Supporting Information

PABA/NO as an Anticancer Lead: Analogue Synthesis, Structure Revision, Solution Chemistry, Reactivity toward Glutathione, and In Vitro Activity

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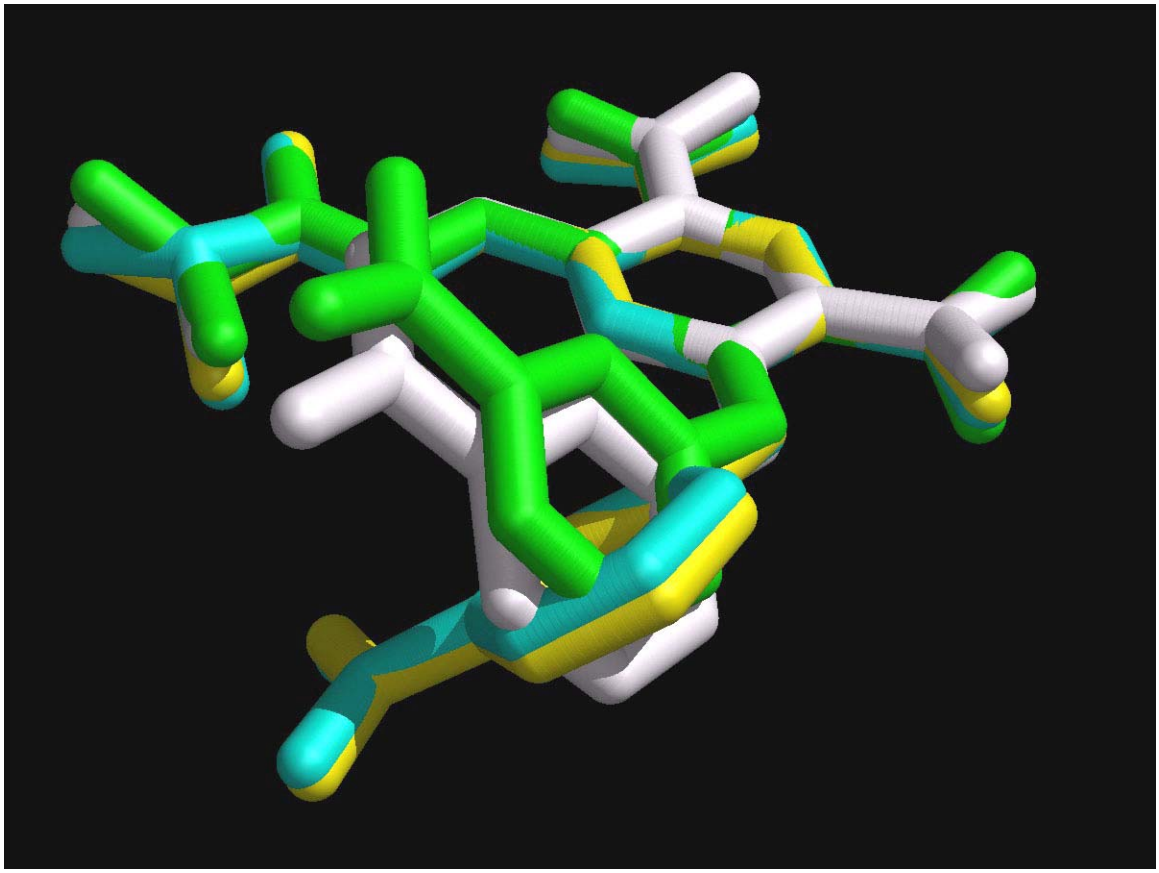

Figure S1. Conformational differences in **6c** after superimposing the carbon atoms of the dinitrobenzene ring. Note the good agreement in the structures except in the area of the benzoate ring, which shows two distinct orientations.

Table S1. Crystal data and structure refinement for **6a**.

Empirical formula	$C_{16}H_{16}N_6O_8$	
Formula weight	420.35	
Temperature	103(2) °K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 14.153(4) Å	α= 90°
	b = 7.881(2) Å	β= 112.336(5)°
	c = 18.163(5) Å	γ = 90°
Volume	1873.8(8) Å3	
Z	4	
Density (calculated)	1.490 Mg/m^3	
Absorption coefficient	0.122 mm^{-1}	
F(000)	872	
Crystal size	0.43 x 0.09 x 0.08 mm^3	
Theta range for data collection	2.31 to 25.42°	
Index ranges	-17<=h<=17, -9<=k<=6, -21<=l<=21	
Reflections collected	7933	
Independent reflections	3419 [R(int) = 0.0466]	
Completeness to θ = 25.42°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.990 and 0.832	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3419 / 0 / 271	
Goodness-of-fit on F2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1379	
R indices (all data)	R1 = 0.1240, wR2 = 0.1620	
Largest diff. peak and hole	0.315 and -0.297 $eÅ^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **6a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	11656(2)	-1598(4)	4035(2)	34(1)
O(1)	12394(2)	-1718(4)	3829(2)	53(1)
N(2)	10807(2)	-825(4)	3668(2)	34(1)
O(2)	10911(2)	-86(4)	2986(1)	37(1)
N(3)	11756(2)	-2320(5)	4768(2)	40(1)
C(3')	10811(3)	-2286(6)	4926(2)	39(1)
C(3")	12302(3)	-3912(5)	4904(2)	39(1)
C(1)	10027(3)	666(5)	2509(2)	31(1)
C(2)	9938(3)	1232(5)	1756(2)	30(1)
N(2')	10754(2)	991(5)	1448(2)	41(1)
O(2')	11609(2)	608(5)	1914(2)	79(1)
O(2")	10529(2)	1172(5)	737(2)	57(1)
C(3)	9057(3)	2014(5)	1245(2)	31(1)
C(4)	8242(3)	2244(5)	1476(2)	28(1)
N(4)	7345(2)	3131(4)	925(2)	32(1)
O(4)	7195(2)	3112(4)	214(2)	43(1)
O(4')	6796(2)	3883(4)	1199(2)	40(1)
C(5)	8304(2)	1621(5)	2217(2)	26(1)
C(6)	9183(3)	852(5)	2719(2)	29(1)
O(7)	7522(2)	1744(3)	2493(1)	31(1)
C(8)	6623(2)	877(5)	2057(2)	27(1)
O(8)	6517(2)	160(3)	1443(1)	36(1)
C(9)	5892(3)	946(5)	2445(2)	28(1)
C(10)	6091(3)	1700(5)	3183(2)	36(1)
C(11)	5370(3)	1685(5)	3522(2)	42(1)
C(12)	4420(3)	910(6)	3131(2)	40(1)
N(12)	3684(3)	859(5)	3447(2)	57(1)
C(12A)	3806(4)	1576(7)	4208(3)	71(2)
C(13)	4216(3)	139(5)	2388(2)	36(1)
C(14)	4941(3)	153(5)	2056(2)	32(1)

Table S3. Bond lengths [Å] and angles [°] for **6a**.

N(1)-O(1)	1.239(3)	N(1)-N(2)	1.284(4)
N(1)-N(3)	1.405(4)	N(2)-O(2)	1.426(3)
O(2)-C(1)	1.358(4)	N(3)-C(3")	1.444(5)
N(3)-C(3')	1.472(4)	C(3')-H(3'A)	0.9800
C(3')-H(3'B)	0.9800	C(3')-H(3'C)	0.9800
C(3")-H(3"A)	0.9800	C(3")-H(3"B)	0.9800
C(3")-H(3"C)	0.9800	C(1)-C(6)	1.392(4)
C(1)-C(2)	1.399(5)	C(2)-C(3)	1.385(5)
C(2)-N(2')	1.473(4)	N(2')-O(2")	1.216(4)
N(2')-O(2')	1.223(4)	C(3)-C(4)	1.382(4)
C(3)-H(3A)	0.9500	C(4)-C(5)	1.404(5)
C(4)-N(4)	1.461(5)	N(4)-O(4')	1.224(3)
N(4)-O(4)	1.227(4)	C(5)-C(6)	1.372(5)
C(5)-O(7)	1.381(4)	C(6)-H(6A)	0.9500
O(7)-C(8)	1.395(4)	C(8)-O(8)	1.207(4)
C(8)-C(9)	1.458(4)	C(9)-C(10)	1.392(5)
C(9)-C(14)	1.407(5)	C(10)-C(11)	1.378(5)
C(10)-H(10A)	0.9500	C(11)-C(12)	1.400(6)
C(11)-H(11A)	0.9500	C(12)-N(12)	1.367(4)
C(12)-C(13)	1.406(5)	N(12)-C(12A)	1.443(5)
N(12)-H(12)	0.8800	C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800	C(12A)-H(12C)	0.9800
C(13)-C(14)	1.373(4)	C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500		
O(1)-N(1)-N(2)	127.5(3)	O(1)-N(1)-N(3)	117.5(3)
N(2)-N(1)-N(3)	114.9(3)	N(1)-N(2)-O(2)	105.0(2)
C(1)-O(2)-N(2)	111.0(2)	N(1)-N(3)-C(3")	111.7(3)
N(1)-N(3)-C(3')	113.9(3)	C(3")-N(3)-C(3')	116.7(3)
N(3)-C(3')-H(3'A)	109.5	N(3)-C(3')-H(3'B)	109.5
H(3'A)-C(3')-H(3'B)	109.5	N(3)-C(3')-H(3'C)	109.5
H(3'A)-C(3')-H(3'C)	109.5	H(3'B)-C(3')-H(3'C)	109.5
N(3)-C(3")-H(3"A)	109.5	N(3)-C(3")-H(3"B)	109.5
H(3"A)-C(3")-H(3"B)	109.5	N(3)-C(3")-H(3"C)	109.5
H(3"A)-C(3")-H(3"C)	109.5	H(3"B)-C(3")-H(3"C)	109.5
O(2)-C(1)-C(6)	123.4(3)	O(2)-C(1)-C(2)	118.8(3)
C(6)-C(1)-C(2)	117.8(3)	C(3)-C(2)-C(1)	121.4(3)
C(3)-C(2)-N(2')	116.0(3)	C(1)-C(2)-N(2')	122.6(3)
O(2")-N(2')-O(2')	123.7(3)	O(2")-N(2')-C(2)	117.5(3)
O(2')-N(2')-C(2)	118.8(3)	C(4)-C(3)-C(2)	119.8(3)
C(4)-C(3)-H(3A)	120.1	C(2)-C(3)-H(3A)	120.1
C(3)-C(4)-C(5)	119.4(3)	C(3)-C(4)-N(4)	117.5(3)
C(5)-C(4)-N(4)	123.1(3)	O(4')-N(4)-O(4)	123.4(3)
O(4')-N(4)-C(4)	118.3(3)	O(4)-N(4)-C(4)	118.3(3)
C(6)-C(5)-O(7)	116.1(3)	C(6)-C(5)-C(4)	120.1(3)
O(7)-C(5)-C(4)	123.8(3)	C(5)-C(6)-C(1)	121.3(3)

Table S3. (continued).

C(5)-C(6)-H(6A)	119.3	C(1)-C(6)-H(6A)	119.3
C(5)-O(7)-C(8)	116.4(3)	O(8)-C(8)-O(7)	121.3(3)
O(8)-C(8)-C(9)	127.0(3)	O(7)-C(8)-C(9)	111.7(3)
C(10)-C(9)-C(14)	118.5(3)	C(10)-C(9)-C(8)	124.0(3)
C(14)-C(9)-C(8)	117.4(3)	C(11)-C(10)-C(9)	120.8(4)
C(11)-C(10)-H(10A)	119.6	C(9)-C(10)-H(10A)	119.6
C(10)-C(11)-C(12)	120.6(4)	C(10)-C(11)-H(11A)	119.7
C(12)-C(11)-H(11A)	119.7	N(12)-C(12)-C(11)	122.5(4)
N(12)-C(12)-C(13)	118.6(4)	C(11)-C(12)-C(13)	118.9(3)
C(12)-N(12)-C(12A)	124.0(4)	C(12)-N(12)-H(12)	118.0
C(12A)-N(12)-H(12)	118.0	N(12)-C(12A)-H(12A)	109.5
N(12)-C(12A)-H(12B)	109.5	H(12A)-C(12A)-H(12B)	109.5
N(12)-C(12A)-H(12C)	109.5	H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5	C(14)-C(13)-C(12)	120.1(4)
C(14)-C(13)-H(13A)	119.9	C(12)-C(13)-H(13A)	119.9
C(13)-C(14)-C(9)	121.0(3)	C(13)-C(14)-H(14A)	119.5
C(9)-C(14)-H(14A)	119.5		

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **6a**. 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}
N(1)	31(2)	27(2)	45(2)	4(2)	16(2)	-1(2)
O(1)	41(2)	56(2)	75(2)	25(2)	35(2)	15(2)
N(2)	33(2)	32(2)	36(2)	9(2)	14(1)	1(2)
O(2)	31(1)	38(2)	46(2)	17(1)	19(1)	5(1)
N(3)	49(2)	35(2)	37(2)	7(2)	18(2)	0(2)
C(3')	48(2)	42(3)	33(2)	3(2)	21(2)	7(2)
C(3")	45(2)	39(3)	32(2)	7(2)	13(2)	12(2)
C(1)	29(2)	24(2)	41(2)	2(2)	14(2)	-4(2)
C(2)	27(2)	26(2)	39(2)	3(2)	18(2)	-1(2)
N(2')	35(2)	49(2)	46(2)	9(2)	23(2)	0(2)
O(2')	35(2)	139(4)	73(2)	53(2)	32(2)	26(2)
O(2")	37(2)	94(3)	45(2)	-2(2)	22(1)	4(2)
C(3)	39(2)	25(2)	35(2)	-2(2)	21(2)	-6(2)
C(4)	27(2)	23(2)	36(2)	0(2)	15(2)	0(2)
N(4)	36(2)	30(2)	37(2)	0(2)	22(2)	2(2)
O(4)	49(2)	50(2)	34(2)	8(2)	21(1)	10(2)
O(4')	44(2)	38(2)	48(2)	7(1)	28(1)	14(1)
C(5)	26(2)	23(2)	33(2)	-4(2)	16(2)	-3(2)
C(6)	33(2)	22(2)	38(2)	3(2)	20(2)	-2(2)
O(7)	29(1)	34(2)	34(1)	-1(1)	17(1)	2(1)
C(8)	30(2)	27(2)	27(2)	4(2)	12(2)	3(2)
O(8)	39(1)	38(2)	36(1)	-7(1)	21(1)	-5(1)
C(9)	31(2)	21(2)	36(2)	9(2)	16(2)	7(2)
C(10)	44(2)	27(2)	43(2)	-2(2)	25(2)	-1(2)
C(11)	56(3)	38(3)	41(2)	1(2)	30(2)	4(2)
C(12)	47(2)	39(3)	46(2)	6(2)	30(2)	8(2)
N(12)	63(2)	68(3)	59(2)	-12(2)	44(2)	-14(2)
C(12A)	93(4)	74(4)	76(3)	-24(3)	66(3)	-25(3)
C(13)	28(2)	39(3)	42(2)	7(2)	13(2)	-2(2)
C(14)	34(2)	33(3)	33(2)	11(2)	16(2)	8(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **6a**.

	x	y	z	U(eq)
H(3'A)	10509	-1149	4814	59
H(3'B)	10968	-2569	5485	59
H(3'C)	10326	-3116	4584	59
H(3"A)	12914	-3785	4779	59
H(3"B)	11859	-4789	4561	59
H(3"C)	12501	-4243	5463	59
H(3A)	9013	2391	736	37
H(6A)	9217	439	3219	35
H(10A)	6732	2232	3455	43
H(11A)	5519	2205	4026	50
H(12)	3102	357	3169	69
H(12A)	3182	1387	4310	106
H(12B)	3934	2798	4205	106
H(12C)	4384	1032	4628	106
H(13A)	3575	-393	2115	43
H(14A)	4798	-380	1556	39

Table S6. Torsion angles [°] for **6a**.

O(1)-N(1)-N(2)-O(2)	-1.9(5)	N(3)-N(1)-N(2)-O(2)	175.3(3)
N(1)-N(2)-O(2)-C(1)	175.2(3)	O(1)-N(1)-N(3)-C(3")	-38.8(5)
N(2)-N(1)-N(3)-C(3")	143.6(3)	O(1)-N(1)-N(3)-C(3')	-173.7(3)
N(2)-N(1)-N(3)-C(3')	8.8(5)	N(2)-O(2)-C(1)-C(6)	7.2(5)
N(2)-O(2)-C(1)-C(2)	-170.5(3)	O(2)-C(1)-C(2)-C(3)	-179.8(4)
C(6)-C(1)-C(2)-C(3)	2.5(6)	O(2)-C(1)-C(2)-N(2')	2.2(6)
C(6)-C(1)-C(2)-N(2')	-175.6(4)	C(3)-C(2)-N(2')-O(2")	-14.3(6)
C(1)-C(2)-N(2')-O(2")	163.9(4)	C(3)-C(2)-N(2')-O(2')	166.4(4)
C(1)-C(2)-N(2')-O(2')	-15.4(6)	C(1)-C(2)-C(3)-C(4)	-0.1(6)
N(2')-C(2)-C(3)-C(4)	178.1(3)	C(2)-C(3)-C(4)-C(5)	-2.4(6)
C(2)-C(3)-C(4)-N(4)	177.8(3)	C(3)-C(4)-N(4)-O(4')	-153.9(3)
C(5)-C(4)-N(4)-O(4')	26.4(5)	C(3)-C(4)-N(4)-O(4)	24.6(5)
C(5)-C(4)-N(4)-O(4)	-155.1(3)	C(3)-C(4)-C(5)-C(6)	2.6(6)
N(4)-C(4)-C(5)-C(6)	-177.7(3)	C(3)-C(4)-C(5)-O(7)	-178.1(3)
N(4)-C(4)-C(5)-O(7)	1.6(6)	O(7)-C(5)-C(6)-C(1)	-179.5(3)
C(4)-C(5)-C(6)-C(1)	-0.2(6)	O(2)-C(1)-C(6)-C(5)	-180.0(4)
C(2)-C(1)-C(6)-C(5)	-2.3(6)	C(6)-C(5)-O(7)-C(8)	-117.0(4)
C(4)-C(5)-O(7)-C(8)	63.6(5)	C(5)-O(7)-C(8)-O(8)	-5.0(5)
C(5)-O(7)-C(8)-C(9)	174.0(3)	O(8)-C(8)-C(9)-C(10)	175.4(4)
O(7)-C(8)-C(9)-C(10)	-3.5(5)	O(8)-C(8)-C(9)-C(14)	-2.7(6)
O(7)-C(8)-C(9)-C(14)	178.5(3)	C(14)-C(9)-C(10)-C(11)	-0.5(6)
C(8)-C(9)-C(10)-C(11)	-178.6(4)	C(9)-C(10)-C(11)-C(12)	-0.1(6)
C(10)-C(11)-C(12)-N(12)	179.7(4)	C(10)-C(11)-C(12)-C(13)	0.4(6)
C(11)-C(12)-N(12)-C(12A)	-0.4(7)	C(13)-C(12)-N(12)-C(12A)	178.9(4)
N(12)-C(12)-C(13)-C(14)	-179.4(4)	C(11)-C(12)-C(13)-C(14)	-0.1(6)
C(12)-C(13)-C(14)-C(9)	-0.5(6)	C(10)-C(9)-C(14)-C(13)	0.9(6)
C(8)-C(9)-C(14)-C(13)	179.0(4)		

Table S7. Crystal data and structure refinement for **6c**.

Empirical formula	$C_{15}H_{13}N_6O_8$	
Formula weight	405.31	
Temperature	293(2) °K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.2367(11) Å	α= 89.451(5)°
	b = 12.8743(10) Å	β= 88.172(6)°
	c = 25.143(2) Å	γ = 87.516(5)°
Volume	3631.9(6) $Å^3$	
Z	8	
Density (calculated)	1.483 Mg/m^3	
Absorption coefficient	1.063 mm^{-1}	
F(000)	1672	
Crystal size	0.36 x 0.06 x 0.04 mm^3	
θ range for data collection	1.76 to 67.20°	
Index ranges	-12<=h<=12, -15<=k<=14, -25<=l<=29	
Reflections collected	18729	
Independent reflections	10961 [R(int) = 0.0415]	
Completeness to θ = 67.20°	84.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.958 and 0.682	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10961 / 9 / 1130	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2s (I)]	R1 = 0.0857, wR2 = 0.2660	
R indices (all data)	R1 = 0.1318, wR2 = 0.3146	
Extinction coefficient	0.0026(4)	
Largest diff. peak and hole	1.320 and -1.142 $e.Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **6c**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(9)	-2378(5)	-1593(4)	3498(2)	79(2)
C(10)	-2752(5)	-2534(4)	3315(2)	75(1)
O(15)	-4209(4)	-3372(3)	2825(2)	102(1)
C(14)	-3800(5)	-2514(5)	2973(2)	82(2)
O(14)	-4257(4)	-1641(3)	2846(2)	114(2)
C(11)	-2138(5)	-3456(4)	3443(2)	83(2)
C(12)	-1165(5)	-3450(4)	3751(2)	83(2)
C(13)	-762(5)	-2516(4)	3927(2)	84(2)
C(8)	-1371(6)	-1584(4)	3803(2)	84(2)
N(7)	-957(5)	-651(4)	4009(2)	107(2)
C(5)	-933(5)	316(4)	3791(2)	87(2)
C(4)	-658(8)	1207(5)	4060(2)	119(3)
O(4')	-667(15)	351(6)	4878(3)	690(20)
O(4)	-150(6)	1889(4)	4852(2)	168(3)
N(4)	-460(5)	1128(4)	4632(2)	233(6)
C(3)	-620(6)	2178(4)	3818(2)	97(2)
C(2)	-894(5)	2290(4)	3307(2)	77(1)
O(2")	-916(7)	4057(4)	3391(2)	161(3)
N(2')	-909(5)	3342(4)	3097(3)	105(2)
C(1)	-1160(5)	1425(4)	3006(2)	72(1)
O(2')	-882(7)	3462(4)	2623(3)	175(3)
C(6)	-1170(5)	457(4)	3243(2)	71(1)
O(2)	-1428(4)	1600(3)	2486(1)	85(1)
N(2)	-1781(5)	690(3)	2246(2)	91(2)
N(1)	-2009(5)	937(4)	1767(2)	97(2)
O(1)	-1894(5)	1782(4)	1554(2)	127(2)
N(3')	-1980(40)	40(20)	1448(6)	115(9)
C(3")	-2100(70)	-880(20)	1731(12)	180(17)
C(3"")	-2650(30)	370(30)	968(11)	98(7)
N(3)	-2770(40)	234(14)	1505(7)	103(8)
C(3')	-2980(30)	-720(20)	1765(10)	123(10)
C(3")	-2470(40)	100(40)	901(15)	165(18)
C(9A)	2240(5)	-1320(4)	1485(2)	69(1)
C(10A)	2598(5)	-2298(4)	1667(2)	70(1)
O(14A)	4119(4)	-1565(3)	2144(2)	107(1)
C(14A)	3659(5)	-2405(4)	2008(2)	77(1)
O(15A)	4031(4)	-3287(3)	2160(2)	102(1)
C(11A)	1984(5)	-3161(4)	1543(2)	76(1)
C(12A)	989(6)	-3033(4)	1229(2)	86(2)
C(13A)	614(5)	-2066(4)	1058(2)	76(1)
C(8A)	1237(5)	-1195(4)	1179(2)	72(1)
N(7A)	865(4)	-227(3)	966(2)	77(1)

Table S8. (continued).

C(5A)	943(5)	723(3)	1193(2)	65(1)
C(4A)	810(4)	1669(3)	901(2)	66(1)
N(4A)	590(4)	1711(3)	341(2)	80(1)
O(4'A)	231(5)	931(3)	132(2)	129(2)
O(4A)	779(4)	2487(3)	87(2)	103(1)
C(3A)	929(4)	2614(4)	1138(2)	67(1)
C(2A)	1187(5)	2678(3)	1666(2)	66(1)
N(2'A)	1381(5)	3696(3)	1871(2)	88(1)
O(2"A)	1213(6)	4444(3)	1595(2)	133(2)
C(1A)	1329(4)	1756(4)	1969(2)	65(1)
O(2'A)	1770(8)	3789(4)	2294(2)	190(4)
C(6A)	1171(4)	822(4)	1733(2)	65(1)
O(2A)	1604(3)	1851(3)	2489(1)	76(1)
N(2A)	1748(4)	862(3)	2729(2)	81(1)
N(1A)	2106(5)	1018(4)	3198(2)	86(1)
O(1A)	2316(5)	1850(4)	3391(2)	134(2)
N(3A)	2155(7)	123(5)	3511(2)	128(2)
C(3"A)	2994(10)	133(9)	3910(4)	201(6)
C(3'A)	1998(9)	-833(6)	3231(3)	149(3)
C(9B)	6494(5)	2928(4)	4039(2)	71(1)
C(10B)	6081(5)	2012(4)	3820(2)	74(1)
O(14B)	5684(5)	2872(3)	3004(2)	108(2)
C(14B)	5716(5)	2027(4)	3253(2)	82(2)
O(15B)	5494(5)	1161(3)	3050(2)	106(1)
C(11B)	6023(6)	1126(4)	4123(2)	87(2)
C(12B)	6339(6)	1130(4)	4644(2)	96(2)
C(13B)	6752(6)	2024(4)	4859(2)	88(2)
C(8B)	6834(5)	2918(4)	4561(2)	76(1)
N(7B)	7351(4)	3768(3)	4802(2)	84(1)
C(5B)	7028(5)	4790(4)	4780(2)	76(1)
C(4B)	7656(5)	5567(4)	5043(2)	77(1)
O(4'B)	9049(5)	4392(4)	5401(2)	127(2)
O(4B)	9143(5)	5990(4)	5593(2)	142(2)
N(4B)	8680(5)	5293(5)	5368(2)	101(2)
C(3B)	7337(5)	6587(4)	5004(2)	80(2)
C(2B)	6385(5)	6928(4)	4707(2)	77(2)
N(2'B)	6150(5)	8047(3)	4666(2)	95(2)
O(2"B)	6679(6)	8609(3)	4953(2)	139(2)
C(1B)	5725(5)	6178(4)	4453(2)	71(1)
O(2'B)	5453(4)	8376(3)	4333(2)	101(1)
C(6B)	6029(5)	5152(4)	4496(2)	69(1)
O(2B)	4736(4)	6542(3)	4189(2)	88(1)
N(2B)	4228(5)	5715(3)	3919(2)	90(2)
O(1B)	2863(5)	6990(3)	3782(2)	133(2)
N(1B)	3258(5)	6096(4)	3727(2)	93(2)
N(3B)	2517(18)	5338(14)	3518(7)	100(4)

Table S8. (continued).

C(3'B)	3320(30)	4460(20)	3331(14)	188(14)
C(3"B)	1670(20)	5760(15)	3130(8)	96(6)
N(3'B)	2980(60)	5630(40)	3300(30)	110(18)
C(3'E)	3040(40)	4270(30)	3385(18)	71(10)
C(3"E)	1910(60)	5890(50)	3120(20)	130(20)
C(9C)	3874(5)	3011(4)	1033(2)	73(1)
C(10C)	4246(5)	2075(4)	1270(2)	75(1)
O(14C)	4791(5)	2918(3)	2049(2)	110(2)
C(14C)	4643(5)	2063(4)	1827(2)	79(2)
O(15C)	4801(5)	1206(3)	2060(2)	115(2)
C(11C)	4243(5)	1154(4)	985(2)	80(2)
C(12C)	3890(5)	1176(4)	465(2)	86(2)
C(13C)	3532(5)	2099(4)	231(2)	78(1)
C(8C)	3507(5)	3023(4)	515(2)	71(1)
N(7C)	2992(4)	3913(3)	254(2)	81(1)
C(5C)	3240(5)	4930(4)	294(2)	73(1)
C(4C)	2582(5)	5720(4)	16(2)	78(2)
N(4C)	1628(5)	5505(4)	-324(2)	101(2)
O(4'C)	1283(5)	4611(4)	-360(2)	123(2)
O(4C)	1174(5)	6216(4)	-580(2)	150(2)
C(3C)	2855(5)	6746(4)	61(2)	81(2)
C(2C)	3748(6)	7043(4)	370(2)	79(2)
O(2"C)	3297(5)	8738(3)	148(2)	125(2)
N(2'C)	3936(5)	8155(3)	415(2)	90(1)
C(1C)	4482(5)	6269(4)	623(2)	73(1)
O(2'C)	4633(4)	8458(3)	728(2)	101(1)
C(6C)	4202(5)	5250(4)	580(2)	72(1)
O(2C)	5413(4)	6590(3)	897(2)	87(1)
N(2C)	5962(5)	5747(4)	1171(2)	97(2)
O(1C)	7260(5)	6970(4)	1308(3)	155(3)
N(1C)	6884(5)	6096(4)	1374(2)	100(2)
N(3C)	7310(30)	5490(30)	1789(18)	111(9)
C(3'C)	6900(50)	4470(30)	1776(19)	170(20)
C(3"C)	8290(40)	5780(30)	1980(15)	134(13)
N(3'C)	7710(40)	5344(15)	1576(14)	98(8)
C(3'F)	7170(50)	4330(30)	1741(17)	131(13)
C(3"F)	8550(30)	5690(30)	1925(17)	136(14)

Table S9. Bond lengths [Å] and angles [°] for **6c**.

C(9)-C(10)	1.387(7)	C(9)-C(8)	1.388(7)
C(9)-H(9)	0.9300	C(10)-C(11)	1.387(7)
C(10)-C(14)	1.479(7)	O(15)-C(14)	1.277(7)
C(14)-O(14)	1.258(6)	C(11)-C(12)	1.361(7)
C(11)-H(11)	0.9300	C(12)-C(13)	1.385(7)
C(12)-H(12)	0.9300	C(13)-C(8)	1.393(7)
C(13)-H(13)	0.9300	C(8)-N(7)	1.416(7)
N(7)-C(5)	1.356(7)	N(7)-H(7)	0.8600
C(5)-C(4)	1.389(7)	C(5)-C(6)	1.421(6)
C(4)-C(3)	1.387(8)	C(4)-N(4)	1.463(6)
O(4')-N(4)	1.1990(11)	O(4)-N(4)	1.1997(10)
C(3)-C(2)	1.335(7)	C(3)-H(3)	0.9300
C(2)-C(1)	1.401(7)	C(2)-N(2')	1.448(7)
O(2")-N(2')	1.186(7)	N(2')-O(2')	1.202(7)
C(1)-O(2)	1.366(6)	C(1)-C(6)	1.376(7)
C(6)-H(6)	0.9300	O(2)-N(2)	1.401(5)
N(2)-N(1)	1.273(6)	N(1)-O(1)	1.218(6)
N(1)-N(3')	1.41(2)	N(1)-N(3)	1.45(2)
N(3')-C(3")	1.39(3)	N(3')-C(3"")	1.49(4)
C(3")-H(3AA)	0.9600	C(3")-H(3AB)	0.9600
C(3")-H(3AC)	0.9600	C(3"")-H(3AD)	0.9600
C(3"")-H(3AE)	0.9600	C(3"")-H(3AF)	0.9600
N(3)-C(3')	1.41(3)	N(3)-C(3")	1.56(5)
C(3')-H(3'A)	0.9600	C(3')-H(3'B)	0.9600
C(3')-H(3'C)	0.9600	C(3")-H(3"A)	0.9600
C(3")-H(3"B)	0.9600	C(3")-H(3"C)	0.9600
C(9A)-C(10A)	1.382(6)	C(9A)-C(8A)	1.389(7)
C(9A)-H(9A)	0.9300	C(10A)-C(11A)	1.377(7)
C(10A)-C(14A)	1.491(7)	O(14A)-C(14A)	1.273(6)
C(14A)-O(15A)	1.254(6)	C(11A)-C(12A)	1.392(7)
C(11A)-H(11A)	0.9300	C(12A)-C(13A)	1.367(7)
C(12A)-H(12A)	0.9300	C(13A)-C(8A)	1.389(7)
C(13A)-H(13A)	0.9300	C(8A)-N(7A)	1.405(6)
N(7A)-C(5A)	1.362(5)	N(7A)-H(7A)	0.8600
C(5A)-C(6A)	1.398(6)	C(5A)-C(4A)	1.421(6)
C(4A)-C(3A)	1.373(6)	C(4A)-N(4A)	1.437(6)
N(4A)-O(4A)	1.204(5)	N(4A)-O(4'A)	1.229(5)
C(3A)-C(2A)	1.371(6)	C(3A)-H(3A)	0.9300
C(2A)-C(1A)	1.411(6)	C(2A)-N(2'A)	1.441(6)
N(2'A)-O(2'A)	1.172(6)	N(2'A)-O(2"A)	1.193(6)
C(1A)-O(2A)	1.361(5)	C(1A)-C(6A)	1.367(6)
C(6A)-H(6A)	0.9300	O(2A)-N(2A)	1.409(5)
N(2A)-N(1A)	1.279(5)	N(1A)-O(1A)	1.215(6)
N(1A)-N(3A)	1.389(7)	N(3A)-C(3"A)	1.399(8)
N(3A)-C(3'A)	1.443(9)	C(3"A)-H(3AG)	0.9600
C(3"A)-H(3AH)	0.9600	C(3"A)-H(3AI)	0.9600

Table S9. (continued)

C(3'A)-H(3AJ)	0.9600	C(3'A)-H(3AK)	0.9600
C(3'A)-H(3AL)	0.9600	C(9B)-C(8B)	1.377(6)
C(9B)-C(10B)	1.408(7)	C(9B)-H(9B)	0.9300
C(10B)-C(11B)	1.369(7)	C(10B)-C(14B)	1.496(7)
O(14B)-C(14B)	1.250(6)	C(14B)-O(15B)	1.269(6)
C(11B)-C(12B)	1.368(7)	C(11B)-H(11B)	0.9300
C(12B)-C(13B)	1.381(7)	C(12B)-H(12B)	0.9300
C(13B)-C(8B)	1.373(7)	C(13B)-H(13B)	0.9300
C(8B)-N(7B)	1.412(6)	N(7B)-C(5B)	1.351(6)
N(7B)-H(7B)	0.8600	C(5B)-C(6B)	1.409(7)
C(5B)-C(4B)	1.427(7)	C(4B)-C(3B)	1.350(7)
C(4B)-N(4B)	1.461(7)	O(4'B)-N(4B)	1.219(6)
O(4B)-N(4B)	1.211(6)	C(3B)-C(2B)	1.377(7)
C(3B)-H(3B)	0.9300	C(2B)-C(1B)	1.413(7)
C(2B)-N(2'B)	1.457(6)	N(2'B)-O(2"B)	1.214(6)
N(2'B)-O(2'B)	1.224(6)	C(1B)-C(6B)	1.354(7)
C(1B)-O(2B)	1.375(6)	C(6B)-H(6B)	0.9300
O(2B)-N(2B)	1.418(5)	N(2B)-N(1B)	1.283(6)
O(1B)-N(1B)	1.223(6)	N(1B)-N(3'B)	1.28(4)
N(1B)-N(3B)	1.425(18)	N(3B)-C(3"B)	1.47(3)
N(3B)-C(3'B)	1.48(3)	C(3'B)-H(3BA)	0.9600
C(3'B)-H(3BB)	0.9600	C(3'B)-H(3BC)	0.9600
C(3"B)-H(3BD)	0.9600	C(3"B)-H(3BE)	0.9600
C(3"B)-H(3BF)	0.9600	N(3'B)-C(3"E)	1.33(7)
N(3'B)-C(3'E)	1.76(6)	C(3'E)-H(3BG)	0.9600
C(3'E)-H(3BH)	0.9600	C(3'E)-H(3BI)	0.9600
C(3"E)-H(3BJ)	0.9600	C(3"E)-H(3BK)	0.9600
C(3"E)-H(3BL)	0.9600	C(9C)-C(8C)	1.378(7)
C(9C)-C(10C)	1.394(7)	C(9C)-H(9C)	0.9300
C(10C)-C(11C)	1.391(7)	C(10C)-C(14C)	1.483(7)
O(14C)-C(14C)	1.260(6)	C(14C)-O(15C)	1.253(6)
C(11C)-C(12C)	1.378(7)	C(11C)-H(11C)	0.9300
C(12C)-C(13C)	1.371(7)	C(12C)-H(12C)	0.9300
C(13C)-C(8C)	1.391(7)	C(13C)-H(13C)	0.9300
C(8C)-N(7C)	1.426(6)	N(7C)-C(5C)	1.356(6)
N(7C)-H(7C)	0.8600	C(5C)-C(6C)	1.396(7)
C(5C)-C(4C)	1.423(7)	C(4C)-C(3C)	1.375(7)
C(4C)-N(4C)	1.431(7)	N(4C)-O(4C)	1.217(6)
N(4C)-O(4'C)	1.235(6)	C(3C)-C(2C)	1.359(8)
C(3C)-H(3C)	0.9300	C(2C)-C(1C)	1.424(7)
C(2C)-N(2'C)	1.463(7)	O(2"C)-N(2'C)	1.227(6)
N(2'C)-O(2'C)	1.207(6)	C(1C)-O(2C)	1.352(6)
C(1C)-C(6C)	1.368(7)	C(6C)-H(6C)	0.9300
O(2C)-N(2C)	1.411(6)	N(2C)-N(1C)	1.270(7)
O(1C)-N(1C)	1.227(6)	N(1C)-N(3C)	1.38(2)
N(1C)-N(3'C)	1.41(2)	N(3C)-C(3"C)	1.28(4)

Table S9. (continued)

N(3C)-C(3'C)	1.42(4)	C(3'C)-H(3CA)	0.9600
C(3'C)-H(3CB)	0.9600	C(3'C)-H(3CC)	0.9600
C(3"C)-H(3CD)	0.9600	C(3"C)-H(3CE)	0.9600
C(3"C)-H(3CF)	0.9600	N(3'C)-C(3"F)	1.40(4)
N(3'C)-C(3'F)	1.52(5)	C(3'F)-H(3CG)	0.9600
C(3'F)-H(3CH)	0.9600	C(3'F)-H(3CI)	0.9600
C(3"F)-H(3CJ)	0.9600	C(3"F)-H(3CK)	0.9600
C(3"F)-H(3CL)	0.9600		
C(10)-C(9)-C(8)	119.2(5)	C(10)-C(9)-H(9)	120.4
C(8)-C(9)-H(9)	120.4	C(9)-C(10)-C(11)	120.4(5)
C(9)-C(10)-C(14)	117.9(5)	C(11)-C(10)-C(14)	121.7(5)
O(14)-C(14)-O(15)	123.0(5)	O(14)-C(14)-C(10)	117.7(5)
O(15)-C(14)-C(10)	119.3(5)	C(12)-C(11)-C(10)	120.5(5)
C(12)-C(11)-H(11)	119.8	C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	120.0(5)	C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0	C(12)-C(13)-C(8)	120.2(5)
C(12)-C(13)-H(13)	119.9	C(8)-C(13)-H(13)	119.9
C(13)-C(8)-C(9)	119.8(5)	C(13)-C(8)-N(7)	118.3(5)
C(9)-C(8)-N(7)	121.8(5)	C(5)-N(7)-C(8)	130.3(4)
C(5)-N(7)-H(7)	114.9	C(8)-N(7)-H(7)	114.9
N(7)-C(5)-C(4)	125.0(4)	N(7)-C(5)-C(6)	119.5(4)
C(4)-C(5)-C(6)	115.5(5)	C(3)-C(4)-C(5)	123.0(5)
C(3)-C(4)-N(4)	118.4(5)	C(5)-C(4)-N(4)	118.5(5)
O(4')-N(4)-O(4)	120.9(5)	O(4')-N(4)-C(4)	121.2(5)
O(4)-N(4)-C(4)	117.7(5)	C(2)-C(3)-C(4)	119.9(5)
C(2)-C(3)-H(3)	120.1	C(4)-C(3)-H(3)	120.1
C(3)-C(2)-C(1)	120.5(5)	C(3)-C(2)-N(2')	116.0(5)
C(1)-C(2)-N(2')	123.5(5)	O(2")-N(2')-O(2')	121.6(6)
O(2")-N(2')-C(2)	120.1(6)	O(2')-N(2')-C(2)	118.3(6)
O(2)-C(1)-C(6)	123.1(4)	O(2)-C(1)-C(2)	117.1(5)
C(6)-C(1)-C(2)	119.7(4)	C(1)-C(6)-C(5)	121.3(4)
C(1)-C(6)-H(6)	119.3	C(5)-C(6)-H(6)	119.3
C(1)-O(2)-N(2)	111.2(4)	N(1)-N(2)-O(2)	106.1(4)
O(1)-N(1)-N(2)	127.0(5)	O(1)-N(1)-N(3')	118.9(9)
N(2)-N(1)-N(3')	110.3(11)	O(1)-N(1)-N(3)	116.2(8)
N(2)-N(1)-N(3)	114.6(9)	N(3')-N(1)-N(3)	37.4(8)
C(3")-N(3')-N(1)	114.1(16)	C(3")-N(3')-C(3"")	126(2)
N(1)-N(3')-C(3"")	105(3)	N(3')-C(3")-H(3AA)	109.5
N(3')-C(3")-H(3AB)	109.5	H(3AA)-C(3")-H(3AB)	109.5
N(3')-C(3")-H(3AC)	109.5	H(3AA)-C(3")-H(3AC)	109.5
H(3AB)-C(3")-H(3AC)	109.5	N(3')-C(3"")-H(3AD)	109.4
N(3')-C(3"")-H(3AE)	109.5	H(3AD)-C(3"")-H(3AE)	109.5
N(3')-C(3"")-H(3AF)	109.5	H(3AD)-C(3"")-H(3AF)	109.5
H(3AE)-C(3"")-H(3AF)	109.5	C(3')-N(3)-N(1)	117.1(12)
C(3')-N(3)-C(3")	112(2)	N(1)-N(3)-C(3")	114(3)

Table S9. (continued)

N(3)-C(3')-H(3'A)	109.5	N(3)-C(3')-H(3'B)	109.5
H(3'A)-C(3')-H(3'B)	109.5	N(3)-C(3')-H(3'C)	109.5
H(3'A)-C(3')-H(3'C)	109.5	H(3'B)-C(3')-H(3'C)	109.5
N(3)-C(3")-H(3"A)	109.5	N(3)-C(3")-H(3"B)	109.4
H(3"A)-C(3")-H(3"B)	109.5	N(3)-C(3")-H(3"C)	109.5
H(3"A)-C(3")-H(3"C)	109.5	H(3"B)-C(3")-H(3"C)	109.5
C(10A)-C(9A)-C(8A)	120.0(4)	C(10A)-C(9A)-H(9A)	120.0
C(8A)-C(9A)-H(9A)	120.0	C(11A)-C(10A)-C(9A)	121.0(5)
C(11A)-C(10A)-C(14A)	120.1(4)	C(9A)-C(10A)-C(14A)	118.9(4)
O(15A)-C(14A)-O(14A)	123.3(5)	O(15A)-C(14A)-C(10A)	120.1(5)
O(14A)-C(14A)-C(10A)	116.5(5)	C(10A)-C(11A)-C(12A)	118.7(5)
C(10A)-C(11A)-H(11A)	120.7	C(12A)-C(11A)-H(11A)	120.7
C(13A)-C(12A)-C(11A)	120.5(5)	C(13A)-C(12A)-H(12A)	119.7
C(11A)-C(12A)-H(12A)	119.7	C(12A)-C(13A)-C(8A)	120.9(5)
C(12A)-C(13A)-H(13A)	119.6	C(8A)-C(13A)-H(13A)	119.5
C(13A)-C(8A)-C(9A)	118.7(4)	C(13A)-C(8A)-N(7A)	118.9(4)
C(9A)-C(8A)-N(7A)	122.3(4)	C(5A)-N(7A)-C(8A)	127.1(4)
C(5A)-N(7A)-H(7A)	116.4	C(8A)-N(7A)-H(7A)	116.5
N(7A)-C(5A)-C(6A)	121.5(4)	N(7A)-C(5A)-C(4A)	122.7(4)
C(6A)-C(5A)-C(4A)	115.8(4)	C(3A)-C(4A)-C(5A)	121.3(4)
C(3A)-C(4A)-N(4A)	115.4(4)	C(5A)-C(4A)-N(4A)	123.2(4)
O(4A)-N(4A)-O(4'A)	121.5(4)	O(4A)-N(4A)-C(4A)	120.3(4)
O(4'A)-N(4A)-C(4A)	118.2(4)	C(2A)-C(3A)-C(4A)	121.2(4)
C(2A)-C(3A)-H(3A)	119.4	C(4A)-C(3A)-H(3A)	119.4
C(3A)-C(2A)-C(1A)	119.2(4)	C(3A)-C(2A)-N(2'A)	117.2(4)
C(1A)-C(2A)-N(2'A)	123.4(4)	O(2'A)-N(2'A)-O(2"A)	119.9(5)
O(2'A)-N(2'A)-C(2A)	120.3(5)	O(2"A)-N(2'A)-C(2A)	119.6(4)
O(2A)-C(1A)-C(6A)	123.4(4)	O(2A)-C(1A)-C(2A)	117.5(4)
C(6A)-C(1A)-C(2A)	119.1(4)	C(1A)-C(6A)-C(5A)	123.2(4)
C(1A)-C(6A)-H(6A)	118.4	C(5A)-C(6A)-H(6A)	118.4
C(1A)-O(2A)-N(2A)	110.2(3)	N(1A)-N(2A)-O(2A)	106.1(4)
O(1A)-N(1A)-N(2A)	126.9(5)	O(1A)-N(1A)-N(3A)	119.8(4)
N(2A)-N(1A)-N(3A)	113.1(5)	N(1A)-N(3A)-C(3"A)	114.1(6)
N(1A)-N(3A)-C(3'A)	115.3(5)	C(3"A)-N(3A)-C(3'A)	118.9(7)
N(3A)-C(3"A)-H(3AG)	109.5	N(3A)-C(3"A)-H(3AH)	109.5
H(3AG)-C(3"A)-H(3AH)	109.5	N(3A)-C(3"A)-H(3AI)	109.5
H(3AG)-C(3"A)-H(3AI)	109.5	H(3AH)-C(3"A)-H(3AI)	109.5
N(3A)-C(3'A)-H(3AJ)	109.5	N(3A)-C(3'A)-H(3AK)	109.5
H(3AJ)-C(3'A)-H(3AK)	109.5	N(3A)-C(3'A)-H(3AL)	109.5
H(3AJ)-C(3'A)-H(3AL)	109.5	H(3AK)-C(3'A)-H(3AL)	109.5
C(8B)-C(9B)-C(10B)	119.1(5)	C(8B)-C(9B)-H(9B)	120.4
C(10B)-C(9B)-H(9B)	120.4	C(11B)-C(10B)-C(9B)	120.2(4)
C(11B)-C(10B)-C(14B)	120.9(5)	C(9B)-C(10B)-C(14B)	118.9(5)
O(14B)-C(14B)-O(15B)	124.0(5)	O(14B)-C(14B)-C(10B)	119.0(5)
O(15B)-C(14B)-C(10B)	117.0(5)	C(12B)-C(11B)-C(10B)	120.2(5)
C(12B)-C(11B)-H(11B)	119.9	C(10B)-C(11B)-H(11B)	119.9

Table S9. (continued)

C(11B)-C(12B)-C(13B)	119.8(5)	C(11B)-C(12B)-H(12B)	120.1
C(13B)-C(12B)-H(12B)	120.1	C(8B)-C(13B)-C(12B)	121.0(5)
C(8B)-C(13B)-H(13B)	119.5	C(12B)-C(13B)-H(13B)	119.5
C(13B)-C(8B)-C(9B)	119.7(5)	C(13B)-C(8B)-N(7B)	116.9(4)
C(9B)-C(8B)-N(7B)	123.3(5)	C(5B)-N(7B)-C(8B)	129.4(4)
C(5B)-N(7B)-H(7B)	115.3	C(8B)-N(7B)-H(7B)	115.3
N(7B)-C(5B)-C(6B)	121.3(4)	N(7B)-C(5B)-C(4B)	122.9(5)
C(6B)-C(5B)-C(4B)	115.8(4)	C(3B)-C(4B)-C(5B)	121.9(5)
C(3B)-C(4B)-N(4B)	116.7(5)	C(5B)-C(4B)-N(4B)	121.4(5)
O(4B)-N(4B)-O(4'B)	122.1(5)	O(4B)-N(4B)-C(4B)	117.7(6)
O(4'B)-N(4B)-C(4B)	120.2(5)	C(4B)-C(3B)-C(2B)	121.4(5)
C(4B)-C(3B)-H(3B)	119.3	C(2B)-C(3B)-H(3B)	119.3
C(3B)-C(2B)-C(1B)	118.2(4)	C(3B)-C(2B)-N(2'B)	117.3(5)
C(1B)-C(2B)-N(2'B)	124.4(5)	O(2"B)-N(2'B)-O(2'B)	123.2(5)
O(2"B)-N(2'B)-C(2B)	118.4(5)	O(2'B)-N(2'B)-C(2B)	118.4(5)
C(6B)-C(1B)-O(2B)	122.5(4)	C(6B)-C(1B)-C(2B)	120.8(5)
O(2B)-C(1B)-C(2B)	116.6(4)	C(1B)-C(6B)-C(5B)	121.8(5)
C(1B)-C(6B)-H(6B)	119.1	C(5B)-C(6B)-H(6B)	119.1
C(1B)-O(2B)-N(2B)	110.0(4)	N(1B)-N(2B)-O(2B)	106.0(4)
O(1B)-N(1B)-N(3'B)	116.9(18)	O(1B)-N(1B)-N(2B)	125.7(5)
N(3'B)-N(1B)-N(2B)	112.1(19)	O(1B)-N(1B)-N(3B)	119.3(8)
N(3'B)-N(1B)-N(3B)	35(3)	N(2B)-N(1B)-N(3B)	114.0(7)
N(1B)-N(3B)-C(3"B)	113.8(13)	N(1B)-N(3B)-C(3'B)	107(2)
C(3"B)-N(3B)-C(3'B)	116.0(17)	N(3B)-C(3'B)-H(3BA)	109.6
N(3B)-C(3'B)-H(3BB)	109.7	H(3BA)-C(3'B)-H(3BB)	109.5
N(3B)-C(3'B)-H(3BC)	109.2	H(3BA)-C(3'B)-H(3BC)	109.5
H(3BB)-C(3'B)-H(3BC)	109.5	N(3B)-C(3"B)-H(3BD)	109.5
N(3B)-C(3"B)-H(3BE)	109.5	H(3BD)-C(3"B)-H(3BE)	109.5
N(3B)-C(3"B)-H(3BF)	109.4	(3BD)-C(3"B)-H(3BF)	109.5
H(3BE)-C(3"B)-H(3BF)	109.5	N(1B)-N(3'B)-C(3"E)	115(5)
N(1B)-N(3'B)-C(3'E)	112(4)	C(3"E)-N(3'B)-C(3'E)	107(4)
N(3'B)-C(3'E)-H(3BG)	109.2	N(3'B)-C(3'E)-H(3BH)	109.5
H(3BG)-C(3'E)-H(3BH)	109.5	N(3'B)-C(3'E)-H(3BI)	109.8
H(3BG)-C(3'E)-H(3BI)	109.5	H(3BH)-C(3'E)-H(3BI)	109.5
N(3'B)-C(3"E)-H(3BJ)	109.4	N(3'B)-C(3"E)-H(3BK)	109.7
H(3BJ)-C(3"E)-H(3BK)	109.5	N(3'B)-C(3"E)-H(3BL)	109.2
H(3BJ)-C(3"E)-H(3BL)	109.5	H(3BK)-C(3"E)-H(3BL)	109.5
C(8C)-C(9C)-C(10C)	119.8(5)	C(8C)-C(9C)-H(9C)	120.1
C(10C)-C(9C)-H(9C)	120.1	C(11C)-C(10C)-C(9C)	120.0(5)
C(11C)-C(10C)-C(14C)	120.2(5)	C(9C)-C(10C)-C(14C)	119.8(4)
O(15C)-C(14C)-O(14C)	122.6(5)	O(15C)-C(14C)-C(10C)	118.8(5)
O(14C)-C(14C)-C(10C)	118.6(5)	C(12C)-C(11C)-C(10C)	119.7(5)
C(12C)-C(11C)-H(11C)	120.1	C(10C)-C(11C)-H(11C)	120.1
C(13C)-C(12C)-C(11C)	120.1(5)	C(13C)-C(12C)-H(12C)	119.9
C(11C)-C(12C)-H(12C)	119.9	C(12C)-C(13C)-C(8C)	120.8(5)
C(12C)-C(13C)-H(13C)	119.6	C(8C)-C(13C)-H(13C)	119.6

Table S9. (continued)

C(9C)-C(8C)-C(13C)	119.5(5)	C(9C)-C(8C)-N(7C)	124.3(4)
C(13C)-C(8C)-N(7C)	115.9(4)	C(5C)-N(7C)-C(8C)	129.8(4)
C(5C)-N(7C)-H(7C)	115.1	C(8C)-N(7C)-H(7C)	115.1
N(7C)-C(5C)-C(6C)	121.9(4)	N(7C)-C(5C)-C(4C)	121.5(5)
C(6C)-C(5C)-C(4C)	116.5(4)	C(3C)-C(4C)-C(5C)	120.5(5)
C(3C)-C(4C)-N(4C)	116.6(5)	C(5C)-C(4C)-N(4C)	122.9(5)
O(4C)-N(4C)-O(4'C)	121.0(5)	O(4C)-N(4C)-C(4C)	118.7(6)
O(4'C)-N(4C)-C(4C)	120.3(5)	C(2C)-C(3C)-C(4C)	121.8(5)
C(2C)-C(3C)-H(3C)	119.1	C(4C)-C(3C)-H(3C)	119.1
C(3C)-C(2C)-C(1C)	119.3(5)	C(3C)-C(2C)-N(2'C)	118.0(5)
C(1C)-C(2C)-N(2'C)	122.7(5)	O(2'C)-N(2'C)-O(2"C)	123.5(5)
O(2'C)-N(2'C)-C(2C)	120.1(5)	O(2"C)-N(2'C)-C(2C)	116.2(5)
O(2C)-C(1C)-C(6C)	123.8(5)	O(2C)-C(1C)-C(2C)	117.6(4)
C(6C)-C(1C)-C(2C)	118.5(5)	C(1C)-C(6C)-C(5C)	123.1(5)
C(1C)-C(6C)-H(6C)	118.4	C(5C)-C(6C)-H(6C)	118.4
C(1C)-O(2C)-N(2C)	110.4(4)	N(1C)-N(2C)-O(2C)	106.1(4)
O(1C)-N(1C)-N(2C)	126.3(5)	O(1C)-N(1C)-N(3C)	118.6(11)
N(2C)-N(1C)-N(3C)	113.3(10)	O(1C)-N(1C)-N(3'C)	115.6(14)
N(2C)-N(1C)-N(3'C)	116.0(11)	N(3C)-N(1C)-N(3'C)	29.5(12)
C(3"C)-N(3C)-N(1C)	115(2)	C(3"C)-N(3C)-C(3'C)	127(3)
N(1C)-N(3C)-C(3'C)	112(2)	N(3C)-C(3'C)-H(3CA)	109.5
N(3C)-C(3'C)-H(3CB)	109.5	H(3CA)-C(3'C)-H(3CB)	109.5
N(3C)-C(3'C)-H(3CC)	109.4	H(3CA)-C(3'C)-H(3CC)	109.5
H(3CB)-C(3'C)-H(3CC)	109.5	N(3C)-C(3"C)-H(3CD)	109.5
N(3C)-C(3"C)-H(3CE)	109.4	H(3CD)-C(3"C)-H(3CE)	109.5
N(3C)-C(3"C)-H(3CF)	109.5	H(3CD)-C(3"C)-H(3CF)	109.5
H(3CE)-C(3"C)-H(3CF)	109.5	N(1C)-N(3'C)-C(3"F)	117(2)
N(1C)-N(3'C)-C(3'F)	115(3)	C(3"F)-N(3'C)-C(3'F)	114(3)
N(3'C)-C(3'F)-H(3CG)	109.5	N(3'C)-C(3'F)-H(3CH)	109.5
H(3CG)-C(3'F)-H(3CH)	109.5	N(3'C)-C(3'F)-H(3CI)	109.5
H(3CG)-C(3'F)-H(3CI)	109.5	H(3CH)-C(3'F)-H(3CI)	109.5
N(3'C)-C(3"F)-H(3CJ)	109.4	N(3'C)-C(3"F)-H(3CK)	109.5
H(3CJ)-C(3"F)-H(3CK)	109.5	N(3'C)-C(3"F)-H(3CL)	109.5
H(3CJ)-C(3"F)-H(3CL)	109.5	H(3CK)-C(3"F)-H(3CL)	109.5

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **6c**. 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}
C(9)	97(4)	65(3)	75(3)	3(2)	-23(3)	9(3)
C(10)	89(4)	62(3)	74(3)	0(2)	-18(3)	5(3)
O(15)	106(3)	73(3)	127(3)	-3(2)	-32(3)	1(2)
C(14)	89(4)	68(3)	89(4)	0(3)	-17(3)	6(3)
O(14)	124(4)	75(3)	147(4)	11(2)	-59(3)	7(2)
C(11)	102(4)	67(3)	78(3)	-6(2)	-20(3)	13(3)
C(12)	90(4)	72(3)	85(3)	1(3)	-20(3)	13(3)
C(13)	102(4)	78(4)	73(3)	5(3)	-27(3)	8(3)
C(8)	119(5)	72(3)	63(3)	-1(2)	-27(3)	-3(3)
N(7)	169(5)	73(3)	81(3)	1(2)	-59(3)	-3(3)
C(5)	112(5)	77(4)	74(3)	-4(3)	-36(3)	2(3)
C(4)	196(8)	82(4)	84(4)	-2(3)	-69(5)	-22(4)
O(4')	1680(60)	129(7)	298(12)	67(8)	-630(30)	-148(17)
O(4)	267(8)	154(5)	94(3)	-12(3)	-61(4)	-79(5)
N(4)	462(16)	103(5)	147(6)	-36(5)	-194(9)	3(7)
C(3)	123(5)	83(4)	89(4)	-20(3)	-33(4)	-10(4)
C(2)	86(4)	57(3)	91(4)	-10(2)	-24(3)	-1(3)
O(2")	279(8)	70(3)	135(4)	-30(3)	-32(5)	-13(4)
N(2')	125(5)	78(4)	114(4)	-1(3)	-37(4)	-9(3)
C(1)	77(3)	69(3)	71(3)	-12(2)	-19(3)	8(3)
O(2')	294(9)	90(4)	147(5)	22(3)	-81(6)	-27(4)
C(6)	76(3)	64(3)	71(3)	-10(2)	-20(2)	6(2)
O(2)	117(3)	70(2)	71(2)	1(2)	-25(2)	-8(2)
N(2)	145(4)	68(3)	61(2)	-8(2)	-20(3)	-5(3)
N(1)	133(5)	87(3)	72(3)	-2(3)	-21(3)	-3(3)
O(1)	185(5)	109(4)	89(3)	25(3)	-36(3)	-20(3)
N(3')	150(20)	130(14)	66(7)	-17(7)	-9(10)	-12(15)
C(3")	290(50)	109(17)	149(19)	-63(16)	-50(30)	-30(30)
C(3"")	100(13)	134(16)	62(12)	-27(12)	-26(11)	-4(13)
N(3)	130(20)	106(10)	70(7)	-29(6)	-29(9)	-4(10)
C(3')	190(30)	85(12)	102(11)	1(9)	-58(15)	-44(14)
C(3")	190(30)	220(40)	79(13)	-65(18)	5(13)	50(20)
C(9A)	86(4)	51(3)	70(3)	-8(2)	-15(2)	-2(2)
C(10A)	82(4)	59(3)	68(3)	-4(2)	-9(2)	6(2)
O(14A)	108(3)	73(3)	143(4)	-4(2)	-50(3)	4(2)
C(14A)	84(4)	57(3)	90(4)	-5(2)	-16(3)	6(3)
O(15A)	113(3)	65(2)	127(3)	6(2)	-32(3)	16(2)
C(11A)	106(4)	47(3)	76(3)	0(2)	-13(3)	-3(3)
C(12A)	126(5)	60(3)	75(3)	-2(2)	-25(3)	-14(3)
C(13A)	100(4)	65(3)	65(3)	-1(2)	-20(3)	-9(3)
C(8A)	107(4)	49(3)	60(3)	-4(2)	-21(3)	-3(3)
N(7A)	115(4)	52(2)	65(2)	-8(2)	-32(2)	6(2)
C(5A)	80(3)	53(3)	62(3)	-5(2)	-18(2)	3(2)

Table S10. (continued)

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(4A)	82(3)	54(3)	62(3)	-3(2)	-25(2)	2(2)
N(4A)	109(4)	63(3)	70(3)	-2(2)	-35(2)	0(2)
O(4'A)	242(6)	72(3)	80(3)	0(2)	-73(3)	-30(3)
O(4A)	156(4)	82(3)	75(2)	21(2)	-46(2)	-28(3)
C(3A)	78(3)	51(3)	73(3)	0(2)	-24(2)	5(2)
C(2A)	82(3)	50(3)	67(3)	-9(2)	-20(2)	2(2)
N(2'A)	125(4)	59(3)	79(3)	-15(2)	-28(3)	8(3)
O(2"A)	227(6)	53(2)	122(4)	0(2)	-55(4)	-3(3)
C(1A)	70(3)	67(3)	59(3)	-7(2)	-16(2)	7(2)
O(2'A)	368(10)	83(3)	126(4)	-18(3)	-125(6)	-17(5)
C(6A)	82(3)	54(3)	60(3)	-4(2)	-15(2)	6(2)
O(2A)	104(3)	66(2)	59(2)	-7(2)	-19(2)	9(2)
N(2A)	115(4)	70(3)	59(2)	4(2)	-17(2)	7(2)
N(1A)	106(4)	87(3)	66(3)	-3(2)	-25(2)	5(3)
O(1A)	201(6)	115(4)	92(3)	-10(3)	-65(3)	-21(4)
N(3A)	194(7)	108(4)	83(3)	23(3)	-50(4)	1(4)
C(3"A)	245(12)	213(11)	156(8)	95(8)	-131(8)	-69(9)
C(3'A)	230(10)	91(5)	123(6)	26(5)	-26(6)	27(6)
C(9B)	94(4)	51(3)	69(3)	-3(2)	-11(3)	6(2)
C(10B)	97(4)	52(3)	73(3)	-13(2)	-10(3)	13(3)
O(14B)	181(5)	69(2)	76(2)	-1(2)	-28(3)	0(3)
C(14B)	104(4)	63(3)	78(3)	-10(3)	-16(3)	9(3)
O(15B)	165(4)	68(2)	85(2)	-18(2)	-24(3)	-6(2)
C(11B)	122(5)	54(3)	86(4)	-5(2)	-13(3)	-2(3)
C(12B)	149(6)	55(3)	87(4)	1(3)	-25(4)	0(3)
C(13B)	126(5)	60(3)	77(3)	-1(2)	-22(3)	8(3)
C(8B)	97(4)	54(3)	78(3)	-4(2)	-20(3)	8(3)
N(7B)	116(4)	54(2)	85(3)	-7(2)	-38(3)	8(2)
C(5B)	102(4)	55(3)	71(3)	-1(2)	-20(3)	-1(3)
C(4B)	101(4)	60(3)	71(3)	-10(2)	-24(3)	-2(3)
O(4'B)	151(4)	91(3)	142(4)	2(3)	-79(3)	8(3)
O(4B)	160(5)	109(4)	165(5)	-22(3)	-82(4)	-20(3)
N(4B)	114(4)	90(4)	102(4)	-7(3)	-48(3)	-9(3)
C(3B)	106(4)	61(3)	75(3)	-8(2)	-18(3)	-15(3)
C(2B)	114(4)	48(3)	70(3)	-8(2)	-12(3)	-1(3)
N(2'B)	139(5)	54(3)	92(3)	-10(2)	-14(3)	-2(3)
O(2"B)	204(6)	62(3)	155(4)	-32(3)	-68(4)	-10(3)
C(1B)	89(4)	55(3)	69(3)	-9(2)	-17(3)	5(2)
O(2'B)	135(4)	61(2)	106(3)	2(2)	-18(3)	6(2)
C(6B)	88(4)	52(3)	69(3)	-8(2)	-15(3)	-3(2)
O(2B)	111(3)	57(2)	97(3)	-16(2)	-32(2)	7(2)
N(2B)	113(4)	64(3)	96(3)	-25(2)	-38(3)	16(3)
O(1B)	159(5)	72(3)	171(5)	-30(3)	-80(4)	38(3)
N(1B)	108(4)	66(3)	104(3)	-22(2)	-39(3)	16(3)

Table S10. (continued)

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(3B)	113(10)	73(8)	116(9)	-22(6)	-38(7)	-3(6)
C(3'B)	230(30)	98(15)	250(30)	-86(16)	-150(20)	22(15)
C(3"B)	83(11)	94(8)	113(10)	-32(8)	-28(8)	12(8)
N(3'B)	120(30)	72(19)	140(40)	-28(19)	-80(30)	3(17)
C(3'E)	87(18)	25(11)	100(20)	-20(12)	-21(17)	13(11)
C(3"E)	100(30)	170(40)	120(30)	60(30)	-60(20)	-60(30)
C(9C)	92(4)	53(3)	74(3)	-2(2)	-6(3)	3(2)
C(10C)	91(4)	59(3)	76(3)	-3(2)	-10(3)	3(3)
O(14C)	182(5)	69(2)	80(2)	0(2)	-30(3)	-3(3)
C(14C)	101(4)	61(3)	75(3)	-1(3)	-5(3)	7(3)
O(15C)	188(5)	68(2)	89(3)	11(2)	-30(3)	8(3)
C(11C)	93(4)	60(3)	88(4)	-2(3)	-8(3)	7(3)
C(12C)	101(4)	56(3)	100(4)	-14(3)	-15(3)	2(3)
C(13C)	93(4)	62(3)	77(3)	-10(2)	-8(3)	4(3)
C(8C)	79(4)	58(3)	77(3)	-10(2)	-10(3)	6(2)
N(7C)	106(4)	59(2)	79(3)	-2(2)	-23(2)	-1(2)
C(5C)	99(4)	51(3)	68(3)	-5(2)	-11(3)	7(3)
C(4C)	91(4)	66(3)	76(3)	-3(2)	-12(3)	19(3)
N(4C)	112(4)	85(4)	107(4)	8(3)	-33(3)	7(3)
O(4'C)	139(4)	98(3)	136(4)	10(3)	-62(3)	-13(3)
O(4C)	158(5)	107(4)	190(5)	27(4)	-94(4)	17(3)
C(3C)	97(4)	60(3)	85(4)	5(3)	-8(3)	14(3)
C(2C)	115(5)	48(3)	75(3)	0(2)	-5(3)	7(3)
O(2"C)	191(5)	58(2)	125(4)	14(2)	-36(3)	18(3)
N(2'C)	128(4)	55(3)	85(3)	3(2)	1(3)	10(3)
C(1C)	95(4)	56(3)	66(3)	-2(2)	-7(3)	2(3)
O(2'C)	134(4)	65(2)	102(3)	-9(2)	-3(3)	0(2)
C(6C)	95(4)	53(3)	68(3)	-2(2)	-11(3)	8(3)
O(2C)	114(3)	57(2)	92(2)	2(2)	-23(2)	0(2)
N(2C)	129(4)	72(3)	92(3)	10(2)	-35(3)	-16(3)
O(1C)	157(5)	80(3)	236(7)	23(4)	-85(5)	-30(3)
N(1C)	126(5)	73(3)	105(4)	5(3)	-29(3)	-9(3)
N(3C)	93(15)	131(15)	114(18)	-6(14)	-39(14)	-30(10)
C(3'C)	140(20)	130(20)	250(40)	120(30)	-100(20)	-25(17)
C(3"C)	160(30)	120(19)	116(18)	44(14)	-11(18)	12(19)
N(3'C)	140(18)	70(9)	84(13)	4(7)	-26(11)	20(10)
C(3'F)	160(30)	68(13)	170(20)	1(16)	-80(18)	-27(15)
C(3"F)	62(12)	130(20)	220(30)	-28(18)	-63(16)	1(10)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **6c**.

	x	y	z	U(eq)
H(9)	-2797	-976	3417	95
H(11)	-2394	-4083	3317	99
H(12)	-770	-4073	3842	99
H(13)	-83	-2510	4129	101
H(7)	-676	-706	4323	128
H(3)	-404	2749	4011	117
H(6)	-1336	-116	3040	85
H(3AA)	-1724	-828	2067	270
H(3AB)	-1730	-1442	1531	270
H(3AC)	-2931	-999	1791	270
H(3AD)	-2435	1057	862	147
H(3AE)	-3486	364	1048	147
H(3AF)	-2444	-105	683	147
H(3'A)	-3048	-614	2142	184
H(3'B)	-2331	-1210	1686	184
H(3'C)	-3707	-988	1643	184
H(3"A)	-2997	-385	755	248
H(3"B)	-1661	-163	852	248
H(3"C)	-2569	757	723	248
H(9A)	2672	-747	1568	82
H(11A)	2229	-3817	1666	91
H(12A)	575	-3611	1135	103
H(13A)	-66	-1991	858	91
H(7A)	555	-234	657	92
H(3A)	833	3220	937	81
H(6A)	1218	222	1942	78
H(3AG)	2735	631	4176	301
H(3AH)	3750	320	3758	301
H(3AI)	3072	-545	4071	301
H(3AJ)	1263	-783	3046	223
H(3AK)	1977	-1400	3482	223
H(3AL)	2650	-953	2980	223
H(9B)	6536	3531	3834	86
H(11B)	5767	519	3974	104
H(12B)	6277	533	4852	116
H(13B)	6977	2020	5212	105
H(7B)	7960	3612	4990	101
H(3B)	7770	7069	5180	96
H(6B)	5566	4672	4334	83
H(3BA)	2857	3927	3191	281
H(3BB)	3768	4190	3624	281
H(3BC)	3859	4707	3058	281
H(3BD)	1128	6259	3301	144

Table S11. (continued)

	x	y	z	U(eq)
H(3BE)	1228	5206	2992	144
H(3BF)	2096	6091	2843	144
H(3BG)	3729	4058	3581	107
H(3BH)	3082	3945	3042	107
H(3BI)	2334	4060	3577	107
H(3BJ)	1785	6637	3135	193
H(3BK)	1306	5577	3343	193
H(3BL)	1854	5664	2764	193
H(9C)	3873	3627	1223	87
H(11C)	4477	527	1144	96
H(12C)	3895	563	272	103
H(13C)	3303	2108	-121	93
H(7C)	2439	3785	37	98
H(3C)	2416	7250	-125	98
H(6C)	4675	4746	750	86
H(3CA)	6193	4458	1569	259
H(3CB)	6711	4234	2132	259
H(3CC)	7505	4011	1619	259
H(3CD)	8472	6449	1836	200
H(3CE)	8916	5282	1887	200
H(3CF)	8200	5823	2361	200
H(3CG)	7758	3892	1914	197
H(3CH)	6909	3980	1431	197
H(3CI)	6501	4461	1981	197
H(3CJ)	8782	6374	1817	204
H(3CK)	9238	5222	1916	204
H(3CL)	8210	5719	2280	204

Table S12. Torsion angles [°] for **6c**.

C(8)-C(9)-C(10)-C(11)	1.0(9)
C(8)-C(9)-C(10)-C(14)	-177.6(5)
C(9)-C(10)-C(14)-O(14)	3.4(9)
C(11)-C(10)-C(14)-O(14)	-175.2(6)
C(9)-C(10)-C(14)-O(15)	-175.8(6)
C(11)-C(10)-C(14)-O(15)	5.6(9)
C(9)-C(10)-C(11)-C(12)	0.3(9)
C(14)-C(10)-C(11)-C(12)	178.8(6)
C(10)-C(11)-C(12)-C(13)	-1.7(9)
C(11)-C(12)-C(13)-C(8)	1.8(9)
C(12)-C(13)-C(8)-C(9)	-0.5(9)
C(12)-C(13)-C(8)-N(7)	177.5(6)
C(10)-C(9)-C(8)-C(13)	-0.9(9)
C(10)-C(9)-C(8)-N(7)	-178.8(6)
C(13)-C(8)-N(7)-C(5)	144.5(7)
C(9)-C(8)-N(7)-C(5)	-37.6(11)
C(8)-N(7)-C(5)-C(4)	170.5(7)
C(8)-N(7)-C(5)-C(6)	-11.3(11)
N(7)-C(5)-C(4)-C(3)	178.6(7)
C(6)-C(5)-C(4)-C(3)	0.4(11)
N(7)-C(5)-C(4)-N(4)	-4.7(12)
C(6)-C(5)-C(4)-N(4)	177.1(6)
C(3)-C(4)-N(4)-O(4')	168.0(9)
C(5)-C(4)-N(4)-O(4')	-8.9(11)
C(3)-C(4)-N(4)-O(4)	-7.7(10)
C(5)-C(4)-N(4)-O(4)	175.4(6)
C(5)-C(4)-C(3)-C(2)	2.3(12)
N(4)-C(4)-C(3)-C(2)	-174.5(6)
C(4)-C(3)-C(2)-C(1)	-3.3(10)
C(4)-C(3)-C(2)-N(2')	175.9(7)
C(3)-C(2)-N(2')-O(2")	-14.5(10)
C(1)-C(2)-N(2')-O(2")	164.7(7)
C(3)-C(2)-N(2')-O(2')	163.5(7)
C(1)-C(2)-N(2')-O(2')	-17.3(10)
C(3)-C(2)-C(1)-O(2)	-179.7(6)
N(2')-C(2)-C(1)-O(2)	1.0(9)
C(3)-C(2)-C(1)-C(6)	1.7(9)
N(2')-C(2)-C(1)-C(6)	-177.5(5)
O(2)-C(1)-C(6)-C(5)	-177.4(5)
C(2)-C(1)-C(6)-C(5)	1.0(8)
N(7)-C(5)-C(6)-C(1)	179.7(6)
C(4)-C(5)-C(6)-C(1)	-2.0(9)
C(6)-C(1)-O(2)-N(2)	3.9(7)
C(2)-C(1)-O(2)-N(2)	-174.6(5)
C(1)-O(2)-N(2)-N(1)	179.9(5)
O(2)-N(2)-N(1)-O(1)	2.8(9)

Table S12. (continued)

O(2)-N(2)-N(1)-N(3')	160(2)
O(2)-N(2)-N(1)-N(3)	-159.4(17)
O(1)-N(1)-N(3')-C(3'')	179(2)
N(2)-N(1)-N(3')-C(3'')	20(2)
N(3)-N(1)-N(3')-C(3'')	-85(3)
O(1)-N(1)-N(3')-C(3''')	-39(4)
N(2)-N(1)-N(3')-C(3''')	161(2)
N(3)-N(1)-N(3')-C(3''')	57(4)
O(1)-N(1)-N(3)-C(3')	-175.7(15)
N(2)-N(1)-N(3)-C(3')	-11(2)
N(3')-N(1)-N(3)-C(3')	80(2)
O(1)-N(1)-N(3)-C(3'')	50(4)
N(2)-N(1)-N(3)-C(3'')	-146(3)
N(3')-N(1)-N(3)-C(3'')	-54(4)
C(8A)-C(9A)-C(10A)-C(11A)	1.0(8)
C(8A)-C(9A)-C(10A)-C(14A)	-178.2(5)
C(11A)-C(10A)-C(14A)-O(15A)	3.7(8)
C(9A)-C(10A)-C(14A)-O(15A)	-177.1(5)
C(11A)-C(10A)-C(14A)-O(14A)	-174.1(5)
C(9A)-C(10A)-C(14A)-O(14A)	5.1(8)
C(9A)-C(10A)-C(11A)-C(12A)	0.0(8)
C(14A)-C(10A)-C(11A)-C(12A)	179.2(5)
C(10A)-C(11A)-C(12A)-C(13A)	-1.4(9)
C(11A)-C(12A)-C(13A)-C(8A)	1.9(9)
C(12A)-C(13A)-C(8A)-C(9A)	-0.9(8)
C(12A)-C(13A)-C(8A)-N(7A)	175.8(5)
C(10A)-C(9A)-C(8A)-C(13A)	-0.5(8)
C(10A)-C(9A)-C(8A)-N(7A)	-177.2(5)
C(13A)-C(8A)-N(7A)-C(5A)	148.0(5)
C(9A)-C(8A)-N(7A)-C(5A)	-35.4(9)
C(8A)-N(7A)-C(5A)-C(6A)	-14.7(9)
C(8A)-N(7A)-C(5A)-C(4A)	164.7(5)
N(7A)-C(5A)-C(4A)-C(3A)	-178.0(5)
C(6A)-C(5A)-C(4A)-C(3A)	1.5(8)
N(7A)-C(5A)-C(4A)-N(4A)	-0.4(8)
C(6A)-C(5A)-C(4A)-N(4A)	179.0(5)
C(3A)-C(4A)-N(4A)-O(4A)	16.5(8)
C(5A)-C(4A)-N(4A)-O(4A)	-161.2(5)
C(3A)-C(4A)-N(4A)-O(4'A)	-165.0(5)
C(5A)-C(4A)-N(4A)-O(4'A)	17.3(8)
C(5A)-C(4A)-C(3A)-C(2A)	0.3(8)
N(4A)-C(4A)-C(3A)-C(2A)	-177.4(5)
C(4A)-C(3A)-C(2A)-C(1A)	-0.2(8)
C(4A)-C(3A)-C(2A)-N(2'A)	175.6(5)
C(3A)-C(2A)-N(2'A)-O(2'A)	-169.0(7)
C(1A)-C(2A)-N(2'A)-O(2'A)	6.6(10)

Table S12. (continued)

C(3A)-C(2A)-N(2'A)-O(2"A)	6.4(9)
C(1A)-C(2A)-N(2'A)-O(2"A)	-178.0(6)
C(3A)-C(2A)-C(1A)-O(2A)	178.9(5)
N(2'A)-C(2A)-C(1A)-O(2A)	3.5(8)
C(3A)-C(2A)-C(1A)-C(6A)	-1.9(8)
N(2'A)-C(2A)-C(1A)-C(6A)	-177.3(5)
O(2A)-C(1A)-C(6A)-C(5A)	-176.9(5)
C(2A)-C(1A)-C(6A)-C(5A)	3.9(8)
N(7A)-C(5A)-C(6A)-C(1A)	175.8(5)
C(4A)-C(5A)-C(6A)-C(1A)	-3.6(8)
C(6A)-C(1A)-O(2A)-N(2A)	2.6(7)
C(2A)-C(1A)-O(2A)-N(2A)	-178.3(4)
C(1A)-O(2A)-N(2A)-N(1A)	174.4(5)
O(2A)-N(2A)-N(1A)-O(1A)	-2.1(8)
O(2A)-N(2A)-N(1A)-N(3A)	172.8(5)
O(1A)-N(1A)-N(3A)-C(3"A)	-31.8(11)
N(2A)-N(1A)-N(3A)-C(3"A)	153.0(8)
O(1A)-N(1A)-N(3A)-C(3'A)	-174.6(7)
N(2A)-N(1A)-N(3A)-C(3'A)	10.1(10)
C(8B)-C(9B)-C(10B)-C(11B)	-0.2(9)
C(8B)-C(9B)-C(10B)-C(14B)	-179.8(5)
C(11B)-C(10B)-C(14B)-O(14B)	173.9(6)
C(9B)-C(10B)-C(14B)-O(14B)	-6.4(9)
C(11B)-C(10B)-C(14B)-O(15B)	-8.4(9)
C(9B)-C(10B)-C(14B)-O(15B)	171.3(5)
C(9B)-C(10B)-C(11B)-C(12B)	1.5(9)
C(14B)-C(10B)-C(11B)-C(12B)	-178.8(6)
C(10B)-C(11B)-C(12B)-C(13B)	-1.9(10)
C(11B)-C(12B)-C(13B)-C(8B)	1.0(10)
C(12B)-C(13B)-C(8B)-C(9B)	0.4(10)
C(12B)-C(13B)-C(8B)-N(7B)	-175.3(6)
C(10B)-C(9B)-C(8B)-C(13B)	-0.8(9)
C(10B)-C(9B)-C(8B)-N(7B)	174.6(5)
C(13B)-C(8B)-N(7B)-C(5B)	-139.7(6)
C(9B)-C(8B)-N(7B)-C(5B)	44.8(9)
C(8B)-N(7B)-C(5B)-C(6B)	1.5(10)
C(8B)-N(7B)-C(5B)-C(4B)	-179.1(6)
N(7B)-C(5B)-C(4B)-C(3B)	178.1(6)
C(6B)-C(5B)-C(4B)-C(3B)	-2.4(9)
N(7B)-C(5B)-C(4B)-N(4B)	-1.8(9)
C(6B)-C(5B)-C(4B)-N(4B)	177.6(5)
C(3B)-C(4B)-N(4B)-O(4B)	2.5(9)
C(5B)-C(4B)-N(4B)-O(4B)	-177.5(6)
C(3B)-C(4B)-N(4B)-O(4'B)	-176.7(6)
C(5B)-C(4B)-N(4B)-O(4'B)	3.3(9)
C(5B)-C(4B)-C(3B)-C(2B)	0.1(9)

Table S12. (continued)

N(4B)-C(4B)-C(3B)-C(2B)	-180.0(5)
C(4B)-C(3B)-C(2B)-C(1B)	1.5(9)
C(4B)-C(3B)-C(2B)-N(2'B)	-176.8(5)
C(3B)-C(2B)-N(2'B)-O(2"B)	-10.8(9)
C(1B)-C(2B)-N(2'B)-O(2"B)	171.0(6)
C(3B)-C(2B)-N(2'B)-O(2'B)	167.2(6)
C(1B)-C(2B)-N(2'B)-O(2'B)	-11.0(9)
C(3B)-C(2B)-C(1B)-C(6B)	-0.7(9)
N(2'B)-C(2B)-C(1B)-C(6B)	177.5(5)
C(3B)-C(2B)-C(1B)-O(2B)	176.0(5)
N(2'B)-C(2B)-C(1B)-O(2B)	-5.8(8)
O(2B)-C(1B)-C(6B)-C(5B)	-178.3(5)
C(2B)-C(1B)-C(6B)-C(5B)	-1.8(9)
N(7B)-C(5B)-C(6B)-C(1B)	-177.3(5)
C(4B)-C(5B)-C(6B)-C(1B)	3.3(8)
C(6B)-C(1B)-O(2B)-N(2B)	-8.3(7)
C(2B)-C(1B)-O(2B)-N(2B)	175.1(5)
C(1B)-O(2B)-N(2B)-N(1B)	174.0(5)
O(2B)-N(2B)-N(1B)-O(1B)	-1.3(9)
O(2B)-N(2B)-N(1B)-N(3'B)	152(4)
O(2B)-N(2B)-N(1B)-N(3B)	-169.9(11)
O(1B)-N(1B)-N(3B)-C(3"B)	32(2)
N(3'B)-N(1B)-N(3B)-C(3"B)	-64(3)
N(2B)-N(1B)-N(3B)-C(3"B)	-158.2(13)
O(1B)-N(1B)-N(3B)-C(3'B)	162(2)
N(3'B)-N(1B)-N(3B)-C(3'B)	66(4)
N(2B)-N(1B)-N(3B)-C(3'B)	-29(3)
O(1B)-N(1B)-N(3'B)-C(3"E)	-33(7)
N(2B)-N(1B)-N(3'B)-C(3"E)	172(4)
N(3B)-N(1B)-N(3'B)-C(3"E)	71(6)
O(1B)-N(1B)-N(3'B)-C(3'E)	-155(3)
N(2B)-N(1B)-N(3'B)-C(3'E)	49(6)
N(3B)-N(1B)-N(3'B)-C(3'E)	-52(4)
C(8C)-C(9C)-C(10C)-C(11C)	-0.3(9)
C(8C)-C(9C)-C(10C)-C(14C)	179.9(5)
C(11C)-C(10C)-C(14C)-O(15C)	-10.6(9)
C(9C)-C(10C)-C(14C)-O(15C)	169.3(6)
C(11C)-C(10C)-C(14C)-O(14C)	170.5(6)
C(9C)-C(10C)-C(14C)-O(14C)	-9.7(9)
C(9C)-C(10C)-C(11C)-C(12C)	1.2(9)
C(14C)-C(10C)-C(11C)-C(12C)	-179.0(6)
C(10C)-C(11C)-C(12C)-C(13C)	-0.7(9)
C(11C)-C(12C)-C(13C)-C(8C)	-0.6(9)
C(10C)-C(9C)-C(8C)-C(13C)	-1.1(8)
C(10C)-C(9C)-C(8C)-N(7C)	173.0(5)
C(12C)-C(13C)-C(8C)-C(9C)	1.6(9)

Table S12. (continued)

C(12C)-C(13C)-C(8C)-N(7C)	-173.0(5)
C(9C)-C(8C)-N(7C)-C(5C)	36.2(9)
C(13C)-C(8C)-N(7C)-C(5C)	-149.5(6)
C(8C)-N(7C)-C(5C)-C(6C)	7.4(9)
C(8C)-N(7C)-C(5C)-C(4C)	-176.9(5)
N(7C)-C(5C)-C(4C)-C(3C)	-179.7(5)
C(6C)-C(5C)-C(4C)-C(3C)	-3.8(8)
N(7C)-C(5C)-C(4C)-N(4C)	-0.5(9)
C(6C)-C(5C)-C(4C)-N(4C)	175.4(5)
C(3C)-C(4C)-N(4C)-O(4C)	5.0(9)
C(5C)-C(4C)-N(4C)-O(4C)	-174.2(6)
C(3C)-C(4C)-N(4C)-O(4'C)	-175.5(6)
C(5C)-C(4C)-N(4C)-O(4'C)	5.2(10)
C(5C)-C(4C)-C(3C)-C(2C)	-0.3(9)
N(4C)-C(4C)-C(3C)-C(2C)	-179.6(6)
C(4C)-C(3C)-C(2C)-C(1C)	4.9(9)
C(4C)-C(3C)-C(2C)-N(2'C)	-177.0(5)
C(3C)-C(2C)-N(2'C)-O(2'C)	172.2(6)
C(1C)-C(2C)-N(2'C)-O(2'C)	-9.7(9)
C(3C)-C(2C)-N(2'C)-O(2"C)	-3.2(8)
C(1C)-C(2C)-N(2'C)-O(2"C)	174.9(5)
C(3C)-C(2C)-C(1C)-O(2C)	175.4(5)
N(2'C)-C(2C)-C(1C)-O(2C)	-2.7(8)
C(3C)-C(2C)-C(1C)-C(6C)	-5.2(8)
N(2'C)-C(2C)-C(1C)-C(6C)	176.8(5)
O(2C)-C(1C)-C(6C)-C(5C)	-179.6(5)
C(2C)-C(1C)-C(6C)-C(5C)	1.0(8)
N(7C)-C(5C)-C(6C)-C(1C)	179.3(5)
C(4C)-C(5C)-C(6C)-C(1C)	3.4(8)
C(6C)-C(1C)-O(2C)-N(2C)	-6.1(7)
C(2C)-C(1C)-O(2C)-N(2C)	173.3(5)
C(1C)-O(2C)-N(2C)-N(1C)	174.0(5)
O(2C)-N(2C)-N(1C)-O(1C)	-4.8(10)
O(2C)-N(2C)-N(1C)-N(3C)	160(3)
O(2C)-N(2C)-N(1C)-N(3'C)	-167(2)
O(1C)-N(1C)-N(3C)-C(3"C)	-19(5)
N(2C)-N(1C)-N(3C)-C(3"C)	175(3)
N(3'C)-N(1C)-N(3C)-C(3"C)	73(4)
O(1C)-N(1C)-N(3C)-C(3'C)	-173(3)
N(2C)-N(1C)-N(3C)-C(3'C)	21(5)
N(3'C)-N(1C)-N(3C)-C(3'C)	-81(6)
O(1C)-N(1C)-N(3'C)-C(3"F)	32(4)
N(2C)-N(1C)-N(3'C)-C(3"F)	-163(3)
N(3C)-N(1C)-N(3'C)-C(3"F)	-71(3)
O(1C)-N(1C)-N(3'C)-C(3'F)	170(2)
N(2C)-N(1C)-N(3'C)-C(3'F)	-25(3)

Table S12. (continued)

N(3C)-N(1C)-N(3'C)-C(3'F)	67(5)

Table S13. IC_{50} Values (μM) for Compounds **6a** – **6d** in the HL-60 and NIH 3T3 Cell Lines

Compound	HL-60	NIH3T3
6a	6.3	5.6
6b	9.1	73
6c	10.1	80
6d	11.6	83

Descriptions of Methods Used to Collect Data for Table S13

Cell Culture for the HL-60 Screen. Human myeloid leukemia HL-60 cells (ATCC, Manassas, VA) were cultured in RPMI-1640 medium supplemented with 10% fetal bovine serum and penicillin/streptomycin. Cells were cultured at 37 °C in a 5% CO_2- humidified atmosphere. Cultures were initiated in 96-well plates in a total volume of 100 μL. Five millimolar stock solutions of each compound were made in dimethyl sulfoxide (DMSO) and serially diluted in phosphate buffered saline (PBS) before addition to the cultures. Dose-response cultures were established with concentrations ranging from 0 to 100 μM. The final concentration of DMSO added to the cultures was 0.1% or less. For each experiment, compounds were added to cells in logarithmic phase growth. Three days after addition of the compounds, cell viability was measured as described below. For each compound screened, at least three replicates were collected.

Cell Viability Assay for the HL-60 Screen. Cell viability was determined using the CellTiter 96 assay from Promega (Madison, WI) using 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium, inner salt (MTS), mixed with an electron coupling reagent, phenazine ethosulfate (PES). Seventy two hours after adding compounds to the cultures, 20 μL of the MTS reagent was added to each well and the plate was further incubated for 3-4 hours at 37 ^{o}C, whereupon spectrophotometric absorbance of samples was measured at 495 nm. The IC_{50} of each compound was determined from growth curves generated by expressing the absorbance of each variable as a percentage of untreated controls.

Cytotoxicity Assays in NIH3T3 Cells. Ten thousand NIH3T3 cells were seeded in 96-well plates in 50 μL of medium. Increasing drug concentrations were added to a

final volume of 100 μL and the cells were maintained in drug for 72 h. Following drug exposure, cell viability was assayed by the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) conversion assay. Each drug concentration was represented in quadruplicate and the experiments were repeated in three independent replicates. Mean values and S.E. were computed for each group.

Table S14. Dependence of First-Order Rate Constants for Reaction of **6a** - **6d** with Glutathione in 0.10 M Phosphate Buffer on Glutathione Concentration.

6a		**6b**		**6c**		**6d**	
[GSH] (mM)	k_{obs} (s^{-1}) [a]	[GSH] (mM)	k_{obs} (s^{-1}) [b]	[GSH] (mM)	k_{obs} (s^{-1}) [b]	[GSH] (mM)	k_{obs} (s^{-1}) [b]
2.50	1.36×10^{-3}	0.50	4.16×10^{-5}	2.00	6.58×10^{-5}	0.50	1.76×10^{-4}
5.00	1.72×10^{-3}	2.00	7.51×10^{-5}	5.00	1.74×10^{-4}	1.00	2.11×10^{-4}
10.0	3.75×10^{-3}	5.00	2.51×10^{-4}	10.0	4.66×10^{-4}	2.00	3.58×10^{-4}
20.0	6.50×10^{-3}	7.50	3.42×10^{-4}	15.0	7.76×10^{-4}	3.00	4.74×10^{-4}
		10.0	4.27×10^{-4}	20.0	9.38×10^{-4}	5.00	7.47×10^{-4}

[a] Measured by following loss of substrate by HPLC at room temperature. [b] Measured by UV spectrophotometry at the λ_{max} of the glutathione conjugate (**6b** at 341 nm, **6c** at 335 nm, **6d** at 346 nm) at 37 °C. Data fitting and statistical analysis ($k_{obs} = k_{GSH}[GSH] + k_{hydrolysis}$) using Microsoft EXCEL.

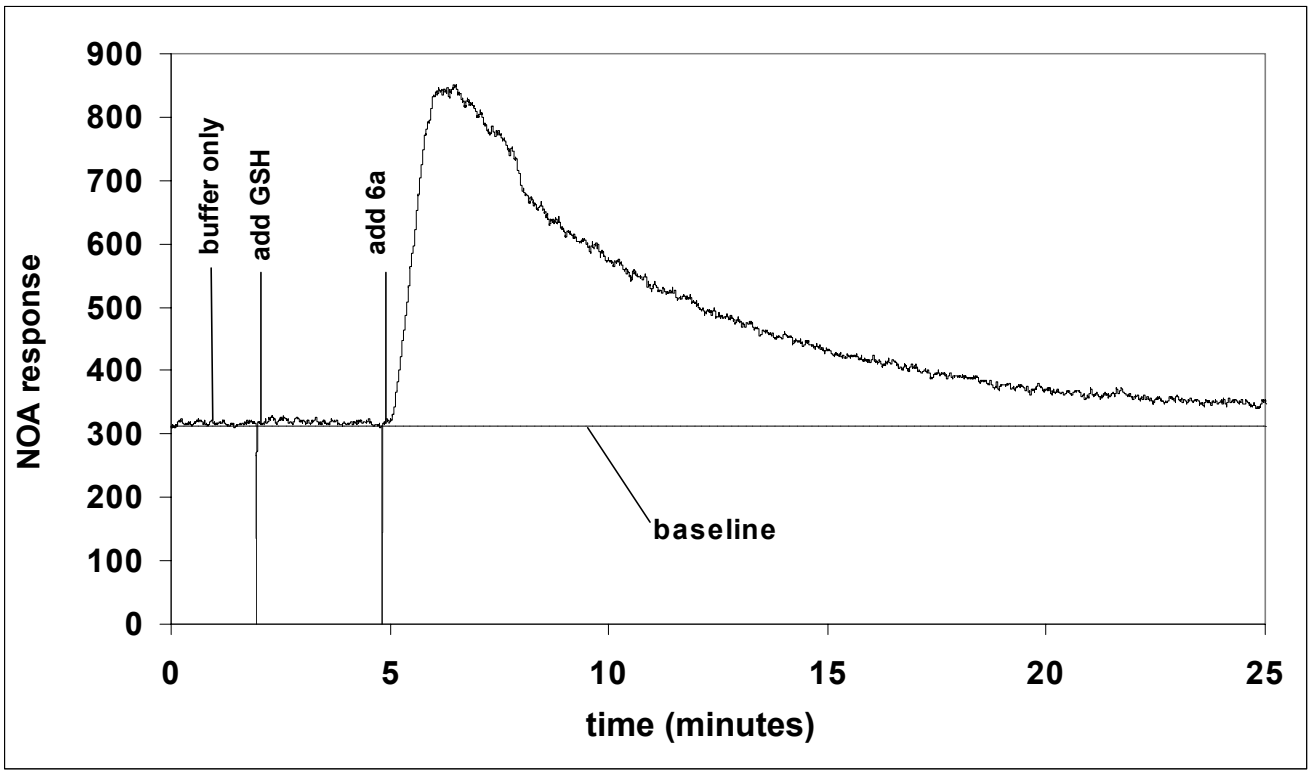

Figure S2. Nitric oxide generation during reaction of the GSH with **6a**. Buffer (1.8 mL of 0.1 M sodium phosphate, pH 7.4) at 37 °C was purged with argon beginning at time 0 to remove oxygen, with effluent gases being passed into a chemiluminescence detector (NOA = Nitric Oxide Analyzer) for quantitation of NO production in the solution. GSH (final concentration 200 μM) and **6a** at a final concentration of 0.5 μM were injected into the reaction chamber at the indicated times. NO was detected only when GSH and **6a** were present in the reaction mixture at the same time.

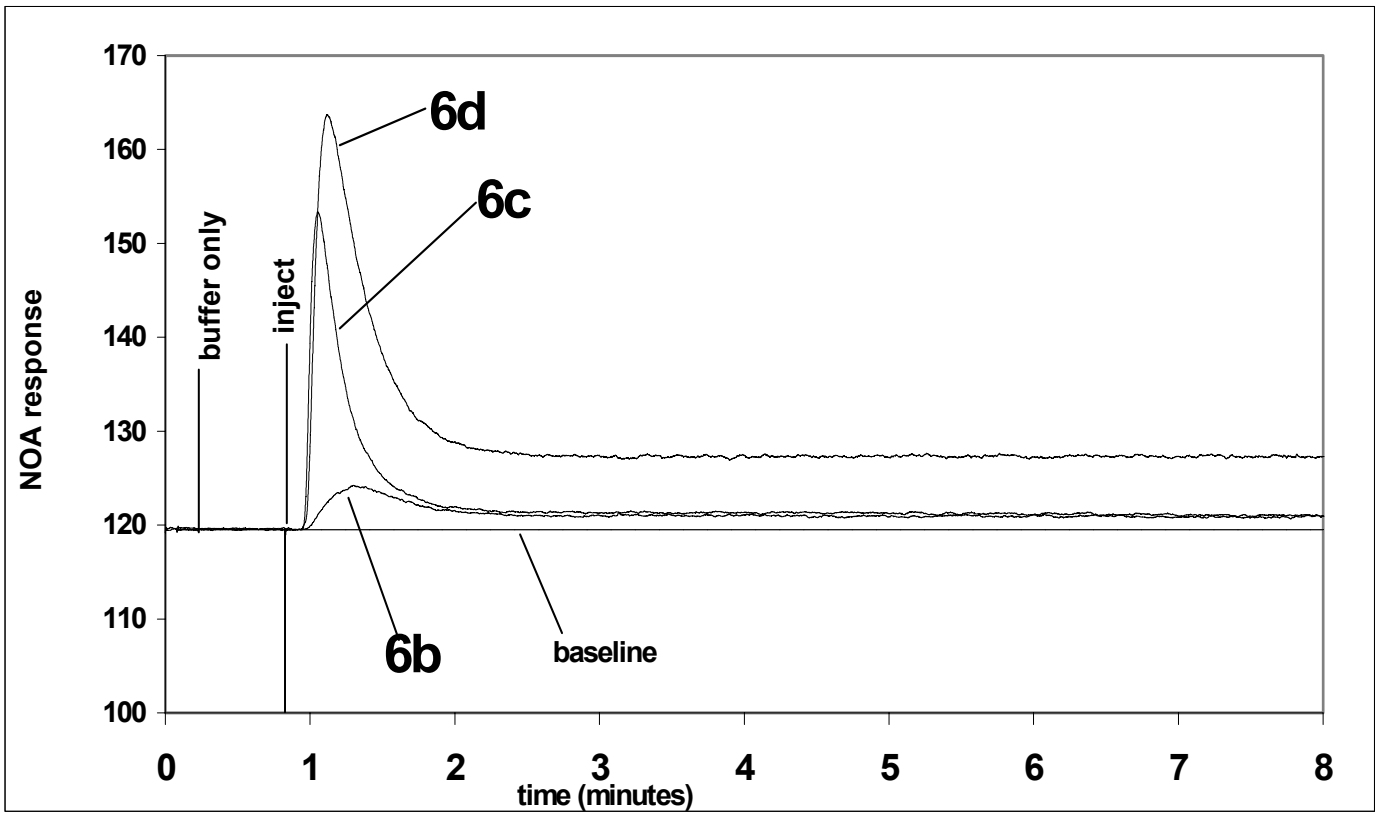

Figure S3. Nitric oxide generation during reaction of the GSH with **6b – 6d**. Buffer (1.8 mL of 0.1 M sodium phosphate, pH 7.4) at 37 °C was purged with argon beginning at time 0 to remove oxygen, with effluent gases being passed into a chemiluminescence detector (NOA = Nitric Oxide Analyzer) for quantitation of NO production in the solution. Solutions of GSH with **6b**, **6c**, and **6d** were prepared individually in buffer and injected (within 20 s of dissolution) into the purging buffer as indicated by the arrow, such that the final concentrations were 100 μM in GSH and 10 μM in **6b**, **6c**, or **6d**. NO was detected only when GSH and the PABA/NO analogues were present in the reaction mixture at the same time.