3-Methyl-1-phenyl-1-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-2 butanone (5a). Microcrystals from hexane-ethyl acetate (96%), mp 44–45 °C; ^{1}H NMR δ 7.37–7.20 (m, 3H), 7.16 (d, *J* = 6.4 Hz, 2H), 6.43 (d, *J* = 8.5 Hz, 1H), 6.34 (d, *J* = 8.2 Hz, 1H), 5.18–5.15 (m, 1H), 4.64 (m, 1H), 3.81–3.68 (m, 2H), 2.63–2.54 (m, 1H), 1.08 (d, *J* = 7.3 Hz, 3H), 0.90 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR δ 212.3, 134.3, 129.0, 128.9, 127,9, 121.9, 121.8, 119.3 (CF_3, q, *J* = 321 Hz), 112.5, 111.7, 64.8, 40.2, 34.6, 18.5, 17.8; Anal. Calcd for $C_{17}H_{18}F_3NO_3S$: C, 54.68; H, 4.86; N, 3.75. Found: C, 54.94; H, 4.87; N, 3.61.

1-(4-Methoxyphenyl)-1-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}acetone (5b). Yellow prisms from hexane (86%), mp 47–48 °C; ^{1}H NMR δ 7.07 (d, *J* = 8.5 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 2H), 6.41 (d, *J* = 8.2 Hz, 2H), 6.32 (d, *J* = 8.5 Hz, 1H), 5.22 (d, *J* = 8.5 Hz, 1H), 4.70 (d, *J* = 7.0 Hz, 1H), 3.81 (s, 3H), 3.64–3.58 (m, 2H), 2.06 (s, 3H); ^{13}C NMR δ 206.6, 159.3, 130.3, 129.8, 126.3, 121.8, 119.3 (CF_3, q, *J* = 322 Hz), 114.5, 112.4, 111.5, 66.0, 55.3, 34.1, 29.9, Anal. Calcd for $C_{16}H_{16}F_3NO_4S$: C, 51.20; H, 4.30; N, 3.73. Found: C, 51.59; H, 4.31; N, 3.52.

1-(4-Bromophenyl)-2-phenyl-2-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-1-ethanone (5c). Needles from hexane-ethyl acetate (88%), mp 104–105 °C; ^{1}H NMR δ 7.78 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.34–7.21 (m, 5H), 6.41 (t, *J* = 9.6 Hz, 2H), 5.25–5.22 (m, 1H), 4.74 (br s, 1H), 4.46 (d, *J* = 9.1 Hz, 1H), 3.91–3.88 (m, 1H); ^{13}C NMR δ 196.9, 135.0, 134.5, 131.9, 130.1, 129.2, 128.7, 128.5, 127.9, 122.2, 122.1, 119.0 (CF_3, q, *J* = 320 Hz), 112.2, 111.4, 61.5, 35.3; Anal. Calcd for $C_{20}H_{15}BrF_3NO_3S$: C, 49.40; H, 3.11; N, 2.88. Found: C, 49.46; H, 3.16; N, 2.78.

1,2-Diphenyl-2-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-1-ethanone (5d). Microcrystals from hexane-ethyl acetate (98%), mp 119–120 °C; ^{1}H NMR δ 7.93 (d, J = 7.5 Hz, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.46–7.20 (m, 7H), 6.40 (t, J = 8.3 Hz, 2H), 5.27 (m, 1H), 4.75 (m, 1H), 4.54 (d, J = 9.4 Hz, 1H), 3.92 (m, 1H); ^{13}C NMR δ 198.0, 136.4, 134.9, 133.2, 128.9, 128.7, 128.6, 127.7, 122.0, 119.7 (CF_3, q, J = 324 Hz), 112.3, 111.6, 61.5, 35.4. Anal. Calcd for $C_{20}H_{16}F_3NO_3S$: C, 58.96; H, 3.96; N, 3.44. Found: C, 58.47; H, 3.86; N, 3.49.

1-{1-[(Trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-3,4-dihydro-2(1*H*)-naphthalenone (5e). Unstable solid (81%); ^{1}H NMR δ 8.07–7.99 (m, 3H), 7.91–7.88 (m, 1H), 7.24 (d, J = 8.4 Hz, 1H), 7.12 (d, J = 8.2 Hz, 1H), 5.91–5.86 (m, 1H), 5.71–5.66 (m, 1H), 4.63 (br s, 1H), 4.19 (d, J = 5.6 Hz, 1H), 3.93 (ddd, J = 16.3, 10.2, 5.4 Hz, 1H), 3.71 (ddd, J = 16.0, 6.2, 4.4 Hz, 1H), 3.44 (ddd, J = 16.5, 5.1, 4.5 Hz, 1H), 3.27 (ddd, J = 17.3, 10.1, 6.4 Hz, 1H); ^{13}C NMR δ 209.9, 136.6, 133.5, 129.4, 127.9, 127.8, 127.0, 126.3, 122.4, 122.1, 119.1 (CF_3, q, J = 320 Hz), 110.9, 110.1, 58.7, 38.3, 27.4.

2-(Benzotriazol-1-yl)-1-phenyl-2-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-1-ethanone (5f). White needles from hexane-ethyl acetate (95%), mp 125–126 °C; ^{1}H NMR δ 8.04 (dd, J = 8.3, 1.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 2H), 7.59–7.45 (m, 3H), 7.40–7.34 (m, 3H), 6.56 (d, J = 8.6 Hz, 1H), 6.53 (dd, J = 8.6, 7.3 Hz, 2H), 5.33–5.28 (m, 1H), 4.59 (br s, 1H), 4.47–4.44 (m, 1H); ^{13}C NMR δ 193.6, 145.9, 135.7, 134.5, 134.2, 129.6, 128.9, 128.7, 125.1, 123.9, 123.8, 120.1, 119.2 (CF_3, q, J = 320 Hz), 111.8, 111.7, 110.7, 66.3, 35.2; Anal. Calcd for $C_{20}H_{15}F_3N_4O_3S$: C, 53.57; H, 3.37; N, 12.49. Found: C, 53.45; H, 3.20; N, 12.42.

2-(Benzotriazol-1-yl)-1-(2-thienyl)-2-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-1-ethanone (5g). Yellow needles from hexane-ethyl acetate (85%), mp 138 °C; ^{1}H NMR δ 8.06 (d, *J* = 8.4 Hz, 1H), 7.67–7.62 (m, 3H), 7.49 (dd, *J* = 8.1, 7.0 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.02 (dd, *J* = 4.5, 4.2 Hz, 1H), 6.56 (d, *J* = 8.4 Hz, 1H), 6.42 (d, *J* = 8.6 Hz, 1H), 6.25 (d, *J* = 8.7 Hz, 1H), 5.35–5.30 (m, 1H), 4.58 (br s, 1H), 4.48–4.45 (m, 1H); ^{13}C NMR δ 184.2, 146.5, 141.3, 136.3, 134.2, 131.9, 128.8, 128.4, 124.5, 124.0, 123.8, 120.4, 119.5 (CF_3, q, *J* = 323 Hz), 110.3, 108.6, 107.8, 68.5, 33.1; Anal. Calcd for $C_{18}H_{13}F_3N_4O_3S_2$: C, 47.57; H, 2.88; N, 12.33. Found: C, 47.54; H, 2.87; N, 12.12.

2-(Benzotriazol-1-yl)-1-(2-furyl)-2-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-1-ethanone (5h). White needles from hexane-ethyl acetate (76%), mp 114–115 °C; ^{1}H NMR δ 8.06 (d, *J* = 8.5 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.51 (dd, *J* = 8.1, 7.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 4.0 Hz, 1H), 6.55 (d, *J* = 8.2 Hz, 1H), 6.50–6.49 (m, 1H), 6.41 (d, *J* = 8.2 Hz, 1H), 6.17 (d, *J* = 9.0 Hz, 1H), 5.33–5.28 (m, 1H), 4.59 (br s, 1H), 4.50–4.47 (m, 1H); ^{13}C NMR δ 180.3, 151.1, 148.5, 146.8, 132.8, 128.6, 124.9, 124.5, 124.3, 120.9, 120.7, 119.5(CF_3, q, *J* = 322 Hz), 113.5, 110.7, 109.1, 108.3, 67.9, 33.5; Anal. Calcd for $C_{18}H_{13}F_3N_4O_4S$: C, 49.32; H, 2.99; N, 12.78. Found: C, 49.36; H, 2.96; N, 12.67.

1-(Benzotriazol-1-yl)-3,3-dimethyl-1-{1-[(trifluoromethyl)sulfonyl]-1,4-dihydro-4-pyridinyl}-2-butanone (5i). White needles from hexane-ethyl acetate (72%), mp 125–126 °C; ^{1}H NMR δ 8.11 (d, *J* = 8.5 Hz, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.52 (dd, *J* = 7.9, 7.3 Hz, 1H), 7.41 (dd, *J* = 7.6, 7.3 Hz, 1H), 6.60 (d, *J* = 8.2 Hz, 1H), 6.41 (d, *J* = 7.9 Hz, 1H), 5.94 (d, *J* = 9.6 Hz, 1H), 5.11–5.08 (m, 1H), 4.28–4.25 (m, 1H), 1.06 (s, 9H);

^{13}C NMR δ 207.1, 146.4, 131.8, 128.3, 124.5, 124.1, 123.5, 120.4, 119.4 (CF_3, q, J = 321 Hz), 110.7, 108.5, 108.1, 66.0, 45.2, 33.2, 25.8; Anal. Calcd for $C_{18}H_{19}F_3N_4O_3S$: C, 50.46; H, 4.47; N, 13.08. Found: C, 50.64; H, 4.55; N, 13.08.

3-Methyl-1-phenyl-1-(4-pyridinyl)-2-butanone (6a). White needles from hexane-ethyl acetate (91%), mp 167–168 °C; ^{1}H NMR δ 8.51 (br s, 2H), 7.36–7.22 (m, 5H), 7.19 (d, J = 4.7 Hz, 2H), 5.38 (s, 1H), 2.82–2.78 (m, 1H), 1.14 (d, J = 6.7 Hz, 3H), 1.06 (d, J = 6.4 Hz, 3H); ^{13}C NMR δ 209.9, 148.7, 147.4, 135.9, 128.3, 128.2, 127.1, 123.5, 60.4, 40.4, 18.0, 17.5. HRMS (FAB) Calcd for $C_{16}H_{18}NO$ [M^++1]: 240.1388. Found: 240.1382.

1-(4-Methoxyphenyl)-1-(4-pyridinyl)acetone (6b). White needles from hexane-ethyl acetate (81%), mp 114–115 °C; ^{1}H NMR δ 8.51 (br d, J = 4.3 Hz, 2H), 7.18–7.10 (m, 4H), 6.91 (dd, J = 7.1, 1.5 Hz, 2H), 5.04 (s, 1H), 3.78 (s, 3H), 2.24 (s, 3H); ^{13}C NMR δ 205.0, 159.0, 149.6, 147.4, 129.8, 128.2, 123.8, 114.4, 63.0, 55.0, 29.8. HRMS (FAB) Calcd for $C_{15}H_{16}NO$ [M^++1]: 242.1181. Found: 242.1184.

1-(4-Bromophenyl)-2-phenyl-2-(4-pyridinyl)-1-ethanone (6c). White plates from hexane-ethyl acetate (97%), mp 235–236 °C; ^{1}H NMR δ 8.53 (d, J = 5.2 Hz, 2H), 7.83 (d, J = 8.2 Hz, 2H), 7.51 (d, J = 7.9 Hz, 2H), 7.33–7.25 (m, 5H), 7.15 (d, J = 5.3 Hz, 2H), 5.96 (s, 1H); ^{13}C NMR δ 195.5, 149.6, 147.8, 136.6, 134.5, 131.8, 130.2, 129.1, 128.7, 128.6, 127.7, 124.1, 58.4. HRMS (FAB) Calcd for $C_{19}H_{15}BrNO$ [M^++1]: 352.0337. Found: 352.0335.

1,2-Diphenyl-2-(4-pyridyl)-1-ethanone (6d). White microcrystals from hexane-ethyl acetate (95%), mp 116–117 °C (lit.[10] 119–120 °C); ^{1}H NMR δ 8.54 (d, J = 6.1 Hz, 2H), 7.98 (d, J = 7.3 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.52–7.26 (m, 7H), 7.18 (d, J = 6.1 Hz,

2H), 6.01 (s, 1H); ^{13}C NMR δ 196.7, 149.8, 148.1, 137.1, 136.1, 133.4, 129.1, 128.9, 128.8, 128.7, 127.7, 124.3, 58.8.

2-(Benzotriazol-1-yl)-1-phenyl-2-(4-pyridinyl)-1-ethanone (6f). White prisms from hexane-ethyl acetate (90%), mp 154–155 °C; ^{1}H NMR δ 8.65 (d, J = 4.4 Hz, 2H), 8.09 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 7.2 Hz, 2H), 7.81 (s, 1H), 7.62 (dd, J = 6.6, 6.3 Hz, 1H), 7.50–7.29 (m, 5H), 7.19 (d, J = 4.4 Hz, 2H); ^{13}C NMR δ 191.1, 150.6, 146.6, 142.2, 134.8, 134.3, 132.6, 129.3, 128.9, 128, 124.4, 123.1, 120.4, 110.8, 66.0. HRMS (FAB) Calcd for $C_{19}H_{15}N_4O$ [M^++1]: 315.1231. Found: 315.1246.

2-(Benzotriazol-1-yl)-2-(4-pyridinyl)-1-(2-thienyl)-1-ethanone (6g). Yellow foam from ethyl acetate (91%); ^{1}H NMR δ 8.64 (d, J = 5.9 Hz, 2H), 8.09 (d, J = 8.0 Hz, 1H), 7.78 (d, J = 4.4 Hz, 1H), 7.76 (d, J = 5.9 Hz, 1H), 7.67 (s, 1H), 7.45–7.35 (m, 3H), 7.20 (d, J = 6.0 Hz, 2H), 7.13 (t, J = 4.4 Hz, 1H); ^{13}C NMR δ 183.7, 150.5, 146.6, 141.9, 141.1, 136.7, 134.2, 132.5, 128.9, 128.3, 124.5, 122.9, 120.3, 111.0, 66.7. HRMS (FAB) Calcd for $C_{17}H_{13}N_4OS$ [M^++1]: 321.0810. Found: 321.0808.

2-(Benzotriazol-1-yl)-1-(2-furyl)-2-(4-pyridinyl)-1-ethanone (6h). Yellow microcrystals from ethyl acetate-hexane (94%), mp 211–212 °C; ^{1}H NMR δ 8.65 (d, J = 5.5 Hz, 2H), 8.09 (d, J = 7.9 Hz, 1H), 7.62 (s, 1H), 7.61 (br s, 1H), 7.45–7.36 (m, 4H), 7.21 (d, J = 5.9 Hz, 2H), 7.13 (dd, J = 3.5, 1.5 Hz, 1H); ^{13}C NMR δ 179.6, 150.8, 150.5, 148.2, 146.5, 141.6, 132.7, 128.2, 124.4, 123.0, 120.5, 120.3, 113.4, 108.9, 65.7. Anal Calcd for $C_{17}H_{12}N_4O_2$: C, 67.10; H, 3.97; N, 18.41. Found: C, 67.21; H, 4.08; N, 18.32.

1-(Benzotriazol-1-yl)-3,3-dimethyl-1-(4-pyridinyl)-2-butanone (6i). White needles from hexane-ethyl acetate (95%), mp 153–154 °C; ^{1}H NMR δ 8.64 (br s, 2H), 8.06–8.03 (m, 1H), 7.35 (br s, 4H), 7.16 (br s, 2H), 1.24 (s, 9H); ^{13}C NMR δ 206.9, 150.4, 146.3,

142.1, 132.2, 128.0, 124.2, 122.9, 120.0, 111.0, 63.8, 45.4, 25.9. Anal Calcd for $C_{17}H_{18}N_4O$: C, 69.37; H, 6.16; N, 19.03. Found: C, 69.42; H, 6.46; N, 19.04.

4-Benzylpyridine (7). (lit.[11]) Oil (95%); ^{1}H NMR δ 8.47 (d, J = 5.9 Hz, 2H), 7.33–7.10 (m, 7H), 3.95 (s, 2H); ^{13}C NMR δ 150.0, 149.5, 138.7, 128.9, 128.6, 126.5, 124.1, 41.1.

4-[(Benzotriazol-1-yl)methyl]pyridine (8). White needles from hexane-ethyl acetate (60%), mp 115–116 °C; ^{1}H NMR δ 8.59 (d, J = 5.9 Hz, 2H), 8.12 (d, J = 8.3 Hz, 1H), 7.50–7.34 (m, 3H), 7.10 (d, J = 5.8 Hz, 2H), 5.87 (s, 2H); ^{13}C NMR δ 150.3, 146.1, 143.6, 132.6, 127.8, 124.1, 121.7, 120.1, 109.1, 50.5. Anal Calcd for $C_{12}H_{10}N_4$: C, 68.56; H, 4.79; N, 26.65. Found: C, 68.45; H, 4.94; N, 27.00.

Table S1. Crystal data and structure refinement for **5f**.

Identification code	3fyb	
Empirical formula	C20 H15 F3 N4 O3 S	
Formula weight	448.42	
Temperature	168(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 16.035(11) Å	α= 90°.
	b = 8.478(5) Å	β= 90°.
	c = 29.206(19) Å	γ = 90°.
Volume	3970(4) $Å^3$	
Z	8	
Density (calculated)	1.500 Mg/m^3	
Absorption coefficient	0.222 mm^{-1}	
F(000)	1840	
Crystal size	0.59 x 0.09 x 0.03 mm^3	
Theta range for data collection	2.50 to 20.00°.	
Index ranges	-15<=h<=15, -8<=k<=7, -28<=l<=28	
Reflections collected	26855	
Independent reflections	3689 [R(int) = 0.1203]	
Completeness to theta = 20.00°	99.8 %	
Max. and min. transmission	0.9934 and 0.8802	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3689 / 1 / 559	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1685	
R indices (all data)	R1 = 0.1069, wR2 = 0.1972	
Absolute structure parameter	0.0(2)	
Largest diff. peak and hole	0.909 and -0.419 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1B)	586(2)	4451(4)	2082(1)	41(1)
O(1B)	1151(7)	4971(12)	1756(4)	52(2)
O(2B)	224(5)	2946(10)	2085(3)	55(2)
C(1B)	1144(9)	4614(16)	2618(6)	50(4)
F(1B)	1478(5)	5976(9)	2688(3)	64(2)
F(2B)	635(6)	4296(11)	2982(3)	77(3)
F(3B)	1776(5)	3554(9)	2629(3)	72(2)
N(1B)	-140(6)	5750(10)	2141(4)	32(3)
C(2B)	-4(9)	7386(13)	2047(5)	41(3)
C(3B)	-549(8)	8487(17)	2159(4)	34(4)
C(4B)	-1352(8)	8175(13)	2433(4)	32(3)
C(5B)	-1505(10)	6450(15)	2443(5)	47(4)
C(6B)	-922(9)	5327(14)	2329(4)	33(3)
C(7B)	-1377(7)	8820(12)	2927(4)	29(3)
C(8B)	-1386(8)	10581(15)	2971(5)	40(3)
O(3B)	-1329(6)	11433(9)	2626(3)	44(2)
N(1'B)	-661(6)	8216(9)	3209(3)	23(2)
N(2'B)	-830(8)	7018(12)	3505(4)	47(3)
N(3'B)	-125(8)	6743(13)	3740(4)	47(3)
C(3'B)	492(8)	7684(15)	3583(5)	32(3)
C(4'B)	1314(9)	7808(16)	3729(5)	48(4)
C(5'B)	1821(9)	8958(16)	3511(5)	45(4)
C(6'B)	1470(8)	9916(15)	3171(5)	46(4)
C(7'B)	643(8)	9870(15)	3025(5)	40(4)
C(8'B)	151(8)	8670(13)	3247(4)	32(3)
C(1"B)	-1555(8)	11346(18)	3435(5)	44(4)
C(2"B)	-1846(8)	10464(15)	3800(5)	41(4)
C(3"B)	-2031(9)	11200(17)	4209(6)	60(5)
C(4"B)	-1825(9)	12739(18)	4286(6)	53(4)
C(5"B)	-1486(8)	13598(15)	3931(5)	39(3)
C(6"B)	-1353(7)	12879(15)	3504(5)	39(4)

S(1)	2147(2)	-460(4)	1449(1)	43(1)
O(1)	2485(6)	-2022(10)	1445(3)	55(2)
O(2)	1573(6)	45(10)	1793(3)	57(3)
C(1)	1581(8)	-328(18)	899(5)	48(4)
F(1)	1258(5)	1158(9)	859(3)	75(3)
F(2)	2071(5)	-553(10)	558(3)	66(3)
F(3)	943(5)	-1334(10)	899(3)	81(3)
N(1)	2895(6)	823(11)	1394(4)	33(3)
C(2)	3691(8)	386(15)	1208(4)	32(3)
C(3)	4248(8)	1502(15)	1103(4)	33(3)
C(4)	4039(8)	3279(12)	1123(4)	27(3)
C(5)	3265(9)	3612(15)	1374(4)	38(4)
C(6)	2706(9)	2444(16)	1506(5)	45(4)
C(7)	4078(7)	3910(12)	618(4)	23(3)
C(8)	4117(7)	5722(14)	569(5)	38(3)
O(3)	4059(5)	6549(10)	921(3)	48(2)
N(1')	3373(6)	3367(10)	342(4)	31(3)
N(2')	3525(7)	2212(12)	12(4)	44(3)
N(3')	2852(7)	1923(11)	-202(3)	33(3)
C(3A')	2238(8)	2921(15)	-60(5)	33(4)
C(4')	1397(10)	2995(18)	-182(5)	56(4)
C(5')	930(10)	4046(19)	27(6)	61(5)
C(6')	1262(9)	5057(15)	396(6)	53(5)
C(7')	2058(9)	4964(15)	528(5)	42(4)
C(7A')	2560(8)	3835(13)	308(4)	26(3)
C(1")	4210(8)	6410(13)	105(4)	26(3)
C(2")	3998(9)	8045(18)	41(5)	49(4)
C(3")	4121(8)	8696(15)	-391(5)	46(4)
C(4")	4418(9)	7745(16)	-746(6)	52(4)
C(5")	4645(7)	6222(15)	-687(6)	47(4)
C(6")	4559(8)	5542(14)	-252(5)	42(4)

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Table S3. Bond lengths [Å] and angles [°] for **5f**.

S(1B)-O(1B)	1.386(11)
S(1B)-O(2B)	1.402(9)
S(1B)-N(1B)	1.613(9)
S(1B)-C(1B)	1.808(15)
C(1B)-F(1B)	1.289(14)
C(1B)-F(3B)	1.355(14)
C(1B)-F(2B)	1.367(17)
N(1B)-C(6B)	1.414(15)
N(1B)-C(2B)	1.431(14)
C(2B)-C(3B)	1.320(17)
C(3B)-C(4B)	1.538(17)
C(4B)-C(5B)	1.483(17)
C(4B)-C(7B)	1.544(17)
C(5B)-C(6B)	1.375(17)
C(7B)-C(8B)	1.498(17)
C(7B)-N(1'B)	1.504(14)
C(8B)-O(3B)	1.242(14)
C(8B)-C(1"B)	1.528(19)
N(1'B)-N(2'B)	1.361(13)
N(1'B)-C(8'B)	1.363(15)
N(2'B)-N(3'B)	1.344(15)
N(3'B)-C(3'B)	1.351(15)
C(3'B)-C(4'B)	1.390(18)
C(3'B)-C(8'B)	1.401(17)
C(4'B)-C(5'B)	1.420(19)
C(5'B)-C(6'B)	1.401(18)
C(6'B)-C(7'B)	1.394(17)
C(7'B)-C(8'B)	1.442(17)
C(1"B)-C(6"B)	1.355(17)
C(1"B)-C(2"B)	1.381(18)
C(2"B)-C(3"B)	1.38(2)
C(3"B)-C(4"B)	1.364(18)
C(4"B)-C(5"B)	1.378(19)
C(5"B)-C(6"B)	1.406(18)

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S(1)-O(2)	1.426(10)
S(1)-O(1)	1.431(9)
S(1)-N(1)	1.628(10)
S(1)-C(1)	1.849(14)
C(1)-F(2)	1.282(15)
C(1)-F(3)	1.333(14)
C(1)-F(1)	1.367(15)
N(1)-C(2)	1.435(15)
N(1)-C(6)	1.445(16)
C(2)-C(3)	1.337(15)
C(3)-C(4)	1.545(16)
C(4)-C(5)	1.469(17)
C(4)-C(7)	1.570(15)
C(5)-C(6)	1.391(17)
C(7)-N(1')	1.462(14)
C(7)-C(8)	1.544(16)
C(8)-O(3)	1.250(15)
C(8)-C(1")	1.482(18)
N(1')-C(7A')	1.366(15)
N(1')-N(2')	1.397(14)
N(2')-N(3')	1.271(13)
N(3')-C(3A')	1.362(15)
C(3A')-C(4')	1.396(19)
C(3A')-C(7A')	1.423(16)
C(4')-C(5')	1.31(2)
C(5')-C(6')	1.48(2)
C(6')-C(7')	1.335(17)
C(7')-C(7A')	1.405(18)
C(1")-C(6")	1.393(16)
C(1")-C(2")	1.439(19)
C(2")-C(3")	1.392(19)
C(3")-C(4")	1.396(19)
C(4")-C(5")	1.353(16)
C(5")-C(6")	1.402(18)

O(1B)-S(1B)-O(2B)	124.4(6)

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O(1B)-S(1B)-N(1B)	109.2(6)
O(2B)-S(1B)-N(1B)	108.8(5)
O(1B)-S(1B)-C(1B)	104.3(7)
O(2B)-S(1B)-C(1B)	105.6(7)
N(1B)-S(1B)-C(1B)	102.2(6)
F(1B)-C(1B)-F(3B)	106.2(11)
F(1B)-C(1B)-F(2B)	107.6(12)
F(3B)-C(1B)-F(2B)	107.2(12)
F(1B)-C(1B)-S(1B)	114.3(11)
F(3B)-C(1B)-S(1B)	109.9(10)
F(2B)-C(1B)-S(1B)	111.3(9)
C(6B)-N(1B)-C(2B)	117.1(9)
C(6B)-N(1B)-S(1B)	120.6(8)
C(2B)-N(1B)-S(1B)	122.1(9)
C(3B)-C(2B)-N(1B)	122.5(12)
C(2B)-C(3B)-C(4B)	124.1(12)
C(5B)-C(4B)-C(3B)	108.6(11)
C(5B)-C(4B)-C(7B)	109.0(10)
C(3B)-C(4B)-C(7B)	116.5(10)
C(6B)-C(5B)-C(4B)	124.4(14)
C(5B)-C(6B)-N(1B)	121.4(11)
C(8B)-C(7B)-N(1'B)	107.4(9)
C(8B)-C(7B)-C(4B)	115.7(10)
N(1'B)-C(7B)-C(4B)	111.9(9)
O(3B)-C(8B)-C(7B)	120.6(12)
O(3B)-C(8B)-C(1"B)	119.0(11)
C(7B)-C(8B)-C(1"B)	120.1(12)
N(2'B)-N(1'B)-C(8'B)	110.5(10)
N(2'B)-N(1'B)-C(7B)	116.8(10)
C(8'B)-N(1'B)-C(7B)	132.7(9)
N(3'B)-N(2'B)-N(1'B)	106.6(10)
N(2'B)-N(3'B)-C(3'B)	109.9(11)
N(3'B)-C(3'B)-C(4'B)	129.5(13)
N(3'B)-C(3'B)-C(8'B)	107.7(11)
C(4'B)-C(3'B)-C(8'B)	122.7(13)
C(3'B)-C(4'B)-C(5'B)	117.2(13)

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C(6'B)-C(5'B)-C(4'B)	119.1(13)
C(7'B)-C(6'B)-C(5'B)	125.7(13)
C(6'B)-C(7'B)-C(8'B)	113.7(12)
N(1'B)-C(8'B)-C(3'B)	105.1(10)
N(1'B)-C(8'B)-C(7'B)	133.3(12)
C(3'B)-C(8'B)-C(7'B)	121.6(13)
C(6"B)-C(1"B)-C(2"B)	119.2(13)
C(6"B)-C(1"B)-C(8B)	119.7(13)
C(2"B)-C(1"B)-C(8B)	120.9(13)
C(1"B)-C(2"B)-C(3"B)	119.7(12)
C(4"B)-C(3"B)-C(2"B)	121.4(14)
C(3"B)-C(4"B)-C(5"B)	118.6(15)
C(4"B)-C(5"B)-C(6"B)	119.9(12)
C(1"B)-C(6"B)-C(5"B)	120.7(12)
O(2)-S(1)-O(1)	121.9(6)
O(2)-S(1)-N(1)	110.2(6)
O(1)-S(1)-N(1)	109.7(6)
O(2)-S(1)-C(1)	106.1(7)
O(1)-S(1)-C(1)	103.6(6)
N(1)-S(1)-C(1)	103.5(6)
F(2)-C(1)-F(3)	112.1(13)
F(2)-C(1)-F(1)	107.6(12)
F(3)-C(1)-F(1)	107.4(10)
F(2)-C(1)-S(1)	111.4(9)
F(3)-C(1)-S(1)	109.8(10)
F(1)-C(1)-S(1)	108.4(10)
C(2)-N(1)-C(6)	121.2(10)
C(2)-N(1)-S(1)	121.4(8)
C(6)-N(1)-S(1)	117.3(9)
C(3)-C(2)-N(1)	119.9(11)
C(2)-C(3)-C(4)	122.4(11)
C(5)-C(4)-C(3)	112.9(10)
C(5)-C(4)-C(7)	116.0(10)
C(3)-C(4)-C(7)	106.7(9)
C(6)-C(5)-C(4)	123.1(11)
C(5)-C(6)-N(1)	118.6(12)

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N(1')-C(7)-C(8)	107.0(9)
N(1')-C(7)-C(4)	112.2(9)
C(8)-C(7)-C(4)	115.3(9)
O(3)-C(8)-C(1")	122.7(11)
O(3)-C(8)-C(7)	118.6(12)
C(1")-C(8)-C(7)	118.7(11)
C(7A')-N(1')-N(2')	108.7(10)
C(7A')-N(1')-C(7)	133.4(9)
N(2')-N(1')-C(7)	117.8(10)
N(3')-N(2')-N(1')	109.0(10)
N(2')-N(3')-C(3A')	110.2(10)
N(3')-C(3A')-C(4')	130.4(12)
N(3')-C(3A')-C(7A')	107.8(10)
C(4')-C(3A')-C(7A')	121.2(13)
C(5')-C(4')-C(3A')	117.6(15)
C(4')-C(5')-C(6')	121.7(14)
C(7')-C(6')-C(5')	121.4(14)
C(6')-C(7')-C(7A')	117.2(13)
N(1')-C(7A')-C(7')	135.3(12)
N(1')-C(7A')-C(3A')	104.1(11)
C(7')-C(7A')-C(3A')	120.5(12)
C(6")-C(1")-C(2")	120.5(12)
C(6")-C(1")-C(8)	121.1(11)
C(2")-C(1")-C(8)	118.3(10)
C(3")-C(2")-C(1")	117.8(13)
C(2")-C(3")-C(4")	119.5(13)
C(5")-C(4")-C(3")	123.3(15)
C(4")-C(5")-C(6")	118.7(13)
C(1")-C(6")-C(5")	120.0(12)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5f**. 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}
S(1B)	35(2)	42(2)	45(2)	-3(2)	3(2)	3(2)
O(1B)	40(5)	66(6)	49(5)	8(4)	23(5)	8(4)
O(2B)	52(6)	43(5)	69(7)	-19(5)	1(6)	9(5)
C(1B)	34(9)	38(9)	79(13)	-6(8)	-19(9)	-9(8)
F(1B)	52(5)	64(5)	75(6)	-15(5)	-7(5)	-11(5)
F(2B)	76(7)	110(8)	45(6)	7(5)	8(6)	-9(6)
F(3B)	42(5)	76(6)	97(7)	-3(5)	-14(5)	14(5)
N(1B)	17(6)	23(6)	54(7)	1(5)	14(6)	14(5)
C(2B)	63(9)	24(8)	37(9)	-2(7)	-3(8)	-2(8)
C(3B)	17(8)	61(10)	24(9)	9(7)	-5(7)	-8(8)
C(4B)	26(8)	37(9)	32(8)	5(6)	-18(7)	6(6)
C(5B)	63(11)	33(8)	47(9)	-5(7)	-23(9)	-15(8)
C(6B)	55(10)	8(6)	35(8)	-4(6)	-3(7)	3(7)
C(7B)	18(8)	16(7)	52(9)	1(6)	-7(6)	-6(5)
C(8B)	29(8)	51(9)	39(9)	10(8)	-22(7)	9(7)
O(3B)	57(7)	47(5)	28(5)	0(5)	-11(5)	5(4)
N(1'B)	20(7)	19(6)	30(6)	6(5)	2(5)	8(5)
N(2'B)	62(10)	34(7)	46(8)	8(6)	33(7)	-13(6)
N(3'B)	34(8)	59(8)	48(8)	-1(6)	-18(7)	16(6)
C(3'B)	40(9)	31(8)	24(8)	2(6)	-3(7)	1(8)
C(4'B)	41(9)	60(10)	44(10)	-7(8)	-18(8)	42(9)
C(5'B)	31(9)	36(8)	69(11)	-14(8)	-2(9)	-3(7)
C(6'B)	22(9)	56(9)	60(10)	2(8)	7(8)	-9(7)
C(7'B)	35(10)	35(8)	48(10)	2(7)	1(8)	-10(7)
C(8'B)	33(9)	24(7)	39(9)	-11(7)	1(8)	4(7)
C(1"B)	23(9)	68(12)	42(11)	5(8)	4(7)	-25(7)
C(2"B)	38(9)	35(8)	51(10)	3(8)	16(8)	-4(7)
C(3"B)	68(12)	46(10)	65(12)	-4(9)	14(10)	-39(8)
C(4"B)	52(9)	65(10)	42(12)	-16(9)	15(8)	0(9)
C(5"B)	52(10)	31(8)	34(9)	-11(7)	-2(8)	2(7)
C(6"B)	36(8)	23(8)	59(11)	24(7)	11(7)	-13(7)

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S(1)	40(2)	43(2)	46(2)	10(2)	6(2)	0(2)
O(1)	63(6)	42(5)	58(6)	0(5)	-16(6)	5(5)
O(2)	61(6)	57(6)	52(6)	7(5)	31(6)	-7(5)
C(1)	17(8)	71(11)	57(11)	4(9)	2(8)	10(8)
F(1)	43(5)	73(6)	107(8)	20(5)	-17(5)	17(5)
F(2)	62(6)	101(7)	37(5)	-8(5)	-2(5)	-5(5)
F(3)	51(5)	89(6)	105(7)	16(6)	-23(6)	-28(5)
N(1)	32(7)	33(6)	36(7)	-4(5)	9(6)	-6(5)
C(2)	25(8)	38(7)	33(8)	3(6)	-2(6)	15(7)
C(3)	27(9)	45(8)	27(8)	-5(6)	-6(7)	12(7)
C(4)	35(9)	28(8)	18(8)	-4(6)	6(6)	-1(6)
C(5)	52(11)	43(9)	18(8)	-19(7)	-10(8)	2(8)
C(6)	61(10)	49(10)	23(9)	1(7)	1(7)	2(9)
C(7)	12(7)	31(8)	25(7)	-6(6)	6(6)	4(6)
C(8)	20(8)	23(8)	72(11)	-15(8)	12(7)	-2(6)
O(3)	40(6)	39(5)	64(7)	-22(5)	4(5)	0(4)
N(1')	29(7)	18(6)	45(7)	-3(5)	12(6)	4(5)
N(2')	60(9)	40(7)	31(7)	-9(6)	7(7)	-26(6)
N(3')	23(7)	46(7)	31(7)	-2(5)	-17(6)	-18(6)
C(3A')	27(10)	31(7)	40(10)	0(7)	-16(7)	20(7)
C(4')	66(13)	64(10)	37(10)	-1(8)	11(9)	13(9)
C(5')	45(10)	72(11)	65(11)	15(9)	-32(10)	-16(10)
C(6')	34(10)	41(9)	85(13)	29(9)	25(9)	21(8)
C(7')	55(11)	31(8)	41(9)	2(7)	2(8)	-9(7)
C(7A')	34(9)	22(7)	22(7)	-3(6)	-5(7)	-1(7)
C(1")	40(9)	16(6)	21(8)	-5(6)	6(6)	-16(6)
C(2")	54(10)	64(11)	29(9)	18(8)	2(7)	-19(8)
C(3")	17(8)	39(8)	81(13)	4(10)	-10(8)	2(6)
C(4")	91(11)	32(10)	32(10)	-4(7)	-1(8)	-7(8)
C(5")	33(9)	33(9)	74(12)	-13(8)	18(8)	-11(6)
C(6")	52(10)	31(7)	43(10)	-4(8)	9(8)	-11(7)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5f**.

	x	y	z	U(eq)
H(2BA)	497	7691	1898	50
H(3BA)	-439	9539	2065	41
H(4BA)	-1824	8670	2261	38
H(5BA)	-2042	6096	2535	57
H(6BA)	-1047	4244	2377	39
H(7BA)	-1901	8419	3071	34
H(4'A)	1529	7150	3965	58
H(5'A)	2390	9076	3595	55
H(6'A)	1827	10663	3028	55
H(7'A)	424	10564	2799	48
H(2"A)	-1918	9357	3769	49
H(3"A)	-2308	10622	4443	72
H(4"A)	-1913	13207	4577	64
H(5"A)	-1342	14675	3976	47
H(6"A)	-1118	13475	3260	47
H(2A)	3822	-694	1160	39
H(3A)	4793	1190	1012	40
H(4A)	4502	3803	1295	32
H(5A)	3141	4676	1450	45
H(6A)	2210	2706	1667	53
H(7A)	4596	3473	476	27
H(4'B)	1171	2311	-407	67
H(5'B)	363	4160	-63	73
H(6'B)	902	5788	543	64
H(7'B)	2276	5634	759	51
H(2"B)	3781	8659	286	59
H(3"B)	4003	9779	-445	55
H(4"B)	4463	8191	-1043	62
H(5"B)	4859	5624	-936	56
H(6"B)	4738	4489	-201	50