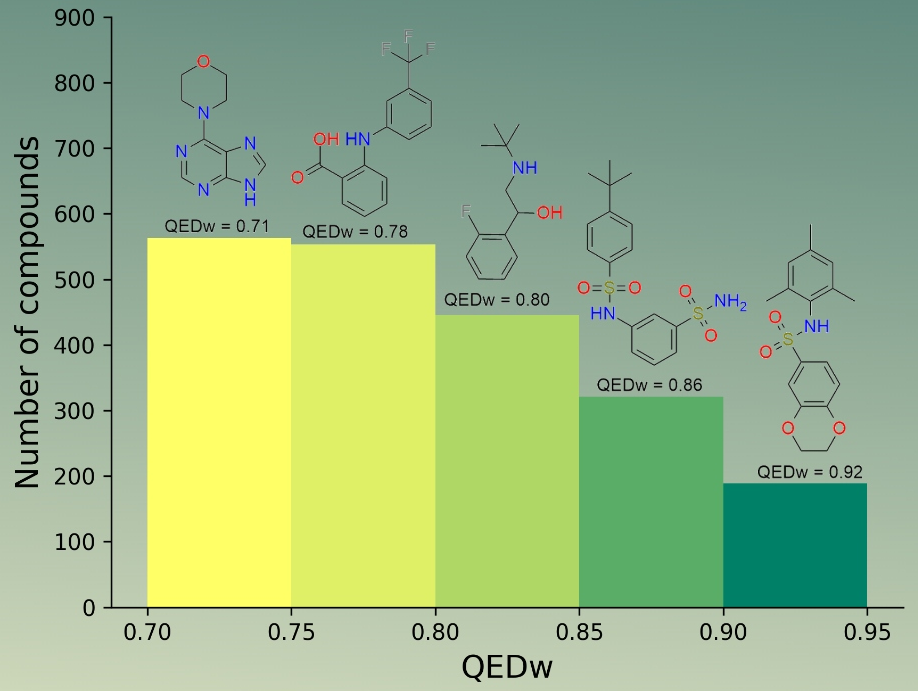
EBCL-0006

QED Bioactive Compounds

Nowadays, several rules and equations are commonly used for the description of the "attractiveness" of molecules for successive research in medicinal chemistry. One of them is the quantitative estimate of drug-likeness(QED) parameter proposed by Bickerton et al in 2012. It is a desirability function of several parameters: molecular weight, octanol-water partition coefficient, polar surface area, number of hydrogen bond donors and acceptors, number of rotatable bonds, number of aromatic rings, and number of chemical alerts(undesirable structural fragments). QED parameter is also known as a measure of the “chemical beauty” of the molecule and can take values from 0 to 1. More than 75% of orally bioavailable drugs have QED values greater than 0.50 and their median value is 0.65 (Warner et al). Also, it was proved that drugs with high QED values have greater absorption and bioavailability score(T.J. Ritchie et al). So this parameter can be used for the prediction of important pharmacological properties of potential hits for HTS.

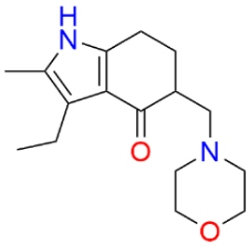
We offer a library of “chemically beautiful” bioactive compounds, where we have selected 2071 compounds with QED values greater than 0.70 and sub-ten micromolar activity coefficient values.



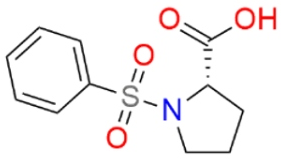
Distribution of molecules from the QED Bioactive library according to their QEDw.

Related terms: *G protein-coupled receptor, GPCR, carbonic anhydrase, ligand-gated ion channels, catecholamine turnover, receptor tyrosine kinase, RTK, nRTK, eicosanoid turnover*

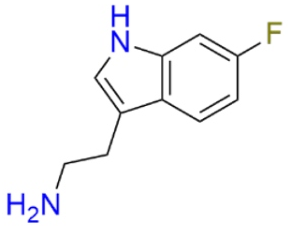
Highlights



EBC-08260
CAS: 7416-34-4
QEDw = 0.92



EBC-03738
CAS: 88425-46-1
QEDw = 0.87



EBC-44086
CAS: 575-85-9
QEDw = 0.72

Library Composition

Name	Occurrence in the library, times
G protein-coupled receptors	749
Carbonic anhydrases	400
Ligand-gated ion channels	149
Catecholamine turnover	93
Receptor tyrosine kinases (RTKs)	91
Non-receptor tyrosine kinases (nRTKs)	86
Eicosanoid turnover	80
Voltage-gated ion channels	77
1.-.-.- Oxidoreductases	76
Steroid hormone receptors	76
SLC6 neurotransmitter transporter family	68

Cytochrome P450	62
Potassium channels	59
Hydrolases	57
Acetylcholine turnover	48
Mitogen-activated protein kinases (MAP kinases)	41
Sigma receptors	40
CAMK: Calcium/calmodulin-dependent protein kinases	34
SLC superfamily of solute carriers	33
Orphan and other 7TM receptors	28
MG: Metallo (M) Peptidases	23
ATP-binding cassette transporter family	22
Poly ADP-ribose polymerases	22
Chloride channels	21

Chromatin modifying enzymes	•	21
CAMK-like (CAMKL) family	•	19
Nuclear hormone receptors	•	19
MA: Metallo (M) Peptidases	•	18
CK1: Casein kinase 1	•	17
AGC: Containing PKA, PKG, PKC families	•	16
SLC22 family of organic cation and anion transporters	•	15
CMGC: Containing CDK, MAPK, GSK3, CLK families	•	15
Endocannabinoid turnover	•	15
Cyclin-dependent kinase (CDK) family	•	14
STE20 family	•	14
IKK family	•	14
CA: Cysteine (C) Peptidases	•	13

Dual-specificity tyrosine-(Y)-phosphorylation regulated kinase (DYRK) family	•	12
Cyclic nucleotide turnover/signalling	•	12
DMPK family	•	11
Aryl hydrocarbon receptor complex	•	11
Glycogen synthase kinase (GSK) family	•	9
Glycerophospholipid turnover	•	9
SC: Serine (S) Peptidases	•	9
NADPH oxidases	•	8
PA: Serine (S) Peptidases	•	8
L-Arginine turnover	•	7
1.13.11.- Dioxygenases	•	6
RSK family	•	6
Alpha kinase family	•	6

Bromodomain-containing proteins	•	6
Pattern recognition receptors	•	6
Carrier proteins	•	5
Receptor serine/threonine kinase (RSTK) family	•	5
Aurora kinase (Aur) family	•	5
STE: Homologs of yeast Sterile 7, Sterile 11, Sterile 20 kinases	•	5
MAPK-Activated Protein Kinase (MAPKAPK) family	•	5
3.2.1.- Glycosidases	•	4
Tubulins	•	4
CD: Cysteine (C) Peptidases	•	4
Heat shock proteins	•	4
Leucine-rich repeat kinase (LRRK) family	•	4
Phosphatidyl inositol 3' kinase-related kinases (PIKK) family	•	4

5.2.-.- Cis-trans-isomerases	•	3
AA: Aspartic (A) Peptidases	•	3
G protein-coupled receptor kinases (GRKs)	•	3
Lipid modifying kinases	•	3
Protein kinase C (PKC) family	•	3
LIM domain kinase (LISK) family	•	3
Transcription factors	•	3
1.14.13.9 Kynurenine 3-monooxygenase	•	2
1.4.3.13 Lysyl oxidases	•	2
2.6.1.42 Branched-chain-amino-acid transaminase	•	2
Atypical	•	2
Bromodomain kinase (BRDK) family	•	2
Catalytic receptors	•	2

Ceramide turnover	•	2
Mixed Lineage Kinase (MLK) family	•	2
Immunoglobulin like domain containing proteins	•	2
IRE family	•	2
Lanosterol biosynthesis pathway	•	2
MC: Metallo (M) Peptidases	•	2
RAF family	•	2
NIMA (never in mitosis gene a)- related kinase (NEK) family	•	2
Casein kinase 2 (CK2) family	•	2
Polo-like kinase (PLK) family	•	2
2.1.1.- Methyltransferases	•	1
2.3.1.- Acyltransferases	•	1
Adenosine turnover	•	1

Haspin family	•	1
Fatty acid-binding proteins	•	1
Mitochondrial-associated proteins	•	1
SLC3 and SLC7 families of heteromeric amino acid transporters (HATs)	•	1
Sphingosine 1-phosphate turnover	•	1
Interleukin-1 receptor-associated kinase (IRAK) family	•	1
Inositol phosphate turnover	•	1
Viral protein targets	•	1
MH: Metallo (M) Peptidases	•	1
Other ion channels	•	1
P-type ATPases	•	1
P2C P-type ATPases	•	1
SB: Serine (S) Peptidases	•	1

SLC17 phosphate and organic anion transporter family	•	1
SLC2 family of hexose and sugar alcohol transporters	•	1
SLC5 family of sodium-dependent glucose transporters	•	1
WEE family	•	1