Supporting Information for
Complexity-Enhancing Acid-Promoted Rearrangement of Tricyclic Products
of Tandem Ugi 4CC/ Intramolecular Diels-Alder Reaction

Alexei Ilyin,^a Volodymyr Kysil,^b Mikhail Krasavin,^a Irina Kurashvili,^a and
Alexandre V. Ivachtchenko^{b}*

^a Chemical Diversity Research Institute, Khimki, Moscow Reg., 141400 Russia

^b ChemDiv, Inc., 11558 Sorrento Valley Rd., Suite 5, San Diego, CA 92121, USA

Contents

Experimental Procedures and Characterization Data
(including ORTEP plots of X-ray structures for compounds **1d** and **3d**) S2 – S8

¹H and ¹³C NMR spectra of compounds **1a-f**, **3a-f**, **7**, **8** S9 – S38

S-2

General Methods

All reactions were run in oven-dried glassware in atmosphere of nitrogen. Melting points were not corrected. Analytical thin-layer chromatography was carried out on F₂₅₄ silica gel plates. Compounds were visualized with short-wavelength UV light. All solvents and reagents were obtained from commercial sources and used without purification.

1b:

White solid, mp = 234-236 °C (decomp.). ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.67 (s, 1H), 8.40 (d, *J* = 6.7 Hz, 1H), 7.30 (m, 1H), 7.11 (t, *J* = 8.5 Hz, 2H), 7.03 (s, 1H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.41 (s, 2H), 4.52 (s, 1H), 4.05 (m, 1H), 2.95 (d, *J* = 8.6 Hz, 1H), 2.90 (d, *J* = 8.6 Hz, 1H), 2.24 (s, 3H), 2.13 (s, 3H), 1.85 (m, 1H), 1.76 (m, 1H), 1.62 (s, 3H), 1.49 – 1.60 (m, 4H), 1.41 (m, 1H), 1.28 (m, 1H) – a number of signals broadened due to restricted N-Ar bond rotation; ¹³C NMR (125 MHz, DMSO-*d*₆) δ 170.1, 167.2, 167.1, 157.6 (dd, *J* = 247.8, 5.5 Hz), 140.2, 137.1, 136.5, 135.7, 133.9, 130.9, 127.7, 127.4 (t, *J* = 9.6 Hz), 126.6, 114.6 (t, *J* = 16.9 Hz), 111.6 (d, *J* = 23.7 Hz), 89.3 (d, *J* = 25.1 Hz), 64.6, 52.5, 50.6, 47.8, 32.2, 31.8, 23.2, 23.1, 20.5, 17.1, 15.3 – a number of signals broadened due to restricted N-Ar bond rotation; LCMS *m/z* 536 (M+H); HRMS calcd for C₃₀H₃₂O₄N₃F₂ (M+H) 536.2355, found 536.2361.

1c:

White solid, mp = 186 - 188 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.73 (s, 1H), 9.08 (t, *J* = 5.5 Hz, 1H), 7.26 – 7.36 (m, 5H), 7.12 (t, *J* = 8.6 Hz, 2H), 7.01 (s, 1H), 6.85 (d, *J* = 9.2 Hz, 1H), 6.69 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.36 (d, *J* = 5.5 Hz, 1H), 6.30 (d, *J* = 5.5 Hz, 1H), 4.64 (d, *J* = 17.1 Hz, 1H), 4.36 (m, 3H), 3.80 (d, *J* = 17.1 Hz, 1H), 3.70 (s, 3H), 3.64 (s, 3H), 3.56 (m, 1H),

S-3

7:

This compound was prepared according to the Typical Procedure 1 using monoethyl fumarate as the acid component in Ugi 4CC/Diels-Alder reaction. After cooling down to rt, the reaction mixture was partitioned between ethyl acetate and water. The organic layer was separated, washed successively with sat. aq. NaHCO₃, brine, and water, dried over anhydrous MgSO₄, filtered, and concentrated *in vacuo* to provide brown viscous oil. The latter was chromatographed on silica gel using 20→ 50% ethyl acetate in heaxanes to afford the adduct **7** in 78% yield:

beige solid, mp = 98-99 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.09 (s, 4H), 6.37 (d, *J* = 5.8 Hz, 1H), 6.10 (d, *J* = 7.3 Hz, 1H), 6.09 (d, *J* = 5.8 Hz, 1H), 4.61 (d, *J* = 14.6 Hz, 1H), 4.24 (d, *J* = 14.6 Hz, 1H), 4.05 – 4.12 (m, 3H), 4.02 (s, 1H), 3.14 (d, *J* = 3.9 Hz, 1H), 3.07 (d, *J* = 3.9 Hz, 1H), 2.29 (s, 3H), 1.83 – 1.90 (m, 2H), 2.29 (s, 3H), 1.83 – 1.90 (m, 2H), 1.73 (s, 3H), 1.54 (m, 4H), 1.23 (t, *J* = 7.3 Hz, 3H), 1.10 – 1.20 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 174.3, 170.6, 166.5, 138.2, 137.9, 134.6, 132.7, 129.8, 128.6, 91.1, 89.4, 64.4, 61.4, 53.8 51.6, 46.7, 33.1, 32.9, 24.0, 21.3, 18.6, 14.4; LCMS *m/z* 453 (M+H); HRMS calcd for C₂₆H₃₃N₂O₅ (M+H) 453.2384, found 453.2389.

3b:

White solid, mp = 146 - 148 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.21 (d, *J* = 7.3 Hz, 1H), 7.07 (s, 1H), 7.03 (d, *J* = 7.9 Hz, 1H), 4.83 (s, 1H), 4.36 (d, *J* = 10.4 Hz, 1H), 3.78 (m, 2H), 3.06 (m, 2H), 2.95 (d, *J* = 18.3 Hz, 1H), 2.28 (s, 3H), 2.13 (s, 3H), 1.97 (s, 3H), 1.66 – 1.92 (m, 6H), 1.48 (m, 2H) – a number of signals broadened due to restricted N-Ar bond rotation; ¹³C NMR (125 MHz, DMSO-*d*₆) δ 206.6, 170.9, 166.5, 137.2, 135.3, 133.2, 130.9, 126.8, 85.6, 66.4, 57.9, 55.0, 46.0, 42.8, 30.0, 29.4, 29.0, 28.2, 23.6, 23.5, 20.5, 17.1 – a number of signals broadened due to restricted N-Ar bond rotation; LCMS *m/z* 425 (M+H); HRMS calcd for C₂₄H₂₉O₅N₂ (M+H) 425.2071, found 425.2070.

S-4

2.91 (d, $J = 9.2$ Hz, 1H), 2.85 (d, $J = 9.2$ Hz, 1H), 1.58 (s, 3H); ^{13}C NMR (125 MHz, DMSO- d_6) δ 171.5, 167.3, 167.1, 157.5 (dd, $J = 247.3, 5.5$ Hz), 153.4, 150.4, 139.9, 138.7, 135.6, 128.3, 127.4, 127.3 (unresolved t), 127.0, 124.7, 114.6 (t, $J = 9.6$ Hz), 126.6, 114.6 (t, $J = 16.9$ Hz), 89.0 (d, $J = 13.2$ Hz), 61.4, 55.7, 55.1, 52.6, 47.6, 42.5, 38.7, 15.1; LCMS m/z 604 (M+H); HRMS calcd for $\text{C}_{33}\text{H}_{32}\text{O}_6\text{N}_3\text{F}_2$ (M+H) 604.2254, found 604.2262.

1d:

White solid, mp = 199 - 201 °C (decomp.). ^1H NMR (500 MHz, DMSO- d_6) δ 9.69 (s, 1H), 8.95 (t, $J = 6.1$ Hz, 1H), 7.09 – 7.33 (m, 9H), 7.05 (t, $J = 7.4$ Hz, 1H), 6.90 (d, $J = 8.0$ Hz, 1H), 6.39 (d, $J = 5.5$ Hz, 1H), 6.35 (d, $J = 5.5$ Hz, 1H), 4.58 (br s, 1H), 4.37 (dd, $J = 5.5, 14.7$ Hz, 1H), 4.28 (dd, $J = 5.5, 14.7$ Hz, 1H), 2.98 (br s, 1H), 2.91 (d, $J = 8.6$ Hz, 1H), 2.22 (s, 3H), 2.07 (s, 3H), 1.62 (s, 3H) – a number of signals broadened due to restricted N-Ar bond rotation; ^{13}C NMR (125 MHz, DMSO- d_6) δ 170.9, 167.8, 167.2, 157.6 (dd, $J = 247.3, 5.5$ Hz), 140.1, 138.4, 137.4, 136.3, 135.7, 135.3, 129.2, 128.2, 127.5, 127.0, 126.1, 125.4, 114.6 (t, $J = 16.9$ Hz), 111.5 (d, $J = 23.2$ Hz), 89.3 (d, $J = 17.3$ Hz), 64.7, 52.6, 47.7, 42.3, 19.8, 15.3, 13.3 – a number of signals broadened due to restricted N-Ar bond rotation; LCMS m/z 558 (M+H); HRMS calcd for $\text{C}_{32}\text{H}_{30}\text{O}_4\text{N}_3\text{F}_2$ (M+H) 558.2199, found 558.2202.

X-ray structure of the compound **1d**.

S-5

1e:

White solid, mp = 164 - 165 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.91 (s, 1H), 7.41 (d, J = 7.3 Hz, 2H), 7.31 (t, J = 7.3 Hz, 2H), 7.10 (t, J = 7.3 Hz, 1H), 6.99 (s, 4H), 6.41 (d, J = 5.5 Hz, 1H), 6.15 (d, J = 5.5 Hz, 1H), 6.03 (d, J = 7.3 Hz, 1H), 4.90 (d, J = 14.6 Hz, 1H), 4.20 (m, 1H), 4.12 (s, 1H), 3.78 (d, J = 14.6 Hz, 1H), 3.16 (d, J = 9.2 Hz, 1H), 2.77 (d, J = 9.2 Hz, 1H), 2.29 (s, 3H), 1.96 (s, 3H), 1.69 (s, 3H), 1.59 (m, 3H), 1.32 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.4, 166.4, 139.6, 138.0, 137.6, 135.7, 132.6, 129.8, 129.1, 128.8, 124.6, 120.8, 90.3, 89.9, 62.9, 54.4, 51.9, 51.3, 46.0, 33.2, 33.1, 23.9, 21.3, 16.3; LCMS m/z 500 (M+H); HRMS calcd for $\text{C}_{30}\text{H}_{34}\text{N}_3\text{O}_4$ (M+H) 500.2544, found 500.2548.

1f:

White solid, mp = 214 - 216 °C (decomp.). ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 9.71 (s, 1H), 8.45 (d, J = 8.0 Hz, 1H), 7.27 – 7.34 (m, 3H), 7.12 (t, J = 7.9 Hz, 2H), 7.04 (s, 1H), 6.45 (d, J = 5.5 Hz, 1H), 6.42 (d, J = 5.5 Hz, 1H), 4.60 (s, 1H), 3.84 (m, 1H), 2.97 (d, J = 9.0 Hz, 1H), 2.93 (d, J = 9.0 Hz, 1H), 2.16 (s, 3H), 1.84 (m, 1H), 1.70 (m, 1H), 1.62 (s, 3H), 1.30 – 1.59 (m, 12H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) δ 170.9, 167.2, 166.2, 157.6 (dd, J = 247.3, 5.5 Hz), 140.2, 137.6, 136.1, 135.6, 132.0, 129.7, 127.8, 127.7, 127.5 (t, J = 9.6 Hz), 114.6 (t, J = 16.4 Hz), 111.6 (dd, J = 4.1, 19.6 Hz), 89.3 (d, J = 18.2 Hz), 64.3, 52.4, 50.0, 47.9, 34.0, 27.6, 27.5, 23.4, 23.2, 16.7, 15.3; LCMS m/z 584 (M+H); HRMS calcd for $\text{C}_{31}\text{H}_{33}\text{O}_4\text{N}_3\text{F}_2\text{Cl}$ (M+H) 584.2122, found 584.2126.

S-6

3c:

White solid, mp = 142 - 143 °C. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.35 (t, J = 6.7 Hz, 2H), 7.29 (t, J = 7.3 Hz, 1H), 7.25 (d, J = 7.3 Hz, 2H), 6.94 (d, J = 9.2 Hz, 1H), 6.84 (dd, J = 9.2, 3.1 Hz, 1H), 6.53 (d, J = 2.5 Hz, 1H), 4.85 (d, J = 15.3 Hz, 1H), 4.57 (d, J = 15.3 Hz, 1H), 4.48 (d, J = 15.3 Hz, 1H), 4.37 (s, 1H), 4.28 (d, J = 15.3 Hz, 1H), 4.10 (dd, J = 9.2, 3.1 Hz, 1H), 3.68 (s, 3H), 3.65 (s, 3H), 3.40 (d, J = 10.4 Hz, 1H), 3.00 (m, 2H), 2.88 (dd, J = 18.3, 3.1 Hz, 1H), 2.60 (d, J = 18.3 Hz, 1H), 1.97 (s, 3H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 206.7, 173.7, 171.1, 167.8, 152.9, 151.1, 136.1, 128.6, 127.6, 127.4, 133.7, 114.2, 113.0, 112.0, 84.7, 62.2, 58.3, 55.7, 55.1, 46.8, 44.0, 41.0, 29.8, 29.4; LCMS m/z 493 (M+H); HRMS calcd for $\text{C}_{27}\text{H}_{29}\text{O}_7\text{N}_2$ (M+H) 493.1969, found 493.1969.

3d:

White solid, mp = 155 - 156 °C. ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ 7.37 (t, J = 7.3 Hz, 2H), 7.30 (m, 4H), 7.16 (m, 2H), 4.97 (br s, 1H), 4.61 (d, J = 15.3 Hz, 1H), 4.30 (br d, J = 14.7 Hz, 1H), 4.18 (t, J = 6.7 Hz, 1H), 3.55 (d, J = 10.4 Hz, 1H), 3.17 (d, J = 4.9 Hz, 1H), 3.06 (m, 1H), 2.98 (d, J = 6.7 Hz, 1H), 2.63 (d, J = 18.3 Hz, 1H), 2.27 (s, 3H), 2.04 (s, 3H), 1.92 (br s, 3H) – a number of signals broadened due to restricted N-Ar bond rotation; ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) δ 206.7, 173.7, 166.9 (br), 137.2, 136.1, 129.2, 128.6, 127.5, 127.4, 125.6, 94.5, 82.1, 66.9, 58.4, 46.6, 44.0, 41.2, 29.8, 29.4, 19.9 – a number of signals failed to appear in the spectrum due to significant line broadening; LCMS m/z 447 (M+H); HRMS calcd for $\text{C}_{26}\text{H}_{27}\text{O}_5\text{N}_2$ (M+H) 447.1914, found 447.1893.

S-7

Figure 2. X-ray structure of the compound **3d**.

3e:

White solid, mp = 144 - 145 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.11 (s, 4H), 5.14 (d, J = 14.7 Hz, 1H), 4.40 (d, J = 14.3 Hz, 1H), 4.31 (d, J = 11.0 Hz, 1H), 3.95 (s, 1H), 3.86 (m, 1H), 3.23 (d, J = 9.9 Hz, 1H), 2.98 (m, 1H), 2.92 (s, 1H), 2.82 (m, 1H), 2.68 (d, J = 19.8 Hz, 1H), 2.31 (s, 3H), 2.16 (s, 3H), 1.56 – 1.98 (m, 8H); ^{13}C NMR (100 MHz, CDCl_3) δ 206.3, 173.1, 170.9, 167.7, 138.1, 131.7, 129.9, 128.8, 84.5, 62.5, 59.8, 55.8, 48.3, 45.2, 44.2, 30.4, 29.5, 29.2, 24.1, 21.3; LCMS m/z 425 ($\text{M}+\text{H}$); HRMS calcd for $\text{C}_{24}\text{H}_{29}\text{N}_2\text{O}_5$ ($\text{M}+\text{H}$) 425.2071, found 425.2075. (A compound with identical ^1H and ^{13}C NMR as well as LC MS data was isolated from the same reaction of the compound **7**).

3f:

White solid, mp = 211 - 213 °C (decomp.). ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 7.52 (s, 1H), 7.33 (m, 2H), 4.21 (s, 1H), 4.38 (dd, J = 7.4, 4.9 Hz, 1H), 3.83 (d, J = 10.9 Hz, 1H), 3.49 (m, 1H), 2.98 – 3.06 (m, 3H), 2.66 (d, J = 18.3 Hz, 1H), 2.13 (s, 3H), 2.00 (s, 3H), 1.34 – 1.92 (m, 12H) – a number of signals broadened due to restricted N-Ar bond rotation; ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) δ 207.7, 173.6, 170.9 (br), 165.8, 137.1, 134.9, 131.9, 129.9, 127.8, 85.5, 66.3, 57.9,

S-8

55.7, 46.1, 42.7, 32.2, 31.1, 30.0, 29.4, 26.8, 26.5, 24.7, 24.5, 16.8 – a number of signals broadened due to restricted N-Ar bond rotation; LCMS m/z 473 (M+H); HRMS calcd for C₂₅H₃₀O₅N₂Cl (M+H) 473.1838, found 473.1828.

8:

The compound **1b** (310 mg, 0.58 mmol) was placed in 5 mL microwave vials dissolved in dioxane (2 mL). BF₃ etherate (0.12 mmol, 15 μ L) was added and the reaction mixture was irradiated at 150 °C for 90 min using Biotage Emrys Optimizer[®] in a sealed reaction vessel. After cooling down to rt, the reaction mixtures were partitioned between chloroform and water, organic layer was separated, further washed with sat. aq. NaHCO₃, brine, water, dried over anhydrous MgSO₄, filtered and concentrated *in vacuo* to provide the crude product. The latter was purified by column chromatography on silica gel using 20→100% ethyl acetate in hexanes as eluent to provide 225 mg of the compound **8** (75%):

white solid, mp = 166-167 °C. ^1H NMR (300 MHz, DMSO- d_6) δ 10.24 (s, 1H), 8.54 (d, J = 6.8 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.37 (m, 1H), 7.04 – 7.19 (m, 5H), 5.58 (s, 1H), 3.92 (m, 1H), 2.46 (s, 3H), 2.30 (s, 3H), 2.20 (s, 3H), 1.27 – 1.78 (m, 8H); ^{13}C NMR (75 MHz, DMSO- d_6) δ 166.4, 165.5, 158.3 (d, J = 5.1, 248.6 Hz), 140.3, 137.0 (d, J = 50.7 Hz), 135.7, 134.2, 134.0, 131.7, 128.3, 127.8, 127.2, 122.8, 114.6 (t, J = 17.1 Hz), 112.1 (d, J = 23.4 Hz), 65.3, 51.2, 32.8, 32.2, 23.8, 21.0, 18.3, 15.6; LCMS m/z 518 (M+H); HRMS calcd for $\text{C}_{30}\text{H}_{30}\text{O}_3\text{N}_3\text{F}_2$ (M+H) 518.2250, found 518.2253.

¹H NMR (400 MHz, DMSO-d₆): δ 7.82 (d, 1H, J = 8.0 Hz, H-6), 7.72 (d, 1H, J = 8.0 Hz, H-5), 7.62 (d, 1H, J = 8.0 Hz, H-4), 7.52 (d, 1H, J = 8.0 Hz, H-3), 7.42 (d, 1H, J = 8.0 Hz, H-2), 7.32 (d, 1H, J = 8.0 Hz, H-1), 7.22 (d, 1H, J = 8.0 Hz, H-10), 7.12 (d, 1H, J = 8.0 Hz, H-9), 7.02 (d, 1H, J = 8.0 Hz, H-8), 6.92 (d, 1H, J = 8.0 Hz, H-7), 6.82 (d, 1H, J = 8.0 Hz, H-6), 6.72 (d, 1H, J = 8.0 Hz, H-5), 6.62 (d, 1H, J = 8.0 Hz, H-4), 6.52 (d, 1H, J = 8.0 Hz, H-3), 6.42 (d, 1H, J = 8.0 Hz, H-2), 6.32 (d, 1H, J = 8.0 Hz, H-1), 6.22 (d, 1H, J = 8.0 Hz, H-10), 6.12 (d, 1H, J = 8.0 Hz, H-9), 6.02 (d, 1H, J = 8.0 Hz, H-8), 5.92 (d, 1H, J = 8.0 Hz, H-7), 5.82 (d, 1H, J = 8.0 Hz, H-6), 5.72 (d, 1H, J = 8.0 Hz, H-5), 5.62 (d, 1H, J = 8.0 Hz, H-4), 5.52 (d, 1H, J = 8.0 Hz, H-3), 5.42 (d, 1H, J = 8.0 Hz, H-2), 5.32 (d, 1H, J = 8.0 Hz, H-1), 5.22 (d, 1H, J = 8.0 Hz, H-10), 5.12 (d, 1H, J = 8.0 Hz, H-9), 5.02 (d, 1H, J = 8.0 Hz, H-8), 4.92 (d, 1H, J = 8.0 Hz, H-7), 4.82 (d, 1H, J = 8.0 Hz, H-6), 4.72 (d, 1H, J = 8.0 Hz, H-5), 4.62 (d, 1H, J = 8.0 Hz, H-4), 4.52 (d, 1H, J = 8.0 Hz, H-3), 4.42 (d, 1H, J = 8.0 Hz, H-2), 4.32 (d, 1H, J = 8.0 Hz, H-1), 4.22 (d, 1H, J = 8.0 Hz, H-10), 4.12 (d, 1H, J = 8.0 Hz, H-9), 4.02 (d, 1H, J = 8.0 Hz, H-8), 3.92 (d, 1H, J = 8.0 Hz, H-7), 3.82 (d, 1H, J = 8.0 Hz, H-6), 3.72 (d, 1H, J = 8.0 Hz, H-5), 3.62 (d, 1H, J = 8.0 Hz, H-4), 3.52 (d, 1H, J = 8.0 Hz, H-3), 3.42 (d, 1H, J = 8.0 Hz, H-2), 3.32 (d, 1H, J = 8.0 Hz, H-1), 3.22 (d, 1H, J = 8.0 Hz, H-10), 3.12 (d, 1H, J = 8.0 Hz, H-9), 3.02 (d, 1H, J = 8.0 Hz, H-8), 2.92 (d, 1H, J = 8.0 Hz, H-7), 2.82 (d, 1H, J = 8.0 Hz, H-6), 2.72 (d, 1H, J = 8.0 Hz, H-5), 2.62 (d, 1H, J = 8.0 Hz, H-4), 2.52 (d, 1H, J = 8.0 Hz, H-3), 2.42 (d, 1H, J = 8.0 Hz, H-2), 2.32 (d, 1H, J = 8.0 Hz, H-1), 2.22 (d, 1H, J = 8.0 Hz, H-10), 2.12 (d, 1H, J = 8.0 Hz, H-9), 2.02 (d, 1H, J = 8.0 Hz, H-8), 1.92 (d, 1H, J = 8.0 Hz, H-7), 1.82 (d, 1H, J = 8.0 Hz, H-6), 1.72 (d, 1H, J = 8.0 Hz, H-5), 1.62 (d, 1H, J = 8.0 Hz, H-4), 1.52 (d, 1H, J = 8.0 Hz, H-3), 1.42 (d, 1H, J = 8.0 Hz, H-2), 1.32 (d, 1H, J = 8.0 Hz, H-1), 1.22 (d, 1H, J = 8.0 Hz, H-10), 1.12 (d, 1H, J = 8.0 Hz, H-9), 1.02 (d, 1H, J = 8.0 Hz, H-8), 0.92 (d, 1H, J = 8.0 Hz, H-7), 0.82 (d, 1H, J = 8.0 Hz, H-6), 0.72 (d, 1H, J = 8.0 Hz, H-5), 0.62 (d, 1H, J = 8.0 Hz, H-4), 0.52 (d, 1H, J = 8.0 Hz, H-3), 0.42 (d, 1H, J = 8.0 Hz, H-2), 0.32 (d, 1H, J = 8.0 Hz, H-1), 0.22 (d, 1H, J = 8.0 Hz, H-10), 0.12 (d, 1H, J = 8.0 Hz, H-9), 0.02 (d, 1H, J = 8.0 Hz, H-8).

F068-0016

FW: $C_2H_5O_4N_5P_3$
MW: 521.57

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz {13C} SI=128K SW=30027 Ol=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=21000 SR=123.903 TE=297K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0016

ppm

171.37
167.29
166.49

158.63
158.59
156.65
156.61

139.93
136.41
135.79
128.24
128.03
127.59
127.51
127.44
127.18
126.90

114.77
114.63
114.50
111.74
111.56

89.15
88.99

61.29

52.74

50.56

47.59

44.17

40.34

40.02

39.93

39.85

39.76

39.69

39.60

39.52

39.43

39.35

39.26

39.10

38.93

32.28

31.90

23.27

-0.00

1a

FW: C₂₉H₂₉O₄N₃F₂
MW: 521.57

ppm

The Best Applied NMR

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DEX500 SP-500.13 MHz ¹H} SI=16K SW=10000 OI=4006 FN=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0038

FM: C₃₀ H₃₁ O₄ N₃ F₂
MW: 535.59

Found protons = 31 impurity * = 0.2 %

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP-125.76 MHz (13C) SI=128K SW=30027 OI=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=2274 SR=123.903 TE=299K 27 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0038

15.35
17.13
20.48
23.14
23.19
31.81
32.24
38.92
39.09
39.26
39.43
39.52
39.59
39.69
39.76
39.85
39.93
40.01
47.78
50.56
52.52

64.57

89.42
89.21

111.69
111.68
114.51
114.64
114.77

126.57
127.34
127.42
127.50
127.70
130.93
133.93
135.72
136.48
137.09
140.18

156.55
156.60
158.53
158.58
167.19
170.66

ppm

FW: C₃₀H₃₁O₄N₃F₂
MW: 535.59

ppm

The Best Applied NMR

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP-500.13 MHz ¹H} SI=16K SW=10000 O1=4006 PM=12.0 AQ=1.6385 RD=0.00 MS=1 SR=6.184 TE=301K 25 April 2006 Opr: Strelenko Yu A.; Prep: L-6482; Solv: DMSO-d6;

F068-0111

FM: C₃₃ H₃₁ O₈ N₃ P₃
MW: 603.62

Found protons = 34 impurity * = 1.5 %

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz (13C) SI=128K SN=30027 O1=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=1490 SR=123.903 TE=296K 28 April 2006 Opr: Strelenko Yu A.; Prep: L-6482; Solv: DMSO-d6;

F068-0111

15.15

38.67

38.90

39.07

39.24

39.40

39.49

39.57

39.66

39.74

39.83

39.90

39.99

42.49

47.60

52.61

55.05

55.70

61.64

89.13

89.02

111.52

111.58

111.64

111.71

111.91

113.65

114.44

114.57

114.70

124.74

127.01

127.26

127.35

127.43

127.51

127.99

128.06

128.31

135.57

138.70

139.88

150.38

153.43

156.50

156.55

159.48

159.53

167.09

167.29

171.52

ppm

FW: C₂₃H₂₁O₂N₂F₂
MW: 403.52

ppm

The Best Applied NMR

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=500.13 MHz (1H) SI=16K SW=10000 OI=4006 PW=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2005 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0113

FM: C₁₂H₂₅O₄N₃F₂
MW: 557.60

Found protons = 29 impurity * = 0.3 %

Top. Test Applied NMR

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF-125.76 MHz (13C) SI-128K SN-30027 O1-12918 PN-8.0 AQ-0.5456 RD-0.50 NS-1451 SR-123.903 TE-296K 28 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0113

170.96
167.36
167.20
158.60
158.55
156.62
156.57
140.12
138.39
137.42
136.26
135.72
135.32
129.16
128.21
127.53
127.45
126.97
126.14
125.96
125.40
114.76
114.63
114.49
111.67
111.49
89.36
89.23
64.75
52.60
47.71
42.28
40.33
39.91
39.83
39.74
39.67
39.57
39.50
39.41
39.24
39.07
38.91
19.84
15.34
13.35
0.01

ppm

FM: C₃₂H₂₉O₄N₃F₂
MW: 557.60

The End Applied NMR

217c

24 May 2006

Acquisition Time (sec)	2.6664	Comment	STANDARD 1H OBSERVE	Date	May 18 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDiv\Doc\API\Reamgm\217cH			Frequency (MHz)	399.95
Nucleus	1H	Number of Transients	16	Points Count	16384
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	6000.60
Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
31	7.25	2898.5	0.1830
32	7.28	2913.5	0.1405
33	7.31	2921.9	0.2416
34	7.32	2929.2	0.1615
35	7.40	2960.0	0.2476
36	7.42	2967.3	0.1813
37	7.91	3162.6	0.1418

No.	(ppm)	(Hz)	Height
21	4.89	1955.3	0.1129
22	4.93	1970.0	0.1057
23	6.02	2408.0	0.0718
24	6.04	2415.4	0.0690
25	6.15	2458.2	0.1690
26	6.16	2463.7	0.1896
27	6.40	2560.4	0.1758
28	6.42	2565.9	0.1545
29	6.99	2794.8	1.0000
30	7.10	2838.8	0.1141

No.	(ppm)	(Hz)	Height
11	2.29	915.5	0.9858
12	2.77	1107.4	0.1568
13	2.79	1116.6	0.1754
14	3.16	1262.0	0.1238
15	3.18	1271.1	0.1086
16	3.77	1507.4	0.0942
17	3.81	1522.0	0.0999
18	4.12	1646.9	0.4216
19	4.18	1671.1	0.0400
20	4.23	1692.0	0.0379

No.	(ppm)	(Hz)	Height
1	-0.02	-6.4	0.3408
2	1.29	514.4	0.0413
3	1.30	521.4	0.0608
4	1.35	541.2	0.0385
5	1.59	634.2	0.1752
6	1.60	639.7	0.1654
7	1.62	646.3	0.0872
8	1.69	675.2	0.9474
9	1.95	778.1	0.0739
10	1.99	796.1	0.0795

217c

24 May 2006

Acquisition Time (sec)	2.0006	Comment	13C OBSERVE	Date	May 18 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDivDoc\APIReamgmt\217cC				
Nucleus	13C	Original Points Count	50016	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	25000.00	Pulse Sequence	s2pul
				Frequency (MHz)	100.58
				Temperature (degree C)	25.000

1e

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	16.31	1640.7	0.2169	8	51.89	5218.6	0.2570	15	90.35	9087.1	0.2132	22	132.63	13339.4	0.2974
2	21.35	2146.9	0.3227	9	54.41	5472.6	0.1887	16	120.83	12152.6	0.2168	23	135.71	13649.6	0.1760
3	23.89	2402.9	0.3633	10	62.91	6327.5	0.1547	17	124.53	12525.0	0.0505	24	137.57	13836.5	0.2302
4	33.13	3332.6	0.2110	11	76.92	7735.9	0.9680	18	124.56	12528.0	0.1026	25	137.96	13875.4	0.1976
5	33.22	3340.9	0.2137	12	77.23	7768.0	1.0000	19	128.78	12952.6	0.6153	26	139.57	14037.1	0.1130
6	45.98	4625.0	0.1013	13	77.55	7800.0	0.9715	20	129.09	12983.5	0.3408	27	166.39	16735.3	0.1602
7	51.27	5156.8	0.0968	14	89.99	9050.5	0.2603	21	129.85	13059.8	0.5725	28	171.35	17233.9	0.0949

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=500.13 MHz {1H} SI=16K SW=10000 OI=4006 PM=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0091

FM: C₃₁H₃₂O₄N₃F₂Cl
MW: 584.06

Found protons = 32 impurity * = 0.2 %

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF-125.76 MHz (13C) SI-128K SW-30027 Q1-12918 PM-8.0 AQ-0.5456 RD-0.50 NS-1920 SR-123.903 TB-299K 27 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0091

ppm

170.85	167.16	166.18	158.60	158.55	156.62	156.58
140.21	137.65	136.12	135.64	132.04	129.67	127.75
127.66	127.59	127.51	127.43	114.70	114.57	114.43
111.70	111.51	89.39	89.24	64.33	52.43	49.97
47.87	40.02	39.93	39.86	39.76	39.69	39.60
39.52	39.43	39.26	39.10	38.93	34.00	27.59
27.57	23.41	23.28	16.69	15.33

FM: C₃₁H₃₂O₄N₃F₂Cl
MW: 584.06

The Best Applied NMR

217e

24 May 2006

Acquisition Time (sec)	2.6664	Comment	STANDARD 1H OBSERVE	Date	May 17 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDivDoc\APIReamgmt\217-1fr	Number of Transients	16	Frequency (MHz)	399.95
Nucleus	1H	Original Points Count	16000	Points Count	16384
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	6000.60
Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.11	442.3	0.0213	10	1.73	690.6	0.6236	19	4.02	1608.1	0.2658	28	4.63	1853.5	0.0923
2	1.12	448.9	0.0262	11	1.83	731.3	0.0209	20	4.07	1627.9	0.0647	29	6.09	2436.6	0.1448
3	1.19	476.0	0.0242	12	1.84	737.1	0.0352	21	4.08	1631.2	0.1158	30	6.10	2439.5	0.0576
4	1.21	483.7	0.2085	13	1.89	757.3	0.0229	22	4.09	1635.6	0.0643	31	6.11	2442.1	0.1699
5	1.23	490.6	0.3975	14	2.29	914.0	0.6658	23	4.10	1638.1	0.1621	32	6.37	2546.5	0.1283
6	1.25	497.9	0.1905	15	3.07	1226.5	0.1151	24	4.11	1645.5	0.1057	33	6.38	2552.4	0.1162
7	1.52	608.2	0.0604	16	3.08	1230.1	0.1380	25	4.22	1687.6	0.0901	34	7.09	2834.4	1.0000
8	1.53	613.3	0.1079	17	3.14	1256.5	0.1257	26	4.26	1702.2	0.1058				
9	1.55	618.4	0.1050	18	3.15	1260.2	0.0966	27	4.60	1838.5	0.1133				

5-(m-UreidoPh)-NOSCAPINE

24 May 2006

Acquisition Time (sec)	2.0006	Comment	13C OBSERVE	Date	May 17 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDiv\Doc\APIReamgmnt\217e1frC				
Nucleus	13C	Original Points Count	50016	Points Count	65536
Solvent	CHLOROFORM-D	Sweep Width (Hz)	25000.00	Temperature (degree C)	25.000

Frequency (MHz)	100.58
Pulse Sequence	s2pul

7

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.39	1447.7	0.2022	8	46.71	4697.5	0.2773	15	77.28	7772.2	0.4871
2	18.64	1874.9	0.3130	9	51.59	5188.8	0.5078	16	77.59	7803.8	0.4739
3	21.29	2141.6	0.4260	10	52.20	5250.6	0.3181	17	89.40	8991.4	0.6154
4	23.96	2410.1	0.5344	11	53.81	5412.0	0.4022	18	91.09	9161.1	0.6294
5	23.99	2412.4	0.4493	12	61.35	6170.7	0.3477	19	128.58	12932.0	1.0000
6	32.85	3304.3	0.3572	13	64.38	6475.1	0.3517	20	129.77	13052.2	0.8617
7	33.12	3330.6	0.3895	14	76.96	7740.1	0.4850	21	132.66	13342.5	0.3435

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=500.13 MHz {1H} SI=16K SW=10000 OI=4006 PW=12.0 AQ=1.6365 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0005

FM: C₂₃H₂₄O₅N₂
MW: 410.47

3a

The Best Applied NMR

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP-125.76 MHz (13C) SI-128K SM-30027 O1-12918 PM-8.0 AQ-0.5456 RD-0.50 NS-2870 SR-124.081 TE-300K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0005

ppm

206.69

173.55
171.34
167.18135.50
128.66
128.65
128.63
127.58
127.56
127.54

84.85

62.12
58.32
54.77
46.28
44.25
42.53
39.94
39.77
39.70
39.61
39.44
39.27
39.11
38.94
29.88
29.17
29.14
28.14
23.61
23.49

FW: C₂₃ H₂₆ O₅ N₂
MW: 410.47

ppm

The Best Applied NMR

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP=500.13 MHz [1H] SI=16K SW=10000 OI=4006 PW=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2006 Opt: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0040

FM: C₂₄ H₂₈ O₅ N₂
MW: 424.50

3b

The Best Applied NMR

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz (13C) SI=128K SW=30027 O1=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=3304 SR=124.081 TE=300K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0040

ppm 206.60 173.65 170.87 166.45 137.23 135.30 133.22 130.89 126.77 85.64 66.36 57.86 54.97 45.96 42.79 40.02 39.93 39.85 39.76 39.69 39.60 39.52 39.43 39.36 39.26 39.10 38.93 29.96 29.39 29.02 28.21 23.59 23.57 23.56 23.54 23.52 23.51 20.47 17.10 0.00

FW: C₂₄ H₂₈ O₅ N₂
MR: 424.50

TH: East Applied NMR I

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=500.13 MHz (1H) SI=16K SW=10000 OI=4006 PM=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TE=301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0144

3c

FM: C₂₅H₂₈O₇N₂
MW: 492.53

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP-125.76 MHz {13C} ST-128K SW-30027 O1=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=2769 SR=123.903 TE=299K 26 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0144

62.22
58.33
55.69
55.08
46.76
43.98
40.97
40.26
39.93
39.76
39.68
39.59
39.52
39.42
39.26
39.09
38.93
29.77
29.37

84.73

114.17
112.97
111.99

128.61
127.55
127.42
123.68

136.06

152.91
151.10

173.68
171.09
167.84

206.68

FW: C₂₅H₂₈O₇N₂
MR: 492.55

The Best Applied NMR

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP-500.13 MHz {1H} SI-16K SW-10000 O1-4006 PW-12.0 AQ-1.6385 RD=0.00 NS-1 SR-6.184 TE-301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0143

3d

FM: C₂₆H₂₆O₄N₂
MW: 446.50

8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Found protons = 26 impurity * = 1.3 %

The Best Applied NMR

© Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP=125.76 MHz (13C) SI=128K SW=30027 01=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=2472 SR=123.903 TE=300K 27 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0143

ppm
206.65

173.69

137.25
136.12
128.62
127.53
127.46
125.56

44.00
41.19
40.03
39.94
39.87
39.77
39.69
39.60
39.53
39.44
39.27
39.10
38.94
29.84
29.43
19.92

FM: C₂₅H₂₆O₅N₂
MW: 446.50

ppm

The Best Applied VNA

Acquisition Time (sec)	2.6684	Comment	STANDARD 1H OBSERVE	Date	May 24 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDivDoc\APIRearmgmt\219rr				
Nucleus	1H	Number of Transients	16	Original Points Count	16384
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D	Sweep Width (Hz)	6000.60
Temperature (degree C) 25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.02	-7.1	0.1118	10	2.16	865.3	0.7399	19	2.95	1180.7	0.0888	28	4.32	1728.6	0.0812
2	1.56	625.8	0.0941	11	2.31	923.2	0.7476	20	2.98	1190.9	0.1018	29	4.33	1730.4	0.0803
3	1.58	632.7	0.0976	12	2.59	1036.0	0.0949	21	3.22	1288.0	0.0929	30	4.38	1752.1	0.1120
4	1.66	665.7	0.0527	13	2.66	1062.7	0.0590	22	3.25	1297.9	0.0761	31	4.42	1766.3	0.1204
5	1.75	700.9	0.0729	14	2.70	1080.3	0.1051	23	3.81	1525.0	0.0139	32	5.12	2049.1	0.1223
6	1.78	713.3	0.1172	15	2.79	1116.2	0.0781	24	3.85	1541.8	0.0719	33	5.16	2063.7	0.1116
7	1.82	727.2	0.0738	16	2.82	1127.2	0.0795	25	3.90	1558.7	0.0149	34	7.11	2845.4	1.0000
8	1.92	769.7	0.0507	17	2.86	1145.5	0.0749	26	3.95	1580.3	0.2407	35	7.25	2899.6	0.1079
9	1.98	792.4	0.0355	18	2.92	1166.8	0.1245	27	4.30	1719.5	0.0850				

Acquisition Time (sec)	2.0006	13C OBSERVE	Date	May 24 2006	
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDiv\Doc\AP\Reamgmnt\219rrC				
Nucleus	13C	Number of Transients	16960	Original Points Count	50016
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Temperature (degree C)	25.000				
			Frequency (MHz)	100.58	
			Points Count	65536	
			Sweep Width (Hz)	25000.00

Acquisition Time (sec)	2.6664	Comment	STANDARD 1H OBSERVE	Date	May 24 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDivDoc\AP\Reamgmt\218rr				
Nucleus	1H	Number of Transients	16	Original Points Count	16000
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Temperature (degree C)	25.000				
				Frequency (MHz)	399.95
				Points Count	16384
				Sweep Width (Hz)	6000.60

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	-0.02	-6.8	0.1208	10	1.93	770.5	0.0479	19	2.95	1181.0	0.0882	28	4.32	1729.0	0.0788
2	1.57	626.1	0.0904	11	2.17	866.0	0.7320	20	2.98	1191.3	0.1014	29	4.33	1730.8	0.0814
3	1.58	633.5	0.0946	12	2.31	923.6	0.7313	21	3.22	1288.0	0.0876	30	4.38	1752.8	0.1094
4	1.60	638.2	0.0725	13	2.66	1062.7	0.0581	22	3.24	1297.5	0.0731	31	4.42	1767.1	0.1190
5	1.75	701.6	0.0700	14	2.70	1080.7	0.1006	23	3.84	1534.1	0.0463	32	5.13	2050.2	0.1216
6	1.79	714.0	0.1139	15	2.79	1116.6	0.0770	24	3.86	1542.2	0.0713	33	5.16	2064.5	0.1115
7	1.80	720.6	0.0836	16	2.82	1127.6	0.0785	25	3.88	1550.6	0.0499	34	7.12	2845.7	1.0000
8	1.82	728.0	0.0729	17	2.87	1146.2	0.0649	26	3.95	1580.6	0.2443	35	7.25	2899.6	0.1028
9	1.84	737.9	0.0636	18	2.92	1167.5	0.1226	27	4.30	1719.8	0.0872				

Acquisition Time (sec)	2.0006	Comment	13C OBSERVE	Date	May 24 2006
File Name	C:\Documents and Settings\Volodymyr\My Documents\ChemDiv\Doc\APIRearmgmt\218rrc				
Nucleus	13C	Number of Transients	16960	Original Points Count	50016
Pulse Sequence	s2pul	Solvent	CHLOROFORM-D		
Temperature (degree C)	25.000				
		Frequency (MHz)	100.58	Points Count	65536
		Sweep Width (Hz)	25000.00

3e
(from 7)

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	21.33	2145.8	0.1818	10	48.27	4854.6	0.1893	19	129.86	13061.3	0.3785
2	24.13	2426.5	0.2500	11	55.78	5610.0	0.1436	20	131.75	13250.9	0.1459
3	24.15	2429.2	0.2299	12	59.78	6012.4	0.1556	21	138.10	13889.5	0.1222
4	29.16	2932.8	0.1638	13	62.46	6282.1	0.1939	22	167.71	16868.1	0.1312
5	29.54	2970.9	0.1448	14	76.92	7736.7	0.9887	23	170.86	17184.3	0.1242
6	30.27	3044.2	0.1669	15	77.24	7768.7	1.0000	24	173.09	17408.6	0.1336
7	30.40	3057.9	0.1907	16	77.56	7800.4	0.9634	25	206.26	20744.6	0.1059
8	44.21	4446.5	0.1231	17	84.49	8497.3	0.1767				
9	45.16	4541.8	0.1521	18	128.81	12955.7	0.3872				

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SP=500.13 MHz {1H} SI=16K SW=10000 OI=4006 PW=12.0 AQ=1.6385 RD=0.00 NS=1 SR=6.184 TB=301K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0122

FW: C₂₅H₂₉O₅N₂Cl
MW: 472.97

Zelinsky Institute of Organic Chemistry, Moscow; Bruker DRX500 SF=125.76 MHz [13C] SI=128K SW=30027 Ol=12918 PW=8.0 AQ=0.5456 RD=0.50 NS=3297 SR=124.081 TE=298K 25 April 2006 Opr: Strelenko Yu.A.; Prep: L-6482; Solv: DMSO-d6;

F068-0122

0.00

66.27
57.82
55.66
46.06
42.75
40.02
39.92
39.85
39.76
39.68
39.59
39.52
39.42
39.25
39.09
38.92
32.15
31.13
29.96
29.40
26.81
26.79
26.77
26.55
24.70
24.53
24.51
16.81

85.48

137.06
134.93
131.87
129.95
127.78

165.84

173.62
170.87

206.71

ppm

FN: C₂₅H₂₉O₅N₂Cl
MW: 472.97

200 180 160 140 120 100 80 60 40 20 0

ppm

The Best Applied NMR

8

F068-0057

8