Supplementary Material for Organic & Biomolecular Chemistry

CIF Data Item	Description
_publ_contact_author_name _publ_contact_author_address	Yuefei Hu, Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China.
_publ_requested_journal	Org. Biomol. Chem.
_publ_section_title	**3-Aryl-Carbolin-1-Ones as A New Class of Potent Inhibitors of Tumor Cell Proliferation: Synthesis and Biological Evaluation**
_publ_section_exptl_refinement _computing_data_collection _computing_cell_refinement _computing_data_reduction _computing_structure_solution _computing_structure_refinement _computing_molecular_graphics _computing_publication_material	_computing_data_collection 'Bruker SMART' _computing_cell_refinement 'Bruker SMART' _computing_data_reduction 'Bruker SHELXTL' _computing_structure_solution 'SHELXS-97 (Sheldrick, 1990)' _computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)' _computing_molecular_graphics 'ORTEP-3 for Windows V1.05(Farrugia, 1999)' _computing_publication_material 'SHELXL-97 (Sheldrick, 1997)'
_chemical_formula_sum	C19 H15 N2 O3, C H4 O
_chemical_formula_weight	351.37
_symmetry_cell_setting	Monoclinic
_symmetry_space_group_name_H-M	P21/n

_symmetry_equiv_pos_as_xyz	'x, y, z' '-x+1/2, y+1/2, -z+1/2' '-x, -y, -z' 'x-1/2, -y-1/2, z-1/2'
_cell_length_a _cell_length_b _cell_length_c _cell_angle_alpha _cell_angle_beta _cell_angle_gamma	_cell_length_a 9.2371(6) _cell_length_b 7.4210(5) _cell_length_c 25.1558(17) _cell_angle_alpha 90.00 _cell_angle_beta 96.0020(10) _cell_angle_gamma 90.00
_cell_volume	1714.9(2)
_cell_formula_units_Z	4
_exptl_crystal_density_diffrn	1.361
_diffrn_radiation_type	MoK\a
_diffrn_radiation_wavelength	0.71073
_cell_measurement_reflns_used	
_cell_measurement_theta_min _cell_measurement_theta_max	
_diffrn_ambient_temperature	293(2)
_exptl_cryst_F_000	740
_exptl_absorpt_coefficient_mu	0.096
_exptl_crystal_description	prismatic
_exptl_crystal_size_max _exptl_crystal_size_mid _exptl_crystal_size_min _exptl_crystal_size_rad	_exptl_crystal_size_max 1.10 _exptl_crystal_size_mid 0.75 _exptl_crystal_size_min 0.65

_exptl_crystal_colour	colorless
_diffrn_measurement_device_type _diffrn_measurement_device (old)	CCD area detector
_diffrn_measurement_method	phi and omega scans
_exptl_absorpt_correction_type _exptl_absorpt_correction_T_min _exptl_absorpt_correction_T_max	multiscans 0.9019 0.9403
_diffrn_radiation_monochromator	graphite
_diffrn_reflns_number	10057
_reflns_number_total	3970
_diffrn_reflns_theta_max	28.24
_diffrn_reflns_av_R_equivalents	0.0438
_diffrn_reflns_limit_h_min _diffrn_reflns_limit_h_max _diffrn_reflns_limit_k_min _diffrn_reflns_limit_k_max _diffrn_reflns_limit_l_min _diffrn_reflns_limit_l_max	_diffrn_reflns_limit_h_min -12 _diffrn_reflns_limit_h_max 11 _diffrn_reflns_limit_k_min -9 _diffrn_reflns_limit_k_max 8 _diffrn_reflns_limit_l_min -31 _diffrn_reflns_limit_l_max 32
_refine_ls_structure_factor_coef	Fsqd
_refine_ls_R_factor_gt _refine_ls_R_factor_obs (old)	0.0646
_refine_ls_wR_factor_ref _refine_ls_wR_factor_obs (old)	0.2036
_refine_ls_goodness_of_fit_ref _refine_ls_goodness_of_fit_obs(old)	1.081
_refine_ls_number_reflns _refine_ls_number_parameters	_refine_ls_number_reflns 3970 _refine_ls_number_parameters 235
_refine_ls_weighting_scheme	calc

_refine_ls_hydrogen_treatment	mixed
_refine_ls_shift/su_max _refine_ls_shift/esd_max(old)	0.001
_refine_diff_density_max _refine_diff_density_min	0.842 -0.776
_refine_ls_abs_structure_details _refine_ls_abs_structure_Flack _refine_ls_abs_structure_Rogers	
_atoms_sites_solution_primary	direct
_atoms_sites_solution_secondary	difmap
_atom_site_label	
_atom_site_fract_x _atom_site_fract_y _atom_site_fract_z	_atom_site_label _atom_site_type_symbol _atom_site_fract_x _atom_site_fract_y _atom_site_fract_z _atom_site_U_iso_or_equiv _atom_site_adp_type _atom_site_occupancy _atom_site_calc_flag _atom_site_refinement_flags _atom_site_disorder_assembly _atom_site_disorder_group N1 N 0.79422(18) 0.6265(2) 1.01201(6) 0.0328(4) Uani 1 d . . . H1 H 0.8749 0.5897 1.0286 0.039 Uiso 1 calc

	R . . N2 N 0.80485(18) 0.6791(2) 0.86855(7) 0.0345(4) Uani 1 d . . . H2 H 0.8605 0.6695 0.8433 0.041 Uiso 1 calc R . . O1 O 0.46221(18) 0.6977(2) 1.15081(6) 0.0478(4) Uani 1 d . . . O2 O 0.26509(18) 0.8038(2) 1.07916(6) 0.0474(4) Uani 1 d . . . O3 O 0.99535(15) 0.5853(2) 0.92696(6) 0.0406(4) Uani 1 d . . . O4 O 0.1804(3) 0.7439(4) 0.86100(11) 0.0894(8) Uiso 1 d . . . H4 H 0.2312 0.7191 0.8887 0.107 Uiso 1 calc R . . C1 C 0.6687(2) 0.6666(3) 1.03481(8) 0.0307(4) Uani 1 d . . . C2 C 0.6414(2) 0.6549(3) 1.08844(8) 0.0348(5) Uani 1 d . . . H2A H 0.7128 0.6159 1.1147 0.042 Uiso 1 calc R . . C3 C 0.5055(2) 0.7029(3) 1.10076(8) 0.0347(5) Uani 1 d . . . C4 C 0.3952(2) 0.7628(3) 1.06072(8) 0.0350(5) Uani 1 d . . . C5 C 0.4231(2) 0.7746(3) 1.00836(8) 0.0341(5) Uani 1 d . . . C6 C 0.5614(2) 0.7254(3) 0.99503(8) 0.0308(4) Uani 1 d . . . C7 C 0.6255(2) 0.7181(3) 0.94581(7)

	0.0298(4) Uani 1 d . . . C8 C 0.5727(2) 0.7581(3) 0.89212(8) 0.0332(5) Uani 1 d . . . H8 H 0.4776 0.7977 0.8834 0.040 Uiso 1 calc R . . C9 C 0.6644(2) 0.7373(3) 0.85399(8) 0.0324(5) Uani 1 d . . . C10 C 0.8649(2) 0.6350(3) 0.91901(8) 0.0314(4) Uani 1 d . . . C11 C 0.7672(2) 0.6558(3) 0.95811(8) 0.0302(4) Uani 1 d . . . C12 C 0.6225(2) 0.7696(3) 0.79631(8) 0.0333(5) Uani 1 d . . . C13 C 0.6917(3) 0.6817(3) 0.75699(8) 0.0407(5) Uani 1 d . . . H13 H 0.7674 0.6020 0.7670 0.049 Uiso 1 calc R . . C14 C 0.6494(3) 0.7115(3) 0.70343(9) 0.0466(6) Uani 1 d . . . H14 H 0.6978 0.6539 0.6776 0.056 Uiso 1 calc R . . C15 C 0.5357(3) 0.8263(4) 0.68834(9) 0.0473(6) Uani 1 d . . . H15 H 0.5059 0.8445 0.6523 0.057 Uiso 1 calc R . . C16 C 0.4663(3) 0.9140(4) 0.72631(9) 0.0485(6) Uani 1 d . . . H16 H 0.3895 0.9916 0.7160 0.058 Uiso 1 calc R . . C17 C 0.5104(2) 0.8871(3) 0.78021(9)

	0.0422(5) Uani 1 d . . . H17 H 0.4639 0.9488 0.8058 0.051 Uiso 1 calc R . . C18 C 0.5665(3) 0.6393(4) 1.19286(9) 0.0507(6) Uani 1 d . . . H18A H 0.5987 0.5200 1.1853 0.076 Uiso 1 calc R . . H18B H 0.5230 0.6386 1.2259 0.076 Uiso 1 calc R . . H18C H 0.6482 0.7200 1.1958 0.076 Uiso 1 calc R . . C19 C 0.1516(3) 0.8607(4) 1.04075(10) 0.0498(6) Uani 1 d . . . H19A H 0.1808 0.9683 1.0235 0.075 Uiso 1 calc R . . H19B H 0.0659 0.8848 1.0581 0.075 Uiso 1 calc R . . H19C H 0.1311 0.7676 1.0145 0.075 Uiso 1 calc R . . C20 C 0.1540(4) 0.9232(5) 0.85933(17) 0.0911(12) Uani 1 d . . . H20A H 0.0538 0.9447 0.8643 0.137 Uiso 1 calc R . . H20B H 0.1738 0.9700 0.8253 0.137 Uiso 1 calc R . . H20C H 0.2155 0.9820 0.8872 0.137 Uiso 1 calc R . .
_atom_site_U_iso_or_equiv	
_atom_site_aniso_label	

_atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_12 _atom_site_aniso_U_13 _atom_site_aniso_U_23	_atom_site_aniso_label _atom_site_aniso_U_11 _atom_site_aniso_U_22 _atom_site_aniso_U_33 _atom_site_aniso_U_23 _atom_site_aniso_U_13 _atom_site_aniso_U_12 N1 0.0275(8) 0.0460(10) 0.0246(8) 0.0012(7) 0.0017(6) 0.0030(7) N2 0.0302(9) 0.0492(10) 0.0249(8) 0.0015(7) 0.0062(6) 0.0042(7) O1 0.0451(9) 0.0730(12) 0.0269(8) -0.0006(7) 0.0111(6) 0.0047(8) O2 0.0360(9) 0.0706(11) 0.0375(9) -0.0034(8) 0.0124(7) 0.0071(8) O3 0.0285(7) 0.0633(10) 0.0300(8) 0.0047(7) 0.0029(6) 0.0075(7) C1 0.0301(10) 0.0355(10) 0.0269(10) -0.0021(8) 0.0047(7) -0.0013(8) C2 0.0353(11) 0.0435(11) 0.0253(9) -0.0003(8) 0.0014(8) -0.0001(9) C3 0.0384(11) 0.0414(11) 0.0251(9) -0.0023(8) 0.0065(8) -0.0027(9) C4 0.0319(10) 0.0407(11) 0.0335(10) -0.0042(8) 0.0084(8) 0.0004(8) C5 0.0325(10) 0.0396(11) 0.0303(10)

	-0.0009(8) 0.0045(8) 0.0015(8) C6 0.0311(10) 0.0347(10) 0.0270(9) 0.0003(7) 0.0048(8) -0.0009(8) C7 0.0295(10) 0.0343(10) 0.0261(9) 0.0002(7) 0.0048(7) 0.0003(8) C8 0.0307(10) 0.0403(11) 0.0283(10) 0.0032(8) 0.0019(8) 0.0058(8) C9 0.0321(10) 0.0379(10) 0.0265(10) 0.0021(8) 0.0001(8) 0.0014(8) C10 0.0296(10) 0.0389(10) 0.0259(9) 0.0001(8) 0.0032(7) 0.0006(8) C11 0.0306(10) 0.0348(10) 0.0250(9) 0.0000(7) 0.0021(7) -0.0003(8) C12 0.0322(10) 0.0428(11) 0.0247(9) 0.0052(8) 0.0016(8) -0.0010(8) C13 0.0408(12) 0.0527(13) 0.0288(10) 0.0040(9) 0.0050(9) 0.0058(10) C14 0.0507(14) 0.0614(15) 0.0281(11) -0.0001(10) 0.0059(9) -0.0046(11) C15 0.0498(14) 0.0609(15) 0.0288(11) 0.0115(10) -0.0069(9) -0.0126(11) C16 0.0428(13) 0.0573(14) 0.0426(13) 0.0153(11) -0.0093(10) 0.0015(11) C17 0.0404(12) 0.0504(13) 0.0359(11) 0.0058(9) 0.0039(9) 0.0065(10) C18 0.0569(15) 0.0682(16) 0.0275(11) 0.0042(10) 0.0069(10) -0.0012(12) C19 0.0353(12) 0.0626(15) 0.0525(14) -0.0067(12) 0.0096(10) 0.0083(11) C20 0.082(2) 0.061(2) 0.134(4) 0.019(2)

	0.034(2) 0.0091(18)
_geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2	_geom_bond_atom_site_label_1 _geom_bond_atom_site_label_2 _geom_bond_distance _geom_bond_site_symmetry_2 _geom_bond_publ_flag N1 C11 1.370(2) . ? N1 C1 1.378(2) . ? N1 H1 0.8600 . ? N2 C10 1.371(2) . ? N2 C9 1.380(3) . ? N2 H2 0.8600 . ? O1 C3 1.361(2) . ? O1 C18 1.422(3) . ? O2 C4 1.367(2) . ? O2 C19 1.414(3) . ? O3 C10 1.256(2) . ? O4 C20 1.352(4) . ? O4 H4 0.8200 . ? C1 C2 1.401(3) . ? C1 C6 1.403(3) . ? C2 C3 1.371(3) . ?

	C2 H2A 0.9300 . ? C3 C4 1.427(3) . ? C4 C5 1.371(3) . ? C5 C6 1.402(3) . ? C6 C7 1.428(3) . ? C7 C11 1.392(3) . ? C7 C8 1.419(3) . ? C8 C9 1.353(3) . ? C8 H8 0.9300 . ? C9 C12 1.482(3) . ? C10 C11 1.411(3) . ? C12 C17 1.381(3) . ? C12 C13 1.395(3) . ? C13 C14 1.381(3) . ? C13 H13 0.9300 . ? C14 C15 1.375(4) . ? C14 H14 0.9300 . ? C15 C16 1.369(4) . ? C15 H15 0.9300 . ? C16 C17 1.389(3) . ? C16 H16 0.9300 . ? C17 H17 0.9300 . ? C18 H18A 0.9599 . ?

	C18 H18B 0.9599 . ? C18 H18C 0.9599 . ? C19 H19A 0.9599 . ? C19 H19B 0.9599 . ? C19 H19C 0.9599 . ? C20 H20A 0.9599 . ? C20 H20B 0.9599 . ? C20 H20C 0.9599 . ?
_geom_bond_distance	
_geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3	geom_angle_atom_site_label_1 _geom_angle_atom_site_label_2 _geom_angle_atom_site_label_3 _geom_angle _geom_angle_site_symmetry_1 _geom_angle_site_symmetry_3 _geom_angle_publ_flag C11 N1 C1 107.66(16) . . ? C11 N1 H1 126.2 . . ? C1 N1 H1 126.2 . . ? C10 N2 C9 126.77(17) . . ? C10 N2 H2 116.6 . . ? C9 N2 H2 116.6 . . ? C3 O1 C18 117.08(18) . . ?

	C4 O2 C19 116.73(18) . . ? C20 O4 H4 109.5 . . ? N1 C1 C2 129.17(18) . . ? N1 C1 C6 109.44(16) . . ? C2 C1 C6 121.39(18) . . ? C3 C2 C1 117.60(19) . . ? C3 C2 H2A 121.2 . . ? C1 C2 H2A 121.2 . . ? O1 C3 C2 124.49(19) . . ? O1 C3 C4 113.87(19) . . ? C2 C3 C4 121.63(18) . . ? O2 C4 C5 124.9(2) . . ? O2 C4 C3 114.72(18) . . ? C5 C4 C3 120.39(19) . . ? C4 C5 C6 118.71(19) . . ? C5 C6 C1 120.27(17) . . ? C5 C6 C7 133.44(18) . . ? C1 C6 C7 106.28(17) . . ? C11 C7 C8 120.18(18) . . ? C11 C7 C6 106.58(17) . . ? C8 C7 C6 133.23(19) . . ? C9 C8 C7 118.18(18) . . ? C9 C8 H8 120.9 . . ?

	C7 C8 H8 120.9 . . ? C8 C9 N2 119.25(18) . . ? C8 C9 C12 123.84(19) . . ? N2 C9 C12 116.90(18) . . ? O3 C10 N2 120.41(18) . . ? O3 C10 C11 126.44(18) . . ? N2 C10 C11 113.14(18) . . ? N1 C11 C7 110.03(17) . . ? N1 C11 C10 127.49(18) . . ? C7 C11 C10 122.45(18) . . ? C17 C12 C13 118.18(19) . . ? C17 C12 C9 120.03(19) . . ? C13 C12 C9 121.78(19) . . ? C14 C13 C12 120.9(2) . . ? C14 C13 H13 119.6 . . ? C12 C13 H13 119.6 . . ? C15 C14 C13 119.9(2) . . ? C15 C14 H14 120.0 . . ? C13 C14 H14 120.0 . . ? C16 C15 C14 120.1(2) . . ? C16 C15 H15 119.9 . . ? C14 C15 H15 119.9 . . ? C15 C16 C17 120.1(2) . . ?

	C15 C16 H16 119.9 . . ? C17 C16 H16 119.9 . . ? C12 C17 C16 120.8(2) . . ? C12 C17 H17 119.6 . . ? C16 C17 H17 119.6 . . ? O1 C18 H18A 109.5 . . ? O1 C18 H18B 109.5 . . ? H18A C18 H18B 109.5 . . ? O1 C18 H18C 109.5 . . ? H18A C18 H18C 109.5 . . ? H18B C18 H18C 109.5 . . ? O2 C19 H19A 109.5 . . ? O2 C19 H19B 109.5 . . ? H19A C19 H19B 109.5 . . ? O2 C19 H19C 109.5 . . ? H19A C19 H19C 109.5 . . ? H19B C19 H19C 109.5 . . ? O4 C20 H20A 109.5 . . ? O4 C20 H20B 109.5 . . ? H20A C20 H20B 109.5 . . ? O4 C20 H20C 109.5 . . ? H20A C20 H20C 109.5 . . ? H20B C20 H20C 109.5 . . ?

_geom_angle	