Search Overview

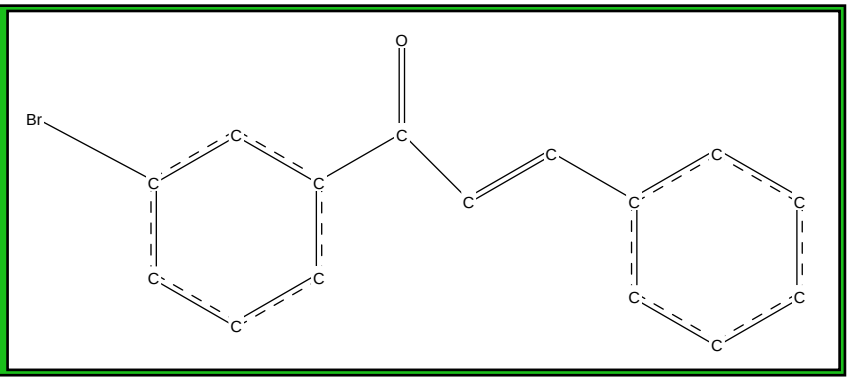
Search:	search2
Date/Time done:	Tue Jan 22 16:03:13 2019
Database(s):	CSD version 5.40 (November 2018)
Restriction Info:	No refcode restrictions applied
Filters:	None
Percentage Completed:	100%
Number of Hits:	31

Single query used. Search found structures that:

match

Query 1

Query 1



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 1

AJUFAO

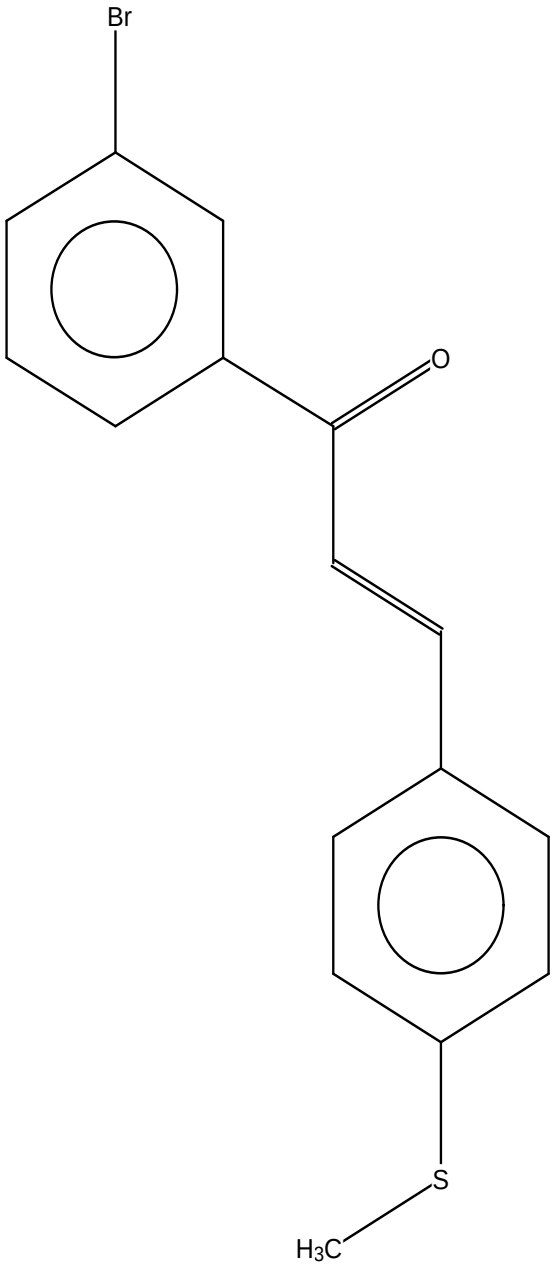
Reference: E.D.Dsilva, D.Narayan Rao, Reji Philip, R.J.Butcher, Rajnikant, S.M.Dharmaprakash (2011)
*Physica B: Condensed Matter(Amsterdam) ,***406,**2206

Formula: $C_{16}\,H_{13}\,Br_1\,O_1\,S_1$

Compound Name: (2E)-3-[4-(Methylsulfanyl)phenyl]-1-(3-bromophenyl)prop-2-en-1-one

Space Group:	Pbca	***Cell:***	***a***	13.941(1)	***b***	5.802(0)	***c***	33.496(4)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 0.00 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.634



Parameters

Fragment 1
ANG1 (A) 50.030

Search: search2 (Tue Jan 22 16:03:13 2019): Hit 2

CICLUW

Reference: M.M.Rosli, P.S.Patil, Hoong-Kun Fun, I.A.Razak, S.M.Dharmaprakash (2007) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**63,**o2501

Formula: $C_{15}\ H_{11}\ Br_1\ O_1$

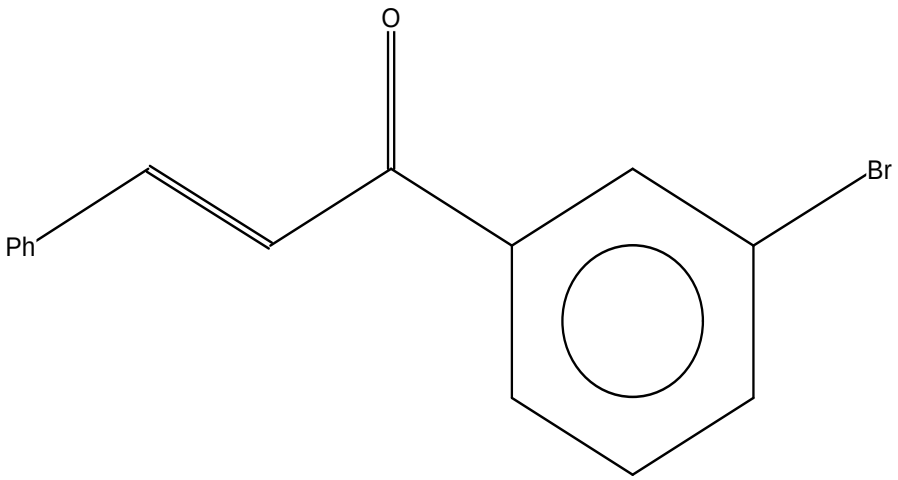
Compound Name: (2E)-1-(3-Bromophenyl)-3-phenylprop-2-en-1-one

Space Group:	P-1	***Cell:***	***a***	5.825(0)	***b***	7.633(0)	***c***	13.337(0)
Space Group No.:	2	***(Å,°)***	α	83.05(0)	β	89.92(0)	γ	87.38(0)

R-Factor (%): 2.59 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.622

Parameters

Fragment 1
ANG1 (A) 49.933



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 3

GASBEK

Reference: S.Rajendraprasad, C.S.Chidan Kumar, C.K.Quah, S.Chandraju, N.K.Lokanath, S.Naveen, I.Warad (2017) *IUCrData ,***2,** x170379

Formula: $C_{15}\,H_{10}\,Br_1\,F_1\,O_1$

Compound Name: (E)-1-(3-Bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one

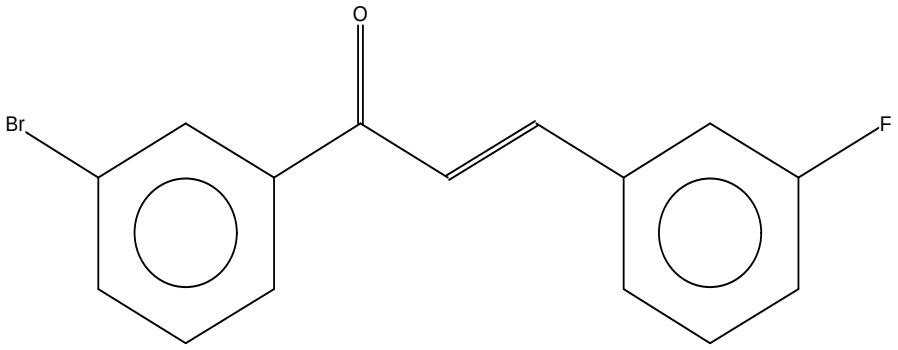
Space Group:	P21/n	***Cell:***	***a***	7.603(0)	***b***	5.928(0)	***c***	27.600(3)
Space Group No.:	14	***(Å,°)***	α	90.00	β	93.18(0)	γ	90.00

R-Factor (%): 3.35 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.632

Parameters

Fragment 1

ANG1 (A) 48.923



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 4

JOFKAR

Reference: H.-K.Fun, S.Chantrapromma, P.S.Patil, S.M.Dharmaprakash (2008) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**64,**o1356

Formula: $C_{17}\,H_{15}\,Br_1\,O_2$

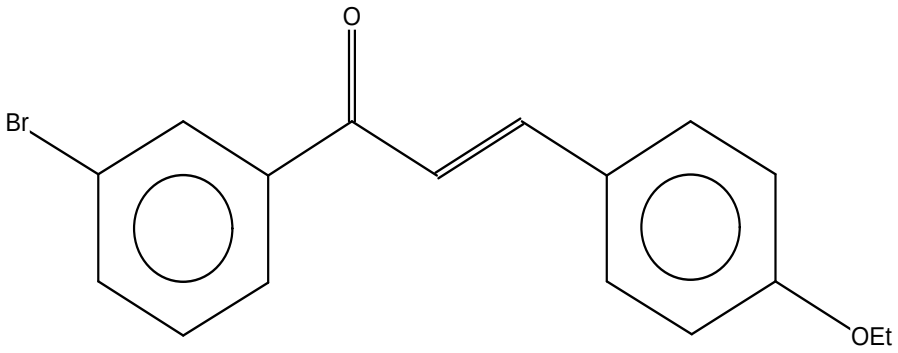
Compound Name: 1-(3-Bromophenyl)-3-(4-ethoxyphenyl)prop-2-en-1-one

Space Group:	P21	***Cell:***	***a***	4.052(0)	***b*** 9.650(0)	***c***	17.912(0)
Space Group No.:	4	***(Å,°)***	α	90.00	β 92.40(0)	γ	90.00

R-Factor (%): 3.43 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.572

Parameters

Fragment 1
ANG1 (A) 10.087



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 5

LAQWUX

Reference: C.A.Escobar, A.Trujillo, J.A.K.Howard, M.Fuentealba (2012) *Acta Crystallogr.,Sect.E:Struct.Rep.Online ,***68,**o887

Formula: $C_{17}\ H_{15}\ Br_1\ O_3$

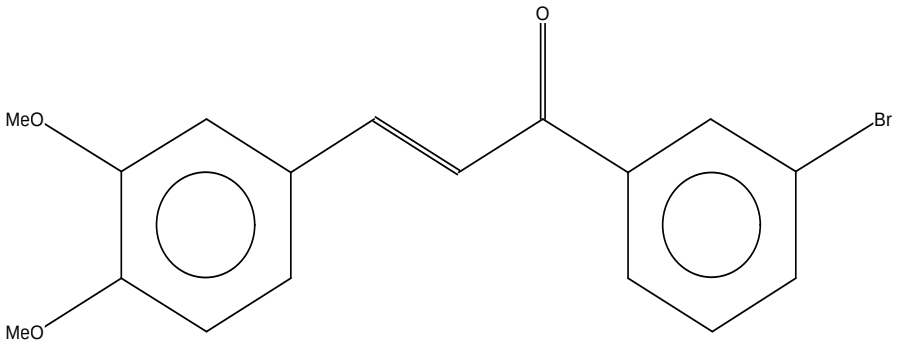
Compound Name: (E)-1-(3-Bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one

Space Group:	P21/c	***Cell:***	***a***	12.795(0)	***b*** 3.937(0)	***c***	29.821(1)
Space Group No.:	14	***(Å,°)***	α	90.00	β 109.22(0)	γ	90.00

R-Factor (%): 4.05 ***Temperature(K):*** 120 ***Density(g/cm^3):*** 1.626

Parameters

Fragment 1
ANG1 (A) 26.582



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 6

OBIYUW

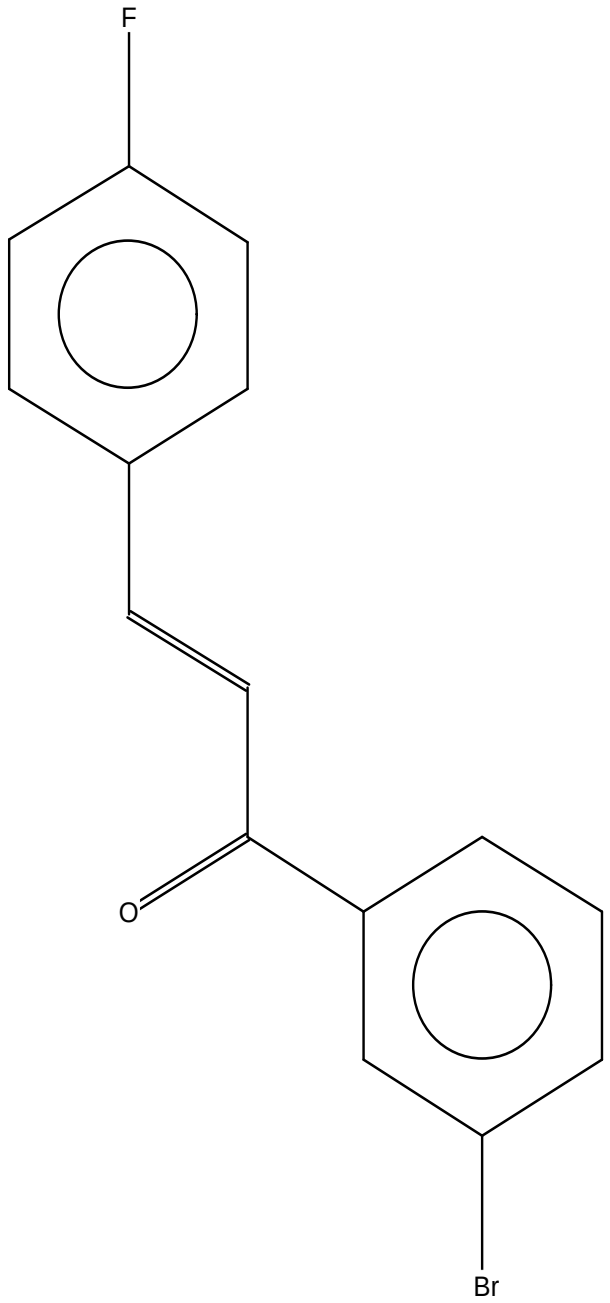
Reference: Anusha Ekbote, P.S.Patil, S.R.Maidur, Tze Shyang Chia, Ching Kheng Quah (2017) *Dyes Pigm.* ,**139,**720

Formula: $C_{15}\ H_{10}\ Br_1\ F_1\ O_1$

Compound Name: 1-(3-bromophenyl)-3-(4-fluorophenyl)prop-2-en-1-one

Space Group:	P-1	***Cell:***	***a***	5.865(0)	***b*** 7.417(0)	***c***	14.032(0)
Space Group No.:	2	***(Å,°)***	α	90.81(0)	β 97.03(0)	γ	92.57(0)

R-Factor (%): 3.53 ***Temperature(K):*** 100 ***Density(g/cm^3):*** 1.675



Parameters

Fragment 1

ANG1 (A) 47.741

Search: search2 (Tue Jan 22 16:03:13 2019): Hit 7

PUGVAP

Reference: G.Dutkiewicz, C.S.C.Kumar, H.S.Yathirajan, B.Narayana, M.Kubicki (2009) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**65,**o2856

Formula: $C_{21}\ H_{15}\ Br_1\ O_1$

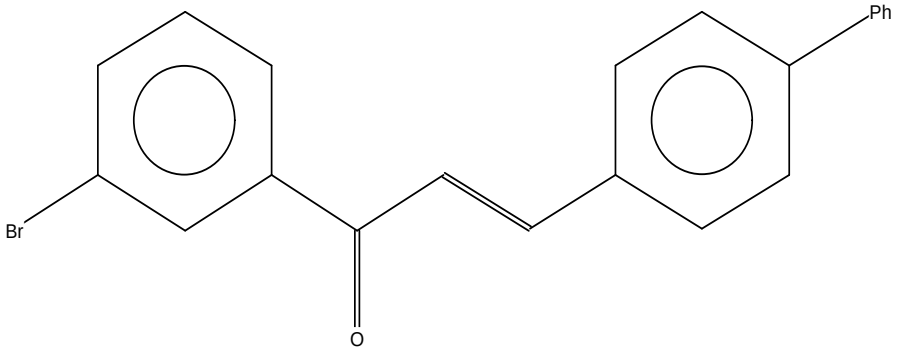
Compound Name: (E)-3-(Biphenyl-4-yl)-1-(3-bromophenyl)prop-2-en-1-one

Space Group:	Pca21	***Cell:***	***a*** 6.092(1)	***b*** 7.295(1)	***c*** 36.619(2)
Space Group No.:	29	***(Å,°)***	α 90.00	β 90.00	γ 90.00

R-Factor (%): 3.45 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.483

Parameters

Fragment 1
ANG1 (A) 47.080



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 8

VABXIH

Reference: J.P.Jasinski, R.J.Butcher, C.S.Chidan Kumar, H.S.Yathirajan, A.N.Mayekar (2010) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**66,**o2936

Formula: $C_{17}\ H_{14}\ Br_1\ N_1\ O_5$

Compound Name: (2E)-1-(3-Bromophenyl)-3-(4,5-dimethoxy-2-nitrophenyl)prop-2-en-1-one

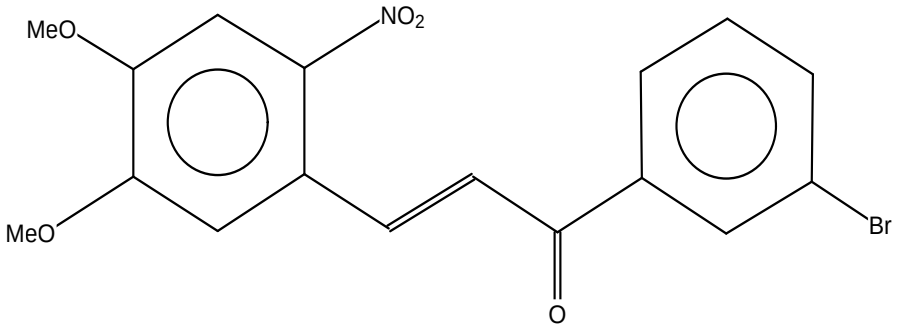
Space Group:	P212121	***Cell:***	***a***	6.855(0)	***b***	8.321(0)	***c*** 27.151(0)
Space Group No.:	19	***(Å,°)***	α	90.00	β	90.00	γ 90.00

R-Factor (%): 3.22 ***Temperature(K):*** 123 ***Density(g/cm^3):*** 1.682

Parameters

Fragment 1

ANG1 (A) 15.197



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 9

VIDFEU

Reference: J.Bee-Jan Teh, P.S.Patil, H.-K.Fun, Y.E.Satheesh, I.A.Razak, S.M.Dharmaprakash (2007) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**63,**o1844

Formula: $C_{15}\,H_{10}\,Br_1\,Cl_1\,O_1$

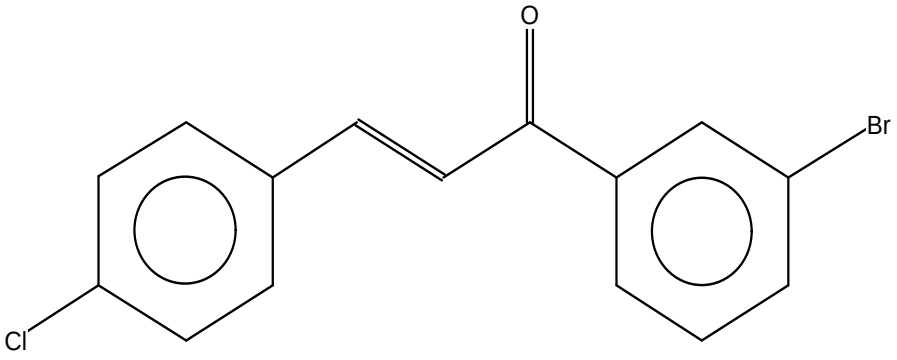
Compound Name: (2E)-1-(3-Bromophenyl)-3-(4-chlorophenyl)prop-2-en-1-one

Space Group:	P-1	***Cell:***	***a***	5.916(0)	***b*** 7.264(0)	***c***	14.663(0)
Space Group No.:	2	***(Å,°)***	α	86.45(0)	β 83.24(0)	γ	87.86(0)

R-Factor (%): 3.21 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.711

Parameters

Fragment 1
ANG1 (A) 46.709



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 10

VIDJIC

Reference: P.S.Patil, S.Chantrapromma, H.-K.Fun, S.M.Dharmaprakash (2007) *Acta Crystallogr.,Sect.E:Struct.Rep.Online* ,**63,**o1738

Formula: $C_{17}\ H_{16}\ Br_1\ N_1\ O_1$

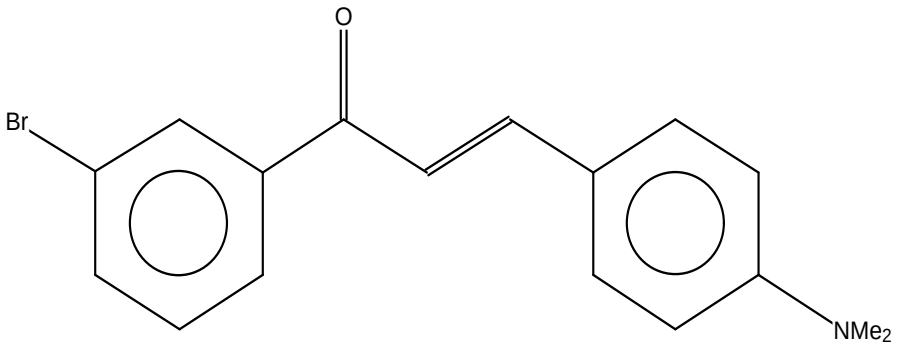
Compound Name: 1-(3-Bromophenyl)-3-(4-dimethylaminophenyl)prop-2-en-1-one

Space Group:	Pbca	***Cell:***	***a***	13.959(0)	***b***	6.070(0)	***c***	33.350(1)
Space Group No.:	61	***(Å,°)***	α	90.00	β	90.00	γ	90.00

R-Factor (%): 4.56 ***Temperature(K):*** 295 ***Density(g/cm^3):*** 1.552

Parameters

Fragment 1
ANG1 (A) 49.170



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 11

XALQAF

Reference: K.S.Harini, C.K.Quah, C.S.Chidan Kumar, S.Chandraju, N.K.Lokanath, S.Naveen, I.Warad (2017) *IUCrData* ,**2,**x170287

Formula: $C_{15}\ H_{10}\ Br_1\ N_1\ O_3$

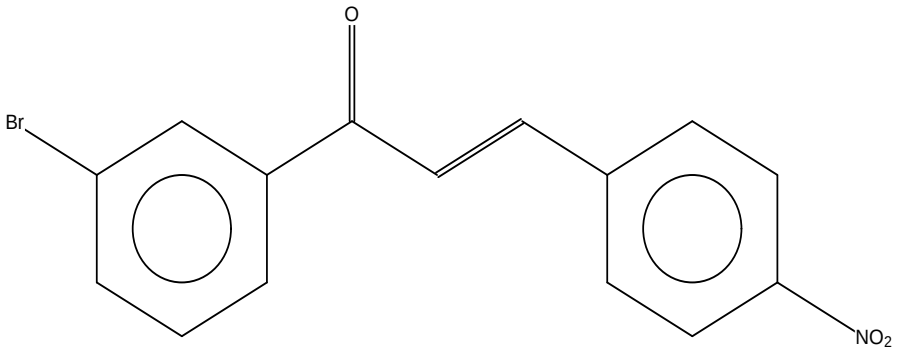
Compound Name: (E)-1-(3-Bromophenyl)-3-(4-nitrophenyl)prop-2-en-1-one

Space Group:	P21	***Cell:***	***a***	6.051(0)	***b***	5.054(0)	***c***	21.841(3)
Space Group No.:	4	***(Å,°)***	α	90.00	β	95.78(0)	γ	90.00

R-Factor (%): 3.32 ***Temperature(K):*** 294 ***Density(g/cm^3):*** 1.660

Parameters

Fragment 1
ANG1 (A) 3.318



Search: search2 (Tue Jan 22 16:03:13 2019): Hit 12

ZAQCUR

Reference: Guang-Bing Li, Lu Li, Guo-Xi Wang (2012)
Acta Crystallogr.,Sect.E:Struct.Rep.Online ,**68,**o1446

Formula: $C_{17}\ H_{16}\ Br_1\ N_1\ O_2$

Compound Name: (E)-1-(5-Bromo-2-hydroxyphenyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one

Space Group:	P21/c	***Cell:***	***a***	15.191(0)	***b*** 5.450(0)	***c***	19.757(0)
Space Group No.:	14	***(Å,°)***	α	90.00	β 106.00(2)	γ	90.00

R-Factor (%): 8.89 ***Temperature(K):*** 123 ***Density(g/cm^3):*** 1.463

Parameters

Fragment 1
ANG1 (A) 7.416