Supporting information

Novel Cyano- and *N*-isopropylamidino-Substituted Derivatives of Benzo[b]thiophene-2-carboxanilides and Benzo[b]thieno[2,3-*c*]quinolones: Synthesis, Photochemical Synthesis, Crystal Structure Determination and Antitumor Evaluation. Part 2.

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Contents:

1.

Compound	Elemental Analysis		
		calcd. (%)	found (%)
2a	C	59.05	59.27
	H	3.50	3.61
	N	4.05	3.86
3a	C	66.01	66.23
	H	3.58	3.69
	N	4.53	4.68
4a	C	61.38	61.24
	H	2.90	3.00
	N	8.96	9.20
4b	C	60.45	55.72
	H	2.39	2.26
	N	12.44	12.21
5a	C	55.88	55.66
	H	4.69	4.47
	N	10.29	10.19
5b	C	56.87	56.72
	H	5.01	4.95
	N	9.95	10.04

5c	C	54.80	53.68
	H	4.54	4.34
	N	9.59	9.41
5d	C	54.08	53.78
	H	4.83	4.97
	N	9.01	9.03
5e	C	46.84	46.90
	H	3.72	3.71
	N	8.62	8.64
5f	C	55.43	55.21
	H	4.19	3.88
	N	12.93	12.76
5g	C	52.23	52.00
	H	5.33	5.03
	N	13.24	13.13
6a	C	61.36	61.15
	H	4.88	4.67
	N	11.30	11.11
6b	C	62.24	61.75
	H	5.22	5.10
	N	10.89	10.68
6c	C	59.77	59.50
	H	5.02	4.96
	N	10.45	10.10
6d	C	58.67	58.78
	H	4.69	4.82
	N	9.77	10.03
6e	C	50.62	50.67
	H	3.80	3.58
	N	9.32	9.44
6f	C	60.52	60.68
	H	4.32	4.45
	N	14.12	14.18
6g	C	56.09	56.42
	H	5.53	5.79
	N	14.22	14.13
7a	C	61.38	61.46
	H	2.90	3.18
	N	8.96	8.90
7b	C	62.48	62.42
	H	3.39	3.27
	N	8.57	8.29
7c	C	59.56	59.54
	H	3.23	3.13
	N	8.17	8.03
7d	C	58.30	58.02
	H	2.99	3.04
	N	7.55	7.70
	C	50.22	50.34

7e	H	2.11	1.85
	N	7.32	7.16
8a	C	55.88	55.65
	H	4.69	4.61
	N	10.29	10.23
8b	C	56.87	56.53
	H	5.01	4.79
	N	9.95	9.85
8c	C	54.80	54.43
	H	4.83	4.63
	N	9.59	9.53
8d	C	54.08	54.14
	H	4.54	4.71
	N	9.01	8.87
8e	C	46.84	46.86
	H	3.72	3.88
	N	8.62	8.39
9a	C	61.36	61.25
	H	4.88	4.87
	N	11.30	11.31
9b	C	62.24	62.08
	H	5.22	5.31
	N	10.89	11.00
9b	C	62.24	62.08
	H	5.22	5.31
	N	10.89	11.00
9c	C	58.67	58.41
	H	4.69	4.64
	N	9.77	9.55
9d	C	50.62	50.68
	H	3.80	3.97
	N	9.32	9.45

2.

X-ray crystal structure analysis

Data were collected on Oxford Diffraction Xcalibur2 diffractometer with Sapphire 3 CCD detector at ambient temperature and controlled by the program CrysAlis Software system, Version 1.4, 2004. Data reduction has been applied by the same program. The data have been corrected for Lorentz-polarization, but not for absorption effects.

The structures were solved by direct methods. Due to the poorer crystal quality only reflections up to $2\theta \leq 45^{o}$ have been included into the refinement process. Refinement procedure by full-matrix least squares methods based on F^2 values against all reflections included anisotropic displacement parameters for all non-H atoms. The positions of hydrogen atoms belonging to the phenyl Csp^2 and methyl Csp^3 atoms were geometrically optimized applying the riding model [Csp^2-H, Csp^3-H, 0.93 and 0.96 Å, respectively; U_{iso}(H) = 1.2 (for Csp^2 and 1.5 for Csp^3 Ueq(C)]. The hydrogen atoms belonging to the all nitrogen N atoms have been found in the electron-density Fourier maps and refined freely (being in the range N- H = 0.74(7) - 1.04(9) Å).

Calculations were performed with SHELXS97 and SHELXL97. The molecular graphics were done with PLATON98.

3.

Selected crystallographic data

	9a
Compound	
Formula	C19 H18 N3 O S, Cl
M_r	371.88
Diffractometer	Oxford Diffraction Xcalibur2 diffractometer with Sapphire 3 CCD detector
Crystal system, space group	Monoclinic, *P* 2_1/c (No. 14)
Unit cell parameters:	
a (Å)	13.465(3)
b (Å)	21.422(4)
c (Å)	14.034(4)
β/°	107.97(2)
V (Å^3)	3850.6(16)
Z	8
D_c (gcm^{-3})	1.283
Radiation, λ (Å)	MoK$_\alpha$ = 0.71073
No. measured reflections	28658
No. independent reflections (R_{int})	4954, 0.080
No. observed reflections, $I \geq 2\sigma(I)$	4312
Method of collection of intenisty data	combination of ω and φ scan
Methods of structure solution and and refinemnet	Direct methods (SHELXS97) Least-squares method (SHELXL97)
R, wR, S	0.1082, 0.2895, 1.12
Min., max. electron density (e Å^{-3})	-0.53, 0.64

Parameters of the non-Hydrogen atoms for: 9a

Atom	x	y	z	U(eq) [Ang^2]
S1	0.02434(12)	0.29607(8)	0.77999(12)	0.0661(6)
O1	-0.0321(3)	0.1593(2)	0.7548(4)	0.0793(17)
N11	0.1346(4)	0.1236(3)	0.8223(4)	0.0666(19)
N12	0.1341(5)	0.5413(3)	0.7895(5)	0.078(2)
N13	0.2824(4)	0.5458(2)	0.9232(4)	0.074(2)
C11	0.2097(5)	0.5142(3)	0.8572(5)	0.068(2)
C12	0.2159(4)	0.4446(3)	0.8578(4)	0.0571(17)
C13	0.1252(4)	0.4102(3)	0.8236(4)	0.0608(19)
C14	0.1306(4)	0.3448(3)	0.8227(4)	0.0519(17)
C15	0.2269(4)	0.3129(3)	0.8573(4)	0.0516(19)
C16	0.3181(4)	0.3493(3)	0.8913(4)	0.0557(19)
C17	0.3125(4)	0.4140(3)	0.8910(4)	0.0596(19)
C18	0.2097(4)	0.2453(3)	0.8504(4)	0.0510(19)
C19	0.1069(4)	0.2319(3)	0.8100(4)	0.055(2)
C110	0.0631(5)	0.1705(3)	0.7926(4)	0.060(2)
C111	0.2416(5)	0.1336(3)	0.8613(4)	0.061(2)
C112	0.2827(4)	0.1944(3)	0.8779(4)	0.0547(19)
C113	0.3926(5)	0.1995(3)	0.9197(5)	0.068(2)
C114	0.4552(6)	0.1490(4)	0.9426(6)	0.083(3)
C115	0.4125(6)	0.0882(4)	0.9235(6)	0.085(3)
C116	0.3070(6)	0.0809(3)	0.8851(5)	0.077(3)
C117	0.2872(6)	0.6138(3)	0.9301(7)	0.096(3)
C118	0.3968(6)	0.6353(4)	0.9755(6)	0.094(3)
C119	0.2184(8)	0.6341(6)	0.9902(13)	0.182(8)
S2	0.48791(12)	0.32480(8)	0.70978(12)	0.0650(6)
O2	0.5445(3)	0.1877(2)	0.7344(4)	0.0774(17)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms (continued) for: 9a

Atom	x	y	z	U(eq) [Ang^2]
N21	0.3779(4)	0.1537(3)	0.6647(4)	0.0666(19)
N22	0.3701(5)	0.5689(3)	0.7049(5)	0.0717(19)
N23	0.2339(6)	0.5731(3)	0.5630(6)	0.107(3)
C21	0.3008(5)	0.5417(3)	0.6313(5)	0.065(2)
C22	0.2960(4)	0.4728(3)	0.6281(4)	0.0585(17)
C23	0.3870(5)	0.4389(2)	0.6647(4)	0.0547(17)
C24	0.3815(4)	0.3748(3)	0.6649(4)	0.0565(19)
C25	0.2862(4)	0.3410(3)	0.6288(4)	0.0496(19)
C26	0.1953(5)	0.3773(3)	0.5933(4)	0.062(2)
C27	0.2006(5)	0.4407(3)	0.5943(4)	0.063(2)
C28	0.3031(4)	0.2741(3)	0.6371(4)	0.0484(17)
C29	0.4068(5)	0.2615(3)	0.6788(4)	0.059(2)
C210	0.4505(5)	0.1983(3)	0.6965(4)	0.062(2)
C211	0.2716(5)	0.1623(3)	0.6240(4)	0.059(2)
C212	0.2297(5)	0.2227(3)	0.6081(4)	0.056(2)
C213	0.1214(5)	0.2279(3)	0.5661(4)	0.065(2)
C214	0.0573(6)	0.1768(3)	0.5416(5)	0.076(3)
C215	0.1008(6)	0.1181(4)	0.5599(5)	0.082(3)
C216	0.2055(5)	0.1106(3)	0.5991(5)	0.069(3)
C217	0.2218(11)	0.6419(4)	0.5598(11)	0.187(6)
C218	0.1126(13)	0.6581(6)	0.5427(12)	0.212(9)
C219	0.2461(13)	0.6650(8)	0.470(3)	0.38(2)
Cl1	-0.07289(17)	0.48337(10)	0.63685(17)	0.1100(8)
Cl2	0.56412(15)	0.50947(8)	0.87124(13)	0.0863(7)

Table S4 - (An)isotropic Displacement Parameters
for: 9a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
S1	0.0491(9)	0.0636(11)	0.0694(10)	0.0021(8)	-0.0056(7)	-0.0070(7)
O1	0.060(3)	0.064(3)	0.096(3)	-0.011(2)	-0.002(2)	-0.012(2)
N11	0.069(4)	0.051(3)	0.067(3)	-0.001(3)	0.002(3)	-0.008(3)
N12	0.061(4)	0.059(4)	0.080(4)	0.008(3)	-0.027(3)	0.000(3)
N13	0.072(4)	0.038(3)	0.080(4)	0.003(3)	-0.022(3)	0.000(3)
C11	0.054(4)	0.063(4)	0.069(4)	0.005(3)	-0.009(3)	-0.005(3)
C12	0.052(3)	0.046(3)	0.057(3)	0.009(3)	-0.007(3)	0.000(3)
C13	0.045(3)	0.072(4)	0.053(3)	0.010(3)	-0.003(3)	0.000(3)
C14	0.055(3)	0.042(3)	0.051(3)	0.007(2)	0.005(3)	-0.003(3)
C15	0.047(3)	0.061(4)	0.041(3)	0.008(3)	0.005(2)	-0.008(3)
C16	0.049(3)	0.052(4)	0.057(3)	-0.003(3)	0.003(3)	-0.004(3)
C17	0.049(3)	0.060(4)	0.056(3)	0.002(3)	-0.004(3)	-0.013(3)
C18	0.051(3)	0.054(4)	0.041(3)	0.006(2)	0.004(2)	-0.004(3)
C19	0.060(4)	0.052(4)	0.044(3)	-0.004(3)	0.003(3)	-0.011(3)
C110	0.071(4)	0.051(4)	0.051(3)	-0.004(3)	0.007(3)	-0.009(3)
C111	0.077(4)	0.047(4)	0.053(3)	0.001(3)	0.012(3)	-0.002(3)
C112	0.056(3)	0.060(4)	0.043(3)	0.004(3)	0.008(3)	0.000(3)
C113	0.064(4)	0.070(4)	0.067(4)	0.010(3)	0.015(3)	0.001(3)
C114	0.068(4)	0.085(6)	0.093(5)	0.022(4)	0.019(4)	0.015(4)
C115	0.092(6)	0.065(5)	0.096(5)	0.018(4)	0.024(4)	0.018(4)
C116	0.083(5)	0.063(4)	0.082(5)	0.011(3)	0.019(4)	0.001(4)
C117	0.070(5)	0.060(4)	0.116(6)	-0.004(4)	-0.033(4)	0.007(4)
C118	0.094(5)	0.065(5)	0.104(6)	-0.006(4)	0.002(4)	-0.017(4)
C119	0.091(7)	0.112(9)	0.34(2)	-0.084(11)	0.063(10)	-0.002(6)
S2	0.0537(10)	0.0500(10)	0.0748(11)	0.0017(7)	-0.0043(8)	0.0074(7)
O2	0.061(3)	0.055(3)	0.095(3)	0.005(2)	-0.007(2)	0.013(2)

Table S4 - (An)isotropic Displacement Parameters (continued)
for: 9a

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
N21	0.074(4)	0.044(3)	0.070(3)	0.005(3)	0.005(3)	0.016(3)
N22	0.059(3)	0.043(3)	0.085(4)	-0.003(3)	-0.019(3)	0.004(3)
N23	0.106(5)	0.059(4)	0.098(5)	-0.011(4)	-0.052(4)	0.014(4)
C21	0.058(4)	0.049(4)	0.068(4)	-0.003(3)	-0.011(3)	0.009(3)
C22	0.052(3)	0.047(3)	0.060(3)	-0.008(3)	-0.007(3)	0.003(3)
C23	0.055(3)	0.033(3)	0.063(3)	0.000(2)	-0.001(3)	0.004(3)
C24	0.046(3)	0.067(4)	0.048(3)	0.000(3)	0.002(3)	0.006(3)
C25	0.045(3)	0.054(4)	0.042(3)	-0.001(2)	0.002(2)	0.007(3)
C26	0.051(3)	0.064(4)	0.060(4)	-0.010(3)	-0.001(3)	0.001(3)
C27	0.050(3)	0.055(4)	0.066(4)	-0.010(3)	-0.009(3)	0.010(3)
C28	0.054(3)	0.042(3)	0.045(3)	0.001(2)	0.009(2)	0.006(3)
C29	0.066(4)	0.052(4)	0.052(3)	0.001(3)	0.006(3)	-0.002(3)
C210	0.066(4)	0.058(4)	0.049(3)	0.003(3)	0.000(3)	0.008(3)
C211	0.066(4)	0.061(4)	0.043(3)	-0.002(3)	0.008(3)	0.003(3)
C212	0.067(4)	0.056(4)	0.043(3)	-0.008(3)	0.012(3)	0.000(3)
C213	0.067(4)	0.060(4)	0.064(4)	-0.006(3)	0.015(3)	-0.006(3)
C214	0.065(4)	0.073(5)	0.084(5)	-0.005(4)	0.016(3)	-0.004(4)
C215	0.079(5)	0.086(6)	0.078(5)	-0.005(4)	0.018(4)	-0.022(4)
C216	0.078(5)	0.058(4)	0.065(4)	-0.007(3)	0.014(3)	0.002(3)
C217	0.167(11)	0.049(5)	0.222(13)	0.034(7)	-0.120(10)	0.002(6)
C218	0.29(2)	0.138(11)	0.229(15)	0.054(10)	0.113(14)	0.149(13)
C219	0.135(12)	0.119(13)	0.90(7)	0.17(3)	0.18(2)	0.044(10)
Cl1	0.0921(14)	0.0730(13)	0.1102(15)	-0.0186(11)	-0.0490(12)	0.0174(10)
Cl2	0.0825(12)	0.0575(11)	0.0831(12)	0.0082(8)	-0.0269(9)	-0.0064(9)

Table S5 - Bond Distances (Angstrom)
for: 9a

S1	-C14	1.722(6)	C14	-C15	1.413(8)
S1	-C19	1.736(6)	C15	-C18	1.465(9)
S2	-C29	1.711(7)	C15	-C16	1.408(8)
S2	-C24	1.744(6)	C16	-C17	1.388(9)
O1	-C110	1.250(8)	C18	-C19	1.355(8)
O2	-C210	1.233(8)	C18	-C112	1.439(9)
N11	-C110	1.365(9)	C19	-C110	1.431(9)
N11	-C111	1.391(9)	C111	-C112	1.406(9)
N12	-C11	1.296(10)	C111	-C116	1.407(10)
N13	-C11	1.310(8)	C112	-C113	1.418(9)
N13	-C117	1.460(8)	C13	-H13	0.9294
N11	-H3	1.04(9)	C113	-C114	1.348(11)
N12	-H2	0.77(6)	C114	-C115	1.416(12)
N12	-H8	0.99(9)	C115	-C116	1.364(12)
N13	-H5	0.88(8)	C16	-H16	0.9296
N21	-C211	1.380(9)	C117	-C118	1.489(12)
N21	-C210	1.341(9)	C117	-C119	1.497(16)
N22	-C21	1.297(10)	C17	-H17	0.9299
N23	-C21	1.284(10)	C113	-H113	0.9304
N23	-C217	1.482(11)	C114	-H114	0.9304
N21	-H1	0.79(4)	C115	-H115	0.9307
N22	-H7	0.96(6)	C116	-H116	0.9294
N22	-H6	0.74(7)	C117	-H117	0.9801
N23	-H4	0.78(6)	C118	-H11B	0.9599
C11	-C12	1.493(9)	C118	-H11A	0.9604
C12	-C17	1.402(8)	C118	-H11C	0.9608
C12	-C13	1.380(8)	C119	-H11F	0.9593
C13	-C14	1.403(9)	C119	-H11D	0.9609

Table S5 - Bond Distances (Angstrom) (continued)
for: 9a

C119	-H11E	0.9591	C212	-C213	1.399(10)
C21	-C22	1.477(9)	C213	-C214	1.371(10)
C22	-C27	1.404(9)	C214	-C215	1.377(11)
C22	-C23	1.380(8)	C215	-C216	1.356(11)
C23	-C24	1.375(8)	C217	-C218	1.46(2)
C24	-C25	1.424(8)	C217	-C219	1.48(4)
C25	-C28	1.450(9)	C213	-H213	0.9296
C25	-C26	1.405(9)	C214	-H214	0.9312
C26	-C27	1.360(9)	C215	-H215	0.9301
C28	-C29	1.364(9)	C216	-H216	0.9299
C28	-C212	1.451(9)	C217	-H217	0.9808
C29	-C210	1.467(9)	C218	-H21A	0.9606
C23	-H23	0.9308	C218	-H21B	0.9595
C26	-H26	0.9298	C218	-H21C	0.9600
C27	-H27	0.9299	C219	-H21D	0.9566
C211	-C216	1.396(9)	C219	-H21E	0.9598
C211	-C212	1.402(9)	C219	-H21F	0.9591

Table S6 - Bond Angles (Degrees)
for: 9a

C14	-S1	-C19	89.7(3)	S1	-C14	-C13	124.6(4)
C24	-S2	-C29	90.3(3)	C13	-C14	-C15	121.6(5)
C110	-N11	-C111	123.7(6)	C14	-C15	-C16	117.4(6)
C11	-N13	-C117	124.8(6)	C16	-C15	-C18	132.3(5)
C111	-N11	-H3	115(5)	C14	-C15	-C18	110.2(5)
C110	-N11	-H3	121(5)	C15	-C16	-C17	120.7(5)
C11	-N12	-H2	126(5)	C12	-C17	-C16	120.8(5)
C11	-N12	-H8	118(4)	C19	-C18	-C112	118.5(6)
H2	-N12	-H8	113(7)	C15	-C18	-C112	130.6(5)
C117	-N13	-H5	127(5)	C15	-C18	-C19	110.9(5)
C11	-N13	-H5	107(6)	S1	-C19	-C18	115.4(5)
C210	-N21	-C211	126.8(6)	S1	-C19	-C110	119.1(4)
C21	-N23	-C217	126.1(9)	C18	-C19	-C110	125.5(6)
C211	-N21	-H1	117(3)	O1	-C110	-N11	121.5(6)
C210	-N21	-H1	116(3)	O1	-C110	-C19	124.3(6)
H6	-N22	-H7	116(6)	N11	-C110	-C19	114.2(6)
C21	-N22	-H6	118(5)	N11	-C111	-C112	121.0(6)
C21	-N22	-H7	125(3)	N11	-C111	-C116	117.8(6)
C217	-N23	-H4	109(5)	C112	-C111	-C116	121.2(6)
C21	-N23	-H4	124(5)	C18	-C112	-C113	126.3(6)
N12	-C11	-N13	122.3(6)	C111	-C112	-C113	116.6(6)
N12	-C11	-C12	118.8(6)	C18	-C112	-C111	117.1(5)
N13	-C11	-C12	118.9(6)	C112	-C113	-C114	122.2(7)
C11	-C12	-C13	119.3(5)	C12	-C13	-H13	120.23
C13	-C12	-C17	119.8(6)	C14	-C13	-H13	120.18
C11	-C12	-C17	120.9(6)	C113	-C114	-C115	120.4(8)
C12	-C13	-C14	119.6(5)	C114	-C115	-C116	119.5(7)
S1	-C14	-C15	113.7(5)	C17	-C16	-H16	119.60

Table S6 - Bond Angles (Degrees) (continued)
for: 9a

C111	-C116	-C115	120.1(7)	H11D	-C119	-H11E	109.52
C15	-C16	-H16	119.66	C117	-C119	-H11D	109.43
C12	-C17	-H17	119.64	N22	-C21	-N23	121.7(7)
N13	-C117	-C119	107.7(7)	N22	-C21	-C22	119.1(6)
N13	-C117	-C118	110.8(6)	N23	-C21	-C22	119.1(6)
C118	-C117	-C119	111.9(8)	C21	-C22	-C23	119.3(5)
C16	-C17	-H17	119.56	C21	-C22	-C27	121.8(6)
C114	-C113	-H113	118.82	C23	-C22	-C27	118.9(6)
C112	-C113	-H113	118.98	C22	-C23	-C24	118.9(6)
C115	-C114	-H114	119.76	S2	-C24	-C23	125.1(5)
C113	-C114	-H114	119.86	S2	-C24	-C25	111.5(5)
C116	-C115	-H115	120.13	C23	-C24	-C25	123.4(6)
C114	-C115	-H115	120.33	C26	-C25	-C28	132.3(6)
C115	-C116	-H116	120.04	C24	-C25	-C28	111.9(5)
C111	-C116	-H116	119.90	C24	-C25	-C26	115.8(6)
C119	-C117	-H117	108.77	C25	-C26	-C27	120.8(6)
N13	-C117	-H117	108.77	C22	-C27	-C26	122.2(6)
C118	-C117	-H117	108.80	C25	-C28	-C29	110.2(5)
C117	-C118	-H11C	109.44	C25	-C28	-C212	130.6(5)
C117	-C118	-H11B	109.50	C29	-C28	-C212	119.2(6)
H11B	-C118	-H11C	109.62	S2	-C29	-C28	116.2(5)
H11A	-C118	-H11B	109.50	S2	-C29	-C210	119.8(5)
H11A	-C118	-H11C	109.35	C28	-C29	-C210	124.0(6)
C117	-C118	-H11A	109.41	C22	-C23	-H23	120.52
C117	-C119	-H11E	109.46	C24	-C23	-H23	120.53
C117	-C119	-H11F	109.45	C25	-C26	-H26	119.70
H11D	-C119	-H11F	109.42	C27	-C26	-H26	119.51
H11E	-C119	-H11F	109.55	C26	-C27	-H27	118.86
C22	-C27	-H27	118.99	C215	-C214	-H214	120.56
O2	-C210	-N21	123.9(6)	C214	-C215	-H215	119.68
N21	-C210	-C29	112.8(6)	C216	-C215	-H215	119.45
O2	-C210	-C29	123.2(6)	C211	-C216	-H216	119.64
N21	-C211	-C212	120.3(6)	C215	-C216	-H216	119.66
C212	-C211	-C216	119.9(6)	N23	-C217	-H217	111.37
N21	-C211	-C216	119.8(6)	C218	-C217	-H217	111.39
C28	-C212	-C213	126.1(6)	C219	-C217	-H217	111.33
C28	-C212	-C211	116.7(6)	C217	-C218	-H21A	109.48

C211	-C212	-C213	117.2(6)	C217	-C218	-H21B	109.49
C212	-C213	-C214	122.4(6)	C217	-C218	-H21C	109.49
C213	-C214	-C215	118.9(7)	H21A	-C218	-H21B	109.51
C214	-C215	-C216	120.9(7)	H21A	-C218	-H21C	109.44
C211	-C216	-C215	120.7(7)	H21B	-C218	-H21C	109.42
C218	-C217	-C219	104.9(14)	C217	-C219	-H21D	109.40
N23	-C217	-C219	107.9(12)	C217	-C219	-H21E	109.24
N23	-C217	-C218	109.7(10)	C217	-C219	-H21F	109.26
C212	-C213	-H213	118.70	H21D	-C219	-H21E	109.74
C214	-C213	-H213	118.87	H21D	-C219	-H21F	109.70
C213	-C214	-H214	120.51	H21E	-C219	-H21F	109.49