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Structure of novel *N*-fluorosilylmethyl-*N*-isopropylureas

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Experimental

1.1. Materials and methods

^{1}H, ^{13}C, ^{29}Si NMR spectra were recorded on a Bruker DPX 400 spectrometer (400.13, 100.61 and 79.5 MHz, respectively) with cyclohexane or $(Me_3Si)_2O$ as an internal standard. FTIR spectra were taken on a FT-IR Varian 3100 spectrometer. All reactions and other manipulations were carried out in thoroughly dried glassware in argon atmosphere. Elemental analysis is performed on the Thermo Scientific Flash 2000 Automatic CHNS Analyzer. Melting points were determined using the Boetius Block apparatus. The solvents were purified by standard procedures prior to use [W. L. F. Armarego, C. L. L. Chai, *Purification of Laboratory Chemicals*, 6th ed., Elsevier, 2009, p. 760].

X-ray study

Crystal data were collected on a Bruker D8 Venture diffractometer with MoKa radiation (λ = 0.71073) using the φ and ω scans. The structures were solved and refined by direct methods using the SHELX programs set. Data were corrected for absorption effects using the multi-scan method (SADABS). Nonhydrogen atoms were refined anisotropically using SHELX programs set [G. M. Sheldrick, *Acta Crystallogr*. 2008, **D64**, 112]. **CCDC 2141508** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre viawww.ccdc.cam.ac.uk/data_request/cif.

1.2. Synthetic procedures for compounds 1a-c

***N*-[(Triethoxysilyl)methyl]isopropylamine 1a.** Chloromethyl(triethoxy)silane (21.3 g, 100 mmol) was slowly added to a solution of 6 equiv. Pr^iNH_2 (35.46 g, 600 mmol) in hexane (100 ml). The resulting mixture was refluxed with stirring for 3 days. Isopropylamine hydrochloride was filtered off. Amine **1a** was isolated by vacuum distillation as the colorless liquid. Yield 9.61g (41%). B.p. 73 °C/ 5 Torr. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.84 (q, 6H, -$\underline{CH_2}CH_3$, ^{3}J = 7.0 Hz), 2.62 (septet, 1H, -$\underline{CH}(CH_3)_2$, ^{3}J = 6.3 Hz), 2.10 (s, 2H, CH_2), 1.22 (t, 9H, -$CH_2\underline{CH_3}$, ^{3}J = 7.0 Hz), 1.01 (d, 6H, -$CH(\underline{CH_3})_2$, ^{3}J = 6.3 Hz). ^{13}C NMR ($CDCl_3$, δ, ppm): 57.93 (-$\underline{CH_2}CH_3$), 51.64 (-$\underline{CH}(CH_3)_2$), 30.87 (CH_2), 21.78 (-$CH(\underline{CH_3})_2$), 17.62 (-$CH_2\underline{CH_3}$). ^{29}Si NMR ($CDCl_3$, δ, ppm): -50.55. Found, %: C, 50.70; H, 10.28; N, 5.70. $C_{10}H_{25}NO_3Si$. Calculated, %: C, 51.02; H, 10.71; N, 5.95.

***N*-[(Methyl(diethoxy)silyl)methyl]isopropylamine 1b** was obtained by the above method. Colorless liquid, yield 9.61g, 53%. B.p. 54 °C/ 5 Torr. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.79 (q, 4H, -$\underline{CH_2}CH_3$), ^{3}J = 7.0 Hz), 2.64 (septet, 1H, -$\underline{CH}(CH_3)_2$, ^{3}J = 6.2 Hz), 2.09 (s, 2H, CH_2), 1.22 (t, 6H, -$CH_2\underline{CH_3}$, ^{3}J = 7.0 Hz) 1.02 (d, 6H, -$CH(\underline{CH_3})_2$, ^{3}J = 6.2 Hz), 0.18 (s, 3H, CH_3). ^{13}C NMR ($CDCl_3$, δ, ppm): 58.30 (-$\underline{CH_2}CH_3$), 52.31 (-$\underline{CH}(CH_3)_2$), 34.39 (CH_2), 22.35 (-$CH(\underline{CH_3})_2$), 18.33,

(-CH($\underline{CH_3}$)$_2$), -5.31 (-CH_3). ^{29}Si NMR ($CDCl_3$, δ, ppm): -8.69. Found, %: C, 52.71; H, 10.92; N, 6.82. $C_9H_{23}NO_2Si$. Calculated, %: C, 52.64; H, 11.29; N, 6.82.

***N*-[(Dimethyl(ethoxy)silyl)methyl]isopropylamine 1c** was obtained by the above method. Colorless liquid, yield 12.59 g, 65%. B.p. 162 °C. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.69 (q, 2H, -$\underline{CH_2}CH_3$, ^3J = 6.9 Hz), 2.65 (septet, 1H, -$\underline{CH}(CH_3)_2$, ^3J = 6.3 Hz), 2.09 (s, 2H, CH_2), 1.19 (t, 3H, $CH_2\underline{CH_3}$, ^3J = 6.9 Hz), 1.03 (d, 6H, -CH($\underline{CH_3}$)$_2$), ^3J = 6.3 Hz), 0.15 (s, 6H, Me). ^{13}C NMR ($CDCl_3$, δ, ppm): 58.44 (-$\underline{CH_2}CH_3$), 52.39 (-$\underline{CH}(CH_3)_2$), 36.84 (CH_2), 22.42 (-CH($\underline{CH_3}$)$_2$), 18.50 (-$CH_2\underline{CH_3}$), -2.78 (s, CH_3). ^{29}Si NMR ($CDCl_3$, δ, ppm): 14.32. Found, %: C, 54.45; H, 11.6; N, 8.15. $C_8H_{21}NOSi$. Calculated, %: C, 54.80; H, 12.07; N, 7.99.

1.3. Synthetic procedures for compounds 2a-c

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(triethoxysilyl)methyl]urea 2a.** *N*,*N*-Dimethylcarbamoyl chloride (1.27 g, 11.8 mmol) was added slowly to a solution of the mixture of compound **1a** (2.8 g, 11.8 mmol) and excess of triethylamine (5.97 g, 59 mmol) in hexane (35 ml). The mixture was refluxed with stirring for 3 days. The white crystalline precipitate was filtered off, and the solvent removed. The colorless liquid product was purified by distillation under reduced pressure. Yield 1.85 g (51%). B.p. 120 °C/ 5 Torr. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.85-3.76 (q, 6H, -$\underline{CH_2}CH_3$, ^3J = 7.0 Hz + septet, 1H, $\underline{CH}CH_3$), 2.79 (s, 6H, N(CH_3)$_2$), 2.46 (s, 2H, CH_2), 1.20 (t, 9H, -$CH_2\underline{CH_3}$, ^3J = 7.0 Hz), 1.12 (d, 6H, -$CH\underline{CH_3}$, ^3J = 6.4 Hz). ^{13}C NMR ($CDCl_3$, δ, ppm): 166.01 (C=O), 58.42 (-$\underline{CH_2}CH_3$), 50.44 (-$\underline{CH}(CH_3)_2$), 38.73 (NCH_3)$_2$), 26.06 (NCH_2), 19.66 (-CH($\underline{CH_3}$)$_2$), 18.11 (-$CH_2\underline{CH_3}$). ^{29}Si NMR ($CDCl_3$, δ, ppm): -53.96. IR (film from chloroform, ν, cm^{-1}): 1648 (C=O). Found, %: C, 50.94; H, 9.69; N, 8.79. $C_{13}H_{30}N_2O_4Si$. Calculated, %: C, 50.95; H, 9.87; N, 9.14.

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(diethoxy)silyl)methyl]urea 2b** was obtained by the above method for compound **2a**. Yield 0.63 g (23%). B.p. 115 °C/ 5 Torr. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.91-3.63 (q, -$\underline{CH_2}CH_3$, ^3J = 6.5 Hz, 4H + septet, -$\underline{CH}(CH_3)_2$, 1H,), 2.78 (s, 6H, N(CH_3)$_2$), 2.39 (s, 2H, CH_2), 1.19 (t, 6H, -$CH_2\underline{CH_3}$, ^3J = 7.1 Hz), 1.12 (d, 6H, -CH($\underline{CH_3}$)$_2$, ^3J = 6.7 Hz). ^{13}C NMR ($CDCl_3$, δ, ppm): 166.28 (C=O), 58.16 (-$\underline{CH_2}CH_3$), 50.55 (-$\underline{CH}(CH_3)_2$), 38.94 (NCH_3)$_2$), 28.86 (CH_2), 19.83 (-CH($\underline{CH_3}$)$_2$), 18.36 (-$CH_2\underline{CH_3}$), -4.36 (CH_3). ^{29}Si NMR ($CDCl_3$, δ, ppm): -11.41. IR (film from chloroform, ν, cm^{-1}): 1645 (C=O). Found, %: C, 51.91; H, 9.68; N, 10.39. $C_{12}H_{28}N_2O_3Si$. Calculated, %: C, 52.14; H, 10.21; N, 10.13.

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(ethoxy)silyl)methyl]urea 2c** was obtained by the above method for compound **2a**. Colorless liquid, yield 2.02 g (41%). B.p. 80 °C/5 Torr. ^{1}H NMR ($CDCl_3$, δ, ppm): 3.84 (septet, 1H, -$\underline{CH}(CH_3)_2$, ^3J = 6.5 Hz), 3.65 (q, 2H, -$\underline{CH_2}CH_3$, ^3J = 6.8 Hz), 2.76 (s, 6H, N(CH_3)$_2$), 2.39 (s, 2H, CH_2), 1.18 (t, 3H, -$CH_2\underline{CH_3}$, ^3J = 6.8 Hz), 1.12 (d, 6H, -CH($\underline{CH_3}$)$_2$, ^3J = 6.5 Hz), 0.15 (s, 6H, -CH_3). ^{13}C NMR ($CDCl_3$, δ, ppm): 166.35 (C=O), 58.09 (-$\underline{CH_2}CH_3$), 50.53 (-$\underline{CH}(CH_3)_2$), 38.95 (N(CH_3)$_2$), 30.52 (CH_2), 19.91 (-CH($\underline{CH_3}$)$_2$), 18.57 (-$CH_2\underline{CH_3}$), -2.08 (CH_3). ^{29}Si NMR ($CDCl_3$, δ, ppm): 13.27. IR (film from chloroform, ν, cm^{-1}):

1642 (C=O). Found, %: C, 53.61; H, 10.42; N, 11.64. $C_{10}H_{24}N_2O_2Si$. Calculated, %: C, 53.61; H, 10.64; N, 11.37.

1.4. Synthetic procedures for compounds 3a-c

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(trifluorosilyl)methyl]urea 3a.** Boron trifluoride etherate (0.43 g, 3 mmol) was added dropwise to a solution of compound **2a** (0.92 g, 3 mmol) in hexane (5 ml) at stirring. The mixture was refluxed for 3 days. The precipitate was filtered off, washed with hexane and pentane and dried in vacuum. The white crystals were obtained by recrystallization from benzene. Yield 0.58 g (84%). M. p. 112 °C. ^{1}H NMR ($CDCl_3$, δ, ppm): δ 4.03 (septet, 1H, -CH$(CH_3)_2$, ^3J = 6.4 Hz), 2.95 (s, 6H, N$(CH_3)_2$), 2.50 (s, 2H, CH_2), 1.19 (d, 6H, -CH(C$H_3)_2$, ^3J = 6.3 Hz). ^{13}C NMR ($CDCl_3$, δ, ppm): 164.56 (C=O), 49.15 (-CH$(CH_3)_2$), 40.15 (N$CH_3)_2$), 26.08 (q, ^2J = 27.3 Hz), 20.05 (-CH(C$H_3)_2$). ^{29}Si NMR ($CDCl_3$, δ, ppm): -104.23 (q, $^1J_{Si\text{-}F}$ = 210.6 Hz). IR (film from chloroform, ν, cm^{-1}): 1537 (C=O). Found, %: C, 37.30; H, 6.61; N, 11.77. $C_7H_{15}F_3N_2OSi$. Calculated, %: C, 36.83; H, 6.62; N, 12.27.

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(difluoro)silyl)methyl]urea 3b** was obtained by the above method for compound **3a**. The substance was purified by heating under reduce pressure. Attempts to obtain crystals of compound **3b** were unsuccessful. Compound **3b** is white-yellow oil. Yield 0.3 g (67%). ^{1}H NMR ($CDCl_3$, δ, ppm): 3.96 (septet, 1H, (-CH$(CH_3)_2$, ^3J = 6.5 Hz), 2.89 (s, 6H, N$(CH_3)_2$), 2.41 (s, 2H, CH_2), 1.19 (d, 6H, -CH(C$H_3)_2$, ^3J = 6.5 Hz), 0.26 (t, 3H, CH_3, ^3J = 5.0 Hz). ^{13}C NMR ($CDCl_3$, δ, ppm): 165.52 (C=O), 48.94 (-CH$(CH_3)_2$), 39.93 N$(CH_3)_2$, 29.07 (t, CH_2, ^2J = 31.7 Hz), 19.97 (-CH(C$H_3)_2$), 0.58 (t, CH_3, ^2J = 23.1 Hz). ^{29}Si NMR ($CDCl_3$, δ ppm): -59.57 (t, ^1J = 252.3 Hz). IR (film from chloroform, ν, cm^{-1}): 1573, 1533 (C=O). Found, %: C, 42.98; H, 7.59; N, 12.07. $C_8H_{18}F_2N_2OSi$. Calculated, %: C, 42.83; H, 8.09; N, 12.49.

***N*-Isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(fluoro)silyl)methyl]urea 3c** was obtained by the above method for compound **3a**. The substance was purified by heating under reduce pressure. Attempts to obtain crystals of compound **3c** were unsuccessful. Compound **3c** is yellow oil, yield 0.66 g (95%). ^{1}H NMR ($CDCl_3$, δ, ppm): 3.90 (septet, 1H, -CH$(CH_3)_2$, ^3J = 6.6 Hz), 2.78 (s, 6H, N$(CH_3)_2$), 2.33 (s, 2H, CH_2), 1.17 (d, 6H, -CH(C$H_3)_2$, ^3J = 6.6 Hz), 0.22 (d, 6H, CH_3, ^3J = 8.5 Hz). ^{13}C NMR ($CDCl_3$): 166.21 (C=O), 49.09 (-CH$(CH_3)_2$), 39.74 (N$(CH_3)_2$), 30.16 (d, CH_2, ^2J = 40.3 Hz,), 19.93 (-CH(C$H_3)_2$), 1.20 (d, CH_3, ^2J = 25.0 Hz). ^{29}Si NMR ($CDCl_3$, δ, ppm): -17.75 (d, $^1J_{Si\text{-}F}$ = 242.8 Hz). IR (film from chloroform, ν, cm^{-1}): 1583,1520 (C=O). Found, %: C, 48.83; H, 9.14; N, 12.60. $C_9H_{21}FN_2OSi$. Calculated: C, 49.05; H, 9.61; N, 12.71.

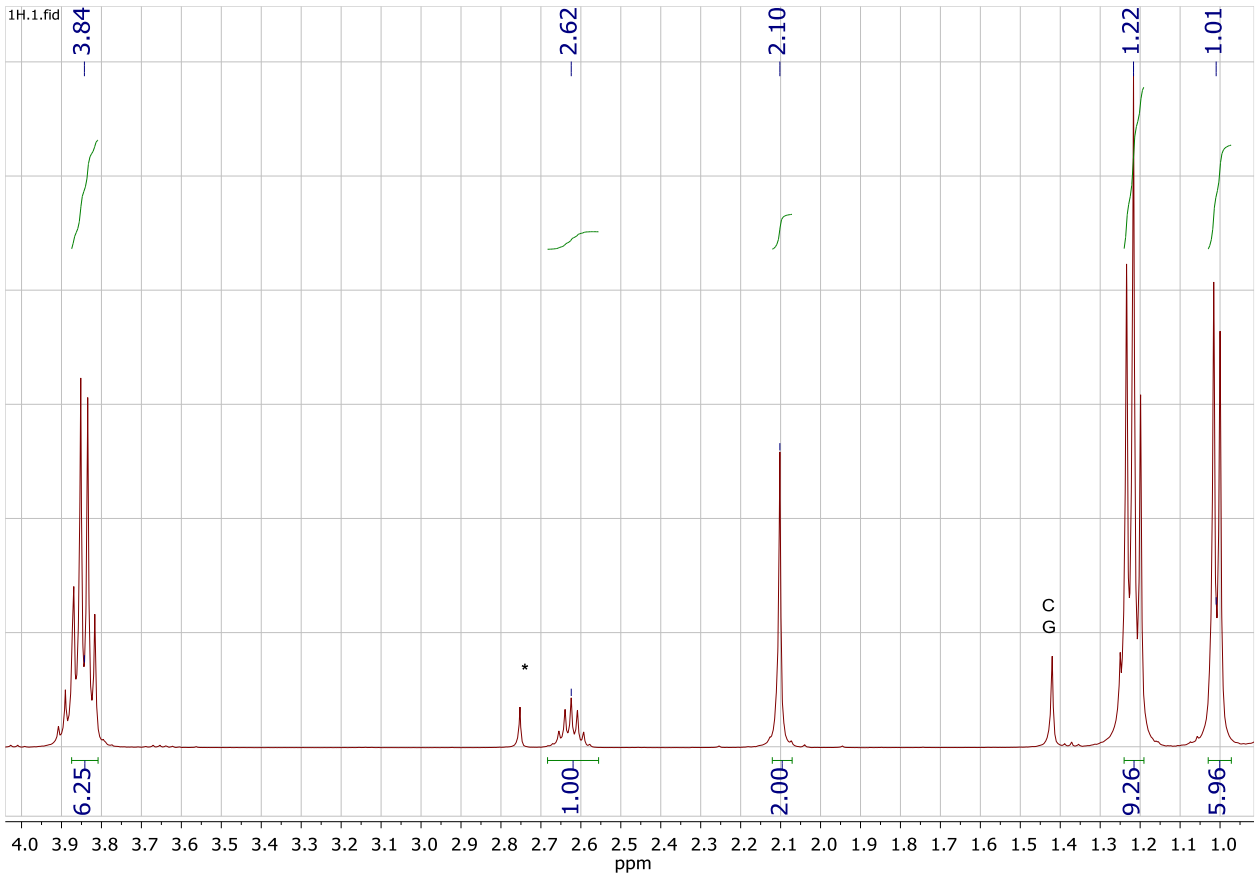

Fig. S1. NMR ^{1}H spectrum of N-[(triethoxysilyl)methyl]isopropylamine 1a.

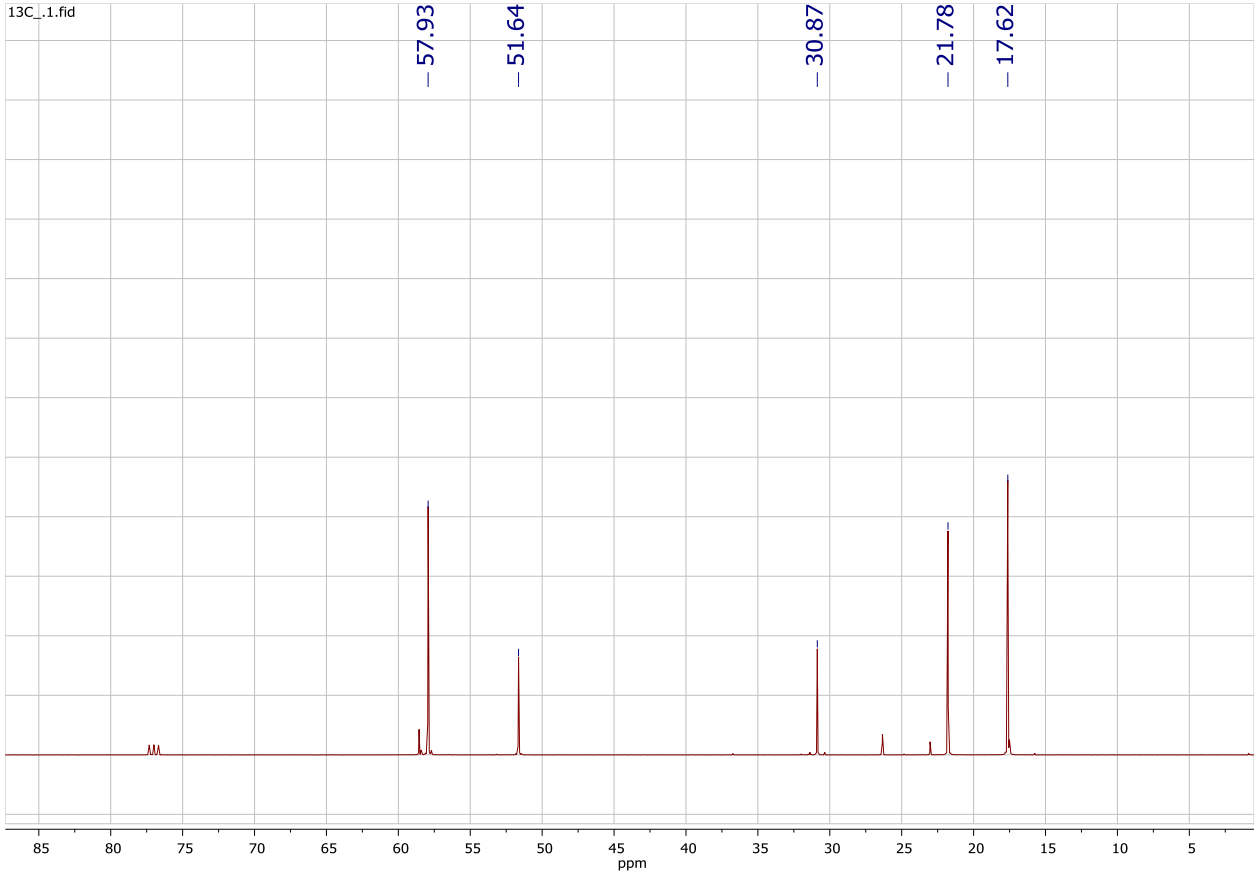

Fig. S2. NMR ^{13}C spectrum of N-[(triethoxysilyl)methyl]isopropylamine 1a.

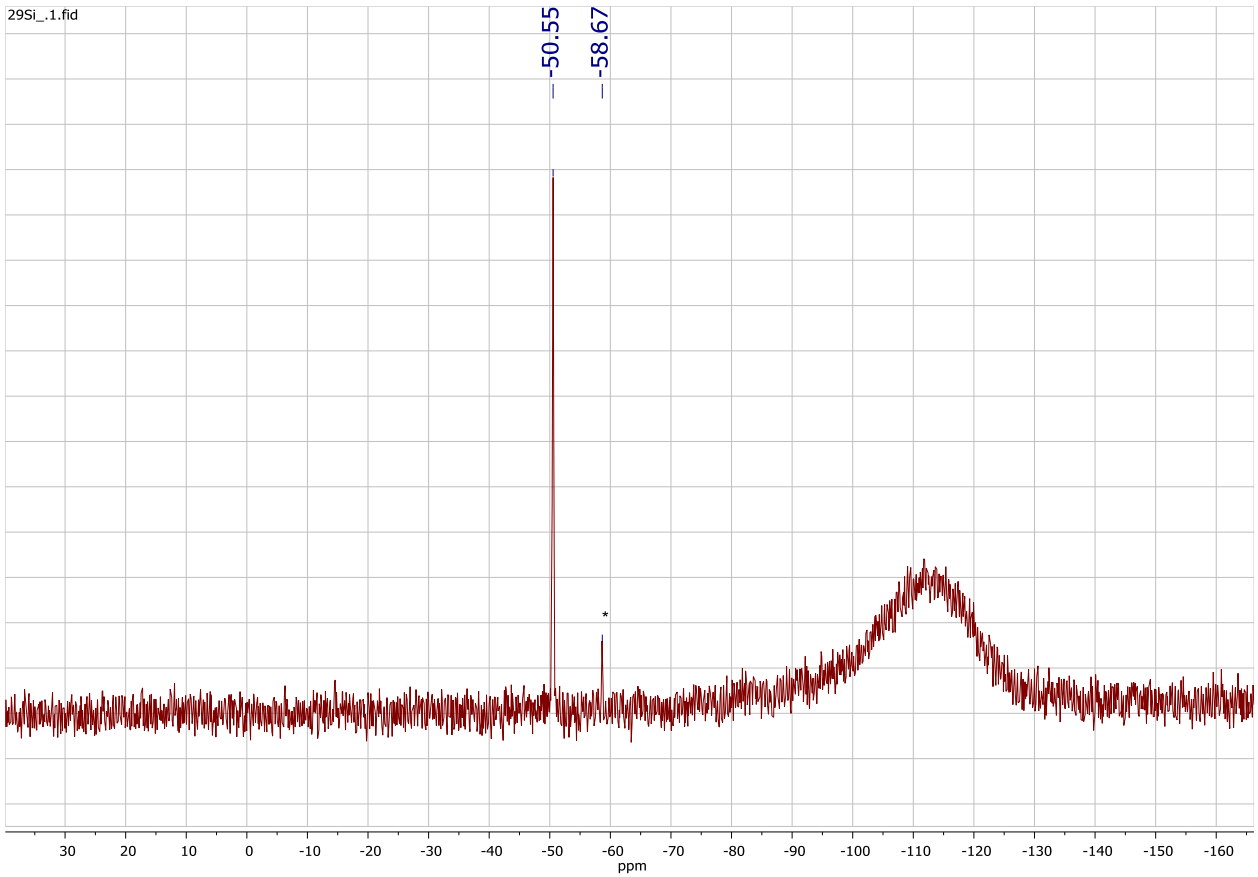

Fig. S3. NMR ^{29}Si spectrum of N-[(triethoxysilyl)methyl]isopropylamine 1a.

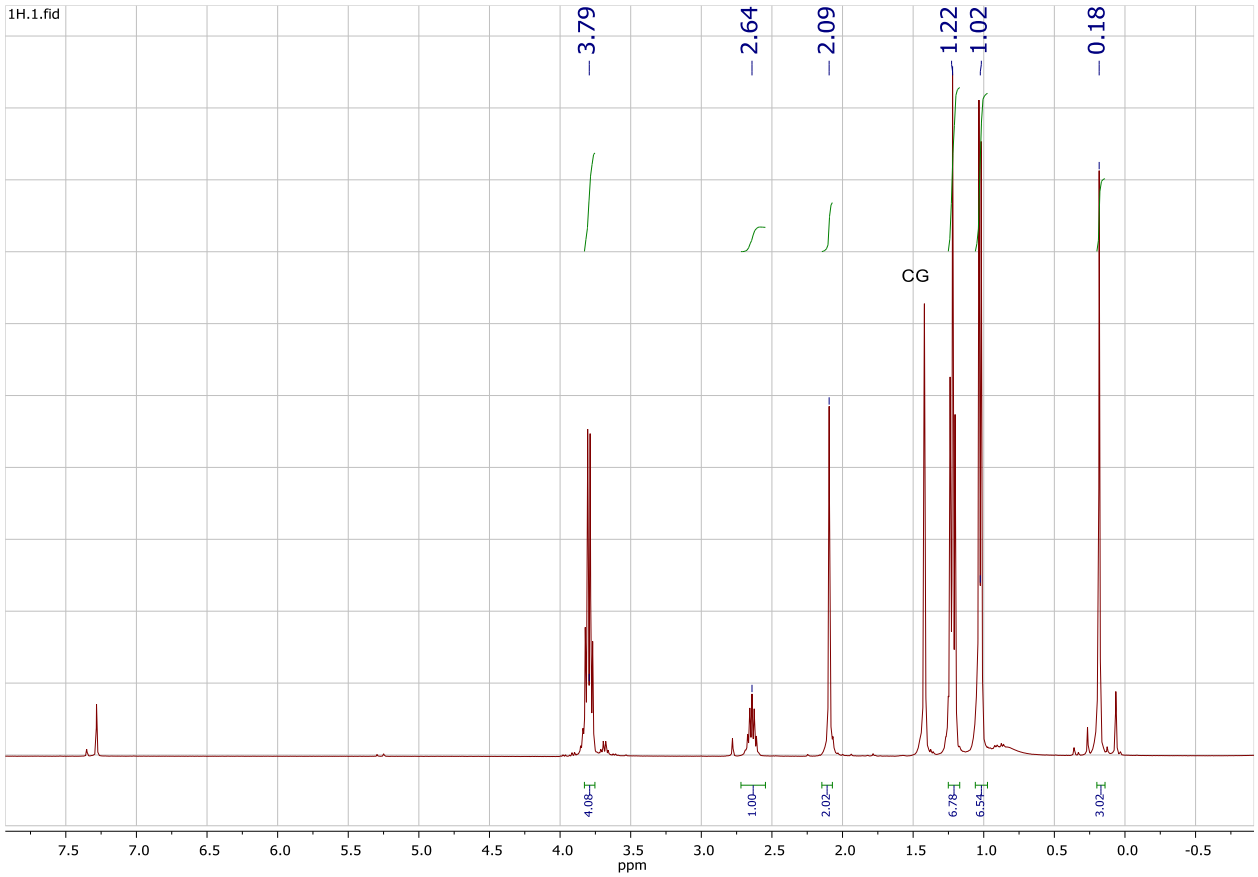

Fig. S4. NMR ^{1}H spectrum of N-[(methyl(diethoxy)silyl)methyl]isopropylamine 1b.

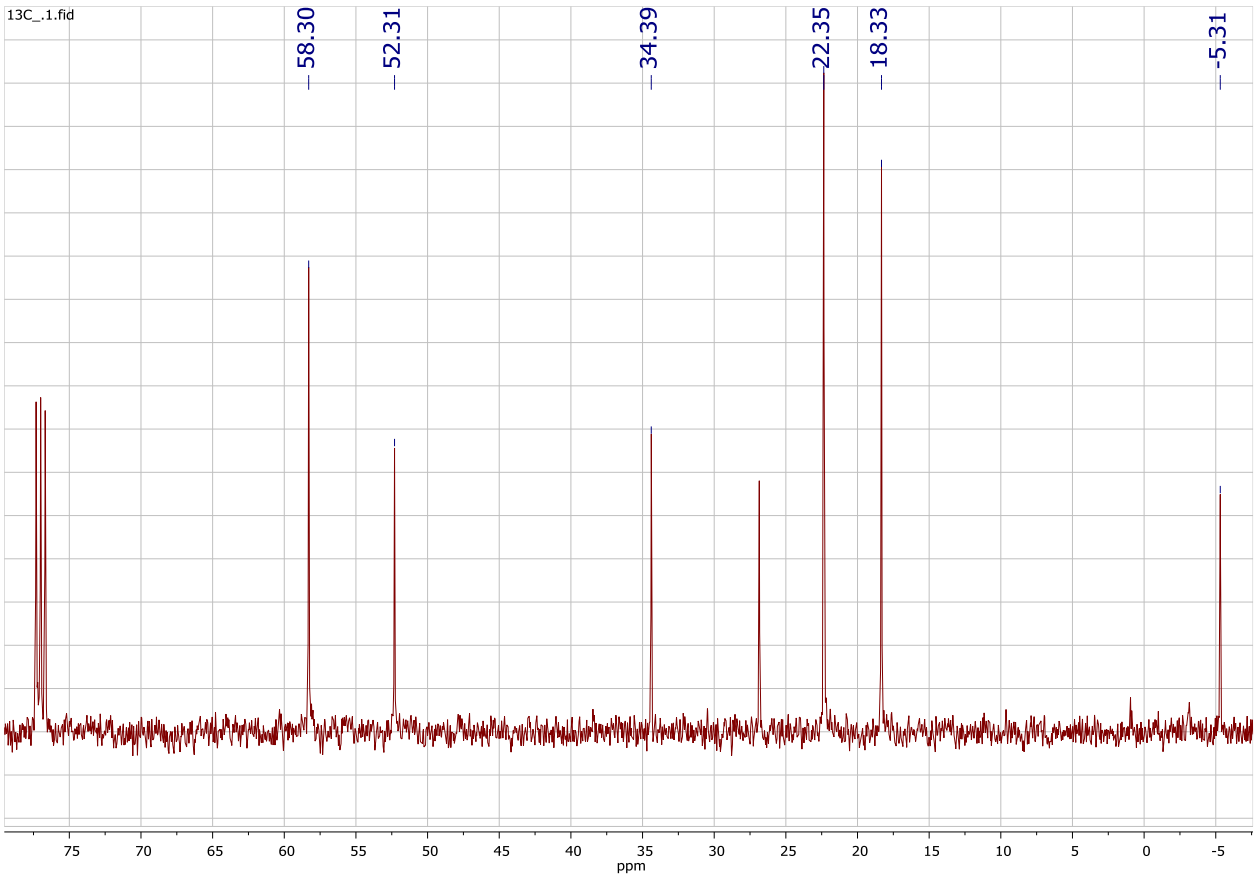

Fig S5. NMR ^{13}C spectrum of N-[(methyl(diethoxy)silyl)methyl]isopropylamine 1b.

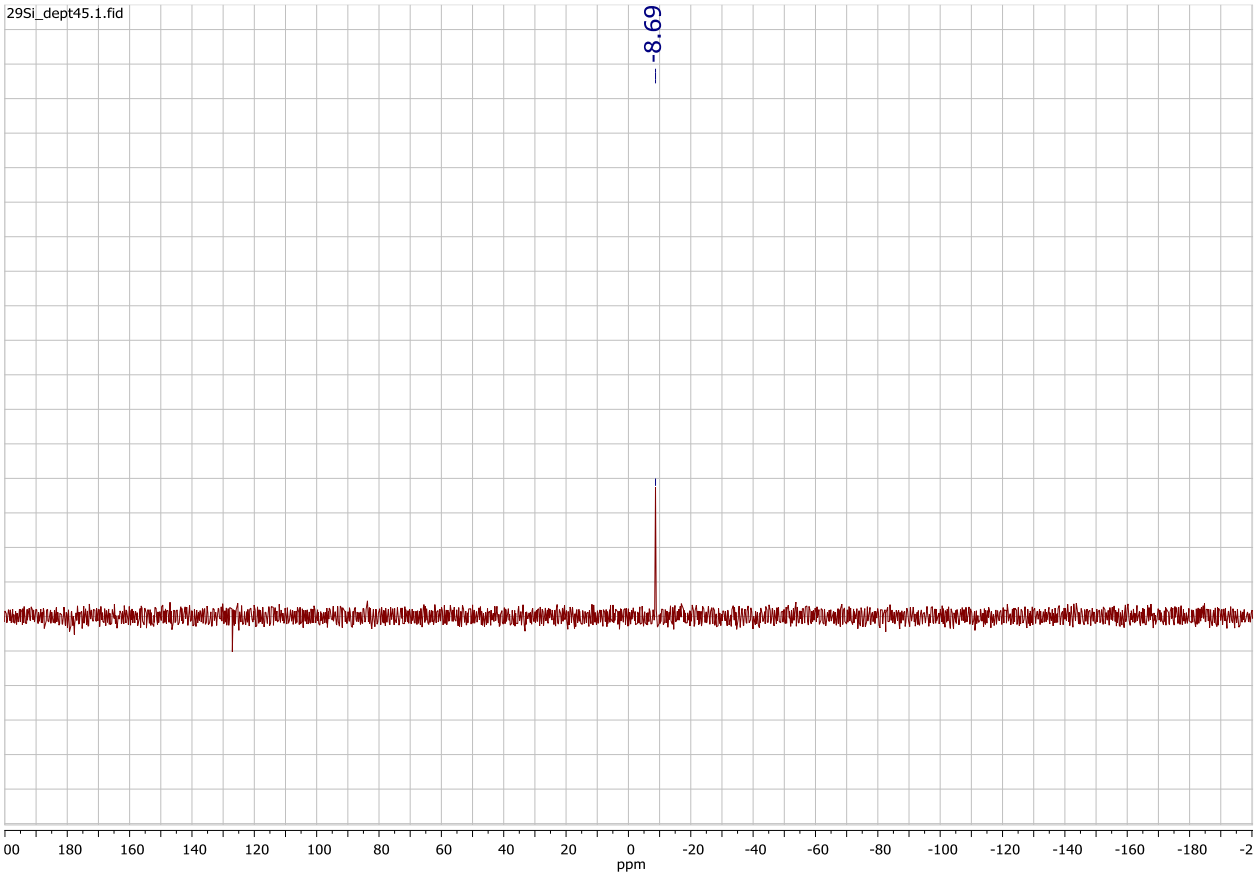

Fig. S6. NMR ^{29}Si spectrum of N-[(methyl(diethoxy)silyl)methyl]isopropylamine 1b.

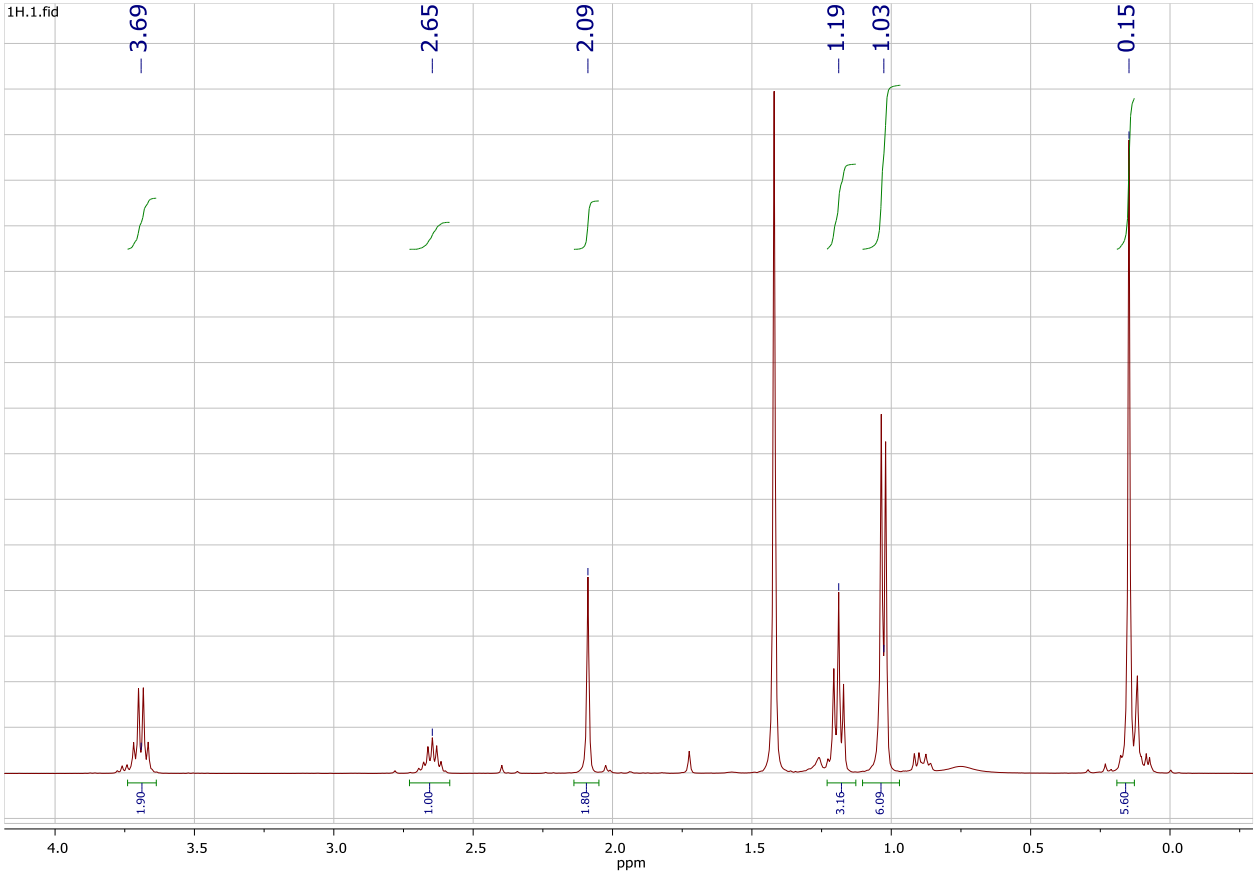

Fig. S7. NMR ^{1}H spectrum of N-[(dimethyl(ethoxy)silyl)methyl]isopropylamine 1c.

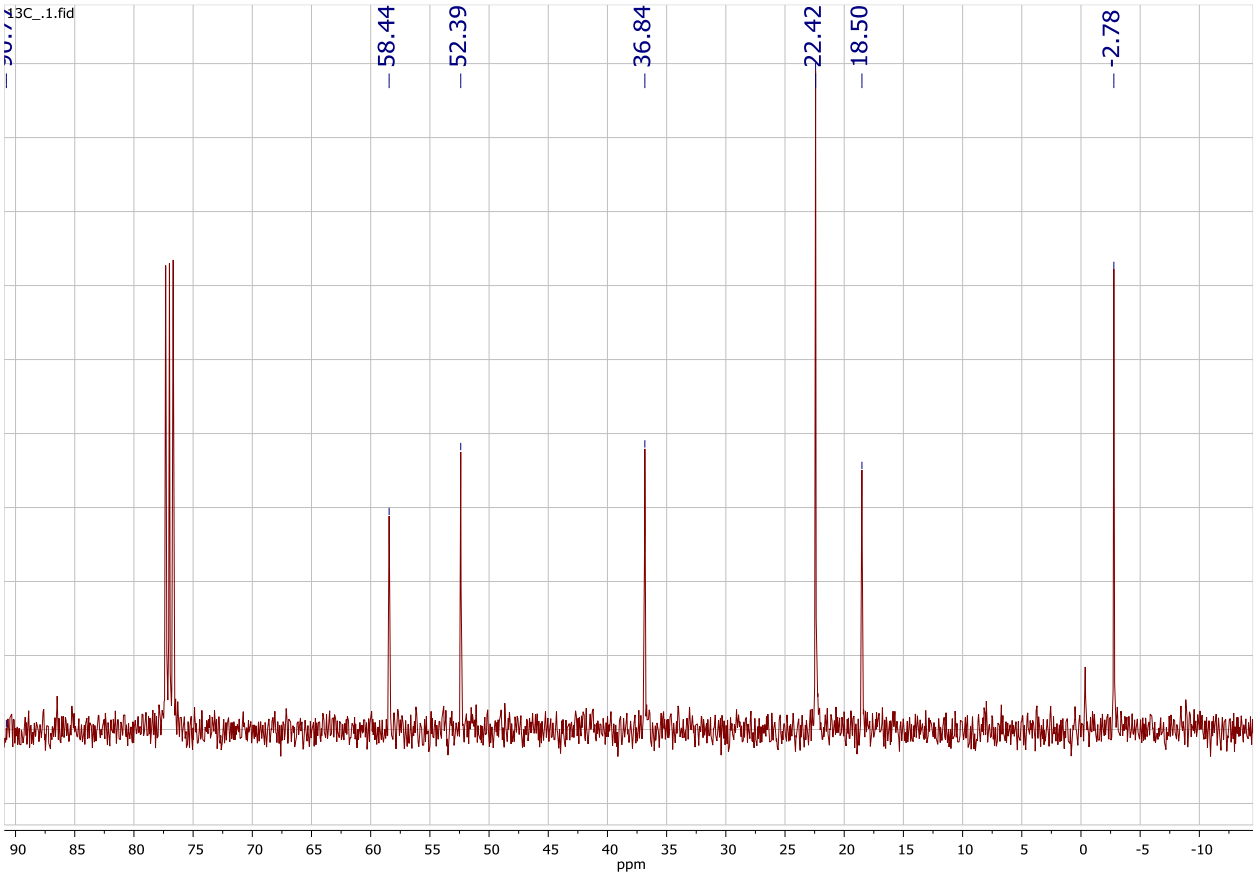

Fig. S8. NMR ^{13}C spectrum of N-[(dimethyl(ethoxy)silyl)methyl]isopropylamine 1c.

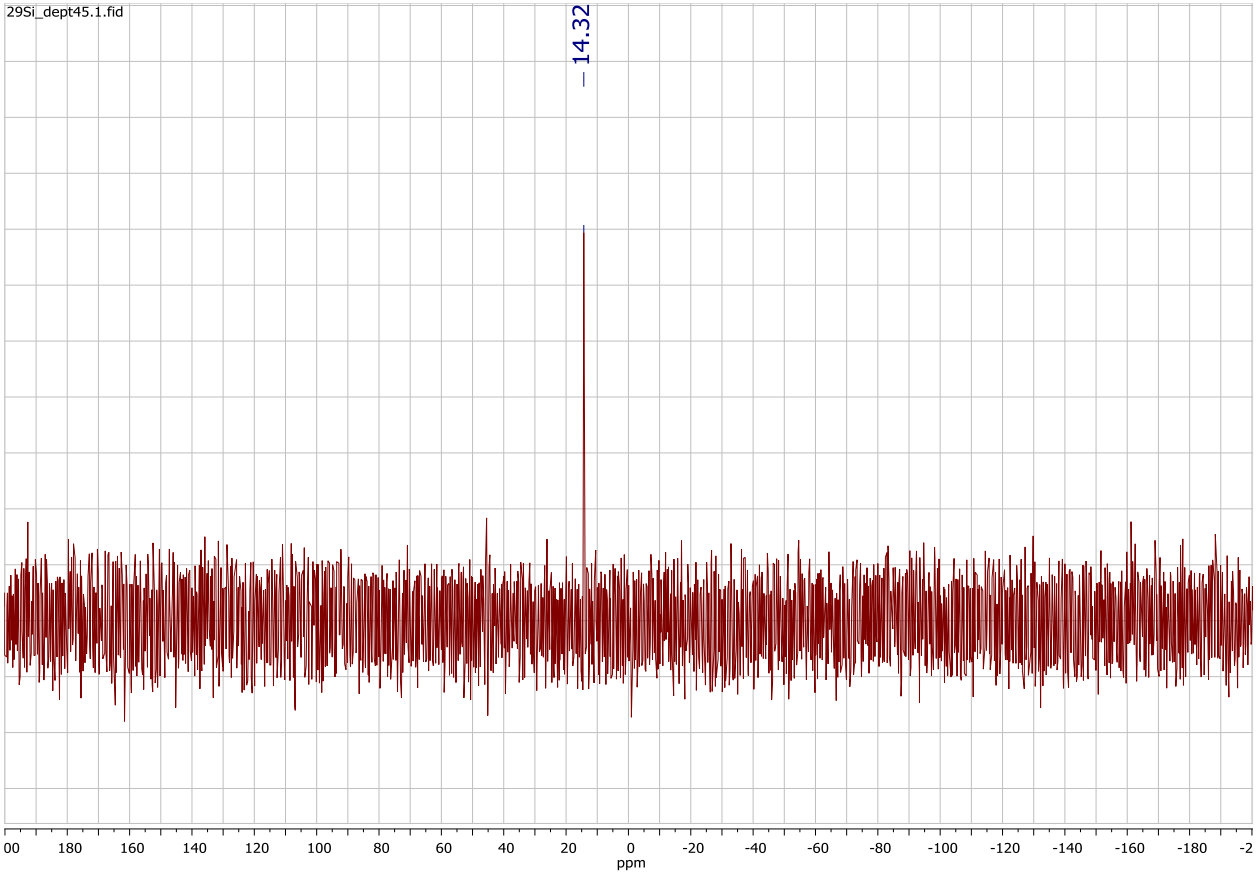

Fig. S9. NMR ^{29}Si spectrum of N-[(dimethyl(ethoxy)silyl)methyl]isopropylamine 1c.

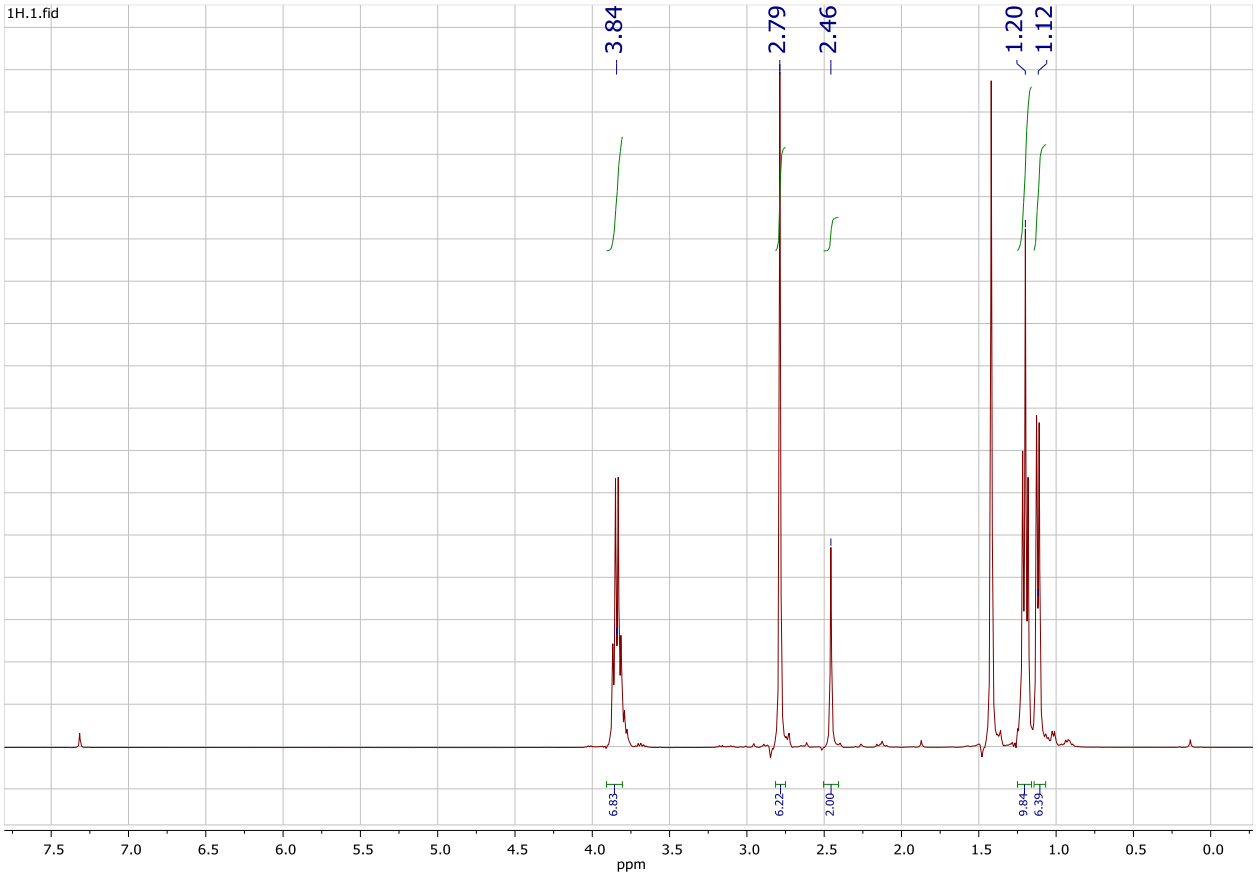

Fig. S10. NMR ^{1}H spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(triethoxysilyl)methyl]urea 2a.

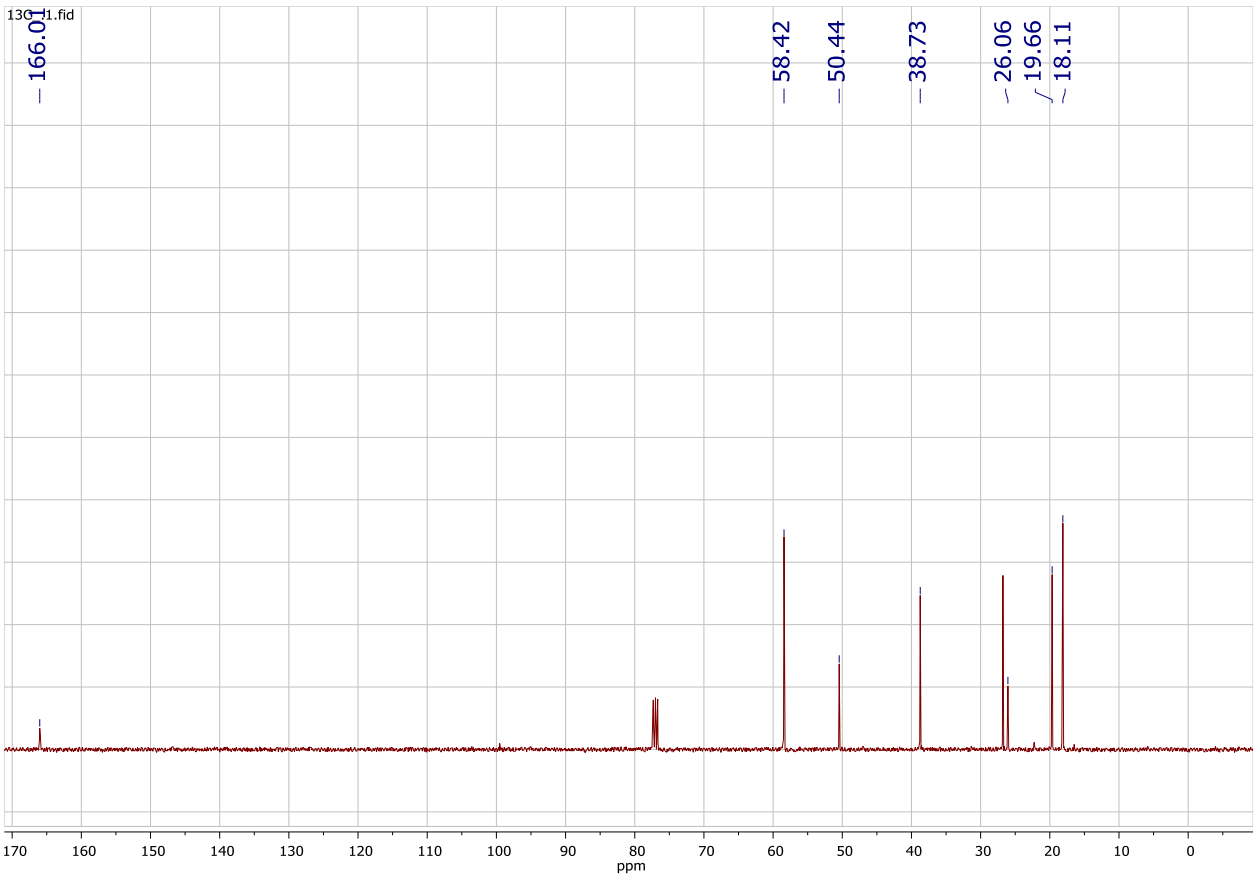

Fig. S11. NMR ^{13}C *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(triethoxysilyl)methyl]urea 2a.

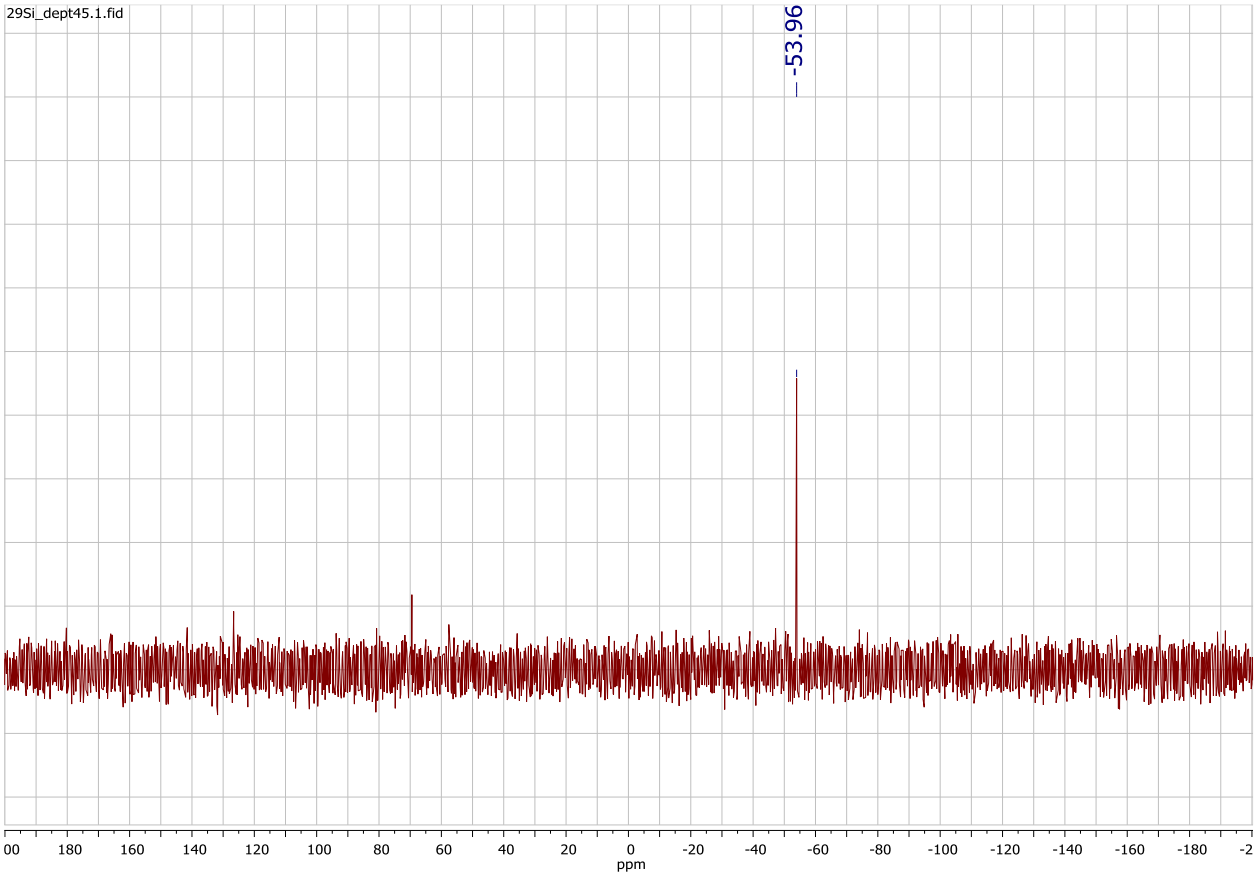

Fig. S12. NMR ^{29}Si of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(triethoxysilyl)methyl]urea 2a.

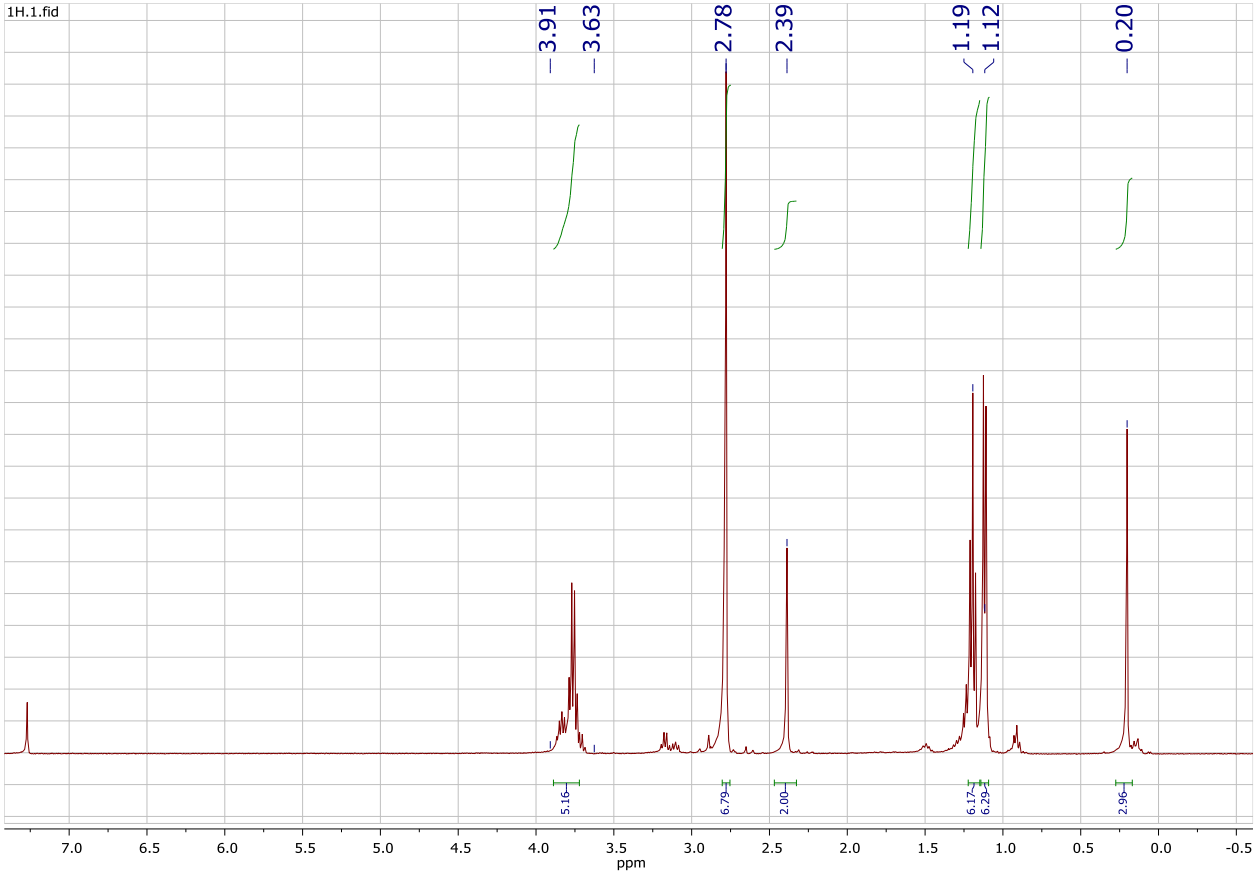

Fig. S13. NMR ^{1}H of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(diethoxy)silyl)methyl]urea 2b.

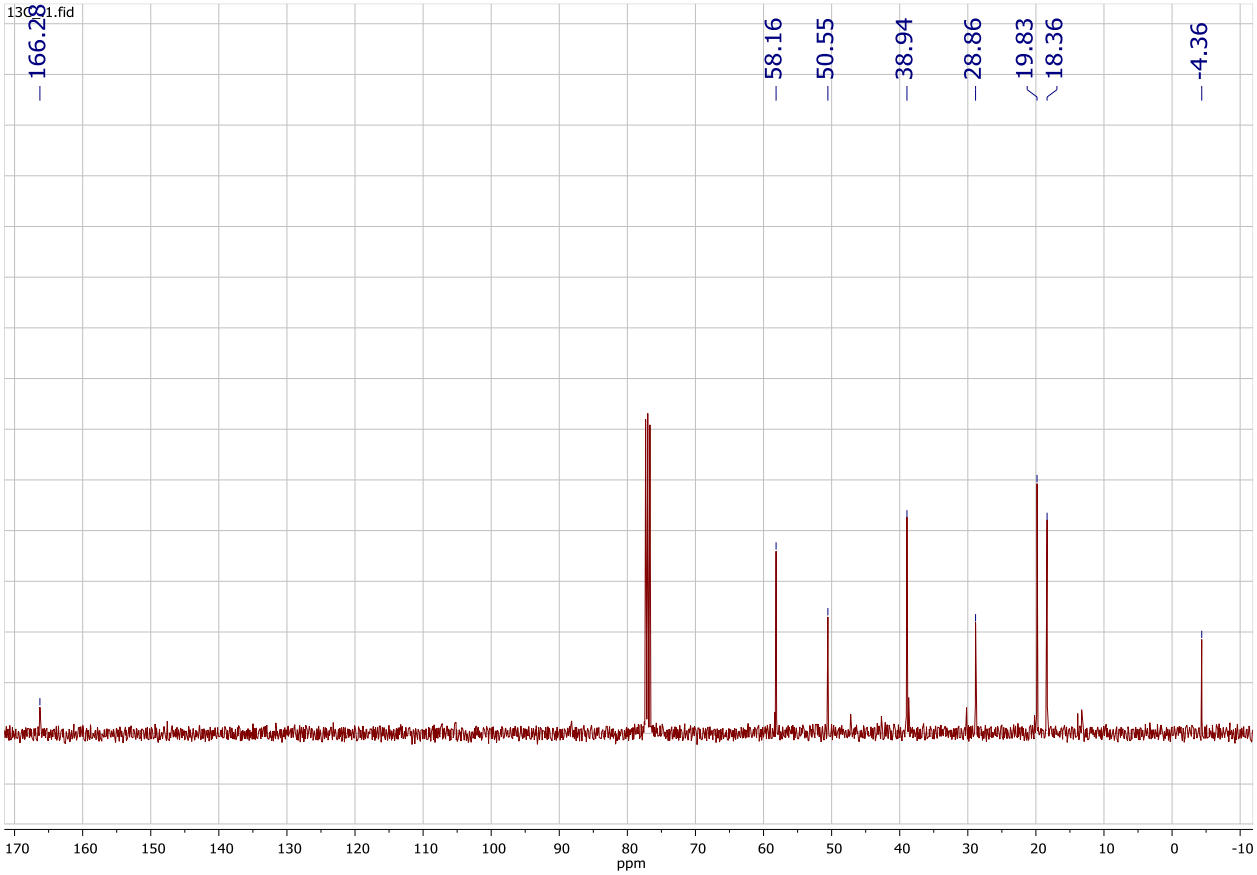

Fig. S14. NMR ^{13}C of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(diethoxy)silyl)methyl]urea 2b.

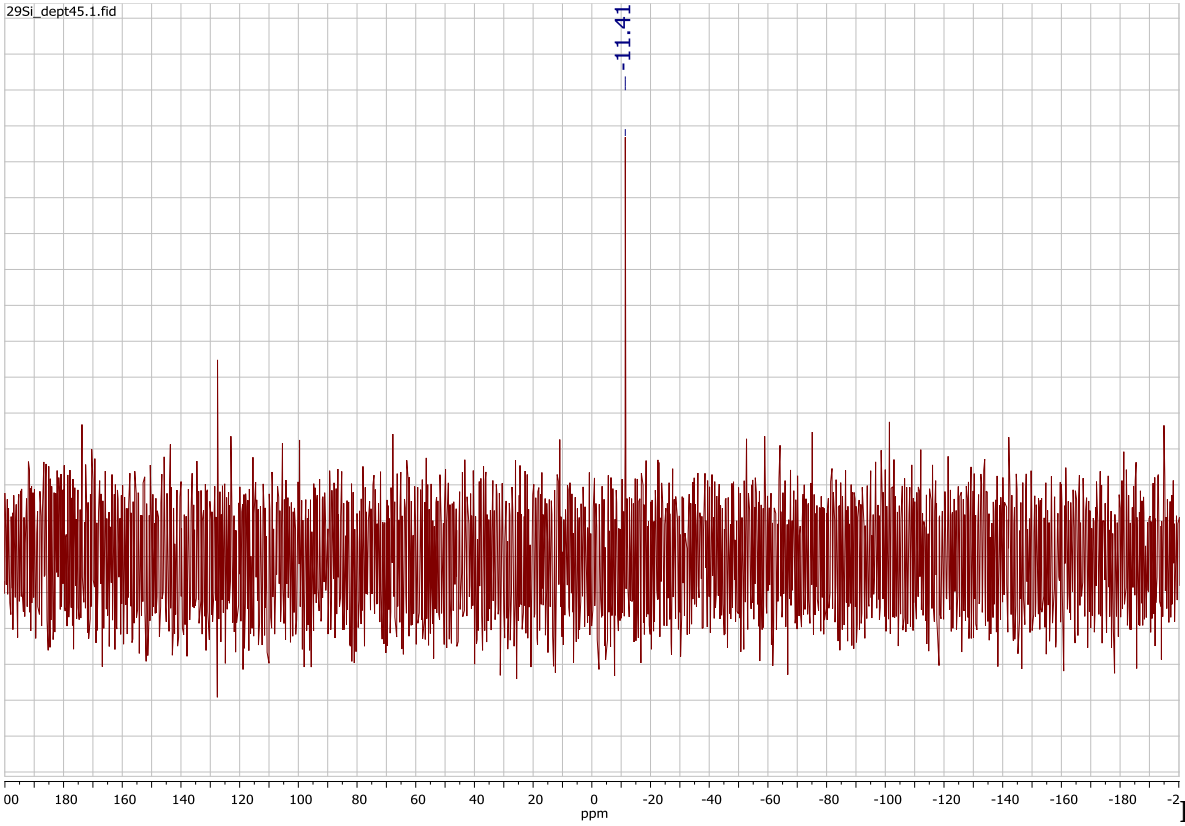

Fig. S15. NMR ^{29}Si of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(diethoxy)silyl)methyl]urea 2b.

Fig. S16. NMR ^{1}H of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(ethoxy)silyl)methyl]urea 2c.

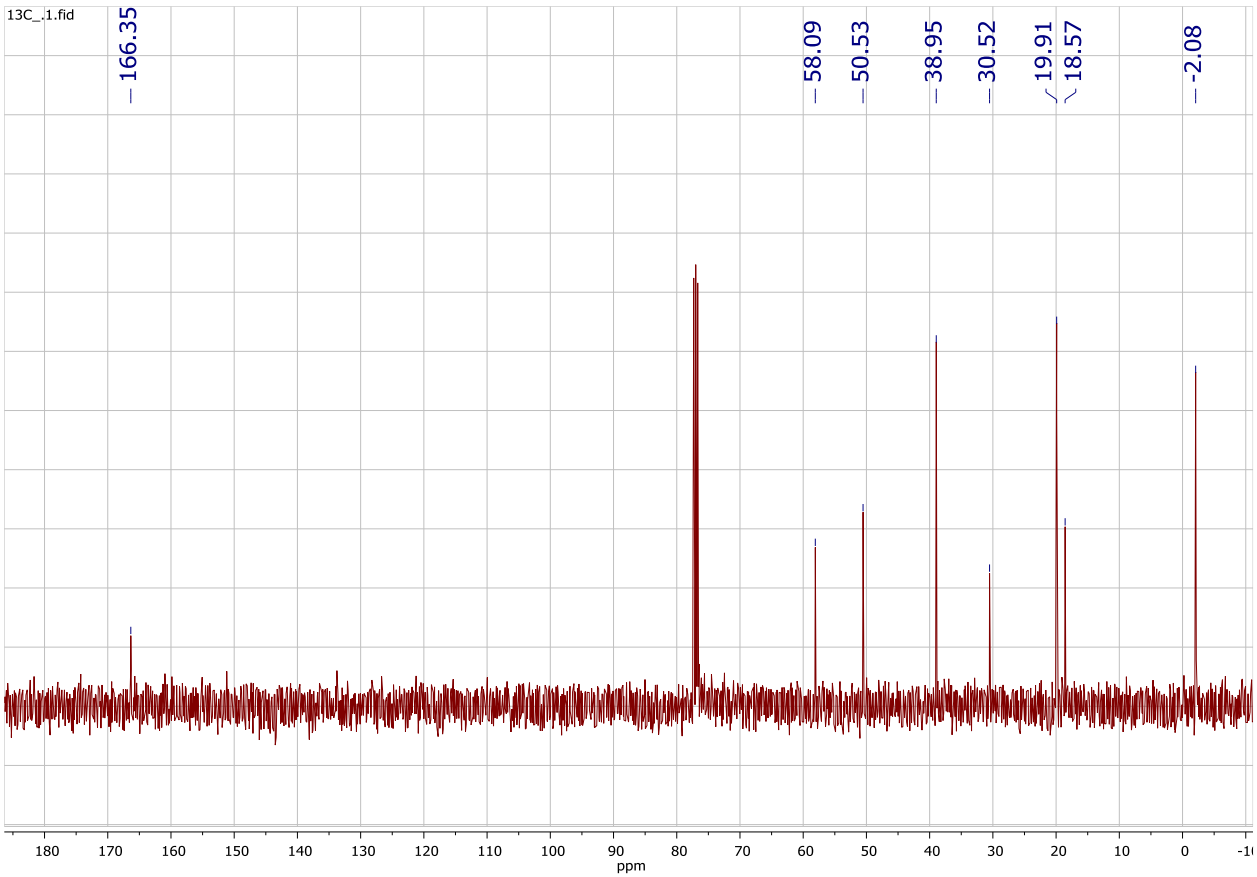

Fig. S17. NMR ^{13}C of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(ethoxy)silyl)methyl]urea 2c.

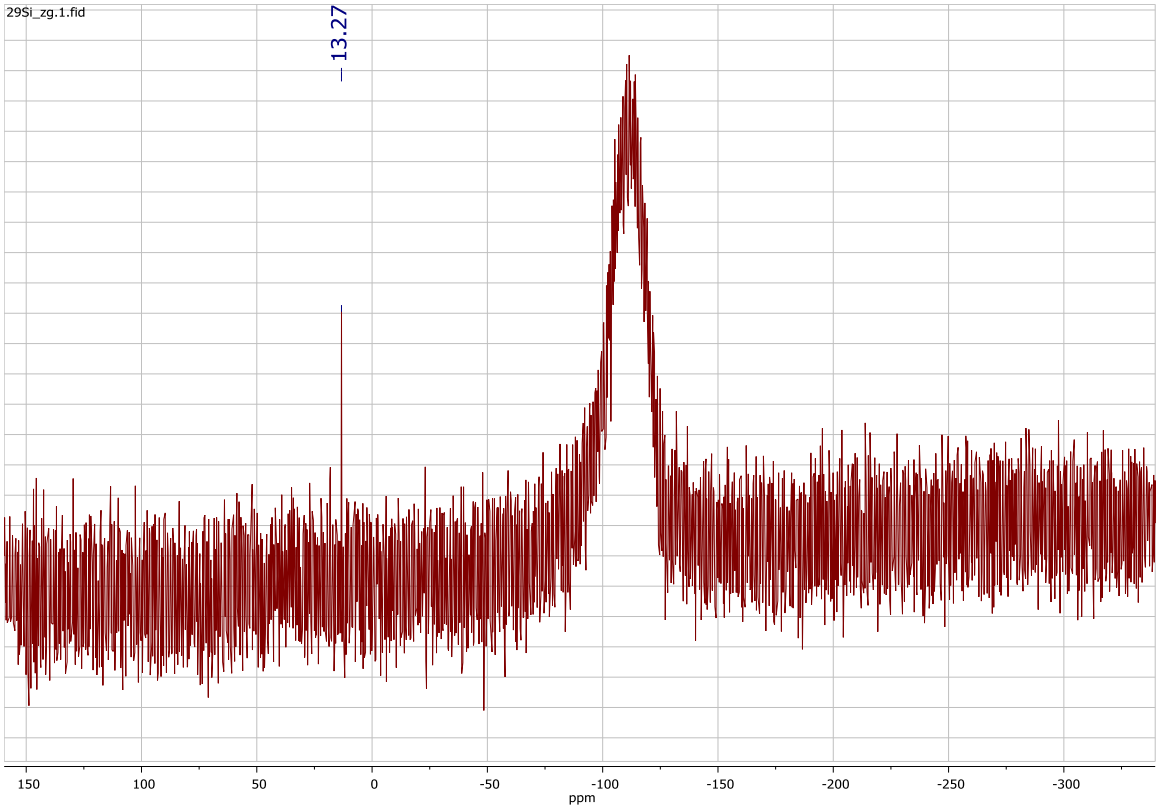

Fig. S18. NMR ^{29}Si *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(ethoxy)silyl)methyl]urea 2c.

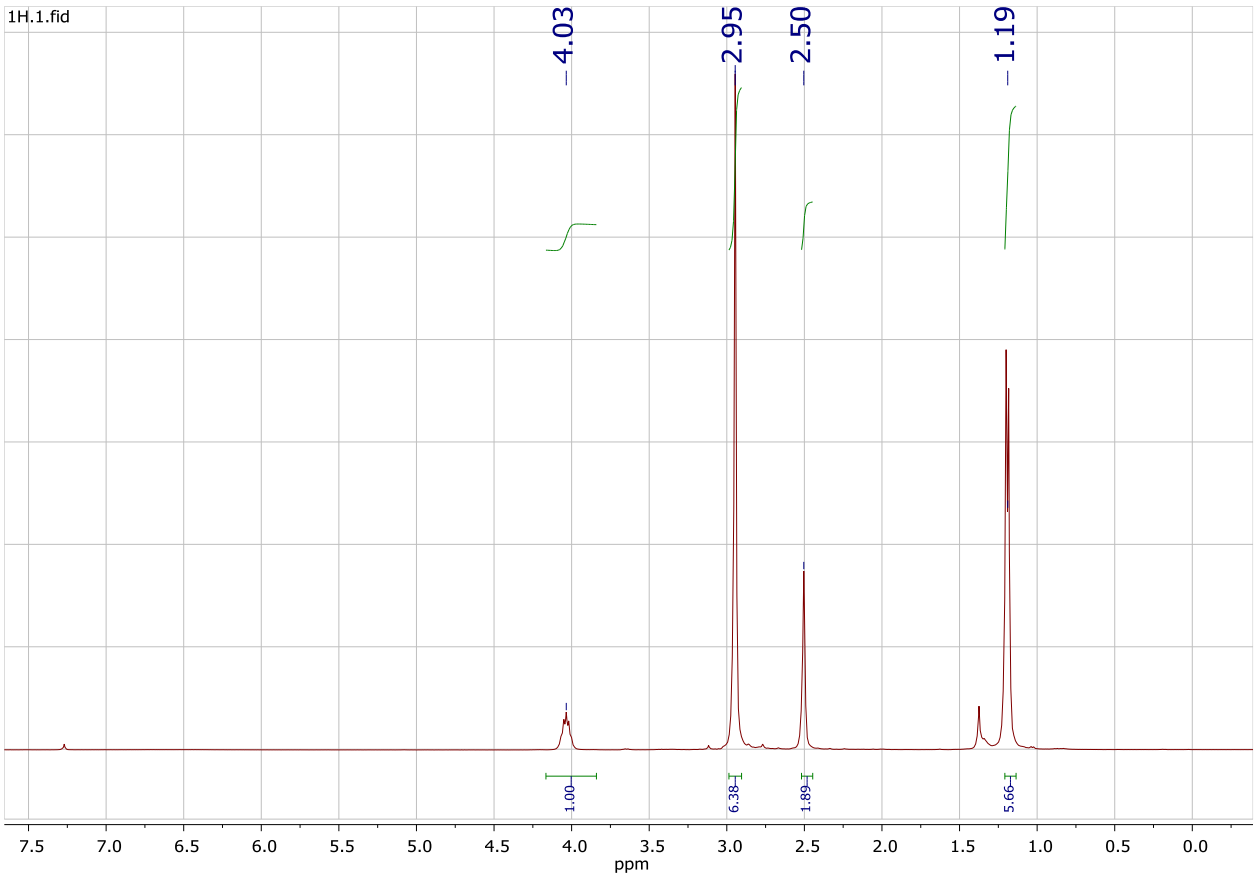

Fig. S19. NMR ^{1}H of *N*-isopropyl-*N′*,*N′*-dimethyl-*N*-[(trifluorosilyl)methyl]urea 3a.

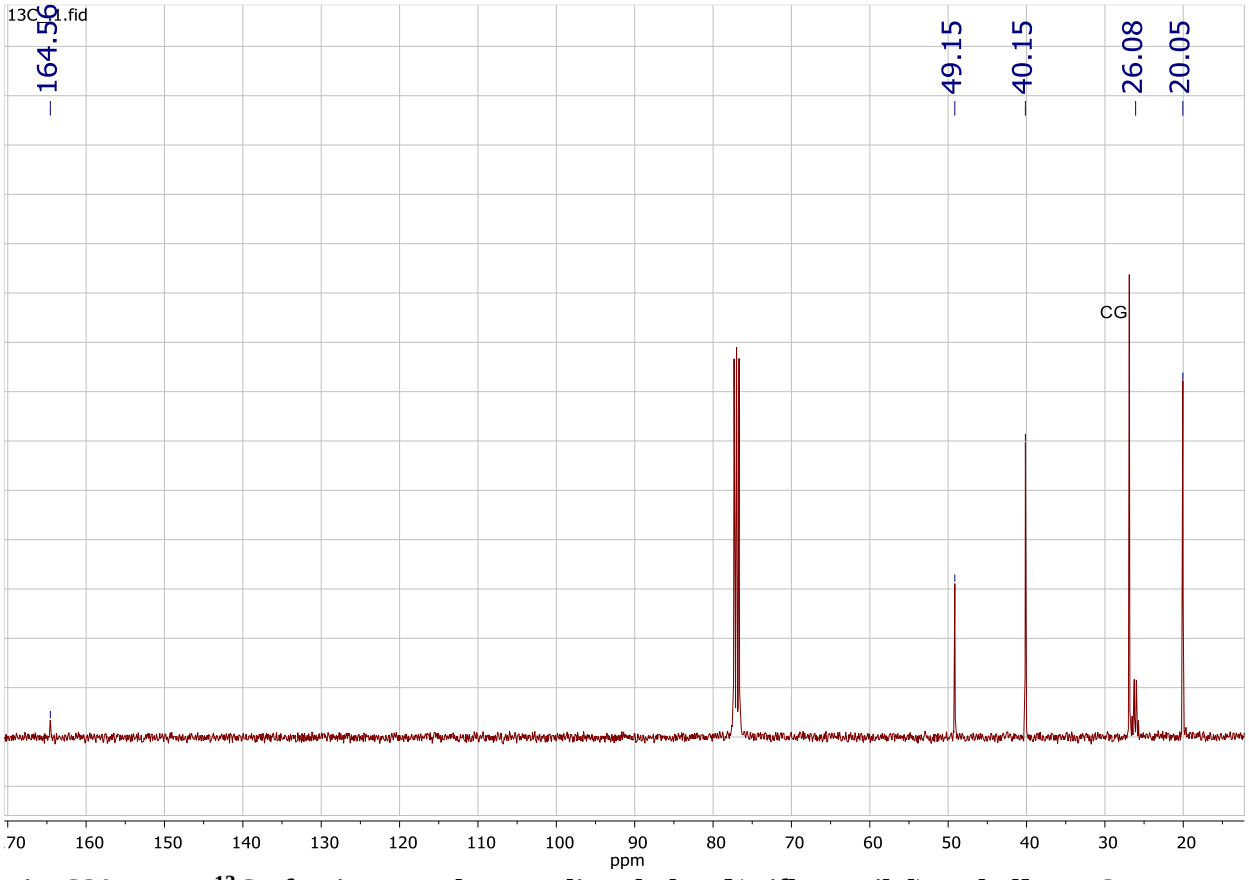

Fig. S20. NMR ^{13}C of *N*-isopropyl-*N′*,*N′*-dimethyl-*N*-[(trifluorosilyl)methyl]urea 3a.

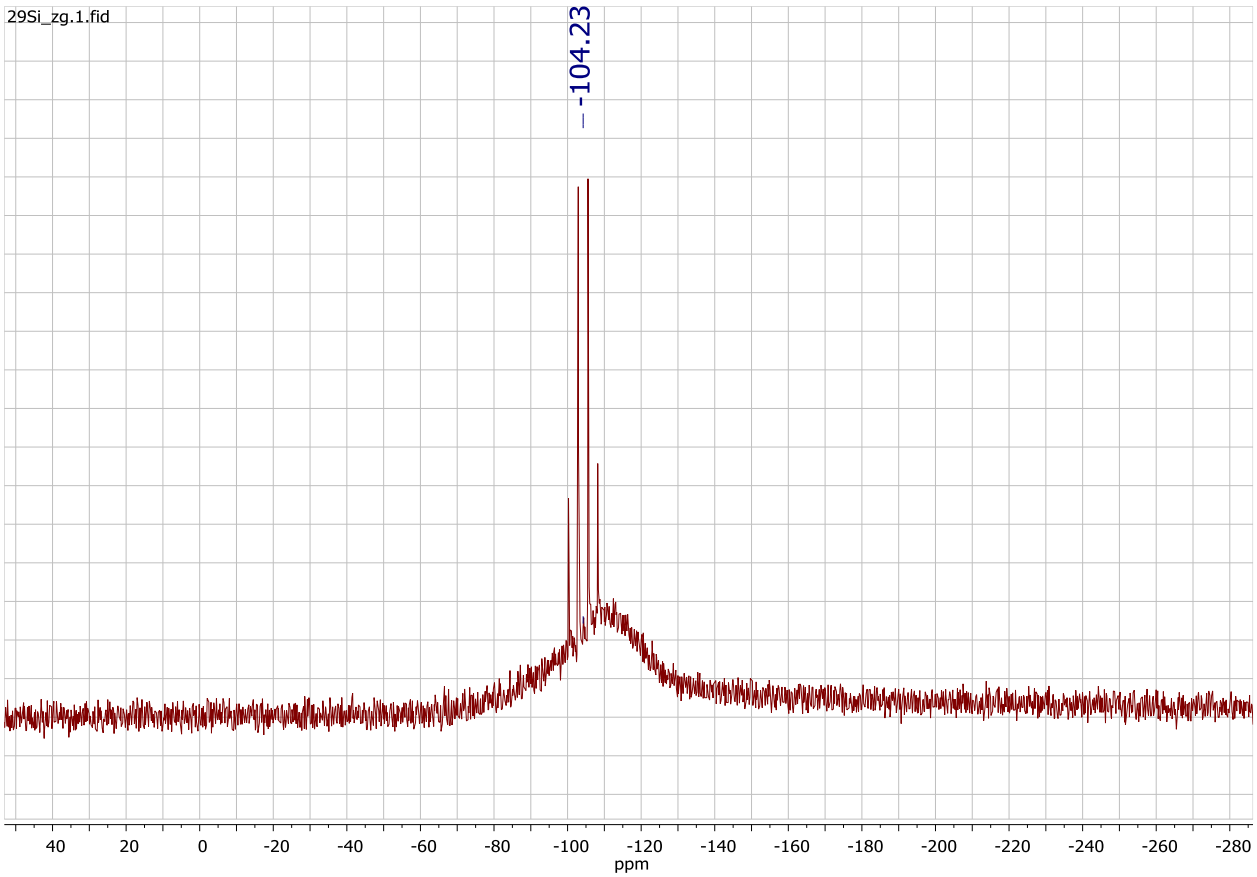

Fig. S21. NMR ^{29}Si of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(trifluorosilyl)methyl]urea 3a.

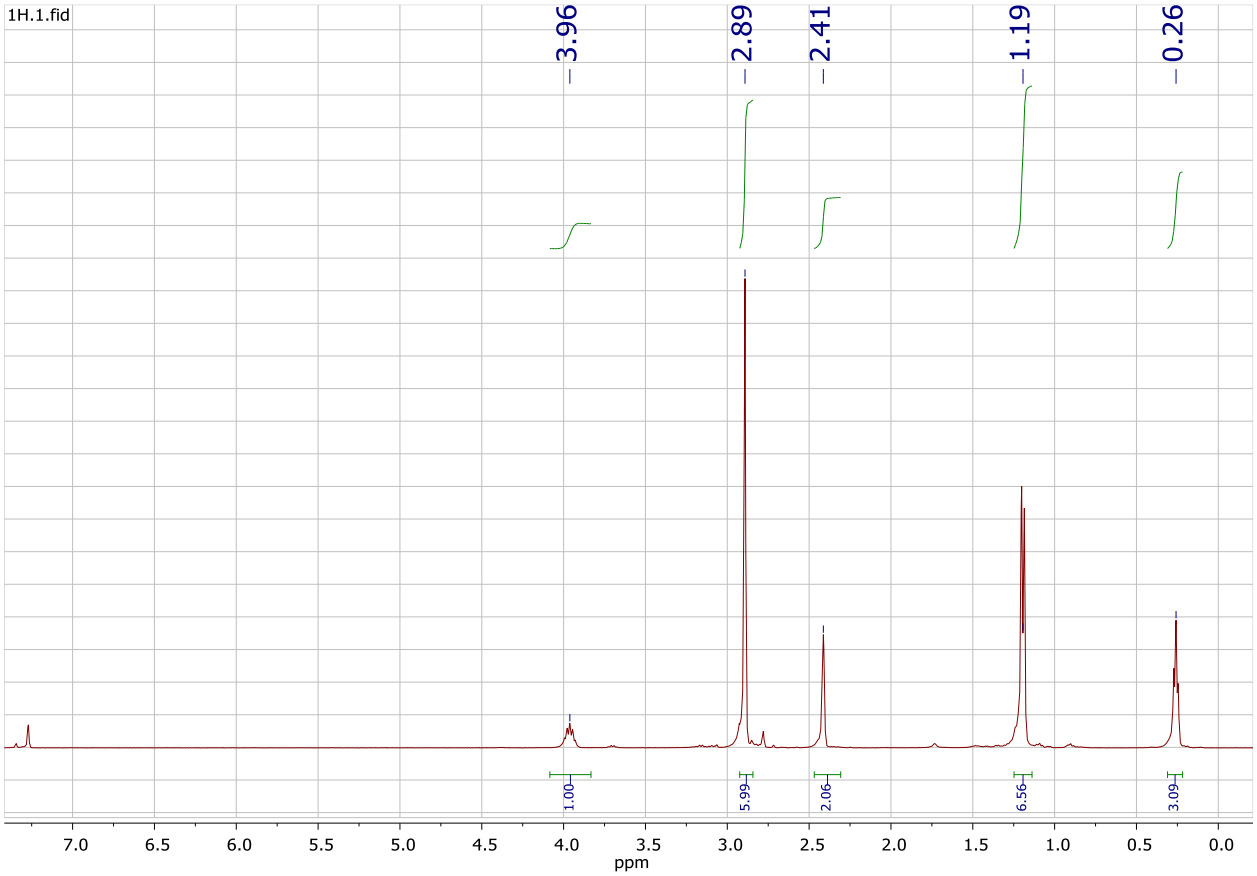

Fig. S22. NMR ^{1}H *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(difluoro)silyl)methyl]urea 3b.

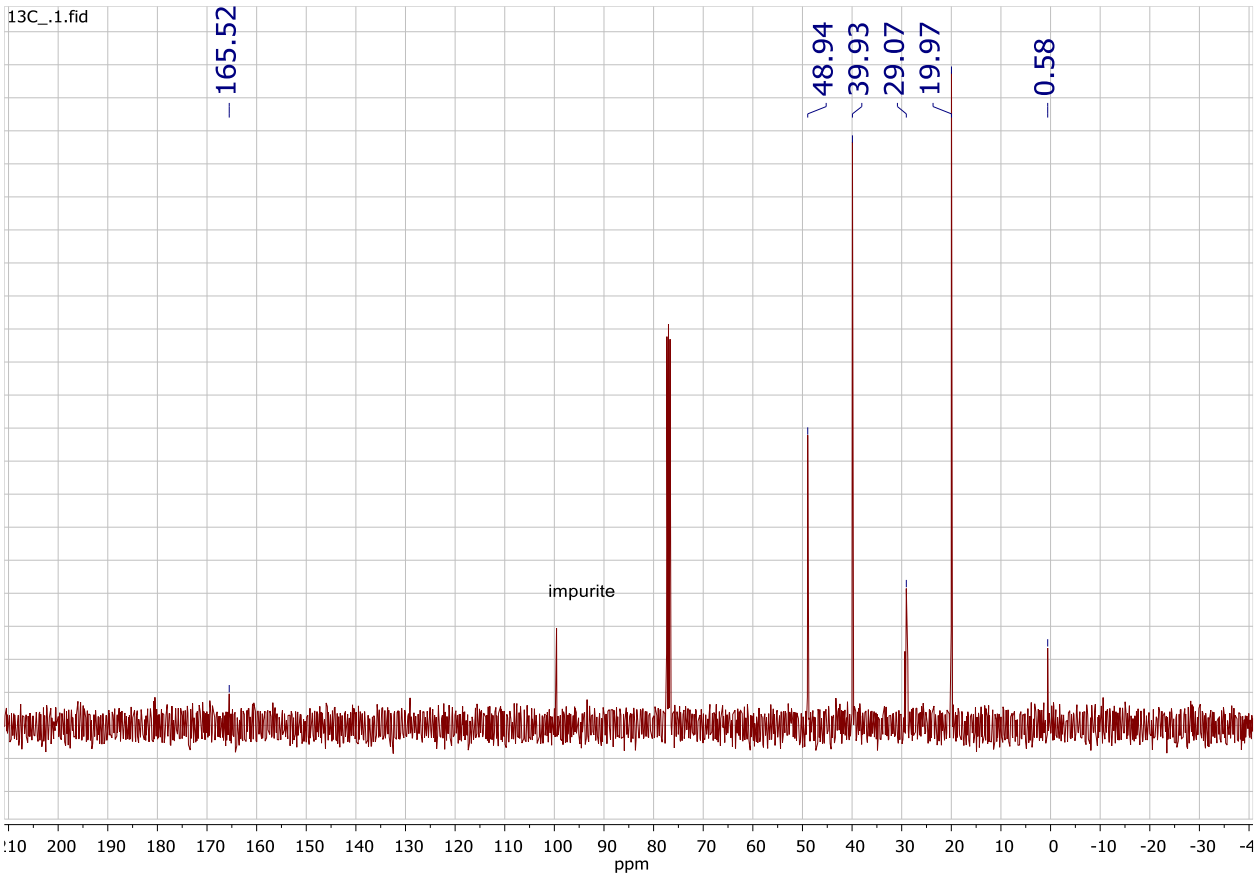

Fig. S23. NMR ^{13}C of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(difluoro)silyl)methyl]urea 3b.

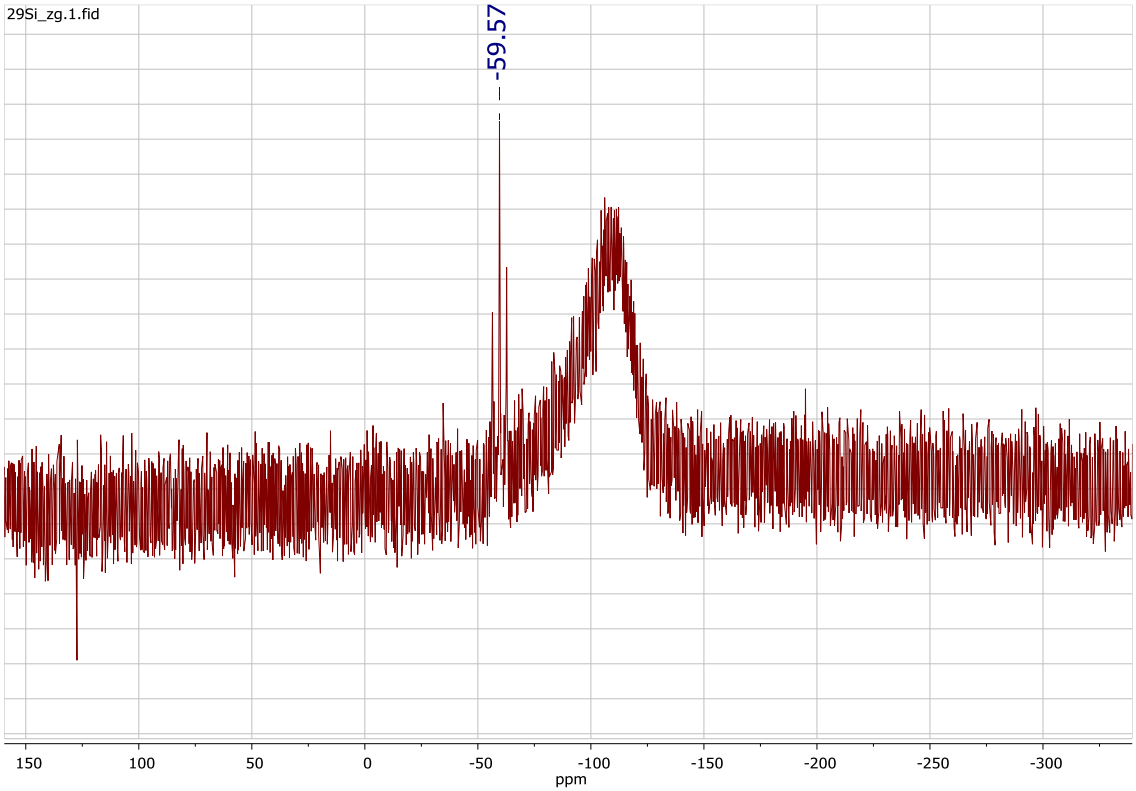

Fig. S24. NMR ^{29}Si of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(difluoro)silyl)methyl]urea 3b.

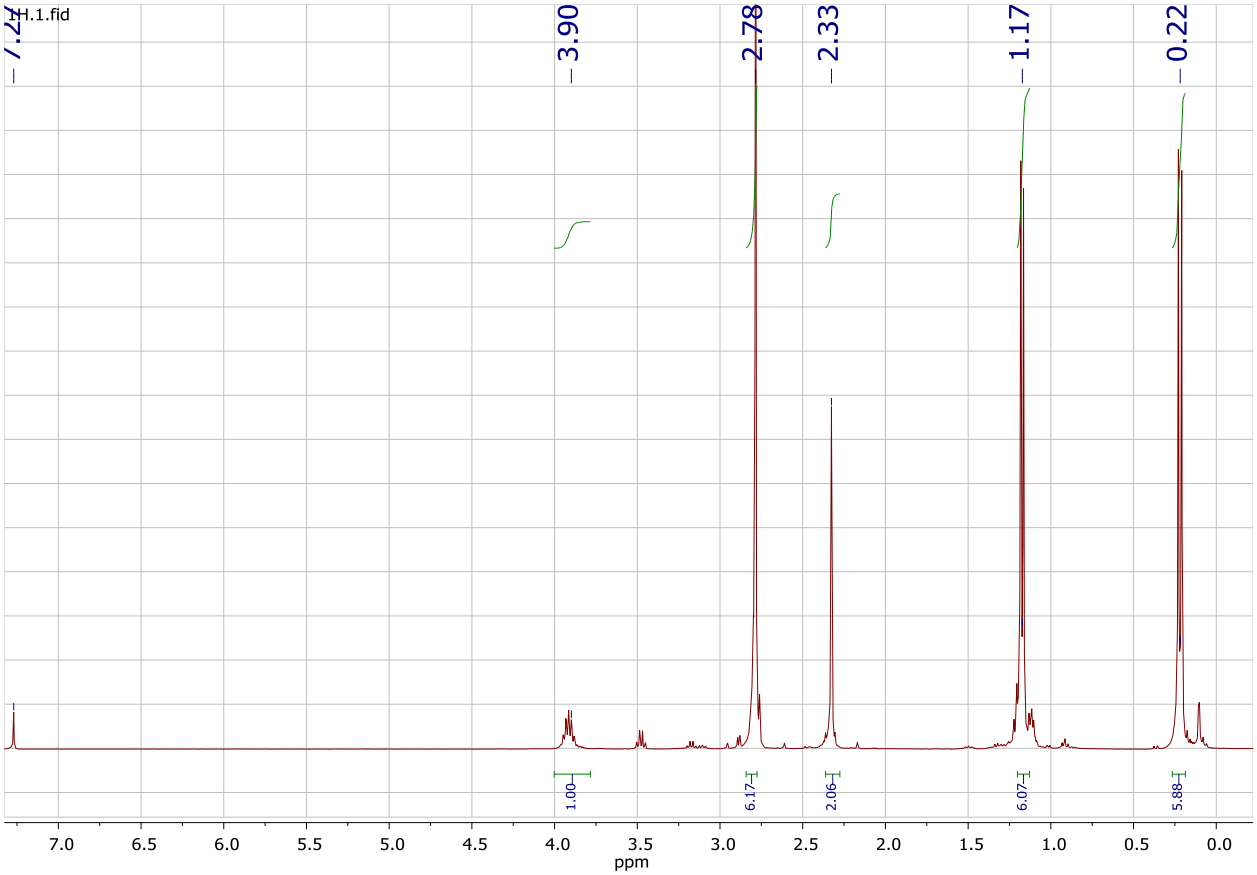

Fig. S25. NMR ^{1}H of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(fluoro)silyl)methyl]urea 3c.

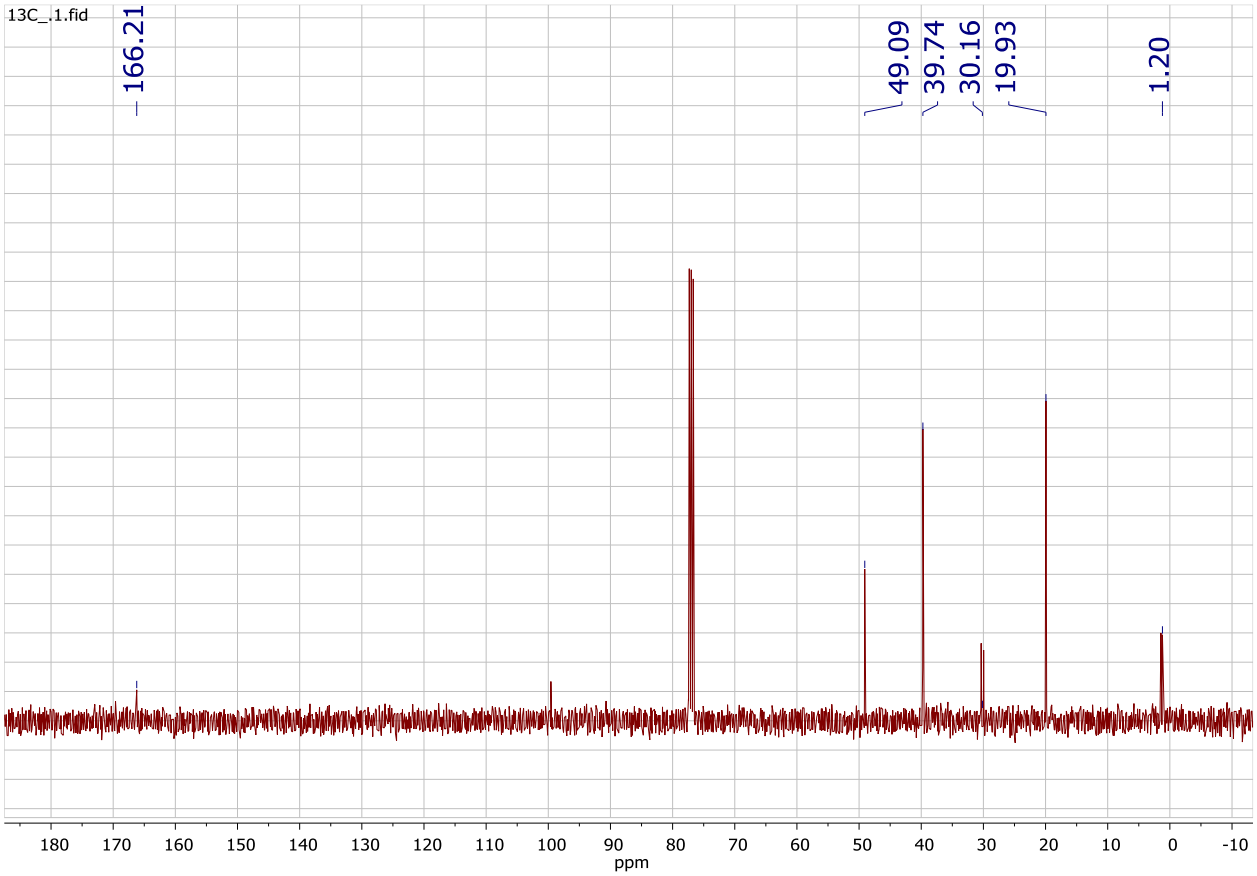

Fig. S26. NMR ^{13}C of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(fluoro)silyl)methyl]urea 3c.

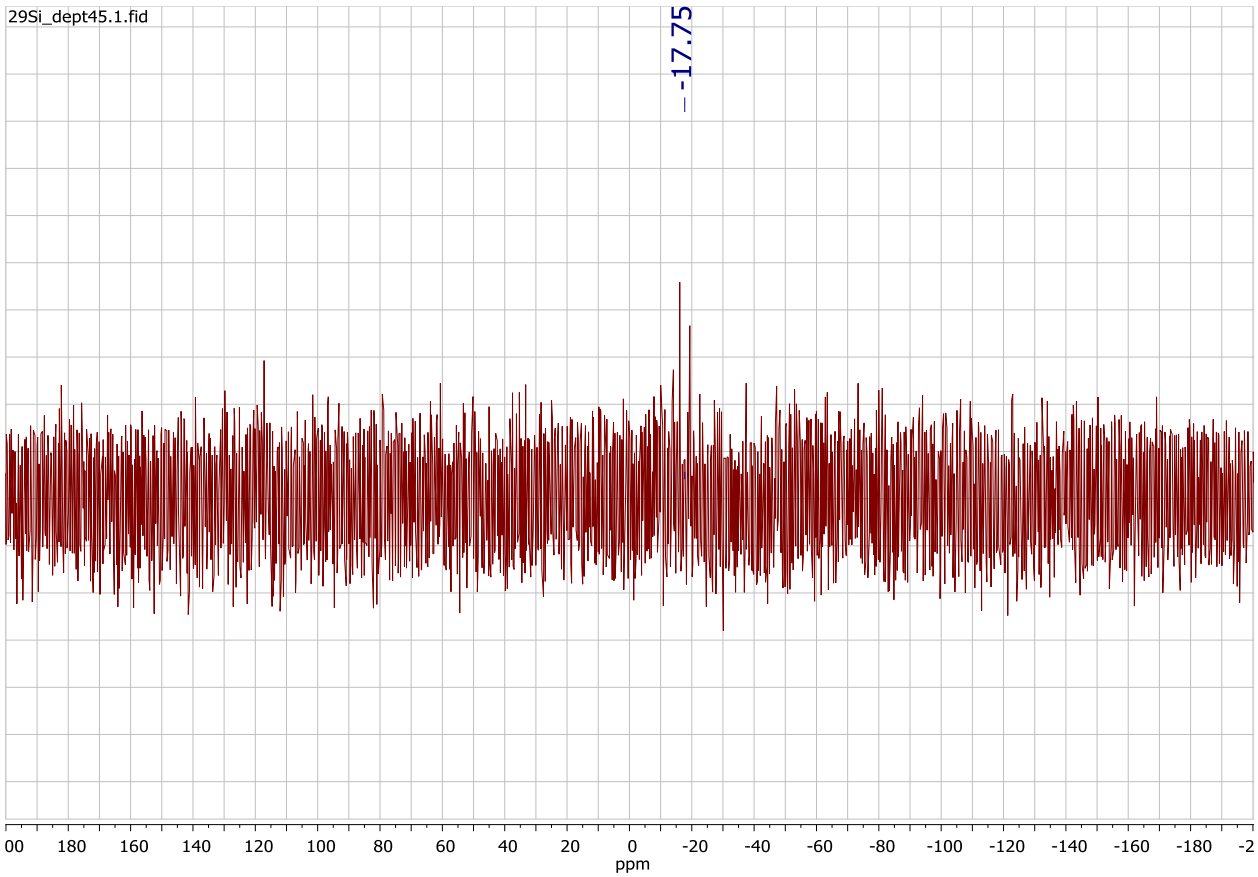

Fig. S27. NMR ^{29}Si of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(fluoro)silyl)methyl]urea 3c.

3. X-Ray analysis of compound 3a.

The single crystals of compound **3a** were obtained by re-crystallization from benzene solution. In order to investigate the molecular structure and intermolecular interactions in the solid state, X-ray structure analysis of the single crystal of compound **3a** was carried out. Crystal data, data collection and structure refinement details are summarized in Table S1. Principal bond distances, bond angles and torsion angles are presented in Table S2.

Table S1. Crystal data, details of intensity measurements, and structure refinement for compound **3a.**

Empirical formula	$C_7H_{15}F_3N2OSi$
Formula weight / g·mol^{-1}	228.3
Crystal system	monoclinic
Space group	P 2_1/c
a / Å	5.8697(3)
b / Å	23.6229(11)
c / Å	8.1910(4)
α, β, γ / °	90, 108.347(2), 90
Volume / Å^3	1078.03(9)
Z	4
Density (calculated) / g·cm^{-3}	1.388
Absorptions coefficient / mm^{-1}	0.232
Radiation (λ / Å)	MoKα (0.71073)
Temperature / K	293(2)
2Θ range / °	5.23 – 60.33
Crystal size / mm	0.200 × 0.200 × 0.400
Crystal habit	colorless prism
F(000)	468
Index ranges	$-7 \le h \le 8$, $-33 \le k \le 33$, $-11 \le l \le 11$
Reflections collected	30692
Independent reflections	3172
Max. and min. transmission	0.6775 / 0.7460
Number of ref. parameters	150
R_1 / wR_2 [$I > 2\sigma(I)$]	0.0442 / 0.1052
R_1 / wR_2 (all data)	0.0857 / 0.1222
Goodness-of-fit on F^2	1.015
Largest diff. peak and hole / e·Å^{-3}	0.220/ -0.321
Weight scheme	$w=1/[\sigma^2(F_o^2)+(0.0586P)^2+$ 0.2151P] where $P=(F_o^2+2F_c^2)/3$

Table S2. Selected bond lengths, bond and torsion angles in compound **3a.**

Bond	*l*, Å	Angle	φ, °	Torsion angle	θ, °
Si1-F1	1.585(1)	F1-Si1-O1	86.6(1)	F1-Si1-O1-C4	131.7(1)
Si1-F2	1.633(1)	F2-Si1-O1	176.3(1)	F3-Si1-O1-C4	-117.5(1)
Si1-F3	1.581(2)	F3-Si1-O1	88.6(1)	C6-Si1-O1-C4	4.2(1)
Si1-O1	1.880(1)	F1-Si1-C6	126.7(1)	C7-C2-N1-C4	-96.5(2)
Si1-C6	1.858(2)	F2-Si1-C6	92.9(1)	C1-C2-N1-C4	139.2(2)
O1-C4	1.284(2)	F3-Si1-C6	121.4(1)	C7-C2-N1-C6	64.6(2)
N1-C4	1.331(2)	F1-Si1-F2	93.6(1)	C1-C2-N1-C6	-59.7(2)
N2-C4	1.345(2)	F3-Si1-F2	94.7(1)	Si1-O1-C4-N1	1.2(2)
N1-C6	1.463(2)	F3-Si1-F1	110.6(1)	Si1-O1-C4-N2	-178.8(1)
N1-C2	1.483(2)	C6-Si1-O1	84.0(1)	C6-N1-C4-O1	-7.9(2)
C1-C2	1.511(3)	C4-O1-Si1	114.7(1)	C2-N1-C4-O1	154.2(2)
C2-C7	1.509(3)	C4-N2-C5	123.2(2)	C6-N1-C4-N2	172.2(2)
N2-C3	1.463(3)	C4-N2-C3	117.6(2)	C2-N1-C4-N2	-25.7(3)
N2-C5	1.458(2)	O1-C4-N1	117.4(1)	C5-N2-C4-O1	146.1(2)

4. IR spectra

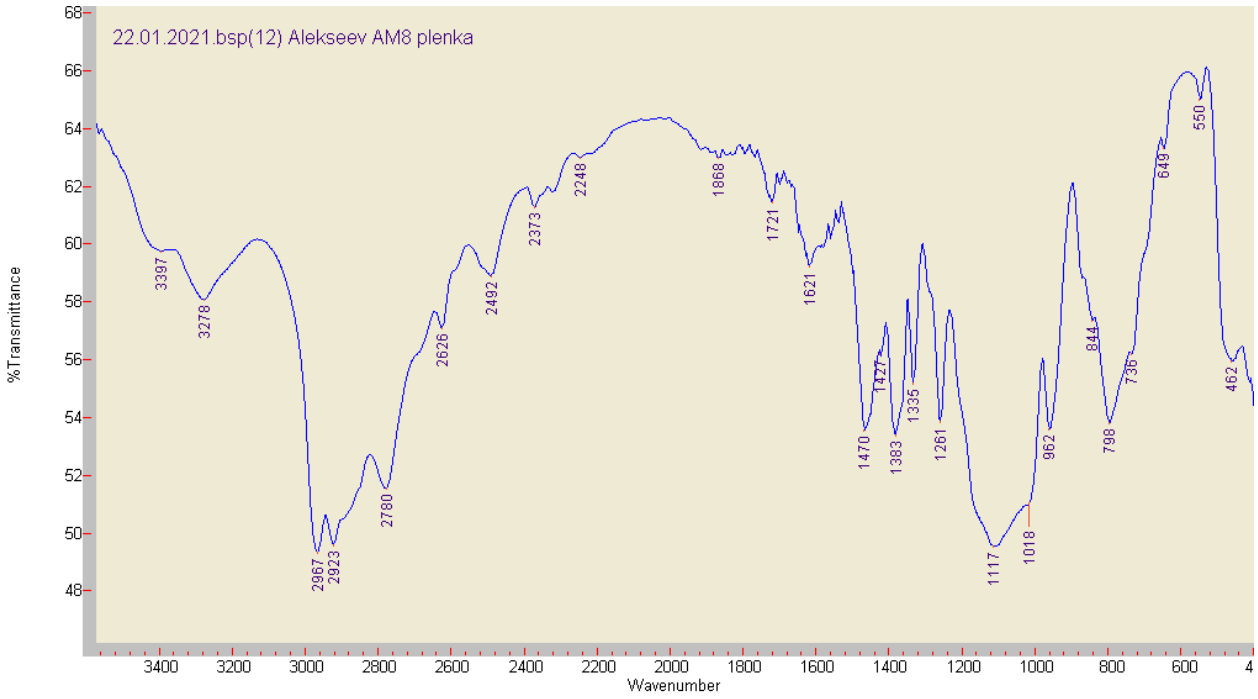

Fig. S28. IR spectrum of *N*-[(triethoxysilyl)methyl]isopropylamine 1a.

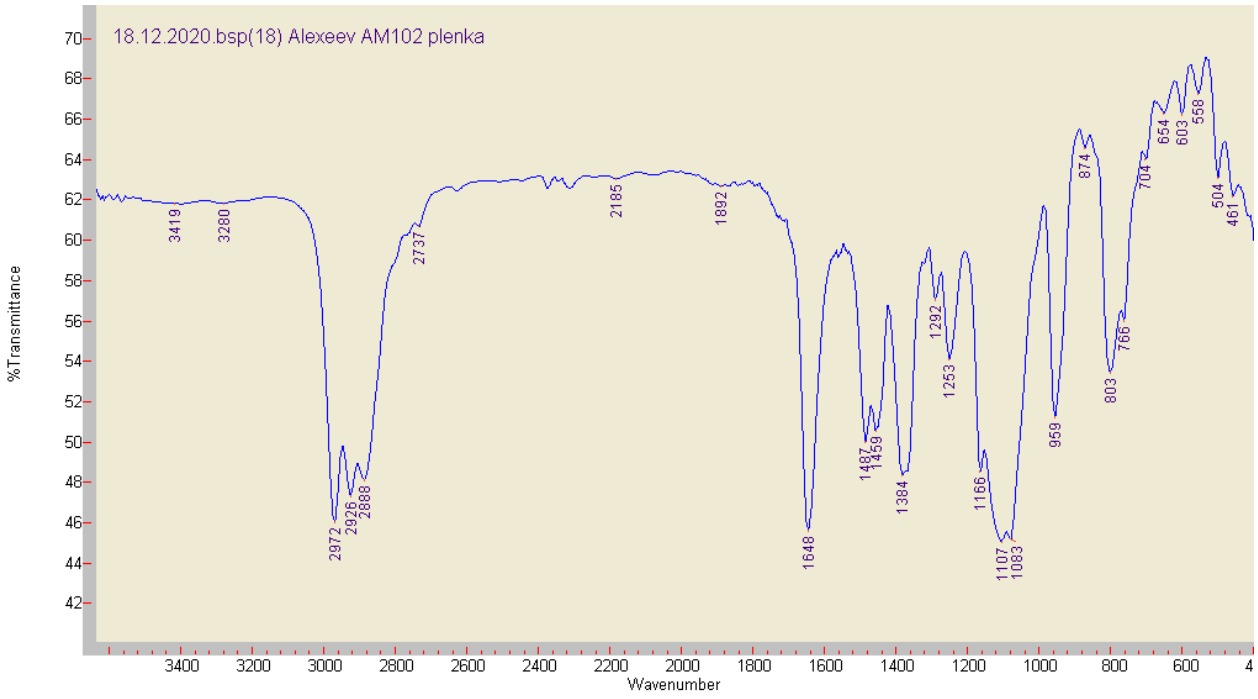

Fig. S29. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(triethoxysilyl)methyl]urea 2a.

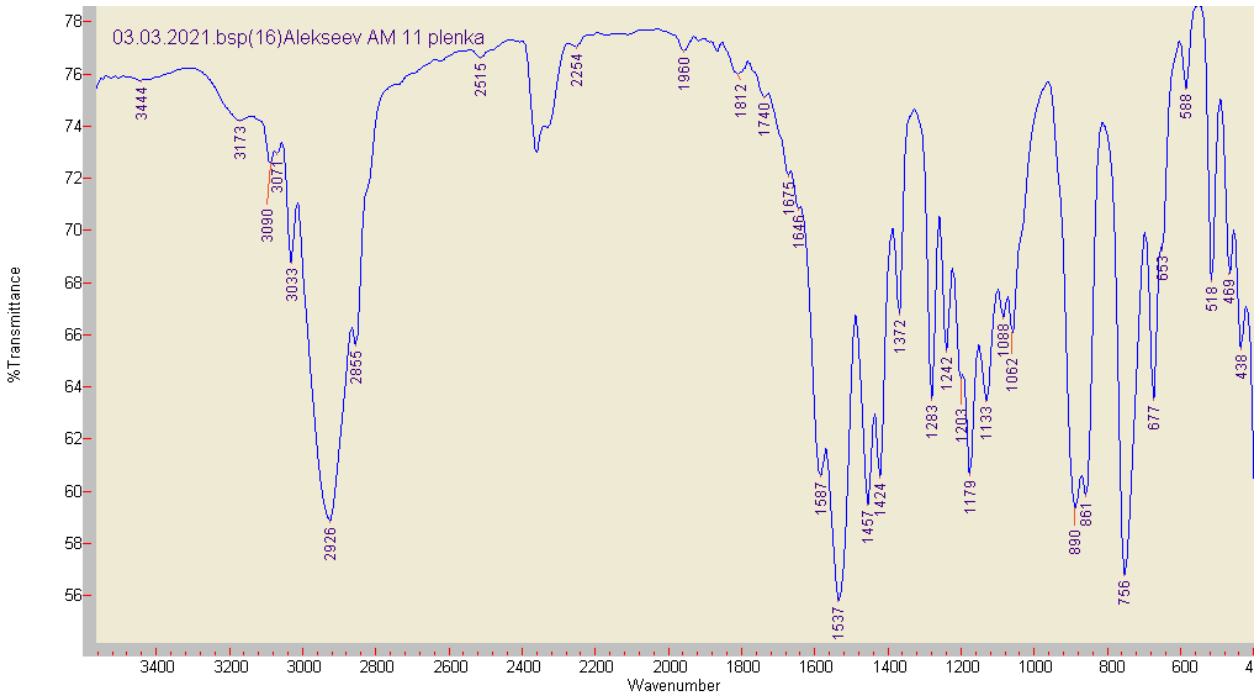

Fig. S30. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(trifluoroxysilyl)methyl]urea 3a.

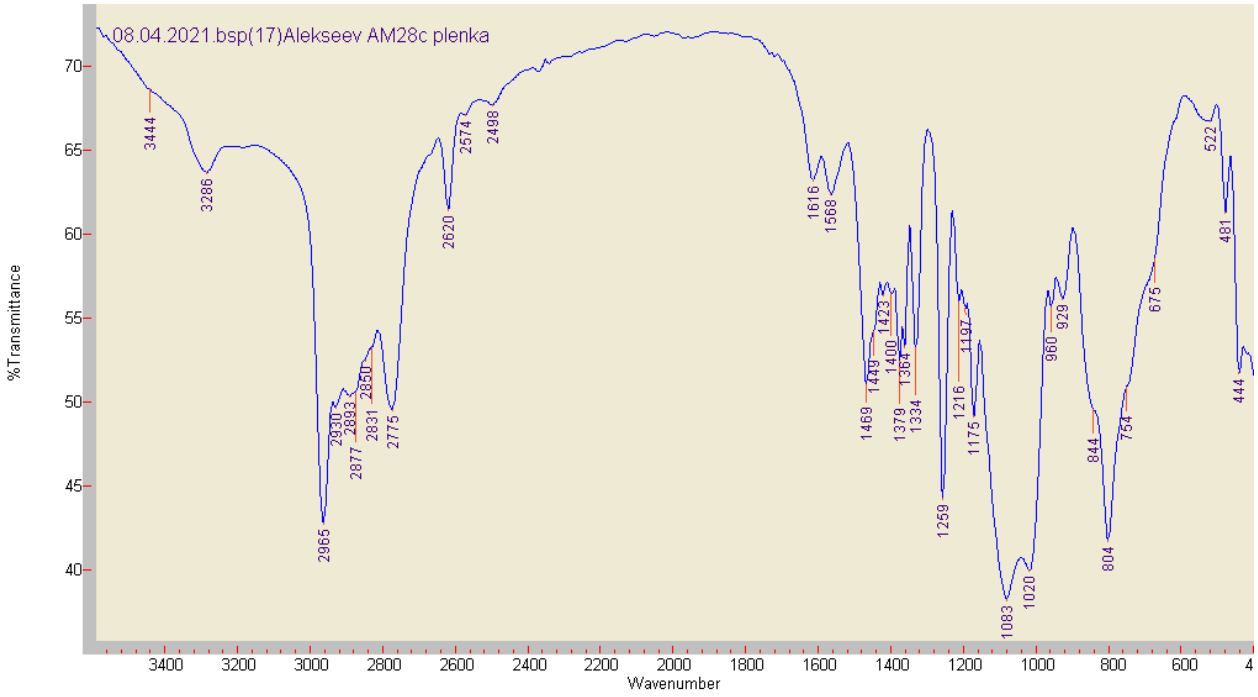

Fig. S31. IR spectrum of *N*-[(methyl(diethoxy)silyl)methyl]isopropylamine 1b.

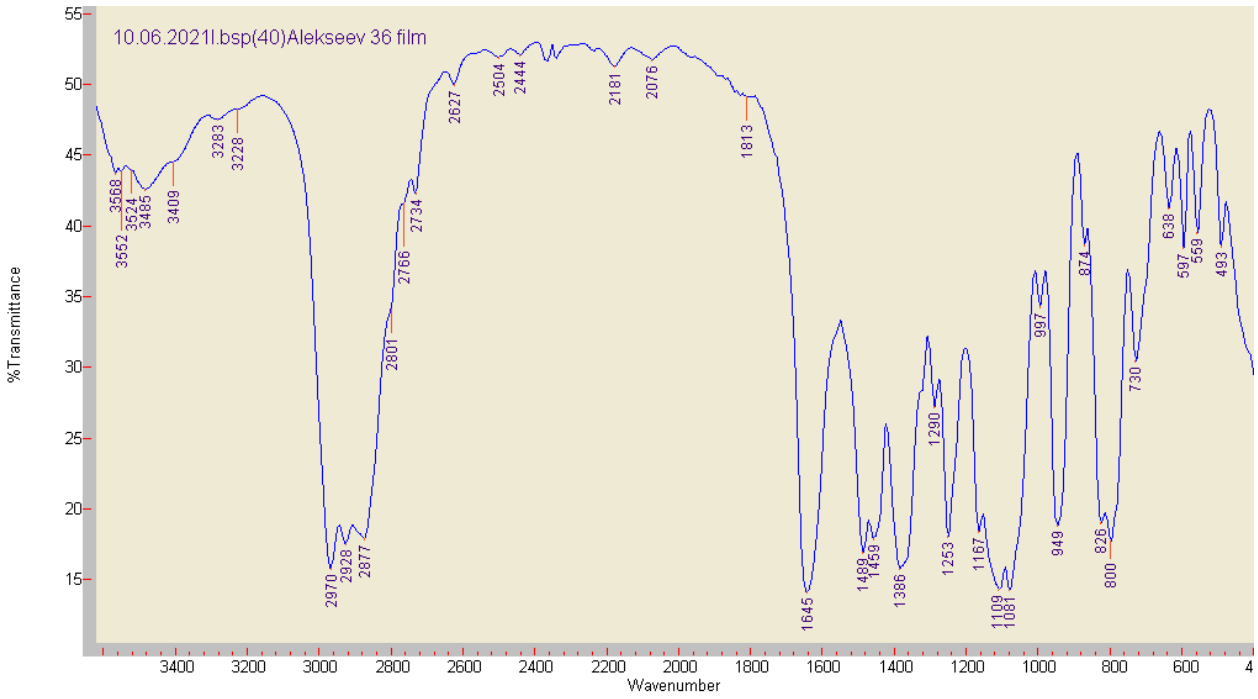

Fig. S32. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(diethoxysilyl)methyl]urea 2b.

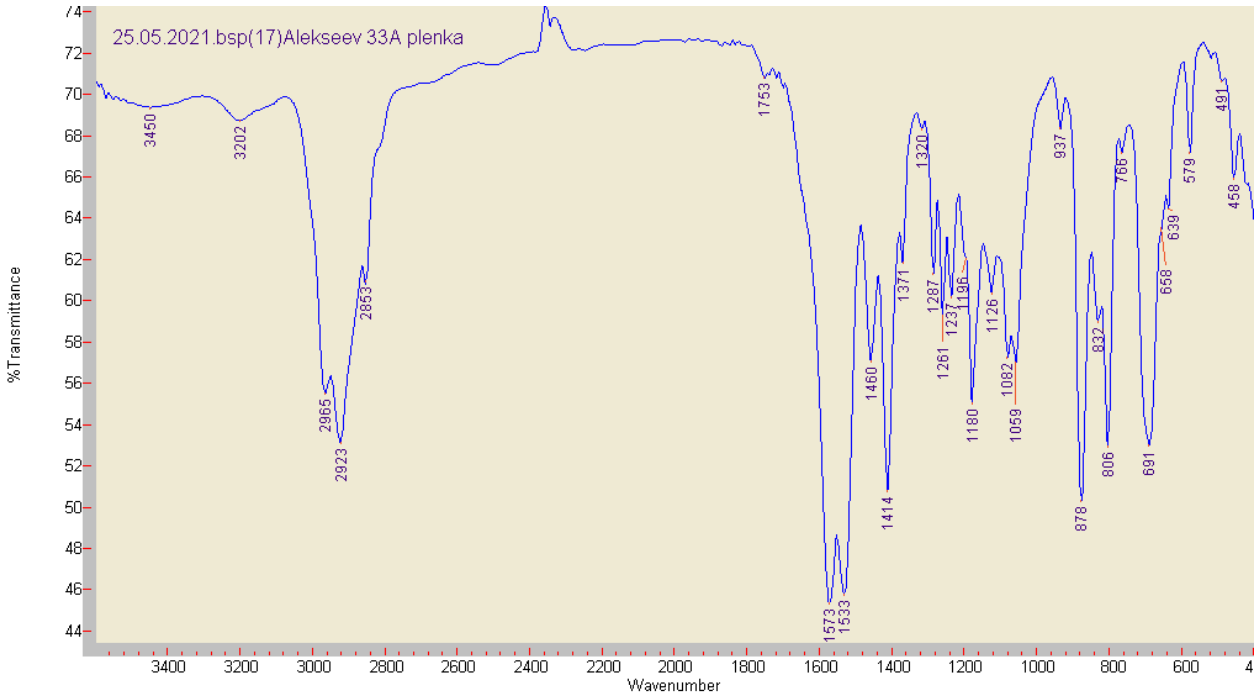

Fig. S33. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(methyl(difluoro)silyl)methyl]urea 3b.

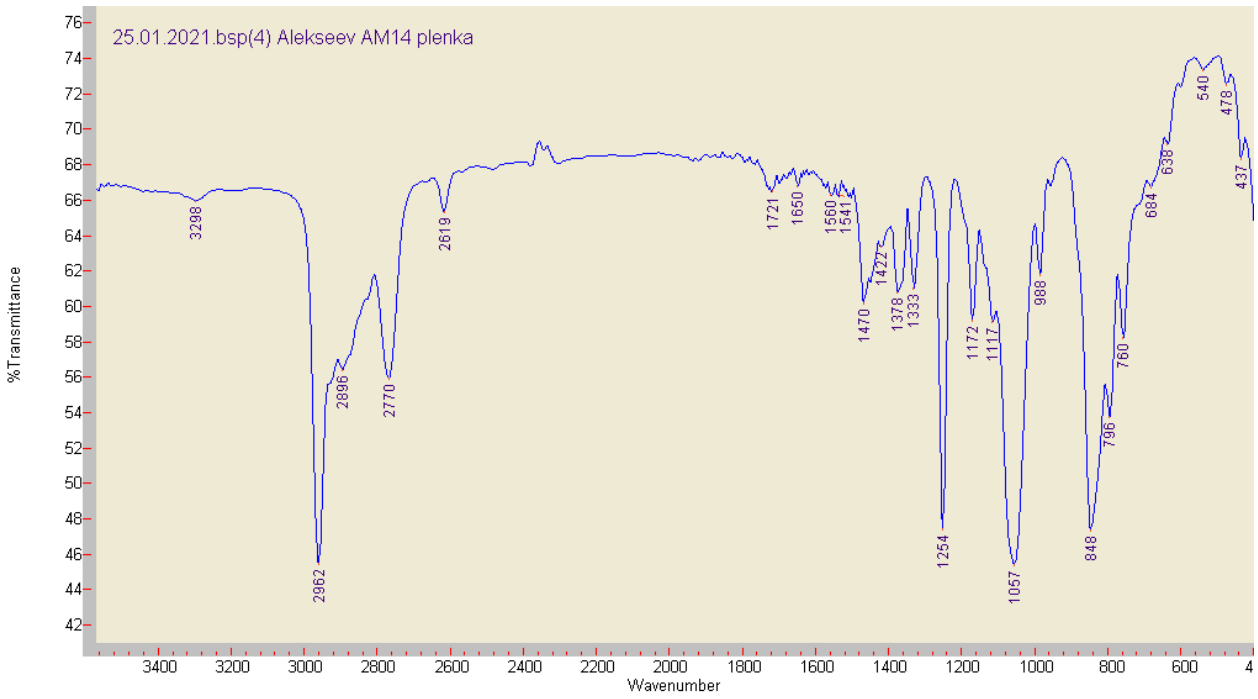

Fig. S34. IR spectrum of *N*-[(dimethyl(ethoxy)silyl)methyl]isopropylamine 1c.

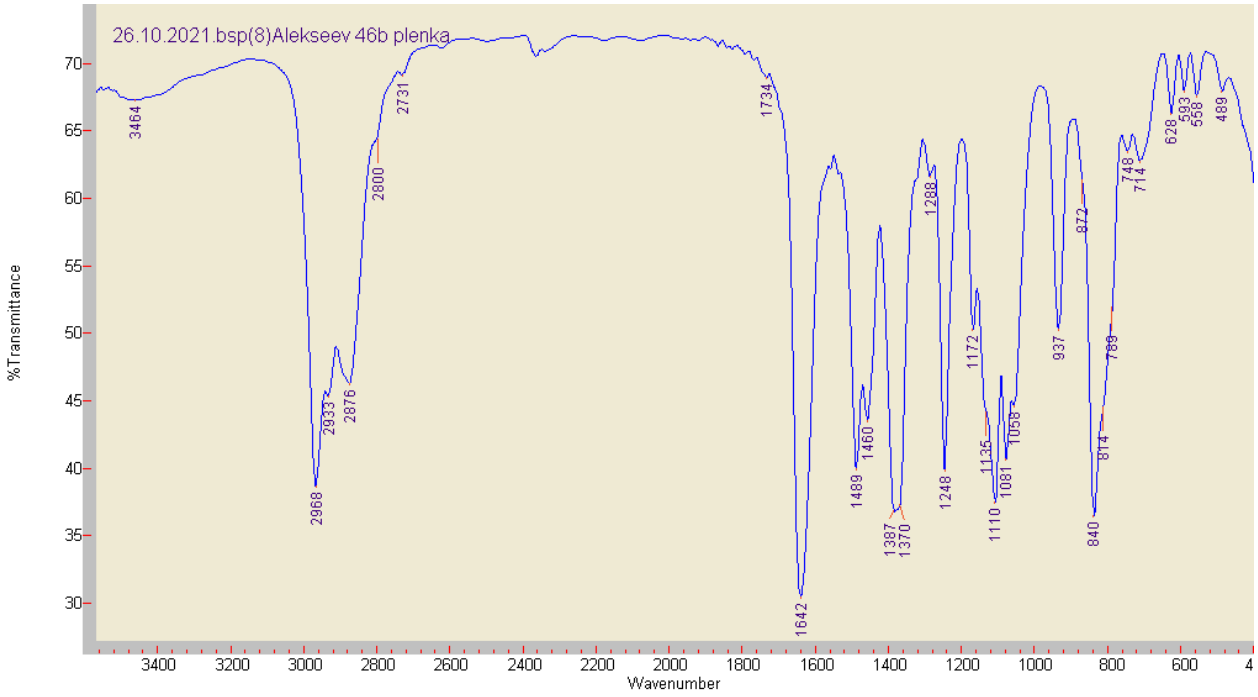

Fig. S35. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(ethoxysilyl)methyl]urea 2c.

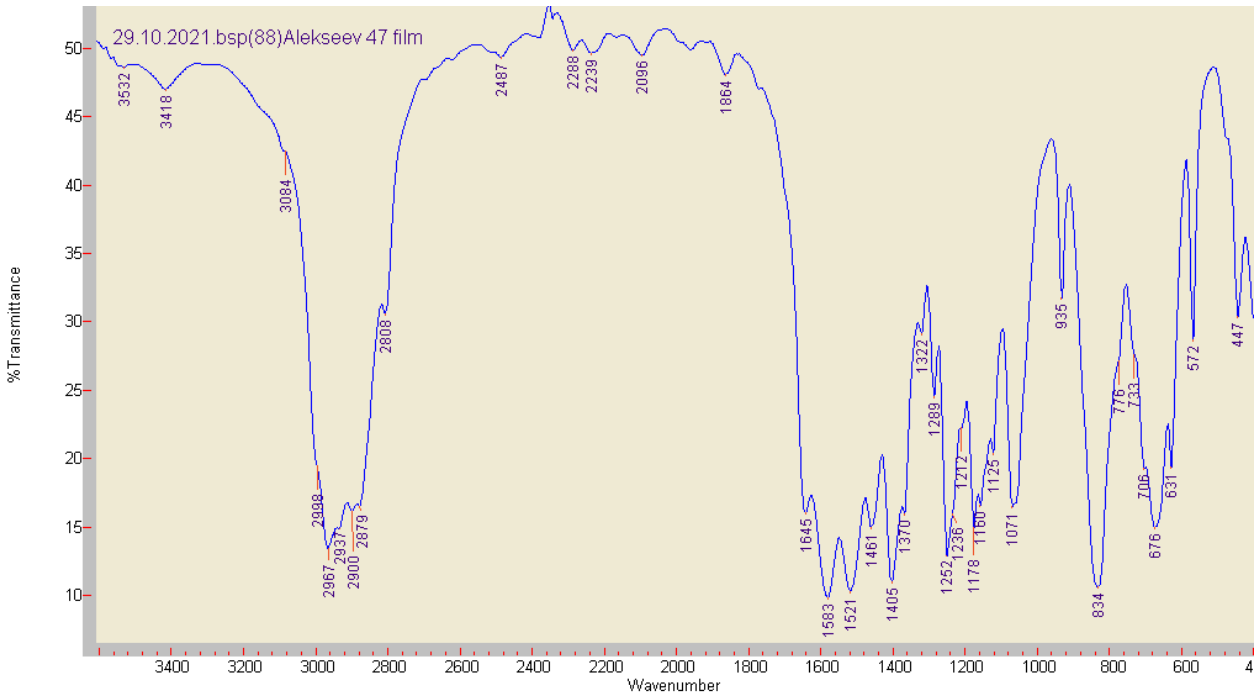

Fig. S36. IR spectrum of *N*-isopropyl-*N'*,*N'*-dimethyl-*N*-[(dimethyl(fluorosilyl)methyl]urea 3c.