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Guidelines for NMR, IR, UV spectroscopy, mass spectrometry and elemental analysis.

Presentation of NMR, IR, UV spectroscopy, mass spectrometry and elemental analysis in the Manuscript. Details of the data collection should be given in the Supplementary Materials. These signals of NMR, UV, IR and MS are presented as a sample that is using in *Mendeleev Communications* and are not relevant to this substance.

*3,4,5-Trimethoxybenzyl 5-aminoisoxazole-3-carboxylate* **1a**: colourless solid, mp 144–145 °C, *R*f 0.4 (light petroleum–EtOAc, 1:1). 1H NMR (400 MHz, CDCl3–CD3OD) **: 0.51 (s, 12H), 0.89 (t, ~3H, 2Me in **3f**, *J*7.2 Hz), 0.91 (t, ~3H, 2Me in **2f**, *J*6.6 Hz), 1.05–1.25 (m, 4H, 2 -CH2), 1.07 (s, 12H, *p*-Me), 1.75–1.77 (m, 2H, 6-CH2), 2.03–2.10 (m, 8H, =CH–C*H*2), 2.43 (s, 24H, *o*-Me) 3.20 (br.s, 2H, NH2), 3.74 (s, 3H, OMe), 4.02 (s, 8H, Ar–C*H*2–Ar), 5.80 (s, 4H, H-5), 5.79 (d, 1H, C9H, 3*J* 8.2 Hz), 6.58 (s, 2H, 2CHAr), 6.75 (s, 1H, H5), 6.87 (dd, 1H, C8H, 3*J* 8.2 Hz, 3*J* 7.5 Hz), 6.88 (d, 8H, H-7, 3*J*HH 8.0 Hz), 7.17–7.27 (m, 5H, Ph), 7.34–7.42 (m, 6H, 4H*m*, 2H*p*), 7.46 (s, 2H, H-4v), 7.82–7.92 (m, 3H, naphthyl). 8.67 (d, 2 H, H4.4*'*, *J* 9.0 Hz). 1H{11B} NMR (400.13 MHz, CDCl3) **: –3.52 (d, 2H, Ru–H–B, *J* 24.7 Hz), 0.35 (br. s, extra-H), 0.75, 2.76, 3.37 and 3.68 (all br.s, 2H, 1H, 2H, 1H, B–H), 6.18 (br. s, 1H, PhC=CH). 13C NMR (101 MHz, CDCl3–CD3OD, 25°C) **: 14.1 (Me), 29.1–29.7 (7C, CH2), 37.3 (*C*Me3), 44.4 (*C*H2Ph), 56.0 (2OMe), 58.59 (4-OMe), 58.82 (4-OMe), 67.5 (CH2), 105.8 (2CHAr), 107.3 (C5) 108.86 (tm, 4CF2, 1*J*CF ≈ 267 Hz), 126.7 (*p-*C), 128.7 (2*m*-C), 129.3 (2*o*-C), 127.1 (=CH), 127.69, 129.3 (*o*-C), 130.6 (CAr), 133.3 (=C), 134.8 (C7), 138.1 (*i*-C), 138.94 (t, C4a(10a), *J*CF 23.9 Hz), 156.9 (C), 160.4 (C=O). 15N NMR (acetone-*d*6) **: –81.8, –138.8 (N3), –143.0 (N4), –145.2 (N1), –306.3 (NH2). 19F NMR (470.5 MHz, CDCl3) **: 27.95–28.09 (m, 4 F, F2,3), 29.4 (m, 8 F, F7,7*'*,8,8*'*), 43.5 (s, NF2), 52.07 and 52.30 (2m, 2F, F1,4) 54.3 (m, 8 F, F6,6*'*,9,9*'*), –119.2 (dd, JH,F 12.2 and 8.7 Hz). 31P NMR (242.9 MHz, DMSO-*d*6, 30°C) d: 49.68 (s) 54.2. 31P {1H} NMR (161.98 MHz, CD2Cl2) **: 44.92 (d, as, J 31.22 Hz), 48.80 (s, 1s), 49.68 (s), 52.82 (br. s, as). 11B NMR (CD2Cl2) **: –1.12, –9.56 (br. s), –14.24 (br. s), –19.29 (s), –20.16, –27.11 and –35.72 (all br. s).1H–1H NOESY (the most important cross-peaks): H1/H3, H1/H4, H2/H1, H3/H4, H7/H6, H7/H3. IR (KBr, *ν*/cm–1): 3487, 3345 (NH), 3398, 3325, 3317, 3062, 3069 (NH), 3028, 2962, 2982 (CH2, CH2Me), 2928, 2920 (C–H), 2870, 1953, 1885, 1811, 1751 (C=O), 1740 (C=O), 1668 [NHC(O)], 1613, 1577, 1552, 1487, 1448, 1393 (C=C, C=N), 1396, 1359, 1237, 1201, 1190 (ArOCH2), 1174, 1155, 1076, 1029, 1004 (P–O–C) 965, 994 (C–F) 926, 853, 829 (P=S), 804, 758, 703, 574, 552, 524. UV (CHCl3, **/nm): 333 (3.7), 400 (Soret), 586 (3.5). MS (EI, 70 eV), *m*/*z* (%): 394 (M+, 7), 362 (5), 330 (27), 229 (25). MS (ESI), *m*/*z*: 188 [M–2NO2]+, 193.0707 [M+H+], 210.0973 [M+NH4+], 215.0522, [M+Na+], 231.0264 [M+K+], 234 [M–NO2]+, (calc. for C7H12O6, *m*/*z*: 193.0707, 210.0972, 215.0526, 231.0265). MS (MALDI-TOF), *m*/*z*: 376 [M]+, 2301 [M+H]+, 2323 [M+Na]+, 2339 [M+K]+. HRMS (ESI), *m*/*z*: 331.0901 [M+Na]+, (calc. for C14H16N2O6Na+, *m*/*z*: 331.0901). Found (%): C, 74.60; H, 7.98; N, 17.36. Calc. for C15H19N3 (%): C, 74.65; H, 7.94; N, 17.41.

The authors should provide all data required to understand and verify the research presented in their article. In manuscripts reporting the syntheses of compounds, fully convincing evidence for the identity and purity (homogeneity) of all new compounds or known compounds made by a new/improved method should be provided. Data associated with particular compounds (the name of the compound, yield, melting point, optical rotation, refractive index, elemental analysis, UV and IR absorptions, NMR and mass spectra) should follow the description of their preparation procedure. High-resolution images of all spectra should be provided in Online Supplementary Materials.

In the articles including computational results, methods and software used for calculations should be properly cited. Equa tions, data, geometric parameters/coordinates, or other numerical parameters essential to reproduction of the computational results should be provided. When the results of electronic structure calculations in relative energies are reported, the absolute energies obtained directly from the computational output files and XYZ coordinates of corresponding structures should also be included in Online Supplementary Materials.