

## **Supporting information**

# **Metal Chelation Therapy and Parkinson's Disease: A Critical Review on the Thermodynamics of Complex Formation Between Relevant Metal Ions and Promising or Established Drugs**

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### **Method and database used for the bibliographic search.**

The used database was Web of Science

([http://apps.webofknowledge.com/UA\\_GeneralSearch\\_input.do?product=UA&SID=D6Y2B9Fsbyg9IOPYezY&search\\_mode=GeneralSearch](http://apps.webofknowledge.com/UA_GeneralSearch_input.do?product=UA&SID=D6Y2B9Fsbyg9IOPYezY&search_mode=GeneralSearch)).

The year span was from 2014 until April 2019

The following subsequent bibliographic searches were performed (\* = wildcard character):

- 1) anti *and* parkinson *and* drug\*
- 2) parkinson *and* neuroprotective *and* agent\*
- 3) parkinson *and* therapeutic *and* agent\*

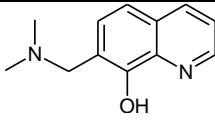
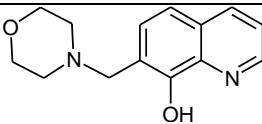
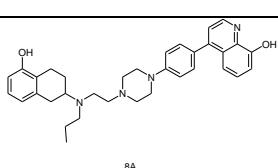
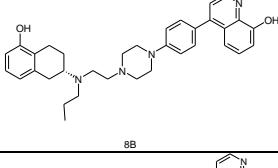
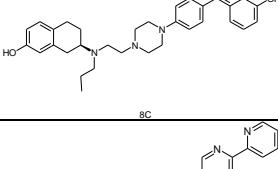
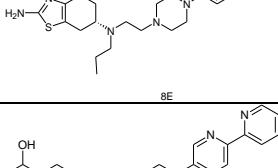
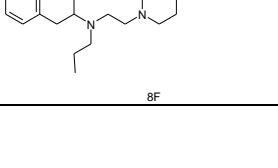
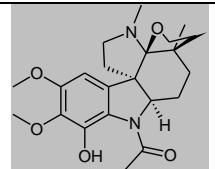
Spot cross-comparisons were performed with bibliographic results obtained in the databases Scopus

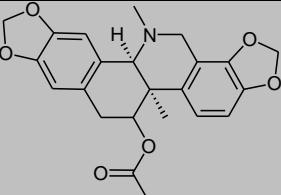
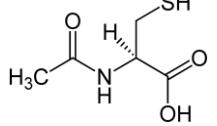
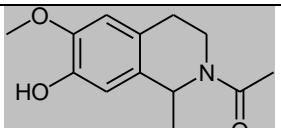
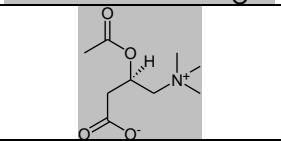
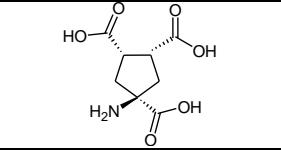
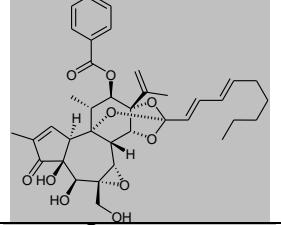
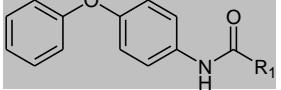
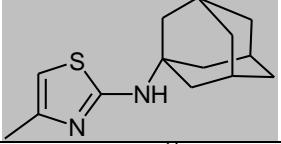
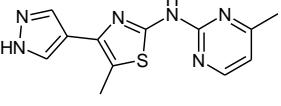
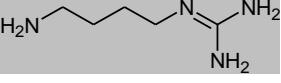
(<https://www.scopus.com/search/form.uri?display=basic>) and Pubmed

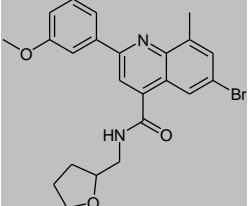
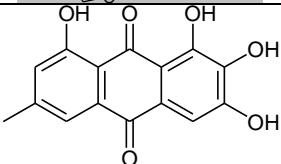
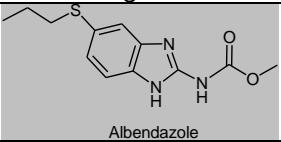
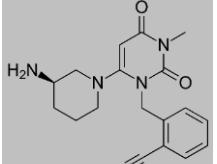
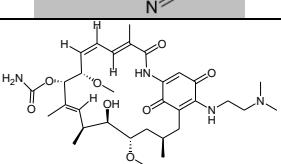
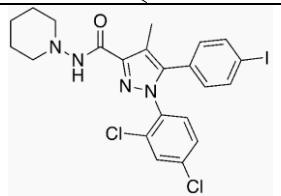
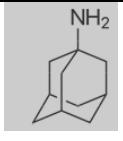
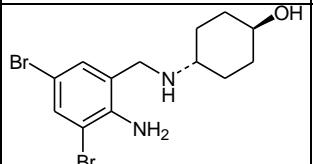
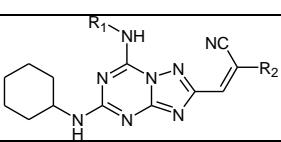
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**TABLE S1**

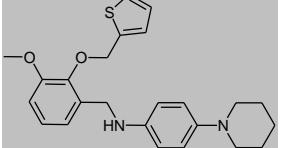
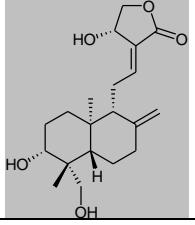
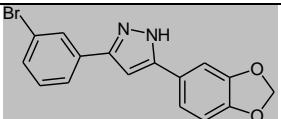
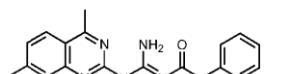
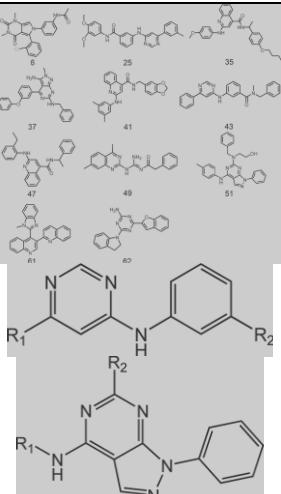
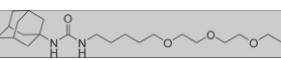
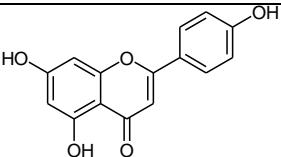
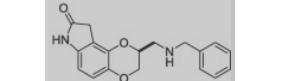
Compounds used, tested or proposed for the therapy against Parkinson's disease, as obtained from a Literature survey in the year range 2014–2019 (April). For each substance, name(s), structure and latest reference(s) are given (if a reference is a review, it is explicitly indicated). Compounds highlighted in grey do not have metal chelation properties. Compounds highlighted in blue likely have metal chelation properties, but to the best of our knowledge their metal speciation has neither been studied nor can be estimated due to complicated and/or peptidic structure (in these cases structures were often omitted). These highlighted substances have not been further considered in the present review.

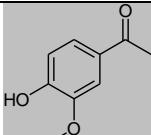
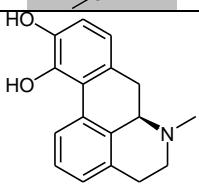
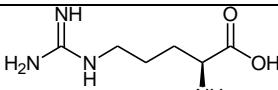
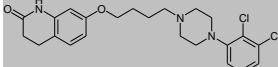
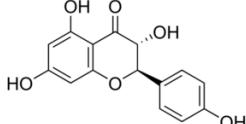
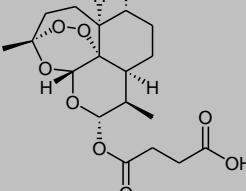
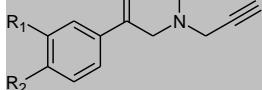
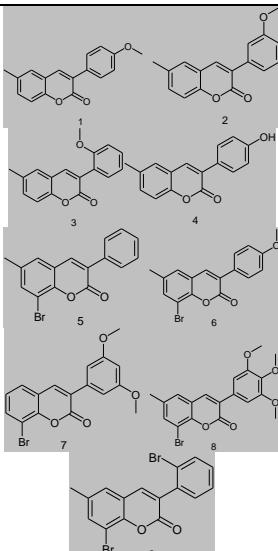
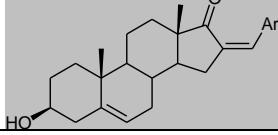
7DH		Iron Chelators and Antioxidants Regenerate Neuritic Tree and Nigrostriatal Fibers of MPP plus /MPTP-Lesioned Dopaminergic Neurons, Aguirre, P; Mena, NP; Carrasco, CM; Munoz, Y; Perez-Henriquez, P; Morales, RA; Cassels, BK; Mendez-Galvez, C; Garcia-Beltran, O; Gonzalez-Billault, C et al, PLOS ONE, 10, 12, Article Number: e0144848, DOI: 10.1371/journal.pone.0144848, DEC 14 2015
7MH		Iron Chelators and Antioxidants Regenerate Neuritic Tree and Nigrostriatal Fibers of MPP plus /MPTP-Lesioned Dopaminergic Neurons, Aguirre, P; Mena, NP; Carrasco, CM; Munoz, Y; Perez-Henriquez, P; Morales, RA; Cassels, BK; Mendez-Galvez, C; Garcia-Beltran, O; Gonzalez-Billault, C et al, PLOS ONE, 10, 12, Article Number: e0144848, DOI: 10.1371/journal.pone.0144848, DEC 14 2015
8A		A review on iron chelators as potential therapeutic agents for the treatment of Alzheimer's and Parkinson's diseases. Singh, YP; Pandey, A; Vishwakarma, S; Modi, G, Molecular diversity, DOI:10.1007/s11030-018-9878-4, 2018-Oct-06. <b>Document type: review</b>
8B		A review on iron chelators as potential therapeutic agents for the treatment of Alzheimer's and Parkinson's diseases. Singh, YP; Pandey, A; Vishwakarma, S; Modi, G, Molecular diversity, DOI:10.1007/s11030-018-9878-4, 2018-Oct-06. <b>Document type: review</b>
8C		A review on iron chelators as potential therapeutic agents for the treatment of Alzheimer's and Parkinson's diseases. Singh, YP; Pandey, A; Vishwakarma, S; Modi, G, Molecular diversity, DOI:10.1007/s11030-018-9878-4, 2018-Oct-06. <b>Document type: review</b>
8E		A review on iron chelators as potential therapeutic agents for the treatment of Alzheimer's and Parkinson's diseases. Singh, YP; Pandey, A; Vishwakarma, S; Modi, G, Molecular diversity, DOI:10.1007/s11030-018-9878-4, 2018-Oct-06. <b>Document type: review</b>
8F		A review on iron chelators as potential therapeutic agents for the treatment of Alzheimer's and Parkinson's diseases. Singh, YP; Pandey, A; Vishwakarma, S; Modi, G, Molecular diversity, DOI:10.1007/s11030-018-9878-4, 2018-Oct-06. <b>Document type: review</b>
AADC		Advances in non-dopaminergic treatments for Parkinson's disease. Stayte, S; Vissel, B ; FRONTIERS IN NEUROSCIENCE, 8, Article Number: 113, DOI: 10.3389/fnins.2014.00113, MAY 22 2014
Ac-[Phe(6), Nle(17)]PACAP(1-27)		Characterizations of a synthetic pituitary adenylate cyclase-activating polypeptide analog displaying potent neuroprotective activity and reduced in vivo cardiovascular side effects in a Parkinson's disease model, Lamine, A; Letourneau, M; Doan, ND; Maucotel, J; Couvineau, A; Vaudry, H; Chatenet, D; Vaudry, D; Fournier, A, NEUROPHARMACOLOGY, 108, 440-450, DOI: 10.1016/j.neuropharm.2015.05.014, SEP 2016
1-Acetyl-19,21-epoxy- 15,16-dimethoxy aspidospermidine-17-ol		Identification of an aspidospermine derivative from borage extract as an anti-amyloid compound: A possible link between protein aggregation and antimalarial drugs, Kalhor, HR; Ashrafiyan, H, PHYTOCHEMISTRY, 140, 134-140, DOI: 10.1016/j.phytochem.2017.05.001, AUG 2017

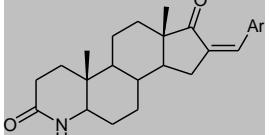
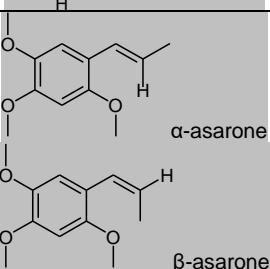
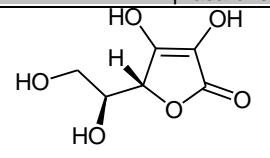
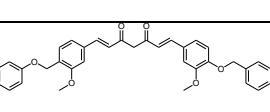
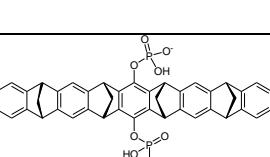
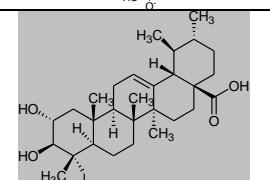
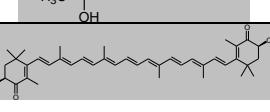
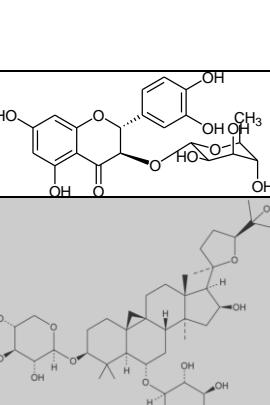
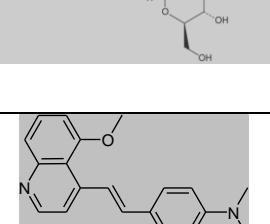
Acetylcorynoline		Acetylcorynoline attenuates dopaminergic neuron degeneration and alpha-synuclein aggregation in animal models of Parkinson's disease, Fu, RH; Wang, YC; Chen, CS; Tsai, RT; Liu, SP; Chang, WL; Lin, HL; Lu, CH; Wei, JR; Wang, ZW, et al, NEUROPHARMACOLOGY, 82, 108-120, DOI: 10.1016/j.neuropharm.2013.08.007, JUL 2014
N-acetylcysteine		<b>1)</b> N-acetylcysteine protects against motor, optomotor and morphological deficits induced by 6- in zebrafish larvae, Benvenutti, R; Marcon, M; Reis, CG; Nery, LR; Miguel, C; Herrmann, AP; Vianna, MRM; Piatto, A, PEERJ, 6, Article Number: e4957, DOI: 10.7717/peerj.4957, JUN 1 2018, <b>2)</b> 17 beta-Estradiol/N-Acetylcysteine Interaction Enhances the Neuroprotective Effect on Dopaminergic Neurons in the Weaver Model of Dopamine Deficiency, Botsakis, K; Theodoritis, S; Grintzalis, K; Angelatou, F; Antonopoulos, I; Georgiou, CD; Margarity, M; Matsokis, NA; Panagopoulos, NT, NEUROSCIENCE, 320, 221-229, DOI: 10.1016/j.neuroscience.2016.01.068, APR 21 2016, <b>3)</b> et cetera
2-Acetyl-7-hydroxy-6-methoxy-1-methyl-1,2,3,4-tetrahydroisoquinoline		2-Acetyl-7-hydroxy-6-methoxy-1-methyl-1,2,3,4-tetrahydroisoquinoline exhibits anti-inflammatory properties and protects the nigral dopaminergic neurons, Son, HJ; Han, SH; Lee, JA Lee, CS; Seo, JW; Chi, DY; Hwang, O, EUROPEAN JOURNAL OF PHARMACOLOGY, 771, 152-161, DOI: 10.1016/j.ejphar.2015.12.009, JAN 15 2016
Acetyl-L-carnitine		Redox-based therapeutics in neurodegenerative disease. McBean, GJ; Lopez, MG; Wallner, FK. BRITISH JOURNAL OF PHARMACOLOGY, 174, 12, 1750-1770, DOI: 10.1111/bph.13551, JUN 2017
Achyranthes bidentata polypeptides		<b>1)</b> Achyranthes bidentata polypeptide protects dopaminergic neurons from apoptosis induced by rotenone and 6-hydroxydopamine, Peng, S; Xu, L; Ma, JY; Gu, XS; Sun, C, NEURAL REGENERATION RESEARCH, 13, 11, 1981-1987, DOI: 10.4103/1673-5374.239446, NOV 2018, <b>2)</b> Achyranthes bidentata polypeptide protects dopaminergic neurons from apoptosis in Parkinson's disease models both in vitro and in vivo, Peng, S; Wang, CP; Ma, JY; Jiang, KT; Jiang, YH; Gu, XS; Sun, C; BRITISH JOURNAL OF PHARMACOLOGY, 175, 4, 631-643, DOI: 10.1111/bph.14110, FEB 2018
ACPT-I		Neuroprotective effects of metabotropic glutamate receptor group II and III activators against MPP-induced cell death in human neuroblastoma SH-SY5Y cells: The impact of cell differentiation state, Jantas, D; Greda, A; Golda, S; Korostynski, M; Grygier, B; Roman, A; Pilc, A; Lason, W; NEUROPHARMACOLOGY, 83, 36-53, DOI: 10.1016/j.neuropharm.2014.03.019, AUG 2014
Acutilonine F		<b>1)</b> Daphnane and Phorbol Diterpenes, Anti-neuroinflammatory Compounds with Nurr1 Activation from the Roots and Stems of Daphne genkwa, Han, BS; Van Minh, N; Choi, HY; Byun, JS; Kim, WG, BIOLOGICAL & PHARMACEUTICAL BULLETIN, 40, 12, 2205-2212, DEC 2017, <b>2)</b> Diterpenes: Advances in Neurobiological Drug Research, Islam, MT; da Silva, CB; de Alencar, MVOB (Oliveira Barros de Alencar, Marcus Vinicius); Paz, MFCJ; Almeida, FRD; Melo-Cavalcante, AAD (de Carvalho Melo-Cavalcante, Ana Amelia), PHYTOTHERAPY RESEARCH, 30, 6, 915-928, DOI: 10.1002/ptr.5609, JUN 2016, Document Type: Review
N-Acyl Derivatives of 4-Phenoxyaniline		N-Acyl Derivatives of 4-Phenoxyaniline as Neuroprotective Agents, Barbo, MT; Oppermann, S; Schrader, FC; Degenhardt, I; Elsasser, K; Wegscheid-Gerlach, C; Culmsee, C; Schlitzer, M; CHEMMEDCHEM, 9, 10, 2260-2273, DOI: 10.1002/cmdc.201402195, OCT 2014
N-Adamantyl-4-methylthiazol-2-amine		Anti-inflammatory mechanisms of N-adamantyl-4-methylthiazol-2-amine in lipopolysaccharide-stimulated BV-2 microglial cells, Kim, EA; Han, AR; Choi, J; Ahn, JY; Choi, SY; Cho, SW; INTERNATIONAL IMMUNOPHARMACOLOGY, 22, 1, 73-83, DOI: 10.1016/j.intimp.2014.06.022, SEP 2014
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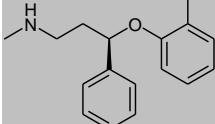
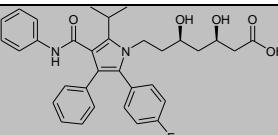
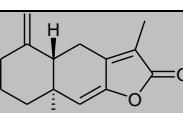
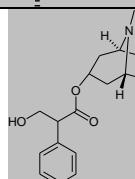
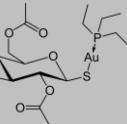
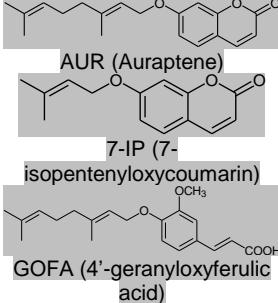
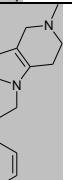
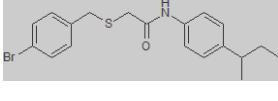
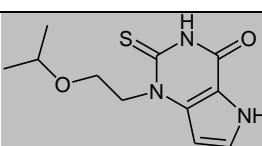
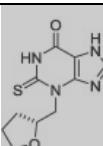
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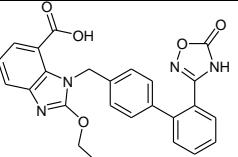
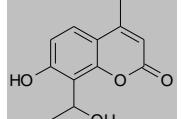
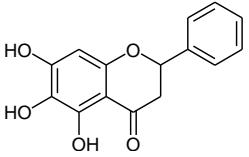
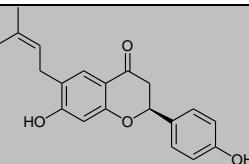
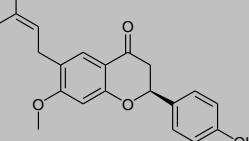
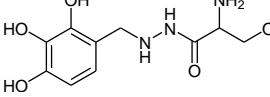
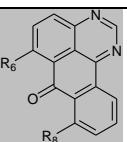
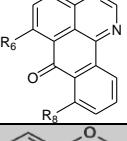
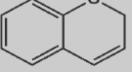
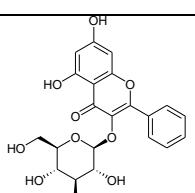
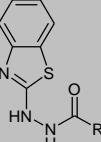
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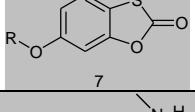
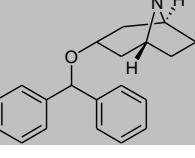
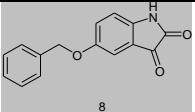
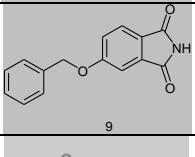
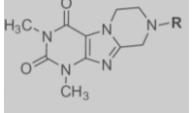
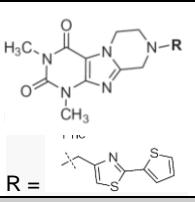
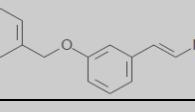
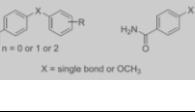
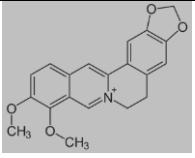
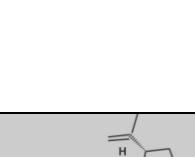
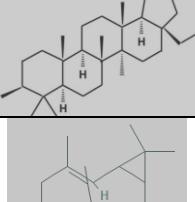
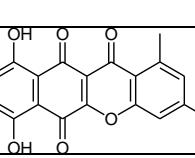
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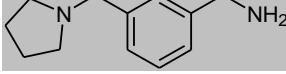
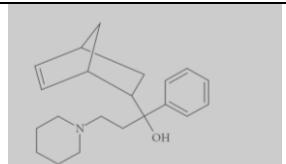
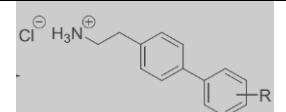
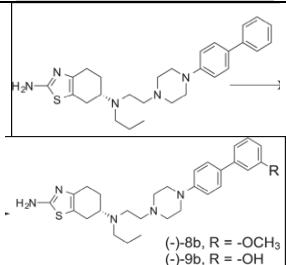
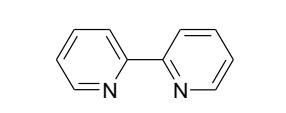
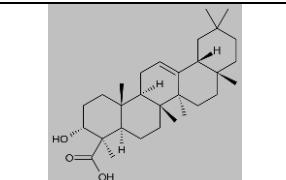
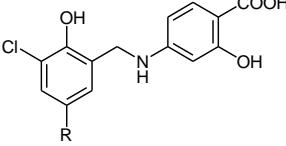
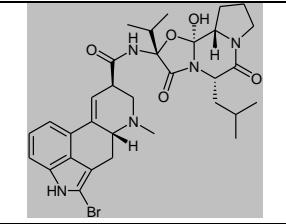
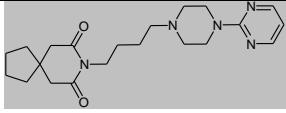
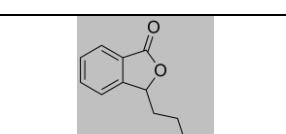
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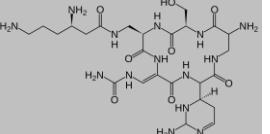
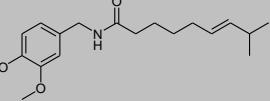
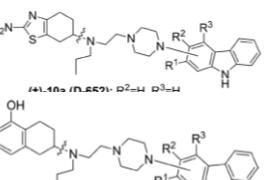
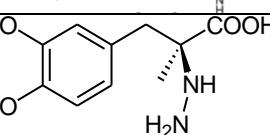
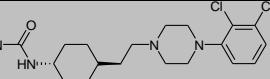
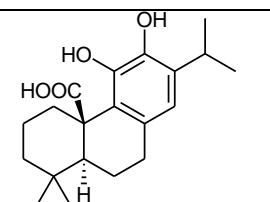
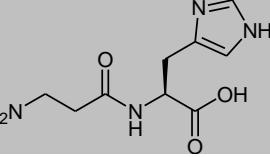
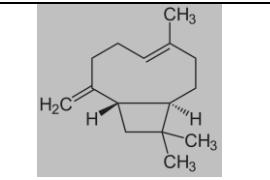
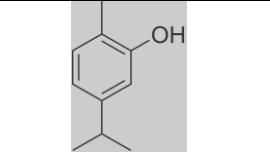
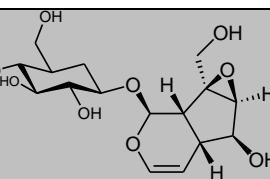
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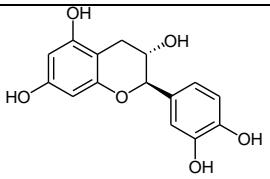
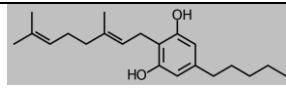
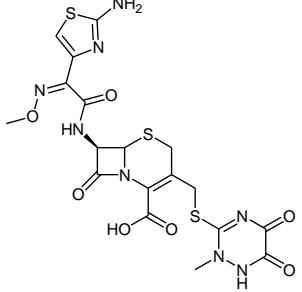
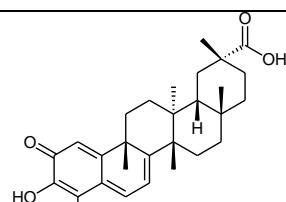
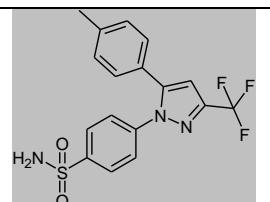
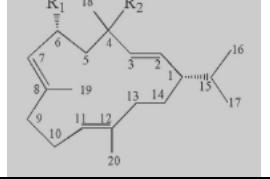
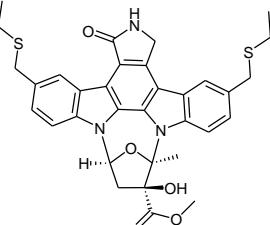
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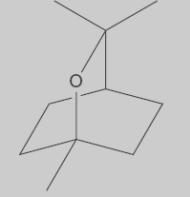
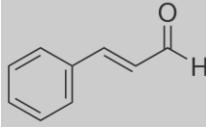
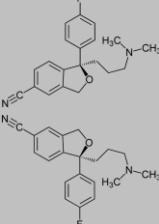
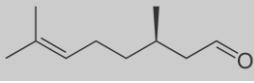
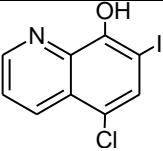
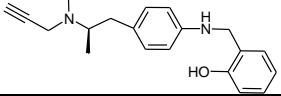
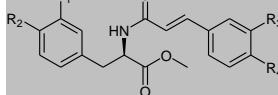
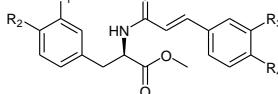
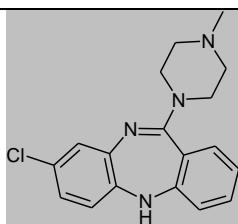
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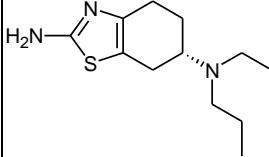
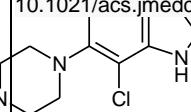
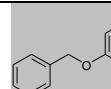
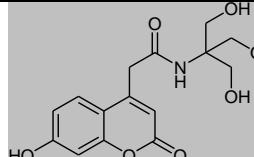
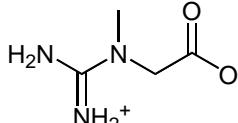
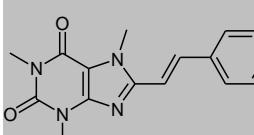
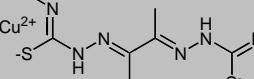
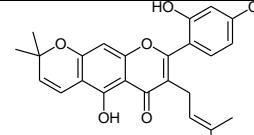
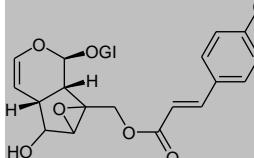
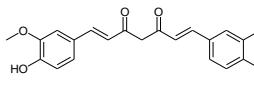
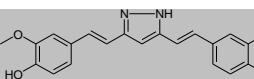
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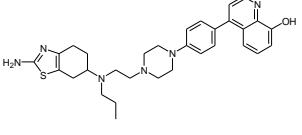
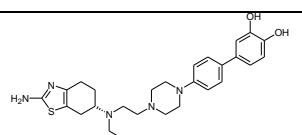
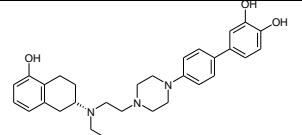
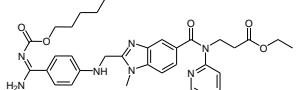
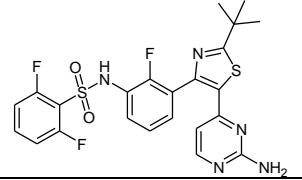
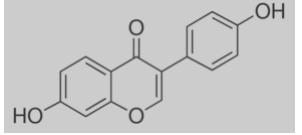
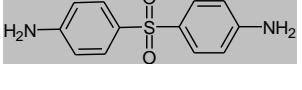
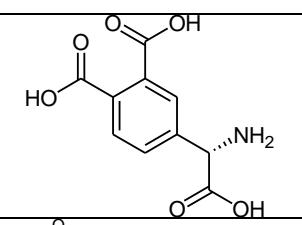
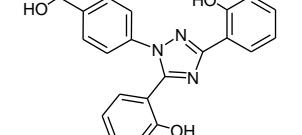
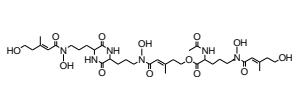
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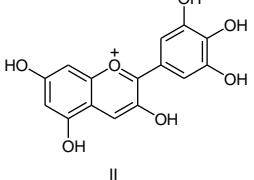
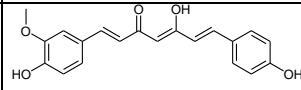
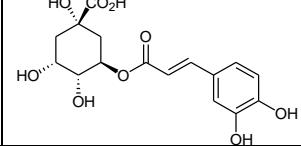
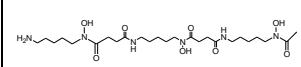
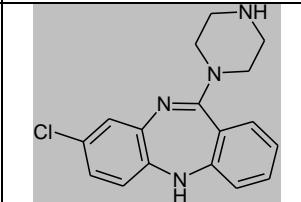
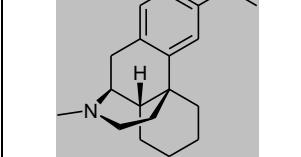
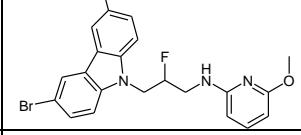
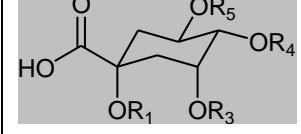
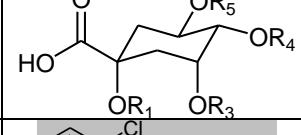
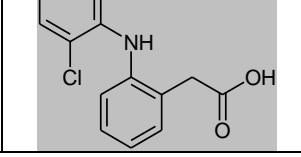
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Clovamide analogues (R <sub>1</sub> and R <sub>2</sub> = OH, and/or R <sub>3</sub> and R <sub>4</sub> = OH)		Synthesis and biological evaluation of clovamide analogues with catechol functionality as potent Parkinson's disease agents in vitro and in vivo, Feng, JH; Hu, XL; Lv, XY; Wang, BL; Lin, J; Zhang, XQ; Ye, WC; Xiong, F; Wang, H; BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, 29, 2, 302-312, DOI: 10.1016/j.bmcl.2018.11.030, JAN 15 2019
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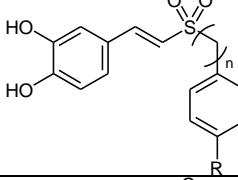
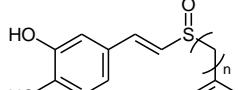
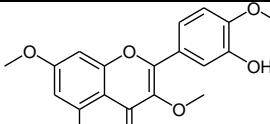
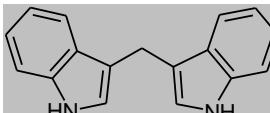
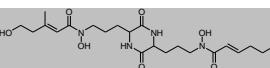
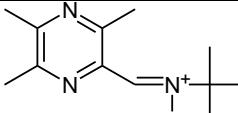
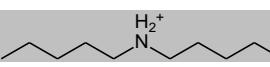
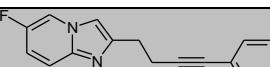
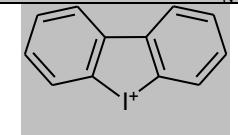
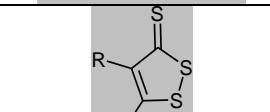
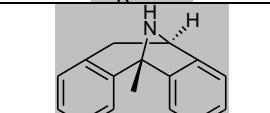
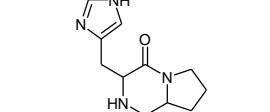
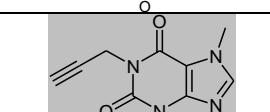
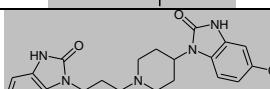
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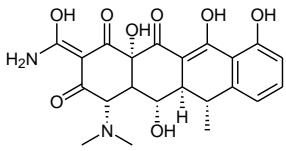
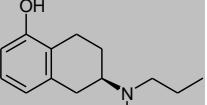
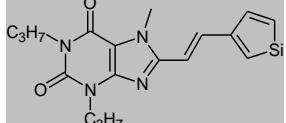
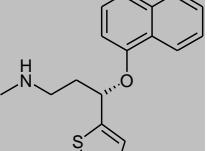
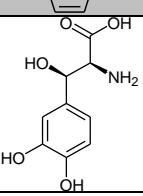
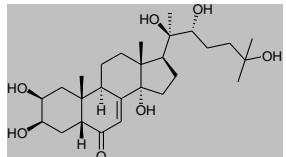
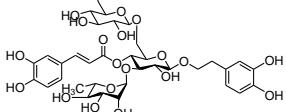
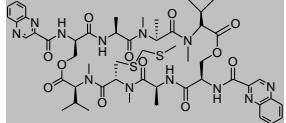
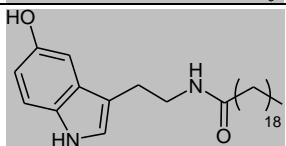
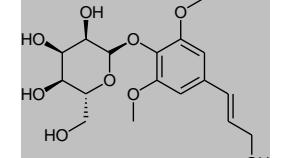
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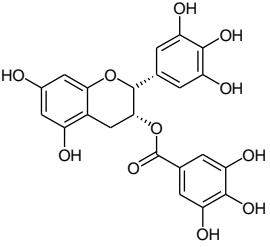
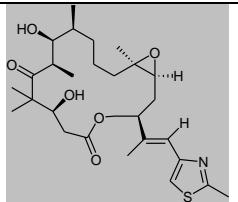
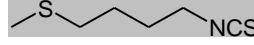
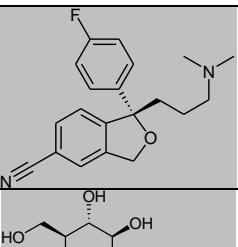
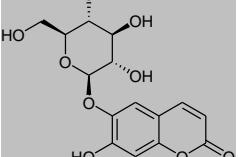
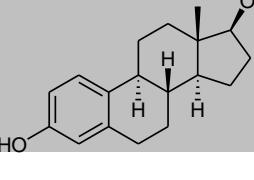
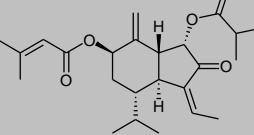
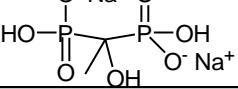
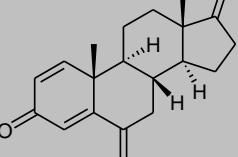
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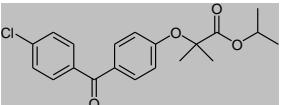
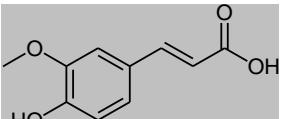
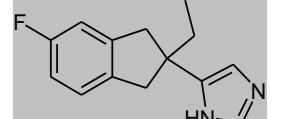
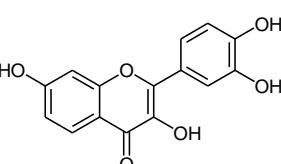
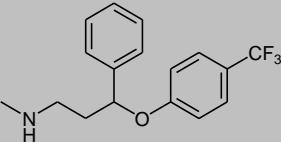
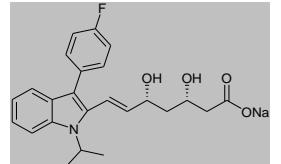
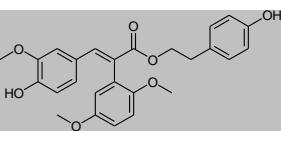
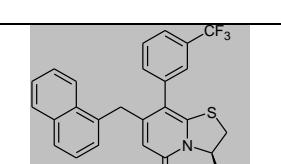
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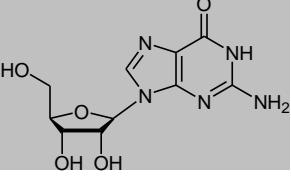
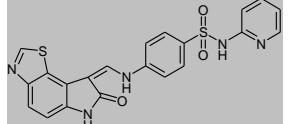
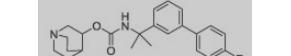
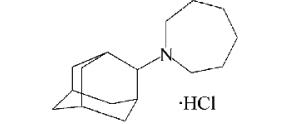
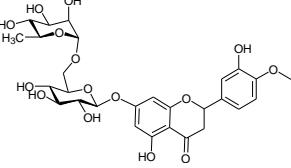
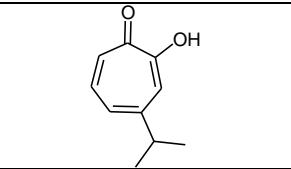
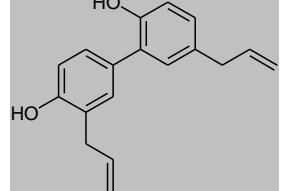
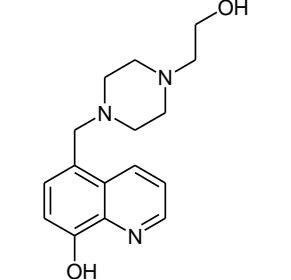
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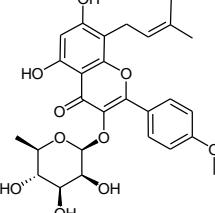
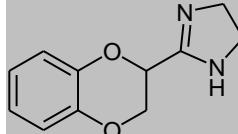
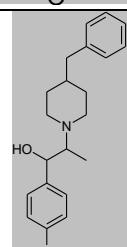
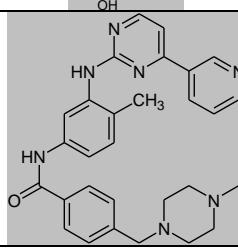
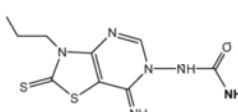
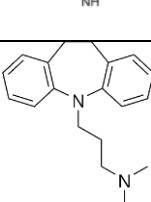
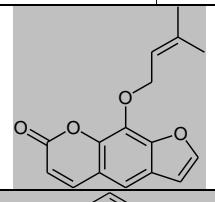
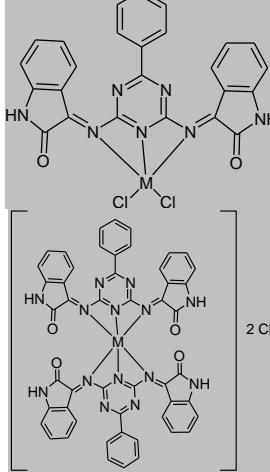
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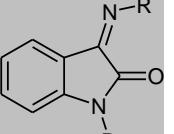
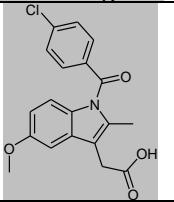
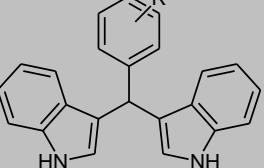
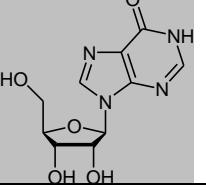
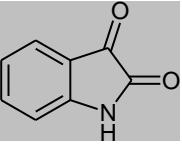
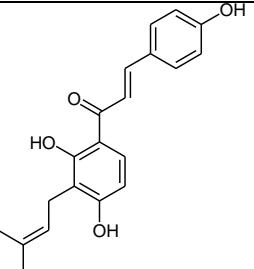
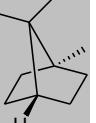
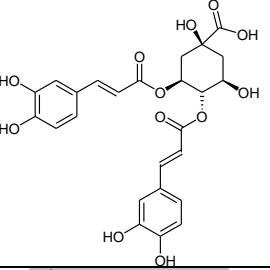
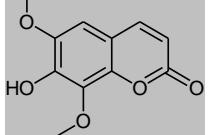
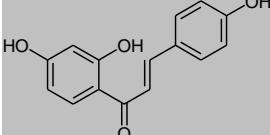
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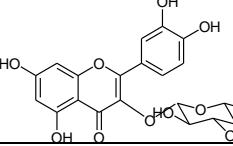
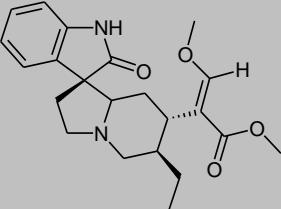
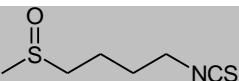
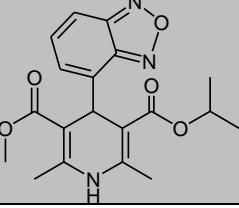
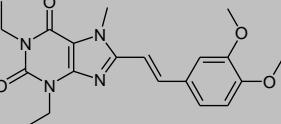
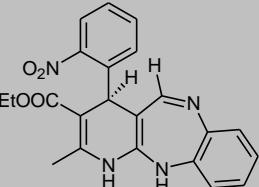
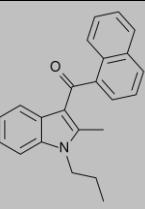
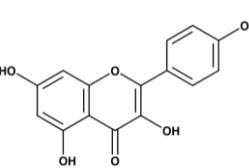
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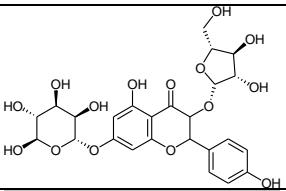
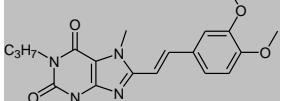
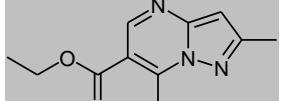
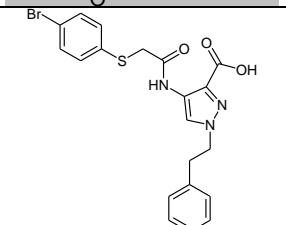
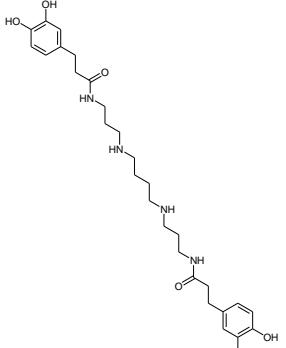
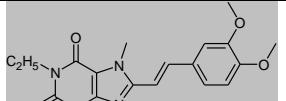
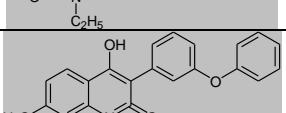
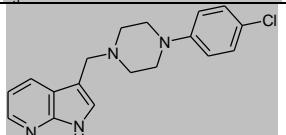
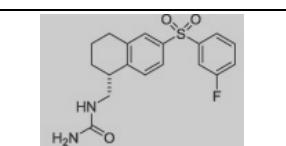
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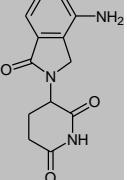
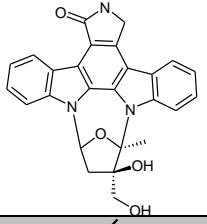
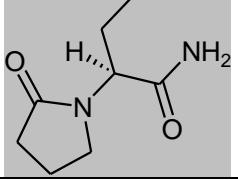
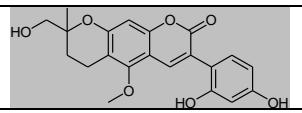
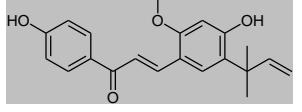
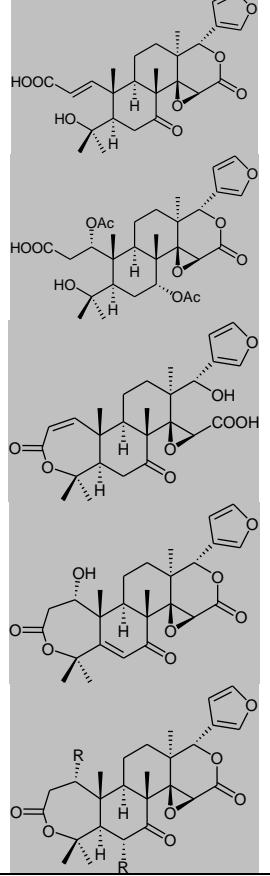
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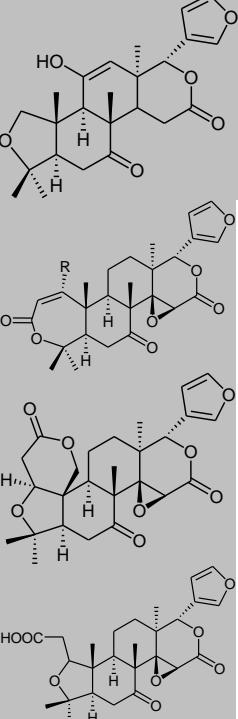
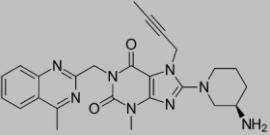
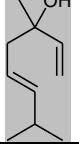
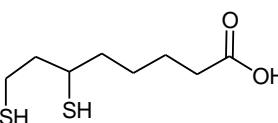
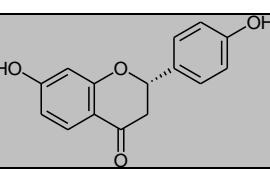
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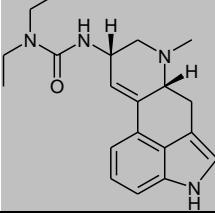
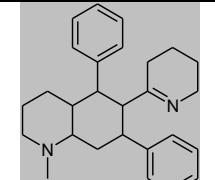
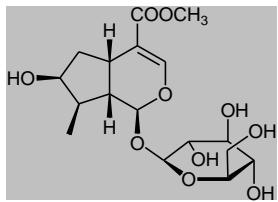
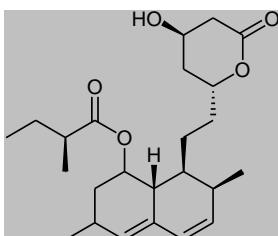
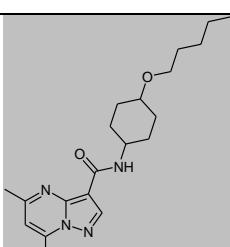
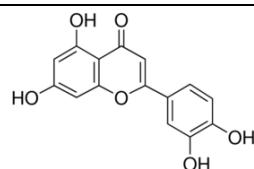
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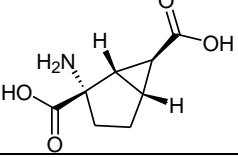
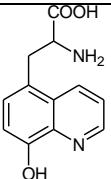
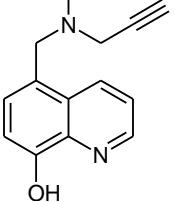
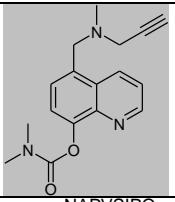
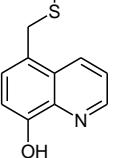
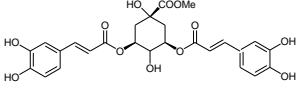
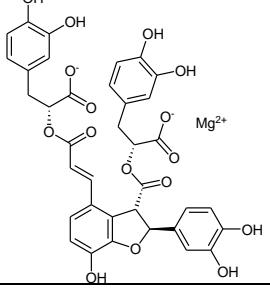
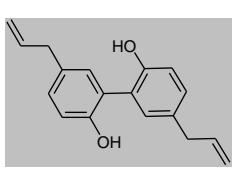
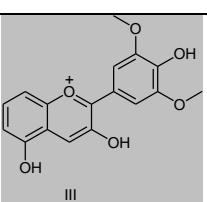
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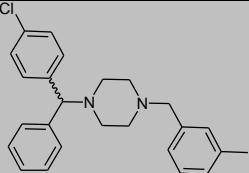
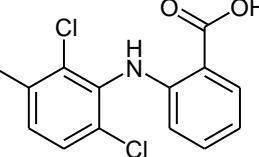
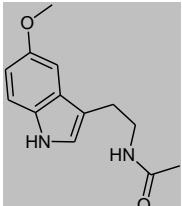
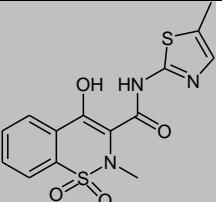
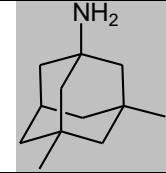
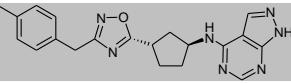
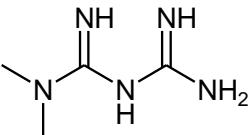
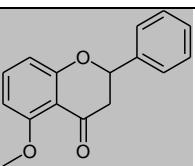
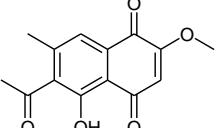
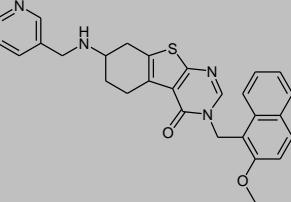
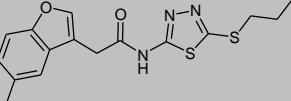
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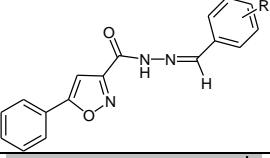
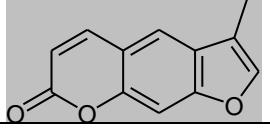
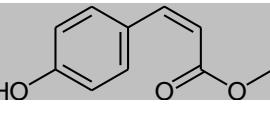
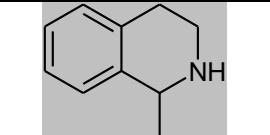
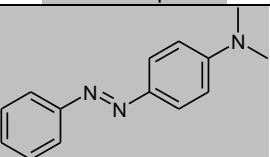
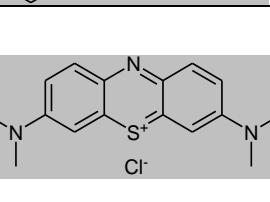
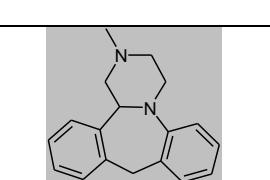
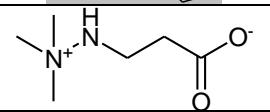
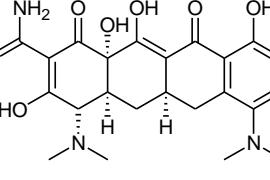
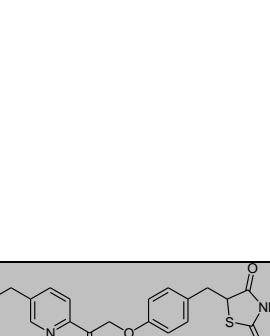
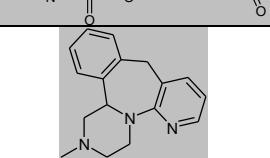
		
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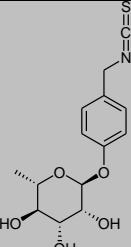
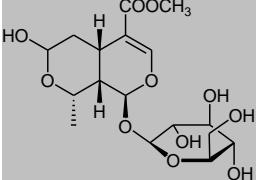
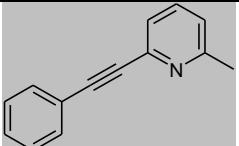
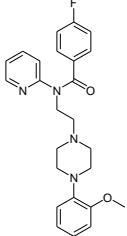
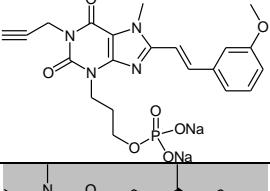
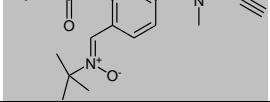
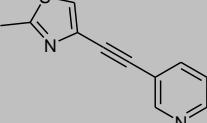
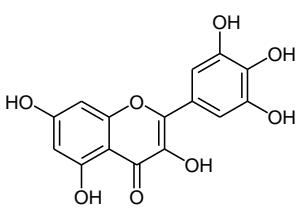
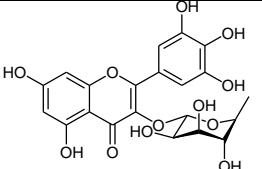
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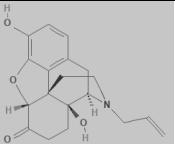
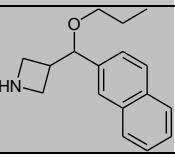
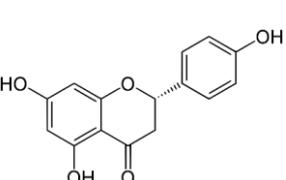
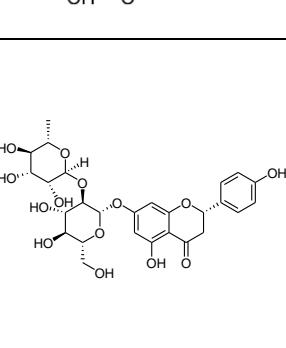
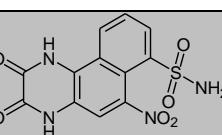
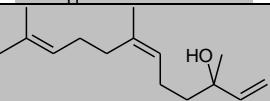
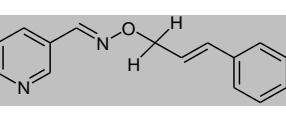
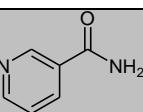
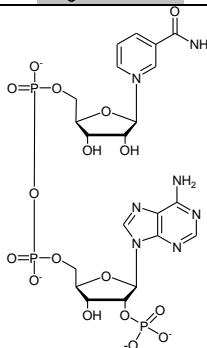
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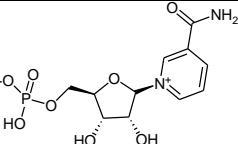
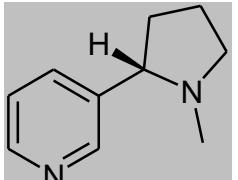
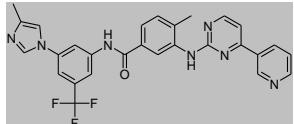
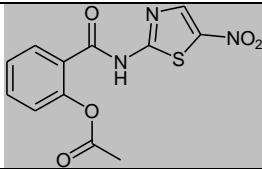
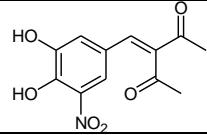
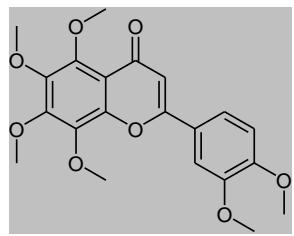
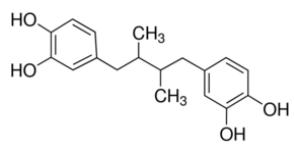
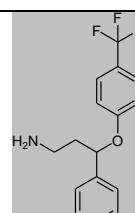
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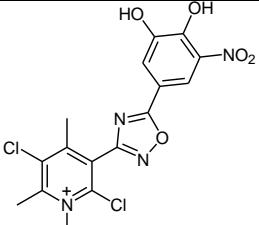
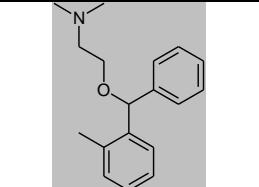
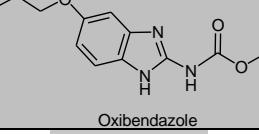
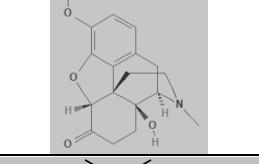
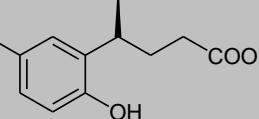
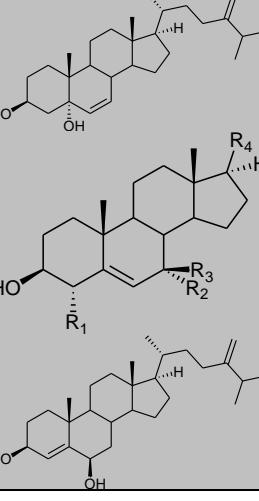
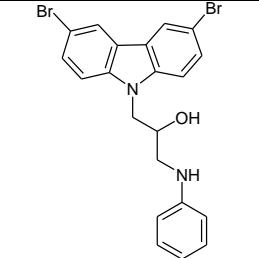
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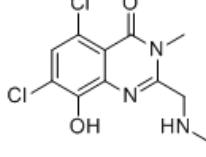
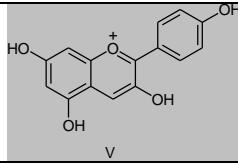
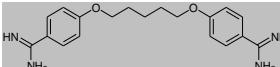
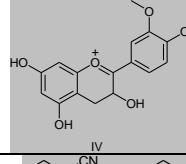
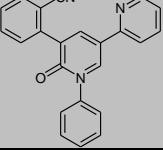
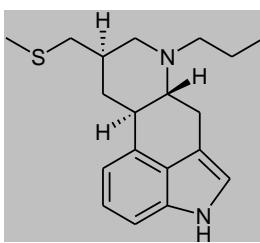
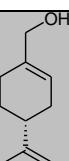
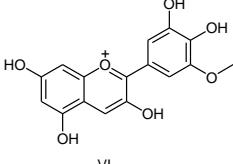
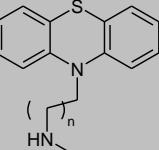
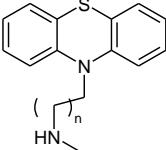
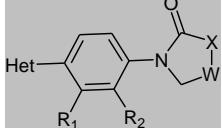
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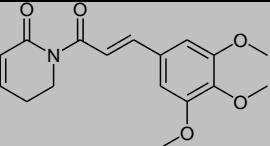
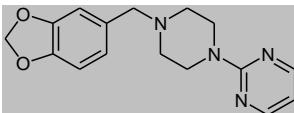
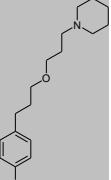
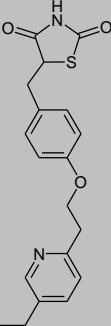
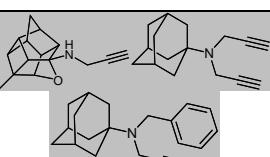
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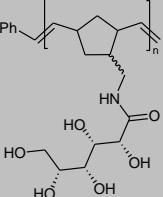
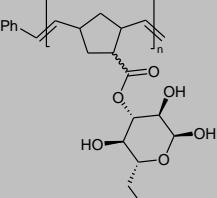
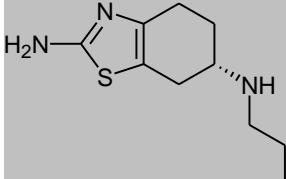
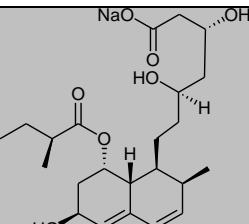
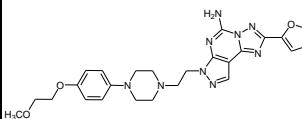
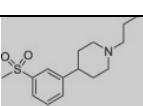
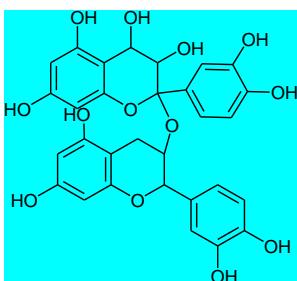
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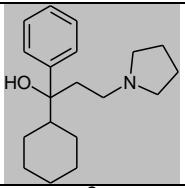
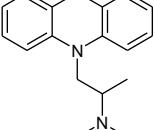
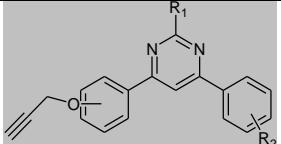
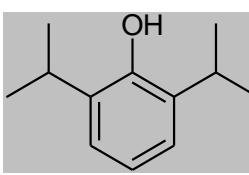
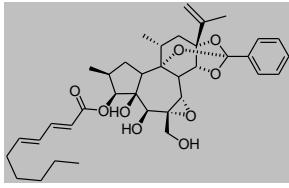
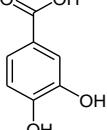
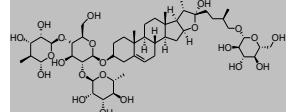
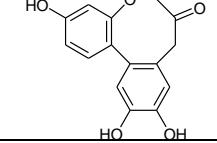
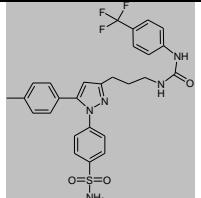
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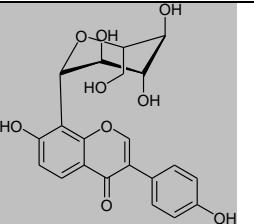
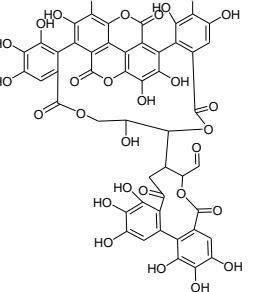
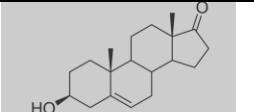
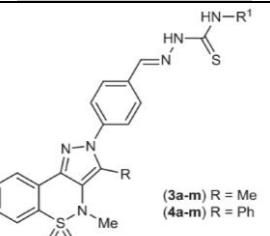
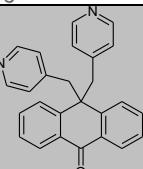
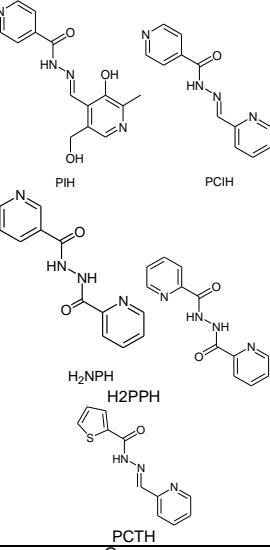
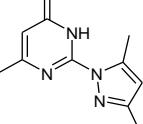
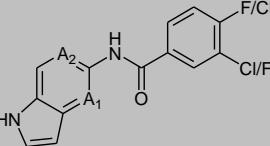
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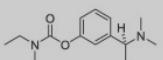
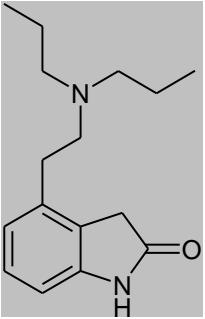
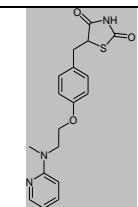
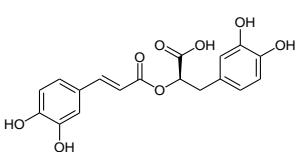
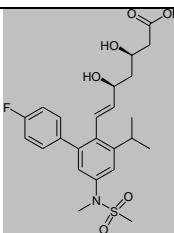
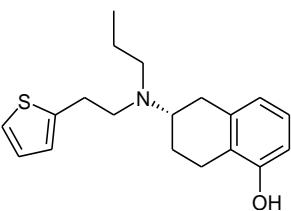
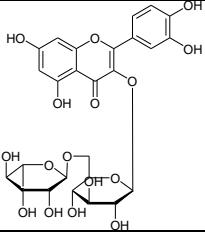
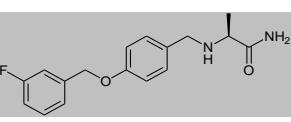
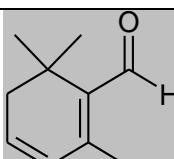
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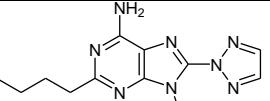
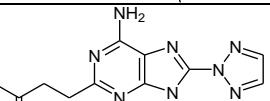
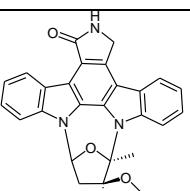
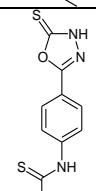
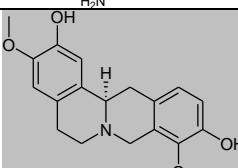
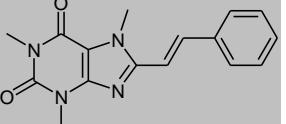
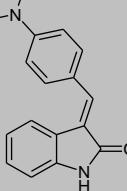
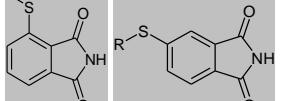
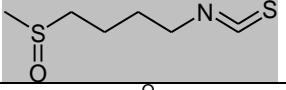
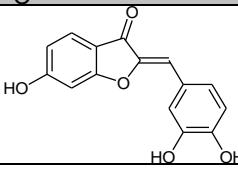
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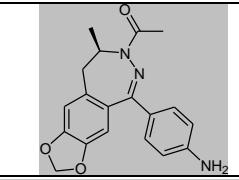
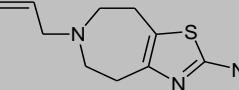
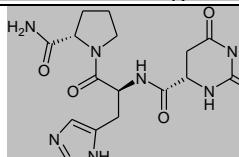
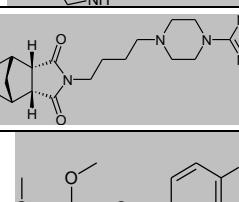
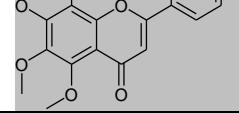
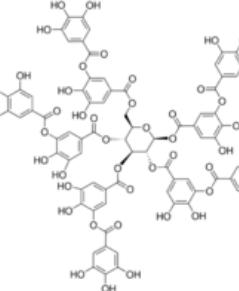
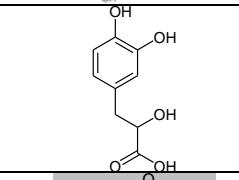
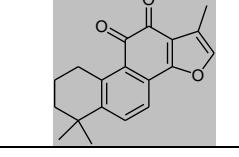
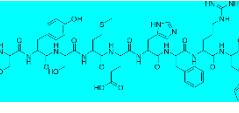
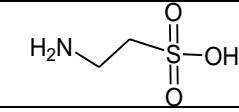
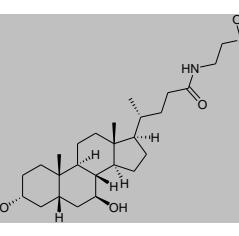
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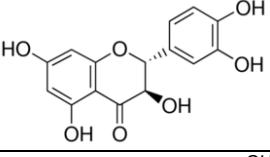
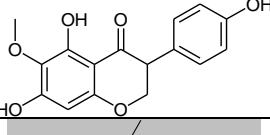
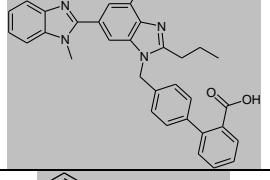
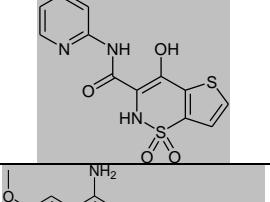
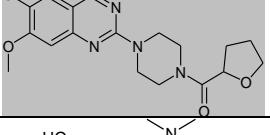
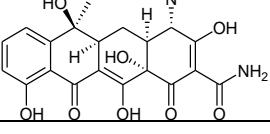
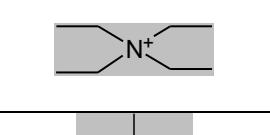
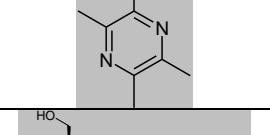
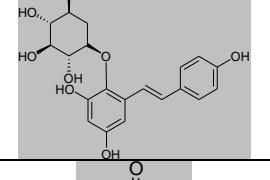
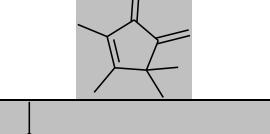
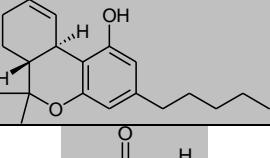
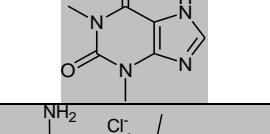
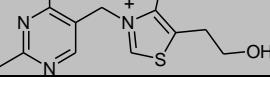
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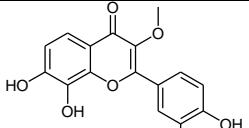
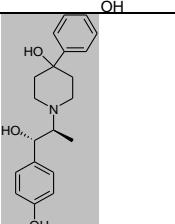
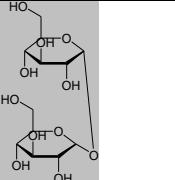
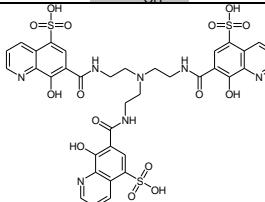
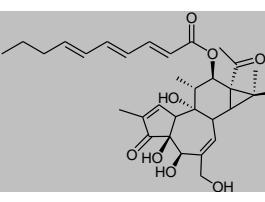
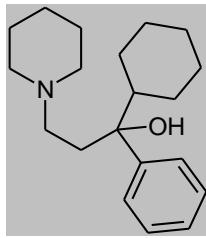
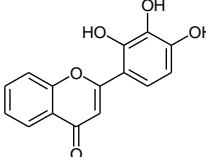
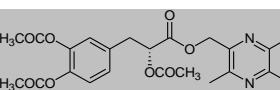
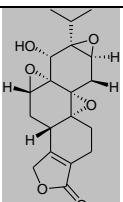
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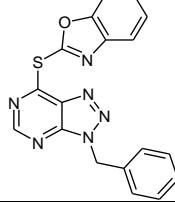
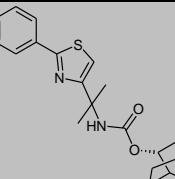
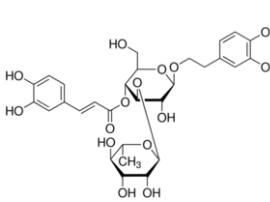
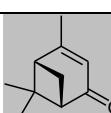
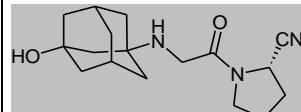
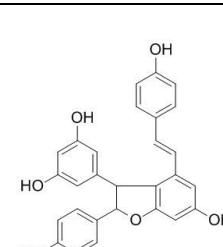
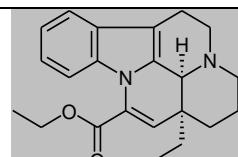
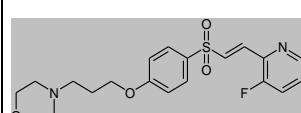
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TABLE S2

Acid-base and metal chelation properties of the compounds listed in Table 2. The formulas in the column marked “H<sup>+</sup>” represent the acid-base species, those in the other columns are the metal-ligand complexes, and the numbers are the corresponding values of log $\beta$  (see equation 2 in main text for the definition of  $\beta$ ). If not differently specified in the notes, values have been obtained at 25 °C and at a 0.1 M (= mol/L) ionic strength, and they have been taken from the IUPAC stability constants database (Academic Software, version 5.84).

Ligand	H <sup>+</sup>	Cu(II)	Cu(I)	Fe(III)	Fe(II)	Mn(II)	Zn(II)	Notes
7DH 7MH	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
8A 8B 8C	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
8E 8F	HL 4.23 H <sub>2</sub> L 5.55	CuL 9.00 CuL <sub>2</sub> 14.724	(23 °C, 0.0 M) CuL 4.59 CuL <sub>2</sub> 9.18	FeL 9.13 FeH <sub>-1</sub> L 6.96 FeH <sub>-2</sub> L 5.11 FeL <sub>2</sub> 18.11 FeH <sub>-1</sub> L <sub>2</sub> 14.74 FeH <sub>-2</sub> L <sub>2</sub> 10.76	FeL 3.98 FeL <sub>2</sub> 9.09 FeL <sub>3</sub> 12.63	MnL 2.62 MnL <sub>2</sub> 4.62 MnL <sub>3</sub> 5.72	ZnL 5.13 ZnL <sub>2</sub> 9.50	tentative, from 2,2'-bipyridine, charges unknown
N-Acetyl cysteine	HL <sup>-</sup> 9.62 H <sub>2</sub> L 12.70	CuHL <sup>+</sup> 13.35 CuL 6.64 CuL <sub>2</sub> <sup>2-</sup> 12.70		FeL <sup>+</sup> 10.58 FeL <sub>2</sub> <sup>-</sup> 18.80		MnHL <sup>+</sup> 12.66 MnL 3.64 MnL <sub>2</sub> <sup>2-</sup> 7.47	ZnL 4.90 ZnHL <sub>2</sub> <sup>-</sup> 18.39 ZnL <sub>2</sub> <sup>2-</sup> 11.48 ZnH <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 2.71	Fe(III) data (0.12 M) from [Guzeloglu 1998], Cu(II) and Mn(II) data (37 °C, 0.15 M) from [Santoso 2014]
ACPT-I	HL 10.31 H <sub>2</sub> L 12.71						ZnL 4.76 ZnL <sub>2</sub> 9.16	tentative, from 1-Amino-cyclopentane-carboxylic acid (20 °C), charges unknown
	HL 9.60 H <sub>2</sub> L 11.93	CuL 8.38 CuL <sub>2</sub> 15.25	(0.3 M) CuL <sub>2</sub> 10.0	FeL 10.83 FeL <sub>2</sub> 20.48	FeL 4.13 FeL <sub>2</sub> 7.65	MnL 2.85		tentative, from glycine, charges unknown
ADX88178	HL 9.74 H <sub>2</sub> L 16.30	CuL 8.77 CuL <sub>2</sub> 14.82						tentative, from 2,2'-Aminoethyl-pyrrolidine (30 °C, → 0 M), charges unknown
	HL 10.84 H <sub>2</sub> L 19.96		(20 °C, 1 M) CuL 11.92 CuL <sub>2</sub> 15.12					tentative, from 3-amino-propane-1-thiol, charges unknown
Alaternin	(0.0 M) HL 12.46 H <sub>2</sub> L 20.76	CuL 6.45 CuL <sub>2</sub> 12.30					ZnL 5.80	tentative, from 1,8-dihydroxy-anthraquinone (100% org. solv.), charges unknown
Alvespimycin	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
AM-251	HL 10.77	CuL 9.77					(20 °C)	tentative, from 1,3-diamino-

	H <sub>2</sub> L 19.62	CuL <sub>2</sub> 16.94				ZnHL 14.96 ZnHL <sub>2</sub> 20.22	propane, charges unknown	
Ambroxol	HL <sup>+</sup> 10.70 H <sub>2</sub> L <sup>2+</sup> 18.3	CuL <sup>+</sup> 11.95		FeL <sup>2+</sup> 18.54	MnL <sup>+</sup> 9.32	ZnL <sup>+</sup> 10.08 ZnL <sub>2</sub> 18.99 ZnL <sub>3</sub> <sup>-</sup> 24.94	data from [Naggar 2018]	
3-(7-Amino-5-(cyclohexylamino)-[1,2,4]triazolo[1,5-a][1,3,5]triazin-2-yl)-2-cyanoacrylamide	HL 9.35 H <sub>2</sub> L 14.08	CuL 9.22 CuL <sub>2</sub> 17.17					tentative, from 4(5)-Amino-methyl-imidazole, charges unknown	
	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80		(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Aminothiazoles derivatives as SUMOylation activators	HL 8.93 H <sub>2</sub> L 10.87	CuL 9.69 CuL <sub>2</sub> 16.90	(50% mix solv.) CuL <sub>2</sub> 10.66		(0.15 M) FeL 4.105 FeL <sub>2</sub> 7.441 FeL <sub>3</sub> 10.116	(20 °C) MnL 2.66	ZnL 5.2	tentative, from 2-(amino-methyl)pyridine, charges unknown
AMN082	0.0 M HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	0.0 M ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
Amodiaquine	HL 10.85 H <sub>2</sub> L 19.05	CuHL 13.54						tentative, from 2-dimethyl-amino-methyl-phenol (20 °C, 40% mix solv.), charges unknown
Antagonist of the A(2A) adenosine receptor derivative 49	HL 9.59 H <sub>2</sub> L 13.51	CuL 7.3 CuL <sub>2</sub> 12.90	(20 °C, 1 M) CuL <sub>2</sub> 10.90					tentative, from 2-(2'-amino-ethyl)pyridine, charges unknown
							(20 °C) ZnHL 14.96 ZnHL <sub>2</sub> 20.22	tentative, from 1,3-diaminopropane
Apigenin	HL <sup>2-</sup> 13.14 H <sub>2</sub> L <sup>-</sup> 21.68 H <sub>3</sub> L 31.61	CuH <sub>2</sub> L <sup>+</sup> 29.86 CuH <sub>4</sub> L <sub>2</sub> 58.38						50% mix solv.
	HL 11.34			FeL <sup>2+</sup> 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.)
	H <sub>3</sub> L 10.18 H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52						ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.), charges unknown
Apomorphine	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71	(1.0 M) FeHL 16.57 FeL 7.948	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

				$\text{FeL}_3$ 43.75	$\text{FeL}_2$ 13.488		
L-Arginine	HL <sup>+</sup> 9.104 H <sub>2</sub> L <sub>2</sub> <sup>+</sup> 11.099	CuL <sup>2+</sup> 7.652 CuL <sub>2</sub> <sup>2+</sup> 14.128 CuL <sub>2</sub> H <sub>-1</sub> 3.14		(20 °C, 1 M) $\text{FeL}^{3+}$ 8.7	20 °C, 0.01 M $\text{FeL}^{2+}$ 3.20	MnL <sup>2+</sup> 2.55	ZnL <sup>2+</sup> 4.11 ZnL <sub>2</sub> <sup>2+</sup> 8.07
Aromadendrin	HL 11.34	CuL 14.12		FeL 14.12			tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Ascorbic acid	HL 4.045	CuHL <sup>2+</sup> 3.94 CuL <sup>+</sup> 2.32 Cu <sub>2</sub> L <sub>2</sub> <sup>2+</sup> 6.33 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 0.05		(0.05 M) $\text{FeL}_2^+$ 6.36	(20 °C, 1 M) $\text{FeL}^+$ -0.27 $\text{FeL}_2$ 1.54		(20 °C, 1 M) ZnL <sup>+</sup> 4.34 ZnL <sub>2</sub> 7.50
ASI-1	HL 10.69 H <sub>2</sub> L 19.99 H <sub>3</sub> L 28.53			FeH <sub>2</sub> L 29.13 FeL 22.06			tentative, from curcumin (50% mix solv.), charges unknown
	HL 8.83	CuL <sup>+</sup> 8.0 CuL <sub>2</sub> 14.8			FeL <sup>+</sup> 5.2	MnL <sup>+</sup> 3.91 MnL <sub>2</sub> 6.82	ZnL <sup>+</sup> 4.70 ZnL <sub>2</sub> 8.3
ASI-5	HL 5.85	CuL 2.77				MnL 2.12	ZnL 2.07
	HL 10.17 H <sub>2</sub> L 17.08 H <sub>3</sub> L 19.79			FeL 19.9 FeL <sub>2</sub> 26.6	FeHL 16.77 FeL 12.6 FeH <sub>2</sub> L <sub>2</sub> 32.24 FeL <sub>2</sub> 18.8 Fe <sub>2</sub> HL 19.27 Fe <sub>2</sub> L 15.4		tentative, from methane-diphosphonic acid, charges unknown
Astilbin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) $\text{FeL}$ 20.05 FeL <sub>2</sub> 34.71 $\text{FeL}_3$ 43.75	FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20
Azilsartan	HL 5.34	CuL 3.45 CuL <sub>2</sub> 6.30					(35 °C, 50 % mix solv.) ZnL 3.3 ZnL <sub>2</sub> 5.8
	HL 10.098 H <sub>2</sub> L 13.660				(20 °C, 0.01 M) FeL <sub>2</sub> 4.0	(20 °C) MnL 2.13	tentative, from $\beta$ -alanine, charges unknown
Baicalein	HL <sup>-</sup> 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> <sup>2-</sup> 23.01			FeL 12.88 FeL <sub>2</sub> <sup>2-</sup> 23.66	MnL 6.41 MnL <sub>2</sub> <sup>2-</sup> 10.82	ZnL 8.41 ZnL <sub>2</sub> <sup>2-</sup> 14.87
	HL 11.34			FeL <sup>2+</sup> 14.12			tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.)
Benserazide	HL <sup>-</sup> 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> 23.01			FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82	ZnL 8.41 ZnL <sub>2</sub> 14.87
7H-Benzo[e] perimidin-7-	HL 8.75	(30 °C, 75% mix solv.)					ZnL 4.21
							tentative, from 5-hydroxy-1,4-

one derivatives (R <sub>6</sub> = OH)		CuL 11.24 CuL <sub>2</sub> 20.91				ZnL <sub>2</sub> 12.07	naphtho-quinone (50% mix solv.), charges unknown	
4H-1-Benzopyran-4-one	HL 11.34	CuL <sup>2+</sup> 14.12		FeL <sup>2+</sup> 14.12			tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.)	
	H <sub>3</sub> L 10.18 H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52					ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.), charges unknown	
8-Benzyl-tetrahydropyrazino[2,1-f]purinedione (derivative n. 57)	HL 3.80	CuL 2.58				ZnL 1.10	tentative, from 2-(2'-Pyridyl)-thiophene, charges unknown	
	HL 10.69 H <sub>2</sub> L 18.87		(20 °C, 1.0 M) CuL 10.80 CuL <sub>2</sub> 13.50				tentative, from 2-aminoethanethiol, charges unknown	
Bikaverin	HL <sup>-</sup> 11.35 H <sub>2</sub> L 16.91					ZnL 8.23 ZnH <sub>-2</sub> L <sup>2-</sup> -5.95	tentative, from 5,8-dihydroxy-1,4-naphtho-quinone (25 °C, 50% mix solv.)	
	HL 8.75	(30 °C, 75% mix solv.) CuL 11.24 CuL <sub>2</sub> 20.91					tentative, from 5-hydroxy-1,4-naphtho-quinone (50% mix solv.), charges unknown	
(-)N6-(2-(4-(Biphenyl-4-yl)piperazin-1-yl)-ethyl)-N6-propyl-4,5,6,7-tetrahydrobenzo[d]thiazole-2,6-diamine derivatives	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
2,2'-Bipyridyl	HL <sup>+</sup> 4.23 H <sub>2</sub> L <sup>2+</sup> 5.55	CuL <sup>2+</sup> 9.00 CuL <sub>2</sub> <sup>2+</sup> 14.724	(23 °C, 0.0 M) CuL <sup>+</sup> 4.59 CuL <sub>2</sub> <sup>+</sup> 9.18	FeL <sup>3+</sup> 9.13 FeH <sub>-1</sub> L <sup>2+</sup> 6.96 FeH <sub>-2</sub> L <sup>+</sup> 5.11 FeL <sub>2</sub> <sup>3+</sup> 18.11 FeH <sub>-1</sub> L <sub>2</sub> <sup>2+</sup> 14.74 FeH <sub>-2</sub> L <sub>2</sub> <sup>+</sup> 10.76	FeL <sup>2+</sup> 3.98 FeL <sub>2</sub> <sup>2+</sup> 9.09 FeL <sub>3</sub> <sup>2+</sup> 12.63	MnL <sup>2+</sup> 2.62 MnL <sub>2</sub> <sup>2+</sup> 4.62 MnL <sub>3</sub> <sup>2+</sup> 5.72	ZnL <sup>2+</sup> 5.13 ZnL <sub>2</sub> <sup>2+</sup> 9.50	
4-((5-Bromo-3-chloro-2-hydroxybenzyl) amino)-2-hydroxybenzoic acid (LX007, ZL006)	HL 13.74 H <sub>2</sub> L 17.82 H <sub>3</sub> L 18.10	(37 °C, 0.15 M) CuHL 15.57 CuL 10.63		FeL 16.97 FeL <sub>2</sub> 29.01 FeL <sub>3</sub> 36.05			(37 °C, 0.15 M) ZnH <sub>-1</sub> L -0.95	tentative, from 5-amino-salicylic acid (3.0 M), charges unknown
	HL 13.44 H <sub>2</sub> L 16.22				(20 °C) FeL 6.55 FeL <sub>2</sub> 11.25	MnL 6.10		tentative, from salicylic acid, charges unknown
C-3 ( $\alpha$ carboxyfullerene)	HL 5.29 H <sub>2</sub> L 8.05	CuL 5.81 CuL <sub>2</sub> 7.73		FeL 8.04 FeL <sub>2</sub> 13.54	(1.0 M) FeL 2.17 FeL <sub>2</sub> 3.21	(0.16 M) MnL 2.30	ZnL 2.7	tentative, from malonic acid, charges unknown

Caffeic acid amide analogues	HL 8.72 H <sub>2</sub> L 13.13	CuHL 10.46 CuL 6.02 CuH <sub>-1</sub> L 0.25 Cu <sub>2</sub> H <sub>-1</sub> L 3.54 Cu <sub>2</sub> H <sub>-3</sub> L <sub>3</sub> 0.97 Cu <sub>3</sub> H <sub>-2</sub> L <sub>2</sub> 7.41			FeL 3.86 FeH <sub>-1</sub> L -3.83 FeH <sub>-1</sub> L <sub>2</sub> -0.36 FeH <sub>-2</sub> L <sub>3</sub> -6.14 Fe <sub>2</sub> L 6.69	MnH <sub>-1</sub> L -4.88 MnH <sub>-2</sub> L -15.55	ZnL 2.99 ZnH <sub>-1</sub> L -3.03 ZnH <sub>-1</sub> L <sub>2</sub> -0.39 ZnH <sub>-2</sub> L <sub>2</sub> -8.21 ZnH <sub>-2</sub> L <sub>3</sub> -5.51	tentative, from caffeic acid, charges unknown
	HL 12.8 H <sub>2</sub> L 22.17		(22 °C)	FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				tentative, from catechol (1 M), charges unknown
Carbazole-derived compounds	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
Carbidopa	HL 9.77 H <sub>2</sub> L 18.61 H <sub>3</sub> L 20.78	CuHL 17.25 CuH <sub>2</sub> L <sub>2</sub> 33.70 CuH L <sub>2</sub> 26.9 CuH <sub>-1</sub> L 9.35 CuH <sub>-2</sub> L 3.20 Cu <sub>2</sub> L <sub>2</sub> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22		(0.12 M) FeH <sub>2</sub> L 31.92 FeL 18.39	FeL 8.80	(0.2 M) MnHL 17.76 MnL 8.14 MnH <sub>2</sub> L <sub>2</sub> 33.43 MnHL <sub>2</sub> 23.75 MnL <sub>2</sub> 12.43	ZnHL 13.77 ZnL <sub>2</sub> 11.07 Zn <sub>2</sub> L <sub>2</sub> 16.55	tentative, from L-dopa, charges unknown
Carnosic acid	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Catechin	HL <sup>3-</sup> 13.26 H <sub>2</sub> L <sup>2-</sup> 24.52 H <sub>3</sub> L <sup>-</sup> 33.93 H <sub>4</sub> L 42.57			FeHL 21.8 FeH <sub>2</sub> L <sub>2</sub> <sup>3-</sup> 37.5 FeH <sub>3</sub> L <sub>3</sub> <sup>6-</sup> 47.4				unspecified ionic strength
	HL <sup>3-</sup> 11.50 H <sub>2</sub> L <sup>2-</sup> 22.36 H <sub>3</sub> L <sup>-</sup> 31.56 H <sub>4</sub> L 39.72	CuH <sub>2</sub> L 31.81 CuHL <sup>-</sup> 23.84 CuL <sup>2-</sup> 14.45						data from [Teixeira 2005]
	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51			(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Ceftriaxone	HL <sup>-</sup> 4.35 H <sub>2</sub> L 7.54 H <sub>3</sub> L <sup>+</sup> 9.88	CuL 2.5					ZnL 4.45	data from [Mayakova 2016]
	HL 9.60		(0.3 M)	FeL 10.83	FeL 4.13	MnL 2.85		tentative, from glycine, charges

	H <sub>2</sub> L 11.93		CuL <sub>2</sub> 10.0	FeL <sub>2</sub> 20.48	FeL <sub>2</sub> 7.65			unknown
Celastrol	HL 12.5 H <sub>2</sub> L 21.18	(30 °C, 0.2 M) CuL 11.78 CuL <sub>2</sub> 20.86		(unspecified temperature) FeL 20.85 FeL <sub>2</sub> 36.15 FeL <sub>3</sub> 45.95				tentative, from 2,3-dihydroxy-naphthalene (20 °C), charges unknown
	HL 12.8 H <sub>2</sub> L 22.17				(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
CEP-1347	HL 10.098 H <sub>2</sub> L 13.660				(20 °C, 0.01 M) FeL <sub>2</sub> 4.0	(20 °C) MnL 2.13		tentative, from $\beta$ -alanine, charges unknown
Chebulagic acid	HL 12 H <sub>2</sub> L 23.2 H <sub>3</sub> L 31.8 H <sub>4</sub> L 36.2	(40% mix solv.) CuHL 21.90 CuH <sub>2</sub> L <sub>2</sub> 43.04		FeH <sub>2</sub> L 33.7 FeHL 30.05 FeL 22.28 FeH <sub>4</sub> L <sub>2</sub> 64.7 FeH <sub>2</sub> L <sub>2</sub> 50.01 FeL <sub>2</sub> 33.89 FeH <sub>6</sub> L <sub>3</sub> 94.4 FeH <sub>3</sub> L <sub>3</sub> 69.16 FeL <sub>3</sub> 42.15			Zn <sub>2</sub> L 11.4	tentative, from gallic acid, charges unknown
	HL 10.85 H <sub>2</sub> L 19.61				FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82		tentative, from pyrogallol (30 °C), charges unknown
Chlorogenic acid	HL <sup>2-</sup> 12.06 H <sub>2</sub> L <sup>-</sup> 20.36 H <sub>3</sub> L 23.71	CuHL 16.92 CuL <sup>-</sup> 12.74 CuL <sub>2</sub> <sup>4-</sup> 23.35		FeL 17.64 FeHL <sup>+</sup> 22.20		MnL <sup>-</sup> 7.02 MnL <sub>2</sub> <sup>4-</sup> 12.13	ZnL <sup>-</sup> 8.79 ZnL <sub>2</sub> <sup>4-</sup> 16.20	(20 °C, 1.0 M)
	HL 12.20 H <sub>2</sub> L 21.45				FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488			tentative, from catechol (1.0 M), charges unknown
3'-O-(3-Chloropivaloyl)quercetin	HL 11.34	CuL 14.12		FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
	H <sub>3</sub> L 10.18 H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52						ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.), charges unknown
Chlorpromazine	HL <sup>+</sup> 10.77 H <sub>2</sub> L <sup>2+</sup> 19.62	CuL <sup>2+</sup> 9.77 CuL <sub>2</sub> <sup>2+</sup> 16.94					(20 °C) ZnHL <sup>3+</sup> 14.96 ZnHL <sub>2</sub> <sup>3+</sup> 20.22	tentative, from 1,3-diamino-propane
Chrysins	(50% mix solv.) HL <sup>-</sup> 12.37 H <sub>2</sub> L 20.74	(50% mix solv.) CuHL <sup>+</sup> 23.01		FeL <sup>+</sup> 11.40				data for Fe(III) (44.6% mix solv.) from [Engelmann 2005]
	H <sub>3</sub> L 10.18						ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.)

	H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52							solv.), charges unknown
Clioquinol	HL 9.07 H <sub>2</sub> L <sup>+</sup> 10.57				FeL <sup>+</sup> 7.61 FeL <sub>2</sub> 15.41 FeL <sub>3</sub> 20.23			(50% mix solv., 0.3 M)
	HL 9.684 H <sub>2</sub> L <sup>+</sup> 14.70	CuL <sup>+</sup> 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> <sup>-</sup> 14.7	FeL <sup>2+</sup> 13.69 FeL <sub>2</sub> <sup>+</sup> 26.3 FeL <sub>3</sub> 36.9		MnL <sup>+</sup> 7.85 MnL <sub>2</sub> 14.40	ZnL <sup>+</sup> 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline
Clioquinol-selegiline hybrid	HL 10.25 H <sub>2</sub> L 18.11 H <sub>3</sub> L 22.52 H <sub>4</sub> L 25.47			FeH <sub>4</sub> L 52.11 FeH <sub>2</sub> L 27.04 FeH <sub>2</sub> L <sub>2</sub> 45.3 FeHL <sub>2</sub> 39.25 FeL <sub>2</sub> 34.0	FeH <sub>4</sub> L <sub>2</sub> 43.2 FeH <sub>2</sub> L <sub>2</sub> 32.97			tentative, from pyridoxal isonicotinoyl hydrazone, charges unknown
Clovamide analogues (R <sub>1</sub> and R <sub>2</sub> = OH, and/or R <sub>3</sub> and R <sub>4</sub> = OH)	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
"Compound 1"	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
"Compound (-) -8a"	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
"Compound 8"	HL 10.69 H <sub>2</sub> L 18.87	(0.26 M) CuL <sub>2</sub> 16.74	(20 °C, 1.0 M) CuL 10.80 CuL <sub>2</sub> 13.50				ZnL 8.77 ZnH <sub>-1</sub> L 1.94 ZnL <sub>2</sub> 15.72	tentative, from 2-aminoethanethiol, charges unknown
"Compound 21", derivative of 3-methyl-1-(2,4,6-trihydroxyphenyl) butan-1-one	HL 9.60 H <sub>2</sub> L <sup>+</sup> 11.93	CuL <sup>+</sup> 8.38 CuL <sub>2</sub> 15.25	(0.3 M) CuL <sub>2</sub> <sup>-</sup> 10.0	FeL <sup>2+</sup> 10.83 FeL <sub>2</sub> <sup>+</sup> 20.48	FeL <sup>+</sup> 4.13 FeL <sub>2</sub> 7.65	MnL <sup>+</sup> 2.85	ZnL <sup>+</sup> 5.03 ZnL <sub>2</sub> 9.30	tentative, from glycine
"Compound (-) - 21 a", derivative of N-6-(2-(4-(1H-indol-5-yl)piperazin-1-yl)ethyl)-N-6-propyl-4,5,6,7-tetrahydrobenzo[d]thiazole-2,6-diamine	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
Creatine	HL 11.04 H <sub>2</sub> L 15.29	CuHL 14.41 CuL 7.89 CuH <sub>-1</sub> L 1.97						tentative, from phospho-creatine, charges unknown

	HL 9.60 H <sub>2</sub> L <sup>+</sup> 11.93		(0.3 M) CuL <sub>2</sub> <sup>-</sup> 10.0	FeL <sup>2+</sup> 10.83 FeL <sub>2</sub> <sup>+</sup> 20.48	FeL <sup>+</sup> 4.13 FeL <sub>2</sub> 7.65	MnL <sup>+</sup> 2.85	ZnL <sup>+</sup> 5.03 ZnL <sub>2</sub> 9.30	tentative, from glycine
Cudraflavone B	HL 11.34	CuL 14.12		FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
	H <sub>3</sub> L 10.18 H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52						ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.), charges unknown
Curcumin	HL <sup>2-</sup> 10.51 H <sub>2</sub> L <sup>-</sup> 20.39 H <sub>3</sub> L 28.77			FeL 22.25 FeH <sub>-1</sub> L <sup>-</sup> 12.14	FeH <sub>2</sub> L <sup>+</sup> 28.11 FeHL 19.76 FeL <sup>-</sup> 9.20			unspecified ionic strength; data from [Bernabé-Pineda 2004]
	HL 8.83	CuL 8.0 CuL <sub>2</sub> 14.8				MnL 3.91 MnL <sub>2</sub> 6.82	ZnL 4.70 ZnL <sub>2</sub> 8.3	tentative, from acetyl-acetone, charges unknown
Cyanidin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
D512	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diamino-ethane (1.0 M)
D607 (bipyridyl-D2R/D3R agonist hybrid)	HL 4.23 H <sub>2</sub> L 5.55	CuL 9.00 CuL <sub>2</sub> 14.724	(23 °C, 0.0 M) CuL 4.59 CuL <sub>2</sub> 9.18	FeL 9.13 FeH <sub>-1</sub> L 6.96 FeH <sub>-2</sub> L 5.11 FeL <sub>2</sub> 18.11 FeH <sub>-1</sub> L <sub>2</sub> 14.74 FeH <sub>-2</sub> L <sub>2</sub> 10.76	FeL 3.98 FeL <sub>2</sub> 9.09 FeL <sub>3</sub> 12.63	MnL 2.62 MnL <sub>2</sub> 4.62 MnL <sub>3</sub> 5.72	ZnL 5.13 ZnL <sub>2</sub> 9.50	tentative, from 2,2'-bipyridine, charges unknown
DA-2 (8D)	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
DA-3	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diamino-ethane (1.0 M), charges unknown
	HL 12.20 H <sub>2</sub> L 21.45			(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				tentative, from catechol (1.0 M), charges unknown
DA-4	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diamino-ethane (1.0 M), charges unknown
	HL 12.20 H <sub>2</sub> L 21.45			(22 °C) FeL 20.05				tentative, from catechol (1.0 M), charges unknown

				FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				
Dabigatran etexilate	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Dabrafenib	HL 3.80	CuL 2.58					ZnL 1.10	tentative, from 2-(2'-pyridyl)-thiophene, charges unknown
	HL 10.84 H <sub>2</sub> L 19.96		(20 °C, 1 M) CuL 11.92 CuL <sub>2</sub> 15.12					tentative, from 3-amino-propane-1-thiol, charges unknown
(S)-3,4-DCPG	HL 4.967 H <sub>2</sub> L 7.71	CuL 3.45				MnL 2.23	ZnL 2.18	tentative, from phthalic acid, charges unknown
Deferasirox (Exjade)	HL <sup>2-</sup> 10.61 H <sub>2</sub> L <sup>-</sup> 19.41			FeHL <sup>+</sup> 24.3 FeL 22.0 FeH <sub>2</sub> L <sub>2</sub> <sup>-</sup> 43.4 FeHL <sub>2</sub> <sup>2-</sup> 41.2 FeL <sub>2</sub> <sup>3-</sup> 36.90				
Deferricoprogen	HL <sup>2-</sup> 9.84 H <sub>2</sub> L <sup>-</sup> 18.84 H <sub>3</sub> L 26.84	CuH <sub>2</sub> L <sup>+</sup> 26.89 CuHL 23.70 CuL <sup>-</sup> 15.25		FeL 29.35			ZnH <sub>2</sub> L <sup>+</sup> 23.60 ZnHL 19.23 ZnL <sup>-</sup> 11.80	(0.2 M)
Delphinidin	HL 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> 23.01			FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82	ZnL 8.41 ZnL <sub>2</sub> 14.87	tentative, from pyrogallol (30 °C), charges unknown
	HL 12.8 H <sub>2</sub> L 22.17			FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				tentative, from catechol (22 °C), charges unknown
Demethoxycurcumin	HL <sup>2-</sup> 10.69 H <sub>2</sub> L <sup>-</sup> 19.99 H <sub>3</sub> L 28.53			FeH <sub>2</sub> L <sup>2+</sup> 29.13 FeL 22.06				tentative, from curcumin (50% mix solv.)
	HL 8.83	CuL 8.0 CuL <sub>2</sub> 14.8			FeL 5.2	MnL 3.91 MnL <sub>2</sub> 6.82	ZnL 4.70 ZnL <sub>2</sub> 8.3	tentative, from acetyl-acetone, charges unknown
Dendropanax morbifera active compound	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Desferrioxamine (deferoxamine, DFO)	HL <sup>2-</sup> 10.89 H <sub>2</sub> L <sup>-</sup> 20.44 H <sub>3</sub> L 29.42 H <sub>4</sub> L <sup>+</sup> 37.74	CuH <sub>3</sub> L <sup>2+</sup> 37.08 CuH <sub>2</sub> L <sup>+</sup> 33.38 CuHL 24.43 Cu <sub>2</sub> HL <sup>2+</sup> 32.14		FeHL <sup>+</sup> 41.39 FeL 30.99	FeH <sub>3</sub> L <sup>2+</sup> 33.22 FeH <sub>2</sub> L <sup>+</sup> 27.64		ZnH <sub>3</sub> L <sup>2+</sup> 33.71 ZnH <sub>2</sub> L <sup>+</sup> 28.32 ZnHL 20.44	
(S)-N-(3-(3,6-Dibromo-9H-carbazol-9-yl)-2-fluoropropyl)-6-	HL 10.77 H <sub>2</sub> L 19.62	CuL 9.77 CuL <sub>2</sub> 16.94					(20 °C) ZnHL 14.96 ZnHL <sub>2</sub> 20.22	tentative, from 1,3-diaminopropane, charges unknown

methoxypyridin-2-amine								
4,5-O-Dicaffeoyl-1-O-(malic acid methyl ester)-quinic acid derivatives (R <sub>1</sub> , R <sub>2</sub> , R <sub>3</sub> , R <sub>4</sub> , or R <sub>5</sub> = caffeoyl)	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Dihydromyricetin	HL 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> 23.01			FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82	ZnL 8.41 ZnL <sub>2</sub> 14.87	tentative, from pyrogallol (30 °C), charges unknown
	HL 12.8 H <sub>2</sub> L 22.17			FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				tentative, from catechol (22 °C), charges unknown
5-(3,4-Dihydroxybenzylidene)-2,2-dimethyl-1,3-dioxane-4,6-dione	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
7,8-Dihydroxycoumarin derivative DHC12	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
3',4'-Dihydroxyflavone	HL <sup>-</sup> 13.43 H <sub>2</sub> L 21.82			FeL <sup>+</sup> 20.87				data for Fe(III) (44.6% mix solv.) from [Engelmann 2005]
	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51			(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
7,8-Dihydroxyflavone	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
5,7-Dihydroxy-4'-methoxyflavone	HL 11.79	CuL 9.83						tentative, from 5-hydroxy-7-methoxy-flavone (50% mix solv.), charges unknown
	HL 7.74			(20 °C, 10% mix solv.) FeL 12.74 FeL <sub>2</sub> 23.25				tentative, from 5-hydroxy-chromone, charges unknown
(E)-3,4-Dihydroxystyryl aralkyl sulfones	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
(E)-3,4-Dihydroxystyryl aralkyl sulfoxides	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05	(1.0 M) FeHL <sup>+</sup> 16.57	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol

				FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488			
5,3'-Dihydroxy-3,7,4'-trimethoxyflavone	HL 11.79	CuL 9.83						tentative, from 5-hydroxy-7-methoxy-flavone (50% mix solv.), charges unknown
	HL 7.74			(20 °C, 10% mix solv.) FeL 12.74 FeL <sub>2</sub> 23.25				tentative, from 5-hydroxy-chromone, charges unknown
2-[(1,1-Dimethylethyl)oxidoimino]-methyl]-3,5,6-trimethylpyrazine	HL 10.01 H <sub>2</sub> L 13.60	CuHL 13.94 CuL 10.91 CuH <sub>2</sub> L <sub>2</sub> 27.50 CuHL <sub>2</sub> 25.45 CuL <sub>2</sub> 18.49 Cu <sub>3</sub> H <sub>-1</sub> L <sub>3</sub> 35.6 Cu <sub>3</sub> H <sub>-2</sub> L <sub>3</sub> 29.06	(20 °C, 0.5 M) CuH <sub>2</sub> L <sub>2</sub> 31.07 CuL <sub>2</sub> 14.4	(24 °C) FeL 11.40 FeL <sub>2</sub> 21.70 FeL <sub>3</sub> 30.10	(24 °C) FeL 9.40 FeL <sub>2</sub> 17.40 FeL <sub>3</sub> 22.50	(0.3 M) MnL 5.20 MnL <sub>2</sub> 9.10	ZnHL 11.912 ZnL 5.20 ZnHL <sub>2</sub> 17.52 ZnL <sub>2</sub> 10.58 ZnL <sub>3</sub> 12.94 Zn <sub>2</sub> L <sub>2</sub> 13.26 Zn <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> 6.724 Zn <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> -2.64	tentative, from pyridine-2-aldoxime, charges unknown
DKP	HL 9.81 H <sub>2</sub> L 15.88	CuHL 12.88 CuL 9.56 CuHL <sub>2</sub> 21.82 CuL <sub>2</sub> 16.06	CuL 8.87 CuH <sub>2</sub> L <sub>2</sub> 20.13	FeL <sub>2</sub> 7.05	(0.058 M) FeL 5.80 FeL <sub>2</sub> 10.06	(35 °C) MnHL 12.83	ZnHL 11.72 ZnL 5.21 ZnL <sub>2</sub> 10.13	tentative, from histamine, charges unknown
L-DOPA (levodopa, CVT-301)	HL <sup>2-</sup> 9.77 H <sub>2</sub> L <sup>-</sup> 18.61 H <sub>3</sub> L 20.78	CuHL 17.25 CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.70 CuH L <sub>2</sub> <sup>3-</sup> 26.9 CuH <sub>-1</sub> L <sup>2-</sup> 9.35 CuH <sub>-2</sub> L <sup>3-</sup> 3.20 Cu <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22		(0.12 M) FeH <sub>2</sub> L <sup>2+</sup> 31.92 FeL 18.39	FeL <sup>-</sup> 8.80	(0.2 M) MnHL 17.76 MnL <sup>-</sup> 8.14 MnH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.43 MnHL <sub>2</sub> <sup>3-</sup> 23.75 MnL <sub>2</sub> <sup>4-</sup> 12.43	ZnHL 13.77 ZnL <sub>2</sub> <sup>4-</sup> 11.07 Zn <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 16.55	
DOPA-derived peptido-mimetics (deprotected)	HL 9.77 H <sub>2</sub> L 18.61 H <sub>3</sub> L 20.78	CuHL 17.25 CuH <sub>2</sub> L <sub>2</sub> 33.70 CuH L <sub>2</sub> 26.9 CuH <sub>-1</sub> L 9.35 CuH <sub>-2</sub> L 3.20 Cu <sub>2</sub> L <sub>2</sub> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22		(0.12 M) FeH <sub>2</sub> L 31.92 FeL 18.39	FeL 8.80	(0.2 M) MnHL 17.76 MnL 8.14 MnH <sub>2</sub> L <sub>2</sub> 33.43 MnHL <sub>2</sub> 23.75 MnL <sub>2</sub> 12.43	ZnHL 13.77 ZnL <sub>2</sub> 11.07 Zn <sub>2</sub> L <sub>2</sub> 16.55	tentative, from L-dopa, charges unknown
DOPA-derived peptido-mimetics (protected)	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
L-DOPA deuterated	HL <sup>2-</sup> 9.77	CuHL 17.25		(0.12 M)	FeL <sup>-</sup> 8.80	(0.2 M)	ZnHL 13.77	tentative, from L-dopa

	H <sub>2</sub> L <sup>-</sup> 18.61 H <sub>3</sub> L 20.78	CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.70 CuH L <sub>2</sub> <sup>3-</sup> 26.9 CuH <sub>-1</sub> L <sup>2-</sup> 9.35 CuH <sub>-2</sub> L <sup>3-</sup> 3.20 Cu <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22		FeH <sub>2</sub> L <sup>2+</sup> 31.92 FeL 18.39		MnHL 17.76 MnL <sup>-</sup> 8.14 MnH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.43 MnHL <sub>2</sub> <sup>3-</sup> 23.75 MnL <sub>2</sub> <sup>4-</sup> 12.43	ZnL <sub>2</sub> <sup>4-</sup> 11.07 Zn <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 16.55	
Doxycycline	HL 13.00 H <sub>2</sub> L 18.35	CuL 13.45 CuL <sub>2</sub> 23.71	(30 °C) Cu <sub>2</sub> L 22.68	FeL 20.6 FeL <sub>2</sub> 33.50	(27 °C) FeL 6.00 FeL <sub>2</sub> 9.45		ZnL 10.03	tentative, from chromotropic acid, charges unknown
Droxidopa	HL <sup>2-</sup> 9.77 H <sub>2</sub> L <sup>-</sup> 18.61 H <sub>3</sub> L 20.78	CuHL 17.25 CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.70 CuH L <sub>2</sub> <sup>3-</sup> 26.9 CuH <sub>-1</sub> L <sup>2-</sup> 9.35 CuH <sub>-2</sub> L <sup>3-</sup> 3.20 Cu <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22		(0.12 M) FeH <sub>2</sub> L <sup>2+</sup> 31.92 FeL 18.39	FeL <sup>-</sup> 8.80	(0.2 M) MnHL 17.76 MnL <sup>-</sup> 8.14 MnH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.43 MnHL <sub>2</sub> <sup>3-</sup> 23.75 MnL <sub>2</sub> <sup>4-</sup> 12.43	ZnHL 13.77 ZnL <sub>2</sub> <sup>4-</sup> 11.07 Zn <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 16.55	tentative, from L-dopa
Echinacoside	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Ellagic acid	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Entacapone (comtan, ASI-6)	HL <sup>-</sup> 9.0 H <sub>2</sub> L 13.5			FeL <sup>+</sup> 11.9 FeL <sub>2</sub> <sup>-</sup> 22.9 FeL <sub>3</sub> <sup>3-</sup> 33.6				[Orama 1997]
	HL <sup>-</sup> 11.40 H <sub>2</sub> L 17.87	CuL 12.30 CuL <sub>2</sub> <sup>2-</sup> 22.33				MnL 7.22 MnL <sub>2</sub> <sup>2-</sup> 12.5	ZnL 8.64 ZnL <sub>2</sub> <sup>2-</sup> 15.80	tentative, from 3-nitro-catechol
	(30 °C) HL <sup>-</sup> 10.67 H <sub>2</sub> L 17.19				(30 °C) FeL 13.53 FeL <sub>2</sub> <sup>2-</sup> 23.52			tentative, from 4-nitro-catechol
Enzastaurin	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4	FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83		tentative, from 1,2-diamino-ethane (1.0 M), charges unknown
Epicatechin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

Epigallocatechin-3-gallate	HL 12 H <sub>2</sub> L 23.2 H <sub>3</sub> L 31.8 H <sub>4</sub> L 36.2	(40% mix solv.) CuLH 21.90 CuL <sub>2</sub> H <sub>2</sub> 43.04		FeH <sub>2</sub> L 33.7 FeHL 30.05 FeL 22.28 FeH <sub>4</sub> L <sub>2</sub> 64.7 FeH <sub>2</sub> L <sub>2</sub> 50.01 FeL <sub>2</sub> 33.89 FeH <sub>6</sub> L <sub>3</sub> 94.4 FeH <sub>3</sub> L <sub>3</sub> 69.16 FeL <sub>3</sub> 42.15			Zn <sub>2</sub> L 11.4	tentative, from gallic acid, charges unknown
Etidronate (HEDPA)	HL <sup>3-</sup> 11.2 H <sub>2</sub> L <sup>2-</sup> 18.22 H <sub>3</sub> L <sup>-</sup> 20.92	CuH <sub>2</sub> L 20.4 CuHL <sup>-</sup> 17.4 CuL <sup>2-</sup> 12.0		FeHL 27.4 FeL <sup>-</sup> 24.2 FeH <sup>-1</sup> L 19.1	FeH <sub>2</sub> L 21.07 FeHL <sup>-</sup> 17.77 FeL <sup>2-</sup> 12.9	MnH <sub>2</sub> L 14.54 MnHL <sup>-</sup> 11.36 MnL <sup>2-</sup> 6.94	ZnH <sub>2</sub> L 20.37 ZnHL <sup>-</sup> 16.57 ZnL <sup>2-</sup> 10.3	
Exifone	HL 12 H <sub>2</sub> L 23.2 H <sub>3</sub> L 31.8 H <sub>4</sub> L 36.2	(40% mix solv.) CuHL 21.90 CuH <sub>2</sub> L <sub>2</sub> 43.04		FeH <sub>2</sub> L 33.7 FeHL 30.05 FeL 22.28 FeH <sub>4</sub> L <sub>2</sub> 64.7 FeH <sub>2</sub> L <sub>2</sub> 50.01 FeL <sub>2</sub> 33.89 FeH <sub>6</sub> L <sub>3</sub> 94.4 FeH <sub>3</sub> L <sub>3</sub> 69.16 FeL <sub>3</sub> 42.15			Zn <sub>2</sub> L 11.4	tentative, from gallic acid, charges unknown
F13714, F15599	HL 8.93 H <sub>2</sub> L 10.87	CuL 9.69 CuL <sub>2</sub> 16.90	(50% mix solv.) CuL <sub>2</sub> 10.66		(0.15 M) FeL 4.105 FeL <sub>2</sub> 7.441 FeL <sub>3</sub> 10.116	(20 °C) MnL 2.66	ZnL 5.2	tentative, from 2-(amino-methyl) pyridine, charges unknown
Farrerol	HL 11.34	CuL 14.12		FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Fisetin (3,3',4',7-tetra-hydroxy-flavone)	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Fraxetin	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
Galangin	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37		FeH <sub>2</sub> L 43.54 FeHL 38.59 FeL 32.30 FeH <sub>-1</sub> L 25.54 FeH <sub>-2</sub> L 16.66				tentative from quercetin (20 °C), charges unknown

		Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09 Cu <sub>2</sub> H <sub>-3</sub> L -5.09 Cu <sub>2</sub> H <sub>-4</sub> L -15.31		Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L 29.90 Fe <sub>2</sub> H <sub>-3</sub> L 23.82 Fe <sub>2</sub> H <sub>-4</sub> L 17.09 Fe <sub>2</sub> H <sub>-5</sub> L 8.85 Fe <sub>2</sub> H <sub>-6</sub> L -0.50				
Gallic acid and derivatives	HL <sup>3-</sup> 12 H <sub>2</sub> L <sup>2-</sup> 23.2 H <sub>3</sub> L <sup>-</sup> 31.8 H <sub>4</sub> L 36.2	(40% mix solv.) CuHL <sup>-</sup> 21.90 CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 43.04		FeHL <sup>+</sup> 33.7 FeHL 30.05 FeL <sup>-</sup> 22.28 FeH <sub>4</sub> L <sub>2</sub> <sup>+</sup> 64.7 FeH <sub>2</sub> L <sub>2</sub> <sup>3+</sup> 50.01 FeL <sub>2</sub> <sup>5+</sup> 33.89 FeH <sub>6</sub> L <sub>3</sub> <sup>3+</sup> 94.4 FeH <sub>3</sub> L <sub>3</sub> <sup>6+</sup> 69.16 FeL <sub>3</sub> <sup>9+</sup> 42.15			Zn <sub>2</sub> L 11.4	
Gallocatechin	HL 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> 23.01		FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82	ZnL 8.41 ZnL <sub>2</sub> 14.87	tentative, from pyrogallol (30 °C), charges unknown	
	HL 12.8 H <sub>2</sub> L 22.17			FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75			tentative, from catechol (22 °C), charges unknown	
Garcinol	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Genistein	HL 11.34	CuL 14.12		FeL 14.12			tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown	
Glutamine	HL 8.68 H <sub>2</sub> L <sup>+</sup> 10.864	CuL <sup>+</sup> 7.475 CuL <sub>2</sub> 13.59			(3.0 M) FeL <sup>+</sup> 4.43 FeL <sub>2</sub> 7.26	MnL <sup>+</sup> 2.94	ZnL <sup>+</sup> 4.38 ZnL <sub>2</sub> 8.38 ZnL <sub>3</sub> <sup>-</sup> 10.24	
Glutathione derivatives	HL <sup>2-</sup> 9.63 H <sub>2</sub> L <sup>-</sup> 18.06 H <sub>3</sub> L 21.58 H <sub>4</sub> L <sup>+</sup> 23.68	CuL <sup>-</sup> 7.545	(0.5 M) CuHL <sup>-</sup> 24.9 CuH <sub>2</sub> L <sub>2</sub> <sup>3-</sup> 38.8			MnL <sup>-</sup> 6.69	ZnHL 14.74 ZnL <sup>-</sup> 8.31 ZnH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 29.50 ZnHL <sub>2</sub> <sup>3-</sup> 22.533 ZnL <sub>2</sub> <sup>4-</sup> 13.62 ZnH <sub>-1</sub> L <sub>2</sub> <sup>5-</sup> 3.817 ZnH <sub>-2</sub> L <sub>2</sub> <sup>6-</sup> -6.485	tentative for derivatives
Glutathione - hydroxy-quinoline compound	HL <sup>+</sup> 4.56	CuH <sub>-1</sub> L <sup>+</sup> 1.0		FeH <sub>-1</sub> L <sup>2+</sup> 6.37 FeH <sub>-2</sub> L <sup>+</sup> 2.24			ZnH <sub>-1</sub> L <sup>+</sup> -0.52	(0.15 M). Data from [Cacciatore 2013]
	HL 9.684 H <sub>2</sub> L <sup>+</sup> 14.70		(50% mix solv., 0.3 M) CuL <sub>2</sub> <sup>-</sup> 14.7		(20 °C, 0.01 M) FeL <sup>+</sup> 8.0	MnL <sup>+</sup> 7.85 MnL <sub>2</sub> 14.40		tentative, from 8-hydroxy-quinoline

				FeL <sub>2</sub> 15.0				
Glutathione - L-DOPA compound	HL 9.3	CuH <sub>-1</sub> L 7.0 CuH <sub>-2</sub> L <sup>-</sup> 2.4				ZnH <sub>-1</sub> L 0.72 ZnH <sub>-2</sub> L <sup>-</sup> 8.49 ZnH <sub>-2</sub> L <sub>2</sub> <sup>2-</sup> 2.84	(0.15 M). Data from [Cacciatore 2018]	
	HL 12.8 H <sub>2</sub> L 22.17		(22 °C)	FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	tentative, from catechol, charges unknown	
Gly-N-C-DOPA	HL <sup>2-</sup> 9.77 H <sub>2</sub> L <sup>-</sup> 18.61 H <sub>3</sub> L 20.78	CuHL 17.25 CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.70 CuH <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 26.9 CuH <sub>-1</sub> L <sup>2-</sup> 9.35 CuH <sub>-2</sub> L <sup>3-</sup> 3.20 Cu <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 25.7 Cu <sub>2</sub> H <sub>-1</sub> L <sub>2</sub> <sup>3-</sup> 20.83 Cu <sub>2</sub> H <sub>-2</sub> L <sub>2</sub> 15.22	(0.12 M)	FeL <sup>-</sup> 8.80 FeH <sub>2</sub> L <sup>2+</sup> 31.92 FeL 18.39	(0.2 M) MnHL 17.76 MnL <sup>-</sup> 8.14 MnH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 33.43 MnHL <sub>2</sub> <sup>3-</sup> 23.75 MnL <sub>2</sub> <sup>4-</sup> 12.43	ZnHL 13.77 ZnL <sub>2</sub> <sup>4-</sup> 11.07 Zn <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 16.55	tentative, from L-dopa	
GSK2795039	HL 10.01 H <sub>2</sub> L 13.73 H <sub>3</sub> L 15.60	CuL 11.96 CuL <sub>2</sub> 21.40				ZnL 9.65 ZnL <sub>2</sub> 19.11	tentative (50% mixed solvent), from 2-Methyl-8-(toluene-4-sulfonamide)-6-quinolylethanoic acid, charges unknown	
Guanabenz	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4	FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown	
Hesperidin	HL 11.34	CuL 14.12		FeL 14.12			tentative, from 5-hydroxyflavone (20 °C, 50% mix solv.), charges unknown	
Hinokitiol	HL 7.66	CuL <sup>+</sup> 6.71 CuL <sub>2</sub> 10.71				ZnL <sup>+</sup> 5.15 ZnL <sub>2</sub> 8.05	50% mixed solvent (data from [Pan 1955])	
	HL 6.68		(2.0 M) FeL <sup>2+</sup> 10.50		MnL <sup>+</sup> 4.60		tentative, from tropolone	
8-HQ-MC-5 (VK-28)	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxyquinoline, charges unknown
4-Hydroxyisophthalic acid	HL 13.44 H <sub>2</sub> L 16.22	CuL 10.83 CuL <sub>2</sub> 18.88		FeL 16.45 FeL <sub>2</sub> 29.12 FeL <sub>3</sub> 40.89	(20 °C) FeL 6.55 FeL <sub>2</sub> 11.25	MnL 6.10	(35 °C) ZnL 7.10	tentative, from salicylic acid, charges unknown
1-Hydroxy-2-pyridinone derivatives	HL 5.78	CuL 6.84 CuL <sub>2</sub> 12.46	(0.1 M)	FeL 10.61 FeL <sub>2</sub> 20.11 FeL <sub>3</sub> 27.21			ZnL 4.97 ZnL <sub>2</sub> 9.09 ZnL <sub>3</sub> 12.00	tentative, from 1-hydroxypyridin-2-one (0.2 M), charges unknown
3-Hydroxy-	HL 9.77	CuL <sup>+</sup> 10.42		FeL <sup>2+</sup> 15.10			ZnL <sup>+</sup> 7.19	

4(1H)pyridinone (deferiprone, ferriprox)	H <sub>2</sub> L <sup>+</sup> 13.45	CuHL <sub>2</sub> <sup>+</sup> 21.98 CuL <sub>2</sub> 19.09 CuH <sub>-1</sub> L <sub>2</sub> <sup>+</sup> 8.49		FeL <sub>2</sub> <sup>+</sup> 26.61 FeL <sub>3</sub> 35.88			ZnL <sub>2</sub> 13.53	
3-Hydroxy- 4(1H)pyridinone derivatives (R = H)	HL 9.77 H <sub>2</sub> L 13.45	CuL 10.42 CuHL <sub>2</sub> 21.98 CuL <sub>2</sub> 19.09 CuH <sub>-1</sub> L <sub>2</sub> <sup>+</sup> 8.49		FeL 15.10 FeL <sub>2</sub> 26.61 FeL <sub>3</sub> 35.88			ZnL 7.19 ZnL <sub>2</sub> 13.53	tentative, from deferiprone, charges unknown
8-Hydroxyquinoline	HL 9.684 H <sub>2</sub> L <sup>+</sup> 14.70	CuL <sup>+</sup> 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> <sup>-</sup> 14.7	FeL <sup>2+</sup> 13.69 FeL <sub>2</sub> <sup>+</sup> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL <sup>+</sup> 8.0 FeL <sub>2</sub> 15.0	MnL <sup>+</sup> 7.85 MnL <sub>2</sub> 14.40	ZnL <sup>+</sup> 8.52 ZnL <sub>2</sub> 15.84	
8-Hydroxyquinoline-2- carboxaldehyde isonicotinoyl hydrazone	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy- quinoline, charges unknown
Hydroxyquinoline- propargyl hybrid (HLA 20)	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy- quinoline, charges unknown
Hydroxytyrosol butyrate	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
Hyperoside	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37 Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09 Cu <sub>2</sub> H <sub>-3</sub> L -5.09 Cu <sub>2</sub> H <sub>-4</sub> L -15.31		FeH <sub>2</sub> L 43.54 FeHL 38.59 FeL 32.30 FeH <sub>-1</sub> L 25.54 FeH <sub>-2</sub> L 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L 29.90 Fe <sub>2</sub> H <sub>-3</sub> L 23.82 Fe <sub>2</sub> H <sub>-4</sub> L 17.09 Fe <sub>2</sub> H <sub>-5</sub> L 8.85 Fe <sub>2</sub> H <sub>-6</sub> L -0.50				tentative, from quercetin (20 °C), charges unknown
IC87201	HL 10.85 H <sub>2</sub> L 19.05	CuHL 13.54						tentative, from 2-dimethyl- amino-methyl-phenol (20 °C, 40% mix solv.), charges unknown
Icariin	HL 11.79	CuL 9.83						tentative, from 5-hydroxy-7- methoxy-flavone (50% mix solv.), charges unknown
	HL 7.74			(20 °C, 10% mix solv.) FeL 12.74 FeL <sub>2</sub> 23.25				tentative, from 5-hydroxy- chromone, charges unknown

Icariside II	HL 11.79 HL 7.74	CuL 9.83 CuL <sub>2</sub> 16.74					tentative, from 5-hydroxy-7-methoxy-flavone (50% mix solv.), charges unknown tentative, from 5-hydroxy-chromone, charges unknown
			(20 °C, 10% mix solv.) FeL 12.74 FeL <sub>2</sub> 23.25				
1-(7-Imino-3-propyl-2,3-dihydrothiazolo [4, 5-d]pyrimidin-6(7H)-yl)urea	HL 10.69 H <sub>2</sub> L 18.87	(0.26 M) CuL <sub>2</sub> 16.74	(20 °C, 1.0 M) CuL 10.80 CuL <sub>2</sub> 13.50			ZnL 8.77 ZnH <sub>-1</sub> L 1.94 ZnL <sub>2</sub> 15.72	tentative, from 2-aminoethanethiol, charges unknown
Imipramine	HL <sup>+</sup> 10.77 H <sub>2</sub> L <sup>2+</sup> 19.62	CuL <sup>2+</sup> 9.77 CuL <sub>2</sub> <sup>2+</sup> 16.94				(20 °C) ZnHL <sup>3+</sup> 14.96 ZnHL <sub>2</sub> <sup>3+</sup> 20.22	tentative, from 1,3-diaminopropane
Isobavachalcone	HL 10.01	CuL <sup>+</sup> 6.80 CuL <sub>2</sub> 12.55		(27 °C, 75% mix solv.) FeL <sup>2+</sup> 11.56 FeL <sub>2</sub> <sup>+</sup> 20.76	(30 °C, 75% mix solv.) MnL <sup>+</sup> 7.42	(40 °C, 50% mix solv.) ZnL <sup>+</sup> 6.30	tentative, from 2-hydroxyacetophenone
Isochlorogenic acid	HL <sup>2-</sup> 12.06 H <sub>2</sub> L <sup>-</sup> 20.36 H <sub>3</sub> L 23.71	CuHL 16.92 CuL <sup>-</sup> 12.74 CuL <sub>2</sub> <sup>4-</sup> 23.35		FeL 17.64 FeHL <sup>+</sup> 22.20	MnL <sup>-</sup> 7.02 MnL <sub>2</sub> <sup>4-</sup> 12.13	ZnL <sup>-</sup> 8.79 ZnL <sub>2</sub> <sup>4-</sup> 16.20	tentative, from chlorogenic acid (20 °C, 1 M)
	HL 12.20 H <sub>2</sub> L 21.45				FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488		tentative, from catechol (1.0 M), charges unknown
Isoquercetin (isoquercitrin)	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37 Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09 Cu <sub>2</sub> H <sub>-3</sub> L -5.09 Cu <sub>2</sub> H <sub>-4</sub> L -15.31		FeH <sub>2</sub> L 43.54 FeHL 38.59 FeL 32.30 FeH <sub>-1</sub> L 25.54 FeH <sub>-2</sub> L 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L 29.90 Fe <sub>2</sub> H <sub>-3</sub> L 23.82 Fe <sub>2</sub> H <sub>-4</sub> L 17.09 Fe <sub>2</sub> H <sub>-5</sub> L 8.85 Fe <sub>2</sub> H <sub>-6</sub> L -0.50			tentative, from quercetin (20 °C), charges unknown
	H <sub>4</sub> L 9.22 H <sub>5</sub> L 17.07					ZnH <sub>4</sub> L 14.02	tentative, from quercetin (50% mix solv.), charges unknown
Kaempferol	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37 Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09		FeH <sub>2</sub> L 43.54 FeHL 38.59 FeL 32.30 FeH <sub>-1</sub> L 25.54 FeH <sub>-2</sub> L 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L 29.90			Tentative, from quercetin (20 °C), charges unknown

		Cu <sub>2</sub> H <sub>3</sub> L -5.09 Cu <sub>2</sub> H <sub>4</sub> L -15.31		Fe <sub>2</sub> H <sub>3</sub> L 23.82 Fe <sub>2</sub> H <sub>4</sub> L 17.09 Fe <sub>2</sub> H <sub>5</sub> L 8.85 Fe <sub>2</sub> H <sub>6</sub> L -0.50				
Kaempferol, 3-O-a-L-arabino-furanoside-7-O-a-L-rhamno-pyranoside	HL 11.34			FeL <sup>2+</sup> 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.)
	H <sub>3</sub> L 10.18 H <sub>4</sub> L 18.55 H <sub>5</sub> L 23.52					ZnH <sub>3</sub> L 14.46	tentative, from morin (50% mix solv.), charges unknown	
KR33493	HL 9.60 H <sub>2</sub> L 11.93	CuL 8.38 CuL <sub>2</sub> 15.25	(0.3 M) CuL <sub>2</sub> 10.0	FeL 10.83 FeL <sub>2</sub> 20.48	FeL 4.13 FeL <sub>2</sub> 7.65	MnL 2.85	ZnL 5.03 ZnL <sub>2</sub> 9.30	tentative, from glycine, charges unknown
Kukoamine	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Lestaurtinib	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diamino-ethane (1.0 M), charges unknown
Lipoic acid	HL 6.37	CuL <sup>+</sup> 3.50				MnL <sup>+</sup> 2.06	ZnL <sup>+</sup> 2.47	
Luteolin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
LY354740	HL 10.31 H <sub>2</sub> L 12.71						ZnL 4.76 ZnL <sub>2</sub> 9.16	tentative, from 1-Amino-cyclopentane-carboxylic acid (20 °C), charges unknown
M10 M30 (VAR10303) M99	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
Macranthoin G	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Magnesium lithospermate B	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
α-Mangostin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71	(1.0 M) FeHL 16.57 FeL 7.948	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

				FeL <sub>3</sub> 43.75 (22 °C)	FeL <sub>2</sub> 13.488 (1.0 M)			
γ-Mangostin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
MAOI-1	HL 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> 23.01			FeL 12.88 FeL <sub>2</sub> 23.66	MnL 6.41 MnL <sub>2</sub> 10.82	ZnL 8.41 ZnL <sub>2</sub> 14.87	tentative, from pyrogallol (30 °C), charges unknown
MAOI-2	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
MAOI-4	HL 10.77 H <sub>2</sub> L 19.62	CuL 9.77 CuL <sub>2</sub> 16.94					(20 °C) ZnHL 14.96 ZnHL <sub>2</sub> 20.22	tentative, from 1,3-diaminopropane, charges unknown
MAOI-8	HL 10.85 H <sub>2</sub> L 19.05	CuHL 13.54						tentative, from 2-dimethylamino-methyl-phenol (20 °C, 40% mix solv.), charges unknown
Meclofenamic acid	HL 10.098 H <sub>2</sub> L 13.660				(20 °C, 0.01 M) FeL <sub>2</sub> 4.0	(20 °C) MnL 2.13		tentative, from β-alanine, charges unknown
Metformin (Met)	HL 11.10 H <sub>2</sub> L <sup>+</sup> 14.00	CuL <sup>+</sup> 8.595 CuL <sub>2</sub> 14.949		FeL <sup>2+</sup> 11.872 FeL <sub>2</sub> <sup>+</sup> 22.318			ZnL <sup>+</sup> 6.444 ZnL <sub>2</sub> 11.637	20% mixed solvent (data from [Thakur 2012])
Methoxy-6-acetyl-7-methylijuglone	HL 8.75	(30 °C, 75% mix solv.) CuL <sup>+</sup> 11.24 CuL <sub>2</sub> 20.91					ZnL <sup>+</sup> 4.21 ZnL <sub>2</sub> 12.07	tentative, from 5-hydroxy-1,4-naphtho-quinone (50% mix solv.)
N'-(4-Methylbenzylidene)-5-phenylisoxazole-3-carbohydrazide	HL 4.14 H <sub>2</sub> L 6.24	CuL 4.92 CuL <sub>2</sub> 8.97					ZnL 2.77	tentative, from carbohydrazide (20 °C), charges unknown
Mildronate	HL 10.098 H <sub>2</sub> L 13.660				(20 °C, 0.01 M) FeL <sub>2</sub> 4.0	(20 °C) MnL 2.13		tentative, from β-alanine, charges unknown
Minocycline	HL 8.968 H <sub>2</sub> L 16.392 H <sub>3</sub> L 21.268 H <sub>4</sub> L 24.311	CuH <sub>3</sub> L 25.391 CuH <sub>2</sub> L 23.065 CuHL 18.316 CuL 12.523 Cu <sub>2</sub> H <sub>4</sub> L 41.730					ZnH <sub>2</sub> L 19.165 ZnHL 14.267 ZnH <sub>3</sub> L <sub>2</sub> 33.803 ZnH <sub>2</sub> L <sub>2</sub> 28.225 Zn <sub>2</sub> HL 16.811	37 °C, 0.15 M, charges unknown
Mitomycin C	HL 9.87 H <sub>2</sub> L 14.61	CuL 8.49 CuL <sub>2</sub> 15.52			(20 °C, 0.0 M) FeL 3.66 FeL <sub>2</sub> 6.34	(20 °C, 0.0 M) MnL 3.60	(0.2 M) ZnL 4.945 ZnL <sub>2</sub> 8.86	tentative, from 2-aminophenol, charges unknown
MitoQ	HL 6.06 H <sub>2</sub> L 9.11			FeL 7.26 FeL <sub>2</sub> 13.30		MnL 3.91	ZnL 6.04 ZnL <sub>2</sub> 10.22	tentative, from 2,5-dihydroxy-1,4-benzoquinone (30 °C, 25% mix solv.), charges unknown
Morin	(0.05 M)	CuH <sub>3</sub> L 15.95					ZnH <sub>3</sub> L 14.46	(50% mix solv.)

	H <sub>3</sub> L <sup>2-</sup> 10.18 H <sub>4</sub> L <sup>-</sup> 18.55 H <sub>5</sub> L 23.52							
	HL 7.74			(20 °C, 10% mix solv.) FeL 12.74 FeL <sub>2</sub> 23.25				tentative, from 5-hydroxy-chromone, charges unknown
[18F]MPPF	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
MSX-3	HL 6.23	CuL 2.83				MnL 2.21	ZnL 2.13	tentative, from glycerol-1-phosphate, charges unknown
Myricetin Myricitrin	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37 Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09 Cu <sub>2</sub> H <sub>-3</sub> L -5.09 Cu <sub>2</sub> H <sub>-4</sub> L -15.31		FeH <sub>2</sub> L 43.54 FeHL 38.59 FeL 32.30 FeH <sub>-1</sub> L 25.54 FeH <sub>-2</sub> L 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L 29.90 Fe <sub>2</sub> H <sub>-3</sub> L 23.82 Fe <sub>2</sub> H <sub>-4</sub> L 17.09 Fe <sub>2</sub> H <sub>-5</sub> L 8.85 Fe <sub>2</sub> H <sub>-6</sub> L -0.50				tentative, from quercetin (20 °C), charges unknown
Naringenin	HL <sup>2-</sup> 11.12 H <sub>2</sub> L <sup>-</sup> 19.61 H <sub>3</sub> L 27.08	CuH <sub>2</sub> L <sup>+</sup> 25.3 CuHL 18.31 CuL <sup>-</sup> 6.25 CuH <sub>4</sub> L <sub>2</sub> 49.15 CuH <sub>3</sub> L <sub>2</sub> <sup>-</sup> 41.17 CuH <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 32.21 CuHL <sub>2</sub> <sup>3-</sup> 21.2 CuL <sub>2</sub> <sup>4-</sup> 10.13						data (27 °C, 70% mix solv.) from [Brodowska 2013]
	HL 11.34			FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Naringin	HL 11.12 H <sub>2</sub> L 19.61 H <sub>3</sub> L 27.08	CuH <sub>2</sub> L 25.3 CuHL 18.31 CuL 6.25 CuH <sub>4</sub> L <sub>2</sub> 49.15 CuH <sub>3</sub> L <sub>2</sub> 41.17 CuH <sub>2</sub> L <sub>2</sub> 32.21 CuHL <sub>2</sub> 21.2 CuL <sub>2</sub> 10.13						tentative, from Naringenin (27 °C, 70% mix solv.), charges unknown

	HL 11.34			FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Nicotinamide adenine dinucleotide phosphate (NADPH)	HL 9.95 H <sub>2</sub> L 14.63	CuL 7.70 CuL <sub>2</sub> 13.26		FeL 9.32 FeL <sub>2</sub> 18.37		MnL 4.25	ZnL 6.92 ZnL <sub>2</sub> 13.77	tentative, from adenine, charges unknown
Nicotinamide mononucleotide	HL 6.23	CuL 2.83				MnL 2.21	ZnL 2.13	tentative, from glycerol-1-phosphate, charges unknown
Nitecapone	HL <sup>-</sup> 11.40 H <sub>2</sub> L 17.87	CuL 12.30 CuL <sub>2</sub> <sup>2-</sup> 22.33		FeL <sup>+</sup> 15.71 FeL <sub>2</sub> <sup>-</sup> 28.92		MnL 7.22 MnL <sub>2</sub> <sup>2-</sup> 12.5	ZnL 8.64 ZnL <sub>2</sub> <sup>2-</sup> 15.80	tentative, from 3-nitro-catechol
	(30 °C) HL <sup>-</sup> 10.67 H <sub>2</sub> L 17.19				(30 °C) FeL 13.53 FeL <sub>2</sub> <sup>2-</sup> 23.52			tentative, from 4-nitro-catechol
Nordihydroguaiaretic acid	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Oleuropein	HL <sup>-</sup> 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> <sup>2-</sup> 24.51		(22 °C) FeL <sup>+</sup> 20.05 FeL <sub>2</sub> <sup>-</sup> 34.71 FeL <sub>3</sub> <sup>3-</sup> 43.75	(1.0 M) FeHL <sup>+</sup> 16.57 FeL 7.948 FeL <sub>2</sub> <sup>2-</sup> 13.488	MnL 7.52 MnL <sub>2</sub> <sup>2-</sup> 13.22	ZnL 9.50 ZnL <sub>2</sub> <sup>2-</sup> 17.20	tentative, from catechol
Opicapone	HL <sup>-</sup> 11.40 H <sub>2</sub> L 17.87	CuL 12.30 CuL <sub>2</sub> <sup>2-</sup> 22.33		FeL <sup>+</sup> 15.71 FeL <sub>2</sub> <sup>-</sup> 28.92		MnL 7.22 MnL <sub>2</sub> <sup>2-</sup> 12.5	ZnL 8.64 ZnL <sub>2</sub> <sup>2-</sup> 15.80	tentative, from 3-nitro-catechol
	(30 °C) HL <sup>-</sup> 10.67 H <sub>2</sub> L 17.19				(30 °C) FeL 13.53 FeL <sub>2</sub> <sup>2-</sup> 23.52			tentative, from 4-nitro-catechol
P7C3	HL <sup>+</sup> 9.54 H <sub>2</sub> L <sup>2+</sup> 17.59	CuL <sup>2+</sup> 8.37 CuL <sub>2</sub> <sup>2+</sup> 14.77 Cu <sub>2</sub> H <sub>2</sub> L <sub>2</sub> <sup>2+</sup> 10.25					(30 °C, 1 M) ZnL <sup>2+</sup> 4.60 ZnL <sub>2</sub> <sup>2+</sup> 9.02	tentative, from 1,3-diamino-propane-2-ol (0.2 M)
PBF-509	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80		(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
PBT2	HL 9.49 H <sub>2</sub> L <sup>+</sup> 15.97	CuL <sup>+</sup> 13.61 CuL <sub>2</sub> 19.56						data from [Sgarlata 2018]
	HL 9.684 H <sub>2</sub> L 14.70		(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
PBT434	HL 9.685 H <sub>2</sub> L <sup>+</sup> 15.804	CuL <sup>+</sup> 12.42 CuL <sub>2</sub> 19.33		FeL <sup>2+</sup> 11.86 FeL <sub>2</sub> <sup>+</sup> 15.30	FeL <sup>+</sup> 7.06 FeL <sub>2</sub> 11.06		ZnL <sup>+</sup> 8.57 ZnL <sub>2</sub> 16.54	[Finkelstein 2017]
Petunidin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05	(1.0 M) FeHL 16.57	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

				FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	FeL 7.948 FeL <sub>2</sub> 13.488			
Phenothiazine 2Bc (n=0)	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
Phenothiazine 2Bc (n=1)	HL <sup>+</sup> 10.77 H <sub>2</sub> L <sup>2+</sup> 19.62	CuL <sup>2+</sup> 9.77 CuL <sub>2</sub> <sup>2+</sup> 16.94					(20 °C) ZnHL <sup>3+</sup> 14.96 ZnHL <sub>2</sub> <sup>3+</sup> 20.22	tentative, from 1,3-diaminopropane
Phenylhydroxamates	HL 8.63	CuL 7.07 CuL <sub>2</sub> 12.88		FeL 11.25 FeL <sub>2</sub> 21.60	(37 °C, 30% mix solv.) FeL <sub>2</sub> 8.74	MnL 3.49 MnL <sub>2</sub> 6.98	ZnL 4.95 ZnL <sub>2</sub> 9.21	tentative, from benzohydroxamic acid, charges unknown
Piceatannol	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Pinostrobin (5-hydroxy-7-methoxy-flavone)	HL 11.79	CuL <sup>+</sup> 9.83						(50% mix solv.)
	HL 7.74			(20 °C, 10% mix solv.) FeL <sup>+</sup> 12.74 FeL <sub>2</sub> 23.25				tentative, from 5-hydroxy-chromone
Piperazine-8-OH-quinolone hybrid	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxy-quinoline, charges unknown
Preladenant	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Promethazine	HL <sup>+</sup> 8.49 H <sub>2</sub> L <sup>2+</sup> 11.21	CuL <sup>2+</sup> 8.32						data from [Shoukry 2011]
	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80		(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
Protocatechuic acid	HL <sup>2-</sup> 13.1 H <sub>2</sub> L <sup>-</sup> 21.77 H <sub>3</sub> L 26.02	CuHL 19.22 CuL <sup>-</sup> 13.95 CuH <sub>1</sub> L <sup>2-</sup> 6.32 CuL <sub>2</sub> <sup>4-</sup> 25.02 Cu <sub>2</sub> L <sup>+</sup> 16.50 Cu <sub>2</sub> L <sub>2</sub> <sup>2-</sup> 30.00 Cu <sub>2</sub> L <sub>3</sub> <sup>5-</sup> 41.30		(1.0 M) FeHL <sup>+</sup> 25.32 FeH <sub>2</sub> L <sub>2</sub> <sup>-</sup> 46.04 FeL <sub>2</sub> <sup>3-</sup> 40.34 FeL <sub>3</sub> <sup>6-</sup> 50.91		(1.0 M) MnL <sup>-</sup> 7.43 MnL <sub>2</sub> <sup>4-</sup> 12.64	ZnL <sup>-</sup> 8.91 ZnL <sub>2</sub> <sup>4-</sup> 15.62	(0.2 M)
Protosappanin A	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

Punicalagin	—	CuL 7.26		FeL 7.00				[Kulkarni 2007]. Values are conditional constants at pH = 7.5, charges unknown
Pyrazolobenzothiazine-based carbothioamides	HL 1.87	CuL 3.30 CuL <sub>2</sub> 7.87					ZnL 1.34 ZnL <sub>2</sub> 2.58 ZnL <sub>3</sub> 3.71	tentative, from thiosemicarbazide (0.5 M), charges unknown
Pyridoxal isonicotinoyl hydrazone (PIH)	HL 10.25 H <sub>2</sub> L <sup>+</sup> 18.11 H <sub>3</sub> L <sup>2+</sup> 22.52 H <sub>4</sub> L <sup>3+</sup> 25.47			FeH <sub>4</sub> L <sup>6+</sup> 52.11 FeH <sub>2</sub> L <sup>4+</sup> 27.04 FeH <sub>2</sub> L <sub>2</sub> <sup>3+</sup> 45.3 FeHL <sub>2</sub> <sup>2+</sup> 39.25 FeL <sub>2</sub> <sup>+</sup> 34.0	FeH <sub>4</sub> L <sub>2</sub> <sup>5+</sup> 43.2 FeH <sub>2</sub> L <sub>2</sub> <sup>2+</sup> 32.97			
Pyridoxal isonicotinoyl hydrazone derivatives: PCIH PCTH H2NPH H2PPH	HL 10.25 H <sub>2</sub> L 18.11 H <sub>3</sub> L 22.52 H <sub>4</sub> L 25.47			FeH <sub>4</sub> L 52.11 FeH <sub>2</sub> L 27.04 FeH <sub>2</sub> L <sub>2</sub> 45.3 FeHL <sub>2</sub> 39.25 FeL <sub>2</sub> 34.0	FeH <sub>4</sub> L <sub>2</sub> 43.2 FeH <sub>2</sub> L <sub>2</sub> 32.97			tentative, from PIH <sup>(1)</sup>
Pyrimidinone 8	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Q1 Q4	HL 9.684 H <sub>2</sub> L 14.70	CuL 12.10 CuL <sub>2</sub> 23.00	(50% mix solv., 0.3 M) CuL <sub>2</sub> 14.7	FeL 13.69 FeL <sub>2</sub> 26.3 FeL <sub>3</sub> 36.9	(20 °C, 0.01 M) FeL 8.0 FeL <sub>2</sub> 15.0	MnL 7.85 MnL <sub>2</sub> 14.40	ZnL 8.52 ZnL <sub>2</sub> 15.84	tentative, from 8-hydroxyquinoline, charges unknown
Quercetin	HL <sup>4-</sup> 11.0 H <sub>2</sub> L <sup>3-</sup> 20.77 H <sub>3</sub> L <sup>2-</sup> 28.98 H <sub>4</sub> L <sup>-</sup> 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L <sup>-</sup> 28.09 CuHL <sup>2-</sup> 22.22 CuL <sup>3-</sup> 14.85 CuH <sub>-1</sub> L <sup>4-</sup> 5.53 Cu <sub>2</sub> L <sup>-</sup> 17.37 Cu <sub>2</sub> H <sub>-1</sub> L <sup>2-</sup> 11.62 Cu <sub>2</sub> H <sub>-2</sub> L <sup>3-</sup> 4.09 Cu <sub>2</sub> H <sub>-3</sub> L <sup>4-</sup> -5.09 Cu <sub>2</sub> H <sub>-4</sub> L <sup>5-</sup> -15.31		FeH <sub>2</sub> L 43.54 FeHL <sup>-</sup> 38.59 FeL <sup>2-</sup> 32.30 FeH <sub>-1</sub> L <sup>3-</sup> 25.54 FeH <sub>-2</sub> L <sup>4-</sup> 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L <sup>-</sup> 29.90 Fe <sub>2</sub> H <sub>-3</sub> L <sup>2-</sup> 23.82 Fe <sub>2</sub> H <sub>-4</sub> L <sup>3-</sup> 17.09 Fe <sub>2</sub> H <sub>-5</sub> L <sup>4-</sup> 8.85 Fe <sub>2</sub> H <sub>-6</sub> L <sup>5-</sup> -0.50				(20 °C)
	H <sub>4</sub> L <sup>-</sup> 9.22 H <sub>5</sub> L 17.07						ZnH <sub>4</sub> L <sup>+</sup> 14.02	tentative, from quercetin (50% mix solv.), charges unknown
Quinoline derivatives as SUMOylation activators	HL <sup>+</sup> 4.04	CuL <sup>2+</sup> 6.06 CuL <sub>2</sub> <sup>2+</sup> 10.79 CuL <sub>3</sub> <sup>2+</sup> 14.75		FeL <sup>3+</sup> 3.0			ZnL <sup>2+</sup> 2.42	tentative, from 8-amino-quinoline (20 °C)
Radotinib	HL 4.23 H <sub>2</sub> L 5.55	CuL 9.00 CuL <sub>2</sub> 14.724	(23 °C, 0.0 M) CuL 4.59	FeL 9.13 FeH <sub>-1</sub> L 6.96	FeL 3.98 FeL <sub>2</sub> 9.09	MnL 2.62 MnL <sub>2</sub> 4.62	ZnL 5.13 ZnL <sub>2</sub> 9.50	tentative, from 2,2'-bipyridine, charges unknown

			CuL <sub>2</sub> 9.18	FeH <sub>-2</sub> L 5.11 FeL <sub>2</sub> 18.11 FeH <sub>-1</sub> L <sub>2</sub> 14.74 FeH <sub>-2</sub> L <sub>2</sub> 10.76	FeL <sub>3</sub> 12.63	MnL <sub>3</sub> 5.72		
Riboflavin	HL <sup>+</sup> 10.58	(35 °C) CuHL <sup>3+</sup> 14.32 CuL <sup>2+</sup> 6.53			(20 °C, 0.01 M) FeL <sup>2+</sup> 7.1	(35 °C) MnHL <sup>3+</sup> 13.82 MnL <sup>2+</sup> 3.72	(35 °C) ZnHL <sup>3+</sup> 14.26 ZnL <sup>2+</sup> 4.16	
Rifampicin (ASI-3)	HL 10.97 H <sub>2</sub> L 18.00	CuL 8.98 CuL <sub>2</sub> 15.58				MnL 6.71 MnL <sub>2</sub> 11.93	ZnL 7.89 ZnL <sub>2</sub> 14.23	30 °C, 50% mix solv., charges unknown
	HL 13.00 H <sub>2</sub> L 18.35		(30 °C) Cu <sub>2</sub> L 22.68	FeL 20.6 FeL <sub>2</sub> 33.50	(27 °C) FeL 6.00 FeL <sub>2</sub> 9.45			tentative, from chromotropic acid, charges unknown
Rimonabant	HL 9.81 H <sub>2</sub> L 15.88	CuHL 12.88 CuL 9.56 CuHL <sub>2</sub> 21.82 CuL <sub>2</sub> 16.06	CuL 8.87 CuH <sub>2</sub> L <sub>2</sub> 20.13	FeL <sub>2</sub> 7.05	(0.058 M) FeL 5.80 FeL <sub>2</sub> 10.06	(35 °C) MnHL 12.83	ZnHL 11.72 ZnL 5.21 ZnL <sub>2</sub> 10.13	tentative, from histamine, charges unknown
Rosmarinic acid	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Rotigotine	HL 10.84 H <sub>2</sub> L 19.96	(0.17 M) CuL <sub>2</sub> 16.28	(20 °C, 1 M) CuL 11.92 CuL <sub>2</sub> 15.12					tentative, from 3-amino-propane-1-thiol, charges unknown
Rutin	H <sub>4</sub> L 9.22 H <sub>5</sub> L 17.07						ZnH <sub>4</sub> L 14.02	tentative, from quercetin (50% mix solv.), charges unknown
	HL 11.0 H <sub>2</sub> L 20.77 H <sub>3</sub> L 28.98 H <sub>4</sub> L 35.93 H <sub>5</sub> L 41.47	CuH <sub>2</sub> L 28.09 CuHL 22.22 CuL 14.85 CuH <sub>-1</sub> L 5.53 Cu <sub>2</sub> L 17.37 Cu <sub>2</sub> H <sub>-1</sub> L 11.62 Cu <sub>2</sub> H <sub>-2</sub> L 4.09 Cu <sub>2</sub> H <sub>-3</sub> L -5.09 Cu <sub>2</sub> H <sub>-4</sub> L -15.31		FeH <sub>2</sub> L 43.54 FeHL <sup>-</sup> 38.59 FeL <sup>2-</sup> 32.30 FeH <sub>-1</sub> L <sup>3-</sup> 25.54 FeH <sub>-2</sub> L <sup>4-</sup> 16.66 Fe <sub>2</sub> H <sub>-1</sub> L 35.40 Fe <sub>2</sub> H <sub>-2</sub> L <sup>-</sup> 29.90 Fe <sub>2</sub> H <sub>-3</sub> L <sup>2-</sup> 23.82 Fe <sub>2</sub> H <sub>-4</sub> L <sup>3-</sup> 17.09 Fe <sub>2</sub> H <sub>-5</sub> L <sup>4-</sup> 8.85 Fe <sub>2</sub> H <sub>-6</sub> L <sup>5-</sup> -0.50				tentative, from quercetin, charges unknown
Salicylate, sodium salt	HL <sup>-</sup> 13.44 H <sub>2</sub> L 16.22	CuL 10.83 CuL <sub>2</sub> <sup>2-</sup> 18.88		FeL <sup>+</sup> 16.45 FeL <sub>2</sub> <sup>-</sup> 29.12 FeL <sub>3</sub> <sup>3-</sup> 40.89	(20 °C) FeL 6.55 FeL <sub>2</sub> <sup>-</sup> 11.25	MnL 6.10	(35 °C) ZnL 7.10	
Salvianolic acid B	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05	(1.0 M) FeHL 16.57	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown

				FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	FeL 7.948 FeL <sub>2</sub> 13.488			
SCH58261 SCH412348	HL 9.35 H <sub>2</sub> L 14.08	CuL 9.22 CuL <sub>2</sub> 17.17						tentative, from 4(5)-amino-methyl-imidazole, charges unknown
	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80		(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Silibinin (silybin) A, B	HL <sup>2-</sup> 13.67 H <sub>2</sub> L <sup>-</sup> 26.97 H <sub>3</sub> L 37.27			FeH <sub>3</sub> L <sup>3+</sup> 37.03				(100% org. solv.)
Silydianin	HL <sup>2-</sup> 13.67 H <sub>2</sub> L <sup>-</sup> 26.97 H <sub>3</sub> L 37.27			FeH <sub>3</sub> L <sup>3+</sup> 37.03				tentative, from silibinin (100% org. solv.)
ST1535 ST4206	HL 9.35 H <sub>2</sub> L 14.08	CuL 9.22 CuL <sub>2</sub> 17.17						tentative, from 4(5)-amino-methyl-imidazole, charges unknown
	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80		(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Staurosporine	(0.0 M) HL 9.94 H <sub>2</sub> L 16.80	(0.5 M) CuL 10.60 CuL <sub>2</sub> 19.75	(0.3 M) CuL <sub>2</sub> 11.4		FeL 4.34 FeL <sub>2</sub> 7.65 FeL <sub>3</sub> 9.70	MnL 2.77 MnL <sub>2</sub> 4.87 MnL <sub>3</sub> 5.79	(0.0 M) ZnL 5.77 ZnL <sub>2</sub> 10.83	tentative, from 1,2-diaminoethane (1.0 M), charges unknown
Stemazole	HL 1.87	CuL 3.30 CuL <sub>2</sub> 7.87					ZnL 1.34 ZnL <sub>2</sub> 2.58 ZnL <sub>3</sub> 3.71	tentative, from thiosemicarbazide (0.5 M), charges unknown
Sulfuretin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Tannic acid	—	CuL 3.84		Fe <sub>4</sub> L 17.45			ZnL 3.93	[Sungur 2008] Unknown temperature and ionic strength; values are conditional constants at pH=8; charges unknown
Tanshinol	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
Taurine	HL 8.93 H <sub>2</sub> L <sup>+</sup> 10.61	CuL <sup>+</sup> 3.56 CuL <sub>2</sub> 6.52				MnL <sub>2</sub> 5.28	ZnL <sub>2</sub> 5.00	data (20 °C) from [Petrova 2013]
Taxifolin	HL <sup>3-</sup> 11.68	CuH <sub>3</sub> L <sup>+</sup> 36.6						data from [Teixeira 2005]

	H <sub>2</sub> L <sup>2-</sup> 22.63 H <sub>3</sub> L <sup>-</sup> 31.52 H <sub>4</sub> L 38.2	CuH <sub>2</sub> L 31.13 CuHL <sup>-</sup> 25.65 CuL <sup>2-</sup> 18.72 CuH <sub>4</sub> L <sub>2</sub> <sup>2-</sup> 24.1 Cu <sub>2</sub> L 23.69						
	HL 11.34			FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Tectorigenin	HL 11.34	CuL 14.12		FeL 14.12				tentative, from 5-hydroxy-flavone (20 °C, 50% mix solv.), charges unknown
Tetracycline	HL <sup>-</sup> 9.57 H <sub>2</sub> L 17.39 H <sub>3</sub> L <sup>+</sup> 20.74	CuL 7.8 CuL <sub>2</sub> <sup>2-</sup> 12.80		FeL <sup>+</sup> 9.9 FeL <sub>2</sub> <sup>-</sup> 18.50 FeL <sub>3</sub> <sup>3-</sup> 25.3	FeL 5.3 FeL <sub>2</sub> <sup>2-</sup> 9.30	MnL 4.4	ZnL 4.9	(20 °C, 0.01 M)
Tolcapone (ASI-7)	HL <sup>-</sup> 11.40 H <sub>2</sub> L 17.87	CuL 12.30 CuL <sub>2</sub> <sup>2-</sup> 22.33		FeL <sup>+</sup> 15.71 FeL <sub>2</sub> <sup>-</sup> 28.92		MnL 7.22 MnL <sub>2</sub> <sup>2-</sup> 12.5	ZnL 8.64 ZnL <sub>2</sub> <sup>2-</sup> 15.80	tentative, from 3-nitro-catechol
	(30 °C) HL <sup>-</sup> 10.67 H <sub>2</sub> L 17.19				(30 °C) FeL 13.53 FeL <sub>2</sub> <sup>2-</sup> 23.52			tentative, from 4-nitro-catechol
Tozadenant	HL 7.90						ZnL 7.33 ZnL <sub>2</sub> 14.10	tentative, from 2-amino-thiophenol (50% mix solv.), charges unknown
Transilitin	HL 12.8 H <sub>2</sub> L 22.17	CuL 13.76 CuL <sub>2</sub> 24.51		(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75	(1.0 M) FeHL 16.57 FeL 7.948 FeL <sub>2</sub> 13.488	MnL 7.52 MnL <sub>2</sub> 13.22	ZnL 9.50 ZnL <sub>2</sub> 17.20	tentative, from catechol, charges unknown
o-Trensox	HL <sup>5-</sup> 8.62 H <sub>2</sub> L <sup>4-</sup> 16.80 H <sub>3</sub> L <sup>3-</sup> 24.24 H <sub>4</sub> L <sup>2-</sup> 30.6 H <sub>5</sub> L <sup>-</sup> 33.61 H <sub>6</sub> L 36.16 H <sub>7</sub> L <sup>+</sup> 37.99	CuH <sub>3</sub> L <sup>-</sup> 38.16 CuH <sub>2</sub> L <sup>2-</sup> 35.60 CuHL <sup>3-</sup> 30.99 CuL <sup>4-</sup> 24.20		FeH <sub>5</sub> L <sup>2+</sup> 42.2 FeHL <sup>2-</sup> 36.5 FeL <sup>3-</sup> 30.9			ZnH <sub>3</sub> L <sup>-</sup> 32.76 ZnH <sub>2</sub> L <sup>2-</sup> 29.83 ZnHL <sup>3-</sup> 27.06 ZnL <sub>4</sub> <sup>-</sup> 23.10	
2', 3', 4' Trihydroxyflavone	HL <sup>-</sup> 10.85 H <sub>2</sub> L 19.61	CuL 12.54 CuL <sub>2</sub> <sup>2-</sup> 23.01			FeL 12.88 FeL <sub>2</sub> <sup>2-</sup> 23.66	MnL 6.41 MnL <sub>2</sub> <sup>2-</sup> 10.82	ZnL 8.41 ZnL <sub>2</sub> <sup>2-</sup> 14.87	tentative, from pyrogallol (30 °C)
2,3,3-Trisphosphonate	HL 10.17 H <sub>2</sub> L 17.08 H <sub>3</sub> L 19.79	CuHL 16.95 CuL 13.29 CuH <sub>2</sub> L <sub>2</sub> 33.22 CuL <sub>2</sub> 23.98 Cu <sub>2</sub> HL 21.74 Cu <sub>2</sub> L 18.54		FeL 19.9 FeL <sub>2</sub> 26.6	FeHL 16.77 FeL 12.6 FeH <sub>2</sub> L <sub>2</sub> 32.24 FeL <sub>2</sub> 18.8 Fe <sub>2</sub> HL 19.27 Fe <sub>2</sub> L 15.4		ZnHL 17.67 ZnL 13.99 ZnH <sub>2</sub> L <sub>2</sub> 33.88 ZnL <sub>2</sub> 20.55 Zn <sub>2</sub> HL 21.4 Zn <sub>2</sub> L 18.16	tentative, from methane-diphosphonic acid, charges unknown

V81444	HL 8.93 H <sub>2</sub> L 10.87	CuL 9.69 CuL <sub>2</sub> 16.90	(50% mix solv.) CuL <sub>2</sub> 10.66		(0.15 M) FeL 4.105 FeL <sub>2</sub> 7.441 FeL <sub>3</sub> 10.116	(20 °C) MnL 2.66	ZnL 5.2	tentative, from 2-(amino-methyl) pyridine, charges unknown
VAS3947 VAS2870	HL 10.69 H <sub>2</sub> L 18.87	(0.26 M) CuL <sub>2</sub> 16.74	(20 °C, 1.0 M) CuL 10.80 CuL <sub>2</sub> 13.50				ZnL 8.77 ZnH <sub>-1</sub> L 1.94 ZnL <sub>2</sub> 15.72	tentative, from 2-aminoethanethiol, charges unknown
Verbascoside	HL 8.72 H <sub>2</sub> L 13.13	CuHL 10.46 CuL 6.02 CuH <sub>-1</sub> L 0.25 Cu <sub>2</sub> H <sub>-1</sub> L 3.54 Cu <sub>2</sub> H <sub>-3</sub> L <sub>3</sub> 0.97 Cu <sub>3</sub> H <sub>-2</sub> L <sub>2</sub> 7.41			FeL 3.86 FeH <sub>-1</sub> L -3.83 FeH <sub>-1</sub> L <sub>2</sub> -0.36 FeH <sub>-2</sub> L <sub>3</sub> -6.14 Fe <sub>2</sub> L 6.69	MnH <sub>-1</sub> L -4.88 MnH <sub>-2</sub> L -15.55	ZnL 2.99 ZnH <sub>-1</sub> L -3.03 ZnH <sub>-1</sub> L <sub>2</sub> -0.39 ZnH <sub>-2</sub> L <sub>2</sub> -8.21 ZnH <sub>-2</sub> L <sub>3</sub> -5.51	tentative, from caffeic acid, charges unknown
	HL 12.8 H <sub>2</sub> L 22.17			(22 °C) FeL 20.05 FeL <sub>2</sub> 34.71 FeL <sub>3</sub> 43.75				tentative, from catechol (1 M), charges unknown
WIN 55,212-2	(0.0 M) HL <sup>+</sup> 9.94 H <sub>2</sub> L <sup>2+</sup> 16.80	(0.5 M) CuL <sup>2+</sup> 10.60 CuL <sub>2</sub> <sup>2+</sup> 19.75	(0.3 M) CuL <sub>2</sub> <sup>+</sup> 11.4		FeL <sup>2+</sup> 4.34 FeL <sub>2</sub> <sup>2+</sup> 7.65 FeL <sub>3</sub> <sup>2+</sup> 9.70	MnL <sup>2+</sup> 2.77 MnL <sub>2</sub> <sup>2+</sup> 4.87 MnL <sub>3</sub> <sup>2+</sup> 5.79	(0.0 M) ZnL <sup>2+</sup> 5.77 ZnL <sub>2</sub> <sup>2+</sup> 10.83	tentative, from 1,2-diaminoethane (1.0 M)
WR-1065	HL <sup>+</sup> 10.139 H <sub>2</sub> L <sup>2+</sup> 19.30	CuHL <sup>3+</sup> 14.805 CuL <sup>2+</sup> 10.035 CuH <sub>-1</sub> L <sup>+</sup> 0.865 CuHL <sub>2</sub> <sup>3+</sup> 22.6 CuL <sub>2</sub> <sup>2+</sup> 12.90						tentative, from 1,6-diamino-3-thia-hexane (0.5 M)
	HL 10.69 H <sub>2</sub> L 18.87		(20 °C, 1.0 M) CuL 10.80 CuL <sub>2</sub> 13.50					tentative, from 2-aminoethanethiol, charges unknown
	HL <sup>+</sup> 10.77 H <sub>2</sub> L <sup>2+</sup> 19.62						(20 °C) ZnHL <sup>3+</sup> 14.96 ZnHL <sub>2</sub> <sup>3+</sup> 20.22	tentative, from 1,3-diaminopropane
Zonisamide	HL 12.49 H <sub>2</sub> L 15.63	CuL 11.47 CuL <sub>2</sub> 20.73		FeL 11.70 FeL <sub>2</sub> 22.94			ZnL 12.16	tentative, from 2-(methane-sulfonamido-methyl)pyridine (30 °C, 45% mix solv.), charges unknown

<sup>(1)</sup> Coordination chemistry similarity is suggested from the data of [Bernhardt 2005]

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**TABLE S3**

Ionic product of water and stability constants for hydrolysis products of Cu(II), Cu(I), Fe(III), Fe(II), Mn(II), and Zn(II). The ionic product of water (column marked "H<sup>+</sup>") has been taken from Nordin et al (Nordin, J; Persson, P; Nordin, A; Sjoberg, S, Langmuir 1998, 14 (13), 3655-3662) and it is valid at 25 °C and at an ionic strength of NaCl 0.1 M. The formulas in the columns marked "Cu(II)", "Cu(I)", etc. represent the hydrolysis products of each metal ion. Numbers are the corresponding values of log $\beta$  (see equation 2 in main text for the definition of  $\beta$ ). If not differently specified in the notes, values for metal hydrolysis products have been taken from Baes and Mesmer (Baes, CF; Mesmer, RE, *The Hydrolysis of cations*, John Wiley and Sons, 1976).

ligand	H <sup>+</sup>	Cu(II)	Cu(I)	Fe(III)	Fe(II)	Mn(II)	Zn(II)
hydroxide (OH <sup>-</sup> )	H <sub>2</sub> O -13.775	Cu(OH) <sup>+</sup> -8 Cu(OH) <sub>2</sub> -17.3 Cu(OH) <sub>3</sub> <sup>-</sup> -27.8 Cu <sub>2</sub> (OH) <sub>2</sub> <sup>2+</sup> -10.36	-	Fe(OH) <sub>2</sub> <sup>2+</sup> -2.87 <sup>(1)</sup> Fe(OH) <sub>2</sub> <sup>+</sup> -6.16 <sup>(1)</sup> Fe(OH) <sub>3</sub> -12.16 <sup>(2)</sup> Fe(OH) <sub>4</sub> <sup>-</sup> -22.16 <sup>(2)</sup> Fe <sub>2</sub> (OH) <sub>2</sub> <sup>4+</sup> -2.9 <sup>(2)</sup> Fe <sub>3</sub> (OH) <sub>4</sub> <sup>5+</sup> -6.3 <sup>(2)</sup>	Fe(OH) <sup>+</sup> -9.3 Fe(OH) <sub>2</sub> -20.5 Fe(OH) <sub>3</sub> <sup>-</sup> -29.4	Mn(OH) <sup>+</sup> -10.59	Zn(OH) <sup>+</sup> -8.96 Zn(OH) <sub>2</sub> -16.9 Zn(OH) <sub>3</sub> <sup>-</sup> -28.4 Zn(OH) <sub>4</sub> <sup>2-</sup> -41.2

<sup>(1)</sup> data from Di Marco, VB; Tapparo, A; Bombi, GG, Ann. Chim. 2001, 91, 595.

<sup>(2)</sup> data from Flynn, CM Jr., Chem. Rev. 1984, 84, 31