Supplementary Material (ESI) for Chemical Communications

Supplementary information

Demonstration of the existence of the intermolecular lone pair•••π interaction between alcoholic oxygen and C_6F_5 group in organic solvent

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General Experimental Methods.

All reactions were carried out under an argon atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. Dehydrated tetrahydrofuran (THF), diethyl ether, and toluene were purchased from Kanto Chemical Co. and then were stored in Schlenk tubes under an argon atmosphere. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. ^{1}H NMR and ^{13}C NMR spectra were measured at 200, 300 or 500 MHz (for ^{1}H NMR) and 75 or 126 MHz (for ^{13}C NMR), respectively, and chemical shifts are given relative to tetramethylsilane (TMS). ^{19}F NMR spectra were measured at 282 MHz, and chemical shifts are given relative to CCl_3F using C_6F_6 as secondary reference (–162.9 ppm). ^{31}P NMR spectra were measured at 121 MHz, and chemical shifts are given relative to 85% H_3PO_4 externally.

Preparation of amines 1.

***N*,*N*-Dimethyl-2,3,4,5,6-pentafluorobenzeneethanamine (1a)**.

To a mixture of formic acid (0.63 mL, 16.6mmol) and 2,3,4,5,6-pentafluorobenzeneethanamine[1] (0.70 g, 3.32 mmol) was added a 37% aqueous formaldehyde solution (0.69 mL, 6.64 mmol) at 0°C. After being stirred at 0°C for 5 h, the solution was heated at 100°C for 5h. The reaction mixture was poured into 25% NaOH aqueous solution, and then was extracted with diethyl ether. The extract was dried over $MgSO_4$ and was concentrated under reduced pressure to give yellow oil, which was purified by distillation using Kugelrohr apparatus to give **1a** (0.25 g, 32%) as colorless oil.

^{1}H NMR (200 MHz, $CDCl_3$): δ 2.27 (s, 6H), 2.50 (t, *J* = 7.4 Hz, 2H), 2.86 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): 21.0, 45.3, 58.4, 113.6 (m), 137.6 (m), 139.8 (m), 145.4 (m). ^{19}F NMR (282 MHz, $CDCl_3$): -164.1 (dt, *J* = 7.9, 21.4 Hz, 2F), -158.9 (t, *J* = 21.4 Hz, 1F), -145.0 (dd, *J* = 7.9, 21.4 Hz, 2F). IR (neat): 1123, 1151, 1265, 1377, 1502 and 2949 cm^{-1}.

The elemental analysis of **1a** was performed after conversion of **1a** to its hydrochloride salt: Anal. calc. for $C_{10}H_{11}NF_5Cl$: C 43.57, H 4.02, N 5.08%. Found: C 43.25, H 3.85, N, 4.95.

***N*,*N*-Dimethyl-3,4,5-trifluorobenzeneethanamine (1b)**.

Compound **1b** (3.05 g, 63 %) was prepared from 3,4,5-trifluorobenzeneethanamine[2] by the procedure described for **1a**.

Colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 2.26 (s, 6H), 2.49 (t, *J* = 7.8 Hz, 2H), 2.70 (t, *J* = 7.8 Hz, 2H), 6.81 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 33.8, 45.6, 60.8, 112.7 (m), 136.9 (m), 138.4 (dt, *J* = 15.1, 249 Hz), 151.3 (dm, *J* = 249 Hz). ^{19}F NMR (282 MHz, $CDCl_3$): -165.6 (m, 1F), -136.4 (m, 2F). IR (neat): 1142, 1448, 1537, 1620, 2773 and 2945 cm^{-1}.

The elemental analysis of **1b** was performed after conversion of **1b** to its hydrochloride salt: Anal. calc. for $C_{10}H_{13}NF_3Cl$: C 50.11, H 5.47, N 5.84%. Found: C 50.35, H 5.31, N, 5.69.

***N*,*N*-Dimethyl-4-trifluoromethyl-benzeneethanamine (1c).**[3]

Compound **1c** (0.41 g, 36 %) was prepared from 4-trifluoromethyl-benzeneethanamine[4] by the procedure described for **1a**.

Colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.32 (s, 6H), 2.57 (t, *J* = 8.0 Hz, 2H), 2.85 (t, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 33.8, 44.9, 60.6, 124.1 (q, *J* = 272 Hz), 124.9, 128.0 (q, *J* = 32.5 Hz), 128.6, 144.4. ^{19}F NMR (282 MHz, $CDCl_3$): -64.3 (s). IR (neat): 829, 1020, 1167, 1325, 1375, 1618, 2860 and 2947 cm^{-1}.

***N*,*N*-Dimethyl-4-fluorobenzeneethanamine (1d)**.[5]

Compound **1d** (1.13 g, 89 %) was prepared from commercially available 4-fluorobenzeneethanamine by the procedure described for **1a**.

Colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$): δ 2.30 (s, 6H), 2.50 (t, *J* = 8.0 Hz, 2H), 2.75 (t, *J* = 8.0 Hz, 2H), 6.96 (m, 2H), 7.15 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 33.2, 45.0, 61.2, 114.7 (d, *J* = 20.9 Hz), 129.6 (d, *J* = 7.7 Hz), 135.7 (d, *J* = 3.2 Hz), 161.0 (d, *J* = 243 Hz). ^{19}F NMR (282 MHz, $CDCl_3$): -119.1 (m). IR (neat): 1016, 1221, 1265, 1445, 1510, 1601 and 2725 cm^{-1}.

***N*,*N*-Dimethylphenethylamine (1e)**.[6]

Compound **1e** (4.96 g, 42 %) was prepared from commercially available phenethylamine by the procedure described for **1a**.

Colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.30 (s, 6H), 2.53 (t, *J* = 8.0 Hz, 2H), 2.78 (t, *J* = 8.0 Hz, 2H), 7.18-7.21 (m, 3H), 7.27-7.30 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 34.2, 45.2, 61.4, 125.7, 128.1, 128.4, 140.1. IR (neat): 864, 1263, 1373, 1454, 1605, 2856 and 2943 cm^{-1}.

***N*,*N*-Dimethyl-4-methoxy-benzeneethanamine (1f)**.[7]

Compound **1f** (0.78 g, 64 %) was prepared from commercially available 4-methoxy-benzeneethanamine by the procedure described for **1a**.

Colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$): δ 2.29 (s, 6H), 2.49 (t, *J* = 8.0 Hz, 2H), 2.72 (t, *J* = 8.0 Hz, 2H), 3.78 (s, 3H), 6.83 (d, *J* = 9.0 Hz, 2H), 7.12 (d, *J* = 9.0 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 33.0, 44.9, 54.3, 61.3, 113.2, 129.0, 131.8, 157.4. IR (neat): 870, 1248, 1371, 1464, 1614, 2856 and 3030 cm^{-1}.

Estimation of Association Constants by ^{1}H NMR Titrations.

All amines **1** and $CDCl_3$ were stored with activated MS-3A under argon atmosphere after being filtered through basic almina column, respectively. All amines **1** were distilled by Kugelrohr apparatus before NMR titration.

As a typical example, the titration between **1a** and MeOH is described here. Six portion of 0.25 mL of 0.966M MeOH solutions in $CDCl_3$ were added to 0.000, 50.88, 96.78, 143.39, 191.73, or 239.45 mg of **1a**, respectively. All solutions were diluted with $CDCl_3$ until 1.00 mL accurately. Each of the resulting solutions was placed in six NMR tubes, and then the NMR tubes were sealded. ^{1}H NMR spectra were taken for each tube at 27, 37, and 47 °C. Association constants (K_a) were calculated by nonlinear curve-fitting method.

NMR titration between 1a and MeOH.

Concentration of MeOH is 0.2415 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

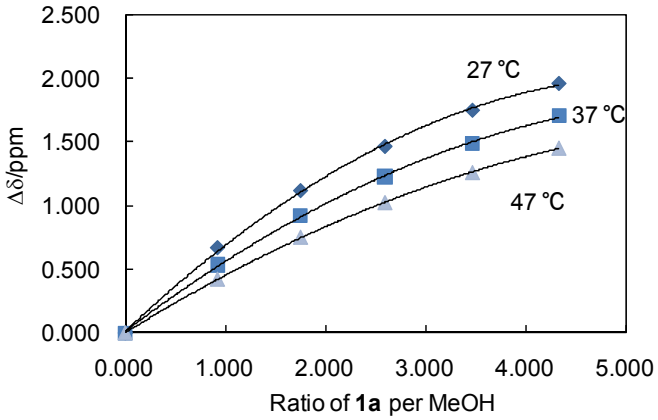
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2a**.

Results of NMR titration.

Ratio of **1a** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm
0.000	1.188	0.000	1.100	0.000	1.028	0.000
0.919	1.859	0.671	1.632	0.532	1.449	0.421
1.748	2.308	1.120	2.019	0.919	1.778	0.750
2.590	2.656	1.468	2.326	1.226	2.050	1.022
3.463	2.940	1.752	2.582	1.482	2.285	1.257
4.325	3.151	1.963	2.801	1.701	2.477	1.449
K_a/M^{-1}	**1.343±0.011**		**0.9477±0.022**		**0.7060±0.041**	
δ_c/ppm	**4.38**		**4.81**		**4.75**	

Graph of NMR titration.



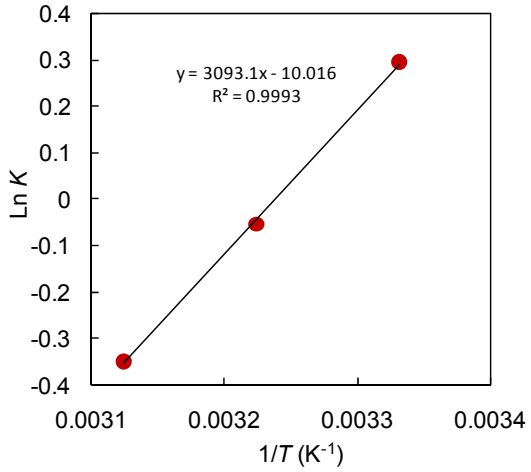
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 2.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –6.15 kcal mol^{-1}

ΔS_{obs} = –19.9 cal mol^{-1} K^{-1}

van't Hoff plot



NMR titration between 1b and MeOH.

Concentration of MeOH is 0.1957 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

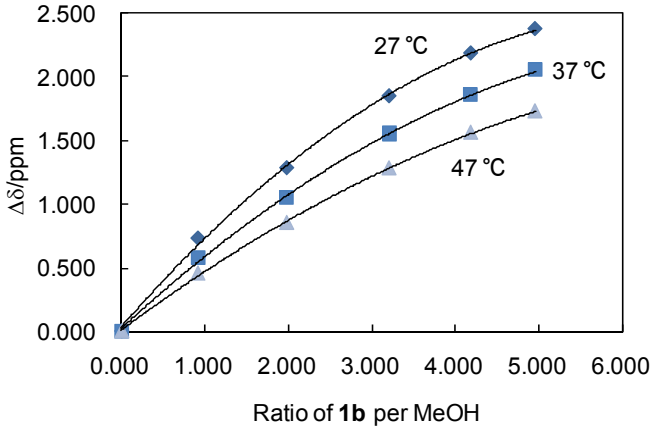
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2b**.

Results of NMR titration.

Ratio of **1b** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm
0.000	1.147	0.000	1.068	0.000	1.001	0.000
0.914	1.878	0.731	1.646	0.578	1.456	0.455
1.979	2.432	1.285	2.121	1.053	1.854	0.853
3.208	2.998	1.851	2.619	1.551	2.284	1.283
4.188	3.335	2.188	2.930	1.862	2.564	1.563
4.959	3.527	2.380	3.121	2.053	2.732	1.731
K_a/M^{-1}	**1.138±0.104**		**0.8227±0.068**		**0.6253±0.057**	
δ_c/ppm	**5.94**		**5.94**		**6.08**	

Graph of NMR titration.



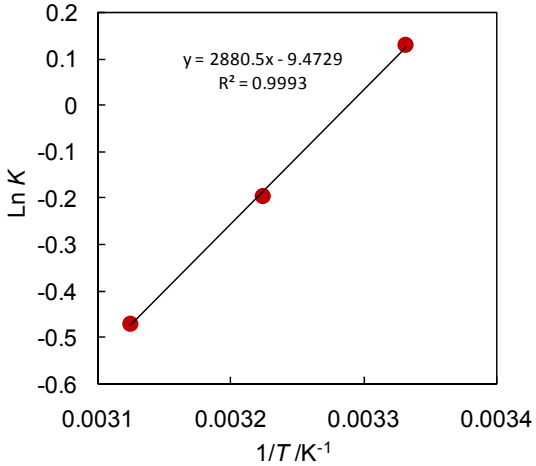
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 1.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –5.72 kcal mol^{-1}

ΔS_{obs} = –18.8 cal mol^{-1} K^{-1}

van't Hoff plot



NMR titration between 1c and MeOH.

Concentration of MeOH is 0.2255 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

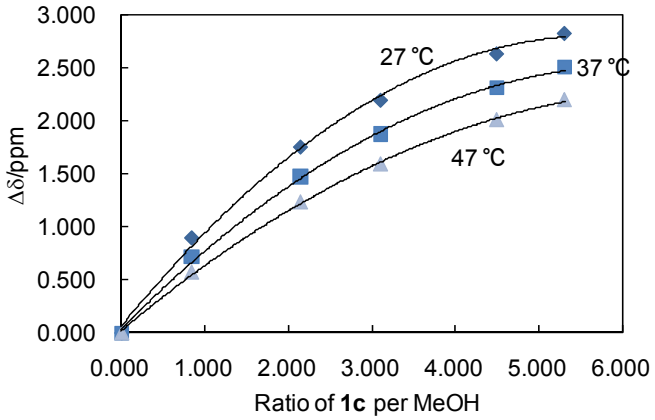
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2c**.

Results of NMR titration.

Ratio of **1c** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm
0.000	1.155	0.000	1.076	0.000	1.007	0.000
0.839	2.053	0.898	1.793	0.717	1.579	0.572
2.145	2.911	1.756	2.550	1.474	2.238	1.231
3.105	3.353	2.198	2.950	1.874	2.595	1.588
4.499	3.791	2.636	3.390	2.314	3.011	2.004
5.312	3.984	2.829	3.577	2.501	3.199	2.192
K_a/M^{-1}	**1.138±0.104**		**0.8227±0.068**		**0.6253±0.057**	
δ_c/ppm	**5.52**		**5.43**		**5.40**	

Graph of NMR titration.



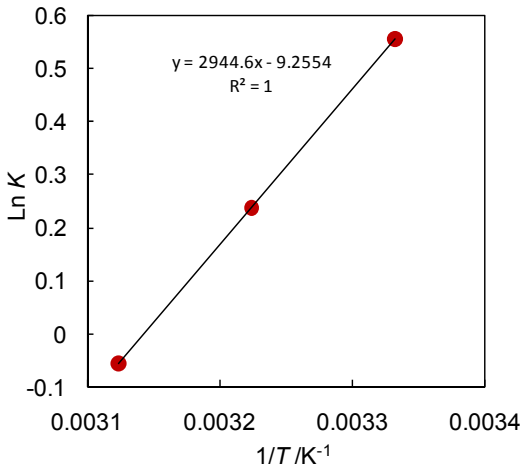
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 1.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –5.85 kcal mol^{-1}

ΔS_{obs} = –18.4 cal mol^{-1} K^{-1}

van't Hoff plot



NMR titration between 1d and MeOH.

Concentration of MeOH is 0.2395 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

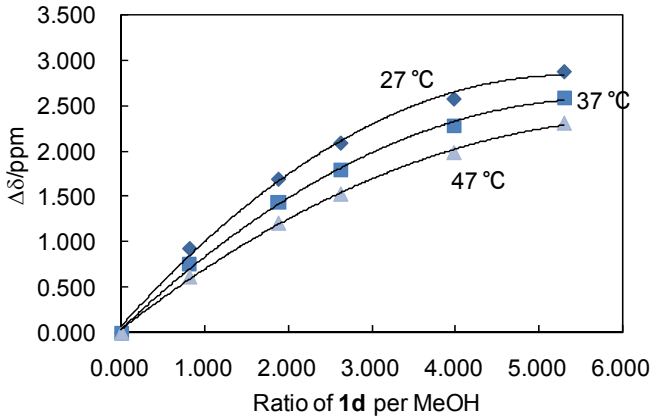
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2d**.

Results of NMR titration.

Ratio of **1d** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm	δ_{obs}/ppm	$\Delta\delta$/ppm
0.000	1.228	0.000	1.133	0.000	1.054	0.000
0.814	2.153	0.925	1.888	0.755	1.668	0.614
1.878	2.915	1.687	2.563	1.430	2.259	1.205
2.624	3.311	2.083	2.922	1.789	2.578	1.524
3.980	3.796	2.568	3.410	2.277	3.034	1.980
5.301	4.095	2.867	3.711	2.578	3.357	2.303
K_a/M^{-1}	**2.092±0.064**		**1.531±0.044**		**1.126±0.019**	
δ_c/ppm	**5.42**		**5.33**		**5.27**	

Graph of NMR titration.



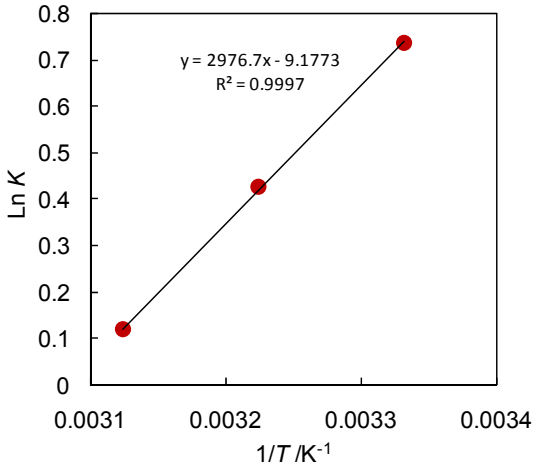
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 1.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –5.92 kcal mol^{-1}

ΔS_{obs} = –18.6 cal mol^{-1} K^{-1}

van't Hoff plot



NMR titration between 1e and MeOH.

Concentration of MeOH is 0.2243 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

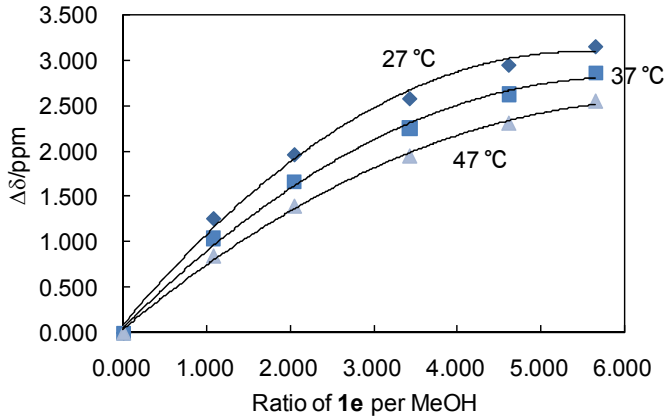
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2e**.

Results of NMR titration.

Ratio of **1e** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm
0.000	1.182	0.000	1.096	0.000	1.024	0.000
1.078	2.441	1.259	2.133	1.037	1.867	0.843
2.048	3.145	1.963	2.753	1.657	2.414	1.390
3.429	3.762	2.580	3.343	2.247	2.964	1.940
4.617	4.132	2.950	3.716	2.620	3.324	2.300
5.658	4.336	3.154	3.947	2.851	3.566	2.542
K_a/M^{-1}	**2.169±0.047**		**1.568±0.038**		**1.154±0.022**	
δ_c/ppm	**5.64**		**5.55**		**5.48**	

Graph of NMR titration.



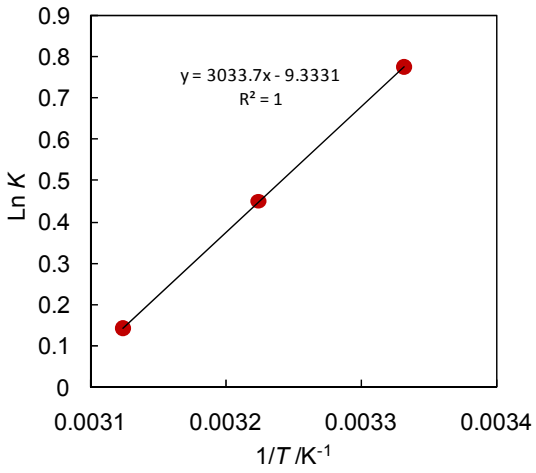
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 1.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –6.03 kcal mol^{-1}

ΔS_{obs} = –18.5 cal mol^{-1} K^{-1}

van't Hoff plot



NMR titration between 1f and MeOH.

Concentration of MeOH is 0.2217 M.

δ_{obs} is the chemical shifts at the H atom of MeOH's hydroxy proton.

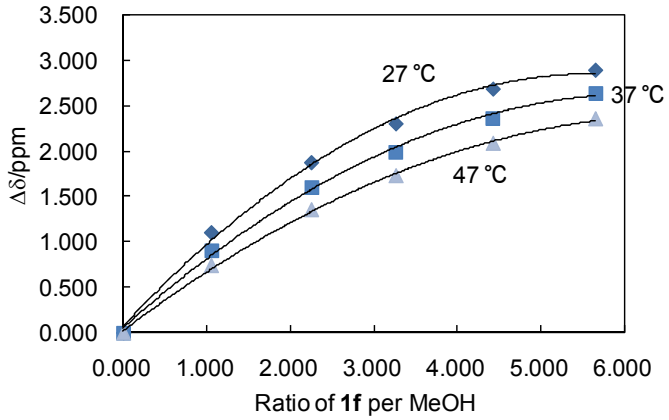
$\Delta\delta = \delta_{obs} - \delta_{obs}^{amine/MeOH=0}$.

δ_c is the predicted chemical shift of the complex **2f**.

Results of NMR titration.

Ratio of **1f** per MeOH	27/°C		37/°C		47/°C	
	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm	δ_{obs}/ppm	Δδ/ppm
0.000	1.174	0.000	1.091	0.000	1.021	0.000
1.052	2.275	1.101	1.995	0.904	1.762	0.741
2.252	3.044	1.870	2.688	1.597	2.376	1.355
3.266	3.470	2.296	3.084	1.993	2.750	1.729
4.431	3.852	2.678	3.452	2.361	3.106	2.085
5.659	4.059	2.885	3.726	2.635	3.376	2.355
K_a/M^{-1}	**2.006±0.090**		**1.411±0.034**		**1.060±0.020**	
δ_c/ppm	**5.39**		**5.39**		**5.34**	

Graph of NMR titration.



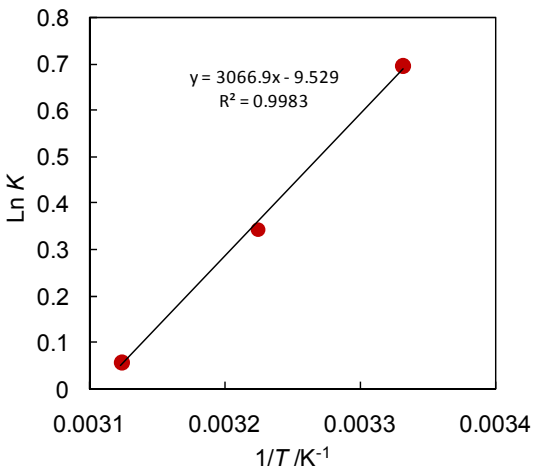
ΔH_{obs} and ΔS_{obs} were determined from van't Hoff plot and eq. 1.

$$\ln K_a = -(\Delta H / R)\cdot(1 / T) + \Delta S / R \qquad (2)$$

ΔH_{obs} = –6.09 kcal mol^{-1}

ΔS_{obs} = –18.9 cal mol^{-1} K^{-1}

van't Hoff plot



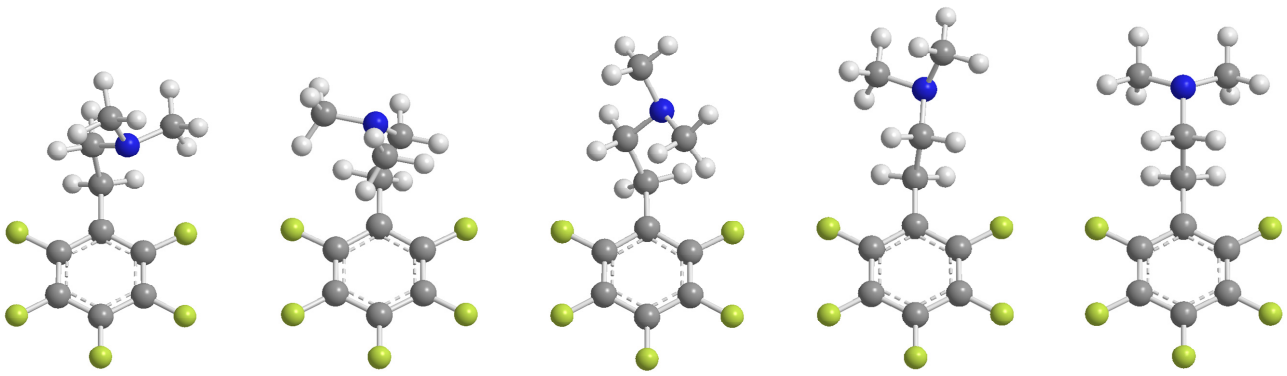
Computational studies of 1a and 2a.

Geometry optimizations and energy calculations of **1a** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2a** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

Summary of energies.

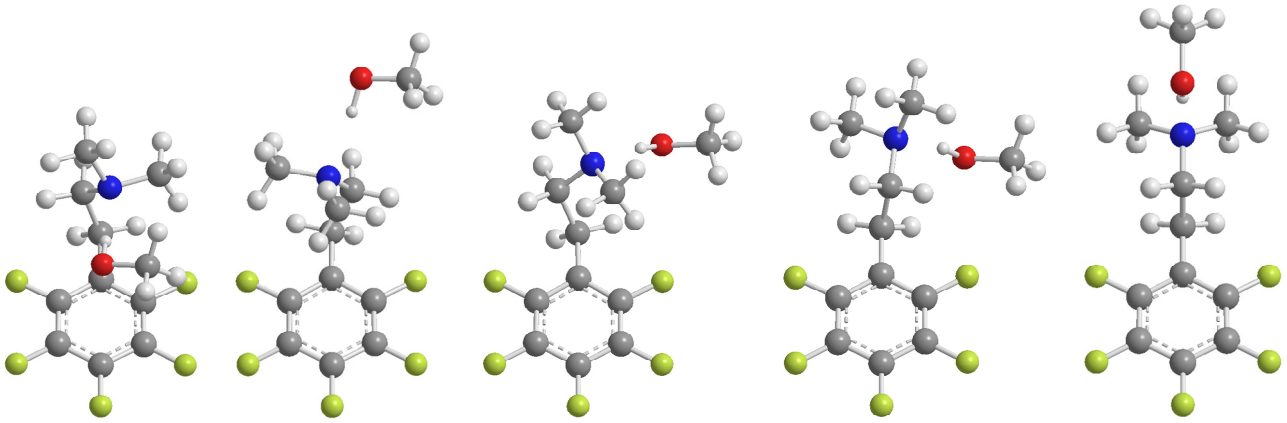
Conformation	**1a** (Hartree)	**2a** (Hartree)
A	**-938.51027**	**-1053.91142**
B	-938.50606	-1053.90608
C	-938.50560	-1053.90649
D	-938.50680	-1053.90739
E	-938.50616	-1053.90591

Results of **1a**.



Conformation A Conformation B Conformation C Conformation D Conformation E

Results of **2a**.



Conformation A Conformation B Conformation C Conformation D Conformation E

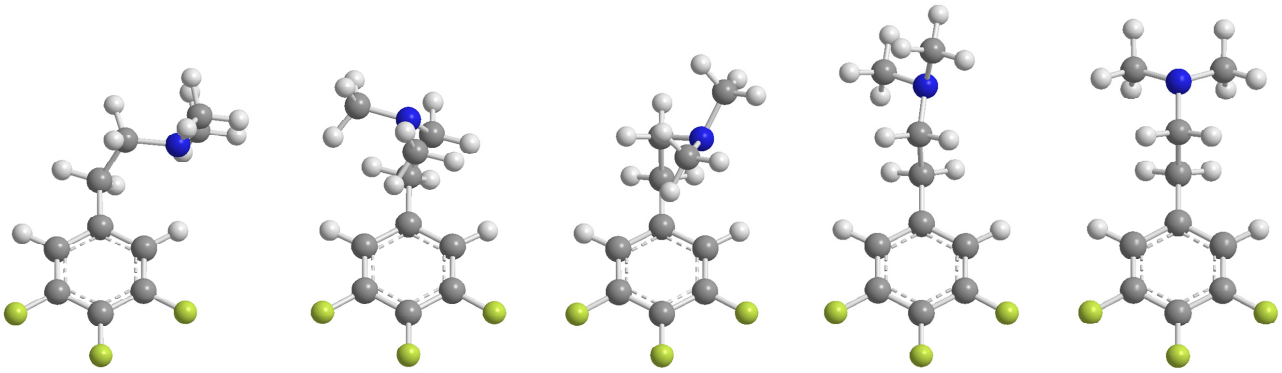
Computational studies of 1b and 2b.

Geometry optimizations and energy calculations of **1b** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2b** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

Summary of energies.

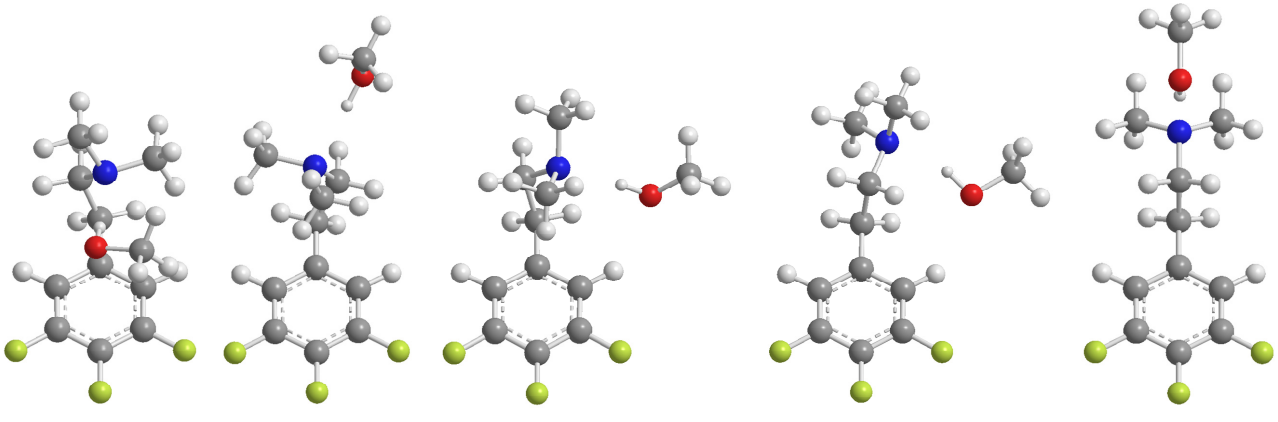
Conformation	**1b** (Hartree)	**2b** (Hartree)
A	**-740.49910**	-855.89892
B	-740.49554	-855.89573
C	-740.49724	-855.89948
D	-740.49778	**-855.89954**
E	-740.49678	-855.89657

Results of **1b**.



Conformation A Conformation B Conformation C Conformation D Conformation E

Results of **2b**.



Conformation A Conformation B Conformation C Conformation D Conformation E

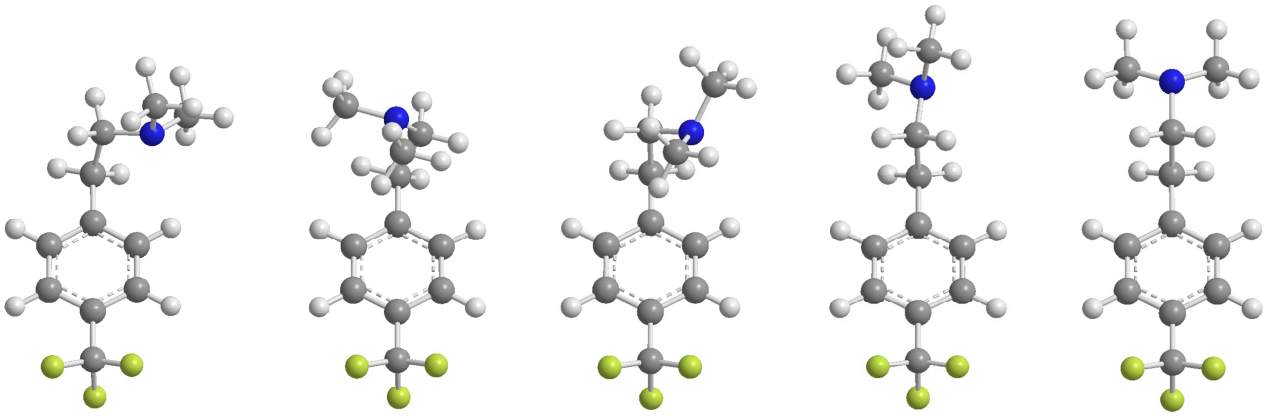
Computational studies of 1c and 2c.

Geometry optimizations and energy calculations of **1c** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2c** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

Summary of energies.

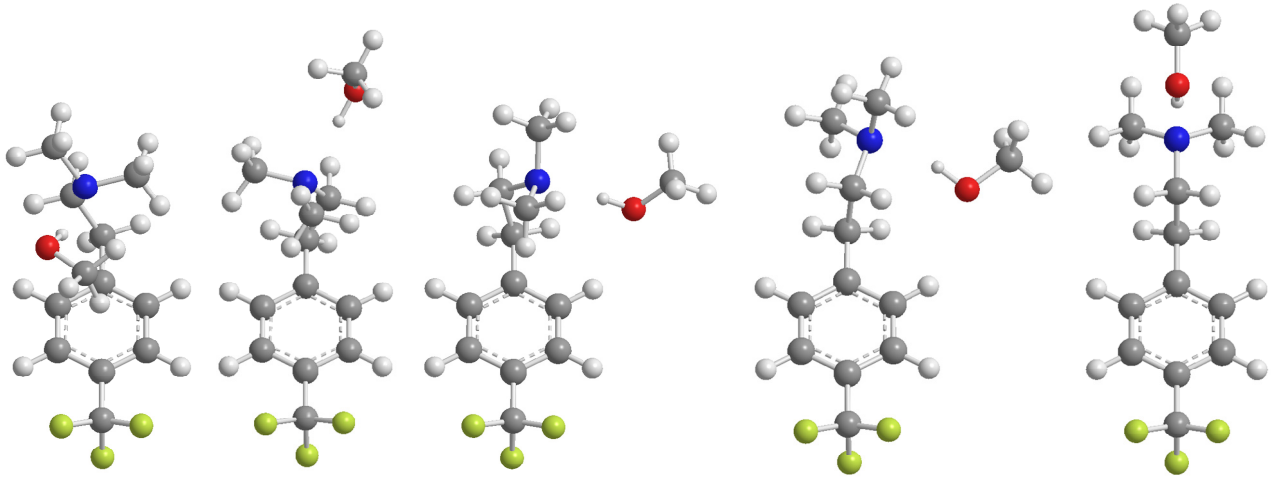
Conformation	**1c** (Hartree)	**2c** (Hartree)
A	**-779.73629**	-895.13626
B	-779.73316	-895.13355
C	-779.73482	-895.13685
D	-779.73542	**-895.13698**
E	-779.73445	-895.13439

Results of **1c**.



Conformation A Conformation B Conformation C Conformation D Conformation E

Results of **2c**.



Conformation A Conformation B Conformation C Conformation D Conformation E

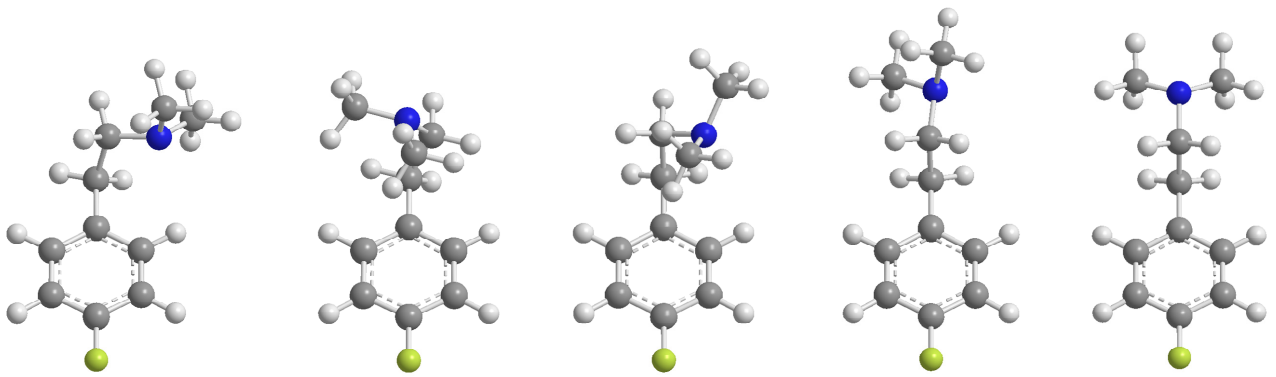
Computational studies of 1d and 2d.

Geometry optimizations and energy calculations of **1d** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2d** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

Summary of energies.

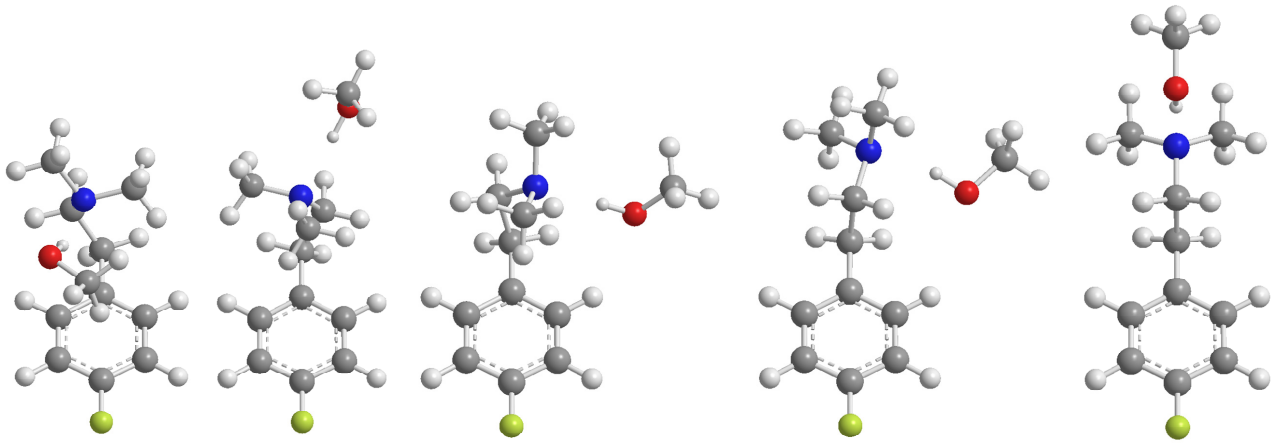
Conformation	**1d** (Hartree)	**2d** (Hartree)
A	**-542.48683**	-657.88709
B	-542.48401	-657.88465
C	-542.48547	-657.88761
D	-542.48631	**-657.88775**
E	-542.48525	-657.88543

Results of **1d**.



Conformation A Conformation B Conformation C Conformation D Conformation E

Results of **2d**.



Conformation A Conformation B Conformation C Conformation D Conformation E

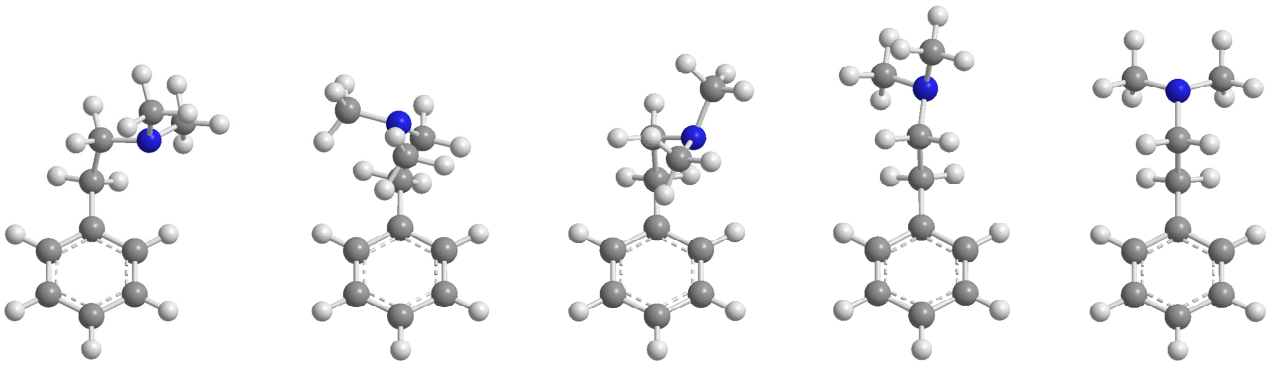
Computational studies of 1e and 2e.

Geometry optimizations and energy calculations of **1e** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2e** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

Summary of energies.

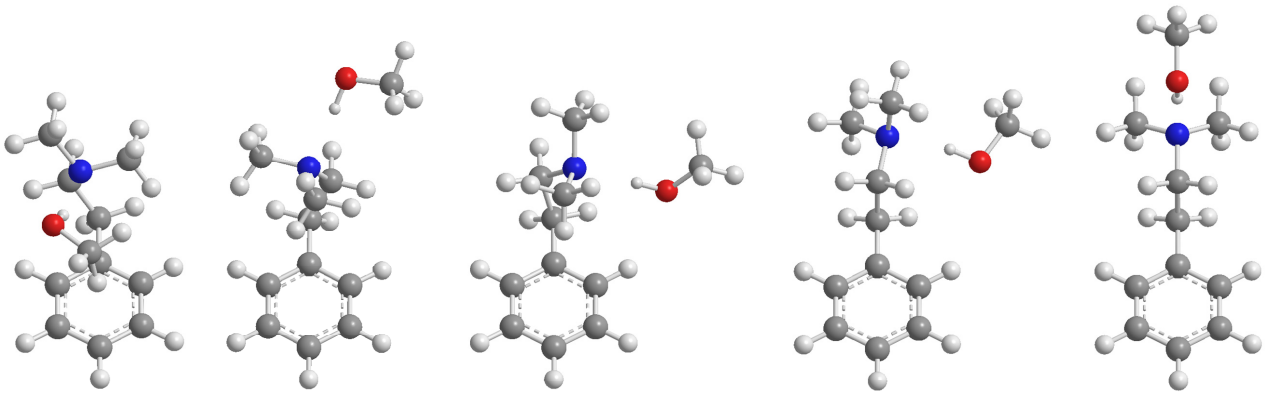
Conformation	**1e** (Hartree)	**2e** (Hartree)
A	**-443.47335**	-558.87415
B	-443.47102	-558.87193
C	-443.47225	-558.87434
D	-443.47323	**-558.87454**
E	-443.47224	-558.87257

Results of **1e**.



Conformation A Conformation B Conformation C Conformation D Conformation E

Results of **2e**.



Conformation A Conformation B Conformation C Conformation D Conformation E

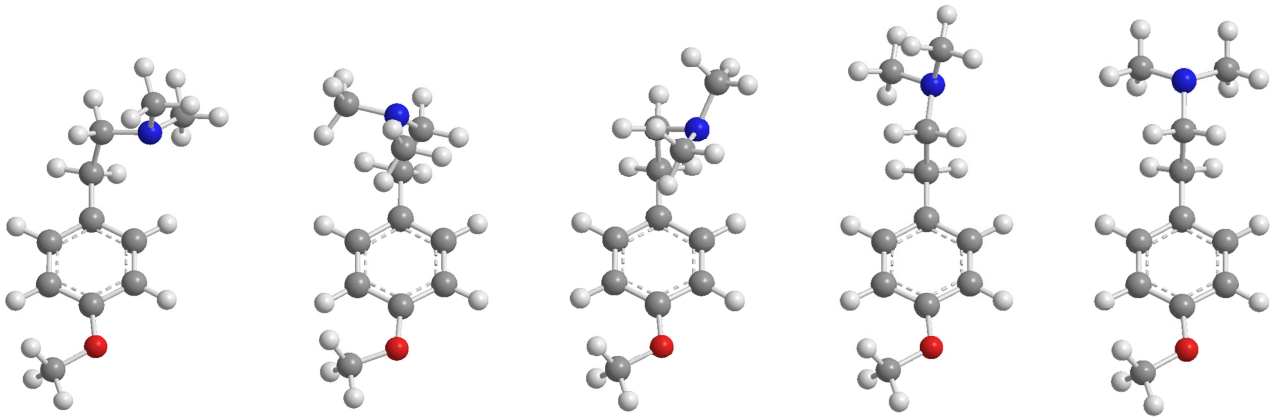
Computational studies of 1f and 2f.

Geometry optimizations and energy calculations of **1f** for each conformations were performed at the MP2(full)/6-31G(d,p). Geometry optimizations and energy calculations of **2f** for each conformations were performed at the CP-MP2(full)/6-31G(d,p).

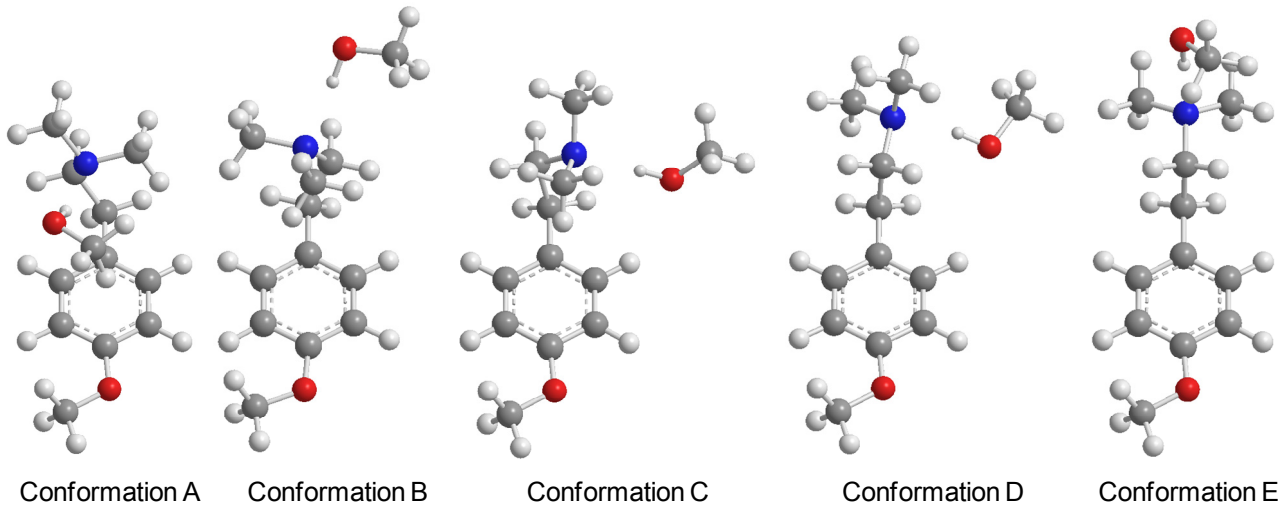
Summary of energies.

Conformation	**1f** (Hartree)	**2f** (Hartree)
A	**-557.68567**	-673.08692
B	-557.68351	-673.08436
C	-557.68455	-673.08661
D	-557.68554	**-673.08695**
E	-557.68450	-673.08524

Results of **1f**.



Results of **2f**.



Calculations of association enthalpies (ΔH_{calc}).

The frequency calculations of **2a** (conformation A) and **2b-f** (conformation D) were performed at the CP-MP2(full)/6-31G(d,p). The frequency calculations of **2a-f** (conformation A) and MeOH were performed at the MP2(full)/6-31G(d,p). No imaginary frequencies appeared in all results. All frequency calculations resulted in Zero point energy (ZPE) corrected energies and Enthalpies (H) in Gaussian's output file. The association enthalpies (ΔH_{calc}) of intermolecular interactions for **2a-f** were given by the eq 1.

$$\Delta H_{calc} = H_{complex} - (H_{amine} + H_{MeOH}) \qquad (1)$$

Ar of amine	Complex **2**		Amine **1**		MeOH		ΔH_{calc} (kcal/mol)
	ZPE corrected E (Hartree)	$H_{complex}$ (Hartree)	ZPE corrected E (Hartree)	H_{amine} (Hartree)	ZPE corrected E (Hartree)	H_{MeOH} (Hartree)	
C_6F_5	**2a** (conformation A)		**1a** (conformation A)				
	-1053.67589	-1053.64059	-938.32678	-938.29925			-5.50
3,4,5-F_3-C_6H_2	**2b** (conformation D)		**1b** (conformation A)				
	-855.64869	-855.61418	-740.30031	-740.27367			-4.98
4-CF_3-C_6H_4	**2c** (conformation D)		**1c** (conformation A)				
	-664.56905	-664.54135	-549.22057	-549.20076			-5.03
4-F-C_6H_4	**2d** (conformation D)		**1d** (conformation A)		-115.33986	-115.33258	
	-657.62143	-657.58771	-542.27260	-542.24680			-5.22
Ph	**2e** (conformation D)		**1e** (conformation A)				
	-558.60050	-558.56706	-443.25134	-443.22588			-5.39
4-MeO-C_6H_4	**2f** (conformation D)		**1f** (conformation A)				
	-672.78128	-672.74320	-557.43199	-557.40204			-5.38

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