Supplementary Information

Diversity oriented synthesis of 6-Nitro- and 6-Aminoquinolones and their activity as alkaline phosphatase inhibitors

Mariia Miliutina,¹ Anton Ivanov,¹ Syeda Abida Ejaz,² Jamshed Iqbal,² Alexander Villinger,¹ Viktor O. Iaroshenko,²,³,*, Peter Langer¹,d,*

¹ Institut für Chemie, Universität Rostock, Albert Einstein Str. 3a, 18059 Rostock, Germany; peter.langer@uni-rostock.de; iva108@googlemail.com
² Centre for Advanced Drug Research, COMSATS Institute of Information Technology, Abbottabad, Pakistan
³ National Taras Shevchenko University, 62 Volodymyrska Str., 01033 Kyiv, Ukraine.
⁴ Leibniz Institut für Katalyse an der Universität Rostock e.V., Albert Einstein Str. 29a, 18059 Rostock, Germany

Copies of ¹H and ¹³C NMR spectras

X-Ray structure of compound 7ab

X-Ray structure of compound 7ac

X-Ray structure of compound 7bd

X-Ray structure of compound 15

X-Ray structure of compound 16

Copies of ¹H and ¹³C NMR spectras
1-(2-Chloro-5-nitrophenyl)-3-p-tolylprop-2-yn-1-one (6a).
1-(2-Chloro-5-nitrophenyl)-3-p-tolyprop-2-yn-1-one (6a).
1-(2-Chloro-5-nitrophenyl)-3-phenylprop-2-yn-1-one (6b).
1-(2-Chloro-5-nitrophenyl)-3-phenylprop-2-yn-1-one (6b).
1-(2-chloro-5-nitrophenyl)hept-2-yn-1-one (6c).
1-(2-chloro-5-nitrophenyl)hept-2-yn-1-one (6c).
1-(2-chloro-5-nitrophenyl)oct-2-yn-1-one (6d).
1-(2-chloro-5-nitrophenyl)oct-2-yn-1-one (6d).
1-(3,4-Dimethoxyphenethyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7aa).
1-(3,4-Dimethoxyphenethyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7aa).
1-(4-Methoxybenzyl)-6-nitro-2-<i>p</i>-tolylquinolin-4(<i>1H</i>)-one (7ab).
1-(4-methoxybenzyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ab).
(R)-6-Nitro-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (7ac).
(R)-6-Nitro-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (7ac).
1-Heptyl-6-nitro-2-p-tolyquinolin-4(1H)-one (7ad).
1-Heptyl-6-nitro-2-p-tolylquinolin-4(1H)-one (7ad).
1-Hexyl-6-nitro-2-\textit{p}-tolylquinolin-4(1\textit{H})-one (7ae).
1-Hexyl-6-nitro-2-p-tolyquinolin-4(1H)-one (7ae).
6-Nitro-1-cyclohexyl-2-p-tolyl-4-quinolone (7af).
6-Nitro-1-cyclohexyl-2-p-tolyl-4-quinolone (7af).
6-Nitro-1-pentyl-2-p-tolylquinolin-4(1H)-one (7ag).
6-Nitro-1-pentyl-2-p-tolyquinolin-4(1H)-one (7ag).
1-n-Butyl-6-nitro-2-p-tolyl-4-quinolone (7ah).
1-\textit{n-Butyl}-6-nitro-2-\textit{p-toly}-4-quinolone (7ah).
6-Nitro-1-n-propyl-2-p-tolyl-4-quinolone (7ai).
6-Nitro-1-n-propyl-2-p-tolyl-4-quinolone (7ai).
1-iso-Propyl-6-nitro-2-p-tolyl-4-quinolone (7aj).
1-iso-Propyl-6-nitro-2-p-tolyl-4-quinolone (7aj).
6-Nitro-1-phenyl-2-p-tolyl-4-quinolone (7ak).
6-Nitro-1-phenyl-2-p-toly1-4-quinolone (7ak).
6-Nitro-2-\(p\)-tolyl-2,4,6-trimethylphenyl-4-quinolone (7al).
6-Nitro-2-\(p\)-tolyl-2,4,6-trimethylphenyl-4-quinolone (7al).
1-(3,5-Dimethylphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7am).
1-(3,5-Dimethylphenyl)-6-nitro-2-p-tolyquinolin-4(1H)-one (7am).
1-(2,3-Dihydro-1H-inden-5-yl)-6-nitro-2-\text{-}\text{p-}tolyquinolin-4(1H)-one (7an).
1-(2,3-Dihydro-1H-inden-5-yl)-6-nitro-2-p-tolyquinolin-4(1H)-one (7an).
1-(3-Methoxyphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ao).
1-(3-Methoxyphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ao).
1-(4-Methoxyphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ap).
1-(4-Methoxyphenyl)-6-nitro-2-p-tolylquinolin-4(1H)-one (7ap).
6-Nitro-1-(3-bromophenyl)-2-p-tolyl-4-quinolone (7aq).
6-Nitro-1-(3-bromphenyl)-2-p-tolyl-4-quinolone (7a q).
1-(3,4-Dimethoxyphenethyl)-6-nitro-2-phenylquinolin-4(1H)-one (7ba).
1-(3,4-Dimethoxyphenethyl)-6-nitro-2-phenylquinolin-4(1H)-one (7ba).
1-[(4-Methoxybenzyl)-6-nitro-2-phenylquinolin-4(1H)-one (7bb).
1-(4-Methoxybenzyl)-6-nitro-2-phenylquinolin-4(1H)-one (7bb).
6-Nitro-1-phenethyl-2-phenylquinolin-4(1H)-one (7bc).
6-Nitro-1-phenethyl-2-phenylquinolin-4(1H)-one (7bc).
6-Nitro-4-oxo-2-phenyl-1-(3-phenylpropyl)quinoline (7bd).
6-Nitro-4-oxo-2-phenyl-1-(3-phenylpropyl)quinoline (7bd).
1-Heptyl-6-nitro-2-phenylquinolin-4(1H)-one (7be).
1-Heptyl-6-nitro-2-phenylquinolin-4(1H)-one (7be).
1-cyclohexane-6-nitro-4-oxo-2-phenylquinoline (7bf).
1-cyclohexane-6-nitro-4-oxo-2-phenylquinoline (7bf).
1-Hexyl-6-nitro-2-phenylquinolin-4(1H)-one (7bg).
1-Hexyl-6-nitro-2-phenylquinolin-4(1H)-one (7bg).

Millitins, Me-94, DMSO, 13C
1-(3,5-dimethoxybenzen)-6-nitro-4-oxo-2-phenylquinoline (7bh).
1-(3,5-dimethoxybenzen)-6-nitro-4-oxo-2-phenylquinoline (7bh).
6-Nitro-1-(3,4-dimethoxyphenethyl)-2-p-tolyl-4-quinolone (7ca).
6-Nitro-1-(3,4-dimethoxyphenethyl)-2-p-tolyl-4-quinolone (7ca).
2-Butyl-1-(3,5-dimethoxyphenyl)-6-nitroquinolin-4(1H)-one (7cb).
2-Butyl-1-(3,5-dimethoxyphenyl)-6-nitroquinolin-4(1H)-one (7cb).
2-Butyl-1-(4-methoxyphenyl)-6-nitroquinolin-4(1H)-one (7cc).
2-Butyl-1-(4-methoxyphenyl)-6-nitroquinolin-4(1H)-one (7cc).

Millistina, NM-98, DMSO, 13C
2-Butyl-1-(4-tert-butylphenyl)-6-nitroquinolin-4(1H)-one (7cd).
2-Butyl-1-(4-tert-butyphenyl)-6-nitroquinolin-4(1H)-one (7cd).
6-Nitro-(3,4-dimethoxyphenethyl)-2-pentyl-4-quinolone (7da).
6-Nitro-(3,4-dimethoxyphenethyl)-2-pentyl-4-quinolone (7da).
1-(4-Methoxybenzyl)-6-nitro-2-pentylquinolin-4(1H)-one (7db).
1-(4-Methoxybenzyl)-6-nitro-2-pentylquinolin-4(1H)-one (7db).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-p-tolylquinolin-4(1H)-one (8aa).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-p-tolylquinolin-4(1H)-one (8aa).

Millutima, M=114-2, CDCl3, 13C
6-Amino-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (8_{ab}).
6-Amino-1-(4-methoxybenzyl)-2-\(p\)-tolyquinolin-4(1\(H\))-one (8\(\text{ab}\)).
6-Amino-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (8ac).
6-Amino-1-(1-phenylethyl)-2-p-tolylquinolin-4(1H)-one (8ac).
6-Amino-1-heptyl-2-p-tolylquinolin-4(1H)-one (8ad).

\[
\begin{align*}
\text{H}_2\text{N} & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\text{H}_3 & \quad \text{C} \\
\end{align*}
\]
6-Amino-1-heptyl-2-p-tolylquinolin-4(1H)-one (8ad).
6-Amino-1-hexyl-2-p-tolylquinolin-4(1H)-one (8ae).
6-Amino-1-hexyl-2-p-tolyquinolin-4(1H)-one (8ae).
6-Amino-1-cyclohexyl-2-p-tolyquinolin-4(1H)-one (8af).

**Bruker**

NAME: 1501.25.m304
PROCNO: 10
Date: 298.50.23
Time: 10:52
INSTRU. spect
PROBHD: 5 mm PA6BO B/B-
PULPROG: 10s
TD: 65.5M
SOLVENT: DMSO
NS: 10
DS: 2
SW1: 6.18.11.19 Hz
FIDRESX: 0.094423 Hz
AQ: 5.293587 sec
RG: 5.8
DW: 80.000 nsec
DE: 10.000 nsec
TE: 299.2 K
TH: 1.0000.000 sec
TD0: 1

**CHANNEL 1**

NDC1: 1H
P1: 10.00 nsec
PL: 0.060 Hz
PLW: 1.12532380 W
SFQAM: 0.015385 Hz
SE: 32786
GF: 1.2969 MHz
WDW: 0.00 EM
SSB: 0.00 Hz
GB: 0
PC: 1.00
6-Amino-1-cyclohexyl-2-p-tolylquinolin-4(1H)-one (8af).

![Chemical Structure](image)
6-Amino-1-pentyl-2-p-tolylquinolin-4(1H)-one (8ag).
6-Amino-1-pentyl-2-p-tolylquinolin-4(1H)-one (8ag).
6-Amino-1-n-butyl-2-p-tolyl-4-quinolone (8ah).
6-Amino-1-n-butyl-2-p-tolyl-4-quinolone (8ah).
6-Amino-1-n-propyl-2-p-tolyl-4-quinolone (8ai).
6-Amino-1-n-propyl-2-p-tolyl-4-quinolone (8ai).
6-Amino-1-isopropyl-2-p-tolylquinolin-4(1H)-one (8aj).
6-Amino-1-isopropyl-2-p-tolylquinolin-4(1H)-one (8aj).
6-Amino-1-phenyl-2-p-tolyquinolin-4(1H)-one (8a).
6-Amino-1-phenyl-2-p-tolylquinolin-4(1H)-one (8ak).
6-Amino-1-(3,5-dimethylphenyl)-2-p-tolyquinolin-4(1H)-one (8aml).
6-Amino-1-(3,5-dimethylphenyl)-2-p-tolylquinolin-4(1H)-one (8aml).
6-Amino-1-(2,3-dihydro-1H-inden-5-yl)-2-p-tolylquinolin-4(1H)-one (8anm).
6-Amino-1-(2,3-dihydro-1H-inden-5-yl)-2-p-tolylquinolin-4(1H)-one (8anm).
6-Amino-1-(4-methoxyphenyl)-2-p-tolylquinolin-4(1H)-one (8appa).
6-Amino-1-(4-methoxyphenyl)-2-p-tolylquinolin-4(1H)-one (8apn).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-phenylquinolin-4(1H)-one (8b<sub>de</sub>).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-phenylquinolin-4(1H)-one (8bao).
6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bcp).
6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bcp).
6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bdq).
6-Amino-1-phenethyl-2-phenylquinolin-4(1H)-one (8bdq).
6-Amino-1-heptyl-2-phenylquinolin-4(1H)-one (8\text{bev}).
6-Amino-1-heptyl-2-phenylquinolin-4(1H)-one (8ber).
6-Amino-1-cyclohexyl-2-phenylquinolin-4(1H)-one (8bfs).
6-Amino-1-cyclohexyl-2-phenylquinolin-4(1H)-one (8bfs).
6-Amino-1-hexyl-2-phenylquinolin-4(1H)-one (8bg).

![NMR spectrum of 6-Amino-1-hexyl-2-phenylquinolin-4(1H)-one (8bg)]
6-Amino-1-hexyl-2-phenylquinolin-4(1H)-one (8bgt).
6-Amino-2-butyl-1-(3,4-dimethoxyphenethyl)quinolin-4(1H)-one (8cau).
6-Amino-2-butyl-1-(3,4-dimethoxyphenethyl)quinolin-4(1H)-one (8cau).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-pentylquinolin-4(1H)-one (8da).
6-Amino-1-(3,4-dimethoxyphenethyl)-2-pentylquinolin-4(1H)-one (8da).
6-Amino-1-(4-methoxybenzyl)-2-pentylquinolin-4(1H)-one (8wdb).
6-Amino-1-(4-methoxybenzyl)-2-pentylquinolin-4(1H)-one (8-wdb).
(Z)-3-(4-Methoxybenzylamino)-1-(2-(4-methoxybenzylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9a).
(Z)-3-(4-Methoxybenzylamino)-1-(2-(4-methoxybenzylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9a).
(Z)-3-(Isopropylamino)-1-(2-(isopropylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9b).
(Z)-3-(Isopropylamino)-1-(2-(isopropylamino)-5-nitrophenyl)-3-p-tolylprop-2-en-1-one (9b).
(Z)-3-(3,4-Dimethoxyphenethylamino)-1-(2-(3,4-dimethoxyphenethylamino)-5-nitrophenyl)hept-2-en-1-one (9c).
(Z)-3-(3,4-Dimethoxyphenethylamino)-1-(2-(3,4-dimethoxyphenethylamino)-5-nitrophenyl)hept-2-en-1-one (9c).

Ivanov, AI-42.1, CDC13, 13C
(Z)-3-(Cyclohexylamino)-1-(2-(cyclohexylamino)-5-nitrophenyl)hept-2-en-1-one (9d).
(Z)-3-(Cyclohexylamino)-1-(2-(cyclohexylamino)-5-nitrophenyl)hept-2-en-1-one (9d).
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(3,4-dimethoxyphenethylamino)hept-2-en-1-one (10a).
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(3,4-dimethoxyphenethylamino)hept-2-en-1-one (10a).
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(cyclohexylamino) hept-2-en-1-one (10b).

Anton Ivanov, AI-43.2, 1H in CDCl3
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(cyclohexy lamino) hept-2-en-1-one (10b).

Anton Ivanov, Al-43.2, 13C in CDCl3
(Z)-1-(2-Chloro-5-nitropheryl)-3-(methyl(phenyl)amino)-3-p-tolylprop-2-en-1-one (11).
(Z)-1-(2-Chloro-5-nitrophenyl)-3-(methyl(phenyl)amino)-3-p-tolylprop-2-en-1-one (11).
1,1'-(Butane-1,4-diyl)bis(6-nitro-2-p-tolyquinolin-4(1H)-one) (12a).
1,1'-[(Butane-1,4-diyl)bis(6-nitro-2-p-tolylquinolin-4(1H)-one) (12a).
1,1'-(Hexane-1,6-diyl)bis(6-nitro-2-p-tolyquinolin-4(1H)-one) (12b).
1,1'-((Hexane-1,6-diyl)bis(6-nitro-2-p-tolylquinolin-4(1H)-one) (12b).
6-Nitro-1'-propyl-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13a).
6-Nitro-1'-propyl-2,2'-dip-tolyl-4H-1,6'-biquinoline-4,4'(1'H)-dione (13a).
1'-Isopropyl-6-nitro-2,2'-dip-toly1-4H-1,6'-biquinoline-4,4'(1'H)-dione (13b).
1'-Isopropyl-6-nitro-2,2'-dip-toly1-4H-1,6'-biquinoline-4,4'(1'H)-dione (13b).
3,6-Dibromo-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (14).
3,6-Dibromo-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (14).
3,6-Bis(4-ethylphenyl)-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (15).
3,6-Bis(4-ethylphenyl)-1-(4-methoxybenzyl)-2-p-tolylquinolin-4(1H)-one (15).
3,6-Bis(4-ethylphenyl)-4H-chromen-4-one (16).
3,6-Bis(4-ethylphenyl)-4H-chromen-4-one (16).
X-Ray structure of compound 7ab

Identification code: is_mm127
Empirical formula: C24 H20 N2 O4
Formula weight: 400.42
Temperature: 173(2) K
Wavelength: 0.71073 Å
Crystal system: monoclinic
Space group (H.-M.): P 21/c
Space group (Hall): -P 2ybc
Unit cell dimensions:
- a = 10.4745(6) Å  \quad \alpha = 90.00°
- b = 10.6976(6) Å  \quad \beta = 91.384(3)°
- c = 17.8031(11) Å  \quad \gamma = 90.00°
Volume: 1994.3(2) Å³
Z: 4
Calculated density: 1.334 mg/m³
Absorption coefficient: 0.092 mm⁻¹
F(000): 840
Crystal size: 0.37 x 0.13 x 0.07 mm³
θ range for data collection: 1.94 to 28.00°
Index ranges:
- -13 ≤ h ≤ 13, -9 ≤ k ≤ 14, -23 ≤ l ≤ 22
Reflections collected: 19220
Independent reflections: 4810 [R(int) = 0.0664]
Completeness to θ = 28.00°: 100.0%
Absorption correction: Multi-scan
Max. and min. transmission: 0.9936 and 0.9668
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 2565 / 0 / 273
Goodness-of-fit on F²: 1.000
Final R indices [I>2σ (I)]: R1 = 0.0505, wR2 = 0.1045
R indices (all data): R1 = 0.1164, wR2 = 0.1328
Largest diff. peak and hole: 0.167 and -0.270 e.Å⁻³
X-Ray structure of compound 7ac

Identification code: is_mm115_118
Empirical formula: C24 H20 N2 O3
Formula weight: 384.42
Temperature: 173(2) K
Wavelength: 0.71073 Å
Crystal system: orthorhombic
Space group (H.-M.): P 21 21 21
Space group (Hall): P 2ac 2ab
Unit cell dimensions:

\[ \begin{align*}
  a &= 9.9322(10) \text{ Å} \\
  b &= 13.6154(10) \text{ Å} \\
  c &= 14.4052(15) \text{ Å}
\end{align*} \]

\[ \alpha = 90^\circ, \quad \beta = 90^\circ, \quad \gamma = 90^\circ \]

Volume: 1948.0(3) Å³
Z: 4
Calculated density: 1.311 mg/m³
Absorption coefficient: 0.087 mm⁻¹
F(000): 808
Crystal size: 0.430 x 0.170 x 0.140 mm³
Θ range for data collection: 3.628 to 28.999°
Index ranges:

\[ -13 \leq h \leq 13, \quad -11 \leq k \leq 17, \quad -19 \leq l \leq 19 \]

Reflections collected: 15463
Independent reflections: 5004 [R(int) = 0.0466]
Completeness to Θ = 28.00°: 96.9%
Absorption correction: Multi-scan
Max. and min. transmission: 0.7460 and 0.6977
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 3347 / 0 / 265
Goodness-of-fit on F²: 1.074
Final R indices [I>2σ (I)]: R1 = 0.0414, wR2 = 0.0724
R indices (all data): R1 = 0.0851, wR2 = 0.0959
Largest diff. peak and hole: 0.191 and -0.178 e.Å⁻³
X-Ray structure of compound 7bd

Identification code av_mm89
Empirical formula C24 H20 N2 O3
Formula weight 384.42
Temperature 173(2) K
Wavelength 0.71073 Å
Crystal system orthorhombic
Space group (H.-M.) Pbca
Space group (Hall) -P 2ac 2ab
Unit cell dimensions
  a = 10.4213(5) Å  α = 90.00°
  b = 15.0974(8) Å  β = 90.00°
  c = 24.6279(14) Å  γ = 90.00°
Volume 3874.8(4) Å³
Z 8
Calculated density 1.318 mg/m³
Absorption coefficient 0.088 mm⁻¹
F(000) 1616
Crystal size 0.68 x 0.20 x 0.15 mm³
Θ range for data collection 2.51 to 30.00°
Index ranges -14 ≤ h ≤ 12, -19 ≤ k ≤ 21, -34 ≤ l ≤ 24
Reflections collected 22580
Independent reflections 5541 [R(int) = 0.0292]
Completeness to Θ = 28.00° 98.0%
Absorption correction Multi-scan
Max. and min. transmission 0.9870 and 0.9427
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 3855 / 0 / 262
Goodness-of-fit on F² 1.049
Final R indices [I>2σ(I)] R1 = 0.0493, wR2 = 0.1103
R indices (all data) R1 = 0.0799, wR2 = 0.1234
Largest diff. peak and hole 0.208 and -0.245 e.Å⁻³
X-Ray structure of compound 15

Identification code: is_mm183
Empirical formula: C39.74 H36.71 Br0.03 N O2
Formula weight: 562.69
Temperature: 173(2) K
Wavelength: 0.71073 Å
Crystal system: triclinic

Space group (H.-M.): $\overline{\text{P}}\text{1}$
Space group (Hall): -P 1

Unit cell dimensions:
- $a = 10.5670(5) \text{ Å}$
- $b = 12.7739(5) \text{ Å}$
- $c = 12.9152(5) \text{ Å}$

Volume: 1498.23(11) Å$^3$
Z: 2
Calculated density: 1.247 mg/m$^3$
Absorption coefficient: 0.115 mm$^{-1}$

F(000): 598
Crystal size: 0.24 x 0.22 x 0.05 mm$^3$

$\Theta$ range for data collection: 2.80 to 30.00°
Index ranges: $-14 \leq h \leq 14$, $-17 \leq k \leq 17$, $-18 \leq l \leq 18$
Reflections collected: 39715
Independent reflections: 8694 [R(int) = 0.0471]
Completeness to $\Theta = 28.00°$: 99.6%
Absorption correction: Multi-scan

Max. and min. transmission: 0.9943 and 0.9728
Refinement method: Full-matrix least-squares on F$^2$

Data / restraints / parameters: 5050 / 0 / 396
Goodness-of-fit on F$^2$: 1.013

Final R indices [I>2\sigma (I)]:
- $R_1 = 0.0558$, $wR_2 = 0.1135$
R indices (all data):
- $R_1 = 0.1178$, $wR_2 = 0.1406$

Largest diff. peak and hole:
- 0.445 and -0.255 e.Å$^{-3}$
X-Ray structure of compound 16

Identification code: ch_mm181
Empirical formula: C25 H22 O2
Formula weight: 354.43
Temperature: 173(2) K
Wavelength: 0.71073 Å
Crystal system: monoclinic
Space group (H.-M.): P 2₁/n
Space group (Hall): -P 2yn
Unit cell dimensions:
- a = 5.8177(4) Å  α = 90.00°
- b = 10.2341(6) Å  β = 94.982(2)°
- c = 31.4579(18) Å  γ = 90.00°
Volume: 1865.9(2) Å³
Z: 4
Calculated density: 1.262 m g/m³
Absorption coefficient: 0.079 mm⁻¹
F(000): 752
Crystal size: 0.57 x 0.16 x 0.15 mm³
Θ range for data collection: 1.30 to 28.00°
Index ranges:
- 7 ≤ h ≤ 7
- -13 ≤ k ≤ 13
- -41 ≤ l ≤ 41
Reflections collected: 24058
Independent reflections: 4514 [R(int) = 0.0339]
Completeness to Θ = 28.00°: 99.9%
Absorption correction: Multi-scan
Max. and min. transmission: 0.9883 and 0.9566
Refinement method: Full-matrix least-squares on F²
Data / restraints / parameters: 3522 / 0 / 273
Goodness-of-fit on F²: 1.017
Final R indices [I>2σ (I)]: R1 = 0.0513, wR2 = 0.1247
R indices (all data): R1 = 0.0674, wR2 = 0.1374
Largest diff. peak and hole: 0.488 and -0.350 e.Å⁻³