75796834259994
C	4.04382586647345	4.35497487154407	-2.40109560147505	C	4.10798105289411	-0.82717748663068	-6.08639942233025
C	4.94578066544585	2.12845193711820	-2.24511135140460	H	4.20295815630289	-1.09250525060505	-5.02644337348915
H	5.66416315128998	1.44538909804225	-1.80597852848338	H	3.10145016510073	-0.43322377195105	-6.26200207753058
C	3.05971941224942	3.90458195848595	-3.28021012753068	H	4.21181411953184	-1.75683235484807	-6.66104428682002
C	3.95795726959090	1.65249092975038	-3.13656451205433	C	5.15056050561528	1.12212588082146	-8.29867278427203
C	3.00717994030346	2.56862196470738	-3.63876498624942	H	5.88456168497818	1.91070585617900	-8.50147763382603
H	2.24423628860976	2.24281092470764	-4.33624975562066	H	5.25498527412363	0.36064860031830	-9.08129578677138
H	5.73549834671777	3.81069625372589	-1.18171994155906	C	4.14593984149337	1.55278630541214	-8.37745603491765
C	3.92447627576838	0.26136991886914	-3.53556293706509	H	4.43185655448523	-0.02890709976594	-1.78554859134021
C	2.66547772933437	-0.33906754237927	-4.05985463653939	H	5.39704288875809	-0.34863340695993	-2.18660758414404
H	2.18270674469213	0.31099381976294	-4.79510265385758	H	4.46636667038701	-0.11775080833634	-0.69586350040690
H	2.88789372982023	-1.29355296146602	-4.54302423700079	H	3.65716283784706	-0.70414447570990	-2.15967478695210
H	2.33270414950659	4.60062121092406	-3.68714131080797	N	5.18583395672249	1.66127197342940	-4.29194644420982
H	4.07719205516626	5.40268244638745	-2.11582425741970	Si	7.47137107671221	2.88721013269216	-3.615744666160364
Si	6.05952209446684	-0.33434862436290	-5.18757971337550	C	8.42735101224063	2.48262876796085	-2.07788739867036
C	7.38515341302010	-1.63747014712482	-5.029588669520783	H	9.23492386113296	3.21097768013991	-1.93431826924834
H	8.00521065938843	-1.47544043377291	-4.14107725382513	H	7.78885245591405	2.502876661901750	-1.18774073410853
H	6.95524783537596	-2.64361611544855	-4.97629240074132	H	8.88630161945596	1.48961883611460	-2.1521201887623
C	8.03794056446831	-1.59424495700467	-5.91106927729703	C	8.53044799317983	2.86274578700365	-5.14098401717176
H	4.91397518379042	-0.64749498721000	-6.62253235768042	H	7.94456171767569	3.00718166134713	-6.05482626085749
H	5.49828790929611	-0.60334760246726	-7.55113937778153	H	9.260333788232565	3.68088519274872	-5.08010754610557
				H	9.09156524256201	1.92558558206186	-5.22367680839645

C	6.40248824680330	4.40335179157615	-3.49926522613971
H	7.04476828250124	5.28502445820401	-3.37797525533266
H	5.80728279188469	4.55959324427337	-4.40654238943564
H	5.72628324844863	4.366378056663624	-2.63760099762947
O	6.36493387324895	1.50792673456113	-3.65572476773751
O	5.28310358683664	1.80815082596136	-5.62988406964688

N7_CH3+

C	1.80970426765528	0.57333668001626	-6.12033785143511
C	0.53845831251356	0.54685018854517	-5.53959075423020
C	2.92685052213778	0.70857886029702	-5.32385138925351
H	3.90663089670697	0.73021762200084	-5.78655608869198
C	0.38254124404610	0.67242993983230	-4.15664717127964
C	2.79528342317820	0.85019182860850	-3.91532744298500
C	1.49005393142503	0.83635140349069	-3.35139850190266
H	1.35344517518916	0.93365110481172	-2.28075372990028
H	1.91714481763133	0.48193418231717	-7.19641550969127
C	3.94177619049702	1.00145961699999	-3.09119228376580
C	3.84162163723935	1.25573393590398	-1.63983583213781
H	4.71316209739328	1.84227767056471	-1.32869461204877
H	2.93415662324396	1.79475345882607	-1.36461253188547
H	-0.60944457377193	0.64740016906043	-3.71716505161986
H	-0.33811189203252	0.42889304619681	-6.17067642323055
C	5.30985736996211	0.89561508695845	-3.62550460175625
H	5.58266804936036	1.90108021427961	-3.99267961088039
H	6.02209517953202	0.65956037605171	-2.83111866297070
H	5.41917415523692	0.20236505332864	-4.46030874472689
C	3.88430040003217	-0.10614194819377	-0.89226792746624
H	3.88759146657883	0.09781042230366	0.18180933977314
H	3.00732240954841	-0.71063802244776	-1.13840003942705
H	4.78649587508676	-0.67019861105376	-1.14476718675412

N8_CH3+

C	1.29392519763312	-0.14429985519679	-5.70031863500546
C	0.37758546314567	-0.88673284440201	-4.92909843398257
C	2.36104898209492	0.47512701978712	-5.10143251508212
H	3.07138524081209	1.04815215104787	-5.69095770511954
C	0.56758519445543	-0.99251763325545	-3.53162345032414
C	2.56354980425566	0.37184142462996	-3.69066807339364
H	1.62793156687520	-0.38142649165107	-2.91740163364895
H	1.75542674008517	-0.47041377704388	-1.84410131212075
H	1.14626968305401	-0.06827636005412	-6.77349027105988
C	3.66774653185169	1.00474624165072	-3.14060407106046
C	4.10555311372287	1.02251408752329	-1.74706894392716
H	3.42641105364590	0.49658558784426	-1.07360000424037
H	5.06924465881605	0.48095682366735	-1.73981638252706
H	-0.14412743569009	-1.56743307910415	-2.94611367593410
C	4.38126865206731	2.46027258607712	-1.26121838050551
H	5.10387121404425	2.96568113038739	-1.90876096604012
H	3.45655688568106	3.04360524538539	-1.24435658541708
H	4.78883143826362	2.42140998860034	-0.24783564921207
C	4.29920717567898	1.56235544269991	-3.83551150821721
H	-0.79897027156663	-1.52977481171424	-5.56686824679064
H	-0.65329469313010	-1.67423825220771	-6.63975934097429
H	-1.04215704287407	-2.48177840836905	-5.08521766258311
H	-1.67555746649046	-0.87793957855339	-5.43433745538772

N9_CH3+

C	1.58882779876312	-0.53272669902001	-5.75105185861171
C	0.38378268799895	-0.72678269264287	-5.06740401714653
C	2.68906730543052	-0.07277622892430	-5.06313608788448
H	3.63766692446765	0.08539438898361	-5.56875224171653
C	0.26923009282899	-0.46132330108542	-3.695162205163012
C	2.59893616130473	0.19921979063180	-3.66495845116793
C	1.35801812453605	-0.00117951395204	-2.99214749602566
H	1.27111371214070	0.21268142360607	-1.93282539616247
H	1.65084200546711	-0.74342416454782	-6.81358749128174
C	3.74600402361822	0.64688764304187	-3.01497250370418
C	3.92932462043929	0.95468678214221	-1.60383538277025
H	3.01834369340327	0.85338393652998	-1.01159164362431
H	4.65008359337596	0.19550690193050	-1.2444448240423
H	-0.68050263694596	-0.61694332489225	-3.19384035297979
H	-0.48445872917626	-1.08862214399347	-5.61159237337298
C	4.59038025512608	2.33628713334459	-1.40848627800834
H	5.53271493545804	2.40671826383378	-1.95938203057784
H	3.92155764971064	3.13076517074924	-1.75001726447540
H	4.79530531127296	2.48253957765631	-0.34516565997606
H	4.63159448877985	0.78132110460821	-3.64000196047941

N10_CH3+

C	3.13078225801332	-0.17519844407132	-1.06775300212929
C	1.96703203905301	-0.79628120495632	-1.52339690215109
C	3.99934589259938	0.42149313856108	-1.9623871779833
H	4.89201934519606	0.91297023064523	-1.59436102464703
C	1.67041770962875	-0.81449412860997	-2.88591201854304
C	3.70446875367049	0.43495781782361	-3.34819895074341
C	2.51855777970910	-0.19351484140552	-3.78803344511790
H	2.29684243713994	-0.23561885036349	-4.84868895404253
H	3.35822514155638	-0.15929160559153	-0.00598792504603
C	4.59216797180229	1.05822005777497	-4.30662223242602
C	6.06484389463629	1.03381934726593	-4.04801982339136
H	6.30210492436035	1.18542169443692	-2.99016148047925
H	6.58608691344835	1.80466930036889	-4.62155063524266
H	0.77568900615036	-1.31591668551533	-3.24265805802536
H	1.29317057817174	-1.27050127583943	-0.81536424638195
Si	4.01617730984782	2.03262955028410	-5.73828389397682
C	5.28982970775246	2.39764910247413	-7.05103101400134
H	4.89533989417707	3.17242248925542	-7.71811968480528
H	6.24461704574293	2.74702072198935	-6.64915364095631
H	5.47550609248317	1.50070926486085	-7.65447386162689
C	2.28044977813271	1.87534770913138	-6.4061083210077
H	1.51783374561918	1.81784081539587	-5.62547330450753
H	2.07396940296148	2.75649405215639	-7.02533943518100
H	2.19585282725409	0.99017957753890	-7.04841002402059
Si	3.89346157837082	3.88115890011603	-4.08798469056324
C	2.23902100328086	3.70516194352318	-3.23492822402266
H	1.40954758369675	3.73382131293096	-3.94917316015017
H	2.16765594525161	2.77927197532349	-2.65314921795890
H	2.11299542598072	4.54467434254862	-2.53764050483342
C	5.30549230512981	4.06063466530332	-2.87954380555629
H	6.28048064871299	4.05287171709768	-3.37826930954128
H	5.19925333752168	5.03017271583097	-2.37416388557068
H	5.29715274202174	3.28210789064404	-2.11005186905528
C	3.90646334244254	5.29457008634335	-5.33335419886618

H	4.87553899274252	5.38106701614181	-5.83556837608901	H	3.37388602614325	0.56426477033413	-1.40975060409514
H	3.12248982065185	5.19599780148727	-6.09118988003613	H	4.89745683845472	1.45080784255498	-1.61862090714069
H	3.72647829367125	6.22655113534444	-4.77811398231605	H	-0.06144057989164	-1.32531832393718	-3.36519307980280
C	6.59185567028300	-0.35320168252553	-4.48228585736381	H	-0.48872704728705	-0.81348262696291	-5.75083691331349
H	7.67551145318083	-0.38083594401978	-4.33224128571575	Si	5.32667839354170	1.94293645299935	-4.42141177422477
H	6.13479532245471	-1.15029599967146	-3.88873785113760	C	6.70573618527819	2.35837751636431	-3.22879752507685
H	6.38265178130978	-0.54130696548215	-5.54006732483819	H	7.14782546093356	1.47814725626754	-2.74995853338697
N11_CH3+							
C	1.31094378626418	0.10628167168566	-5.74028953998371	H	7.50207625842061	2.85295062803851	-3.800211110593928
C	0.37883772718672	-0.42272675987021	-4.82542946595262	H	6.38591568763808	3.05724978447481	-2.44768350674108
C	2.52049678935147	0.58494626492455	-5.30720244577035	C	5.98841714002388	0.85163778034956	-5.79533422640577
C	3.21261657437713	0.98888083862109	-6.03542941100906	H	6.83621650279199	1.36492457621464	-6.26730843459679
H	0.71196842085329	-0.45835755037508	-3.45679532148738	H	6.35785562072354	-0.09903093672319	-5.39380328869320
C	2.88266579037045	0.55038014083656	-3.92491822033566	H	5.25195118078825	0.63035456355450	-6.57360684593057
C	1.92607573658802	0.003273403321230	-3.01332263955104	C	5.06082079098201	-0.66714279133563	-2.01295624281257
H	2.14548353149899	-0.04460657059309	-1.95312424854821	H	5.38781856025706	-0.84132730723947	-0.98400143174670
H	1.06082399744910	0.13492958402031	-6.797122890311638	H	4.42719966825964	-1.49564867947365	-2.34013874830587
C	4.11945001820909	1.06475043718697	-3.49616820116145	H	5.94482370191299	-0.62859860354664	-2.65550951929154
C	4.48763496172710	1.06465680622634	-2.06132436962894	C	4.557212685618134	3.54612030090111	-5.02532478455398
H	4.04193164206859	0.24024232566382	-1.49989854098498	H	5.37148098477453	4.22335883073285	-5.31403536037144
H	5.57450662252110	1.00604759701986	-1.95058177034063	H	3.89843617038290	3.42252086375609	-5.88990583761981
H	-0.00455605083995	-0.86476536205017	-2.74884655744459	H	3.98795406244472	4.03499389049698	-4.22637539836406
Si	5.41197880173794	1.89521759800300	-4.68791337765955	N13_CH3+			
C	6.90607839001757	2.40124775710907	-3.68204376523778	C	0.61431828365354	0.37870400877818	-5.51817899886886
H	7.44550106687396	1.53919711474681	-3.27358791970719	C	0.10316216683680	-0.80628177514527	-4.89676402992420
H	7.59742855413806	2.92876854136764	-4.35216923239301	C	1.96387649907827	0.72152109049986	-5.33674742196856
H	6.66683069714756	3.08362387983565	-2.85941886866887	C	0.97970237362602	-1.59784722844955	-4.10756965693501
C	5.95526428961449	0.60728972674236	-5.94266976911250	C	2.80014432145108	-0.04962772185079	-4.52892218560057
H	6.87811245875140	0.96394097730297	-6.41812473654516	C	2.28091436499496	-1.23345320218241	-3.91488079897085
H	6.18393415823517	-0.34576097973239	-5.45161727372039	H	2.92682939287245	-1.89383265414058	-3.34389516423129
H	5.22213103603006	0.41768214727043	-6.73229200642087	C	4.15380351337776	0.39942947120588	-4.29951215494394
C	4.63234752052001	3.41846366029453	-5.45695302696554	C	4.83484520349597	1.33168499738369	-5.23768597467872
H	3.79295684391226	3.19484757514910	-6.12234792386270	H	4.32662859656909	1.29900717254323	-6.20170094880003
H	4.27837846019901	4.10782137272758	-4.68158324534842	H	5.86258983798208	0.98945073798105	-5.38467303003780
H	5.39778541957936	3.94318038660459	-6.04318517512944	H	0.60077446103862	-2.51545982221625	-3.66592050689482
C	-0.93757857751366	-0.91746939920691	-5.30566164872183	H	2.32614360769171	1.62998757017200	-5.80644433594834
H	-1.48273514525806	-1.45558343513779	-4.52767570796735	N	4.75966553023963	-0.02200532569704	-3.19226160279621
H	-1.55039807210710	-0.06580180552315	-5.63326270797625	H	4.19814690782712	-0.56877936538973	-2.54483851955525
H	-0.81308682521367	-1.56064713077581	-6.18413255812954	C	6.12505595451685	0.15110521737700	-2.75704882954920
C	4.01363897225063	2.41085058319370	-1.44530591612426	O	6.92762753106704	0.78543346393013	-3.39499088975670
H	4.36861488284018	2.46069840396631	-0.41197401791322	C	6.38549575157646	-0.53931299403736	-1.46016372812807
H	4.41239947162285	3.27218577994850	-1.98887705741723	H	5.71074298379449	-0.15057777398347	-0.68759873444328
H	2.92176427532298	2.46946770393994	-1.45671038808724	H	6.18825477759454	-1.61371359988716	-1.55739331683260
N12_CH3+							
C	1.33025997076715	0.30544923612875	-6.01937620296681	H	7.42170813021760	-0.37690906706390	-1.16514748355860
C	0.41767646774494	-0.44759591587958	-5.27618165616707	C	-0.24807475031378	1.17719932688312	-6.31309951921466
C	2.48215567735882	0.76615072947783	-5.41985865220412	H	0.14826126278193	2.07533397432894	-6.77929196326145
C	3.18411602998861	1.34416474224776	-6.00732507785720	C	-1.24794996922993	-1.15430081433632	-5.09903743673887
H	0.65614225256694	-0.73639670607502	-3.92744902974585	H	-1.63804509632461	-2.05467020771559	-4.63202568760784
C	2.75297480339484	0.49936354732117	-4.04564666823365	C	-1.56010550851556	0.81210754885413	-6.48783761615856
C	1.79578976060960	-0.26736087223923	-3.313746638213621	H	-2.22006107307688	1.42268030077325	-7.09671754227641
H	1.96120941553777	-0.49784808284964	-2.26802974054419	C	-2.06060863195776	-0.35885295179289	-5.87742618670171
H	1.13422199051893	0.52246329724923	-7.06439077719480	H	-3.10133304687342	-0.63297266771366	-6.02538200659930
C	3.94936617765838	0.96481342876699	-3.45330426711956	C	4.85595919326757	2.77424827974282	-4.692027979879151
C	4.25918953455440	0.66928896853011	-2.04059474344010	H	3.83867702482338	3.15847760817432	-4.57295151080353
				H	5.36884258493339	2.83334667287403	-3.72931650053041
				H	5.38777587474622	3.40888532363580	-5.40603719050721

N14	CH₃⁺			H	4.93600823682739	-2.06757973472235	-3.83308981901276
C	0.55310448254813	-1.03753282719394	-4.37988123392096	H	6.21742628776835	-0.89053723409058	-3.47020672405507
C	-0.24306343943802	0.11310903459633	-4.29207052287938	H	5.75884326401716	-2.10252404433922	-2.25890607714949
C	1.93159785112188	-0.95207248379167	-4.38923623502828				
C	0.39272036683633	1.36140838337955	-4.19995453253485				
C	2.57007957620812	0.30010178211548	-4.26445213408457				
C	1.76846352962027	1.46015767210172	-4.17483452989074				
H	2.21581976186030	2.44983387160386	-4.14736873568520				
C	4.01162862945299	0.36586172767714	-4.21682589883388				
C	4.85177378950406	-0.71394839572732	-4.79991579426166				
H	5.68032045608906	-0.25682563462204	-5.34746580969082				
H	4.25047762357085	-1.28571849120409	-5.50743712580822				
H	-0.20951268172509	2.26491489045018	-4.15904202803738				
H	2.51542930963170	-1.86417529041405	-4.44586765628629				
N	4.56115128239859	1.40895776568264	-3.60008813177525				
H	3.92560347156348	2.04394926212219	-3.12419366080754				
C	5.94321445857654	1.81793806163285	-3.52202483728270				
O	6.83414006787582	1.16728509036388	-4.00801691923578				
C	6.10041806046022	3.10514916210527	-2.78312111891603				
H	5.70632958751726	3.00164230070691	-1.76456736375725				
H	7.15535273380289	3.37521937476071	-2.74742033569183				
H	5.52682223578586	3.89828983027338	-3.27746863530149				
C	-1.73313845289289	0.01932952368551	-4.33811036979849				
H	-2.08570481941840	-0.93497983054278	-3.93730369943789				
C	5.42094074965817	-1.64400649140736	-3.70835660608689				
H	6.04346229930596	-1.09563621163543	-2.99762103209374				
H	4.61415629777241	-2.13980075395970	-3.16094229972867				
H	6.03701143572316	-2.40803152743566	-4.19006826166708				
H	0.07785526549823	-2.01246441154968	-4.44468987656110				
H	-2.20181424483974	0.84114562919939	-3.78953622873732				
H	-2.07697093280446	0.08406992543672	-5.37942305909942				
N15	CH₃⁺						
C	0.72654705742378	-1.38339771069114	-4.66548291304925				
C	0.00340332005950	-0.32596766776403	-5.21296565333583				
C	1.94295963807798	-1.12051661071005	-4.06397284764768				
C	0.47577330331719	0.98590479812246	-5.17568009469448				
C	2.46465473673122	0.18817234444984	-4.03840920484535				
C	1.70551069974506	1.23633986813663	-4.59956260969536				
H	2.03929871729461	2.26819347357806	-4.54127230219283				
C	3.76581461296888	0.42580904220927	-3.44495978645330				
C	4.32394566273580	-0.50455444852854	-2.42998968052010				
H	3.50786808565368	-1.08264427428250	-1.99524400157360				
H	4.79139975037169	0.08073876986784	-1.63390908519780				
H	-0.11740324176610	1.79856942499139	-5.58079436966808				
H	2.50459056688262	-1.95018661137301	-3.64959216761585				
N	4.44888293890774	1.48144920142262	-3.86786887646512				
H	4.04539543769913	2.01109804513811	-4.63697336463875				
C	5.68693931255081	2.04512129789357	-3.36821844941180				
O	6.31892530181736	1.51658057316420	-2.48991057844573				
C	6.04251039888794	3.31246205544689	-4.06899289944460				
H	5.24792921822104	4.055520906664605	-3.92929327895697				
H	6.98288006916993	3.69394757385070	-3.67242488884632				
H	6.13560547780191	3.13096392837646	-5.14686598390574				
H	0.34171166669615	-2.39659920319560	-4.70584260442009				
Cl	-1.54035333316537	-0.64708918052820	-5.95086262983037				
C	5.37850419944539	-1.44821117954529	-3.04779788905148				

8. References

- (S1) G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw, K. I. Goldberg, *Organometallics*, 2010, **29**, 2176.
- (S2) Y.-F. Wang, M. Hu, H. Hayashi, B. Xing, S. Chiba, *Org. Lett.*, 2016, **18**, 992.
- (S3) P. Gu, Y. Su, X.-P. Wu, J. Sun, W. Liu, P. Xue, R. Li, *Org. Lett.*, 2012, **14**, 2246.
- (S4) Z. Liu, P. Liao, X. Bi, *Org. Lett.*, 2014, **16**, 3668.
- (S5) N. S. Y. Loy, S. Kim, C.-M. Park, *Org. Lett.*, 2015, **17**, 395.
- (S6) Y.-F. Wang, K. K. Toh, J.-Y. Lee, S. Chiba, *Angew. Chem. Int. Ed.*, 2011, **50**, 5927.
- (S7) (a) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2012, **2**, 73. (b) F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.*, 2017, **8**, e1327.
- (S8) A.V. Marenich, C.J. Cramer, D.G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.
- (S9) S. Grimme, A. Hansen, S. Ehlert, J.-M. Mewes, *J. Chem. Phys.*, 2021, **154**, 064103.
- (S10) B. de Souza, *Angew. Chem. Int. Ed.*, 2025, **64**, e202500393.
- (S11) C. Bannwarth, S. Ehlert, S. Grimme, *J. Chem. Theory Comput.*, 2019, **15**, 1652.
- (S12) E. C. Meng, T. D. Goddard, E. F. Pettersen, G. S. Couch, Z. J. Pearson, J. H. Morris, T. E. Ferrin, *Protein Sci.* 2023, **32**, e4792.