

***Representative Chemotypes  
from the CMLD-BU Library  
Collection***

# Natural Product Analog Libraries

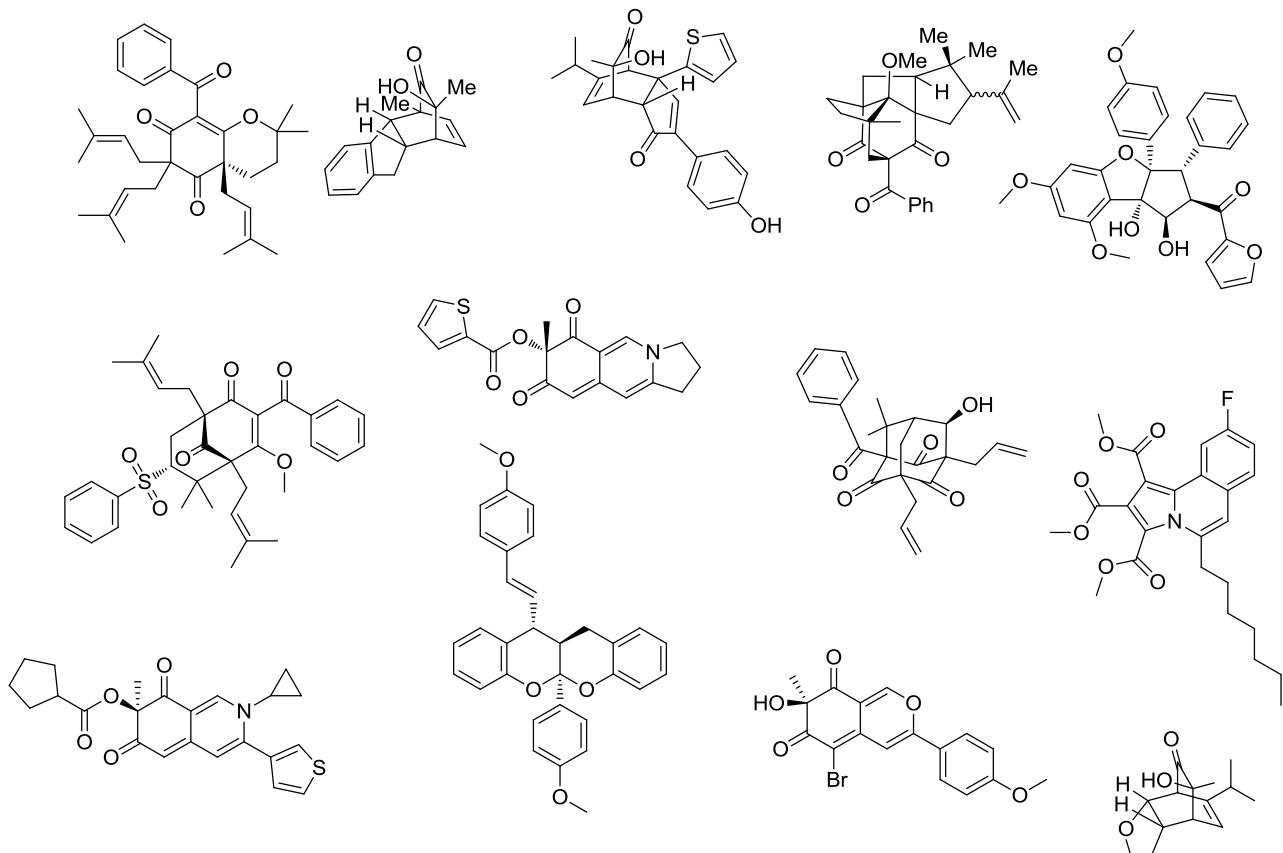
## Selected References:

- Mitasev, B.; Porco, J.A., Jr. *Org. Lett.*, **2009**, *11*, 2285-2288.
- Dong, S.; Hamel, E.; Bai, R.; Covell, D.G.; Beutler, J.A.; Porco, J.A., Jr. *Angew. Chem. Int. Ed.*, **2009**, *48*, 1494-1497.
- Su, S.; Porco, J.A., Jr. *J. Am. Chem. Soc.*, **2007**, *129*, 7744-7745.
- Achard, M.; Beeler, A.B.; Porco, J.A., Jr. *ACS Comb. Sci.*, **2012**, *14*, 236-244.
- Kulkarni, B.A.; Roth, G.P.; Lobkovsky, E.; Porco, J.A., Jr. *J. Comb. Chem.* **2002**, *4*, 56-72.

## Calculated Physical Properties:

- Average MW = 451.3
- Average LogP = 4.1
- Average TPSA = 82.5
- Avg. chiral centers = 3.0
- Average # rings = 4.4

## Representative Structures:

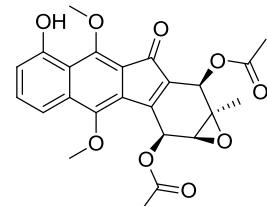
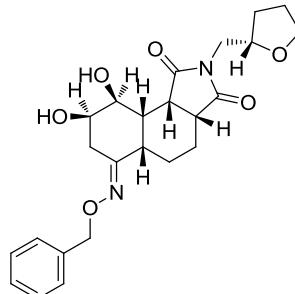
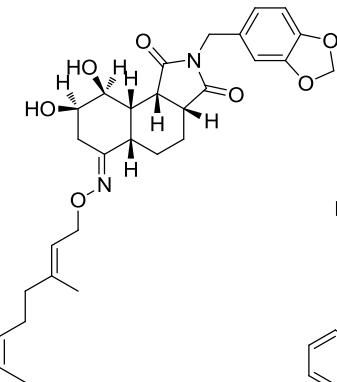
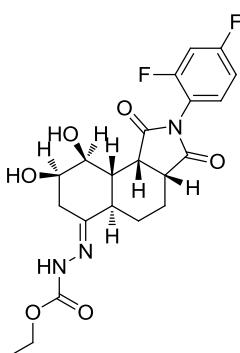


# Epoxyquinols

## Selected References:

- Lei, X.; Zaarur, N.; Sherman, M.Y.; Porco, J.A., Jr. *J. Org. Chem.*, **2005**, *70*, 6474-6483.
- Li, C.; Porco, J.A., Jr. *J. Org. Chem.*, **2005**, *70*, 6053-6065.

## Representative Structures:



## Calculated Physical Properties:

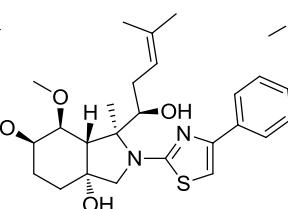
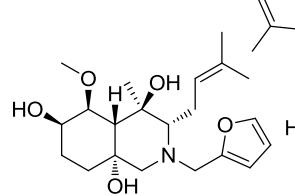
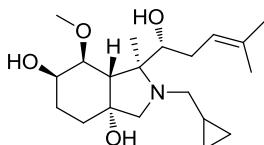
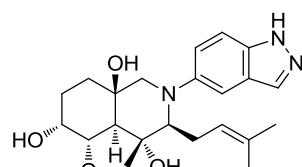
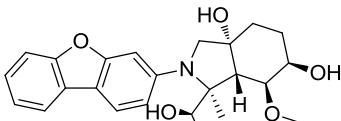
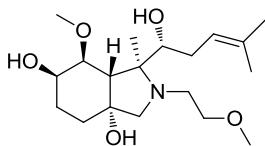
- Average MW = 468.4
- Average LogP = 1.7
- Average TPSA = 115.7
- Avg. chiral centers = 6.1
- Average # rings = 4.5

# Fumagillool-derived alkaloids

## Selected References:

- Balthaser, B.R.; Maloney, M.C.; Beeler, A.B.; Porco, J.A., Jr.; Snyder, J.K. *Nat. Chem.*, **2011**, *3*, 969-973.

## Representative Structures:



## Calculated Physical Properties:

- Average MW = 418.8
- Average LogP = 2.2
- Average TPSA = 84.7
- Avg. chiral centers = 6.1
- Average # rings = 3.2

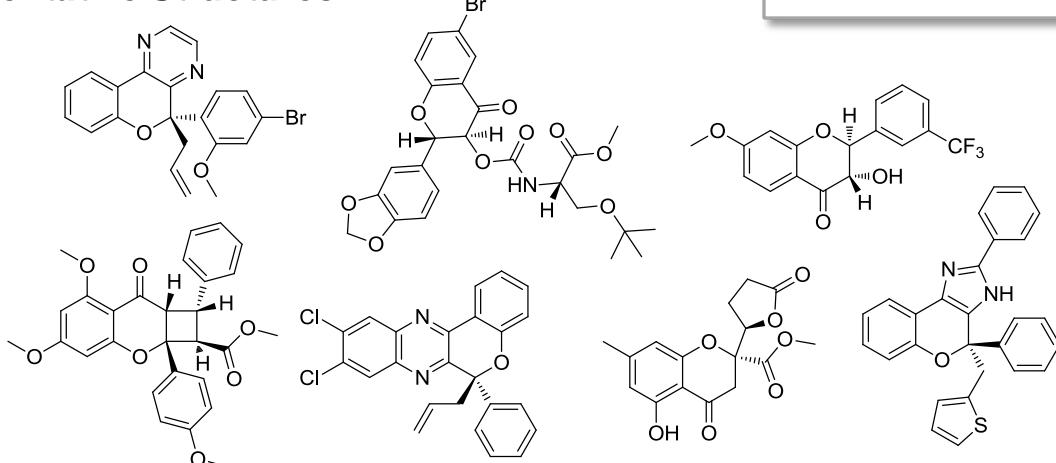
# Chromanone derivatives



## Selected References:

- Marie, J.-C.; Xiong, Y.; Min, G.K.; Yeager, A.R.; Taniguchi, T.; Berova, N.; Schaus, S.E.; Porco, J.A., Jr. *J. Org. Chem.*, **2010**, 75, 4584-4590.
- Quin, T.; Johnson, R.P.; Porco, J.A., Jr. *J. Am. Chem. Soc.*, **2011**, 133, 1714-1717.

## Representative Structures:



## Calculated Physical Properties:

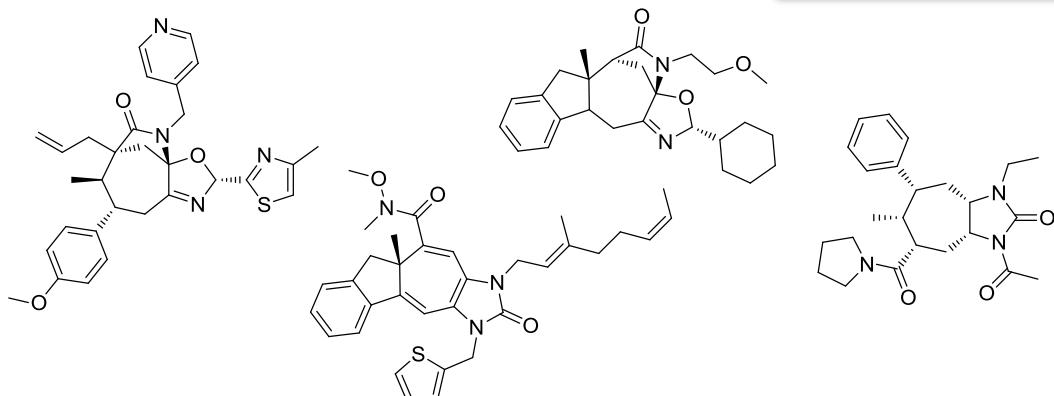
- Average MW = 438.7
- Average LogP = 4.4
- Average TPSA = 80.2
- Avg. chiral centers = 2.1
- Average # rings = 4.1

# Cycloheptyl heterocycles

## Selected References:

- Goodell, J.R.; Leng, B.; Snyder, T.K.; Beeler, A.B.; Porco, J.A., Jr. *Synthesis*, **2010**, 13, 2254-2270.
- Goodell, J.R.; McMullen, J.P.; Zaborenko, N.; Maloney, J.R.; Ho, C.-X.; Jensen, K.; Porco, J.A., Jr.; Beeler, A.B. *J. Org. Chem.*, **2009**, 74, 6169-6180.

## Representative Structures:



## Calculated Physical Properties:

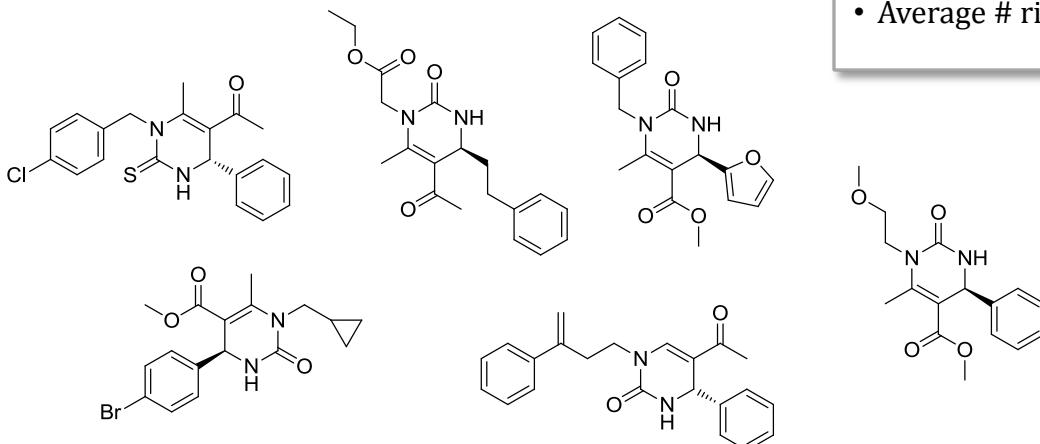
- Average MW = 533.5
- Average LogP = 5.3
- Average TPSA = 61.4
- Avg. chiral centers = 3.8
- Average # rings = 5.7

# Dihydropyrimidinones

## Selected References:

- Lou, S.; Dai, P.; Schaus, S.E. *J. Org. Chem.*, 2007, 72, 9998-10008.
- Lou, S.; Taoka, B.M.; Ting, A.; Schaus, S.E. *J. Am. Chem. Soc.*, 2005, 127, 11256-11257.

## Representative Structures:



## Calculated Physical Properties:

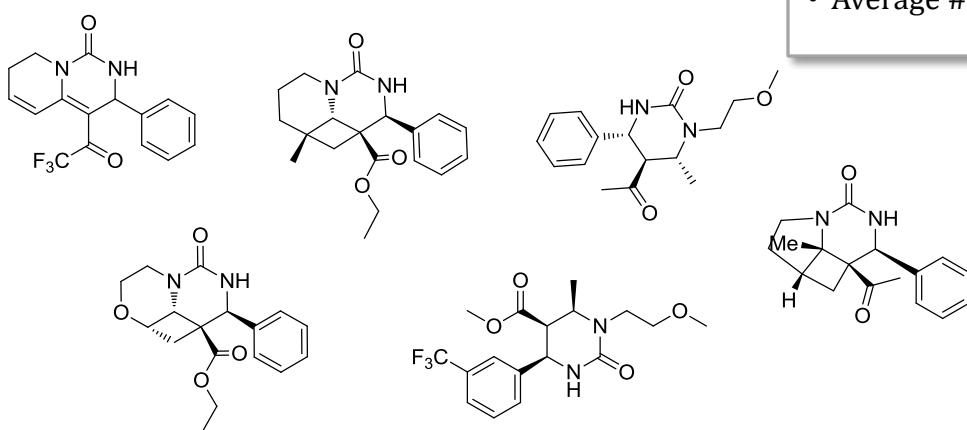
- Average MW = 364.8
- Average LogP = 3.1
- Average TPSA = 51.9
- Avg. chiral centers = 1.0
- Average # rings = 2.5

# Pyrimidinone derivatives

## Selected References:

- Brown, L.E.; Dai, P.; Porco, J.A., Jr.; Schaus, S.E. *Org. Lett.*, 2011, 13, 4228-4231.
- Lou, S.; Dai, P.; Schaus, S.E. *J. Org. Chem.*, 2007, 72, 9998-10008.

## Representative Structures:



## Calculated Physical Properties:

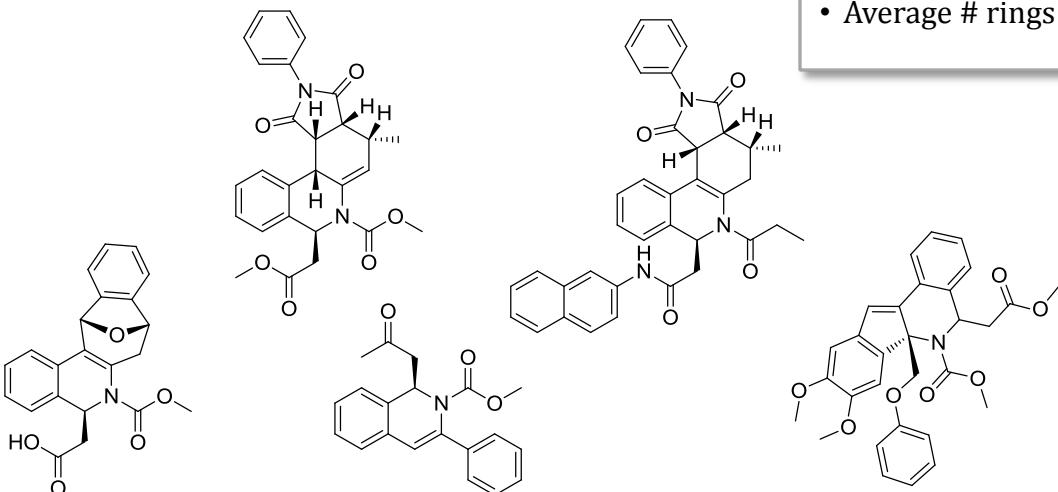
- Average MW = 320.2
- Average LogP = 2.1
- Average TPSA = 55.1
- Avg. chiral centers = 2.2
- Average # rings = 3.0

# Dihydroisoquinolines

## Selected References:

- Su, S.; Porco, J.A. Jr., *Org. Lett.*, **2007**, 9, 4983-4986.

## Representative Structures:



## Calculated Physical Properties:

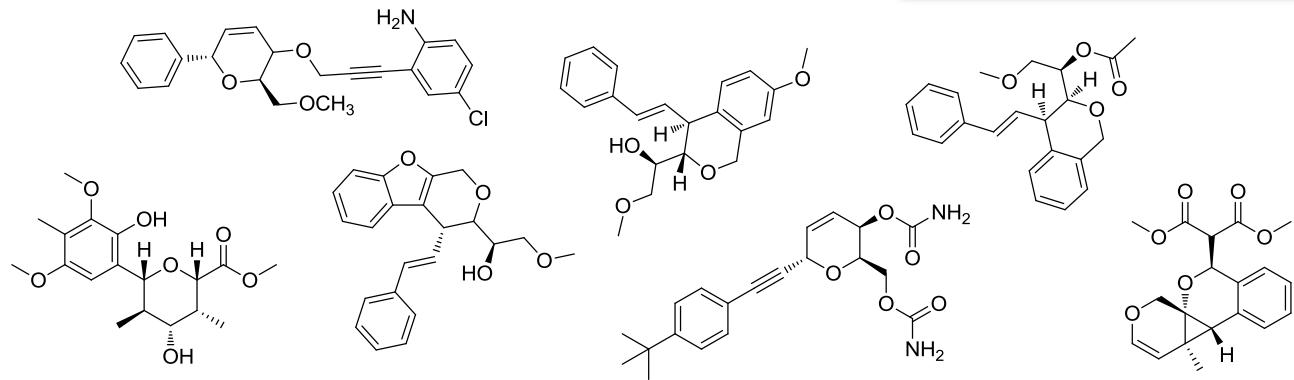
- Average MW = 387.5
- Average LogP = 3.3
- Average TPSA = 70.9
- Avg. chiral centers = 1.8
- Average # rings = 3.2

# Complex Pyrans

## Selected References:

- Medeiros, M.R.; Narayan, R.S.; McDougal, N.T.; Schaus, S.E.; Porco, J.A., Jr. *Org. Lett.*, **2010**, 12, 3222-3225.
- Yeager, A.R.; Min, G.K.; Porco, J.A., Jr.; Schaus, S.E. *Org. Lett.*, **2006**, 8, 5065-5068.

## Representative Structures:



## Calculated Physical Properties:

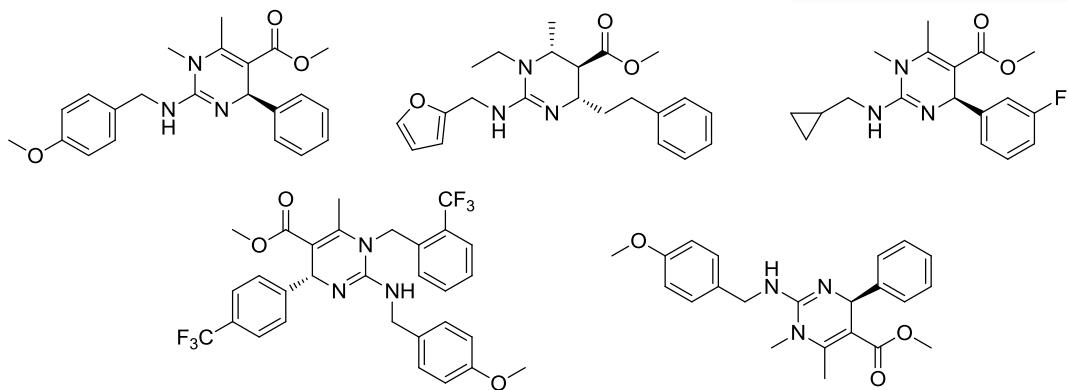
- Average MW = 367.6
- Average LogP = 3.8
- Average TPSA = 59.3
- Avg. chiral centers = 3.0
- Average # rings = 2.8

# Guanidines

## Selected References:

- Brown, L.E.; Cheng, K.C.; Wei, W.; Yuan, P.; Dai, P.; Trilles, R.; Ni, F.; Yuan, J.; MacArthur, R.; Guha, R.; Johnson, R.L.; Su, X.; Dominguez, M.M.; Snyder, J.K.; Beeler, A.B.; Schaus, S.E.; Inglese, J.; Porco, J.A., Jr. *Proc. Nat. Acad. Sci. USA*, **2011**, *108*, 6775-6780.

## Representative Structures:



## Calculated Physical Properties:

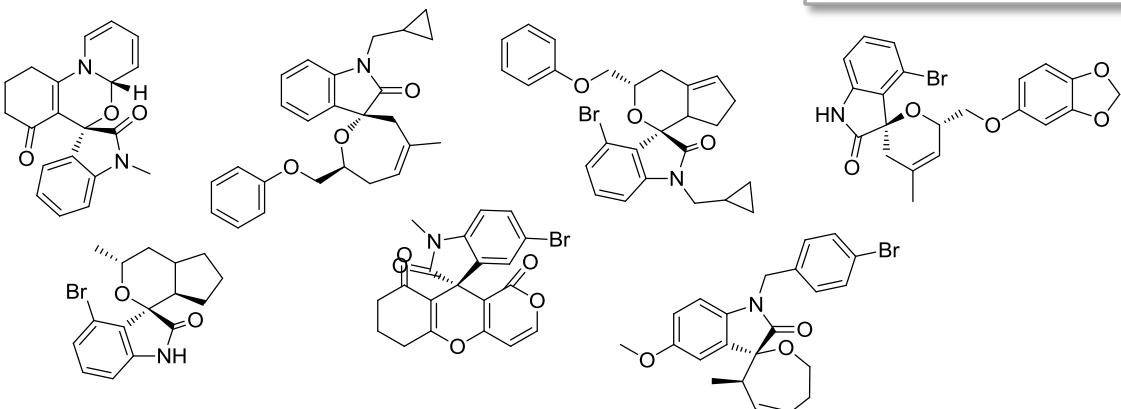
- Average MW = 505.5
- Average LogP = 5.4
- Average TPSA = 60.4
- Avg. chiral centers = 1.05
- Average # rings = 3.6

# Spirooxindoles

## Selected References:

- Liang, B.; Kalidindi, S.; Porco, J.A., Jr.; Stephenson, C.R.J. *Org. Lett.*, **2010**, *12*, 572-575.
- Castaldi, M.P.; Troast, D.M.; Porco, J.A., Jr. *Org. Lett.*, **2009**, *11*, 3362-3365.
- Zhang, Y.; Panek, J.S. *Org. Lett.*, **2009**, *11*, 3366-3369.

## Representative Structures:



## Calculated Physical Properties:

- Average MW = 383.1
- Average LogP = 3.9
- Average TPSA = 47.4
- Avg. chiral centers = 2.1
- Average # rings = 4.3

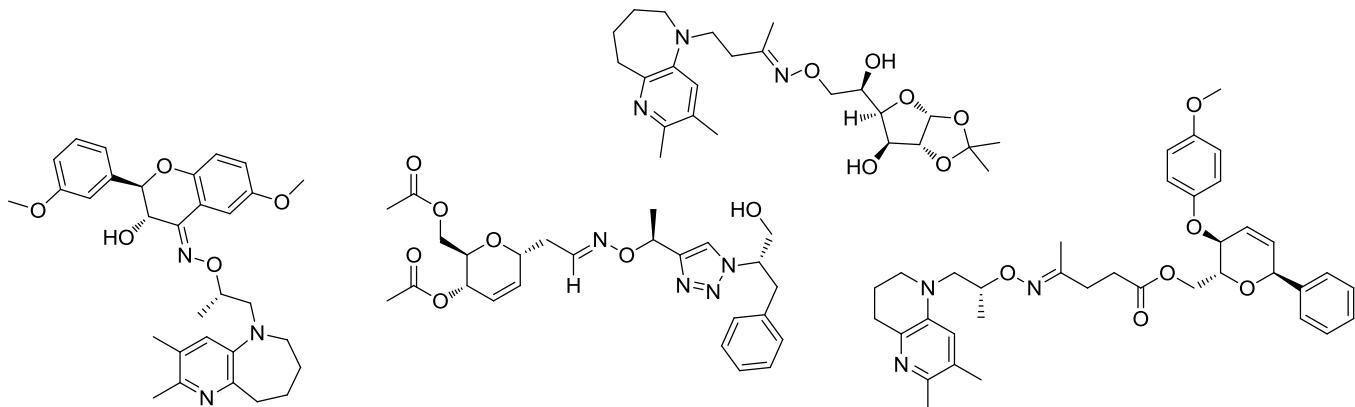
# Domain-Shuffled Oximes



## Selected References:

- Su, S.; Acquilano, D.E.; Arumugasamy, J.; Beeler, A.B.; Eastwood, E.L.; Giguere, J.R.; Lan, P.; Lei, X.; Min, G.K.; Yeager, A.R.; Zhou, Y.; Panek, J.S.; Snyder, J.K.; Schaus, S.E.; Porco, J.A., Jr. *Org. Lett.*, **2005**, 7, 2751-2754.

## Representative Structures:

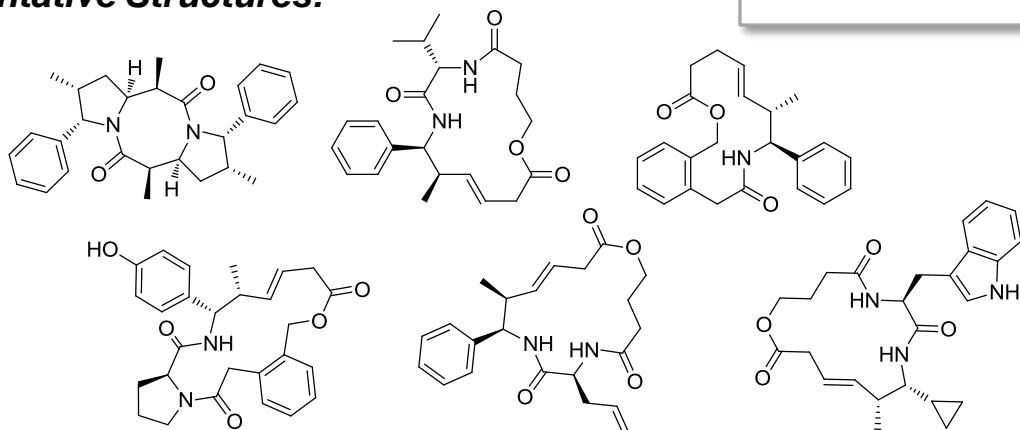


# Macrocycles

## Selected References:

- Han, C.; Rangarajan, S.; Voukides, A.C.; Beeler, A.B.; Johnson, R.; Porco, J.A., Jr. *Org. Lett.* **2009**, 11, 413-416.
- Beeler, A.B. et al. *J. Comb. Chem.*, **2005**, 7, 673-681.
- Su, Q.; Beeler, A.B.; Lobkovsky, E.; Porco, J.A., Jr.; Panek, J.S. *Org. Lett.* **2003**, 5, 2149-2152.

## Representative Structures:



## Calculated Physical Properties:

- Average MW = 546.2
- Average LogP = 3.7
- Average TPSA = 117.8
- Avg. chiral centers = 5.3
- Average # rings = 4.0

# Miscellaneous Heterocycle Libraries

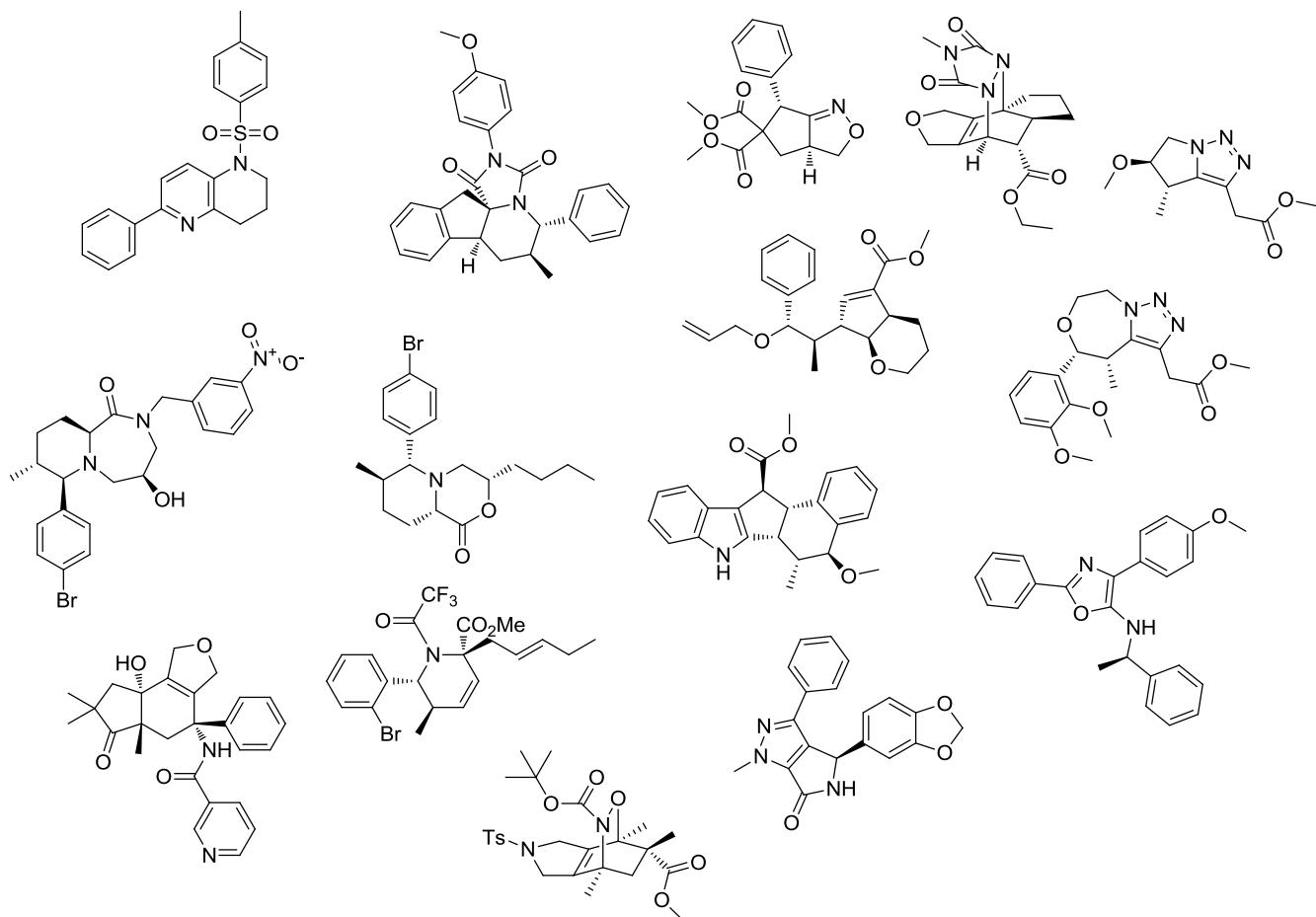
## Selected References:

- Wu, J.; Becerril, J.; Lian, Y.; Davies, H.M.L.; Porco, J.A., Jr.; Panek, J.S. *Angew. Chem. Int. Ed.*, **2011**, *50*, 5938-5942.
- Jones, A.L.; Snyder, J.K. *Org. Lett.*, **2010**, *12*, 1592-1595.
- Brown, R.A.; Welzel, M.; Lowe, J.T.; Panek, J.S. *Org. Lett.*, **2010**, *12*, 336-339.
- Brown, R.A.; Panek, J.S. *Org. Lett.*, **2009**, *11*, 473-476.
- Dandapani, S.; Dudata, M.; Panek, J.S.; Porco, J.A., Jr. *Org. Lett.*, **2007**, *9*, 3849-3852.
- Chen, Y.; Porco, J.A., Jr.; Panek, J.S. *Org. Lett.* **2007**, *9*, 1529-1532.

## Calculated Physical Properties:

- Average MW = 378.8
- Average LogP = 3.7
- Average TPSA = 53.1
- Avg. chiral centers = 1.5
- Average # rings = 3.9

## Representative Structures:

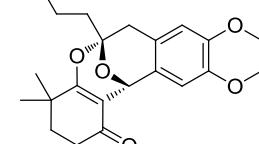
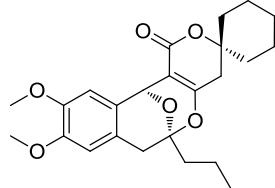
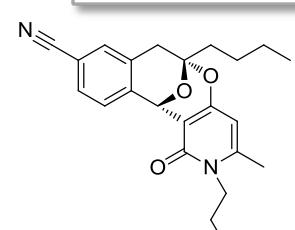
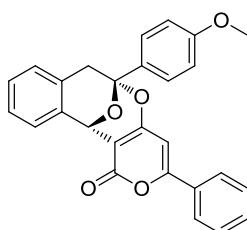
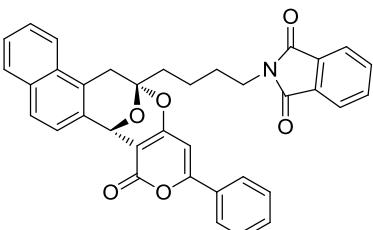


# Polycyclic Ketals

## Selected References:

- Brown, L.E.; Cheng, K.C.; Wei, W.; Yuan, P. et al. *Proc. Nat. Acad. Sci. USA*, **2011**, *108*, 6775-6780.
- Beeler, A.B.; Su, S.; Singleton, C.A.; Porco, J.A., Jr. *J. Am. Chem. Soc.*, **2007**, *129*, 1413-1419.

## Representative Structures:

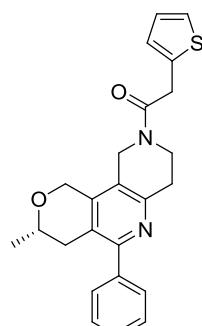
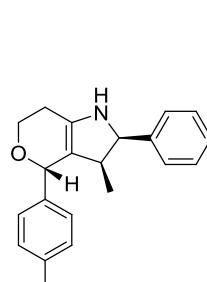
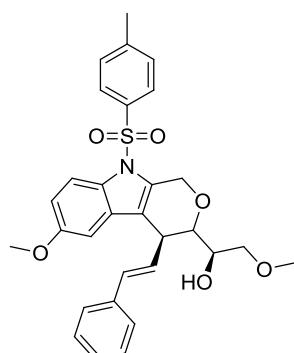
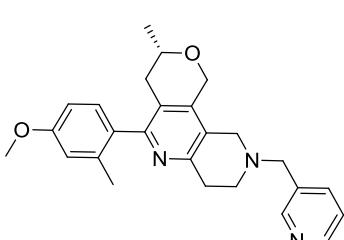


# Pyranoalkaloids

## Selected References:

- Medeiros, M.R.; Schaus, S.E.; Porco, J.A., Jr. *Org. Lett.*, **2011**, *13*, 4012-4015.
- Zhou, Y.; Porco, J.A. Jr.; Snyder, J.K. *Org. Lett.*, **2007**, *9*, 393-396.
- Woo, G.H.C.; Beeler, A.B.; Snyder, J.K. *Tetrahedron*, **2007**, *63*, 5649-5655.

## Representative Structures:



## Calculated Physical Properties:

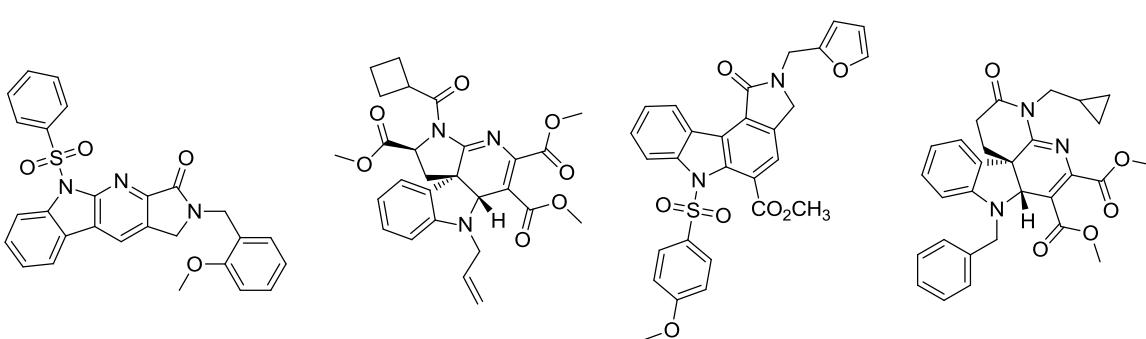
- Average MW = 464.4
- Average LogP = 4.7
- Average TPSA = 69.6
- Avg. chiral centers = 2
- Average # rings = 5.8

# Indole Alkaloids

## Selected References:

- Kota, S.; Takahashi, V.; Ni, F.; Snyder, J.K.; Strosberg, A.D. *PLoS One*, **2012**, 7, e32207.
- Brown, L.E.; Cheng, K.C.; Wei, W.; Yuan, P. *et al. Proc. Nat. Acad. Sci. USA*, **2011**, 108, 6775-6780.
- Ni, F.; Kota, S.; Takahashi, V.; Strosberg, A.D.; Snyder, J.K. *Bioorg. Med. Chem. Lett.*, **2011**, 21, 2198-2202.

## Representative Structures:

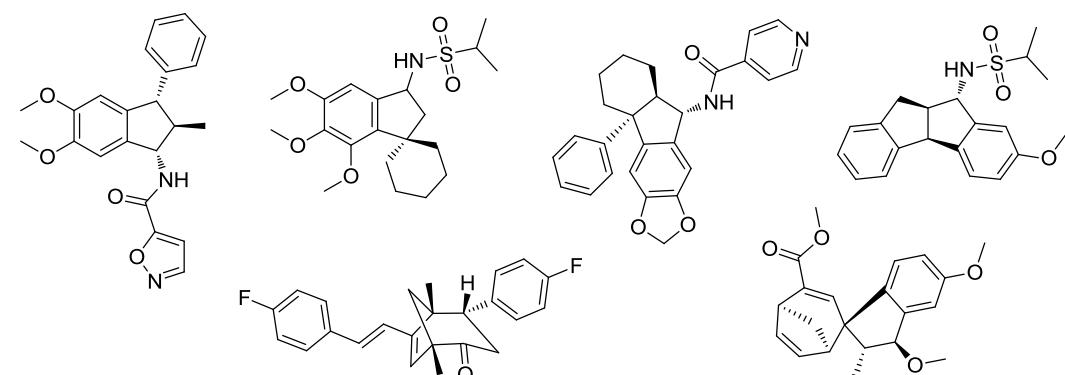


# Complex carbocycles

## Selected References:

- Kinoshita, H.; Ingham, O.J.; Ong, W.W.; Beeler, A.B.; Porco, J.A., Jr. *J. Am. Chem. Soc.*, **2010**, 132, 6412-6418.
- Kesavan, S.; Panek, J.S.; Porco, J.A., Jr. *Org. Lett.* **2007**, 9, 5203-5206.
- McDougal, N.T.; Schaus, S.E. *Angew. Chem. Int. Ed.* **2006**, 45, 3117-3119.

## Representative Structures:



## Calculated Physical Properties:

- Average MW = 547.3
- Average LogP = 4.2
- Average TPSA = 106.8
- Avg. chiral centers = 0.9
- Average # rings = 5.4

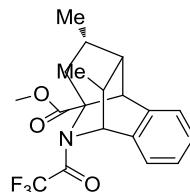
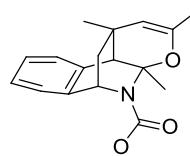
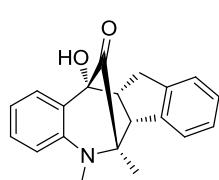
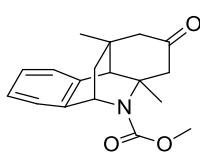
# Azabicyclooctanoids



## Selected References:

- Xia, B.; Gerard, B.; Solano, D.M.; Wan, J.; Jones, G. II; Porco, J.A. Jr. *Org. Lett.*, **2011**, 13, 1346-1349.
- Dandapani, S.; Dudata, M.; Panek, J.S.; Porco, J.A., Jr. *Org. Lett.*, **2007**, 9, 3849-3852.

## Representative Structures:

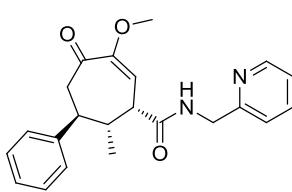
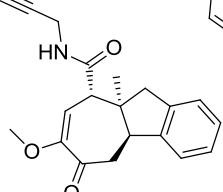
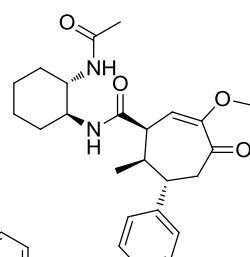
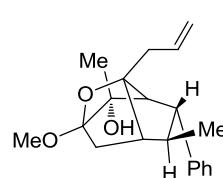
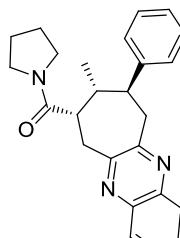
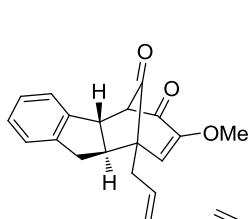


# Bicyclooctanoids and related derivatives

## Selected References:

- Goodell, J.R.; Poole, J.L.; Beeler, A.B.; Porco, J.A., Jr. *J. Org. Chem.*, **2011**, 76, 9792-9800.
- Goodell, J.R.; McMullen, J.P.; Zaborenko, N.; Maloney, J.R.; Ho, C.-X.; Jensen, K.; Porco, J.A., Jr.; Beeler, A.B. *J. Org. Chem.*, **2009**, 74, 6169-6180.

## Representative Structures:



## Calculated Physical Properties:

- Average MW = 359.9
- Average LogP = 3.2
- Average TPSA = 56.5
- Avg. chiral centers = 3.7
- Average # rings = 3.7