

Ecdysteroid Physico-Chemical Data

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This database has been designed as a tool to help the scientific community in research on ecdysteroids. The author wishes it to be an evolving system and would encourage other researchers to submit new data, additional publications, proposals for modifications or comments to the authors for inclusion. All new material will be referenced to its contributor.

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Lafont R., Harmatha J., Marion-Poll F., Dinan L., Wilson I.D.: The Ecdysone Handbook, 3rd edition, on-line, <http://ecdybase.org>

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Please notify Laurie Dinan (dinanlaurence@gmail.com) of any errors or additional data/literature sources.

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Molecular parameters have been calculated using 'molinspiration cheminformatics' (<https://www.molinspiration.com/>) after input of the isomeric SMILES string for each ecdysteroid:

miLogP (Log of the octanol/water partition coefficient): LogP is calculated by the methodology developed by Molinspiration as a sum of fragment-based contributions and correction factors. Method is very robust and is able to process practically all organic, and most organometallic molecules.

TPSA (Topological polar surface area; Molecular Polar Surface Area; units = Å²): is calculated based on the methodology published by Ertl *et al.* [2000] as a sum of fragment contributions. O- and N- centered polar fragments are considered. PSA has been shown to be a very good descriptor characterizing drug absorption, including intestinal absorption, bioavailability, Caco-2 permeability and blood-brain barrier penetration. PSA is a commonly used medicinal chemistry metric for the optimization of a drug's ability to permeate cells. Molecules with a polar surface area of greater than 140 angstroms squared tend to be poor at permeating cell membranes. For molecules to penetrate the blood–brain barrier (and thus act on receptors in the central nervous system), a PSA less than 90 angstroms squared is usually needed.

Natoms (number of atoms): the number of atoms present in the molecule, excluding hydrogens

MW: molecular weight

nON: the number of oxygen and nitrogen atoms (i.e. H-bond donors and acceptors) in the molecule

nOHNH: the number of -OH and -NH groups (i.e. H-bond donors) in the molecule

nviolations (number of violations): the number of violations to Lipinski's Rule of Five (see below; Lipinski *et al.*, 1997; 2001). The parameters assessed are LogP, TPSA, MW, nON, nOHNH & nrotb; 0 violations in black, 1 violation in orange and 2 or more violations in red.

nrotb (number of rotatable bonds): This simple topological parameter is a measure of molecular flexibility. It has been shown to be a very good descriptor of oral bioavailability of drugs [Veber et al., 2002]. Rotatable bond is defined as any single non-ring bond, bounded to nonterminal heavy (i.e., non-hydrogen) atom. Amide C-N bonds are not considered because of their high rotational energy barrier.

volume (molecular volume; van der Waals volume; units = Å³): Method for calculation of molecule volume developed at Molinspiration is based on group contributions. These have been obtained by fitting sum of fragment contributions to "real" 3D volume for a training set of about twelve thousand, mostly drug-like molecules. 3D molecular geometries for a training set were fully optimized by the semiempirical AM1 method.

"Rule of 5" Properties: is set of simple molecular descriptors used by Lipinski in formulating his "Rule of 5" [Ertl et al., 2000]. The rule states, that most "drug-like" molecules have logP ≤ 5, molecular weight ≤ 500, number of hydrogen bond acceptors ≤ 10, and number of hydrogen bond donors ≤ 5. Molecules violating more than one of these rules may have problems with bioavailability. The rule is called "Rule of 5", because the border values are 5, 500, 2*5, and 5.

Colours for the molecular parameters refer to the ADMET Traffic Light System [Lobell et al., 2006], such that green is compatible with bioavailability, orange indicates somewhat impaired bioavailability and red implies a negative impact on bioavailability. The param

Exact/monoisotopic masses from PubChem, where available, or calculated on ChemCalc (<https://www.chemcalc.org/>; Patny & Borel, 2013)

References

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3. D.F. Veber, S.R. Johnson, H.-Y. Cheng, B.R. Smith, K.W. Ward, K.D. Kopple, Molecular properties that influence the oral bioavailability of drug candidates. *J.Med.Chem.* 45, 2615-2623 (2002).
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5. Patiny, Luc; Borel, Alain *Journal of Chemical Information and Modeling* **2013**. DOI: [10.1021/ci300563h](https://doi.org/10.1021/ci300563h)

NB: As time permits, the information in this Table will be transferred to the main data sheets for the ecdysteroids to provide a unified summary of physico-chemical data, chemical identifiers and biological activities for each ecdysteroid.

Ecdysteroid*	
Abutasterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
25-acetoxy-20-hydroxyecdysone 3-O-b-D-glucopyranoside	miLogP 0.36 TPSA 223.67 natoms 48 MW 684.82 nON 13 nOHNH 8 nviolations 3 nrotb 10 volume 633.11 Exact/Monoisotopic Mass = 684.372092 g/mol
Acetypinnasterol	miLogP 4.03 TPSA 104.06 natoms 35 MW 488.67 nON 6 nOHNH 3 nviolations 0

	nrotb 7 volume 479.39 Exact/Monoisotopic Mass = 488.313789 g/mol
Achyranthesterone A	miLogP 0.35 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6 volume 472.74 Exact/Monoisotopic Mass = 496.303618 g/mol
Aervecdysteroid A	miLogP 2.94 TPSA 107.22 natoms 34 MW 476.65 nON 6 nOHNH 4 nviolations 0 nrotb 1 volume 463.17 Exact/Monoisotopic Mass = 476.313789 g/mol
Aervecdysteroid B	miLogP 2.78 TPSA 107.22 natoms 34 MW 474.64 nON 6 nOHNH 4 nviolations 0 nrotb 1 volume 457.51 Exact/Monoisotopic Mass = 474.298139 g/mol

Aervecdysteroid C	miLogP 1.83 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.06 Exact/Monoisotopic Mass = 494.324354 g/mol
Aervecdysteroid D	miLogP 1.67 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 475.41 Exact/Monoisotopic Mass = 492.308704 g/mol
Ajugacetalsterone A	miLogP 1.78 TPSA 147.67 natoms 37 MW 522.68 nON 8 nOHNH 6 nviolations 2 nrotb 3 volume 496.28 Exact/Monoisotopic Mass = 522.319268 g/mol
Ajugacetalsterone B	miLogP 2.52 TPSA 153.75 natoms 40

	MW 564.72 nON 9 nOHNH 5 nviolations 1 nrotb 6 volume 533.14 Exact/Monoisotopic Mass = 564.329833 g/mol
Ajugacetalsterone C	miLogP 2.58 TPSA 116.45 natoms 36 MW 502.65 nON 7 nOHNH 4 nviolations 1 nrotb 2 volume 472.50 Exact/Monoisotopic Mass = 502.293054 g/mol
Ajugacetalsterone D	miLogP 2.43 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 514.15 Exact/Monoisotopic Mass = 536.334918 g/mol
Ajugalactone	miLogP 2.05 TPSA 141.36 natoms 37 MW 516.63 nON 8 nOHNH 4

	nviolations 1 nrotb 3 volume 478.66 Exact/Monoisotopic Mass = 516.272318 g/mol
Ajugalide E	miLogP 1.42 TPSA 150.59 natoms 40 MW 562.70 nON 9 nOHNH 4 nviolations 1 nrotb 6 volume 527.28 Exact/Monoisotopic Mass = 562.314183 g/mol
Ajugasterone B	miLogP 2.11 TPSA 138.44 natoms 36 MW 506.68 nON 7 nOHNH 6 nviolations 2 nrotb 7 volume 492.77 Exact/Monoisotopic Mass = 506.324354 g/mol
Ajugasterone B'	miLogP 2.20 TPSA 138.44 natoms 36 MW 506.68 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 492.56

	Exact/Monoisotopic Mass = 506.324354 g/mol
Ajugasterone C	miLogP 1.65 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
Ajugasterone C 11-acetate	miLogP 2.35 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 501.34 Exact/Monoisotopic Mass = 522.3192684318 g/mol
Ajugasterone C 2-acetate	miLogP 2.35 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 501.34 Exact/Monoisotopic Mass = 522.3192684318 g/mol
Ajugasterone C 3-acetate	miLogP 2.35 TPSA 144.52

	natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 501.34 Exact/Monoisotopic Mass =522.3192684318 g/mol
Ajugasterone C 2,3;20,22-diacetonide	miLogP 5.43 TPSA 94.46 natoms 40 MW 560.77 nON 7 nOHNH 2 nviolations 2 nrotb 4 volume 546.26 Exact/Monoisotopic Mass = 560.371304 g/mol
Ajugasterone C 20,22-ethylidene acetal	miLogP 3.09 TPSA 116.45 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 4 volume 489.31 Exact/Monoisotopic Mass = 506.324354 g/mol
Ajugasterone C 20,22-monoacetone	miLogP 3.54 TPSA 116.45 natoms 37 MW 520.71 nON 7

	nOHNH 4 nviolations 1 nrotb 4 volume 505.55 Exact/Monoisotopic Mass = 520.340004 g/mol
Ajugasterone D	miLogP 1.52 TPSA 127.44 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 2 volume 454.28 Exact/Monoisotopic Mass = 478.293054 g/mol
Alfredensterol	miLogP 5.86 TPSA 89.91 natoms 37 MW 516.72 nON 6 nOHNH 1 nviolations 2 nrotb 9 volume 514.42 Exact/Monoisotopic Mass = 516.3450892568 g/mol
Amarasterone A	miLogP 2.27 TPSA 138.44 natoms 36 MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 7

	volume 498.43 Exact/Monoisotopic Mass = 508.340004 g/mol
Amarasterone B	miLogP 2.80 TPSA 138.44 natoms 36 MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 7 volume 498.43 Exact/Monoisotopic Mass = 508.340004 g/mol
Asterasterol B	miLogP 1.87 TPSA 103.73 natoms 34 MW 495.70 (unprotonated) nON 6 nOHNH 1 nviolations 0 nrotb 8 volume 471.24 Exact/Monoisotopic Mass = 495.278035 g/mol Exact/Monoisotopic Mass (+proton) = 496.28586 g/mol
Atrotosterone A	miLogP 2.62 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.42 Exact/Monoisotopic Mass = 494.324354 g/mol

Atrotosterone B	miLogP 2.81 TPSA 130.74 natoms 35 MW 492.65 nON 7 nOHNH 5 nviolations 0 nrotb 4 volume 471.57 Exact/Monoisotopic Mass = 492.308704 g/mol
Atrotosterone C	miLogP 0.76 TPSA 158.67 natoms 36 MW 508.65 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 483.45 Exact/Monoisotopic Mass = 508.303618 g/mol
B	
Bathoristerone	miLogP 1.30 TPSA 97.98 natoms 26 MW 360.45 nON 5 nOHNH 4 nviolations 0 nrotb 1 volume 336.58 Exact/Monoisotopic Mass = 360.193675 g/mol
Blechnoside A	miLogP 1.51 TPSA 177.13

	natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.86 Exact/ Monoisotopic Mass = 610.371698 g/mol
Blechnoside B	miLogP 1.51 TPSA 177.13 natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.86 Exact/ Monoisotopic Mass = 610.371698 g/mol
Bombycosterol	miLogP 3.43 TPSA 101.14 natoms 32 MW 448.64 nON 5 nOHNH 5 nviolations 0 nrotb 5 volume 448.04 Exact/ Monoisotopic Mass = 448.318875 g/mol
Bombycosterol 3-phosphate	miLogP -0.49 TPSA 153.33 natoms 36 MW 526.61 (unprotonated) nON 8

	nOHNH 4 nviolations 1 nrotb 7 volume 487.90 Exact/ Monoisotopic Mass (protonated) = 528.285205 g/mol
Brahuisterone	miLogP 2.27 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/ Monoisotopic Mass = 464.313789 g/mol
Brainesteroside A	miLogP 1.05 TPSA 189.66 natoms 44 MW 624.77 nON 11 nOHNH 7 nviolations 3 nrotb 8 volume 579.06 Exact/ Monoisotopic Mass = 624.350962 g/mol
Brainesteroside B	miLogP 1.62 TPSA 177.13 natoms 43 MW 608.77 nON 10 nOHNH 7 nviolations 2 nrotb 8

	volume 575.00 Exact/ Monoisotopic Mass = 608.356048 g/mol
Brainesteroside C	miLogP 0.94 TPSA 197.36 natoms 44 MW 622.75 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 576.78 Exact/ Monoisotopic Mass = 622.335312 g/mol
Brainesteroside D	miLogP 1.80 TPSA 177.13 natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 581.21 Exact/ Monoisotopic Mass = 610.371698 g/mol
Brainesteroside E	miLogP 0.86 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/ Monoisotopic Mass = 626.366613 g/mol
Breviflorasterone	miLogP 0.94

	TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
C	
Callecdysterol A	miLogP -0.45 TPSA 118.21 natoms 25 MW 352.43 nON 6 nOHNH 5 nviolations 0 nrotb 0 volume 323.37 Exact/Monoisotopic Mass = 352.188589 g/mol
Callecdysterol B	miLogP -1.39 TPSA 138.44 natoms 26 MW 368.43 nON 7 nOHNH 6 nviolations 1 nrotb 0 volume 331.06 Exact/Monoisotopic Mass = 368.183503 g/mol
Callecdysterol C	miLogP 0.28 TPSA 97.98 natoms 24

	MW 334.41 nON 5 nOHNH 4 nviolations 0 nrotb 0 volume 309.11 Exact/Monoisotopic Mass = 334.178024 g/mol
Calonysterone	miLogP 1.44 TPSA 138.44 natoms 34 MW 476.61 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 452.35 Exact/Monoisotopic Mass = 476.277404 g/mol
Calvasterol A	miLogP 4.77 TPSA 54.37 natoms 31 MW 422.61 nON 3 nOHNH 1 nviolations 0 nrotb 4 volume 425.12 Exact/Monoisotopic Mass = 422.282095 g/mol
Calvasterol B	miLogP 4.01 TPSA 74.60 natoms 32 MW 440.62 nON 4 nOHNH 2

	nviolations 0 nrotb 4 volume 439.02 Exact/Monoisotopic Mass = 440.29266 g/mol
Canescensterone	miLogP 2.60 TPSA 160.31 natoms 41 MW 573.73 nON 9 nOHNH 6 nviolations 2 nrotb 8 volume 540.82 Exact/Monoisotopic Mass = 573.330167 g/mol
Capitasterone	miLogP 4.62 TPSA 104.06 natoms 36 MW 502.69 nON 6 nOHNH 3 nviolations 1 nrotb 3 volume 491.26 Exact/Monoisotopic Mass = 504.308704 g/mol
Carpesterol	miLogP 9.01 TPSA 63.60 natoms 41 MW 562.84 nON 4 nOHNH 1 nviolations 2 nrotb 9 volume 574.69

	Exact/Monoisotopic Mass = 562.40221 g/mol
Carthamoleusterone	miLogP 1.02 TPSA 147.67 atoms 36 MW 508.65 nON 8 nOHNH 6 nviolations 2 nrotb 3 volume 479.48 Exact/Monoisotopic Mass = 508.303618 g/mol
Carthamosterone	miLogP 1.90 TPSA 144.52 atoms 37 MW 518.65 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 484.20 Exact/Monoisotopic Mass = 518.287968 g/mol
Carthamosterone A	miLogP -0.10 TPSA 184.97 atoms 38 MW 540.65 nON 10 nOHNH 7 nviolations 2 nrotb 7 volume 500.14 Exact/Monoisotopic Mass = 540.2934476067 g/mol
Carthamosterone B	miLogP 0.85 TPSA 164.74

	natoms 37 MW 524.65 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 492.45 Exact/Monoisotopic Mass = 524.2985329872 g/mol
Castasterone	miLogP 4.69 TPSA 97.98 natoms 33 MW 464.69 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 472.24 Exact/Monoisotopic Mass = 464.350175 g/mol
Cheilanthone A	miLogP 2.49 TPSA 118.21 natoms 33 MW 466.66 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 463.00 Exact/Monoisotopic Mass = 466.329439 g/mol
Cheilanthone B	miLogP 3.69 TPSA 97.98 natoms 32 MW 450.66 nON 5

	nOHNH 4 nviolations 0 nrotb 5 volume 455.30 Exact/Monoisotopic Mass = 450.334525 g/mol
Cyanosterone A	miLogP 3.48 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.74 Exact/Monoisotopic Mass = 448.3188745089 g/mol
Cyanosterone B	miLogP 2.54 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/Monoisotopic Mass = 464.3137891285 g/mol
Cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4

	volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
Cyasterone 3-acetate	miLogP 1.42 TPSA 150.59 natoms 40 MW 562.70 nON 9 nOHNH 4 nviolations 1 nrotb 6 volume 527.28 Exact/Monoisotopic Mass = 562.3141830513 g/mol
Cyasterone 22-acetate	miLogP 1.42 TPSA 150.59 natoms 40 MW 562.70 nON 9 nOHNH 4 nviolations 1 nrotb 6 volume 527.28 Exact/Monoisotopic Mass = 562.314183 g/mol
Cyasterone 2,3-monoacetone	miLogP 2.60 TPSA 122.53 natoms 40 MW 560.73 nON 8 nOHNH 3 nviolations 1 nrotb 4 volume 531.48 Exact/Monoisotopic Mass = 560.3349184959 g/mol
Cyathisterone	miLogP 6.08

	TPSA 34.14 natoms 30 MW 410.64 nON 2 nOHNH 0 nviolations 1 nrotb 4 volume 429.85 Exact/Monoisotopic Mass = 410.318481 g/mol
Cycleasterone A	miLogP 2.26 TPSA 104.06 natoms 33 MW 458.60 nON 6 nOHNH 3 nviolations 0 nrotb 1 volume 434.54 Exact/Monoisotopic Mass = 458.2668389361 g/mol
D	
Dacryhainansterone	miLogP 2.38 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.57 Exact/Monoisotopic Mass = 462.298139 g/mol
Dacryhainansterone 20,22-acetonide	miLogP 4.27 TPSA 96.22 natoms 36

	MW 502.69 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 491.29 Exact/Monoisotopic Mass = 502.329439 g/mol
Dacrysterone	miLogP 0.89 TPSA 158.67 natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 488.76 Exact/Monoisotopic Mass = 510.319268 g/mol
3-deacetoxyalfredensterol	miLogP 5.16 TPSA 83.83 natoms 34 MW 474.68 nON 5 nOHNH 2 nviolations 1 nrotb 7 volume 477.91 Exact/Monoisotopic Mass = 474.3345245731 g/mol
Decumbesterone A	miLogP 2.20 TPSA 138.44 natoms 36 MW 506.68 nON 7 nOHNH 6

	nviolations 2 nrotb 6 volume 492.56 Exact/Monoisotopic Mass = 506.324354 g/mol
2-dehydroajugalactone	miLogP 1.86 TPSA 138.20 natoms 37 MW 514.62 nON 8 nOHNH 3 nviolations 1 nrotb 3 volume 472.80 Exact/Monoisotopic Mass = 514.256668 g/mol
3-dehydroajugalactone	miLogP 1.86 TPSA 138.20 natoms 37 MW 514.62 nON 8 nOHNH 3 nviolations 1 nrotb 3 volume 472.80 Exact/Monoisotopic Mass = 514.256668 g/mol
24(24 ¹)[Z]-dehydroamarasterone B	miLogP 1.86 TPSA 138.44 natoms 36 MW 506.68 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 492.22

	Exact/Monoisotopic Mass = 506.324354 g/mol
22-dehydrocyasterone 2-glucoside	miLogP -1.18 TPSA 220.51 natoms 48 MW 680.79 nON 13 nOHNH 7 nviolations 3 nrotb 7 volume 617.02 Exact/Monoisotopic Mass = 680.340792 g/mol
22-dehydro-20-deoxyajugasterone C	miLogP 2.41 TPSA 115.05 natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 5 volume 451.27 Exact/Monoisotopic Mass = 462.2981390644 g/mol
22-dehydroecdysone	miLogP 2.12 TPSA 115.05 natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 5 volume 450.92 Exact/Monoisotopic Mass = 462.298139 g/mol
3-dehydroecdysone	miLogP 2.12 TPSA 115.05

	natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 5 volume 450.92 Exact/Monoisotopic Mass = 462.298139 g/mol
2-dehydro-3-epi-20-hydroxyecdysone	miLogP 1.17 TPSA 135.28 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 5 volume 458.62 Exact/Monoisotopic Mass = 478.293054 g/mol
22-dehydro-12-hydroxycysterone	miLogP -0.39 TPSA 161.59 natoms 38 MW 534.65 nON 9 nOHNH 5 nviolations 1 nrotb 4 volume 492.95 Exact/Monoisotopic Mass = 534.282883 g/mol
4-dehydro-20-hydroxyecdysone	miLogP 1.18 TPSA 138.44 natoms 34 MW 478.63 nON 7

	nOHNH 6 nviolations 1 nrotb 5 volume 458.27 Exact/Monoisotopic Mass = 478.293054 g/mol
3-dehydro-20-hydroxyecdysone	miLogP 1.17 TPSA 135.28 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 5 volume 458.62 Exact/Monoisotopic Mass = 478.293054 g/mol
24(24 ¹)-dehydro-24 ² -hydroxymakisterone C	miLogP 0.91 TPSA 158.67 natoms 37 MW 522.68 nON 8 nOHNH 7 nviolations 2 nrotb 6 volume 499.91 Exact/Monoisotopic Mass = 522.319268 g/mol
22-dehydro-12-hydroxy-29-nor-cyasterone	miLogP -0.50 TPSA 161.59 natoms 37 MW 520.62 nON 9 nOHNH 5 nviolations 1 nrotb 4

	volume 476.36 Exact/Monoisotopic Mass = 520.267233 g/mol
22-dehydro-12-hydroxy-29-nor-sengosterone	miLogP -1.44 TPSA 181.81 natoms 38 MW 536.62 nON 10 nOHNH 6 nviolations 2 nrotb 4 volume 484.05 Exact/Monoisotopic Mass = 536.262147 g/mol
22-dehydro-12-hydroxy-sengosterone	miLogP -1.44 TPSA 181.81 natoms 38 MW 536.62 nON 10 nOHNH 6 nviolations 2 nrotb 4 volume 484.05 Exact/Monoisotopic Mass = 536.2621474785 g/mol
25,27-dehydroinokosterone	miLogP 1.13 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 459.39 Exact/Monoisotopic Mass = 478.293054 g/mol
24,25-dehydroinokosterone	miLogP 1.35

	TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 458.83 Exact/Monoisotopic Mass = 478.293054 g/mol
24(28)-dehydromakisterone A	miLogP 1.67 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 475.41 Exact/Monoisotopic Mass = 492.308704 g/mol
2-dehydropoststerone	miLogP 0.84 TPSA 91.67 natoms 26 MW 360.45 nON 5 nOHNH 2 nviolations 0 nrotb 1 volume 336.99 Exact/Monoisotopic Mass = 360.193674 g/mol
3-dehydro-17a,19a-poststerone	miLogP 0.84 TPSA 91.67 natoms 26 MW 360.45

	nON 5 nOHNH 2 nviolations 0 nrotb 1 volume 336.99 Exact/Monoisotopic Mass = 360.193674 g/mol
14(15)-dehydropoststerone 2-acetate	miLogP 2.50 TPSA 80.67 natoms 28 MW 386.49 nON 5 nOHNH 1 nviolations 0 nrotb 3 volume 365.45 Exact/Monoisotopic Mass = 386.2093240599 g/mol
24-dehydroprecyasterone	miLogP 2.00 TPSA 144.52 natoms 37 MW 518.65 nON 8 nOHNH 5 nviolations 1 nrotb 3 volume 484.53 Exact/Monoisotopic Mass = 518.287968 g/mol
2-deoxycastasterone (typhasterol)	miLogP 5.61 TPSA 77.75 natoms 32 MW 448.69 nON 4 nOHNH 3 nviolations 1

	nrotb 5 volume 464.20 Exact/Monoisotopic Mass = 448.35526 g/mol
14-deoxydacryhainansterone	miLogP 3.33 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 442.88 Exact/Monoisotopic Mass = 446.303225 g/mol
22-deoxy-20,21-dehydroecdysone	miLogP 3.29 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 443.08 Exact/Monoisotopic Mass = 446.303224 g/mol
22-deoxy-20,21-dihydroxyecdysone	miLogP 1.50 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 464.69 Exact/Monoisotopic Mass = 480.308704 g/mol

2-deoxy-20,26-dihydroxyecdysone	miLogP 1.27 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 464.69 Exact/Monoisotopic Mass = 480.308704 g/mol
22-deoxy-20,26-dihydroxyecdysone	miLogP 1.50 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 464.69 Exact/Monoisotopic Mass = 480.308704 g/mol
3-deoxy-1 b ,20-dihydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
2-deoxy-5,20-dihydroxyecdysone	miLogP 1.33 TPSA 138.44 natoms 34

	MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.13 Exact/Monoisotopic Mass = 480.308704 g/mol
22-deoxyecdysone	miLogP 3.45 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.74 Exact/Monoisotopic Mass = 448.318875 g/mol
2-deoxyecdysone	miLogP 3.22 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.74 Exact/Monoisotopic Mass = 448.318875 g/mol
14-deoxyecdysone	miLogP 3.25 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4

	nviolations 0 nrotb 5 volume 449.09 Exact/Monoisotopic Mass = 448.318875 g/mol
25-deoxyecdysone	miLogP 3.51 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 449.09 Exact/Monoisotopic Mass = 448.318875 g/mol
2-deoxyecdysone 3-acetate	miLogP 3.92 TPSA 104.06 natoms 35 MW 490.68 nON 6 nOHNH 3 nviolations 0 nrotb 7 volume 485.25 Exact/Monoisotopic Mass = 490.329439 g/mol
2-deoxyecdysone 22-acetate	miLogP 3.92 TPSA 104.06 natoms 35 MW 490.68 nON 6 nOHNH 3 nviolations 0 nrotb 7 volume 485.25

	Exact/Monoisotopic Mass = 490.329439 g/mol
2-deoxyecdysone 22-benzoate	miLogP 5.65 TPSA 104.06 atoms 40 MW 552.75 nON 6 nOHNH 3 nviolations 2 nrotb 8 volume 540.10 Exact/Monoisotopic Mass = 552.345089 g/mol
2-deoxyecdysone 3-[4-(1-b-D-glucopyranosyl)]-ferulate	miLogP 3.39 TPSA 212.67 atoms 56 MW 786.96 nON 13 nOHNH 7 nviolations 3 nrotb 13 volume 733.20 Exact/Monoisotopic Mass = 786.4190420427 g/mol
2-deoxyecdysone 22-b-D-glucoside	miLogP 1.51 TPSA 177.13 atoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.86 Exact/Monoisotopic Mass = 610.371698 g/mol
25-deoxyecdysone 22-O-b-D-glucopyranoside	miLogP 1.80 TPSA 177.13

	natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 581.21 Exact/Monoisotopic Mass = 610.371698 g/mol
2-deoxyecdysone 22-phosphate	miLogP 2.55 TPSA 144.52 natoms 36 MW 528.62 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 494.09 Exact/Monoisotopic Mass = 528.285205 g/mol
2-deoxyecdysone 25-rhamnoside	miLogP 2.52 TPSA 156.91 natoms 42 MW 594.79 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 572.60 Exact/Monoisotopic Mass = 594.376783 g/mol
14-deoxy-25-hydroxydacryhainansterone	miLogP 2.12 TPSA 118.21 natoms 33 MW 462.63 nON 6

	nOHNH 5 nviolations 0 nrotb 5 volume 450.57 Exact/Monoisotopic Mass = 462.29813906 g/mol
(5a)-2-deoxy-21-hydroxyecdysone	miLogP 2.21 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 6 volume 457.00 Exact/Monoisotopic Mass = 464.313789 g/mol
22-deoxy-26-hydroxyecdysone	miLogP 2.45 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 6 volume 457.00 Exact/Monoisotopic Mass = 464.313789 g/mol
2-deoxy-20-hydroxyecdysone	miLogP 2.27 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5

	volume 456.44 Exact/Monoisotopic Mass = 464.313789 g/mol
[14a-H]14-deoxy-20-hydroxyecdysone	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
[14b-H]14-deoxy-20-hydroxyecdysone	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
2-deoxy-21-hydroxyecdysone	miLogP 2.21 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 6 volume 457.00 Exact/Monoisotopic Mass = 464.313789 g/mol
(5a)-2-deoxy-20-hydroxyecdysone 3-acetate	miLogP 2.98

	TPSA 124.29 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 492.95 Exact/Monoisotopic Mass = 506.324354 g/mol
2-deoxy-20-hydroxyecdysone 22-acetate	miLogP 2.98 TPSA 124.29 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 492.95 Exact/Monoisotopic Mass = 506.324354 g/mol
2-deoxy-20-hydroxyecdysone 3-acetate	miLogP 2.98 TPSA 124.29 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 492.95 Exact/Monoisotopic Mass = 506.324354 g/mol
2-deoxy-20-hydroxyecdysone 25-acetate	miLogP 2.98 TPSA 124.29 natoms 36 MW 506.68

	nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 492.95 Exact/Monoisotopic Mass = 506.324354 g/mol
(5a)-2-deoxy-20-hydroxyecdysone 20,22-acetonide	miLogP 4.17 TPSA 96.22 natoms 36 MW 504.71 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 497.15 Exact/Monoisotopic Mass = 504.345089 g/mol
2-deoxy-20-hydroxyecdysone 22-benzoate	miLogP 4.70 TPSA 124.29 natoms 41 MW 568.75 nON 7 nOHNH 4 nviolations 1 nrotb 8 volume 547.79 Exact/Monoisotopic Mass = 568.340004 g/mol
2-deoxy-20-hydroxyecdysone 3-crotonate	miLogP 3.66 TPSA 124.29 natoms 38 MW 532.72 nON 7 nOHNH 4 nviolations 1

	nrotb 8 volume 520.36 Exact/Monoisotopic Mass = 532.340004 g/mol
2-deoxy-20-hydroxyecdysone 3-[4-(1-b-D-glucopyranosyl)]-ferulate	miLogP 2.44 TPSA 232.90 natoms 57 MW 802.96 nON 14 nOHNH 8 nviolations 3 nrotb 13 volume 740.89 Exact/Monoisotopic Mass = 802.4139566623 g/mol
2-deoxy-20-hydroxyecdysone 3,22-diacetate	miLogP 3.68 TPSA 130.37 natoms 39 MW 548.72 nON 8 nOHNH 3 nviolations 1 nrotb 9 volume 529.46 Exact/Monoisotopic Mass = 626.366613 g/mol
2-deoxy-20-hydroxyecdysone 3-glucoside	miLogP 0.57 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.56 Exact/Monoisotopic Mass = 626.366613 g/mol

2-deoxy-20-hydroxyecdysone 25-glucoside	miLogP 0.57 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.56 Exact/Monoisotopic Mass = 626.366613 g/mol
2-deoxy-20-hydroxyecdysone 20,22-monoacetone	miLogP 4.17 TPSA 96.22 natoms 36 MW 504.71 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 497.15 Exact/Monoisotopic Mass = 504.345089 g/mol
2-deoxy-20-hydroxyecdysone 22-phosphate	miLogP 1.61 TPSA 164.74 natoms 37 MW 544.62 (protonated) nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 501.78 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
22-deoxy-20-hydroxyecdysone 3-phosphate	miLogP -1.64 TPSA 170.40 natoms 37

	MW 542.61 (unprotonated) nON 9 nOHNH 4 nviolations 1 nrotb 7 volume 496.30 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
2-deoxy-20-hydroxyecdysone 22-glucoside	miLogP 0.57 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.56 Exact/Monoisotopic Mass = 626.366613 g/mol
2-deoxy-20-hydroxyecdysone 3-O-benzoate	miLogP 4.70 TPSA 124.29 natoms 41 MW 568.75 nON 7 nOHNH 4 nviolations 1 nrotb 8 volume 547.79 Exact/Monoisotopic Mass = 568.340004 g/mol
25-deoxy-20-hydroxyecdysoneic acid	miLogP -1.54 TPSA 158.34 natoms 35 MW 493.62 (unprotonated) nON 8 nOHNH 5

	nviolations 0 nrotb 6 volume 464.48 Exact/Monoisotopic Mass = 494.287968 g/mol (protonated)
22-deoxy-28-hydroxymakisterone C	miLogP 2.11 TPSA 138.44 natoms 36 MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 497.87 Exact/Monoisotopic Mass = 508.340004 g/mol
[14b,22S]14-deoxy-20-hydroxypoststerone	miLogP 2.16 TPSA 77.75 natoms 25 MW 348.48 nON 4 nOHNH 3 nviolations 0 nrotb 1 volume 341.02 Exact/Monoisotopic Mass = 348.230060 g/mol
22-deoxyinokosterone	miLogP 2.45 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 6 volume 457.00

	Exact/Monoisotopic Mass = 464.313789 g/mol
2-deoxyintegristerone A	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
22-deoxyintegristerone	miLogP 1.81 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
(5a)-2-deoxyintegristerone A	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
(5a)-22-deoxyintegristerone A	miLogP 1.81 TPSA 138.44

	natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
5-deoxykaladasteone 20,22-acetonide	miLogP 4.27 TPSA 96.22 natoms 36 MW 502.69 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 491.29 Exact/Monoisotopic Mass = 502.329439 g/mol
20-deoxymakisterone A (24-methylecdysone)	miLogP 2.78 TPSA 118.21 natoms 34 MW 478.67 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 473.37 Exact/Monoisotopic Mass = 478.329439 g/mol
2-deoxypolypodine B 3b-D-glucoside	miLogP -0.38 TPSA 217.59 natoms 45 MW 642.78 nON 12

	nOHNH 9 nviolations 3 nrotb 8 volume 596.25 Exact/Monoisotopic Mass = 642.361527 g/mol
[14b,17a]14-deoxypoststerone	miLogP 1.97 TPSA 74.60 natoms 25 MW 346.47 nON 4 nOHNH 2 nviolations 0 nrotb 1 volume 335.15 Exact/Monoisotopic Mass = 346.214410 g/mol
20-deoxyshidasterone	miLogP 3.41 TPSA 86.99 natoms 32 MW 446.63 nON 5 nOHNH 3 nviolations 0 nrotb 2 volume 438.89 Exact/Monoisotopic Mass = 446.303224 g/mol
2-deoxy-5,20,26-trihydroxyecdysone	miLogP 0.32 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6

	volume 472.39 Exact/Monoisotopic Mass = 496.303618 g/mol
2-deoxy-5,20,26-trihydroxyecdysone 20,22-acetonide	miLogP 2.21 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 513.1 Exact/Monoisotopic Mass = 536.334918 g/mol
Deoxyviperidone	miLogP 6.52 TPSA 37.30 natoms 29 MW 400.65 nON 2 nOHNH 1 nviolations 1 nrotb 5 volume 425.31 Exact/Monoisotopic Mass = 400.334131 g/mol
Diaulusterol A	miLogP 4.40 TPSA 104.06 natoms 37 MW 516.72 nON 6 nOHNH 3 nviolations 1 nrotb 9 volume 512.99 Exact/Monoisotopic Mass = 516.345089 g/mol
Diaulusterol B	miLogP 4.21

	TPSA 77.75 natoms 31 MW 430.63 nON 4 nOHNH 3 nviolations 0 nrotb 5 volume 434.83 Exact/Monoisotopic Mass = 430.30831 g/mol
25,26-didehydroponasterone A	miLogP 2.37 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 451.13 Exact/Monoisotopic Mass = 462.298139 g/mol
20,22-didehydrotaxisterone	miLogP 3.51 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 4 volume 442.53 Exact/Monoisotopic Mass = 446.303224 g/mol
2,22-dideoxyecdysone	miLogP 4.37 TPSA 77.75 natoms 31 MW 432.64

	nON 4 nOHNH 3 nviolations 0 nrotb 5 volume 440.70 Exact/Monoisotopic Mass = 432.32396 g/mol
22,25-dideoxyecdysone	miLogP 4.66 TPSA 77.75 natoms 31 MW 432.64 nON 4 nOHNH 3 nviolations 0 nrotb 5 volume 441.05 Exact/Monoisotopic Mass = 432.32396 g/mol
2,22-dideoxyecdysone 25-O-b-D-glucopyranoside	miLogP 2.66 TPSA 156.91 natoms 42 MW 594.79 nON 9 nOHNH 6 nviolations 2 nrotb 8 volume 572.82 Exact/Monoisotopic Mass = 594.376783 g/mol
2,22-dideoxyecdysone 25-O-b-D-glucopyranosyl-(1→2)-b-D-glucopyranoside	miLogP 0.96 TPSA 236.06 natoms 53 MW 756.93 nON 14 nOHNH 9 nviolations 3

	nrotb 11 volume 704.94 Exact/Monoisotopic Mass = 756.429607 g/mol
(5a)-2,22-dideoxyecdysone 25-O-b-D-glucopyranosyl-(1→2)-b-D-glucopyranoside	miLogP 0.96 TPSA 236.06 natoms 53 MW 756.93 nON 14 nOHNH 9 nviolations 3 nrotb 11 volume 704.94 Exact/Monoisotopic Mass = 756.429607 g/mol
2,22-dideoxy-20-hydroxyecdysone	miLogP 3.42 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.39 Exact/Monoisotopic Mass = 448.318875 g/mol
2,22-dideoxy-23-hydroxyecdysone	miLogP 3.22 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.74 Exact/Monoisotopic Mass = 448.318875 g/mol

2,22-dideoxy-20-hydroxyecdysone 3b-O-b-D-glucopyranoside	miLogP 1.72 TPSA 177.13 natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.51 Exact/Monoisotopic Mass = 610.3716979274 g/mol
2,22-dideoxy-20-hydroxyecdysone 25-O-b-D-glucopyranoside	miLogP 1.72 TPSA 177.13 natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.51 Exact/Monoisotopic Mass = 610.371698 g/mol
2,22-dideoxy-5b-hydroxyecdysone 25-O-b-D-glucopyranosyl-(1→2)-b-D-glucopyranoside	miLogP 0.01 TPSA 256.29 natoms 54 MW 772.93 nON 15 nOHNH 10 nviolations 3 nrotb 11 volume 712.63 Exact/Monoisotopic Mass = 772.424521 g/mol
2,22-dideoxy-20-hydroxyecdysone 3-phosphate	miLogP -0.49 TPSA 150.17 natoms 36

	MW 526.61 (unprotonated) nON 8 nOHNH 3 nviolations 1 nrotb 7 volume 488.25 Exact/Monoisotopic Mass = 528.285205 g/mol (protonated)
2,22-dideoxy-23-hydroxyecdysone 3-phosphate	miLogP -0.69 TPSA 150.17 natoms 36 MW 526.61 (unprotonated) nON 8 nOHNH 3 nviolations 1 nrotb 7 volume 488.61 Exact/Monoisotopic Mass = 528.285205 g/mol (protonated)
24,28-diepi-cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
7,8-dihydroajugasterone C	miLogP 1.83 TPSA 138.44 natoms 34 MW 482.66 nON 7 nOHNH 6

	nviolations 1 nrotb 5 volume 471.04 Exact/Monoisotopic Mass = 482.324354 g/mol
[14b-H]14,15-dihydrocalonysterone	miLogP 1.62 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 458.56 Exact/Monoisotopic Mass = 478.293055 g/mol
7,8-dihydroponasterone A	miLogP 2.75 TPSA 118.21 natoms 33 MW 466.66 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 463.00 Exact/Monoisotopic Mass = 466.329439 g/mol
Dihydropoststerone	miLogP 1.22 TPSA 97.98 natoms 26 MW 364.48 nON 5 nOHNH 4 nviolations 0 nrotb 1 volume 348.71

	Exact/Monoisotopic Mass = 364.2249741241 g/mol
(5a)-dihydrorubrosterone	miLogP 0.47 TPSA 97.98 natoms 24 MW 336.43 nON 5 nOHNH 4 nviolations 0 nrotb 0 volume 315.32 Exact/Monoisotopic Mass = 336.193674 g/mol
dihydrorubrosterone	miLogP 0.47 TPSA 97.98 natoms 24 MW 336.43 nON 5 nOHNH 4 nviolations 0 nrotb 0 volume 315.32 Exact/Monoisotopic Mass = 336.193674 g/mol
5,29-dihydrocapitasterone	miLogP 1.08 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 498.67 Exact/Monoisotopic Mass = 496.303618 g/mol
9b,20-dihydroxyecdysone	miLogP 0.41 TPSA 158.67

	natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303618 g/mol
9a,20-dihydroxyecdysone	miLogP 0.41 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303618 g/mol
(20R)-1a,20-dihydroxyecdysone	miLogP 0.66 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
20,26-dihydroxyecdysone	miLogP 0.35 TPSA 158.67 natoms 35 MW 496.64 nON 8

	nOHNH 7 nviolations 1 nrotb 6 volume 472.74 Exact/Monoisotopic Mass = 496.303618 g/mol
20,26-dihydroxyecdysone 22-acetate	miLogP 1.05 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 8 volume 509.25 Exact/Monoisotopic Mass = 538.314183 g/mol
20,26-dihydroxyecdysone 20,22-acetonide	miLogP 2.24 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 513.46 Exact/Monoisotopic Mass = 536.334918 g/mol
20,26-dihydroxyecdysone 3,22-diacetate	miLogP 1.76 TPSA 170.82 natoms 41 MW 580.72 nON 10 nOHNH 5 nviolations 1 nrotb 10

	volume 545.76 Exact/Monoisotopic Mass = 580.324747735 g/mol
20,26-dihydroxyecdysone 2,22-diacetate	miLogP 1.76 TPSA 170.82 natoms 41 MW 580.72 nON 10 nOHNH 5 nviolations 1 nrotb 10 volume 545.76 Exact/Monoisotopic Mass = 580.324747735 g/mol
20,26-dihydroxyecdysone 22,26-hemiacetal	miLogP 0.80 TPSA 147.67 natoms 35 MW 494.62 nON 8 nOHNH 6 nviolations 1 nrotb 2 volume 462.89 Exact/Monoisotopic Mass = 494.2879683035 g/mol
20,24-dihydroxy-24ξ-hydroxymethylecdysone	miLogP -0.12 TPSA 178.90 natoms 37 MW 526.67 nON 9 nOHNH 8 nviolations 2 nrotb 6 volume 497.02 Exact/Monoisotopic Mass = 526.314185 g/mol
Diploclidine	miLogP 3.40

	TPSA 90.65 natoms 32 MW 439.60 nON 5 nOHNH 3 nviolations 0 nrotb 3 volume 424.21 Exact/Monoisotopic Mass = 439.272259 g/mol
E	
Ecdysone	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
Ecdysone 3-acetate 22-phosphate	miLogP -0.90 TPSA 176.48 natoms 40 MW 584.64 (unprotonated) nON 10 nOHNH 3 nviolations 1 nrotb 9 volume 533.16 Exact/Monoisotopic Mass = 586.290684335 g/mol (protonated)
Ecdysone 2-acetate 22-phosphate	miLogP -0.90

	TPSA 176.48 natoms 40 MW 584.64 (unprotonated) nON 10 nOHNH 3 nviolations 1 nrotb 9 volume 533.16 Exact/Monoisotopic Mass = 586.290684335 g/mol (protonated)
Ecdysone 22-acetate	miLogP 3.01 TPSA 124.29 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 493.30 Exact/Monoisotopic Mass = 506.324354 g/mol
Ecdysone 3-acetate	miLogP 3.01 TPSA 124.29 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 493.30 Exact/Monoisotopic Mass = 506.324354 g/mol
Ecdysone 3-acetate 2-phosphate	miLogP 2.34 TPSA 170.82 natoms 40 MW 586.66

	nON 10 nOHNH 5 nviolations 1 nrotb 9 volume 538.64 Exact/Monoisotopic Mass = 586.290685 g/mol
Ecdysone 2,3-diacetate 22-phosphate	miLogP -0.20 TPSA 182.56 natoms 43 MW 626.68 (unprotonated) nON 11 nOHNH 2 nviolations 2 nrotb 11 volume 569.67 Exact/Monoisotopic Mass = 628.301249 g/mol (protonated)
Ecdysone 22-glucoside	miLogP 0.60 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/Monoisotopic Mass = 626.366613 g/mol
Ecdysone 22-glycolate	miLogP 2.17 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1

	nrotb 8 volume 501.56 Exact/Monoisotopic Mass = 522.319268 g/mol
Ecdysone 22-linoleate	miLogP 9.03 TPSA 124.29 natoms 52 MW 727.08 nON 7 nOHNH 4 nviolations 2 nrotb 21 volume 749.75 Exact/Monoisotopic Mass = 726.543455 g/mol
Ecdysone 3-O-b-D-glucopyranoside	miLogP 0.60 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/Monoisotopic Mass = 626.366613 g/mol
Ecdysone 25-O-b-D-glucopyranoside	miLogP 0.60 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/Monoisotopic Mass = 626.366613 g/mol

Ecdysone 22-oleate	miLogP 9.33 TPSA 133.52 natoms 53 MW 745.10 nON 8 nOHNH 4 nviolations 2 nrotb 23 volume 764.92 Exact/Monoisotopic Mass = 744.554019 g/mol
Ecdysone 22-palmitate	miLogP 9.10 TPSA 124.29 natoms 50 MW 703.06 nON 7 nOHNH 4 nviolations 2 nrotb 21 volume 728.52 Exact/Monoisotopic Mass = 702.543455 g/mol
Ecdysone 22-palmitoleate	miLogP 8.92 TPSA 124.29 natoms 50 MW 701.04 nON 7 nOHNH 4 nviolations 2 nrotb 20 volume 722.34 Exact/Monoisotopic Mass = 700.527805 g/mol
Ecdysone 22-phosphate	miLogP 1.64 TPSA 164.74 natoms 37

	MW 544.62 (protonated) nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 502.13 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
Ecdysone 3-phosphate	miLogP -1.61 TPSA 170.40 natoms 37 MW 542.61 (unprotonated) nON 9 nOHNH 4 nviolations 1 nrotb 7 volume 496.65 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
Ecdysone 2-phosphate	miLogP -1.61 TPSA 170.40 natoms 37 MW 542.61 (unprotonated) nON 9 nOHNH 4 nviolations 1 nrotb 7 volume 496.65 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
Ecdysone 22-stearate	miLogP 9.39 TPSA 124.29 natoms 52 MW 731.11 nON 7 nOHNH 4

	nviolations 2 nrotb 23 volume 762.12 Exact/Monoisotopic Mass = 730.574755 g/mol
Ecdysone 22-sulphate	miLogP -1.08 TPSA 164.42 natoms 37 MW 543.70 (unprotonated) nON 9 nOHNH 4 nviolations 1 nrotb 7 volume 494.46 Exact/Monoisotopic Mass = 543.262779 g/mol (unprotonated)
Ecdysonelactone A	miLogP -0.29 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 5 volume 497.76 Exact/Monoisotopic Mass = 536.298533 g/mol
Ecdysonelactone B	miLogP 0.92 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 490.06

	Exact/Monoisotopic Mass = 520.303618 g/mol
Ecdysonelactone C	miLogP 0.66 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 490.06 Exact/Monoisotopic Mass = 520.303618 g/mol
Ecdysonelactone D	miLogP 0.68 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 5 volume 490.42 Exact/Monoisotopic Mass = 520.303618 g/mol
Ecdysonoic acid	miLogP -1.54 TPSA 158.34 natoms 35 MW 493.62 (unprotonated) nON 8 nOHNH 5 nviolations 0 nrotb 6 volume 464.48 Exact/Monoisotopic Mass = 494.287968 g/mol (protonated)
Ecdysteroside	miLogP -2.05 TPSA 296.74

	natoms 56 MW 804.92 nON 17 nOHNH 12 nviolations 3 nrotb 11 volume 728.72 Exact/Monoisotopic Mass = 804.414351 g/mol
[E]-2-deoxy-20-hydroxyecdysone 3-[4-(1-b-D-glucopyranosyl)]-cafeate	miLogP 2.14 TPSA 243.90 natoms 56 MW 788.93 nON 14 nOHNH 9 nviolations 3 nrotb 12 volume 723.37 Exact/Monoisotopic Mass = 788.3983065981 g/mol
24-epi-abutasterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
22-epi-ajugasterone C	miLogP 1.65 TPSA 138.44 natoms 34 MW 480.64 nON 7

	nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
24-epi-atrotosterone A	miLogP 2.62 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.42 Exact/Monoisotopic Mass = 494.3243538122 g/mol
3-epi-cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
28-epi-cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4

	volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
3-epi-cyasterone 22-acetate	miLogP 1.42 TPSA 150.59 natoms 40 MW 562.70 nON 9 nOHNH 4 nviolations 1 nrotb 6 volume 527.28 Exact/Monoisotopic Mass = 562.314183 g/mol
5-epi-cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
3-epi-22-deoxy-20,26-dihydroxyecdysone	miLogP 1.50 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 464.69 Exact/Monoisotopic Mass = 480.3087037481 g/mol
3-epi-22-deoxy-20,26-dihydroxyecdysone 2-phosphate	miLogP -2.41

	TPSA 190.63 natoms 38 MW 558.61 (unprotonated) nON 10 nOHNH 5 nviolations 1 nrotb 8 volume 504.56 Exact/Monoisotopic Mass = 560.2750342708 g/mol (protonated)
3-epi-2-deoxyecdysone	miLogP 3.22 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.74 Exact/Monoisotopic Mass = 448.318875 g/mol
3-epi-2-deoxyecdysone 22-phosphate	miLogP -0.69 TPSA 150.17 natoms 36 MW 526.61 (unprotonated) nON 8 nOHNH 3 nviolations 1 nrotb 7 volume 488.61 Exact/Monoisotopic Mass = 528.285205 g/mol (protonated)
3-epi-2-deoxyecdysone 3-phosphate	miLogP -0.69 TPSA 150.17 natoms 36 MW 526.61 (unprotonated)

	nON 8 nOHNH 3 nviolations 1 nrotb 7 volume 488.61 Exact/Monoisotopic Mass = 528.285205 g/mol (protonated)
3-epi-2-deoxy-20-hydroxyecdysone	miLogP 2.27 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/Monoisotopic Mass = 464.313789 g/mol
3-epi-22-deoxy-20-hydroxyecdysone	miLogP 2.51 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/Monoisotopic Mass = 464.313789 g/mol
3-epi-22-deoxy-20-hydroxyecdysone 2-phosphate	miLogP -1.40 TPSA 170.40 natoms 37 MW 542.61 (unprotonated) nON 9 nOHNH 4 nviolations 1

	nrotb 7 volume 496.30 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
3-epi-22-deoxy-16b, 20-dihydroxyecdysone	miLogP 1.59 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.3087037481 g/mol
3-epi-22-deoxy-16b,20-dihydroxyecdysone 2-phosphate	miLogP -2.32 TPSA 190.63 natoms 38 MW 558.61 nON 10 nOHNH 5 nviolations 1 nrotb 7 volume 504.34 Exact/Monoisotopic Mass = 560.2750342708 g/mol
3-epi-20,26-dihydroxyecdysone	miLogP 0.35 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6 volume 472.74 Exact/Monoisotopic Mass = 496.3036183676 g/mol

3-epi-ecdysone	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
3-epi-ecdysone 22-phosphate	miLogP -1.61 TPSA 170.40 natoms 37 MW 542.61 (unprotonated) nON 9 nOHNH 4 nviolations 1 nrotb 7 volume 496.65 Exact/Monoisotopic Mass = 544.28012 g/mol (protonated)
25,28-diepi-cyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
22-epi-20-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34

	MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
3-epi-26-hydroxyecdysone	miLogP 1.30 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 465.04 Exact/Monoisotopic Mass = 480.308704 g/mol
14-epi-20-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
3-epi-20-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6

	nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
3-epi-20-hydroxyecdysone 3-phosphate	miLogP -2.55 TPSA 190.63 natoms 38 MW 558.61 (unprotonated) nON 10 nOHNH 5 nviolations 1 nrotb 7 volume 504.34 Exact/Monoisotopic Mass = 560.275035 g/mol (protonated)
22-epi-14-hydroxypinnasterol 2-acetate	miLogP 3.08 TPSA 124.29 natoms 36 MW 504.66 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 487.08 Exact/Monoisotopic Mass = 504.3087037481 g/mol
24-epi-makisterone A	miLogP 1.83 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.06

	Exact/Monoisotopic Mass = 494.324354 g/mol
24-epi-pinnatasterone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
14-epi-polypodine B	miLogP 0.41 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303620 g/mol
14-epi-ponasterone A 22-glucoside	miLogP 0.86 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/Monoisotopic Mass = 626.366613 g/mol
3-epi-poststerone	miLogP 1.03 TPSA 94.83

	natoms 26 MW 362.47 nON 5 nOHNH 3 nviolations 0 nrotb 1 volume 342.85 Exact/Monoisotopic Mass = 362.209324 g/mol
24-epi-pterosterone	miLogP 1.39 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
3-epi-rubrosterone	miLogP 0.28 TPSA 94.83 natoms 24 MW 334.41 nON 5 nOHNH 3 nviolations 0 nrotb 0 volume 309.46 Exact/Monoisotopic Mass = 334.178024 g/mol
28-epi-sengosterone	miLogP -0.23 TPSA 164.74 natoms 38 MW 536.66 nON 9

	nOHNH 6 nviolations 2 nrotb 4 volume 498.46 Exact/Monoisotopic Mass = 536.298533 g/mol
3-epi-shidasterone	miLogP 2.47 TPSA 107.22 natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 446.59 Exact/Monoisotopic Mass = 462.2981390644 g/mol
Polyporusterone H	miLogP 2.97 TPSA 107.22 natoms 34 MW 476.65 nON 6 nOHNH 4 nviolations 0 nrotb 3 volume 463.52 Exact/Monoisotopic Mass = 476.313789 g/mol
Polyporusterone I	miLogP 2.88 TPSA 107.22 natoms 34 MW 476.65 nON 6 nOHNH 4 nviolations 0 nrotb 3

	volume 463.74 Exact/Monoisotopic Mass = 476.313789 g/mol
Polyporusterone J	miLogP 2.94 TPSA 110.51 natoms 34 MW 476.65 nON 6 nOHNH 4 nviolations 0 nrotb 4 volume 463.17 Exact/Monoisotopic Mass = 476.313789 g/mol
Ergosta-4,7,22-triene-3,6-dione	miLogP 5.90 TPSA 34.14 natoms 30 MW 408.63 nON 2 nOHNH 0 nviolations 1 nrotb 4 volume 423.63 Exact/Monoisotopic Mass = 408.302831 g/mol
F	
Fibrauecdyside A	miLogP 0.13 TPSA 217.59 natoms 46 MW 656.81 nON 12 nOHNH 9 nviolations 3 nrotb 8

	volume 613.19 Exact/Monoisotopic Mass = 656.377177 g/mol
G	
Geradiasterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Glutinoesterone	miLogP 0.97 TPSA 158.67 natoms 36 MW 508.65 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 483.45 Exact/Monoisotopic Mass = 508.3036183676 g/mol
Gymnasterone B	miLogP 5.33 TPSA 46.67 natoms 31 MW 424.62 nON 3 nOHNH 0 nviolations 1 nrotb 4

	volume 427.69 Exact/Monoisotopic Mass = 424.297745 g/mol
H	
Herkesterone	miLogP 0.23 TPSA 158.67 natoms 35 MW 494.62 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 465.96 Exact/Monoisotopic Mass = 494.287968 g/mol
3b,4a,14a,20R,22R,25-hexahydroxy-5a-cholest-7-en-6-one	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.3087037481 g/mol
3b,14a,17a,20,24,25-hexahydroxy-5a-ergosta-7,22-dien-6-one	miLogP 1.75 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 4 volume 474.18

	Exact/Monoisotopic Mass = 492.308704 g/mol
5-hydroxyabutasterone	miLogP -0.50 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 5 volume 480.22 Exact/Monoisotopic Mass = 512.298533 g/mol
14-hydroxyacetylpinnasterol	miLogP 3.08 TPSA 124.29 natoms 36 MW 504.66 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 487.08 Exact/Monoisotopic Mass = 504.3087037481 g/mol
14a-hydroxyalfredensterol	miLogP 4.92 TPSA 110.14 natoms 38 MW 532.72 nON 7 nOHNH 2 nviolations 1 nrotb 9 volume 522.11 Exact/Monoisotopic Mass = 532.3400038763 g/mol
25-hydroxyatrosterone A	miLogP 0.92 TPSA 158.67

	natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 489.11 Exact/Monoisotopic Mass = 510.319268 g/mol
25-hydroxyatrotosterone B	miLogP 1.11 TPSA 150.97 natoms 36 MW 508.65 nON 8 nOHNH 6 nviolations 2 nrotb 4 volume 479.26 Exact/Monoisotopic Mass = 508.303618 g/mol
14-hydroxycarpesterol	miLogP 8.59 TPSA 83.83 natoms 42 MW 578.83 nON 5 nOHNH 2 nviolations 2 nrotb 9 volume 582.38 Exact/Monoisotopic Mass = 578.3971248296 g/mol
23-hydroxycyasterone	miLogP -0.20 TPSA 164.74 natoms 38 MW 536.66 nON 9

	nOHNH 6 nviolations 2 nrotb 4 volume 498.81 Exact/Monoisotopic Mass = 536.2985329872 g/mol
11-hydroxycyasterone	miLogP -0.20 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 498.81 Exact/Monoisotopic Mass = 536.2985329872 g/mol
24-hydroxycyasterone	miLogP -0.23 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 498.46 Exact/Monoisotopic Mass = 536.2985329872 g/mol
25-hydroxydacryhainansterone	miLogP 1.18 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5

	volume 458.27 Exact/Monoisotopic Mass = 478.293054 g/mol
11-hydroxy-24-dehydrocapitasterone	miLogP 2.23 TPSA 144.52 natoms 37 MW 518.65 nON 8 nOHNH 5 nviolations 1 nrotb 3 volume 484.53 Exact/Monoisotopic Mass = 518.2879683035 g/mol
5b-hydroxy-24(28)-dehydromakisterone A	miLogP 0.73 TPSA 158.67 natoms 36 MW 508.65 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 483.10 Exact/Monoisotopic Mass = 508.303618 g/mol
1b-hydroxy-22-deoxy-20,21-dehydroecdysone	miLogP 2.59 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 451.13 Exact/Monoisotopic Mass = 462.298139 g/mol
11b-hydroxy-20-deoxyshidasterone	miLogP 2.50

	TPSA 107.22 natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 446.94 Exact/Monoisotopic Mass = 462.298139 g/mol
1b-hydroxy-20,22-didehydrotaxisterone	miLogP 2.81 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 4 volume 450.57 Exact/Monoisotopic Mass = 462.298139 g/mol
24-hydroxy-24,28-dihydrocarthamosterone	miLogP -0.54 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 498.11 Exact/Monoisotopic Mass = 536.298533 g/mol
11a-hydroxyecdysone	miLogP 1.39 TPSA 138.44 natoms 34 MW 480.64

	nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
26-hydroxyecdysone	miLogP 1.30 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 465.04 Exact/Monoisotopic Mass = 480.308704 g/mol
24-hydroxyecdysone	miLogP 1.39 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
5-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1

	nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
20-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
20-hydroxyecdysone 3-acetate 22-phosphate	miLogP -1.85 TPSA 196.71 natoms 41 MW 600.64 (unprotonated) nON 11 nOHNH 4 nviolations 2 nrotb 9 volume 540.85 Exact/Monoisotopic Mass = 602.2855989545 g/mol (protonated)
20-hydroxyecdysone 3-phosphate	miLogP -2.55 TPSA 190.63 natoms 38 MW 558.61 nON 10 nOHNH 5 nviolations 1 nrotb 7 volume 504.34 Exact/Monoisotopic Mass = 560.275035 g/mol

[5a-H]20-hydroxyecdysone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
20-hydroxyecdysone 3-acetate	miLogP 2.06 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 500.99 Exact/Monoisotopic Mass = 522.319268 g/mol
20-hydroxyecdysone 2-acetate	miLogP 2.06 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 500.99 Exact/Monoisotopic Mass = 522.319268 g/mol
20-hydroxyecdysone 22-acetate	miLogP 2.06 TPSA 144.52 natoms 37

	MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 500.99 Exact/Monoisotopic Mass = 522.319268 g/mol
20-hydroxyecdysone 3-acetate 2-phosphate	miLogP -1.85 TPSA 196.71 natoms 41 MW 600.64 (unprotonated) nON 11 nOHNH 4 nviolations 2 nrotb 9 volume 540.85 Exact/Monoisotopic Mass = 602.2855989545 (protonated)
24-hydroxyecdysone 2,3-acetonide	miLogP 3.28 TPSA 116.45 natoms 37 MW 520.71 nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 505.55 Exact/Monoisotopic Mass = 520.340004 g/mol
20-hydroxyecdysone 22-benzoate	miLogP 3.79 TPSA 144.52 natoms 42 MW 584.75 nON 8 nOHNH 5

	nviolations 1 nrotb 8 volume 555.84 Exact/Monoisotopic Mass = 584.334918 g/mol
20-hydroxyecdysone 20-benzoate	miLogP 3.79 TPSA 144.52 natoms 42 MW 584.75 nON 8 nOHNH 5 nviolations 1 nrotb 8 volume 555.84 Exact/Monoisotopic Mass = 584.334918 g/mol
[5a-H])20-hydroxyecdysone 22-benzoate	miLogP 3.79 TPSA 144.52 natoms 42 MW 584.75 nON 8 nOHNH 5 nviolations 1 nrotb 8 volume 555.84 Exact/Monoisotopic Mass = 584.334918 g/mol
20-hydroxyecdysone 22-benzoate 25-glucoside	miLogP 2.08 TPSA 223.67 natoms 53 MW 746.89 nON 13 nOHNH 8 nviolations 3 nrotb 11 volume 687.96

	Exact/Monoisotopic Mass = 746.387742 g/mol
20-hydroxyecdysone 2-cinnamate	miLogP 4.21 TPSA 144.52 atoms 44 MW 610.79 nON 8 nOHNH 5 nviolations 1 nrotb 9 volume 583.25 Exact/Monoisotopic Mass = 610.350569 g/mol
20-hydroxyecdysone 2-glucoside	miLogP -0.35 TPSA 217.59 atoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.361527 g/mol
20-hydroxyecdysone 3-glucoside	miLogP -0.35 TPSA 217.59 atoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.361527 g/mol
20-hydroxyecdysone 25-glucoside	miLogP -0.35 TPSA 217.59

	natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.361527 g/mol
20-hydroxyecdysone 2,22-diacetate	miLogP 2.77 TPSA 150.59 natoms 40 MW 564.72 nON 9 nOHNH 4 nviolations 1 nrotb 9 volume 537.50 Exact/Monoisotopic Mass = 564.329833 g/mol
20-hydroxyecdysone 3,22-diacetate	miLogP 2.77 TPSA 150.59 natoms 40 MW 564.72 nON 9 nOHNH 4 nviolations 1 nrotb 9 volume 537.50 Exact/Monoisotopic Mass = 564.329833 g/mol
20-hydroxyecdysone 2,3-diacetate 22-benzoate	miLogP 5.20 TPSA 156.67 natoms 48 MW 668.82 nON 10

	nOHNH 3 nviolations 2 nrotb 12 volume 628.86 Exact/Monoisotopic Mass = 668.3560478633 g/mol
20-hydroxyecdysone 2,3:20,22-diacetonide	miLogP 5.14 TPSA 94.46 natoms 40 MW 560.77 nON 7 nOHNH 2 nviolations 2 nrotb 4 volume 545.91 Exact/Monoisotopic Mass = 560.371304 g/mol
20-hydroxyecdysone 22,25-dibenzoate	miLogP 6.21 TPSA 150.59 natoms 50 MW 688.86 nON 9 nOHNH 4 nviolations 2 nrotb 11 volume 647.20 Exact/Monoisotopic Mass = 688.361133 g/mol
20-hydroxyecdysone 20,22-ethylidene	miLogP 2.80 TPSA 116.45 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 4

	volume 488.96 Exact/Monoisotopic Mass = 506.324354 g/mol
26-hydroxyecdysone 22-glucoside	miLogP -0.41 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 9 volume 597.16 Exact/Monoisotopic Mass = 642.361527 g/mol
20-hydroxyecdysone 22-glycolate	miLogP 1.22 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 8 volume 509.25 Exact/Monoisotopic Mass = 538.314183 g/mol
20-hydroxyecdysone 22-linoleate	miLogP 8.61 TPSA 144.52 natoms 53 MW 743.08 nON 8 nOHNH 5 nviolations 2 nrotb 21 volume 757.45 Exact/Monoisotopic Mass = 742.538369 g/mol
20-hydroxyecdysone 20,22-acetonide	miLogP 3.25

	TPSA 116.45 natoms 37 MW 520.71 nON 7 nOHNH 4 nviolations 1 nrotb 4 volume 505.20 Exact/Monoisotopic Mass = 520.340004 g/mol
20-hydroxyecdysone 2,3-acetonide	miLogP 3.25 TPSA 116.45 natoms 37 MW 520.71 nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 505.20 Exact/Monoisotopic Mass = 520.340004 g/mol
20-hydroxyecdysone 2-galactoside	miLogP -0.35 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.3615271666 g/mol
20-hydroxyecdysone 22-oleate	miLogP 8.94 TPSA 144.52 natoms 53 MW 745.10

	nON 8 nOHNH 5 nviolations 2 nrotb 22 volume 763.63 Exact/Monoisotopic Mass = 743.5461943618 g/mol
20-hydroxyecdysone 22-palmitate	miLogP 8.72 TPSA 144.52 natoms 51 MW 719.06 nON 8 nOHNH 5 nviolations 2 nrotb 21 volume 736.22 Exact/Monoisotopic Mass = 718.538369 g/mol
20-hydroxyecdysone 3-p-coumarate	miLogP 3.73 TPSA 164.74 natoms 45 MW 626.79 nON 9 nOHNH 6 nviolations 2 nrotb 9 volume 591.27 Exact/Monoisotopic Mass = 626.345483 g/mol
26-hydroxyecdysone 26-phosphate	miLogP -2.62 TPSA 190.63 natoms 38 MW 558.61 (unprotonated) nON 10 nOHNH 5 nviolations 1

	nrotb 8 volume 504.91 Exact/Monoisotopic Mass = 560.275035 g/mol (protonated)
26-hydroxyecdysone 2-phosphate	miLogP -2.62 TPSA 190.63 natoms 38 MW 558.61 (unprotonated) nON 10 nOHNH 5 nviolations 1 nrotb 8 volume 504.91 Exact/Monoisotopic Mass = 560.275035 g/mol (protonated)
20-hydroxyecdysone 22-phosphate	miLogP -2.55 TPSA 190.63 natoms 38 MW 558.61 (unprotonated) nON 10 nOHNH 5 nviolations 1 nrotb 7 volume 504.34 Exact/Monoisotopic Mass = 560.275035 g/mol (protonated)
20-hydroxyecdysone 22-stearate	miLogP 9.12 TPSA 144.52 natoms 53 MW 747.11 nON 8 nOHNH 5 nviolations 2 nrotb 23 volume 769.82 Exact/Monoisotopic Mass = 746.569669 g/mol

20-hydroxyecdysone 20,25-acetonide 25-acetate	miLogP 3.95 TPSA 122.53 natoms 40 MW 562.74 nON 8 nOHNH 3 nviolations 1 nrotb 6 volume 541.71 Exact/Monoisotopic Mass = 562.350569 g/mol
20-hydroxyecdysone 20,22-butyldiene acetal	miLogP 3.87 TPSA 116.45 natoms 38 MW 534.73 nON 7 nOHNH 4 nviolations 1 nrotb 6 volume 522.56 Exact/Monoisotopic Mass = 534.3556539405 g/mol
20-hydroxyecdysone 20,25-acetonide 25-acetate	miLogP 0.23 TPSA 175.74 natoms 36 MW 510.62 (protonated) nON 9 nOHNH 7 nviolations 2 nrotb 6 volume 474.92 Exact/Monoisotopic Mass = 510.282883 g/mol (protonated)
[24R]24-(2-hydroxyethyl)-20-hydroxyecdysone	miLogP 1.10 TPSA 158.67 natoms 37

	MW 524.70 nON 8 nOHNH 7 nviolations 2 nrotb 7 volume 506.13 Exact/Monoisotopic Mass = 524.334918 g/mol
20-hydroxy-24-hydroxymethylecdysone	miLogP 0.83 TPSA 158.67 natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 6 volume 489.32 Exact/Monoisotopic Mass = 510.319268 g/mol
26-hydroxyintegristerone A	miLogP -0.35 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 6 volume 480.78 Exact/Monoisotopic Mass = 512.2985329872 g/mol
1b-hydroxymakisterone C	miLogP 1.64 TPSA 158.67 natoms 37 MW 524.70 nON 8 nOHNH 7

	nviolations 2 nrotb 6 volume 505.91 Exact/Monoisotopic Mass = 524.334918 g/mol
26-hydroxymakisterone C	miLogP 1.33 TPSA 158.67 natoms 37 MW 524.70 nON 8 nOHNH 7 nviolations 2 nrotb 7 volume 506.13 Exact/Monoisotopic Mass = 524.334918 g/mol
25-hydroxypanuosterone	miLogP 0.89 TPSA 158.67 natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 488.76 Exact/Monoisotopic Mass = 510.319268 g/mol
14-hydroxypinnasterol	miLogP 2.38 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.57

	Exact/Monoisotopic Mass = 462.2981390644 g/mol
14-hydroxypinnasterol 3-acetate	miLogP 3.08 TPSA 124.29 natoms 36 MW 504.66 nON 7 nOHNH 4 nviolations 1 nrotb 7 volume 487.08 Exact/Monoisotopic Mass = 504.3087037481 g/mol
26-hydroxypinnatasterone	miLogP 0.35 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6 volume 472.74 Exact/Monoisotopic Mass = 496.3036183676
5-hydroxypodecdysone B	miLogP 1.01 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 458.24 Exact/Monoisotopic Mass = 478.2931
26-hydroxypolypodine B	miLogP -0.59 TPSA 178.90

	natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 6 volume 480.43 Exact/Monoisotopic Mass = 512.298533 g/mol
15-hydroxyponasterone A	miLogP 1.65 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
5b-hydroxypoststerone	miLogP 0.09 TPSA 115.05 natoms 27 MW 378.46 nON 6 nOHNH 4 nviolations 0 nrotb 1 volume 350.54 Exact/Monoisotopic Mass = 378.204239 g/mol
11a-hydroxypoststerone	miLogP 0.11 TPSA 115.05 natoms 27 MW 378.46 nON 6

	nOHNH 4 nviolations 0 nrotb 1 volume 350.89 Exact/Monoisotopic Mass = 378.204239 g/mol
11a-hydroxyrubrosterone	miLogP -0.63 TPSA 115.05 natoms 25 MW 350.41 nON 6 nOHNH 4 nviolations 0 nrotb 0 volume 317.50 Exact/Monoisotopic Mass = 350.172939 g/mol
5b-hydroxyrubrosterone	miLogP -0.66 TPSA 115.05 natoms 25 MW 350.41 nON 6 nOHNH 4 nviolations 0 nrotb 0 volume 317.15 Exact/Monoisotopic Mass = 350.172939 g/mol
21-hydroxyshidasterone	miLogP 1.46 TPSA 127.44 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0

	nrotb 3 volume 454.84 Exact/Monoisotopic Mass = 478.293054 g/mol
11a-hydroxyshidasterone	miLogP 1.55 TPSA 127.44 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 2 volume 454.63 Exact/Monoisotopic Mass = 478.293054 g/mol
11a-hydroxysidisterone	miLogP 1.25 TPSA 124.29 natoms 31 MW 432.51 nON 7 nOHNH 4 nviolations 0 nrotb 1 volume 392.95 Exact/Monoisotopic Mass = 432.2148033632 g/mol
16a-hydroxytaxisterone	miLogP 1.59 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308705 g/mol

Hyosterone A	miLogP 3.27 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 442.53 Exact/Monoisotopic Mass = 446.303224 g/mol
Hyosterone B	miLogP 3.27 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 442.53 Exact/Monoisotopic Mass = 446.303224 g/mol
Hyosterone C	miLogP 2.33 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.22 Exact/Monoisotopic Mass = 462.298139 g/mol
Hyosterone D	miLogP 2.33 TPSA 118.21 natoms 33

	MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.22 Exact/Monoisotopic Mass = 462.298139 g/mol
I	
Inokosterone	miLogP 1.30 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 465.04 Exact/Monoisotopic Mass = 480.308704 g/mol
Inokosterone 26-acetate	miLogP 2.00 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 8 volume 501.56 Exact/Monoisotopic Mass = 522.319268 g/mol
Inokosterone 20,22-acetonide	miLogP 3.19 TPSA 116.45 natoms 37 MW 520.71

	nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 505.76 Exact/Monoisotopic Mass = 520.340004 g/mol
Integristerone A	miLogP 0.66 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Integristerone A 25-acetate	miLogP 1.37 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 509.03 Exact/Monoisotopic Mass = 538.314183 g/mol
Integristerone A 20,22-acetonide	miLogP 2.55 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1

	nrotb 4 volume 513.24 Exact/Monoisotopic Mass = 536.334918 g/mol
Integristerone B	miLogP -0.28 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 5 volume 480.22 Exact/Monoisotopic Mass = 512.2985329872 g/mol
Isocyasterone	miLogP 0.71 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
Isocyasterone 2,3-acetonide	miLogP 2.60 TPSA 122.53 natoms 40 MW 560.73 nON 8 nOHNH 3 nviolations 1 nrotb 4 volume 531.48 Exact/Monoisotopic Mass = 560.3349184959 g/mol

isovitexirone	miLogP 1.46 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 459.17 Exact/Monoisotopic Mass = 478.293054 g/mol
J	
Japonicone (24-methyleneshidasterone)	miLogP 2.78 TPSA 107.22 natoms 34 MW 474.64 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 457.51 Exact/Monoisotopic Mass = 474.298139 g/mol
K	
Kaladasterone	miLogP 1.44 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 5

	volume 458.27 Exact/Monoisotopic Mass = 478.293054 g/mol
Kancollosterone	miLogP 1.61 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 475.97 Exact/Monoisotopic Mass = 492.308704 g/mol
L	
Lesterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Leuzeasterone	miLogP 1.90 TPSA 144.52 natoms 37 MW 518.65 nON 8 nOHNH 5 nviolations 1 nrotb 3 volume 484.20

	Exact/Monoisotopic Mass = 518.2879683035 g/mol
Limnantheoside A	miLogP 0.08 TPSA 197.36 natoms 43 MW 612.76 nON 11 nOHNH 8 nviolations 3 nrotb 7 volume 571.75 Exact/Monoisotopic Mass = 612.350962 g/mol
Limnantheoside B	miLogP 1.28 TPSA 177.13 natoms 42 MW 596.76 nON 10 nOHNH 7 nviolations 2 nrotb 7 volume 564.06 Exact/Monoisotopic Mass = 596.356048 g/mol
Limnantheoside C	miLogP -1.85 TPSA 276.51 natoms 54 MW 774.90 nON 16 nOHNH 11 nviolations 3 nrotb 10 volume 703.88 Exact/Monoisotopic Mass = 774.4037859014 g/mol
Lygodiumsteroside A	miLogP 1.55 TPSA 203.44

	natoms 47 MW 666.80 nON 12 nOHNH 7 nviolations 3 nrotb 6 volume 614.84 Exact/Monoisotopic Mass = 666.361527 g/mol
M	
Makisterone A	miLogP 1.83 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.06 Exact/Monoisotopic Mass = 494.324354 g/mol
Makisterone B	miLogP 1.77 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 481.63 Exact/Monoisotopic Mass = 494.324354 g/mol
Makisterone C	miLogP 2.34 TPSA 138.44 natoms 36

	MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 497.87 Exact/Monoisotopic Mass = 508.340004 g/mol
Makisterone C 20,22-acetonide	miLogP 4.23 TPSA 116.45 natoms 39 MW 548.76 nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 538.59 Exact/Monoisotopic Mass = 548.371304 g/mol
Makisterone C 2,3;20,22-diacetonide	miLogP 6.12 TPSA 94.46 natoms 42 MW 588.83 nON 7 nOHNH 2 nviolations 2 nrotb 5 volume 579.30 Exact/Monoisotopic Mass = 588.402604 g/mol
Makisterone D	miLogP 2.89 TPSA 138.44 natoms 36 MW 508.70 nON 7 nOHNH 6

	nviolations 2 nrotb 6 volume 498.22 Exact/Monoisotopic Mass = 508.340004 g/mol
Malacosterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Melandrioside	miLogP 0.36 TPSA 223.67 natoms 48 MW 684.82 nON 13 nOHNH 8 nviolations 3 nrotb 10 volume 633.11 Exact/Monoisotopic Mass = 684.372092 g/mol
26-methoxypolypodosaponin	miLogP 2.76 TPSA 193.84 natoms 53 MW 752.94 nON 13 nOHNH 6 nviolations 3 nrotb 8 volume 705.27

	Exact/Monoisotopic Mass = 752.434692 g/mol
24-methyleneshidasterone (japonicone)	miLogP 2.78 TPSA 107.22 natoms 34 MW 474.64 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 457.51 Exact/Monoisotopic Mass = 474.298139 g/mol
24-methylshidasterone	miLogP 2.94 TPSA 107.22 natoms 34 MW 476.65 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 463.17 Exact/Monoisotopic Mass = 476.3137891285 g/mol
Muristerone A	miLogP 0.70 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
N	

Niuxinsterone A	miLogP 3.33 TPSA 149.82 natoms 43 MW 602.76 nON 9 nOHNH 5 nviolations 1 nrotb 6 volume 566.78 Exact/Monoisotopic Mass = 602.3454831796 g/mol
Niuxinsterone B	miLogP 3.62 TPSA 129.59 natoms 41 MW 570.72 nON 8 nOHNH 4 nviolations 1 nrotb 6 volume 536.29 Exact/Monoisotopic Mass = 570.3192684318 g/mol
Niuxinsterone C	miLogP 1.85 TPSA 170.05 natoms 43 MW 604.74 nON 10 nOHNH 6 nviolations 2 nrotb 7 volume 558.45 Exact/Monoisotopic Mass = 604.324747735 g/mol
Niuxinsterone D	miLogP 3.27 TPSA 149.82 natoms 43

	MW 602.76 nON 9 nOHNH 5 nviolations 1 nrotb 7 volume 567.35 Exact/Monoisotopic Mass = 602.3454831796
29-norcyasterone	miLogP 0.60 TPSA 144.52 natoms 36 MW 506.64 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 474.18 Exact/Monoisotopic Mass = 506.287968 g/mol
29-norcyasterone 2-acetate	miLogP 1.31 TPSA 150.59 natoms 39 MW 548.67 nON 9 nOHNH 4 nviolations 1 nrotb 6 volume 510.69 Exact/Monoisotopic Mass = 548.2985329872 g/mol
29-norcyasterone 3-acetate	miLogP 1.31 TPSA 150.59 natoms 39 MW 548.67 nON 9 nOHNH 4

	nviolations 1 nrotb 6 volume 510.69 Exact/Monoisotopic Mass = 548.2985329872 g/mol
29-norsengosterone	miLogP -0.34 TPSA 164.74 natoms 37 MW 522.63 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 481.87 Exact/Monoisotopic Mass = 522.282883 g/mol
Nusilsterone	miLogP -0.25 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 5 volume 480.57 Exact/Monoisotopic Mass = 512.298533 g/mol
O	
24-O-acetyl-epi-abutasterone	miLogP 1.15 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2

	nrotb 7 volume 509.03 Exact/Monoisotopic Mass = 538.3141830513 g/mol
3-O-acetyl-20-hydroxyecdysone 2-galactoside	miLogP 0.36 TPSA 223.67 natoms 48 MW 684.82 nON 13 nOHNH 8 nviolations 3 nrotb 10 volume 633.11 Exact/Monoisotopic Mass = 684.3720918503 g/mol
3-O-acetyl-20-hydroxyecdysone 2-glucoside	miLogP 0.36 TPSA 223.67 natoms 48 MW 684.82 nON 13 nOHNH 8 nviolations 3 nrotb 10 volume 633.11 Exact/Monoisotopic Mass = 684.3720918503 g/mol
[25S]20,22-O-(R-ethylidene)inokosterone	miLogP 2.74 TPSA 116.45 natoms 36 MW 506.68 nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 489.52 Exact/Monoisotopic Mass = 506.3243538122 g/mol

20,22-O-(R-3-methoxycarbonyl)propylidene-20-hydroxyecdysone	miLogP 2.52 TPSA 142.76 natoms 41 MW 578.74 nON 9 nOHNH 4 nviolations 1 nrotb 8 volume 550.53 Exact/Monoisotopic Mass = 578.345483 g/mol
Osladin	miLogP 1.63 TPSA 263.76 natoms 62 MW 887.07 nON 17 nOHNH 9 nviolations 3 nrotb 9 volume 817.82 Exact/Monoisotopic Mass = 886.4926009058 g/mol
22-oxo-ajugasterone C	miLogP 1.46 TPSA 135.28 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 5 volume 458.97 Exact/Monoisotopic Mass = 478.2930536839 g/mol
22-oxo-cyasterone	miLogP 0.53 TPSA 141.36 natoms 37

	MW 518.65 nON 8 nOHNH 4 nviolations 1 nrotb 4 volume 484.90 Exact/Monoisotopic Mass = 518.287968 g/mol
22-oxo-dacryhainansterone	miLogP 2.19 TPSA 115.05 natoms 33 MW 460.61 nON 6 nOHNH 4 nviolations 0 nrotb 5 volume 444.71 Exact/Monoisotopic Mass = 460.282490 g/mol
22-oxo-20-hydroxyecdysone	miLogP 1.17 TPSA 135.28 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0 nrotb 5 volume 458.62 Exact/Monoisotopic Mass = 478.293054 g/mol
22-oxo-polypodine B	miLogP 0.23 TPSA 155.51 natoms 35 MW 494.62 nON 8 nOHNH 6 nviolations 1

	nrotb 5 volume 466.31 Exact/Monoisotopic Mass = 494.287970 g/mol
22-oxo-turkesterone	miLogP 0.26 TPSA 155.51 natoms 35 MW 494.62 nON 8 nOHNH 6 nviolations 1 nrotb 5 volume 466.66 Exact/Monoisotopic Mass = 494.2879683035 g/mol
P	
Palythoalone A	miLogP 0.83 TPSA 158.67 natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 6 volume 489.32 Exact/Monoisotopic Mass = 510.319268 g/mol
Palythoalone B	miLogP 0.35 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6

	volume 472.74 Exact/Monoisotopic Mass = 496.303618 g/mol
Palythone A	miLogP 2.51 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/Monoisotopic Mass = 464.313789 g/mol
Panuosterone	miLogP 1.83 TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.06 Exact/Monoisotopic Mass = 494.324354 g/mol
Paristerone	miLogP 1.36 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
Paxillosterone	miLogP 0.92

	TPSA 158.67 natoms 36 MW 510.67 nON 8 nOHNH 7 nviolations 2 nrotb 5 volume 489.11 Exact/Monoisotopic Mass = 510.319268 g/mol
Paxillosterone 20,22-p-hydroxybenzylidene acetal	miLogP 3.10 TPSA 156.91 natoms 44 MW 614.78 nON 9 nOHNH 6 nviolations 2 nrotb 5 volume 576.46 Exact/Monoisotopic Mass = 614.345483 g/mol
2b,3b,6a,22R,25-pentahydroxy-5b-cholestane	miLogP 3.62 TPSA 101.14 natoms 32 MW 452.68 nON 5 nOHNH 5 nviolations 0 nrotb 5 volume 461.17 Exact/Monoisotopic Mass = 452.350175 g/mol
2b,3a,6a,22R,25-pentahydroxy-5b-cholestane	miLogP 3.62 TPSA 101.14 natoms 32 MW 452.68

	nON 5 nOHNH 5 nviolations 0 nrotb 5 volume 461.17 Exact/Monoisotopic Mass = 452.350175 g/mol
(2b,3a,5b,14b,22R)2,3,20,22,25-pentahydroxycholest-7-en-6-one	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
(2b,3a,5b,14a,22R)2,3,20,22,25-pentahydroxycholest-7-en-6-one	miLogP 2.30 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
2b,3b,14a,20,24-pentahydroxy-6,26-dioxo-stigmast-7-en-22,26-olide	miLogP 2.32 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1

	nrotb 3 volume 490.42 Exact/Monoisotopic Mass = 520.303618 g/mol
2,3,20,22,26-pentahydroxy-14-methyl-18-norcholesta-7,12-dien-6-one	miLogP 2.06 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 6 volume 451.14 Exact/Monoisotopic Mass = 462.2981390644 g/mol
2b,3b,14a,20,26-pentahydroxy-6-oxo-stigmast-7-ene-22,26-lactol	miLogP 2.73 TPSA 127.44 natoms 36 MW 506.68 nON 7 nOHNH 5 nviolations 1 nrotb 3 volume 488.58 Exact/Monoisotopic Mass = 506.324354 g/mol
Pfaffiaglycoside C	miLogP 0.80 TPSA 197.36 natoms 44 MW 626.78 (Ecdybase structure) nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.56 Exact/Monoisotopic Mass = 610.371698 g/mol (PubChem structure)

Pfaffiaglicoside D	miLogP 0.63 TPSA 217.59 natoms 47 MW 670.84 nON 12 nOHNH 9 nviolations 3 nrotb 9 volume 629.99 Exact/Monoisotopic Mass = 670.392827 g/mol
Pfaffiaglicoside E (Pfaffioside E in PubChem)	miLogP -0.27 TPSA 217.59 natoms 45 MW 638.75 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 584.47 Exact/Monoisotopic Mass = 638.330227 g/mol
Pinnasterol	miLogP 3.33 TPSA 97.98 natoms 32 MW 446.63 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 442.88 Exact/Monoisotopic Mass = 446.303224 g/mol
Pinnatasterone	miLogP 1.36 TPSA 138.44 natoms 34

	MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
Podecdysone B	miLogP 1.96 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.55 Exact/Monoisotopic Mass = 462.298139 g/mol
Podecdysone B 25-glucoside	miLogP 0.25 TPSA 197.36 natoms 44 MW 624.77 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 582.67 Exact/Monoisotopic Mass = 624.3509624829 g/mol
[5a-OH]polypodine B	miLogP 0.41 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7

	nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303618 g/mol
Polypodine B	miLogP 0.41 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303618 g/mol
Polypodine B 22-acetate	miLogP 1.12 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 508.68 Exact/Monoisotopic Mass = 538.314183 g/mol
Polypodine B 20,22-acetonide	miLogP 2.31 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 512.89

	Exact/Monoisotopic Mass = 536.334918 g/mol
Polypodine B 22-benzoate	miLogP 2.84 TPSA 164.74 natoms 43 MW 600.75 nON 9 nOHNH 6 nviolations 2 nrotb 8 volume 563.53 Exact/Monoisotopic Mass = 600.329833 g/mol
Polypodine B 2-cinnamate	miLogP 3.26 TPSA 164.74 natoms 45 MW 626.79 nON 9 nOHNH 6 nviolations 2 nrotb 9 volume 590.95 Exact/Monoisotopic Mass = 626.3454831796 g/mol
Polypodine B 3-glucoside	miLogP -1.29 TPSA 237.82 natoms 46 MW 658.78 nON 13 nOHNH 10 nviolations 3 nrotb 8 volume 604.29 Exact/Monoisotopic Mass = 658.356442 g/mol
Polypodine B 2-glucoside	miLogP -0.61 TPSA 228.59

	natoms 46 MW 656.81 nON 12 nOHNH 10 nviolations 3 nrotb 8 volume 612.11 Exact/Monoisotopic Mass = 658.356442 g/mol
[5a-OH]]polypodine B 3-glucoside	miLogP -1.29 TPSA 237.82 natoms 46 MW 658.78 nON 13 nOHNH 10 nviolations 3 nrotb 8 volume 604.29 Exact/Monoisotopic Mass = 658.356442 g/mol
Polypodaurein	miLogP 1.98 TPSA 127.44 natoms 35 MW 494.67 nON 7 nOHNH 5 nviolations 0 nrotb 6 volume 482.01 Exact/Monoisotopic Mass = 494.324354 g/mol
Polypodogenin	miLogP 4.55 TPSA 66.76 natoms 31 MW 430.63 nON 4

	nOHNH 2 nviolations 0 nrotb 2 volume 431.76 Exact/Monoisotopic Mass = 430.30831 g/mol
Polypodosaponin	miLogP 2.15 TPSA 204.84 natoms 52 MW 738.91 nON 13 nOHNH 7 nviolations 3 nrotb 7 volume 687.75 Exact/Monoisotopic Mass = 738.419042 g/mol
Polypodoside A	miLogP 1.45 TPSA 263.76 natoms 62 MW 885.05 nON 17 nOHNH 9 nviolations 3 nrotb 9 volume 811.61 Exact/Monoisotopic Mass = 884.476951 g/mol
Polypodoside B	iLogP 2.15 TPSA 204.84 natoms 52 MW 738.91 nON 13 nOHNH 7 nviolations 3 nrotb 7

	volume 687.75 Exact/Monoisotopic Mass = 738.419042 g/mol
Polypodoside C	miLogP 2.55 TPSA 193.84 natoms 53 MW 752.94 nON 13 nOHNH 6 nviolations 3 nrotb 8 volume 705.27 Exact/Monoisotopic Mass = 752.434692 g/mol
Polyporoid A	miLogP 2.81 TPSA 127.44 natoms 35 MW 492.65 nON 7 nOHNH 5 nviolations 0 nrotb 3 volume 471.57 Exact/Monoisotopic Mass = 492.308704 g/mol
Polyporoid B	miLogP 1.97 TPSA 127.44 natoms 35 MW 492.65 nON 7 nOHNH 5 nviolations 0 nrotb 3 volume 471.78 Exact/Monoisotopic Mass = 492.308704 g/mol
Polyporoid C	miLogP 2.62

	TPSA 138.44 natoms 35 MW 494.67 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 481.42 Exact/Monoisotopic Mass = 494.324354 g/mol
Polyporusterone A	miLogP 3.54 TPSA 118.21 natoms 34 MW 478.67 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 473.37 Exact/Monoisotopic Mass = 478.329439 g/mol
Polyporusterone B	miLogP 2.62 TPSA 118.21 natoms 34 MW 476.65 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 467.71 Exact/Monoisotopic Mass = 476.313789 g/mol
Polyporusterone C	miLogP 3.73 TPSA 110.51 natoms 34 MW 476.65

	nON 6 nOHNH 4 nviolations 0 nrotb 4 volume 463.52 Exact/Monoisotopic Mass = 476.313789 g/mol
Polyporusterone D	miLogP 4.32 TPSA 97.98 natoms 33 MW 460.65 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 460.02 Exact/Monoisotopic Mass = 460.318875 g/mol
Polyporusterone E	miLogP 4.67 TPSA 90.28 natoms 33 MW 460.65 nON 5 nOHNH 3 nviolations 0 nrotb 4 volume 455.83 Exact/Monoisotopic Mass = 460.318875 g/mol
Polyporusterone F	miLogP 4.48 TPSA 97.98 natoms 33 MW 462.67 nON 5 nOHNH 4 nviolations 0

	nrotb 5 volume 465.68 Exact/Monoisotopic Mass = 462.334525 g/mol
Polyporusterone G	miLogP 3.56 TPSA 97.98 natoms 33 MW 460.65 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 460.02 Exact/Monoisotopic Mass = 460.318875 g/mol
Ponasterone A	miLogP 2.56 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mol
Ponasterone A 20,22-acetonide	miLogP 4.46 TPSA 96.22 natoms 36 MW 504.71 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 497.50 Exact/Monoisotopic Mass = 504.345089 g/mol

Ponasterone A 22-apioside	miLogP 1.15 TPSA 177.13 natoms 42 MW 596.76 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 563.71 Exact/Monoisotopic Mass = 596.3560478633 g/mol
Ponasterone A 22-glycolate	miLogP 2.43 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 8 volume 501.56 Exact/Monoisotopic Mass = 522.319268 g/mol
Ponasterone A 20,22-p-hydroxybenzylidene acetal	miLogP 4.75 TPSA 116.45 natoms 41 MW 568.75 nON 7 nOHNH 4 nviolations 1 nrotb 5 volume 544.13 Exact/Monoisotopic Mass = 568.340004 g/mol
Ponasterone B	miLogP 2.56 TPSA 118.21 natoms 33

	MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.79 Exact/Monoisotopic Mass = 464.313789 g/mo
Ponasterone C	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Ponasterone C 2-cinnamate	miLogP 3.29 TPSA 164.74 natoms 45 MW 626.79 nON 9 nOHNH 6 nviolations 2 nrotb 9 volume 591.30 Exact/Monoisotopic Mass = 626.345483 g/mol
Ponasterone F	miLogP 3.51 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4

	nviolations 0 nrotb 5 volume 449.09 Exact/Monoisotopic Mass = 448.3188745089 g/mol
Ponasteroside A	miLogP 0.86 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.9 Exact/Monoisotopic Mass = 626.366613 g/mol
Ponasteroside B	miLogP 0.86 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.91 Exact/Monoisotopic Mass = 626.366613 g/mol
Poststerone	miLogP 1.03 TPSA 94.83 natoms 26 MW 362.47 nON 5 nOHNH 3 nviolations 0 nrotb 1 volume 342.85

	Exact/Monoisotopic Mass = 362.209324 g/mol
Poststerone 2-acetate	miLogP 1.73 TPSA 100.90 natoms 29 MW 404.50 nON 6 nOHNH 2 nviolations 0 nrotb 3 volume 379.36 Exact/Monoisotopic Mass = 404.219889 g/mol
Praemixerone	miLogP 3.06 TPSA 97.98 natoms 32 MW 448.64 nON 5 nOHNH 4 nviolations 0 nrotb 5 volume 448.71 Exact/Monoisotopic Mass = 448.3188745089 g/mol
Precyasterone	miLogP 2.12 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 3 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
Pterosterone	miLogP 1.39 TPSA 138.44

	natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol
Pterosterone 3-glucoside	miLogP -0.32 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.95 Exact/Monoisotopic Mass = 642.361527 g/mol
Pterosterone 24-glucoside	miLogP -0.32 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.95 Exact/Monoisotopic Mass = 642.361527 g/mol
R	
Rapisterone	miLogP 3.12 TPSA 138.44 natoms 36

	MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 498.22 Exact/Monoisotopic Mass = 508.3400038763 g/mol
Rapisterone B	miLogP 0.47 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.87 Exact/Monoisotopic Mass = 480.308704 g/mol (PubChem structure)
Rapisterone C	miLogP 2.34 TPSA 138.44 natoms 36 MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 6 volume 497.87 Exact/Monoisotopic Mass = 508.3400038763 g/mol
Rapisterone D	miLogP 0.41 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7

	nviolations 1 nrotb 5 volume 472.17 Exact/Monoisotopic Mass = 496.303618 g/mol
Rapisterone D 20-acetate	miLogP 1.12 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 508.68 Exact/Monoisotopic Mass = 538.3141830513 g/mol
Reptanslactone A	miLogP 2.35 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 3 volume 490.76 Exact/Monoisotopic Mass = 520.303618 g/mol
Reptanslactone B	miLogP 0.94 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.76

	Exact/Monoisotopic Mass = 520.303618 g/mol
Reptansterone	miLogP 2.02 TPSA 144.52 natoms 37 MW 520.66 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 490.98 Exact/Monoisotopic Mass = 520.3036183676 g/mol
Rhapontisterone	miLogP 0.47 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.87 Exact/Monoisotopic Mass = 496.303618 g/mol
Rhapontisterone R1	miLogP 0.99 TPSA 164.74 natoms 38 MW 534.65 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 492.25 Exact/Monoisotopic Mass = 534.282882923 g/mol
Rubrosterone	miLogP 0.28 TPSA 94.83

	natoms 24 MW 334.41 nON 5 nOHNH 3 nviolations 0 nrotb 0 volume 309.46 Exact/Monoisotopic Mass = 334.178024 g/mol
S	
Scabraesterone	miLogP 1.59 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.48 Exact/Monoisotopic Mass = 480.308704 g/mol
Schizaeasterone A	miLogP 3.54 TPSA 118.21 natoms 34 MW 478.67 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 473.37 Exact/Monoisotopic Mass = 478.329439 g/mol
Schizaeasterone B	miLogP 2.27 TPSA 138.44 natoms 36

	MW 508.70 nON 7 nOHNH 6 nviolations 2 nrotb 7 volume 498.43 Exact/Monoisotopic Mass = 508.340004 g/mol
Sendreisterone	miLogP 2.40 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 513.80 Exact/Monoisotopic Mass = 552.329833 g/mol (PubChem structure)
Sengosterone	miLogP -0.23 TPSA 164.74 natoms 38 MW 536.66 nON 9 nOHNH 6 nviolations 2 nrotb 4 volume 498.46 Exact/Monoisotopic Mass = 536.298533 g/mol
Septanoecdysone	miLogP 0.13 TPSA 206.60 natoms 46 MW 656.81 nON 12 nOHNH 8

	nviolations 3 nrotb 8 volume 613.78 Exact/Monoisotopic Mass = 656.3771772307 g/mol
Serfurostereone A	miLogP 2.86 TPSA 149.82 natoms 42 MW 588.74 nON 9 nOHNH 5 nviolations 1 nrotb 6 volume 550.19 Exact/Monoisotopic Mass = 588.329833 g/mol
Serfurosterone B	miLogP 3.15 TPSA 149.82 natoms 42 MW 588.74 nON 9 nOHNH 5 nviolations 1 nrotb 6 volume 550.54 Exact/Monoisotopic Mass = 588.329833 g/mol
Shidasterone	miLogP 2.47 TPSA 107.22 natoms 33 MW 462.63 nON 6 nOHNH 4 nviolations 0 nrotb 2 volume 446.59

	Exact/Monoisotopic Mass = 462.298139 g/mol
Shidasterone 3-acetate	miLogP 3.17 TPSA 113.29 natoms 36 MW 504.66 nON 7 nOHNH 3 nviolations 1 nrotb 4 volume 483.10 Exact/Monoisotopic Mass = 504.3087037481 g/mol
Sidasterone A	miLogP 1.61 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 6 volume 475.97 Exact/Monoisotopic Mass = 492.3087037481 g/mol
Sidasterone B	miLogP 1.89 TPSA 138.44 natoms 35 MW 492.65 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 475.39 Exact/Monoisotopic Mass = 492.308704 g/mol
Sidisterone	miLogP 2.16 TPSA 104.06

	natoms 30 MW 416.51 nON 6 nOHNH 3 nviolations 0 nrotb 1 volume 384.91 Exact/Monoisotopic Mass = 416.219889 g/mol
Sileneoside A	miLogP -0.35 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.361527 g/mol
Sileneoside B	miLogP -2.05 TPSA 296.74 natoms 56 MW 804.92 nON 17 nOHNH 12 nviolations 3 nrotb 11 volume 728.72 Exact/Monoisotopic Mass = 804.414351 g/mol
Sileneoside C	miLogP -1.04 TPSA 237.82 natoms 46 MW 658.78 nON 13

	nOHNH 10 nviolations 3 nrotb 8 volume 604.64 Exact/Monoisotopic Mass = 658.356442 g/mol
Silenoside D	miLogP -0.35 TPSA 217.59 natoms 45 MW 642.78 nON 12 nOHNH 9 nviolations 3 nrotb 8 volume 596.60 Exact/Monoisotopic Mass = 642.361527 g/mol
Sileneoside F	miLogP 0.57 TPSA 197.36 natoms 44 MW 626.78 nON 11 nOHNH 8 nviolations 3 nrotb 8 volume 588.56 Exact/Monoisotopic Mass = 626.366613 g/mol
Sileneoside G	miLogP -3.00 TPSA 316.97 natoms 57 MW 820.92 nON 18 nOHNH 13 nviolations 3 nrotb 11

	volume 736.41 Exact/Monoisotopic Mass = 804.4143505851
Sileneoside H	miLogP -0.34 TPSA 243.90 natoms 49 MW 700.82 nON 14 nOHNH 9 nviolations 3 nrotb 10 volume 641.15 Exact/Monoisotopic Mass = 700.367006 g/mol
(5a)sileneoside E	miLogP 1.51 TPSA 177.13 natoms 43 MW 610.78 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 580.86 Exact/Monoisotopic Mass = 610.371698 g/mol
Silenosterone (3-dehydro-2-deoxyecdysone)	miLogP 3.03 TPSA 94.83 natoms 32 MW 446.63 nON 5 nOHNH 3 nviolations 0 nrotb 5 volume 442.88 Exact/Monoisotopic Mass = 446.303224 g/mol
Sogdisterone	miLogP 0.18

	TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 6 volume 472.74 Exact/Monoisotopic Mass = 496.303618 g/mol
Sphenocentrioxide A	miLogP 0.44 TPSA 200.52 natoms 44 MW 626.78 nON 11 nOHNH 9 nviolations 3 nrotb 8 volume 588.53 Exact/Monoisotopic Mass = 626.366612547 g/mol
Sphenocentrioxide B	miLogP -0.51 TPSA 220.75 natoms 45 MW 642.78 nON 12 nOHNH 10 nviolations 3 nrotb 8 volume 596.22 Exact/Monoisotopic Mass = 642.3615271666 g/mol
Stachysterone A	miLogP 2.12 TPSA 118.21 natoms 33 MW 462.63

	nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.57 Exact/Monoisotopic Mass = 462.298139 g/mol
Stachysterone A 20,22-acetonide	miLogP 4.01 TPSA 96.22 natoms 36 MW 502.69 nON 6 nOHNH 3 nviolations 1 nrotb 4 volume 491.29 Exact/Monoisotopic Mass = 502.329439 g/mol
Stachysterone B	miLogP 2.12 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 450.57 Exact/Monoisotopic Mass = 462.298139 g/mol
Stachysterone B 14a,15a-epoxide	miLogP 1.55 TPSA 130.74 natoms 34 MW 478.63 nON 7 nOHNH 5 nviolations 0

	nrotb 5 volume 454.63 Exact/Monoisotopic Mass = 478.293054 g/mol
Stachysterone C	miLogP 2.59 TPSA 118.21 natoms 33 MW 462.63 nON 6 nOHNH 5 nviolations 0 nrotb 4 volume 450.57 Exact/Monoisotopic Mass = 462.298139 g/mol
T	
Taxisterone	miLogP 2.51 TPSA 118.21 natoms 33 MW 464.64 nON 6 nOHNH 5 nviolations 0 nrotb 5 volume 456.44 Exact/Monoisotopic Mass = 464.313789 g/mol
Tenuifolioside A	miLogP 1.96 TPSA 177.13 natoms 43 MW 612.80 nON 10 nOHNH 7 nviolations 2 nrotb 8

	volume 587.08 Exact/Monoisotopic Mass = 612.387348 g/mol
Tenuifolioside B	miLogP 1.96 TPSA 177.13 natoms 43 MW 612.80 nON 10 nOHNH 7 nviolations 2 nrotb 8 volume 587.08 Exact/Monoisotopic Mass = 612.387348 g/mol
2,14,22,25-tetradexyecdysone	miLogP 6.52 TPSA 37.30 natoms 29 MW 400.65 nON 2 nOHNH 1 nviolations 1 nrotb 5 volume 425.31 Exact/Monoisotopic Mass = 400.334131 g/mol
3b,5a,9a,14a-tetrahydroxyergosta-7,22[E]-dien-6-one	miLogP 3.43 TPSA 97.98 natoms 33 MW 460.65 nON 5 nOHNH 4 nviolations 0 nrotb 4 volume 458.79 Exact/Monoisotopic Mass = 460.318875 g/mol
2,3,14,20-tetrahydroxy-26-methoxy-6-oxo-stigmast-7-ene-22,26-lactol	miLogP 3.34

	TPSA 116.45 natoms 37 MW 520.71 nON 7 nOHNH 4 nviolations 1 nrotb 4 volume 506.11 Exact/Monoisotopic Mass = 520.340004 g/mol
Tomentesterone A	miLogP 6.35 TPSA 110.14 natoms 43 MW 594.79 nON 7 nOHNH 2 nviolations 2 nrotb 10 volume 576.61 Exact/Monoisotopic Mass = 594.355654 g/mol
Tomentesterone B	miLogP 5.65 TPSA 104.06 natoms 40 MW 552.75 nON 6 nOHNH 3 nviolations 2 nrotb 8 volume 540.10 Exact/Monoisotopic Mass = 552.3450892568 g/mol
2,22,25-trideoxyecdysone	miLogP 5.57 TPSA 57.53 natoms 30 MW 416.65

	nON 3 nOHNH 2 nviolations 1 nrotb 5 volume 433.00 Exact/Monoisotopic Mass = 416.329045 g/mol
2,14,22-trideoxyecdysone 3,25-diglucoside	miLogP 1.90 TPSA 215.83 natoms 52 MW 740.93 nON 13 nOHNH 8 nviolations 3 nrotb 11 volume 697.25 Exact/Monoisotopic Mass = 740.4346921068 g/mol
2,22,25-trihydroxyecdysone	miLogP 5.57 TPSA 57.53 natoms 30 MW 416.65 nON 3 nOHNH 2 nviolations 1 nrotb 5 volume 433.00 Exact/Monoisotopic Mass = 416.329045 g/mol
11a,20,26-trihydroxyecdysone	miLogP -0.56 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2

	nrotb 6 volume 480.78 Exact/Monoisotopic Mass = 512.298533 g/mol
[24R]11a,20,24-trihydroxyecdysone	miLogP -0.47 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 5 volume 480.57 Exact/Monoisotopic Mass = 512.298533 g/mol
5b,11a,20-trihydroxyecdysone	miLogP -0.50 TPSA 178.90 natoms 36 MW 512.64 nON 9 nOHNH 8 nviolations 2 nrotb 5 volume 480.22 Exact/Monoisotopic Mass = 512.298533 g/mol
5b,20,26-trihydroxyecdysone 20,22-acetonide	miLogP 1.30 TPSA 156.91 natoms 39 MW 552.71 nON 9 nOHNH 6 nviolations 2 nrotb 5 volume 521.15 Exact/Monoisotopic Mass = 552.329833 g/mol

3b,5a,14a-trihydroxyergosta-7,22[E]-dien-6-one	miLogP 4.38 TPSA 77.75 natoms 32 MW 444.66 nON 4 nOHNH 3 nviolations 0 nrotb 4 volume 451.10 Exact/Monoisotopic Mass = 444.32396 g/mol
3b,5a,9a-trihydroxyergosta-7,22(E)-dien-6-one	miLogP 4.38 TPSA 77.75 natoms 32 MW 444.66 nON 4 nOHNH 3 nviolations 0 nrotb 4 volume 451.10 Exact/Monoisotopic Mass = 444.32396 g/mol
Turkesterone	miLogP 0.44 TPSA 158.67 natoms 35 MW 496.64 nON 8 nOHNH 7 nviolations 1 nrotb 5 volume 472.52 Exact/Monoisotopic Mass = 496.303618 g/mol
Turkesterone 22-acetate	miLogP 1.15 TPSA 164.74 natoms 38

	MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 509.03 Exact/Monoisotopic Mass = 538.3141830513 g/mol
Turkesterone 20,22-acetonide	miLogP 2.33 TPSA 136.68 natoms 38 MW 536.71 nON 8 nOHNH 5 nviolations 1 nrotb 4 volume 513.24 Exact/Monoisotopic Mass = 536.3349184959 g/mol
Turkesterone 2-O-cinnamate	miLogP 3.29 TPSA 164.74 natoms 45 MW 626.79 nON 9 nOHNH 6 nviolations 2 nrotb 9 volume 591.30 Exact/Monoisotopic Mass = 626.3454831796 g/mol
U	
Uniflorsterone	miLogP 1.65 TPSA 138.44 natoms 34 MW 480.64

	nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.3087037481 g/mol
V	
Venustone	miLogP 1.55 TPSA 164.74 natoms 40 MW 566.73 nON 9 nOHNH 6 nviolations 2 nrotb 9 volume 542.64 Exact/Monoisotopic Mass = 566.3454831796 g/mol
Viperidinone	miLogP 4.63 TPSA 77.75 natoms 31 MW 432.64 nON 4 nOHNH 3 nviolations 0 nrotb 5 volume 440.70 Exact/Monoisotopic Mass = 432.3239598894 g/mol
Viperidone	miLogP 5.57 TPSA 57.53 natoms 30 MW 416.65 nON 3

	nOHNH 2 nviolations 1 nrotb 5 volume 433.00 Exact/Monoisotopic Mass = 416.329045 g/mol
Vitexirone	miLogP 1.67 TPSA 138.44 natoms 34 MW 478.63 nON 7 nOHNH 6 nviolations 1 nrotb 4 volume 458.62 Exact/Monoisotopic Mass = 478.293054 g/mol
Viticosterone E	miLogP 2.06 TPSA 144.52 natoms 37 MW 522.68 nON 8 nOHNH 5 nviolations 1 nrotb 7 volume 500.99 Exact/Monoisotopic Mass = 522.319268 g/mol
Viticosterone E 22-benzoate	miLogP 4.49 TPSA 150.59 natoms 45 MW 626.79 nON 9 nOHNH 4 nviolations 1 nrotb 10

	volume 592.35 Exact/Monoisotopic Mass = 626.345483 g/mol
Z	
Zoanthone A	miLogP 1.15 TPSA 164.74 natoms 38 MW 538.68 nON 9 nOHNH 6 nviolations 2 nrotb 7 volume 509.03 Exact/Monoisotopic Mass = 538.314183 g/mol
Zoanthusterone	miLogP 1.87 TPSA 138.44 natoms 34 MW 480.64 nON 7 nOHNH 6 nviolations 1 nrotb 5 volume 464.83 Exact/Monoisotopic Mass = 480.308704 g/mol