Gary L Grunewald

List of Publications by Year
in descending order

46 papers	1,103 citations	279701 23 h-index	414303 32 g-index
46 all docs	46 docs citations	46 times ranked	864 citing authors

#	Article	IF	Citations
1	Structure-Based Drug Design of Bisubstrate Inhibitors of Phenylethanolamine N-Methyltransferase Possessing Low Nanomolar Affinity at Both Substrate Binding Domains¹. Journal of Medicinal Chemistry, 2020, 63, 13878-13898.	2.9	2
2	Fragment-based screening by X-ray crystallography, MS and isothermal titration calorimetry to identify PNMT (phenylethanolamine N-methyltransferase) inhibitors. Biochemical Journal, 2010, 431, 51-61.	1.7	41
3	Molecular recognition of physiological substrate noradrenaline by the adrenaline-synthesizing enzyme PNMT and factors influencing its methyltransferase activity. Biochemical Journal, 2009, 422, 463-471.	1.7	30
4	Eulogy to Mathias P. Mertes, 1932-1989. Medicinal Research Reviews, 2009, 29, 1-2.	5.0	0
5	Synthesis of 4,5,6,7-tetrahydrothieno[3,2-c]pyridines and comparison with their isosteric 1,2,3,4-tetrahydroisoquinolines as inhibitors of phenylethanolamine N-methyltransferase. Bioorganic and Medicinal Chemistry, 2008, 16, 542-559.	1.4	22
6	Enzyme Adaptation to Inhibitor Binding:â€‰ A Cryptic Binding Site in Phenylethanolamine N-Methyltransferase. Journal of Medicinal Chemistry, 2007, 50, 4845-4853.	2.9	26
7	Exploring the active site of phenylethanolamine N-methyltransferase with 1,2,3,4-tetrahydrobenz[h]isoquinoline inhibitorsâ˜†. Bioorganic and Medicinal Chemistry, 2007, 15, 1298-1310.	1.4	9
8	Application of the Goldilocks Effect to the Design of Potent and Selective Inhibitors of Phenylethanolamine N-Methyltransferase:â€‰ Balancing pKa and Steric Effects in the Optimization of 3-Methyl-1,2,3,4-tetrahydroisoquinoline Inhibitors by Î²-Fluorination. Journal of Medicinal Chemistry, 2006, 49, 2939-2952.	2.9	44
9	Comparison of the Binding of 3-Fluoromethyl-7-sulfonyl-1,2,3,4-tetrahydroisoquinolines with Their Isosteric Sulfonamides to the Active Site of PhenylethanolamineN-Methyltransferase1. Journal of Medicinal Chemistry, 2006, 49, 5424-5433.	2.9	40
10	Exploring the active site of phenylethanolamine N-methyltransferase: 3-alkyl-7-substituted-1,2,3,4-tetrahydroisoquinoline inhibitors. Bioorganic and Medicinal Chemistry, 2005, 13, 1261-1273.	1.4	9
11	Exploring the active site of phenylethanolamine N-methyltransferase with 3-hydroxyethyl- and 3-hydroxypropyl-7-substituted-1,2,3,4-tetrahydroisoquinolines. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1143-1147.	1.0	8
12	Inhibitors of phenylethanolamine N-methyltransferase devoid of Î±2-adrenoceptor affinity. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5319-5323.	1.0	34
13	Mode of Binding of Methyl Acceptor Substrates to the Adrenaline-Synthesizing Enzyme Phenylethanolamine N-Methyltransferase:â€‰ Implications for Catalysis. Biochemistry, 2005, 44, 16875-16885.	1.2	24
14	Nanomolar Inhibitors of CNS Epinephrine Biosynthesis:Â (R)-(+)-3-Fluoromethyl-7-(N-substituted) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2 PhenylethanolamineN-Methyltransferase1. Journal of Medicinal Chemistry, 2005, 48, 1806-1812.	2.9	15
15	Structural, Mutagenic, and Kinetic Analysis of the Binding of Substrates and Inhibitors of Human Phenylethanolamine N-Methyltransferase. Journal of Medicinal Chemistry, 2005, 48, 7243-7252.	2.9	26
16	3-Hydroxymethyl-7-(N-substituted aminosulfonyl)-1,2,3,4-tetrahydroisoquinoline Inhibitors of Phenylethanolamine N-Methyltransferase that Display Remarkable Potency and Selectivity. Journal of Medicinal Chemistry, 2005, 48, 134-140.	2.9	17
17	Phenylethanolamine N-methyltransferase inhibition: re-evaluation of kinetic data. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4217-4220.	1.0	15
18	Molecular Recognition of Sub-micromolar Inhibitors by the Epinephrine-Synthesizing Enzyme Phenylethanolamine N-Methyltransferase. Journal of Medicinal Chemistry, 2004, 47, 37-44.	2.9	25

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19	Inhibitors of PhenylethanolamineN-Methyltransferase That Are Predicted To Penetrate the Bloodâ"Brain Barrier:Â Design, Synthesis, and Evaluation of 3-Fluoromethyl-7-(N-substituted) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf Î±2-Adrenoceptor1. Journal of Medicinal Chemistry, 2004, 47, 4483-4493.	2.9	28
20	Role of epinephrine stimulation of CNS ?1-adrenoceptors in motor activity in mice. Synapse, 2003, 49, 67-76.	0.6	34
21	The NH---FC Dipole Orientation Effect for Pendant Exocyclic CH2F. Organic Letters, 2002, 4, 3557-3560.	2.4	38
22	Synthesis and Evaluation of 4-Fluoro-8-substituted-2,3,4,5-tetrahydro-1H-2-benzazapines as Selective Inhibitors of PhenylethanolamineN-Methyltransferase versus the Î±2-Adrenoceptor. Journal of Medicinal Chemistry, 2001, 44, 2849-2856.	2.9	27
23	Effects of a 3-Alkyl-, 4-Hydroxy- and/or 8-Aromatic-substituent on the Phenylethanolamine N-Methyltransferase Inhibitor Potency and Î±2-Adrenoceptor Affinity of 2,3,4,5-Tetrahydro-1H-2-benzazepines. Bioorganic and Medicinal Chemistry, 2001, 9, 1957-1965.	1.4	19
24	Getting the Adrenaline Going. Structure, 2001, 9, 977-985.	1.6	60
25	Comparative molecular field analysis (CoMFA) models of phenylethanolamine N-methyltransferase (PNMT) and the Î±2-adrenoceptor: The development of new, highly selective inhibitors of PNMT. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 481-486.	1.0	15
26	3,7-Disubstituted-1,2,3,4-tetrahydroisoquinolines Display Remarkable Potency and Selectivity as Inhibitors of PhenylethanolamineN-Methyltransferase versus the Î±2-Adrenoceptor1a. Journal of Medicinal Chemistry, 1999, 42, 1982-1990.	2.9	33
27	Synthesis, Biochemical Evaluation, and Classical and Three-Dimensional Quantitative Structureâ"Activity Relationship Studies of 7-Substituted-1,2,3,4-tetrahydroisoquinolines and Their Relative Affinities toward Phenylethanolamine N-Methyltransferase and the Î±2-Adrenoceptor,1. Journal of Medicinal Chemistry, 1999, 42, 118-134.	2.9	33
28	Synthesis and Evaluation of 3-Trifluoromethyl-7-substituted- 1,2,3,4-tetrahydroisoquinolines as Selective Inhibitors of Phenylethanolamine N-Methyltransferase versus the Î±2-Adrenoceptor. Journal of Medicinal Chemistry, 1999, 42, 3315-3323.	2.9	39
29	Synthesis and Biochemical Evaluation of 3-Fluoromethyl-1,2,3,4-tetrahydroisoquinolines as Selective Inhibitors of PhenylethanolamineN-Methyltransferase versus the Î±2-Adrenoceptor1. Journal of Medicinal Chemistry, 1999, 42, 3588-3601.	2.9	55
30	Enantiospecific Synthesis of 3-Fluoromethyl-, 3-Hydroxymethyl-, and 3-Chloromethyl-1,2,3,4-tetrahydroisoquinolines as Selective Inhibitors of PhenylethanolamineN-Methyltransferase versus the Î±2-Adrenoceptor1. Journal of Medicinal Chemistry, 1999, 42, 4351-4361.	2.9	22
31	Examination of the Role of the Acidic Hydrogen in Imparting Selectivity of 7-(Aminosulfonyl)-1,2,3,4-tetrahydroisoquinoline (SK&F 29661) Toward Inhibition of PhenylethanolamineN-Methyltransferasevsthe Î±2-Adrenoceptor1a. Journal of Medicinal Chemistry, 1997, 40, 3997-4005.	2.9	26
32	Effect of Ring Size or an Additional Heteroatom on the Potency and Selectivity of Bicyclic Benzylamine-Type Inhibitors of PhenylethanolamineN-Methyltransferase1a. Journal of Medicinal Chemistry, 1996, 39, 3539-3546.	2.9	75
33	Recombinant Human PhenylethanolamineN-Methyltransferase: Overproduction inEscherichia coli,Purification, and Characterization. Protein Expression and Purification, 1996, 8, 160-166.	0.6	20
34	Design and stereoselective synthesis of conformationally constrained analogues of Zimeldine. Archives of Pharmacal Research, 1996, 19, 168-170.	2.7	1
35	Synthesis of 3â€alkylâ€8â€substitutedâ€and 4â€hydroxyâ€8â€substitutedâ€2,3,4,5â€tetrahydroâ€1Hâ€2â€benzazepines. Journal of Heterocyclic Chemistry, 1994, 31, 1609-1617.	1.4	24
36	A new procedure for regioselective synthesis of 8,9-dichloro-2,3,4,5-tetrahydro-1H-2-benzazepine (LY134046) and its 3-methyl analogue as inhibitors of phenylethanolamineN-methyltransferase (PNMT). Journal of Heterocyclic Chemistry, 1991, 28, 1587-1592.	1.4	7

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37	Conformational preferences in alkylbenzenes and aryl-alkylamines: A comparative study using CAMSEQ, MM2 and molecular dynamics methods. Journal of Computational Chemistry, 1988, 9, 315-326.	1.5	16
38	Synthesis and evaluation of 3-substituted analogs of 1,2,3,4-tetrahydroisoquinoline as inhibitors of phenylethanolamine N-methyltransferase. Journal of Medicinal Chemistry, 1988, 31, 824-830.	2.9	39
39	Conformationally defined adrenergic agents. 13. Conformational and steric aspects of the inhibition of phenylethanolamine N-methyltransferase by benzylamines. Journal of Medicinal Chemistry, 1988, 31, 433-444.	2.9	37
40	Inhibition of phenylethanolamine N-methyltransferase (PNMT) by aromatic hydroxy-substituted 1,2,3,4-tetrahydroisoquinolines. Further studies on the hydrophilic pocket of the aromatic ring binding region of the active site. Journal of Medicinal Chemistry, 1987, 30, 2208-2216.	2.9	36
41	Carbon-13 nuclear magnetic resonance examination of benzonorbornene derivatives. Assignment of site of aromatic ring substitution in benzonorbornen-2-ones. Magnetic Resonance in Chemistry, 1983, 21, 596-601.	0.7	5
42	Importance of the aromatic ring in adrenergic amines. 7. Comparison of the stereoselectivity of norepinephrine N-methyltransferase for aromatics. Nonaromatic substrates and inhibitors. Journal of Medicinal Chemistry, 1982, 25, 1198-1204.	2.9	13
43	Stereochemical aspects of binding of aromatic and non-aromatic substrates and inhibitors to phenylethanolamine N-methyltransferase. , 1981, , 691-699.		1
44	Application of CNDO/2 Calculations and X-Ray Crystallographic Analysis to the Design of Conformationally Defined Analogs of Methamphetamine. ACS Symposium Series, 1979, , 439-487.	0.5	4
45	SOME NEW INHIBITORS OF EPINEPHRINE BIOSYNTHESIS. IMPORTANCE OF THE AROMATIC RING IN ADRENERGIC AMINES. 4. (Ref. 1). , 1979, , 189-191.		1
46	A RAPID, CONVENIENT, HIGH YIELD PROCEDURE FOR THE REGENERATION OF 2,3-DICHLORO-5,6-DICYANOBENZOQUINONE (DDQ) FROM THE CORRESPONDING HYDROQUINONE (DDHQ). Organic Preparations and Procedures International, 1976, 8, 141-143.	0.6	13