Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Prediction of Enantiomeric Excess Values for Asymmetric Transfer Hydrogenation Based on Machine Learning

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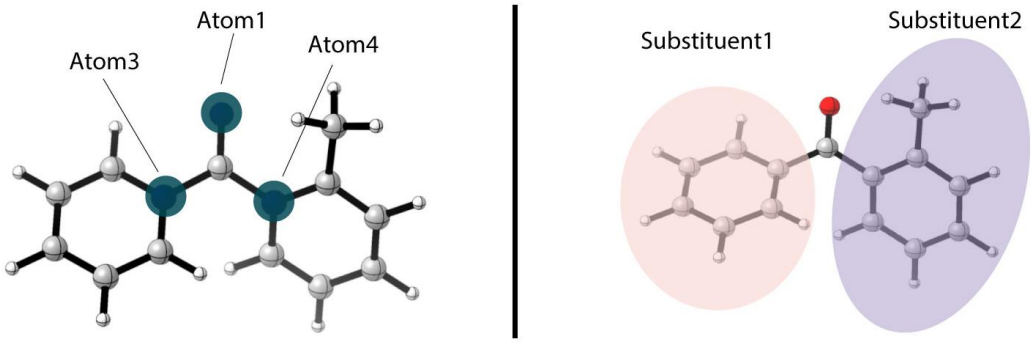
Content

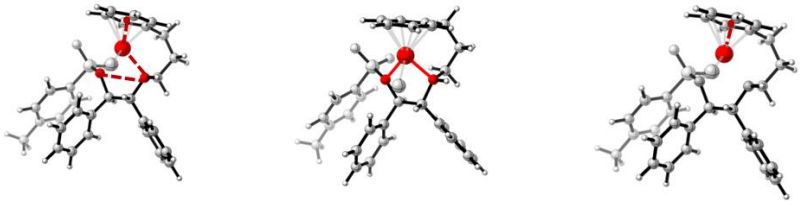
1. Details for Descriptors

1.1 Substrate



Symbol	Notes
Atom1 NBO charge	NBO charge of oxygen or nitrogen atom (atom1)
Atom3 NBO charge	NBO charge of atom 3 and atom 4, whichever is numerically larger
Atom4 NBO charge	NBO charge of atom 3 and atom 4, whichever is numerically smaller
C=O/C=N Vibration Frequency	The vibration frequency with the largest vibration amplitude of C=O or C=N
Sterimol L1	*Max*(L+Bmax) corresponds to the sterimol parameter of the substituent
Sterimol Bmin1	*Max*(L+Bmin) corresponds to the sterimol parameter of the substituent
Sterimol Bmax1	*Max*(L+Bmax) corresponds to the sterimol parameter of the substituent
Sterimol L2	*Min*(L+Bmax) corresponds to the sterimol parameter of the substituent
Sterimol Bmin2	*Min*(L+Bmin) corresponds to the sterimol parameter of the substituent
Sterimol Bmax2	*Min*(L+Bmax) corresponds to the sterimol parameter of the substituent

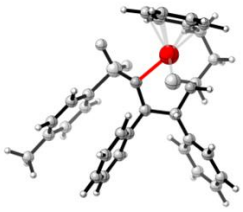
1.2 Catalyst



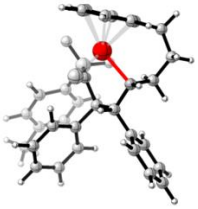
Dihedral Angle
Symbol: C_Di_HA

Bite Angle

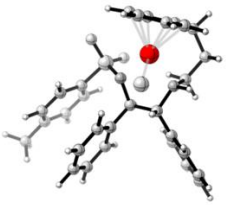
Distance
Symbol: Ph_distance



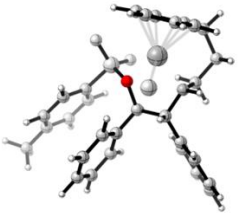
Bond Length
Symbol: C_BL1



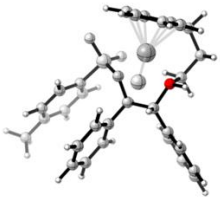
Bond Length
Symbol: C_BL2



Buried volume
Symbol: %V_bur



NBO Charge
Symbol: N_Q1



NBO Charge
Symbol: N_Q2

NBO Charge
Symbol: M_Q (M=Ru/Rh)

Symbol	Notes
C_Di_HA	Catalyst dihedral angle
Bite Angle	Bite angle between nitrogen atoms and metal atom
Ph_distance	Distance from metal atom to the center of aromatic ring
C_BL1	Distance from metal atom to nitrogen atom
C_BL2	Distance from metal atom to nitrogen atom
%V_bur	Buried volume of metal atoms (%)
N_Q1	NBO charge of chiral diamine nitrogen atom
N_Q2	NBO charge of chiral diamine nitrogen atom
M_Q	NBO charge of metal atoms

Notes:

Structure optimization with reference to the single crystal structure (X-ray) of the catalyst.[1-2]

References:

1. A. Fujii, S. Hashiguchi, N. Uematsu, T. Ikariya, R. Noyori, *J. Am. Chem. Soc.*, 1996, **118**, 2521-2522.
2. J. Hannedouche, G. J. Clarkson, M. Wills, *J. Am. Chem. Soc.*, 2004, **126**, 986-987.

1.3 Conditions

Symbol	Notes
Temperature	Numerical value of reaction temperature
S_C	Ratio of substrate to catalyst
H_logP	Partition coefficient (Hydrogen source)
H_TPSA	Topological molecular polar surface area (Hydrogen source)

2. Computational Methods and Programming Detail

All the DFT calculations in this work were performed with Gaussian 16.[1] Geometries of chiral catalyst families and substrates at the SMD(solvent) model, B3LYP-D3(BJ) functional[2] with the basis set lanz2dz for metal atom,[3] 6-31G** for other main group atoms.[4]

The data processing and computing software used in this study are as follows.

Download and install the following programs:

- Python 3.7 (Download at https://www.anaconda.com/download/)
- Multiwfn 3.8 (We use this software to convert log files into xyz files.)[5]
- DBSTEP (Calculate Sterimol parameters, %Buried Volume)[6]
- CYLview (Draw molecular diagrams)[7]
- RDkit package[8]

References:

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Na-katsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cam-mi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16, Revision A.03, Gaussian, Inc., Wallingford CT, 2016.
2. (a) Becke, A. D., Phys. Rev. A, 1988, **38**, 3098-3100; (b) Lee, C.; Yang, W.; Parr, R. G., Phys. Rev. B, 1988, **37**, 785-789; (c) Miehlich, B.; Savin, A.; Stoll, H.; Preuss, H., Chem. Phys. Lett., 1989, **157**, 200-206; (d) Grimme, S.; Ehrlich, S.; Goerigk, L., J. Comput. Chem.,2011, **32**, 1456-1465.
3. (a) Hay, P. J.; Wadt, W. R., *J. Chem. Phys.*, 1985, **82**, 270-283; (b) Wadt, W. R.; Hay, P. J., *J. Chem. Phys.*, 1985, **82**, 284-298; (c) Hay, P. J.; Wadt, W. R., *J. Chem. Phys.*, 1985, **82**, 299-310.
4. (a) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J., J. Chem. Phys., 1988, **89**, 2193-2218; (b) Petersson, G. A.; Al-Laham, M. A., J. Chem. Phys., 1991, **94**, 6081-6090..
5. Tian Lu, Feiwu Chen, *J. Comput. Chem.*, 33, 580-592 (2012)
6. https://github.com/patonlab/DBSTEP
7. CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)
8. RDKit: open-source chemoinformatics and machine learning. http://www.rdkit.org.

3. Machine Learning Model

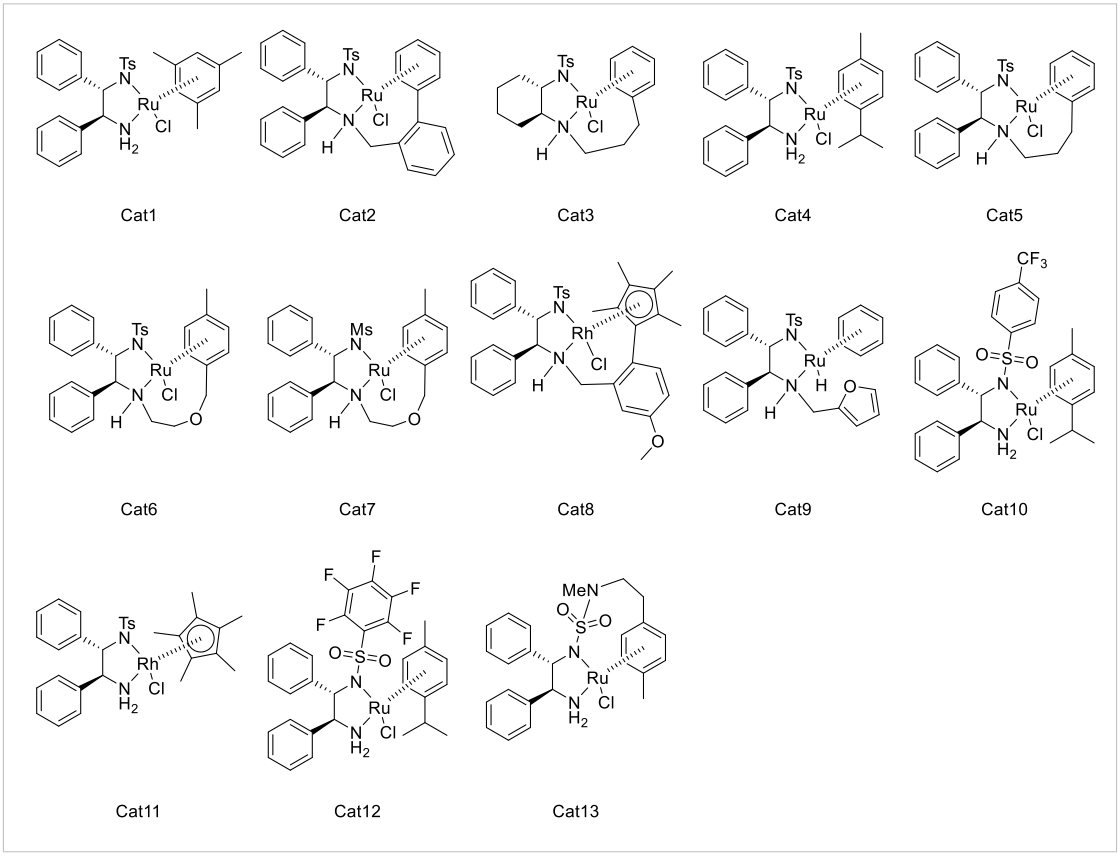
Model	Parameters
SVM	kernel='rbf'
KNN	k=2
DT	random_state = 42
RF	n_estimators = 750, criterion='mse', random_state = 42
AdaBoost	n_estimators = 100, random_state = 42
XGB	n_estimators = 20, random_state = 42

Note: The above settings are optimized with hyperparameters.

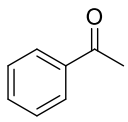
4. Dataset and Code

The dataset is in the file **dataset.xlsx**. The code is in the **SVM42.html, KNN42.html, DT42.html, RF42.html, AdaBoost42.html, XGB42.html (https://github.com/UchihaBen/ML_ATH)**.

4.1 Catalyst family



4.2 Substrate family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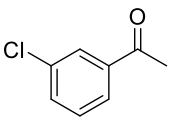
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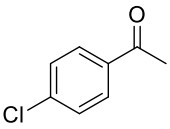
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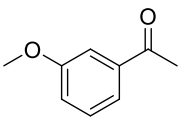
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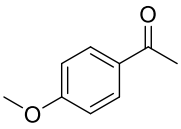
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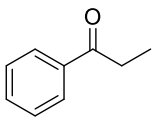
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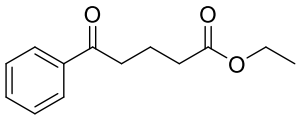
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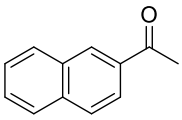
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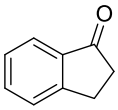
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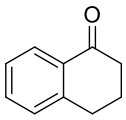
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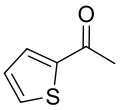
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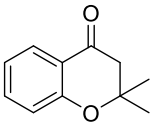
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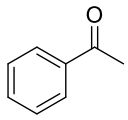
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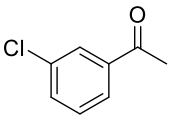
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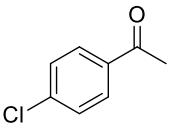
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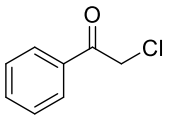
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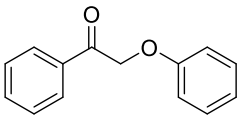
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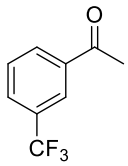
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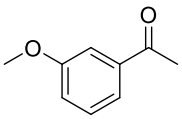
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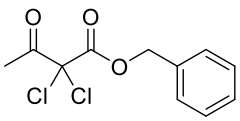
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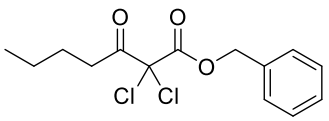
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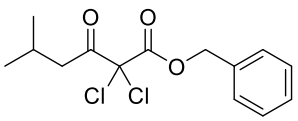
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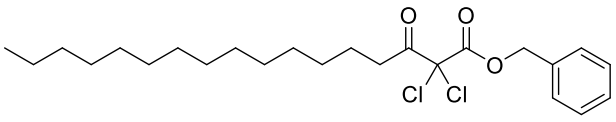
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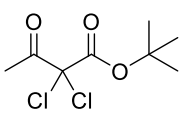
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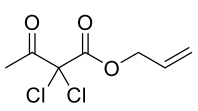

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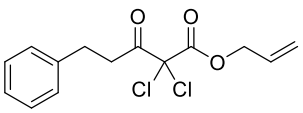

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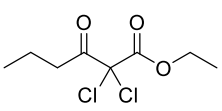

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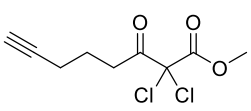

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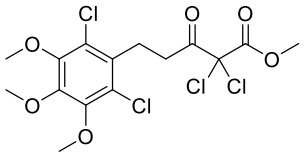

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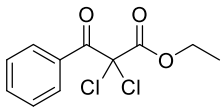

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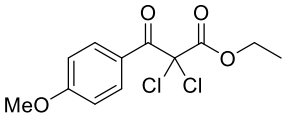

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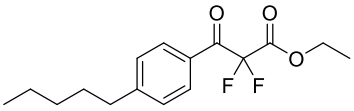

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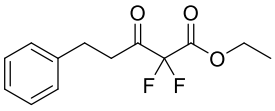

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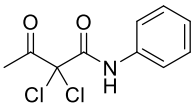

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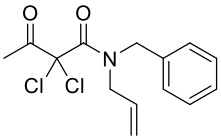

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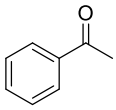

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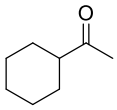

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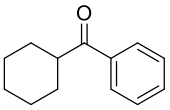

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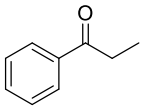

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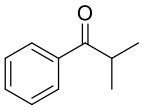

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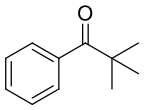

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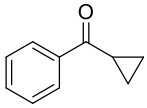

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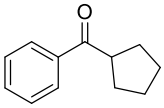

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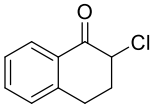

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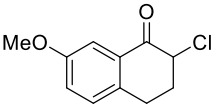

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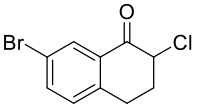

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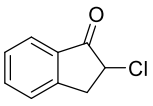

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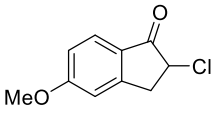

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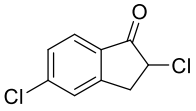

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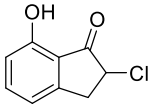

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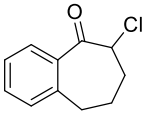

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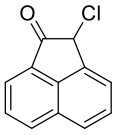

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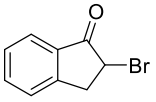

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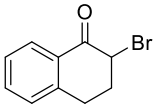

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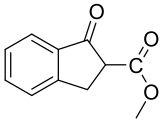

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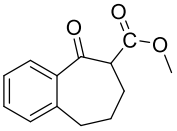

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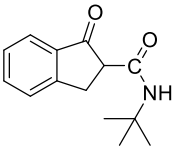

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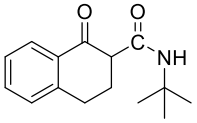

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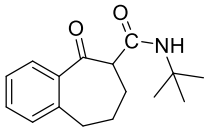

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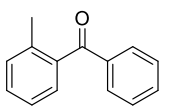

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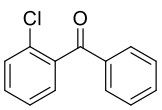

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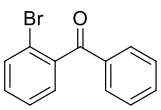

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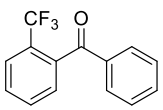

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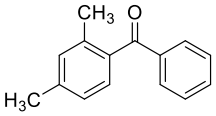

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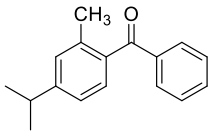

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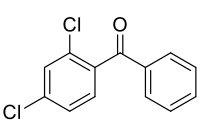

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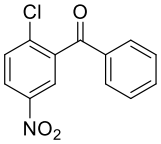

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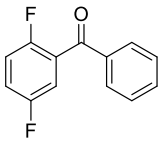

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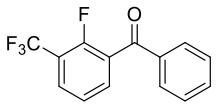

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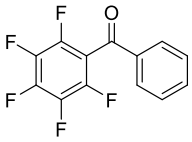

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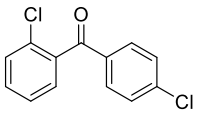

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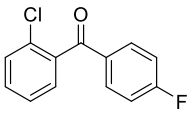

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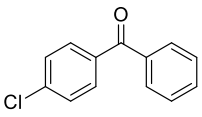

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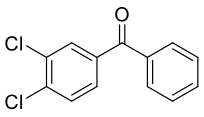

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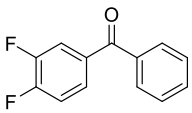

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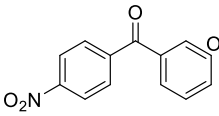

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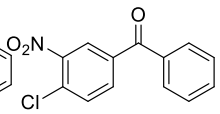

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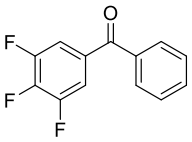

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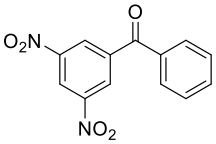

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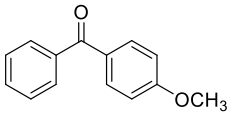

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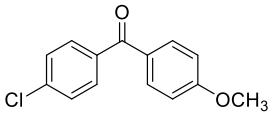

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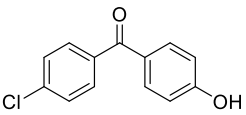

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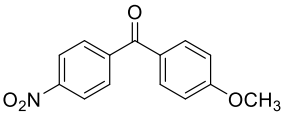

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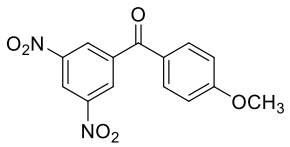

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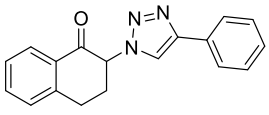

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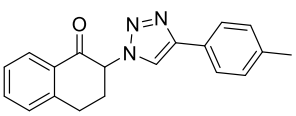

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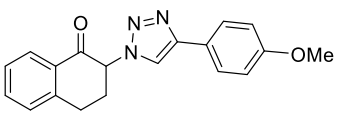

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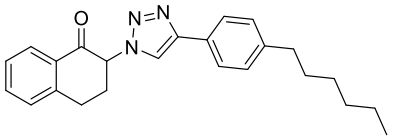

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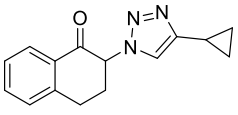

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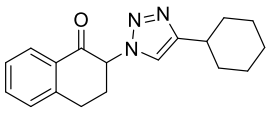

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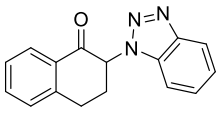

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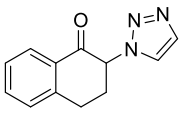

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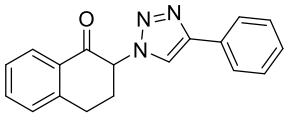

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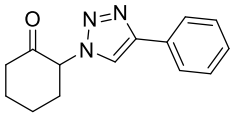

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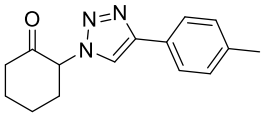

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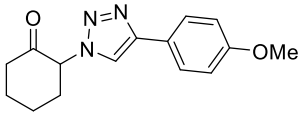
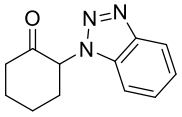


07_12



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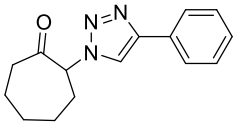

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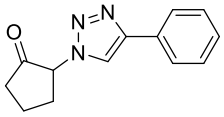

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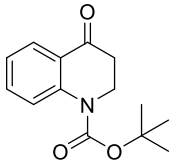

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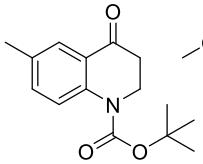

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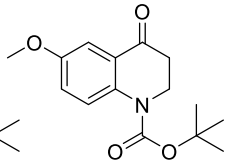

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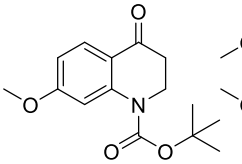

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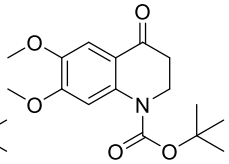

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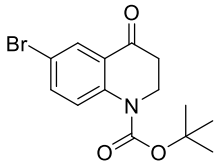

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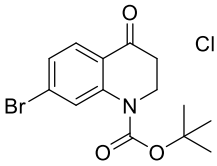

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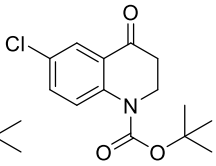

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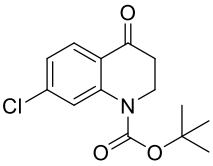

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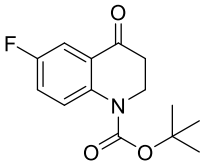

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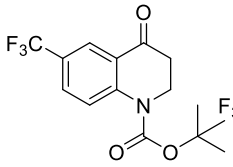

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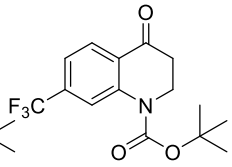

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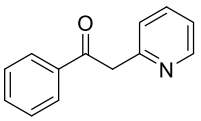

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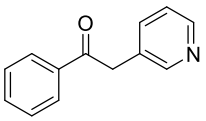

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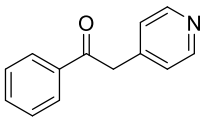

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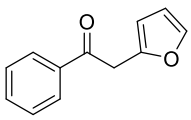

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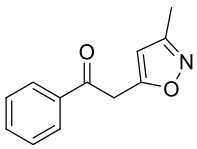

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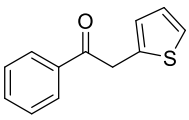

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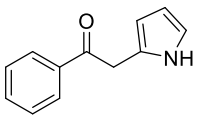

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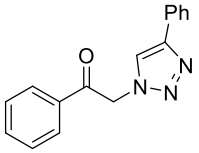

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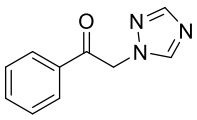

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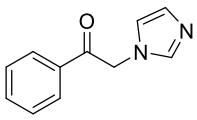

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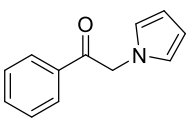

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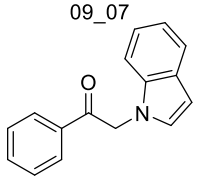

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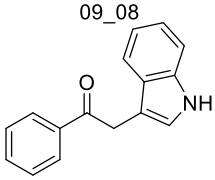

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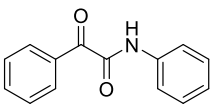
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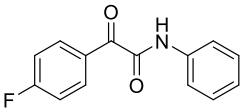
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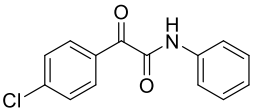
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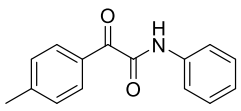
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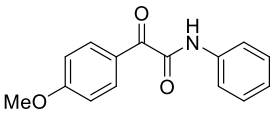
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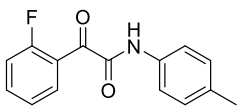
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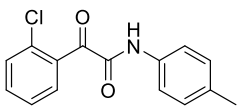
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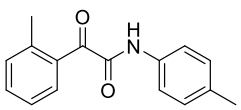
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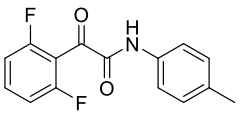
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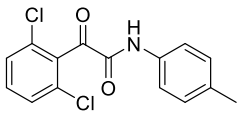
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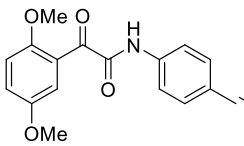
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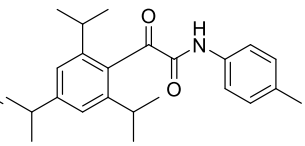
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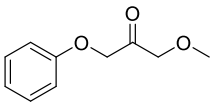
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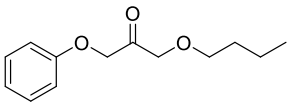
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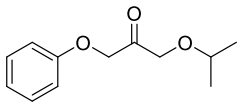
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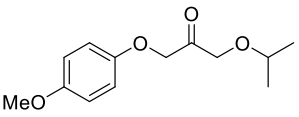
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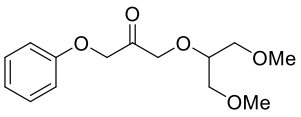
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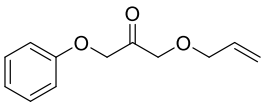
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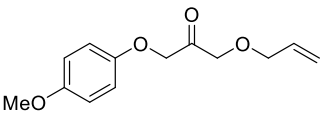
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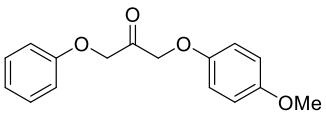
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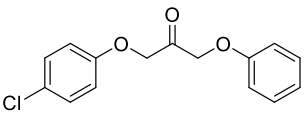
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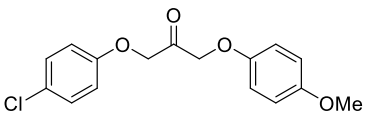
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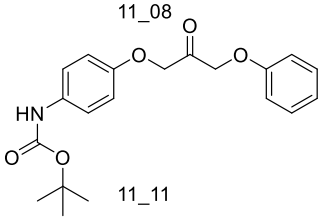
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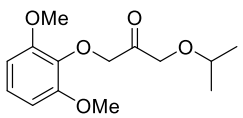
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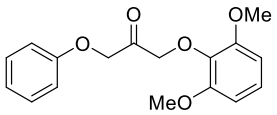
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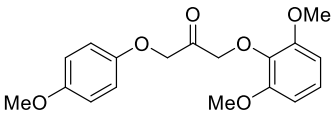
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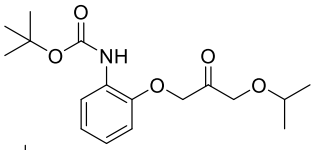
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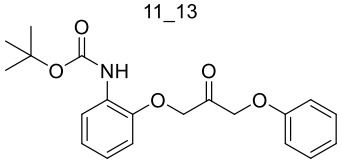
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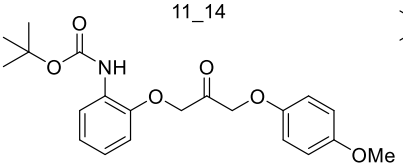
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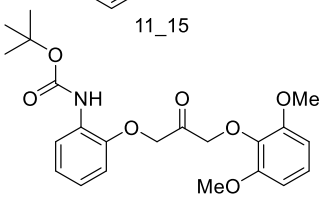
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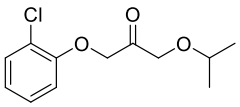
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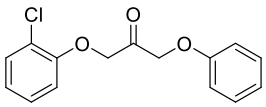
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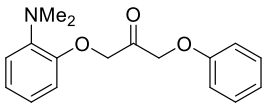
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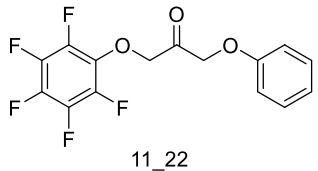

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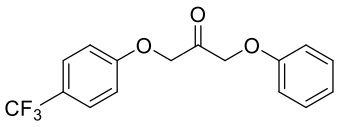

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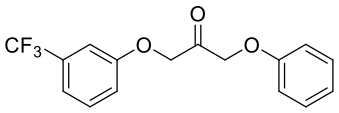

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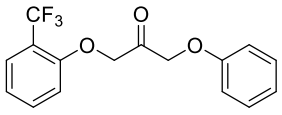

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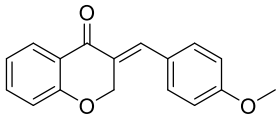

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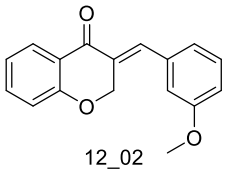

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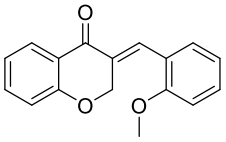

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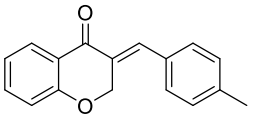

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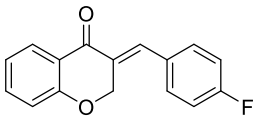

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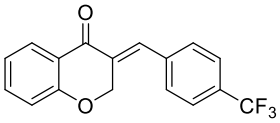

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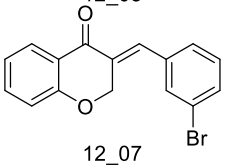

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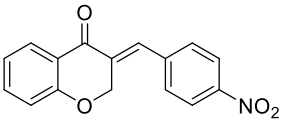

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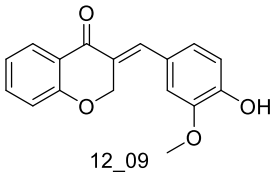

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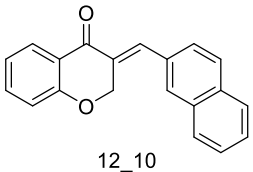

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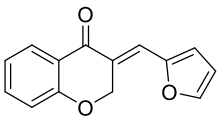

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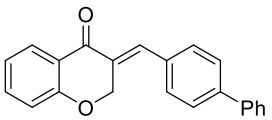

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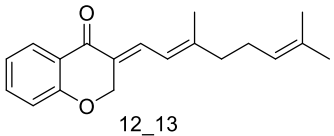

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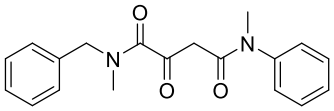

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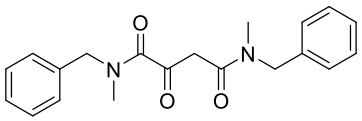

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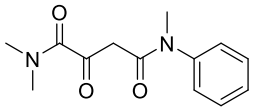

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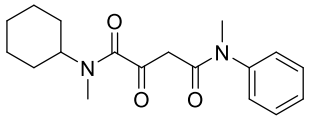

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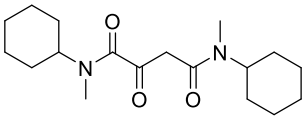

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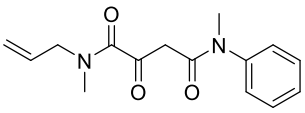

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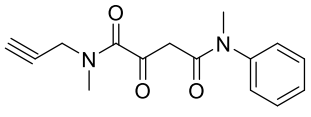

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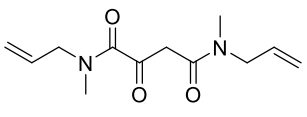

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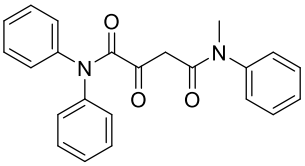

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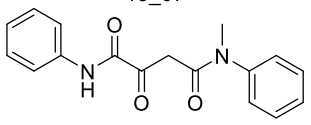

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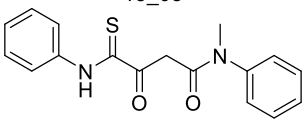

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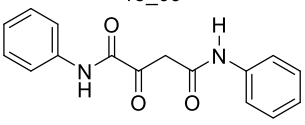

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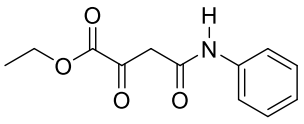

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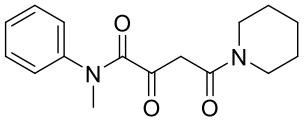

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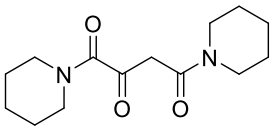

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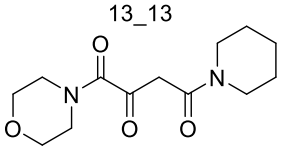

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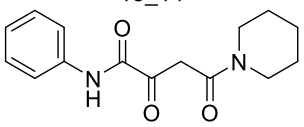

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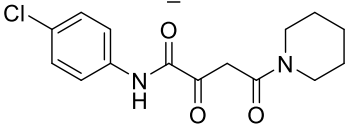

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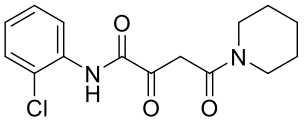

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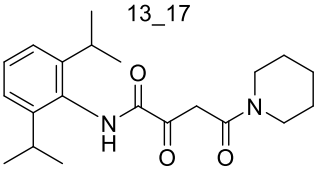

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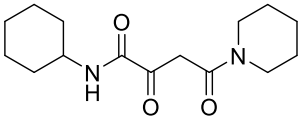

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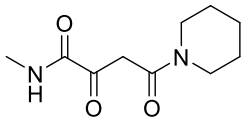

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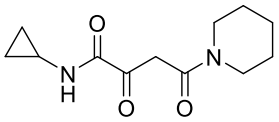

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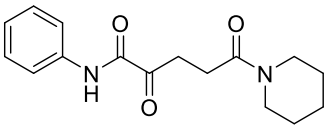

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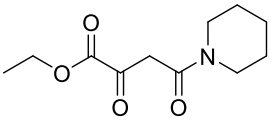

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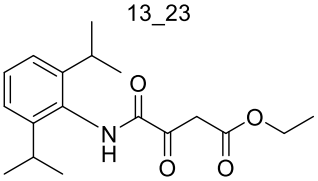

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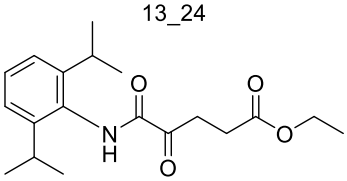

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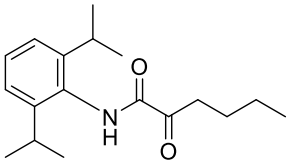

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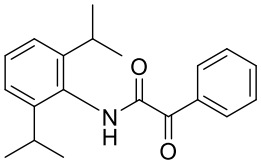

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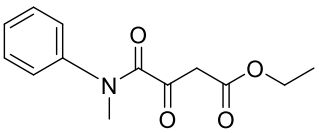

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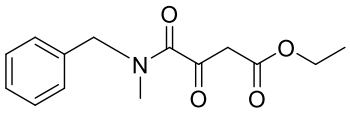

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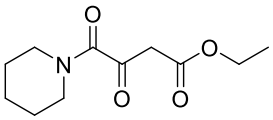

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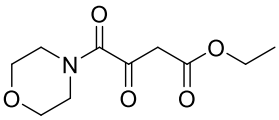

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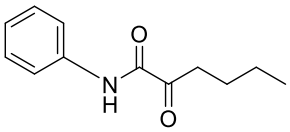

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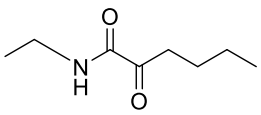

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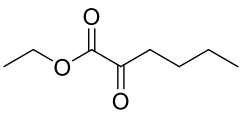

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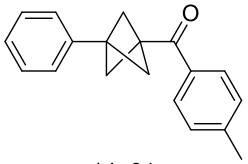

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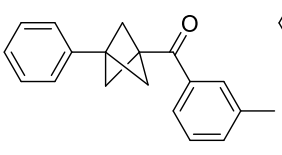

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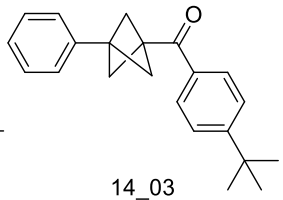

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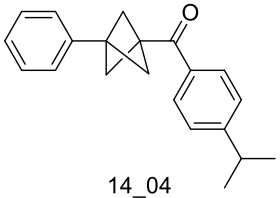

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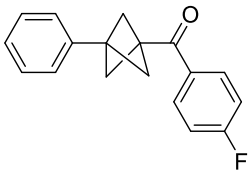

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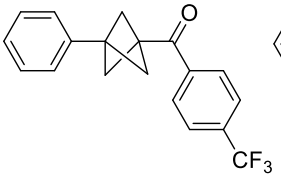
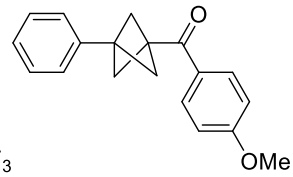


14_06



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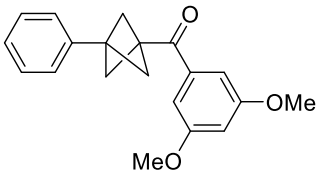

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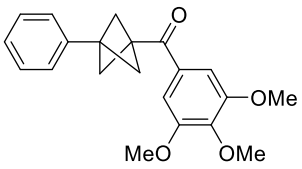

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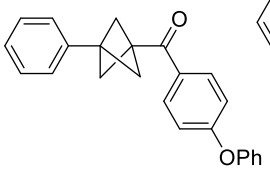

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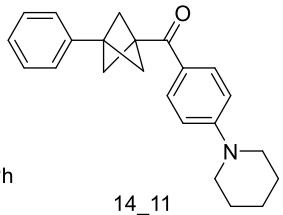

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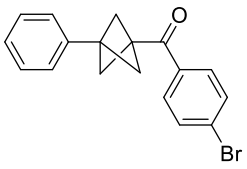

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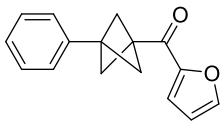

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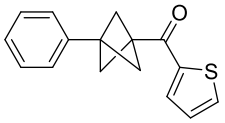

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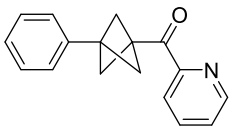

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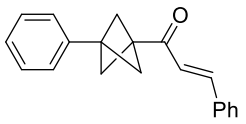

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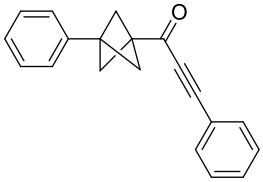

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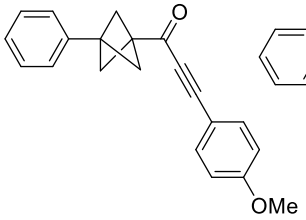

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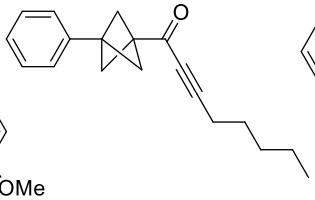

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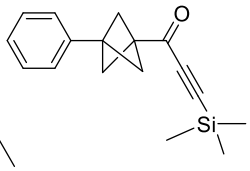

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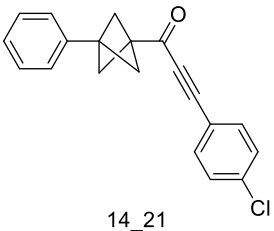

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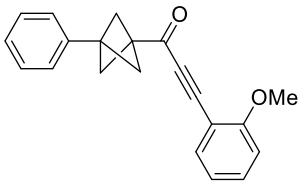

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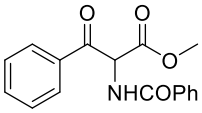

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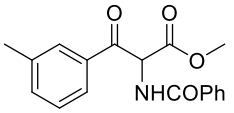

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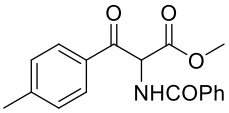

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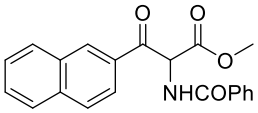

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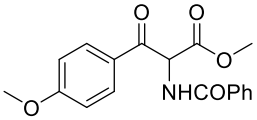

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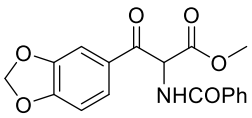

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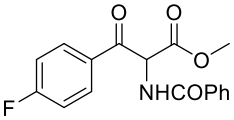

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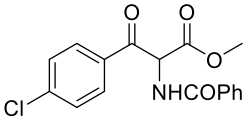

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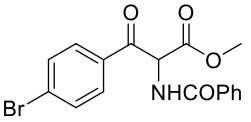

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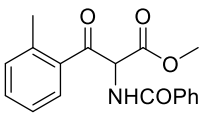

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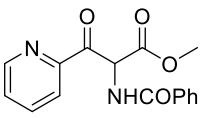

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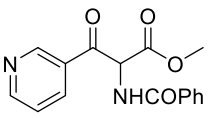

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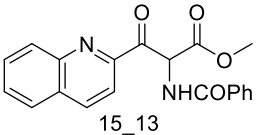

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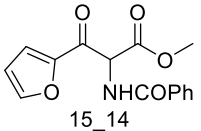

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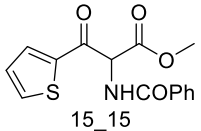

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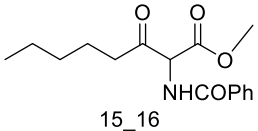

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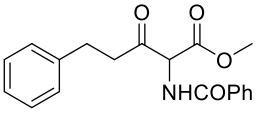

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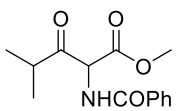

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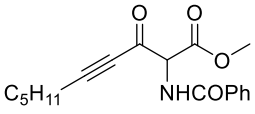

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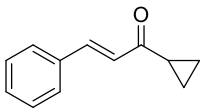
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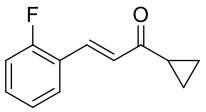
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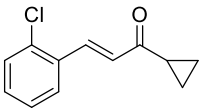
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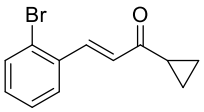
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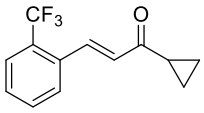
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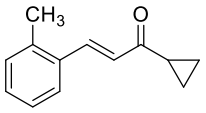
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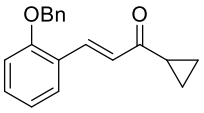
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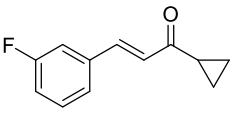
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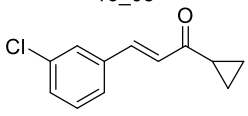
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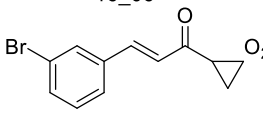
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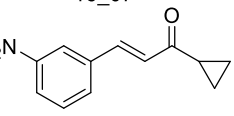
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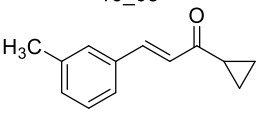
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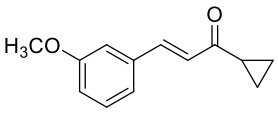
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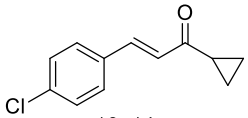
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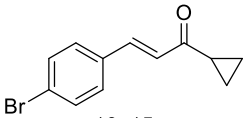
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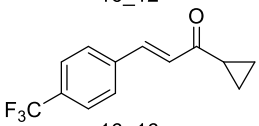
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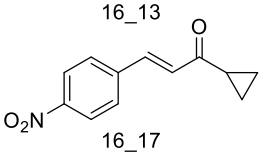
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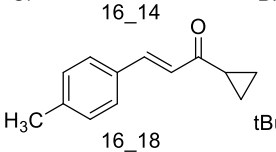
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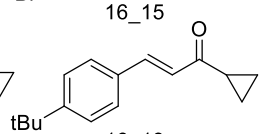
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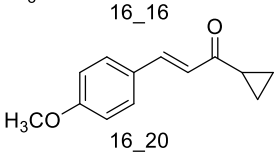
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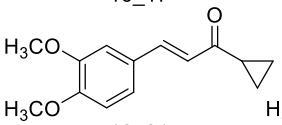
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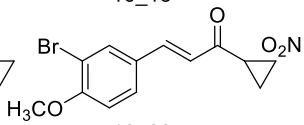
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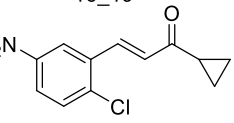
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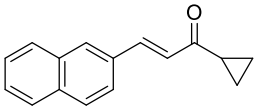
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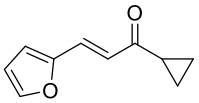
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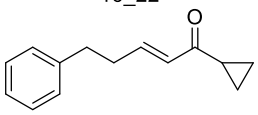
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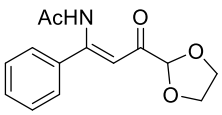
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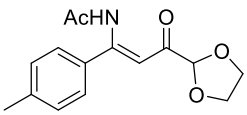
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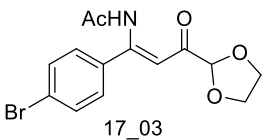
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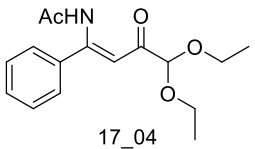
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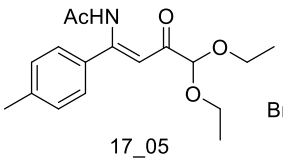
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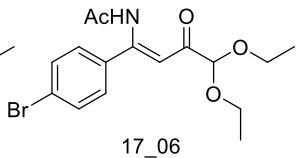
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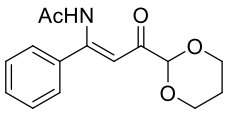
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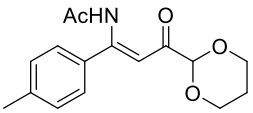
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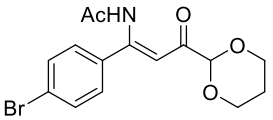
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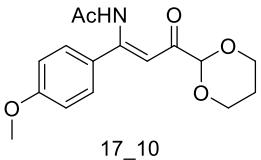
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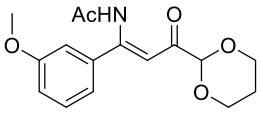
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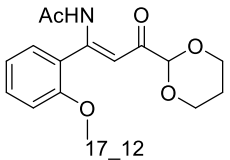
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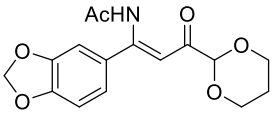
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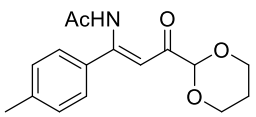
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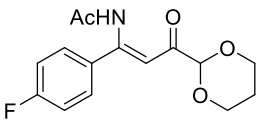
17_17



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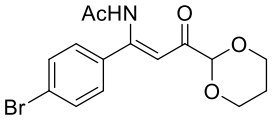

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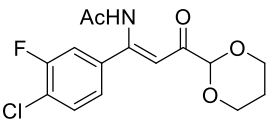

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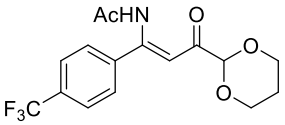

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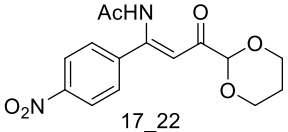

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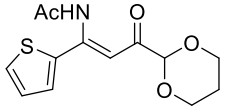

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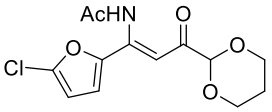

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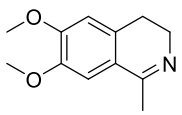

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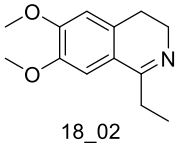

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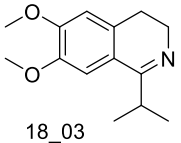

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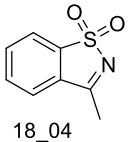

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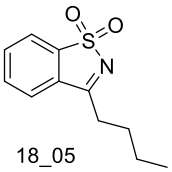

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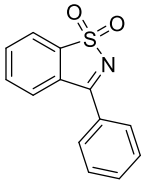

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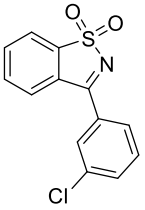

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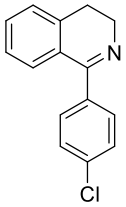

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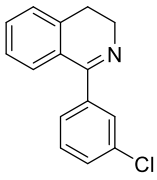

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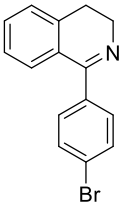

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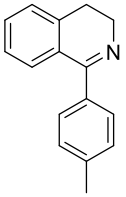

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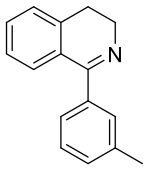

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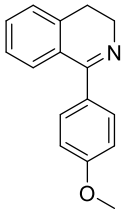

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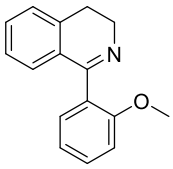

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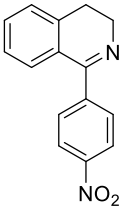

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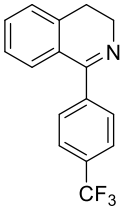

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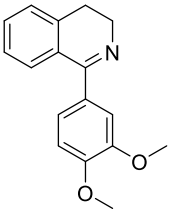

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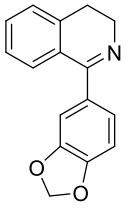

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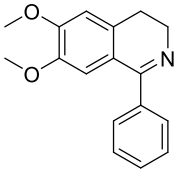

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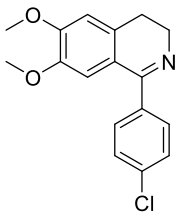

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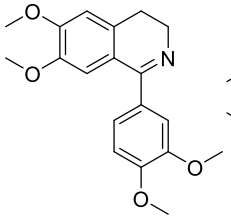

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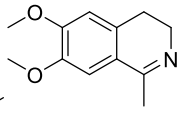

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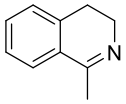

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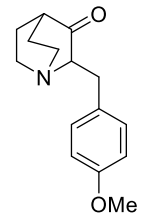

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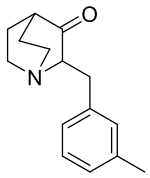

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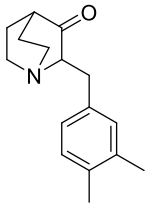

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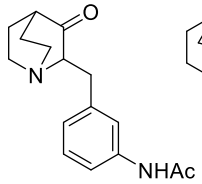

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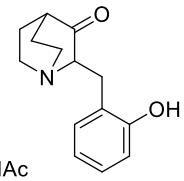

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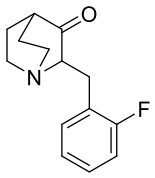

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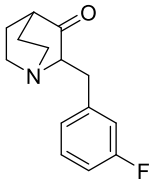

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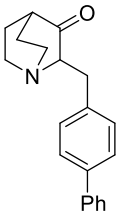

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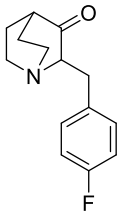

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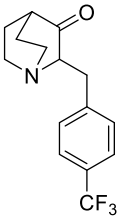

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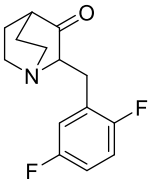

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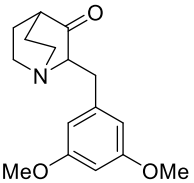

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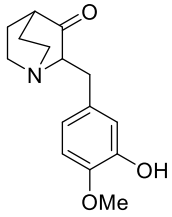

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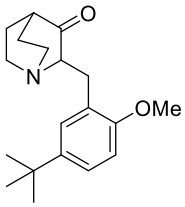

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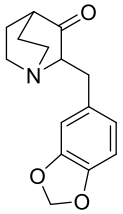
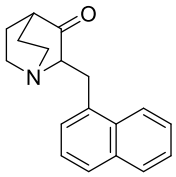
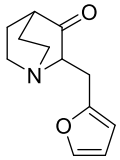


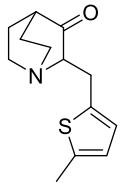
20_15



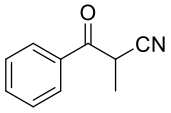
20_16



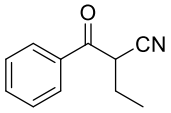
20_17



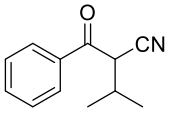
20_18



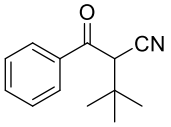
21_01



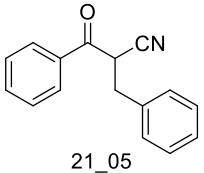
21_02



21_03



21_04



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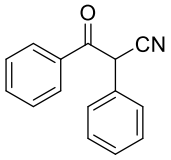
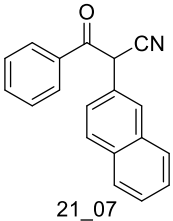
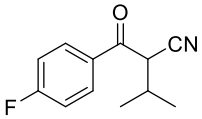


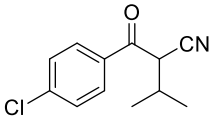
21_06



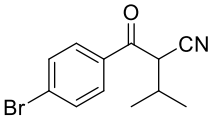
21_07



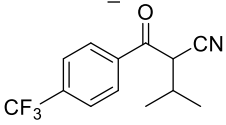
21_08



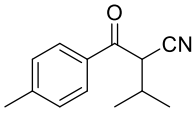
21_09



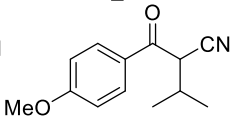
21_10



21_11



21_12



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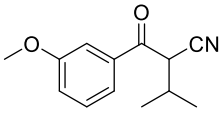
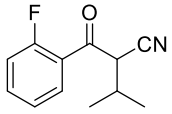
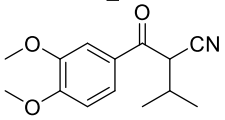


21_14



21_15



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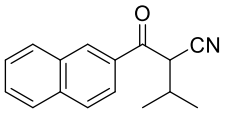

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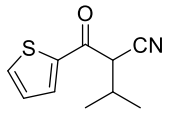

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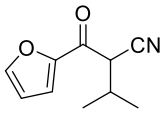
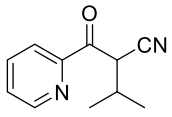
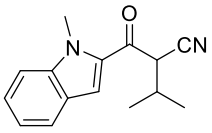


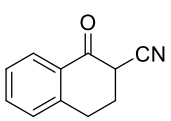
21_19



21_20



21_21

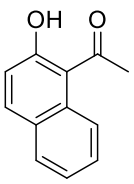


21_22

21_23

21_24

21_25



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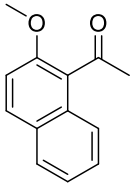
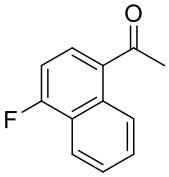
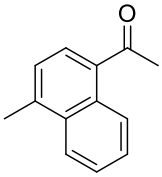


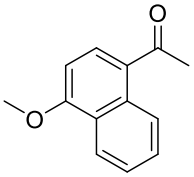
22_02



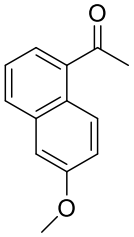
22_03



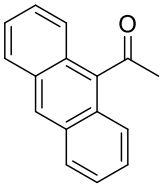
22_04



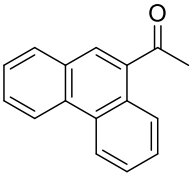
22_05



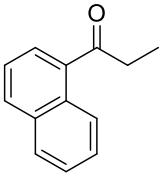
22_06



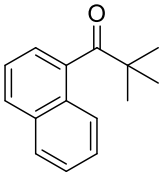
22_07



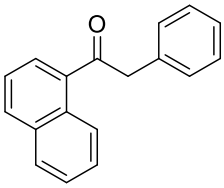
22_08



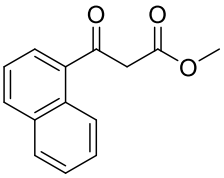
22_09



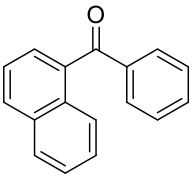
22_10



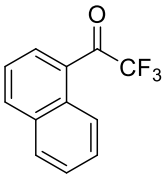
22_11



22_12



22_13



22_14

5. Reactions

Number	Temperature(K)	Hydrogen Source	Solvent	Sub.	Cat.	ee(%)
01_01Cat01301	301	FA/TEA=5:2	/	01_01	Cat01	98
01_02Cat01301	301	FA/TEA=5:2	/	01_02	Cat01	97
01_03Cat01301	301	FA/TEA=5:2	/	01_03	Cat01	95
01_04Cat01301	301	FA/TEA=5:2	/	01_04	Cat01	98
01_05Cat01301	301	FA/TEA=5:2	/	01_05	Cat01	97
01_06Cat01301	301	FA/TEA=5:2	/	01_06	Cat01	97
01_07Cat01301	301	FA/TEA=5:2	/	01_07	Cat01	95
01_08Cat01301	301	FA/TEA=5:2	/	01_08	Cat01	96
01_09Cat01301	301	FA/TEA=5:2	/	01_09	Cat01	99
01_10Cat01301	301	FA/TEA=5:2	/	01_10	Cat01	99
01_11Cat01301	301	FA/TEA=5:2	/	01_11	Cat01	98
01_12Cat01301	301	FA/TEA=5:2	/	01_12	Cat01	97
01_01Cat01333	333	FA/TEA=5:2	/	01_01	Cat01	96
01_10Cat01333	333	FA/TEA=5:2	/	01_10	Cat01	98
02_01Cat02313	313	FA/TEA=5:2	/	02_01	Cat02	95
02_02Cat02301	301	FA/TEA=5:2	/	02_02	Cat02	88
02_03Cat02313	313	FA/TEA=5:2	/	02_03	Cat02	92
02_04Cat02301	301	FA/TEA=5:2	/	02_04	Cat02	93
02_05Cat02301	301	FA/TEA=5:2	/	02_05	Cat02	89
02_02Cat03301	301	FA/TEA=5:2	/	02_02	Cat03	86
02_03Cat03301	301	FA/TEA=5:2	/	02_03	Cat03	86
02_04Cat03301	301	FA/TEA=5:2	/	02_04	Cat03	83
02_05Cat03301	301	FA/TEA=5:2	/	02_05	Cat03	85
02_06Cat03301	301	FA/TEA=5:2	/	02_06	Cat03	88
02_07Cat03301	301	FA/TEA=5:2	/	02_07	Cat03	83
03_01Cat04303	303	FA/TEA=5:2	DCM	03_01	Cat04	99
03_02Cat04303	303	FA/TEA=5:2	DCM	03_02	Cat04	99
03_03Cat04303	303	FA/TEA=5:2	DCM	03_03	Cat04	98
03_04Cat04303	303	FA/TEA=5:2	DCM	03_04	Cat04	99
03_05Cat04303	303	FA/TEA=5:2	DCM	03_05	Cat04	99
03_06Cat04303	303	FA/TEA=5:2	DCM	03_06	Cat04	99
03_07Cat04303	303	FA/TEA=5:2	DCM	03_07	Cat04	99
03_08Cat04303	303	FA/TEA=5:2	DCM	03_08	Cat04	99
03_09Cat04303	303	FA/TEA=5:2	DCM	03_09	Cat04	98.5
03_10Cat04303	303	FA/TEA=5:2	DCM	03_10	Cat04	98
03_11Cat04303	303	FA/TEA=5:2	DCM	03_11	Cat04	70
03_12Cat04303	303	FA/TEA=5:2	DCM	03_12	Cat04	71

03_13Cat04303	303	FA/TEA=5:2	DCM	03_13	Cat04	98
03_14Cat04303	303	FA/TEA=5:2	DCM	03_14	Cat04	98
03_15Cat04303	303	FA/TEA=5:2	DCM	03_15	Cat04	98.5
03_16Cat04303	303	FA/TEA=5:2	DCM	03_16	Cat04	98
04_01Cat05301	301	FA/TEA=5:2	/	04_01	Cat05	96
04_01Cat05313	313	FA/TEA=5:2	/	04_01	Cat05	96
04_01Cat05353	353	FA/TEA=5:2	/	04_01	Cat05	94
04_02Cat05287	287	FA/TEA=5:2	/	04_02	Cat05	72
04_02Cat05301	301	FA/TEA=5:2	/	04_02	Cat05	69
04_03Cat05313	313	FA/TEA=5:2	/	04_03	Cat05	94
04_04Cat05301	301	FA/TEA=5:2	/	04_04	Cat05	95
04_04Cat05313	313	FA/TEA=5:2	/	04_04	Cat05	95
04_05Cat05313	313	FA/TEA=5:2	/	04_05	Cat05	95
04_06Cat05313	313	FA/TEA=5:2	/	04_06	Cat05	77
04_07Cat05313	313	FA/TEA=5:2	/	04_07	Cat05	78
04_08Cat05313	313	FA/TEA=5:2	/	04_08	Cat05	78
05_01Cat06333	333	FA/TEA=5:2	EtOAc	05_01	Cat06	99.9
05_02Cat06333	333	FA/TEA=5:2	EtOAc	05_02	Cat06	99.9
05_03Cat06333	333	FA/TEA=5:2	EtOAc	05_03	Cat06	99.9
05_04Cat06333	333	FA/TEA=5:2	EtOAc	05_04	Cat06	99.8
05_05Cat06333	333	FA/TEA=5:2	EtOAc	05_05	Cat06	99.7
05_06Cat06333	333	FA/TEA=5:2	EtOAc	05_06	Cat06	99.5
05_07Cat06333	333	FA/TEA=5:2	EtOAc	05_07	Cat06	99.8
05_12Cat06303	303	FA/TEA=5:2	EtOAc	05_12	Cat06	99.6
05_14Cat06333	333	FA/TEA=5:2	EtOAc	05_14	Cat06	99.9
05_15Cat06333	333	FA/TEA=5:2	EtOAc	05_15	Cat06	99.9
05_08Cat06333	333	FA/TEA=5:2	EtOAc	05_08	Cat06	97
05_10Cat06313	313	FA/TEA=5:2	EtOAc	05_10	Cat06	99.5
05_11Cat06313	313	FA/TEA=5:2	EtOAc	05_11	Cat06	99.9
05_13Cat06333	333	FA/TEA=5:2	EtOAc	05_13	Cat06	98.9
05_16Cat06333	333	FA/TEA=5:2	EtOAc	05_16	Cat06	99.9
05_01Cat06333	333	FA/TEA=5:2	EtOAc	05_01	Cat06	99.9
06_01Cat06333	333	FA/TEA=5:2	/	06_01	Cat06	98
06_02Cat06313	313	FA/TEA=5:2	/	06_02	Cat06	98
06_03Cat06333	333	FA/TEA=5:2	/	06_03	Cat06	99
06_04Cat06333	333	FA/TEA=5:2	/	06_04	Cat06	99
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06_06Cat06333	333	FA/TEA=5:2	/	06_06	Cat06	98
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06_09Cat06283	283	FA/TEA=5:2	/	06_09	Cat06	91
06_10Cat06303	303	FA/TEA=5:2	/	06_10	Cat06	90
06_11Cat06333	333	FA/TEA=5:2	/	06_11	Cat06	99

06_12Cat06303	303	FA/TEA=5:2	/	06_12	Cat06	97
06_13Cat06313	313	FA/TEA=5:2	/	06_13	Cat06	97
06_15Cat06303	303	FA/TEA=5:2	/	06_15	Cat06	76
06_16Cat06303	303	FA/TEA=5:2	/	06_16	Cat06	77
06_17Cat06303	303	FA/TEA=5:2	/	06_17	Cat06	76
06_18Cat06303	303	FA/TEA=5:2	/	06_18	Cat06	93
06_19Cat06283	283	FA/TEA=5:2	/	06_19	Cat06	95
06_20Cat06303	303	FA/TEA=5:2	/	06_20	Cat06	99
06_24Cat06303	303	FA/TEA=5:2	/	06_24	Cat06	79
06_25Cat06303	303	FA/TEA=5:2	/	06_25	Cat06	99
07_01Cat05300	300	FA/TEA=5:2	DCM	07_01	Cat05	99.9
07_02Cat05300	300	FA/TEA=5:2	DCM	07_02	Cat05	99.2
07_03Cat05300	300	FA/TEA=5:2	DCM	07_03	Cat05	99.9
07_04Cat05300	300	FA/TEA=5:2	DCM	07_04	Cat05	94.3
07_05Cat05300	300	FA/TEA=5:2	DCM	07_05	Cat05	97.7
07_06Cat05300	300	FA/TEA=5:2	DCM	07_06	Cat05	87.6
07_07Cat05300	300	FA/TEA=5:2	DCM	07_07	Cat05	88.3
07_08Cat05300	300	FA/TEA=5:2	DCM	07_08	Cat05	99.5
07_09Cat05300	300	FA/TEA=5:2	DCM	07_09	Cat05	91.8
07_10Cat05300	300	FA/TEA=5:2	DCM	07_10	Cat05	95.4
07_11Cat05300	300	FA/TEA=5:2	DCM	07_11	Cat05	95.2
07_12Cat05300	300	FA/TEA=5:2	DCM	07_12	Cat05	89.6
07_13Cat05300	300	FA/TEA=5:2	DCM	07_13	Cat05	88.1
07_14Cat05300	300	FA/TEA=5:2	DCM	07_14	Cat05	95.5
07_15Cat05300	300	FA/TEA=5:2	DCM	07_15	Cat05	91.5
08_01Cat08303	303	FA/TEA=5:2	DCM	08_01	Cat08	99
08_02Cat08303	303	FA/TEA=5:2	DCM	08_02	Cat08	99
08_03Cat08303	303	FA/TEA=5:2	DCM	08_03	Cat08	99
08_04Cat08303	303	FA/TEA=5:2	DCM	08_04	Cat08	99
08_05Cat08303	303	FA/TEA=5:2	DCM	08_05	Cat08	97
08_06Cat08303	303	FA/TEA=5:2	DCM	08_06	Cat08	99
08_07Cat08303	303	FA/TEA=5:2	DCM	08_07	Cat08	99
08_08Cat08303	303	FA/TEA=5:2	DCM	08_08	Cat08	99
08_09Cat08303	303	FA/TEA=5:2	DCM	08_09	Cat08	99
08_10Cat08303	303	FA/TEA=5:2	DCM	08_10	Cat08	99
08_11Cat08303	303	FA/TEA=5:2	DCM	08_11	Cat08	99
08_12Cat08303	303	FA/TEA=5:2	DCM	08_12	Cat08	99
09_01Cat09298	298	FA/TEA=5:2	DCM	09_01	Cat09	98
09_02Cat09298	298	FA/TEA=5:2	DCM	09_02	Cat09	94
09_03Cat09298	298	FA/TEA=5:2	DCM	09_03	Cat09	95
09_04Cat09298	298	FA/TEA=5:2	DCM	09_04	Cat09	96
09_05Cat09298	298	FA/TEA=5:2	DCM	09_05	Cat09	94
09_06Cat09298	298	FA/TEA=5:2	DCM	09_06	Cat09	94

09_07Cat09298	298	FA/TEA=5:2	DCM	09_07	Cat09	92
09_08Cat09298	298	FA/TEA=5:2	DCM	09_08	Cat09	95
09_09Cat09298	298	FA/TEA=5:2	DCM	09_09	Cat09	96
09_10Cat09298	298	FA/TEA=5:2	DCM	09_10	Cat09	90
09_11Cat09298	298	FA/TEA=5:2	DCM	09_11	Cat09	95
09_12Cat09298	298	FA/TEA=5:2	DCM	09_12	Cat09	97
09_13Cat09298	298	FA/TEA=5:2	DCM	09_13	Cat09	96
10_01Cat05300	300	FA/TEA=5:2	DCM	10_01	Cat05	43.6
10_02Cat05300	300	FA/TEA=5:2	DCM	10_02	Cat05	52.04
10_03Cat05300	300	FA/TEA=5:2	DCM	10_03	Cat05	45.4
10_04Cat05300	300	FA/TEA=5:2	DCM	10_04	Cat05	24.6
10_05Cat05300	300	FA/TEA=5:2	DCM	10_05	Cat05	34.9
10_06Cat05300	300	FA/TEA=5:2	DCM	10_06	Cat05	95.3
10_07Cat05300	300	FA/TEA=5:2	DCM	10_07	Cat05	29.5
10_08Cat05300	300	FA/TEA=5:2	DCM	10_08	Cat05	79.1
10_10Cat05300	300	FA/TEA=5:2	DCM	10_10	Cat05	50
10_11Cat05300	300	FA/TEA=5:2	DCM	10_11	Cat05	77.9
10_12Cat05300	300	FA/TEA=5:2	DCM	10_12	Cat05	94.42
11_01Cat05298	298	FA/TEA=5:2	/	11_01	Cat05	30
11_02Cat05298	298	FA/TEA=5:2	/	11_02	Cat05	41
11_03Cat05298	298	FA/TEA=5:2	/	11_03	Cat05	39
11_04Cat05298	298	FA/TEA=5:2	/	11_04	Cat05	27
11_05Cat05298	298	FA/TEA=5:2	/	11_05	Cat05	46
11_06Cat05298	298	FA/TEA=5:2	/	11_06	Cat05	37
11_07Cat05298	298	FA/TEA=5:2	/	11_07	Cat05	31
11_08Cat05298	298	FA/TEA=5:2	/	11_08	Cat05	7
11_09Cat05298	298	FA/TEA=5:2	/	11_09	Cat05	6
11_10Cat05298	298	FA/TEA=5:2	/	11_10	Cat05	12
11_11Cat05298	298	FA/TEA=5:2	/	11_11	Cat05	0
11_12Cat05298	298	FA/TEA=5:2	/	11_12	Cat05	16
11_13Cat05298	298	FA/TEA=5:2	/	11_13	Cat05	42
11_14Cat05298	298	FA/TEA=5:2	/	11_14	Cat05	33
11_15Cat05298	298	FA/TEA=5:2	/	11_15	Cat05	68
11_16Cat05298	298	FA/TEA=5:2	/	11_16	Cat05	46
11_17Cat05298	298	FA/TEA=5:2	/	11_17	Cat05	65
11_18Cat05298	298	FA/TEA=5:2	/	11_18	Cat05	59
11_19Cat05298	298	FA/TEA=5:2	/	11_19	Cat05	21
11_21Cat05298	298	FA/TEA=5:2	/	11_21	Cat05	0
11_22Cat05298	298	FA/TEA=5:2	/	11_22	Cat05	27
11_23Cat05298	298	FA/TEA=5:2	/	11_23	Cat05	28
11_24Cat05298	298	FA/TEA=5:2	/	11_24	Cat05	28
11_25Cat05298	298	FA/TEA=5:2	/	11_25	Cat05	50
12_01Cat08323	323	FA/TEA=5:2	MeCN	12_01	Cat08	99

12_02Cat08323	323	FA/TEA=5:2	MeCN	12_02	Cat08	99
12_03Cat08323	323	FA/TEA=5:2	MeCN	12_03	Cat08	97
12_04Cat08323	323	FA/TEA=5:2	MeCN	12_04	Cat08	99
12_05Cat08323	323	FA/TEA=5:2	MeCN	12_05	Cat08	99
12_06Cat08323	323	FA/TEA=5:2	MeCN	12_06	Cat08	99
12_07Cat08323	323	FA/TEA=5:2	MeCN	12_07	Cat08	99
12_08Cat08323	323	FA/TEA=5:2	MeCN	12_08	Cat08	99
12_09Cat08323	323	FA/TEA=5:2	MeCN	12_09	Cat08	99
12_10Cat08323	323	FA/TEA=5:2	MeCN	12_10	Cat08	98
12_11Cat08323	323	FA/TEA=5:2	MeCN	12_11	Cat08	99
12_12Cat08323	323	FA/TEA=5:2	MeCN	12_12	Cat08	99
12_13Cat08323	323	FA/TEA=5:2	MeCN	12_13	Cat08	99
13_01Cat05298	298	FA/TEA=5:2	DCM	13_01	Cat05	77
13_02Cat05298	298	FA/TEA=5:2	DCM	13_02	Cat05	94
13_04Cat05298	298	FA/TEA=5:2	DCM	13_04	Cat05	79
13_06Cat05298	298	FA/TEA=5:2	DCM	13_06	Cat05	77
13_07Cat05298	298	FA/TEA=5:2	DCM	13_07	Cat05	88
13_08Cat05298	298	FA/TEA=5:2	DCM	13_08	Cat05	94
13_10Cat05298	298	FA/TEA=5:2	DCM	13_10	Cat05	91
13_11Cat05298	298	FA/TEA=5:2	DCM	13_11	Cat05	89
13_12Cat05298	298	FA/TEA=5:2	DCM	13_12	Cat05	95
13_14Cat05298	298	FA/TEA=5:2	DCM	13_14	Cat05	89
13_15Cat05298	298	FA/TEA=5:2	DCM	13_15	Cat05	92
13_16Cat05298	298	FA/TEA=5:2	DCM	13_16	Cat05	92
13_17Cat05298	298	FA/TEA=5:2	DCM	13_17	Cat05	97
13_18Cat05298	298	FA/TEA=5:2	DCM	13_18	Cat05	97
13_19Cat05298	298	FA/TEA=5:2	DCM	13_19	Cat05	98
13_20Cat05298	298	FA/TEA=5:2	DCM	13_20	Cat05	99
13_21Cat05298	298	FA/TEA=5:2	DCM	13_21	Cat05	97
13_22Cat05298	298	FA/TEA=5:2	DCM	13_22	Cat05	95
13_23Cat05298	298	FA/TEA=5:2	DCM	13_23	Cat05	98
13_24Cat05298	298	FA/TEA=5:2	DCM	13_24	Cat05	94
13_25Cat05298	298	FA/TEA=5:2	DCM	13_25	Cat05	98
13_26Cat05298	298	FA/TEA=5:2	DCM	13_26	Cat05	98
13_28Cat05298	298	FA/TEA=5:2	DCM	13_28	Cat05	97
13_31Cat05298	298	FA/TEA=5:2	DCM	13_31	Cat05	90
13_32Cat05298	298	FA/TEA=5:2	DCM	13_32	Cat05	94
13_33Cat05298	298	FA/TEA=5:2	DCM	13_33	Cat05	92
13_34Cat05298	298	FA/TEA=5:2	DCM	13_34	Cat05	93
13_35Cat05298	298	FA/TEA=5:2	DCM	13_35	Cat05	90
13_36Cat05298	298	FA/TEA=5:2	DCM	13_36	Cat05	80
14_01Cat05298	298	FA/TEA=5:2	DCM	14_01	Cat05	99
14_02Cat05298	298	FA/TEA=5:2	DCM	14_02	Cat05	93

14_03Cat05298	298	FA/TEA=5:2	DCM	14_03	Cat05	99
14_04Cat05298	298	FA/TEA=5:2	DCM	14_04	Cat05	99
14_05Cat05298	298	FA/TEA=5:2	DCM	14_05	Cat05	84
14_06Cat05298	298	FA/TEA=5:2	DCM	14_06	Cat05	70
14_07Cat05298	298	FA/TEA=5:2	DCM	14_07	Cat05	98
14_08Cat05298	298	FA/TEA=5:2	DCM	14_08	Cat05	90
14_09Cat05298	298	FA/TEA=5:2	DCM	14_09	Cat05	88
14_10Cat05298	298	FA/TEA=5:2	DCM	14_10	Cat05	85
14_11Cat05298	298	FA/TEA=5:2	DCM	14_11	Cat05	97
14_12Cat05298	298	FA/TEA=5:2	DCM	14_12	Cat05	81
14_13Cat05298	298	FA/TEA=5:2	DCM	14_13	Cat05	99
14_14Cat05298	298	FA/TEA=5:2	DCM	14_14	Cat05	99
14_15Cat05298	298	FA/TEA=5:2	DCM	14_15	Cat05	91
14_16Cat05298	298	FA/TEA=5:2	DCM	14_16	Cat05	41
14_17Cat05298	298	FA/TEA=5:2	DCM	14_17	Cat05	95
14_18Cat05298	298	FA/TEA=5:2	DCM	14_18	Cat05	95
14_19Cat05298	298	FA/TEA=5:2	DCM	14_19	Cat05	97
14_20Cat05298	298	FA/TEA=5:2	DCM	14_20	Cat05	99
14_21Cat05298	298	FA/TEA=5:2	DCM	14_21	Cat05	96
14_22Cat05298	298	FA/TEA=5:2	DCM	14_22	Cat05	97
15_01Cat08273	273	FA/TEA=5:2	DCM	15_01	Cat08	99
15_02Cat08273	273	FA/TEA=5:2	DCM	15_02	Cat08	99
15_03Cat08273	273	FA/TEA=5:2	DCM	15_03	Cat08	99
15_04Cat08273	273	FA/TEA=5:2	DCM	15_04	Cat08	99
15_05Cat08273	273	FA/TEA=5:2	DCM	15_05	Cat08	99
15_06Cat08273	273	FA/TEA=5:2	DCM	15_06	Cat08	99
15_07Cat08273	273	FA/TEA=5:2	DCM	15_07	Cat08	99
15_08Cat08273	273	FA/TEA=5:2	DCM	15_08	Cat08	99
15_09Cat08273	273	FA/TEA=5:2	DCM	15_09	Cat08	99
15_10Cat08273	273	FA/TEA=5:2	DCM	15_10	Cat08	99
15_11Cat08273	273	FA/TEA=5:2	DCM	15_11	Cat08	99
15_12Cat08273	273	FA/TEA=5:2	DCM	15_12	Cat08	99
15_13Cat08273	273	FA/TEA=5:2	DCM	15_13	Cat08	99
15_14Cat08273	273	FA/TEA=5:2	DCM	15_14	Cat08	99
15_16Cat08273	273	FA/TEA=5:2	DCM	15_16	Cat08	99
15_17Cat08273	273	FA/TEA=5:2	DCM	15_17	Cat08	99
15_18Cat08273	273	FA/TEA=5:2	DCM	15_18	Cat08	99
15_19Cat08273	273	FA/TEA=5:2	DCM	15_19	Cat08	99
15_01_02Cat14273	273	FA/TEA=5:2	DCM	15_01_02	Cat14	28
15_01_03Cat06273	273	FA/TEA=5:2	DCM	15_01_03	Cat06	25
15_01_04Cat05273	273	FA/TEA=5:2	DCM	15_01_04	Cat05	36
16_01Cat10313	313	FA/TEA=5:2	/	16_01	Cat10	81
16_02Cat10313	313	FA/TEA=5:2	/	16_02	Cat10	77

16_03Cat10313	313	FA/TEA=5:2	/	16_03	Cat10	85
16_04Cat10313	313	FA/TEA=5:2	/	16_04	Cat10	83
16_05Cat10313	313	FA/TEA=5:2	/	16_05	Cat10	86
16_06Cat10313	313	FA/TEA=5:2	/	16_06	Cat10	81
16_07Cat10313	313	FA/TEA=5:2	/	16_07	Cat10	70
16_08Cat10313	313	FA/TEA=5:2	/	16_08	Cat10	85
16_09Cat10313	313	FA/TEA=5:2	/	16_09	Cat10	85
16_10Cat10313	313	FA/TEA=5:2	/	16_10	Cat10	84
16_11Cat10313	313	FA/TEA=5:2	/	16_11	Cat10	85
16_12Cat10313	313	FA/TEA=5:2	/	16_12	Cat10	74
16_13Cat10313	313	FA/TEA=5:2	/	16_13	Cat10	81
16_14Cat10313	313	FA/TEA=5:2	/	16_14	Cat10	79
16_15Cat10313	313	FA/TEA=5:2	/	16_15	Cat10	79
16_16Cat10313	313	FA/TEA=5:2	/	16_16	Cat10	82
16_17Cat10313	313	FA/TEA=5:2	/	16_17	Cat10	78
16_18Cat10313	313	FA/TEA=5:2	/	16_18	Cat10	78
16_19Cat10313	313	FA/TEA=5:2	/	16_19	Cat10	82
16_20Cat10313	313	FA/TEA=5:2	/	16_20	Cat10	73
16_21Cat10313	313	FA/TEA=5:2	/	16_21	Cat10	74
16_22Cat10313	313	FA/TEA=5:2	/	16_22	Cat10	78
16_23Cat10313	313	FA/TEA=5:2	/	16_23	Cat10	87
16_24Cat10313	313	FA/TEA=5:2	/	16_24	Cat10	82
16_25Cat10313	313	FA/TEA=5:2	/	16_25	Cat10	85
16_26Cat10313	313	FA/TEA=5:2	/	16_26	Cat10	83
16_01_02Cat06313	313	FA/TEA=5:2	/	16_01_02	Cat06	60
16_01_03Cat04313	313	FA/TEA=5:2	/	16_01_03	Cat04	61
16_01_04Cat04313	313	FA/TEA=5:2	/	16_01_04	Cat04	79
16_01_05Cat04313	313	FA/TEA=5:2	/	16_01_05	Cat04	77
16_01_06Cat04313	313	FA/TEA=5:2	/	16_01_06	Cat04	79
16_01_07Cat04313	313	FA/TEA=5:2	/	16_01_07	Cat04	77
16_01_08Cat04313	313	FA/TEA=5:2	/	16_01_08	Cat04	73
17_01Cat08298	298	FA/TEA=5:2	DCM	17_01	Cat08	77
17_02Cat08298	298	FA/TEA=5:2	DCM	17_02	Cat08	76
17_04Cat08298	298	FA/TEA=5:2	DCM	17_04	Cat08	96
17_05Cat08298	298	FA/TEA=5:2	DCM	17_05	Cat08	97
17_06Cat08298	298	FA/TEA=5:2	DCM	17_06	Cat08	97
17_07Cat08298	298	FA/TEA=5:2	DCM	17_07	Cat08	99
17_08Cat08298	298	FA/TEA=5:2	DCM	17_08	Cat08	96
17_09Cat08298	298	FA/TEA=5:2	DCM	17_09	Cat08	97
17_10Cat08298	298	FA/TEA=5:2	DCM	17_10	Cat08	98
17_11Cat08298	298	FA/TEA=5:2	DCM	17_11	Cat08	99
17_12Cat08298	298	FA/TEA=5:2	DCM	17_12	Cat08	99
17_13Cat08298	298	FA/TEA=5:2	DCM	17_13	Cat08	98

17_14Cat08298	298	FA/TEA=5:2	DCM	17_14	Cat08	96
17_15Cat08298	298	FA/TEA=5:2	DCM	17_15	Cat08	98
17_16Cat08298	298	FA/TEA=5:2	DCM	17_16	Cat08	95
17_17Cat08298	298	FA/TEA=5:2	DCM	17_17	Cat08	98
17_18Cat08298	298	FA/TEA=5:2	DCM	17_18	Cat08	96
17_19Cat08298	298	FA/TEA=5:2	DCM	17_19	Cat08	97
17_20Cat08298	298	FA/TEA=5:2	DCM	17_20	Cat08	94
17_21Cat08298	298	FA/TEA=5:2	DCM	17_21	Cat08	94
17_22Cat08298	298	FA/TEA=5:2	DCM	17_22	Cat08	88
17_23Cat08298	298	FA/TEA=5:2	DCM	17_23	Cat08	99
17_24Cat08298	298	FA/TEA=5:2	DCM	17_24	Cat08	98
18_01Cat11293	293	FA/TEA=5:2	DCM	18_01	Cat11	90
18_02Cat11293	293	FA/TEA=5:2	DCM	18_02	Cat11	83
18_03Cat11293	293	FA/TEA=5:2	DCM	18_03	Cat11	89
18_04Cat11293	293	FA/TEA=5:2	DCM	18_04	Cat11	68
18_05Cat11293	293	FA/TEA=5:2	DCM	18_05	Cat11	67
18_07Cat11293	293	FA/TEA=5:2	DCM	18_07	Cat11	81
19_01Cat09298	298	FA/TEA=5:2	DCM	19_01	Cat09	88
19_02Cat09298	298	FA/TEA=5:2	DCM	19_02	Cat09	91
19_03Cat09298	298	FA/TEA=5:2	DCM	19_03	Cat09	93
19_04Cat09298	298	FA/TEA=5:2	DCM	19_04	Cat09	90
19_05Cat09298	298	FA/TEA=5:2	DCM	19_05	Cat09	92
19_06Cat09298	298	FA/TEA=5:2	DCM	19_06	Cat09	92
19_07Cat09298	298	FA/TEA=5:2	DCM	19_07	Cat09	90
19_08Cat09298	298	FA/TEA=5:2	DCM	19_08	Cat09	89
19_09Cat09298	298	FA/TEA=5:2	DCM	19_09	Cat09	91
19_10Cat09298	298	FA/TEA=5:2	DCM	19_10	Cat09	91
19_11Cat09298	298	FA/TEA=5:2	DCM	19_11	Cat09	90
19_12Cat09298	298	FA/TEA=5:2	DCM	19_12	Cat09	92
19_13Cat09298	298	FA/TEA=5:2	DCM	19_13	Cat09	97
19_14Cat09298	298	FA/TEA=5:2	DCM	19_14	Cat09	93
19_15Cat09298	298	FA/TEA=5:2	DCM	19_15	Cat09	81
19_16Cat09298	298	FA/TEA=5:2	DCM	19_16	Cat09	80
20_01Cat12323	323	HCOONH4	IPA/DCM	20_01	Cat12	99
20_02Cat12323	323	HCOONH4	IPA/DCM	20_02	Cat12	99
20_03Cat12323	323	HCOONH4	IPA/DCM	20_03	Cat12	99
20_04Cat12323	323	HCOONH4	IPA/DCM	20_04	Cat12	99
20_05Cat12323	323	HCOONH4	IPA/DCM	20_05	Cat12	99
20_06Cat12323	323	HCOONH4	IPA/DCM	20_06	Cat12	97
20_07Cat12323	323	HCOONH4	IPA/DCM	20_07	Cat12	98
20_08Cat12323	323	HCOONH4	IPA/DCM	20_08	Cat12	99
20_09Cat12323	323	HCOONH4	IPA/DCM	20_09	Cat12	99
20_10Cat12323	323	HCOONH4	IPA/DCM	20_10	Cat12	98

20_11Cat12323	323	HCOONH4	IPA/DCM	20_11	Cat12	95
20_12Cat12323	323	HCOONH4	IPA/DCM	20_12	Cat12	99
20_13Cat12323	323	HCOONH4	IPA/DCM	20_13	Cat12	99
20_14Cat12323	323	HCOONH4	IPA/DCM	20_14	Cat12	99
20_15Cat12323	323	HCOONH4	IPA/DCM	20_15	Cat12	98
20_16Cat12323	323	HCOONH4	IPA/DCM	20_16	Cat12	99
20_17Cat12323	323	HCOONH4	IPA/DCM	20_17	Cat12	97
20_18Cat12323	323	HCOONH4	IPA/DCM	20_18	Cat12	99
21_01Cat08298	298	FA/TEA=5:2	toluene	21_01	Cat08	99
21_02Cat08298	298	FA/TEA=5:2	toluene	21_02	Cat08	99
21_03Cat08298	298	FA/TEA=5:2	toluene	21_03	Cat08	99
21_04Cat08298	298	FA/TEA=5:2	toluene	21_04	Cat08	99
21_05Cat08298	298	FA/TEA=5:2	toluene	21_05	Cat08	98
21_06Cat08298	298	FA/TEA=5:2	toluene	21_06	Cat08	99
21_07Cat08298	298	FA/TEA=5:2	toluene	21_07	Cat08	99
21_08Cat08298	298	FA/TEA=5:2	toluene	21_08	Cat08	99
21_09Cat08298	298	FA/TEA=5:2	toluene	21_09	Cat08	99
21_10Cat08298	298	FA/TEA=5:2	toluene	21_10	Cat08	99
21_11Cat08298	298	FA/TEA=5:2	toluene	21_11	Cat08	99
21_12Cat08298	298	FA/TEA=5:2	toluene	21_12	Cat08	99
21_13Cat08298	298	FA/TEA=5:2	toluene	21_13	Cat08	99
21_14Cat08298	298	FA/TEA=5:2	toluene	21_14	Cat08	99
21_15Cat08298	298	FA/TEA=5:2	toluene	21_15	Cat08	99
21_16Cat08298	298	FA/TEA=5:2	toluene	21_16	Cat08	99
21_17Cat08298	298	FA/TEA=5:2	toluene	21_17	Cat08	99
21_18Cat08298	298	FA/TEA=5:2	toluene	21_18	Cat08	99
21_19Cat08298	298	FA/TEA=5:2	toluene	21_19	Cat08	99
21_20Cat08298	298	FA/TEA=5:2	toluene	21_20	Cat08	99
21_21Cat08298	298	FA/TEA=5:2	toluene	21_21	Cat08	99
21_22Cat08298	298	FA/TEA=5:2	toluene	21_22	Cat08	99
21_23Cat08298	298	FA/TEA=5:2	toluene	21_23	Cat08	99
21_24Cat08298	298	FA/TEA=5:2	toluene	21_24	Cat08	99
21_01_02Cat08298	298	FA/TEA=5:2	toluene	21_01_02	Cat08	77
22_01Cat13313	313	FA/TEA=5:2	/	22_01	Cat13	97.2
22_01Cat13333	333	FA/TEA=5:2	/	22_01	Cat13	95
22_03Cat13313	313	FA/TEA=5:2	/	22_03	Cat13	97.8
22_03Cat13333	333	FA/TEA=5:2	/	22_03	Cat13	97.2
22_04Cat13333	333	FA/TEA=5:2	/	22_04	Cat13	98.4
22_05Cat13333	333	FA/TEA=5:2	/	22_05	Cat13	92.3
22_06Cat13333	333	FA/TEA=5:2	/	22_06	Cat13	97.6
22_08Cat13313	313	FA/TEA=5:2	/	22_08	Cat13	99.9
22_08Cat13333	333	FA/TEA=5:2	/	22_08	Cat13	98.1
22_09Cat13333	333	FA/TEA=5:2	/	22_09	Cat13	97.8

22_10Cat13333	333	FA/TEA=5:2	/	22_10	Cat13	97
22_11Cat13313	313	FA/TEA=5:2	/	22_11	Cat13	99
22_11Cat13333	333	FA/TEA=5:2	/	22_11	Cat13	98.5
22_12Cat13313	313	FA/TEA=5:2	/	22_12	Cat13	98.2
22_12Cat13333	333	FA/TEA=5:2	/	22_12	Cat13	98.1

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