Supporting information

Identification of Cyanamide-Based Janus Kinase 3 (JAK3) Covalent Inhibitors

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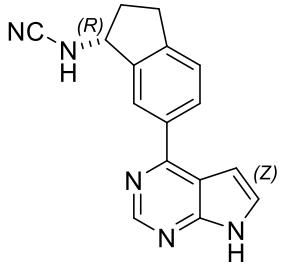
S-Table 1. Crystallographic data collection and refinement statistics

Compound	**10**	**12**	**23**	**34**
PDB entry	**6DA4**	**6DUD**	**6DB3**	**6DB4**
A. Data collection				
Space Group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Unit Cell	a= 46.4	a= 47.6	A= 47.2	a= 48.1
	b=75.5	b=75.5	B=75.8	b= 75.1
	c=89.6	c=88.9	C=90.1	c= 88.6
Resolution (Å)	24-2.90	75-1.66	90-1.72	88.6-1.66
(high res)	(2.64-2.60)	(1.663-1.658)	(1.73-1.72)	(1.75-1.66)
Completeness (%)	97.8 (98.4)	88.9 (100)	99.3 (75.4)	99.8 (99.9)
Rsym[a]	0.09 (0.90)	0.06 (0.93)	0.03 (0.37)	0.03 (0.27)
Redundancy	5.0 (4.0)	6.1 (6.8)	6.1 (3.6)	6.1 (5.1)
$\langle I \rangle / \langle \sigma(I) \rangle$	25.3 (2.0)	15.8 (1.9)	28.8 (2.6)	31.9 (4.4)
B. Refinement				
Rwork[b]	0.227	0.184	0.197	0.185
Rfree[b]	0.263	0.215	0.212	0.216
Amino Acid Residues (#)	279	273	275	277
Waters (#)	18	310	230	294
RMSD bond length (Å)	0.01	0.01	0.01	0.01
RMSD angles (degrees)	1.08	0.93	0.97	0.94
Average B (Å2)	50.2	37.4	38.8	32.52
Ramachandran (%)	99.3	100.0	99.6	99.6
Ramachandran outliers (%)	0.7	0.0	0.4	0.4

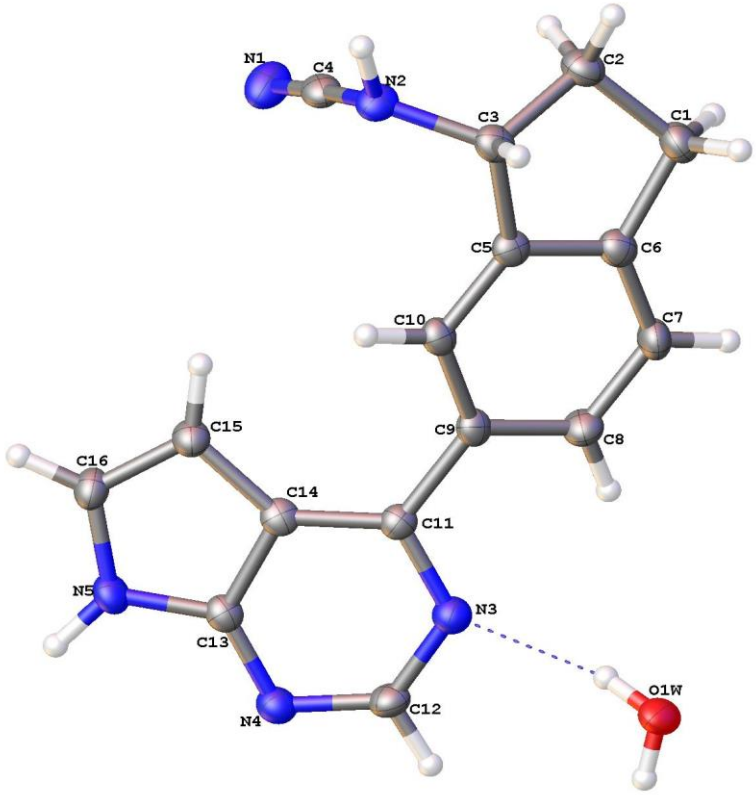
[a] $R_{sym} = \Sigma_{hkl}(|I_{hkl} - \langle I_{hkl} \rangle|)/\Sigma_{hkl}\langle I_{hkl} \rangle$, where I_{hkl} is the intensity of reflection hkl, and $\langle I_{hkl} \rangle$ is the average intensity of multiple observations.

[b] $R_{work} = \Sigma|F_o - F_c|/\Sigma F_o$, where F_o and F_c are the observed and calculated structure factor amplitudes, respectively. R_{free} is the R-factor for a randomly selected 5% of reflections which were not used in the refinement.

Single Molecule X-ray crystallography for 13



13



S-Figure 1. Asymmetric unit with displacement parameters drawn at 50% probability for **13**.

Experimental for 13

Data collection was performed on a Bruker APEX diffractometer at -150 °C temperature. Data collection consisted of omega and phi scans. The structure was solved by direct methods using SHELX software suite in the Monoclinic class space group $P2_1$. The

structure was subsequently refined by the full-matrix least squares method. All non-hydrogen atoms were found and refined using anisotropic displacement parameters. The structure refined as a monohydrate. The hydrogen atoms located on nitrogen and oxygen were found from the Fourier difference map and refined with distances restrained. The remaining hydrogen atoms were placed in calculated positions and were allowed to ride on their carrier atoms. The final refinement included isotropic displacement parameters for all hydrogen atoms. Analysis of the absolute structure using likelihood methods (Hooft 2008) was performed using PLATON (Spek 2010). Assuming the sample submitted is enantiopure, the results indicate that the absolute structure has been correctly assigned. The method calculates that the probability that the structure is correctly assigned is 1.000. The Hooft parameter is reported as -0.13 with an esd of 0.015. The final R-index was 3.7%. A final difference Fourier revealed no missing or misplaced electron density. Pertinent crystal, data collection and refinement for **13** are summarized in S-Table 2. Atomic coordinates, bond lengths, bond angles and displacement parameters are listed in S-Tables 3 –5.

Software and References

SHELXTL, Version 5.1, Bruker AXS, 1997

PLATON, A.L. Spek, J. Appl. Cryst. 2003, 36, 7-13.

MERCURY, C.F. Macrae, P.R. Edington, P. McCabe, E. Pidcock, G.P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.* **39**, 453-457, 2006.

OLEX2, Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., (2009). J. Appl. Cryst., 42, 339-341.

R.W.W. Hooft et al. *J. Appl. Cryst.* (2008). 41. 96-103.

H.D. Flack, *Acta Cryst.* 1983, **A**39, 867-881.

S-Table 2. Crystal data and structure refinement for **13.**

Identification code	Z688	
Crystallization	Ethanol / Acetone	
Empirical formula	C16 H13 N5. H2 O	
Formula weight	293.33	
Temperature	123(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 4.9212(2) Å	α= 90°.
	b = 7.6041(3) Å	β= 90.973(3)°.
	c = 18.6105(8) Å	γ = 90°.
Volume	696.33(5) $Å^3$	
Z	2	
Density (calculated)	1.399 Mg/m^3	
Absorption coefficient	0.752 mm^{-1}	
F(000)	308	
Crystal size	0.380 x 0.240 x 0.040 mm^3	
Theta range for data collection	2.374 to 67.942°.	
Index ranges	-5<=h<=5, -9<=k<=9, -21<=l<=22	
Reflections collected	7704	
Independent reflections	2399 [R(int) = 0.0325]	
Completeness to theta = 67.679°	99.3 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2399 / 3 / 211	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0978	
R indices (all data)	R1 = 0.0386, wR2 = 0.0991	
Absolute structure parameter	-0.1(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.222 and -0.250 e.$Å^{-3}$	

S-Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **13.** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	481(5)	9901(4)	4296(2)	32(1)
N(2)	-4109(5)	9155(3)	3824(1)	24(1)
N(3)	3008(5)	5193(3)	1202(1)	24(1)
N(4)	6204(5)	7117(3)	642(1)	24(1)
N(5)	6398(5)	9995(3)	1158(1)	24(1)
C(1)	-4498(6)	4244(4)	4024(2)	28(1)
C(2)	-5092(6)	6102(4)	4309(2)	27(1)
C(3)	-4833(5)	7325(4)	3654(2)	23(1)
C(4)	-1665(6)	9524(4)	4095(2)	24(1)
C(5)	-2826(6)	6365(4)	3188(1)	21(1)
C(6)	-2724(6)	4604(4)	3387(1)	23(1)
C(7)	-1141(6)	3454(4)	2998(2)	26(1)
C(8)	371(6)	4069(4)	2432(2)	26(1)
C(9)	352(5)	5854(4)	2243(1)	20(1)
C(10)	-1305(5)	7009(4)	2621(1)	21(1)
C(11)	2239(5)	6439(4)	1673(1)	19(1)
C(12)	4920(6)	5586(4)	722(2)	24(1)
C(13)	5387(5)	8346(4)	1101(1)	20(1)
C(14)	3382(5)	8116(4)	1636(2)	21(1)
C(15)	3286(5)	9749(4)	2022(2)	23(1)
C(16)	5120(6)	10836(4)	1711(2)	24(1)
O(1W)	-120(4)	2335(3)	485(1)	32(1)

S-Table 4. Bond lengths [Å] and angles [°] for **13**.

N(1)-C(4)	1.150(4)
N(2)-C(4)	1.327(4)
N(2)-C(3)	1.469(4)
N(3)-C(12)	1.342(4)
N(3)-C(11)	1.349(4)
N(4)-C(13)	1.332(4)
N(4)-C(12)	1.334(4)

N(5)-C(13)	1.353(4)
N(5)-C(16)	1.373(4)
C(1)-C(6)	1.509(4)
C(1)-C(2)	1.539(4)
C(2)-C(3)	1.542(4)
C(3)-C(5)	1.512(4)
C(5)-C(6)	1.390(4)
C(5)-C(10)	1.394(4)
C(6)-C(7)	1.384(4)
C(7)-C(8)	1.381(4)
C(8)-C(9)	1.402(4)
C(9)-C(10)	1.397(4)
C(9)-C(11)	1.490(4)
C(11)-C(14)	1.396(4)
C(13)-C(14)	1.424(4)
C(14)-C(15)	1.436(4)
C(15)-C(16)	1.361(4)

C(4)-N(2)-C(3)	119.8(2)
C(12)-N(3)-C(11)	118.9(2)
C(13)-N(4)-C(12)	113.1(2)
C(13)-N(5)-C(16)	108.5(2)
C(6)-C(1)-C(2)	102.8(2)
C(1)-C(2)-C(3)	105.2(2)
N(2)-C(3)-C(5)	115.0(2)
N(2)-C(3)-C(2)	115.1(2)
C(5)-C(3)-C(2)	103.1(2)
N(1)-C(4)-N(2)	176.1(3)
C(6)-C(5)-C(10)	121.5(3)
C(6)-C(5)-C(3)	109.5(2)
C(10)-C(5)-C(3)	129.0(3)
C(7)-C(6)-C(5)	119.2(3)
C(7)-C(6)-C(1)	129.4(3)
C(5)-C(6)-C(1)	111.4(3)
C(8)-C(7)-C(6)	120.0(3)
C(7)-C(8)-C(9)	121.2(3)
C(10)-C(9)-C(8)	118.9(3)
C(10)-C(9)-C(11)	123.2(3)
C(8)-C(9)-C(11)	117.8(2)
C(5)-C(10)-C(9)	119.1(3)
N(3)-C(11)-C(14)	119.5(2)
N(3)-C(11)-C(9)	116.0(2)
C(14)-C(11)-C(9)	124.3(2)
N(4)-C(12)-N(3)	127.4(3)
N(4)-C(13)-N(5)	125.9(3)
N(4)-C(13)-C(14)	125.6(3)

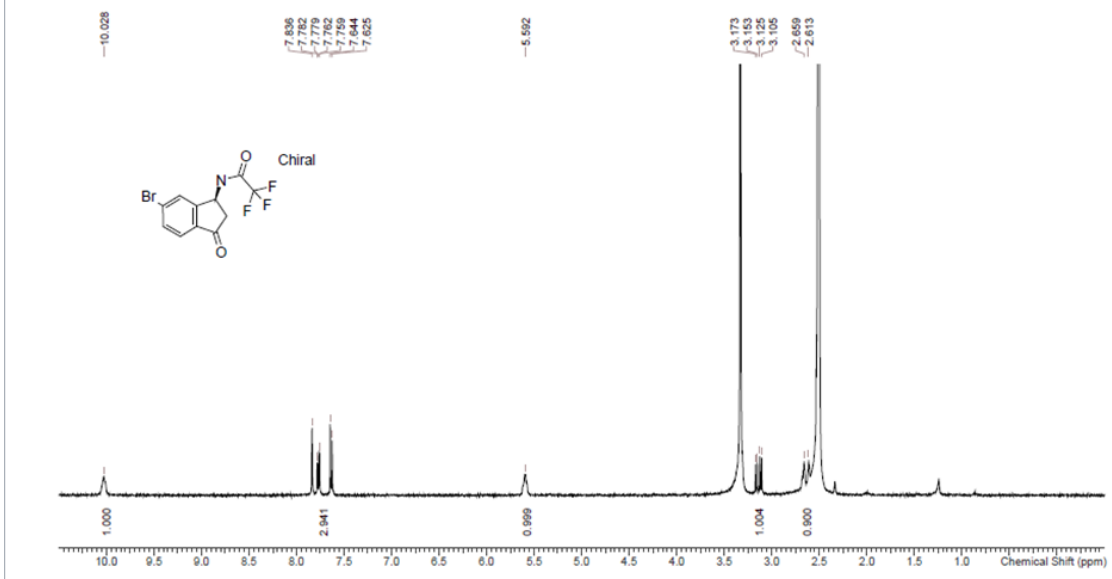
N(5)-C(13)-C(14)	108.5(2)
C(11)-C(14)-C(13)	115.5(2)
C(11)-C(14)-C(15)	138.5(3)
C(13)-C(14)-C(15)	105.9(2)
C(16)-C(15)-C(14)	106.5(2)
C(15)-C(16)-N(5)	110.6(3)

Symmetry transformations used to generate equivalent atoms:

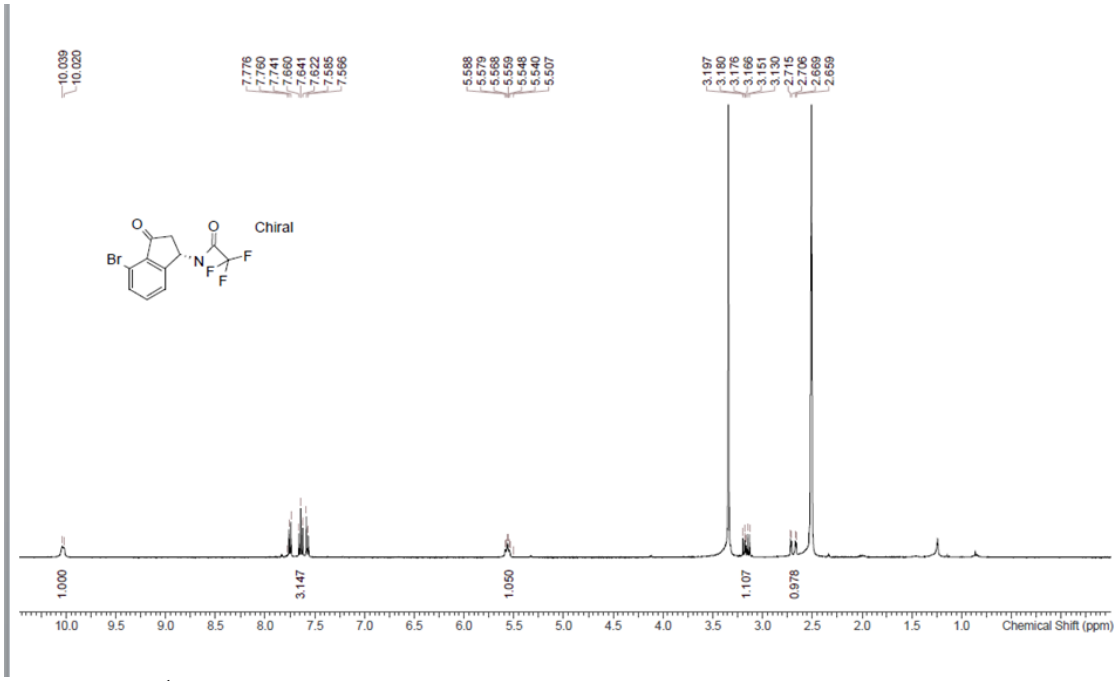
S-Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **13**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	19(1)	31(1)	47(2)	-9(1)	3(1)	2(1)
N(2)	17(1)	26(1)	29(1)	-4(1)	2(1)	3(1)
N(3)	21(1)	24(1)	26(1)	-2(1)	3(1)	1(1)
N(4)	21(1)	25(1)	25(1)	1(1)	3(1)	1(1)
N(5)	18(1)	25(1)	29(1)	3(1)	4(1)	-3(1)
C(1)	28(2)	25(1)	30(2)	3(1)	7(1)	-3(1)
C(2)	25(2)	29(2)	27(1)	1(1)	7(1)	0(1)
C(3)	17(1)	27(2)	26(1)	0(1)	2(1)	-2(1)
C(4)	23(2)	23(1)	27(1)	-2(1)	6(1)	4(1)
C(5)	16(1)	23(1)	24(1)	0(1)	-1(1)	-1(1)
C(6)	18(1)	26(2)	25(1)	1(1)	2(1)	-2(1)
C(7)	29(2)	18(1)	32(2)	3(1)	5(1)	-2(1)
C(8)	25(2)	24(1)	30(1)	-1(1)	7(1)	3(1)
C(9)	16(1)	21(1)	24(1)	0(1)	-1(1)	-2(1)
C(10)	16(1)	23(1)	23(1)	1(1)	1(1)	-3(1)
C(11)	16(1)	20(1)	22(1)	1(1)	0(1)	1(1)
C(12)	24(1)	24(1)	24(1)	-4(1)	4(1)	2(1)
C(13)	16(1)	22(1)	24(1)	2(1)	0(1)	0(1)
C(14)	15(1)	23(1)	24(1)	2(1)	0(1)	4(1)
C(15)	20(1)	21(1)	28(1)	-1(1)	4(1)	1(1)
C(16)	21(1)	18(1)	34(2)	-1(1)	2(1)	-1(1)
O(1W)	29(1)	34(1)	32(1)	-6(1)	13(1)	-10(1)

^{1}H NMR spectra for 90 and 91

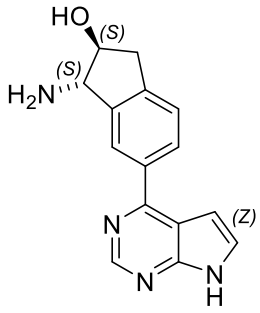


S-Figure 2. ^{1}H NMR of **90**.



S-Figure 3. ^{1}H NMR of **91**.

Single Molecule X-ray crystallography for 105



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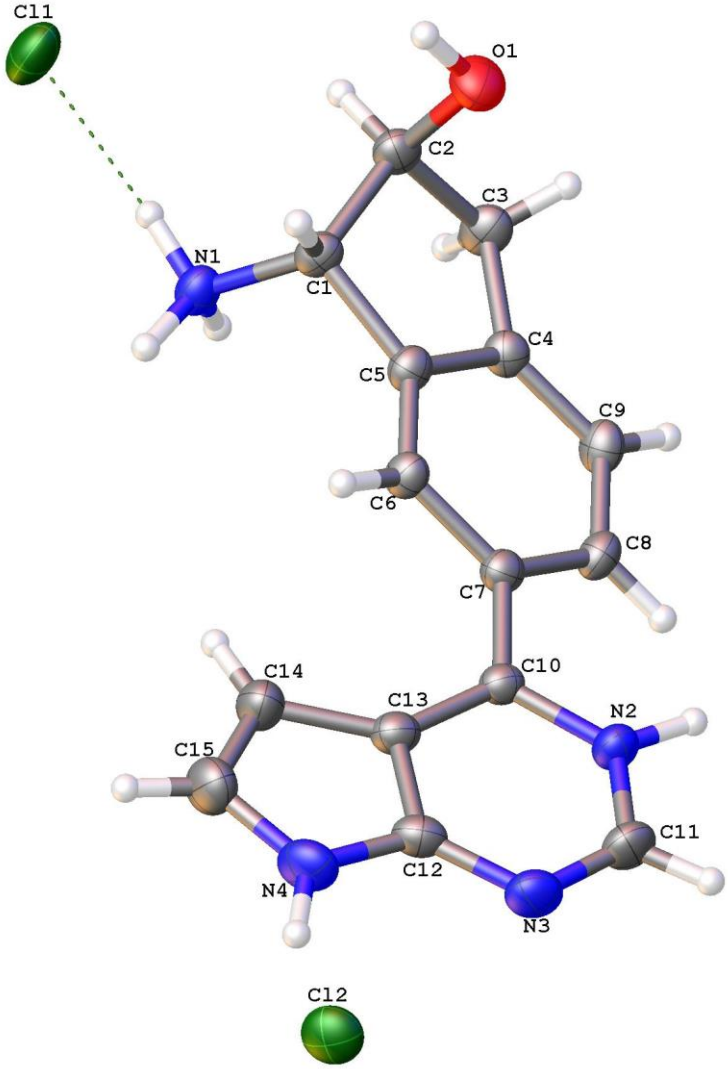


S-Figure 4. Asymmetric unit with displacement parameters drawn at 50% probability for **105**.

Experimental for 105

Data collection was performed on a Bruker APEX diffractometer at room temperature. Data collection consisted of omega and phi scans. The structure was solved by direct methods using SHELX software suite in the Orthorhombic class space group $P2_12_12_1$. The structure was subsequently refined by the full-matrix least squares method. All non-hydrogen atoms were found and refined using anisotropic displacement parameters. The hydrogen atoms located on nitrogen and oxygen were found from the Fourier difference map and refined with distances restrained. The remaining hydrogen atoms were placed in calculated positions and were allowed to ride on their carrier atoms. The final refinement included isotropic displacement parameters for all hydrogen atoms. Asymmetric unit consisits of one API molecule (+2) and two Cl(-1). Analysis of the absolute structure using likelihood methods (Hooft 2008) was performed using PLATON (Spek 2010). Assuming the sample submitted is enantiopure, the results indicate that the absolute structure has been correctly assigned. The method calculates that the probability that the structure is correctly assigned is 1.000 and the probability that the structure is incorrect to be 0.000. The Hooft parameter is reported as 0.013 with an esd of 0.008. The final R-index was 2.9%. A final difference Fourier revealed no missing or misplaced electron density. Pertinent crystal, data collection and refinement for **105** are summarized in S-Table 6. Atomic coordinates, bond lengths, bond angles and displacement parameters are listed in S-Tables 7 –9.

Software and References

SHELXTL, Version 5.1, Bruker AXS, 1997

PLATON, A.L. Spek, J. Appl. Cryst. 2003, 36, 7-13.

MERCURY, C.F. Macrae, P.R. Edington, P. McCabe, E. Pidcock, G.P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.* **39**, 453-457, 2006.

OLEX2, Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., (2009). J. Appl. Cryst., 42, 339-341.

R.W.W. Hooft et al. *J. Appl. Cryst.* (2008). 41. 96-103.

H.D. Flack, *Acta Cryst.* 1983, **A**39, 867-881.

S-Table 6. Crystal data and structure refinement for **105**.

Identification code	Z719	
Crystallization	Methanol / Water	
Empirical formula	C15 H16 N4 O Cl2	
Formula weight	339.22	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.7406(3) Å	α= 90°.
	b = 11.4288(5) Å	β= 90°.
	c = 23.8713(10) Å	γ = 90°.
Volume	1566.15(13) $Å^3$	
Z	4	
Density (calculated)	1.439 Mg/m^3	
Absorption coefficient	3.789 mm^{-1}	
F(000)	704	
Crystal size	0.220 x 0.200 x 0.030 mm^3	
Theta range for data collection	3.703 to 70.220°.	
Index ranges	-6<=h<=6, -13<=k<=13, -29<=l<=29	
Reflections collected	18942	
Independent reflections	2942 [R(int) = 0.0736]	
Completeness to theta = 67.679°	99.2 %	
Absorption correction	Empirical	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2942 / 6 / 218
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0654
R indices (all data)	R1 = 0.0476, wR2 = 0.0676
Absolute structure parameter	0.020(7)
Extinction coefficient	0.0008(3)
Largest diff. peak and hole	0.368 and -0.397 e.$Å^{-3}$

S-Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **105**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	8972(1)	1392(1)	5759(1)	44(1)
Cl(2)	6567(1)	9101(1)	8290(1)	39(1)
N(1)	8365(4)	3953(2)	6121(1)	28(1)
N(2)	5656(4)	9802(2)	6478(1)	28(1)
N(3)	2501(5)	10282(2)	7060(1)	35(1)
N(4)	766(4)	8601(2)	7481(1)	39(1)
O(1)	8420(4)	4961(2)	4648(1)	38(1)
C(1)	7741(4)	4738(2)	5641(1)	25(1)
C(2)	9498(5)	4606(2)	5155(1)	27(1)
C(3)	11384(5)	5506(2)	5283(1)	30(1)
C(4)	10093(4)	6448(2)	5600(1)	24(1)
C(5)	7999(4)	6009(2)	5812(1)	24(1)
C(6)	6511(5)	6699(2)	6123(1)	24(1)
C(7)	7143(4)	7867(2)	6234(1)	23(1)
C(8)	9244(5)	8300(2)	6021(1)	26(1)
C(9)	10712(4)	7597(2)	5702(1)	27(1)
C(10)	5553(4)	8621(2)	6556(1)	23(1)
C(11)	4177(6)	10574(2)	6717(1)	36(1)
C(12)	2370(5)	9127(3)	7157(1)	29(1)
C(13)	3857(5)	8249(2)	6931(1)	27(1)
C(14)	3064(6)	7161(3)	7157(1)	37(1)
C(15)	1203(6)	7409(3)	7482(1)	41(1)

S-Table 8. Bond lengths [Å] and angles [°] for **105**.

N(1)-C(1)	1.499(3)
N(1)-H(1X)	0.93(2)
N(1)-H(1Y)	0.97(2)
N(1)-H(1Z)	0.94(2)
N(2)-C(11)	1.352(4)
N(2)-C(10)	1.364(3)
N(2)-H(2X)	0.95(2)
N(3)-C(11)	1.306(4)
N(3)-C(12)	1.343(4)
N(4)-C(12)	1.344(4)
N(4)-C(15)	1.385(4)
N(4)-H(4X)	0.96(2)
O(1)-C(2)	1.418(3)
O(1)-H(1XX)	0.93(2)
C(1)-C(5)	1.516(4)
C(1)-C(2)	1.545(4)
C(1)-H(1)	0.9800
C(2)-C(3)	1.525(4)
C(2)-H(2)	0.9800
C(3)-C(4)	1.510(4)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(9)	1.382(4)
C(4)-C(5)	1.396(3)
C(5)-C(6)	1.380(3)
C(6)-C(7)	1.408(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.400(4)
C(7)-C(10)	1.472(3)
C(8)-C(9)	1.390(4)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(13)	1.390(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.423(4)
C(13)-C(14)	1.429(4)
C(14)-C(15)	1.351(4)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300

C(1)-N(1)-H(1X)	111(2)
C(1)-N(1)-H(1Y)	109.7(18)
H(1X)-N(1)-H(1Y)	112(3)
C(1)-N(1)-H(1Z)	109.0(18)
H(1X)-N(1)-H(1Z)	107(3)
H(1Y)-N(1)-H(1Z)	108(3)
C(11)-N(2)-C(10)	124.1(2)
C(11)-N(2)-H(2X)	114.9(19)
C(10)-N(2)-H(2X)	121.0(19)
C(11)-N(3)-C(12)	113.6(2)
C(12)-N(4)-C(15)	108.4(2)
C(12)-N(4)-H(4X)	125(2)
C(15)-N(4)-H(4X)	126(2)
C(2)-O(1)-H(1XX)	108(2)
N(1)-C(1)-C(5)	110.2(2)
N(1)-C(1)-C(2)	111.1(2)
C(5)-C(1)-C(2)	103.4(2)
N(1)-C(1)-H(1)	110.6
C(5)-C(1)-H(1)	110.6
C(2)-C(1)-H(1)	110.6
O(1)-C(2)-C(3)	106.7(2)
O(1)-C(2)-C(1)	109.1(2)
C(3)-C(2)-C(1)	104.3(2)
O(1)-C(2)-H(2)	112.1
C(3)-C(2)-H(2)	112.1
C(1)-C(2)-H(2)	112.1
C(4)-C(3)-C(2)	103.5(2)
C(4)-C(3)-H(3A)	111.1
C(2)-C(3)-H(3A)	111.1
C(4)-C(3)-H(3B)	111.1
C(2)-C(3)-H(3B)	111.1
H(3A)-C(3)-H(3B)	109.0
C(9)-C(4)-C(5)	119.9(2)
C(9)-C(4)-C(3)	129.7(2)
C(5)-C(4)-C(3)	110.4(2)
C(6)-C(5)-C(4)	121.5(2)
C(6)-C(5)-C(1)	129.2(2)
C(4)-C(5)-C(1)	109.3(2)
C(5)-C(6)-C(7)	118.9(2)
C(5)-C(6)-H(6)	120.5
C(7)-C(6)-H(6)	120.5
C(8)-C(7)-C(6)	119.2(2)
C(8)-C(7)-C(10)	121.1(2)
C(6)-C(7)-C(10)	119.6(2)
C(9)-C(8)-C(7)	121.1(2)
C(9)-C(8)-H(8)	119.4

C(7)-C(8)-H(8)	119.4
C(4)-C(9)-C(8)	119.3(2)
C(4)-C(9)-H(9)	120.3
C(8)-C(9)-H(9)	120.3
N(2)-C(10)-C(13)	114.9(2)
N(2)-C(10)-C(7)	118.8(2)
C(13)-C(10)-C(7)	126.3(2)
N(3)-C(11)-N(2)	124.2(2)
N(3)-C(11)-H(11)	117.9
N(2)-C(11)-H(11)	117.9
N(3)-C(12)-N(4)	125.3(2)
N(3)-C(12)-C(13)	126.4(3)
N(4)-C(12)-C(13)	108.3(2)
C(10)-C(13)-C(12)	116.7(2)
C(10)-C(13)-C(14)	137.1(2)
C(12)-C(13)-C(14)	106.2(2)
C(15)-C(14)-C(13)	106.6(3)
C(15)-C(14)-H(14)	126.7
C(13)-C(14)-H(14)	126.7
C(14)-C(15)-N(4)	110.4(3)
C(14)-C(15)-H(15)	124.8
N(4)-C(15)-H(15)	124.8

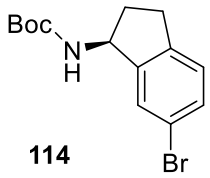
Symmetry transformations used to generate equivalent atoms

S-Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **105**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

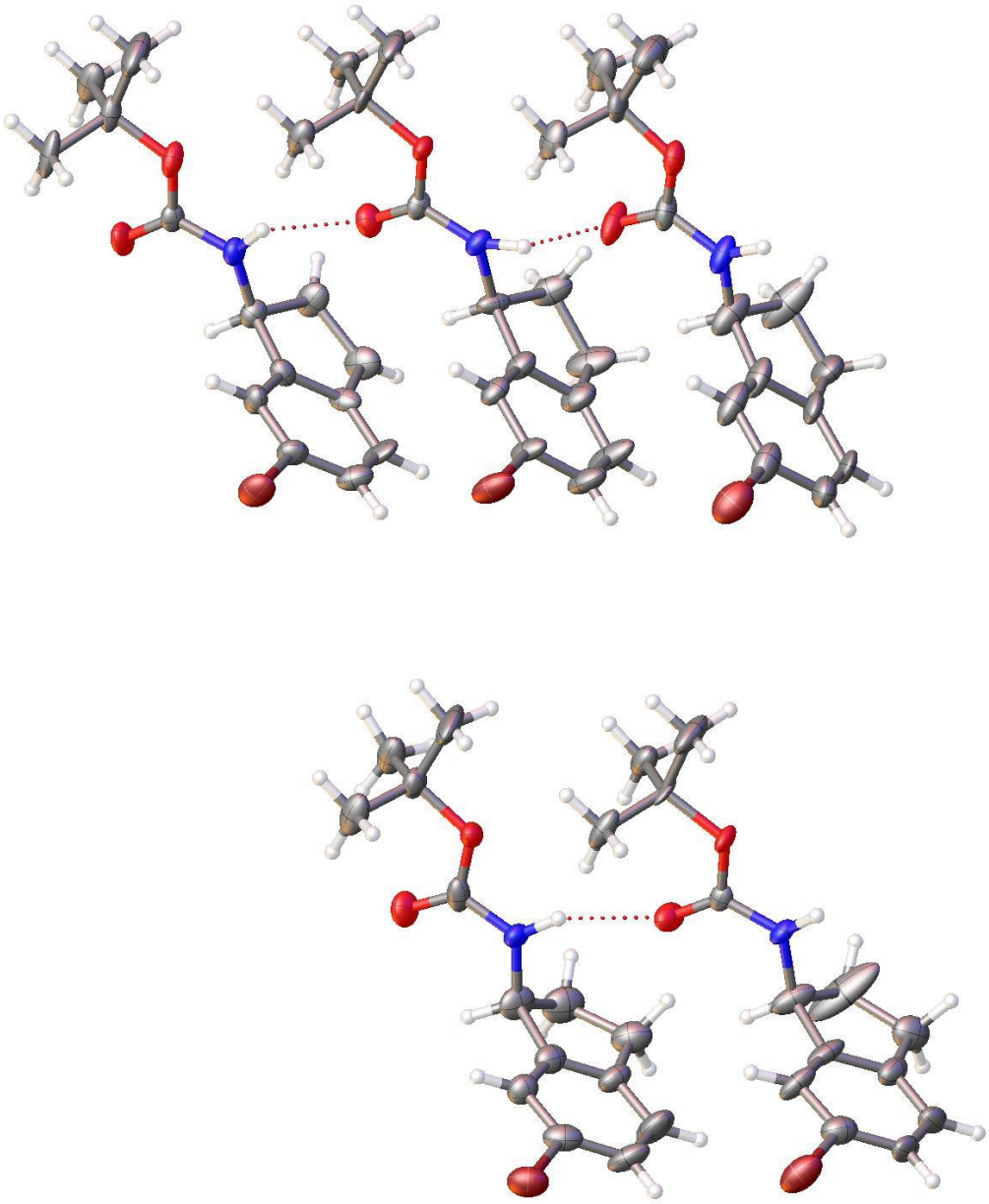
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	47(1)	24(1)	62(1)	-2(1)	13(1)	-3(1)
Cl(2)	28(1)	46(1)	42(1)	-3(1)	9(1)	3(1)
N(1)	28(1)	22(1)	34(1)	0(1)	5(1)	1(1)
N(2)	34(1)	21(1)	30(1)	-2(1)	5(1)	1(1)
N(3)	41(2)	30(1)	35(1)	-5(1)	5(1)	9(1)
N(4)	35(1)	44(1)	36(1)	-7(1)	14(1)	-1(1)
O(1)	44(1)	40(1)	31(1)	2(1)	-6(1)	-3(1)
C(1)	21(1)	23(1)	30(1)	-3(1)	2(1)	2(1)
C(2)	30(1)	23(1)	28(1)	-2(1)	3(1)	5(1)
C(3)	23(1)	30(1)	37(1)	-3(1)	7(1)	2(1)
C(4)	20(1)	25(1)	26(1)	1(1)	2(1)	2(1)
C(5)	22(1)	21(1)	27(1)	1(1)	-1(1)	2(1)
C(6)	20(1)	23(1)	28(1)	-1(1)	4(1)	-1(1)

C(7)	25(1)	22(1)	23(1)	0(1)	0(1)	2(1)
C(8)	27(1)	20(1)	31(1)	1(1)	-2(1)	-3(1)
C(9)	20(1)	27(1)	34(1)	4(1)	2(1)	-2(1)
C(10)	25(1)	21(1)	22(1)	-2(1)	-1(1)	2(1)
C(11)	47(2)	22(1)	38(2)	-4(1)	5(1)	5(1)
C(12)	30(1)	32(1)	25(1)	-6(1)	2(1)	3(1)
C(13)	30(2)	26(1)	25(1)	-4(1)	1(1)	1(1)
C(14)	48(2)	28(1)	35(1)	-1(1)	11(1)	-3(1)
C(15)	44(2)	39(2)	40(2)	1(1)	14(1)	-8(1)

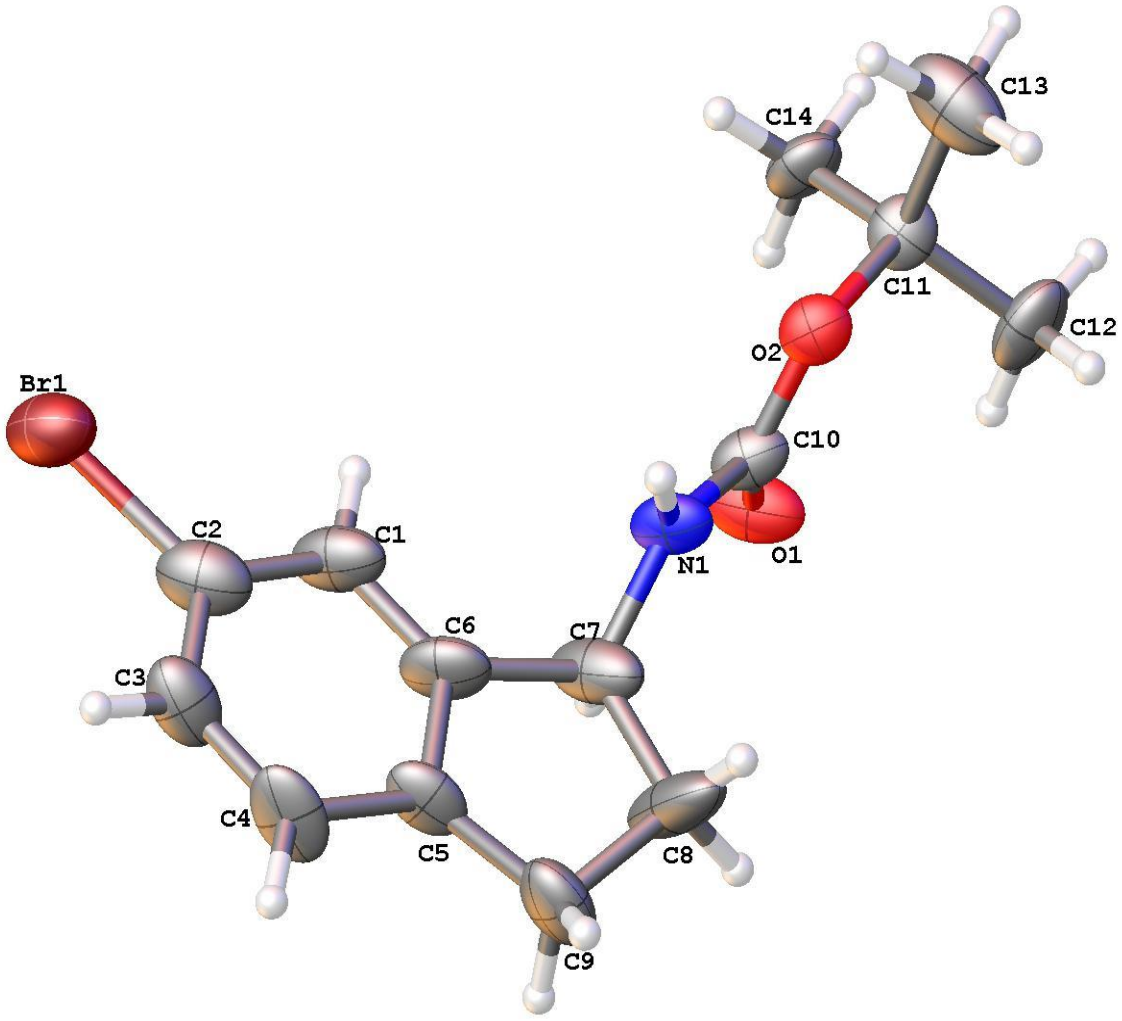
Single Molecule X-ray crystallography for 114



114



S-Figure 5. Five molecules per asymmetric unit with displacement parameters drawn at 50% probability for **114**.



S-Figure 6. Shown only one out of five molecule per asymmetric unit with displacement parameters drawn at 50% probability for **114**.

Experimental for 114

Data collection was performed on a Bruker D8 Venture diffractometer at -150 °C temperature. Data collection consisted of omega and phi scans. The structure was solved by intrinsic phasing using SHELX software suite in the Triclinic class space group P1 as unusual five identical molecules per asymmetric unit. The structure was subsequently refined by the full-matrix least squares method. All non-hydrogen atoms were found and refined using anisotropic displacement parameters. Structure was likely twinned with

several domains. Possible P21 solution could be examined as this appears a likely solution. The hydrogen atoms located on nitrogen were found from the Fourier difference map and refined with distances restrained. The remaining hydrogen atoms were placed in calculated positions and were allowed to ride on their carrier atoms. The final refinement included isotropic displacement parameters for all hydrogen atoms. Analysis of the absolute structure using likelihood methods (Hooft 2008) was performed using PLATON (Spek 2010). Assuming the sample submitted is enantiopure, the results indicate that the absolute structure has been correctly assigned. The method calculates that the probability that the structure is correctly assigned is 100.0. The Hooft parameter is reported as 0.111 with an Esd of 0.012 of and the Parson's parameter is reported as 0.118 with an Esd of 0.010. The final R-index was 7.6%. A final difference Fourier revealed no missing or misplaced electron density. Pertinent crystal, data collection and refinement for **114** are summarized in S-Table 10. Atomic coordinates, bond lengths, bond angles and displacement parameters are listed in S-Tables 11 – 13.

Software and References

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MERCURY, C.F. Macrae, P.R. Edington, P. McCabe, E. Pidcock, G.P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.* **39**, 453-457, 2006.

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S-Table 10. Crystal data and structure refinement for **114**.

Identification code	Z850	
Crystallization	Ethyl Acetate	
Empirical formula	C70 H88 Br5 N5 O10	
Formula weight	1559.00	
Temperature	123(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 18.295(3) Å	α= 90°.
	b = 9.7771(13) Å	β= 95.534(4)°.
	c = 19.931(3) Å	γ = 90°.
Volume	3548.5(8) $Å^3$	
Z	2	
Density (calculated)	1.459 Mg/m^3	
Absorption coefficient	3.903 mm^{-1}	
F(000)	1596	
Crystal size	0.160 x 0.140 x 0.060 mm^3	
Theta range for data collection	2.426 to 70.536°.	
Index ranges	-22<=h<=21, -11<=k<=11, -24<=l<=24	
Reflections collected	20581	
Independent reflections	10790 [R(int) = 0.0659]	
Completeness to theta = 67.679°	92.0 %	
Absorption correction	Empirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10790 / 6 / 842	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0764, wR2 = 0.2005	
R indices (all data)	R1 = 0.0868, wR2 = 0.2120	
Absolute structure parameter	0.110(17)	
Extinction coefficient	0.0035(6)	
Largest diff. peak and hole	1.313 and -1.219 $e.Å^{-3}$	

S-Table 11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **114**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	7947(1)	8266(2)	6552(1)	62(1)
Br(2)	6113(1)	8059(2)	4582(1)	53(1)
Br(3)	4201(1)	8027(1)	2726(1)	46(1)
Br(4)	2032(1)	8204(2)	10770(1)	57(1)
Br(5)	-100(1)	8532(2)	8657(1)	51(1)
N(1)	8563(5)	3400(10)	5101(4)	40(2)
N(2)	6666(4)	3190(10)	3105(3)	28(2)
N(3)	4605(4)	3083(11)	1227(3)	29(2)
N(4)	2468(4)	3181(10)	9284(3)	27(2)
N(5)	407(4)	3431(10)	7204(4)	32(2)
O(1)	7919(4)	3167(13)	4071(3)	51(2)
O(2)	9139(4)	3509(8)	4189(3)	35(2)
O(3)	5936(4)	2976(11)	2120(3)	41(2)
O(4)	7172(3)	3313(8)	2152(3)	27(2)
O(5)	3811(4)	3000(11)	275(3)	42(2)
O(6)	5054(4)	3247(9)	237(3)	34(2)
O(7)	1711(4)	3183(12)	8309(3)	45(2)
O(8)	2952(3)	3323(8)	8324(3)	30(2)
O(9)	-235(4)	3398(10)	6178(4)	45(2)
O(10)	1000(4)	3383(8)	6298(3)	35(2)
C(1)	7958(8)	5556(16)	6007(6)	52(4)
C(2)	7922(7)	6329(17)	6597(6)	54(4)
C(3)	7883(7)	5688(16)	7209(6)	49(3)
C(5)	7850(7)	3490(15)	6654(5)	42(3)
C(6)	7930(8)	4169(15)	6057(6)	48(3)
C(7)	7962(7)	3143(18)	5494(5)	56(4)
C(8)	8047(13)	1742(17)	5874(7)	81(7)
C(9)	7800(8)	1988(17)	6559(6)	54(4)
C(10)	8496(6)	3329(12)	4418(5)	35(3)
C(11)	9206(6)	3537(13)	3456(5)	36(3)
C(12)	10019(8)	3740(20)	3438(7)	72(5)
C(13)	8958(9)	2194(13)	3131(7)	53(4)
C(14)	8786(7)	4742(12)	3138(6)	42(3)
C(15)	6117(6)	5333(13)	4056(5)	34(2)
C(16)	6087(7)	6102(12)	4647(5)	40(3)
C(17)	6049(8)	5511(14)	5273(6)	51(3)
C(18)	5981(10)	4082(14)	5325(6)	60(4)

C(19)	6017(7)	3295(15)	4742(6)	47(3)
C(20)	6085(7)	3945(13)	4118(5)	36(3)
C(21)	6099(5)	2895(12)	3561(5)	31(2)
C(4)	7823(8)	4300(16)	7249(5)	53(4)
C(22)	6217(8)	1539(13)	3944(6)	44(3)
C(23)	5938(9)	1796(15)	4645(8)	60(4)
C(24)	6538(5)	3164(11)	2431(4)	24(2)
C(25)	7194(6)	3377(11)	1409(4)	32(2)
C(26)	7996(6)	3599(19)	1348(5)	56(4)
C(27)	6914(7)	2059(12)	1082(6)	41(3)
C(28)	6762(7)	4600(12)	1130(6)	38(3)
C(29)	4124(6)	5303(11)	2210(5)	32(2)
C(30)	4175(6)	6076(12)	2797(6)	35(2)
C(31)	4226(7)	5494(12)	3425(6)	40(3)
C(32)	4181(8)	4081(13)	3484(6)	44(3)
C(33)	4134(5)	3281(11)	2912(5)	30(2)
C(34)	4109(5)	3883(11)	2279(5)	29(2)
C(35)	4078(5)	2835(11)	1718(5)	29(2)
C(36)	4215(8)	1491(12)	2105(6)	40(3)
C(37)	4094(7)	1748(12)	2848(7)	43(3)
C(38)	4444(5)	3087(12)	554(4)	26(2)
C(39)	5041(6)	3353(11)	-505(5)	34(2)
C(40)	5856(8)	3500(20)	-627(6)	72(6)
C(41)	4731(8)	2042(12)	-835(6)	45(3)
C(42)	4596(8)	4603(12)	-760(6)	47(4)
C(43)	1931(7)	5486(14)	10240(5)	43(3)
C(44)	2070(7)	6234(14)	10827(6)	44(3)
C(45)	2214(6)	5642(14)	11451(5)	41(3)
C(46)	2218(6)	4233(14)	11500(6)	41(3)
C(47)	2091(6)	3435(16)	10919(5)	42(3)
C(48)	1968(7)	4100(15)	10293(6)	44(3)
C(49)	1866(7)	3063(16)	9738(6)	48(3)
C(50)	1865(17)	1690(20)	10093(9)	125(12)
C(51)	2078(7)	1914(15)	10849(7)	50(3)
C(52)	2322(5)	3225(10)	8613(4)	23(2)
C(53)	2950(5)	3398(12)	7583(4)	32(3)
C(54)	3748(7)	3520(20)	7482(5)	69(6)
C(55)	2550(8)	4663(12)	7316(5)	43(3)
C(56)	2638(7)	2108(12)	7253(6)	40(3)
C(57)	-181(6)	5852(12)	8102(6)	37(3)
C(58)	-76(7)	6572(14)	8686(7)	45(3)
C(59)	49(8)	5978(14)	9313(6)	51(3)
C(60)	57(9)	4548(17)	9352(6)	61(4)
C(61)	-54(7)	3801(16)	8763(6)	38(3)
C(62)	-162(6)	4431(14)	8153(6)	38(3)
C(63)	-243(6)	3400(13)	7577(6)	42(3)

C(64)	-353(9)	2082(17)	7950(8)	58(4)
C(65)	-57(9)	2270(16)	8669(7)	52(4)
C(66)	340(6)	3427(11)	6523(5)	35(3)
C(67)	1062(6)	3426(12)	5564(5)	36(3)
C(68)	1881(7)	3380(30)	5526(5)	78(7)
C(69)	740(9)	4749(13)	5265(6)	50(3)
C(70)	702(8)	2160(13)	5226(7)	50(3)

S-Table 12. Bond lengths [Å] and angles [°] for **114**.

Br(1)-C(2)	1.896(16)	C(6)-C(7)	1.51(2)
Br(2)-C(16)	1.918(11)	C(7)-C(8)	1.57(2)
Br(3)-C(30)	1.914(11)	C(7)-H(7)	1.0000
Br(4)-C(44)	1.931(14)	C(8)-C(9)	1.499(19)
Br(5)-C(58)	1.917(14)	C(8)-H(8A)	0.9900
N(1)-C(10)	1.355(12)	C(8)-H(8B)	0.9900
N(1)-C(7)	1.434(15)	C(9)-H(9A)	0.9900
N(1)-H(1X)	1.00(3)	C(9)-H(9B)	0.9900
N(2)-C(24)	1.342(10)	C(11)-C(12)	1.503(18)
N(2)-C(21)	1.471(12)	C(11)-C(14)	1.512(16)
N(2)-H(2X)	0.99(3)	C(11)-C(13)	1.514(17)
N(3)-C(38)	1.346(11)	C(12)-H(12A)	0.9800
N(3)-C(35)	1.459(13)	C(12)-H(12B)	0.9800
N(3)-H(3X)	0.99(3)	C(12)-H(12C)	0.9800
N(4)-C(52)	1.339(10)	C(13)-H(13A)	0.9800
N(4)-C(49)	1.496(13)	C(13)-H(13B)	0.9800
N(4)-H(4X)	1.00(3)	C(13)-H(13C)	0.9800
N(5)-C(66)	1.352(12)	C(14)-H(14A)	0.9800
N(5)-C(63)	1.462(15)	C(14)-H(14B)	0.9800
N(5)-H(5X)	1.00(3)	C(14)-H(14C)	0.9800
O(1)-C(10)	1.215(12)	C(15)-C(20)	1.365(17)
O(2)-C(10)	1.316(13)	C(15)-C(16)	1.404(15)
O(2)-C(11)	1.478(12)	C(15)-H(15)	0.9500
O(3)-C(24)	1.225(11)	C(16)-C(17)	1.382(16)
O(4)-C(24)	1.343(11)	C(17)-C(18)	1.407(19)
O(4)-C(25)	1.487(9)	C(17)-H(17)	0.9500
O(5)-C(38)	1.237(11)	C(18)-C(19)	1.401(18)
O(6)-C(38)	1.344(12)	C(18)-H(18)	0.9500
O(6)-C(39)	1.479(11)	C(19)-C(20)	1.412(16)
O(7)-C(52)	1.219(11)	C(19)-C(23)	1.48(2)
O(8)-C(52)	1.341(11)	C(20)-C(21)	1.514(15)
O(8)-C(53)	1.478(9)	C(21)-C(22)	1.535(17)
O(9)-C(66)	1.201(13)	C(21)-H(21)	1.0000
O(10)-C(66)	1.328(14)	C(4)-H(4)	0.9500
O(10)-C(67)	1.479(11)	C(22)-C(23)	1.552(17)
C(1)-C(6)	1.36(2)	C(22)-H(22A)	0.9900
C(1)-C(2)	1.404(19)	C(22)-H(22B)	0.9900
C(1)-H(1)	0.9500	C(23)-H(23A)	0.9900
C(2)-C(3)	1.380(17)	C(23)-H(23B)	0.9900
C(3)-C(4)	1.36(2)	C(25)-C(26)	1.499(16)
C(3)-H(3)	0.9500	C(25)-C(28)	1.509(15)
C(5)-C(6)	1.383(16)	C(25)-C(27)	1.510(16)
C(5)-C(4)	1.430(18)	C(26)-H(26A)	0.9800
C(5)-C(9)	1.48(2)	C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800	C(49)-C(50)	1.52(3)
C(27)-H(27A)	0.9800	C(49)-H(49)	1.0000
C(27)-H(27B)	0.9800	C(50)-C(51)	1.54(2)
C(27)-H(27C)	0.9800	C(50)-H(50A)	0.9900
C(28)-H(28A)	0.9800	C(50)-H(50B)	0.9900
C(28)-H(28B)	0.9800	C(51)-H(51A)	0.9900
C(28)-H(28C)	0.9800	C(51)-H(51B)	0.9900
C(29)-C(30)	1.389(15)	C(53)-C(54)	1.498(16)
C(29)-C(34)	1.395(15)	C(53)-C(55)	1.507(17)
C(29)-H(29)	0.9500	C(53)-C(56)	1.508(16)
C(30)-C(31)	1.369(16)	C(54)-H(54A)	0.9800
C(31)-C(32)	1.390(17)	C(54)-H(54B)	0.9800
C(31)-H(31)	0.9500	C(54)-H(54C)	0.9800
C(32)-C(33)	1.379(16)	C(55)-H(55A)	0.9800
C(32)-H(32)	0.9500	C(55)-H(55B)	0.9800
C(33)-C(34)	1.390(15)	C(55)-H(55C)	0.9800
C(33)-C(37)	1.506(15)	C(56)-H(56A)	0.9800
C(34)-C(35)	1.513(14)	C(56)-H(56B)	0.9800
C(35)-C(36)	1.531(15)	C(56)-H(56C)	0.9800
C(35)-H(35)	1.0000	C(57)-C(58)	1.358(16)
C(36)-C(37)	1.540(17)	C(57)-C(62)	1.393(18)
C(36)-H(36)	0.9500	C(57)-H(57)	0.9500
C(37)-H(37)	0.9500	C(58)-C(59)	1.378(19)
C(39)-C(41)	1.525(15)	C(59)-C(60)	1.40(2)
C(39)-C(42)	1.528(16)	C(59)-H(59)	0.9500
C(39)-C(40)	1.542(18)	C(60)-C(61)	1.380(17)
C(40)-H(40A)	0.9800	C(60)-H(60)	0.9500
C(40)-H(40B)	0.9800	C(61)-C(62)	1.361(18)
C(40)-H(40C)	0.9800	C(61)-C(65)	1.509(19)
C(41)-H(41A)	0.9800	C(62)-C(63)	1.524(15)
C(41)-H(41B)	0.9800	C(63)-C(64)	1.51(2)
C(41)-H(41C)	0.9800	C(63)-H(63)	1.0000
C(42)-H(42A)	0.9800	C(64)-C(65)	1.49(2)
C(42)-H(42B)	0.9800	C(64)-H(64A)	0.9900
C(42)-H(42C)	0.9800	C(64)-H(64B)	0.9900
C(43)-C(48)	1.36(2)	C(65)-H(65A)	0.9900
C(43)-C(44)	1.382(16)	C(65)-H(65B)	0.9900
C(43)-H(43)	0.9500	C(67)-C(68)	1.507(17)
C(44)-C(45)	1.375(18)	C(67)-C(69)	1.520(16)
C(45)-C(46)	1.380(19)	C(67)-C(70)	1.527(17)
C(45)-H(45)	0.9500	C(68)-H(68A)	0.9800
C(46)-C(47)	1.398(16)	C(68)-H(68B)	0.9800
C(46)-H(46)	0.9500	C(68)-H(68C)	0.9800
C(47)-C(48)	1.404(18)	C(69)-H(69A)	0.9800
C(47)-C(51)	1.49(2)	C(69)-H(69B)	0.9800
C(48)-C(49)	1.499(16)	C(69)-H(69C)	0.9800

C(70)-H(70A)	0.9800	C(9)-C(8)-H(8A)	110.5
C(70)-H(70B)	0.9800	C(7)-C(8)-H(8A)	110.5
C(70)-H(70C)	0.9800	C(9)-C(8)-H(8B)	110.5
		C(7)-C(8)-H(8B)	110.5
C(10)-N(1)-C(7)	122.7(9)	H(8A)-C(8)-H(8B)	108.7
C(10)-N(1)-H(1X)	125(7)	C(5)-C(9)-C(8)	104.8(12)
C(7)-N(1)-H(1X)	112(7)	C(5)-C(9)-H(9A)	110.8
C(24)-N(2)-C(21)	123.3(8)	C(8)-C(9)-H(9A)	110.8
C(24)-N(2)-H(2X)	142(6)	C(5)-C(9)-H(9B)	110.8
C(21)-N(2)-H(2X)	95(6)	C(8)-C(9)-H(9B)	110.8
C(38)-N(3)-C(35)	125.1(8)	H(9A)-C(9)-H(9B)	108.9
C(38)-N(3)-H(3X)	109(6)	O(1)-C(10)-O(2)	125.2(9)
C(35)-N(3)-H(3X)	126(6)	O(1)-C(10)-N(1)	124.6(10)
C(52)-N(4)-C(49)	121.3(8)	O(2)-C(10)-N(1)	110.2(8)
C(52)-N(4)-H(4X)	117(6)	O(2)-C(11)-C(12)	101.7(8)
C(49)-N(4)-H(4X)	121(6)	O(2)-C(11)-C(14)	110.0(9)
C(66)-N(5)-C(63)	120.8(9)	C(12)-C(11)-C(14)	110.6(12)
C(66)-N(5)-H(5X)	119(7)	O(2)-C(11)-C(13)	110.8(10)
C(63)-N(5)-H(5X)	121(6)	C(12)-C(11)-C(13)	111.1(12)
C(10)-O(2)-C(11)	120.6(7)	C(14)-C(11)-C(13)	112.2(8)
C(24)-O(4)-C(25)	121.7(7)	C(11)-C(12)-H(12A)	109.5
C(38)-O(6)-C(39)	122.9(7)	C(11)-C(12)-H(12B)	109.5
C(52)-O(8)-C(53)	120.8(6)	H(12A)-C(12)-H(12B)	109.5
C(66)-O(10)-C(67)	119.5(7)	C(11)-C(12)-H(12C)	109.5
C(6)-C(1)-C(2)	118.1(12)	H(12A)-C(12)-H(12C)	109.5
C(6)-C(1)-H(1)	121.0	H(12B)-C(12)-H(12C)	109.5
C(2)-C(1)-H(1)	121.0	C(11)-C(13)-H(13A)	109.5
C(3)-C(2)-C(1)	120.4(15)	C(11)-C(13)-H(13B)	109.5
C(3)-C(2)-Br(1)	119.9(11)	H(13A)-C(13)-H(13B)	109.5
C(1)-C(2)-Br(1)	119.7(10)	C(11)-C(13)-H(13C)	109.5
C(4)-C(3)-C(2)	121.0(13)	H(13A)-C(13)-H(13C)	109.5
C(4)-C(3)-H(3)	119.5	H(13B)-C(13)-H(13C)	109.5
C(2)-C(3)-H(3)	119.5	C(11)-C(14)-H(14A)	109.5
C(6)-C(5)-C(4)	117.5(13)	C(11)-C(14)-H(14B)	109.5
C(6)-C(5)-C(9)	112.1(12)	H(14A)-C(14)-H(14B)	109.5
C(4)-C(5)-C(9)	130.4(12)	C(11)-C(14)-H(14C)	109.5
C(1)-C(6)-C(5)	123.3(13)	H(14A)-C(14)-H(14C)	109.5
C(1)-C(6)-C(7)	127.1(12)	H(14B)-C(14)-H(14C)	109.5
C(5)-C(6)-C(7)	109.6(13)	C(20)-C(15)-C(16)	116.8(10)
N(1)-C(7)-C(6)	112.1(11)	C(20)-C(15)-H(15)	121.6
N(1)-C(7)-C(8)	111.8(14)	C(16)-C(15)-H(15)	121.6
C(6)-C(7)-C(8)	103.4(10)	C(17)-C(16)-C(15)	122.9(11)
N(1)-C(7)-H(7)	109.8	C(17)-C(16)-Br(2)	118.8(9)
C(6)-C(7)-H(7)	109.8	C(15)-C(16)-Br(2)	118.3(8)
C(8)-C(7)-H(7)	109.8	C(16)-C(17)-C(18)	119.7(12)
C(9)-C(8)-C(7)	106.0(14)	C(16)-C(17)-H(17)	120.2

C(18)-C(17)-H(17)	120.2	C(25)-C(27)-H(27A)	109.5
C(19)-C(18)-C(17)	118.1(12)	C(25)-C(27)-H(27B)	109.5
C(19)-C(18)-H(18)	120.9	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18)	120.9	C(25)-C(27)-H(27C)	109.5
C(18)-C(19)-C(20)	120.0(13)	H(27A)-C(27)-H(27C)	109.5
C(18)-C(19)-C(23)	129.7(12)	H(27B)-C(27)-H(27C)	109.5
C(20)-C(19)-C(23)	110.2(11)	C(25)-C(28)-H(28A)	109.5
C(15)-C(20)-C(19)	122.3(11)	C(25)-C(28)-H(28B)	109.5
C(15)-C(20)-C(21)	127.1(10)	H(28A)-C(28)-H(28B)	109.5
C(19)-C(20)-C(21)	110.5(11)	C(25)-C(28)-H(28C)	109.5
N(2)-C(21)-C(20)	112.5(9)	H(28A)-C(28)-H(28C)	109.5
N(2)-C(21)-C(22)	113.8(9)	H(28B)-C(28)-H(28C)	109.5
C(20)-C(21)-C(22)	103.4(9)	C(30)-C(29)-C(34)	117.3(10)
N(2)-C(21)-H(21)	109.0	C(30)-C(29)-H(29)	121.4
C(20)-C(21)-H(21)	109.0	C(34)-C(29)-H(29)	121.4
C(22)-C(21)-H(21)	109.0	C(31)-C(30)-C(29)	122.5(11)
C(3)-C(4)-C(5)	119.5(12)	C(31)-C(30)-Br(3)	118.8(8)
C(3)-C(4)-H(4)	120.2	C(29)-C(30)-Br(3)	118.6(9)
C(5)-C(4)-H(4)	120.2	C(30)-C(31)-C(32)	119.4(11)
C(21)-C(22)-C(23)	105.4(10)	C(30)-C(31)-H(31)	120.3
C(21)-C(22)-H(22A)	110.7	C(32)-C(31)-H(31)	120.3
C(23)-C(22)-H(22A)	110.7	C(33)-C(32)-C(31)	119.5(10)
C(21)-C(22)-H(22B)	110.7	C(33)-C(32)-H(32)	120.2
C(23)-C(22)-H(22B)	110.7	C(31)-C(32)-H(32)	120.2
H(22A)-C(22)-H(22B)	108.8	C(32)-C(33)-C(34)	120.3(10)
C(19)-C(23)-C(22)	103.9(10)	C(32)-C(33)-C(37)	129.3(10)
C(19)-C(23)-H(23A)	111.0	C(34)-C(33)-C(37)	110.3(10)
C(22)-C(23)-H(23A)	111.0	C(33)-C(34)-C(29)	120.8(10)
C(19)-C(23)-H(23B)	111.0	C(33)-C(34)-C(35)	112.3(9)
C(22)-C(23)-H(23B)	111.0	C(29)-C(34)-C(35)	126.9(10)
H(23A)-C(23)-H(23B)	109.0	N(3)-C(35)-C(34)	113.7(9)
O(3)-C(24)-N(2)	124.9(8)	N(3)-C(35)-C(36)	113.2(9)
O(3)-C(24)-O(4)	125.2(8)	C(34)-C(35)-C(36)	102.6(8)
N(2)-C(24)-O(4)	109.9(7)	N(3)-C(35)-H(35)	109.0
O(4)-C(25)-C(26)	101.9(7)	C(34)-C(35)-H(35)	109.0
O(4)-C(25)-C(28)	109.6(8)	C(36)-C(35)-H(35)	109.0
C(26)-C(25)-C(28)	109.7(11)	C(35)-C(36)-C(37)	108.2(10)
O(4)-C(25)-C(27)	110.7(9)	C(35)-C(36)-H(36)	125.9
C(26)-C(25)-C(27)	112.5(11)	C(37)-C(36)-H(36)	125.9
C(28)-C(25)-C(27)	111.9(8)	C(33)-C(37)-C(36)	103.5(9)
C(25)-C(26)-H(26A)	109.5	C(33)-C(37)-H(37)	128.2
C(25)-C(26)-H(26B)	109.5	C(36)-C(37)-H(37)	128.2
H(26A)-C(26)-H(26B)	109.5	O(5)-C(38)-O(6)	125.5(8)
C(25)-C(26)-H(26C)	109.5	O(5)-C(38)-N(3)	123.6(9)
H(26A)-C(26)-H(26C)	109.5	O(6)-C(38)-N(3)	110.9(7)
H(26B)-C(26)-H(26C)	109.5	O(6)-C(39)-C(41)	110.0(9)

O(6)-C(39)-C(42)	110.2(9)	C(50)-C(49)-H(49)	109.5
C(41)-C(39)-C(42)	111.4(8)	C(49)-C(50)-C(51)	108.5(13)
O(6)-C(39)-C(40)	104.0(7)	C(49)-C(50)-H(50A)	110.0
C(41)-C(39)-C(40)	109.6(12)	C(51)-C(50)-H(50A)	110.0
C(42)-C(39)-C(40)	111.4(11)	C(49)-C(50)-H(50B)	110.0
C(39)-C(40)-H(40A)	109.5	C(51)-C(50)-H(50B)	110.0
C(39)-C(40)-H(40B)	109.5	H(50A)-C(50)-H(50B)	108.4
H(40A)-C(40)-H(40B)	109.5	C(47)-C(51)-C(50)	103.6(13)
C(39)-C(40)-H(40C)	109.5	C(47)-C(51)-H(51A)	111.0
H(40A)-C(40)-H(40C)	109.5	C(50)-C(51)-H(51A)	111.0
H(40B)-C(40)-H(40C)	109.5	C(47)-C(51)-H(51B)	111.0
C(39)-C(41)-H(41A)	109.5	C(50)-C(51)-H(51B)	111.0
C(39)-C(41)-H(41B)	109.5	H(51A)-C(51)-H(51B)	109.0
H(41A)-C(41)-H(41B)	109.5	O(7)-C(52)-N(4)	125.4(9)
C(39)-C(41)-H(41C)	109.5	O(7)-C(52)-O(8)	125.1(8)
H(41A)-C(41)-H(41C)	109.5	N(4)-C(52)-O(8)	109.5(7)
H(41B)-C(41)-H(41C)	109.5	O(8)-C(53)-C(54)	103.2(7)
C(39)-C(42)-H(42A)	109.5	O(8)-C(53)-C(55)	110.4(8)
C(39)-C(42)-H(42B)	109.5	C(54)-C(53)-C(55)	109.5(11)
H(42A)-C(42)-H(42B)	109.5	O(8)-C(53)-C(56)	111.0(9)
C(39)-C(42)-H(42C)	109.5	C(54)-C(53)-C(56)	109.8(11)
H(42A)-C(42)-H(42C)	109.5	C(55)-C(53)-C(56)	112.4(8)
H(42B)-C(42)-H(42C)	109.5	C(53)-C(54)-H(54A)	109.5
C(48)-C(43)-C(44)	117.2(12)	C(53)-C(54)-H(54B)	109.5
C(48)-C(43)-H(43)	121.4	H(54A)-C(54)-H(54B)	109.5
C(44)-C(43)-H(43)	121.4	C(53)-C(54)-H(54C)	109.5
C(45)-C(44)-C(43)	123.2(13)	H(54A)-C(54)-H(54C)	109.5
C(45)-C(44)-Br(4)	118.4(9)	H(54B)-C(54)-H(54C)	109.5
C(43)-C(44)-Br(4)	118.4(10)	C(53)-C(55)-H(55A)	109.5
C(44)-C(45)-C(46)	118.9(11)	C(53)-C(55)-H(55B)	109.5
C(44)-C(45)-H(45)	120.6	H(55A)-C(55)-H(55B)	109.5
C(46)-C(45)-H(45)	120.6	C(53)-C(55)-H(55C)	109.5
C(45)-C(46)-C(47)	119.9(12)	H(55A)-C(55)-H(55C)	109.5
C(45)-C(46)-H(46)	120.0	H(55B)-C(55)-H(55C)	109.5
C(47)-C(46)-H(46)	120.0	C(53)-C(56)-H(56A)	109.5
C(46)-C(47)-C(48)	118.5(14)	C(53)-C(56)-H(56B)	109.5
C(46)-C(47)-C(51)	129.3(12)	H(56A)-C(56)-H(56B)	109.5
C(48)-C(47)-C(51)	112.2(11)	C(53)-C(56)-H(56C)	109.5
C(43)-C(48)-C(47)	122.2(11)	H(56A)-C(56)-H(56C)	109.5
C(43)-C(48)-C(49)	127.9(12)	H(56B)-C(56)-H(56C)	109.5
C(47)-C(48)-C(49)	109.9(13)	C(58)-C(57)-C(62)	117.1(12)
N(4)-C(49)-C(48)	110.4(10)	C(58)-C(57)-H(57)	121.5
N(4)-C(49)-C(50)	112.6(15)	C(62)-C(57)-H(57)	121.5
C(48)-C(49)-C(50)	105.1(12)	C(57)-C(58)-C(59)	123.8(13)
N(4)-C(49)-H(49)	109.5	C(57)-C(58)-Br(5)	119.4(10)
C(48)-C(49)-H(49)	109.5	C(59)-C(58)-Br(5)	116.8(10)

C(58)-C(59)-C(60)	118.1(12)	C(67)-C(69)-H(69B)	109.5
C(58)-C(59)-H(59)	121.0	H(69A)-C(69)-H(69B)	109.5
C(60)-C(59)-H(59)	121.0	C(67)-C(69)-H(69C)	109.5
C(61)-C(60)-C(59)	118.8(13)	H(69A)-C(69)-H(69C)	109.5
C(61)-C(60)-H(60)	120.6	H(69B)-C(69)-H(69C)	109.5
C(59)-C(60)-H(60)	120.6	C(67)-C(70)-H(70A)	109.5
C(62)-C(61)-C(60)	121.2(15)	C(67)-C(70)-H(70B)	109.5
C(62)-C(61)-C(65)	109.8(12)	H(70A)-C(70)-H(70B)	109.5
C(60)-C(61)-C(65)	129.0(14)	C(67)-C(70)-H(70C)	109.5
C(61)-C(62)-C(57)	121.1(12)	H(70A)-C(70)-H(70C)	109.5
C(61)-C(62)-C(63)	111.7(12)	H(70B)-C(70)-H(70C)	109.5
C(57)-C(62)-C(63)	127.2(12)		
N(5)-C(63)-C(64)	114.8(11)		
N(5)-C(63)-C(62)	110.1(9)		
C(64)-C(63)-C(62)	101.6(10)		
N(5)-C(63)-H(63)	110.0		
C(64)-C(63)-H(63)	110.0		
C(62)-C(63)-H(63)	110.0		
C(65)-C(64)-C(63)	108.3(11)		
C(65)-C(64)-H(64A)	110.0		
C(63)-C(64)-H(64A)	110.0		
C(65)-C(64)-H(64B)	110.0		
C(63)-C(64)-H(64B)	110.0		
H(64A)-C(64)-H(64B)	108.4		
C(64)-C(65)-C(61)	103.8(13)		
C(64)-C(65)-H(65A)	111.0		
C(61)-C(65)-H(65A)	111.0		
C(64)-C(65)-H(65B)	111.0		
C(61)-C(65)-H(65B)	111.0		
H(65A)-C(65)-H(65B)	109.0		
O(9)-C(66)-O(10)	125.5(10)		
O(9)-C(66)-N(5)	124.4(11)		
O(10)-C(66)-N(5)	110.1(8)		
O(10)-C(67)-C(68)	102.7(7)		
O(10)-C(67)-C(69)	110.3(9)		
C(68)-C(67)-C(69)	110.8(13)		
O(10)-C(67)-C(70)	110.0(10)		
C(68)-C(67)-C(70)	110.1(12)		
C(69)-C(67)-C(70)	112.5(9)		
C(67)-C(68)-H(68A)	109.5		
C(67)-C(68)-H(68B)	109.5		
H(68A)-C(68)-H(68B)	109.5		
C(67)-C(68)-H(68C)	109.5		
H(68A)-C(68)-H(68C)	109.5		
H(68B)-C(68)-H(68C)	109.5		
C(67)-C(69)-H(69A)	109.5		

Symmetry transformations used to generate equivalent atoms:

S-Table 13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **114**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

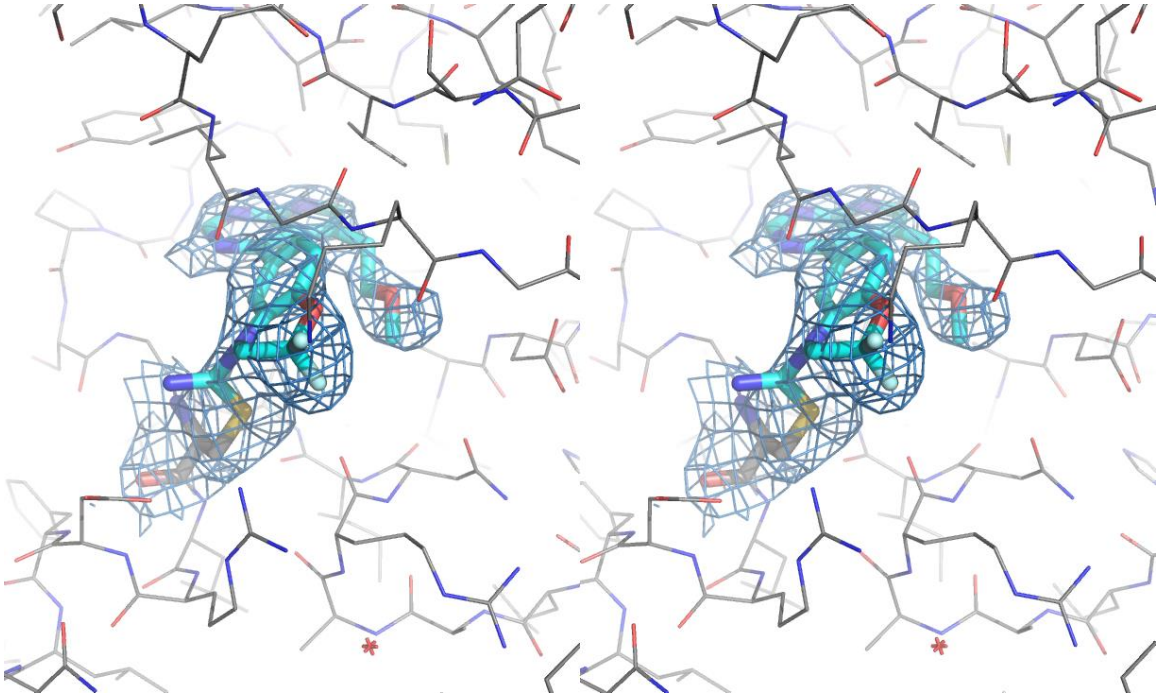
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	79(1)	61(1)	47(1)	0(1)	12(1)	-22(1)
Br(2)	89(1)	32(1)	44(1)	-5(1)	28(1)	1(1)
Br(3)	72(1)	24(1)	44(1)	-5(1)	11(1)	4(1)
Br(4)	88(1)	47(1)	39(1)	-8(1)	16(1)	-14(1)
Br(5)	53(1)	43(1)	59(1)	-10(1)	16(1)	1(1)
N(1)	50(5)	48(7)	19(4)	7(4)	-4(4)	-16(5)
N(2)	34(4)	30(5)	18(3)	-2(4)	4(3)	-3(4)
N(3)	31(4)	34(4)	22(3)	-2(4)	-5(3)	2(4)
N(4)	34(4)	33(5)	15(3)	0(4)	6(3)	-2(4)
N(5)	31(4)	46(6)	20(3)	-7(4)	0(3)	7(4)
O(1)	44(4)	84(7)	24(3)	8(5)	-11(3)	-22(5)
O(2)	38(4)	41(4)	24(3)	3(3)	-11(3)	-4(3)
O(3)	32(4)	50(5)	37(4)	-2(5)	-10(3)	1(4)
O(4)	27(3)	40(4)	14(3)	-1(3)	-2(2)	3(3)
O(5)	36(4)	53(5)	32(3)	-11(4)	-16(3)	8(4)
O(6)	37(4)	43(5)	21(3)	5(3)	-9(3)	-9(4)
O(7)	27(3)	75(7)	31(3)	-13(5)	-4(3)	1(5)
O(8)	26(3)	51(5)	11(2)	-1(3)	-2(2)	-4(3)
O(9)	39(4)	56(7)	37(4)	-7(4)	-13(3)	-1(4)
O(10)	30(3)	50(5)	23(3)	-5(4)	-5(3)	13(3)
C(1)	64(8)	66(9)	23(5)	5(6)	-1(5)	-27(7)
C(2)	49(7)	80(10)	31(6)	8(6)	-5(6)	-15(7)
C(3)	50(7)	70(9)	27(6)	7(6)	1(5)	19(7)
C(5)	41(6)	67(9)	17(4)	13(6)	0(4)	7(6)
C(6)	58(8)	62(9)	22(6)	13(6)	-1(5)	-18(7)
C(7)	66(8)	75(10)	28(5)	-8(7)	6(5)	-37(8)
C(8)	156(18)	52(10)	40(8)	-6(7)	29(10)	-54(11)
C(9)	62(8)	74(10)	29(6)	6(7)	15(6)	14(8)
C(10)	41(6)	38(7)	25(4)	6(5)	-12(4)	-11(5)
C(11)	36(5)	43(7)	24(4)	0(5)	-13(4)	0(5)
C(12)	53(8)	128(16)	35(6)	-9(9)	1(6)	-6(9)
C(13)	89(10)	26(6)	41(7)	6(5)	-12(7)	4(6)
C(14)	62(8)	30(6)	31(6)	10(5)	-2(5)	-7(6)
C(15)	35(6)	45(7)	21(5)	1(5)	8(4)	-8(5)

C(16)	64(8)	29(6)	31(6)	5(5)	27(6)	6(5)
C(17)	78(9)	47(7)	33(6)	-1(5)	28(6)	10(7)
C(18)	118(13)	33(7)	36(7)	3(5)	44(8)	-1(7)
C(19)	58(7)	53(9)	32(5)	4(6)	19(5)	2(7)
C(20)	46(6)	39(7)	24(5)	0(5)	8(5)	-3(5)
C(21)	24(4)	40(6)	31(5)	-17(5)	11(4)	-6(5)
C(4)	66(9)	79(11)	13(5)	11(5)	0(5)	24(8)
C(22)	64(8)	30(6)	43(7)	-7(5)	23(6)	-13(6)
C(23)	86(11)	44(8)	59(9)	1(7)	46(8)	-11(7)
C(24)	27(4)	23(5)	22(4)	-2(4)	-2(3)	-8(4)
C(25)	45(6)	41(7)	9(3)	-1(4)	-7(4)	5(5)
C(26)	38(6)	112(13)	19(4)	9(7)	8(4)	4(7)
C(27)	66(8)	33(6)	24(5)	-4(5)	5(5)	14(6)
C(28)	61(8)	24(6)	27(5)	0(5)	-2(5)	1(5)
C(29)	41(6)	27(6)	27(5)	2(4)	-2(4)	6(5)
C(30)	38(6)	32(6)	35(6)	-9(5)	6(5)	3(5)
C(31)	47(7)	37(6)	38(6)	-5(5)	19(5)	-1(5)
C(32)	64(8)	48(7)	23(5)	5(5)	26(5)	6(6)
C(33)	31(5)	23(6)	40(5)	9(5)	18(4)	1(4)
C(34)	25(5)	26(6)	34(5)	-3(4)	-3(4)	2(4)
C(35)	33(5)	27(6)	27(4)	-3(4)	2(4)	-5(4)
C(36)	64(8)	20(5)	37(6)	2(5)	5(6)	-3(5)
C(37)	57(8)	26(6)	49(7)	7(5)	13(6)	-1(5)
C(38)	31(5)	20(4)	25(4)	-5(5)	-7(4)	-2(5)
C(39)	47(6)	27(6)	24(4)	3(4)	-13(4)	-5(5)
C(40)	60(8)	131(18)	25(5)	15(8)	-3(5)	-9(10)
C(41)	78(9)	21(6)	34(6)	1(5)	-8(6)	5(6)
C(42)	85(10)	27(6)	24(5)	10(5)	-25(6)	-15(6)
C(43)	61(8)	51(8)	20(5)	-10(5)	11(5)	-19(6)
C(44)	41(7)	50(8)	44(7)	-12(6)	10(6)	-1(6)
C(45)	36(6)	62(8)	23(5)	-18(5)	-7(4)	10(6)
C(46)	38(6)	53(8)	31(6)	-17(5)	-5(5)	12(6)
C(47)	31(5)	69(10)	27(5)	-9(6)	1(4)	-1(6)
C(48)	43(7)	67(9)	24(5)	-16(6)	16(5)	-17(6)
C(49)	63(7)	47(7)	39(5)	-19(6)	24(5)	-24(7)
C(50)	250(30)	82(14)	58(11)	-22(10)	78(15)	-97(18)
C(51)	41(7)	52(8)	55(8)	-16(7)	-3(6)	-5(6)
C(52)	33(5)	14(5)	21(4)	-1(4)	1(4)	-2(4)
C(53)	33(5)	55(8)	7(3)	2(4)	5(3)	-8(5)
C(54)	46(7)	142(18)	19(5)	-6(8)	5(5)	-15(9)
C(55)	79(9)	30(6)	18(5)	0(4)	1(5)	-13(6)
C(56)	61(8)	34(6)	24(5)	0(5)	2(5)	10(6)
C(57)	38(6)	37(6)	34(6)	-6(5)	2(5)	-4(5)
C(58)	40(6)	42(7)	54(7)	-11(6)	15(6)	-2(5)
C(59)	73(9)	48(8)	35(6)	-13(5)	25(6)	-6(7)
C(60)	93(12)	61(9)	29(6)	-12(6)	12(7)	7(8)

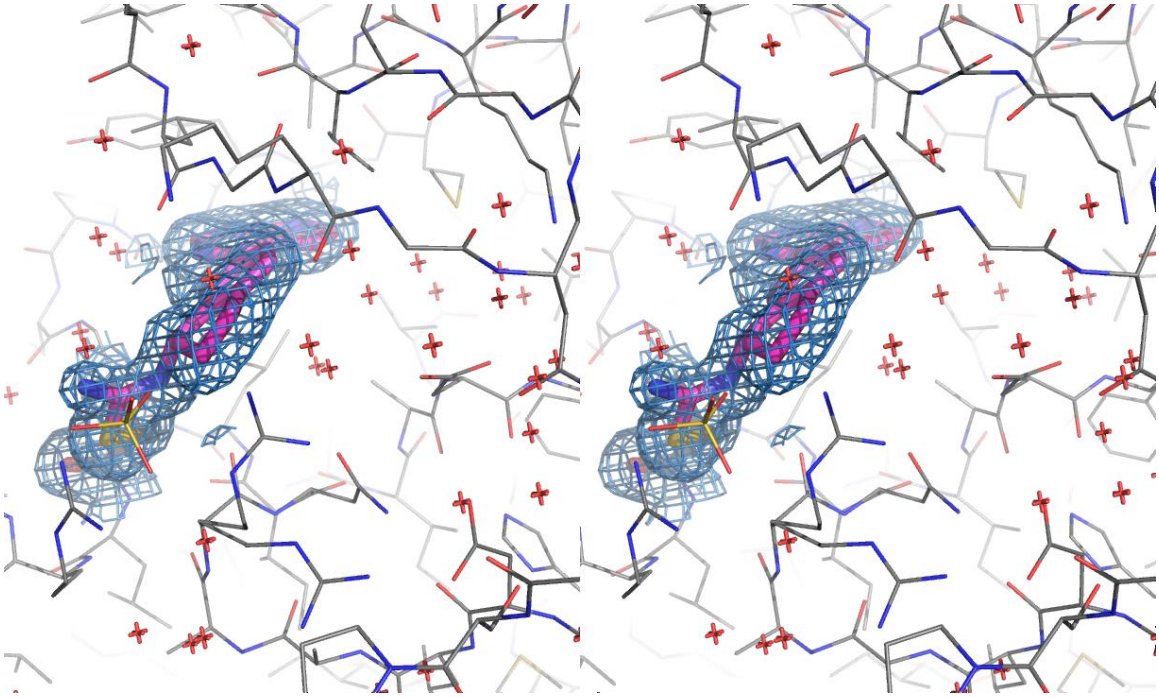
C(61)	39(6)	51(8)	26(5)	-10(5)	9(5)	-6(6)
C(62)	30(6)	49(7)	36(6)	-9(5)	0(5)	-4(5)
C(63)	39(6)	45(8)	40(5)	-17(6)	0(5)	-14(5)
C(64)	57(9)	59(9)	58(9)	-21(7)	6(7)	-15(7)
C(65)	57(8)	46(9)	55(9)	-7(6)	19(7)	-4(7)
C(66)	47(6)	24(6)	31(5)	-6(5)	-14(5)	6(5)
C(67)	42(6)	38(7)	24(4)	-4(5)	-8(4)	3(5)
C(68)	51(7)	170(20)	19(5)	15(10)	3(5)	11(11)
C(69)	89(10)	26(6)	34(6)	2(5)	-8(6)	2(6)
C(70)	84(10)	30(7)	35(6)	-2(5)	-8(6)	16(6)

Electron density of 10, 12, 23, and 34 in complex with JAK3

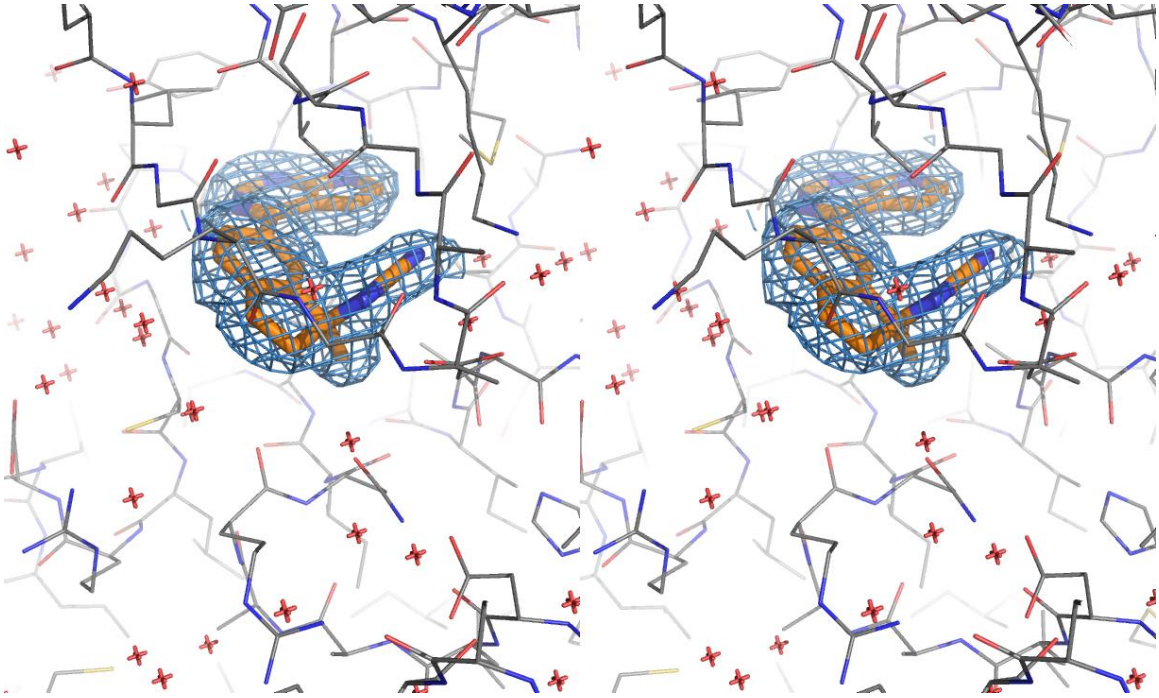
S-Figure 7. Electron density for compound **10** in the complex with JAK3.



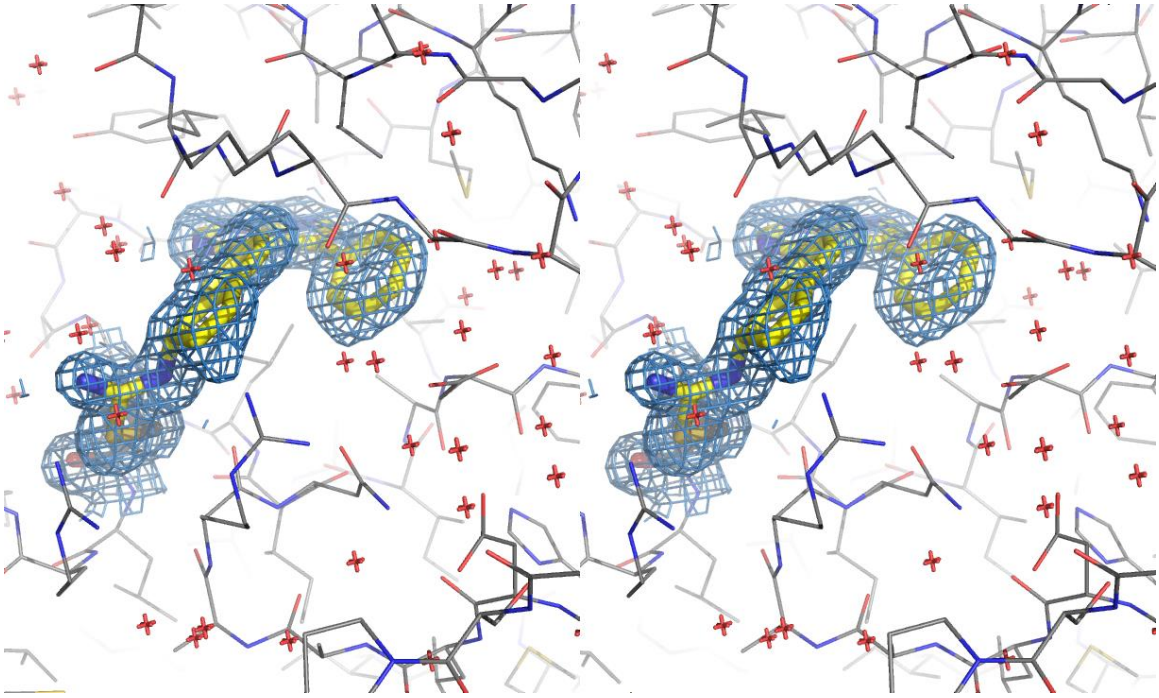
S-Figure 8. Electron density for compounds **12** in the complex with JAK3.



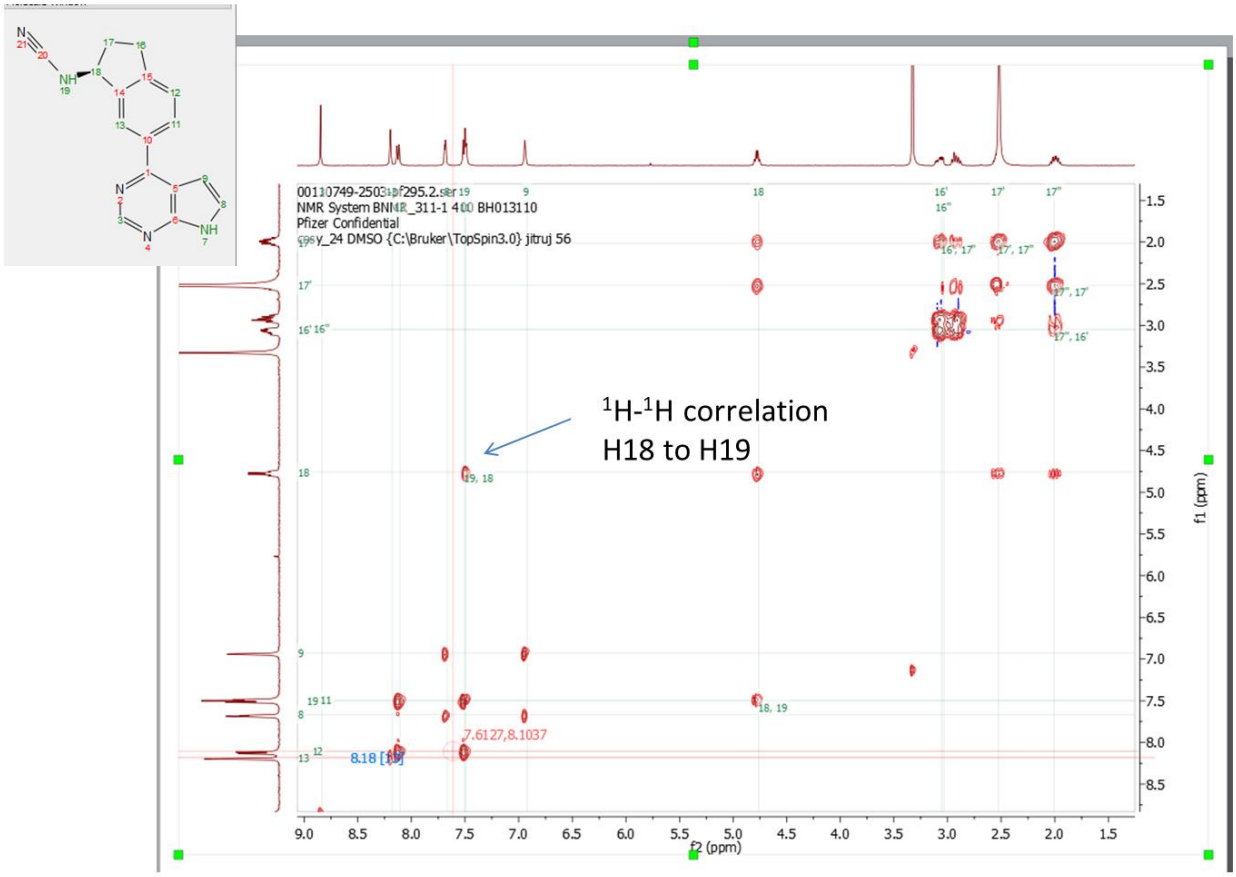
S-Figure 9. Electron density for compounds **23** in the complex with JAK3.



S-Figure 10. Electron density for compounds **34** in the complex with JAK3.

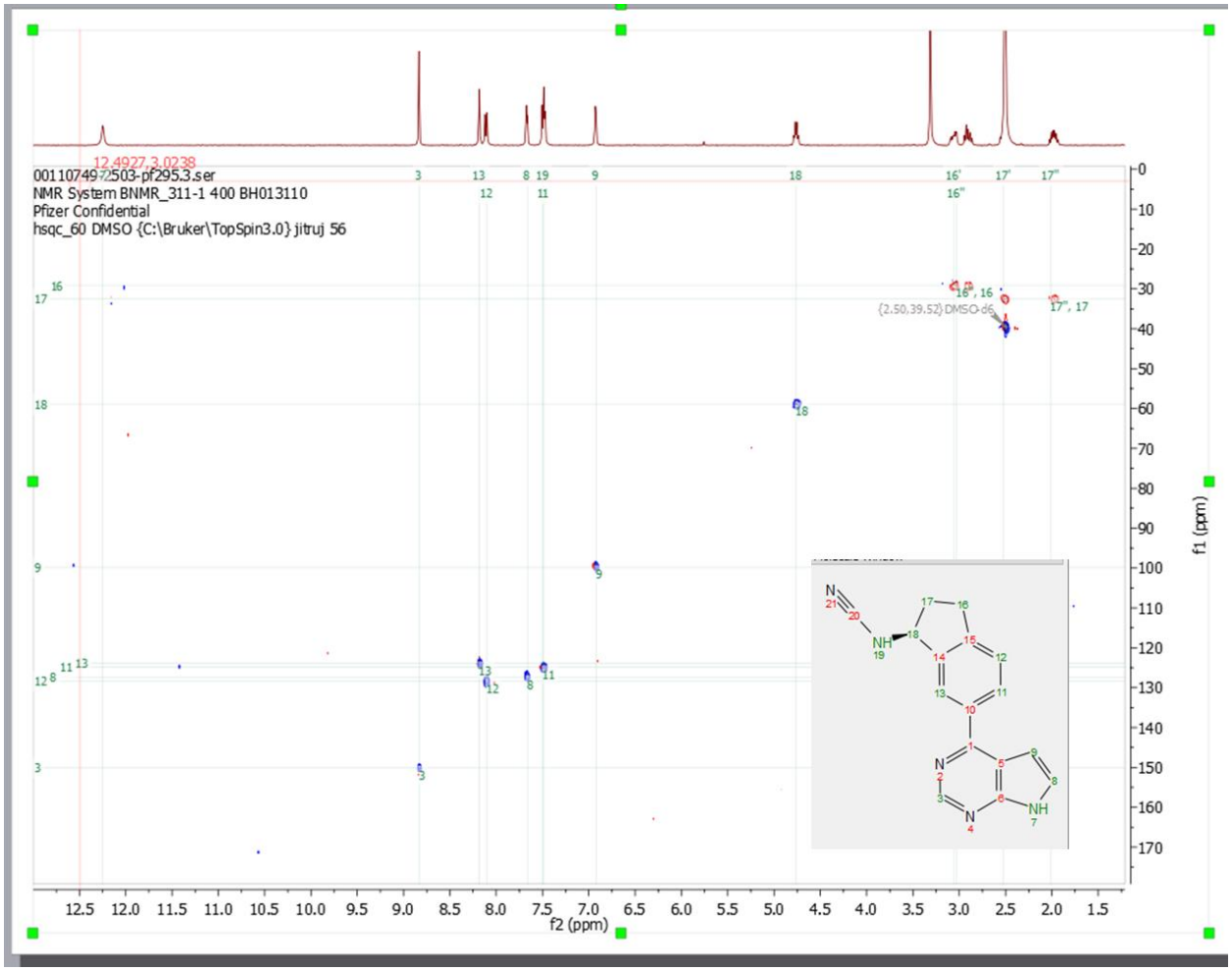


Determination of preferred tautomer form of 12 using 2D NMR.

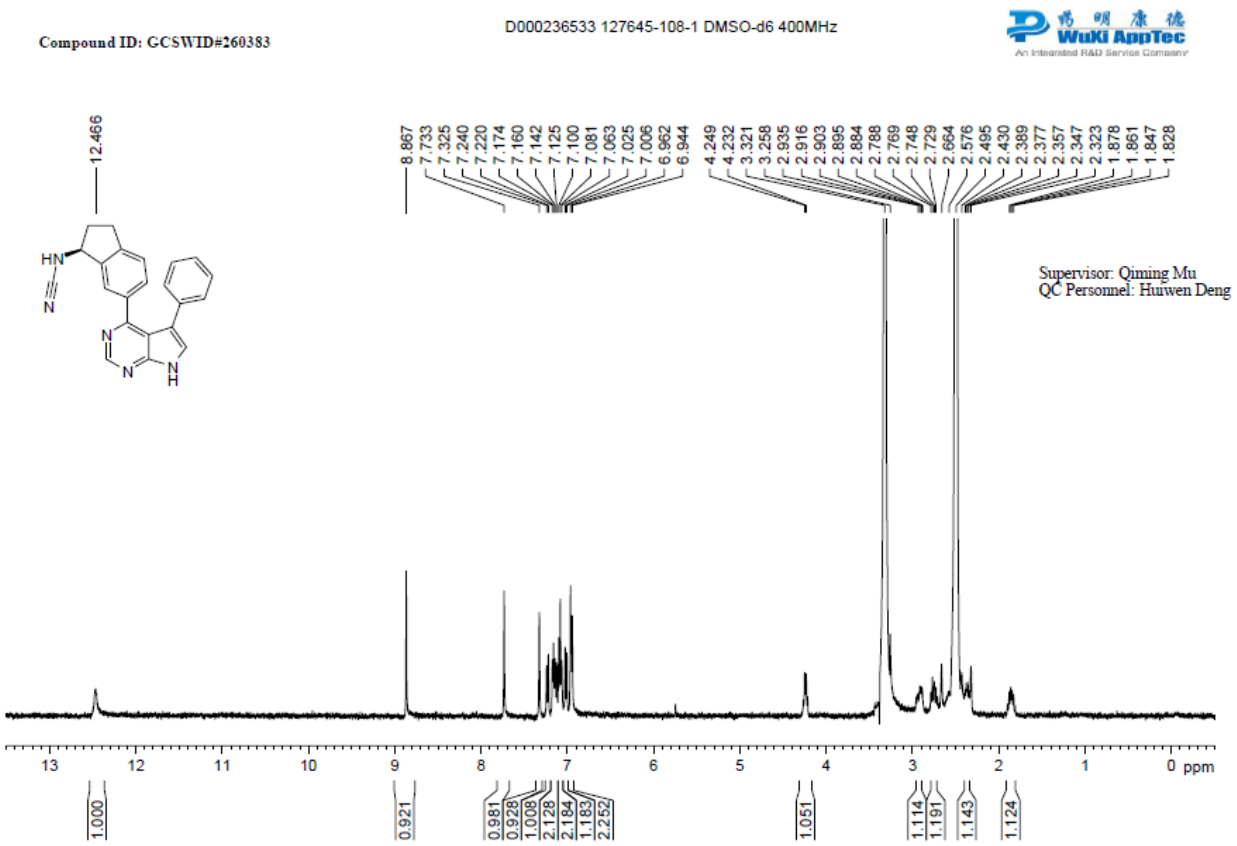


S-Figure 11. COSY experiment with **12**.

S-Figure 12. ^{1}H NMR spectrum of **12**.



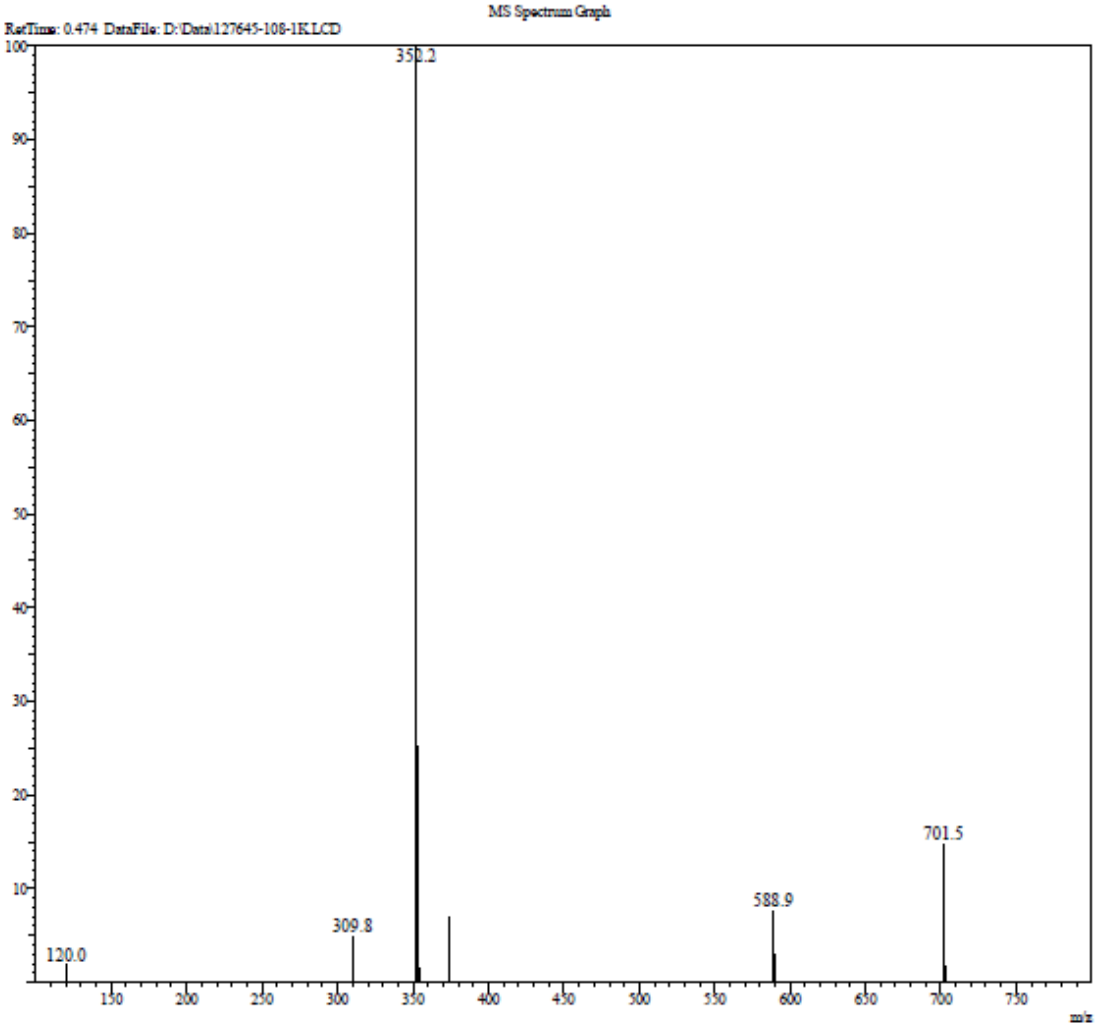
S-Figure 13. HSQC spectrum of **12**.



S-Figure 14. ^{1}H NMR data for **34**.

MS REPORT

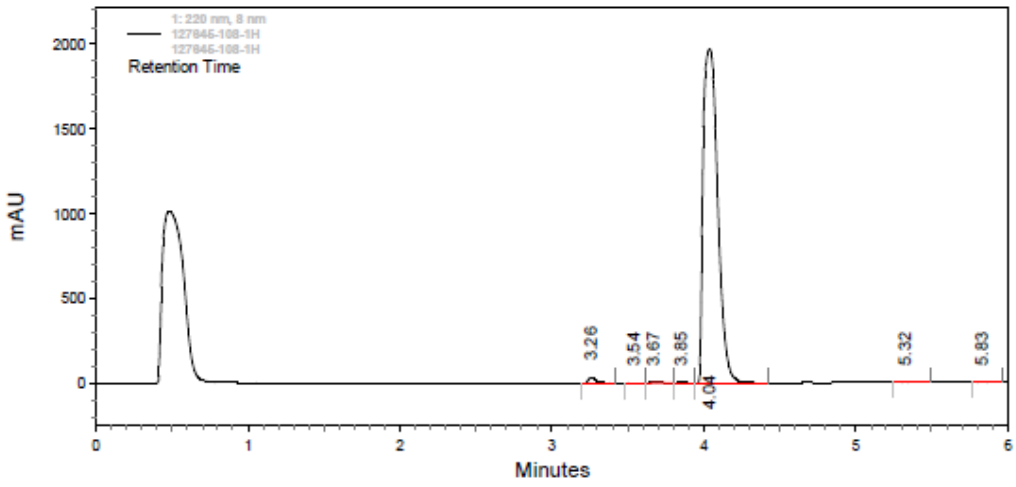
Compound ID :GCSWID#260383
Sample ID : 127645-108-1K
Injection Date : 2011-11-17 16:48:09
Injection Vol : 6ul
Location : tray1 vial94
Acq Method : D:\METHOD\UFLC\MS_UFLC.lcm
Org DataFile : D:\DATA\1111\17\127645-108-1K.lcd
Instrument & Column: LCMS-AB(4#-302) Ultimate XB-C18 2.1*30



S-Figure 15. MS data for **34.**

HPLC REPORT

Compound ID	: GCSWID#260383
Filename/Sample ID	: D:\DATA\1111\FTE-PFSD\127645-108-1H
Method Name	: D:\Method of 5cm\0-60_AB_1.2ml.met
Instrument & Column	: Ultimate XB-C18 3pm 3.0*50mm
Run Time	: 11/17/2011 16:03:15



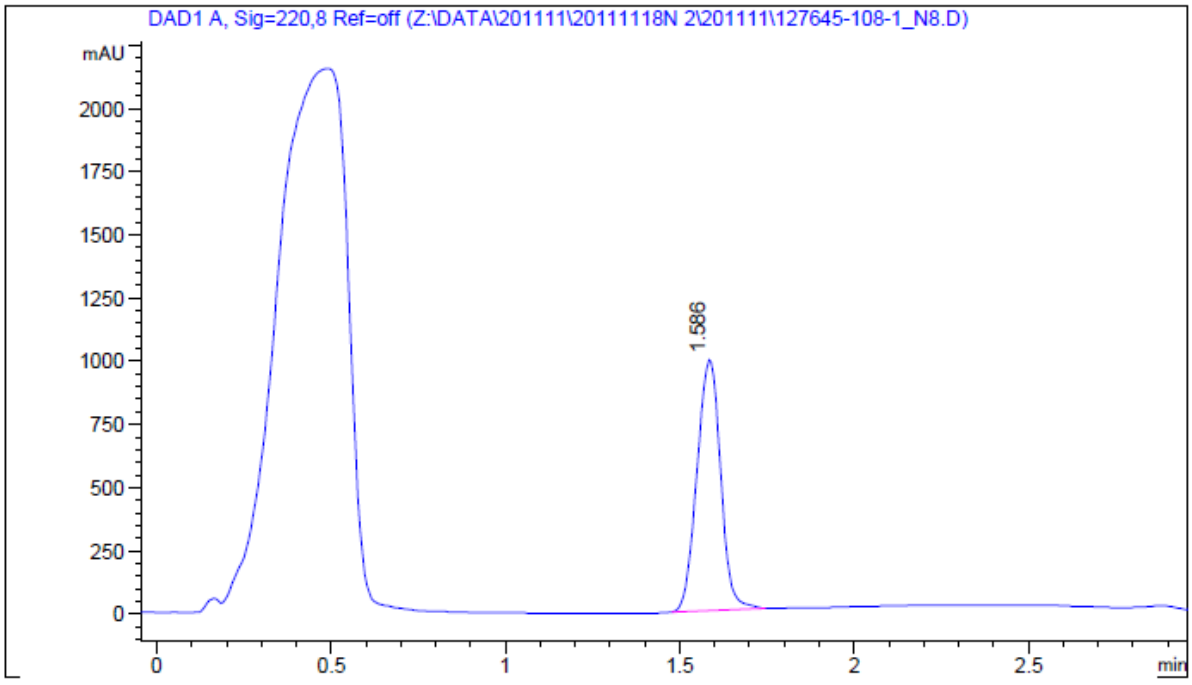
1: 220 nm, 8 nm

Retention Time	*Height*	*Area*	*Area Percent*
3.26	33248	131655	0.99
3.54	2323	8256	0.06
3.67	7206	35302	0.26
3.85	4946	16674	0.12
4.04	1965296	13115280	98.31
5.32	3444	16484	0.12
5.83	3327	16495	0.12

S-Figure 16. HPLC data for **34.**

CHIRAL SFC-MS REPORT

Compound ID :GCSWID#260383 ->
Filename/Sample ID:127645-108-1_N8
Injection Date :19. Nov. 2011
Acq Method :C:\DATA\201111\20111118N 2\AD-H_3UM_5_5_40_4ML_3MIN.M
Data Filename :Z:\DATA\201111\20111118N 2\201111\127645-108-1_N8.D
Instrument :SFC-MS(1#-310)



Integration Result

Signal 1 : DAD1 A, Sig=220,8 Ref=off

Peak #	RT [min]	Area	Height	Height %	Width [min]	Area %
1	1.586	4666.058	996.507	100.000	0.078	100.000

S-Figure 17. Chiral HPLC data for **34.**

CHIRAL SFC-MS REPORT

```
Compound ID        :GCSWID#260383                                          ->
Filename/Sample ID:127645-108-1_N5
Injection Date     :18. Nov. 2011
Acq  Method        :C:\DATA\201111\20111118N 2\AS-H_S_5_5_40_3ML_8MIN_   ->
Data Filename      :Z:\DATA\201111\20111118N 2\201111\127645-108-1_N5.D
Instrument         :SFC-MS(1#-310)
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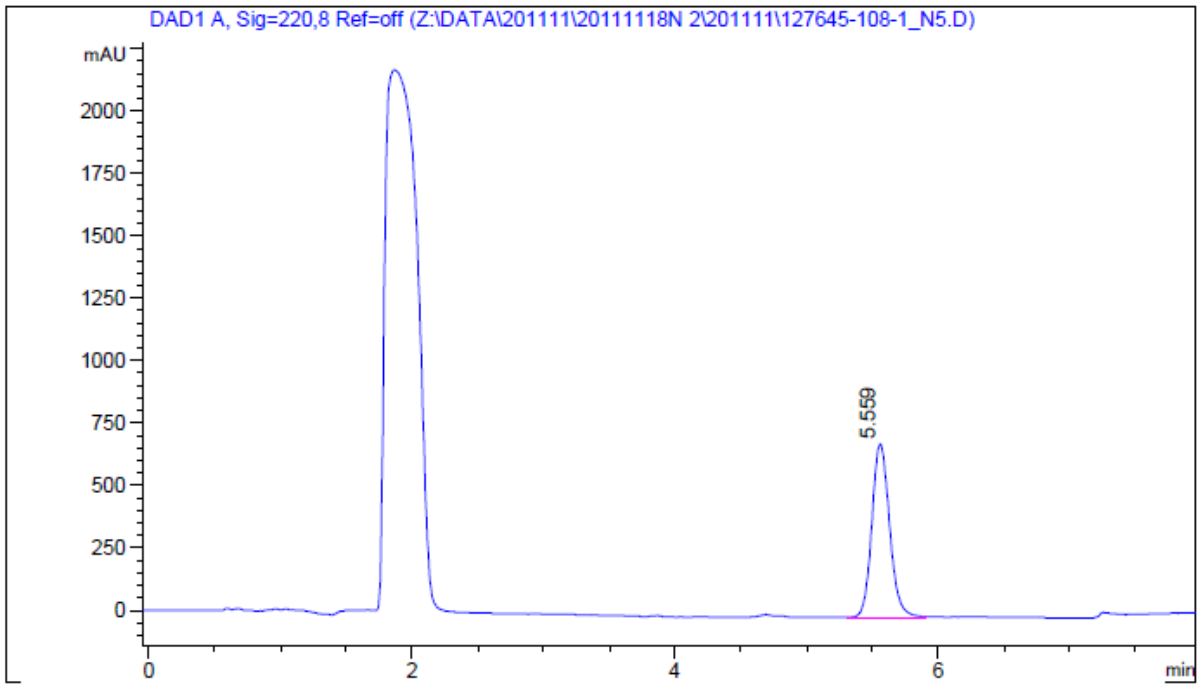
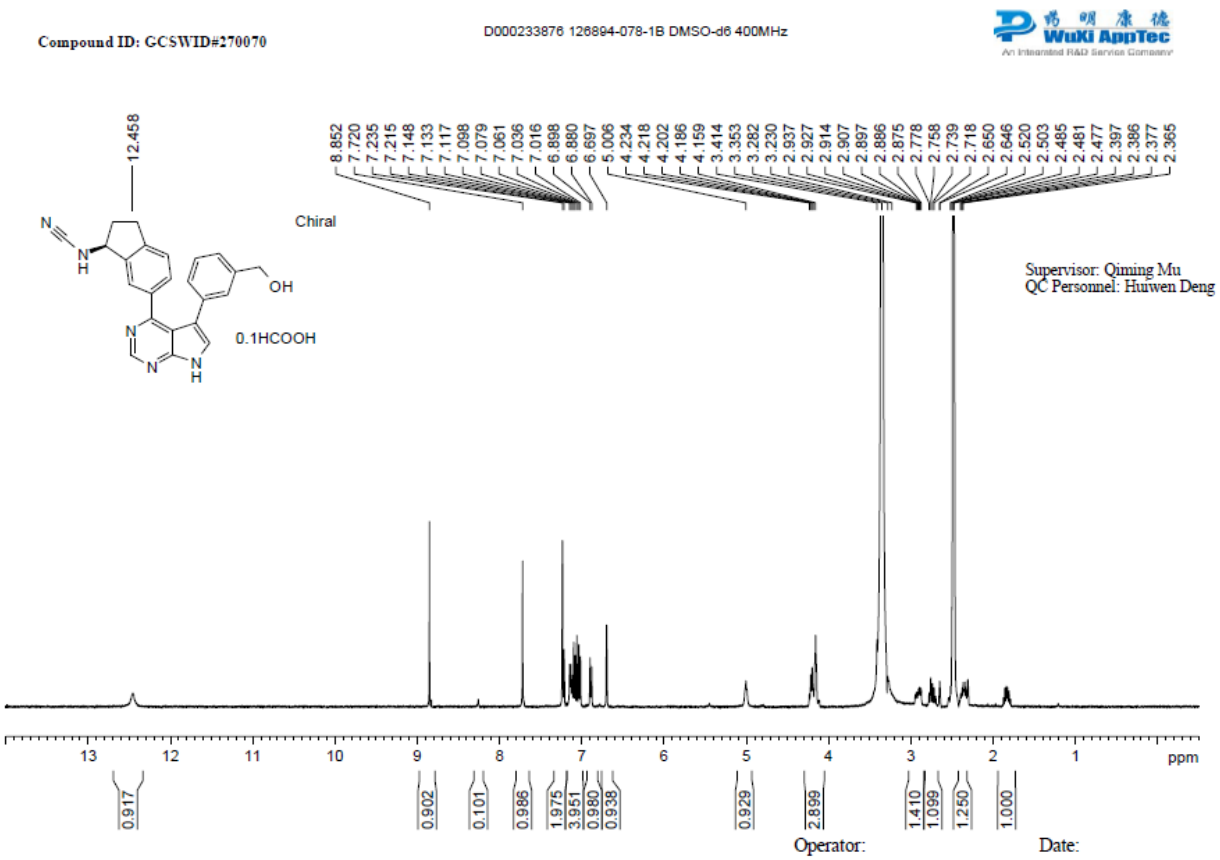


Integration Result

Signal 1 : DAD1 A, Sig=220,8 Ref=off

Peak #	RT [min]	Area	Height	Height %	Width [min]	Area %
1	5.559	6508.706	693.746	100.000	0.145	100.000

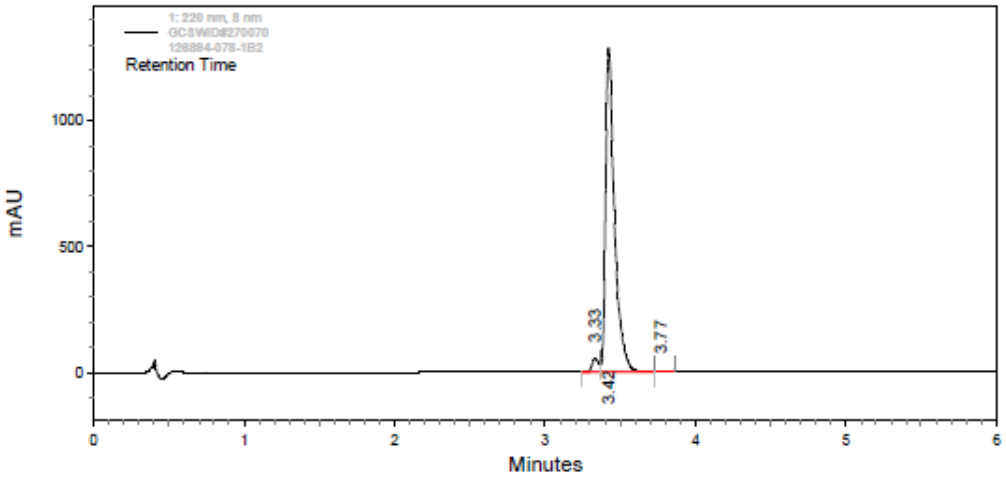
S-Figure 18. Chiral HPLC data for **34.**



S-Figure 19. ^{1}H NMR data for **35**.

HPLC REPORT

Compound ID	: GCSWID#270070
Filename/Sample ID	: D:\DATA\1111\FTE-PFGT\126894-078-1B2
Method Name	: D:\Method of 5cm\0-60_AB_1.2ml.met
Instrument & Column	: Ultimate XB-C18 3pm 3.0*50mm
Run Time	: 11/3/2011 13:25:40



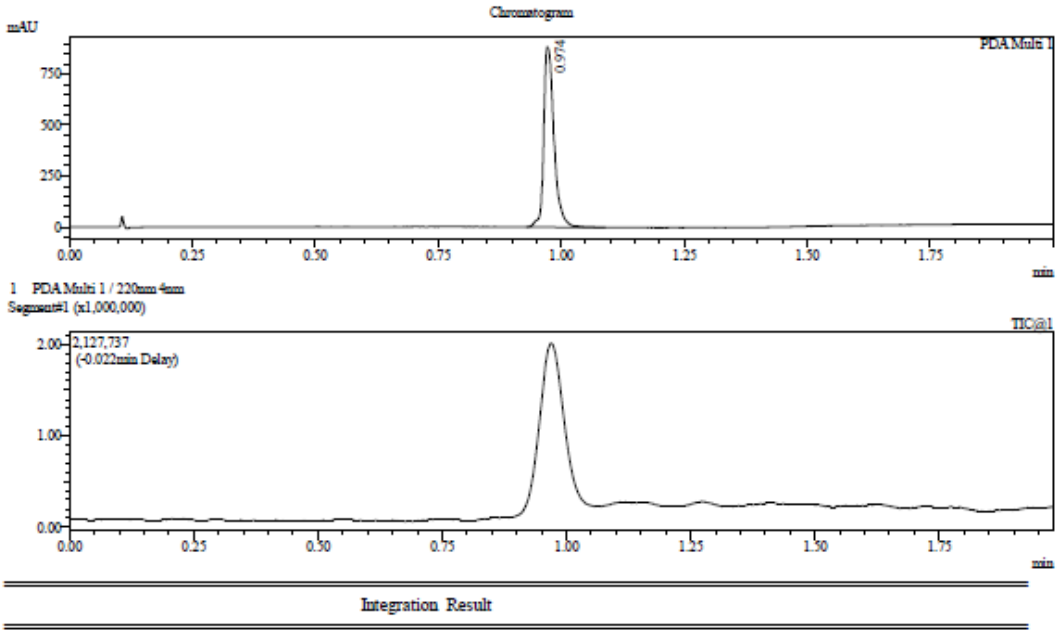
1: 220 nm, 8 nm

Retention Time	*Height*	*Area*	*Area Percent*
3.33	53698	163604	3.04
3.42	1277047	5215952	96.77
3.77	3255	10424	0.19

S-Figure 20. HPLC data for **35**.

LCMS REPORT

Compound ID : GCSWID#270070
Sample ID : 126894-078-1B
Injection Date : 11/3/2011 13:48:45
Injection Vol : 5ul
Location : tray1 vial23
Acq Method : D:\METHOD\UFLC\10-80AB_2min.lcm
Org DataFile : D:\DATA\1111\03\126894-078-1B.lcd
Instrument & Column: LCMS-AB(4#-302) Ultimate XB-C18 2.1*30mm

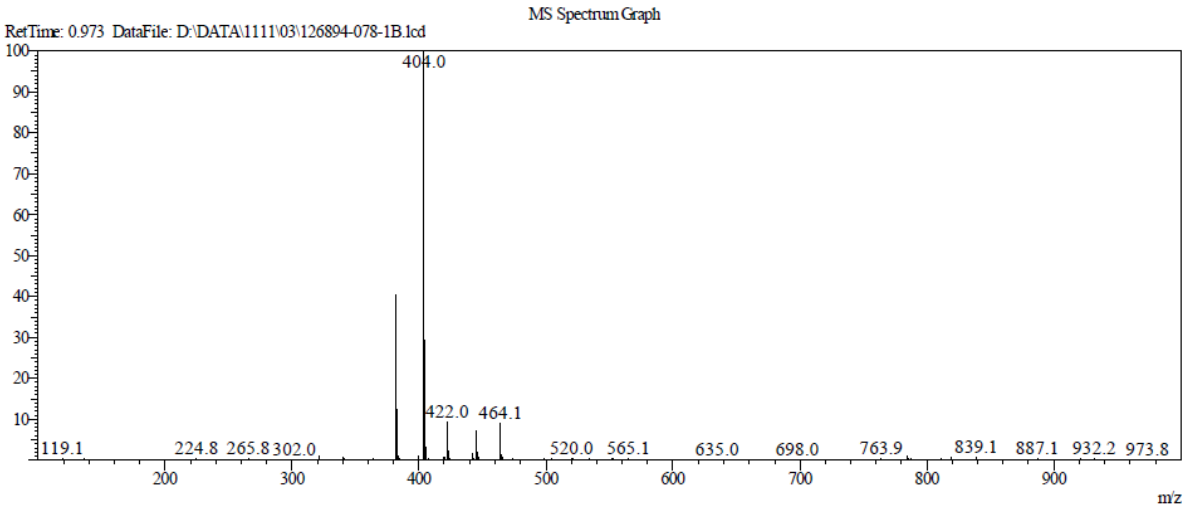


Integration Result

PDA Ch1 220nm 4nm

Peak#	Ret. Time	Height	Height %	USP Width	Area	Area %
1	0.974	876877	100.000	0.034	1291075	100.000

S-Figure 21. LCMS data for **35**.



S-Figure 22. MS spectrum of **35**.

CHIRAL SFC-MS REPORT

```
Compound ID        :GCSWID#270070                                          ->
Filename/Sample ID:126894-078-1_N1
Injection Date     :1. Nov. 2011
Acq  Method        :C:\DATA\201111\20111101\AS-H_S_5_5_40_3ML_8MIN_15CM.M
Data Filename      :Z:\DATA\201111\20111101\126894-078-1_N1.D
Instrument         :SFC-MS(1#-310)
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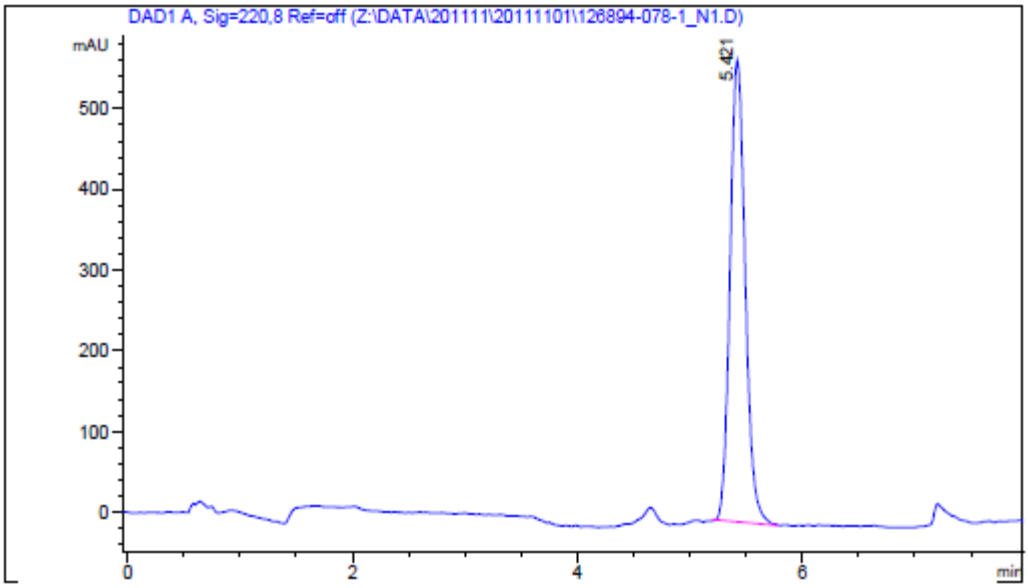

Integration Result

Signal 1 : DAD1 A, Sig=220,8 Ref=off

Peak #	RT [min]	Area	Height	Height %	Width [min]	Area %
1	5.421	5380.135	572.807	100.000	0.157	100.000

S-Figure 23. Chiral HPLC data for **35**.