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Supporting Information

# A GFP-Chromophore-Based $C_{3V}$-symmetric Tripodal Receptor with Selective Recognition of Hg(II), Fe(III) and Cr(III)

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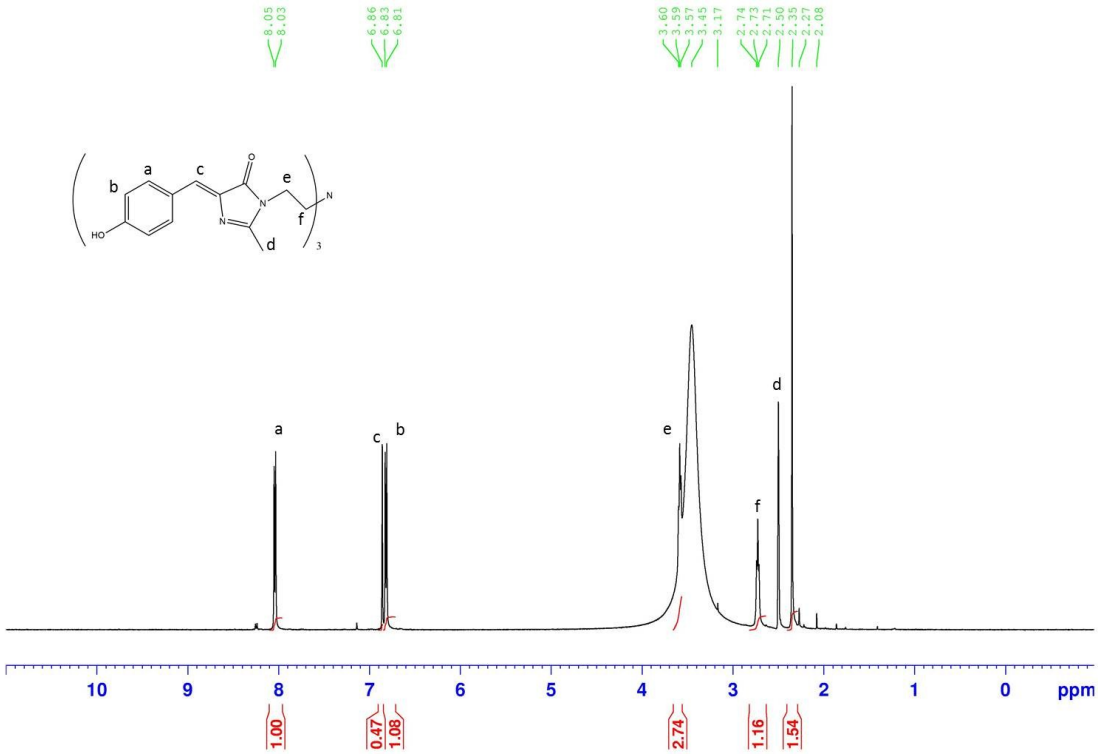


**Figure S1.** $^{1}$H-NMR spectrum of **1** in DMSO-$d_6$

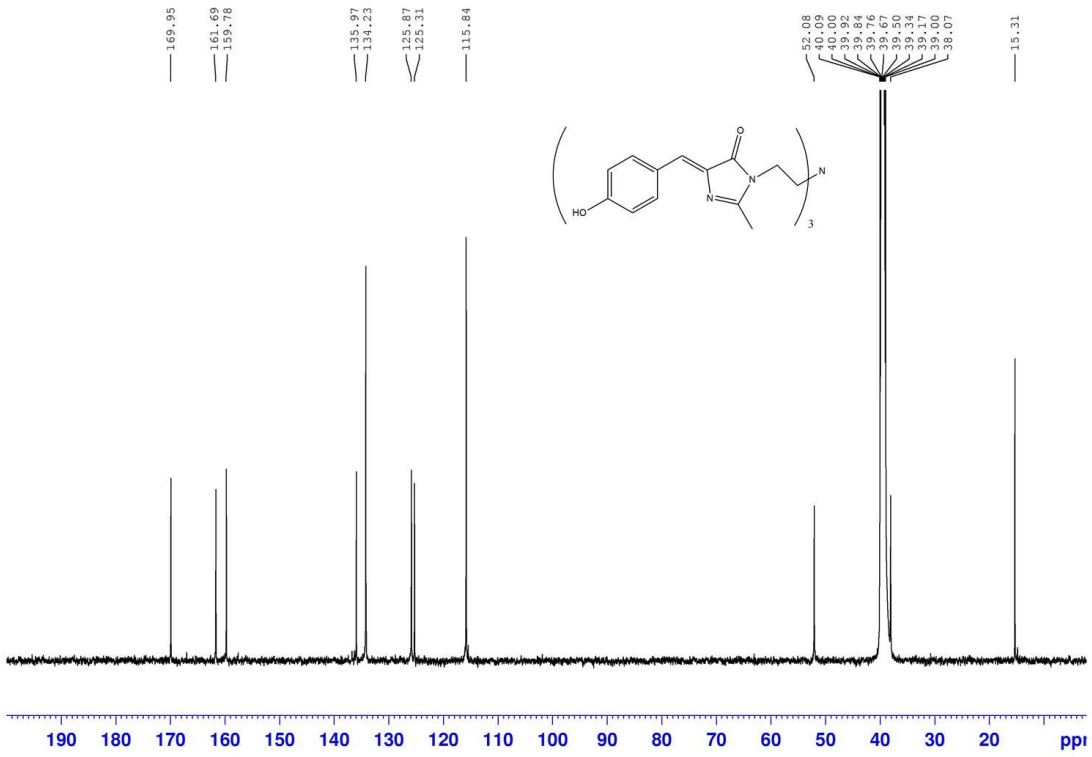


**Figure S2.** $^{13}$C-NMR spectrum of **1** in DMSO-$d_6$

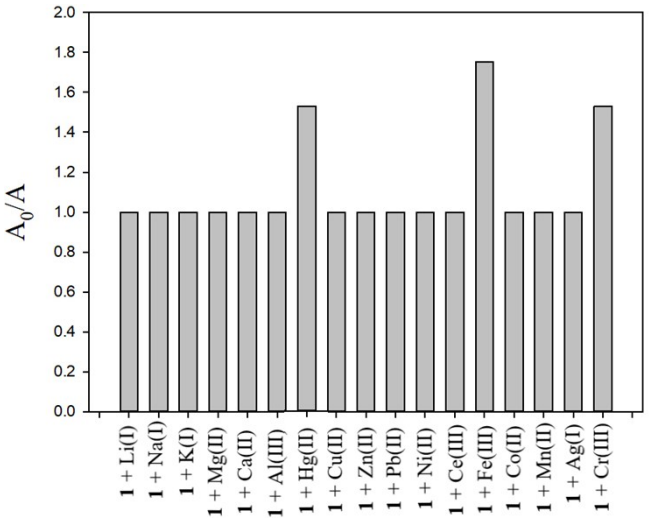


**Figure S3.** Relative absorbance ($A_0/A$) at λ=370 nm (selectivity test) between **1** (20 μM) and **1** with one equivalent of various cations in $CH_3CN$

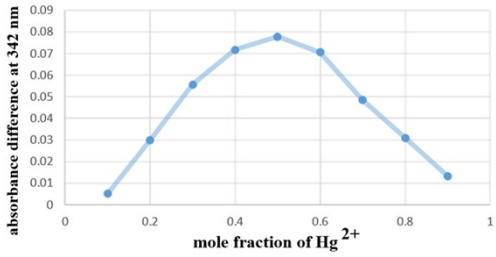


**Figure S4.** Job plot for the complex of the tripodal receptor **1** with $Hg(NO_3)_2$ in $CH_3CN$

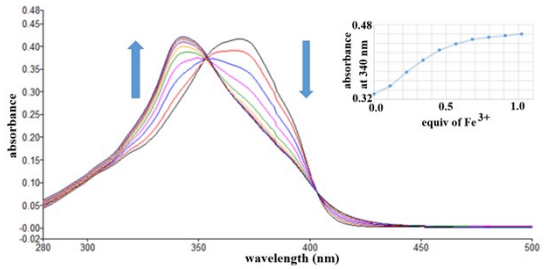


**Figure S5.** Electronic absorption spectra for the titration of the tripodal receptor **1** with various concentrations of $Fe(NO_3)_3$ in $CH_3CN$

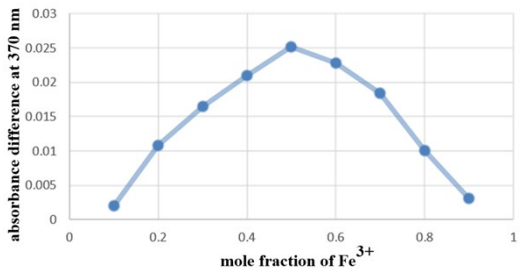


**Figure S6.** Job plot for the complex of the tripodal receptor **1** with $Fe(NO_3)_3$ in $CH_3CN$

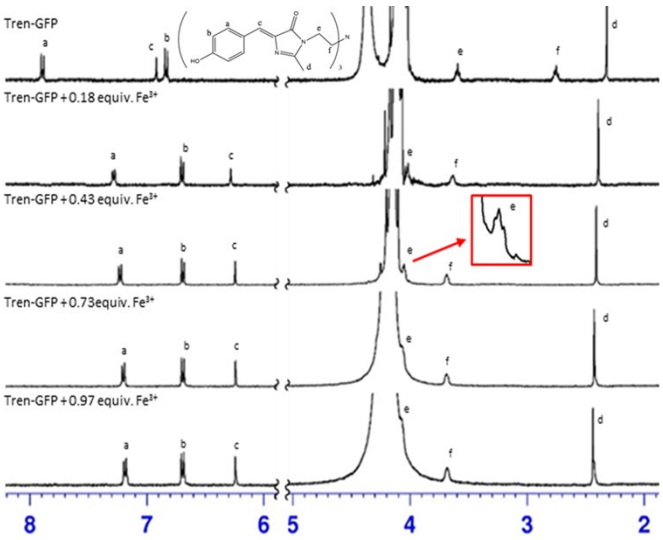


**Figure S7.** $^1H$ NMR spectra for the titration of the tripodal receptor **1** with 0.18, 0.43, 0.73 and 0.97 equivalent of $Fe^{3+}$ in 1:1 of $CD_3CN$ and $D_2O$

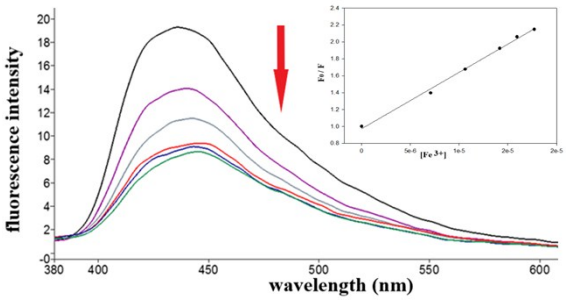


**Figure S8.** Fluorescence spectra for the titration of the tripodal receptor **1** with various concentrations of $Fe(NO_3)_3$ in $CH_3CN$ with excitation wavelength of 350 nm. Inset: their Stern-Volmer plot

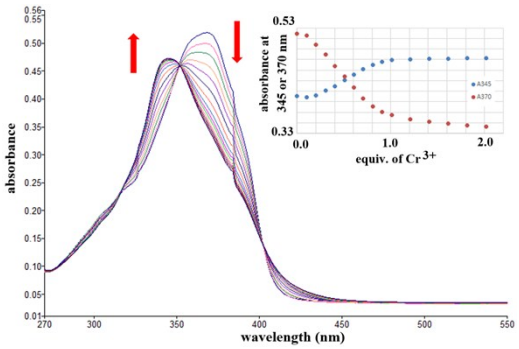


**Figure S9.** Electronic absorption spectra for the titration of the tripodal receptor **1** with various concentrations of $Cr(NO_3)_3$ in $CH_3CN$

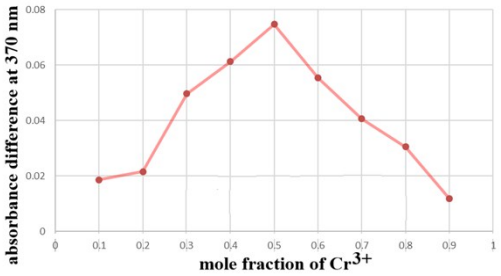


**Figure S10.** Electronic absorption spectra for the titration of the tripodal receptor **1** with various concentrations of $Cr(NO_3)_3$ in $CH_3CN$

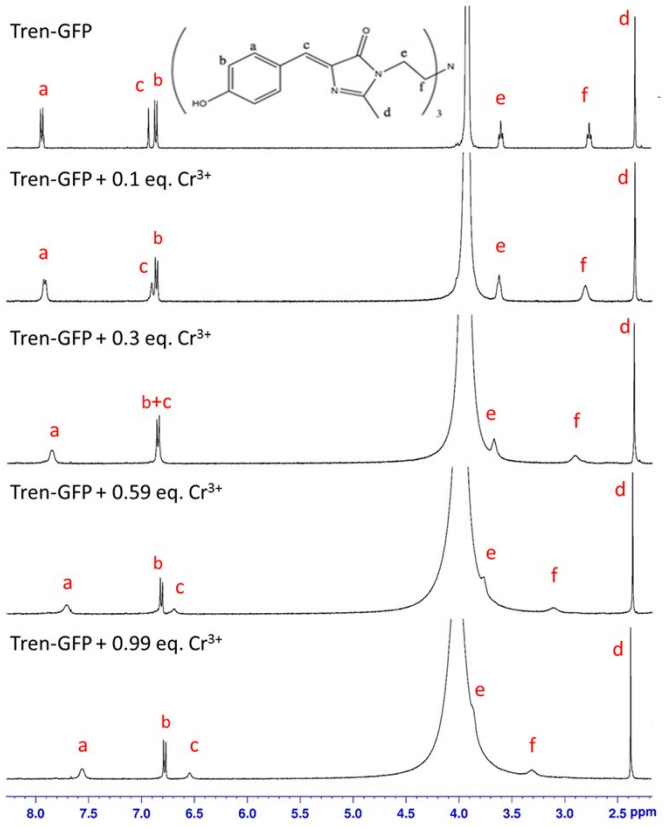


**Figure S11.** $^{1}$H NMR spectra for the titration of the tripodal receptor **1** with 0.1, 0.3, 0.59 and 0.99 equivalent of $Cr^{3+}$ in 1:1 of $CD_3CN$ and $D_2O$

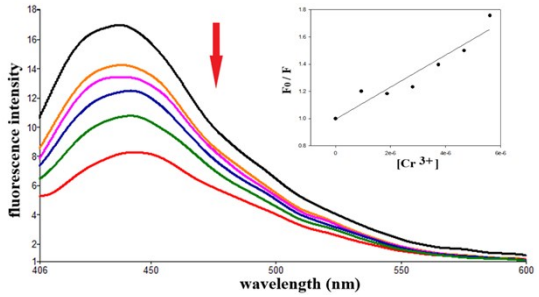


**Figure S12.** Fluorescence spectra for the titration of the tripodal receptor **1** with various concentrations of $Cr(NO_3)_3$ in $CH_3CN$ with excitation wavelength of 350 nm. Inset: their Stern-Volmer plot

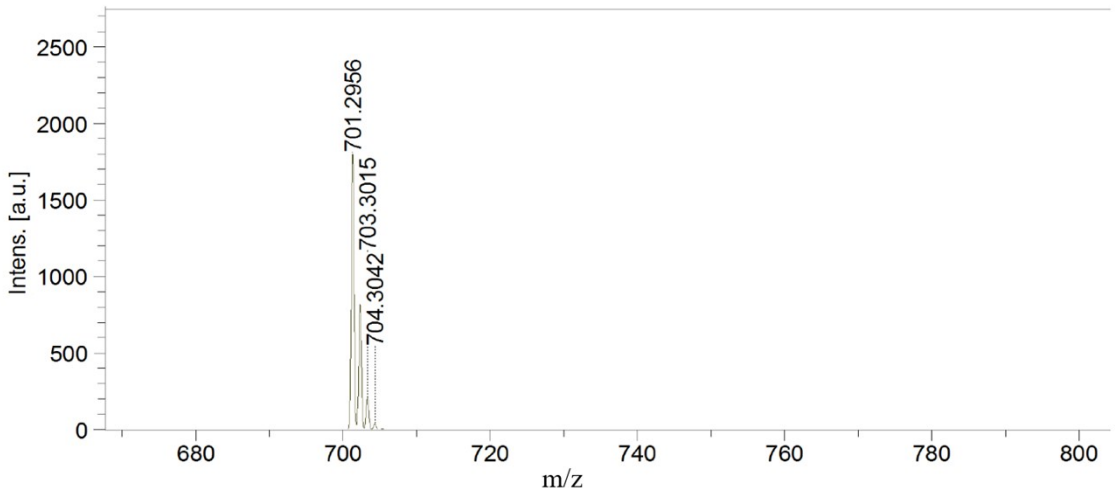


**Figure S13.** MALDI graph for the high-resolution mass of the tripodal receptor **1** [HRMS (MALDI) m/z calcd. for $C_{39}H_{39}N_7O_6^+(M^+)$ 701.2961, found: 701.2956.]

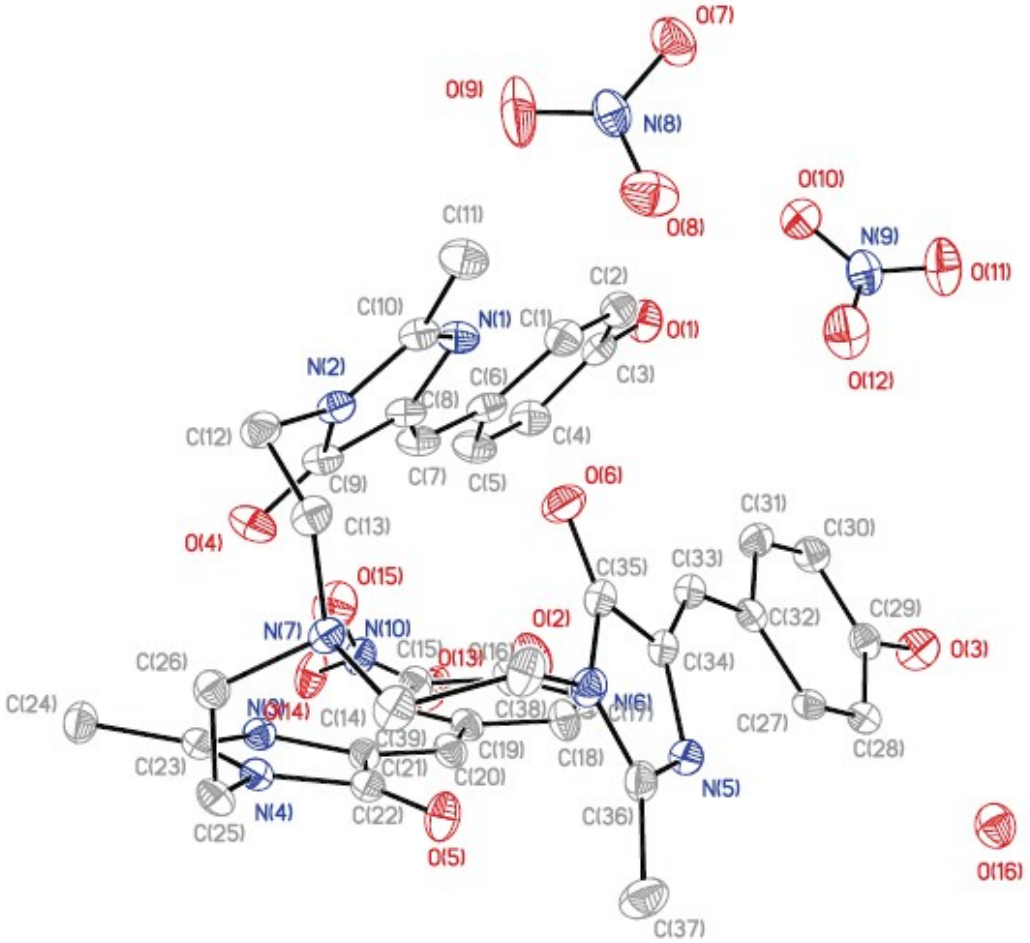


**Figure S14.** Single crystal X-ray diffraction structure of the tripodal receptor **1**•3 $HNO_3$ with thermal ellipsoids at the 50% probability level

Table S1. Crystal data and structure refinement for **1**.

| | | |
|---|---|---|
| Identification code | **1** | |
| Empirical formula | C39 H44 N10 O16 | |
| Formula weight | 908.84 | |
| Temperature | 298(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | $P2_12_12_1$ | |
| Unit cell dimensions | a = 13.4659(9) Å | α= 90°. |
| | b = 14.4044(12) Å | β= 90°. |
| | c = 22.0460(18) Å | γ = 90°. |
| Volume | 4276.2(6) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.412 $Mg/m^3$ | |
| Absorption coefficient | 0.111 $mm^{-1}$ | |
| F(000) | 1904 | |
| Crystal size | 0.500 x 0.340 x 0.240 $mm^3$ | |
| Theta range for data collection | 2.828 to 26.435°. | |
| Index ranges | -16<=h<=16, -18<=k<=18, -27<=l<=27 | |
| Reflections collected | 48343 | |
| Independent reflections | 8699 [R(int) = 0.0480] | |
| Completeness to theta = 25.242° | 99.3 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.9281 and 0.8075 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 8699 / 0 / 609 | |
| Goodness-of-fit on $F^2$ | 1.025 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0593, wR2 = 0.1477 | |
| R indices (all data) | R1 = 0.0904, wR2 = 0.1695 | |
| Absolute structure parameter | 0.4(4) | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.241 and -0.222 $e.Å^{-3}$ | |

Table S2. Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$x $10^3$) for crgfp. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| O(1) | 1057(3) | 2525(3) | 604(2) | 68(1) |
| O(2) | 1269(3) | 6007(3) | 1302(3) | 85(2) |
| O(3) | 1137(3) | 3308(3) | 3361(2) | 71(1) |
| O(4) | 7112(3) | 4346(3) | 643(2) | 65(1) |
| O(5) | 7193(3) | 5159(3) | 2560(2) | 60(1) |
| O(6) | 7037(3) | 2351(3) | 2106(2) | 63(1) |
| N(1) | 6136(3) | 2151(3) | 843(2) | 49(1) |
| N(2) | 7578(3) | 2820(3) | 823(2) | 44(1) |
| N(3) | 6448(3) | 6143(3) | 1206(2) | 42(1) |
| N(4) | 7823(3) | 5743(3) | 1653(2) | 42(1) |
| N(5) | 6298(3) | 3642(3) | 3350(2) | 46(1) |
| N(6) | 7673(3) | 3176(3) | 2922(2) | 46(1) |
| N(7) | 8825(3) | 3867(3) | 1798(2) | 39(1) |
| C(1) | 3727(4) | 2328(4) | 819(3) | 56(1) |
| C(2) | 2750(4) | 2084(4) | 793(3) | 59(1) |
| C(3) | 2037(4) | 2739(4) | 667(2) | 50(1) |
| C(4) | 2305(4) | 3658(4) | 593(3) | 61(1) |
| C(5) | 3292(4) | 3900(4) | 612(3) | 61(1) |
| C(6) | 4039(4) | 3241(4) | 717(2) | 49(1) |
| C(7) | 5061(4) | 3545(4) | 710(2) | 52(1) |
| C(8) | 5918(4) | 3087(3) | 764(2) | 45(1) |
| C(9) | 6898(4) | 3542(4) | 739(2) | 48(1) |
| C(10) | 7104(4) | 2013(3) | 883(2) | 45(1) |
| C(11) | 7550(4) | 1102(4) | 985(3) | 63(2) |
| C(12) | 8663(4) | 2969(4) | 815(2) | 51(1) |
| C(13) | 9124(3) | 3039(4) | 1442(2) | 46(1) |
| C(14) | 3973(4) | 6210(4) | 1262(2) | 50(1) |
| C(15) | 2993(4) | 6318(4) | 1092(2) | 54(1) |
| C(16) | 2241(4) | 5927(4) | 1448(3) | 58(1) |
| C(17) | 2488(4) | 5453(4) | 1966(3) | 65(2) |
| C(18) | 3455(4) | 5354(4) | 2134(3) | 58(1) |
| C(19) | 4228(4) | 5718(3) | 1781(2) | 46(1) |
| C(20) | 5239(4) | 5563(3) | 1988(2) | 47(1) |

| | | | | |
|---|---|---|---|---|
| C(21) | 6137(4) | 5744(3) | 1750(2) | 42(1) |
| C(22) | 7060(4) | 5485(3) | 2067(2) | 43(1) |
| C(23) | 7424(4) | 6124(3) | 1160(2) | 43(1) |
| C(24) | 7994(4) | 6459(4) | 629(2) | 59(1) |
| C(25) | 8885(4) | 5602(3) | 1780(2) | 48(1) |
| C(26) | 9275(4) | 4699(4) | 1529(2) | 46(1) |
| C(27) | 3839(4) | 3473(3) | 3386(2) | 45(1) |
| C(28) | 2862(4) | 3580(4) | 3567(2) | 49(1) |
| C(29) | 2102(4) | 3263(4) | 3192(2) | 49(1) |
| C(30) | 2329(4) | 2868(4) | 2634(3) | 56(1) |
| C(31) | 3304(4) | 2781(4) | 2461(2) | 55(1) |
| C(32) | 4091(3) | 3087(3) | 2830(2) | 43(1) |
| C(33) | 5080(4) | 2931(3) | 2617(2) | 46(1) |
| C(34) | 5992(4) | 3150(3) | 2836(2) | 44(1) |
| C(35) | 6902(4) | 2829(4) | 2550(2) | 47(1) |
| C(36) | 7277(4) | 3663(4) | 3380(2) | 48(1) |
| C(37) | 7849(5) | 4167(5) | 3845(3) | 68(2) |
| C(38) | 8720(4) | 2999(4) | 2793(2) | 53(1) |
| C(39) | 9216(3) | 3760(4) | 2418(2) | 51(1) |
| O(7) | 4406(4) | -676(4) | 548(2) | 88(2) |
| O(8) | 5024(4) | 377(4) | 1079(3) | 97(2) |
| O(9) | 5084(5) | 531(5) | 138(3) | 129(2) |
| N(8) | 4831(4) | 76(4) | 569(3) | 65(1) |
| O(10) | 226(4) | 906(3) | 938(2) | 85(1) |
| O(11) | -406(4) | 542(5) | 1804(3) | 110(2) |
| O(12) | 936(4) | 1332(5) | 1757(3) | 109(2) |
| N(9) | 251(4) | 925(4) | 1507(3) | 70(1) |
| O(13) | 422(5) | 7412(4) | 651(2) | 105(2) |
| O(14) | 465(4) | 8235(4) | -153(2) | 87(2) |
| O(15) | 1394(5) | 7012(5) | -58(3) | 112(2) |
| N(10) | 754(4) | 7544(4) | 147(2) | 69(1) |
| O(16) | 869(3) | 4275(4) | 4390(2) | 84(1) |

Table S3. Bond lengths [Å] and angles [°] for **1**.

| | |
|---|---|
| O(1)-C(3) | 1.363(6) |
| O(1)-H(1B) | 0.99(9) |
| O(2)-C(16) | 1.353(7) |
| O(2)-H(2B) | 1.08(9) |
| O(3)-C(29) | 1.353(6) |
| O(3)-H(3B) | 0.8200 |
| O(4)-C(9) | 1.212(6) |
| O(5)-C(22) | 1.196(6) |
| O(6)-C(35) | 1.211(6) |
| N(1)-C(10) | 1.322(7) |
| N(1)-C(8) | 1.391(7) |
| N(1)-H(1A) | 0.76(6) |
| N(2)-C(10) | 1.332(7) |
| N(2)-C(9) | 1.398(6) |
| N(2)-C(12) | 1.476(6) |
| N(3)-C(23) | 1.318(6) |
| N(3)-C(21) | 1.395(6) |
| N(3)-H(3A) | 0.84(5) |
| N(4)-C(23) | 1.331(6) |
| N(4)-C(22) | 1.424(6) |
| N(4)-C(25) | 1.471(6) |
| N(5)-C(36) | 1.320(7) |
| N(5)-C(34) | 1.399(7) |
| N(5)-H(5A) | 0.87(7) |
| N(6)-C(36) | 1.342(7) |
| N(6)-C(35) | 1.415(7) |
| N(6)-C(38) | 1.460(6) |
| N(7)-C(26) | 1.468(6) |
| N(7)-C(39) | 1.473(6) |
| N(7)-C(13) | 1.482(6) |
| C(1)-C(2) | 1.363(8) |
| C(1)-C(6) | 1.399(8) |
| C(1)-H(1C) | 0.9300 |
| C(2)-C(3) | 1.374(8) |
| C(2)-H(2A) | 0.9300 |
| C(3)-C(4) | 1.383(8) |

| | |
|---|---|
| C(4)-C(5) | 1.375(8) |
| C(4)-H(4A) | 0.9300 |
| C(5)-C(6) | 1.401(7) |
| C(5)-H(5B) | 0.9300 |
| C(6)-C(7) | 1.444(7) |
| C(7)-C(8) | 1.334(7) |
| C(7)-H(7A) | 0.9300 |
| C(8)-C(9) | 1.474(7) |
| C(10)-C(11) | 1.461(7) |
| C(11)-H(11A) | 0.9600 |
| C(11)-H(11B) | 0.9600 |
| C(11)-H(11C) | 0.9600 |
| C(12)-C(13) | 1.518(7) |
| C(12)-H(12A) | 0.9700 |
| C(12)-H(12B) | 0.9700 |
| C(13)-H(13A) | 0.9700 |
| C(13)-H(13B) | 0.9700 |
| C(14)-C(15) | 1.381(7) |
| C(14)-C(19) | 1.390(7) |
| C(14)-H(14A) | 0.9300 |
| C(15)-C(16) | 1.399(8) |
| C(15)-H(15A) | 0.9300 |
| C(16)-C(17) | 1.372(9) |
| C(17)-C(18) | 1.361(8) |
| C(17)-H(17A) | 0.9300 |
| C(18)-C(19) | 1.401(7) |
| C(18)-H(18A) | 0.9300 |
| C(19)-C(20) | 1.454(7) |
| C(20)-C(21) | 1.343(7) |
| C(20)-H(20A) | 0.9300 |
| C(21)-C(22) | 1.474(7) |
| C(23)-C(24) | 1.481(7) |
| C(24)-H(24A) | 0.9600 |
| C(24)-H(24B) | 0.9600 |
| C(24)-H(24C) | 0.9600 |
| C(25)-C(26) | 1.508(7) |
| C(25)-H(25A) | 0.9700 |
| C(25)-H(25B) | 0.9700 |

| | |
|---|---|
| C(26)-H(26A) | 0.9700 |
| C(26)-H(26B) | 0.9700 |
| C(27)-C(28) | 1.384(7) |
| C(27)-C(32) | 1.387(7) |
| C(27)-H(27A) | 0.9300 |
| C(28)-C(29) | 1.392(7) |
| C(28)-H(28A) | 0.9300 |
| C(29)-C(30) | 1.390(8) |
| C(30)-C(31) | 1.372(8) |
| C(30)-H(30A) | 0.9300 |
| C(31)-C(32) | 1.407(7) |
| C(31)-H(31A) | 0.9300 |
| C(32)-C(33) | 1.431(7) |
| C(33)-C(34) | 1.356(7) |
| C(33)-H(33A) | 0.9300 |
| C(34)-C(35) | 1.454(7) |
| C(36)-C(37) | 1.474(7) |
| C(37)-H(37A) | 0.9600 |
| C(37)-H(37B) | 0.9600 |
| C(37)-H(37C) | 0.9600 |
| C(38)-C(39) | 1.527(8) |
| C(38)-H(38A) | 0.9700 |
| C(38)-H(38B) | 0.9700 |
| C(39)-H(39A) | 0.9700 |
| C(39)-H(39B) | 0.9700 |
| O(7)-N(8) | 1.226(7) |
| O(8)-N(8) | 1.232(7) |
| O(9)-N(8) | 1.203(7) |
| O(10)-N(9) | 1.255(7) |
| O(11)-N(9) | 1.232(7) |
| O(12)-N(9) | 1.224(7) |
| O(13)-N(10) | 1.214(7) |
| O(14)-N(10) | 1.256(7) |
| O(15)-N(10) | 1.238(7) |
| O(16)-H(16A) | 1.1021 |
| O(16)-H(16B) | 1.0911 |
| C(3)-O(1)-H(1B) | 103(5) |
| C(16)-O(2)-H(2B) | 106(5) |

| | |
|---|---|
| C(29)-O(3)-H(3B) | 109.5 |
| C(10)-N(1)-C(8) | 111.2(5) |
| C(10)-N(1)-H(1A) | 123(5) |
| C(8)-N(1)-H(1A) | 124(5) |
| C(10)-N(2)-C(9) | 110.3(4) |
| C(10)-N(2)-C(12) | 127.0(4) |
| C(9)-N(2)-C(12) | 122.6(4) |
| C(23)-N(3)-C(21) | 110.8(4) |
| C(23)-N(3)-H(3A) | 124(3) |
| C(21)-N(3)-H(3A) | 125(3) |
| C(23)-N(4)-C(22) | 109.8(4) |
| C(23)-N(4)-C(25) | 127.2(4) |
| C(22)-N(4)-C(25) | 122.9(4) |
| C(36)-N(5)-C(34) | 110.3(4) |
| C(36)-N(5)-H(5A) | 118(4) |
| C(34)-N(5)-H(5A) | 131(4) |
| C(36)-N(6)-C(35) | 109.2(4) |
| C(36)-N(6)-C(38) | 128.4(4) |
| C(35)-N(6)-C(38) | 122.3(4) |
| C(26)-N(7)-C(39) | 108.2(4) |
| C(26)-N(7)-C(13) | 109.4(4) |
| C(39)-N(7)-C(13) | 108.1(4) |
| C(2)-C(1)-C(6) | 121.7(5) |
| C(2)-C(1)-H(1C) | 119.1 |
| C(6)-C(1)-H(1C) | 119.1 |
| C(1)-C(2)-C(3) | 120.3(6) |
| C(1)-C(2)-H(2A) | 119.8 |
| C(3)-C(2)-H(2A) | 119.8 |
| O(1)-C(3)-C(2) | 122.8(5) |
| O(1)-C(3)-C(4) | 117.2(5) |
| C(2)-C(3)-C(4) | 120.0(5) |
| C(5)-C(4)-C(3) | 119.4(5) |
| C(5)-C(4)-H(4A) | 120.3 |
| C(3)-C(4)-H(4A) | 120.3 |
| C(4)-C(5)-C(6) | 121.8(5) |
| C(4)-C(5)-H(5B) | 119.1 |
| C(6)-C(5)-H(5B) | 119.1 |
| C(1)-C(6)-C(5) | 116.6(5) |

| | |
|---|---|
| C(1)-C(6)-C(7) | 124.9(5) |
| C(5)-C(6)-C(7) | 118.4(5) |
| C(8)-C(7)-C(6) | 132.4(5) |
| C(8)-C(7)-H(7A) | 113.8 |
| C(6)-C(7)-H(7A) | 113.8 |
| C(7)-C(8)-N(1) | 132.2(5) |
| C(7)-C(8)-C(9) | 123.5(5) |
| N(1)-C(8)-C(9) | 104.3(4) |
| O(4)-C(9)-N(2) | 125.3(5) |
| O(4)-C(9)-C(8) | 130.0(5) |
| N(2)-C(9)-C(8) | 104.6(4) |
| N(1)-C(10)-N(2) | 109.6(4) |
| N(1)-C(10)-C(11) | 123.4(5) |
| N(2)-C(10)-C(11) | 126.9(4) |
| C(10)-C(11)-H(11A) | 109.5 |
| C(10)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 |
| C(10)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 |
| H(11B)-C(11)-H(11C) | 109.5 |
| N(2)-C(12)-C(13) | 113.8(4) |
| N(2)-C(12)-H(12A) | 108.8 |
| C(13)-C(12)-H(12A) | 108.8 |
| N(2)-C(12)-H(12B) | 108.8 |
| C(13)-C(12)-H(12B) | 108.8 |
| H(12A)-C(12)-H(12B) | 107.7 |
| N(7)-C(13)-C(12) | 115.1(4) |
| N(7)-C(13)-H(13A) | 108.5 |
| C(12)-C(13)-H(13A) | 108.5 |
| N(7)-C(13)-H(13B) | 108.5 |
| C(12)-C(13)-H(13B) | 108.5 |
| H(13A)-C(13)-H(13B) | 107.5 |
| C(15)-C(14)-C(19) | 121.1(5) |
| C(15)-C(14)-H(14A) | 119.4 |
| C(19)-C(14)-H(14A) | 119.4 |
| C(14)-C(15)-C(16) | 119.6(5) |
| C(14)-C(15)-H(15A) | 120.2 |
| C(16)-C(15)-H(15A) | 120.2 |

| | |
|---|---|
| O(2)-C(16)-C(17) | 118.3(5) |
| O(2)-C(16)-C(15) | 122.2(5) |
| C(17)-C(16)-C(15) | 119.5(5) |
| C(18)-C(17)-C(16) | 120.7(5) |
| C(18)-C(17)-H(17A) | 119.7 |
| C(16)-C(17)-H(17A) | 119.7 |
| C(17)-C(18)-C(19) | 121.4(5) |
| C(17)-C(18)-H(18A) | 119.3 |
| C(19)-C(18)-H(18A) | 119.3 |
| C(14)-C(19)-C(18) | 117.7(5) |
| C(14)-C(19)-C(20) | 124.6(5) |
| C(18)-C(19)-C(20) | 117.7(5) |
| C(21)-C(20)-C(19) | 133.7(5) |
| C(21)-C(20)-H(20A) | 113.1 |
| C(19)-C(20)-H(20A) | 113.1 |
| C(20)-C(21)-N(3) | 133.3(5) |
| C(20)-C(21)-C(22) | 121.6(4) |
| N(3)-C(21)-C(22) | 105.1(4) |
| O(5)-C(22)-N(4) | 125.1(5) |
| O(5)-C(22)-C(21) | 131.1(5) |
| N(4)-C(22)-C(21) | 103.8(4) |
| N(3)-C(23)-N(4) | 110.5(4) |
| N(3)-C(23)-C(24) | 124.8(5) |
| N(4)-C(23)-C(24) | 124.7(5) |
| C(23)-C(24)-H(24A) | 109.5 |
| C(23)-C(24)-H(24B) | 109.5 |
| H(24A)-C(24)-H(24B) | 109.5 |
| C(23)-C(24)-H(24C) | 109.5 |
| H(24A)-C(24)-H(24C) | 109.5 |
| H(24B)-C(24)-H(24C) | 109.5 |
| N(4)-C(25)-C(26) | 112.8(4) |
| N(4)-C(25)-H(25A) | 109.0 |
| C(26)-C(25)-H(25A) | 109.0 |
| N(4)-C(25)-H(25B) | 109.0 |
| C(26)-C(25)-H(25B) | 109.0 |
| H(25A)-C(25)-H(25B) | 107.8 |
| N(7)-C(26)-C(25) | 114.3(4) |
| N(7)-C(26)-H(26A) | 108.7 |

| | |
|---|---|
| C(25)-C(26)-H(26A) | 108.7 |
| N(7)-C(26)-H(26B) | 108.7 |
| C(25)-C(26)-H(26B) | 108.7 |
| H(26A)-C(26)-H(26B) | 107.6 |
| C(28)-C(27)-C(32) | 122.1(4) |
| C(28)-C(27)-H(27A) | 118.9 |
| C(32)-C(27)-H(27A) | 118.9 |
| C(27)-C(28)-C(29) | 119.4(5) |
| C(27)-C(28)-H(28A) | 120.3 |
| C(29)-C(28)-H(28A) | 120.3 |
| O(3)-C(29)-C(30) | 118.3(5) |
| O(3)-C(29)-C(28) | 121.8(5) |
| C(30)-C(29)-C(28) | 119.8(5) |
| C(31)-C(30)-C(29) | 119.6(5) |
| C(31)-C(30)-H(30A) | 120.2 |
| C(29)-C(30)-H(30A) | 120.2 |
| C(30)-C(31)-C(32) | 122.1(5) |
| C(30)-C(31)-H(31A) | 118.9 |
| C(32)-C(31)-H(31A) | 118.9 |
| C(27)-C(32)-C(31) | 116.9(5) |
| C(27)-C(32)-C(33) | 125.5(4) |
| C(31)-C(32)-C(33) | 117.5(5) |
| C(34)-C(33)-C(32) | 133.6(5) |
| C(34)-C(33)-H(33A) | 113.2 |
| C(32)-C(33)-H(33A) | 113.2 |
| C(33)-C(34)-N(5) | 132.3(5) |
| C(33)-C(34)-C(35) | 122.3(5) |
| N(5)-C(34)-C(35) | 105.4(4) |
| O(6)-C(35)-N(6) | 124.0(5) |
| O(6)-C(35)-C(34) | 131.2(5) |
| N(6)-C(35)-C(34) | 104.8(4) |
| N(5)-C(36)-N(6) | 110.3(5) |
| N(5)-C(36)-C(37) | 124.7(5) |
| N(6)-C(36)-C(37) | 125.0(5) |
| C(36)-C(37)-H(37A) | 109.5 |
| C(36)-C(37)-H(37B) | 109.5 |
| H(37A)-C(37)-H(37B) | 109.5 |
| C(36)-C(37)-H(37C) | 109.5 |

| | |
|---|---|
| H(37A)-C(37)-H(37C) | 109.5 |
| H(37B)-C(37)-H(37C) | 109.5 |
| N(6)-C(38)-C(39) | 113.7(4) |
| N(6)-C(38)-H(38A) | 108.8 |
| C(39)-C(38)-H(38A) | 108.8 |
| N(6)-C(38)-H(38B) | 108.8 |
| C(39)-C(38)-H(38B) | 108.8 |
| H(38A)-C(38)-H(38B) | 107.7 |
| N(7)-C(39)-C(38) | 114.9(4) |
| N(7)-C(39)-H(39A) | 108.5 |
| C(38)-C(39)-H(39A) | 108.5 |
| N(7)-C(39)-H(39B) | 108.5 |
| C(38)-C(39)-H(39B) | 108.5 |
| H(39A)-C(39)-H(39B) | 107.5 |
| O(9)-N(8)-O(8) | 118.0(6) |
| O(9)-N(8)-O(7) | 125.7(7) |
| O(8)-N(8)-O(7) | 116.3(6) |
| O(12)-N(9)-O(11) | 121.1(7) |
| O(12)-N(9)-O(10) | 118.7(6) |
| O(11)-N(9)-O(10) | 120.2(6) |
| O(13)-N(10)-O(15) | 119.5(6) |
| O(13)-N(10)-O(14) | 119.4(6) |
| O(15)-N(10)-O(14) | 121.0(6) |
| H(16A)-O(16)-H(16B) | 103.6 |

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Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| O(1) | 45(2) | 87(3) | 72(3) | 7(2) | 1(2) | 1(2) |
| O(2) | 46(2) | 85(3) | 123(4) | 28(3) | -8(2) | -4(2) |
| O(3) | 43(2) | 97(3) | 74(3) | -6(2) | -9(2) | 0(2) |
| O(4) | 62(2) | 41(2) | 92(3) | -10(2) | -8(2) | -2(2) |
| O(5) | 59(2) | 74(3) | 49(2) | 23(2) | 1(2) | 9(2) |
| O(6) | 64(2) | 75(3) | 49(2) | -18(2) | 8(2) | -4(2) |
| N(1) | 44(2) | 46(2) | 56(3) | -12(2) | -8(2) | 2(2) |
| N(2) | 40(2) | 50(2) | 41(2) | -11(2) | 0(2) | 2(2) |
| N(3) | 46(2) | 37(2) | 43(2) | 1(2) | -1(2) | 3(2) |
| N(4) | 44(2) | 38(2) | 45(2) | -4(2) | 2(2) | -5(2) |
| N(5) | 52(3) | 44(2) | 41(2) | 1(2) | 1(2) | -2(2) |
| N(6) | 48(2) | 54(2) | 37(2) | 5(2) | -3(2) | -1(2) |
| N(7) | 28(2) | 50(2) | 38(2) | -4(2) | -1(2) | 2(2) |
| C(1) | 49(3) | 56(3) | 63(3) | -2(3) | 4(3) | 15(2) |
| C(2) | 52(3) | 62(3) | 64(3) | -3(3) | 9(3) | 6(3) |
| C(3) | 44(3) | 69(3) | 38(3) | -6(2) | -1(2) | 7(2) |
| C(4) | 53(3) | 59(3) | 72(4) | -6(3) | -4(3) | 14(3) |
| C(5) | 58(3) | 48(3) | 78(4) | -13(3) | -11(3) | 12(3) |
| C(6) | 45(3) | 55(3) | 48(3) | -15(2) | -6(2) | 11(2) |
| C(7) | 50(3) | 47(3) | 60(3) | -15(2) | -13(3) | 11(2) |
| C(8) | 46(3) | 41(3) | 49(3) | -12(2) | -7(2) | 6(2) |
| C(9) | 46(3) | 49(3) | 47(3) | -15(2) | -4(2) | 4(2) |
| C(10) | 43(3) | 49(3) | 44(3) | -12(2) | -5(2) | 5(2) |
| C(11) | 62(3) | 49(3) | 76(4) | -6(3) | -6(3) | 13(3) |
| C(12) | 42(3) | 59(3) | 53(3) | -14(2) | 8(2) | -1(2) |
| C(13) | 30(2) | 57(3) | 50(3) | -5(2) | 1(2) | 7(2) |
| C(14) | 43(3) | 50(3) | 56(3) | 4(2) | 8(2) | 1(2) |
| C(15) | 58(3) | 47(3) | 55(3) | 9(2) | -4(2) | 4(2) |
| C(16) | 43(3) | 45(3) | 86(4) | 7(3) | 4(3) | 2(2) |
| C(17) | 46(3) | 56(3) | 95(5) | 19(3) | 14(3) | -4(3) |
| C(18) | 52(3) | 51(3) | 69(4) | 17(3) | 5(3) | 3(2) |
| C(19) | 44(3) | 36(2) | 58(3) | -1(2) | 3(2) | 2(2) |
| C(20) | 49(3) | 36(2) | 57(3) | 4(2) | 3(2) | 1(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(21) | 49(3) | 34(2) | 44(3) | 2(2) | 4(2) | 1(2) |
| C(22) | 49(3) | 36(2) | 45(3) | -1(2) | 2(2) | 1(2) |
| C(23) | 50(3) | 33(2) | 45(3) | -2(2) | 2(2) | -4(2) |
| C(24) | 63(3) | 67(3) | 48(3) | 7(3) | 6(3) | -8(3) |
| C(25) | 39(3) | 46(3) | 59(3) | -1(2) | -6(2) | -13(2) |
| C(26) | 35(2) | 53(3) | 50(3) | -1(2) | 2(2) | -5(2) |
| C(27) | 48(3) | 43(3) | 44(3) | -3(2) | -7(2) | -12(2) |
| C(28) | 52(3) | 43(3) | 51(3) | -2(2) | 0(2) | -5(2) |
| C(29) | 45(3) | 47(3) | 55(3) | 10(2) | -5(2) | -2(2) |
| C(30) | 51(3) | 61(3) | 56(3) | 1(3) | -15(2) | -10(3) |
| C(31) | 59(3) | 62(3) | 43(3) | -3(2) | -1(2) | -10(3) |
| C(32) | 44(3) | 37(2) | 48(3) | 6(2) | -3(2) | -7(2) |
| C(33) | 55(3) | 45(3) | 39(2) | 1(2) | 4(2) | -7(2) |
| C(34) | 49(3) | 45(3) | 36(2) | 6(2) | 4(2) | -4(2) |
| C(35) | 53(3) | 51(3) | 37(3) | 4(2) | 6(2) | -5(2) |
| C(36) | 52(3) | 50(3) | 41(3) | 11(2) | 1(2) | -4(2) |
| C(37) | 64(4) | 91(5) | 49(3) | -16(3) | -8(3) | -8(3) |
| C(38) | 43(3) | 72(4) | 45(3) | 12(3) | -2(2) | 9(3) |
| C(39) | 32(2) | 73(4) | 49(3) | 2(3) | -7(2) | 2(2) |
| O(7) | 83(3) | 82(3) | 100(4) | 4(3) | -7(3) | -34(3) |
| O(8) | 116(4) | 73(3) | 101(4) | -3(3) | -33(3) | 16(3) |
| O(9) | 126(5) | 121(5) | 141(5) | 75(4) | 47(4) | 5(4) |
| N(8) | 52(3) | 64(3) | 79(4) | 17(3) | -5(3) | -5(2) |
| O(10) | 95(4) | 86(3) | 73(3) | -2(2) | 1(3) | -4(3) |
| O(11) | 96(4) | 130(5) | 105(4) | 52(4) | -8(3) | -14(4) |
| O(12) | 95(4) | 138(5) | 95(4) | 24(4) | -36(3) | -30(4) |
| N(9) | 63(3) | 70(3) | 79(4) | 26(3) | -12(3) | 12(3) |
| O(13) | 141(5) | 116(4) | 58(3) | 15(3) | 18(3) | 3(4) |
| O(14) | 84(3) | 113(4) | 64(3) | 35(3) | 11(2) | 24(3) |
| O(15) | 100(4) | 120(5) | 116(5) | 11(4) | 17(3) | 33(4) |
| N(10) | 67(3) | 87(4) | 53(3) | 6(3) | 2(3) | -4(3) |
| O(16) | 72(3) | 86(3) | 93(3) | 5(3) | 12(3) | -2(2) |

Table S5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$) for **1**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1B) | 1010(60) | 1920(60) | 810(40) | 110(30) |
| H(2B) | 1240(60) | 6450(60) | 910(40) | 120(30) |
| H(3B) | 1093 | 3577 | 3687 | 170(50) |
| H(1A) | 5770(50) | 1760(50) | 790(30) | 70(20) |
| H(3A) | 6080(30) | 6390(30) | 950(20) | 28(12) |
| H(5A) | 5960(50) | 3960(50) | 3620(30) | 80(20) |
| H(1C) | 4199 | 1876 | 906 | 67 |
| H(2A) | 2564 | 1471 | 862 | 71 |
| H(4A) | 1821 | 4109 | 530 | 73 |
| H(5B) | 3470 | 4517 | 554 | 74 |
| H(7A) | 5136 | 4181 | 658 | 63 |
| H(11A) | 8260 | 1162 | 999 | 94 |
| H(11B) | 7316 | 853 | 1363 | 94 |
| H(11C) | 7368 | 692 | 660 | 94 |
| H(12A) | 8804 | 3535 | 594 | 62 |
| H(12B) | 8974 | 2459 | 599 | 62 |
| H(13A) | 8947 | 2488 | 1671 | 55 |
| H(13B) | 9841 | 3043 | 1399 | 55 |
| H(14A) | 4471 | 6471 | 1025 | 60 |
| H(15A) | 2833 | 6649 | 743 | 64 |
| H(17A) | 1990 | 5197 | 2206 | 78 |
| H(18A) | 3606 | 5038 | 2490 | 69 |
| H(20A) | 5272 | 5278 | 2366 | 57 |
| H(24A) | 8691 | 6373 | 702 | 88 |
| H(24B) | 7802 | 6114 | 276 | 88 |
| H(24C) | 7860 | 7106 | 566 | 88 |
| H(25A) | 8988 | 5612 | 2216 | 58 |
| H(25B) | 9260 | 6111 | 1606 | 58 |
| H(26A) | 9160 | 4689 | 1095 | 55 |
| H(26B) | 9987 | 4676 | 1594 | 55 |
| H(27A) | 4344 | 3665 | 3645 | 54 |
| H(28A) | 2714 | 3861 | 3936 | 58 |

| | | | | |
|---|---|---|---|---|
| H(30A) | 1824 | 2664 | 2379 | 67 |
| H(31A) | 3449 | 2511 | 2089 | 66 |
| H(33A) | 5104 | 2613 | 2250 | 56 |
| H(37A) | 8546 | 4080 | 3774 | 103 |
| H(37B) | 7693 | 4816 | 3825 | 103 |
| H(37C) | 7681 | 3932 | 4240 | 103 |
| H(38A) | 8777 | 2415 | 2577 | 64 |
| H(38B) | 9074 | 2935 | 3174 | 64 |
| H(39A) | 9140 | 4346 | 2630 | 62 |
| H(39B) | 9921 | 3628 | 2393 | 62 |
| H(16A) | 325 | 4040 | 4730 | 90(20) |
| H(16B) | 449 | 4763 | 4112 | 170(40) |