7 Abkürzungsverzeichnis

Abb.	Abbildung
AKT	= PBK
ATP	Adenosintriphosphat
BAD	Proapoptotisches Protein der Bc1-Familie
Bcl-X_L	Antiapoptotisches Protein der Bc1-Familie
ber.	berechnet
BTC	Betacellulin
bzw.	beziehungsweise
ca.	circa
Caspase	Cysteinyl-Aspartase
CDK	Cyclinkinase
CHN	Verbrennungsanalyse
d	Tag
d	Duplett
δ	Chemische Verschiebung
dd	Duplett vom Duplett
DMSO	Dimethylsulfoxid
DNA	Desoxyribonucleinsäure
EGF	epidermal growth factor
EGFR	epidermal growth factor receptor
EI	Elektronenstoßionisation
ErbB1/2/3/4	= HER1/2/3/4 (Rezeptoren der EGFR-Familie)
et al.	et alii (und andere)
FAB	fast atom bombardment
fos, jun	Transkriptionsfaktoren
GDP	Guanosindiphosphat
gef.	gefunden
GRB	growth factor receptor-bound protein
GTP	Guanosintriphosphat
h	Stunden
HER1/2/3/4	human epidermal growth factor-like receptor type 1/2/3/4
IP_3	Inositol-1,4,5-triphosphat
IR	Infrarot
J	Kopplungskonstante
Jak	just another kinase

Kap.	Kapitel
m	Multiplett
M	molar (mol/L)
MAPK	Mitogen-activated protein kinase
MAPKK	Mitogen-activated protein kinase kinase
MAPKKK	Mitogen-activated protein kinase kinase kinase
MEK	= MAPKK
min	Minuten
MS	Massenspektrum
m/z	Ionenmasse/Ionenladung
mTOR	mammalian target of rapamycin
NCI	National Cancer Institute
NMR	Kernmagnetische Resonanz
NRG	Neuregulin
PKC	Proteinkinase C
PI3K	Phosphatidylinositol-3-Kinase
PLC-γ	Phospholipase C-γ
ppm	parts per million
PTK	Proteintyrosinkinase
Ras	Ras-Protein
RT	Raumtemperatur
s	Singulett
SC	Säulenchromatographie
Smp.	Schmelzpunkt
SH	src-homolog
SOS	son-of-evenless guanine nucleotide exchange factor
STAT	signal transduction and activation of transcription
ΔT	unter Erhitzen
t	Triplett
TGF	transforming growth factor
TK	Tyrosinkinase
z. B.	zum Beispiel

8 Publikationsverzeichnis

Posterpräsentationen

Anja Lüth, Werner Löwe, Manuela Weber und Peter Luger
„Syntheses of Substituted 4-(Indol-3-yl)quinazolines, a New Class of EGFR-Tyrosinkinase Inhibitors“

20th International Congress of Heterocylic Chemistry,
31. Juli - 03. August 2005, Palermo

DPhG – Jahrestagung
05. Oktober - 08. Oktober 2005, Mainz

Postervorträge

Anja Lüth, Werner Löwe, Manuela Weber und Peter Luger
„Syntheses of Substituted 4-(Indol-3-yl)quinazolines, a New Class of EGFR-Tyrosinkinase Inhibitors“

akzeptiert zum 27. Deutscher Krebskongress
22. März - 26. März 2006, Berlin

Patente

Substitutierte 4-(Indol-3-yl)chinazoline und ihre Verwendung
Deutsches Patent- und Markenamt, Akten-Zeichen: 10 2005 007 151.1, (09.02.2005)

Röntgenstrukturdaten von 51

Formel	$C_{24}H_{24}ClFN_4O_3$
Molekulargewicht	470.92
Temperatur	298 (2) K
Wellenlänge	0.71073 A
Kristallsystem	monoklinisch
Raumgruppe	P 21/c
Gitterkonstanten	a = 13.6285 (11) Å
	b = 15.7825 (12) Å
	c = 11.3541 (7) Å
	α = 90.000°
	β = 110.284 (2)°
	γ = 90.000°
Zellvolumen	2290.7 (3) $Å^3$
Z	4
Dichte ρ (berechnet)	1.365 mg/m^3
Absorptionskoeffizient μ	0.209 mm^{-1}
F (000)	984
Kristallabmessungen	0.60 x 0.15 x 0.10
ɵ - Bereich der Datenerfassung	2.05 bis 27.99°
h, k, l – Grenzen	-17≤h≤13, -20≤k≤20, -14≤l≤7
gemessene Reflexzahl	13474
Verfeinerungsmethode	Full-matrix least-square bzgl. F^2
Goodness-of-fit bzgl. F^2	0.873<41
Endgültige *R*-Werte [I>2σ (I)]	R1 = 0.0446, wR2 = 0.1052
R-Werte (alle Daten)	R1 = 0.0895, wR2 = 0.1177
Größtes Differenzdichtemaximum und –minimum	0.307 and -0.188 e. $Å^3$

Tabelle 1: Kristalldaten und Strukturverfeinerung von **51**

	x	y	z	U (eq)
N (1)	1391 (1)	8531 (1)	4008 (2)	54 (1)
C (2)	1949 (2)	9052 (1)	3604 (2)	64 (1)
N (3)	2457 (2)	8903 (1)	2804 (2)	58 (1)
C (4)	2389 (2)	8122 (1)	2330 (2)	43 (1)
C (5)	1596 (1)	6662 (1)	2145 (2)	42 (1)
C (6)	1039 (2)	6089 (1)	2559 (2)	43 (1)
O (6)	868 (1)	5268 (1)	2176 (1)	53 (1)
C (7)	562 (2)	6348 (1)	3439 (2)	46 (1)
O (7)	-17 (1)	5741 (1)	3746 (2)	63 (1)
C (71)	-525 (2)	5983 (2)	4606 (3)	78 (1)
C (8)	688 (2)	7150 (1)	3897 (2)	48 (1)
C (9)	1292 (2)	7737 (1)	3510 (2)	44 (1)
C (10)	1766 (1)	7493 (1)	2641 (2)	40 (1)
N (11)	3982 (1)	7427 (1)	488 (2)	50 (1)
C (12)	3464 (2)	7268 (1)	1288 (2)	47 (1)
C (13)	2991 (1)	7984 (1)	1509 (2)	41 (1)
C (14)	3006 (2)	9497 (1)	584 (2)	48 (1)
C (15)	3347 (2)	9938 (1)	-245 (2)	51 (1)
Cl (15)	3072 (1)	11010 (1)	-480 (1)	76 (1)
C (16)	3929 (2)	9531 (2)	-867 (2)	55 (1)
F (16)	4236 (1)	9985 (1)	-1697 (1)	79 (1)
C (17)	4210 (2)	8706 (1)	-682 (2)	52 (1)
C (18)	3855 (2)	8259 (1)	150 (2)	44 (1)
C (19)	3251 (1)	8636 (1)	779 (2)	41 (1)
C (21)	1361 (2)	4972 (1)	1319 (2)	51 (1)
C (22)	1192 (2)	4031 (1)	1161 (2)	60 (1)
C (23)	1467 (2)	3682 (1)	65 (2)	67 (1)
N (24)	2505 (1)	3907 (1)	76 (2)	57 (1)
C (25)	2647 (2)	3662 (2)	-1095 (2)	79 (1)
C (26)	3685 (2)	3957 (2)	-1108 (3)	99 (1)
O (27)	4517 (2)	3622 (1)	-66 (2)	109 (1)
C (28)	4381 (2)	3849 (2)	1083 (3)	100 (1)
C (29)	3346 (2)	3539 (2)	1116 (2)	75 (1)

Tabelle 2: Atomkoordinaten (x 10^4) und äquivalente isotrope Verschiebungsparameter (Å^2 x 10^3) von **51** (U_{eq} = 1/3 $\Sigma_i\Sigma_j U_{ij} a^*_i a^*_j a^*_i a^*_j$)

N (1)-C (2)	1.307 (3)
N (1)-C (9)	1.363 (2)
C (2)-N (3)	1.341 (3)
C (2)-H (2)	0.9300
N (3)-C (4)	1.335 (2)
C (4)-C (10)	1.428 (3)
C (4)-C (13)	1.456 (3)
C (5)-C (6)	1.365 (3)
C (5)-C (10)	1.415 (2)
C (5)-H (5)	0.9300
C (6)-O (6)	1.362 (2)
C (6)-C (7)	1.427 (3)
O (6)-C (21)	1.438 (2)
C (7)-C (8)	1.357 (3)
C (7)-O (7)	1.361 (2)
O (7)-C (71)	1.431 (3)
C (71)-H (71A)	0.9600
C (71-H (72B)	0.9600
C (71)-H (73C)	0.9600
C (8)-C (9)	1.406 (3)
C (8)-H (8)	0.9300
C (9)-C (10)	1.407 (3)
N (11)-C (12)	1.353 (2)
N (11)-C (18)	1.363 (2)
N (11)-H (11)	0.8600
C (12)-C (13)	1.366 (3)
C (12)-H (12)	0.9300
C (13)-C (19)	1.440 (3)
C (14)-C (15)	1.374 (3)
C (14)-C (19)	1.399 (3)
C (14)-H (14)	0.9300
C (15)-C (16)	1.388 (3)
C (15)-Cl (15)	1.735 (2)
C (16)-C (17)	1.353 (3)
C (16)-F (16)	1.360 (2)
C (17)-C (18)	1.392 (3)
C (17)-H (17)	0.9300
C (18)-C (19)	1.397 (3)
C (21)-C (22)	1.505 (3)
C (21)-H (21A)	0.9700
C (21)-H (21B)	0.9700

C (22)-C (23)	1.521 (3)
C (22)-H (22A)	0.9700
C (22)-H (22B)	0.9700
C (23)-N (24)	1.455 (3)
C (23)-H (23A)	0.9700
C (23)-H (23B)	0.9700
N (24)-C (29)	1.452 (3)
N (24)-C (25)	1.461 (3)
C (25)-C (26)	1.494 (4)
C (25)-H (25A)	0.9700
C (25)-H (25B)	0.9700
C (26)-O (27)	1.427 (3)
C (26)-H (26A)	0.9700
C (26)-H (26B)	0.9700
O (27)-C (28)	1.426 (3)
C (28)-C (29)	1.505 (4)
C (28)-H (28A)	0.9700
C (28)-H (28B)	0.9700
C (29)-H (29A)	0.9700
C (29)-H (29B)	0.9700

Tabelle 3: Bindungslängen (Å) von **51**

C (2)-N (1)-C (9)	114.74 (18)
N (1)-C (2)-N (3)	128.91 (19)
N (1)-C (2)-H (2)	115.5
N (3)-C (2)-H (2)	115.5
C (4)-N (3)-C (2)	117.08 (18)
N (3)-C (4)-C (10)	120.40 (19)
N (3)-C (4)-C (13)	114.84 (17)
C (10)-C(4)-C (13)	124.76 (17)
C (6)-C (5)-C (10)	120.67 (19)
C (6)-C (5)-H (5)	119.7
C (10)-C (5)-H (5)	119.7
O (6)-C (6)-C (5)	125.03 (18)
O (6)-C (6)-C (7)	115.30 (17)
C (5)-C (6)-C (1)	119.66 (17)
C (6)-O (6)-C (21)	117.19 (15)
C (8)-C (7)-O (7)	124.4 (2)
C (8)-C (7)-C (6)	120.51 (19)
O (7)-C (7)-C (6)	115.04 (18)
C (7)-O (7)-C (71)	116.65 (17)
O (7)-C (71)-H (71A)	109.5
O (7)-C (71)-H (72B)	109.5
H (71A)-C (71)-H (72B)	109.5
O (7)-C (71)-H (73C)	109.5
H (71A)-C (71)-H (73C)	109.5
H (72B)-C (71)-H (73C)	109.5
C (7)-C (8)-C (9)	120.3 (2)
C (7)-C (8)-H (8)	119.9
C (9)-C (8)-H (8)	119.9
N (1)-C (9)-C (8)	117.38 (19)
N (1)-C (9)-C (10)	122.60 (18)
C (8)-C (9)-C (10)	120.02 (18)
C (9)-C (10)-C (5)	118.75 (17)
C (9)-C (10)-C (4)	116.17 (17)
C (5)-C (10)-C (4)	125.08 (19)
C (12)-N (11)-C (18)	108.89 (17)
C (12)-N (11)-H (11)	125.6
C (18)-N (11)-H (11)	125.6
N (11)-C (12)-C (13)	111.03 (18)
N (11)-C (12)-H (12)	124.5
C (13)-C (12)-H (12)	124.5
C (12)-C (13)-C (19)	105.05 (17)

C (12)-C (13)-C (4)	130.32 (18)
C (19)-C (13)-C (4)	124.57 (17)
C (15)-C (14)-C (19)	118.79 (19)
C (15)-C (14)-H (14)	120.6
C (19)-C (14)-H (14)	120.6
C (14)-C (15)-C (16)	120.18 (19)
C (14)-C (15)-Cl (15)	119.54 (18)
C (16)-C (15)-Cl (15)	120.26 (16)
C (17)-C (16)-F (16)	118.4 (2)
C (17)-C (16)-C (15)	123.15 (19)
F (16)-C (16)-C (15)	118.4 (2)
C (16)-C (17)-C (18)	116.6(2)
C (16)-C (17)-H (17)	121.7
C (18)-C (17)-H (17)	121.7
N (11)-C (18)-C (17)	129.8 (2)
N (11)-C (18)-C (19)	107.76 (17)
C (17)-C (18)-C (19)	122.39 (19)
C (18)-C (19)-C (14)	118. 89 (17)
C (18)-C (19)-C (13)	107.26 (17)
C (14)-C (19)-C (13)	133.83 (18)
O (6)-C (21)-C (22)	108.23 (17)
O (6)-C (21)-H (21A)	110.1
C (22)-C (21)-H (21A)	110.1
O (6)-C (21)-H (21B)	110.1
C (22)-C (21)-H (21B)	110.1
H (21A)-C (21)-H (21B)	108.4
C (21)-C (22)-C (23)	112.57 (18)
C (21)-C (22)-H (22A)	109.1
C (23)-C (22)-H (22A)	109.1
C (21)-C (22)-H (22B)	109.1
C (23)-C (22)-H (22B)	109.1
H (22A)-C (22)-H (22B)	107.8
N (24)-C (23)-C (22)	114.81 (18)
N (24)-C (23)-H (23A)	108.6
C (22)-C (23)-H (23A)	108.6
N (24)-O (23)-H (23B)	108.6
C (22)-C (23)-H (23B)	108.6
H (23A)-C (23)-H (23B)	107.5
O (29)-N (24)-O (23)	113.7 (2)
O (29)-N (24)-O (25)	108.56 (18)
O (23)-N (24)-O (25)	111.28 (18)

N (24)-C (25)-O (26)	110.5 (2)
N (24)-C (25)-H (25A)	109.5
O (26)-C (25)-H (25A)	109.5
N (24)-C (25)-H (25B)	109.5
O (26)-C (25)-H (25B)	109.5
H (25A)-O (25)-H (25B)	108.1
O (27)-C (26)-C (25)	111.1 (3)
O (27)-C (26)-H (26A)	109.4
O (25)-C (26)-H (26A)	109.4
O (27)-C (26)-H (26B)	109.4
C (25)-C (26)-H (26B)	109.4
H (26A)-C (26)-H (26B)	108.0
O (28)-O (27)-C (26)	110.35 (19)
O (27)-O (28)-C (29)	111.2 (2)
O (27)-C (28)-H (28A)	109.4
O (29)-C (28)-H (28A)	109.4
O (27)-C (28)-H (28B)	109.4
C (29)-C (28)-H (28B)	109.4
H (28A)-C (28)-H (28B)	108.0
N (24)-O (29)-O (28)	109.4 (2)
N (24)-O (29)-H (29A)	109.8
C (28)-C (29)-H (29A)	109.8
N (24)-C (29)-H (29B)	109.8
O (28)-O (29)-H (29B)	109.8
H (29A)-O (29)-H (29B)	108.2

Tabelle 4: Bindungswinkel (°) von **51**

	U 11	U 22	U 33	U 23	U 13	U 12
N (1)	66 (1)	47 (1)	64 (1)	-2 (1)	40 (1)	-1 (1)
C (2)	88 (2)	42 (1)	82 (2)	-11 (1)	54 (2)	-7 (1)
N (3)	75 (1)	45 (1)	74 (1)	-9 (1)	52 (1)	-9 (1)
C (4)	43 (1)	39 (1)	52 (1)	1 (1)	22 (1)	0 (1)
C (5)	39 (1)	42 (1)	49 (1)	0 (1)	18 (1)	2 (1)
C (6)	36 (1)	39 (1)	54 (1)	4 (1)	17 (1)	2 (1)
O (6)	53 (1)	42 (1)	74 (1)	-2 (1)	35 (1)	-5 (1)
C (7)	39 (1)	49 (1)	54 (1)	11 (1)	21 (1)	0 (1)
O (7)	67 (1)	54 (1)	86 (1)	7 (1)	50 (1)	-7 (1)
C (71)	86 (2)	69 (2)	111 (2)	10 (1)	73 (2)	-6 (1)
C (9)	42 (1)	43 (1)	50 (1)	3 (1)	21 (1)	2 (1)
C (10)	37 (1)	39 (1)	48 (1)	2 (1)	18 (1)	4 (1)
N (11)	45 (1)	55 (1)	58 (1)	-5 (1)	28 (1)	6 (1)
C (12)	45 (1)	48 (1)	51 (1)	1 (1)	21 (1)	0 (1)
C (13)	37 (1)	43 (1)	47 (1)	-3 (1)	19 (1)	-2 (1)
C (14)	42 (1)	48 (1)	55 (1)	-1 (1)	18 (1)	-4 (1)
C (15)	46 (1)	54 (1)	51 (1)	5 (1)	13 (1)	-9 (1)
Cl (15)	79 (1)	56 (1)	90 (1)	18 (1)	25 (1)	-7 (1)
C (16)	51 (1)	69 (2)	44 (1)	7 (1)	16 (1)	-17 (1)
F (16)	82 (1)	98 (1)	64 (1)	17 (1)	35 (1)	-21 (1)
C (17)	41 (1)	77 (2)	45 (1)	-8 (1)	22 (1)	-10 (1)
C (18)	36 (1)	53 (1)	44 (1)	-3 (1)	16 (1)	-3 (1)
C (19)	34 (1)	48 (1)	44 (1)	-3 (1)	16 (1)	-5 (1)
C (21)	47 (1)	43 (1)	69 (1)	-2 (1)	28 (1)	-2 (1)
C (22)	52 (1)	44 (1)	83 (2)	-5 (1)	24 (1)	-6 (1)
C (23)	64 (2)	48 (1)	81 (2)	-16 (1)	15 (1)	-5 (1)
N (24)	56 (1)	53 (1)	60 (1)	-9 (1)	16 (1)	12 (1)
C (25)	84 (2)	79 (2)	65 (2)	-15 (1)	14 (2)	28 (1)
C (26)	87 (2)	134 (3)	84 (2)	-7 (2)	40 (2)	39 (1)
O (27)	79 (1)	163 (2)	87 (1)	-22 (1)	32 (1)	56 (1)
C (28)	65 (2)	154 (3)	79 (2)	-29 (2)	22 (2)	36 (1)
C (29)	75 (2)	81 (2)	63 (1)	-8 (1)	18 (1)	28 (1)

Tabelle 5: Anisotrope Verschiebungsparameter (Åx10^3) von **51**

Der Exponent des anisotropen Verschiebungsfaktors hat die Formel:

$-2\pi^2 (h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}+...)$

	x	y	z	U (eq)
H (2)	2000	9602	3913	77
H (5)	1868	6504	1530	51
H (71A)	-10	6157	5385	118
H (72B)	-911	5509	4751	118
H (73C)	-996	6444	4257	118
H (8)	374	7313	4470	57
H (11)	4333	7062	234	60
H (12)	3434	6741	1642	56
H (14)	2619	9766	1006	58
H (17)	4619	8451	-1089	63
H (21A)	2104	5097	1648	61
H (21B)	1058	5254	515	61
H (22A)	465	3905	1028	72
H (22B)	1617	3749	1926	72
H (23A)	1411	3070	66	80
H (23B)	955	3887	-711	80
H (25A)	2094	3908	-1800	95
H (25B)	2603	3050	-1184	95
H (26A)	3772	3779	-1884	119
H (26B)	3709	4571	-1078	119
H (28A)	4417	4460	1176	120
H (28B)	4943	3605	1781	120
H (29A)	3316	2926	1054	90
H (29B)	3270	3700	1904	90

Tabelle 6: Wasserstoffkoordinaten (x 10^4) und isotrope Verschiebungsparameter (Å^2 x 10^3) von **51**

C (9)-N (1)-C (2)-N (3)	-2.3 (4)
N (1)-C (2)-N (3)-C (4)	0.8 (4)
C (2)-N (3)-C (4)-C (10)	2.3 (3)
C (2)-N (3)-C (4)-C (13)	-177.57 (18)
C (10)-C (5)-C (6)-O (6)	-177.36 (16)
C (10)-C (5)-C (6)-C (7)	4.2 (3)
C (5)-C (6)-C (6)-C (21)	3.4 (3)
C (7)-C (6)-O (6)-C (21)	-178.14 (16)
O (6)-C (6)-C (7)-C (8)	179.27 (17)
C (5)-C (6)-C (7)-C (8)	-2.2 (3)
O (6)-C (6)-C (7)-O (7)	-1.6 (2)
C (5)-C (6)-C (7)-O (7)	176.97 (16)
C (8)-C (7)-O (7)-C (71)	0.4 (3)
C (6)-C (7)-O (7)-C (71)	-178.72 (17)
O (7)-C (7)-C (8)-C (9)	-179.11 (17)
C (6)-C (7)-C (8)-C (9)	0.0 (3)
C (2)-N (1)-C (9)-C (8)	-179.21 (18)
C (2)-N (1)-C (9)-C (10)	0.9 (3)
C (7)-C (8)-C (9)-N (1)	-179.76 (17)
C (7)-C (8)-C (9)-C (10)	0.2 (3)
N (1)-C (9)-C (10)-C (5)	-178.24 (17)
C (8)-C (9)-C (10)-C (5)	1.8 (3)
N (1)-C (9)-C (10)-C (4)	1.8 (3)
C (8)-C (9)-C (10)-C (4)	-178.16 (17)
C (6)-C (5)-C (10)-C (9)	-4.1 (3)
C (6)-C (5)-C (10)-C (4)	175.91 (17)
N (3)-C (4)-C (10)-C (9)	-3.4 (3)
C (13)-C (4)-C (10)-C (9)	176.43 (16)
N (3)-C (4)-C (10)-C (5)	176.64 (18)
C (13)-C (4)-C (10)-C (5)	-3.6 (3)
C (18)-N (11)-C (12)-C (13)	-0.4 (2)
N (11)-C (12)-C (13)-C (19)	-0.3 (2)
N (11)-C (12)-C (13)-C (4)	-177.46 (17)
N (3)-C (4)-C (13)-C (12)	149.2 (2)
C (10)-C (4)-C (13)-C (12)	-30.6 (3)
N (3)-C (4)-C (13)-C (19)	-27.5 (3)
C (10)-C (4)-C (13)-C (19)	152.73 (18)
C (19)-C (14)-C (15)-C (16)	-0.3 (3)
C (19)-C (14)-C (15)-Cl (15)	-178.82 (14)
C (14)-C (15)-C (16)-C (17)	-1.6 (3)
Cl (15)-C (15)-C (16)-C (17)	176.93 (16)

C (14)-C (15)-C (16)-F (16)	178.77 (16)
Cl (15)-C (15)-C (16)-F (16)	-2.7 (2)
F (16)-C (16)-C (17)-C (18)	-178.27 (16)
C (15)-C (16)-C (17)-C (18)	2.1 (3)
C (12)-N (11)-C (18)-C (17)	-177.59 (18)
C (12)-N (11)-C (18)-C (19)	1.0 (2)
C (16)-C (17)-C (18)-N (11)	177.66 (19)
C (16)-C (17)-C (18)-C (19)	-0.8 (3)
N (11)-C (18)-C (19)-C (14)	-179.72 (16)
C (17)-C (18)-C (19)-C (14)	-1.0 (3)
N (11)-C (18)-C (19)-C (13)	-1.2 (2)
C (17)-C (18)-C (19)-C (13)	177.52 (16)
C (15)-C (14)-C (19)-C (18)	1.5 (3)
C (15)-C (14)-C (19)-C (13)	-176.52 (19)
C (12)-C (13)-C (19)-C (18)	0.9 (2)
C (4)-C (13)-C (19)-C (18)	178.28 (16)
C (12)-C (13)-C (19)-C (14)	179.13 (19)
C (4)-C (13)-C (19)-C (14)	-3.5 (3)
C (6)-O (6)-C (21)-C (22)	172.44 (16)
C (6)-C (21)-C (22)-C (23)	167.35 (17)
C (21)-C (22)-C (23)-N (24)	52.5 (3)
C (22)-C (23)-N (24)-C (29)	65.9 (2)
C (22)-C (23)-N (24)-C (25)	-171.21 (18)
C (29)-N (24)-C (25)-C (26)	-58.6 (3)
C (23)-N (24)-C (25)-C (26)	175.5 (2)
N (24)-C (25)-C (26)-O (27)	57.9 (3)
C (25)-C (26)-O (27)-C (28)	-56.8 (3)
C (26)-O (27)-C (28)-C (29)	57.7 (3)
C (23)-N (24)-C (29)-C (28)	-176.77 (19)
C (25)-N (24)-C (29)-C (28)	58.8 (2)
O (27)-C (28)-C (29)-N (24)	-59.4 (3)

Tabelle 7: Torsionswinkel (°) von **51**

D-H...A	D-H	H...A	D...A	DHA-Winkel	Sym.op. für A
N 11-H 11...O 27	0.86	1.97	2.799 (2)	163	1-x, q1-y, -z

Tabelle 8: Intra- und intermolekulare Bindungen von **51**