Electronic Supplementary Material (ESI) for ChemComm.

N-Heterocyclic Carbene Induced Transmethylation in Tungsten Imido Alkylidene Bistriflates: Unexpected Formation of an *N*-Heterocyclic Olefin Complex

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Experimental

General. All manipulations of moisture and air sensitive materials were performed under nitrogen atmosphere applying standard Schlenk techniques or in a N_2-filled glove box (*Lab Master 130*, *MBraun*, Garching, Germany). Methylene chloride, diethyl ether, toluene, *n*-pentane and tetrahydrofuran were dried by a solvent purification system (SPS, MBraun). 1,2-Dimethoxyethane (DME) and benzene were vacuum-distilled from a dark purple solution of sodium benzophenone ketyl and then degassed by three consecutive freeze-pump-thaw cycles. Starting materials and all reagents were purchased from *Sigma-Aldrich* (Munich, Germany), *Alfa Aesar* (Karlsruhe, Germany), *ABCR* (Karlsruhe, Germany) and *TCI* (Geel, Belgium), dried and where appropriate, distilled prior to use. NMR measurements were recorded on a *Bruker Avance III 400*. Chemical shifts are reported in ppm relative to the solvent signal. GC-MS data were recorded on an *Agilent Technologies* device consisting of a *7693 autosampler, a 7890 A GC and a 5975C quadrupole MS*. *n*-Dodecan was used as internal standard. An SPB-5 fused silica column (34.13 m x 0.25 mm x 0.25 mm film thickness) was used. The injection temperature was set to 150°C. The column temperature ramped from 45°C to 250°C within eight minutes and was then held for further five minutes. The column flow was 1.05 mL per minute. All substrates for HM, CM, RCM, and SM were either distilled from CaH_2 or recrystallized and stored under nitrogen.

W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)(IMesH$_2$)(κ^2-O(CH$_2$)$_2$OMe) (**2**). W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME) (292 mg, 0.33 mmol) was dissolved in 5 mL benzene. To this stirred solution, IMesH$_2$ (204 mg, 0.67 mmol), dissolved in 1 mL benzene, was added drop wise. The reaction mixture was stirred for 3 h at room temperature. After partial removal of the benzene under reduced pressure, the reaction mixture was filtered through a pad of celite and the residual solvent was removed *in vacuo* from the obtained clear solution. The residual yellow solid was dissolved in 1 mL CH_2Cl_2 and a mixture of 1,3-bis(2,4,6-trimethylphenyl)-2-H-imidazolidinium triflate (**1**), [W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)(IMesH$_2$)(κ^2-O(CH$_2$)$_2$OMe)] (**2**) and 1,3-bis(2,4,6-trimethylphenyl)2-methylimidazolidinium triflate (**3**) was precipitated upon addition of diethyl ether. The liquid phase was decanted off and the solid was dried *in vacuo*. The

yellow powder was suspended in 1 mL benzene and filtered over a pad of celite. The solvent was removed from the obtained clear solution and the received yellow solid was crystallized in a mixture of CH_2Cl_2 and diethyl ether to get the product with residual compound **1** and **3**: ^{1}H NMR (400 MHz, CD_2Cl_2) δ = 12.58 (s, 1H, W=CH, $^1J_{C\text{-}H}$ = 139.26 Hz), 7.29 - 7.06 (m, 8H, Ar), 6.97 (s, 2H, Ar), 6.86 (s, 2H, Ar), 4.08 - 3.83 (m, 5H), 3.76 - 3.65 (m, 1H), 3.37 - 3.29 (m, 1H), 3.07 - 2.96 (m, 1H), 2.96 - 2.87 (m, 1H), 2.73 (s, 3H, Me), 2.63 - 2.51 (m, 1H), 2.23 (s, 6H, Me), 2.15 (s, 6H, Me), 2.12 (s, 6H, Me), 1.73 (s, 3H, Me), 1.57 (s, 3H, Me), 1.28 (d, 3H, ^{i}Pr, $^3J_{H\text{-}H}$ = 6.67 Hz), 1.08 (d, 6H, ^{i}Pr, $^3J_{H\text{-}H}$ = 6.71 Hz), 1.03 (d, 3H, ^{i}Pr, $^3J_{H\text{-}H}$ = 6.79 Hz) ppm; ^{19}F NMR (376 MHz, CD_2Cl_2) δ = -78.95 ppm; ^{13}C NMR (101 MHz, CD_2Cl_2) δ = 302.7 (W=CH, $^1J_{C\text{-}H}$ = 139.26 Hz), 212.2 (N-C-N), 151.8 (*ipso*-CMe_2Ph), 151.1 (*ipso*-N-Mes), 146.6 (CAr), 144.7 (CAr), 139.2 (CAr), 136.9 (CAr), 135.7 (CAr), 134.7 (CAr), 130.9 (CAr), 130.4 (CAr), 129.7 (CAr), 129.1 (CAr), 128.8 (CAr), 128.5 (CAr), 127.1 (CAr), 126.1 (CAr), 123.7 (CAr), 123.3 (CAr), 121.5 (q, OTf, $^1J_{C\text{-}F}$ = 320.6 Hz), 73.6, 70.3, 66.9, 62.2, 53.1, 50.4, 33.2 (Me), 32.6 (Me), 31.1 (Me), 28.4 (Me), 25.2 (Me), 24.3 (Me), 24.0 (Me), 23.8 (Me), 21.4 (Me), 18.8 (Me), 18.5 (Me) ppm.

W(*N*-2,6-^{i}Pr2C_6H_3)(CHCMe$_2$Ph)(OTf)$_2$(DME*) (6). W(*N*-2,6-^{i}Pr$_2C_6H_3$)$_2$(CH_2CMe_2Ph)$_2$ (2.57 g, 3.21 mmol) was dissolved in a mixture of 30% ^{13}C labelled DME (2.57 g, 28.5 mmol) and 50 mL toluene. This mixture was cooled to -30 °C and a -30 °C cooled mixture of triflic acid (1.45 g, 9.63 mmol) diluted with 5 mL toluene was added slowly. The reaction mixture was stirred at room temperature overnight. The resulting suspension was passed through a pad of celite and all volatiles were removed *in vacuo*. The resulting solid was suspended in 20 mL benzene and again passed over a pad of celite. All volatiles were removed *in vacuo*. The resulting orange solid was suspended in 20 mL cold diethyl ether and filtered off. The orange solid was dried *in vacuo* to yield the product as light orange powder. Analytical data were identical to the unlabelled compound **6**.

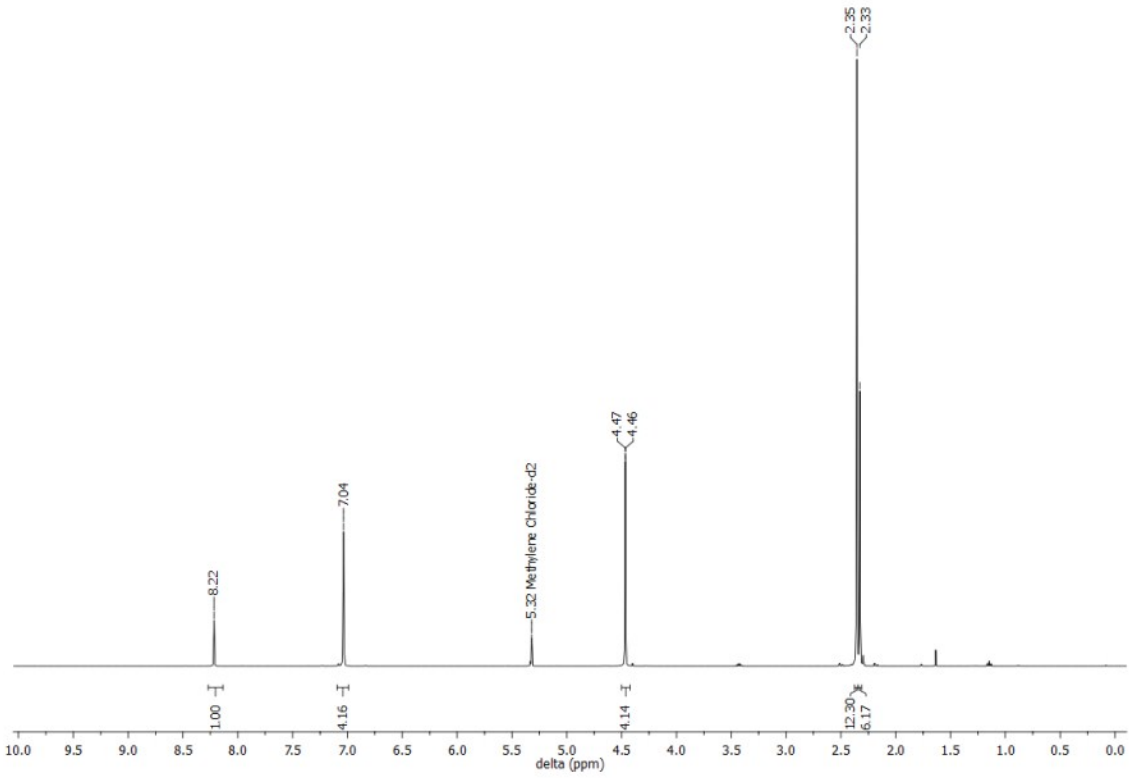

Figure S1. ^{1}H NMR (400 MHz, CD_2Cl_2) of **1.**

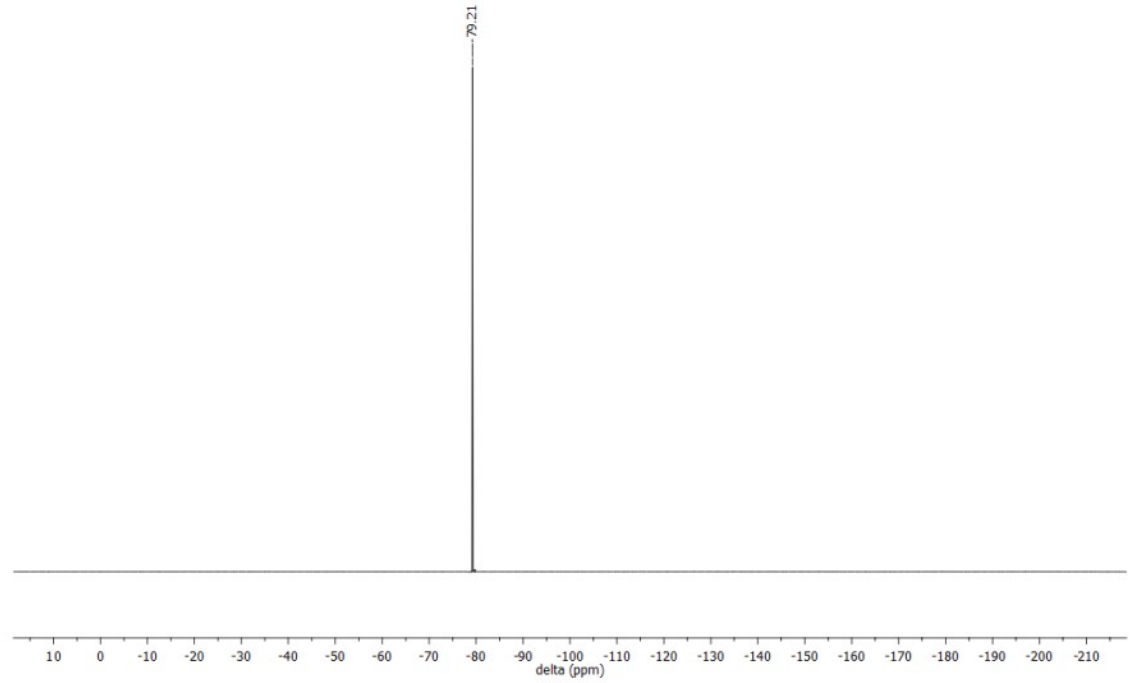

Figure S2. ^{19}F NMR (376 MHz, CD_2Cl_2) of **1**.

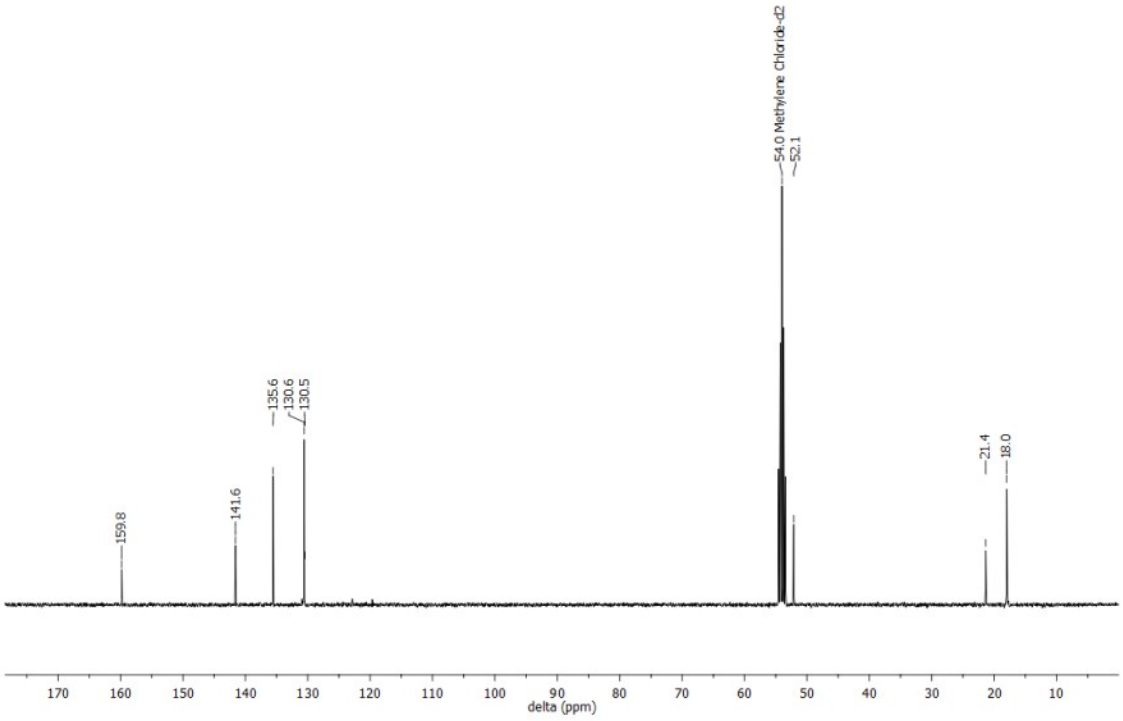

Figure S3. ^{13}C NMR (101 MHz, CD_2Cl_2) of **1**.

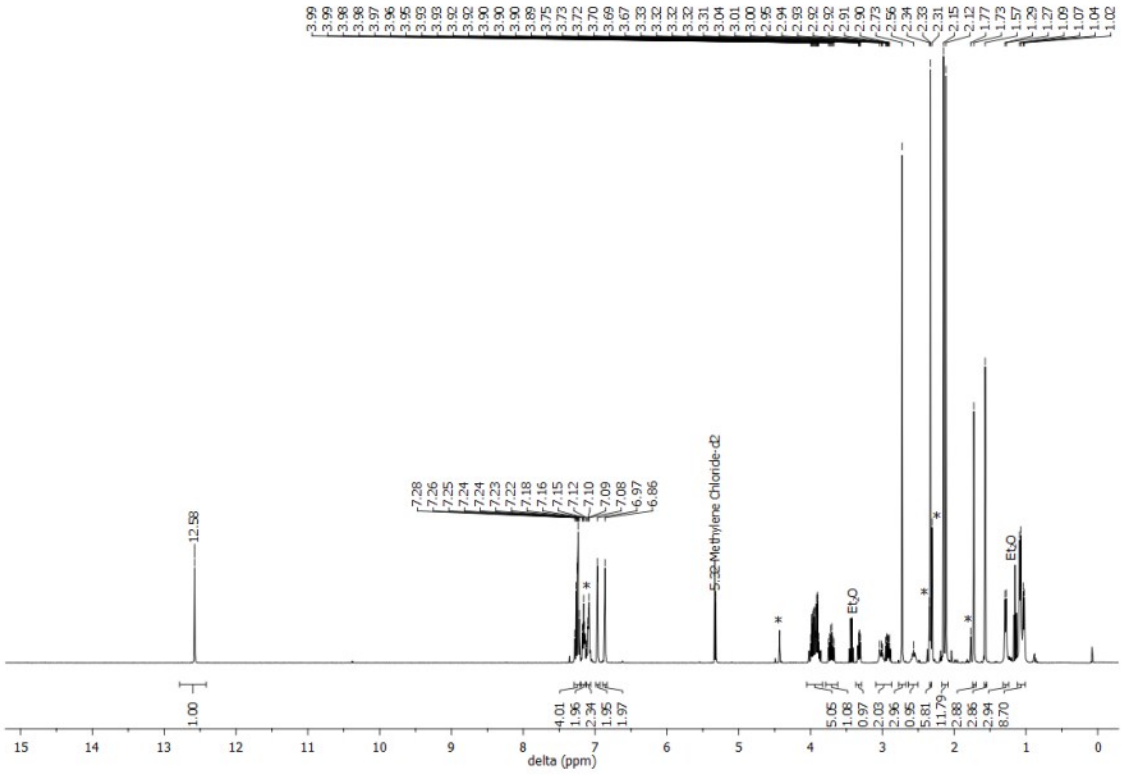

Figure S4. ^{1}H NMR (400 MHz, CD_2Cl_2) of **2** (* residual compound **3**).

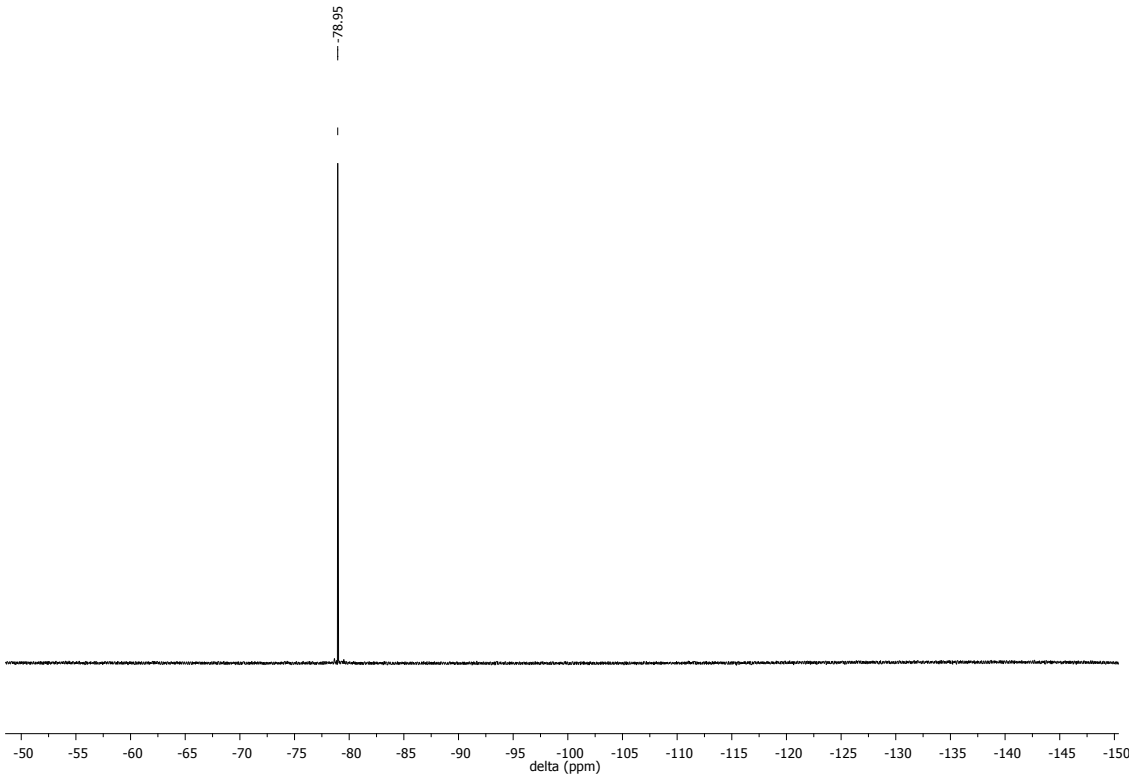

Figure S5. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2**.

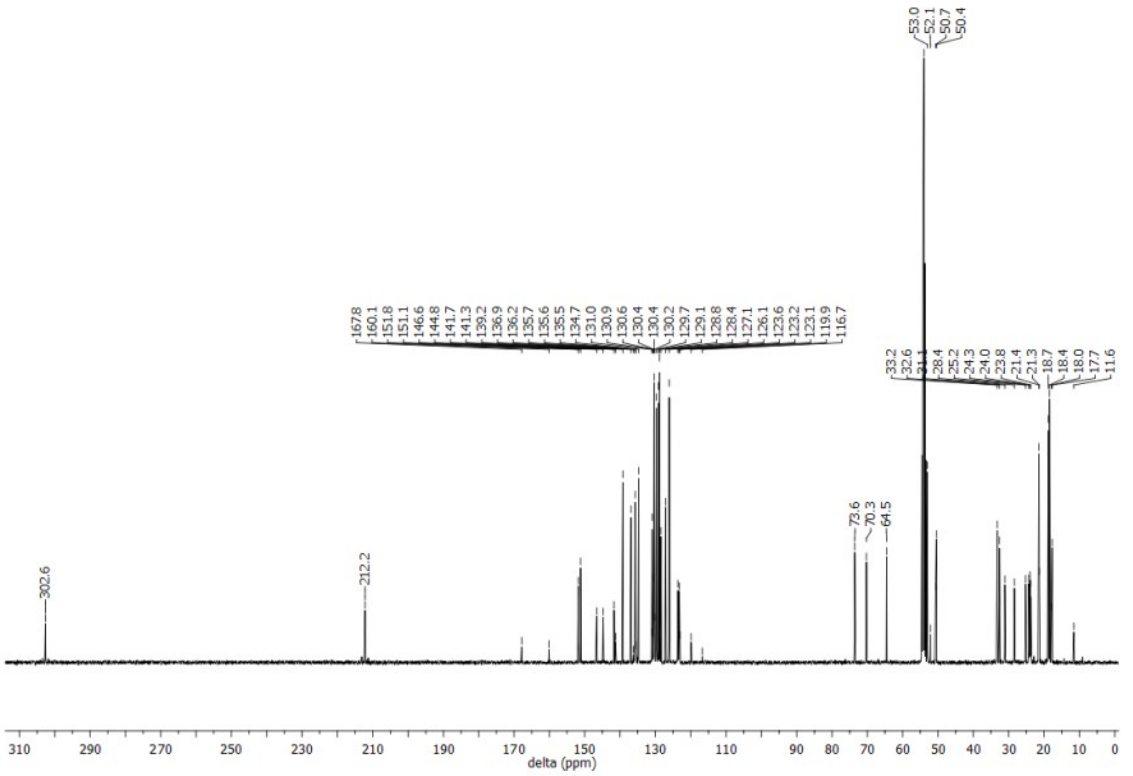

Figure S6. ^{13}C NMR (101 MHz, CD_2Cl_2) of **2**.

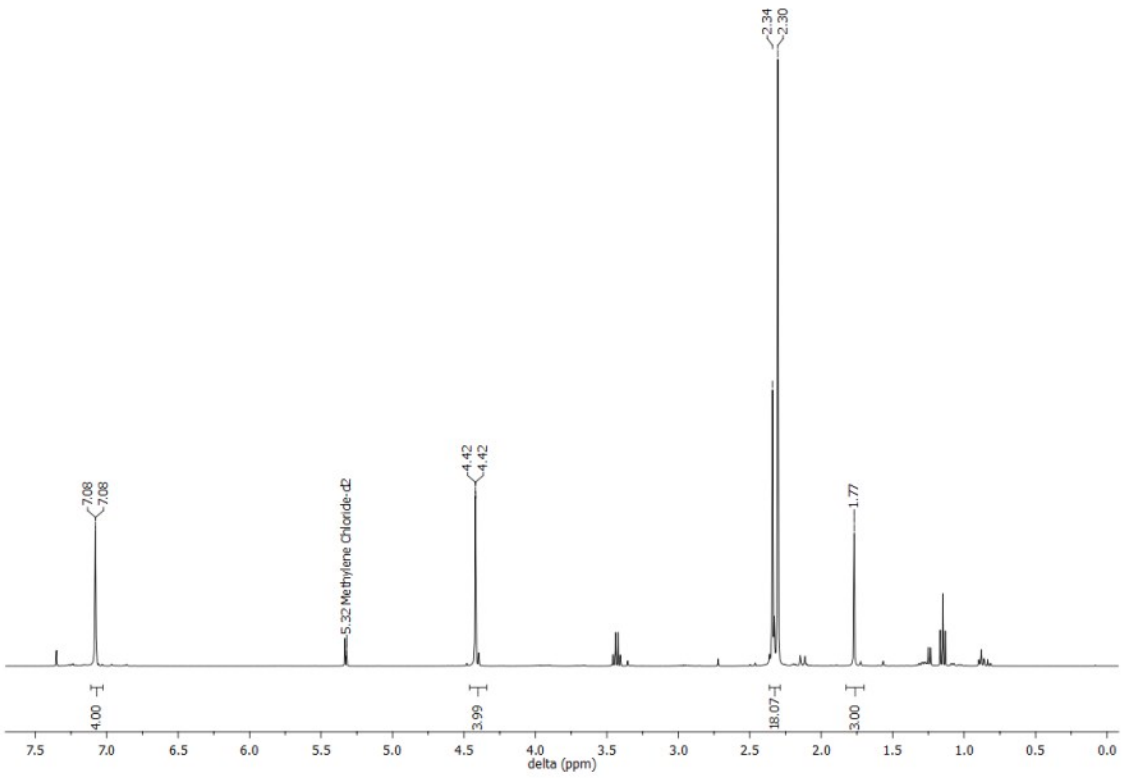

Figure S7. ^{1}H NMR (400 MHz, CD_2Cl_2) of **3**.

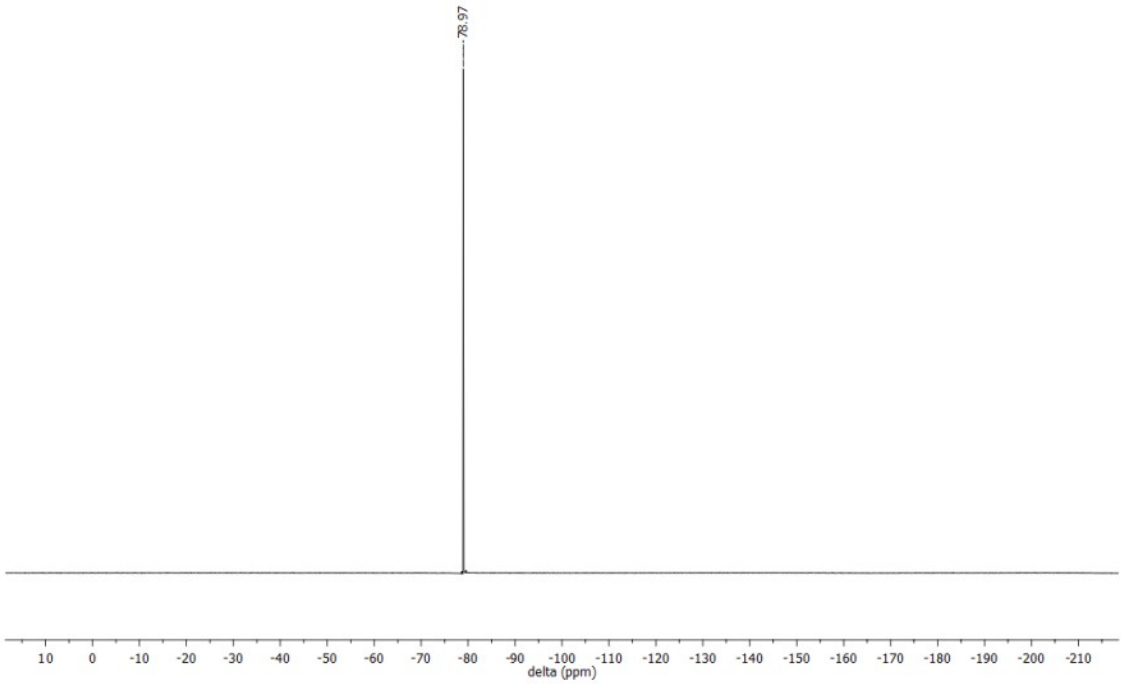

Figure S8. ^{19}F NMR (376 MHz, CD_2Cl_2) of **3**.

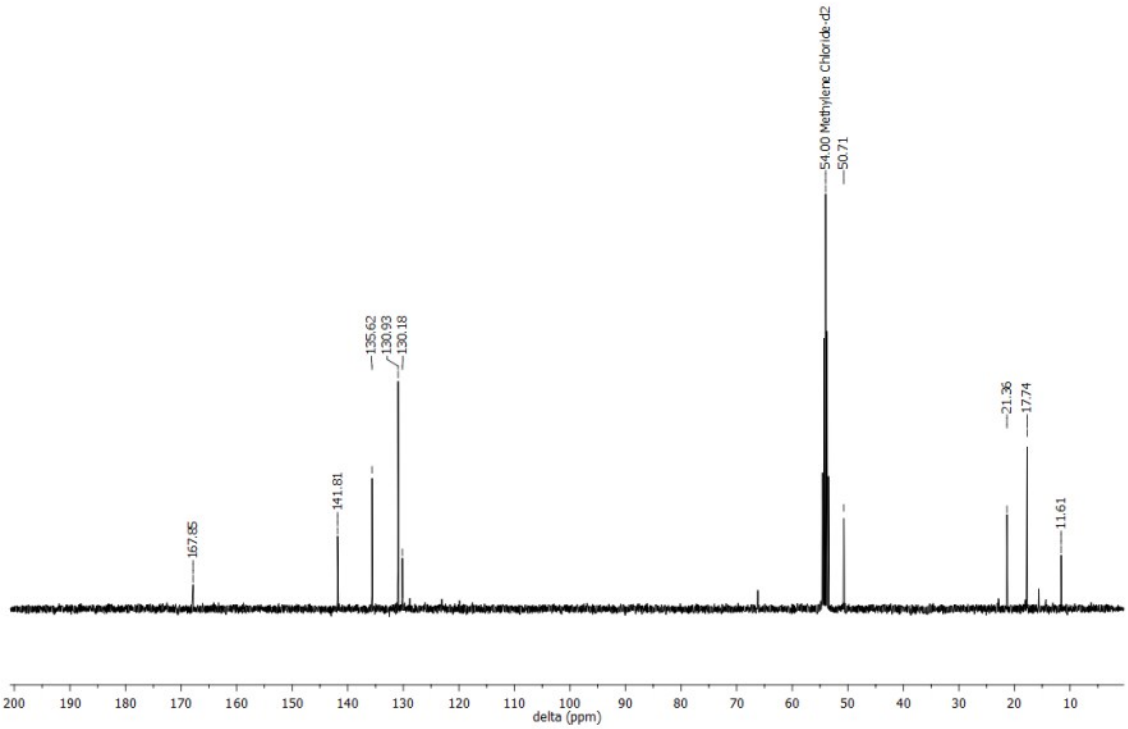

Figure S9. ^{13}C NMR (101 MHz, CD_2Cl_2) of **3.**

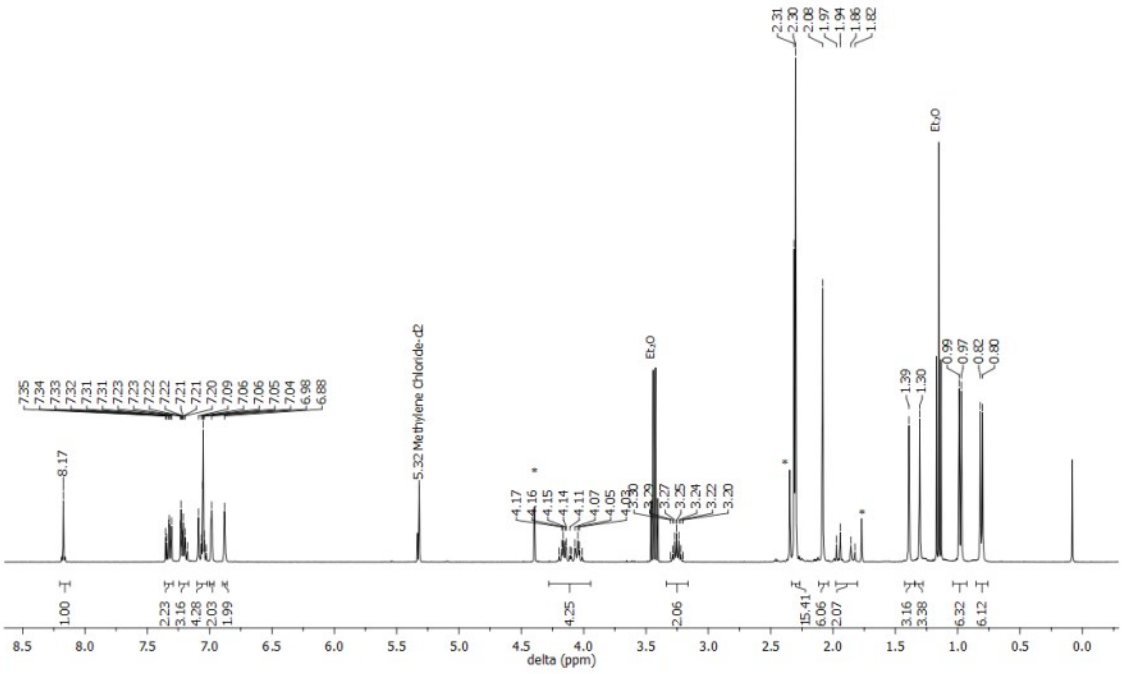

Figure S10. ^{1}H NMR (400 MHz, CD_2Cl_2) of **4** (* residual compound **3**).

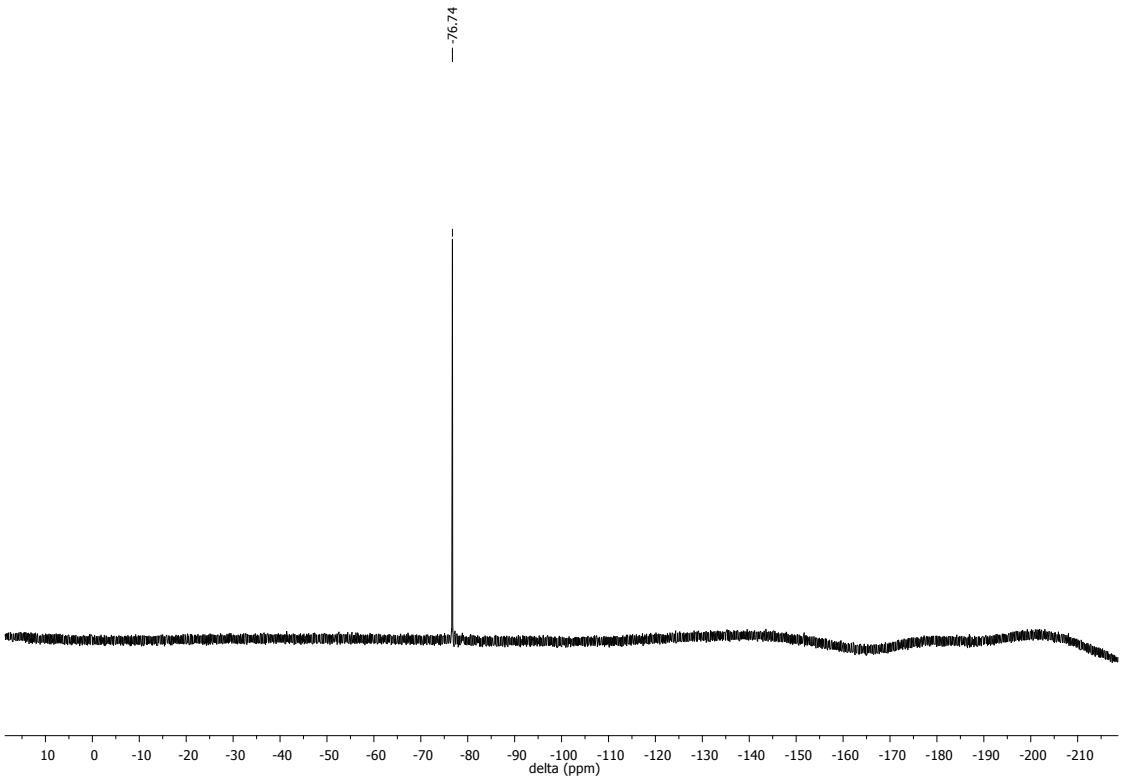

Figure S1

1. ^{19}F NMR (376 MHz, CD_2Cl_2) of **4.**

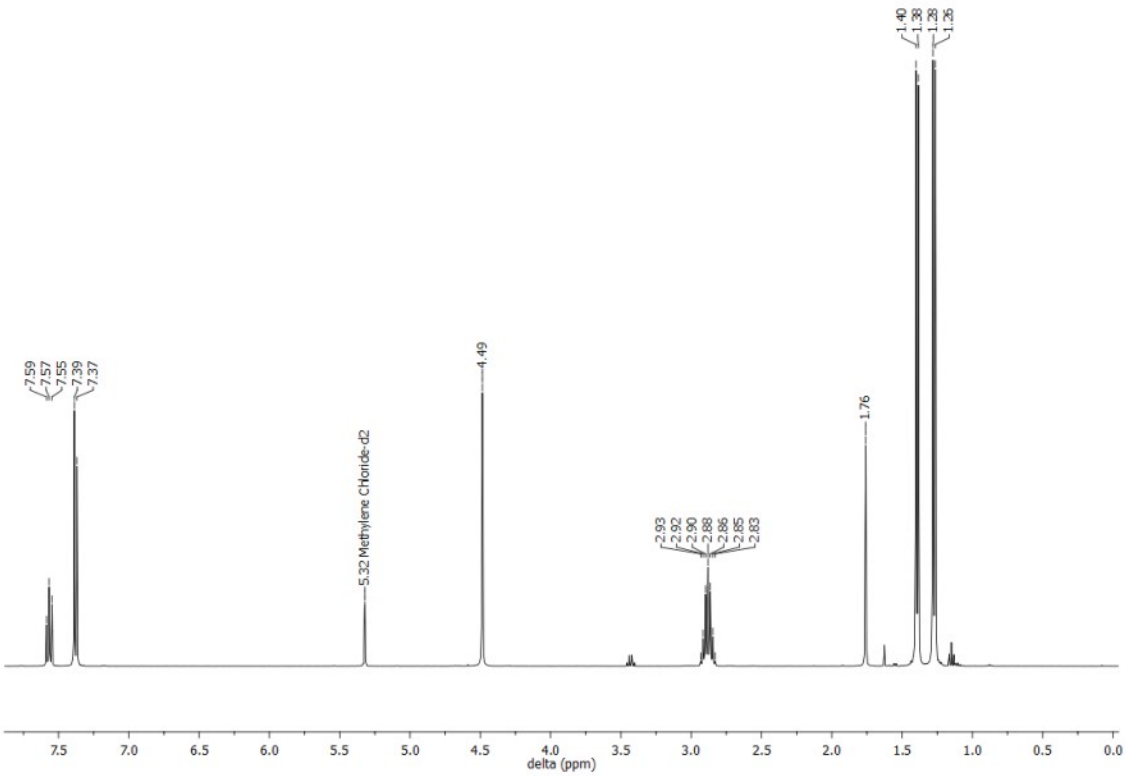

Figure S1

2. ^{1}H NMR (400 MHz, CD_2Cl_2) of **5**.

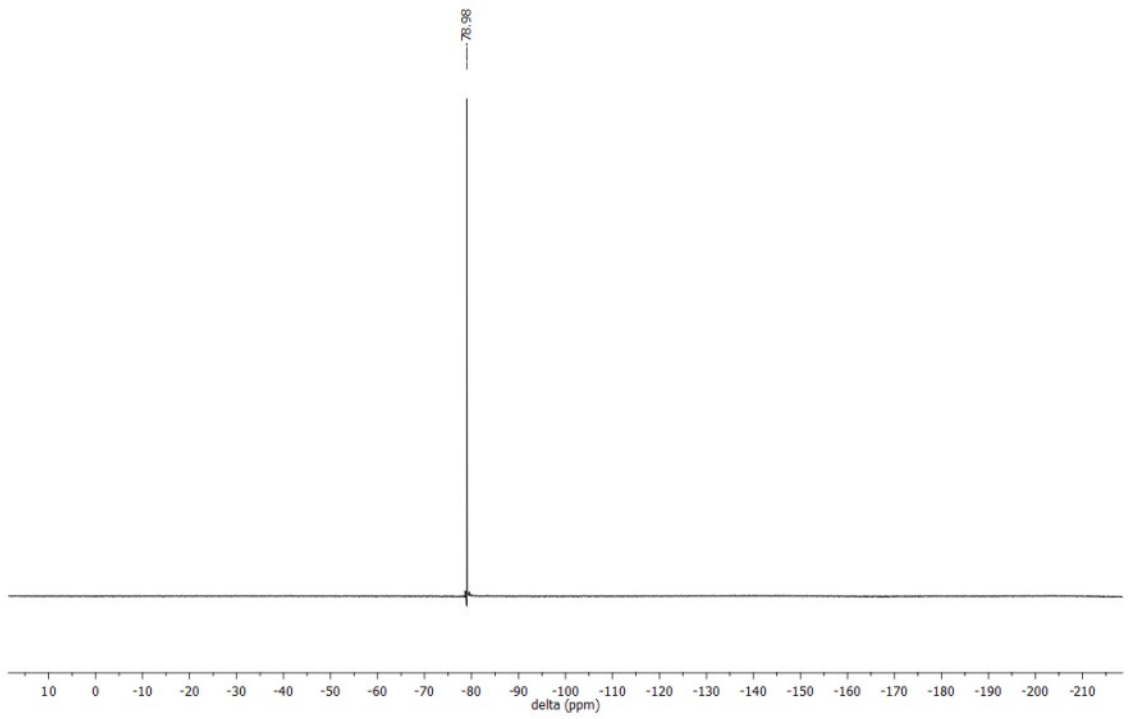

Figure S1

3. ^{19}F NMR (376 MHz, CD_2Cl_2) of **5**.

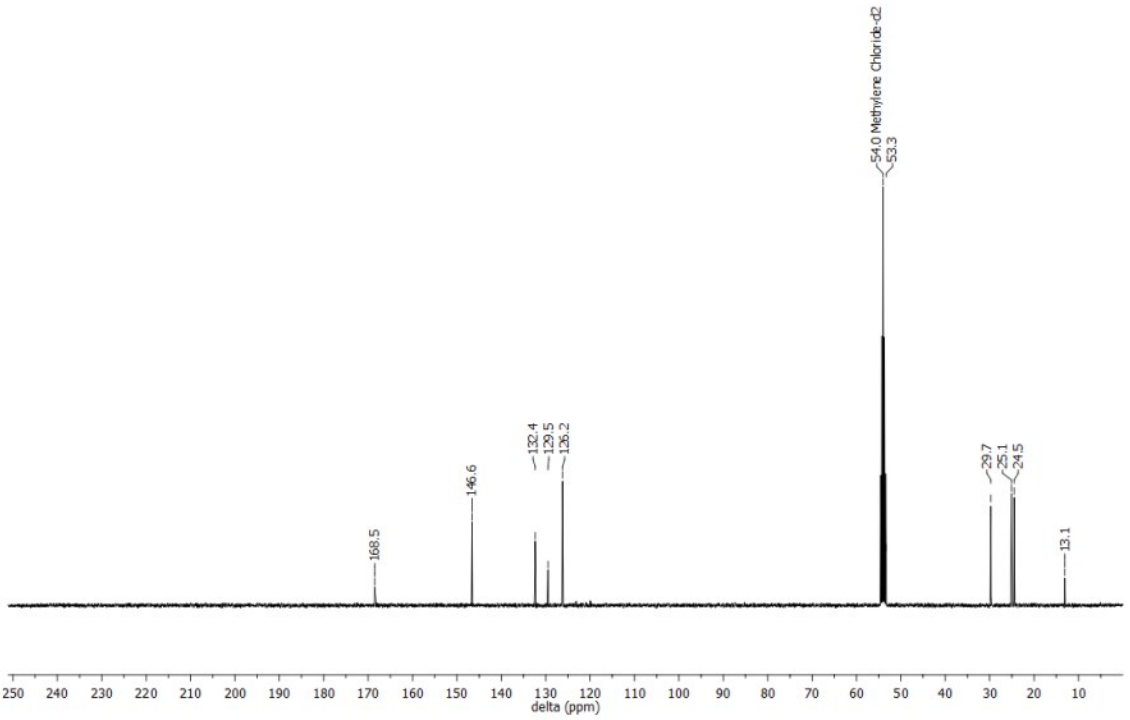

Figure S1

4. ^{13}C NMR (101 MHz, CD_2Cl_2) of **5**.

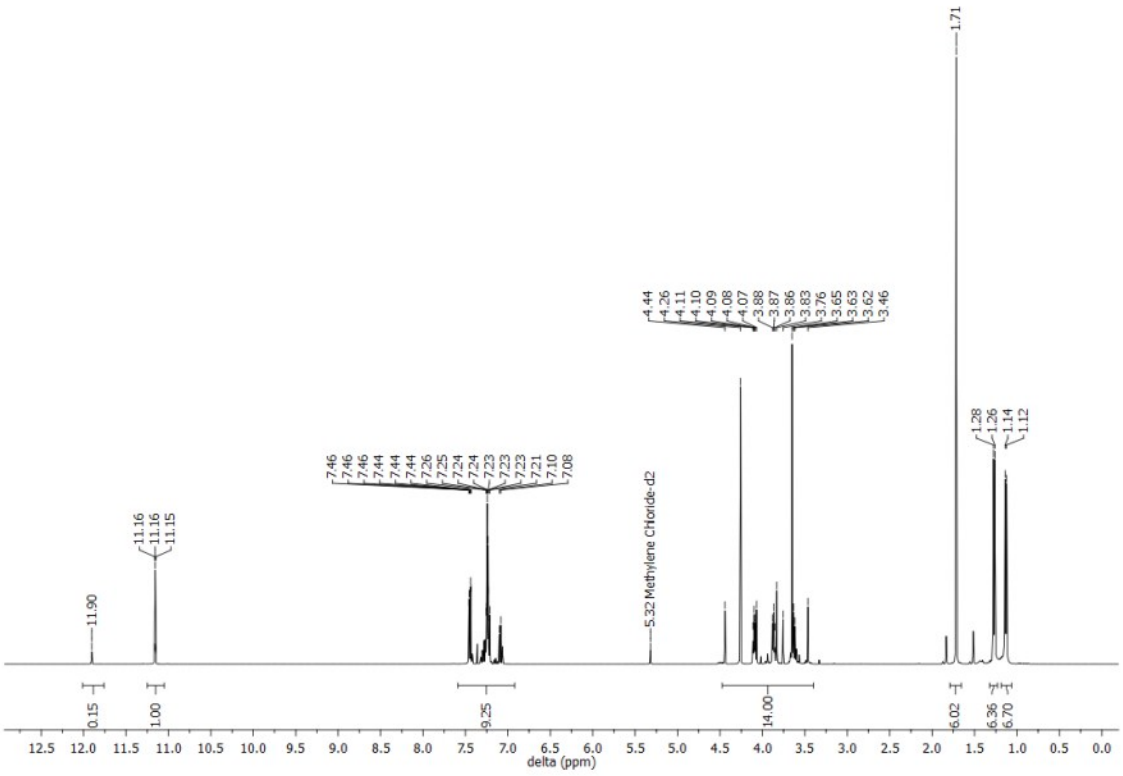

Figure S1

5. ^{1}H NMR (400 MHz, CD_2Cl_2) of ^{13}C labeled [W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME*)].

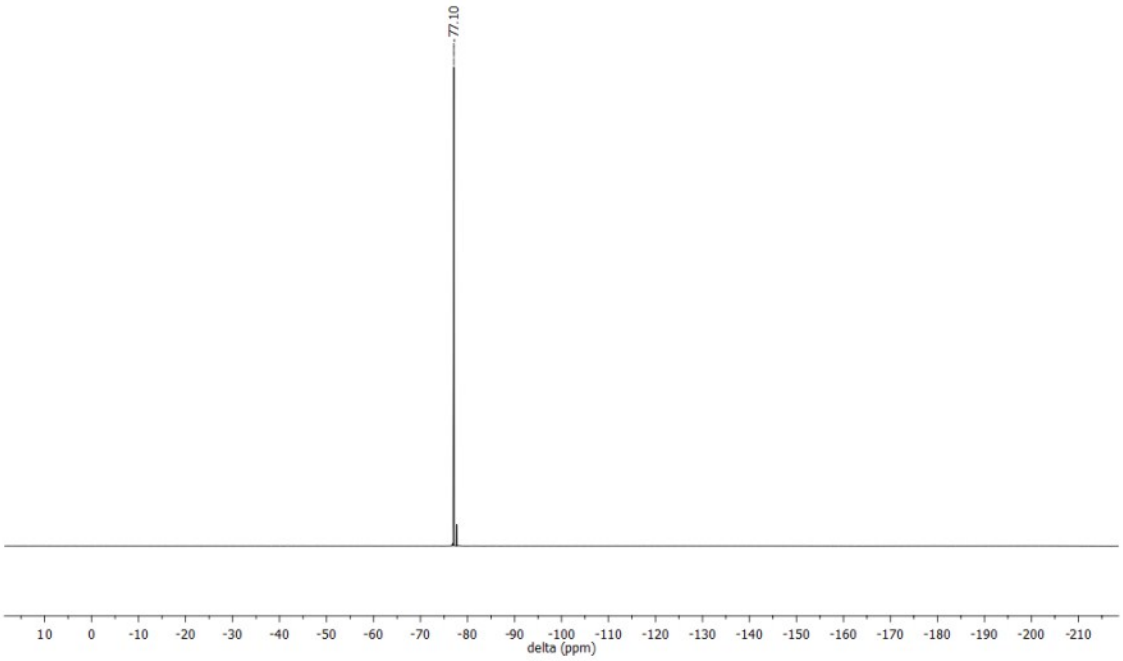

Figure S1

6. ^{19}F NMR (376 MHz, CD_2Cl_2) of ^{13}C labeled [W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME*)].

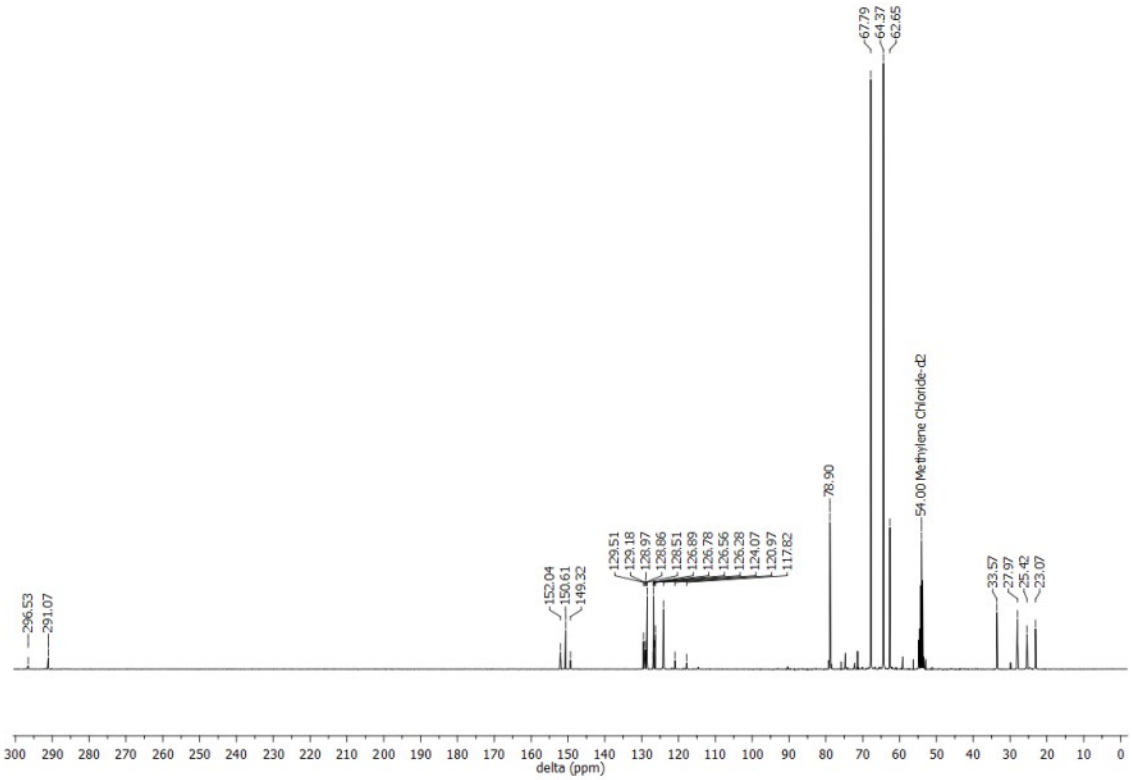

Figure S1

7. ^{13}C NMR (101 MHz, CD_2Cl_2) of ^{13}C labeled [W(*N*-2,6-$^{i}Pr_2C_6H_3$)(CHCMe$_2$Ph)(OTf)$_2$(DME*)].

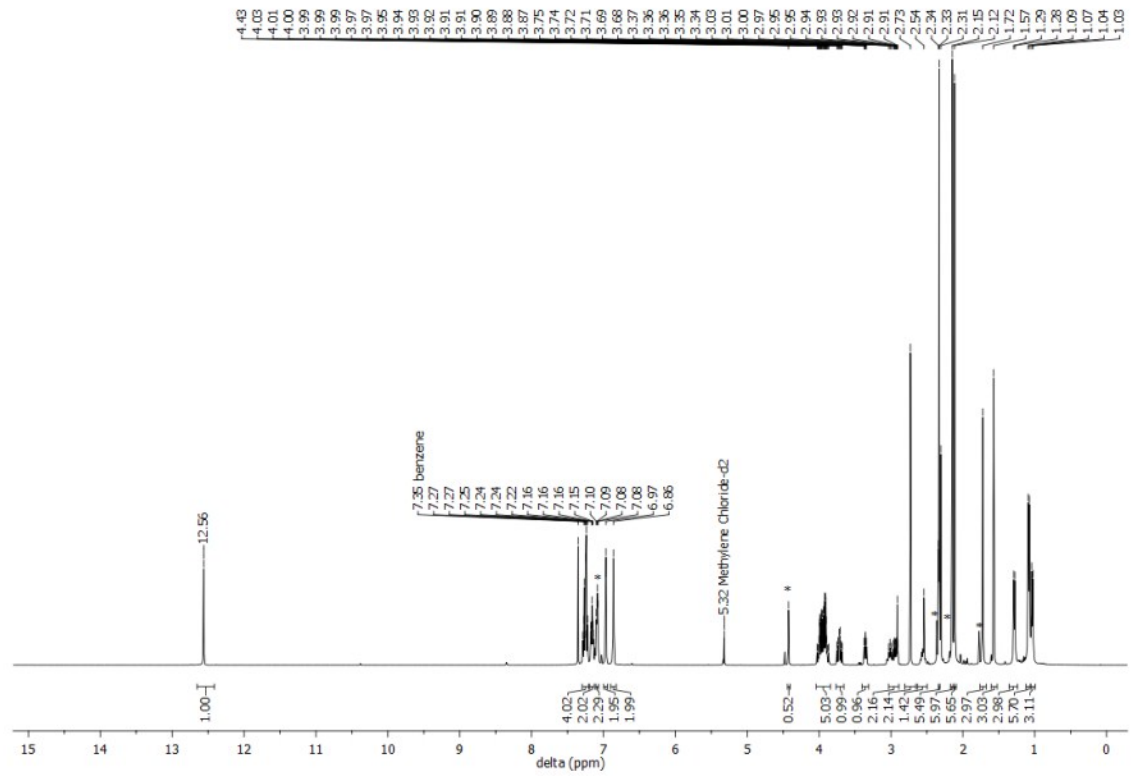

Figure S1

8. ^{1}H NMR (400 MHz, CD_2Cl_2) of ^{13}C labeled **2** (* residual compound **3**).

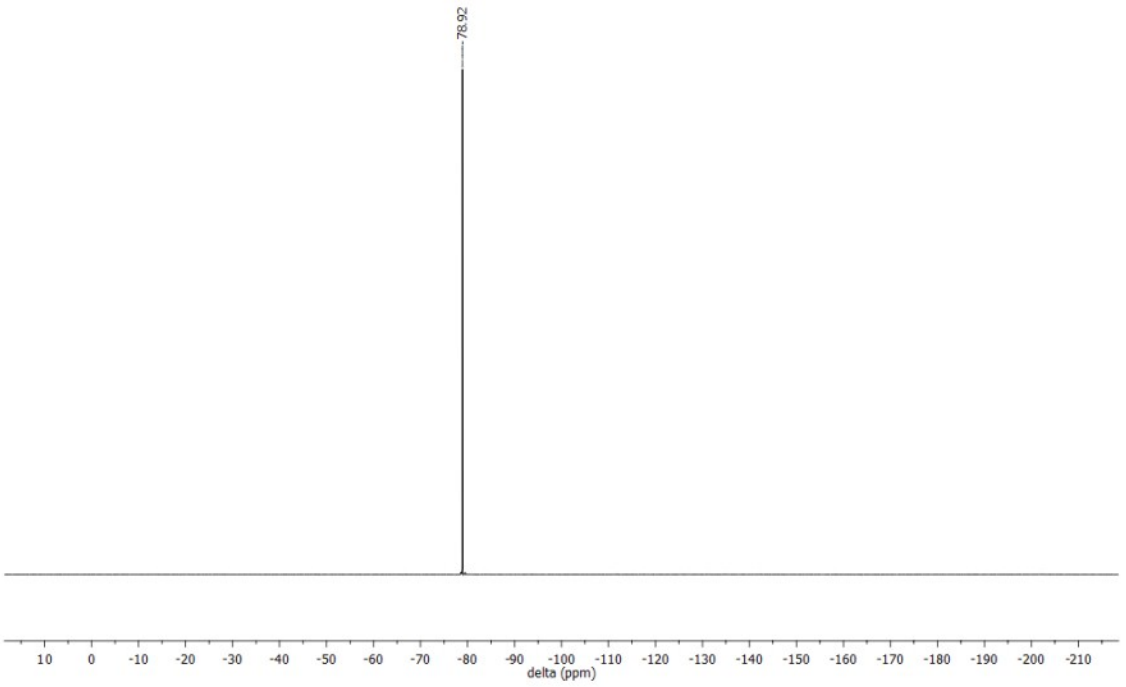

Figure S1

9. ^{19}F NMR (376 MHz, CD_2Cl_2) of ^{13}C labeled **2**.

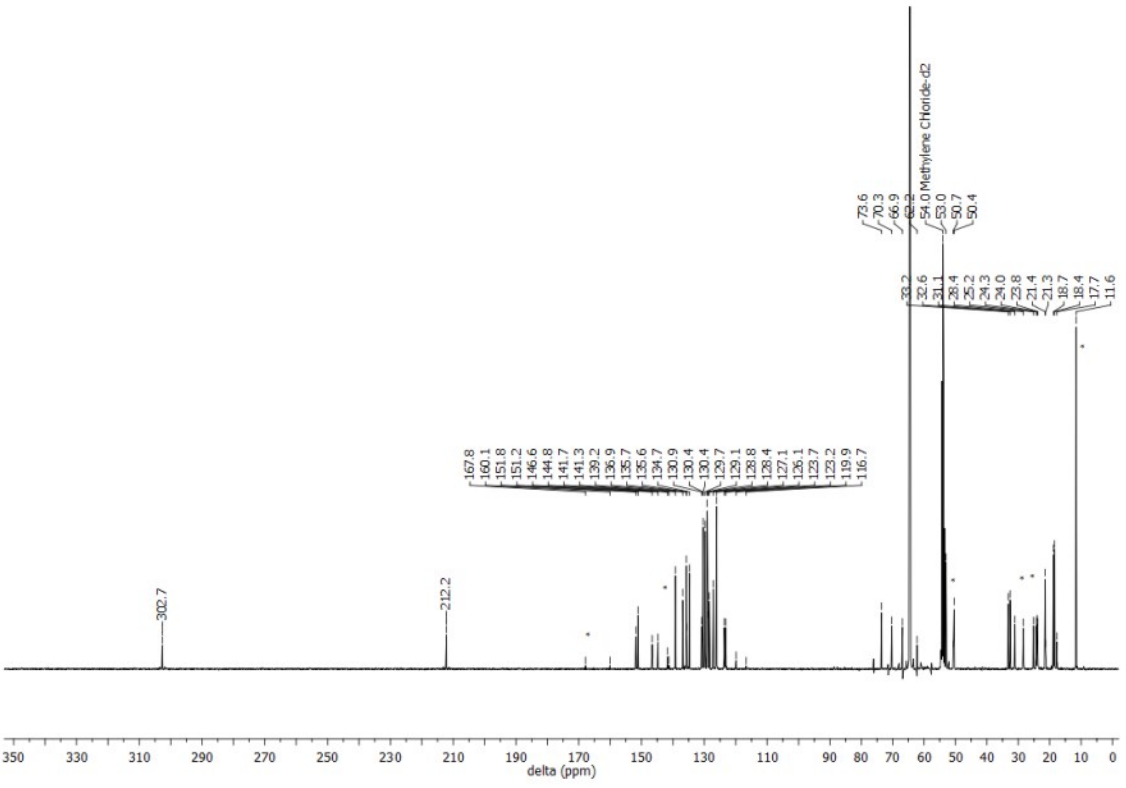

Figure S2

0. ^{13}C NMR (101 MHz, CD_2Cl_2) of ^{13}C labeled **2** (* residual compound **3**).

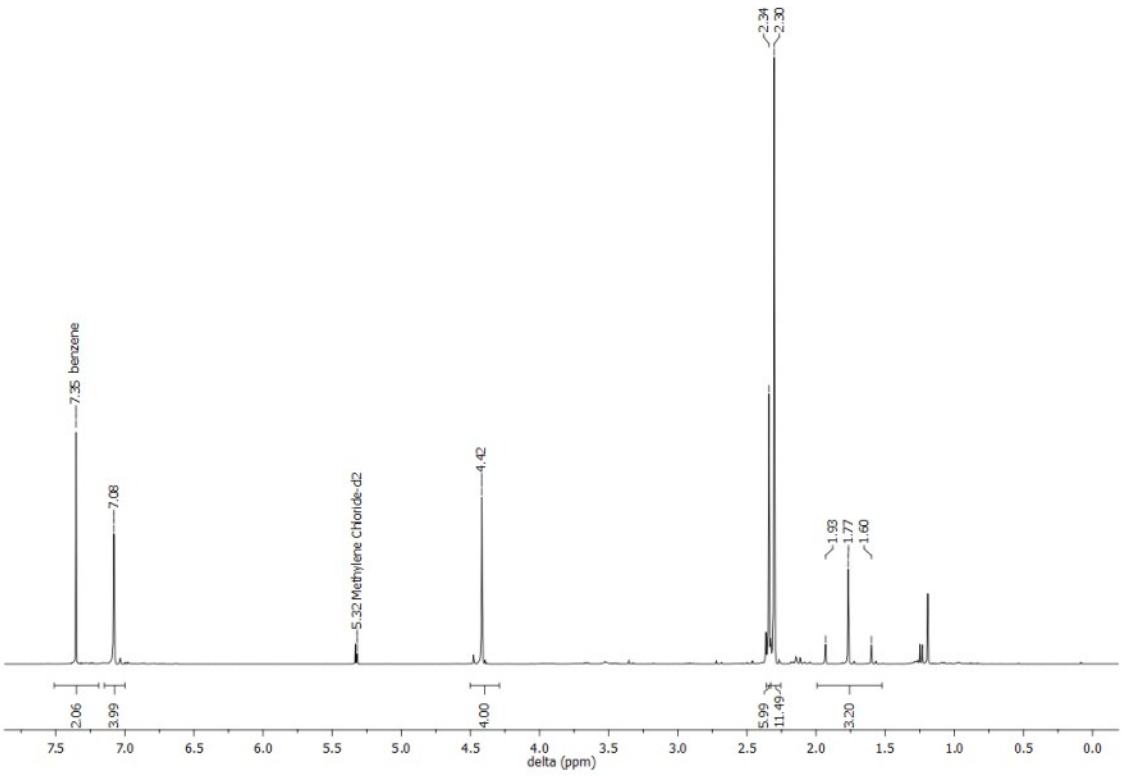

Figure S2

1. ^{1}H NMR (400 MHz, CD_2Cl_2) of ^{13}C labeled compound **3**.

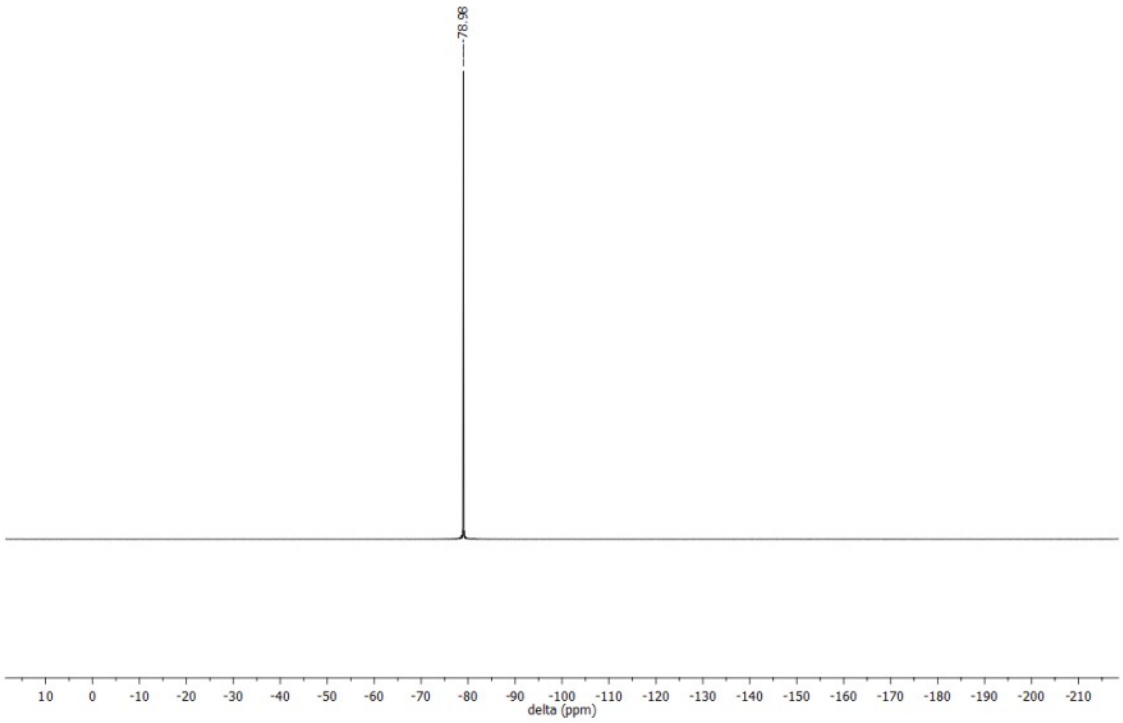

Figure S22. ^{19}F NMR (376 MHz, CD_2Cl_2) of ^{13}C labeled compound **3**.

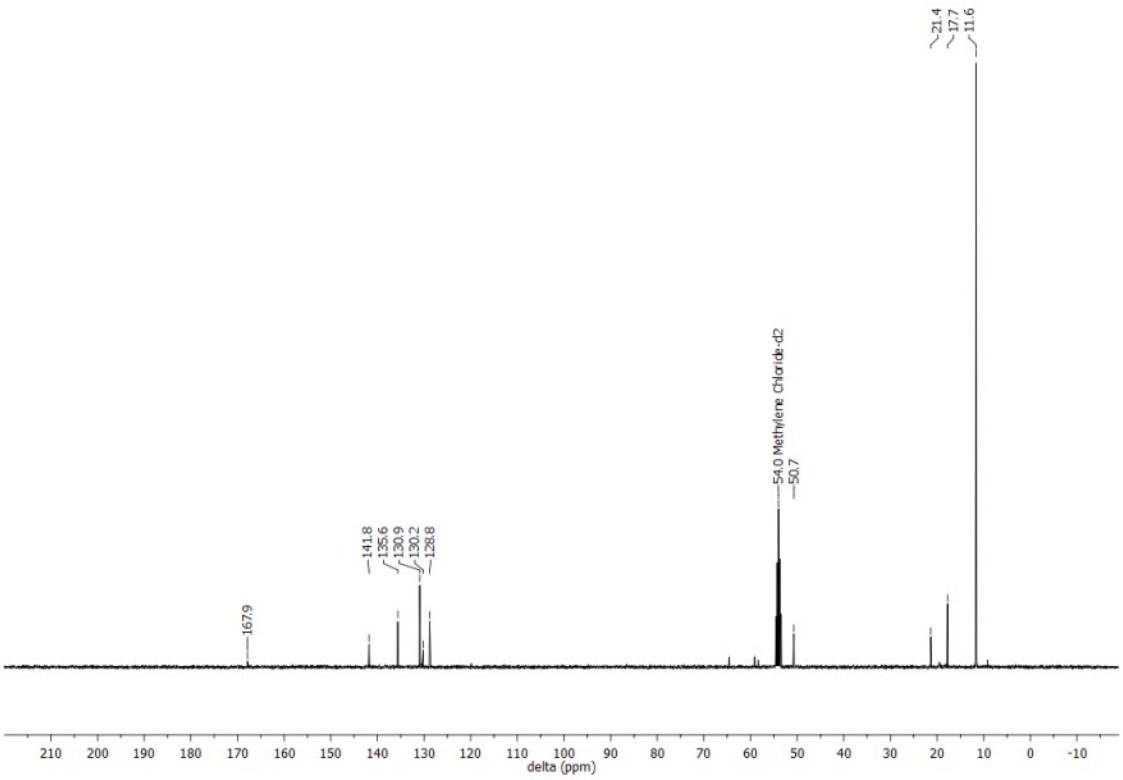

Figure S23. ^{13}C NMR (101 MHz, CD_2Cl_2) of ^{13}C labeled **3**.

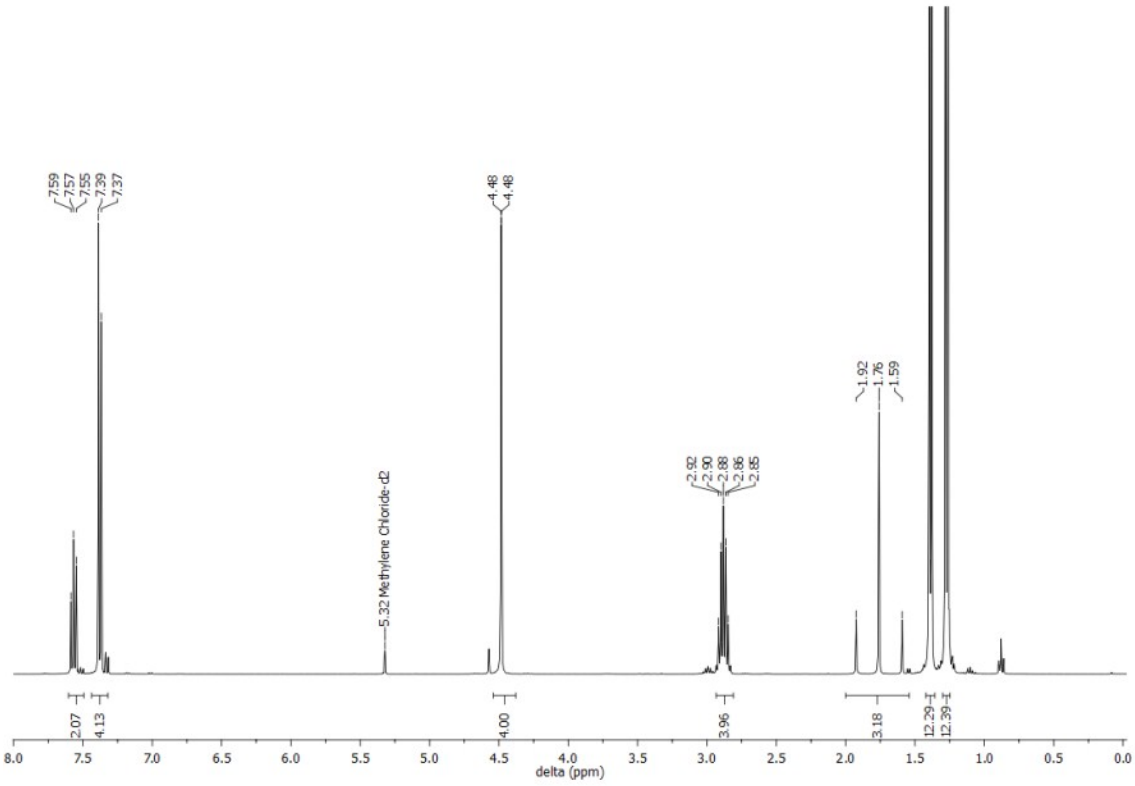

Figure S24. ^{1}H NMR (400 MHz, CD_2Cl_2) of ^{13}C labeled **5**.

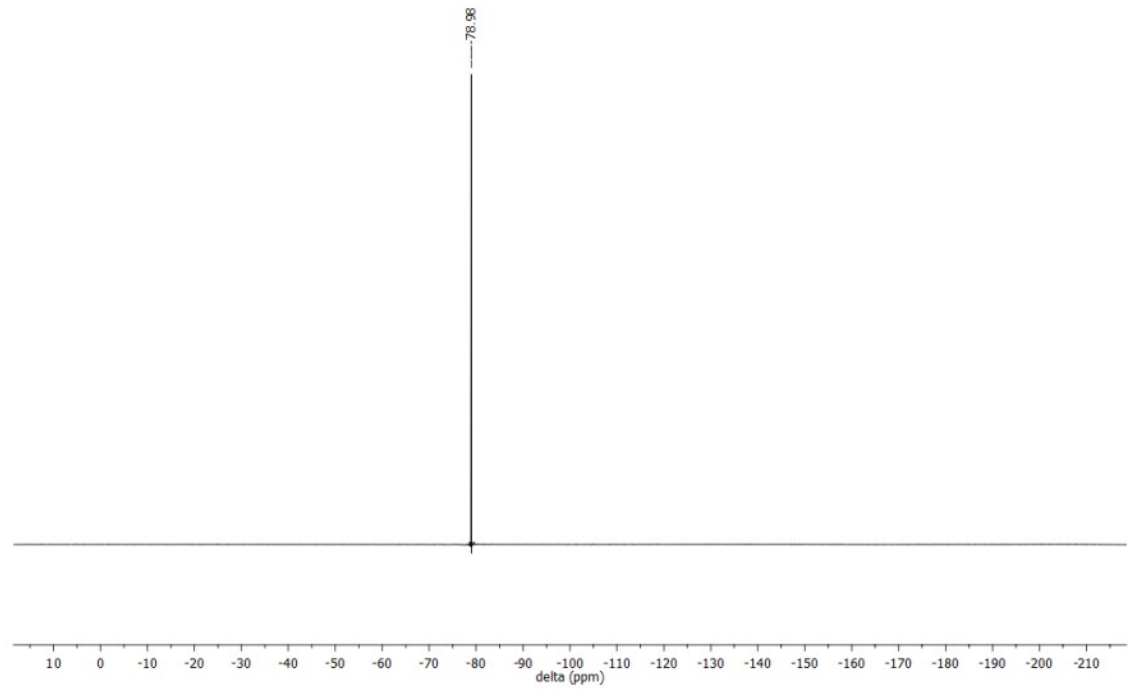

Figure S25. ^{19}F NMR (376 MHz, CD_2Cl_2) of ^{13}C labeled **5**.

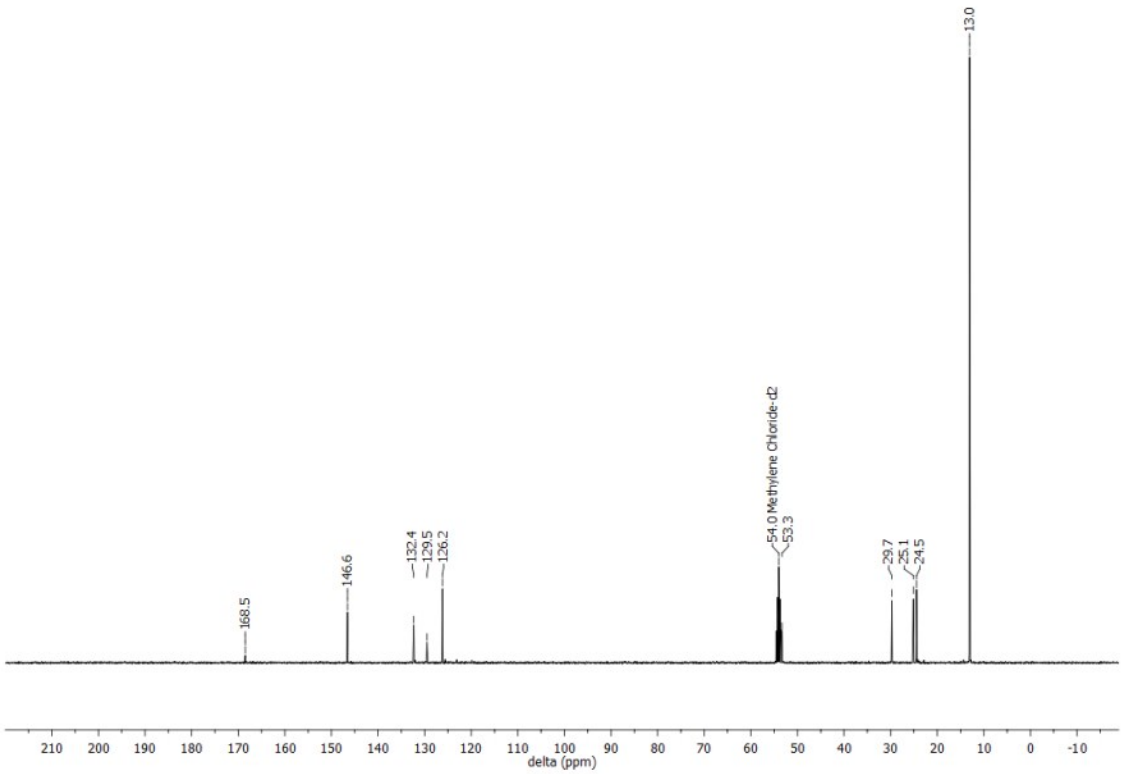

Figure S26. ^{13}C NMR (101 MHz, CD_2Cl_2) of ^{13}C labeled **5**.

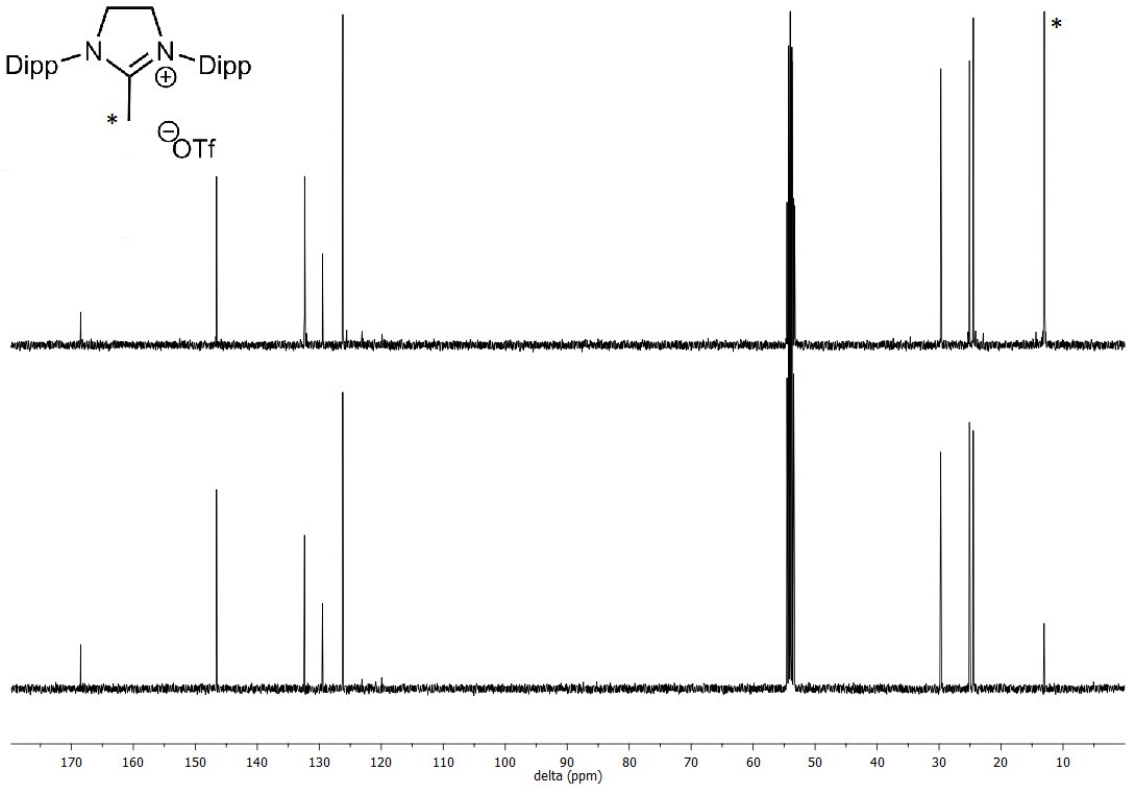

Figure S27. Comparison of ^{13}C NMR spectra of ^{13}C labeled and unlabeled **5**.

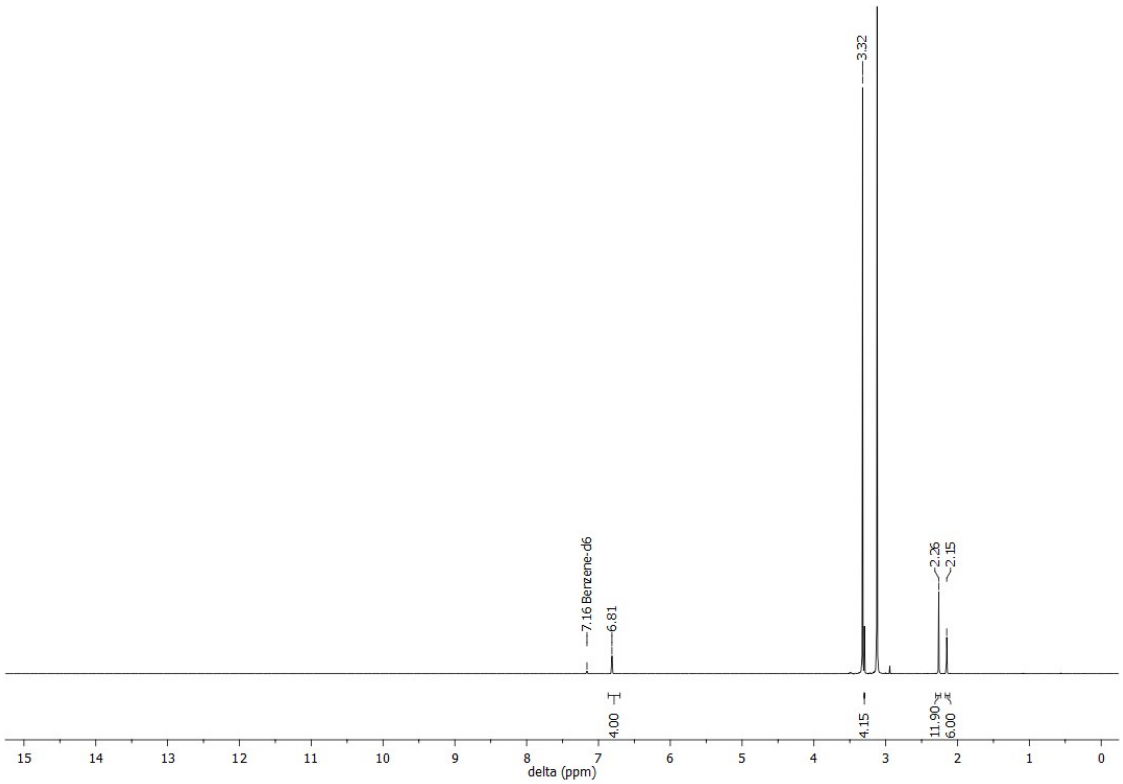

Figure S28. ^{1}H NMR (400 MHz, C_6D_6) of control experiment.

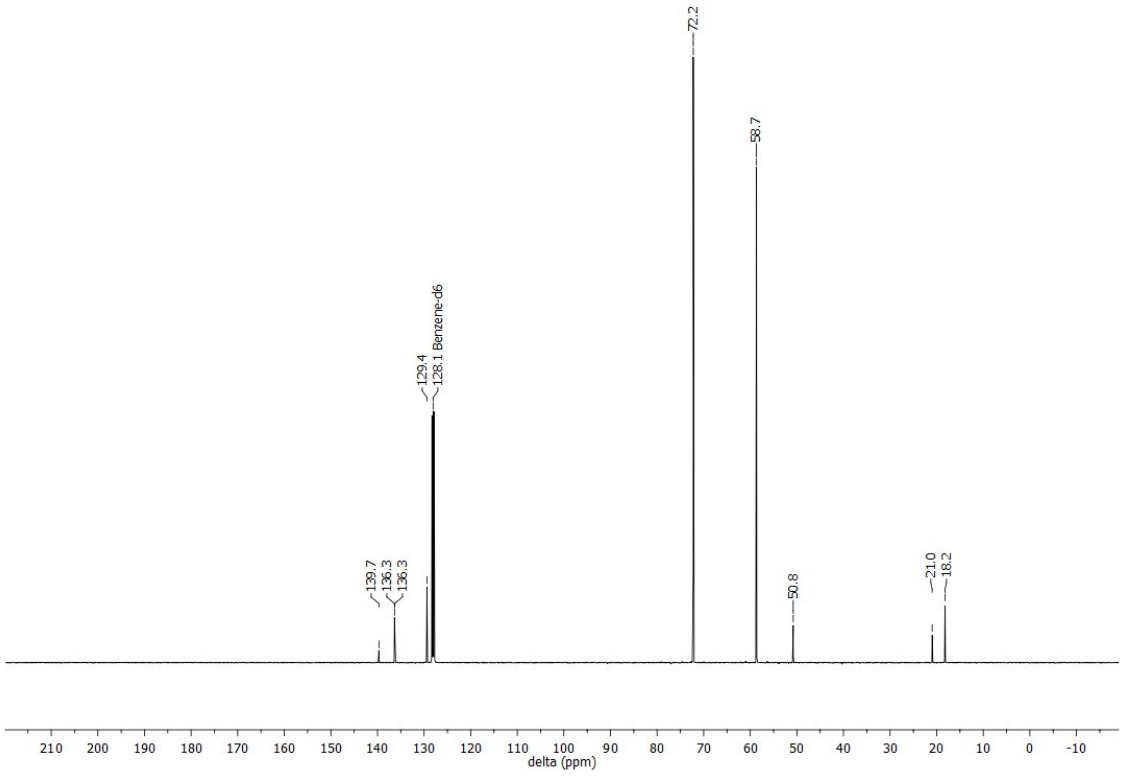

Figure S29. ^{13}C NMR (400 MHz, C_6D_6) of control experiment.

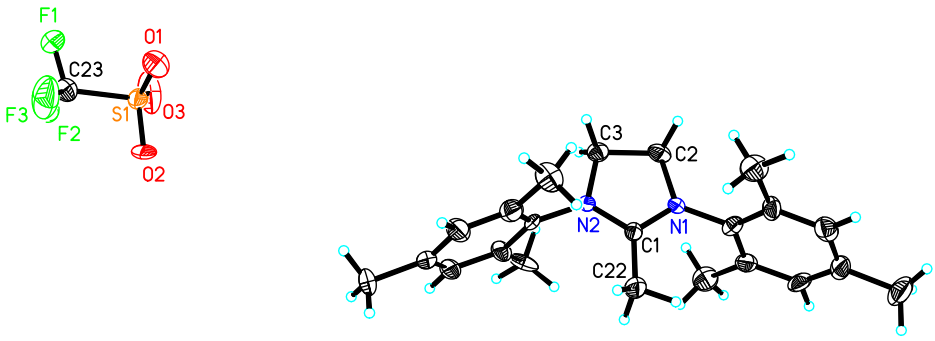

Figure S30. Single crystal X-ray structure of compound **3**. Relevant bond lengths (pm) and angles (°): N(1)-C(1) 130.6(7), N(1)-C(4) 1.437(7), N(1)-C(2) 148.8(7), C(1)-N(2) 133.0(7), C(1)-C(22) 147.4(8), N(2)-C(13) 143.9(7), N(2)-C(3) 147.0(7), C(2)-C(3) 152.6(8), C(1)-N(1)-C(4) 125.6(5), C(1)-N(1)-C(2) 111.0(4), C(4)-N(1)-C(2) 123.3(4), N(1)-C(1)-N(2) 112.3(5), N(1)-C(1)-C(22) 124.8(5), N(2)-C(1)-C(22) 122.9(5).

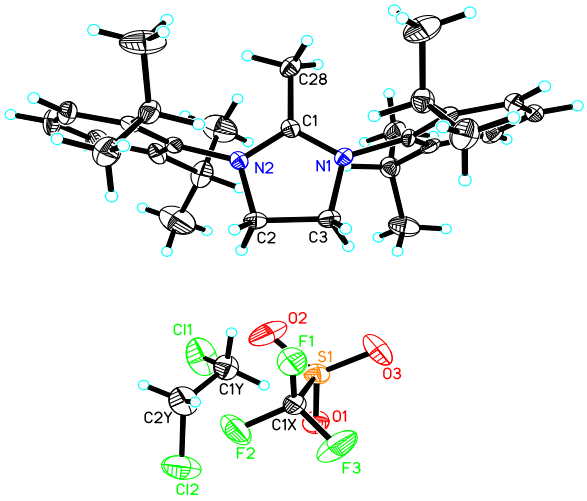

Figure S31. Single crystal X-ray structure of compound **5**. Relevant bond lengths (pm) and angles (°): N(1)-C(1) 132.3(4), N(1)-C(4) 144.1(4), N(1)-C(3) 148.3(4), C(1)-N(2) 131.0(4), C(1)-C(28) 148.4(4), N(2)-C(16) 145.1(4), N(2)-C(2) 148.5(4), C(2)-C(3) 152.0(4), C(1)-N(1)-C(4) 126.7(3), C(1)-N(1)-C(3) 110.7(2), C(4)-N(1)-C(3) 121.6(2), N(2)-C(1)-N(1) 112.6(3), N(2)-C(1)-C(28) 124.6(3), N(1)-C(1)-C(28) 122.8(3).

Table S1. Crystal data and structure refinement for compound **2**.

Empirical formula	$C_{47}H_{62}F_3N_3O_5SW$
Formula weight	1021.91
Temperature	130(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 16.2173(8) Å, α = 90° b = 17.5402(9) Å, β = 109.557(2)° c = 17.1966(9) Å, γ = 90°
Volume	4609.4(4) $Å^3$
Z, Calculated density	4, 1.473 Mg/m^3
Absorption coefficient	2.611 mm^{-1}
F(000)	2088
Crystal size	0.43 x 0.38 x 0.29 mm
θ range for data collection	1.71 to 30.48°
Limiting indices	-21<=h<=23, -25<=k<=18, -24<=l<=24
Reflections collected/unique	52954/13998 [R(int) = 0.0280]
Completeness to θ = 30.48	99.8 %
Absorption correction	Numerical
Max. and min. transmission	0.6048 and 0.4304
Refinement method	Full-matrix least-squares on F^2
Data/restraints / parameters	13998/0/554
Goodness-of-fit on F^2	1.040
Final R indices [I>2σ(I)]	R1 = 0.0447, wR2 = 0.1046
R indices (all data)	R1 = 0.0631, wR2 = 0.1112
Largest diff. peak and hole	9.946 and -2.192 $e.Å^{-3}$

REMARK: B-Alert in cif-Report: High Residual Density. Not critical - side-peak of W, depended on crystal quality.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	132(1)	2366(1)	7957(1)	13(1)
O(1)	-1061(2)	2564(2)	7833(2)	20(1)
N(1)	874(2)	4041(2)	7728(2)	19(1)
C(1)	386(3)	3605(2)	8050(2)	18(1)
O(2)	-457(2)	1259(2)	8142(2)	24(1)
N(2)	32(2)	4064(2)	8474(2)	21(1)
C(2)	886(3)	4858(3)	7960(3)	28(1)
N(3)	1144(2)	2025(2)	8652(2)	16(1)
C(3)	237(4)	4880(3)	8420(3)	30(1)
C(4)	1465(3)	3832(2)	7290(3)	19(1)
C(5)	2312(3)	3610(3)	7744(3)	21(1)
C(6)	2913(3)	3529(3)	7326(3)	24(1)
C(7)	2677(3)	3665(3)	6476(3)	25(1)
C(8)	1813(3)	3872(3)	6039(3)	22(1)
C(9)	1204(3)	3979(2)	6442(3)	19(1)
C(10)	2610(3)	3511(3)	8669(3)	29(1)
C(11)	3356(4)	3652(3)	6052(4)	37(1)
C(12)	307(3)	4292(3)	5968(3)	27(1)
C(13)	-453(3)	3861(2)	9003(3)	20(1)
C(14)	-1365(3)	3902(3)	8708(3)	22(1)
C(15)	-1805(3)	3718(3)	9257(3)	25(1)
C(16)	-1369(3)	3524(3)	10073(3)	27(1)
C(17)	-461(3)	3520(3)	10357(3)	27(1)
C(18)	17(3)	3692(3)	9833(3)	23(1)
C(19)	-1872(3)	4153(3)	7834(3)	29(1)
C(20)	-1884(5)	3353(4)	10646(4)	43(1)
C(21)	999(3)	3747(4)	10172(3)	36(1)
C(22)	-1606(3)	2078(3)	8124(3)	27(1)
C(23)	-1400(3)	1270(3)	7948(3)	29(1)
C(24)	-127(4)	516(3)	8021(3)	31(1)
C(25)	1740(3)	1558(2)	9231(2)	17(1)
C(26)	1616(3)	1355(3)	9981(2)	20(1)
C(27)	2191(3)	824(3)	10493(3)	25(1)
C(28)	2868(3)	504(3)	10286(3)	27(1)
C(29)	2996(3)	724(3)	9562(3)	24(1)
C(30)	2442(3)	1243(2)	9021(3)	19(1)
C(31)	892(3)	1688(3)	10248(3)	31(1)
C(32)	1251(5)	2014(5)	11134(3)	58(2)
C(33)	171(5)	1107(5)	10187(5)	54(2)

C(34)	2566(3)	1428(3)	8198(3)	22(1)
C(35)	3513(3)	1600(3)	8289(3)	30(1)
C(36)	2229(3)	757(3)	7603(3)	28(1)
C(37)	283(3)	2152(2)	6907(2)	17(1)
C(38)	-384(3)	2051(3)	6030(3)	21(1)
C(39)	57(3)	2281(3)	5392(3)	26(1)
C(40)	-1202(3)	2555(3)	5892(3)	26(1)
C(41)	-618(3)	1203(3)	5938(3)	23(1)
C(42)	35(3)	661(3)	5988(3)	26(1)
C(43)	-151(4)	-115(3)	5918(3)	32(1)
C(44)	-1001(4)	-369(3)	5787(4)	38(1)
C(45)	-1647(4)	154(3)	5719(4)	39(1)
C(46)	-1459(3)	934(3)	5799(3)	29(1)
S(1)	1278(1)	3659(1)	3250(1)	32(1)
O(3)	1380(3)	3743(3)	2448(3)	46(1)
O(4)	2096(3)	3592(3)	3919(3)	58(2)
O(5)	639(3)	4136(3)	3424(3)	52(1)
C(47)	802(4)	2710(3)	3185(4)	34(1)
F(1)	46(2)	2669(2)	2553(3)	57(1)
F(2)	1336(2)	2175(2)	3057(2)	39(1)
F(3)	629(4)	2520(3)	3855(3)	75(2)

Table S3. Bond lengths [Å] and angles [°] for compound **2**.

W(1)-N(3)	1.779(3)
W(1)-O(1)	1.906(3)
W(1)-C(37)	1.939(4)
W(1)-C(1)	2.207(4)
W(1)-O(2)	2.233(3)
O(1)-C(22)	1.434(5)
N(1)-C(1)	1.347(5)
N(1)-C(4)	1.450(5)
N(1)-C(2)	1.486(6)
C(1)-N(2)	1.337(5)
O(2)-C(24)	1.450(6)
O(2)-C(23)	1.452(6)
N(2)-C(13)	1.433(5)
N(2)-C(3)	1.480(6)
C(2)-C(3)	1.515(7)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(3)-C(25)	1.398(5)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.389(6)
C(4)-C(9)	1.399(6)
C(5)-C(6)	1.398(6)
C(5)-C(10)	1.511(6)
C(6)-C(7)	1.402(7)
C(6)-H(6)	0.9500
C(7)-C(8)	1.398(7)
C(7)-C(11)	1.511(6)
C(8)-C(9)	1.396(6)
C(8)-H(8)	0.9500
C(9)-C(12)	1.514(6)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.396(6)
C(13)-C(18)	1.405(6)

C(14)-C(15)	1.397(6)
C(14)-C(19)	1.518(6)
C(15)-C(16)	1.386(7)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(7)
C(16)-C(20)	1.521(7)
C(17)-C(18)	1.404(7)
C(17)-H(17)	0.9500
C(18)-C(21)	1.505(7)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.509(7)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.416(6)
C(25)-C(30)	1.416(6)
C(26)-C(27)	1.401(6)
C(26)-C(31)	1.513(6)
C(27)-C(28)	1.382(7)
C(27)-H(27)	0.9500
C(28)-C(29)	1.383(7)
C(28)-H(28)	0.9500
C(29)-C(30)	1.394(6)
C(29)-H(29)	0.9500
C(30)-C(34)	1.530(6)
C(31)-C(33)	1.528(9)
C(31)-C(32)	1.548(8)
C(31)-H(31)	10.000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800

C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.521(6)
C(34)-C(36)	1.536(7)
C(34)-H(34)	10.000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-C(38)	1.544(6)
C(37)-H(37)	0.9500
C(38)-C(41)	1.530(6)
C(38)-C(40)	1.545(7)
C(38)-C(39)	1.552(6)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-C(46)	1.386(7)
C(41)-C(42)	1.405(7)
C(42)-C(43)	1.391(7)
C(42)-H(42)	0.9500
C(43)-C(44)	1.394(8)
C(43)-H(43)	0.9500
C(44)-C(45)	1.368(9)
C(44)-H(44)	0.9500
C(45)-C(46)	1.398(7)
C(45)-H(45)	0.9500
C(46)-H(46)	0.9500
S(1)-O(5)	1.438(4)
S(1)-O(4)	1.440(5)
S(1)-O(3)	1.450(5)
S(1)-C(47)	1.821(6)
C(47)-F(3)	1.316(6)
C(47)-F(2)	1.344(6)
C(47)-F(1)	1.341(7)

N(3)-W(1)-O(1)	144.09(14)

N(3)-W(1)-C(37)	100.63(16)
O(1)-W(1)-C(37)	111.81(16)
N(3)-W(1)-C(1)	100.02(16)
O(1)-W(1)-C(1)	89.20(14)
C(37)-W(1)-C(1)	100.35(16)
N(3)-W(1)-O(2)	87.40(15)
O(1)-W(1)-O(2)	73.05(13)
C(37)-W(1)-O(2)	99.07(15)
C(1)-W(1)-O(2)	157.51(14)
C(22)-O(1)-W(1)	125.0(3)
C(1)-N(1)-C(4)	130.7(4)
C(1)-N(1)-C(2)	113.2(4)
C(4)-N(1)-C(2)	115.6(3)
N(2)-C(1)-N(1)	107.5(4)
N(2)-C(1)-W(1)	121.9(3)
N(1)-C(1)-W(1)	130.6(3)
C(24)-O(2)-C(23)	113.0(4)
C(24)-O(2)-W(1)	124.3(3)
C(23)-O(2)-W(1)	115.0(3)
C(1)-N(2)-C(13)	128.5(4)
C(1)-N(2)-C(3)	113.8(4)
C(13)-N(2)-C(3)	117.5(4)
N(1)-C(2)-C(3)	102.5(4)
N(1)-C(2)-H(2A)	111.3
C(3)-C(2)-H(2A)	111.3
N(1)-C(2)-H(2B)	111.3
C(3)-C(2)-H(2B)	111.3
H(2A)-C(2)-H(2B)	109.2
C(25)-N(3)-W(1)	159.7(3)
N(2)-C(3)-C(2)	102.5(4)
N(2)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
N(2)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2
C(5)-C(4)-C(9)	122.3(4)
C(5)-C(4)-N(1)	118.7(4)
C(9)-C(4)-N(1)	118.2(4)
C(4)-C(5)-C(6)	117.9(4)
C(4)-C(5)-C(10)	122.1(4)
C(6)-C(5)-C(10)	119.8(4)
C(5)-C(6)-C(7)	121.6(4)
C(5)-C(6)-H(6)	119.2

C(7)-C(6)-H(6)	119.2
C(8)-C(7)-C(6)	118.7(4)
C(8)-C(7)-C(11)	120.4(5)
C(6)-C(7)-C(11)	120.8(5)
C(7)-C(8)-C(9)	121.1(4)
C(7)-C(8)-H(8)	119.5
C(9)-C(8)-H(8)	119.5
C(8)-C(9)-C(4)	118.3(4)
C(8)-C(9)-C(12)	119.6(4)
C(4)-C(9)-C(12)	122.0(4)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	121.9(4)
C(14)-C(13)-N(2)	119.7(4)
C(18)-C(13)-N(2)	118.1(4)
C(13)-C(14)-C(15)	117.5(4)
C(13)-C(14)-C(19)	122.1(4)
C(15)-C(14)-C(19)	120.4(4)
C(16)-C(15)-C(14)	122.5(4)
C(16)-C(15)-H(15)	118.8
C(14)-C(15)-H(15)	118.8
C(17)-C(16)-C(15)	118.7(4)
C(17)-C(16)-C(20)	121.3(5)
C(15)-C(16)-C(20)	120.0(5)
C(16)-C(17)-C(18)	121.4(4)
C(16)-C(17)-H(17)	119.3
C(18)-C(17)-H(17)	119.3

C(17)-C(18)-C(13)	118.0(4)
C(17)-C(18)-C(21)	120.4(4)
C(13)-C(18)-C(21)	121.5(4)
0C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(1)-C(22)-C(23)	106.6(4)
O(1)-C(22)-H(22A)	110.4
C(23)-C(22)-H(22A)	110.4
O(1)-C(22)-H(22B)	110.4
C(23)-C(22)-H(22B)	110.4
H(22A)-C(22)-H(22B)	108.6
O(2)-C(23)-C(22)	104.7(4)
O(2)-C(23)-H(23A)	110.8
C(22)-C(23)-H(23A)	110.8
O(2)-C(23)-H(23B)	110.8
C(22)-C(23)-H(23B)	110.8
H(23A)-C(23)-H(23B)	108.9
O(2)-C(24)-H(24A)	109.5
O(2)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(2)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(3)-C(25)-C(26)	121.4(4)
N(3)-C(25)-C(30)	118.1(4)
C(26)-C(25)-C(30)	120.4(4)
C(27)-C(26)-C(25)	118.1(4)

C(27)-C(26)-C(31)	119.2(4)
C(25)-C(26)-C(31)	122.7(4)
C(28)-C(27)-C(26)	121.9(4)
C(28)-C(27)-H(27)	119.1
C(26)-C(27)-H(27)	119.1
C(27)-C(28)-C(29)	119.3(4)
C(27)-C(28)-H(28)	120.3
C(29)-C(28)-H(28)	120.3
C(28)-C(29)-C(30)	121.7(4)
C(28)-C(29)-H(29)	119.2
C(30)-C(29)-H(29)	119.2
C(29)-C(30)-C(25)	118.6(4)
C(29)-C(30)-C(34)	120.1(4)
C(25)-C(30)-C(34)	121.2(4)
C(26)-C(31)-C(33)	112.0(5)
C(26)-C(31)-C(32)	111.5(5)
C(33)-C(31)-C(32)	109.9(5)
C(26)-C(31)-H(31)	107.7
C(33)-C(31)-H(31)	107.7
C(32)-C(31)-H(31)	107.7
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-C(30)	112.8(4)
C(35)-C(34)-C(36)	110.0(4)
C(30)-C(34)-C(36)	109.1(4)
C(35)-C(34)-H(34)	108.3
C(30)-C(34)-H(34)	108.3
C(36)-C(34)-H(34)	108.3
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5

H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-W(1)	131.8(3)
C(38)-C(37)-H(37)	114.1
W(1)-C(37)-H(37)	114.1
C(41)-C(38)-C(37)	106.3(3)
C(41)-C(38)-C(40)	111.7(4)
C(37)-C(38)-C(40)	111.7(4)
C(41)-C(38)-C(39)	109.7(4)
C(37)-C(38)-C(39)	108.8(4)
C(40)-C(38)-C(39)	108.5(4)
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(46)-C(41)-C(42)	117.3(4)
C(46)-C(41)-C(38)	123.0(4)
C(42)-C(41)-C(38)	119.7(4)
C(43)-C(42)-C(41)	121.4(5)
C(43)-C(42)-H(42)	119.3
C(41)-C(42)-H(42)	119.3
C(42)-C(43)-C(44)	120.0(5)
C(42)-C(43)-H(43)	120.0
C(44)-C(43)-H(43)	120.0
C(45)-C(44)-C(43)	119.1(5)
C(45)-C(44)-H(44)	120.4
C(43)-C(44)-H(44)	120.4
C(44)-C(45)-C(46)	120.9(5)
C(44)-C(45)-H(45)	119.5
C(46)-C(45)-H(45)	119.5

C(41)-C(46)-C(45)	121.3(5)
C(41)-C(46)-H(46)	119.4
C(45)-C(46)-H(46)	119.4
O(5)-S(1)-O(4)	114.6(3)
O(5)-S(1)-O(3)	117.2(3)
O(4)-S(1)-O(3)	113.5(3)
O(5)-S(1)-C(47)	103.0(3)
O(4)-S(1)-C(47)	103.5(3)
O(3)-S(1)-C(47)	102.5(3)
F(3)-C(47)-F(2)	107.7(5)
F(3)-C(47)-F(1)	106.9(5)
F(2)-C(47)-F(1)	107.1(5)
F(3)-C(47)-S(1)	112.8(4)
F(2)-C(47)-S(1)	111.4(4)
F(1)-C(47)-S(1)	110.6(4)

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

	U11	U22	U33	U23	U13	U12
W(1)	13(1)	13(1)	13(1)	1(1)	6(1)	1(1)
O(1)	14(1)	20(2)	27(2)	0(1)	9(1)	1(1)
N(1)	22(2)	13(2)	25(2)	0(1)	11(1)	-1(1)
C(1)	22(2)	15(2)	16(2)	3(1)	7(1)	5(1)
O(2)	27(2)	14(2)	36(2)	4(1)	19(1)	0(1)
N(2)	26(2)	14(2)	26(2)	-1(1)	14(2)	-3(1)
C(2)	37(3)	14(2)	44(3)	-6(2)	26(2)	-4(2)
N(3)	17(2)	18(2)	15(1)	1(1)	8(1)	3(1)
C(3)	44(3)	12(2)	43(3)	-1(2)	26(2)	-1(2)
C(4)	20(2)	13(2)	25(2)	-1(2)	11(2)	-2(2)
C(5)	23(2)	20(2)	22(2)	1(2)	10(2)	-1(2)
C(6)	20(2)	25(2)	31(2)	4(2)	11(2)	3(2)
C(7)	27(2)	22(2)	31(2)	0(2)	17(2)	-2(2)
C(8)	30(2)	17(2)	21(2)	1(2)	12(2)	-3(2)
C(9)	22(2)	14(2)	22(2)	1(2)	7(2)	-4(2)
C(10)	27(2)	32(3)	26(2)	3(2)	6(2)	1(2)
C(11)	42(3)	35(3)	49(3)	2(2)	36(3)	3(2)
C(12)	23(2)	23(2)	29(2)	5(2)	3(2)	0(2)
C(13)	24(2)	15(2)	22(2)	-1(2)	11(2)	-1(2)
C(14)	27(2)	18(2)	22(2)	-4(2)	9(2)	-1(2)
C(15)	25(2)	21(2)	32(2)	-5(2)	16(2)	1(2)
C(16)	40(3)	18(2)	30(2)	-3(2)	21(2)	0(2)
C(17)	42(3)	20(2)	19(2)	-1(2)	12(2)	2(2)
C(18)	24(2)	20(2)	24(2)	-3(2)	7(2)	-2(2)
C(19)	31(2)	28(3)	25(2)	2(2)	6(2)	8(2)
C(20)	62(4)	38(3)	46(3)	7(3)	40(3)	6(3)
C(21)	27(2)	44(3)	29(2)	-3(2)	0(2)	-5(2)
C(22)	26(2)	22(2)	44(3)	0(2)	23(2)	-2(2)
C(23)	30(2)	23(2)	42(3)	-2(2)	22(2)	-6(2)
C(24)	44(3)	17(2)	41(3)	4(2)	26(2)	4(2)
C(25)	19(2)	13(2)	16(2)	-1(1)	4(1)	3(1)
C(26)	25(2)	20(2)	14(2)	1(1)	5(2)	3(2)
C(27)	33(2)	20(2)	18(2)	4(2)	5(2)	4(2)
C(28)	33(2)	19(2)	22(2)	3(2)	0(2)	7(2)
C(29)	25(2)	19(2)	25(2)	-2(2)	6(2)	7(2)
C(30)	20(2)	17(2)	20(2)	-3(2)	6(2)	2(2)
C(31)	36(3)	40(3)	20(2)	11(2)	15(2)	17(2)
C(32)	83(5)	71(5)	19(2)	3(3)	16(3)	44(4)
C(33)	50(4)	70(5)	58(4)	26(4)	38(3)	7(3)
C(34)	22(2)	23(2)	21(2)	0(2)	9(2)	5(2)

C(35)	23(2)	34(3)	38(3)	-3(2)	15(2)	1(2)
C(36)	27(2)	32(3)	25(2)	-7(2)	10(2)	1(2)
C(37)	20(2)	17(2)	17(2)	1(1)	9(1)	-4(2)
C(38)	26(2)	19(2)	18(2)	3(2)	6(2)	-4(2)
C(39)	33(2)	33(3)	14(2)	-1(2)	8(2)	-9(2)
C(40)	25(2)	21(2)	29(2)	0(2)	4(2)	0(2)
C(41)	30(2)	21(2)	15(2)	0(2)	5(2)	-3(2)
C(42)	31(2)	26(2)	21(2)	-4(2)	10(2)	-2(2)
C(43)	44(3)	23(2)	30(2)	-1(2)	13(2)	3(2)
C(44)	53(3)	21(3)	38(3)	-5(2)	12(3)	-9(2)
C(45)	35(3)	27(3)	48(3)	3(2)	5(2)	-12(2)
C(46)	28(2)	23(2)	32(2)	1(2)	5(2)	-5(2)
S(1)	29(1)	28(1)	39(1)	-10(1)	11(1)	5(1)
O(3)	54(3)	36(2)	56(3)	11(2)	29(2)	7(2)
O(4)	31(2)	89(4)	49(3)	-35(3)	5(2)	9(2)
O(5)	33(2)	37(2)	84(4)	-26(2)	20(2)	7(2)
C(47)	37(3)	33(3)	42(3)	1(2)	26(2)	4(2)
F(1)	29(2)	60(3)	79(3)	-25(2)	16(2)	-8(2)
F(2)	48(2)	25(2)	53(2)	4(1)	28(2)	12(1)
F(3)	114(4)	68(3)	79(3)	26(2)	79(3)	17(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **2**.

	x	y	z	U(eq)
H(2A)	696	5189	7466	34
H(2B)	1477	5017	8319	34
H(3A)	501	5107	8976	36
H(3B)	-293	5173	8111	36
H(6)	3496	3377	7626	29
H(8)	1638	3942	5459	26
H(10A)	2423	3952	8918	43
H(10B)	3250	3472	8886	43
H(10C)	2352	3046	8804	43
H(11A)	3098	3436	5498	55
H(11B)	3854	3339	6373	55
H(11C)	3555	4173	6011	55
H(12A)	-131	4046	6162	40
H(12B)	171	4188	5378	40
H(12C)	299	4843	6056	40
H(15)	-2427	3725	9063	30
H(17)	-156	3397	10918	32
H(19A)	-1760	4695	7770	43
H(19B)	-2499	4075	7724	43
H(19C)	-1684	3852	7443	43
H(20A)	-1479	3212	11192	65
H(20B)	-2289	2930	10421	65
H(20C)	-2216	3806	10696	65
H(21A)	1254	3370	9898	54
H(21B)	1201	3647	10767	54
H(21C)	1182	4260	10071	54
H(22A)	-2231	2193	7833	33
H(22B)	-1480	2151	8723	33
H(23A)	-1581	904	8299	35
H(23B)	-1703	1139	7362	35
H(24A)	-227	151	8411	46
H(24B)	502	552	8114	46
H(24C)	-431	343	7455	46
H(27)	2114	681	10997	30
H(28)	3241	136	10637	32
H(29)	3473	515	9430	28
H(31)	624	2119	9866	37
H(32A)	1452	1594	11529	86
H(32B)	786	2296	11255	86
H(32C)	1741	2358	11180	86

H(33A)	-37	888	9631	81
H(33B)	-316	1360	10300	81
H(33C)	404	701	10592	81
H(34)	2205	1888	7958	26
H(35A)	3729	2016	8685	45
H(35B)	3549	1750	7753	45
H(35C)	3870	1144	8488	45
H(36A)	2315	869	7077	42
H(36B)	1604	680	7508	42
H(36C)	2553	294	7843	42
H(37)	876	2099	6938	21
H(39A)	617	2013	5517	39
H(39B)	159	2832	5419	39
H(39C)	-326	2142	4836	39
H(40A)	-1621	2460	5339	39
H(40B)	-1030	3093	5941	39
H(40C)	-1474	2432	6306	39
H(42)	615	828	6070	31
H(43)	303	-473	5961	38
H(44)	-1131	-899	5745	46
H(45)	-2230	-14	5617	47
H(46)	-1917	1287	5756	35

Table S6. Torsion angles [°] for compound **2**.

N(3)-W(1)-O(1)-C(22)	-41.4(5)
C(37)-W(1)-O(1)-C(22)	111.7(4)
C(1)-W(1)-O(1)-C(22)	-147.5(4)
O(2)-W(1)-O(1)-C(22)	18.5(3)
C(4)-N(1)-C(1)-N(2)	173.0(4)
C(2)-N(1)-C(1)-N(2)	1.8(5)
C(4)-N(1)-C(1)-W(1)	-7.5(7)
C(2)-N(1)-C(1)-W(1)	-178.6(3)
N(3)-W(1)-C(1)-N(2)	-104.7(3)
O(1)-W(1)-C(1)-N(2)	40.4(3)
C(37)-W(1)-C(1)-N(2)	152.4(3)
O(2)-W(1)-C(1)-N(2)	3.1(6)
N(3)-W(1)-C(1)-N(1)	75.8(4)
O(1)-W(1)-C(1)-N(1)	-139.1(4)
C(37)-W(1)-C(1)-N(1)	-27.1(4)
O(2)-W(1)-C(1)-N(1)	-176.3(3)
N(3)-W(1)-O(2)-C(24)	-54.3(4)
O(1)-W(1)-O(2)-C(24)	156.3(4)
C(37)-W(1)-O(2)-C(24)	46.1(4)
C(1)-W(1)-O(2)-C(24)	-164.5(4)
N(3)-W(1)-O(2)-C(23)	158.4(3)
O(1)-W(1)-O(2)-C(23)	9.0(3)
C(37)-W(1)-O(2)-C(23)	-101.2(3)
C(1)-W(1)-O(2)-C(23)	48.2(5)
N(1)-C(1)-N(2)-C(13)	-172.0(4)
W(1)-C(1)-N(2)-C(13)	8.4(6)
N(1)-C(1)-N(2)-C(3)	3.1(5)
W(1)-C(1)-N(2)-C(3)	-176.5(3)
C(1)-N(1)-C(2)-C(3)	-5.7(6)
C(4)-N(1)-C(2)-C(3)	-178.2(4)
O(1)-W(1)-N(3)-C(25)	46.9(10)
C(37)-W(1)-N(3)-C(25)	-107.7(8)
C(1)-W(1)-N(3)-C(25)	149.6(8)
O(2)-W(1)-N(3)-C(25)	-9.0(8)
C(1)-N(2)-C(3)-C(2)	-6.5(6)
C(13)-N(2)-C(3)-C(2)	169.2(4)
N(1)-C(2)-C(3)-N(2)	6.6(5)
C(1)-N(1)-C(4)-C(5)	-81.7(6)
C(2)-N(1)-C(4)-C(5)	89.3(5)
C(1)-N(1)-C(4)-C(9)	108.4(5)
C(2)-N(1)-C(4)-C(9)	-80.6(5)
C(9)-C(4)-C(5)-C(6)	-0.5(7)

N(1)-C(4)-C(5)-C(6)	-169.9(4)
C(9)-C(4)-C(5)-C(10)	175.1(4)
N(1)-C(4)-C(5)-C(10)	5.6(6)
C(4)-C(5)-C(6)-C(7)	0.0(7)
C(10)-C(5)-C(6)-C(7)	-175.7(5)
C(5)-C(6)-C(7)-C(8)	-1.3(7)
C(5)-C(6)-C(7)-C(11)	173.7(5)
C(6)-C(7)-C(8)-C(9)	3.1(7)
C(11)-C(7)-C(8)-C(9)	-172.0(4)
C(7)-C(8)-C(9)-C(4)	-3.5(7)
C(7)-C(8)-C(9)-C(12)	172.9(4)
C(5)-C(4)-C(9)-C(8)	2.2(6)
N(1)-C(4)-C(9)-C(8)	171.7(4)
C(5)-C(4)-C(9)-C(12)	-174.1(4)
N(1)-C(4)-C(9)-C(12)	-4.6(6)
C(1)-N(2)-C(13)-C(14)	-100.2(6)
C(3)-N(2)-C(13)-C(14)	84.8(5)
C(1)-N(2)-C(13)-C(18)	85.6(6)
C(3)-N(2)-C(13)-C(18)	-89.4(5)
C(18)-C(13)-C(14)-C(15)	-4.3(7)
N(2)-C(13)-C(14)-C(15)	-178.3(4)
C(18)-C(13)-C(14)-C(19)	174.3(4)
N(2)-C(13)-C(14)-C(19)	0.3(7)
C(13)-C(14)-C(15)-C(16)	2.1(7)
C(19)-C(14)-C(15)-C(16)	-176.5(4)
C(14)-C(15)-C(16)-C(17)	0.6(7)
C(14)-C(15)-C(16)-C(20)	178.1(5)
C(15)-C(16)-C(17)-C(18)	-1.2(7)
C(20)-C(16)-C(17)-C(18)	-178.7(5)
C(16)-C(17)-C(18)-C(13)	-0.9(7)
C(16)-C(17)-C(18)-C(21)	174.9(5)
C(14)-C(13)-C(18)-C(17)	3.7(7)
N(2)-C(13)-C(18)-C(17)	177.8(4)
C(14)-C(13)-C(18)-C(21)	-172.0(5)
N(2)-C(13)-C(18)-C(21)	2.0(7)
W(1)-O(1)-C(22)-C(23)	-40.5(5)
C(24)-O(2)-C(23)-C(22)	179.3(4)
W(1)-O(2)-C(23)-C(22)	-29.7(5)
O(1)-C(22)-C(23)-O(2)	40.1(5)
W(1)-N(3)-C(25)-C(26)	-54.3(10)
W(1)-N(3)-C(25)-C(30)	121.2(8)
N(3)-C(25)-C(26)-C(27)	173.7(4)
C(30)-C(25)-C(26)-C(27)	-1.6(6)

N(3)-C(25)-C(26)-C(31)	-6.3(7)
C(30)-C(25)-C(26)-C(31)	178.3(4)
C(25)-C(26)-C(27)-C(28)	0.4(7)
C(31)-C(26)-C(27)-C(28)	-179.6(5)
C(26)-C(27)-C(28)-C(29)	1.5(7)
C(27)-C(28)-C(29)-C(30)	-2.1(7)
C(28)-C(29)-C(30)-C(25)	0.8(7)
C(28)-C(29)-C(30)-C(34)	-175.6(4)
N(3)-C(25)-C(30)-C(29)	-174.4(4)
C(26)-C(25)-C(30)-C(29)	1.0(6)
N(3)-C(25)-C(30)-C(34)	1.9(6)
C(26)-C(25)-C(30)-C(34)	177.4(4)
C(27)-C(26)-C(31)-C(33)	-72.0(6)
C(25)-C(26)-C(31)-C(33)	108.0(5)
C(27)-C(26)-C(31)-C(32)	51.6(7)
C(25)-C(26)-C(31)-C(32)	-128.3(5)
C(29)-C(30)-C(34)-C(35)	-47.8(6)
C(25)-C(30)-C(34)-C(35)	135.9(4)
C(29)-C(30)-C(34)-C(36)	74.8(5)
C(25)-C(30)-C(34)-C(36)	-101.5(5)
N(3)-W(1)-C(37)-C(38)	158.5(4)
O(1)-W(1)-C(37)-C(38)	-5.9(4)
C(1)-W(1)-C(37)-C(38)	-99.2(4)
O(2)-W(1)-C(37)-C(38)	69.4(4)
W(1)-C(37)-C(38)-C(41)	-89.5(5)
W(1)-C(37)-C(38)-C(40)	32.7(6)
W(1)-C(37)-C(38)-C(39)	152.5(4)
C(37)-C(38)-C(41)-C(46)	118.4(5)
C(40)-C(38)-C(41)-C(46)	-3.7(6)
C(39)-C(38)-C(41)-C(46)	-124.1(5)
C(37)-C(38)-C(41)-C(42)	-62.2(5)
C(40)-C(38)-C(41)-C(42)	175.7(4)
C(39)-C(38)-C(41)-C(42)	55.3(5)
C(46)-C(41)-C(42)-C(43)	-1.5(7)
C(38)-C(41)-C(42)-C(43)	179.1(4)
C(41)-C(42)-C(43)-C(44)	0.8(8)
C(42)-C(43)-C(44)-C(45)	0.7(8)
C(43)-C(44)-C(45)-C(46)	-1.5(9)
C(42)-C(41)-C(46)-C(45)	0.7(7)
C(38)-C(41)-C(46)-C(45)	-179.9(5)
C(44)-C(45)-C(46)-C(41)	0.8(9)
O(5)-S(1)-C(47)-F(3)	-56.1(5)
O(4)-S(1)-C(47)-F(3)	63.5(5)

O(3)-S(1)-C(47)-F(3)	-178.3(5)
O(5)-S(1)-C(47)-F(2)	-177.4(4)
O(4)-S(1)-C(47)-F(2)	-57.8(5)
O(3)-S(1)-C(47)-F(2)	60.4(5)
O(5)-S(1)-C(47)-F(1)	63.5(4)
O(4)-S(1)-C(47)-F(1)	-176.8(4)
O(3)-S(1)-C(47)-F(1)	-58.6(4)

Table S7. Crystal data and structure refinement for compound **3**.

Empirical formula	$C_{23}H_{29}F_3N_2O_3S$
Formula weight	470.54
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 10.596(3) Å, α = 90°
	b = 10.814(2) Å, β = 90.907(7)°
	c = 23.235(6) Å, γ = 90°
Volume	2662.0(11) $Å^3$
Z, Calculated density	4, 1.174 Mg/m^3
Absorption coefficient	0.166 mm^{-1}
F(000)	992
Crystal size	0.15 x 0.12 x 0.04 mm
θ range for data collection	1.75 to 25.05°
Limiting indices	-12<=h<=12, -12<=k<=9, -27<=l<=27
Reflections collected /unique	16999 / 4645 [R(int) =0.1106]
Completeness to θ = 25.05	98.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7339 and 0.6288
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	4645/24/322
Goodness-of-fit on F^2	1.042
Final R indices [I>2σ(I)]	R1 = 0.0983, wR2 = 0.1981
R indices (all data)	R1 = 0.1828, wR2 = 0.2239
Largest diff. peak and hole	0.693 and -0.411 e. $Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **3**. U(eq) is defined as one third of the trace of the U_{ij} tensor.

	x	y	z	U(eq)
S(1)	5199(2)	9589(2)	7704(1)	33(1)
O(1)	4532(5)	8523(4)	7509(2)	49(1)
O(2)	4530(7)	10706(4)	7603(2)	81(2)
O(3)	6506(12)	9800(20)	7606(17)	62(8)
O(3A)	6475(11)	9270(20)	7591(17)	60(8)
C(23)	5152(6)	9446(6)	8492(3)	39(2)
F(1)	5692(4)	8418(4)	8675(2)	58(1)
F(2)	6015(10)	10234(9)	8719(4)	50(3)
F(2A)	5339(11)	10443(8)	8783(4)	46(3)
F(3)	3968(5)	9308(5)	8667(2)	90(2)
N(1)	-89(5)	9896(4)	1993(2)	24(1)
C(1)	-527(5)	10410(5)	2458(2)	19(1)
N(2)	40(4)	9989(4)	2933(2)	20(1)
C(2)	940(6)	9008(5)	2137(2)	26(2)
C(3)	1015(6)	9076(5)	2793(2)	25(1)
C(4)	-473(5)	10190(5)	1413(2)	23(1)
C(5)	-1350(6)	9440(6)	1137(2)	29(2)
C(6)	-1737(6)	9734(6)	587(3)	35(2)
C(7)	-1249(7)	10793(7)	306(3)	38(2)
C(8)	-371(6)	11509(6)	594(3)	33(2)
C(9)	35(6)	11240(6)	1149(3)	30(2)
C(10)	-1939(6)	8352(6)	1448(3)	40(2)
C(11)	-1714(7)	11115(7)	-300(3)	54(2)
C(12)	990(7)	12033(6)	1460(3)	40(2)
C(13)	-256(5)	10384(5)	3507(2)	21(1)
C(14)	-1244(6)	9797(6)	3803(3)	31(2)
C(15)	-1520(7)	10202(6)	4339(3)	37(2)
C(16)	-851(7)	11166(6)	4601(3)	34(2)
C(17)	116(7)	11722(6)	4300(3)	35(2)
C(18)	430(6)	11353(5)	3757(3)	28(2)
C(19)	-2006(6)	8751(6)	3511(3)	39(2)
C(20)	-1193(8)	11608(7)	5199(3)	56(2)
C(21)	1456(6)	11982(5)	3436(3)	37(2)
C(22)	-1518(7)	11367(6)	2465(3)	35(2)

Table S9. Bond lengths [Å] and angles [°] for compound **3**.

S(1)-O(2)	1.419(5)
S(1)-O(1)	1.422(5)
S(1)-O(3A)	1.423(9)
S(1)-O(3)	1.424(9)
S(1)-C(23)	1.839(7)
C(23)-F(2A)	1.286(8)
C(23)-F(1)	1.317(7)
C(23)-F(3)	1.333(8)
C(23)-F(2)	1.351(8)
N(1)-C(1)	1.306(7)
N(1)-C(4)	1.437(7)
N(1)-C(2)	1.488(7)
C(1)-N(2)	1.330(7)
C(1)-C(22)	1.474(8)
N(2)-C(13)	1.439(7)
N(2)-C(3)	1.470(7)
C(2)-C(3)	1.526(8)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.384(8)
C(4)-C(9)	1.403(8)
C(5)-C(6)	1.373(8)
C(5)-C(10)	1.521(8)
C(6)-C(7)	1.420(9)
C(6)-H(6)	0.9500
C(7)-C(8)	1.376(9)
C(7)-C(11)	1.524(9)
C(8)-C(9)	1.383(8)
C(8)-H(8)	0.9500
C(9)-C(12)	1.502(9)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.397(8)

C(13)-C(14)	1.412(8)
C(14)-C(15)	1.357(8)
C(14)-C(19)	1.541(8)
C(15)-C(16)	1.394(9)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(9)
C(16)-C(20)	1.520(8)
C(17)-C(18)	1.367(8)
C(17)-H(17)	0.9500
C(18)-C(21)	1.493(8)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.960(16)
C(22)-H(22B)	0.95(2)
C(22)-H(22C)	0.95(2)

O(2)-S(1)-O(1)	113.1(3)
O(2)-S(1)-O(3A)	130.4(12)
O(1)-S(1)-O(3A)	102.4(10)
O(2)-S(1)-O(3)	108.9(11)
O(1)-S(1)-O(3)	123.8(11)
O(3A)-S(1)-O(3)	23.1(15)
O(2)-S(1)-C(23)	102.4(3)
O(1)-S(1)-C(23)	103.2(3)
O(3A)-S(1)-C(23)	101.8(17)
O(3)-S(1)-C(23)	102.4(17)
F(2A)-C(23)-F(1)	118.4(7)
F(2A)-C(23)-F(3)	94.1(7)
F(1)-C(23)-F(3)	102.3(6)
F(2A)-C(23)-F(2)	33.8(5)
F(1)-C(23)-F(2)	96.9(7)
F(3)-C(23)-F(2)	125.9(8)
F(2A)-C(23)-S(1)	116.5(7)
F(1)-C(23)-S(1)	111.9(4)
F(3)-C(23)-S(1)	110.7(4)
F(2)-C(23)-S(1)	107.8(6)

C(1)-N(1)-C(4)	125.6(5)
C(1)-N(1)-C(2)	111.0(4)
C(4)-N(1)-C(2)	123.3(4)
N(1)-C(1)-N(2)	112.3(5)
N(1)-C(1)-C(22)	124.8(5)
N(2)-C(1)-C(22)	122.9(5)
C(1)-N(2)-C(13)	124.5(4)
C(1)-N(2)-C(3)	110.9(4)
C(13)-N(2)-C(3)	124.7(4)
N(1)-C(2)-C(3)	102.7(4)
N(1)-C(2)-H(2A)	111.2
C(3)-C(2)-H(2A)	111.2
N(1)-C(2)-H(2B)	111.2
C(3)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
N(2)-C(3)-C(2)	103.2(4)
N(2)-C(3)-H(3A)	111.1
C(2)-C(3)-H(3A)	111.1
N(2)-C(3)-H(3B)	111.1
C(2)-C(3)-H(3B)	111.1
H(3A)-C(3)-H(3B)	109.1
C(5)-C(4)-C(9)	122.0(5)
C(5)-C(4)-N(1)	119.0(5)
C(9)-C(4)-N(1)	119.0(5)
C(6)-C(5)-C(4)	119.0(6)
C(6)-C(5)-C(10)	120.2(6)
C(4)-C(5)-C(10)	120.6(5)
C(5)-C(6)-C(7)	120.6(6)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(8)-C(7)-C(6)	118.6(6)
C(8)-C(7)-C(11)	121.8(7)
C(6)-C(7)-C(11)	119.6(7)
C(7)-C(8)-C(9)	122.3(6)
C(7)-C(8)-H(8)	118.9
C(9)-C(8)-H(8)	118.9
C(8)-C(9)-C(4)	117.5(6)
C(8)-C(9)-C(12)	121.8(6)
C(4)-C(9)-C(12)	120.7(5)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5

H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.3(5)
C(18)-C(13)-N(2)	119.2(5)
C(14)-C(13)-N(2)	119.5(5)
C(15)-C(14)-C(13)	118.3(6)
C(15)-C(14)-C(19)	121.5(6)
C(13)-C(14)-C(19)	120.1(5)
C(14)-C(15)-C(16)	121.7(6)
C(14)-C(15)-H(15)	119.1
C(16)-C(15)-H(15)	119.1
C(17)-C(16)-C(15)	118.6(6)
C(17)-C(16)-C(20)	120.9(6)
C(15)-C(16)-C(20)	120.5(7)
C(18)-C(17)-C(16)	122.1(6)
C(18)-C(17)-H(17)	119.0
C(16)-C(17)-H(17)	119.0
C(17)-C(18)-C(13)	118.0(6)
C(17)-C(18)-C(21)	121.2(6)
C(13)-C(18)-C(21)	120.8(5)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5

H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(1)-C(22)-H(22A)	113(4)
C(1)-C(22)-H(22B)	110(4)
H(22A)-C(22)-H(22B)	107(2)
C(1)-C(22)-H(22C)	109(4)
H(22A)-C(22)-H(22C)	108(3)
H(22B)-C(22)-H(22C)	109(3)

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
S(1)	48(1)	24(1)	26(1)	1(1)	-4(1)	-6(1)
O(1)	58(3)	39(3)	48(3)	-12(2)	-13(3)	-16(2)
O(2)	183(7)	17(3)	43(3)	-5(2)	-13(4)	31(3)
O(3)	39(9)	106(19)	41(11)	-19(16)	-2(6)	-53(8)
O(3A)	29(9)	99(18)	53(14)	26(16)	-2(7)	-40(7)
C(23)	41(5)	40(5)	35(4)	-1(4)	7(3)	7(4)
F(1)	97(4)	41(3)	37(2)	5(2)	-7(2)	18(2)
F(2)	92(6)	27(5)	31(5)	-3(4)	-6(5)	-18(5)
F(2A)	89(6)	23(4)	28(4)	-10(3)	11(5)	2(5)
F(3)	73(4)	146(5)	53(3)	18(3)	23(3)	27(3)
N(1)	35(3)	18(3)	17(3)	-2(2)	1(2)	8(2)
C(1)	22(3)	16(3)	19(3)	0(3)	-2(2)	-5(3)
N(2)	26(3)	16(3)	19(3)	-2(2)	-4(2)	4(2)
C(2)	22(4)	23(3)	34(4)	-6(3)	2(3)	4(3)
C(3)	26(4)	20(3)	29(3)	2(3)	1(3)	-4(3)
C(4)	19(3)	27(4)	22(3)	7(3)	4(3)	5(3)
C(5)	34(4)	37(4)	17(3)	-2(3)	2(3)	4(3)
C(6)	28(4)	41(4)	37(4)	-10(3)	-1(3)	7(3)
C(7)	45(5)	51(5)	18(3)	-1(3)	5(3)	24(4)
C(8)	42(4)	24(4)	32(4)	13(3)	1(3)	5(3)
C(9)	40(4)	24(4)	27(4)	1(3)	6(3)	8(3)
C(10)	37(4)	35(4)	48(4)	2(3)	-5(3)	-7(3)
C(11)	64(6)	69(5)	29(4)	14(4)	0(4)	26(4)
C(12)	50(5)	31(4)	39(4)	8(3)	7(3)	-8(3)
C(13)	31(3)	17(3)	14(3)	5(3)	-3(2)	5(3)
C(14)	33(4)	29(4)	32(4)	3(3)	1(3)	1(3)
C(15)	53(5)	27(4)	30(4)	-1(3)	10(3)	-1(3)
C(16)	53(5)	27(4)	23(3)	1(3)	-2(3)	17(3)
C(17)	53(5)	21(4)	31(4)	-9(3)	-17(3)	2(3)
C(18)	31(4)	22(4)	30(4)	-8(3)	-8(3)	-2(3)
C(19)	33(4)	41(4)	42(4)	-7(3)	7(3)	-12(3)
C(20)	99(7)	50(5)	18(4)	-9(3)	-1(4)	23(5)
C(21)	37(4)	16(3)	58(5)	-14(3)	7(4)	-1(3)
C(22)	40(4)	38(4)	26(4)	-2(3)	-4(3)	13(4)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **3**.

	x	y	z	U(eq)
H(2A)	1746	9263	1964	32
H(2B)	724	8162	2005	32
H(3A)	830	8263	2968	30
H(3B)	1860	9355	2926	30
H(6)	-2337	9224	392	42
H(8)	-33	12211	406	39
H(10A)	-1271	7836	1619	60
H(10B)	-2439	7859	1174	60
H(10C)	-2487	8659	1753	60
H(11A)	-2294	11820	-282	81
H(11B)	-2155	10402	-468	81
H(11C)	-993	11332	-539	81
H(12A)	565	12532	1751	60
H(12B)	1403	12579	1184	60
H(12C)	1624	11504	1648	60
H(15)	-2186	9818	4542	44
H(17)	574	12380	4475	42
H(19A)	-2393	8233	3806	58
H(19B)	-1441	8245	3278	58
H(19C)	-2667	9109	3263	58
H(20A)	-567	12214	5334	83
H(20B)	-1202	10902	5464	83
H(20C)	-2030	11994	5186	83
H(21A)	1882	12582	3689	55
H(21B)	1093	12412	3101	55
H(21C)	2068	11365	3307	55
H(22A)	-1970(40)	11430(50)	2106(12)	52
H(22B)	-1160(50)	12150(30)	2544(19)	52
H(22C)	-2100(40)	11180(50)	2758(15)	52

Table S12. Torsion angles [°] for compound **3**.

O(2)-S(1)-C(23)-F(2A)	-41.9(8)
O(1)-S(1)-C(23)-F(2A)	-159.6(7)
O(3A)-S(1)-C(23)-F(2A)	94.5(12)
O(3)-S(1)-C(23)-F(2A)	70.9(12)
O(2)-S(1)-C(23)-F(1)	177.4(5)
O(1)-S(1)-C(23)-F(1)	59.7(5)
O(3A)-S(1)-C(23)-F(1)	-46.2(10)
O(3)-S(1)-C(23)-F(1)	-69.8(11)
O(2)-S(1)-C(23)-F(3)	64.0(6)
O(1)-S(1)-C(23)-F(3)	-53.7(6)
O(3A)-S(1)-C(23)-F(3)	-159.6(10)
O(3)-S(1)-C(23)-F(3)	176.9(11)
O(2)-S(1)-C(23)-F(2)	-77.2(7)
O(1)-S(1)-C(23)-F(2)	165.1(7)
O(3A)-S(1)-C(23)-F(2)	59.2(11)
O(3)-S(1)-C(23)-F(2)	35.6(12)
C(4)-N(1)-C(1)-N(2)	-177.4(5)
C(2)-N(1)-C(1)-N(2)	-1.2(7)
C(4)-N(1)-C(1)-C(22)	1.4(9)
C(2)-N(1)-C(1)-C(22)	177.6(5)
N(1)-C(1)-N(2)-C(13)	-179.5(5)
C(22)-C(1)-N(2)-C(13)	1.6(9)
N(1)-C(1)-N(2)-C(3)	0.9(7)
C(22)-C(1)-N(2)-C(3)	-178.0(5)
C(1)-N(1)-C(2)-C(3)	1.0(6)
C(4)-N(1)-C(2)-C(3)	177.3(5)
C(1)-N(2)-C(3)-C(2)	-0.2(6)
C(13)-N(2)-C(3)-C(2)	-179.8(5)
N(1)-C(2)-C(3)-N(2)	-0.5(6)
C(1)-N(1)-C(4)-C(5)	-98.6(7)
C(2)-N(1)-C(4)-C(5)	85.7(7)
C(1)-N(1)-C(4)-C(9)	80.2(7)
C(2)-N(1)-C(4)-C(9)	-95.5(7)
C(9)-C(4)-C(5)-C(6)	-0.1(9)
N(1)-C(4)-C(5)-C(6)	178.7(5)
C(9)-C(4)-C(5)-C(10)	-176.4(6)
N(1)-C(4)-C(5)-C(10)	2.4(8)
C(4)-C(5)-C(6)-C(7)	-0.2(9)
C(10)-C(5)-C(6)-C(7)	176.1(6)
C(5)-C(6)-C(7)-C(8)	0.7(9)
C(5)-C(6)-C(7)-C(11)	-178.7(6)
C(6)-C(7)-C(8)-C(9)	-0.9(9)

C(11)-C(7)-C(8)-C(9)	178.5(6)
C(7)-C(8)-C(9)-C(4)	0.6(9)
C(7)-C(8)-C(9)-C(12)	-179.7(6)
C(5)-C(4)-C(9)-C(8)	-0.1(9)
N(1)-C(4)-C(9)-C(8)	-178.9(5)
C(5)-C(4)-C(9)-C(12)	-179.8(6)
N(1)-C(4)-C(9)-C(12)	1.5(8)
C(1)-N(2)-C(13)-C(18)	-93.0(7)
C(3)-N(2)-C(13)-C(18)	86.5(7)
C(1)-N(2)-C(13)-C(14)	86.0(7)
C(3)-N(2)-C(13)-C(14)	-94.4(7)
C(18)-C(13)-C(14)-C(15)	0.3(9)
N(2)-C(13)-C(14)-C(15)	-178.8(5)
C(18)-C(13)-C(14)-C(19)	178.5(5)
N(2)-C(13)-C(14)-C(19)	-0.5(8)
C(13)-C(14)-C(15)-C(16)	-0.4(9)
C(19)-C(14)-C(15)-C(16)	-178.6(6)
C(14)-C(15)-C(16)-C(17)	0.3(10)
C(14)-C(15)-C(16)-C(20)	179.3(6)
C(15)-C(16)-C(17)-C(18)	-0.1(9)
C(20)-C(16)-C(17)-C(18)	-179.1(6)
C(16)-C(17)-C(18)-C(13)	0.0(9)
C(16)-C(17)-C(18)-C(21)	178.7(6)
C(14)-C(13)-C(18)-C(17)	-0.1(9)
N(2)-C(13)-C(18)-C(17)	179.0(5)
C(14)-C(13)-C(18)-C(21)	-178.8(5)
N(2)-C(13)-C(18)-C(21)	0.2(8)

Table S13. Crystal data and structure refinement for compound **4**.

Empirical formula	$C_{50}H_{67}F_6N_3O_7S_2W$
Formula weight	1184.04
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, $P\bar{1}$
Unit cell dimensions	a = 12.0693(8) Å, α = 79.289(3)°
	b = 12.9179(9) Å, β = 83.831(4)°
	c = 18.8210(13) Å, γ = 65.484(3)°
Volume	2621.8(3) $Å^3$
Z, Calculated density	2, 1.500 Mg/m^3
Absorption coefficient	2.355 mm^{-1}
F(000)	1208
Crystal size	0.34 x 0.31 x 0.29mm
θ range for data collection	1.75 to 30.59°
Limiting indices	-17<=h<=17, -18<=k<=18, -26<=l<=26
Reflections collected / unique	76602 / 15994 [R(int) = 0.330]
Completeness to θ = 30.59	99.1 %
Absorption correction	Numerical
Max. and min. transmission	0.9952 and 0.8642
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15994/0/707
Goodness-of-fit on F^2	1.043
Final R indices [I>2σ (I)]	R1 = 0.0255, wR2 = 0.0521
R indices (all data)	R1 = 0.0384, wR2 = 0.0566
Largest diff. peak and hole	2.946 and -1.208 e. $Å^{-3}$

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W(1)	9808(1)	7068(1)	2190(1)	13(1)
O(1)	8623(1)	6289(1)	2105(1)	20(1)
S(1)	8387(1)	5840(1)	1479(1)	18(1)
O(2)	9429(1)	4919(2)	1244(1)	28(1)
O(3)	7641(2)	6732(2)	951(1)	29(1)
O(4)	9344(1)	6495(1)	3312(1)	18(1)
C(44)	7402(2)	5158(2)	1952(1)	24(1)
F(1)	7034(1)	4725(1)	1475(1)	31(1)
F(2)	6423(1)	5894(1)	2254(1)	35(1)
F(3)	7997(2)	4291(1)	2459(1)	39(1)
S(2)	8552(1)	7014(1)	3919(1)	15(1)
O(5)	8905(9)	6290(7)	4593(5)	29(1)
O(6)	8315(5)	8188(5)	3885(3)	36(1)
C(45)	7109(4)	6968(5)	3757(2)	23(1)
F(4)	6641(5)	7638(4)	3143(3)	35(1)
F(5)	7217(3)	5931(4)	3717(2)	38(1)
F(6)	6316(8)	7308(7)	4315(5)	48(2)
S(2A)	8432(1)	6278(1)	3836(1)	21(1)
O(5A)	8851(9)	5942(7)	4559(5)	28(1)
O(6A)	7830(4)	5642(4)	3613(2)	33(1)
C(45A)	7247(5)	7709(5)	3827(3)	40(1)
F(4A)	6367(9)	7708(7)	4296(6)	61(2)
F(5A)	6725(6)	8108(5)	3190(4)	62(2)
F(6A)	7705(5)	8424(5)	3959(4)	68(2)
N(1)	12237(2)	6213(2)	3980(1)	21(1)
N(2)	12390(2)	4906(2)	3337(1)	20(1)
N(3)	9098(2)	8545(2)	1968(1)	16(1)
C(1)	12000(2)	6023(2)	3348(1)	19(1)
C(2)	12922(2)	5116(2)	4447(1)	30(1)
C(3)	12927(2)	4209(2)	4032(1)	24(1)
C(4)	12223(2)	7264(2)	4142(1)	22(1)
C(5)	13090(2)	7672(2)	3805(1)	21(1)
C(6)	13131(2)	8621(2)	4026(1)	32(1)
C(7)	12359(3)	9156(2)	4577(2)	45(1)
C(8)	11510(3)	8725(3)	4894(1)	48(1)
C(9)	11431(2)	7781(3)	4695(1)	37(1)
C(10)	13988(2)	7105(2)	3230(1)	24(1)
C(11)	12482(4)	10145(3)	4829(2)	76(1)
C(12)	10548(3)	7297(4)	5083(2)	63(1)
C(13)	12411(2)	4372(2)	2729(1)	21(1)

C(14)	13314(2)	4312(2)	2179(1)	19(1)
C(15)	13342(2)	3770(2)	1597(1)	24(1)
C(16)	12519(3)	3286(2)	1556(1)	31(1)
C(17)	11679(2)	3324(2)	2121(2)	35(1)
C(18)	11614(2)	3839(2)	2721(1)	28(1)
C(19)	14242(2)	4798(2)	2205(1)	21(1)
C(20)	12536(3)	2745(3)	909(2)	49(1)
C(21)	10744(2)	3758(2)	3353(2)	38(1)
C(22)	8463(2)	9737(2)	1753(1)	16(1)
C(23)	8948(2)	10490(2)	1911(1)	17(1)
C(24)	8292(2)	11668(2)	1710(1)	20(1)
C(25)	7205(2)	12091(2)	1355(1)	23(1)
C(26)	6762(2)	11339(2)	1190(1)	25(1)
C(27)	7367(2)	10154(2)	1381(1)	22(1)
C(28)	10125(2)	10038(2)	2309(1)	22(1)
C(29)	9859(3)	10014(3)	3119(1)	52(1)
C(30)	10923(3)	10691(3)	2019(2)	53(1)
C(31)	6840(2)	9363(2)	1200(1)	31(1)
C(32)	6581(3)	9583(2)	397(2)	38(1)
C(33)	5675(3)	9480(3)	1653(2)	50(1)
C(34)	10724(2)	6652(2)	1331(1)	17(1)
C(35)	11091(2)	7074(2)	565(1)	18(1)
C(36)	11179(2)	6220(2)	71(1)	30(1)
C(37)	10139(2)	8265(2)	267(1)	28(1)
C(38)	12316(2)	7141(2)	633(1)	16(1)
C(39)	12359(2)	7988(2)	981(1)	21(1)
C(40)	13444(2)	8077(2)	1057(1)	28(1)
C(41)	14526(2)	7315(2)	786(1)	30(1)
C(42)	14507(2)	6474(2)	443(1)	29(1)
C(43)	13413(2)	6383(2)	368(1)	23(1)
C(46)	11402(2)	6959(2)	2755(1)	18(1)
O(1X)	5636(2)	2291(2)	3627(1)	36(1)
C(1X)	5779(3)	1382(3)	3252(2)	57(1)
C(2X)	4687(3)	1110(3)	3410(2)	67(1)
C(4X)	6405(2)	3554(3)	3948(2)	40(1)
C(3X)	6648(2)	2592(3)	3532(1)	41(1)

Table S15. Bond lengths [Å] and angles [°] for compound **4**.

W(1)-N(3)	1.7235(18)
W(1)-C(34)	1.890(2)
W(1)-O(1)	2.0950(14)
W(1)-O(4)	2.1977(14)
W(1)-C(46)	2.237(2)
O(1)-S(1)	1.5065(15)
S(1)-O(2)	1.4235(17)
S(1)-O(3)	1.4264(17)
S(1)-C(44)	1.825(2)
O(4)-S(2A)	1.4767(17)
O(4)-S(2)	1.4780(16)
C(44)-F(2)	1.321(3)
C(44)-F(3)	1.328(3)
C(44)-F(1)	1.340(3)
S(2)-O(6)	1.412(6)
S(2)-O(5)	1.418(10)
S(2)-C(45)	1.827(5)
C(45)-F(5)	1.307(7)
C(45)-F(4)	1.330(7)
C(45)-F(6)	1.349(10)
S(2A)-O(5A)	1.429(10)
S(2A)-O(6A)	1.438(5)
S(2A)-C(45A)	1.807(6)
C(45A)-F(4A)	1.306(10)
C(45A)-F(6A)	1.326(8)
C(45A)-F(5A)	1.328(9)
N(1)-C(1)	1.341(3)
N(1)-C(4)	1.439(3)
N(1)-C(2)	1.479(3)
N(2)-C(1)	1.322(3)
N(2)-C(13)	1.435(3)
N(2)-C(3)	1.485(3)
N(3)-C(22)	1.406(3)
C(1)-C(46)	1.475(3)
C(2)-C(3)	1.522(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(9)	1.398(3)
C(4)-C(5)	1.402(3)
C(5)-C(6)	1.388(3)

C(5)-C(10)	1.505(3)
C(6)-C(7)	1.394(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.392(5)
C(7)-C(11)	1.509(5)
C(8)-C(9)	1.382(5)
C(8)-H(8)	0.9500
C(9)-C(12)	1.509(4)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.398(3)
C(13)-C(14)	1.408(3)
C(14)-C(15)	1.394(3)
C(14)-C(19)	1.503(3)
C(15)-C(16)	1.391(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.382(4)
C(16)-C(20)	1.506(4)
C(17)-C(18)	1.391(4)
C(17)-H(17)	0.9500
C(18)-C(21)	1.518(4)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.412(3)
C(22)-C(27)	1.414(3)
C(23)-C(24)	1.392(3)
C(23)-C(28)	1.516(3)
C(24)-C(25)	1.387(3)
C(24)-H(24)	0.9500

C(25)-C(26)	1.381(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.390(3)
C(26)-H(26)	0.9500
C(27)-C(31)	1.510(3)
C(28)-C(29)	1.522(3)
C(28)-C(30)	1.524(4)
C(28)-H(28)	10.000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.527(4)
C(31)-C(33)	1.530(4)
C(31)-H(31)	10.000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.530(3)
C(34)-H(34)	0.9500
C(35)-C(37)	1.534(3)
C(35)-C(36)	1.535(3)
C(35)-C(38)	1.537(3)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(43)	1.387(3)
C(38)-C(39)	1.398(3)
C(39)-C(40)	1.384(3)
C(39)-H(39)	0.9500
C(40)-C(41)	1.383(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.371(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.397(3)

C(42)-H(42)	0.9500
C(43)-H(43)	0.9500
C(46)-H(46A)	0.92(3)
C(46)-H(46B)	0.96(3)
O(1X)-C(3X)	1.412(3)
O(1X)-C(1X)	1.421(4)
C(1X)-C(2X)	1.487(5)
C(1X)-H(1X1)	0.9900
C(1X)-H(1X2)	0.9900
C(2X)-H(2X1)	0.9800
C(2X)-H(2X2)	0.9800
C(2X)-H(2X3)	0.9800
C(4X)-C(3X)	1.502(4)
C(4X)-H(4X1)	0.9800
C(4X)-H(4X2)	0.9800
C(4X)-H(4X3)	0.9800
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900

N(3)-W(1)-C(34)	101.68(8)
N(3)-W(1)-O(1)	111.10(7)
C(34)-W(1)-O(1)	95.43(7)
N(3)-W(1)-O(4)	111.07(7)
C(34)-W(1)-O(4)	147.20(8)
O(1)-W(1)-O(4)	74.97(5)
N(3)-W(1)-C(46)	98.77(8)
C(34)-W(1)-C(46)	93.84(8)
O(1)-W(1)-C(46)	146.07(7)
O(4)-W(1)-C(46)	79.64(6)
S(1)-O(1)-W(1)	130.98(9)
O(2)-S(1)-O(3)	118.94(11)
O(2)-S(1)-O(1)	113.42(9)
O(3)-S(1)-O(1)	112.99(10)
O(2)-S(1)-C(44)	104.79(11)
O(3)-S(1)-C(44)	105.07(11)
O(1)-S(1)-C(44)	98.67(9)
S(2A)-O(4)-S(2)	42.06(7)
S(2A)-O(4)-W(1)	148.04(10)
S(2)-O(4)-W(1)	137.84(10)
F(2)-C(44)-F(3)	108.78(19)
F(2)-C(44)-F(1)	108.12(18)
F(3)-C(44)-F(1)	107.59(19)
F(2)-C(44)-S(1)	112.26(16)

F(3)-C(44)-S(1)	111.22(16)
F(1)-C(44)-S(1)	108.72(15)
O(6)-S(2)-O(5)	117.2(4)
O(6)-S(2)-O(4)	113.2(2)
O(5)-S(2)-O(4)	112.0(4)
O(6)-S(2)-C(45)	106.3(3)
O(5)-S(2)-C(45)	103.9(4)
O(4)-S(2)-C(45)	102.46(16)
F(5)-C(45)-F(4)	107.5(4)
F(5)-C(45)-F(6)	105.8(5)
F(4)-C(45)-F(6)	109.9(5)
F(5)-C(45)-S(2)	112.8(3)
F(4)-C(45)-S(2)	111.0(4)
F(6)-C(45)-S(2)	109.6(4)
O(5A)-S(2A)-O(6A)	116.7(3)
O(5A)-S(2A)-O(4)	111.9(3)
O(6A)-S(2A)-O(4)	115.73(19)
O(5A)-S(2A)-C(45A)	104.4(4)
O(6A)-S(2A)-C(45A)	103.8(3)
O(4)-S(2A)-C(45A)	101.9(2)
F(4A)-C(45A)-F(6A)	110.4(6)
F(4A)-C(45A)-F(5A)	105.2(7)
F(6A)-C(45A)-F(5A)	108.7(6)
F(4A)-C(45A)-S(2A)	111.3(6)
F(6A)-C(45A)-S(2A)	110.4(4)
F(5A)-C(45A)-S(2A)	110.8(5)
C(1)-N(1)-C(4)	127.46(18)
C(1)-N(1)-C(2)	110.95(19)
C(4)-N(1)-C(2)	118.87(18)
C(1)-N(2)-C(13)	126.71(17)
C(1)-N(2)-C(3)	111.81(18)
C(13)-N(2)-C(3)	121.30(19)
C(22)-N(3)-W(1)	175.78(15)
N(2)-C(1)-N(1)	110.80(18)
N(2)-C(1)-C(46)	126.22(19)
N(1)-C(1)-C(46)	123.0(2)
N(1)-C(2)-C(3)	103.33(17)
N(1)-C(2)-H(2A)	111.1
C(3)-C(2)-H(2A)	111.1
N(1)-C(2)-H(2B)	111.1
C(3)-C(2)-H(2B)	111.1
H(2A)-C(2)-H(2B)	109.1
N(2)-C(3)-C(2)	102.49(18)

N(2)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
N(2)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2
C(9)-C(4)-C(5)	121.5(2)
C(9)-C(4)-N(1)	118.6(2)
C(5)-C(4)-N(1)	119.50(18)
C(6)-C(5)-C(4)	118.1(2)
C(6)-C(5)-C(10)	119.2(2)
C(4)-C(5)-C(10)	122.7(2)
C(5)-C(6)-C(7)	122.0(3)
C(5)-C(6)-H(6)	119.0
C(7)-C(6)-H(6)	119.0
C(8)-C(7)-C(6)	117.9(3)
C(8)-C(7)-C(11)	121.8(3)
C(6)-C(7)-C(11)	120.3(4)
C(9)-C(8)-C(7)	122.4(2)
C(9)-C(8)-H(8)	118.8
C(7)-C(8)-H(8)	118.8
C(8)-C(9)-C(4)	118.1(3)
C(8)-C(9)-C(12)	120.8(3)
C(4)-C(9)-C(12)	121.1(3)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	121.3(2)
C(18)-C(13)-N(2)	120.0(2)

C(14)-C(13)-N(2)	118.51(19)
C(15)-C(14)-C(13)	118.1(2)
C(15)-C(14)-C(19)	119.67(19)
C(13)-C(14)-C(19)	122.25(19)
C(16)-C(15)-C(14)	121.9(2)
C(16)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1
C(17)-C(16)-C(15)	118.1(2)
C(17)-C(16)-C(20)	121.0(3)
C(15)-C(16)-C(20)	120.9(3)
C(16)-C(17)-C(18)	122.8(2)
C(16)-C(17)-H(17)	118.6
C(18)-C(17)-H(17)	118.6
C(17)-C(18)-C(13)	117.7(2)
C(17)-C(18)-C(21)	120.0(2)
C(13)-C(18)-C(21)	122.2(2)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	118.80(18)
N(3)-C(22)-C(27)	119.69(19)
C(23)-C(22)-C(27)	121.51(19)
C(24)-C(23)-C(22)	118.00(19)
C(24)-C(23)-C(28)	120.62(19)
C(22)-C(23)-C(28)	121.35(19)
C(25)-C(24)-C(23)	121.1(2)
C(25)-C(24)-H(24)	119.4
C(23)-C(24)-H(24)	119.4

C(26)-C(25)-C(24)	120.0(2)
C(26)-C(25)-H(25)	120.0
C(24)-C(25)-H(25)	120.0
C(25)-C(26)-C(27)	121.7(2)
C(25)-C(26)-H(26)	119.2
C(27)-C(26)-H(26)	119.2
C(26)-C(27)-C(22)	117.6(2)
C(26)-C(27)-C(31)	120.0(2)
C(22)-C(27)-C(31)	122.37(19)
C(23)-C(28)-C(29)	110.30(19)
C(23)-C(28)-C(30)	113.0(2)
C(29)-C(28)-C(30)	112.1(3)
C(23)-C(28)-H(28)	107.0
C(29)-C(28)-H(28)	107.0
C(30)-C(28)-H(28)	107.0
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-C(32)	112.0(2)
C(27)-C(31)-C(33)	110.9(2)
C(32)-C(31)-C(33)	109.8(2)
C(27)-C(31)-H(31)	108.0
C(32)-C(31)-H(31)	108.0
C(33)-C(31)-H(31)	108.0
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5

H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(35)-C(34)-W(1)	146.50(16)
C(35)-C(34)-H(34)	106.7
W(1)-C(34)-H(34)	106.7
C(34)-C(35)-C(37)	111.10(17)
C(34)-C(35)-C(36)	108.67(18)
C(37)-C(35)-C(36)	108.42(19)
C(34)-C(35)-C(38)	105.67(16)
C(37)-C(35)-C(38)	110.09(18)
C(36)-C(35)-C(38)	112.89(18)
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(35)-C(37)-H(37A)	109.5
C(35)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(35)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(43)-C(38)-C(39)	116.9(2)
C(43)-C(38)-C(35)	123.13(19)
C(39)-C(38)-C(35)	119.94(18)
C(40)-C(39)-C(38)	121.8(2)
C(40)-C(39)-H(39)	119.1
C(38)-C(39)-H(39)	119.1
C(41)-C(40)-C(39)	120.2(2)
C(41)-C(40)-H(40)	119.9
C(39)-C(40)-H(40)	119.9
C(42)-C(41)-C(40)	119.1(2)
C(42)-C(41)-H(41)	120.4
C(40)-C(41)-H(41)	120.4
C(41)-C(42)-C(43)	120.7(2)
C(41)-C(42)-H(42)	119.7
C(43)-C(42)-H(42)	119.7
C(38)-C(43)-C(42)	121.3(2)
C(38)-C(43)-H(43)	119.4
C(42)-C(43)-H(43)	119.4
C(1)-C(46)-W(1)	122.72(15)
C(1)-C(46)-H(46A)	106.9(17)

W(1)-C(46)-H(46A)	105.7(16)
C(1)-C(46)-H(46B)	104.1(16)
W(1)-C(46)-H(46B)	107.0(16)
H(46A)-C(46)-H(46B)	110(2)
C(3X)-O(1X)-C(1X)	113.3(2)
O(1X)-C(1X)-C(2X)	108.8(2)
O(1X)-C(1X)-H(1X1)	109.9
C(2X)-C(1X)-H(1X1)	109.9
O(1X)-C(1X)-H(1X2)	109.9
C(2X)-C(1X)-H(1X2)	109.9
H(1X1)-C(1X)-H(1X2)	108.3
C(1X)-C(2X)-H(2X1)	109.5
C(1X)-C(2X)-H(2X2)	109.5
H(2X1)-C(2X)-H(2X2)	109.5
C(1X)-C(2X)-H(2X3)	109.5
H(2X1)-C(2X)-H(2X3)	109.5
H(2X2)-C(2X)-H(2X3)	109.5
C(3X)-C(4X)-H(4X1)	109.5
C(3X)-C(4X)-H(4X2)	109.5
H(4X1)-C(4X)-H(4X2)	109.5
C(3X)-C(4X)-H(4X3)	109.5
H(4X1)-C(4X)-H(4X3)	109.5
H(4X2)-C(4X)-H(4X3)	109.5
O(1X)-C(3X)-C(4X)	109.0(2)
O(1X)-C(3X)-H(3X1)	109.9
C(4X)-C(3X)-H(3X1)	109.9
O(1X)-C(3X)-H(3X2)	109.9
C(4X)-C(3X)-H(3X2)	109.9
H(3X1)-C(3X)-H(3X2)	108.3

Table S16. Anisotropic displacement parameters (A^2 x 10^3) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
W(1)	12(1)	16(1)	12(1)	0(1)	-1(1)	-7(1)
O(1)	21(1)	26(1)	18(1)	-5(1)	2(1)	-16(1)
S(1)	18(1)	23(1)	18(1)	-3(1)	0(1)	-13(1)
O(2)	20(1)	35(1)	34(1)	-13(1)	0(1)	-12(1)
O(3)	35(1)	28(1)	27(1)	3(1)	-10(1)	-17(1)
O(4)	17(1)	23(1)	15(1)	0(1)	3(1)	-10(1)
C(44)	23(1)	27(1)	27(1)	-8(1)	5(1)	-17(1)
F(1)	30(1)	37(1)	39(1)	-16(1)	5(1)	-25(1)
F(2)	26(1)	48(1)	41(1)	-23(1)	14(1)	-24(1)
F(3)	52(1)	35(1)	35(1)	8(1)	-4(1)	-28(1)
S(2)	16(1)	24(1)	9(1)	-4(1)	2(1)	-11(1)
O(5)	33(2)	47(5)	13(2)	4(3)	-3(2)	-27(3)
O(6)	49(3)	36(3)	30(2)	-14(2)	4(2)	-22(3)
C(45)	16(2)	35(3)	17(2)	-1(2)	1(2)	-10(2)
F(4)	22(2)	42(3)	34(2)	1(2)	-10(1)	-6(2)
F(5)	37(2)	53(3)	36(2)	3(2)	-2(2)	-34(2)
F(6)	21(2)	79(6)	36(2)	-1(3)	9(2)	-17(3)
S(2A)	19(1)	26(1)	18(1)	-2(1)	3(1)	-11(1)
O(5A)	26(2)	46(5)	17(2)	7(3)	-1(2)	-23(3)
O(6A)	48(3)	36(2)	30(2)	-12(2)	10(2)	-32(2)
C(45A)	30(3)	34(3)	48(3)	-12(3)	3(2)	-5(2)
F(4A)	33(3)	59(5)	72(4)	-18(3)	35(2)	-6(3)
F(5A)	43(3)	49(4)	61(3)	12(3)	-20(2)	10(3)
F(6A)	79(4)	39(3)	100(4)	-38(3)	11(3)	-28(3)
N(1)	19(1)	29(1)	14(1)	3(1)	-3(1)	-9(1)
N(2)	20(1)	25(1)	14(1)	5(1)	-2(1)	-10(1)
N(3)	16(1)	20(1)	15(1)	-1(1)	-3(1)	-9(1)
C(1)	11(1)	29(1)	14(1)	2(1)	1(1)	-9(1)
C(2)	33(1)	35(1)	19(1)	9(1)	-9(1)	-15(1)
C(3)	21(1)	32(1)	14(1)	7(1)	-3(1)	-10(1)
C(4)	15(1)	31(1)	12(1)	-4(1)	-2(1)	-2(1)
C(5)	20(1)	21(1)	18(1)	-6(1)	-4(1)	-3(1)
C(6)	36(1)	24(1)	31(1)	-10(1)	-13(1)	-3(1)
C(7)	51(2)	31(2)	34(1)	-20(1)	-24(1)	15(1)
C(8)	36(2)	55(2)	21(1)	-21(1)	-10(1)	22(1)
C(9)	19(1)	57(2)	12(1)	-6(1)	-1(1)	7(1)
C(10)	24(1)	29(1)	25(1)	-11(1)	5(1)	-14(1)
C(11)	84(3)	46(2)	78(3)	-43(2)	-44(2)	17(2)
C(12)	23(1)	109(3)	28(1)	1(2)	11(1)	-6(2)
C(13)	22(1)	22(1)	20(1)	5(1)	-6(1)	-11(1)

C(14)	22(1)	18(1)	18(1)	4(1)	-5(1)	-10(1)
C(15)	35(1)	20(1)	19(1)	1(1)	-6(1)	-14(1)
C(16)	48(2)	21(1)	32(1)	5(1)	-19(1)	-19(1)
C(17)	40(1)	27(1)	46(2)	12(1)	-21(1)	-24(1)
C(18)	25(1)	26(1)	34(1)	13(1)	-10(1)	-16(1)
C(19)	22(1)	27(1)	18(1)	-3(1)	2(1)	-14(1)
C(20)	81(2)	37(2)	43(2)	-3(1)	-24(2)	-34(2)
C(21)	27(1)	33(1)	52(2)	17(1)	-4(1)	-19(1)
C(22)	18(1)	16(1)	14(1)	-1(1)	0(1)	-6(1)
C(23)	18(1)	19(1)	13(1)	-3(1)	2(1)	-8(1)
C(24)	26(1)	20(1)	17(1)	-4(1)	2(1)	-11(1)
C(25)	29(1)	15(1)	20(1)	0(1)	-3(1)	-5(1)
C(26)	26(1)	19(1)	26(1)	3(1)	-11(1)	-5(1)
C(27)	24(1)	18(1)	22(1)	1(1)	-8(1)	-9(1)
C(28)	17(1)	21(1)	29(1)	-8(1)	-4(1)	-7(1)
C(29)	34(1)	70(2)	28(1)	-24(1)	-14(1)	13(1)
C(30)	33(2)	28(2)	103(3)	-1(2)	-18(2)	-18(1)
C(31)	32(1)	19(1)	43(1)	7(1)	-25(1)	-10(1)
C(32)	39(1)	30(1)	46(2)	-3(1)	-26(1)	-12(1)
C(33)	55(2)	51(2)	57(2)	11(2)	-14(2)	-38(2)
C(34)	16(1)	20(1)	17(1)	0(1)	-3(1)	-10(1)
C(35)	19(1)	24(1)	13(1)	-2(1)	1(1)	-12(1)
C(36)	43(1)	46(2)	18(1)	-11(1)	4(1)	-31(1)
C(37)	22(1)	39(1)	19(1)	6(1)	-2(1)	-10(1)
C(38)	19(1)	18(1)	12(1)	0(1)	1(1)	-9(1)
C(39)	23(1)	22(1)	20(1)	-5(1)	4(1)	-12(1)
C(40)	35(1)	34(1)	25(1)	-2(1)	-1(1)	-24(1)
C(41)	23(1)	38(1)	31(1)	9(1)	-6(1)	-19(1)
C(42)	16(1)	28(1)	33(1)	5(1)	3(1)	-3(1)
C(43)	23(1)	19(1)	22(1)	-2(1)	2(1)	-5(1)
C(46)	15(1)	25(1)	14(1)	2(1)	-2(1)	-9(1)
O(1X)	26(1)	41(1)	33(1)	-8(1)	7(1)	-7(1)
C(1X)	45(2)	73(3)	54(2)	-38(2)	11(2)	-14(2)
C(2X)	59(2)	53(2)	93(3)	-35(2)	9(2)	-22(2)
C(4X)	29(1)	52(2)	32(1)	5(1)	-10(1)	-13(1)
C(3X)	25(1)	66(2)	24(1)	-3(1)	1(1)	-12(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **4**.

	x	y	z	U(eq)
H(2A)	12509	5069	4928	36
H(2B)	13762	5027	4511	36
H(3A)	13765	3635	3956	29
H(3B)	12422	3806	4288	29
H(6)	13703	8916	3796	38
H(8)	10964	9093	5262	58
H(10A)	13583	7337	2767	36
H(10B)	14296	6266	3364	36
H(10C)	14668	7343	3184	36
H(11A)	11865	10422	5212	114
H(11B)	12365	10771	4422	114
H(11C)	13295	9883	5018	114
H(12A)	10997	6569	5394	94
H(12B)	10108	7160	4727	94
H(12C)	9966	7848	5380	94
H(15)	13940	3731	1219	29
H(17)	11122	2985	2100	42
H(19A)	14947	4433	1890	31
H(19B)	14504	4646	2703	31
H(19C)	13881	5631	2039	31
H(20A)	12596	1958	1071	73
H(20B)	13238	2726	589	73
H(20C)	11784	3199	646	73
H(21A)	9960	3886	3169	57
H(21B)	10622	4343	3652	57
H(21C)	11088	2991	3644	57
H(24)	8593	12192	1819	24
H(25)	6766	12899	1226	27
H(26)	6024	11640	938	30
H(28)	10597	9223	2229	26
H(29A)	9439	10804	3223	78
H(29B)	10626	9629	3374	78
H(29C)	9341	9592	3282	78
H(30A)	11039	10717	1493	79
H(30B)	11716	10297	2245	79
H(30C)	10526	11477	2131	79
H(31)	7452	8552	1321	37
H(32A)	5919	10344	277	56
H(32B)	6341	8991	291	56
H(32C)	7316	9554	108	56

H(33A)	5842	9355	2168	75
H(33B)	5396	8906	1563	75
H(33C)	5042	10254	1521	75
H(34)	11128	5836	1407	20
H(36A)	11769	5450	261	45
H(36B)	11445	6464	-418	45
H(36C)	10378	6202	53	45
H(37A)	9359	8215	232	42
H(37B)	10412	8529	-215	42
H(37C)	10039	8811	591	42
H(39)	11625	8518	1172	25
H(40)	13445	8663	1296	33
H(41)	15272	7373	836	36
H(42)	15246	5948	253	35
H(43)	13421	5791	132	27
H(46A)	11990(20)	6940(20)	2398(14)	27(7)
H(46B)	11140(20)	7650(20)	2968(14)	26(7)
H(1X1)	6520	693	3411	69
H(1X2)	5869	1618	2725	69
H(2X1)	4614	860	3931	100
H(2X2)	4770	491	3148	100
H(2X3)	3957	1798	3255	100
H(4X1)	5701	4236	3751	60
H(4X2)	7121	3739	3907	60
H(4X3)	6233	3316	4459	60
H(3X1)	6783	2840	3012	49
H(3X2)	7389	1916	3708	49

Table S18. Torsion angles [°] for compound **4**.

N(3)-W(1)-O(1)-S(1)	90.82(13)
C(34)-W(1)-O(1)-S(1)	-13.94(14)
O(4)-W(1)-O(1)-S(1)	-162.01(14)
C(46)-W(1)-O(1)-S(1)	-119.13(14)
W(1)-O(1)-S(1)-O(2)	62.18(15)
W(1)-O(1)-S(1)-O(3)	-76.98(14)
W(1)-O(1)-S(1)-C(44)	172.51(12)
N(3)-W(1)-O(4)-S(2A)	74.8(2)
C(34)-W(1)-O(4)-S(2A)	-108.8(2)
O(1)-W(1)-O(4)-S(2A)	-32.44(19)
C(46)-W(1)-O(4)-S(2A)	170.3(2)
N(3)-W(1)-O(4)-S(2)	3.42(16)
C(34)-W(1)-O(4)-S(2)	179.84(14)
O(1)-W(1)-O(4)-S(2)	-103.80(15)
C(46)-W(1)-O(4)-S(2)	98.92(15)
O(2)-S(1)-C(44)-F(2)	175.20(16)
O(3)-S(1)-C(44)-F(2)	-58.69(18)
O(1)-S(1)-C(44)-F(2)	58.07(18)
O(2)-S(1)-C(44)-F(3)	53.06(18)
O(3)-S(1)-C(44)-F(3)	179.17(16)
O(1)-S(1)-C(44)-F(3)	-64.07(17)
O(2)-S(1)-C(44)-F(1)	-65.23(18)
O(3)-S(1)-C(44)-F(1)	60.88(18)
O(1)-S(1)-C(44)-F(1)	177.64(15)
S(2A)-O(4)-S(2)-O(6)	-157.2(3)
W(1)-O(4)-S(2)-O(6)	-25.7(3)
S(2A)-O(4)-S(2)-O(5)	67.6(3)
W(1)-O(4)-S(2)-O(5)	-160.9(3)
S(2A)-O(4)-S(2)-C(45)	-43.14(18)
W(1)-O(4)-S(2)-C(45)	88.4(2)
O(6)-S(2)-C(45)-F(5)	174.9(4)
O(5)-S(2)-C(45)-F(5)	-60.8(5)
O(4)-S(2)-C(45)-F(5)	56.0(3)
O(6)-S(2)-C(45)-F(4)	54.2(4)
O(5)-S(2)-C(45)-F(4)	178.5(5)
O(4)-S(2)-C(45)-F(4)	-64.8(4)
O(6)-S(2)-C(45)-F(6)	-67.4(5)
O(5)-S(2)-C(45)-F(6)	56.9(6)
O(4)-S(2)-C(45)-F(6)	173.6(4)
S(2)-O(4)-S(2A)-O(5A)	-67.3(4)
W(1)-O(4)-S(2A)-O(5A)	-175.6(4)
S(2)-O(4)-S(2A)-O(6A)	155.6(3)

W(1)-O(4)-S(2A)-O(6A)	47.3(3)
S(2)-O(4)-S(2A)-C(45A)	43.8(2)
W(1)-O(4)-S(2A)-C(45A)	-64.5(3)
O(5A)-S(2A)-C(45A)-F(4A)	-59.9(7)
O(6A)-S(2A)-C(45A)-F(4A)	62.9(7)
O(4)-S(2A)-C(45A)-F(4A)	-176.6(6)
O(5A)-S(2A)-C(45A)-F(6A)	63.0(6)
O(6A)-S(2A)-C(45A)-F(6A)	-174.3(5)
O(4)-S(2A)-C(45A)-F(6A)	-53.7(5)
O(5A)-S(2A)-C(45A)-F(5A)	-176.6(5)
O(6A)-S(2A)-C(45A)-F(5A)	-53.8(5)
O(4)-S(2A)-C(45A)-F(5A)	66.8(5)
C(34)-W(1)-N(3)-C(22)	73(2)
O(1)-W(1)-N(3)-C(22)	-27(2)
O(4)-W(1)-N(3)-C(22)	-109(2)
C(46)-W(1)-N(3)-C(22)	169(2)
C(13)-N(2)-C(1)-N(1)	-173.08(19)
C(3)-N(2)-C(1)-N(1)	2.1(2)
C(13)-N(2)-C(1)-C(46)	6.0(3)
C(3)-N(2)-C(1)-C(46)	-178.89(19)
C(4)-N(1)-C(1)-N(2)	164.20(19)
C(2)-N(1)-C(1)-N(2)	3.3(2)
C(4)-N(1)-C(1)-C(46)	-14.9(3)
C(2)-N(1)-C(1)-C(46)	-175.75(19)
C(1)-N(1)-C(2)-C(3)	-7.0(2)
C(4)-N(1)-C(2)-C(3)	-169.69(18)
C(1)-N(2)-C(3)-C(2)	-6.2(2)
C(13)-N(2)-C(3)-C(2)	169.23(19)
N(1)-C(2)-C(3)-N(2)	7.4(2)
C(1)-N(1)-C(4)-C(9)	120.8(2)
C(2)-N(1)-C(4)-C(9)	-79.7(3)
C(1)-N(1)-C(4)-C(5)	-66.5(3)
C(2)-N(1)-C(4)-C(5)	93.1(2)
C(9)-C(4)-C(5)-C(6)	-1.1(3)
N(1)-C(4)-C(5)-C(6)	-173.63(19)
C(9)-C(4)-C(5)-C(10)	177.5(2)
N(1)-C(4)-C(5)-C(10)	4.9(3)
C(4)-C(5)-C(6)-C(7)	1.3(3)
C(10)-C(5)-C(6)-C(7)	-177.3(2)
C(5)-C(6)-C(7)-C(8)	-1.5(4)
C(5)-C(6)-C(7)-C(11)	176.6(2)
C(6)-C(7)-C(8)-C(9)	1.6(4)
C(11)-C(7)-C(8)-C(9)	-176.5(3)

C(7)-C(8)-C(9)-C(4)	-1.4(4)
C(7)-C(8)-C(9)-C(12)	176.3(2)
C(5)-C(4)-C(9)-C(8)	1.1(3)
N(1)-C(4)-C(9)-C(8)	173.7(2)
C(5)-C(4)-C(9)-C(12)	-176.6(2)
N(1)-C(4)-C(9)-C(12)	-4.0(3)
C(1)-N(2)-C(13)-C(18)	-110.0(2)
C(3)-N(2)-C(13)-C(18)	75.3(3)
C(1)-N(2)-C(13)-C(14)	75.4(3)
C(3)-N(2)-C(13)-C(14)	-99.3(2)
C(18)-C(13)-C(14)-C(15)	4.2(3)
N(2)-C(13)-C(14)-C(15)	178.70(19)
C(18)-C(13)-C(14)-C(19)	-175.1(2)
N(2)-C(13)-C(14)-C(19)	-0.6(3)
C(13)-C(14)-C(15)-C(16)	-0.7(3)
C(19)-C(14)-C(15)-C(16)	178.6(2)
C(14)-C(15)-C(16)-C(17)	-1.8(4)
C(14)-C(15)-C(16)-C(20)	177.6(2)
C(15)-C(16)-C(17)-C(18)	0.9(4)
C(20)-C(16)-C(17)-C(18)	-178.5(2)
C(16)-C(17)-C(18)-C(13)	2.4(4)
C(16)-C(17)-C(18)-C(21)	-174.6(2)
C(14)-C(13)-C(18)-C(17)	-5.0(3)
N(2)-C(13)-C(18)-C(17)	-179.4(2)
C(14)-C(13)-C(18)-C(21)	172.0(2)
N(2)-C(13)-C(18)-C(21)	-2.5(3)
W(1)-N(3)-C(22)-C(23)	-167(2)
W(1)-N(3)-C(22)-C(27)	12(2)
N(3)-C(22)-C(23)-C(24)	-178.44(18)
C(27)-C(22)-C(23)-C(24)	2.1(3)
N(3)-C(22)-C(23)-C(28)	-0.4(3)
C(27)-C(22)-C(23)-C(28)	-179.90(19)
C(22)-C(23)-C(24)-C(25)	-1.1(3)
C(28)-C(23)-C(24)-C(25)	-179.12(19)
C(23)-C(24)-C(25)-C(26)	-0.5(3)
C(24)-C(25)-C(26)-C(27)	1.1(4)
C(25)-C(26)-C(27)-C(22)	-0.2(3)
C(25)-C(26)-C(27)-C(31)	179.0(2)
N(3)-C(22)-C(27)-C(26)	179.06(19)
C(23)-C(22)-C(27)-C(26)	-1.5(3)
N(3)-C(22)-C(27)-C(31)	-0.1(3)
C(23)-C(22)-C(27)-C(31)	179.3(2)
C(24)-C(23)-C(28)-C(29)	85.7(3)

C(22)-C(23)-C(28)-C(29)	-92.3(3)
C(24)-C(23)-C(28)-C(30)	-40.7(3)
C(22)-C(23)-C(28)-C(30)	141.3(2)
C(26)-C(27)-C(31)-C(32)	53.9(3)
C(22)-C(27)-C(31)-C(32)	-126.9(2)
C(26)-C(27)-C(31)-C(33)	-69.2(3)
C(22)-C(27)-C(31)-C(33)	110.0(3)
N(3)-W(1)-C(34)-C(35)	1.8(3)
O(1)-W(1)-C(34)-C(35)	114.7(3)
O(4)-W(1)-C(34)-C(35)	-174.8(2)
C(46)-W(1)-C(34)-C(35)	-98.0(3)
W(1)-C(34)-C(35)-C(37)	-23.5(3)
W(1)-C(34)-C(35)-C(36)	-142.7(2)
W(1)-C(34)-C(35)-C(38)	95.9(3)
C(34)-C(35)-C(38)-C(43)	109.1(2)
C(37)-C(35)-C(38)-C(43)	-130.9(2)
C(36)-C(35)-C(38)-C(43)	-9.6(3)
C(34)-C(35)-C(38)-C(39)	-70.1(2)
C(37)-C(35)-C(38)-C(39)	49.9(2)
C(36)-C(35)-C(38)-C(39)	171.25(19)
C(43)-C(38)-C(39)-C(40)	0.5(3)
C(35)-C(38)-C(39)-C(40)	179.7(2)
C(38)-C(39)-C(40)-C(41)	-0.1(3)
C(39)-C(40)-C(41)-C(42)	0.0(4)
C(40)-C(41)-C(42)-C(43)	-0.2(4)
C(39)-C(38)-C(43)-C(42)	-0.6(3)
C(35)-C(38)-C(43)-C(42)	-179.9(2)
C(41)-C(42)-C(43)-C(38)	0.5(3)
N(2)-C(1)-C(46)-W(1)	50.6(3)
N(1)-C(1)-C(46)-W(1)	-130.41(18)
N(3)-W(1)-C(46)-C(1)	149.85(17)
C(34)-W(1)-C(46)-C(1)	-107.70(18)
O(1)-W(1)-C(46)-C(1)	-2.0(3)
O(4)-W(1)-C(46)-C(1)	39.88(17)
C(3X)-O(1X)-C(1X)-C(2X)	178.0(3)
C(1X)-O(1X)-C(3X)-C(4X)	180.0(3)

Table S19. Crystal data and structure refinement for compound **5**.

Empirical formula	$C_{31}H_{45}Cl_2F_3N_2O_3S$
Formula weight	653.65
Temperature	130(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 11.6954(11) Å,α = 90°
	b = 16.0357(14) Å,β = 92.943(2)°
	c = 18.0340(13) Å,γ = 90°
Volume	3377.7(5) $Å^3$
Z, Calculated density	4, 1.285 Mg/m^3
Absorption coefficient	0.304 mm^{-1}
F(000)	1384
Crystal size	0.23 x 0.10 x 0.10 mm
θ range for data collection	1.70 to 25.04°
Limiting indices	-13<=h<=13, -19<=k<=19, -15<=l<=21
Reflections collected / unique	22785 / 5971 [R(int) = 0.707]
Completeness to θ = 25.04	99.9 %
Absorption correction	Numerical
Max. and min. transmission	0.9642 and 0.8894
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5971/0/388
Goodness-of-fit on F^2	1.040
Final R indices [I>2σ(I)]	R1 = 0.0575, wR2 = 0.1242
R indices (all data)	R1 = 0.1161, wR2 = 0.1379
Largest diff. peak and hole	0.805 and -0.884 e. $Å^{-3}$

Table S20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **5**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	8392(2)	6014(2)	1637(1)	18(1)
C(1)	8945(3)	6698(2)	1456(2)	16(1)
N(2)	8404(2)	7380(2)	1632(1)	19(1)
C(2)	7329(3)	7174(2)	1996(2)	22(1)
C(3)	7302(3)	6226(2)	1977(2)	23(1)
C(4)	8651(3)	5173(2)	1419(2)	17(1)
C(5)	8272(3)	4902(2)	708(2)	19(1)
C(6)	8420(3)	4066(2)	540(2)	23(1)
C(7)	8936(3)	3524(2)	1054(2)	23(1)
C(8)	9333(3)	3815(2)	1745(2)	22(1)
C(9)	9204(3)	4644(2)	1945(2)	19(1)
C(10)	7700(3)	5479(2)	133(2)	24(1)
C(11)	8242(3)	5411(2)	-615(2)	30(1)
C(12)	6412(3)	5323(2)	51(2)	35(1)
C(13)	9679(3)	4954(2)	2692(2)	25(1)
C(14)	9202(3)	4470(2)	3330(2)	35(1)
C(15)	10987(3)	4918(2)	2733(2)	41(1)
C(16)	8720(3)	8236(2)	1479(2)	17(1)
C(17)	8373(3)	8581(2)	797(2)	22(1)
C(18)	8643(3)	9409(2)	683(2)	27(1)
C(19)	9215(3)	9878(2)	1225(2)	29(1)
C(20)	9547(3)	9517(2)	1897(2)	26(1)
C(21)	9312(3)	8687(2)	2044(2)	18(1)
C(22)	7730(3)	8085(2)	184(2)	30(1)
C(23)	6665(4)	8528(3)	-140(2)	62(1)
C(24)	8510(3)	7875(3)	-432(2)	51(1)
C(25)	9707(3)	8298(2)	2784(2)	24(1)
C(26)	9184(3)	8737(2)	3433(2)	33(1)
C(27)	11009(3)	8299(3)	2872(2)	51(1)
C(28)	10071(3)	6680(2)	1113(2)	27(1)
S(1)	4004(1)	6544(1)	1536(1)	27(1)
O(1)	2840(2)	6621(1)	1234(1)	34(1)
O(2)	4769(2)	7187(2)	1305(1)	48(1)
O(3)	4470(2)	5714(2)	1549(1)	42(1)
C(1X)	3896(3)	6767(2)	2514(2)	31(1)
F(1)	4917(2)	6729(1)	2885(1)	36(1)
F(2)	3481(2)	7528(1)	2624(1)	56(1)
F(3)	3209(2)	6231(2)	2836(1)	61(1)
Cl(1)	3245(1)	8459(1)	-1006(1)	67(1)
Cl(2)	1477(1)	8648(1)	398(1)	79(1)

C(1Y)	3408(3)	7981(2)	-114(2)	35(1)
C(2Y)	2986(3)	8530(2)	476(2)	44(1)

Table S21. Bond lengths [Å] and angles [°] for compound **5**.

N(1)-C(1)	1.323(4)
N(1)-C(4)	1.441(4)
N(1)-C(3)	1.483(4)
C(1)-N(2)	1.310(4)
C(1)-C(28)	1.484(4)
N(2)-C(16)	1.451(4)
N(2)-C(2)	1.485(4)
C(2)-C(3)	1.520(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.405(4)
C(4)-C(9)	1.405(4)
C(5)-C(6)	1.387(4)
C(5)-C(10)	1.518(4)
C(6)-C(7)	1.387(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.388(4)
C(8)-H(8)	0.9500
C(9)-C(13)	1.515(4)
C(10)-C(11)	1.523(4)
C(10)-C(12)	1.527(4)
C(10)-H(10)	10.000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.517(4)
C(13)-C(15)	1.529(4)
C(13)-H(13)	10.000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.391(4)

C(16)-C(21)	1.403(4)
C(17)-C(18)	1.382(4)
C(17)-C(22)	1.528(4)
C(18)-C(19)	1.379(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.381(4)
C(19)-H(19)	0.9500
C(20)-C(21)	1.387(4)
C(20)-H(20)	0.9500
C(21)-C(25)	1.523(4)
C(22)-C(24)	1.512(5)
C(22)-C(23)	1.524(5)
C(22)-H(22)	10.000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.520(4)
C(25)-C(27)	1.522(5)
C(25)-H(25)	10.000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
S(1)-O(3)	1.437(2)
S(1)-O(2)	1.441(2)
S(1)-O(1)	1.446(2)
S(1)-C(1X)	1.810(4)
C(1X)-F(3)	1.330(4)
C(1X)-F(2)	1.331(4)
C(1X)-F(1)	1.339(4)
Cl(1)-C(1Y)	1.783(3)
Cl(2)-C(2Y)	1.773(4)
C(1Y)-C(2Y)	1.486(5)
C(1Y)-H(1Y1)	0.9900
C(1Y)-H(1Y2)	0.9900

C(2Y)-H(2Y1)	0.9900
C(2Y)-H(2Y2)	0.9900
C(1)-N(1)-C(4)	126.7(3)
C(1)-N(1)-C(3)	110.7(2)
C(4)-N(1)-C(3)	121.6(2)
N(2)-C(1)-N(1)	112.6(3)
N(2)-C(1)-C(28)	124.6(3)
N(1)-C(1)-C(28)	122.8(3)
C(1)-N(2)-C(16)	127.7(3)
C(1)-N(2)-C(2)	110.6(2)
C(16)-N(2)-C(2)	121.6(2)
N(2)-C(2)-C(3)	103.3(2)
N(2)-C(2)-H(2A)	111.1
C(3)-C(2)-H(2A)	111.1
N(2)-C(2)-H(2B)	111.1
C(3)-C(2)-H(2B)	111.1
H(2A)-C(2)-H(2B)	109.1
N(1)-C(3)-C(2)	102.8(2)
N(1)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3A)	111.2
N(1)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1
C(5)-C(4)-C(9)	122.8(3)
C(5)-C(4)-N(1)	118.6(3)
C(9)-C(4)-N(1)	118.5(2)
C(6)-C(5)-C(4)	117.5(3)
C(6)-C(5)-C(10)	119.7(3)
C(4)-C(5)-C(10)	122.8(3)
C(7)-C(6)-C(5)	121.0(3)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(6)-C(7)-C(8)	120.2(3)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(9)-C(8)-C(7)	121.3(3)
C(9)-C(8)-H(8)	119.3
C(7)-C(8)-H(8)	119.3
C(8)-C(9)-C(4)	117.1(3)
C(8)-C(9)-C(13)	120.3(3)
C(4)-C(9)-C(13)	122.5(3)
C(5)-C(10)-C(11)	111.8(3)

C(5)-C(10)-C(12)	111.4(3)
C(11)-C(10)-C(12)	110.9(3)
C(5)-C(10)-H(10)	107.5
C(11)-C(10)-H(10)	107.5
C(12)-C(10)-H(10)	107.5
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
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(9)-C(13)-C(14)	112.0(3)
C(9)-C(13)-C(15)	110.6(3)
C(14)-C(13)-C(15)	110.5(3)
C(9)-C(13)-H(13)	107.9
C(14)-C(13)-H(13)	107.9
C(15)-C(13)-H(13)	107.9
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	123.2(3)
C(17)-C(16)-N(2)	118.6(3)
C(21)-C(16)-N(2)	118.1(2)
C(18)-C(17)-C(16)	117.1(3)
C(18)-C(17)-C(22)	120.1(3)
C(16)-C(17)-C(22)	122.8(3)
C(19)-C(18)-C(17)	121.7(3)
C(19)-C(18)-H(18)	119.2

C(17)-C(18)-H(18)	119.2
C(18)-C(19)-C(20)	119.9(3)
C(18)-C(19)-H(19)	120.1
C(20)-C(19)-H(19)	120.1
C(19)-C(20)-C(21)	121.4(3)
C(19)-C(20)-H(20)	119.3
C(21)-C(20)-H(20)	119.3
C(20)-C(21)-C(16)	116.8(3)
C(20)-C(21)-C(25)	120.4(3)
C(16)-C(21)-C(25)	122.7(3)
C(24)-C(22)-C(23)	109.5(3)
C(24)-C(22)-C(17)	110.7(3)
C(23)-C(22)-C(17)	113.3(3)
C(24)-C(22)-H(22)	107.7
C(23)-C(22)-H(22)	107.7
C(17)-C(22)-H(22)	107.7
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(27)	111.1(3)
C(26)-C(25)-C(21)	111.6(3)
C(27)-C(25)-C(21)	110.3(3)
C(26)-C(25)-H(25)	107.9
C(27)-C(25)-H(25)	107.9
C(21)-C(25)-H(25)	107.9
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(1)-C(28)-H(28A)	109.5
C(1)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(1)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(3)-S(1)-O(2)	115.26(17)
O(3)-S(1)-O(1)	115.76(15)
O(2)-S(1)-O(1)	114.62(14)
O(3)-S(1)-C(1X)	102.25(14)
O(2)-S(1)-C(1X)	102.44(15)
O(1)-S(1)-C(1X)	103.81(15)
F(3)-C(1X)-F(2)	107.1(3)
F(3)-C(1X)-F(1)	107.2(3)
F(2)-C(1X)-F(1)	106.9(3)
F(3)-C(1X)-S(1)	111.8(2)
F(2)-C(1X)-S(1)	111.8(2)
F(1)-C(1X)-S(1)	111.9(2)
C(2Y)-C(1Y)-Cl(1)	111.5(3)
C(2Y)-C(1Y)-H(1Y1)	109.3
Cl(1)-C(1Y)-H(1Y1)	109.3
C(2Y)-C(1Y)-H(1Y2)	109.3
Cl(1)-C(1Y)-H(1Y2)	109.3
H(1Y1)-C(1Y)-H(1Y2)	108.0
C(1Y)-C(2Y)-Cl(2)	111.8(3)
C(1Y)-C(2Y)-H(2Y1)	109.2
Cl(2)-C(2Y)-H(2Y1)	109.2
C(1Y)-C(2Y)-H(2Y2)	109.2
Cl(2)-C(2Y)-H(2Y2)	109.2
H(2Y1)-C(2Y)-H(2Y2)	107.9

Table S22. Anisotropic displacement parameters (A^2 x 10^3) for compound **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

	U11	U22	U33	U23	U13	U12
N(1)	18(2)	16(2)	20(1)	1(1)	3(1)	-2(1)
C(1)	17(2)	16(2)	13(2)	0(1)	-3(1)	2(2)
N(2)	19(2)	15(2)	23(1)	-3(1)	5(1)	1(1)
C(2)	18(2)	24(2)	24(2)	0(1)	7(1)	0(2)
C(3)	18(2)	24(2)	28(2)	-2(1)	6(1)	-2(2)
C(4)	18(2)	10(2)	24(2)	-4(1)	5(1)	-3(1)
C(5)	12(2)	20(2)	24(2)	-2(1)	3(1)	-6(1)
C(6)	21(2)	23(2)	25(2)	-7(2)	4(2)	-8(2)
C(7)	18(2)	16(2)	35(2)	-3(2)	8(2)	0(1)
C(8)	18(2)	17(2)	30(2)	4(1)	4(2)	-1(1)
C(9)	13(2)	18(2)	25(2)	2(1)	2(1)	-2(1)
C(10)	26(2)	21(2)	25(2)	-4(1)	-2(2)	0(2)
C(11)	32(2)	27(2)	33(2)	4(2)	10(2)	-6(2)
C(12)	24(2)	51(2)	30(2)	2(2)	-2(2)	8(2)
C(13)	28(2)	22(2)	23(2)	2(1)	-3(2)	0(2)
C(14)	45(3)	33(2)	28(2)	6(2)	4(2)	-5(2)
C(15)	32(2)	57(3)	33(2)	1(2)	-8(2)	-14(2)
C(16)	15(2)	14(2)	22(2)	2(1)	4(1)	1(1)
C(17)	26(2)	18(2)	21(2)	-3(1)	4(1)	5(2)
C(18)	31(2)	24(2)	25(2)	7(2)	-1(2)	4(2)
C(19)	39(2)	14(2)	33(2)	5(2)	-2(2)	-3(2)
C(20)	27(2)	20(2)	30(2)	-6(2)	-2(2)	-3(2)
C(21)	14(2)	17(2)	22(2)	-1(1)	2(1)	3(1)
C(22)	44(2)	26(2)	19(2)	0(1)	-1(2)	-7(2)
C(23)	44(3)	81(3)	58(3)	-35(2)	-19(2)	18(2)
C(24)	48(3)	70(3)	35(2)	-21(2)	-1(2)	10(2)
C(25)	25(2)	21(2)	26(2)	1(1)	-5(2)	-3(2)
C(26)	40(2)	34(2)	26(2)	-3(2)	1(2)	-5(2)
C(27)	25(2)	83(3)	43(2)	17(2)	-5(2)	7(2)
C(28)	25(2)	21(2)	35(2)	2(2)	8(2)	-5(2)
S(1)	20(1)	31(1)	28(1)	2(1)	-3(1)	3(1)
O(1)	20(1)	35(1)	45(1)	0(1)	-12(1)	-1(1)
O(2)	27(2)	67(2)	50(2)	29(1)	-7(1)	-15(1)
O(3)	51(2)	39(2)	36(1)	-11(1)	-8(1)	23(1)
C(1X)	21(2)	25(2)	46(2)	-11(2)	4(2)	-4(2)
F(1)	36(1)	38(1)	34(1)	-6(1)	-7(1)	0(1)
F(2)	38(1)	46(1)	84(2)	-35(1)	-8(1)	13(1)
F(3)	63(2)	76(2)	45(1)	-10(1)	20(1)	-41(1)
Cl(1)	116(1)	52(1)	34(1)	15(1)	14(1)	16(1)
Cl(2)	60(1)	67(1)	117(1)	55(1)	47(1)	30(1)

C(1Y)	38(2)	33(2)	32(2)	6(2)	-5(2)	2(2)
C(2Y)	51(3)	46(3)	35(2)	4(2)	-4(2)	5(2)

Table S23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **5**.

	x	y	z	U(eq)
H(2A)	6654	7413	1718	26
H(2B)	7350	7383	2513	26
H(3A)	7276	5991	2483	27
H(3B)	6635	6020	1670	27
H(6)	8165	3862	65	27
H(7)	9018	2951	933	27
H(8)	9701	3439	2088	26
H(10)	7815	6063	314	29
H(11A)	9076	5459	-542	45
H(11B)	7951	5859	-942	45
H(11C)	8048	4870	-840	45
H(12A)	6270	4747	-108	53
H(12B)	6067	5706	-321	53
H(12C)	6071	5418	529	53
H(13)	9447	5550	2743	30
H(14A)	8364	4488	3289	53
H(14B)	9476	4721	3802	53
H(14C)	9460	3889	3311	53
H(15A)	11237	4338	2683	62
H(15B)	11281	5140	3212	62
H(15C)	11283	5253	2331	62
H(18)	8430	9661	219	32
H(19)	9380	10448	1136	34
H(20)	9945	9844	2266	31
H(22)	7478	7548	406	36
H(23A)	6888	9054	-368	93
H(23B)	6145	8643	256	93
H(23C)	6279	8172	-517	93
H(24A)	8761	8391	-665	77
H(24B)	8096	7528	-804	77
H(24C)	9179	7570	-226	77
H(25)	9444	7705	2782	29
H(26A)	9461	9313	3462	50
H(26B)	9407	8444	3895	50
H(26C)	8348	8735	3359	50
H(27A)	11326	8055	2428	76
H(27B)	11254	7970	3309	76
H(27C)	11284	8873	2934	76
H(28A)	10311	7250	1005	40
H(28B)	10006	6358	651	40

H(28C)	10639	6418	1457	40
H(1Y1)	2978	7449	-120	41
H(1Y2)	4227	7852	-2	41
H(2Y1)	3351	9085	443	53
H(2Y2)	3210	8290	969	53

Table S24. Torsion angles [°] for compound **5**.

C(4)-N(1)-C(1)-N(2)	169.5(3)
C(3)-N(1)-C(1)-N(2)	1.0(3)
C(4)-N(1)-C(1)-C(28)	-12.3(4)
C(3)-N(1)-C(1)-C(28)	179.2(3)
N(1)-C(1)-N(2)-C(16)	-176.2(3)
C(28)-C(1)-N(2)-C(16)	5.7(4)
N(1)-C(1)-N(2)-C(2)	0.8(3)
C(28)-C(1)-N(2)-C(2)	-177.3(3)
C(1)-N(2)-C(2)-C(3)	-2.2(3)
C(16)-N(2)-C(2)-C(3)	175.0(2)
C(1)-N(1)-C(3)-C(2)	-2.3(3)
C(4)-N(1)-C(3)-C(2)	-171.5(2)
N(2)-C(2)-C(3)-N(1)	2.6(3)
C(1)-N(1)-C(4)-C(5)	-80.3(4)
C(3)-N(1)-C(4)-C(5)	87.0(3)
C(1)-N(1)-C(4)-C(9)	103.9(3)
C(3)-N(1)-C(4)-C(9)	-88.9(3)
C(9)-C(4)-C(5)-C(6)	2.6(5)
N(1)-C(4)-C(5)-C(6)	-173.1(3)
C(9)-C(4)-C(5)-C(10)	-178.5(3)
N(1)-C(4)-C(5)-C(10)	5.8(4)
C(4)-C(5)-C(6)-C(7)	-0.8(5)
C(10)-C(5)-C(6)-C(7)	-179.8(3)
C(5)-C(6)-C(7)-C(8)	-1.1(5)
C(6)-C(7)-C(8)-C(9)	1.4(5)
C(7)-C(8)-C(9)-C(4)	0.2(4)
C(7)-C(8)-C(9)-C(13)	-178.0(3)
C(5)-C(4)-C(9)-C(8)	-2.3(4)
N(1)-C(4)-C(9)-C(8)	173.4(3)
C(5)-C(4)-C(9)-C(13)	175.9(3)
N(1)-C(4)-C(9)-C(13)	-8.4(4)
C(6)-C(5)-C(10)-C(11)	-50.9(4)
C(4)-C(5)-C(10)-C(11)	130.2(3)
C(6)-C(5)-C(10)-C(12)	73.8(4)
C(4)-C(5)-C(10)-C(12)	-105.1(3)
C(8)-C(9)-C(13)-C(14)	-57.3(4)
C(4)-C(9)-C(13)-C(14)	124.7(3)
C(8)-C(9)-C(13)-C(15)	66.4(4)
C(4)-C(9)-C(13)-C(15)	-111.7(3)
C(1)-N(2)-C(16)-C(17)	85.7(4)
C(2)-N(2)-C(16)-C(17)	-91.0(3)
C(1)-N(2)-C(16)-C(21)	-97.6(3)

C(2)-N(2)-C(16)-C(21)	85.7(3)
C(21)-C(16)-C(17)-C(18)	0.5(5)
N(2)-C(16)-C(17)-C(18)	177.1(3)
C(21)-C(16)-C(17)-C(22)	179.9(3)
N(2)-C(16)-C(17)-C(22)	-3.5(4)
C(16)-C(17)-C(18)-C(19)	-1.1(5)
C(22)-C(17)-C(18)-C(19)	179.5(3)
C(17)-C(18)-C(19)-C(20)	1.0(5)
C(18)-C(19)-C(20)-C(21)	-0.4(5)
C(19)-C(20)-C(21)-C(16)	-0.1(5)
C(19)-C(20)-C(21)-C(25)	178.8(3)
C(17)-C(16)-C(21)-C(20)	0.1(5)
N(2)-C(16)-C(21)-C(20)	-176.5(3)
C(17)-C(16)-C(21)-C(25)	-178.8(3)
N(2)-C(16)-C(21)-C(25)	4.6(4)
C(18)-C(17)-C(22)-C(24)	73.9(4)
C(16)-C(17)-C(22)-C(24)	-105.5(4)
C(18)-C(17)-C(22)-C(23)	-49.6(4)
C(16)-C(17)-C(22)-C(23)	131.0(4)
C(20)-C(21)-C(25)-C(26)	60.8(4)
C(16)-C(21)-C(25)-C(26)	-120.4(3)
C(20)-C(21)-C(25)-C(27)	-63.2(4)
C(16)-C(21)-C(25)-C(27)	115.6(3)
O(3)-S(1)-C(1X)-F(3)	-60.5(3)
O(2)-S(1)-C(1X)-F(3)	179.9(2)
O(1)-S(1)-C(1X)-F(3)	60.3(3)
O(3)-S(1)-C(1X)-F(2)	179.5(2)
O(2)-S(1)-C(1X)-F(2)	59.8(3)
O(1)-S(1)-C(1X)-F(2)	-59.7(3)
O(3)-S(1)-C(1X)-F(1)	59.7(3)
O(2)-S(1)-C(1X)-F(1)	-60.0(3)
O(1)-S(1)-C(1X)-F(1)	-179.5(2)
Cl(1)-C(1Y)-C(2Y)-Cl(2)	68.7(3)