– Supporting Information –

J. Org. Chem.

Organocatalytic Activity of Cinchona Alkaloids: Which Nitrogen is More Nucleophilic?

Mahiuddin Baidya, Markus Horn, Hendrik Zipse, and Herbert Mayr*

Department Chemie und Biochemie
Ludwig-Maximilians-Universität München
Butenandtstraße 5-13 (Haus F)
81377 München (Germany)
Fax: (+49) 89-2180-77717
E-mail: herbert.mayr@cup.uni-muenchen.de

Table of contents

Materials

Commercially available acetonitrile (HPLC-gradient grade) and DMSO (>99.8%, extra dry) were used as received. Commercially available CH_2Cl_2 was freshly distilled over CaH_2 before use.

The benzhydrylium tetrafluoroborates $Ar_2CH^+BF_4^-$ were prepared as described before.[S1] The benzhydryl chlorides were synthesized according to literature procedures.[S2] Commercially available benzyl bromide was freshly distilled before all kinetic experiments.

Quinine (**1a,** 99%), quinidine (**1b,** 99%), chinchonidine (**1d,** 99%), and quinuclidine (**1e**, >98%) were purchased and used directly without further purification. Compounds **1c** and **1f** were also synthesized according to literature procedures.[S3] Lepidine (**1g**, 99%) and 6-methoxyquinoline (**1h**, 98%) were purified by distillation.

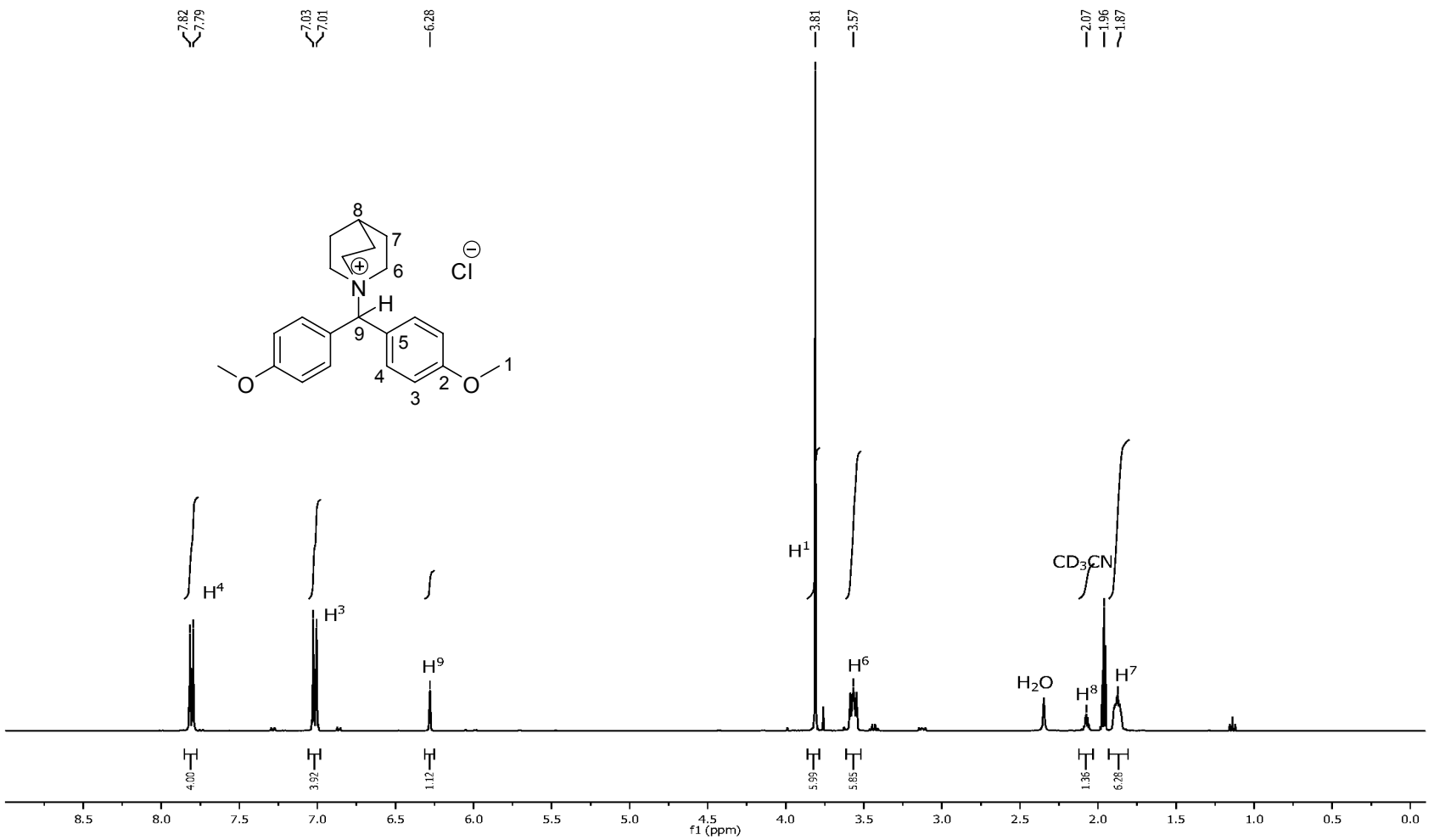
Product Studies

Reactions of cinchona alkaloids and related amines with benzyl bromide have previously been described in literature.[S4-S5] For that reason, only the reactions of amines **1** with benzhydrylium ions have been investigated. For all of the ^1H, ^{13}C NMR, and other 2D-NMR (COSY, HSQC, and HMBC) spectroscopic measurements almost equivalent amount of amines and benzhydrylium ions were used. Chemical shifts are reported in ppm relative to the deuterated solvent as internal standard (δ_H1.96 for CD_3CN in ^1H NMR and δ_c 1.39 for $\underline{C}D_3CN$ in ^{13}C NMR).

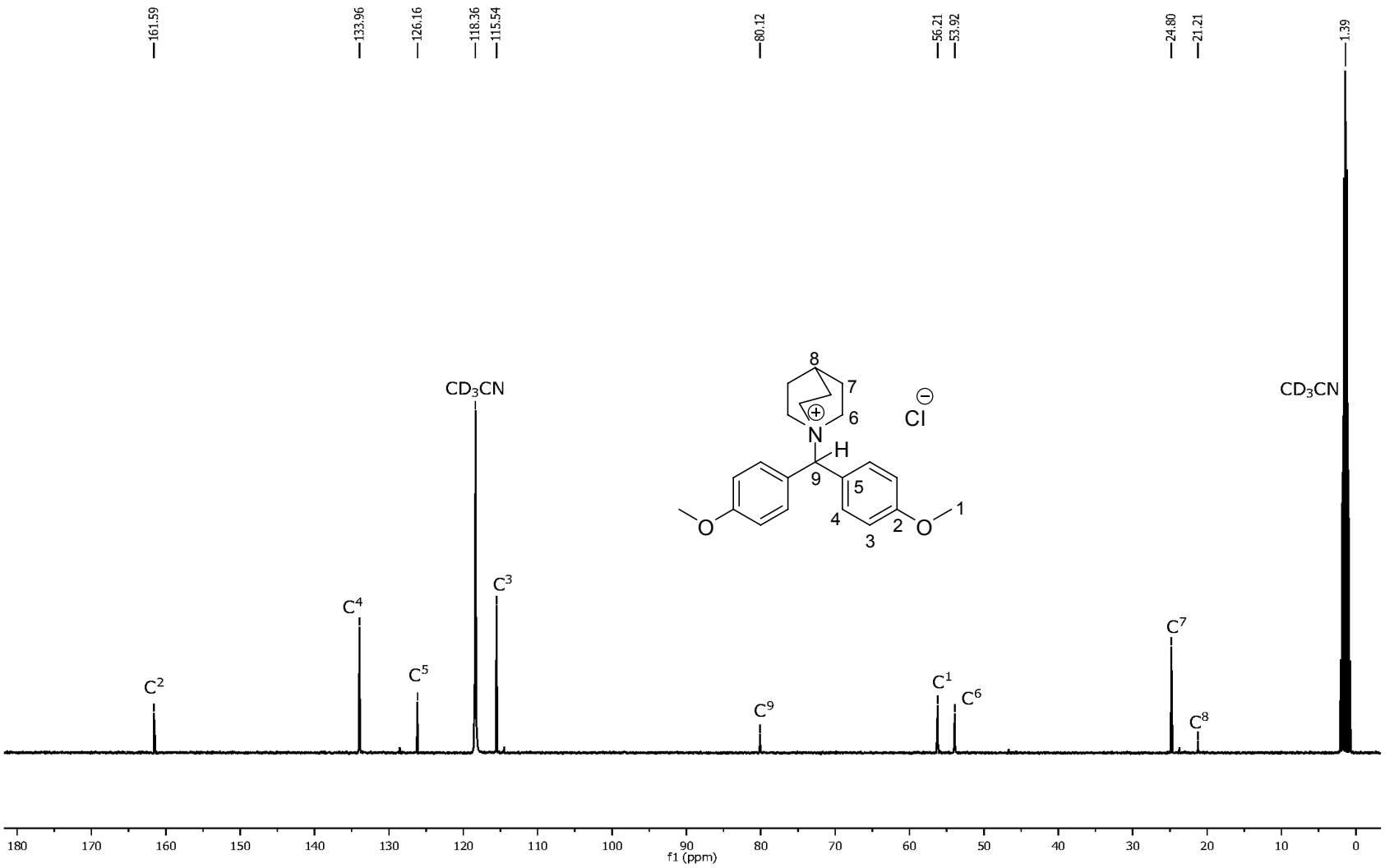
Reaction of $(ani)_2CHCl$ with 1e.

$(ani)_2CHCl$ (58 mg, 0.22 mmol) and quinuclidine **1e** (25 mg, 0.22 mmol) were dissolved in dry THF (4 ml) and stirred for few minutes at ambient temperature. A colorless salt ($(ani)_2CH$-**1e**, 55 mg, 67%) precipitated which was filtered and analyzed by NMR.

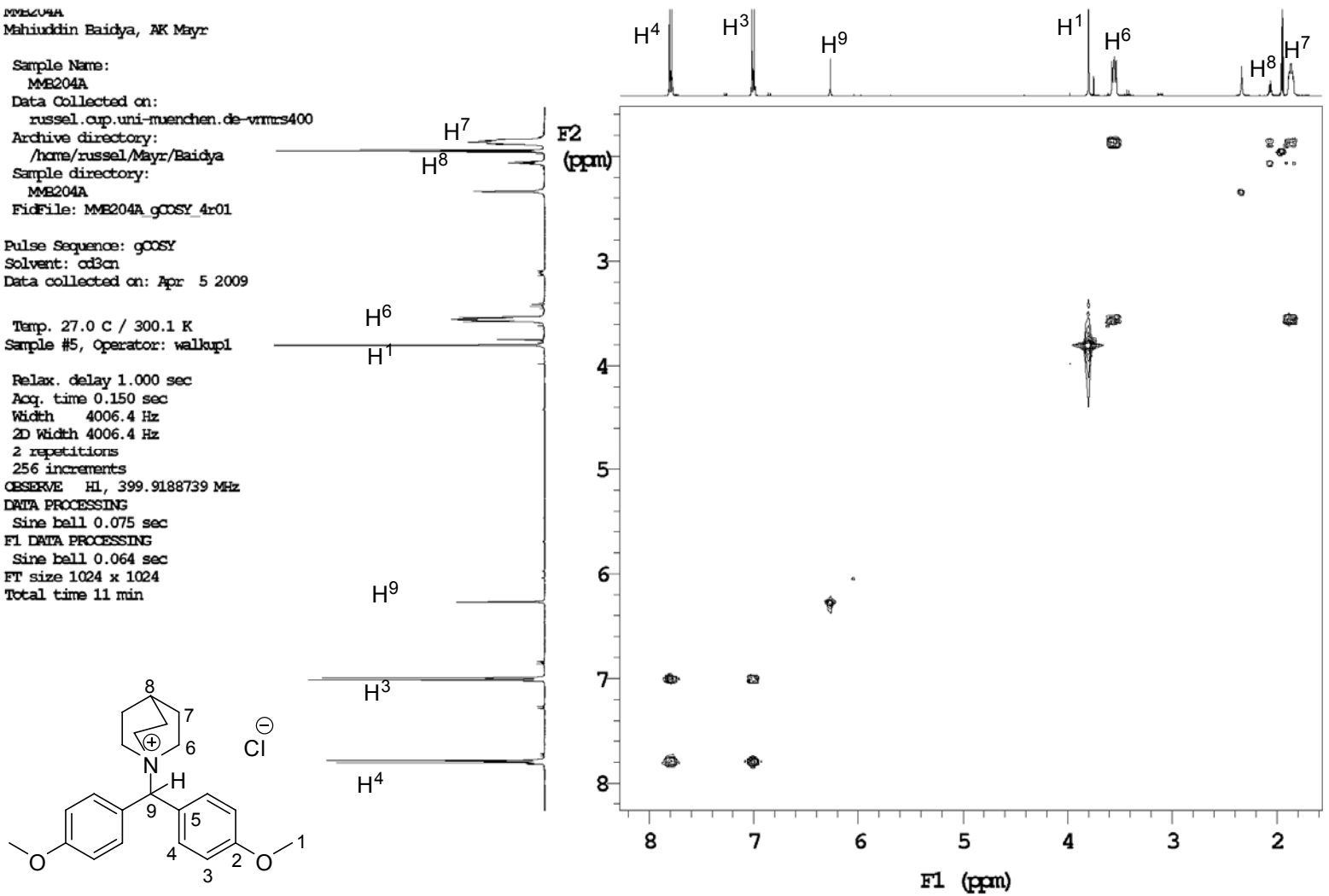
^1H-NMR (CD_3CN, 400 MHz): δ = 1.87 (m, 6 H, CH_2), 2.07 (m, 1 H, CH), 3.57 (m, 6 H, N^+CH_2), 3.81 (s, 6 H, OCH_3), 6.28 (s, 1 H, H^9), 7.02 (d, J = 8.9 Hz, 4 H, Ar), 7.80 (d, J = 8.9 Hz, 4 H, Ar). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 21.2 (C^8), 24.8 (C^7), 53.9 (C^6), 56.2 (C^1), 80.1 (C^9, $Ar_2\underline{C}H$-N^+), 115.5 (C^3), 126.2 (C^5), 134.0 (C^4), 161.6 (C^2).



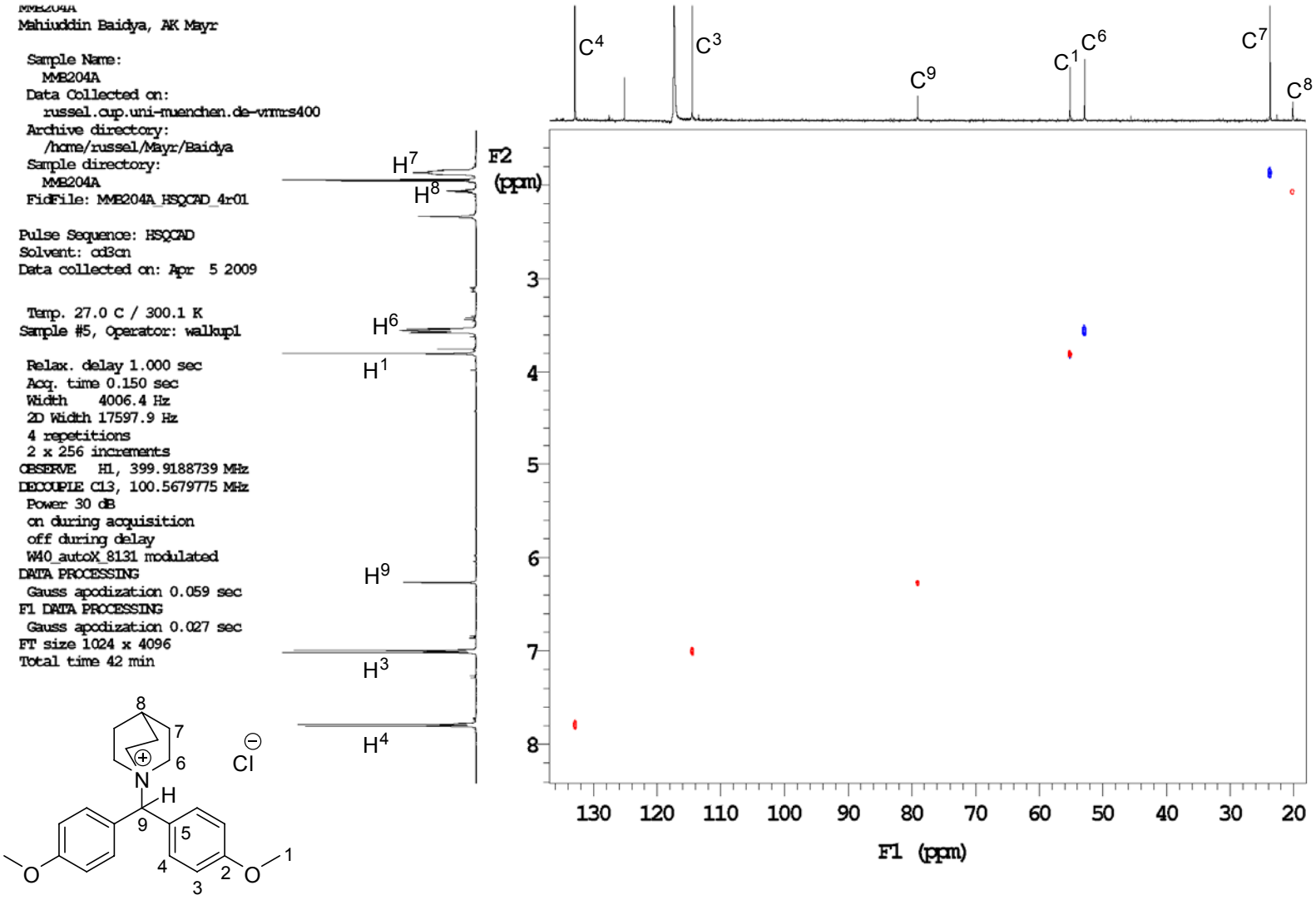
^{1}H-NMR (CD_3CN, 400 HMz) for $(ani)_2CH$-**1e**



^{13}C-NMR (CD_3CN, 100 HMz) for $(ani)_2CH$-**1e**

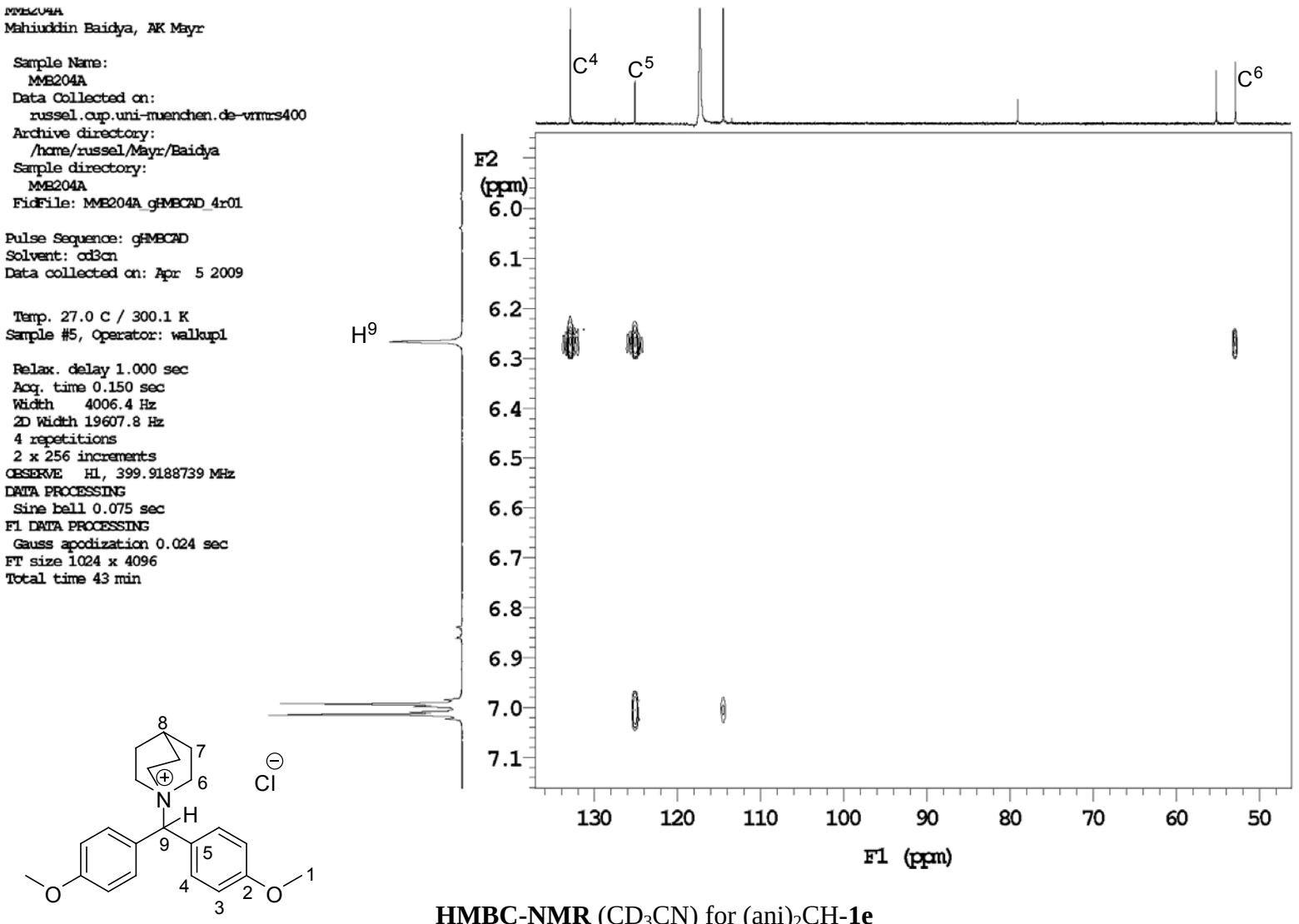


COSY-NMR (CD_3CN) for $(ani)_2CH$-**1e**
[Correlation between protons]



HSQC-NMR (CD_3CN) for $(ani)_2CH$-**1e**

[Correlation between protons and carbons, specially between H^9 and C^9]



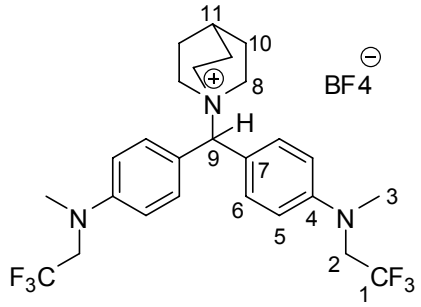
HMBC-NMR (CD_3CN) for $(ani)_2CH$-**1e**

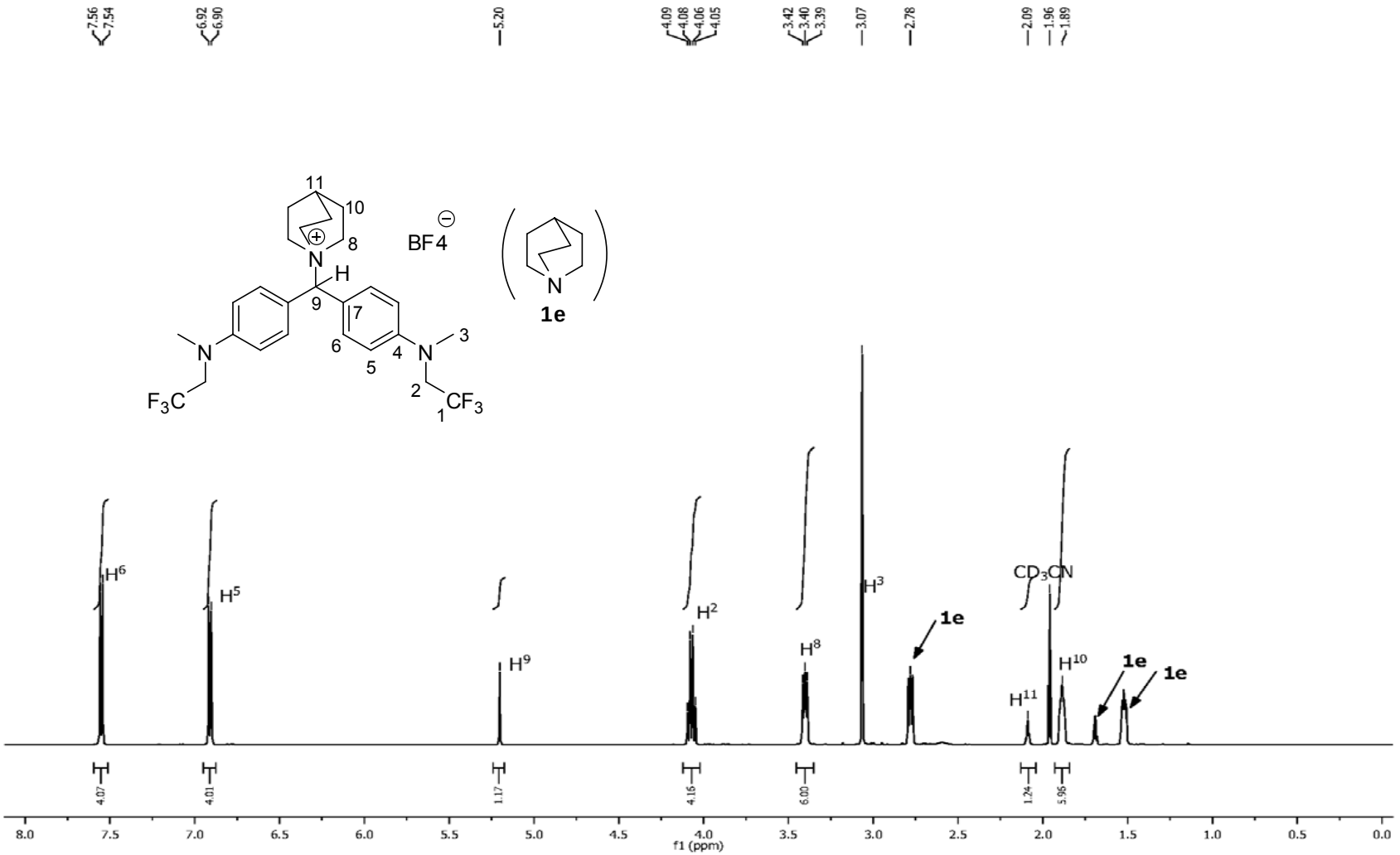
[Correlation shows that C^4 and C^6 is connected via C^9]

Reaction of $(mfa)_2CH\text{-}BF_4$ with 1e.

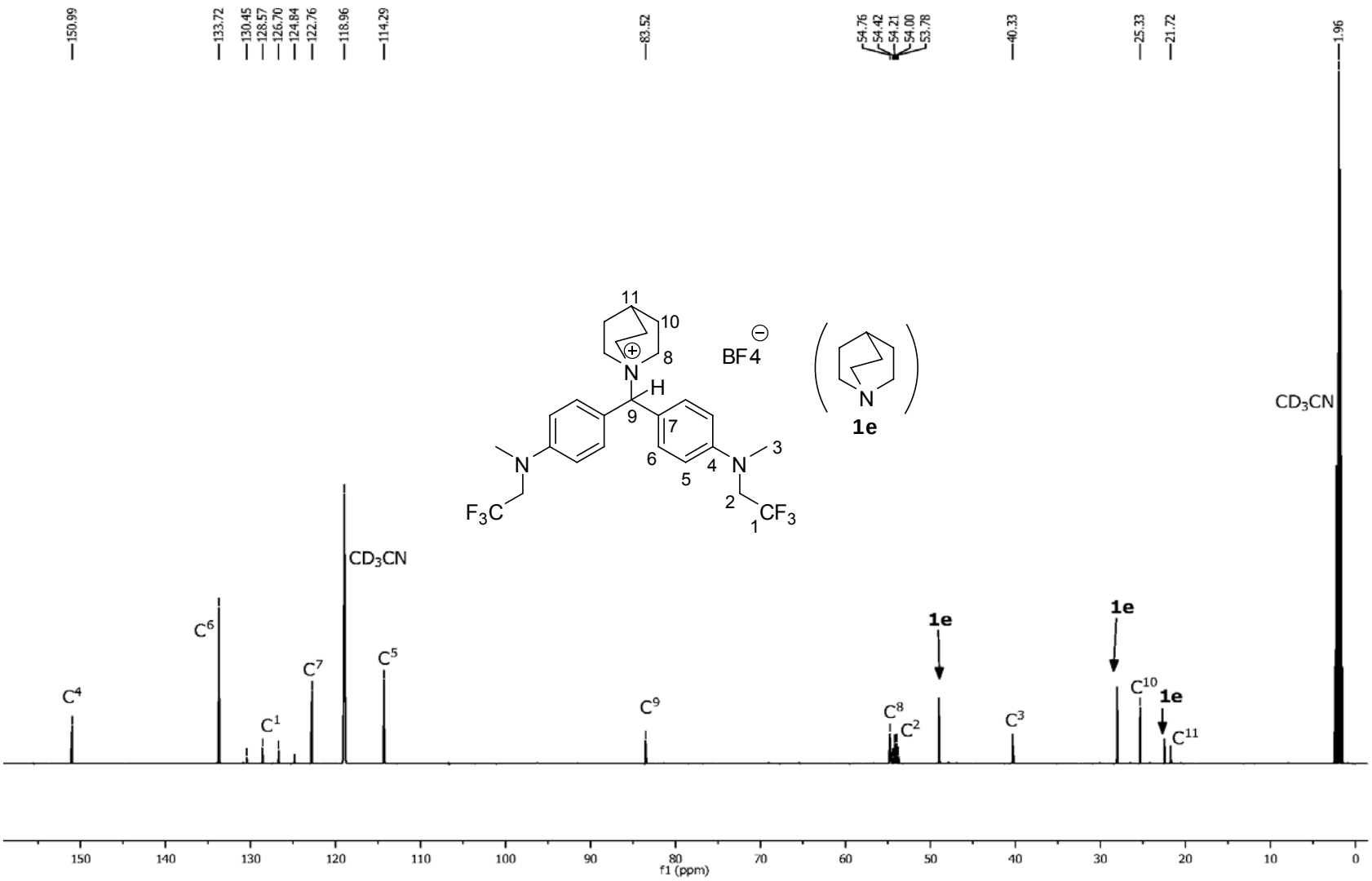
$(mfa)_2CH\text{-}BF_4$ (22 mg, 0.05 mmol) and quinuclidine **1e** (8.0 mg, 0.07 mmol) were mixed in an NMR tube and the mixture was analyzed by NMR.

^{1}H-NMR (CD_3CN, 600 MHz): δ = 1.89 (m, 6 H, H^{10}), 2.09 (m, 1 H, H^{11}), 3.07 (s, 6 H, NCH_3), 3.40 (m, 6 H, N^+CH_2), 4.07 (q, J = 9.2 Hz, 4 H, $C\underline{H}_2CF_3$), 5.20 (s, 1 H, H^9), 6.91 (d, J = 9.0 Hz, 4 H, Ar), 7.55 (d, J = 9.0 Hz, 4 H, Ar). ^{13}C-NMR (CD_3CN, 150 MHz): δ = 21.7 (C^{11}), 25.3 (C^{10}), 40.3 (C^3), 54.1 (q, J = 32 Hz, $\underline{C}H_2CF_3$), 54.8 (C^8), 83.5 (C^9, $Ar_2\underline{C}H\text{-}N^+$), 114.3 ($C^5$), 122.8 ($C^7$), 127.6 (q, J = 282 Hz, CF_3), 133.7 (C^6), 151.0 (C^4).

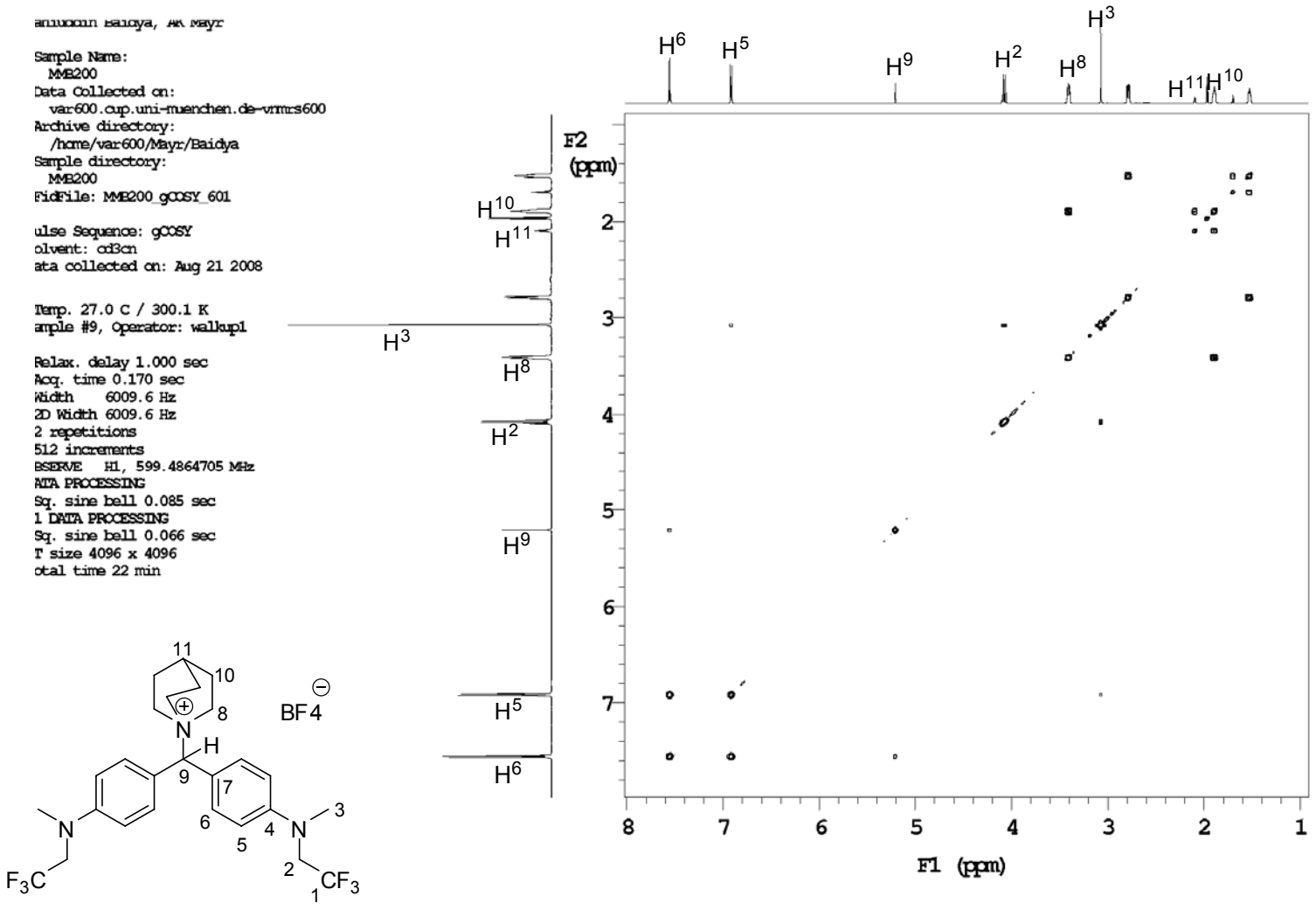




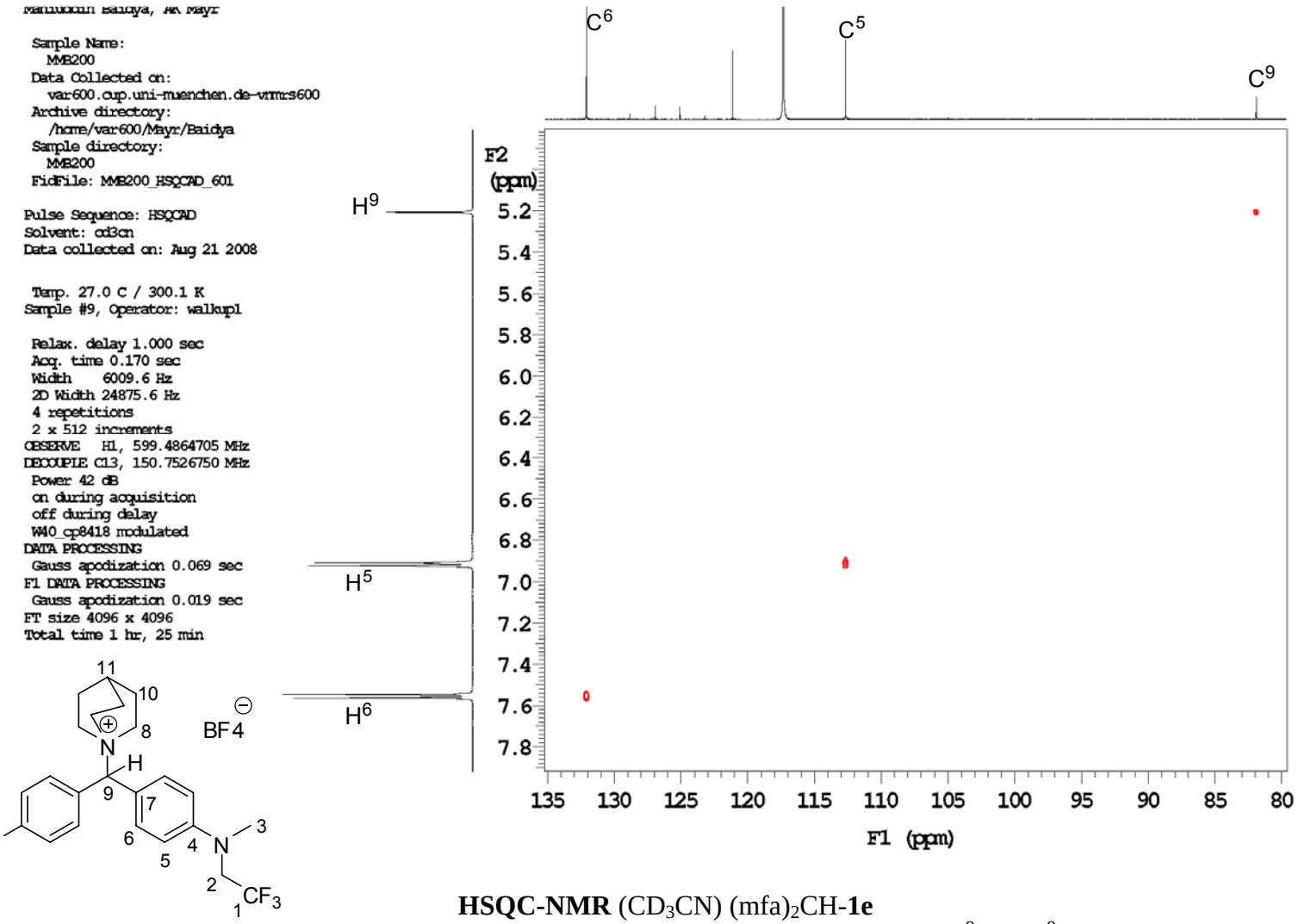
^{1}H-NMR (CD_3CN, 600 HMz) for $(mfa)_2CH$-**1e**



^{13}C-NMR (CD_3CN, 150 HMz) $(mfa)_2CH$-**1e**

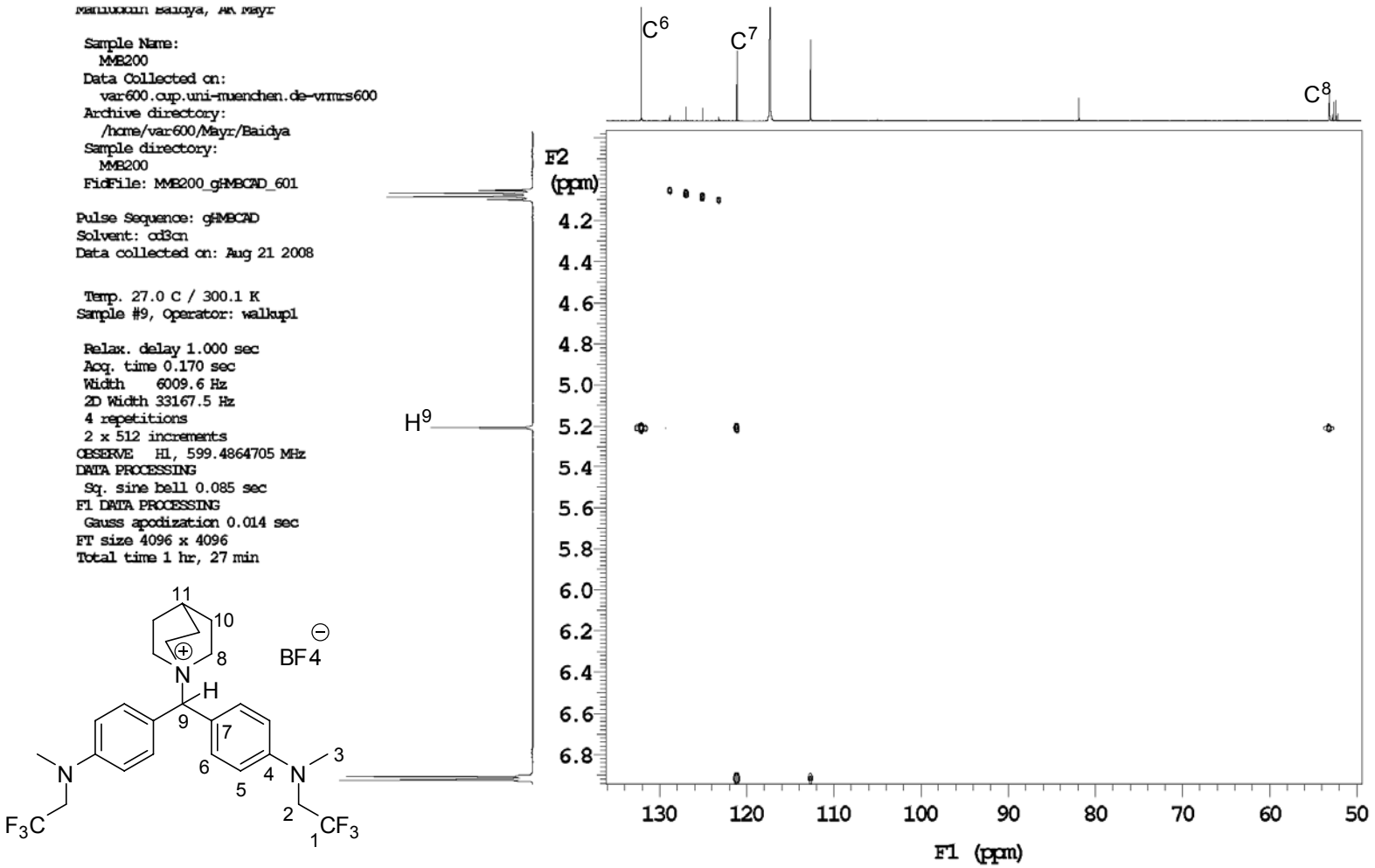


COSY-NMR (CD_3CN) $(mfa)_2CH$-**1e**
[Correlation between protons]



HSQC-NMR (CD_3CN) $(mfa)_2CH$-**1e**

[Correlation between protons and carbons, specially between H^9 and C^9]

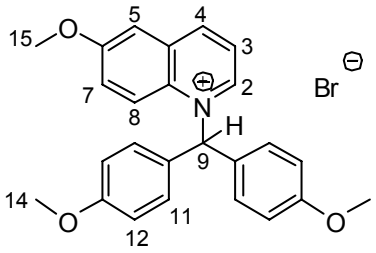


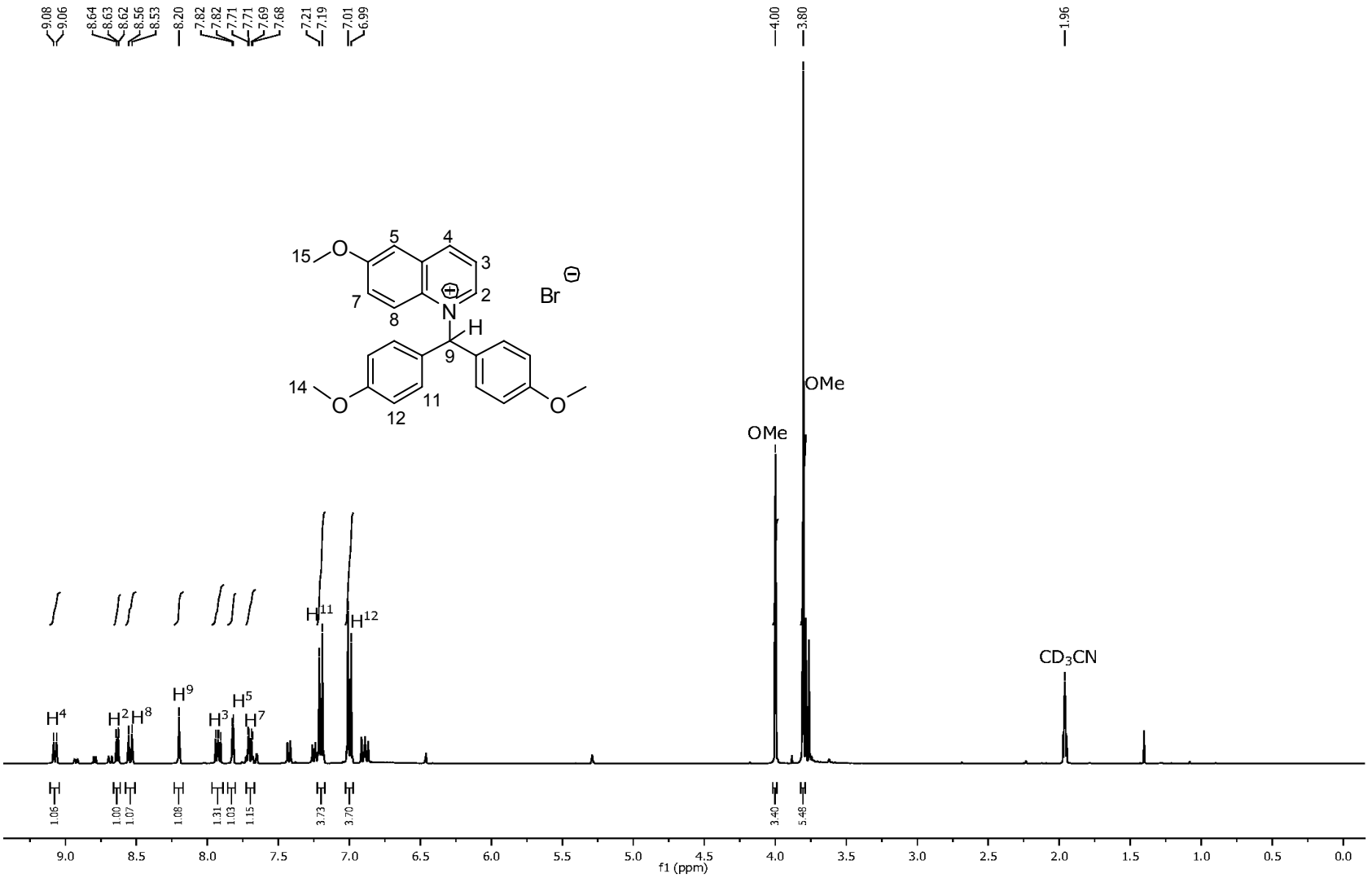
HMBC-NMR (CD_3CN) $(mfa)_2CH$-**1e**
[Correlation shows that C^8 and C^6 is connected via C^9]

Reaction of $(ani)_2CHBr$ with 1h.

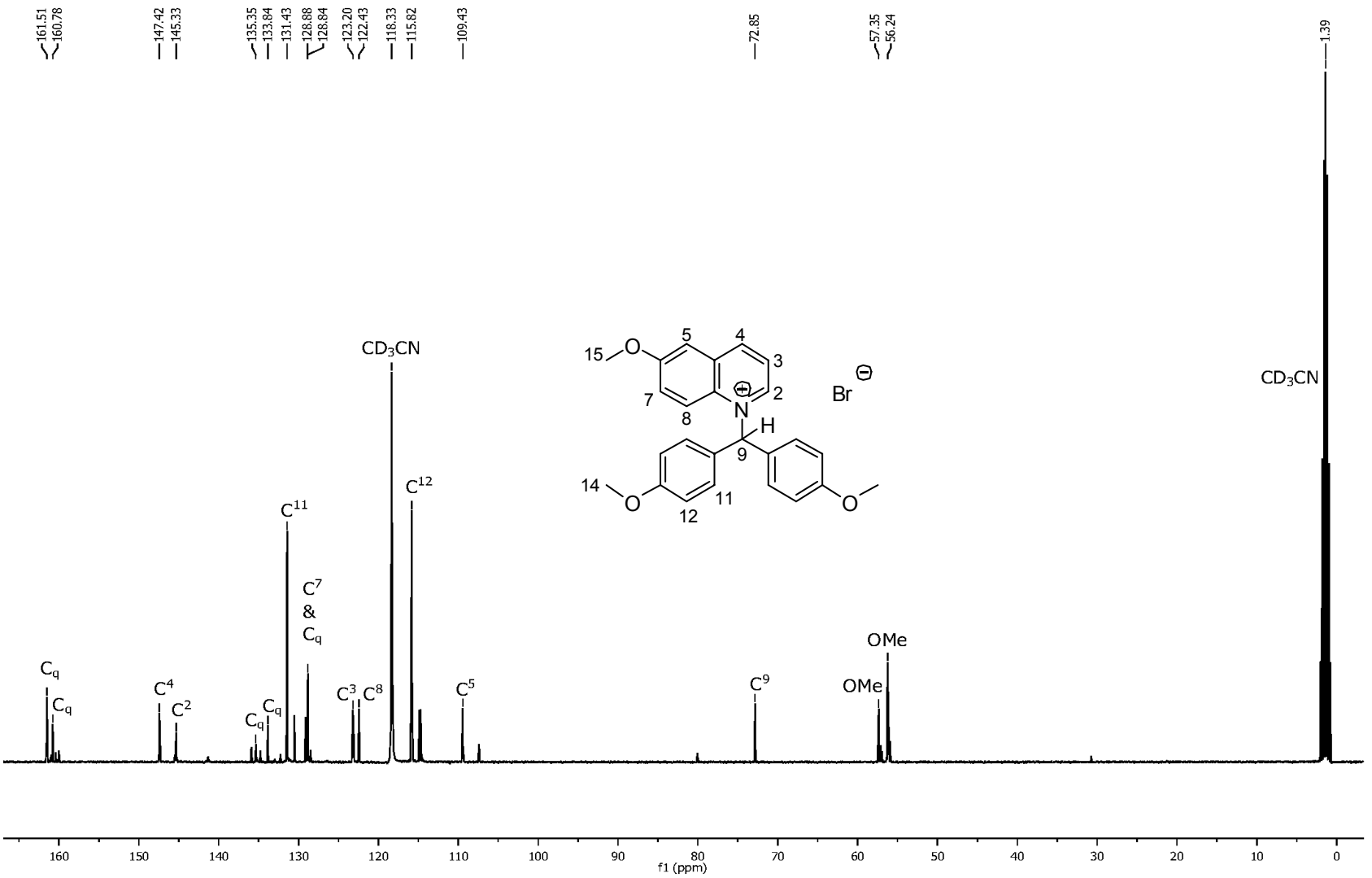
$(ani)_2CHBr$ (26 mg, 0.08 mmol) and **1h** (11 mg, 0.07 mmol) were mixed in an NMR tube and the mixture was analyzed by NMR.

^{1}H-NMR (CD_3CN, 400 MHz): δ = 3.80 (s, 6 H, OCH_3), 4.00 (s, 3 H, OCH_3), 7.00 (d, J = 8.8 Hz, 4 H, H^{12}), 7.20 (d, J = 8.8 Hz, 4 H, H^{11}), 7.69 (dd, ^1J = 9.8 Hz, ^2J = 2.9 Hz, 1 H, H^7), 7.82 (d, J = 2.9 Hz, 1 H, H^5), 7.92 (dd, $J_{3,4}$ = 8.3 Hz, $J_{3,2}$ = 6.0 Hz, 1 H, H^3), 8.20 (s, 1 H, H^9), 8.55 (d, J = 9.8 Hz, 1 H, H^8), 8.63 (d, J = 6.0 Hz, 1 H, H^2), 9.07 (d, J = 8.3 Hz, 1 H, H^4). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 56.2 (OMe), 57.4 (Ome), 72.9 (C^9), 109.4 (C^5), 115.8 (C^{12}), 122.4 (C^8), 123.2 (C^3), 128.8 (C^7), 128.9 (C_q), 131.4 (C^{11}), 133.8 (C_q), 135.4 (C_q), 145.3 (C^2), 147.4 (C^4), 160.8 (C_q), 161.5 (C_q).

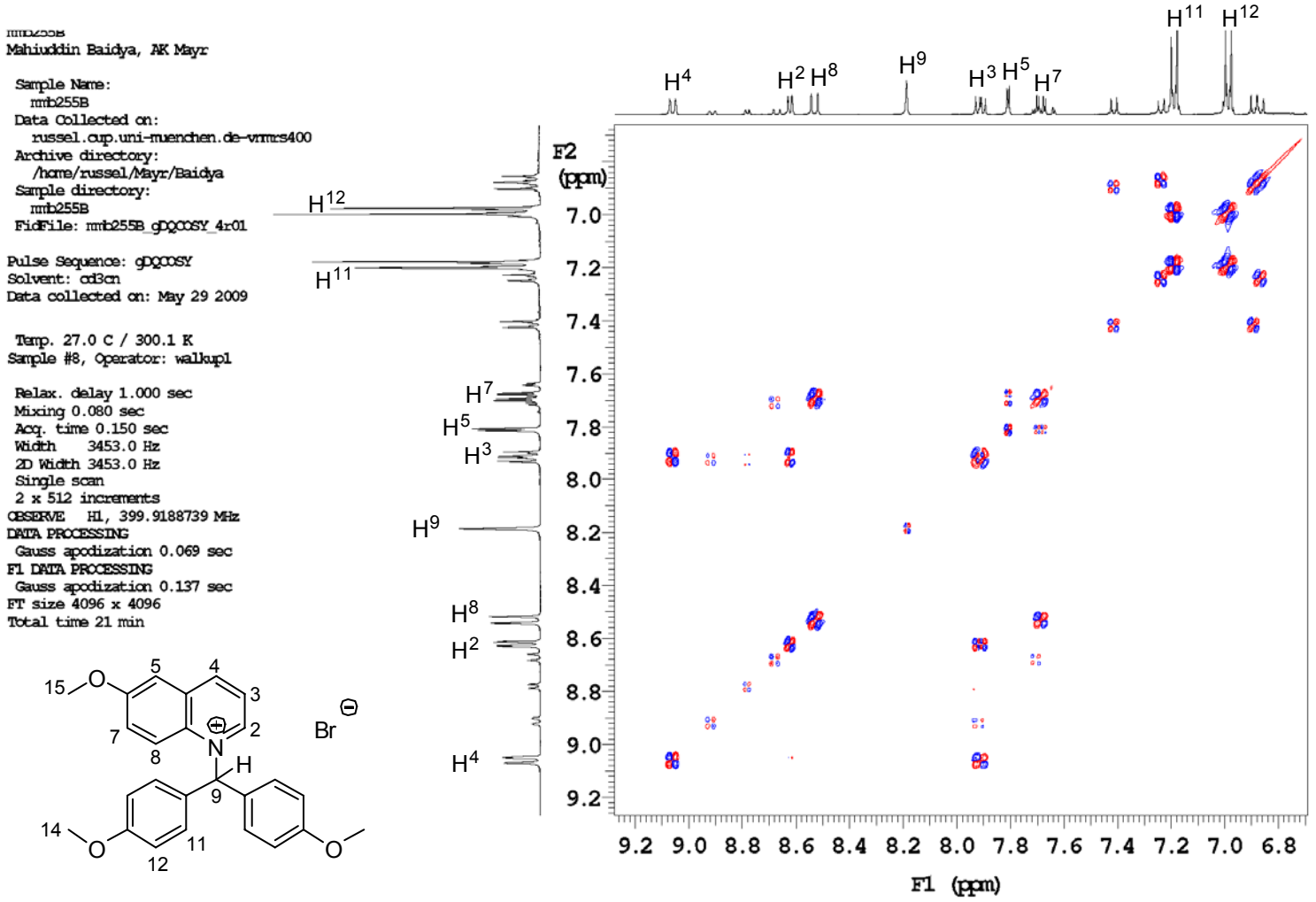




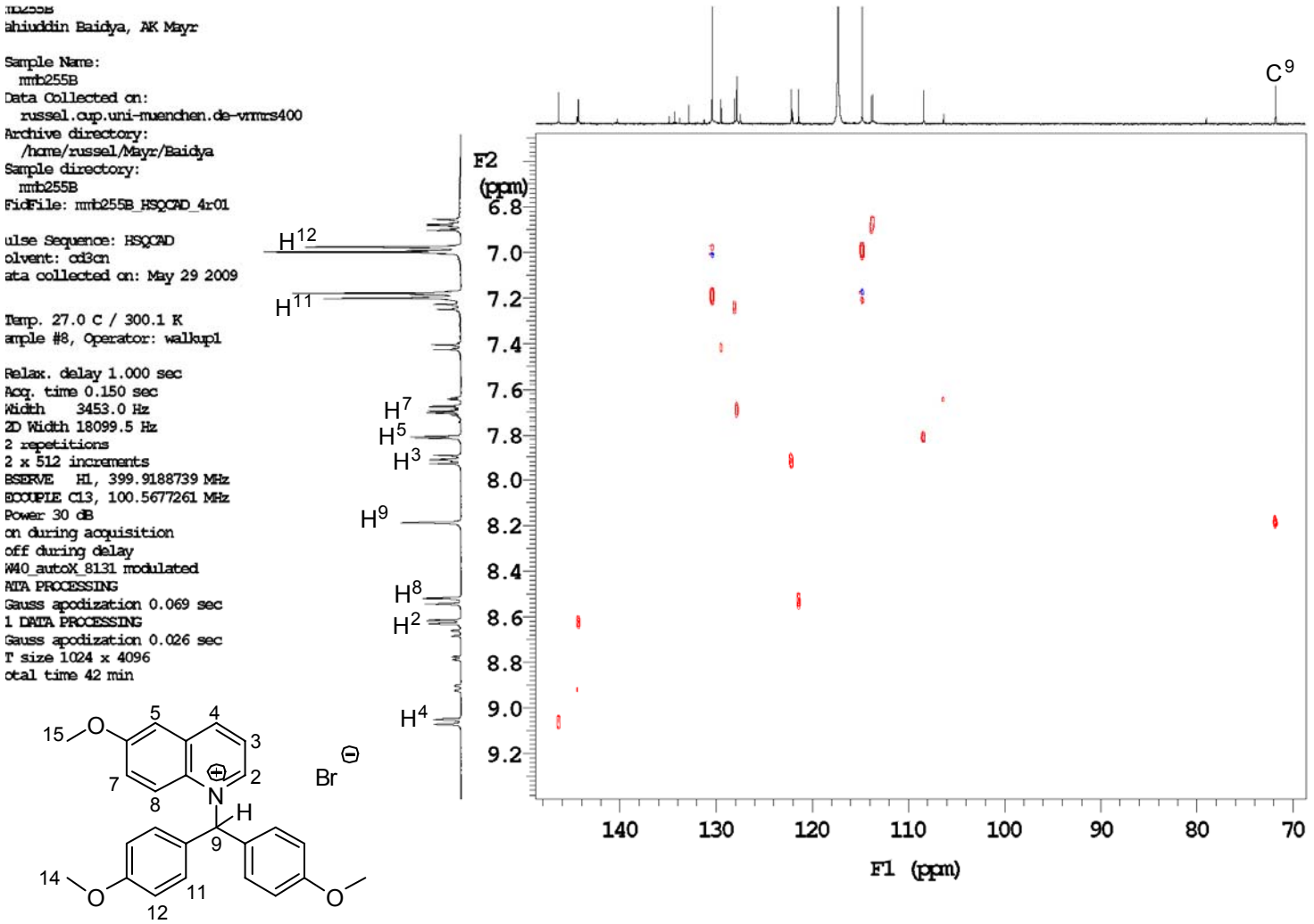
^{1}H-NMR (CD_3CN, 400 MHz) for $(ani)_2CH$-**1h**



^{13}C-NMR (CD_3CN, 100 MHz) for $(ani)_2CH$-**1h**

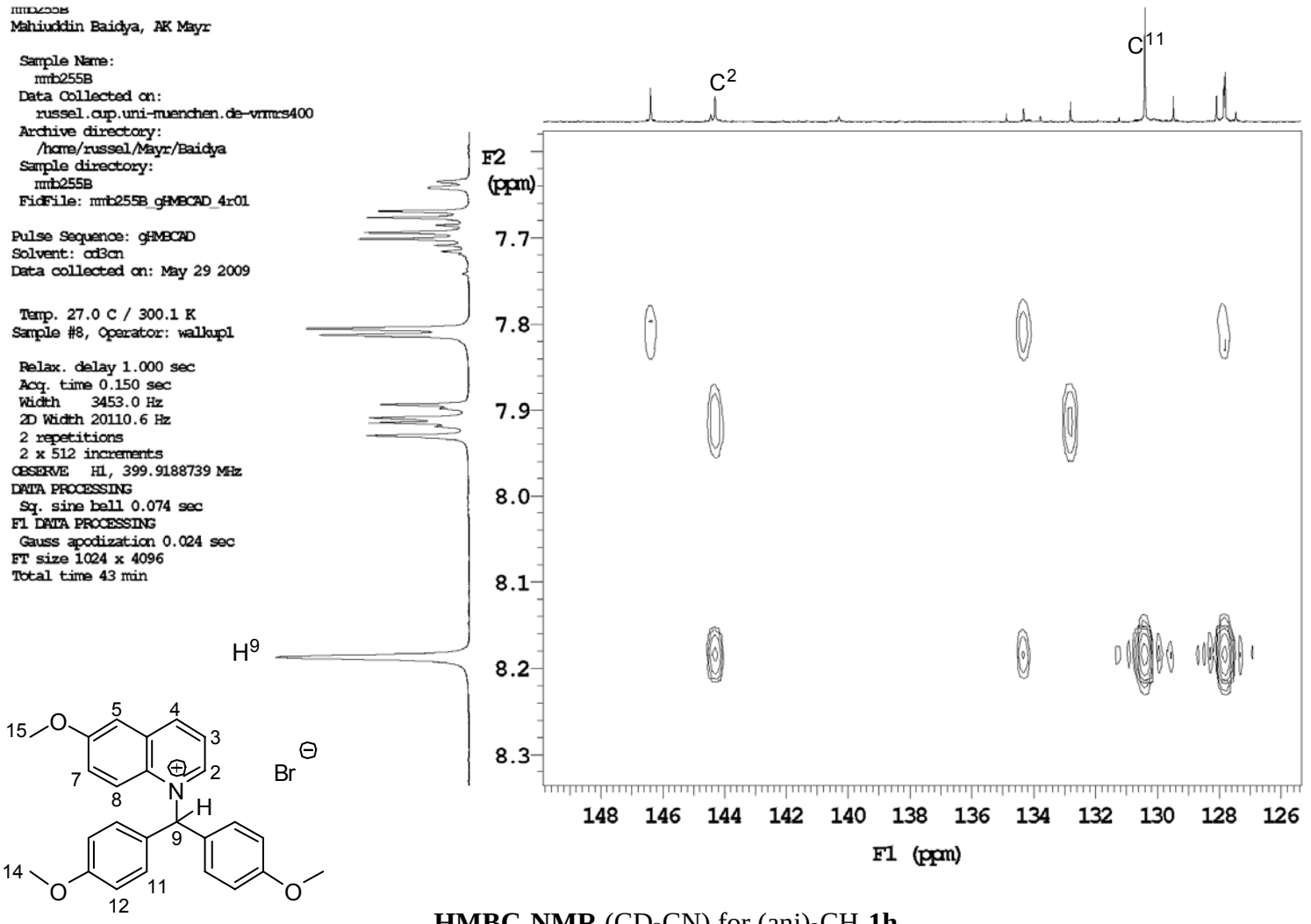


COSY-NMR (CD_3CN) for $(ani)_2CH$-**1h**
[Correlation between protons]



HSQC-NMR (CD_3CN) for $(ani)_2CH$-**1h**

[Correlation between protons and carbons, specially between H^9 and C^9]

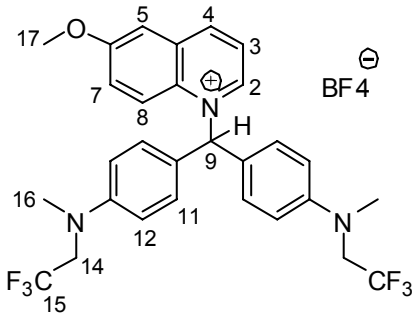


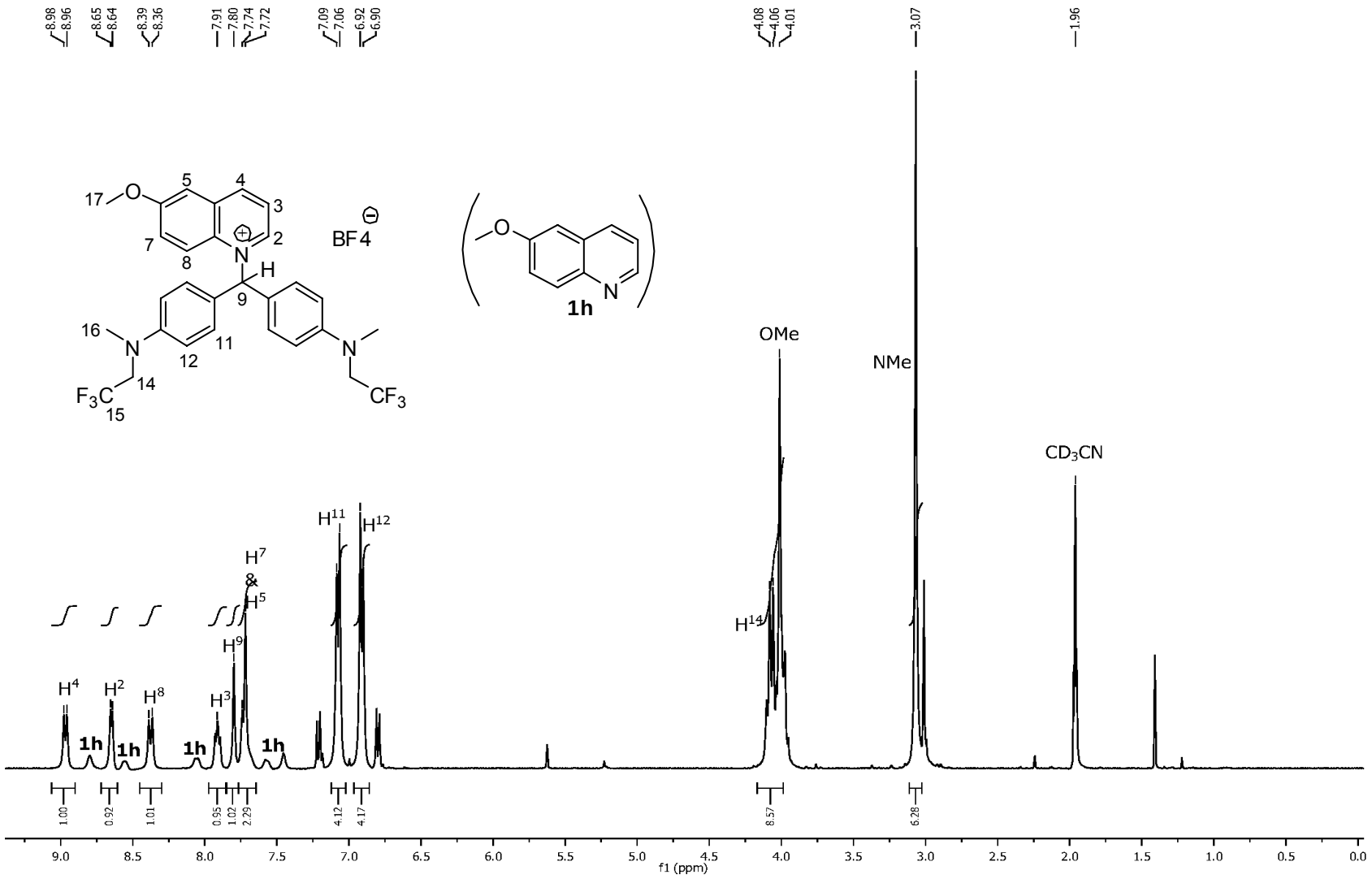
HMBC-NMR (CD_3CN) for $(ani)_2CH$-**1h**
[Correlation shows that C^2 and C^{11} is connected via C^9]

Reaction of $(mfa)_2CH\text{-}BF_4$ with 1h.

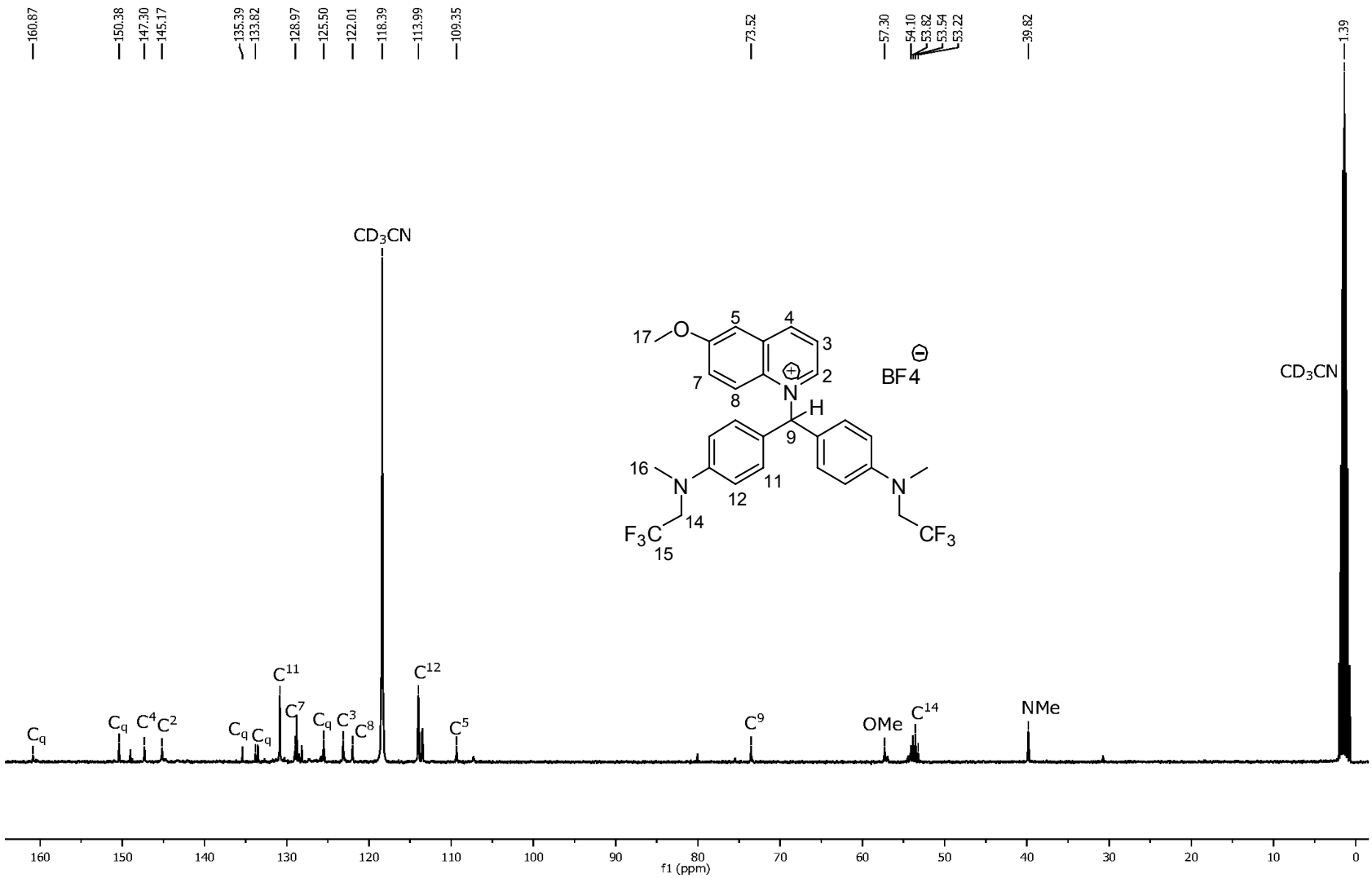
$(mfa)_2CH\text{-}BF_4$ (24 mg, 0.05 mmol) and **1h** (8 mg, 0.05 mmol) were mixed in an NMR tube and the mixture was analyzed by NMR.

^{1}H-NMR (CD_3CN, 400 MHz): δ = 3.07 (s, 6 H, NCH_3), 4.01 (s, 3 H, OCH_3), 4.07 (q, J = 8 Hz, 4 H, $C\underline{H_2}CF_3$), 6.91 (d, J = 8.5 Hz, 4 H, Ar), 7.08 (d, J = 8.5 Hz, 4 H, Ar), 7.72-7.74 (m, 2 H, H^7 & H^5), 7.80 (s, 1 H, H^9), 7.91 (m, 1 H, H^3), 8.38 (d, J = 9.7, 1 H, H^8), 8.65 (d, J = 5.6, 1 H, H^2), 8.97 (d, J = 8.3, 1 H, H^4). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 39.8 (NCH_3), 53.6 (q, J = 32 Hz, $\underline{C}H_2CF_3$), 57.3 (Ome), 73.5 (C^9, $Ar_2\underline{C}H\text{-}N^+$), 109.4 ($C^5$), 114.0 ($C^{12}$), 122.0 ($C^8$), 123.2 ($C^3$), 125.5 ($C_q$), 125.9 (q, J = 280 Hz, CF_3), 129.0 (C^7), 130.8 (C^{11}), 133.8 (C_q), 135.4 (C_q), 145.2 (C^2), 147.3 (C^4), 150.4 (C_q), 160.9 (C_q).

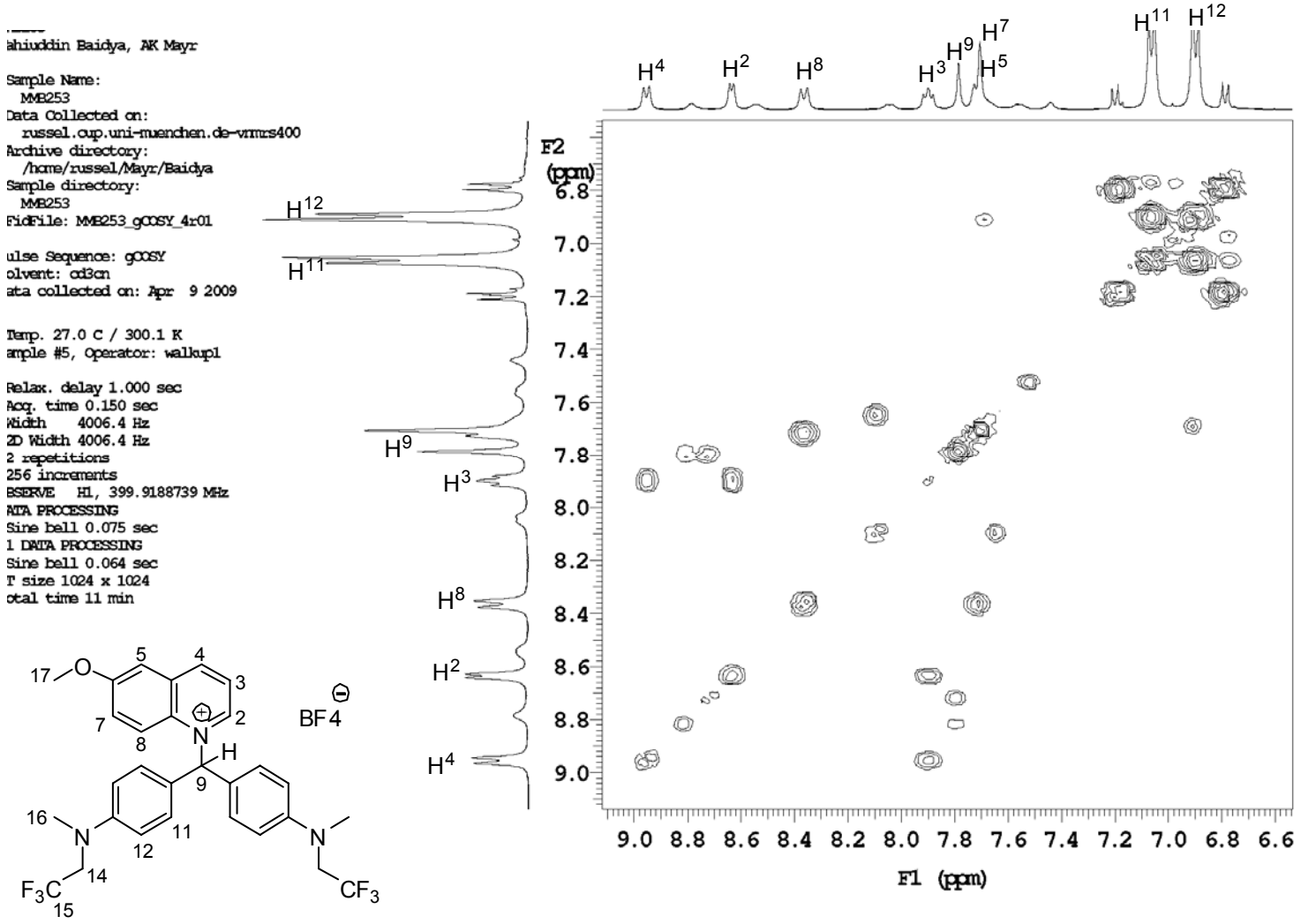




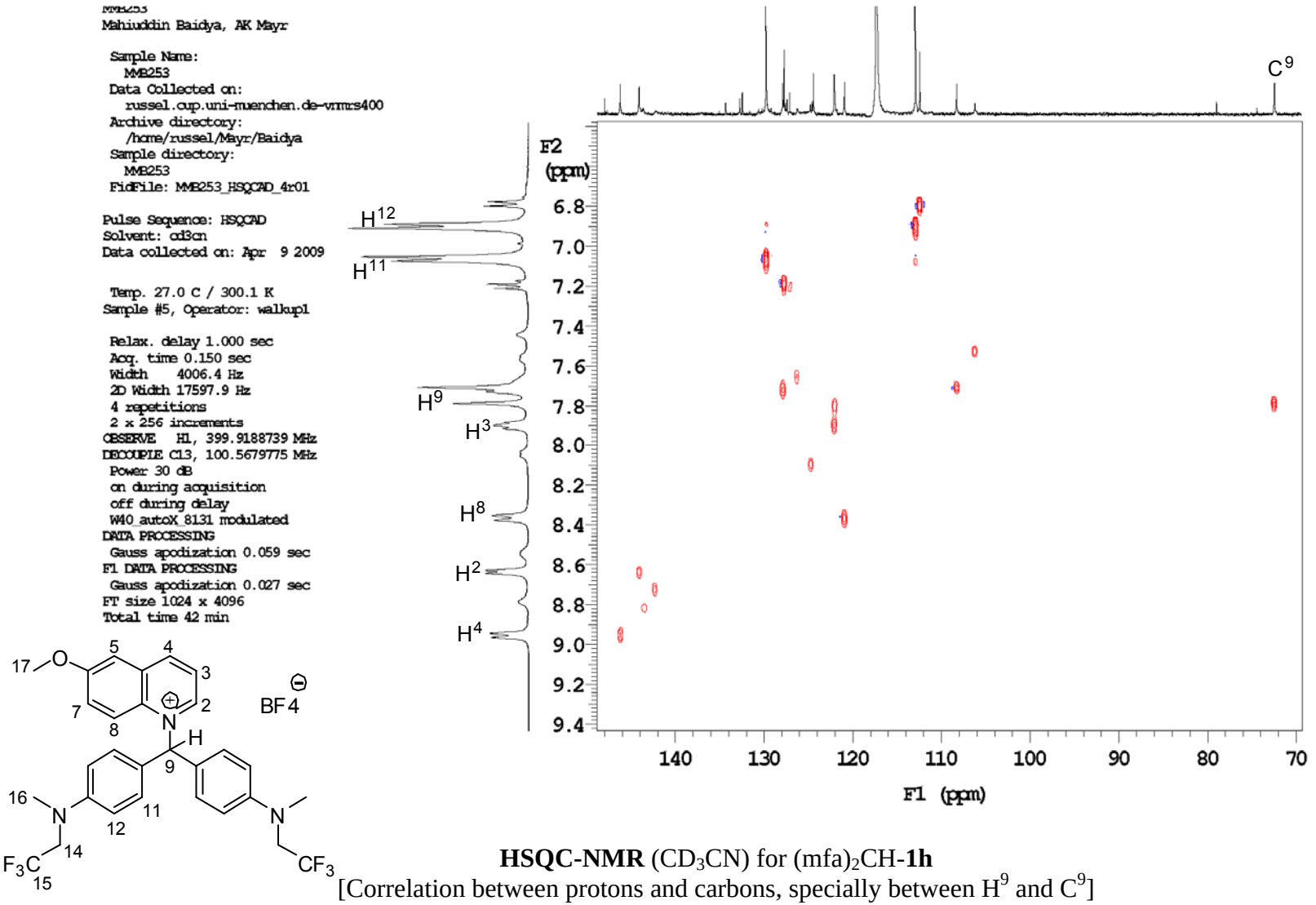
^{1}H-NMR (CD_3CN, 400 MHz) for $(mfa)_2CH$-**1h**



^{13}C-NMR (CD_3CN, 100 MHz) for $(mfa)_2CH$-**1h**

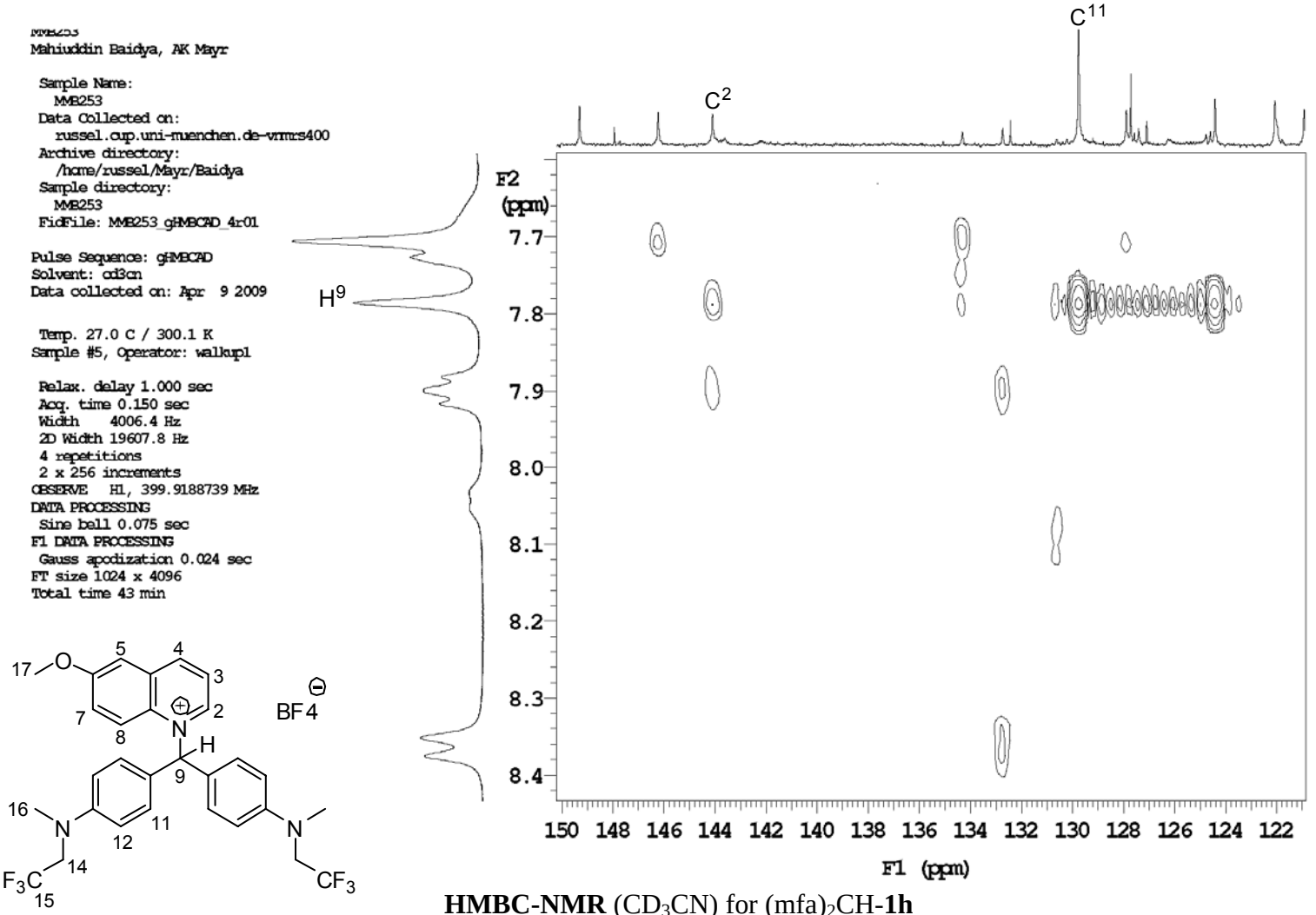


COSY-NMR (CD_3CN) for $(mfa)_2CH$-**1h**
[Correlation between protons]



HSQC-NMR (CD_3CN) for $(mfa)_2CH$-**1h**

[Correlation between protons and carbons, specially between H^9 and C^9]

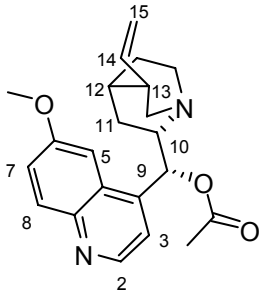


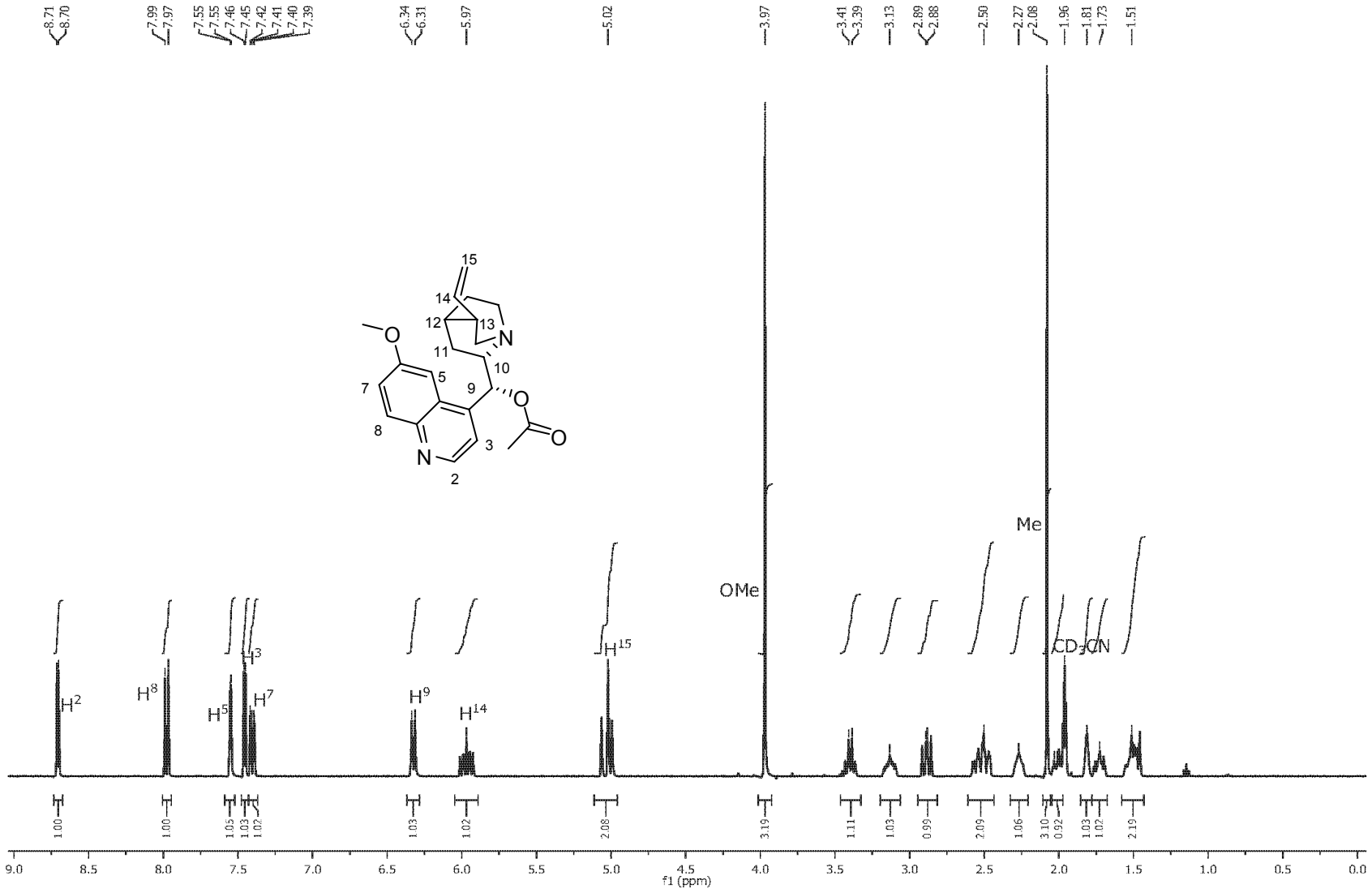
HMBC-NMR (CD_3CN) for $(mfa)_2CH$-**1h**

[Correlation shows that C^2 and C^{11} is connected via C^9]

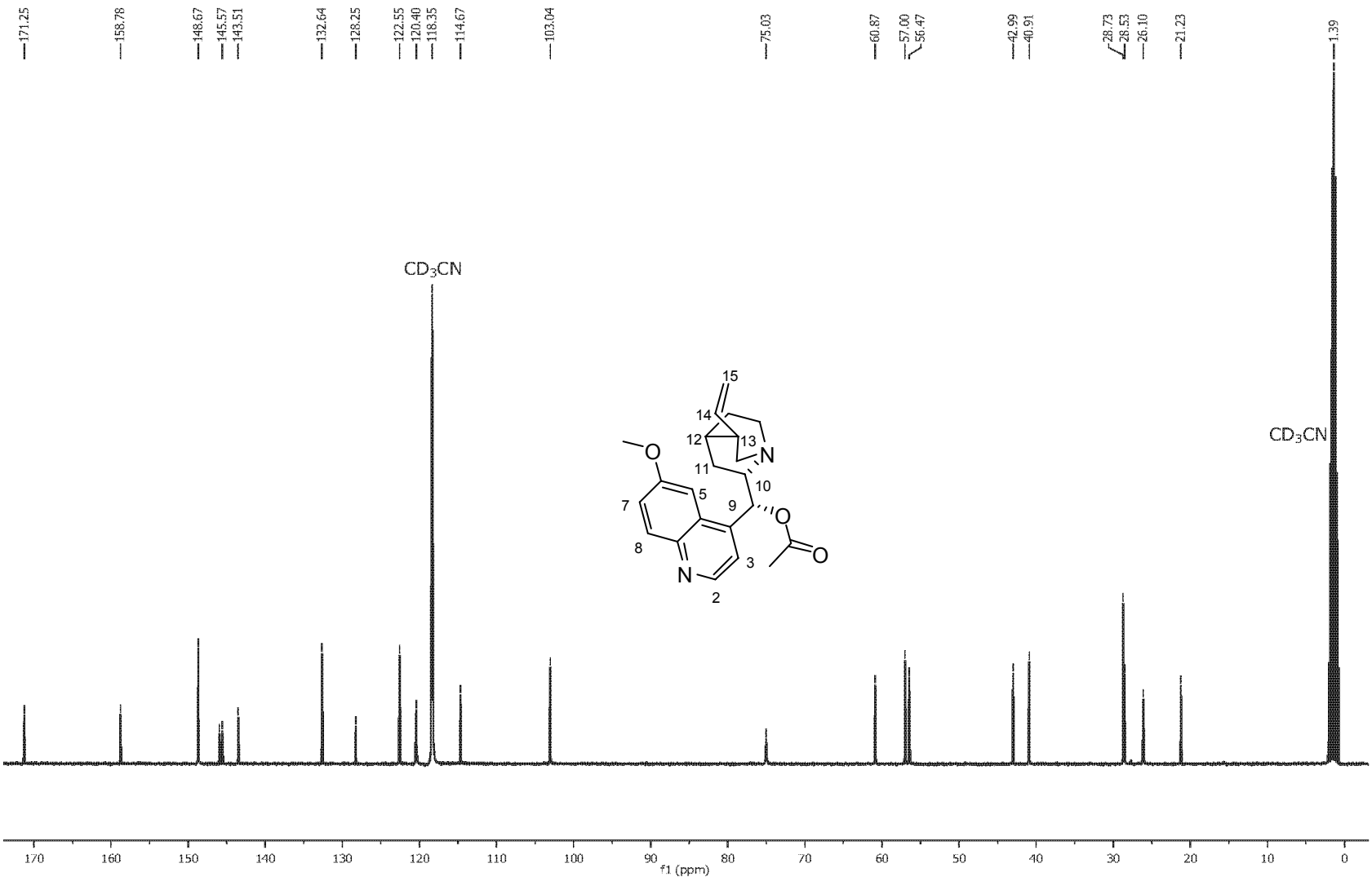
Quinine-Oac (**1c**): **1c** was synthesized by treatment of **1a** with Ac_2O according to ref [S3].

^{1}H-NMR (CD_3CN, 400 MHz): δ = 1.51 (m, 2 H), 1.73 (m, 1 H), 1.81 (m, 1 H), 2.03 (m, 1 H, overlapping with CD_3CN), 2.08 (s, 3 H, CH_3), 2.27 (m, 1 H), 2.50 (m, 2 H), 2.89 (m, 1 H), 3.13 (m, 1 H), 3.40 (q, 1 H), 3.97 (s, 3 H, OCH_3), 5.02 (m, 2 H, CH=C$\underline{H}_2$), 5.97 (m, 1 H, C$\underline{H}$=CH_2), 6.33 (d, *J* = 8.8 Hz, 1 H, C$\underline{H}$OAc), 7.41 (dd, ^{1}J = 2.7 Hz, ^{2}J = 9.2 Hz, 1 H), 7.46 (d, *J* = 4.5 Hz, 1 H), 7.55 (d, *J* = 2.7 Hz, 1 H), 7.98 (d, *J* = 9.2 Hz, 1 H), 8.70 (d, *J* = 4.5 Hz, 1 H). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 21.2, 26.1, 28.5, 28.7, 40.9, 43.0, 56.5, 57.0, 60.9, 75.0, 103.0, 114.7, 120.4, 122.6, 128.3, 132.6, 143.5, 145.6, 145.9, 148.7, 158.78, 171.3.





^{1}H-NMR (CD_3CN, 400 MHz) of **1c**

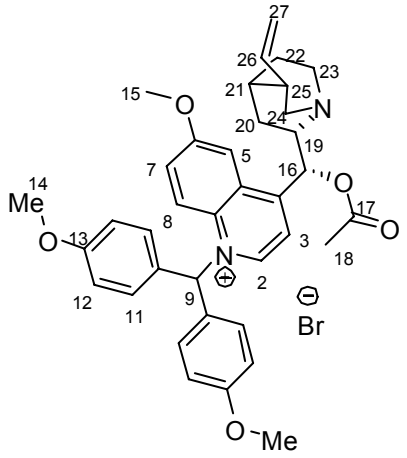


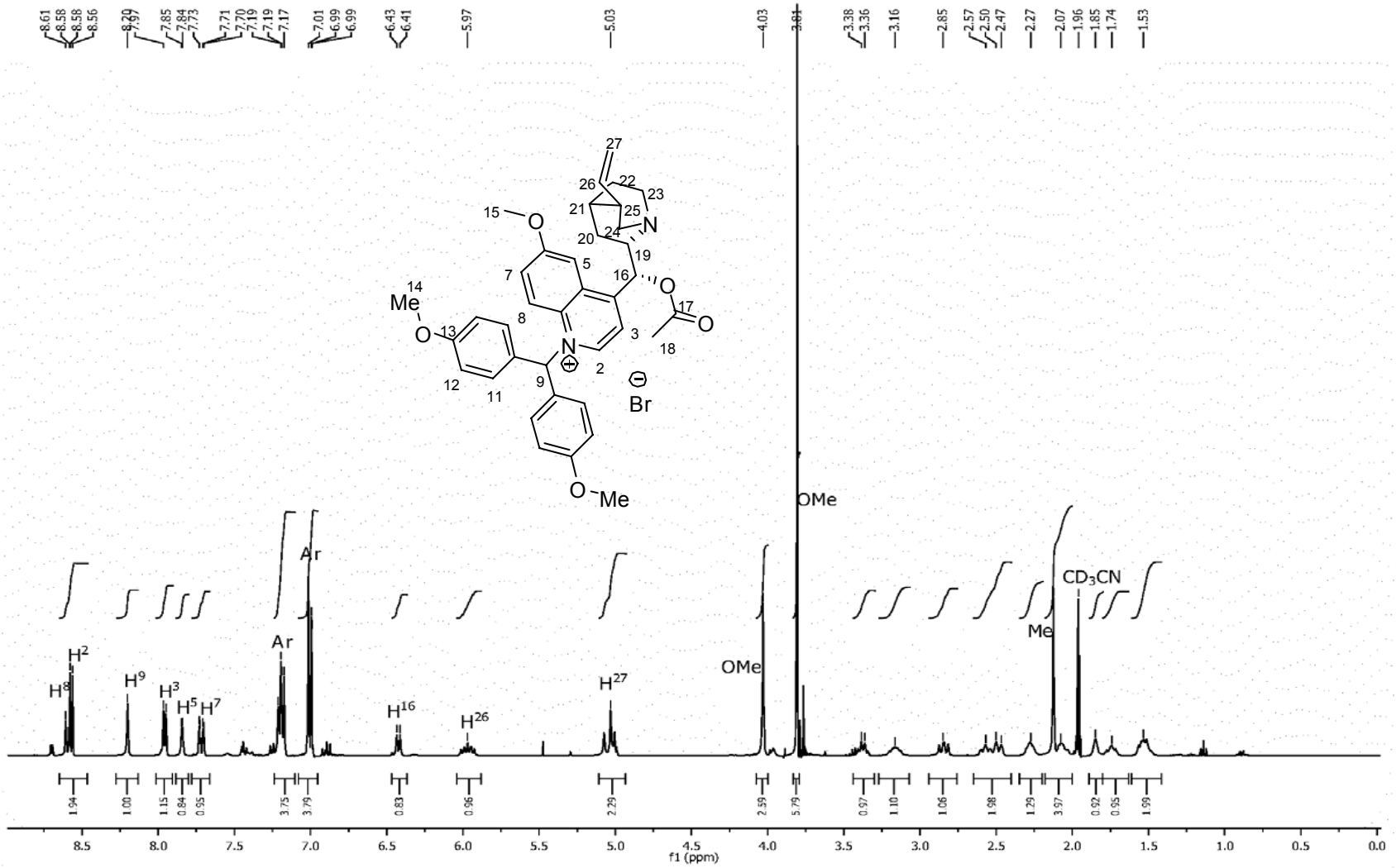
^{13}C-NMR (CD_3CN, 100 MHz) of **1c**

Reaction of $(ani)_2CHBr$ with 1c.

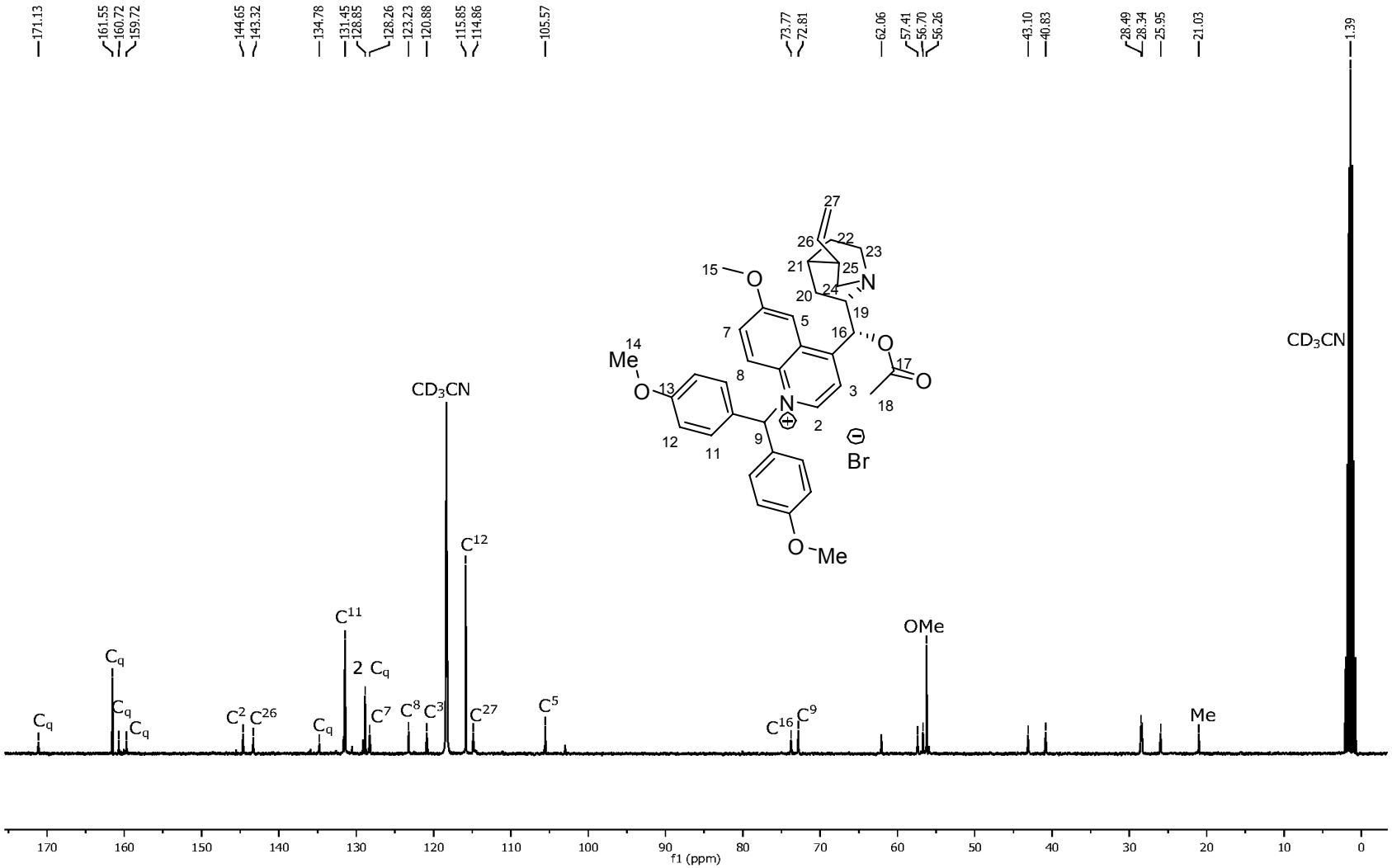
$(ani)_2CHBr$ (19 mg. 0.06 mmol) and **1c** (23 mg, 0,06 mmol) were mixed in an NMR tube and the mixture was analyzed by NMR.

^{1}H-NMR (CD_3CN, 400 MHz): δ = 1.53 (m, 2 H, CH_2), 1.74 (m, 1 H, CH_2), 1.85 (m, 1 H, CH), 2.07 (m, 1 H, CH_2), 2.12 (s, 3 H, Me), 2.27 (m, 1 H, CH), 2.47-2.57 (m, 2 H, CH_2), 2.85 (m, 1 H, CH_2), 3.16 (m, 1 H, CH_2), 3.67 (m, 1 H, CH), 3.81 (s, 6 H, Ome), 4.03 (s, 3 H, Ome), 5.03 (m, 2 H, H^{27}), 5.97 (m, 1 H, H^{26}), 6.42 (d, J = 8.8 Hz, 1 H, H^{16}), 7.00 (m, 4 H, Ar), 7.19 (m, 4 H, Ar), 7.72 (dd, ^1J = 3 Hz, ^2J = 10 Hz, 1 H, H^7), 7.84 (d, J = 3 Hz, 1 H, H^5), 7.96 (d, J = 6.4 Hz, 1 H, H^3), 8.20 (s, 1 H, H^9), 8.57 (d, J = 6.4 Hz, 1 H, H^2), 8.60 (d, J = 10 Hz, 1 H, H^8). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 21.0 (Me), 26.0 (CH_2), 28.3 (CH_2), 28.5 (CH), 40.8 (CH), 43.1 (CH_2), 56.3 (Ome), 56.7 (CH_2), 57.4 (Ome), 62.1 (CH), 72.81 (C^9), 73.8 (C^{16}), 105.6 (C^5), 114.9 (C^{27}), 115.9 (C^{12}), 120.9 (C^3), 123.2 (C^8), 128.3 (C^7), 128.8 (C_q), 128.9 (C_q), 131.5 (C^{11}), 134.8 (C_q), 143.3 (C_{26}), 144.7 (C^2), 159.7 (C_q), 160.7 (C_q), 161.6 (C_q), 171.1 (C_q).

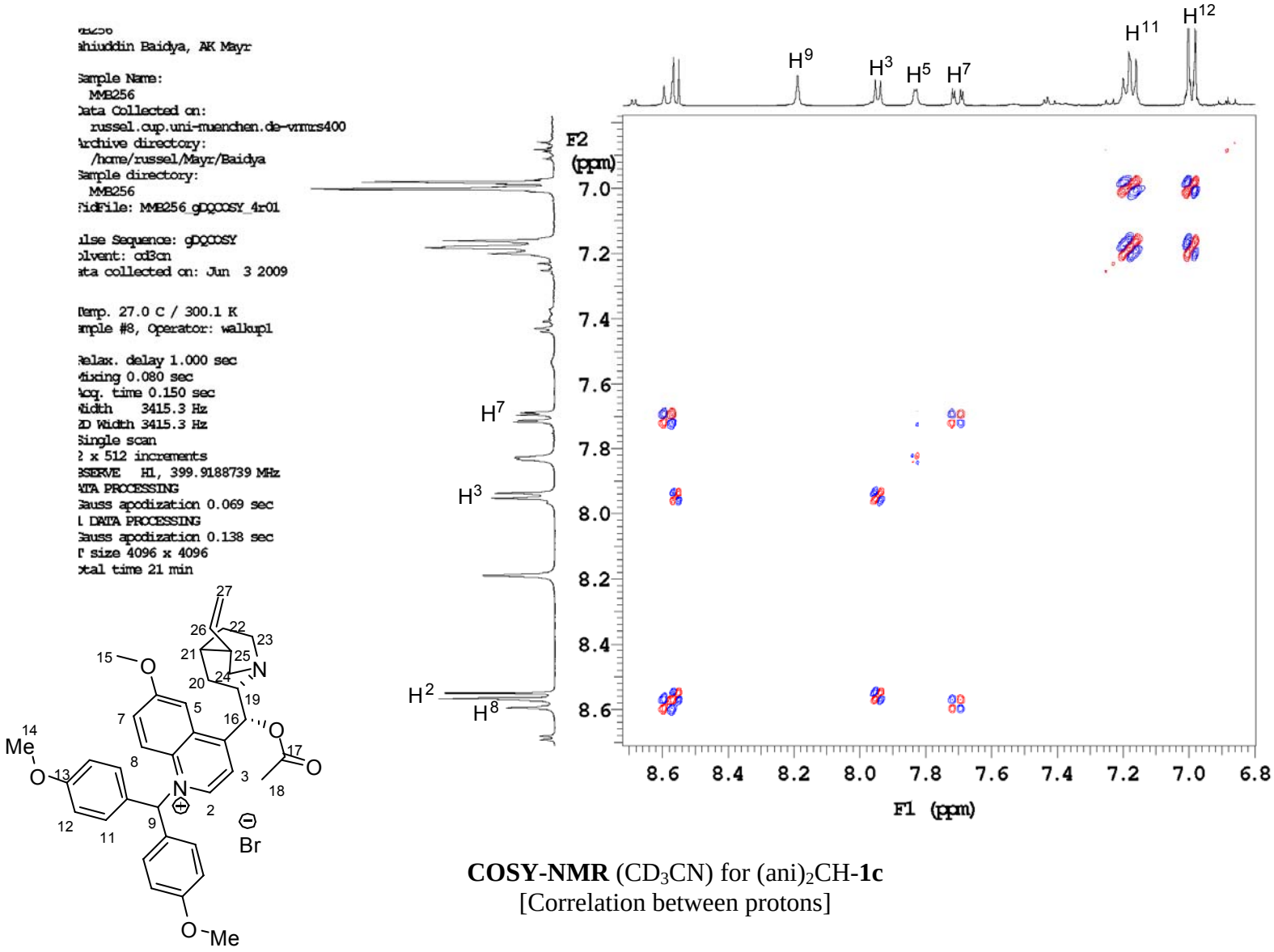




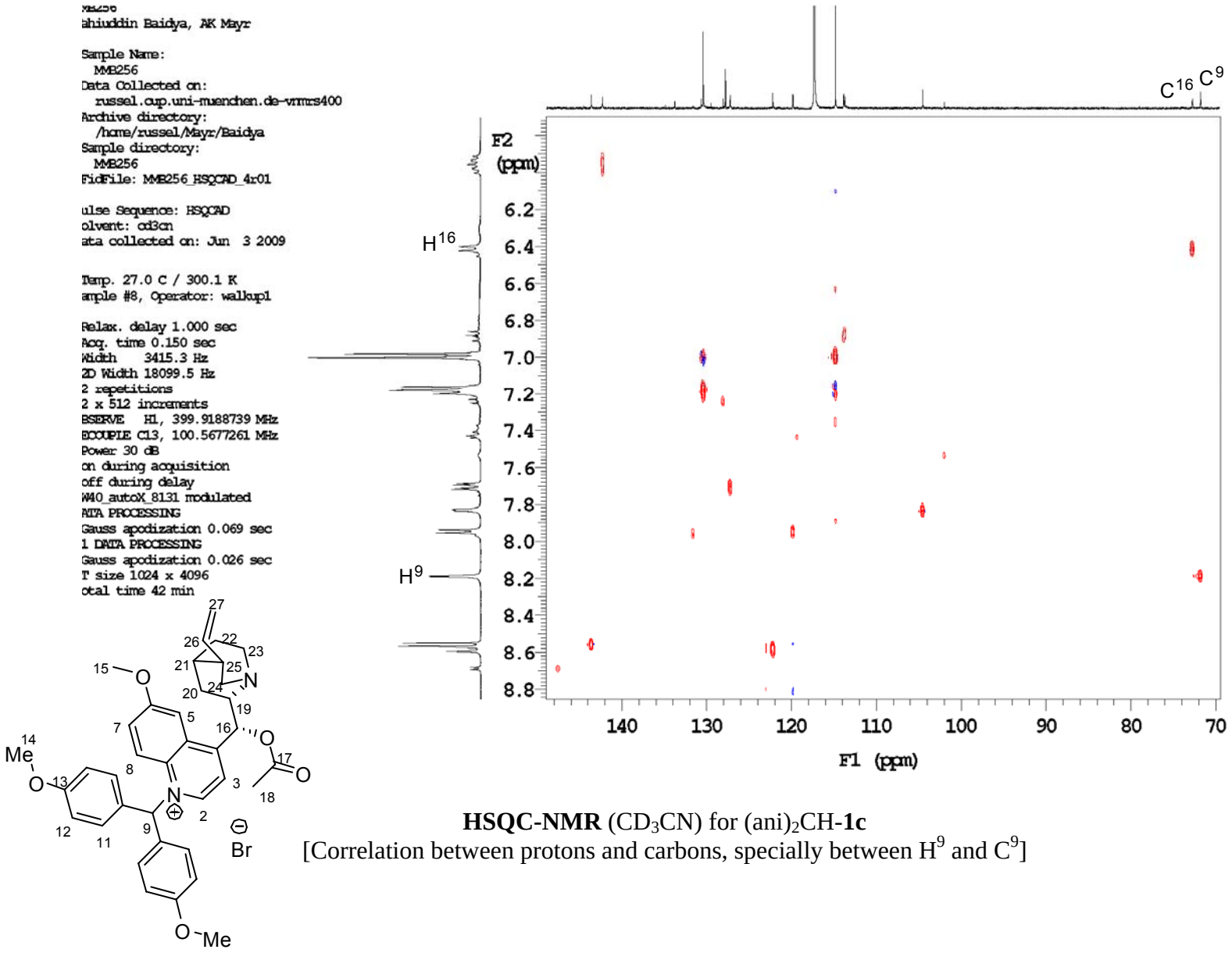
^{1}H-NMR (CD_3CN, 400 MHz) for **(**ani)$_2$CH-**1c**



^{13}C-NMR (CD_3CN, 100 MHz) for $(ani)_2CH$-**1c**

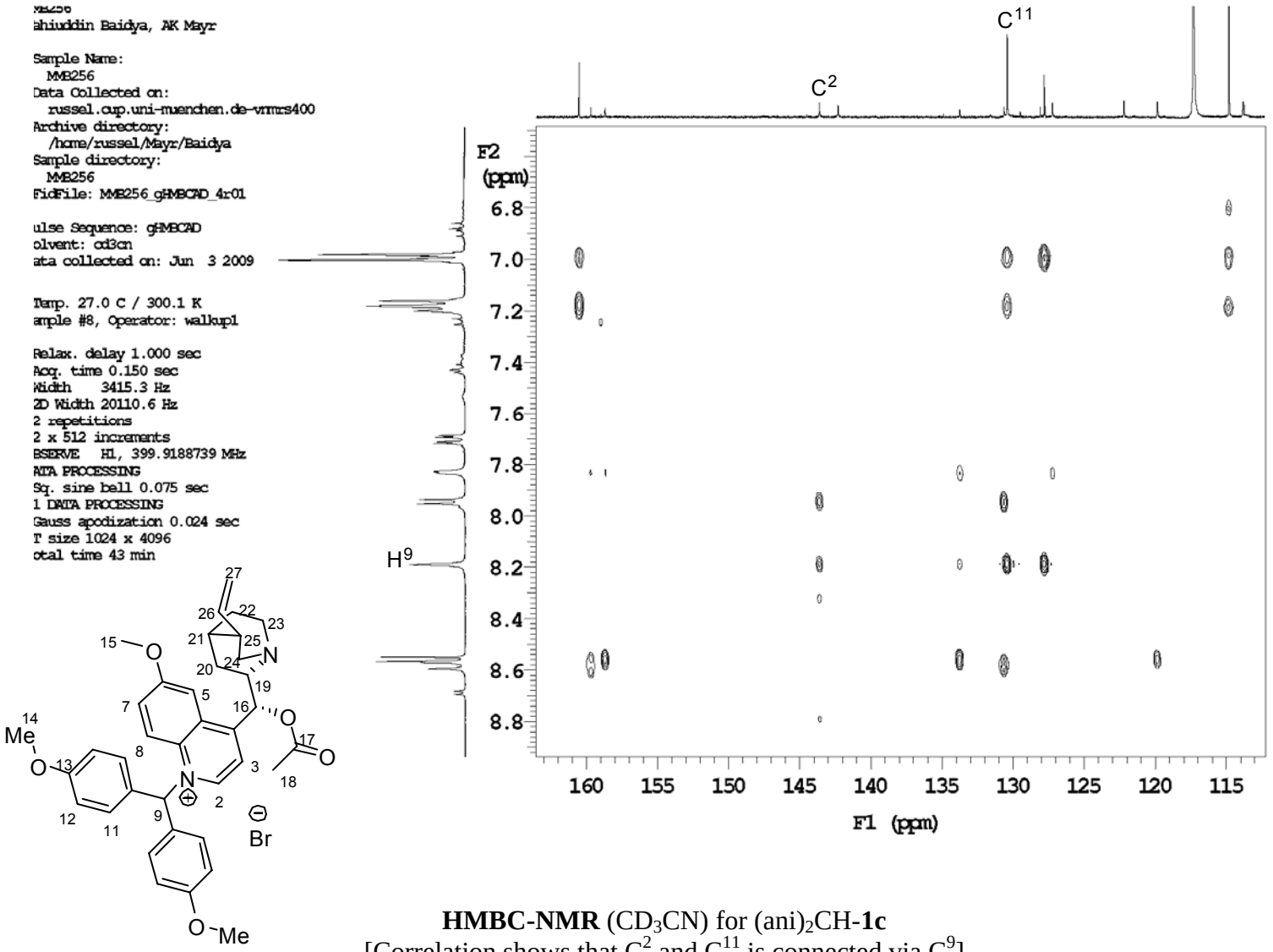


COSY-NMR (CD_3CN) for $(ani)_2CH$-**1c**
[Correlation between protons]



HSQC-NMR (CD_3CN) for $(ani)_2CH$-**1c**

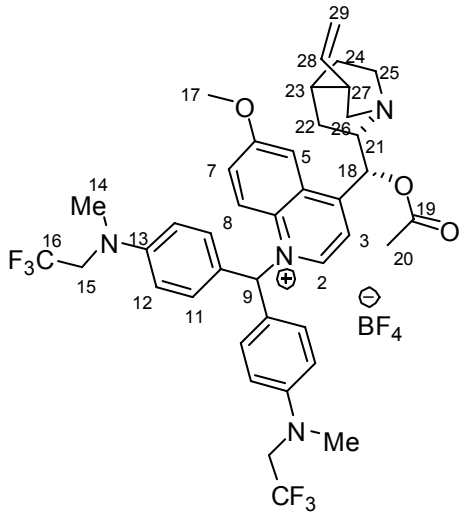
[Correlation between protons and carbons, specially between H^9 and C^9]

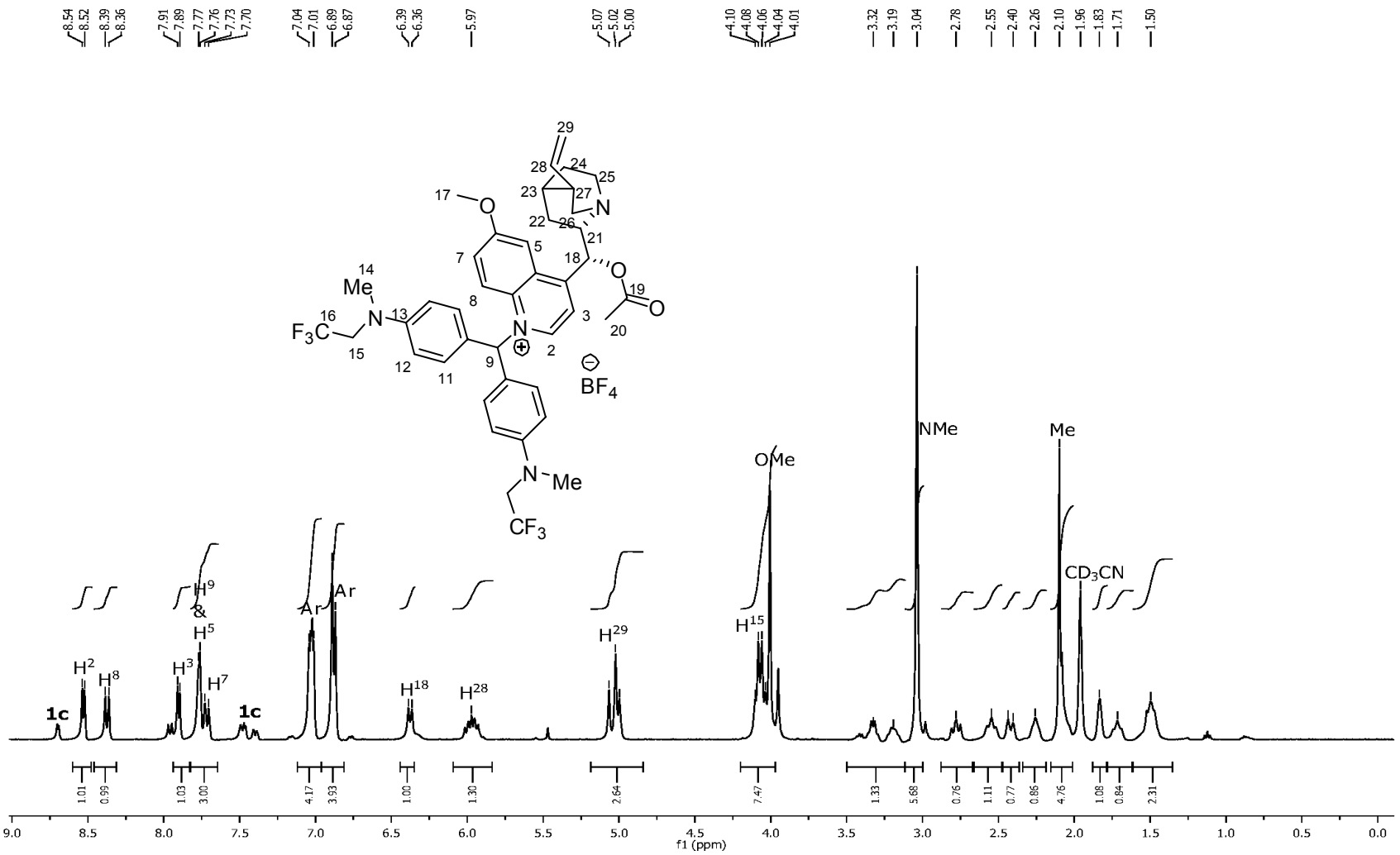


HMBC-NMR (CD_3CN) for $(ani)_2CH$-**1c**
[Correlation shows that C^2 and C^{11} is connected via C^9]

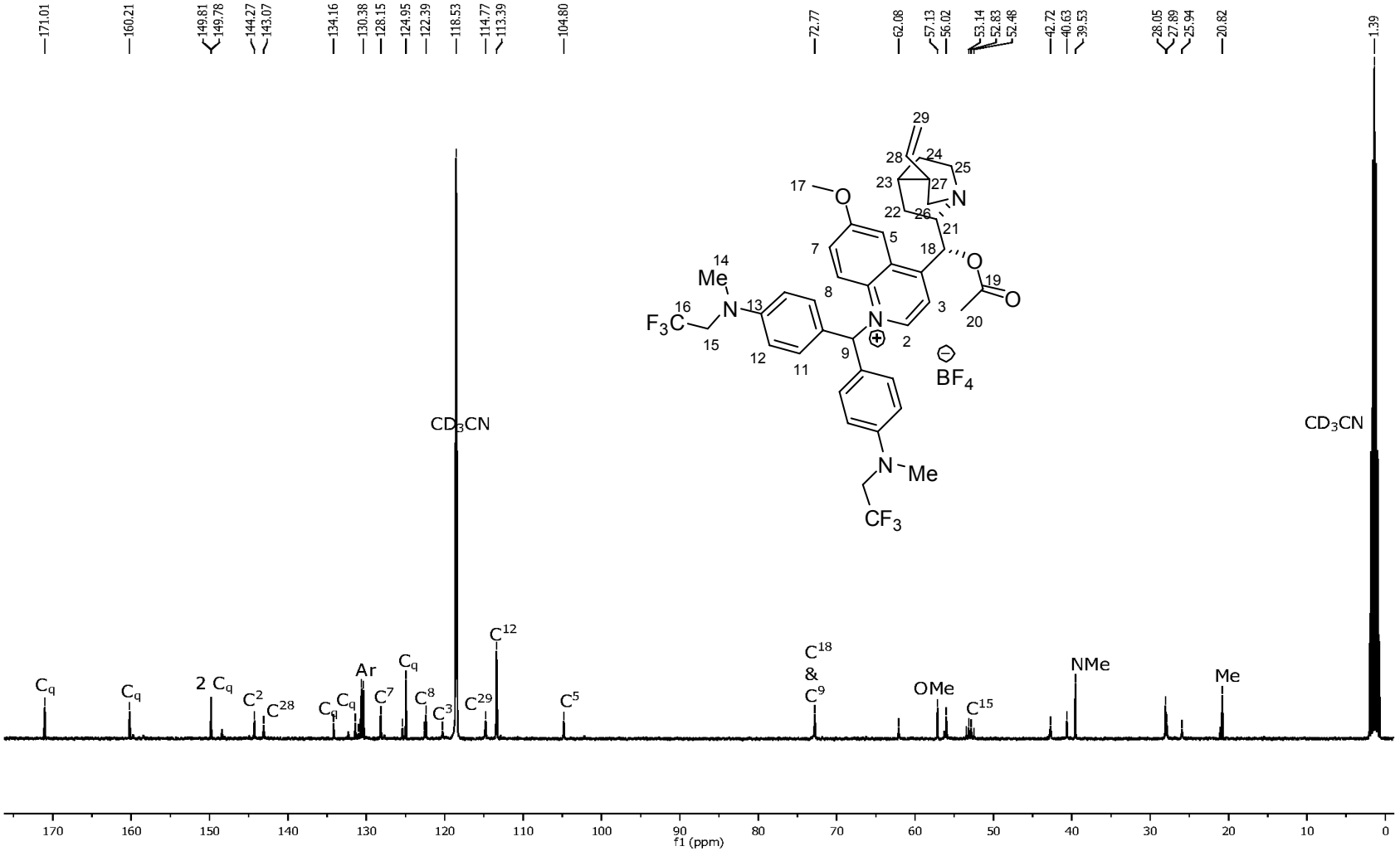
Reaction of $(mfa)_2CH\text{-}BF_4$ with 1c.

$(mfa)_2CH\text{-}BF_4$ (21 mg, 0.04 mmol) and **1c** (16 mg, 0.04 mmol) were mixed in an NMR tube and the mixture was analyzed by NMR at -25 °C. ^{1}H-NMR (CD_3CN, 400 MHz): δ = 1.50 (m, 2 H, CH_2), 1.71 (m, 1 H, CH_2), 1.83 (m, 1 H, CH), 2.08 (m, 1 H, CH_2), 2.10 (s, 3 H, Me), 2.26 (m, 1 H, CH), 2.40 (m, 1 H, CH_2), 2.55 (m, 1 H, CH_2), 2.78 (m, 1 H, CH_2), 3.04 (s, 6 H, Nme), 3.19 (m, 1 H, CH_2), 3.32 (m, 1 H, CH), 4.01 (s, 3 H, Ome), 4.07 (q, J = 8.0 Hz, 4 H, CH_2CF_3), 5.02 (m, 2 H, H^{29}), 5.97 (m, 1 H, H^{28}), 6.37 (d, J = 9.4 Hz, 1 H, CHOAc), 6.88 (d, J = 8.6 Hz, 4 H, Ar), 7.02 (m, 4 H, Ar), 7.71 (d, J = 9.9 Hz, 1 H, H^7), 7.76 (m, 1 H, H^5), 7.77 (s, 1 H, H^9, overlapping with H^5) 7.90 (d, J = 6.3 Hz, 1 H, H^3), 8.37 (d, J = 9.9 Hz, 1 H, H^8), 8.53 (d, J = 6.3 Hz, 1 H, H^2). ^{13}C-NMR (CD_3CN, 100 MHz): δ = 20.8 ($CO\underline{C}H_3$), 25.9 (CH_2), 27.9 (CH_2), 28.1 (CH), 39.5 (Nme), 40.6 (CH), 42.7 (CH_2), 52.8 (q, J = 31 Hz, $\underline{C}H_2CF_3$), 56.0 (CH_2), 57.1 (Ome), 62.1 (CH), 72.8 (2 × C, C^9 & C^{18}), 104.8 (C^5), 113.4 (C^{12}), 114.8 (C^{29}), 120.4 (C^3), 122.3 (C^8), 125.0 (C_q), 126.8 (q, J = 283 Hz, CF_3), 128.2 (C^7), 130.4, 130.6 (Ar), 131.4 (C_q), 134.2 (C_q), 143.1 (C^{28}), 144.3 (C^2), 149.8 (2 × C_q), 160.2 (C_q), 171.1 (C_q).

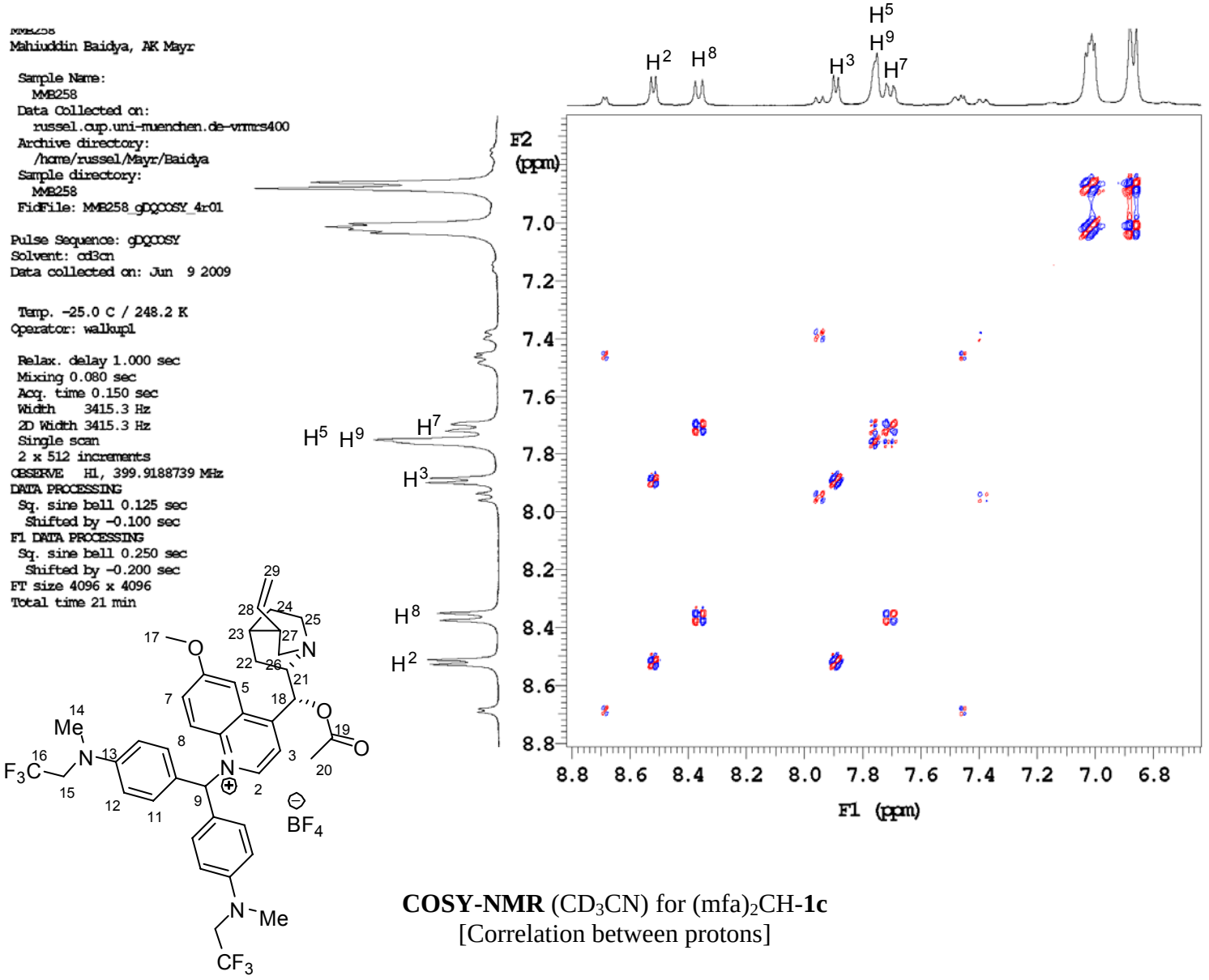




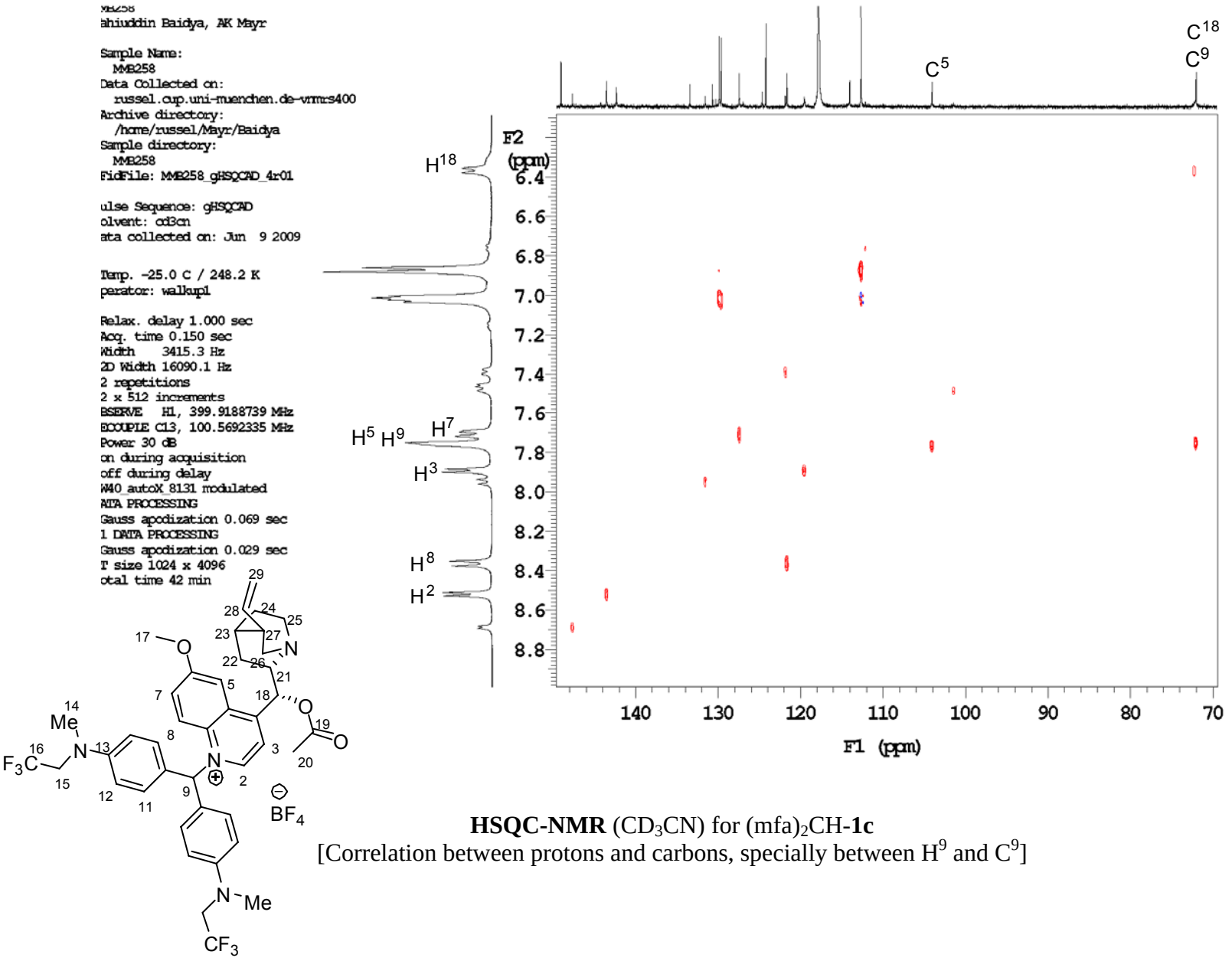
^{1}H-NMR (CD_3CN, 400 MHz) for $(mfa)_2CH$-**1c**



^{13}C-NMR (CD_3CN, 100 MHz) for $(mfa)_2CH$-**1c**



COSY-NMR (CD_3CN) for $(mfa)_2CH$-**1c**
[Correlation between protons]



HSQC-NMR (CD_3CN) for $(mfa)_2CH$-**1c**

[Correlation between protons and carbons, specially between H^9 and C^9]

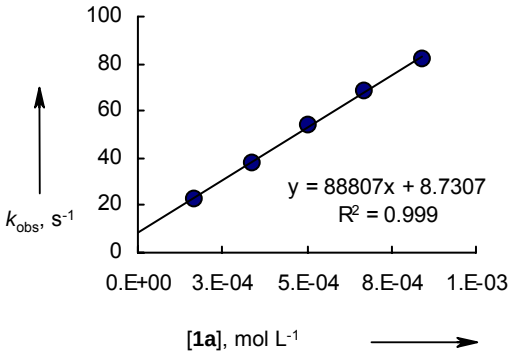
Details of Kinetics

Kinetics of the Reactions of Amines with Benzhydrylium Ions

The reactions of the amines **1a-h** with the colored benzhydrylium ions were followed photometrically at the absorption maxima of Ar_2CH^+ by UV-Vis pectrometry using a stopped flow instrument as described previously.[S1] All experiments were performed under *pseudo*-first-order conditions (excess of amines) at 20 °C in dry acetonitrile or in dry CH_2Cl_2. First order rate constants k_{obs} were obtained by least-squares fitting of the absorbances to the mono-exponential curve $A_t = A_0 \exp(-k_{obs}t) + C$. Because of $k_{obs} = k$[amine], the second-order rate constants k (L mol^{-1} s^{-1}) were derived from the slopes of the linear plots of k_{obs} (s^{-1}) vs. [amine].

Table S1. Kinetics of the Reactions of Quinine (**1a**) with Ar_2CH^+ (20°C, CH_2Cl_2)

$[Ar_2CH^+]$ (mol L^{-1})	[**1a**] (mol L^{-1})	k_{obs} (s^{-1})		k (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 1.8 \times 10^{-5}$, $\lambda_{max} = 593$ nm				
	1.68×10^{-4}	2.30×10^{1}		8.88×10^{4}
	3.35×10^{-4}	3.85×10^{1}		
	5.03×10^{-4}	5.45×10^{1}		
	6.71×10^{-4}	6.85×10^{1}		
	8.38×10^{-4}	8.25×10^{1}		
$[(dpa)_2CH^+] = 2.65 \times 10^{-5}$, $\lambda_{max} = 644$ nm				
	3.69×10^{-4}	1.16×10^{1}		1.76×10^{4}
	5.53×10^{-4}	1.55×10^{1}		
	7.38×10^{-4}	1.93×10^{1}		
	1.11×10^{-3}	2.59×10^{1}		
	1.48×10^{-3}	3.21×10^{1}		
	1.84×10^{-3}	3.77×10^{1}		



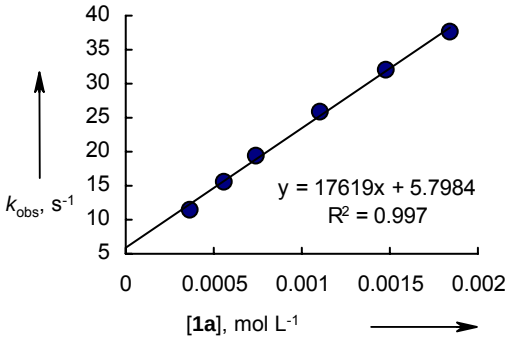
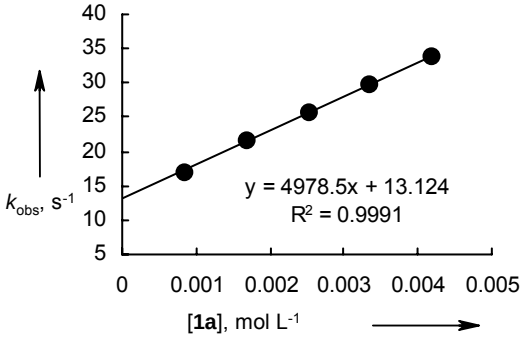


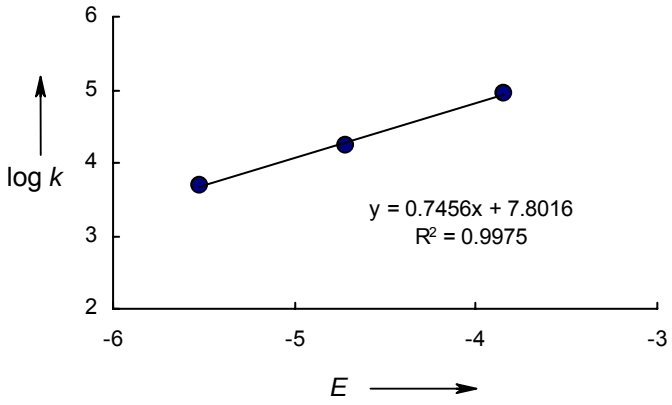
Table S1. Continued

$[Ar_2CH^+]$ (mol L^{-1})	[**1a**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mor)_2CH^+] = 3.48 \times 10^{-5}$, λ_{max} = 612 nm			
	8.38×10^{-4}	1.71×10^{1}	4.98×10^{3}
	1.68×10^{-3}	2.17×10^{1}	
	2.52×10^{-3}	2.58×10^{1}	
	3.35×10^{-3}	2.97×10^{1}	
	4.19×10^{-3}	3.40×10^{1}	



Determination of the Nucleophilicity Parameters *N* and *s* for Quinine (**1a**) in CH_2Cl_2

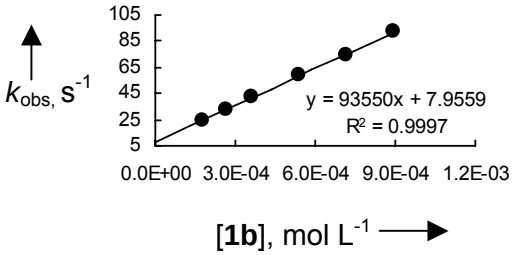
Ar_2CH^+	*E*	*k* (L mol^{-1} s^{-1})	log *k*
$[(mfa)_2CH^+]$	–3.85	8.88×10^{4}	4.95
$[(dpa)_2CH^+]$	–4.72	1.76×10^{4}	4.25
$[(mor)_2CH^+]$	–5.53	4.98×10^{3}	3.70

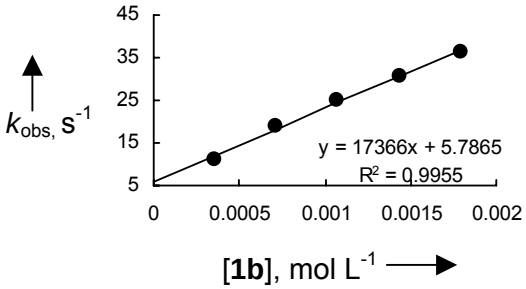


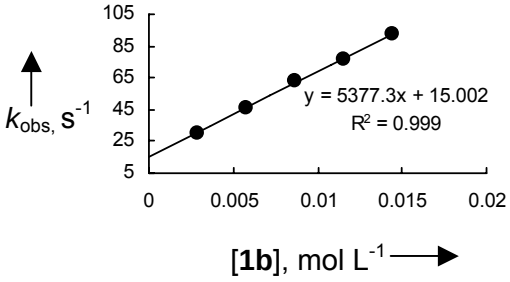
Nucleophilicity parameters for **Quinine (1a) in CH_2Cl_2: *N* = 10.46, *s* = 0.75**

Table S2. Kinetics of the reactions of quinidine (**1b**) with Ar_2CH^+ (20°C, CH_2Cl_2)

$[Ar_2CH^+]$ (mol L^{-1})	[**1b**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 1.8 \times 10^{-5}$, λ_{max} = 593 nm			
	1.79×10^{-4}	2.44×10^{1}	9.36×10^{4}
	2.69×10^{-4}	3.31×10^{1}	
	3.58×10^{-4}	4.18×10^{1}	
	5.37×10^{-4}	5.86×10^{1}	
	7.16×10^{-4}	7.42×10^{1}	
	8.95×10^{-4}	9.20×10^{1}	
$[(dpa)_2CH^+] = 2.8 \times 10^{-5}$, λ_{max} = 672 nm			
	3.58×10^{-4}	1.12×10^{1}	1.74×10^{4}
	7.16×10^{-4}	1.87×10^{1}	
	1.07×10^{-3}	2.52×10^{1}	
	1.43×10^{-3}	3.08×10^{1}	
	1.79×10^{-3}	3.63×10^{1}	
$[(mor)_2CH^+] = 2.9 \times 10^{-5}$, λ_{max} = 620 nm			
	2.89×10^{-3}	3.01×10^{1}	5.38×10^{3}
	5.77×10^{-3}	4.61×10^{1}	
	8.66×10^{-3}	6.27×10^{1}	
	1.15×10^{-2}	7.61×10^{1}	
	1.44×10^{-2}	9.28×10^{1}	

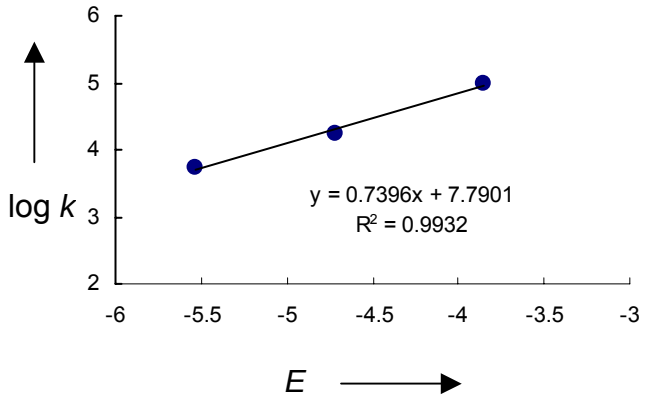






Determination of the Nucleophilicity Parameters *N* and *s* for quinidine **1b** in CH_2CL_2

Ar_2CH^+	*E*	*k* (L mol^{-1} s^{-1})	log *k*
$[(mfa)_2CH^+]$	–3.85	9.36×10^4	4.97
$[(dpa)_2CH^+]$	–4.72	1.74×10^4	4.24
$[(mor)_2CH^+]$	–5.53	5.38×10^3	3.73



Nucleophilicity parameters for **quinidine (1b) in CH_2Cl_2: *N* = 10.54, *s* = 0.74**

Table S3. Kinetics of the Reactions of **1c** with Ar_2CH^+ (20°C, CH_3CN)

$[Ar_2CH^+]$ (mol L^{-1})	[**1c**] (mol L^{-1})	k_{obs} (s^{-1})	*k* (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 1.8 \times 10^{-5}$, λ_{max} = 586 nm			
	3.32×10^{-4}	1.94×10^1	2.68×10^4
	4.98×10^{-4}	2.32×10^1	
	6.64×10^{-4}	2.80×10^1	
	8.30×10^{-4}	3.26×10^1	

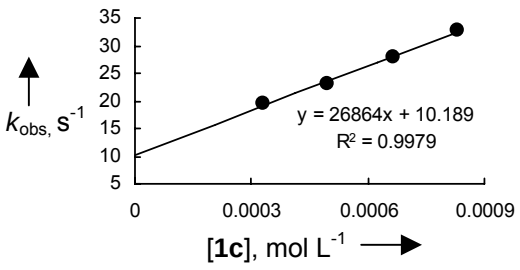


Table S4. Kinetics of the Reactions of **1c** with Ar_2CH^+ (20°C, CH_2Cl_2)

$[Ar_2CH^+]$ (mol L^{-1})	[**1c**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 2.1 \times 10^{-5}$, $\lambda_{max} = 593$ nm			
	2.05×10^{-4}	3.36×10^{1}	8.23×10^{4}
	4.10×10^{-4}	4.79×10^{1}	
	6.15×10^{-4}	6.49×10^{1}	
	8.20×10^{-4}	8.06×10^{1}	
	1.02×10^{-3}	9.91×10^{1}	
	1.23×10^{-3}	1.18×10^{2}	

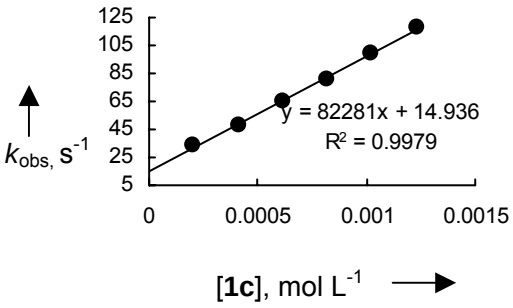
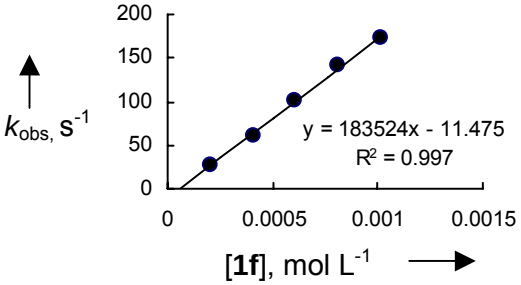


Table S5. Kinetics of the Reactions of **1f** with Ar_2CH^+ (20°C, CH_3CN)

$[Ar_2CH^+]$ (mol L^{-1})	[**1f**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(dma)_2CH^+] = 1.3 \times 10^{-5}$, $\lambda_{max} = 605$ nm			
	2.03×10^{-4}	27.02	1.84×10^{5}
	4.06×10^{-4}	59.78	
	6.08×10^{-4}	100.01	
	8.11×10^{-4}	142.13	
	1.01×10^{-4}	171.93	



$[(pyr)_2CH^+] = 1.2 \times 10^{-5}$, $\lambda_{max} = 605$ nm			
	4.06×10^{-4}	31.48	1.13×10^{5}
	6.08×10^{-4}	51.17	
	8.11×10^{-4}	77.22	
	1.01×10^{-4}	98.90	

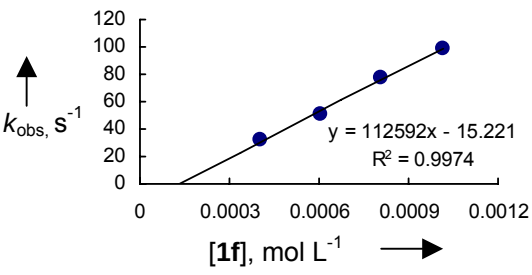
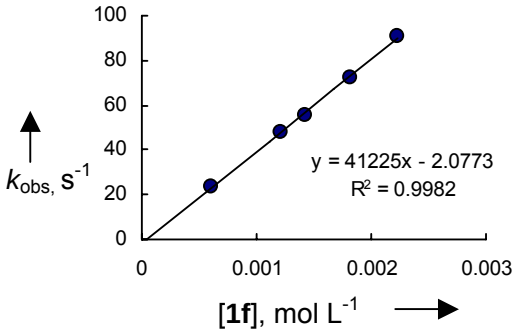
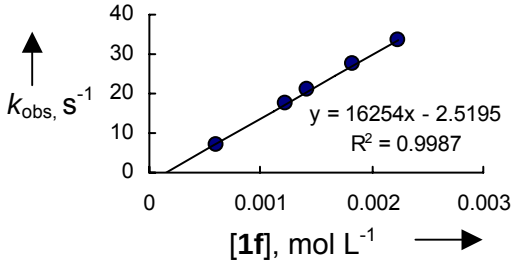


Table S5. Continued

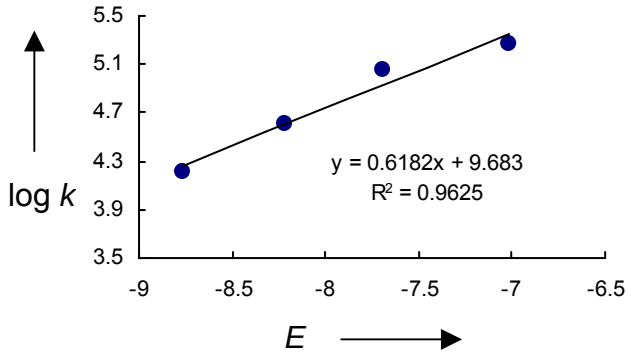
$[Ar_2CH^+]$ (mol L^{-1})	[**1f**] (mol L^{-1})	k_{obs} (s^{-1})		k (L mol^{-1} s^{-1})
$[(thq)_2CH^+] = 4.4 \times 10^{-5}$, $\lambda_{max} = 620$ nm				
	6.08×10^{-4}	23.91		4.12×10^4
	1.22×10^{-3}	47.91		
	1.42×10^{-3}	55.28		
	1.83×10^{-3}	72.30		
	2.23×10^{-3}	91.17		
$[(ind)_2CH^+] = 1.2 \times 10^{-5}$, $\lambda_{max} = 616$ nm				
	6.08×10^{-3}	7.092		1.63×10^4
	1.22×10^{-3}	17.29		
	1.42×10^{-3}	20.89		
	1.83×10^{-3}	27.50		
	2.23×10^{-3}	33.29		





Determination of the Nucleophilicity Parameters *N* and *s* for **1f** in CH_3CN

Ar_2CH^+	*E*	*k* (L mol^{-1} s^{-1})	log *k*
$[(dma)_2CH^+]$	-8.76	1.84×10^5	5.26
$[(pyr)_2CH^+]$	-8.22	1.13×10^5	5.05
$[(thq)_2CH^+]$	-7.69	4.12×10^4	4.62
$[(ind)_2CH^+]$	-7.02	1.63×10^4	4.21



Nucleophilicity parameters for **1f in CH_3CN: *N* = 15.66, *s* = 0.62**

Table S6. Kinetics of the Reactions of Lepidine (**1g**) with Ar_2CH^+ (20°C, CH_3CN)

$[Ar_2CH^+]$ (mol L^{-1})	[**1g**] (mol L^{-1})	k_{obs} (s^{-1})	*k* (L mol^{-1} s^{-1})
$[(pfa)_2CH^+] = 7.66 \times 10^{-6}$, λ_{max} = 592 nm			
	9.45×10^{-5}	23.88	1.78×10^5
	1.89×10^{-4}	41.77	
	2.84×10^{-4}	55.58	
	3.78×10^{-4}	79.88	
	4.73×10^{-4}	89.17	

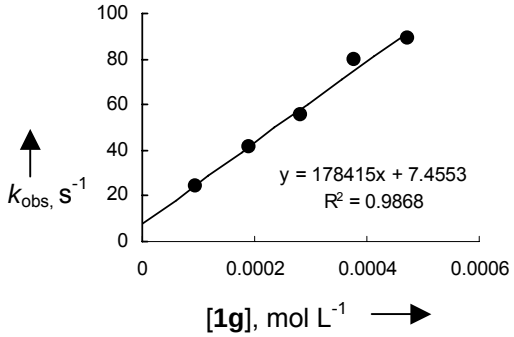
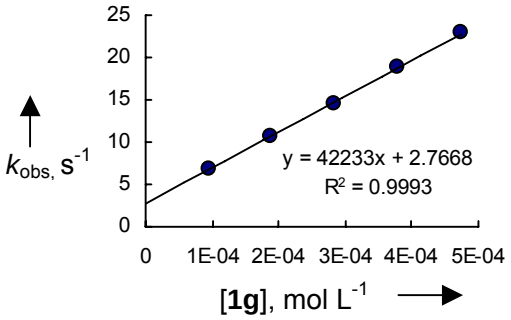
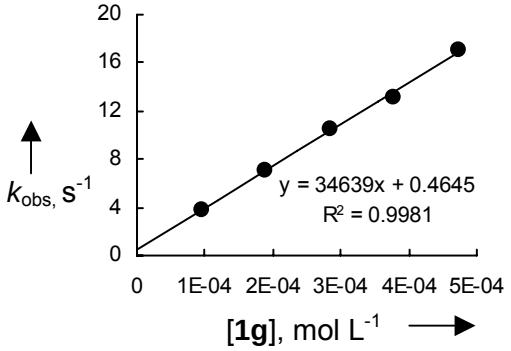


Table S6. Continued.

$[Ar_2CH^+]$ (mol L^{-1})	[**1g**] (mol L^{-1})	k_{obs} (s^{-1})		k (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 7.66 \times 10^{-6}$, λ_{max} = 586 nm				
	9.45×10^{-5}	6.87		4.22×10^4
	1.89×10^{-4}	10.79		
	2.84×10^{-4}	14.45		
	3.78×10^{-4}	18.75		
	4.73×10^{-4}	22.86		
$[(dpa)_2CH^+] = 7.65 \times 10^{-6}$, λ_{max} = 644 nm				
	9.45×10^{-5}	3.74		3.46×10^4
	1.89×10^{-4}	7.03		
	2.84×10^{-4}	10.40		
	3.78×10^{-4}	13.19		
	4.73×10^{-4}	17.03		
$[(mor)_2CH^+] = 9.89 \times 10^{-6}$, λ_{max} = 618 nm				
	1.89×10^{-3}	8.89		3.34×10^3
	2.84×10^{-3}	12.06		
	3.78×10^{-3}	15.28		
	5.67×10^{-3}	21.45		
	7.56×10^{-3}	27.90		





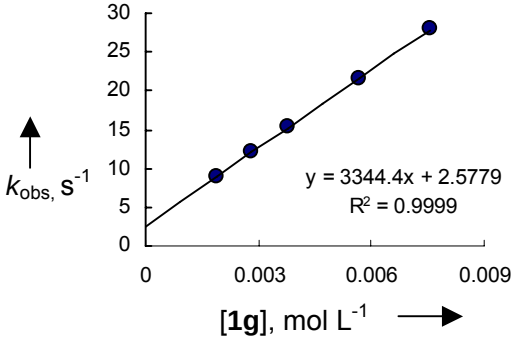
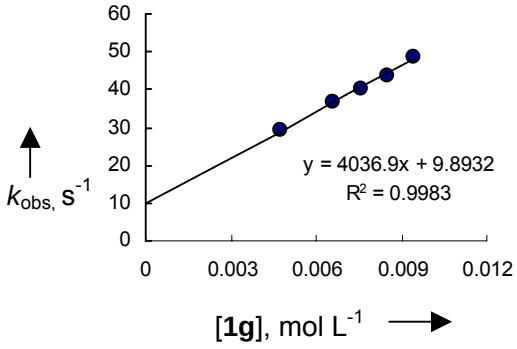


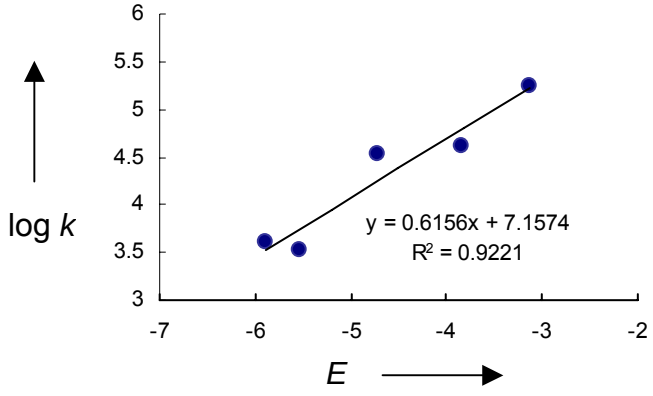
Table S6. Continued.

$[Ar_2CH^+]$ (mol L^{-1})	[**1g**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mpa)_2CH^+] = 9.89 \times 10^{-6}$, λ_{max} = 613 nm			
	4.72×10^{-3}	29.12	4.04×10^3
	6.61×10^{-3}	36.50	
	7.56×10^{-3}	40.40	
	8.50×10^{-3}	43.80	
	9.45×10^{-3}	48.43	



Determination of the Nucleophilicity Parameters *N* and *s* for Lepidine (**1g**) in CH_3CN

Ar_2CH^+	*E*	*k* (L mol^{-1} s^{-1})	log *k*
$[(pfa)_2CH^+]$	-3.14	1.78×10^5	5.25
$[(mfa)_2CH^+]$	-3.85	4.22×10^4	4.63
$[(dpa)_2CH^+]$	-4.72	3.46×10^4	4.54
$[(mor)_2CH^+]$	-5.53	3.34×10^3	3.52
$[(mpa)_2CH^+]$	-5.89	4.04×10^3	3.61



Nucleophilicity parameters for **1g in CH_3CN: *N* = 11.60, *s* = 0.62**

Table S7. Kinetics of the Reaction of Lepidine (**1g**) with Ar_2CH^+ (20°C, CH_2Cl_2)

$[Ar_2CH^+]$ (mol L^{-1})	[**1g**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 7.66 \times 10^{-6}$, $\lambda_{max} = 586$ nm			
	2.40×10^{-4}	36.56	1.23×10^5
	4.81×10^{-4}	62.20	
	7.21×10^{-4}	91.90	
	9.61×10^{-4}	1.25×10^2	

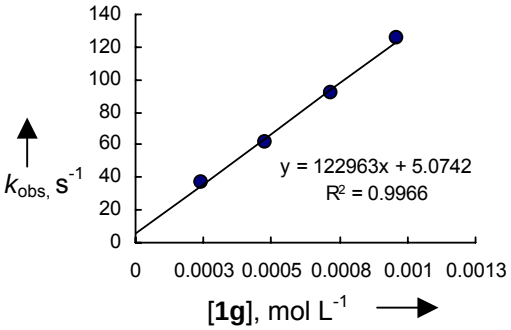
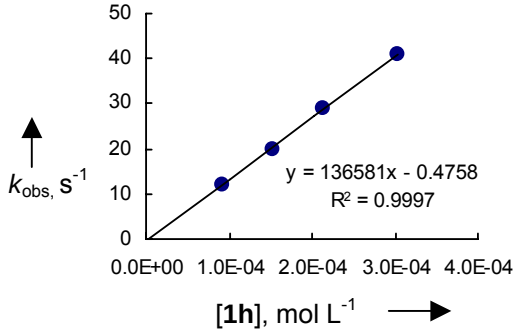


Table S8. Kinetics of the Reactions of **1h** with Ar_2CH^+ (20°C, CH_3CN)

$[Ar_2CH^+]$ (mol L^{-1})	[**1h**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(pfa)_2CH^+] = 1.12 \times 10^{-5}$, $\lambda_{max} = 592$ nm			
	9.12×10^{-5}	12.03	1.37×10^5
	1.52×10^{-4}	20.04	
	2.13×10^{-4}	28.84	
	3.04×10^{-4}	40.95	



$[(mfa)_2CH^+] = 1.27 \times 10^{-5}$, $\lambda_{max} = 586$ nm			
	2.05×10^{-4}	8.94	2.16×10^4
	4.10×10^{-4}	13.81	
	6.15×10^{-4}	18.55	
	8.20×10^{-4}	22.67	
	1.02×10^{-3}	26.86	
	1.23×10^{-3}	31.20	

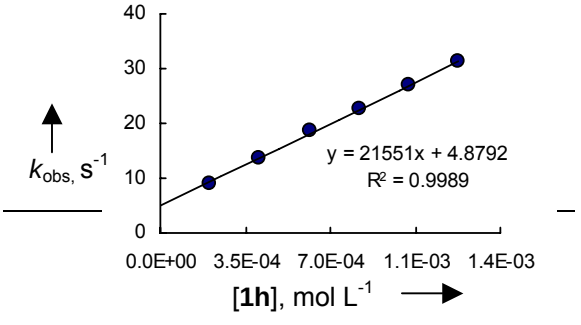
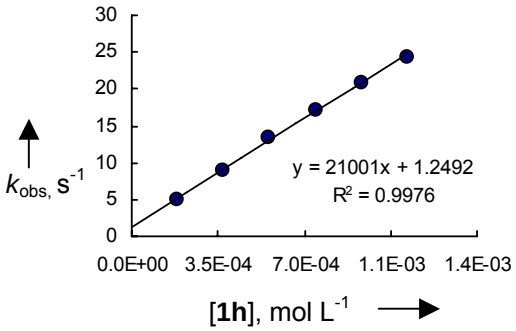
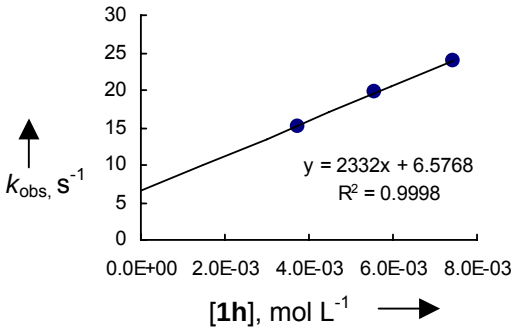


Table S8. Continued.

$[Ar_2CH^+]$ (mol L^{-1})	[**1h**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(dpa)_2CH^+] = 2.45 \times 10^{-5}$, λ_{max} = 644 nm			
	1.86×10^{-4}	4.88	2.10×10^4
	3.72×10^{-4}	8.87	
	5.59×10^{-4}	13.45	
	7.45×10^{-4}	17.21	
	9.31×10^{-4}	20.93	
	1.12×10^{-3}	24.27	

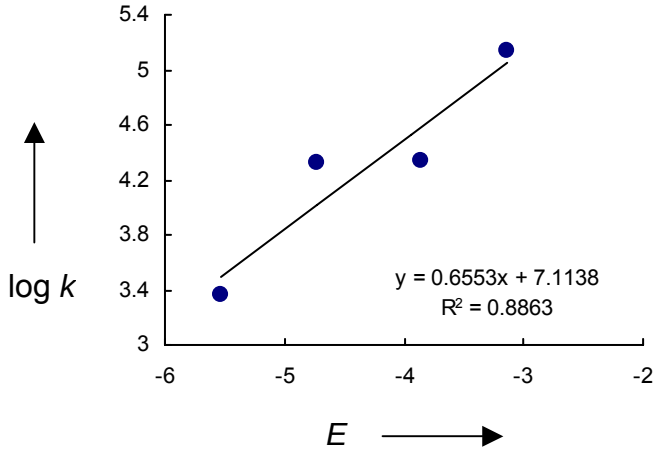


$[Ar_2CH^+]$ (mol L^{-1})	[**1h**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
$[(mor)_2CH^+] = 2.56 \times 10^{-5}$, λ_{max} = 612 nm			
	7.45×10^{-3}	23.91	2.33×10^3
	5.59×10^{-3}	19.68	
	3.72×10^{-3}	15.22	



Determination of the Nucleophilicity Parameters *N* and *s* for **1h** in CH_3CN

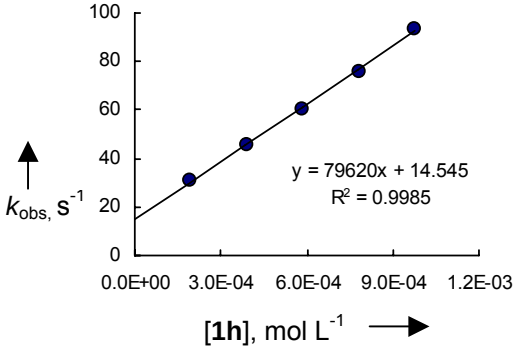
Ar_2CH^+	*E*	*k* (L mol^{-1} s^{-1})	log *k*
$[(pfa)_2CH^+]$	-3.14	1.37×10^5	5.14
$[(mfa)_2CH^+]$	-3.85	2.16×10^4	4.33
$[(dpa)_2CH^+]$	-4.72	2.10×10^4	4.32
$[(mor)_2CH^+]$	-5.53	2.33×10^3	3.37



Nucleophilicity parameters for **1h in CH_3CN: *N* = 10.86, *s* = 0.66**

Table S9. Kinetics of the Reaction of **1h** with Ar_2CH^+ (20°C, CH_2Cl_2)

$[Ar_2CH^+]$ (mol L^{-1})	[**1h**] (mol L^{-1})	k_{obs} (s^{-1})	*k* (L mol^{-1} s^{-1})
$[(mfa)_2CH^+] = 2.18 \times 10^{-5}$, $\lambda_{max} = 593$ nm			
	1.96×10^{-4}	30.88	7.96×10^4
	3.91×10^{-4}	45.46	
	5.87×10^{-4}	60.54	
	7.82×10^{-4}	75.78	
	9.78×10^{-4}	93.55	



Determination of the Rate Constants for the Reactions of Amines with Benzyl Bromides

The reactions of the benzyl bromides with amines in DMSO or in CH_3CN were followed at 20°C by conductometry (conductimeters: WTW LF530 or Tacussel CD 810, Pt electrode: WTW LTA 1/NS). The temperature of the solutions during all kinetic studies was kept constant at 20 °C by using a circulating bath thermostat.

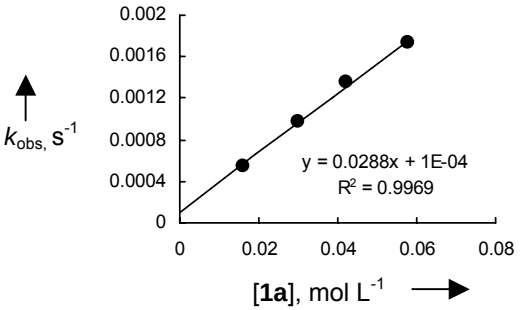
The first order rate constants k_{obs} (s^{-1}) were obtained by least squares fitting of the conductance data to a single-exponential equation shown below.

$dG / dt = G_{max}$ [1-exp(-k_{obs}t] + const

Table S10. Kinetics of the Reactions of amines **1** with $PhCH_2Br$ at 20°C.

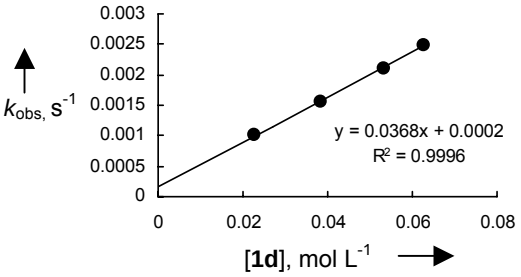
Kinetics of the Reaction of **1a** with $PhCH_2Br$ at 20°C in DMSO

[$PhCH_2Br$] (mol L^{-1})	[**1a**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
1.81×10^{-3}	1.59×10^{-2}	5.395×10^{-4}	2.88×10^{-2}
1.71×10^{-3}	3.02×10^{-2}	9.720×10^{-4}	
1.60×10^{-3}	4.21×10^{-2}	1.350×10^{-4}	
1.64×10^{-3}	5.77×10^{-2}	1.734×10^{-3}	



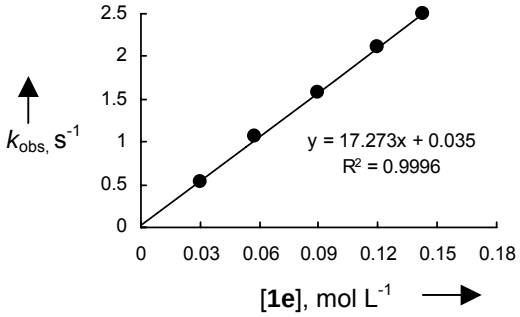
Kinetics of the Reaction of **1d** with $PhCH_2Br$ at 20°C in DMSO

[$PhCH_2Br$] (mol L^{-1})	[**1d**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
1.76×10^{-3}	2.26×10^{-2}	9.968×10^{-4}	3.68×10^{-2}
1.64×10^{-3}	3.83×10^{-2}	1.565×10^{-3}	
1.72×10^{-3}	5.34×10^{-2}	2.107×10^{-3}	
1.69×10^{-3}	6.29×10^{-2}	2.489×10^{-3}	



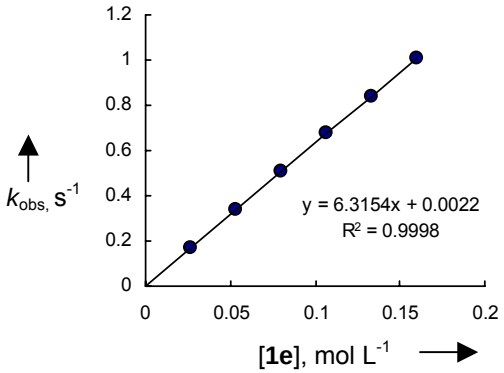
Kinetics of the Reaction of **1e** with $PhCH_2Br$ at 20°C in DMSO

$[PhCH_2Br]$ (mol L^{-1})	[**1e**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
2.54×10^{-3}	3.04×10^{-2}	0.542	17.27
2.54×10^{-3}	5.80×10^{-2}	1.059	
2.54×10^{-3}	8.94×10^{-2}	1.578	
2.54×10^{-3}	1.20×10^{-2}	2.118	
2.54×10^{-3}	1.43×10^{-2}	2.494	



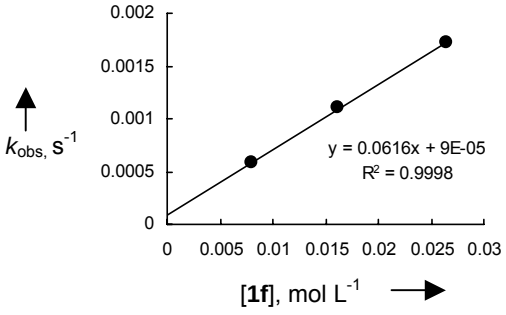
Kinetics of the Reaction of **1e** with $PhCH_2Br$ at 20°C in CH_3CN

$[PhCH_2Br]$ (mol L^{-1})	[**1e**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
2.57×10^{-3}	2.66×10^{-2}	0.165	6.32
2.57×10^{-3}	5.32×10^{-2}	0.339	
2.57×10^{-3}	7.98×10^{-2}	0.510	
2.57×10^{-3}	1.06×10^{-1}	0.679	
2.57×10^{-3}	1.33×10^{-1}	0.841	
2.57×10^{-3}	1.60×10^{-1}	1.006	



Kinetics of the Reaction of **1f** with $PhCH_2Br$ at 20°C in CH_3CN

$[PhCH_2Br]$ (mol L^{-1})	[**1f**] (mol L^{-1})	k_{obs} (s^{-1})	k (L mol^{-1} s^{-1})
8.11×10^{-3}	8.03×10^{-3}	5.835×10^{-5}	6.16×10^{-2}
9.57×10^{-3}	1.62×10^{-2}	1.103×10^{-3}	
7.76×10^{-3}	2.64×10^{-2}	1.717×10^{-3}	



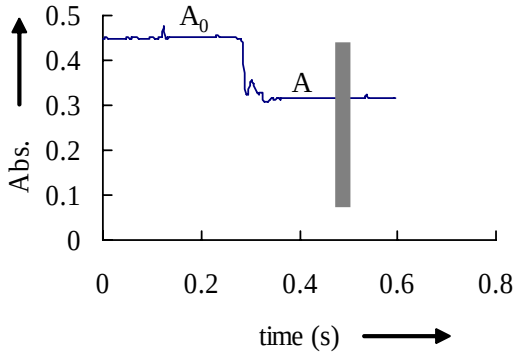
Kinetics of the Reaction of **1g** with $PhCH_2Br$ at 20°C in CH_3CN

$[PhCH_2Br]$ (mol L^{-1})	[**1g**] (mol L^{-1})	k_{obs} (s^{-1})		k (L mol^{-1} s^{-1})
1.66×10^{-3}	3.75×10^{-2}	6.4×10^{-6}		1.7×10^{-4}
			only one point (half life ≈ 30 h)	

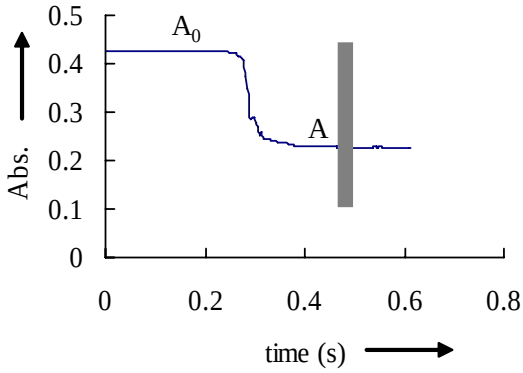
Determination of Equilibrium Constants

Equilibrium constants were determined by UV/Vis spectroscopy in CH_2Cl_2 as follows: To solutions of the benzhydrylium tetrafluoroborate $(mfa)_2CH^+BF_4^-$ in CH_2Cl_2 small volumes of stock solutions of the amines **1a-c** were added, and the absorbances were monitored at λ_{max} (593 nm) of $(mfa)_2CH^+BF_4^-$ before (A_0) and immediately after (A) the addition of the amines. This procedure was carried out with five to six different concentrations of the amines **1a-c**.

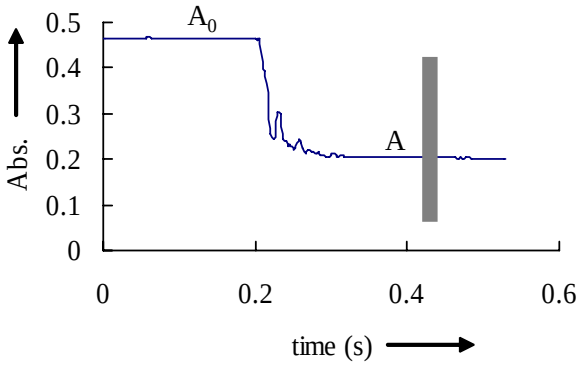
$(mfa)_2CH^+$ with **1c** (9.25×10^{-5} mol L^{-1})



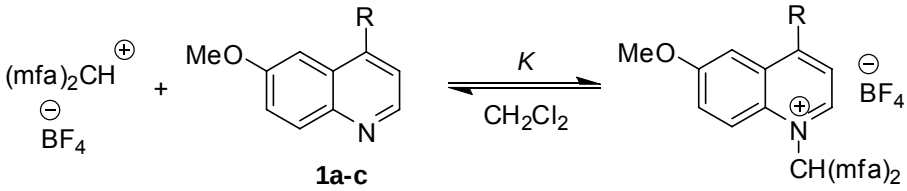
$(mfa)_2CH^+$ with **1c** (1.82×10^{-4} mol L^{-1})



$(mfa)_2CH^+$ with **1c** (2.71×10^{-4} mol L^{-1})



Assuming a proportionality between the absorbances and the concentrations of the benzhydrylium ions, the equilibrium constants can be calculated by the absorbances of the benzhydrylium ions before (A_0) and after (A) the addition of **1a-c** using the following equation.



(4)

$$K = \frac{[(mfa)_2CH\text{-}NR_3^+]}{[(mfa)_2CH^+]\ [\mathbf{1}]} = \frac{A_0\text{-}A}{A\ [\mathbf{1}]} \qquad (5)$$

Equilibrium constant for the reaction of **1a** with $(mfa)_2CH^+BF_4^-$ (20 °C, CH_2Cl_2)
ε [$(mfa)_2CH^+BF_4^-$] at 593 nm] = 1.38×10^5 M^{-1} cm^{-1} and d = 0.5 cm

Entry	[**1a**]$_0$ (mol L^{-1})	A	[$(mfa)_2CH^+BF_4^-$]$_{eq}$ (mol L^{-1})	K (L mol^{-1})
0	0	0.570	8.26×10^{-6}	
1	8.79×10^{-5}	0.292	4.23×10^{-6}	1.13×10^4
0	0	0.621	9.00×10^{-6}	
1	1.28×10^{-4}	0.200	2.89×10^{-6}	1.72×10^4
0	0	0.543	7.87×10^{-6}	
1	1.69×10^{-4}	0.146	2.11×10^{-6}	1.65×10^4
0	0	0.593	8.60×10^{-6}	
1	2.13×10^{-4}	0.133	1.93×10^{-6}	1.65×10^4
0	0	0.609	8.83×10^{-6}	
1	2.61×10^{-4}	0.117	1.70×10^{-6}	1.63×10^4

K_{av}(20 °C) = 1.55×10^4 L mol^{-1}

Equilibrium constant for the reaction of **1b** with $(mfa)_2CH^+BF_4^-$ (20 °C, CH_2Cl_2)
ε [$(mfa)_2CH^+BF_4^-$] at 593 nm] = 1.38×10^5 M^{-1} cm^{-1} and d = 0.5 cm

Entry	[**1b**]$_0$ (mol L^{-1})	A	[$(mfa)_2CH^+BF_4^-$]$_{eq}$ (mol L^{-1})	K (L mol^{-1})
0	0	0.710	1.02×10^{-5}	
1	8.25×10^{-5}	0.297	4.30×10^{-6}	1.81×10^4
0	0	0.630	9.13×10^{-6}	
1	1.23×10^{-4}	0.203	2.94×10^{-6}	1.79×10^4
0	0	0.700	1.02×10^{-5}	
1	1.78×10^{-4}	0.172	2.50×10^{-6}	1.78×10^4
0	0	0.657	9.52×10^{-6}	
1	2.06×10^{-4}	0.142	2.06×10^{-6}	1.81×10^4

0	0	0.654	9.47×10^{-6}	
1	2.46×10^{-4}	0.124	1.79×10^{-6}	1.77×10^{4}

K_{av}(20 °C) = 1.79×10^{4} L mol^{-1}

Equilibrium constant for the reaction of **1c** with $(mfa)_2CH^+BF_4^-$ (20 °C, CH_2Cl_2)
ε [$(mfa)_2CH^+BF_4^-$] at 593 nm] = 1.38×10^{5} M^{-1} cm^{-1} and d = 0.5 cm

Entry	[**1c**]$_0$ (mol L^{-1})	A	[$(mfa)_2CH^+BF_4^-$]$_{eq}$ (mol L^{-1})	K (L mol^{-1})
0	0	0.450	6.52×10^{-6}	
1	9.25×10^{-5}	0.315	4.56×10^{-6}	4.67×10^{3}
0	0	0.404	5.85×10^{-6}	
1	1.36×10^{-4}	0.239	3.46×10^{-6}	5.11×10^{3}
0	0	0.425	6.16×10^{-6}	
1	1.82×10^{-4}	0.227	3.29×10^{-6}	4.80×10^{3}
0	0	0.496	7.19×10^{-6}	
1	2.25×10^{-4}	0.237	3.43×10^{-6}	4.85×10^{3}
0	0	0.466	6.75×10^{-6}	
1	2.71×10^{-4}	0.203	2.95×10^{-6}	4.73×10^{3}
0	0	0.519	7.52×10^{-6}	
1	1.36×10^{-4}	0.309	4.48×10^{-6}	5.03×10^{3}
2	2.70×10^{-4}	0.218	3.15×10^{-6}	5.09×10^{3}
3	4.03×10^{-4}	0.166	2.40×10^{-6}	5.22×10^{3}
4	5.34×10^{-4}	0.133	1.93×10^{-6}	5.30×10^{3}

K_{av}(20 °C) = 4.98×10^{3} L mol^{-1}

Computational Details

The conformational space of quinine (**1a**), hydroxymethylquinuclidine (**1k**) and naphthylmethylquinuclidine (**1f**) as well as their cationic adducts has first been searched using the MM3 force field and the systematic search routine in the TINKER program.[S6] Therefore it was necessary to adapt four additional parameters required for the compounds with a positively charged quinoline adducts. In the case of hydroxymethylquinuclidine, naphthylmethylquinuclidine and their cationic adducts, the best three conformers were optimized at the B3LYP/6-31G(d) level of theory, respectively. Thermochemical corrections (B3LYP/6-31G(d)) to 298.15 K were combined with single-point MP2(FC)/6-31+G(2d,p) energies.

For quinine and its adducts the twenty energetically most favorable conformers according to the force field energies were submitted to single point calculations (B3LYP/6-31G(d)). The seven best conformers according to B3LYP energies were then taken as starting structures for geometry optimizations on the B3LYP/6-31G(d) level. Again, thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this level. The thermochemical corrections have been combined with single-point energies calculated at the MP2(FC)/6-31+G(2d,p)//B3LYP/6-31G(d) level to yield enthalpies H_{298} at 298.15 K.

When two force-field conformations turned into a single conformer during quantum mechanical geometry optimization, one was discarded, so that in each case seven different conformations were taken into account.

The other five smaller and therefore less flexible systems (lepidine, hydroxymethylquinoline, methoxyquinoline, methoxylepidine and quinuclidine) have not been submitted to conformational analyses but the structures were simply drawn in the manner, which was assumed to be the best. Care was only taken of the direction into which the methoxy group in methoxylepidine and -quinoline showed. Both possibilities have been calculated and the better one was taken in each case.

Solvation effects in dichloromethane have been calculated on the HF/6-31G(d) level of theory using the united atom for Hartree-Fock/polarizable continuum model PCM/UAHF. Resulting Gibbs free energies of solvation were combined with the MP2(FC)/6-31+G(2d,p)//B3LYP/6-31G(d) data.

All quantum mechanical calculations have been performed by Gaussian 03.[S7]

Single-point calculations (MP2(FC)/6-31+G(2d,p)//B3LYP/6-31G(d))

Benzyl cation ($PhCH_2^+$):

1\1\GINC-NODE21\SP\RMP2-FC\6-31+G(2d,p)\C7H7(1+)\MAY03\21-Nov-2008\0\\
#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.44368937\C,1,1.4436
5346,2,119.38010526\C,2,1.37588507,1,119.8726165,3,0.0096333,0\H,2,1.0
8619684,1,119.05389432,3,-179.98972038,0\C,3,1.37587835,1,119.871268,2
,-0.0027882,0\H,3,1.08619725,1,119.05600182,2,180.,0\C,4,1.41105857,2,
119.29683443,1,-0.00745762,0\H,4,1.08475191,2,120.80955776,1,179.99387
544,0\H,6,1.08475428,3,120.80950306,1,179.99611224,0\H,8,1.08704101,4,
118.86178288,2,180.,0\C,1,1.37042602,3,120.3126567,6,179.98702931,0\H,
12,1.08762464,1,121.59436693,3,-180.,0\H,12,1.08764282,1,121.58661677,
3,0.,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-268.9107031\MP2=-269.85
92704\RMSD=1.323e-09\Thermal=0.\PG=C01 [X(C7H7)]\\@

Benzhydryl cation (Ph_2CH^+):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C13H11(1+)\MAY03\21-Nov-2008\0
\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.42697722\C,1,1.42
622891,2,118.57003483\C,2,1.38404934,1,120.71100792,3,-3.66882154,0\H,
2,1.08640637,1,119.12934642,3,178.22892657,0\C,3,1.38287356,1,120.1551
9022,2,2.42494007,0\H,3,1.08325722,1,120.0455015,2,-173.40693522,0\C,4
,1.40157239,2,119.50432595,1,2.32681887,0\H,4,1.08496485,2,120.2828241
7,1,-178.52665707,0\H,6,1.08512432,3,120.03840986,1,-178.6711638,0\H,8
,1.08618077,4,119.60298651,2,178.76704649,0\C,1,1.41697689,3,124.44040
507,6,-179.33244762,0\H,12,1.090299,1,114.23410663,3,-162.53488617,0\C
,12,1.41697866,1,131.531484,3,17.45945996,0\C,14,1.42697772,12,116.965
8655,1,-164.25673057,0\C,14,1.42621999,12,124.44193184,1,17.46971883,0
\C,15,1.38405524,14,120.71072742,12,177.95184469,0\H,15,1.08640407,14,
119.13039094,12,-0.14782367,0\C,16,1.38287885,14,120.15517644,12,-179.
32840458,0\H,16,1.08325335,14,120.04629403,12,4.83899553,0\C,17,1.4015
7184,15,119.50417127,14,2.32855344,0\H,17,1.08496271,15,120.28334746,1
4,-178.52838013,0\H,19,1.08512361,16,120.03798344,14,-178.67024215,0\H
,21,1.08618275,17,119.60212226,15,178.76765182,0\\Version=AM64L-G03Rev
D.01\State=1-A\HF=-498.5050119\MP2=-500.2934716\RMSD=1.521e-09\Thermal
=0.\PG=C01 [X(C13H11)]\\@

Methyl cation (CH_3^+):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C1H3(1+)\MAY03\21-Nov-2008\0\\
#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\H,1,1.094601\H,1,1.094601
01,2,120.00002981\H,1,1.09460101,2,120.00002981,3,180.,0\\Version=AM64
L-G03RevD.01\State=1-A'\HF=-39.2382981\MP2=-39.3523833\RMSD=1.649e-09\
Thermal=0.\PG=C03H [O(C1),SGH(H3)]\\@

Quinine (**1a**):

Neutral (**1a**):

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C20H24N2O2\MAY03\19-Nov-2008\0
\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\N\C,1,1.36332144\C,2,1.43
209317,1,123.48623198\C,3,1.43155064,2,117.2614381,1,-0.40681184,0\C,4
,1.38004257,3,117.91434328,2,0.26932941,0\C,1,1.31757441,2,117.2980057
7,3,0.18518523,0\C,2,1.42316986,1,117.69086489,6,-179.75521432,0\C,7,1
.36959492,2,121.09408527,1,-179.89584323,0\C,8,1.42192776,7,120.155879
19,2,-0.05695701,0\C,9,1.38268545,8,120.53820534,7,-0.02093626,0\C,4,1
.52309751,3,121.27692423,2,-179.72392453,0\O,11,1.4293237,4,111.595126
28,3,159.58650503,0\O,9,1.36186076,8,114.48027539,7,179.95270645,0\C,1
3,1.4200636,9,118.26293322,8,-179.95957703,0\C,11,1.54944739,4,111.784
32795,3,-77.91230213,0\C,15,1.56111356,11,114.37843887,4,-80.32782151,
0\C,16,1.54324962,15,108.2082369,11,-130.7370253,0\C,17,1.55590321,16,
111.00885196,15,-56.82660063,0\C,18,1.57423267,17,106.39015563,16,56.3
1610146,0\N,19,1.4717016,18,112.64548213,17,3.48382705,0\C,20,1.478876
48,19,108.46782707,18,58.19209771,0\C,17,1.54135727,16,108.0712069,15,
61.44879745,0\C,18,1.5033077,17,113.85254547,16,-67.88530175,0\C,23,1.
33442257,18,125.17281345,17,-117.23889899,0\H,16,1.09553541,15,110.598
41647,11,107.3250969,0\H,16,1.09398102,15,110.87023879,11,-11.31744245
,0\H,15,1.09506134,11,105.47177935,4,39.24866922,0\H,18,1.09829348,17,
107.31546738,16,173.03665126,0\H,19,1.09595027,18,110.37414632,17,124.
53189849,0\H,17,1.09582269,16,109.91722904,15,-178.04536613,0\H,21,1.0
9621121,20,106.87523502,19,59.84073353,0\H,21,1.09078905,20,108.542479
97,19,175.58189615,0\H,22,1.09735934,17,110.18996104,16,177.01487482,0
\H,22,1.0959011,17,109.55148398,16,59.14482076,0\H,11,1.09917031,4,108
.85087611,3,39.08976205,0\H,5,1.0849063,4,119.98243313,3,-179.83361862
,0\H,10,1.08262783,9,120.14984058,8,179.68172254,0\H,6,1.08977654,1,11
6.46212709,2,-179.87781366,0\H,7,1.08535669,2,117.39037642,1,0.0301341
5,0\H,8,1.08551153,7,121.78993928,2,179.97024569,0\H,12,0.97042366,11,
107.356287,4,-59.46579966,0\H,19,1.09687077,18,110.39747132,17,-117.38
12312,0\H,23,1.09173781,18,116.15838934,17,63.58795712,0\H,24,1.086849
36,23,121.87739853,18,-179.62492633,0\H,24,1.08858908,23,121.65277488,
18,0.39334298,0\H,14,1.0977743,13,111.4431486,9,-61.36647679,0\H,14,1.
097678,13,111.45004376,9,60.75253828,0\H,14,1.09129798,13,105.90375881
,9,179.71344254,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1030.0016757
\MP2=-1033.6585297\RMSD=4.837e-09\Thermal=0.\PG=C01 [X(C20H24N2O2)]\\@

benzyl adduct ($PhCH_2$-**1a**, N_{sp2}):

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C27H31N2O2(1+)\MAY03\20-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.3952348\C,2,1
.39561464,1,120.01071316\C,3,1.39999615,2,120.35730085,1,0.4502058,0\C
,4,1.4000524,3,119.40891397,2,-0.16512549,0\C,5,1.39458102,4,120.15883
421,3,-0.29537511,0\C,4,1.51641248,3,118.93347154,2,176.58507646,0\N,7
,1.49311195,4,114.31458459,3,141.0246644,0\C,8,1.38601028,7,121.266642
48,4,-72.2739549,0\C,9,1.43754246,8,119.56447325,7,-179.41885049,0\C,1
0,1.43216365,9,118.7877326,8,-1.40775855,0\C,11,1.38725868,10,118.0703

4176,9,1.2492769,0\C,8,1.3408626,7,118.09929778,4,107.70729577,0\C,10,
1.42093309,9,118.45927097,8,179.10901944,0\C,14,1.38433073,10,120.7873
3574,9,0.76188583,0\C,15,1.42118817,14,119.82906248,10,-0.12644481,0\C
,16,1.37108252,15,121.01769453,14,-0.34035516,0\C,11,1.52670617,10,124
.44872388,9,-175.21495964,0\C,18,1.55056728,11,110.95971575,10,79.9282
2578,0\C,19,1.55635325,18,112.89116399,11,-176.55739688,0\C,20,1.54461
5,19,107.62195718,18,-140.53811544,0\C,21,1.55670102,20,111.28617368,1
9,-50.03891907,0\C,22,1.5745103,21,106.66735972,20,60.62777561,0\N,19,
1.47708739,18,111.51151101,11,57.23933225,0\C,24,1.48157007,19,111.552
22428,18,78.10465995,0\C,21,1.53947485,20,107.69398905,19,67.97302721,
0\O,15,1.34352133,14,125.45236741,10,179.98954106,0\C,27,1.43068087,15
,118.98764505,14,-0.19396505,0\C,22,1.5054714,21,113.71040566,20,-64.2
3561786,0\C,29,1.33377637,22,124.85154575,21,-115.19698289,0\O,18,1.42
154043,11,113.9750766,10,-40.58239856,0\H,20,1.09382102,19,110.5468194
8,18,96.9428721,0\H,20,1.09692033,19,111.10903331,18,-20.82571062,0\H,
19,1.09666273,18,106.05144202,11,-57.33878948,0\H,22,1.0971738,21,107.
11529756,20,177.08544623,0\H,23,1.09510066,22,110.65189094,21,114.8716
8267,0\H,21,1.09451967,20,109.93642714,19,-171.5269611,0\H,25,1.094993
86,24,107.07847887,19,-175.96027008,0\H,25,1.09567871,24,108.84546899,
19,-61.37787128,0\H,26,1.09608219,21,110.26268892,20,-176.99839502,0\H
,26,1.09642632,21,110.17081492,20,65.24829961,0\H,18,1.09856338,11,107
.26488578,10,-161.78595293,0\H,12,1.08366987,11,120.72545911,10,-179.9
6109205,0\H,14,1.07929903,10,117.91723446,9,-177.47857191,0\H,13,1.083
08652,8,116.40698706,7,0.35093241,0\H,17,1.08109063,16,119.07138762,15
,178.39138567,0\H,16,1.0850475,15,118.16840268,14,179.59364176,0\H,31,
0.97010922,18,109.00443635,11,-72.58121137,0\H,23,1.09608361,22,110.73
090726,21,-126.62389092,0\H,29,1.09209394,22,116.53790349,21,65.271796
62,0\H,30,1.08642451,29,121.86916406,22,-179.9692731,0\H,30,1.08819279
,29,121.70983533,22,0.12270181,0\H,28,1.09575247,27,110.9543948,15,61.
14051509,0\H,28,1.08957157,27,105.52696501,15,179.99144502,0\H,28,1.09
595211,27,110.88322618,15,-61.22016155,0\H,7,1.09277986,4,111.22625297
,3,18.87017297,0\H,7,1.09356139,4,111.06814901,3,-99.79374247,0\H,3,1.
08813764,2,119.65694899,1,179.83130835,0\H,5,1.0873037,4,120.47211925,
3,-179.96232314,0\H,2,1.08586887,1,120.2590559,6,179.97920856,0\H,6,1.
08598033,5,119.66782099,4,-179.76445517,0\H,1,1.08584169,2,120.1047436
6,3,179.73043085,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1298.992510
7\MP2=-1303.6363771\RMSD=3.568e-09\Thermal=0.\PG=C01 [X(C27H31N2O2)]\\
@

benzyl adduct ($PhCH_2$-**1a**, N_{sp3}):

1\1\GINC-NODE15\SP\RMP2-FC\6-31+G(2d,p)\C27H31N2O2(1+)\MAY03\20-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39653341\C,2,
1.39435288,1,120.02924092\C,3,1.40352686,2,120.5701767,1,-0.50268248,0
\C,4,1.40377363,3,118.85466771,2,1.60288209,0\C,5,1.39472431,4,120.581
17169,3,-1.64697278,0\C,4,1.50864844,3,120.6927646,2,177.59986403,0\N,
7,1.5417741,4,116.32888217,3,91.74606477,0\C,8,1.55830643,7,110.545606
6,4,-171.26473424,0\C,9,1.54408654,8,108.02535938,7,-169.51128182,0\C,
10,1.53626651,9,110.2160708,8,-17.76641768,0\C,11,1.54968961,10,110.85
528594,9,-48.00082239,0\C,8,1.52391118,7,110.47123033,4,-54.1110233,0\
C,8,1.52773609,7,110.20139519,4,65.49385034,0\C,11,1.53644073,10,107.9

4827941,9,70.25743902,0\C,9,1.54682852,8,115.11845034,7,-40.78589637,0
\O,16,1.42255332,9,107.77756248,8,-60.3153299,0\C,12,1.50959497,11,114
.07463471,10,-62.25214124,0\C,18,1.33301161,12,123.95607227,11,-114.06
575961,0\C,16,1.52478483,9,109.84790161,8,175.86472524,0\C,20,1.433503
,16,120.94843858,9,-78.68715305,0\C,21,1.43638071,20,116.71027591,16,1
79.49670789,0\N,22,1.36264571,21,123.42274988,20,0.54212835,0\C,23,1.3
1480115,22,117.85632001,21,0.29184311,0\C,20,1.37847199,16,120.5851058
,9,101.7428855,0\C,21,1.41422225,20,124.64830501,16,-0.84515102,0\C,26
,1.38790413,21,121.18871221,20,-179.96555775,0\C,27,1.42005779,26,120.
04461242,21,-0.12547164,0\C,28,1.37562355,27,119.75873628,26,0.3962854
1,0\O,27,1.35677068,26,115.94109029,21,179.89261041,0\C,30,1.42745236,
27,119.11165004,26,-177.8538836,0\H,10,1.09250953,9,108.67992841,8,-14
0.36321397,0\H,10,1.09371518,9,109.79363452,8,102.80455837,0\H,9,1.093
19992,8,102.99464466,7,74.11750141,0\H,12,1.09596556,11,107.41295188,1
0,178.54229274,0\H,13,1.09008004,8,106.30792478,7,62.46603366,0\H,11,1
.09340684,10,110.12060884,9,-169.14591294,0\H,14,1.0900418,8,105.90608
746,7,-51.29147904,0\H,14,1.08824979,8,105.8201868,7,64.76455026,0\H,1
5,1.095033,11,110.42297252,10,-174.43062515,0\H,15,1.09417972,11,110.3
5291856,10,67.24987598,0\H,16,1.09725232,9,108.86181504,8,58.35594223,
0\H,25,1.08536593,20,120.72496315,16,-0.0682174,0\H,26,1.08508297,21,1
21.97369294,20,-1.54862637,0\H,24,1.08858562,23,116.7771098,22,179.574
10401,0\H,29,1.08506338,28,121.11884725,27,179.547567,0\H,28,1.0835241
4,27,120.54912862,26,179.97008987,0\H,17,0.97175972,16,108.18589943,9,
-173.65924227,0\H,13,1.09278751,8,106.67389315,7,-52.6396201,0\H,18,1.
09101563,12,117.03963449,11,65.65198959,0\H,19,1.08589041,18,121.63702
634,12,179.18496532,0\H,19,1.08808699,18,121.8934192,12,-0.60020434,0\
H,31,1.09643465,30,111.4153812,27,-62.66165839,0\H,31,1.09615081,30,11
1.35388309,27,60.17896802,0\H,31,1.09055301,30,105.57037031,27,178.746
90258,0\H,7,1.09333018,4,110.6052083,3,-28.1105546,0\H,7,1.09045573,4,
110.54769245,3,-148.95440547,0\H,3,1.08750047,2,119.45125614,1,178.425
94943,0\H,5,1.08744439,4,119.88936252,3,177.08172501,0\H,2,1.08580523,
1,120.17483309,6,178.64185363,0\H,6,1.08578753,5,119.7939362,4,179.740
07118,0\H,1,1.08587971,6,120.03468358,5,179.56814352,0\\Version=AM64L-
G03RevD.01\State=1-A\HF=-1298.9930231\MP2=-1303.6446802\RMSD=9.754e-09
\Thermal=0.\PG=C01 [X(C27H31N2O2)]\\@

benzhydryl adduct (Ph_2CH-**1a**, N_{sp2}):

1\1\GINC-NODE22\SP\RMP2-FC\6-31+G(2d,p)\C33H35N2O2(1+)\MAY03\21-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39552738\C,2,
1.39636524,1,120.26375892\C,3,1.4013091,2,120.21050037,1,-0.30924623,0
\C,4,1.40324202,3,119.14416581,2,0.58334985,0\C,5,1.39355385,4,120.581
65661,3,-0.48638962,0\C,4,1.5243744,3,122.22552119,2,179.7115195,0\C,7
,1.52374238,4,114.75797316,3,-27.1678002,0\C,8,1.40178357,7,117.976807
46,4,-82.62384135,0\C,9,1.39394186,8,120.47659472,7,177.70443197,0\C,1
0,1.39672425,9,120.0841124,8,0.13472589,0\C,11,1.39480159,10,119.71199
303,9,-0.00853897,0\C,12,1.39687336,11,120.28328072,10,-0.06363906,0\N
,7,1.52559439,4,111.85225738,3,100.08450246,0\C,14,1.38980125,7,120.06
768719,4,156.78482151,0\C,15,1.43737093,14,119.58920588,7,-179.1933604
9,0\C,16,1.43235273,15,118.86784955,14,-2.89653705,0\C,17,1.38450111,1
6,117.89577556,15,2.14609741,0\C,14,1.33773827,7,119.52891379,4,-24.18

369255,0\C,16,1.42098508,15,118.73409587,14,177.9284262,0\C,20,1.38367
329,16,120.83968079,15,1.46869196,0\C,21,1.41981669,20,119.66230995,16
,0.28735913,0\C,22,1.37152263,21,121.07844098,20,-1.1304865,0\C,17,1.5
2656469,16,124.32094821,15,-174.49967625,0\C,24,1.54944845,17,111.3660
6693,16,77.18706167,0\C,25,1.55650178,24,112.70389572,17,-178.15614736
,0\C,26,1.5437166,25,107.70284533,24,-139.92084895,0\C,27,1.55693946,2
6,111.14874346,25,-50.55777727,0\C,28,1.57460479,27,106.63057049,26,60
.61569208,0\N,25,1.47696609,24,111.65662326,17,55.62024659,0\C,30,1.48
128835,25,111.53026053,24,77.50432803,0\C,27,1.53994888,26,107.8221210
9,25,67.46842246,0\O,21,1.34476706,20,125.48811991,16,-179.87976124,0\
C,33,1.42997697,21,118.90208304,20,0.03830153,0\C,28,1.50549637,27,113
.65984226,26,-64.05649214,0\C,35,1.33379185,28,124.90020289,27,-114.78
552363,0\O,24,1.4228097,17,113.82339467,16,-43.17860549,0\H,26,1.09386
844,25,110.5810879,24,97.59859542,0\H,26,1.09704257,25,111.06995595,24
,-20.10488829,0\H,25,1.09642786,24,106.03435427,17,-58.95941397,0\H,28
,1.09724363,27,107.21097928,26,177.17256808,0\H,29,1.09517996,28,110.6
2188711,27,115.14379909,0\H,27,1.09459743,26,109.97105963,25,-171.9721
3298,0\H,31,1.0950449,30,107.07946656,25,-176.10439112,0\H,31,1.095646
28,30,108.82470594,25,-61.54965617,0\H,32,1.0962005,27,110.21677226,26
,-177.11028593,0\H,32,1.09644054,27,110.15688791,26,65.20673017,0\H,24
,1.09861893,17,107.23072757,16,-164.25680151,0\H,18,1.08399895,17,120.
75088694,16,-179.98082215,0\H,20,1.07938392,16,117.87821841,15,-176.78
296157,0\H,19,1.08120835,14,116.27007837,7,1.36162033,0\H,23,1.0805758
9,22,118.54463509,21,178.02845288,0\H,22,1.08506215,21,118.20625524,20
,178.79239355,0\H,37,0.97009197,24,108.95869482,17,-71.45218574,0\H,29
,1.09606668,28,110.68469216,27,-126.3904327,0\H,35,1.09211993,28,116.4
5709353,27,65.73547475,0\H,36,1.08819462,35,121.70425427,28,0.1405429,
0\H,36,1.08645087,35,121.87190094,28,-179.94507547,0\H,34,1.08966546,3
3,105.55243905,21,179.99260535,0\H,34,1.09606624,33,110.92948784,21,-6
1.21782596,0\H,34,1.09584664,33,110.99840461,21,61.13636005,0\H,7,1.09
205602,4,106.201996,3,-147.37627182,0\H,9,1.08790594,8,119.83521545,7,
-1.66108798,0\H,13,1.08665395,12,119.15409419,11,179.47062164,0\H,10,1
.08597159,9,119.69603227,8,179.98453054,0\H,12,1.08607255,11,120.15555
549,10,179.800424,0\H,11,1.08585985,10,120.133274,9,179.81281444,0\H,3
,1.08553673,2,119.78391227,1,178.58271675,0\H,5,1.08814592,4,119.79417
335,3,179.08393037,0\H,2,1.08598573,1,120.13414952,6,179.25795577,0\H,
6,1.08598127,5,119.84069393,4,179.48026284,0\H,1,1.08599758,2,120.0903
3401,3,-179.47200131,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1528.55
34225\MP2=-1534.0449813\RMSD=1.981e-09\Thermal=0.\PG=C01 [X(C33H35N2O2
)]\\@

benzhydryl adduct (Ph_2CH-**1a**, N_{sp3}):

1\1\GINC-NODE15\SP\RMP2-FC\6-31+G(2d,p)\C33H35N2O2(1+)\MAY03\21-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39452828\C,2,
1.39355997,1,119.99838477\C,3,1.40709728,2,121.62088554,1,0.34963313,0
\C,4,1.40497534,3,117.51560706,2,0.98207831,0\C,1,1.39386049,2,119.299
74314,3,-0.91502613,0\C,4,1.52957593,3,115.40695661,2,174.96568813,0\C
,7,1.52704707,4,112.5459752,3,-98.86156056,0\C,8,1.40468077,7,118.2439
2096,4,124.6533621,0\C,9,1.39485786,8,121.07847046,7,-177.17540619,0\C
,10,1.39486204,9,119.96802606,8,0.0727427,0\C,11,1.39620007,10,119.612

38988,9,0.68052142,0\C,12,1.39444526,11,120.35573044,10,-0.21470544,0\
N,7,1.59042517,4,116.82461421,3,128.1467047,0\C,14,1.56259702,7,113.29
360607,4,-47.60337117,0\C,15,1.54770336,14,108.09558163,7,-166.7341015
5,0\C,16,1.53247507,15,110.86969491,14,-17.38858444,0\C,17,1.54718254,
16,109.90969812,15,-48.15054039,0\C,14,1.52500431,7,112.61661228,4,73.
39825492,0\C,14,1.53616511,7,107.37508505,4,-168.98065408,0\C,17,1.532
51967,16,108.12834988,15,69.70390488,0\C,15,1.54926449,14,115.81849751
,7,-38.85352352,0\O,22,1.42697437,15,108.22573371,14,-54.89542863,0\C,
18,1.51405802,17,111.85318307,16,-64.15927769,0\C,24,1.33337581,18,129
.42464768,17,119.25862075,0\C,22,1.52719946,15,110.33714574,14,-178.28
808848,0\C,26,1.4342184,22,121.47824068,15,-77.66374248,0\C,27,1.43722
056,26,116.68799151,22,179.92183187,0\N,28,1.36317485,27,123.54867301,
26,0.65148096,0\C,29,1.31427173,28,117.73595864,27,0.17266353,0\C,26,1
.37902229,22,120.22748712,15,103.22670304,0\C,27,1.41467531,26,124.583
6107,22,-0.3799682,0\C,32,1.38770102,27,120.94709296,26,179.79285805,0
\C,33,1.41949003,32,120.24307661,27,0.02339256,0\C,34,1.37556787,33,11
9.75072226,32,0.38181793,0\O,33,1.36025265,32,116.07390312,27,179.9868
2801,0\C,36,1.42582767,33,118.90483297,32,-179.0410579,0\H,16,1.092412
45,15,108.03717473,14,-139.53103126,0\H,16,1.09361773,15,109.8758338,1
4,103.59875666,0\H,15,1.09081009,14,103.42393534,7,77.04154295,0\H,18,
1.09879017,17,106.92475196,16,179.46619824,0\H,19,1.08958469,14,105.90
228983,7,61.02465567,0\H,17,1.09445138,16,110.21182173,15,-169.4595738
7,0\H,20,1.08803614,14,106.20131654,7,-49.75532122,0\H,20,1.08712495,1
4,105.78734648,7,66.37876991,0\H,21,1.09537088,17,110.49454911,16,-173
.05222492,0\H,21,1.09438231,17,110.42662491,16,68.56116965,0\H,22,1.09
31272,15,108.58185538,14,63.73292699,0\H,31,1.08532223,26,120.7081713,
22,-0.64639076,0\H,32,1.08409113,27,121.85153744,26,-1.38732714,0\H,30
,1.0887619,29,116.79331559,28,179.62089371,0\H,35,1.085058,34,121.1681
8664,33,179.54825946,0\H,34,1.08352579,33,120.60663214,32,179.98196707
,0\H,23,0.97160878,22,107.86168243,15,-173.21355781,0\H,19,1.083875,14
,107.11157271,7,-54.5429276,0\H,24,1.09072636,18,112.67671616,17,-60.9
2310034,0\H,25,1.08566758,24,120.60360975,18,179.81713276,0\H,25,1.087
34227,24,124.08064447,18,0.2211839,0\H,7,1.09044002,4,106.40105797,3,1
7.67713934,0\H,9,1.08759637,8,119.67444054,7,2.29951066,0\H,13,1.08432
22,12,118.71382711,11,177.38729141,0\H,10,1.08589262,9,119.71786507,8,
179.67378182,0\H,12,1.08595288,11,120.11388891,10,178.84555489,0\H,11,
1.08584638,10,120.22479203,9,179.86121161,0\H,3,1.08778161,2,118.97204
406,1,179.48403159,0\H,5,1.08299716,4,121.72882093,3,176.902735,0\H,2,
1.08582946,1,120.38162693,6,179.27122357,0\H,6,1.08572326,1,120.145076
38,2,-179.34023374,0\H,1,1.08541672,6,120.30480048,5,179.80995014,0\H,
37,1.09668498,36,111.53896692,33,-62.01116586,0\H,37,1.09648903,36,111
.49818089,33,60.83168841,0\H,37,1.09091873,36,105.66298638,33,179.4336
5418,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1528.5311886\MP2=-1534.
0467616\RMSD=1.713e-09\Thermal=0.\PG=C01 [X(C33H35N2O2)]\\@

methyl adduct (CH_3-**1a**, N_{sp2}):

1\1\GINC-NODE22\SP\RMP2-FC\6-31+G(2d,p)\C21H27N2O2(1+)\MAY03\24-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.53959048\C,2,
1.54437138,1,107.75731713\C,3,1.55634296,2,107.56389589,1,67.98421733,
0\N,4,1.4762829,3,111.37184126,2,-14.3120447,0\C,5,1.48155757,4,111.56

565636,3,-48.87948271,0\C,5,1.4781521,4,107.34278561,3,69.42810866,0\C
,2,1.55677095,1,107.87987347,6,64.45778022,0\C,4,1.55183027,3,112.7911
2883,2,-140.59977795,0\O,9,1.42097262,4,106.77153967,3,-51.76408729,0\
C,8,1.50566092,2,113.70976136,1,178.07947247,0\C,11,1.33376181,8,124.8
4358617,2,-115.61997966,0\C,9,1.52624913,4,110.84541695,3,-176.4968105
5,0\C,13,1.43241669,9,124.48426523,4,81.38187803,0\C,14,1.43688193,13,
118.67362457,9,-175.72678881,0\N,15,1.38538915,14,119.614155,13,-0.359
11446,0\C,16,1.34102929,15,120.80761013,14,0.,0\C,17,1.38715389,16,121
.52847519,15,0.17884318,0\C,14,1.42068593,13,122.96516351,9,3.64437206
,0\C,19,1.38510528,14,120.82143182,13,-178.82958392,0\C,20,1.42124119,
19,119.85687287,14,-0.51543594,0\C,21,1.37173123,20,120.94245671,19,0.
12407105,0\C,16,1.47750643,15,120.29093638,14,179.86392741,0\O,20,1.34
259841,19,125.45269963,14,179.86000923,0\C,24,1.43132223,20,119.044989
21,19,-0.20524283,0\H,3,1.09374263,2,111.930594,1,-170.40716511,0\H,3,
1.0969793,2,109.44116708,1,-52.87191445,0\H,4,1.0968198,3,108.96920006
,2,101.90953989,0\H,8,1.09715137,2,107.17682356,1,59.34201575,0\H,7,1.
09495832,5,107.8328957,4,-179.10642106,0\H,2,1.09451122,1,110.53665782
,6,-175.85096021,0\H,6,1.09499007,5,107.04572233,4,-175.89844876,0\H,6
,1.09602039,5,108.88876797,4,-61.33978913,0\H,1,1.09605155,2,110.25853
742,3,-176.87801119,0\H,1,1.09635391,2,110.20881178,3,65.35664405,0\H,
9,1.09849393,4,108.42232651,3,66.03709361,0\H,18,1.08347651,17,118.058
4138,16,179.34816867,0\H,19,1.07939982,14,117.93230584,13,2.78079213,0
\H,17,1.08297312,16,116.53394447,15,179.93212796,0\H,22,1.08228014,21,
118.91179621,20,-179.83045755,0\H,21,1.08504417,20,118.19333364,19,-17
9.65988233,0\H,10,0.97008487,9,109.07619847,4,163.10238566,0\H,7,1.096
12202,5,108.18053101,4,65.468478,0\H,11,1.0921223,8,116.53868116,2,64.
96035046,0\H,12,1.0864206,11,121.87253593,8,-179.86678649,0\H,12,1.088
154,11,121.70130613,8,0.21020698,0\H,25,1.09584941,24,110.85480611,20,
-61.12417055,0\H,25,1.0957029,24,110.92419609,20,61.25372733,0\H,25,1.
08948217,24,105.5022798,20,-179.91284226,0\H,23,1.0889187,16,108.66533
584,15,179.92314366,0\H,23,1.09197927,16,109.83520174,15,-60.65693976,
0\H,23,1.09203871,16,109.89011916,15,60.45039572,0\\Version=AM64L-G03R
evD.01\State=1-A\HF=-1069.4276427\MP2=-1073.2331605\RMSD=3.722e-09\The
rmal=0.\PG=C01 [X(C21H27N2O2)]\\@

methyl adduct (CH_3-**1a**, N_{sp3}):

1\1\GINC-NODE17\SP\RMP2-FC\6-31+G(2d,p)\C21H27N2O2(1+)\MAY03\25-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.53791054\C,2,
1.53831112,1,108.06221723\C,3,1.54332045,2,110.12120772,1,70.70792697,
0\N,4,1.5562907,3,107.69632879,2,-18.27469925,0\C,5,1.53119829,4,111.3
3362182,3,-46.76658598,0\C,5,1.52632007,4,106.58293285,3,71.07475448,0
\C,2,1.55153938,1,108.29556848,6,67.92145316,0\C,4,1.54543522,3,114.78
356664,2,-146.95384838,0\O,9,1.42191413,4,107.75585777,3,65.50224368,0
\C,8,1.50962657,2,114.0982293,1,-179.91734688,0\C,11,1.33296423,8,123.
85950359,2,-114.58641957,0\C,5,1.49790218,4,112.31038405,3,-169.512199
09,0\C,9,1.52431279,4,109.79211534,3,-58.39842846,0\C,14,1.43344784,9,
120.96002524,4,-78.17860989,0\C,15,1.43649924,14,116.66986287,9,179.31
195462,0\N,16,1.36243688,15,123.41455011,14,0.60142974,0\C,17,1.314804
45,16,117.90198538,15,0.21766561,0\C,14,1.37853251,9,120.51614862,4,10
2.0269779,0\C,15,1.41417798,14,124.67177498,9,-0.89724942,0\C,20,1.388

11084,15,121.17806673,14,179.83268068,0\C,21,1.4202473,20,120.03542438
,15,-0.05607707,0\C,22,1.37554775,21,119.77402146,20,0.38781984,0\O,21
,1.35602947,20,115.93792838,15,179.94755854,0\C,24,1.42799455,21,119.1
6412876,20,-177.98399404,0\H,3,1.09245064,2,111.55051834,1,-168.516073
39,0\H,3,1.09380642,2,109.49174419,1,-50.15925817,0\H,4,1.09326745,3,1
10.12167272,2,93.47304348,0\H,8,1.09576972,2,107.46017793,1,60.7637334
,0\H,7,1.09292229,5,105.98922157,4,-176.66996041,0\H,2,1.09312512,1,11
0.27576037,6,-172.62327755,0\H,6,1.0926485,5,105.83047787,4,-173.22518
082,0\H,6,1.08777874,5,105.76240612,4,-57.40036939,0\H,1,1.094859,2,11
0.45573222,3,-174.01539303,0\H,1,1.09401234,2,110.37493308,3,67.632574
48,0\H,9,1.09832867,4,108.59678207,3,-175.96706542,0\H,19,1.08540019,1
4,120.76913452,9,0.06429864,0\H,20,1.08512267,15,121.97591057,14,-1.81
013492,0\H,18,1.08851562,17,116.79525709,16,179.59389809,0\H,23,1.0850
5777,22,121.12338985,21,179.55676668,0\H,22,1.083482,21,120.49575893,2
0,179.93792954,0\H,10,0.97183068,9,108.29387316,4,-173.46813504,0\H,7,
1.09277662,5,106.70679997,4,68.17001594,0\H,11,1.09097831,8,117.111262
47,2,65.11197506,0\H,12,1.08583127,11,121.60788533,8,179.22942834,0\H,
12,1.08807618,11,121.9353532,8,-0.57978862,0\H,25,1.09635161,24,111.38
688626,21,-62.52708546,0\H,25,1.0960742,24,111.32967009,21,60.32002061
,0\H,25,1.09046823,24,105.55448601,21,178.88746676,0\H,13,1.09136534,5
,108.44939319,4,-171.31062279,0\H,13,1.09168239,5,109.4575308,4,-51.95
956136,0\H,13,1.08954119,5,109.03604351,4,69.1938472,0\\Version=AM64L-
G03RevD.01\State=1-A\HF=-1069.4316041\MP2=-1073.2424698\RMSD=3.723e-09
\Thermal=0.\PG=C01 [X(C21H27N2O2)]\\@

Quinuclidine (**1e**):

Neutral (**1e**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C7H13N1\MAY03\21-Nov-2008\0\\#
P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\C\C,1,1.54250862\C,1,1.56212
955,2,107.96369196\H,1,1.09718509,2,109.94353623,3,121.32322088,0\H,1,
1.09717028,2,109.99483169,3,-121.34923275,0\H,3,1.09612777,1,111.21979
771,2,120.29176995,0\H,3,1.09608725,1,111.11710965,2,-120.61688557,0\C
,2,1.54244756,1,108.59067409,3,-59.04946861,0\H,8,1.09719602,2,109.983
65682,1,-178.99572928,0\H,8,1.09715678,2,109.95791182,1,-61.68181975,0
\C,8,1.56204517,2,107.97098371,1,59.64500337,0\H,11,1.0961223,8,111.11
739113,2,119.58476565,0\H,11,1.09609512,8,111.21953365,2,-121.33217539
,0\H,2,1.0959069,1,110.21449544,3,-179.8742689,0\C,11,2.40051516,8,92.
17477558,2,29.43332817,0\H,15,1.09612914,11,89.7961974,8,111.80440622,
0\H,15,1.09613159,11,143.07244032,8,-129.43063144,0\C,2,1.54270868,1,1
08.75913022,3,59.18439927,0\H,18,1.09719722,2,109.98339904,1,179.82799
865,0\H,18,1.09720015,2,109.96898692,1,62.5579036,0\N,15,1.47237185,11
,35.41371056,8,-126.29536897,0\\Version=AM64L-G03RevD.01\State=1-A\HF=
-327.1099565\MP2=-328.3435491\RMSD=7.544e-09\Thermal=0.\PG=C01 [X(C7H1
3N1)]\\@

benzyl adduct ($PhCH_2$-**1e**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C14H20N1(1+)\MAY03\21-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,2.51948604\C,2,1.

53734001,1,35.39257475\H,1,1.09303624,3,112.48193378,2,-113.45272779,0
\H,1,1.09020113,3,112.81754308,2,123.81417312,0\H,3,1.09412068,2,110.4
9082669,1,-120.75625513,0\H,3,1.09435369,2,110.24849516,1,121.10816455
,0\C,1,2.47290218,3,91.6322174,2,-26.33322728,0\H,8,1.09268701,1,141.8
334347,3,123.03687627,0\H,8,1.0923947,1,90.01416921,3,-116.88868814,0\
C,2,1.53784794,1,87.87514792,3,-127.82656338,0\H,11,1.09396442,2,110.4
6372942,1,-153.50936069,0\H,11,1.09424383,2,110.33375602,1,88.25349919
,0\H,2,1.09332611,1,145.40596595,3,-4.42888177,0\C,2,1.53768207,1,90.3
2555112,3,123.36298941,0\H,15,1.09436994,2,110.19587752,1,147.08066485
,0\H,15,1.09399001,2,110.47897041,1,-94.8049372,0\C,15,1.54754859,2,10
9.49371089,1,25.91817756,0\H,18,1.09270709,15,112.44606439,2,123.03628
187,0\H,18,1.09042886,15,112.83908972,2,-114.44893645,0\C,18,3.0861293
5,15,156.32135015,2,-48.77811504,0\C,21,1.40374355,18,132.2948368,15,-
5.0947614,0\C,21,1.40382945,18,87.5381806,15,-133.11779878,0\C,22,1.39
466508,21,120.52404631,18,-114.41543492,0\H,22,1.08763604,21,120.00661
367,18,66.94913898,0\C,23,1.39425858,21,120.50381192,18,136.68622223,0
\H,23,1.08758621,21,120.05852474,18,-44.75791982,0\C,24,1.39629383,22,
119.99264657,21,-0.44465129,0\H,24,1.08565923,22,119.80348638,21,-179.
57398176,0\H,26,1.08572554,23,119.7880826,21,179.63696871,0\H,28,1.085
78038,24,120.01505318,22,-179.52019672,0\N,18,1.52104929,15,110.566911
61,2,4.34236877,0\C,21,1.50572104,18,54.42369839,15,95.79237238,0\H,33
,1.09349118,21,111.23324899,18,90.35414253,0\H,33,1.09310249,21,111.10
836668,18,-149.10370376,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-596.
1076118\MP2=-598.3280801\RMSD=5.348e-09\Thermal=0.\PG=C01 [X(C14H20N1)
]\\@

benzhydryl adduct (Ph_2CH-**1e**):

1\1\GINC-NODE21\SP\RMP2-FC\6-31+G(2d,p)\C20H24N1(1+)\MAY03\21-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,2.51021887\C,2,1.
53757587,1,35.59926772\H,1,1.09322482,3,112.18798373,2,-102.52503074,0
\H,1,1.08942894,3,112.65422049,2,135.10694274,0\H,3,1.09429669,2,110.9
4813345,1,-120.18172722,0\H,3,1.09501468,2,110.3525527,1,121.35011915,
0\C,1,2.46619456,3,94.18189504,2,-17.66044774,0\H,8,1.08999472,1,141.7
6277031,3,107.02809836,0\H,8,1.09156218,1,94.2279982,3,-126.77851542,0
\C,2,1.53733762,1,84.27163072,3,-133.14186008,0\H,11,1.09424383,2,110.
90816098,1,-161.19555467,0\H,11,1.09504549,2,110.27827891,1,80.3719241
4,0\H,2,1.09321304,1,145.50946003,3,-14.65385101,0\C,2,1.53692,1,92.60
087883,3,118.70972014,0\H,15,1.09503968,2,110.23837427,1,138.74694548,
0\H,15,1.09422957,2,110.90031936,1,-102.82119669,0\C,15,1.54729995,2,1
09.17475659,1,17.32998412,0\H,18,1.0895896,15,112.04709669,2,134.18954
397,0\H,18,1.08972556,15,112.04319541,2,-102.96532899,0\C,1,2.53774126
,3,146.61395255,2,22.09759528,0\H,21,1.0923398,1,79.8908394,3,-135.135
05374,0\C,21,1.5225985,1,146.02958484,3,-31.27328739,0\C,23,1.40527414
,21,117.25444631,1,-90.3990418,0\C,23,1.40524823,21,124.66183348,1,92.
20306921,0\C,24,1.39431145,23,121.30029567,21,-178.4242572,0\H,24,1.08
776597,23,119.69970642,21,0.5540452,0\C,25,1.39479365,23,120.71702339,
21,178.68905012,0\H,25,1.08337773,23,121.1161448,21,0.28482826,0\C,26,
1.39469425,24,119.92808678,23,-0.13231541,0\H,26,1.08579622,24,119.719
23901,23,179.50178079,0\H,28,1.08588248,25,119.42216007,23,-179.947084
16,0\H,30,1.08576289,26,120.27406335,24,179.92753772,0\C,21,1.52251588

,1,92.10920689,3,118.86590181,0\C,34,1.40529803,21,116.85038871,1,81.7
9849692,0\C,34,1.40594573,21,125.08895283,1,-101.11706575,0\C,35,1.394
63798,34,121.30109446,21,177.4019345,0\H,35,1.08759648,34,119.64820166
,21,-1.71497983,0\C,36,1.39460696,34,120.73546782,21,-177.6285391,0\H,
36,1.08338287,34,121.21562671,21,1.96787748,0\C,37,1.39436095,35,119.9
5728889,34,0.36033865,0\H,37,1.08578359,35,119.69456644,34,-179.500065
3,0\H,39,1.0858993,36,119.40729982,34,-179.98109563,0\H,41,1.0857433,3
7,120.2926545,35,179.98315945,0\N,18,1.51935254,15,110.41489546,2,15.1
4496848,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-825.6575651\MP2=-828
.7281023\RMSD=7.786e-09\Thermal=0.\PG=C01 [X(C20H24N1)]\\@

Hydroxymethylquinuclidine (**1k**):

neutral (**1k**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C8H15N1O1\MAY03\21-Nov-2008\0\
\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\N\C,1,1.47930484\C,2,1.559
25584,1,111.70028405\C,3,1.54077516,2,107.77049594,1,-7.37682251,0\C,4
,1.54414449,3,108.24804366,2,-55.1317353,0\C,1,1.48769122,2,111.096161
74,3,62.70649223,0\C,1,1.47564612,2,108.49230023,3,-56.02535317,0\C,4,
1.54400496,3,108.49478568,2,63.2364654,0\C,6,1.53140128,1,109.39227959
,7,-164.00618699,0\O,9,1.41358306,6,110.64259803,1,51.15321152,0\H,3,1
.09695237,2,110.85836317,1,-128.15959746,0\H,3,1.09728472,2,111.046606
87,1,113.16522043,0\H,2,1.09390045,1,108.30868816,7,-178.85164259,0\H,
2,1.09553679,1,107.42496827,7,66.3481374,0\H,5,1.09665856,4,110.826762
95,3,-172.04674862,0\H,5,1.09940268,4,109.58406637,3,-54.35024429,0\H,
6,1.09705305,1,104.94630461,7,-50.21236739,0\H,4,1.09583009,3,110.3272
5562,2,-175.87696725,0\H,7,1.09550503,1,108.22187696,2,-172.17432919,0
\H,7,1.09597093,1,107.69986093,2,-56.66494708,0\H,8,1.09723988,4,109.9
3256147,3,-175.66318992,0\H,8,1.09683382,4,110.11168106,3,66.88744419,
0\H,9,1.10478732,6,110.22571148,1,-72.53111908,0\H,9,1.0967186,6,109.5
426974,1,170.2109506,0\H,10,0.97695141,9,103.97321938,6,-35.45930037,0
\\Version=AM64L-G03RevD.01\State=1-A\HF=-441.0116755\MP2=-442.6063017\
RMSD=4.587e-09\Thermal=0.\PG=C01 [X(C8H15N1O1)]\\@

benzyl adduct ($PhCH_2$-**1k**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C15H22N1O1(1+)\MAY03\23-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39611163\C,2,
1.39473259,1,120.01358353\C,3,1.40381848,2,120.56808407,1,0.592811,0\C
,4,1.40354107,3,118.85903931,2,-1.66471932,0\C,5,1.39425968,4,120.5778
2076,3,1.620105,0\C,4,1.50786758,3,120.35594237,2,-177.77363769,0\N,7,
1.54195592,4,116.1804356,3,-92.26996207,0\C,8,1.5301975,7,110.50607878
,4,65.89383154,0\C,9,1.54481069,8,110.36934188,7,-171.68551192,0\C,10,
1.53691563,9,108.99659045,8,-14.38584231,0\C,11,1.53707377,10,108.1199
986,9,-50.40574902,0\C,12,1.54571358,11,109.84503127,10,70.94905172,0\
C,8,1.52424867,7,110.92887983,4,-53.65623767,0\C,11,1.53865598,10,108.
55013324,9,67.33229478,0\C,13,1.52940498,12,112.79099042,11,-148.57583
448,0\O,16,1.41796383,13,109.81939486,12,66.22673831,0\H,10,1.09408945
,9,109.02518733,8,-135.29341754,0\H,10,1.09503713,9,110.61199627,8,107
.08213617,0\H,9,1.08836509,8,105.79444873,7,66.22111989,0\H,9,1.090005

44,8,105.9776967,7,-49.91282937,0\H,12,1.0949623,11,111.21258851,10,-1
69.11611588,0\H,12,1.09484262,11,110.26334372,10,-49.84471149,0\H,13,1
.09521138,12,110.25406607,11,92.73820186,0\H,11,1.09328187,10,110.5087
0183,9,-171.41829602,0\H,14,1.09234871,8,106.99947536,7,-48.50549124,0
\H,14,1.09030535,8,106.06106906,7,66.57425958,0\H,15,1.09509278,11,110
.38005555,10,-171.87501461,0\H,15,1.09412793,11,110.81777189,10,69.770
05722,0\H,16,1.10017394,13,105.34755008,12,-54.29831638,0\H,16,1.09772
537,13,111.18375947,12,-169.89437672,0\H,17,0.97003371,16,109.16252073
,13,-168.13223037,0\H,7,1.09349942,4,110.66243815,3,148.08203205,0\H,7
,1.0909898,4,110.80976171,3,27.0741308,0\H,3,1.08751352,2,119.50909526
,1,-178.03268504,0\H,5,1.0875886,4,120.03324804,3,-177.09999607,0\H,2,
1.08574837,1,120.1931143,6,-178.57112147,0\H,6,1.08578381,5,119.790521
85,4,-179.67316586,0\H,1,1.08583584,2,120.04249915,3,179.53748641,0\\V
ersion=AM64L-G03RevD.01\State=1-A\HF=-710.0043699\MP2=-712.5883835\RMS
D=5.729e-09\Thermal=0.\PG=C01 [X(C15H22N1O1)]\\@

benzhydryl adduct (Ph_2CH-**1k**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C21H26N1O1(1+)\MAY03\02-Dec-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39590266\C,2,
1.39290731,1,120.08192962\C,3,1.40659638,2,121.40229071,1,0.47674556,0
\C,4,1.40273069,3,117.81455106,2,0.12353349,0\C,1,1.39317758,2,119.288
30597,3,-0.43521035,0\C,4,1.53134431,3,114.78765879,2,175.8866243,0\C,
7,1.526052,4,112.00097752,3,-87.65388126,0\C,8,1.40386057,7,122.294832
61,4,-46.49764916,0\C,9,1.39388996,8,120.58278844,7,177.80322426,0\C,1
0,1.39684149,9,120.30709938,8,-1.09680573,0\C,11,1.39486498,10,119.700
53282,9,-0.35970814,0\C,12,1.39537674,11,119.95822294,10,0.79803861,0\
N,7,1.58032295,4,116.68737157,3,140.58338241,0\C,14,1.53732698,7,108.1
0663664,4,-162.77635287,0\C,15,1.54503742,14,110.75001249,7,-170.85428
15,0\C,16,1.53602452,15,109.22222306,14,-14.83613214,0\C,17,1.53374613
,16,108.14496182,15,-49.97514338,0\C,18,1.5504779,17,110.45051179,16,6
9.18210651,0\C,14,1.52839359,7,112.74334593,4,80.37477244,0\C,17,1.534
56871,16,108.50613279,15,67.3004543,0\C,19,1.53128382,18,111.1992315,1
7,-145.92791645,0\O,22,1.42198162,19,110.24986043,18,63.84383629,0\H,1
6,1.09425567,15,108.7988265,14,-135.69792858,0\H,16,1.09520755,15,110.
63477789,14,106.82968887,0\H,15,1.08774721,14,105.84058967,7,67.273206
78,0\H,15,1.08875342,14,106.14151917,7,-49.15308155,0\H,18,1.09514275,
17,111.03351487,16,-170.69924986,0\H,18,1.09451483,17,110.07940762,16,
-51.59965674,0\H,19,1.09198199,18,110.5898672,17,96.16009739,0\H,17,1.
09350556,16,110.60850718,15,-171.09227973,0\H,20,1.08599273,14,108.326
27334,7,-49.30567797,0\H,20,1.08969392,14,105.456282,7,65.78278853,0\H
,21,1.09551797,17,110.382248,16,-170.10545931,0\H,21,1.09451306,17,111
.17268566,16,71.30706785,0\H,22,1.10065715,19,104.72009488,18,-56.0069
0178,0\H,22,1.0934839,19,111.49852784,18,-171.82712709,0\H,23,0.969741
34,22,108.79209121,19,-168.98423288,0\H,7,1.09192273,4,106.45736058,3,
29.29240469,0\H,9,1.08541484,8,120.28378111,7,-0.40250296,0\H,13,1.087
68713,12,119.25751863,11,-178.77165869,0\H,10,1.0859446,9,119.58653798
,8,179.96302558,0\H,12,1.08584636,11,120.30676291,10,-178.62668289,0\H
,11,1.085841,10,120.11253593,9,-179.35233142,0\H,3,1.08762472,2,119.14
273367,1,179.67900128,0\H,5,1.08374412,4,121.82127072,3,179.24186521,0
\H,2,1.08589632,1,120.31992784,6,179.76758302,0\H,6,1.08600991,1,120.1

7220194,2,-179.7901825,0\H,1,1.08563292,6,120.32113531,5,179.66923031,
0\\Version=AM64L-G03RevD.01\State=1-A\HF=-939.5486689\MP2=-942.985745\
RMSD=9.978e-09\Thermal=0.\PG=C01 [X(C21H26N1O1)]\\@

Naphtylmethylquinuclidine (**1f**):

Neutral (**1f**):

1\1\GINC-NODE13\SP\RMP2-FC\6-31+G(2d,p)\C18H21N1\MAY03\23-Nov-2008\0\\
#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\C\C,1,1.41417118\C,2,1.3779
8351,1,120.51298767\C,3,1.42378071,2,121.3366415,1,0.,0\C,4,1.43617334
,3,117.88700487,2,-0.44927945,0\C,1,1.37595163,2,119.80890606,3,0.3586
1122,0\C,5,1.42067403,4,119.51822137,3,-179.14438644,0\C,7,1.37365446,
5,120.39655622,4,0.39866676,0\C,8,1.41466867,7,120.1089745,5,-0.412846
09,0\C,9,1.38236989,8,122.04109709,7,-0.25739806,0\C,10,1.51519164,9,1
19.99531576,8,-178.48305191,0\C,11,1.54592538,10,113.63966184,9,102.51
051546,0\C,12,1.56153024,11,113.9223954,10,-68.82152274,0\C,13,1.54278
414,12,108.38350829,11,-136.39527607,0\C,14,1.54219223,13,109.1582478,
12,-52.81410632,0\C,15,1.56193342,14,107.80400501,13,62.44331118,0\N,1
6,1.47443416,15,111.70000788,14,-6.97954362,0\C,17,1.47507905,16,108.4
4602555,15,64.28292742,0\C,14,1.5416873,13,108.36946909,12,65.21001966
,0\H,13,1.09653031,12,110.72001816,11,101.94326554,0\H,13,1.09836229,1
2,110.9836682,11,-16.10215052,0\H,12,1.09598748,11,107.12048058,10,51.
17971044,0\H,15,1.09720584,14,110.20424765,13,-176.24718355,0\H,15,1.0
9750558,14,109.94664145,13,-58.74365176,0\H,16,1.09633888,15,111.06588
148,14,113.04723802,0\H,16,1.09615338,15,111.16361731,14,-127.8902092,
0\H,14,1.09617492,13,110.15577015,12,-174.06193755,0\H,18,1.09603906,1
7,107.50774179,16,65.82091402,0\H,18,1.0942511,17,108.35836529,16,-179
.36622906,0\H,19,1.09753477,14,109.98727387,13,-176.85547343,0\H,19,1.
09735169,14,110.20635495,13,65.59273794,0\H,11,1.09599949,10,110.88661
565,9,-136.09694229,0\H,11,1.09644799,10,108.42925973,9,-19.58176505,0
\H,9,1.0875138,8,118.89838085,7,179.51473283,0\H,3,1.08494555,2,119.13
074045,1,-179.59579302,0\H,8,1.08679094,7,120.39347004,5,179.46206709,
0\H,2,1.08681236,1,119.69845013,6,-179.45487596,0\H,6,1.08772778,1,120
.42064392,2,179.58960066,0\H,7,1.08749402,5,118.82372068,4,-179.980070
5,0\H,1,1.08670515,6,120.29709945,5,-179.94520697,0\\Version=AM64L-G03
RevD.01\State=1-A\HF=-748.3719354\MP2=-751.1535243\RMSD=4.316e-09\Ther
mal=0.\PG=C01 [X(C18H21N1)]\\@

benzyl adduct ($PhCH_2$-**1f**):

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C25H28N1(1+)\MAY03\29-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\N\C,1,1.55657137\C,2,1.
55934375,1,107.59318188\C,3,1.53713366,2,110.90026095,1,13.37886909,0\
C,4,1.53365822,3,108.2733407,2,-67.79318899,0\C,1,1.52810711,2,107.354
58959,3,51.25348323,0\C,1,1.5177338,6,108.35729617,5,49.48169535,0\C,4
,1.53889785,3,109.0441841,2,50.07566079,0\C,2,1.55279871,1,116.5051250
7,7,57.16875181,0\C,9,1.51702336,2,121.08893764,1,63.63614333,0\C,10,1
.43531406,9,121.65428507,2,66.47718767,0\C,11,1.43678597,10,118.660539
23,9,-178.92805151,0\C,12,1.42085388,11,119.64638586,10,-1.70021609,0\

C,13,1.37415409,12,120.68786543,11,-0.7378261,0\C,10,1.38420176,9,119.
06832903,2,-115.74228383,0\C,12,1.42054851,11,119.34451636,10,179.1926
0561,0\C,16,1.37590172,12,121.10098953,11,0.8611931,0\C,17,1.41377279,
16,119.82550995,12,0.59563779,0\C,18,1.378478,17,120.53274017,16,-1.12
143761,0\C,1,1.54802047,7,111.58203461,8,174.15571225,0\C,20,1.5080848
7,1,116.16926178,7,60.73572707,0\C,21,1.40404591,20,120.64529077,1,95.
47576557,0\C,22,1.39461499,21,120.67481396,20,177.41797562,0\C,23,1.39
617017,22,119.99634169,21,-0.37012048,0\C,24,1.39639861,23,119.9074868
8,22,-0.69538575,0\C,25,1.39451442,24,120.04197468,23,0.50046297,0\H,3
,1.0954442,2,110.17451082,1,-108.80417444,0\H,3,1.09418221,2,108.91631
002,1,134.39611257,0\H,2,1.09170433,1,102.90416671,7,176.53161576,0\H,
5,1.09497377,4,110.66100773,3,171.79383553,0\H,5,1.09426781,4,110.9568
9343,3,-69.44525915,0\H,6,1.0890277,1,106.50104021,7,-73.22481075,0\H,
6,1.09300351,1,105.6875998,7,171.83232543,0\H,4,1.09349631,3,110.06259
697,2,171.07848015,0\H,7,1.09081702,1,106.03819257,6,55.87273995,0\H,7
,1.09074137,1,107.1591395,6,170.86527355,0\H,8,1.09425195,4,110.604964
4,3,173.46554346,0\H,8,1.09486471,4,110.2324547,3,55.35931099,0\H,9,1.
09572461,2,109.02852827,1,-64.07779455,0\H,9,1.09836574,2,102.80339719
,1,-174.8545451,0\H,15,1.08873701,10,119.38849201,9,-0.8628997,0\H,19,
1.08576134,18,118.63826646,17,177.82977568,0\H,14,1.08577909,13,120.56
937061,12,-178.30325645,0\H,18,1.08625847,17,119.6523635,16,178.167076
61,0\H,16,1.08682847,12,118.50773728,11,-179.81946979,0\H,13,1.0867126
2,12,118.74266602,11,-179.66292919,0\H,17,1.08578478,16,120.327866,12,
179.62373178,0\H,22,1.08774426,21,119.858097,20,-1.37297798,0\H,26,1.0
8727052,25,119.45168347,24,-177.83902548,0\H,23,1.08582534,22,119.8030
4937,21,-179.646169,0\H,25,1.08585424,24,120.15050106,23,-178.53743267
,0\H,24,1.08588034,23,120.04311587,22,-179.69129288,0\H,20,1.09272055,
1,104.69646075,7,-176.33626525,0\H,20,1.08749225,1,105.33370681,7,-62.
48438074,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1017.3618468\MP2=-1
021.1416367\RMSD=3.742e-09\Thermal=0.\PG=C01 [X(C25H28N1)]\\@

benzhydryl adduct (Ph_2CH-**1f**):

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C31H32N1(1+)\MAY03\25-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39460772\C,2,1.
39469506,1,119.98110454\C,3,1.40542703,2,121.41812246,1,0.52921731,0\C
,4,1.40588113,3,117.84729491,2,0.48255804,0\C,1,1.3954208,2,119.414574
89,3,-0.73975395,0\C,4,1.52497546,3,115.91673468,2,175.65708804,0\C,7,
1.52623617,4,114.21106102,3,-100.821248,0\C,8,1.40444365,7,123.2249009
8,4,-45.43242019,0\C,9,1.39461518,8,120.72013569,7,177.89175906,0\C,10
,1.39590238,9,120.34583277,8,-0.94559841,0\C,11,1.39512941,10,119.6094
8538,9,-0.41536791,0\C,12,1.39458769,11,119.97298574,10,0.74889363,0\N
,7,1.59042268,4,115.19723226,3,126.33289478,0\C,14,1.56186158,7,112.02
904737,4,-46.9985665,0\C,15,1.55714087,14,107.8472686,7,175.11594471,0
\C,16,1.53495629,15,111.27113347,14,13.17159614,0\C,17,1.53363027,16,1
08.90251491,15,-66.54672455,0\C,14,1.52702801,7,112.65132351,4,73.4775
811,0\C,14,1.52757875,7,108.11797558,4,-168.51720329,0\C,17,1.53492908
,16,108.38676899,15,50.82606223,0\C,15,1.55080098,14,112.64376439,7,-5
7.8610607,0\C,22,1.52171402,15,113.45390188,14,-173.93935818,0\C,23,1.
43462434,22,121.94130773,15,-72.11691313,0\C,24,1.43705037,23,118.6613
6944,22,178.4805209,0\C,25,1.42036267,24,119.66804438,23,0.99683136,0\

C,26,1.37362505,25,120.64708946,24,0.34172312,0\C,23,1.383243,22,118.7
9933425,15,108.10103351,0\C,25,1.42049152,24,119.3548031,23,-179.50768
756,0\C,29,1.37586112,25,121.11708274,24,-0.51397148,0\C,30,1.41357627
,29,119.75039509,25,-0.45547533,0\C,31,1.37811445,30,120.62117182,29,0
.73946642,0\H,16,1.0952412,15,109.67280835,14,-109.04723113,0\H,16,1.0
9234334,15,108.87135335,14,134.82785256,0\H,15,1.08975316,14,103.33993
328,7,58.85613434,0\H,18,1.09539736,17,110.65515945,16,170.03003817,0\
H,18,1.09434776,17,111.04786766,16,-71.20627828,0\H,19,1.08927404,14,1
07.06373635,7,43.44408299,0\H,19,1.0883149,14,106.10138069,7,-72.94303
805,0\H,17,1.09356318,16,110.14533425,15,171.83182284,0\H,20,1.0898553
5,14,105.74149858,7,-67.77192833,0\H,20,1.089771,14,107.72554166,7,46.
99743427,0\H,21,1.09460998,17,111.130682,16,171.74458189,0\H,21,1.0950
3958,17,110.28108443,16,53.11350254,0\H,22,1.0943188,15,109.22265445,1
4,63.63224804,0\H,22,1.09489838,15,109.97357943,14,-53.57790391,0\H,28
,1.08814537,23,119.41295092,22,1.38568041,0\H,32,1.08450374,31,118.671
79486,30,-178.38253089,0\H,27,1.08580449,26,120.59594098,25,179.067561
69,0\H,31,1.08639367,30,119.74815393,29,-178.8333916,0\H,29,1.08693216
,25,118.4676024,24,179.82268878,0\H,26,1.08680524,25,118.76964014,24,1
79.76746295,0\H,30,1.08595331,29,120.31793415,25,-179.84708118,0\H,7,1
.0897367,4,106.15261333,3,15.91054659,0\H,9,1.08434788,8,120.49136307,
7,-0.03695547,0\H,13,1.08757791,12,119.04100241,11,-178.72874363,0\H,1
0,1.08589896,9,119.51154242,8,-179.91889395,0\H,12,1.08586282,11,120.2
9964665,10,-178.58908852,0\H,11,1.08581407,10,120.17359779,9,-179.3941
8198,0\H,3,1.08744514,2,118.93066073,1,179.47387697,0\H,5,1.08355896,4
,121.39422332,3,177.89732973,0\H,2,1.08576402,1,120.39551099,6,179.400
21087,0\H,6,1.08595241,1,120.11931668,2,-179.32713583,0\H,1,1.08580663
,2,120.35381751,3,179.8458107,0\\Version=AM64L-G03RevD.01\State=1-A\HF
=-1246.9097726\MP2=-1251.5431541\RMSD=8.432e-10\Thermal=0.\PG=C01 [X(C
31H32N1)]\\@

Lepidine (**1g**):

Neutral (**1g**):

1\1\GINC-NODE22\SP\RMP2-FC\6-31+G(2d,p)\C10H9N1\MAY03\23-Nov-2008\0\\#
P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\C\C,1,1.37661269\C,2,1.41977
141,1,120.70580636\C,3,1.43281879,2,119.25185902,1,0.,0\C,4,1.42058394
,3,118.56402334,2,0.,0\C,5,1.37802667,4,120.839516,3,0.,0\H,1,1.086638
89,2,120.17802704,3,180.,0\H,2,1.08555985,1,121.94356086,6,180.,0\C,4,
1.43120148,3,117.99894877,2,180.,0\H,5,1.08587004,4,119.44918481,3,-18
0.,0\H,6,1.08669488,5,119.89046244,4,-180.,0\C,9,1.37872286,4,117.3756
1484,3,0.,0\C,12,1.41627017,9,120.12291051,4,0.,0\H,12,1.08684617,9,12
0.51365586,4,-180.,0\H,13,1.09031617,12,119.26393653,9,180.,0\N,13,1.3
1592073,12,124.35752316,9,0.,0\C,9,1.50771007,4,121.41122907,3,-180.,0
\H,17,1.09700614,9,111.44828072,4,-59.78039774,0\H,17,1.09700107,9,111
.44948767,4,59.72381146,0\H,17,1.0937351,9,110.87710902,4,179.97257772
,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-438.4247009\MP2=-440.004028
2\RMSD=5.137e-09\Thermal=0.\PG=C01 [X(C10H9N1)]\\@

benzyl adduct ($PhCH_2$-**1g**):

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C17H16N1(1+)\MAY03\23-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.37686265\C,2,1.
41936405,1,121.16158141\C,3,1.4323122,2,118.20732338,1,0.,0\C,4,1.4124
052,3,119.90188757,2,0.,0\C,5,1.38121096,4,119.83951571,3,0.,0\H,1,1.0
850841,2,120.2044877,3,180.,0\H,2,1.08370367,1,119.7808587,6,-180.,0\C
,3,1.4304424,2,121.96053846,1,-180.,0\H,5,1.08150332,4,121.08062778,3,
-180.,0\H,6,1.08549495,5,119.22920316,4,-180.,0\C,4,2.36899305,3,89.81
852647,2,180.,0\C,9,1.38535416,3,117.68424244,2,180.,0\H,12,1.0820016,
4,146.48959185,3,-180.,0\H,13,1.08418405,9,120.97093454,3,-180.,0\C,9,
1.50211746,3,121.81265296,2,0.,0\H,16,1.09628515,9,111.10997715,3,-59.
67208113,0\H,16,1.0962847,9,111.10995845,3,59.6724417,0\H,16,1.0919565
8,9,111.0091844,3,-180.,0\C,12,2.47724593,4,62.31282116,3,-180.,0\H,20
,1.09294769,12,118.81292083,4,-67.80524051,0\H,20,1.09294808,12,118.81
064322,4,67.80988122,0\C,20,1.50432116,12,87.31139548,4,-180.,0\C,23,1
.40274163,20,120.29695288,12,90.63026639,0\C,23,1.40274022,20,120.2969
2395,12,-90.61994049,0\C,24,1.39457464,23,120.27095624,20,179.12564943
,0\H,24,1.08778068,23,119.9189372,20,-0.15388898,0\C,25,1.39457524,23,
120.27092663,20,-179.12559664,0\H,25,1.08778058,23,119.91895267,20,0.1
5391399,0\C,28,1.39685716,25,119.98122264,23,0.10926413,0\H,26,1.08574
868,24,119.83711931,23,-179.48127159,0\H,28,1.08574884,25,119.83704451
,23,179.48116625,0\H,30,1.08590353,28,119.94870392,25,179.56689725,0\N
,12,1.33575853,4,30.44406788,3,-180.,0\\Version=AM64L-G03RevD.01\State
=1-A\HF=-707.4140345\MP2=-709.9745664\RMSD=6.484e-09\Thermal=0.\PG=C01
[X(C17H16N1)]\\@

benzhydryl adduct (Ph_2CH-**1g**):

1\1\GINC-NODE25\SP\RMP2-FC\6-31+G(2d,p)\C23H20N1(1+)\MAY03\23-Nov-2008
\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.38052291\C,2,1.
41291038,1,119.93233449\C,3,1.43333629,2,119.64836326,1,-1.29267408,0\
C,4,1.4199302,3,118.35345902,2,1.38840351,0\C,5,1.37608797,4,121.16062
471,3,-0.46894541,0\H,1,1.08551484,2,119.14163859,3,179.81873524,0\H,2
,1.08064133,1,119.09810636,6,-177.64407221,0\C,4,1.42979007,3,119.9363
3435,2,-178.31700414,0\H,5,1.08373469,4,119.01592883,3,179.64594088,0\
H,6,1.08512838,5,120.2475606,4,179.98709603,0\C,9,1.3850209,4,117.6655
2641,3,-0.26626333,0\C,12,1.39261261,9,120.72469994,4,-1.22509307,0\H,
12,1.08421543,9,121.01261945,4,179.7795991,0\H,13,1.08209285,12,121.44
363674,9,-177.97907607,0\C,9,1.50243031,4,121.85767788,3,179.6802089,0
\H,16,1.09617283,9,111.12185057,4,-59.30906391,0\H,16,1.09628315,9,111
.09932845,4,60.03468568,0\H,16,1.09196729,9,110.98854342,4,-179.660692
98,0\N,13,1.33656281,12,122.5489627,9,1.1247006,0\C,20,1.52892874,13,1
19.74280229,12,-179.64735317,0\H,21,1.0923265,20,103.47049412,13,137.4
7262725,0\C,21,1.52327792,20,111.75683028,13,23.37402978,0\C,23,1.4035
854,21,118.66679883,20,80.90424887,0\C,23,1.40164271,21,122.16045486,2
0,-99.88582621,0\C,24,1.39363768,23,120.54627689,21,179.73305241,0\H,2
4,1.08818565,23,119.84539539,21,0.2508337,0\C,25,1.39633063,23,120.197
42141,21,-179.80881009,0\H,25,1.0855899,23,120.08457594,21,-1.03517698
,0\C,28,1.39555395,25,120.25852354,23,0.30847487,0\H,26,1.08591457,24,

119.82295758,23,-179.44837529,0\H,28,1.08592941,25,119.60488792,23,179
.60966807,0\H,30,1.0859382,28,120.08790611,25,179.46731758,0\C,21,1.52
332201,20,110.76274046,13,-106.1126022,0\C,34,1.40182723,21,117.954100
99,20,-148.15660811,0\C,34,1.39941953,21,122.81661145,20,34.25868788,0
\C,35,1.39400071,34,120.45698637,21,-177.51896667,0\H,35,1.0879016,34,
119.85024327,21,1.73963282,0\C,36,1.39672144,34,120.29387846,21,177.49
297242,0\H,36,1.08679908,34,120.58786387,21,-2.81834349,0\C,39,1.39492
008,36,120.23036537,34,-0.02890051,0\H,37,1.08591151,35,119.69719688,3
4,179.96912532,0\H,39,1.08601702,36,119.60491248,34,179.88729595,0\H,4
1,1.08579593,39,120.1277698,36,179.90240722,0\\Version=AM64L-G03RevD.0
1\State=1-A\HF=-936.9737283\MP2=-940.3835649\RMSD=5.520e-09\Thermal=0.
\PG=C01 [X(C23H20N1)]\\@

Hydroxymethylquinoline (**1i**):

neutral (**1i**):

1\1\GINC-NODE25\SP\RMP2-FC\6-31+G(2d,p)\C10H9N1O1\MAY03\24-Nov-2008\0\
\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\C\C,1,1.37614385\C,2,1.419
7233,1,120.5929725\C,3,1.43347843,2,119.29719839,1,0.00492843,0\C,4,1.
42101376,3,118.6670628,2,-0.47690259,0\C,5,1.3775929,4,120.60118657,3,
0.63067046,0\H,1,1.08675394,2,120.15049706,3,-179.97405309,0\H,2,1.085
48375,1,122.01351157,6,-179.70703237,0\C,4,1.42993305,3,117.56994694,2
,178.85747323,0\H,5,1.0840929,4,119.0311813,3,-177.31397364,0\C,9,1.37
738944,4,117.91995314,3,1.04498813,0\C,11,1.41639665,9,119.95397674,4,
-0.51473244,0\H,11,1.0868456,9,120.5829944,4,179.78490787,0\H,12,1.089
96148,11,119.42014581,9,179.94829282,0\N,12,1.31544051,11,124.11439867
,9,-0.26929882,0\C,9,1.509805,4,121.73978599,3,-176.65187398,0\H,16,1.
10261418,9,109.14970572,4,58.92217222,0\H,16,1.10002451,9,108.92700614
,4,175.82667061,0\H,6,1.08675626,5,119.79105053,4,-179.83581992,0\O,16
,1.4277997,9,109.66047732,4,-62.4661902,0\H,20,0.96999504,16,107.39608
028,9,176.75208244,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-513.27787
8\MP2=-515.0604377\RMSD=5.156e-09\Thermal=0.\PG=C01 [X(C10H9N1O1)]\\@

benzyl adduct ($PhCH_2$-**1i**):

1\1\GINC-NODE10\SP\RMP2-FC\6-31+G(2d,p)\C17H16N1O1(1+)\MAY03\24-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.38113126\C,2,
1.41180282,1,119.75090041\C,3,1.43459371,2,119.95503395,1,-0.10837934,
0\C,4,1.4212848,3,118.24769166,2,-0.21738715,0\C,5,1.37636195,4,120.91
019955,3,0.42538033,0\H,1,1.08557539,2,119.18159413,3,-179.89949439,0\
H,2,1.08136404,1,119.08476418,6,-179.95958631,0\C,4,1.427613,3,119.320
73299,2,178.94328213,0\H,5,1.0821449,4,118.38850839,3,-177.51984792,0\
C,9,1.38316119,4,118.31697778,3,0.27392213,0\C,11,1.39385858,9,120.634
00161,4,0.28111428,0\H,11,1.08419809,9,121.15009724,4,179.68461969,0\H
,12,1.08183297,11,121.82842912,9,179.30602629,0\N,12,1.33479468,11,122
.071524,9,-0.32059803,0\C,9,1.51452078,4,122.2546854,3,-177.63617453,0
\H,16,1.10310538,9,108.22058915,4,66.50482786,0\H,16,1.09818731,9,108.
72424257,4,-177.25826999,0\C,15,1.51729707,12,120.28321044,11,179.7751
6404,0\H,19,1.09264262,15,105.71813379,12,-124.08848045,0\C,19,1.50420
445,15,115.09783232,12,-1.69141759,0\C,21,1.4026888,19,120.34511771,15

,91.50077142,0\C,21,1.4028241,19,120.23927249,15,-89.94131634,0\C,22,1
.39471944,21,120.26305529,19,178.86511083,0\H,22,1.08778174,21,119.923
71699,19,-0.35248608,0\C,23,1.39452251,21,120.27085098,19,-178.8643514
9,0\H,23,1.08775984,21,119.92039556,19,0.38259942,0\C,24,1.39677878,22
,119.98267912,21,-0.09751601,0\H,24,1.085755,22,119.83728183,21,-179.4
4457403,0\H,26,1.08574075,23,119.83512045,21,179.45035245,0\H,28,1.085
91275,24,119.94609788,22,-179.54292635,0\H,6,1.08510239,5,120.06806432
,4,-179.9474374,0\O,16,1.41830189,9,108.99468658,4,-55.2684023,0\H,33,
0.97069664,16,108.20200114,9,-177.25328696,0\H,19,1.09299339,15,105.84
675514,12,120.97208941,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-782.2
663441\MP2=-785.0299946\RMSD=7.309e-09\Thermal=0.\PG=C01 [X(C17H16N1O1
)]\\@

benzhydryl adduct (Ph_2CH-**1i**):

1\1\GINC-NODE26\SP\RMP2-FC\6-31+G(2d,p)\C23H20N1O1(1+)\MAY03\24-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.38041136\C,2,
1.41240723,1,119.82403674\C,3,1.43553676,2,119.72589478,1,1.13216045,0
\C,4,1.42166412,3,118.38220801,2,-1.64974262,0\C,5,1.3756396,4,120.907
98124,3,0.98127381,0\H,1,1.08560474,2,119.10357724,3,-179.65653663,0\H
,2,1.08057395,1,119.12688165,6,177.73412648,0\C,4,1.42701703,3,119.453
13271,2,177.18081066,0\H,5,1.08212366,4,118.37950821,3,-177.14574989,0
\C,9,1.38283137,4,118.2736074,3,0.49672823,0\C,11,1.39357145,9,120.523
92073,4,1.543227,0\H,11,1.08424093,9,121.20676598,4,179.96495922,0\H,1
2,1.08190982,11,121.60443171,9,177.29240487,0\N,12,1.33554546,11,122.3
5124035,9,-1.39614817,0\C,9,1.51447706,4,122.2799188,3,-177.38472175,0
\H,16,1.10301385,9,108.29145822,4,65.71027942,0\H,16,1.09827795,9,108.
72595395,4,-178.01039215,0\C,15,1.52997851,12,119.54657014,11,179.0156
4936,0\H,19,1.09218881,15,103.36648411,12,-137.82606589,0\C,19,1.52379
031,15,111.65715777,12,-23.83185604,0\C,21,1.4013333,19,122.25213646,1
5,101.28862404,0\C,21,1.40370452,19,118.5448568,15,-79.49665662,0\C,22
,1.39658296,21,120.16709068,19,179.77963069,0\H,22,1.08547219,21,120.0
256036,19,0.99539704,0\C,23,1.39333207,21,120.54461463,19,-179.7624325
7,0\H,23,1.08812195,21,119.84189796,19,-0.1753792,0\C,24,1.39548889,22
,120.26185302,21,-0.2522691,0\H,24,1.08593155,22,119.5933446,21,-179.5
9597961,0\H,26,1.08590581,23,119.8393854,21,179.50115345,0\H,28,1.0859
4759,24,120.07387607,22,-179.51065204,0\C,19,1.52303733,15,110.8265192
2,12,105.82180262,0\C,32,1.40191154,19,117.8897995,15,148.04888791,0\C
,32,1.39920052,19,122.88130335,15,-34.23035827,0\C,33,1.39402015,32,12
0.46411044,19,177.68918386,0\H,33,1.08786985,32,119.84017281,19,-1.614
91343,0\C,34,1.39682736,32,120.28355545,19,-177.69890481,0\H,34,1.0867
7714,32,120.60020876,19,2.63626746,0\C,37,1.39492411,34,120.23980894,3
2,0.06793802,0\H,35,1.08591332,33,119.69430229,32,-179.98182295,0\H,37
,1.08601728,34,119.60612458,32,-179.85417532,0\H,39,1.08580449,37,120.
12760476,34,-179.8869994,0\H,6,1.08516142,5,120.11216016,4,-179.971470
75,0\O,16,1.41856057,9,108.97848778,4,-56.07327493,0\H,44,0.97067495,1
6,108.17772997,9,-177.86165706,0\\Version=AM64L-G03RevD.01\State=1-A\H
F=-1011.8259473\MP2=-1015.4389331\RMSD=8.301e-09\Thermal=0.\PG=C01 [X(
C23H20N1O1)]\\@

6-Methoxyquinoline (**1h**):

Neutral (**1h**):

1\1\GINC-NODE9\SP\RMP2-FC\6-31+G(2d,p)\C10H9N1O1\MAY03\23-Nov-2008\0\\
#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\N\C,1,1.36271306\C,2,1.4307
7243,1,122.96645378\C,3,1.41783346,2,117.05398419,1,0.,0\C,4,1.3759018
2,3,119.4129938,2,0.,0\C,1,1.31931156,2,117.73321226,3,0.,0\C,3,1.4213
3154,2,119.96023723,1,180.,0\C,7,1.3809862,3,119.87432651,2,0.,0\C,8,1
.42437656,7,120.31612384,3,0.,0\C,9,1.37021542,8,120.59070341,7,0.,0\O
,8,1.36275438,7,125.26118408,3,180.,0\C,11,1.41895427,8,118.04882947,7
,0.,0\H,9,1.08561334,8,117.76969285,7,180.,0\H,10,1.0854081,9,121.4866
6069,8,180.,0\H,7,1.08473025,3,118.61293599,2,180.,0\H,4,1.08785827,3,
119.50873869,2,180.,0\H,5,1.08612398,4,121.26441607,3,180.,0\H,6,1.089
66496,1,116.34686983,2,180.,0\H,12,1.09802268,11,111.41933047,8,-61.08
030539,0\H,12,1.09802268,11,111.41933047,8,61.08030539,0\H,12,1.091360
07,11,105.98094397,8,180.,0\\Version=AM64L-G03RevD.01\State=1-A'\HF=-5
13.2719338\MP2=-515.0510466\RMSD=8.405e-09\Thermal=0.\PG=CS [SG(C10H7N
1O1),X(H2)]\\@

benzyl adduct ($PhCH_2$-**1h**):

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C17H16N1O1(1+)\MAY03\23-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39687172\C,2,
1.39455959,1,119.98295908\C,3,1.40270632,2,120.27073952,1,-0.08587175,
0\C,4,1.40269838,3,119.39581454,2,0.28828752,0\C,5,1.39455828,4,120.27
102363,3,-0.28749184,0\C,4,1.50387932,3,120.29485171,2,178.81336249,0\
N,7,1.51850191,4,115.23848181,3,90.74617993,0\C,8,1.38803965,7,118.515
51572,4,179.97726804,0\C,9,1.43148258,8,118.86970349,7,-180.,0\C,10,1.
41552051,9,118.4757126,8,0.,0\C,11,1.3778906,10,120.30193721,9,0.,0\C,
8,1.33818628,7,120.20293468,4,-0.0249606,0\C,10,1.41633191,9,119.94991
491,8,180.,0\C,14,1.38517562,10,120.21932731,9,0.,0\C,15,1.4243939,14,
119.25553424,10,0.,0\C,16,1.37319472,15,121.74202371,14,0.,0\O,15,1.34
020582,14,126.02561333,10,-180.,0\C,18,1.43231274,15,119.14621501,14,0
.,0\H,16,1.08511757,15,117.68217797,14,180.,0\H,17,1.0816091,16,118.71
138529,15,180.,0\H,14,1.08336322,10,118.28648196,9,-180.,0\H,11,1.0861
9274,10,119.18104629,9,-180.,0\H,12,1.08369122,11,121.80836821,10,-180
.,0\H,13,1.08142615,8,116.06018331,7,0.,0\H,19,1.09581655,18,110.81552
455,15,61.31635433,0\H,19,1.08932308,18,105.50088793,15,180.,0\H,19,1.
09581693,18,110.81576119,15,-61.31948697,0\H,7,1.0928584,4,110.6987447
1,3,-29.11051311,0\H,7,1.09284407,4,110.69406603,3,-149.40367047,0\H,3
,1.08775655,2,119.80493916,1,179.18324686,0\H,5,1.08775601,4,119.92006
304,3,178.98137691,0\H,2,1.08574865,1,120.18291573,6,179.25358493,0\H,
6,1.08574904,5,119.83109659,4,179.46166562,0\H,1,1.08590622,6,119.9510
5537,5,179.57424283,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-782.2592
168\MP2=-785.0225453\RMSD=8.916e-09\Thermal=0.\PG=C01 [X(C17H16N1O1)]\
\@

benzhydryl adduct (Ph_2CH-**1h**):

1\1\GINC-NODE19\SP\RMP2-FC\6-31+G(2d,p)\C23H20N1O1(1+)\MAY03\23-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39664001\C,2,
1.39404813,1,120.07687022\C,3,1.40197054,2,120.46245262,1,0.16794274,0
\C,4,1.39941322,3,119.2024506,2,-0.15101054,0\C,1,1.39492825,2,119.744
0708,3,-0.06606638,0\C,4,1.52310511,3,117.89993158,2,177.55958507,0\C,
7,1.52323147,4,114.97994056,3,-83.66010836,0\C,8,1.40143425,7,122.1826
9303,4,-27.10442131,0\C,9,1.39637113,8,120.18986288,7,179.76630725,0\C
,10,1.39555253,9,120.25137837,8,-0.30107948,0\C,11,1.39719877,10,119.8
8100483,9,-0.08312566,0\C,12,1.39346256,11,119.94954653,10,0.17738721,
0\N,7,1.53073775,4,110.67431953,3,148.40082552,0\C,14,1.38941335,7,119
.48919795,4,-73.57159992,0\C,15,1.43254824,14,118.80615942,7,-178.2199
0676,0\C,16,1.41479058,15,118.62852276,14,-1.84566593,0\C,17,1.3776895
3,16,120.25253213,15,0.28928703,0\C,14,1.33925636,7,119.4901112,4,106.
17568537,0\C,16,1.41697395,15,120.09054124,14,178.39965073,0\C,20,1.38
417972,16,120.19087015,15,0.437455,0\C,21,1.42420846,20,119.19958929,1
6,0.68727146,0\C,22,1.37256006,21,121.83763535,20,-0.84211471,0\O,21,1
.34113532,20,126.04318699,16,-179.78752783,0\C,24,1.43161059,21,119.02
995016,20,0.28914954,0\H,22,1.08512645,21,117.66531046,20,178.72894459
,0\H,23,1.08083066,22,118.72812509,21,177.73825402,0\H,20,1.08344918,1
6,118.26514787,15,-179.69269222,0\H,17,1.08622823,16,119.1879576,15,-1
79.64619472,0\H,18,1.08373059,17,121.87080007,16,-179.74984784,0\H,19,
1.0814397,14,116.02535226,7,0.51704048,0\H,25,1.09591586,24,110.844813
15,21,-61.56047814,0\H,25,1.09592561,24,110.82635318,21,61.02762259,0\
H,25,1.08939398,24,105.53831253,21,179.73585431,0\H,7,1.09226513,4,108
.7595654,3,35.5127042,0\H,9,1.08549658,8,120.04699951,7,0.94706379,0\H
,13,1.08809816,12,119.61585342,11,-179.46339064,0\H,10,1.08591849,9,11
9.59877027,8,-179.61891307,0\H,12,1.08591477,11,120.21040676,10,-179.1
9256532,0\H,11,1.08594708,10,120.08208719,9,-179.48103901,0\H,3,1.0879
1628,2,119.68974593,1,179.42884176,0\H,5,1.08678545,4,120.61075227,3,-
179.60914204,0\H,2,1.08590166,1,120.22305483,6,-179.92464633,0\H,6,1.0
8602167,1,120.15044156,2,179.89103214,0\H,1,1.08580594,6,120.11818594,
5,-179.9087066,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1011.8191262\
MP2=-1015.4318639\RMSD=6.185e-09\Thermal=0.\PG=C01 [X(C23H20N1O1)]\\@

<u>Methoxylepidine (**1j**):</u>

neutral (**1j**):

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C11H11N1O1\MAY03\23-Nov-2008\0
\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\0,1\C\C,1,1.37012337\C,2,1.42
291001,1,121.06411285\C,3,1.43084406,2,118.713996,1,0.,0\C,4,1.4224449
6,3,119.33733346,2,0.,0\C,5,1.38212226,4,120.24339213,3,0.,0\H,1,1.085
5576,2,121.77492882,3,-180.,0\H,2,1.08540139,1,121.46686678,6,180.,0\C
,4,1.43024262,3,117.68175466,2,-180.,0\H,5,1.08274245,4,119.14698923,3
,-180.,0\C,9,1.37995889,4,117.4595303,3,0.,0\C,11,1.41417154,9,120.281
85999,4,0.,0\H,11,1.08706859,9,120.3235671,4,-180.,0\H,12,1.08986642,1
1,119.49642905,9,-180.,0\N,12,1.31758361,11,124.01274867,9,0.,0\C,9,1.
50740532,4,121.35889299,3,-180.,0\H,16,1.09744584,9,111.49823331,4,-59

.78116181,0\H,16,1.09744472,9,111.4986917,4,59.77008861,0\H,16,1.09375
577,9,110.93459635,4,179.99472522,0\O,6,1.36356189,5,125.12322228,4,-1
80.,0\C,20,1.41840474,6,118.16043315,5,0.,0\H,21,1.09814352,20,111.463
2748,6,61.10074169,0\H,21,1.09140734,20,105.96448157,6,-180.,0\H,21,1.
09814429,20,111.46287305,6,-61.09801575,0\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-552.3137845\MP2=-554.2496712\RMSD=6.108e-09\Thermal=0.\PG=
C01 [X(C11H11N1O1)]\\@

benzyl adduct ($PhCH_2$-**1j**):

1\1\GINC-NODE28\SP\RMP2-FC\6-31+G(2d,p)\C18H18N1O1(1+)\MAY03\23-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.39683575\C,2,
1.39457669,1,119.98285907\C,3,1.40257768,2,120.28533575,1,-0.09419401,
0\C,4,1.4025858,3,119.37737422,2,0.33830624,0\C,5,1.39457952,4,120.284
93773,3,-0.33936669,0\C,4,1.50454324,3,120.30258348,2,178.91772053,0\N
,7,1.51635235,4,115.11946102,3,90.70042348,0\C,8,1.38866966,7,118.9770
8954,4,-179.96973128,0\C,9,1.43109396,8,119.36916944,7,180.,0\C,10,1.4
316126,9,119.24795547,8,0.00298459,0\C,11,1.38471784,10,117.90098814,9
,0.,0\C,8,1.33651733,7,120.38010363,4,0.0368354,0\C,10,1.41714428,9,11
9.13470369,8,-180.,0\C,14,1.38594884,10,120.74163534,9,-0.00415184,0\C
,15,1.42158533,14,119.38873099,10,0.,0\C,16,1.37234558,15,121.24474602
,14,0.00261023,0\O,15,1.34163921,14,125.80246595,10,-180.,0\C,18,1.431
05945,15,119.191908,14,0.,0\H,16,1.0850111,15,117.98404334,14,-179.996
76141,0\H,17,1.08156929,16,118.64424064,15,-179.99517898,0\H,14,1.0813
065,10,118.7966491,9,179.9972062,0\H,12,1.08426753,11,120.79388068,10,
180.,0\H,13,1.08142074,8,116.20008922,7,-0.00413243,0\H,19,1.09602385,
18,110.86580067,15,61.31894078,0\H,19,1.08940699,18,105.53249935,15,18
0.,0\H,19,1.09602348,18,110.86587265,15,-61.31934665,0\H,7,1.09288414,
4,110.6260047,3,-29.21177944,0\H,7,1.09290735,4,110.63372772,3,-149.37
518678,0\H,3,1.0877523,2,119.81296269,1,179.20783778,0\H,5,1.08775371,
4,119.89835561,3,178.96121345,0\H,2,1.08577469,1,120.18026502,6,179.22
932678,0\H,6,1.0857753,5,119.83409911,4,179.47814304,0\H,1,1.08592298,
2,119.9561411,3,-179.58013136,0\C,11,1.50200696,10,121.57076666,9,180.
,0\H,35,1.09655657,11,111.07089215,10,-59.6574715,0\H,35,1.09655674,11
,111.07079382,10,59.6683476,0\H,35,1.0920124,11,111.10344709,10,-179.9
946396,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-821.3052619\MP2=-824.
2244984\RMSD=4.015e-09\Thermal=0.\PG=C01 [X(C18H18N1O1)]\\@

benzhydryl adduct (Ph_2CH-**1j**):

1\1\GINC-NODE20\SP\RMP2-FC\6-31+G(2d,p)\C24H22N1O1(1+)\MAY03\24-Nov-20
08\0\\#P mp2(fc)/6-31+G(2d,p) sp scf=tight\\\1,1\C\C,1,1.37166341\C,2,
1.41775125,1,120.29719075\C,3,1.43212822,2,119.03906408,1,1.33154064,0
\C,4,1.41783,3,119.24696753,2,-1.44760257,0\C,5,1.38495773,4,120.73815
153,3,0.43274587,0\H,1,1.08501504,2,120.68596335,3,-179.70412553,0\H,2
,1.08074533,1,118.65839123,6,177.65558792,0\C,4,1.43097814,3,119.37761
565,2,178.29508725,0\H,5,1.08117469,4,118.77880482,3,-179.7446427,0\C,
9,1.38445312,4,117.85846232,3,0.2020558,0\C,11,1.39268454,9,120.927099
59,4,1.19358324,0\H,11,1.0843275,9,120.85650449,4,-179.74781392,0\H,12
,1.08140082,11,121.72249038,9,178.04261024,0\N,12,1.33747602,11,122.09
22425,9,-1.00830198,0\C,9,1.50226144,4,121.64356942,3,-179.76813307,0\

H,16,1.09654912,9,111.07396427,4,-59.85734414,0\H,16,1.09655263,9,111.
11583089,4,59.47582076,0\H,16,1.0920905,9,111.08454408,4,179.85569515,
0\O,6,1.34250461,5,125.84416773,4,-179.816059,0\C,20,1.43040708,6,119.
15179414,5,0.18523702,0\H,21,1.09613296,20,110.90765274,6,61.02897084,
0\H,21,1.08949231,20,105.55499898,6,179.72928371,0\H,21,1.09612208,20,
110.90280388,6,-61.59217529,0\C,15,1.52875482,12,119.74095614,11,179.4
3666999,0\H,25,1.09234046,15,103.45797621,12,-136.86961069,0\C,25,1.52
348887,15,111.82956309,12,-22.80983951,0\C,27,1.40149831,25,122.188581
59,15,99.80507394,0\C,27,1.40350084,25,118.64785712,15,-80.98462539,0\
C,28,1.39632411,27,120.20013444,25,179.80090278,0\H,28,1.08557413,27,1
20.06827002,25,0.94346425,0\C,29,1.39355845,27,120.56103032,25,-179.72
696551,0\H,29,1.08817554,27,119.80050885,25,-0.14748846,0\C,30,1.39552
45,28,120.26199021,27,-0.29672156,0\H,30,1.08594976,28,119.60249323,27
,-179.63561726,0\H,32,1.08593685,29,119.8310119,27,179.46703606,0\H,34
,1.08596272,30,120.08882236,28,-179.48735723,0\C,25,1.52325142,15,110.
86309407,12,106.68385017,0\C,38,1.40184986,25,117.94844595,15,148.4251
6916,0\C,38,1.39923512,25,122.82544904,15,-33.95434546,0\C,39,1.394024
6,38,120.46378862,25,177.56489897,0\H,39,1.08788667,38,119.8369154,25,
-1.71051075,0\C,40,1.39677273,38,120.29072247,25,-177.55144088,0\H,40,
1.08671944,38,120.54816673,25,2.72531343,0\C,43,1.39497804,40,120.2415
9398,38,0.05110061,0\H,41,1.08593465,39,119.69475645,38,-179.97778281,
0\H,43,1.08604648,40,119.59898863,38,-179.88947329,0\H,45,1.08581922,4
3,120.13872648,40,-179.91271112,0\\Version=AM64L-G03RevD.01\State=1-A\
HF=-1050.8649337\MP2=-1054.6336681\RMSD=6.309e-09\Thermal=0.\PG=C01 [X
(C24H22N1O1)]\\@

Solvation (PCM/UAHF, 6-31G(d)):

Benzyl cation ($PhCH_2^+$):

1\1\GINC-NODE11\SP\RHF\6-31G(d)\C7H7(1+)\MAY03\21-Dec-2008\0\\#P HF/6-
31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1,1\C\C
,1,1.44368937\C,1,1.44365346,2,119.38010526\C,2,1.37588507,1,119.87261
65,3,0.0096333,0\H,2,1.08619684,1,119.05389432,3,-179.98972038,0\C,3,1
.37587835,1,119.871268,2,-0.0027882,0\H,3,1.08619725,1,119.05600182,2,
180.,0\C,4,1.41105857,2,119.29683443,1,-0.00745762,0\H,4,1.08475191,2,
120.80955776,1,179.99387544,0\H,6,1.08475428,3,120.80950306,1,179.9961
1224,0\H,8,1.08704101,4,118.86178288,2,180.,0\C,1,1.37042602,3,120.312
6567,6,179.98702931,0\H,12,1.08762464,1,121.59436693,3,-180.,0\H,12,1.
08764282,1,121.58661677,3,0.,0\\Version=AM64L-G03RevD.01\State=1-A\HF=
-268.9464756\RMSD=1.876e-09\Thermal=0.\Dipole=-0.8505189,0.0001194,-0.
4971424\PG=C01 [X(C7H7)]\\@

Benzhydryl cation (Ph_2CH^+):

1\1\GINC-NODE23\SP\RHF\6-31G(d)\C13H11(1+)\MAY03\21-Dec-2008\0\\#P HF/
6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1,1\C
\C,1,1.42697722\C,1,1.42622891,2,118.57003483\C,2,1.38404934,1,120.711
00792,3,-3.66882154,0\H,2,1.08640637,1,119.12934642,3,178.22892657,0\C
,3,1.38287356,1,120.15519022,2,2.42494007,0\H,3,1.08325722,1,120.04550
15,2,-173.40693522,0\C,4,1.40157239,2,119.50432595,1,2.32681887,0\H,4,

1.08496485,2,120.28282417,1,-178.52665707,0\H,6,1.08512432,3,120.03840
986,1,-178.6711638,0\H,8,1.08618077,4,119.60298651,2,178.76704649,0\C,
1,1.41697689,3,124.44040507,6,-179.33244762,0\H,12,1.090299,1,114.2341
0663,3,-162.53488617,0\C,12,1.41697866,1,131.531484,3,17.45945996,0\C,
14,1.42697772,12,116.9658655,1,-164.25673057,0\C,14,1.42621999,12,124.
44193184,1,17.46971883,0\C,15,1.38405524,14,120.71072742,12,177.951844
69,0\H,15,1.08640407,14,119.13039094,12,-0.14782367,0\C,16,1.38287885,
14,120.15517644,12,-179.32840458,0\H,16,1.08325335,14,120.04629403,12,
4.83899553,0\C,17,1.40157184,15,119.50417127,14,2.32855344,0\H,17,1.08
496271,15,120.28334746,14,-178.52838013,0\H,19,1.08512361,16,120.03798
344,14,-178.67024215,0\H,21,1.08618275,17,119.60212226,15,178.76765182
,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-498.5151728\RMSD=3.132e-09\
Thermal=0.\Dipole=-0.2916366,0.103685,0.2299474\PG=C01 [X(C13H11)]\\@

Methyl cation (CH_3^+):

1\1\GINC-NODE16\SP\RHF\6-31G(d)\C1H3(1+)\MAY03\21-Dec-2008\0\\#P HF/6-
31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1,1\C\H
,1,1.094601\H,1,1.09460101,2,120.00002981\H,1,1.09460101,2,120.0000298
1,3,180.,0\\Version=AM64L-G03RevD.01\State=1-A'\HF=-39.3257282\RMSD=3.
650e-10\Thermal=0.\Dipole=0.,0.,0.\PG=C03H [O(C1),SGH(H3)]\\@

Quinine (**1a**):

neutral (**1a**):

1\1\GINC-NODE11\SP\RHF\6-31G(d)\C20H24N2O2\MAY03\16-Dec-2008\0\\#P HF/
6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\0,1\N
\C,1,1.36332144\C,2,1.43209317,1,123.48623198\C,3,1.43155064,2,117.261
4381,1,-0.40681184,0\C,4,1.38004257,3,117.91434328,2,0.26932941,0\C,1,
1.31757441,2,117.29800577,3,0.18518523,0\C,2,1.42316986,1,117.69086489
,6,-179.75521432,0\C,7,1.36959492,2,121.09408527,1,-179.89584323,0\C,8
,1.42192776,7,120.15587919,2,-0.05695701,0\C,9,1.38268545,8,120.538205
34,7,-0.02093626,0\C,4,1.52309751,3,121.27692423,2,-179.72392453,0\O,1
1,1.4293237,4,111.59512628,3,159.58650503,0\O,9,1.36186076,8,114.48027
539,7,179.95270645,0\C,13,1.4200636,9,118.26293322,8,-179.95957703,0\C
,11,1.54944739,4,111.78432795,3,-77.91230213,0\C,15,1.56111356,11,114.
37843887,4,-80.32782151,0\C,16,1.54324962,15,108.2082369,11,-130.73702
53,0\C,17,1.55590321,16,111.00885196,15,-56.82660063,0\C,18,1.57423267
,17,106.39015563,16,56.31610146,0\N,19,1.4717016,18,112.64548213,17,3.
48382705,0\C,20,1.47887648,19,108.46782707,18,58.19209771,0\C,17,1.541
35727,16,108.0712069,15,61.44879745,0\C,18,1.5033077,17,113.85254547,1
6,-67.88530175,0\C,23,1.33442257,18,125.17281345,17,-117.23889899,0\H,
16,1.09553541,15,110.59841647,11,107.3250969,0\H,16,1.09398102,15,110.
87023879,11,-11.31744245,0\H,15,1.09506134,11,105.47177935,4,39.248669
22,0\H,18,1.09829348,17,107.31546738,16,173.03665126,0\H,19,1.09595027
,18,110.37414632,17,124.53189849,0\H,17,1.09582269,16,109.91722904,15,
-178.04536613,0\H,21,1.09621121,20,106.87523502,19,59.84073353,0\H,21,
1.09078905,20,108.54247997,19,175.58189615,0\H,22,1.09735934,17,110.18
996104,16,177.01487482,0\H,22,1.0959011,17,109.55148398,16,59.14482076
,0\H,11,1.09917031,4,108.85087611,3,39.08976205,0\H,5,1.0849063,4,119.
98243313,3,-179.83361862,0\H,10,1.08262783,9,120.14984058,8,179.681722

54,0\H,6,1.08977654,1,116.46212709,2,-179.87781366,0\H,7,1.08535669,2,
117.39037642,1,0.03013415,0\H,8,1.08551153,7,121.78993928,2,179.970245
69,0\H,12,0.97042366,11,107.356287,4,-59.46579966,0\H,19,1.09687077,18
,110.39747132,17,-117.3812312,0\H,23,1.09173781,18,116.15838934,17,63.
58795712,0\H,24,1.08684936,23,121.87739853,18,-179.62492633,0\H,24,1.0
8858908,23,121.65277488,18,0.39334298,0\H,14,1.0977743,13,111.4431486,
9,-61.36647679,0\H,14,1.097678,13,111.45004376,9,60.75253828,0\H,14,1.
09129798,13,105.90375881,9,179.71344254,0\\Version=AM64L-G03RevD.01\St
ate=1-A\HF=-1029.911368\RMSD=3.697e-09\Thermal=0.\Dipole=1.1292003,-0.
2720887,0.5635321\PG=C01 [X(C20H24N2O2)]\\@

benzyl adduct ($PhCH_2$-**1a**, N_{sp2}):

1\1\GINC-NODE22\SP\RHF\6-31G(d)\C27H31N2O2(1+)\MAY03\16-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1
,1\C\C,1,1.39515158\C,2,1.39570119,1,120.00814247\C,3,1.39996804,2,120
.38096441,1,0.41393755,0\C,4,1.40015747,3,119.3602069,2,-0.07373375,0\
C,5,1.39444652,4,120.20919887,3,-0.36224988,0\C,4,1.51646872,3,119.030
27819,2,176.68312103,0\N,7,1.49326598,4,114.39978753,3,139.20819118,0\
C,8,1.3857746,7,121.24642521,4,-72.7148391,0\C,9,1.43723006,8,119.5207
6693,7,-178.29726676,0\C,10,1.42934927,9,118.82103599,8,-1.84320054,0\
C,11,1.38943564,10,118.23773475,9,0.32945275,0\C,8,1.34222158,7,118.15
913037,4,107.29218839,0\C,10,1.41889492,9,118.48545878,8,179.37303368,
0\C,14,1.384131,10,120.8966768,9,0.26391944,0\C,15,1.42094699,14,119.6
6430001,10,-0.08807024,0\C,16,1.37088346,15,121.14660723,14,-0.1110373
,0\C,11,1.52778817,10,124.69725823,9,179.50480609,0\C,18,1.55668116,11
,110.82587297,10,-91.33031634,0\C,19,1.55572133,18,113.78400014,11,-16
1.8248432,0\C,20,1.54552919,19,107.32436101,18,-145.14737804,0\C,21,1.
55730798,20,111.53599009,19,-47.46445788,0\C,22,1.57474247,21,106.6114
1162,20,61.8761444,0\N,19,1.47542088,18,111.74615114,11,71.52644219,0\
C,24,1.48131875,19,111.19963138,18,81.69056687,0\C,21,1.53914906,20,10
7.41904186,19,70.28163979,0\O,15,1.34451618,14,125.80949666,10,179.648
51633,0\C,27,1.42895351,15,119.18838284,14,-0.8606198,0\C,22,1.5059433
3,21,113.66259462,20,-63.14782108,0\C,29,1.33376246,22,124.76524275,21
,-115.92699396,0\O,18,1.42149659,11,110.04566677,10,151.57809391,0\H,2
0,1.09332795,19,110.37183977,18,92.37914089,0\H,20,1.09623836,19,111.2
670724,18,-25.39169373,0\H,19,1.0965511,18,105.70766643,11,-43.1908042
3,0\H,22,1.09715179,21,107.18041767,20,178.17587115,0\H,23,1.09506272,
22,110.71805903,21,111.63851006,0\H,21,1.09445739,20,109.99187965,19,-
169.21732299,0\H,25,1.09579397,24,107.30321171,19,-173.49799406,0\H,25
,1.09654569,24,108.63502947,19,-58.44811323,0\H,26,1.0962027,21,110.37
367555,20,-174.66405714,0\H,26,1.09620661,21,110.46091559,20,67.228723
25,0\H,18,1.09670811,11,110.21263116,10,30.04692565,0\H,12,1.08308398,
11,119.73460928,10,-178.69265917,0\H,14,1.07824307,10,118.80753706,9,-
178.1951863,0\H,13,1.08324545,8,116.32003219,7,0.15103724,0\H,17,1.080
95449,16,119.09811455,15,178.21510768,0\H,16,1.0850176,15,118.03185711
,14,179.5095119,0\H,31,0.97022625,18,109.0250111,11,-75.21724255,0\H,2
3,1.09564669,22,110.82221312,21,-129.74509633,0\H,29,1.09189053,22,116
.65891447,21,64.42210129,0\H,30,1.08639863,29,121.83532487,22,-179.993
8913,0\H,30,1.08824611,29,121.74295283,22,0.10503387,0\H,28,1.09572821
,27,110.93684686,15,61.85403703,0\H,28,1.08968348,27,105.56699131,15,-

179.33915544,0\H,28,1.09640994,27,110.91068904,15,-60.67378014,0\H,7,1
.09263606,4,111.18102162,3,17.0931471,0\H,7,1.09349715,4,111.0592673,3
,-101.56897427,0\H,3,1.08816787,2,119.66239337,1,179.77603275,0\H,5,1.
08740787,4,120.43275122,3,179.77235114,0\H,2,1.08585983,1,120.25705839
,6,179.89660946,0\H,6,1.08599581,5,119.70884124,4,-179.84285518,0\H,1,
1.08583477,2,120.10513912,3,179.75375663,0\\Version=AM64L-G03RevD.01\S
tate=1-A\HF=-1298.9256144\RMSD=3.813e-09\Thermal=0.\Dipole=-1.8980617,
1.1782613,-0.6868186\PG=C01 [X(C27H31N2O2)]\\@

benzyl adduct ($PhCH_2$-**1a**, N_{sp3}):

1\1\GINC-NODE22\SP\RHF\6-31G(d)\C27H31N2O2(1+)\MAY03\21-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1
,1\C\C,1,1.39653341\C,2,1.39435288,1,120.02924092\C,3,1.40352686,2,120
.5701767,1,-0.50268248,0\C,4,1.40377363,3,118.85466771,2,1.60288209,0\
C,5,1.39472431,4,120.58117169,3,-1.64697278,0\C,4,1.50864844,3,120.692
7646,2,177.59986403,0\N,7,1.5417741,4,116.32888217,3,91.74606477,0\C,8
,1.55830643,7,110.5456066,4,-171.26473424,0\C,9,1.54408654,8,108.02535
938,7,-169.51128182,0\C,10,1.53626651,9,110.2160708,8,-17.76641768,0\C
,11,1.54968961,10,110.85528594,9,-48.00082239,0\C,8,1.52391118,7,110.4
7123033,4,-54.1110233,0\C,8,1.52773609,7,110.20139519,4,65.49385034,0\
C,11,1.53644073,10,107.94827941,9,70.25743902,0\C,9,1.54682852,8,115.1
1845034,7,-40.78589637,0\O,16,1.42255332,9,107.77756248,8,-60.3153299,
0\C,12,1.50959497,11,114.07463471,10,-62.25214124,0\C,18,1.33301161,12
,123.95607227,11,-114.06575961,0\C,16,1.52478483,9,109.84790161,8,175.
86472524,0\C,20,1.433503,16,120.94843858,9,-78.68715305,0\C,21,1.43638
071,20,116.71027591,16,179.49670789,0\N,22,1.36264571,21,123.42274988,
20,0.54212835,0\C,23,1.31480115,22,117.85632001,21,0.29184311,0\C,20,1
.37847199,16,120.5851058,9,101.7428855,0\C,21,1.41422225,20,124.648305
01,16,-0.84515102,0\C,26,1.38790413,21,121.18871221,20,-179.96555775,0
\C,27,1.42005779,26,120.04461242,21,-0.12547164,0\C,28,1.37562355,27,1
19.75873628,26,0.39628541,0\O,27,1.35677068,26,115.94109029,21,179.892
61041,0\C,30,1.42745236,27,119.11165004,26,-177.8538836,0\H,10,1.09250
953,9,108.67992841,8,-140.36321397,0\H,10,1.09371518,9,109.79363452,8,
102.80455837,0\H,9,1.09319992,8,102.99464466,7,74.11750141,0\H,12,1.09
596556,11,107.41295188,10,178.54229274,0\H,13,1.09008004,8,106.3079247
8,7,62.46603366,0\H,11,1.09340684,10,110.12060884,9,-169.14591294,0\H,
14,1.0900418,8,105.90608746,7,-51.29147904,0\H,14,1.08824979,8,105.820
1868,7,64.76455026,0\H,15,1.095033,11,110.42297252,10,-174.43062515,0\
H,15,1.09417972,11,110.35291856,10,67.24987598,0\H,16,1.09725232,9,108
.86181504,8,58.35594223,0\H,25,1.08536593,20,120.72496315,16,-0.068217
4,0\H,26,1.08508297,21,121.97369294,20,-1.54862637,0\H,24,1.08858562,2
3,116.7771098,22,179.57410401,0\H,29,1.08506338,28,121.11884725,27,179
.547567,0\H,28,1.08352414,27,120.54912862,26,179.97008987,0\H,17,0.971
75972,16,108.18589943,9,-173.65924227,0\H,13,1.09278751,8,106.67389315
,7,-52.6396201,0\H,18,1.09101563,12,117.03963449,11,65.65198959,0\H,19
,1.08589041,18,121.63702634,12,179.18496532,0\H,19,1.08808699,18,121.8
934192,12,-0.60020434,0\H,31,1.09643465,30,111.4153812,27,-62.66165839
,0\H,31,1.09615081,30,111.35388309,27,60.17896802,0\H,31,1.09055301,30
,105.57037031,27,178.74690258,0\H,7,1.09333018,4,110.6052083,3,-28.110
5546,0\H,7,1.09045573,4,110.54769245,3,-148.95440547,0\H,3,1.08750047,
2,119.45125614,1,178.42594943,0\H,5,1.08744439,4,119.88936252,3,177.08

172501,0\H,2,1.08580523,1,120.17483309,6,178.64185363,0\H,6,1.08578753
,5,119.7939362,4,179.74007118,0\H,1,1.08587971,6,120.03468358,5,179.56
814352,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1298.9270883\RMSD=2.4
99e-09\Thermal=0.\Dipole=-1.6504071,-0.9246311,-1.9399758\PG=C01 [X(C2
7H31N2O2)]\\@

benzhydryl adduct (Ph_2CH-**1a,** N_{sp2}):

1\1\GINC-NODE20\SP\RHF\6-31G(d)\C33H35N2O2(1+)\MAY03\19-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1
,1\C\C,1,1.39543407\C,2,1.39638824,1,120.26222966\C,3,1.40125949,2,120
.22911872,1,-0.29608461,0\C,4,1.40332722,3,119.12694663,2,0.59666513,0
\C,5,1.39354473,4,120.57740123,3,-0.50903842,0\C,4,1.52442812,3,122.23
963245,2,179.86298685,0\C,7,1.52337343,4,114.72393512,3,-27.16630462,0
\C,8,1.40185762,7,118.01246383,4,-83.76992649,0\C,9,1.39403631,8,120.4
9013232,7,177.78911852,0\C,10,1.39660085,9,120.08578624,8,0.11918494,0
\C,11,1.3949588,10,119.72015563,9,-0.0686795,0\C,12,1.39674777,11,120.
24557455,10,-0.01390438,0\N,7,1.52615866,4,111.79790971,3,100.35625562
,0\C,14,1.38929977,7,120.05411044,4,156.51977489,0\C,15,1.43737258,14,
119.5807433,7,-177.13639773,0\C,16,1.42975905,15,118.88576956,14,-2.61
606605,0\C,17,1.38694366,16,118.03964116,15,-0.20569169,0\C,14,1.33917
875,7,119.62123483,4,-23.82981796,0\C,16,1.41935499,15,118.66788593,14
,178.81974472,0\C,20,1.38340361,16,120.99452959,15,0.61072358,0\C,21,1
.41950617,20,119.52760749,16,0.18882856,0\C,22,1.37118562,21,121.17042
045,20,-0.53621753,0\C,17,1.52776469,16,124.8114498,15,178.91713147,0\
C,24,1.55582054,17,110.74912352,16,-91.54155736,0\C,25,1.5554072,24,11
3.81162447,17,-162.53656927,0\C,26,1.54560877,25,107.30903351,24,-145.
63658388,0\C,27,1.55774881,26,111.45992697,25,-47.23710186,0\C,28,1.57
478219,27,106.60569837,26,62.07669675,0\N,25,1.47579231,24,111.8238578
4,17,70.71377214,0\C,30,1.48117257,25,111.12072135,24,82.0418839,0\C,2
7,1.5389413,26,107.44986475,25,70.39309664,0\O,21,1.34579328,20,125.83
909735,16,179.67189584,0\C,33,1.42818959,21,119.12365979,20,-0.7181040
4,0\C,28,1.50600328,27,113.62263066,26,-62.93309226,0\C,35,1.33381235,
28,124.74047621,27,-115.24499503,0\O,24,1.42199575,17,110.19779228,16,
151.52001367,0\H,26,1.09331693,25,110.3768526,24,91.85876932,0\H,26,1.
09628962,25,111.22101541,24,-25.91117776,0\H,25,1.0965701,24,105.57771
689,17,-43.96818256,0\H,28,1.09725502,27,107.19527393,26,178.42127126,
0\H,29,1.09512192,28,110.70492884,27,111.27774674,0\H,27,1.09444028,26
,110.05391079,25,-168.98846629,0\H,31,1.09583072,30,107.3677248,25,-17
3.16645929,0\H,31,1.09626116,30,108.61141526,25,-58.08678346,0\H,32,1.
09623809,27,110.34983969,26,-174.28303815,0\H,32,1.0962604,27,110.4886
8762,26,67.59074957,0\H,24,1.09678519,17,110.33736495,16,29.96972359,0
\H,18,1.08310369,17,119.7819244,16,-178.22052642,0\H,20,1.07837164,16,
118.84139702,15,-178.16357421,0\H,19,1.08131048,14,116.18683146,7,0.35
8241,0\H,23,1.08051824,22,118.59305133,21,177.60410248,0\H,22,1.085027
86,21,118.08617509,20,178.8954759,0\H,37,0.97020829,24,108.95624283,17
,-74.12060243,0\H,29,1.09575871,28,110.7941333,27,-130.12237158,0\H,35
,1.09187433,28,116.65957281,27,65.05715361,0\H,36,1.08821328,35,121.70
091171,28,0.09255359,0\H,36,1.08643355,35,121.857699,28,179.93117405,0
\H,34,1.08977373,33,105.59409082,21,-179.61866542,0\H,34,1.09655668,33
,110.9484639,21,-60.95688661,0\H,34,1.09590922,33,110.98962847,21,61.5

6665408,0\H,7,1.09223589,4,106.26979473,3,-147.28613231,0\H,9,1.087923
41,8,119.81526798,7,-1.59400506,0\H,13,1.08670499,12,119.20438538,11,1
79.68870664,0\H,10,1.08596191,9,119.7013475,8,179.97351674,0\H,12,1.08
60875,11,120.13944546,10,179.91464853,0\H,11,1.08584882,10,120.1357620
2,9,179.80863916,0\H,3,1.08552016,2,119.72548395,1,178.60784057,0\H,5,
1.08812083,4,119.80343529,3,179.13483939,0\H,2,1.08598722,1,120.139366
14,6,179.25968701,0\H,6,1.08596894,5,119.82469753,4,179.51969611,0\H,1
,1.08598421,2,120.09668501,3,-179.51280684,0\\Version=AM64L-G03RevD.01
\State=1-A\HF=-1528.4619818\RMSD=2.311e-09\Thermal=0.\Dipole=-0.264394
3,0.7774449,1.4229746\PG=C01 [X(C33H35N2O2)]\\@

benzhydryl adduct (Ph_2CH-**1a,** N_{sp3}):

1\1\GINC-NODE11\SP\RHF\6-31G(d)\C33H35N2O2(1+)\MAY03\16-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1
,1\C\C,1,1.39452828\C,2,1.39355997,1,119.99838477\C,3,1.40709728,2,121
.62088554,1,0.34963313,0\C,4,1.40497534,3,117.51560706,2,0.98207831,0\
C,1,1.39386049,2,119.29974314,3,-0.91502613,0\C,4,1.52957593,3,115.406
95661,2,174.96568813,0\C,7,1.52704707,4,112.5459752,3,-98.86156056,0\C
,8,1.40468077,7,118.24392096,4,124.6533621,0\C,9,1.39485786,8,121.0784
7046,7,-177.17540619,0\C,10,1.39486204,9,119.96802606,8,0.0727427,0\C,
11,1.39620007,10,119.61238988,9,0.68052142,0\C,12,1.39444526,11,120.35
573044,10,-0.21470544,0\N,7,1.59042517,4,116.82461421,3,128.1467047,0\
C,14,1.56259702,7,113.29360607,4,-47.60337117,0\C,15,1.54770336,14,108
.09558163,7,-166.73410155,0\C,16,1.53247507,15,110.86969491,14,-17.388
58444,0\C,17,1.54718254,16,109.90969812,15,-48.15054039,0\C,14,1.52500
431,7,112.61661228,4,73.39825492,0\C,14,1.53616511,7,107.37508505,4,-1
68.98065408,0\C,17,1.53251967,16,108.12834988,15,69.70390488,0\C,15,1.
54926449,14,115.81849751,7,-38.85352352,0\O,22,1.42697437,15,108.22573
371,14,-54.89542863,0\C,18,1.51405802,17,111.85318307,16,-64.15927769,
0\C,24,1.33337581,18,129.42464768,17,119.25862075,0\C,22,1.52719946,15
,110.33714574,14,-178.28808848,0\C,26,1.4342184,22,121.47824068,15,-77
.66374248,0\C,27,1.43722056,26,116.68799151,22,179.92183187,0\N,28,1.3
6317485,27,123.54867301,26,0.65148096,0\C,29,1.31427173,28,117.7359586
4,27,0.17266353,0\C,26,1.37902229,22,120.22748712,15,103.22670304,0\C,
27,1.41467531,26,124.5836107,22,-0.3799682,0\C,32,1.38770102,27,120.94
709296,26,179.79285805,0\C,33,1.41949003,32,120.24307661,27,0.02339256
,0\C,34,1.37556787,33,119.75072226,32,0.38181793,0\O,33,1.36025265,32,
116.07390312,27,179.98682801,0\C,36,1.42582767,33,118.90483297,32,-179
.0410579,0\H,16,1.09241245,15,108.03717473,14,-139.53103126,0\H,16,1.0
9361773,15,109.8758338,14,103.59875666,0\H,15,1.09081009,14,103.423935
34,7,77.04154295,0\H,18,1.09879017,17,106.92475196,16,179.46619824,0\H
,19,1.08958469,14,105.90228983,7,61.02465567,0\H,17,1.09445138,16,110.
21182173,15,-169.45957387,0\H,20,1.08803614,14,106.20131654,7,-49.7553
2122,0\H,20,1.08712495,14,105.78734648,7,66.37876991,0\H,21,1.09537088
,17,110.49454911,16,-173.05222492,0\H,21,1.09438231,17,110.42662491,16
,68.56116965,0\H,22,1.0931272,15,108.58185538,14,63.73292699,0\H,31,1.
08532223,26,120.7081713,22,-0.64639076,0\H,32,1.08409113,27,121.851537
44,26,-1.38732714,0\H,30,1.0887619,29,116.79331559,28,179.62089371,0\H
,35,1.085058,34,121.16818664,33,179.54825946,0\H,34,1.08352579,33,120.
60663214,32,179.98196707,0\H,23,0.97160878,22,107.86168243,15,-173.213

55781,0\H,19,1.083875,14,107.11157271,7,-54.5429276,0\H,24,1.09072636,
18,112.67671616,17,-60.92310034,0\H,25,1.08566758,24,120.60360975,18,1
79.81713276,0\H,25,1.08734227,24,124.08064447,18,0.2211839,0\H,7,1.090
44002,4,106.40105797,3,17.67713934,0\H,9,1.08759637,8,119.67444054,7,2
.29951066,0\H,13,1.0843222,12,118.71382711,11,177.38729141,0\H,10,1.08
589262,9,119.71786507,8,179.67378182,0\H,12,1.08595288,11,120.11388891
,10,178.84555489,0\H,11,1.08584638,10,120.22479203,9,179.86121161,0\H,
3,1.08778161,2,118.97204406,1,179.48403159,0\H,5,1.08299716,4,121.7288
2093,3,176.902735,0\H,2,1.08582946,1,120.38162693,6,179.27122357,0\H,6
,1.08572326,1,120.14507638,2,-179.34023374,0\H,1,1.08541672,6,120.3048
0048,5,179.80995014,0\H,37,1.09668498,36,111.53896692,33,-62.01116586,
0\H,37,1.09648903,36,111.49818089,33,60.83168841,0\H,37,1.09091873,36,
105.66298638,33,179.43365418,0\\Version=AM64L-G03RevD.01\State=1-A\HF=
-1528.4462041\RMSD=3.873e-09\Thermal=0.\Dipole=1.581569,1.8978384,0.33
39655\PG=C01 [X(C33H35N2O2)]\\@

methyl adduct (CH_3-**1a**, N_{sp2}):

1\1\GINC-NODE10\SP\RHF\6-31G(d)\C21H27N2O2(1+)\MAY03\21-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1
,1\C\C,1,1.53857676\C,2,1.54510692,1,107.52006192\C,3,1.55535532,2,107
.29194946,1,70.18243832,0\N,4,1.47472826,3,111.07623861,2,-18.06976421
,0\C,5,1.48167825,4,111.18547258,3,-46.41008065,0\C,5,1.47953399,4,107
.29770389,3,71.61588077,0\C,2,1.55718578,1,107.62700373,6,66.71118796,
0\C,4,1.55706916,3,113.57914803,2,-145.19780551,0\O,9,1.4209854,4,106.
05608118,3,-43.5176302,0\C,8,1.506138,2,113.72446994,1,179.33627084,0\
C,11,1.33376191,8,124.73842609,2,-115.47820424,0\C,9,1.52731516,4,110.
71163068,3,-162.93393832,0\C,13,1.42982391,9,124.68734312,4,-90.921232
82,0\C,14,1.43620448,13,118.71347906,9,178.62356074,0\N,15,1.38521682,
14,119.56207377,13,-0.68943082,0\C,16,1.34231176,15,120.78264525,14,0.
9827534,0\C,17,1.38624203,16,121.6380724,15,-0.19582162,0\C,14,1.41845
642,13,122.89184448,9,-2.69435781,0\C,19,1.38492362,14,120.93565587,13
,-178.53504944,0\C,20,1.42104813,19,119.68122809,14,-0.58125007,0\C,21
,1.37147121,20,121.0754625,19,0.40263901,0\C,16,1.47737457,15,120.2740
1784,14,-179.37757512,0\O,20,1.34354854,19,125.8420168,14,179.36138532
,0\C,24,1.42965307,20,119.29784514,19,-1.13616712,0\H,3,1.09324243,2,1
12.13864743,1,-168.50421551,0\H,3,1.09632316,2,109.50281138,1,-50.7687
3486,0\H,4,1.09667986,3,108.25729561,2,97.8110555,0\H,8,1.09714754,2,1
07.18588523,1,60.6153237,0\H,7,1.09498946,5,107.7954619,4,-177.1032379
1,0\H,2,1.09438919,1,110.68970655,6,-173.66010919,0\H,6,1.09581388,5,1
07.293002,4,-173.53424025,0\H,6,1.09665446,5,108.6870055,4,-58.4500050
6,0\H,1,1.09613613,2,110.35311939,3,-174.54443409,0\H,1,1.09618668,2,1
10.45713305,3,67.3623768,0\H,9,1.09675496,4,109.48889038,3,75.19503803
,0\H,18,1.08303816,17,119.3300242,16,178.70748586,0\H,19,1.07821234,14
,118.85207116,13,2.77427537,0\H,17,1.08312855,16,116.44537325,15,179.7
1970773,0\H,22,1.08216101,21,118.9608003,20,179.90894363,0\H,21,1.0850
1309,20,118.04563879,19,-179.75600769,0\H,10,0.97022385,9,109.12417627
,4,163.80587283,0\H,7,1.0956909,5,108.26680706,4,67.42269973,0\H,11,1.
0919257,8,116.66943277,2,64.89863572,0\H,12,1.08638248,11,121.84210123
,8,179.9970782,0\H,12,1.08818403,11,121.71975517,8,0.12227561,0\H,25,1
.08960024,24,105.53138323,20,-179.09587432,0\H,25,1.09632017,24,110.87

807469,20,-60.45828144,0\H,25,1.09569989,24,110.94868217,20,62.1233911
8,0\H,23,1.08896478,16,108.66247781,15,179.45725944,0\H,23,1.09215953,
16,109.91802537,15,-61.07962438,0\H,23,1.09199289,16,109.85125434,15,6
0.03851286,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1069.3808994\RMSD
=3.782e-09\Thermal=0.\Dipole=3.6852571,2.3123462,0.3559025\PG=C01 [X(C
21H27N2O2)]\\@

methyl adduct (CH_3-**1a**, N_{sp3}):

1\1\GINC-NODE9\SP\RHF\6-31G(d)\C21H27N2O2(1+)\MAY03\19-Dec-2008\0\\#P
HF/6-31G(d) scf=tight int=finegrid SCRF=(PCM,Read,Solvent=CH2Cl2)\\\1,
1\C\C,1,1.53791054\C,2,1.53831112,1,108.06221723\C,3,1.54332045,2,110.
12120772,1,70.70792697,0\N,4,1.5562907,3,107.69632879,2,-18.27469925,0
\C,5,1.53119829,4,111.33362182,3,-46.76658598,0\C,5,1.52632007,4,106.5
8293285,3,71.07475448,0\C,2,1.55153938,1,108.29556848,6,67.92145316,0\
C,4,1.54543522,3,114.78356664,2,-146.95384838,0\O,9,1.42191413,4,107.7
5585777,3,65.50224368,0\C,8,1.50962657,2,114.0982293,1,-179.91734688,0
\C,11,1.33296423,8,123.85950359,2,-114.58641957,0\C,5,1.49790218,4,112
.31038405,3,-169.51219909,0\C,9,1.52431279,4,109.79211534,3,-58.398428
46,0\C,14,1.43344784,9,120.96002524,4,-78.17860989,0\C,15,1.43649924,1
4,116.66986287,9,179.31195462,0\N,16,1.36243688,15,123.41455011,14,0.6
0142974,0\C,17,1.31480445,16,117.90198538,15,0.21766561,0\C,14,1.37853
251,9,120.51614862,4,102.0269779,0\C,15,1.41417798,14,124.67177498,9,-
0.89724942,0\C,20,1.38811084,15,121.17806673,14,179.83268068,0\C,21,1.
4202473,20,120.03542438,15,-0.05607707,0\C,22,1.37554775,21,119.774021
46,20,0.38781984,0\O,21,1.35602947,20,115.93792838,15,179.94755854,0\C
,24,1.42799455,21,119.16412876,20,-177.98399404,0\H,3,1.09245064,2,111
.55051834,1,-168.51607339,0\H,3,1.09380642,2,109.49174419,1,-50.159258
17,0\H,4,1.09326745,3,110.12167272,2,93.47304348,0\H,8,1.09576972,2,10
7.46017793,1,60.7637334,0\H,7,1.09292229,5,105.98922157,4,-176.6699604
1,0\H,2,1.09312512,1,110.27576037,6,-172.62327755,0\H,6,1.0926485,5,10
5.83047787,4,-173.22518082,0\H,6,1.08777874,5,105.76240612,4,-57.40036
939,0\H,1,1.094859,2,110.45573222,3,-174.01539303,0\H,1,1.09401234,2,1
10.37493308,3,67.63257448,0\H,9,1.09832867,4,108.59678207,3,-175.96706
542,0\H,19,1.08540019,14,120.76913452,9,0.06429864,0\H,20,1.08512267,1
5,121.97591057,14,-1.81013492,0\H,18,1.08851562,17,116.79525709,16,179
.59389809,0\H,23,1.08505777,22,121.12338985,21,179.55676668,0\H,22,1.0
83482,21,120.49575893,20,179.93792954,0\H,10,0.97183068,9,108.29387316
,4,-173.46813504,0\H,7,1.09277662,5,106.70679997,4,68.17001594,0\H,11,
1.09097831,8,117.11126247,2,65.11197506,0\H,12,1.08583127,11,121.60788
533,8,179.22942834,0\H,12,1.08807618,11,121.9353532,8,-0.57978862,0\H,
25,1.09635161,24,111.38688626,21,-62.52708546,0\H,25,1.0960742,24,111.
32967009,21,60.32002061,0\H,25,1.09046823,24,105.55448601,21,178.88746
676,0\H,13,1.09136534,5,108.44939319,4,-171.31062279,0\H,13,1.09168239
,5,109.4575308,4,-51.95956136,0\H,13,1.08954119,5,109.03604351,4,69.19
38472,0\\Version=AM64L-G03RevD.01\State=1-A\HF=-1069.3882001\RMSD=3.17
2e-09\Thermal=0.\Dipole=-2.3374156,1.2260606,-3.1065784\PG=C01 [X(C21H
27N2O2)]\\@

quinine (**1a**)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
51	-1036.416920	-1036.476349	0.432894	-1033.656662	-1033.223768	3.77	3.707	-3.68	-11.647
9	-1036.418363	-1036.476642	0.433203	-1033.655041	-1033.221838	8.85	1.317	-4.66	-10.680
43	-1036.420258	-1036.479073	0.433327	-1033.658530	-1033.225203	0.00	2.752	-3.53	-14.791
35	-1036.415568	-1036.472949							
21	-1036.414983	-1036.473839							
41	-1036.416611	-1036.474552	0.432806	-1033.655987	-1033.223181	5.32	3.816	-3.89	-10.982
66	-1036.415354								
65	-1036.415070								
19	-1036.412662								
53	-1036.418357	-1036.477154	0.433264	-1033.656642	-1033.223378	4.80	2.863	-3.13	-8.318
2	-1036.416543								
10	-1036.416415								
54	-1036.418192	-1036.476618	0.433285	-1033.656051	-1033.222766	6.41	3.025	-3.58	-8.594
7	-1036.413106								
22	-1036.413859								
153	-1036.413863								
29	-1036.415704								
50	-1036.414964								
37	-1036.413615								
60	-1036.416934	-1036.47683	0.43344	-1033.658229	-1033.224789	1.09	4.634	-3.64	-14.165

quinine (**1a**) (benzyl adduct, N_{sp2})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
71	-1307.170784	-1307.238020	0.562618	-1303.636377	-1303.073759	0.00	6.513	-29.46	-123.437
189	-1307.172260	-1307.238740	0.562719	-1303.635714	-1303.072995	2.01	7.162	-29.78	-122.770
117	-1307.170840	-1307.237861	0.562495	-1303.635777	-1303.073282	1.25	5.552	-30.18	-125.201
22	-1307.170584								
123	-1307.172552	-1307.238785	0.562845	-1303.635678	-1303.072833	2.43	6.444	-30.31	-124.564
1	-1307.170921	-1307.235995	0.562734	-1303.631249	-1303.068515	13.79	8.259	-31.3	-117.359
2	-1307.168913								
17	-1307.170463								
72	-1307.171249	-1307.236261	0.562347	-1303.635953	-1303.073606	0.40	6.144	-29.67	-123.915
12	-1307.168885								
127	-1307.167006								
4	-1307.170722								
80	-1307.166626								
130	-1307.167695								
49	-1307.171548	-1307.23629	0.562305	-1303.635627	-1303.073322	1.15	5.210	-30.29	-125.766
251	-1307.147482								
114	-1307.168544								
7	-1307.166114								
1786	-1307.146235								
6	-1307.166912								

quinine (**1a**) (benzyl adduct, N_{sp3})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
30	-1307.157340	-1307.237017	0.563485	-1303.644680	1303.081195	0.00	6.049	-28.91	-121.133
83	-1307.156635	-1307.236186	0.563546	-1303.644500	1303.080954	0.64	6.154	-28.75	-119.827
410	-1307.155712	-1307.235065	0.563478	-1303.643035	1303.079557	4.31	6.183	-29.48	-119.214
403	-1307.154801	-1307.235065	0.563480	-1303.643036	1303.079556	4.31	6.183		
62	-1307.151971	-1307.232463	0.563714	-1303.642412	1303.078698	6.57	6.757	-29.14	-115.531
1	-1307.154753	-1307.235100	0.563448	-1303.643623	1303.080175	2.68	8.250	-29.29	-120.042
48	-1307.153921	-1307.234194	0.563414	-1303.643298	1303.079884	3.45	8.358	-29.38	-119.654
43	-1307.151078								
429	-1307.149421								
25	-1307.143920								
38	-1307.144548								
112	-1307.149958								
60	-1307.150114								
409	-1307.153131	-1307.233174	0.563445	-1303.641989	1303.078544	6.97	8.357	-29.91	-118.352
78	-1307.143078								
431	-1307.142533								
18	-1307.143940								
37	-1307.143417								
22	-1307.142626								
113	-1307.142631								

quinine (**1a**) (benzhydryl adduct, N_{sp2})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
55	-1538.201378	-1538.288014	0.64807	-1534.044981	1533.396911	0.00	4.512	-23.34	-97.795
65	-1538.202616	-1538.288829	0.648429	-1534.044313	1533.395884	2.70	4.988	-23.79	-96.980
74	-1538.201508	-1538.287847	0.648007	-1534.044259	1533.396252	1.73	3.872	-23.79	-97.947
6	-1538.201086								
64	-1538.203332	-1538.288888	0.648394	-1534.044257	1533.395863	2.76	4.429	-24.06	-98.056
1	-1538.201605	-1538.286083	0.648187	-1534.039759	1533.391572	14.04	6.440	-24.98	-90.627
2	-1538.199487								
15	-1538.200671								
10	-1538.199609								
88	-1538.201446	-1538.286146	0.647789	-1534.04401	1533.396221	1.82	4.229	-23.65	-97.277
4	-1538.201263								
67	-1538.202001	-1538.286243	0.64786	-1534.04424	-1533.39638	1.40	3.572	-23.94	-98.911
102	-1538.200453								
75	-1538.194514								
71	-1538.194345								
7	-1538.194469								
92	-1538.196153								
89	-1538.195932								
20	-1538.194303								
86	-1538.200585								

quinine (**1a**) (benzhydryl adduct, N_{sp3})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
2	-1538.171084	-1538.273364	0.649477	-1534.046466	1533.396989	1.48	5.214	-22.73	-93.761
41	-1538.169975	-1538.272110	0.649211	-1534.046762	1533.397551	0.00	5.296	-22.72	-95.197
668	-1538.169455	-1538.271008	0.649227	-1534.044487	1533.395260	6.02	5.330	-23.21	-91.226
547	-1538.169966	-1538.271413	0.649645	-1534.043884	1533.394239	8.71	5.112	-23.67	-90.470
81	-1538.169495	-1538.272200	0.649606	-1534.044614	1533.395008	6.69	5.079	-22.64	-88.176
27	-1538.166689								
12	-1538.168166	-1538.269343	0.64907	-1534.041442	1533.392372	13.62	5.591	-22.04	-78.731
9	-1538.167142								
331	-1538.164964								
659	-1538.165733								
133	-1538.166358								
13	-1538.168361	-1538.271647	0.649583	-1534.040101	1533.390518	18.49	5.382	-24.09	-82.445
22	-1538.156262								
64	-1538.165961								
1	-1538.165165								
435	-1538.163699								
96	-1538.165354								
981	-1538.164379								
128	-1538.167782								
35	-1538.157322								

quinine (**1a**) (methyl adduct, N_{sp2})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
1	-1076.137306	-1076.185863	0.476597	-1073.233162	1072.756565	0.00	9.690		
5	-1076.137741	-1076.185863	0.476596	-1073.233161	1072.756565	0.00	9.690	-32.66	-136.845
19	-1076.138559	-1076.186592	0.477051	-1073.232838	1072.755787	2.04	10.696		
15	-1076.139139	-1076.186592	0.477051	-1073.232838	1072.755787	2.04	10.694	-32.68	-134.886
44	-1076.136927								
38	-1076.137325	-1076.183768	0.476896	-1073.228343	1072.751447	13.46	12.535	-33.75	-127.957
30	-1076.135412								
37	-1076.135731								
42	-1076.137110								
8	-1076.137957	-1076.184303	0.476502	-1073.232822	1072.756320	0.64	9.444		
57	-1076.137689	-1076.183157	0.476415	-1073.230314	1072.753899	7.01	11.190	-33.15	-131.889
18	-1076.138506	-1076.184303	0.476502	-1073.232825	1072.756323	0.64	9.443	-32.82	-136.880
51	-1076.136515								
59	-1076.137022								
75	-1076.137509	-1076.185542	0.477152	-1073.231838	1072.754686	4.94	10.179		
33	-1076.136007								
63	-1076.138176	-1076.185542	0.477152	-1073.231836	1072.754684	4.95	10.180	-31.88	-128.632
46	-1076.136383								
60	-1076.137290	-1076.184800	0.477064	-1073.230916	1072.753852	7.13	10.497	-32.51	-129.084
27	-1076.131896								

quinine (**1a**) (methyl adduct, N_{sp3})

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)	Dipole moment (debye)	delta G_{solv} (kcal/mol)	delta + delta G_{solv} (kJ/mol)
16	-1076.125253	-1076.185640	0.477506	-1073.242470	-1072.764964	0.00	8.744	-33.58	-140.700
6	-1076.122430	-1076.183547	0.477439	-1073.240881	-1072.763442	4.00	10.829	-33.96	-138.290
17	-1076.112812	-1076.175081	0.477066	-1073.232406	-1072.755340	25.30	6.828		
13	-1076.113233	-1076.175678	0.476966	-1073.233942	-1072.756976	21.00	6.165		
9	-1076.112301	-1076.175334	0.477358	-1073.233008	-1072.755650	24.49	6.890		
10	-1076.119378	-1076.181190	0.477719	-1073.236461	-1072.758742	16.36	9.360	-34.85	-129.664
11	-1076.112788								
19	-1076.111473								
2	-1076.110648								
7	-1076.111133								
1	-1076.110244								
5	-1076.111743								
4	-1076.117592	-1076.180145	0.477533	-1073.2366	-1072.759067	15.50	11.668	-35.87	-134.792
8	-1076.118441	-1076.174521	0.477288	-1073.232967	-1072.755679	24.41	8.899	-35.16	-122.909
18	-1076.117717	-1076.179631	0.477367	-1073.23338	-1072.756013	23.53	8.966	-35.13	-123.660
20	-1076.108857								
12	-1076.116254	-1076.178741	0.477214	-1073.233162	-1072.755948	23.70	11.213	-35.99	-127.093
3	-1076.106386								
15	-1076.099931								
14	-1076.099057								

(naphthylmethyl)quinuclidine (**1f**)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
4	-753.2651427	-753.3165755	0.368887	-751.1535243	-750.7846373	0.00
6	-753.2642904	-753.3154701	0.368842	-751.1527055	-750.7838635	2.03
3	-753.2633652	-753.3144444	0.368701	-751.1512879	-750.7825869	5.39

(naphthylmethyl)quinuclidine (**1f**) (benzhydryl adduct)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
5	-1255.017648	-1255.112466	0.585263	-1251.5419699	-1250.9567069	2.83
8	-1255.011623	-1255.109377	0.585095	-1251.5426503	-1250.9575553	0.60
9	-1255.018632	-1255.113615	0.585369	-1251.5431541	-1250.9577851	0.00

(naphthylmethyl)quinuclidine (**1f**) (benzyl adduct)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
8	-1023.996961	-1024.072854	0.49929	-1021.141637	-1020.6423467	0.00
4	-1023.996823	-1024.072892	0.499323	-1021.1404771	-1020.6411541	3.14
2	-1024.002144	-1024.075018	0.499381	-1021.1407586	-1020.6413776	2.55

(hydroxymethyl)quinuclidine (**1k**)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
6	-443.8296309	-443.8355403	0.239482	-442.6063017	-442.3668197	0.00
1	-443.8229025	-443.8281132	0.23892	-442.5997007	-442.3607807	15.88
3	-443.8204851	-443.8257981	0.238772	-442.5972547	-442.3584827	21.92

(hydroxymethyl)quinuclidine (**1k**) (benzhydryl adduct)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
10	-945.5759989	-945.6290945	0.455626	-942.9853885	-942.5297625	1.25
5	-945.5787217	-945.6285398	0.455506	-942.9857450	-942.5302390	0.00
6	-945.5771193	-945.6283938	0.455453	-942.9838872	-942.5284342	4.75

(hydroxymethyl)quinuclidine (**1k**) (benzyl adduct)

Force-Field-Number	B3LYP/6-31G(d) sp (hartree)	B3LYP/6-31G(d) opt (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	MP2(FC)/6-31+G(2d,p) sp (hartree)	H_{298} (hartree)	delta to best (kJ/mol)
3	-714.5597291	-714.5876988	0.369333	-712.5855074	-712.2161744	6.19
6	-714.5621748	-714.5906121	0.369853	-712.5883835	-712.2185305	0.00
2	-714.5597783	-714.5880062	0.369735	-712.5860423	-712.2163073	5.85

Base	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to free Enthalpy B3LYP/6-31G(d) (hartree)	Cation	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to free Enthalpy B3LYP/6-31G(d) (hartree)	Adduct	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to free Enthalpy B3LYP/6-31G(d) (hartree)	Delta G (kJ/mol)
quinuclidine (**1e**)	-328.3435491	0.16569	benzyl	-269.8592704	0.088482	quinbenzyl	-598.3280801	0.282532	-254.8
	-328.3435491	0.16569	benz	-500.2934716	0.163807	quinbenz	-828.7281023	0.356855	-167.5
hydroxymethylquinuclidine (**1k**)	-442.6063017	0.196412	benzyl	-269.8592704	0.088482	quinohbenzyl	-712.5883835	0.312921	-249.2
	-442.6063017	0.196412	benz	-500.2934716	0.163807	quinohbenz5	-942.985745	0.387371	-154.7
methoxyquinoline (**1h**)	-515.0510466	0.134309	benzyl	-269.8592704	0.088482	meochinbenzyl	-785.0225453	0.248393	-227.8
	-515.0510466	0.134309	benz	-500.2934716	0.163807	meochinbenz	-1015.431864	0.323032	-164.1
lepidine (**1g**)	-440.004028	0.131093	benzyl	-269.8592704	0.088482	chinbenzyl	-709.9745664	0.245215	-225.1
	-440.004028	0.131093	benz	-500.2934716	0.163807	chinbenz	-940.3835649	0.320036	-160.2
Naphthylmethylquinuclidine (**1f**)	-751.1535243	0.310536	benzyl	-269.8592704	0.088482	QNPbenzyl	-1021.141637	0.426734	-265.9
	-751.1535243	0.310536	benz	-500.2934716	0.163807	QNPbenz	-1251.543154	0.503717	-175.6
methoxylepidine (**1j**)	-554.2496712	0.160415	benzyl	-269.8592704	0.088482	MeOLbenzyl	-824.2244984	0.274682	-236.0
	-554.2496712	0.160415	benz	-500.2934716	0.163807	MeOLbenz	-1054.633668	0.349189	-172.4
hydroxymethylquinoline (**1i**)	-515.0604377	0.134282	benzyl	-269.8592704	0.088482	LepOHbenzyl	-785.0299946	0.248524	-222.2
	-515.0604377	0.134282	benz	-500.2934716	0.163807	LepOHbenz	-1015.438933	0.322869	-158.4
quinine (**1a**)	-1033.658530	0.361712	benzyl	-269.8592704	0.088482	QNNbenzyl	-1303.644680	0.478024	-260.4
	-1033.658530	0.361712	benz	-500.2934716	0.163807	QNNbenz	-1534.046762	0.553760	-174.9
	-1033.658530	0.361712	benzyl	-269.8592704	0.088482	QNLbenzyl	-1303.636377	0.475580	-245.0
	-1033.658530	0.361712	benz	-500.2934716	0.163807	QNLbenz	-1534.044981	0.549733	-180.8
	-1033.658530	0.361712	Me	-39.3523833	0.014216	QNNMe	-1073.242470	0.403624	-536.0
	-1033.658530	0.361712	Me	-39.3523833	0.014216	QNLMe	-1073.233162	0.400982	-518.5

Base	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	Cation	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	Adduct	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to Enthalpy B3LYP/6-31G(d) (hartree)	Delta H (kJ/mol)
quinuclidine (**1e**)	-328.3435491	0.203617	benzyl	-269.8592704	0.124198	quinbenzyl	-598.3280801	0.333253	-315.0
	-328.3435491	0.203617	benz	-500.2934716	0.211046	quinbenz	-828.7281023	0.419896	-225.7
hydroxymethylquinuclidine (**1k**)	-442.6063017	0.239482	benzyl	-269.8592704	0.124198	quinohbenzyl	-712.5883835	0.369853	-306.7
	-442.6063017	0.239482	benz	-500.2934716	0.211046	quinohbenz	-942.985745	0.455506	-213.0
methoxyquinoline (**1h**)	-515.0510466	0.178973	benzyl	-269.8592704	0.124198	meochinbenzyl	-785.0225453	0.308705	-280.5
	-515.0510466	0.178973	benz	-500.2934716	0.211046	meochinbenz	-1015.431864	0.394112	-218.9
lepidine (**1g**)	-440.004028	0.173267	benzyl	-269.8592704	0.124198	chinbenzyl	-709.9745664	0.302897	-278.3
	-440.004028	0.173267	benz	-500.2934716	0.211046	chinbenz	-940.3835649	0.388434	-215.5
Naphthylmethylquinuclidine (**1f**)	-751.1535243	0.368887	benzyl	-269.8592704	0.124198	QNPbenzyl	-1021.141637	0.499290	-322.4
	-751.1535243	0.368887	benz	-500.2934716	0.211046	QNPbenz	-1251.543154	0.585369	-238.5
methoxylepidine (**1j**)	-554.2496712	0.208592	benzyl	-269.8592704	0.124198	MeOLbenzyl	-824.2244984	0.338287	-289.4
	-554.2496712	0.208592	benz	-500.2934716	0.211046	MeOLbenz	-1054.633668	0.423731	-227.2
hydroxymethylquinoline (**1i**)	-515.0604377	0.17925	benzyl	-269.8592704	0.124198	LepOHbenzyl	-785.0299946	0.308885	-275.7
	-515.0604377	0.17925	benz	-500.2934716	0.211046	LepOHbenz	-1015.438933	0.394268	-213.1
quinine (**1a**)	-1033.658530	0.433327	benzyl	-269.8592704	0.124198	QNNbenzyl	-1303.644680	0.563485	-317.9
	-1033.658530	0.433327	benz	-500.2934716	0.211046	QNNbenz	-1534.046762	0.649211	-236.4
	-1033.658530	0.433327	benzyl	-269.8592704	0.124198	QNLbenzyl	-1303.636377	0.562618	-298.4
	-1033.658530	0.433327	benz	-500.2934716	0.211046	QNLbenz	-1534.044981	0.648070	-234.7
	-1033.658530	0.433327	Me	-39.3523833	0.035413	QNNMe	-1073.242470	0.477506	-585.8
	-1033.658530	0.433327	Me	-39.3523833	0.035413	QNLMe	-1073.233162	0.476596	-563.7

	Force-Field-Number	MP2(FC)/6-31+G(2d,p) sp (hartree)	Thermal correction to free Enthalpy B3LYP/6-31G(d) (hartree)	delta G_{solv} HF/6-31G(d) (kcal/mol)	Σ (hartree)	Delta G (hartree)	Delta G (kJ/mol)
Methyl		-39.3523833	0.014216	-60.08	-39.43391232		
Benzyl		-269.8592704	0.088482	-38.25	-269.8317446		
Benzhydryl		-500.2934716	0.163807	-33.3	-500.1827323		
Quinine (**1a**)	43	-1033.658530	0.361712	-3.53	-1033.302443		
methyl adduct N_{sp3}	16	-1073.242470	0.403624	-33.58	-1072.89236	-0.156004226	-410.2
methyl adduct N_{sp2}	18	-1073.232825	0.401602	-32.82	-1072.883525	-0.147169871	-386.9
benzyl adduct N_{sp3}	30	-1303.644680	0.478024	-28.91	-1303.212728	-0.07854014	-206.5
benzyl adduct N_{sp2}	49	-1303.635627	0.475494	-30.29	-1303.208404	-0.074216143	-195.1
benzhydryl adduct N_{sp3}	41	-1534.046762	0.55376	-22.72	-1533.529209	-0.044033244	-115.8
benzhydryl adduct N_{sp2}	67	-1534.04424	0.549657	-23.94	-1533.532734	-0.047558467	-125.0

References

[S1] Mayr, H.; Bug, T.; Gotta, M. F.; Hering, N., Irrgang, B.; Janker, B.; Kempf, B.; Loos, R.; Ofial, A. R.; Remennikov, G.; Schimmel, H. *J. Am. Chem. Soc.* **2001**, *123*, 9500-9512.

[S2] a) Denegri, B.; Streiter, A.; Juric, S.; Ofial, A. R.; Kronja, O.; Mayr, H. *Chem. Eur. J.* **2006**, *12*, 1648-1656. b) Baidya, M.; Kobayashi, S.; Brotzel, F.; Schmidhammer, U.; Riedle, E.; Mayr, H. *Angew. Chem., Int. Ed.* **2006**, *46*, 6176-6179.

[S3] For the synthesis of **1f**: Kolb, H. C.; Andersson, P. G.; Sharpless, K. B. *J. Am. Chem. Soc.* **1994**, *116*, 1278-1291. and for the synthesis of **1c**: Pettit, G. R.; Gupta, S. K. *J. Chem. Soc. (C)* **1968,** *10*, 1208-13.

[S4] Maruoka, K.; Ooi, T. *Chem. Rev.* **2003**, *103*, 3013-3028. (b) Maruoka, K.; Ooi, T. *Angew. Chem., Int. Ed.* **2007**, *46*, 4222-4266. (c) Maruoka, K. *Asymmetric Phase Transfer Catalysis;* Wiley-WCH: Weinheim, **2008**. (d) Santoro, S.; Poulsen, T. B.; Jørgensen, K. A. *Chem. Commun.* **2007**, 5155-5157. (e) Dalko, P. I. *Enantioselective Organocatalysis;* Wiley-WCH: Weinheim, **2007**. (f) Berkessel, A.; Gröger, H. *Asymmetric Organocatalysis;* Wiley-WCH: Weinheim, **2005**. (g) Elsner, P.; Bernardi, L.; Salla, G. D.; Overgaard, J.; Jørgensen, K. A. *J. Am. Chem. Soc.* **2008**, *130*, 4897-4905.

[S5] For synthesis of other ammonium salts: (a) Tozawa, T.; Nagao, H.; Yamane, Y.; Mukaiyama. T. *Chem. Asian. J.* **2007**, *2*, 123-134. (b) Matsushita, M.; Yoshida, K.; Yamamoto, N.; Wirsching, P.; Lerner, R. A.; Janda, K. D. *Angew. Chem., Int. Ed.* **2003**, *42*, 5984-5987. (c) Masui, M.; Ando, A.; Shioiri, T. *Tetrahedron Lett.* **1988**, *29*, 2835-2836. (d) Hahn, U.; Kaufmann, A.; Nieger, M.; Julinek, O.; Urbanova, M.; Vögtle, F. *Eur. J. Org. Chem.* **2006**, 1237-1244. (e) Perrin, C. L.; Zhao, C. *Org. Biomol. Chem.* **2008**, *6*, 3349-3353. (f) Robiette, R.; Conza, M.; Aggarwal, V. K. *Org. Biomol. Chem.* **2006**, *4*, 621-623. (g) Lall, S.; Behaj, V.; Mancheno, D.; Casiano, R.; Thomas, M.; Rikin, A.; Gaillard, J.; Raju, R.; Scumpia, A.; Castro, S.; Engel, R.; Cohen, J. I. *Synthesis* **2002**, 1530-1540.

[S6] Ponder, J. W. *TINKER*, 4.2 ed.; **2004**.

[S7] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma,

K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision D. 01, Gaussian, Inc., Wallingford, CT, **2004**.