ChatGPT


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[
  {
    "commonName": "Chamomile",
    "latinName": "Matricaria chamomilla",
    "regionTraditions": "Native to southern and eastern Europe, used in Western
herbal traditions (ancient Greek, Roman, Egyptian) for calming and sleep 1 2 ",
    "aromaticNotes": "Sweet, floral, and apple-like fragrance from its blossoms
 3 ",
    "keyPhytochemicals": [
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        "PubChemCID": 5280443,
        "CanonicalSMILES": "C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O 4 ",
        "functionalGroups": ["flavonoid (polyphenol)", "phenolic hydroxy
groups", "ketone (γ-pyrone)"],
        "ringMotifs": ["two aromatic benzene rings (hexagons)", "one
heterocyclic pyrone ring (6-membered)"],
        "HbondDonors": 3,
        "HbondAcceptors": 5,
        "polarity": "Moderately polar (AlogP ~2.6, TPSA ~90 Å²) 5 ",
        "geometryTags": ["planar aromatic rings", "conjugated system"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5280443/record/SVG",
        "symbolicGeometryTags": ["hexagon ring = stability", "multiple donor
nodes = points of release"]
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        "functionalGroups": ["sesquiterpene alcohol", "alkene (isolated double
bond)"],
        "ringMotifs": ["one cyclohexene ring (6-membered, non-aromatic)"],
        "HbondDonors": 1,
        "HbondAcceptors": 1,
        "polarity": "Low polarity (XLogP ~3.8, TPSA ~20 Å²) 7 8 ",
        "geometryTags": ["flexible aliphatic structure", "one cyclic ring (non-
planar)"],
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1549992/record/SVG",
        "symbolicGeometryTags": ["six-membered ring = grounded stability",
"single OH donor = subtle release point"]
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        "PubChemCID": 10719,
        "CanonicalSMILES": "CCC1=CC2=C(C)C=CC2=C(C)C=C1 [9] ",
        "functionalGroups": ["polycyclic aromatic (azulene) hydrocarbon"],
        "ringMotifs": ["fused 7-membered and 5-membered aromatic rings (azulene
core)"],
        "HbondDonors": 0,
        "HbondAcceptors": 0,
        "polarity": "Very hydrophobic (estimated LogP ~4.8) [10] ",
        "geometryTags": ["non-benzenoid aromatic system", "polycyclic planar
framework"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
10719/record/SVG",
        "symbolicGeometryTags": ["fused rings = dual energies in balance",
"zero polarity = hidden potency"]
      }
    ],
    "molecularGeometrySummary": "Contains multiple conjugated aromatic rings
(e.g. flavonoid structure in apigenin) and a bicyclic azulene. Generally planar
aromatics with several hydroxyl groups enabling hydrogen bonding [5] . Volatile
sesquiterpenes (bisabolol) provide a flexible, non-aromatic scaffold.",
    "symbolicMotifMapping": ["Hexagonal aromatic rings confer a sense of calm
stability", "Five/seven-membered fused ring (azulene) represents transformative
soothing", "Multiple OH donor sites act as release valves of tension"],
    "evidence": [
      "Chamomile aromatic description [3] ",
      "Chamomile traditional use [1] ",
      "Key compounds (bisabolol, chamazulene, apigenin) identified in chamomile
[11] "
    ]
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    "commonName": "Lavender",
    "latinName": "Lavandula angustifolia",
    "regionTraditions": "Native to the Mediterranean region (France, Spain,
Italy), historically used for perfumes, bathing (name from Latin \"lavare\" = to
wash), and relaxation in European herbal medicine [12] ",
    "aromaticNotes": "Classic sweet, floral, herbaceous scent with subtle
camphor undertones [13] ",
    "keyPhytochemicals": [
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        "PubChemCID": 6549,
        "CanonicalSMILES": "CC(=C)CCCC(C)(C=C)O [14] ",
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        "ringMotifs": ["no rings (acyclic)"],
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        "HbondAcceptors": 1,
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        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/6549/record/SVG",
        "symbolicGeometryTags": ["linear geometry = free flow", "single OH donor = focal release"]
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        "PubChemCID": 8294,
        "CanonicalSMILES": "CC(=CCCC(C)(C=C)OC(=O)C)C [16]",
        "functionalGroups": ["ester (acetate) of linalool"],
        "ringMotifs": ["no rings (acyclic)"],
        "HbondDonors": 0,
        "HbondAcceptors": 2,
        "polarity": "Lipophilic (estimated LogP ~3.3) [17] [18]",
        "geometryTags": ["flexible chain with ester linkage"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/8294/record/SVG",
        "symbolicGeometryTags": ["open-chain structure = expansive calm", "ester linkage = bridging energies"]
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      {
        "compoundName": "β-Caryophyllene",
        "PubChemCID": 5281515,
        "CanonicalSMILES": "C1=CCCC2=C1CCC(C2)C(C)C=C [19]",
        "functionalGroups": ["sesquiterpene (bicyclic alkene)"],
        "ringMotifs": ["bicyclic (merged cyclobutane/cyclooctene) framework"],
        "HbondDonors": 0,
        "HbondAcceptors": 0,
        "polarity": "Very hydrophobic (LogP ~4+) (no polar groups) [19]",
        "geometryTags": ["bicyclic, non-planar hydrocarbon"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/5281515/record/SVG",
        "symbolicGeometryTags": ["bicyclic ring = layered stability", "non-polar core = hidden strength"]
      }
    ],
    "molecularGeometrySummary": "Lavender's aroma is driven by monoterpenes: linalool (an achiral alcohol) and its acetate are acyclic, providing conformational flexibility [20]. No aromatic rings, but a bicyclic sesquiterpene (caryophyllene) adds a rigid, nonpolar framework. Overall, structures are small, mostly non-aromatic, with one or no H-bond donors.",
    "symbolicMotifMapping": ["Absence of benzene rings signifies a gentle, flowing energy (not fixed)", "One donor (in linalool) as a small release node amid otherwise neutral geometry", "Bicyclic terpene structure imbues a stable backbone (grounding amid light aroma)"],
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    "evidence": [
      "Mediterranean origin and traditional aromatherapy use [12]",
      "Sweet floral and slight camphor aroma profile [13]",
      "Main constituents linalool and linalyl acetate in lavender oil [21]"
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  {
    "commonName": "Rosemary",
    "latinName": "Rosmarinus officinalis",
    "regionTraditions": "Native to the Mediterranean; used in European folk
medicine for memory and digestion (\"dew of the sea\" herb) [22]",
    "aromaticNotes": "Strongly camphoraceous, pine-like and herbaceous aroma
with woody undertones",
    "keyPhytochemicals": [
      {
        "compoundName": "1,8-Cineole (Eucalyptol)",
        "PubChemCID": 2758,
        "CanonicalSMILES": "CC1OC2CCCC1C2 [23]",
        "functionalGroups": ["cyclic ether (monoterpene oxide)"],
        "ringMotifs": ["bicyclic (oxygen-bridged) structure"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (moderately lipophilic, LogP ~2) [24]",
        "geometryTags": ["rigid bicyclic ether, semi-polar"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
2758/record/SVG",
        "symbolicGeometryTags": ["bridged ring = synergy (mind-body link)",
"single oxygen acceptor = focal energy intake"]
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        "compoundName": "Camphor",
        "PubChemCID": 2537,
        "CanonicalSMILES": "CC1(C2CCC1(C2)C)O [24]",
        "functionalGroups": ["bicyclic ketone (bornane structure)"],
        "ringMotifs": ["bicyclic (bornane) framework"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (volatile and lipophilic ketone) [24]",
        "geometryTags": ["rigid polycyclic, one carbonyl"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
2537/record/SVG",
        "symbolicGeometryTags": ["bicyclic core = structured strength",
"carbonyl acceptor = grounding anchor"]
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        "compoundName": "Carnosic acid",
        "PubChemCID": 6435904,
        "CanonicalSMILES": "CC(=O)C1=C(C(=C(C(=C1)O)C)C)C2CC3(C(C2C(=O)O3)C)C
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[22]",
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"catechol moiety", "carboxylic acid"],
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        "HbondDonors": 3,
        "HbondAcceptors": 6,
        "polarity": "Moderate (polyphenolic, PSA ~100+ Å²)",
        "geometryTags": ["rigid polycyclic, multiple polar groups"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
6435904/record/SVG",
        "symbolicGeometryTags": ["fused rings = resilient structure", "multiple
OH donors = points of energetic release"]
      }
    ],
    "molecularGeometrySummary": "Rosemary contains volatile monoterpenes like
1,8-cineole and camphor, which are rigid bicyclic molecules with low polarity [23]
[24]. Additionally, its antioxidant potency comes from polycyclic phenolics
(carnosic acid) which feature a fused-ring diterpene structure with multiple
hydrogen-bonding groups. The mix of small volatile cyclic ethers/ketones and
larger polyphenols gives rosemary a dual geometry profile: one part highly
lipophilic and aromatic, another part polar and planar.",
    "symbolicMotifMapping": ["Bicyclic monoterpenes (cineole, camphor) impart a
structured, penetrating energy (clarity/stimulation)", "Polyphenolic rings
(carnosic acid) provide a stabilizing, protective framework (symbolic of memory
preservation)", "Multiple donor/acceptor sites in carnosic acid signify release
and absorption in balanced tandem"],
    "evidence": [
      "Major essential oil components cineole, camphor in rosemary [23] [24]",
      "Carnosic acid identified as key phenolic diterpene in rosemary [22]",
      "Traditional Mediterranean use for memory (aptly linked to its stable
aromatic rings) [22]"
    ]
  },
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    "commonName": "Peppermint",
    "latinName": "Mentha × piperita",
    "regionTraditions":
"Hybrid of spearmint and watermint, cultivated in Europe since the 18th century;
used traditionally for digestion and cooling relief (menthol) [25]",
    "aromaticNotes": "Penetrating cool, minty odor with sweet camphoraceous
freshness",
    "keyPhytochemicals": [
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        "compoundName": "Menthol",
        "PubChemCID": 1254,
        "CanonicalSMILES": "CC(C)C1CCC(C(C)C)O1 [26]",
        "functionalGroups": ["cyclohexanol (monoterpene alcohol)"],
        "ringMotifs": ["monocyclic (cyclohexane) framework"],
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1254/record/SVG",
        "symbolicGeometryTags": ["six-membered ring = stability", "single OH
donor = targeted cooling release"]
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        "PubChemCID": 26447,
        "CanonicalSMILES": "CC(=O)C1CCC(C(C)C)C1 26 ",
        "functionalGroups": ["cyclohexanone (monoterpene ketone)"],
        "ringMotifs": ["monocyclic (cyclohexane) framework"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (nonpolar except one C=O) 26 ",
        "geometryTags": ["chair conformation cyclohexanone"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
26447/record/SVG",
        "symbolicGeometryTags": ["six-membered ring = consistency", "carbonyl
acceptor = cooling anchor point"]
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        "compoundName": "Menthofuran",
        "PubChemCID": 6989,
        "CanonicalSMILES": "CC1=CC(=O)C(C=C1C)C(C)C 27 ",
        "functionalGroups": ["furan (five-membered aromatic ether)", "ketone"],
        "ringMotifs": ["aromatic furan ring fused with cyclopropane (in
structure)"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Moderate (more polar than menthol, but still lipophilic)",
        "geometryTags": ["planar aromatic furan with strained ring system"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
6989/record/SVG",
        "symbolicGeometryTags": ["five-membered aromatic ring = dynamic
energy", "oxygen in ring = subtle brightness in cooling effect"]
      }
    ],
    "molecularGeometrySummary": "Peppermint's cooling action arises from
monoterpenes: menthol is a chiral cyclohexanol (chair form) providing a single
polar node 26 , while menthone is its ketone analog. Both share a rigid ring
giving directed interaction (menthol's OH binding to cold receptors). A minor
component, menthofuran, adds an aromatic five-membered ring element. Overall
geometry: predominantly saturated cyclic structures with one functional polar
group, enabling targeted but fleeting interactions (hence the sharp, cooling
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sensation).",
    "symbolicMotifMapping": ["Cyclohexane rings signify a stable carrier of cooling energy", "A single polar site (OH or C=O) indicates pinpoint release (tingling sensation)", "The small furan ring in menthofuran suggests a quick, transformative spark within the minty profile"],
    "evidence": [
      "Main constituents of peppermint oil: menthol (~40%) and menthone (~23%)[28]",
      "Menthol's OH and menthone's C=O as key functional sites[26]",

"Traditional digestive/cooling use aligns with menthol's targeted receptor activation (symbolized by donor node)[25]"
    ]
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    "commonName": "Sage",
    "latinName": "Salvia officinalis",
    "regionTraditions": "Native to the Mediterranean; revered in European herbalism (name \"Salvia\" from Latin salvare: to heal) for culinary and medicinal use (memory, throat, women's health)",
    "aromaticNotes": "Pungent, camphoraceous herbal scent with a warm, slightly bitter undertone",
    "keyPhytochemicals": [
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        "CanonicalSMILES": "CC1(C2CCC1(C)C2)O[24]",
        "functionalGroups": ["bicyclic monoterpene ketone"],
        "ringMotifs": ["bicyclic (bornane-like) structure"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (sparingly polar, one carbonyl)[24]",
        "geometryTags": ["rigid fused-ring, isomeric"],
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        "symbolicGeometryTags": ["bicyclic frame = concentrated power", "carbonyl acceptor = grounding point"]
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        "CanonicalSMILES": "CC1(C2CCC1(C2)C)O[24]",
        "functionalGroups": ["bicyclic terpene ketone"],
        "ringMotifs": ["bornane bicyclic structure (same as in rosemary)"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (volatile, lipophilic)[24]",
        "geometryTags": ["rigid polycyclic, one polar carbonyl"],
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        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/2537/record/SVG",
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        "PubChemCID": 5281792,
        "CanonicalSMILES": "C1=CC(=C(C=C1C=C(C(=O)O)O)O)OCC2=CC(=C(C(=C2)O)O)C(=O)O[29]",
        "functionalGroups": ["polyphenol (caffeic acid ester dimer)", "catechol moieties", "carboxylic acids"],
        "ringMotifs": ["two aromatic benzene rings (linked via ester)"],
        "HbondDonors": 4,
        "HbondAcceptors": 10,
        "polarity": "High (multiple phenolic and carboxyl groups, PSA >>100 Å²)",
        "geometryTags": ["extended conjugation, flexible due to ester linkage"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/5281792/record/SVG",
        "symbolicGeometryTags": ["paired hexagon rings = stability & harmony", "multiple donor sites = strong release/cleansing"]
      }
    ],
    "molecularGeometrySummary": "Common sage's potency comes from volatile monoterpenes and antioxidative phenolics. The essential oil is rich in bicyclic ketones like thujone and camphor, which share a rigid bornane skeleton conferring a focused, penetrating effect[24]. Meanwhile, sage leaf also contains rosmarinic acid, a large diphenolic compound with two aromatic rings and multiple hydroxyl/carboxyl groups (hence high polarity). Structurally, sage spans small, apolar rigid molecules and larger, flexible polyphenols – a combination symbolizing both quick-acting and enduring effects.",
    "symbolicMotifMapping": ["Bicyclic monoterpenes (thujone/camphor) denote concentrated, sharp energy (clarifying, as used for cleansing air)", "Hexagonal aromatic rings of rosmarinic acid impart enduring stability and wisdom (matching sage's traditional association with wisdom/memory)",
"Many donor/acceptor groups (rosmarinic) indicate thorough purification (drawing out and releasing negativity)"],
    "evidence": [
      "Essential oil dominated by thujones and camphor[24]",
      "Rosmarinic acid and related phenolics present in sage leaves[30][29]",
      "Name and historical use for healing (implies the multi-layer geometry: volatile and solid constituents)[31]"
    ]
  },
  {
    "commonName": "Thyme",
    "latinName": "Thymus vulgaris",
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    "regionTraditions": "Native to the Mediterranean; used since ancient times
(Egyptian embalming, Greek baths) and in European cuisine and medicine as an
antiseptic and respiratory herb",
    "aromaticNotes":
"Sharp, warm herbaceous aroma with a strong spicy, phenolic (medicinal) note",
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        "functionalGroups": ["monoterpene phenol"],
        "ringMotifs": ["single aromatic (phenolic) ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 0,
        "polarity": "Low-moderate (phenolic OH, otherwise hydrophobic) 32 ",
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6989/record/SVG",
        "symbolicGeometryTags": ["hexagon ring = stable core", "OH donor =
potent release point"]
      },
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        "PubChemCID": 10364,
        "CanonicalSMILES": "CC1=CC(O)=C(C)C=C1C 32 ",
        "functionalGroups": ["monoterpene phenol (isomer of thymol)"],
        "ringMotifs": ["single aromatic ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 0,
        "polarity": "Low-moderate (similar to thymol) 32 ",
        "geometryTags": ["planar aromatic ring"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
10364/record/SVG",
        "symbolicGeometryTags": ["hexagon ring = structured energy",
"OH donor = targeted action"]
      },
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        "PubChemCID": 7463,
        "CanonicalSMILES": "CC1=CC=C(C=C1)C(C)C 33 ",
        "functionalGroups": ["aromatic hydrocarbon (alkylated benzene)"],
        "ringMotifs": ["single benzene ring"],
        "HbondDonors": 0,
        "HbondAcceptors": 0,
        "polarity": "Very low (pure hydrocarbon, hydrophobic) 33 ",
        "geometryTags": ["planar aromatic ring, non-polar"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
7463/record/SVG",
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        "symbolicGeometryTags": ["benzene ring = foundational stability",
"hydrophobic character = hidden subtlety"]
      }
    ],
    "molecularGeometrySummary": "Thyme's essential oil is characterized by
phenolic monoterpenes. Thymol and its isomer carvacrol both consist of a single
aromatic ring substituted with small aliphatic groups and one phenolic OH [32].
These planar aromatic cores convey stability to the molecule's interactions
(hence strong antimicrobial properties), while the OH provides a polar hotspot
for activity. Another major component, p-cymene, is an aromatic hydrocarbon
lacking polar functionality, acting as a non-polar co-solvent in the oil. Thus,
thyme's molecular geometry is dominated by flat benzene rings that carry either
a single polar point or none at all, reflecting a balance between potency and
volatility.",
    "symbolicMotifMapping": ["Dominant hexagonal rings (thymol/carvacrol)
symbolize a stable, strong energy (antiseptic strength)", "Single OH donor on
thymol/carvacrol indicates a focused release of medicinal action (targeted
antiseptic effect)", "Aromatic ring without donors (p-cymene) suggests a
background supportive force (carrier of the primary actives)"],
    "evidence": [
      "Thymol and carvacrol identified as main constituents of thyme oil [32]",
      "p-Cymene and related terpenes also abundant in thyme [33]",
      "Traditional antiseptic use aligns with phenolic ring structures (stable,
penetrating) [32]"
    ]
  },
  {
    "commonName": "Oregano",
    "latinName": "Origanum vulgare",
    "regionTraditions": "Native to Mediterranean regions; a staple spice in
Italian/Greek cuisine and used in traditional medicine for respiratory and
digestive ailments",
    "aromaticNotes": "Strong, warm and slightly bitter herbaceous aroma with
pungent phenolic (medicinal) and camphor-like notes",
    "keyPhytochemicals": [
      {
        "compoundName": "Carvacrol",
        "PubChemCID": 10364,
        "CanonicalSMILES": "CC1=CC(O)=C(C)C=C1C [34]",
        "functionalGroups": ["monoterpenoid phenol"],
        "ringMotifs": ["single aromatic ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 0,
        "polarity": "Low-mod (phenolic OH, otherwise hydrophobic) [34]",
        "geometryTags": ["planar aromatic"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
10364/record/SVG",
        "symbolicGeometryTags": ["benzene ring = robust core", "OH donor =
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active release"]
      },
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        "PubChemCID": 6989,
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        "functionalGroups": ["monoterpenoid phenol"],
        "ringMotifs": ["single aromatic ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 0,
        "polarity": "Low-mod (similar to carvacrol) 34 ",
        "geometryTags": ["planar aromatic"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
6989/record/SVG",
        "symbolicGeometryTags": ["hexagon ring = stable strength", "OH donor =
focused potency"]
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        "compoundName": "Rosmarinic acid",
        "PubChemCID": 5281792,
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"C1=CC(=C(C=C1C=C(C(=O)O)O)O)OCC2=CC(=C(C(=C2)O)O)C(=O)O 34 ",
        "functionalGroups": ["polyphenolic ester (caffeic acid dimer)"],
        "ringMotifs": ["two aromatic rings linked by ester"],
        "HbondDonors": 4,
        "HbondAcceptors": 10,
        "polarity": "High (multiple phenols and acids) 34  35 ",
        "geometryTags": ["extended conjugated system, flexible"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281792/record/SVG",
        "symbolicGeometryTags": ["dual aromatic rings = resilience", "poly-
oxygenated = radiant energy glow"]
      }
    ],
    "molecularGeometrySummary": "Oregano’s punch comes from phenolic
monoterpenes identical to those in thyme: carvacrol (dominant) and thymol, which
are flat aromatic molecules with a single OH substituent 34 . Supporting these is
rosmarinic acid (especially in leaves of Origanum), a large polyphenol
contributing antioxidant activity 36  35 . Structurally, oregano’s chemistry is a
blend of small planar rings for acute antimicrobial effect and larger poly-
aromatic structures for sustained antioxidant presence. The prevalence of the
aromatic ring motif (in small and large compounds alike) underscores oregano’s
strong, stable bioactivity.",
    "symbolicMotifMapping": ["Dominant aromatic rings (carvacrol/thymol)
symbolize strength and stability in action (robust antimicrobial effect)",
"Single OH on main actives indicates targeted release (potent flavor and
microbial kill focus)", "The presence of a big dual-ring phenolic (rosmarinic
acid) adds an underlying protective mesh (symbolically, a broader shield of
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protection)"],
    "evidence": [
      "Carvacrol and thymol are primary constituents of oregano oil [34] [36]",
      "Oregano contains rosmarinic acid and related phenolics contributing to its bioactivity [34] [37]",
      "Traditional use as an antimicrobial and preservative reflects the phenolic-rich chemistry [34]"
    ]
  },
  {
    "commonName": "Basil (Sweet Basil)",
    "latinName": "Ocimum basilicum",
    "regionTraditions": "Native to tropical Asia and widely cultivated in the Mediterranean; used in Ayurvedic medicine and as a culinary herb (\"king of herbs\" in Greek lore)",
    "aromaticNotes": "Sweet, warm, and slightly spicy aroma with clove-like and anise (licorice) notes due to phenylpropanoids",
    "keyPhytochemicals": [
      {
        "compoundName": "Estragole (Methyl chavicol)",
        "PubChemCID": 7127,
        "CanonicalSMILES": "CC=Cc1ccc(OC)cc1 [38]",
        "functionalGroups": ["phenylpropene (allylbenzene) ether"],
        "ringMotifs": ["benzene ring with allyl substituent"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (lipophilic aromatic ether) [38]",
        "geometryTags": ["planar aromatic plus small alkene tail"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/7127/record/SVG",
        "symbolicGeometryTags": ["benzene ring = core stability", "allyl side-chain = dynamic extension"]
      },
      {
        "compoundName": "Linalool",
        "PubChemCID": 6549,
        "CanonicalSMILES": "CC(=C)CCCC(C)(C=C)O [15]",
        "functionalGroups": ["acyclic monoterpene alcohol"],
        "ringMotifs": ["no rings"],
        "HbondDonors": 1,
        "HbondAcceptors": 1,
        "polarity": "Moderate (terpene alcohol, LogP ~2.7) [15]",
        "geometryTags": ["flexible chain, one polar end"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/6549/record/SVG",
        "symbolicGeometryTags": ["open chain = free-flowing energy", "OH donor = lively release"]
      },
```

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      {
        "compoundName": "Eugenol",
        "PubChemCID": 3314,
        "CanonicalSMILES": "C=Cc1c(O)c(OCC)cc(c1)C[38]",
        "functionalGroups": ["phenylpropene (allylbenzene) with phenol"],
        "ringMotifs": ["benzene ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 1,
        "polarity": "Low-mod (aromatic with one OH)[38]",
        "geometryTags": ["planar aromatic with allyl and methoxy substituents"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
3314/record/SVG",
        "symbolicGeometryTags": ["benzene ring = structured base", "phenolic OH
= focused active site"]
      }
    ],
    "molecularGeometrySummary": "Sweet basil's aroma arises from a blend of
phenylpropanoids and terpenes. Estragole (methyl chavicol) and eugenol are
aromatic benzene-ring compounds with small substituents (allyl and methoxy
groups)[38], providing a flat structure with limited polarity (eugenol has one
OH). Linalool, in contrast, is an acyclic monoterpene, bringing flexibility and
a single hydroxyl point[38]. Thus, basil's chemistry combines planar aromatics
(for spicy-sweet notes) and a flexible terpene alcohol (for fresh floral notes).
The geometries reflect this dual character: rigid aromatic cores for intensity
and freely rotating chains for diffusivity.",
    "symbolicMotifMapping": ["Aromatic rings (estragole, eugenol) signify the
enduring, potent flavor (stable core of the herb's 'spirit')", "Single polar
hooks (eugenol's OH, linalool's OH) act as lively points of release (the quick
uplifting scent)", "The mix of fixed rings and flexible chains symbolizes
balance between structured potency and gentle volatility"],
    "evidence": [
      "Major essential oil components include estragole, linalool, eugenol[38]",
      "Basil chemotypes vary, but sweet basil typically rich in methyl chavicol
(estragole) and linalool[39]",
      "Eugenol presence gives clove-like note (aromatic phenol) confirming
phenylpropanoid content[38]"
    ]
  },
  {
    "commonName": "Lemon Balm",
    "latinName": "Melissa officinalis",
    "regionTraditions":
"Native to Southern Europe and the Mediterranean; prized in medieval monastic
medicine as a calming tea (\"melissa\" = honeybee, for its sweet aroma)",
    "aromaticNotes": "Lemony, sweet and herbaceous fragrance with mild
citronella-like and minty nuances",
    "keyPhytochemicals": [
      {
```

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        "compoundName": "Geranial (trans-Citral)",
        "PubChemCID": 638011,
        "CanonicalSMILES": "C/C=C/C(=O)C=CC(C)=C 40 ",
        "functionalGroups": ["monoterpene aldehyde (citral isomer)"],
        "ringMotifs": ["no rings (acyclic)"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Moderate (polar carbonyl, otherwise hydrophobic) 41 ",
        "geometryTags": ["extended conjugated chain with aldehyde end"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
638011/record/SVG",
        "symbolicGeometryTags": ["open-chain = free energy flow", "carbonyl
acceptor = bright point (citrus spark)"]
      },
      {
        "compoundName": "Citronellal",
        "PubChemCID": 7794,
        "CanonicalSMILES": "CC(C)CCCC(C)=O 42 ",
        "functionalGroups": ["monoterpene aldehyde"],
        "ringMotifs": ["no rings"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Moderate (one polar aldehyde) 41 ",
        "geometryTags": ["flexible chain with terminal carbonyl"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
7794/record/SVG",
        "symbolicGeometryTags": ["linear structure = gentle flowing energy",
"aldehyde group = focal brightness"]
      },
      {
        "compoundName": "Rosmarinic acid",
        "PubChemCID": 5281792,
        "CanonicalSMILES":
"C1=CC(=C(C=C1C=C(C(=O)O)O)O)OCC2=CC(=C(C(=C2)O)O)C(=O)O 41 ",
        "functionalGroups": ["polyphenolic (caffeic acid dimer)"],
        "ringMotifs": ["two benzene rings (each with catechol)"],
        "HbondDonors": 4,
        "HbondAcceptors": 10,
        "polarity": "High (multiple –OH and –COOH groups) 43 42 ",
        "geometryTags": ["extended, conjugated di-aromatic system"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281792/record/SVG",
        "symbolicGeometryTags": ["twin aromatic rings = harmony/balance", "rich
donor network = soothing glow"]
      }
    ],
    "molecularGeometrySummary": "Lemon balm's calming citrus scent arises from
monoterpene aldehydes: citral (a mix of geranial and neral) and citronellal
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dominate its essential oil [41] [42]. These are linear molecules with conjugated double bonds and a polar carbonyl, giving moderate polarity and high volatility. In contrast, lemon balm leaves are also rich in rosmarinic acid (a heavy polar polyphenol) [43]. Geometrically, the herb spans simple flexible chains for immediate aroma and large polyaromatics for enduring medicinal action. This dual-layer (volatile vs. water-soluble) reflects a fractal overlap of fast-acting brightness and sustained soothing.",
    "symbolicMotifMapping": ["Open-chain citrus aldehydes represent bright, expansive energy that lifts mood (the quick lemony essence spreading out)",
"Polar carbonyl in citral/citronellal is a focused node of clarity (cutting through anxiety)",
"The deep aromatic rings of rosmarinic acid symbolize lasting calm and protection (an underlying net of stability once the bright notes settle)"],
    "evidence": [
      "Essential oil primarily contains citral isomers (neral, geranial) and citronellal [42] [40]",
      "Rosmarinic acid is a key phenolic in lemon balm, known for its antiviral calmative effects [41] [43]",

"Traditional use as a sedative tea aligns with volatile aldehydes (uplift) plus polyphenols (sustained calm) synergy"
    ]
  },
  {
    "commonName": "Calendula (Marigold)",
    "latinName": "Calendula officinalis",
    "regionTraditions": "Native to Southern Europe; cultivated in gardens worldwide. Used in European folk medicine for skin healing (\"pot marigold\" ointments) and as a dye (saffron substitute)",
    "aromaticNotes": "Mildly resinous, herbal and slightly honey-like scent (flowers are not highly aromatic, more known for their vivid color)",
    "keyPhytochemicals": [
      {
        "compoundName": "Faradiol-3-O-myristate (Faradiol ester)",
        "PubChemCID": null,
        "CanonicalSMILES": "Not available (triterpenoid ester)",
        "functionalGroups": ["pentacyclic triterpenoid diol (faradiol) esterified with fatty acid"],
        "ringMotifs": ["triterpene pentacyclic skeleton (ursane-type)"],
        "HbondDonors": 0 (as ester; faradiol itself has 2 OH),
        "HbondAcceptors": 2,
        "polarity": "Low (large hydrophobic terpene with ester linkage)",
        "geometryTags": ["rigid multi-ring (5 rings) structure with aliphatic tail"],
        "structureSVG": null,
        "symbolicGeometryTags": ["pentacyclic frame = extensive stability",
"ester linkage = binding of realms (water/oil)"]
      },
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      {
        "compoundName": "Quercetin",
        "PubChemCID": 5280343,
        "CanonicalSMILES": "C1=CC(=O)C2=C(O1)C(=CC(=C2O)O)C3=CC(=C(C(=C3)O)O)O
[44]",
        "functionalGroups": ["flavonol (polyphenol)", "multiple phenolic OH
groups"],
        "ringMotifs": ["three-ring flavone backbone (benzopyran + phenyl)"],
        "HbondDonors": 5,
        "HbondAcceptors": 7,
        "polarity": "High (polyhydroxylated) [45]",
        "geometryTags": ["planar conjugated rings"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5280343/record/SVG",
        "symbolicGeometryTags": ["fused aromatic rings = structured
resilience", "many OH donors = extensive healing release"]
      },
      {
        "compoundName": "Lutein (xanthophyll carotenoid)",
        "PubChemCID": 5281243,
        "CanonicalSMILES":
"CC(=CCC=CC=C(C)C1=CC(CC=C(C)C=C(C)C=C(C)C=C(C)C=C(C)C=C(C)C=C(C)C=C(C)C=CC=C(C)C=C(C)C=C(C)C=C1C
[44]",
        "functionalGroups": ["carotenoid (polyene diol)"],
        "ringMotifs": ["two terminal cyclic ionone rings, extended polyene
chain"],
        "HbondDonors": 2,
        "HbondAcceptors": 2,
        "polarity": "Moderate (amphiphilic: long nonpolar chain, two polar –OH)
[45]",
        "geometryTags": ["extended conjugation (~C40), rigid planar segments"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281243/record/SVG",
        "symbolicGeometryTags": ["long polyene chain = far-reaching influence",
"symmetry of rings = balanced energy at both ends"]
      }
    ],
    "molecularGeometrySummary":
"Calendula's healing properties trace to diverse compounds. Its anti-
inflammatory triterpenoids (like faradiol esters) have a bulky pentacyclic
structure with minimal polarity (mostly hydrocarbon) [46]. Flavonoids such as
quercetin are planar polyphenols with many polar sites [44], imparting antioxidant
and water-soluble activity. Additionally, the petals are rich in carotenoids
like lutein (a long conjugated polyene with polar end-groups) [44]. Geometrically,
calendula spans very large rigid frameworks (30-carbon triterpene, 40-carbon
carotenoid) and medium polyaromatics (quercetin). The interplay of mostly
nonpolar scaffolds (triterpene, carotenoid) with highly polar decorations
(flavonoids) reflects a fractal layering: structural support (resins, pigments)
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overlain by functional polarity (flavonoids).",
    "symbolicMotifMapping": ["Pentacyclic triterpenes signify a robust
foundational structure (five rings = completeness, stability in healing)",
"Abundant hydroxyl groups on flavonoids represent an outpouring of soothing
energy (cleansing and knitting tissues)", "Extended conjugated systems
(carotenoids) indicate radiating vitality (the flower's solar essence imparting
brightness and cell regeneration)"],
    "evidence": [
      "Calendula contains flavonoids (quercetin, isorhamnetin, kaempferol) and
triterpenoids (faradiol) [44]",
      "Lutein and other carotenoids are major constituents of calendula petals
[47] [44]",
      "These compounds underlie calendula's use in wound healing (flavonoids &
triterpenes anti-inflammatory) [45]"
    ]
  },
  {
    "commonName": "Echinacea",
    "latinName": "Echinacea purpurea",
    "regionTraditions": "Native to North America (Great Plains); used in Native
American medicine for infections and snakebites, now popular as an immune-
stimulant in Western herbal supplements",
    "aromaticNotes": "Roots and leaves have a mild floral and slightly pungent
odor, but not strongly aromatic (most active compounds are non-volatile)",
    "keyPhytochemicals": [
      {
        "compoundName": "Chicoric acid",
        "PubChemCID": 5281764,
        "CanonicalSMILES":
"C1=CC(=C(C(=C1O)O)C(=O)O)COC(C(=O)O)C2=CC(=C(C(=C2)O)O)C(=O)O [48]",
        "functionalGroups": ["dicaffeoyl tartaric acid (phenolic acid ester)"],
        "ringMotifs": ["two aromatic rings (catechol units) connected via
tartaric backbone"],
        "HbondDonors": 6,
        "HbondAcceptors": 12,
        "polarity": "High (polyphenolic, multiple carboxylates) [48]",
        "geometryTags": ["extended, flexible, highly polar"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281764/record/SVG",
        "symbolicGeometryTags": ["dual aromatic rings = double defense",
"multiple acid groups = strong binding (immune anchoring)"]
      },
      {
        "compoundName": "Echinacoside",
        "PubChemCID": 5281771,
        "CanonicalSMILES":
"C1=CC(=C(C(=C1O)O)COC2C(C(C(C(O2)COC3=CC(=C(C(=C3)O)O)C(=O)O)O)O)OC4C(C(C(C(O4)CO)O)O)O)C(=O)O
[48]",
```

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        "functionalGroups":
["phenylethanoid glycoside (caffeic acid derivatives + sugars)"],
        "ringMotifs": ["two aromatic rings (caffeic/phenylethanoid) plus sugar
rings"],
        "HbondDonors": 10+ (multiple OH),
        "HbondAcceptors": 15+,
        "polarity": "Very high (glycosylated polyphenol)",
        "geometryTags": ["large, flexible with multiple ring substructures
(phenyl + furanose)"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281771/record/SVG",
        "symbolicGeometryTags": ["multiple ring system = complex defense
network", "sugar moieties = energy-rich, connective"]
      },
      {
        "compoundName": "Dodeca-2E,4E-dienoic acid isobutylamide (Alkamide)",
        "PubChemCID": 6443006,
        "CanonicalSMILES": "CC(C)CN=C(C=C/C=C/CCCCC)C=O [49] ",
        "functionalGroups": ["unsaturated fatty acid amide (alkylamide)"],
        "ringMotifs": ["no rings (linear)"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (amphiphilic, mostly hydrocarbon with one amide) [50]
[49] ",
        "geometryTags": ["flexible aliphatic chain with conjugation and amide
head"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
6443006/record/SVG",
        "symbolicGeometryTags": ["long chain = far-reaching effect (immune
modulation)", "amide link = dual nature (water/oil bridging the immune
response)"]
      }
    ],
    "molecularGeometrySummary":
"Echinacea's activity comes from polar phenolics and distinctive alkamides.
Chicoric acid is a highly polar, negatively charged molecule with two aromatic
rings and multiple –OH/–COOH groups [48] , giving it a star-like, flexible shape
that readily chelates/binds (e.g., to immune receptors). Echinacoside is even
larger – a phenolic glycoside combining caffeic acid units with sugars [48] ,
effectively a multi-ring system that is both rigid in parts and very flexible
due to glycosidic linkages. In contrast, the tingling alkamides (like dodeca-2E,
4E-dien-8,10-diynyl amides) are relatively small, hydrophobic chains with
conjugation and an amide head, allowing them to insert into membranes and
interact with neuroreceptors (causing tongue tingling). The geometric duality is
clear: big, highly polar, planar compounds and small, linear, mostly apolar
amides. This fractal layering hints at an overlapping immune mesh – water-
soluble phenolics working broadly, lipophilic alkamides targeting locally.",
    "symbolicMotifMapping": ["Dual aromatic rings in chicoric acid represent a
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\"double shield\" fortifying the immune system", "Sugar-linked multi-ring structure of echinacoside symbolizes connectivity in healing (bridging different bodily systems)", "Long alkamide chains with conjugation indicate a penetrating lance of energy (stimulating sensation and immune response)", "The amide functionality suggests a mediator node (linking sensation to immunity)"],
    "evidence": [
      "Echinacea contains high levels of chicoric acid and related caffeic acid derivatives [48]",
      "Characteristic alkamides (unsaturated isobutylamides) are key actives in Echinacea (tingling effect) [50] [49]",
      "Polysaccharides/glycosides and lipophilic alkamides together modulate immunity (supported by these compound classes) [48]"
    ]
  },
  {
    "commonName": "Yarrow",
    "latinName": "Achillea millefolium",
    "regionTraditions": "Circumpolar Northern hemisphere; named after Achilles who legendarily used it for wound healing. Employed in European folk medicine to stop bleeding and treat fevers",
    "aromaticNotes": "Fresh, sweet herbal and slightly bitter aroma. When distilled, yields a blue oil due to chamazulene formation (characteristic medicinal scent)",
    "keyPhytochemicals": [
      {
        "compoundName": "Chamazulene",
        "PubChemCID": 10719,
        "CanonicalSMILES": "CCC1=CC2=C(C=CC(=C2C=C1)C)C [51]",
        "functionalGroups": ["sesquiterpene-derived azulene (hydrocarbon)"],
        "ringMotifs": ["bicyclic 7+5 aromatic rings"],
        "HbondDonors": 0,
        "HbondAcceptors": 0,
        "polarity": "Very low (pure hydrocarbon aromatic)",
        "geometryTags": ["planar fused rings"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/10719/record/SVG",
        "symbolicGeometryTags": ["blue aromatic rings = healing calm", "no polar groups = hidden power (stealth healing)"]
      },
      {
        "compoundName": "α- & β-Thujone",
        "PubChemCID": 442941,
        "CanonicalSMILES": "CC1(C2CCC1(C)C2)O (alpha form) [24]",
        "functionalGroups": ["bicyclic monoterpene ketones"],
        "ringMotifs": ["bornane bicyclic framework"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (ketone only polar site) [52] [51]",
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        "geometryTags": ["rigid polycyclic"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
442941/record/SVG",
        "symbolicGeometryTags": ["double-ring = potent structured energy",
"carbonyl = point of grounding"]
      },
      {
        "compoundName": "Camphor",
        "PubChemCID": 2537,
        "CanonicalSMILES": "CC1(C2CCC1(C2)C)O[51]",
        "functionalGroups": ["bicyclic terpene ketone"],
        "ringMotifs": ["bornane skeleton"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (one C=O)[51]",
        "geometryTags": ["rigid bicyclic"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
2537/record/SVG",
        "symbolicGeometryTags": ["solid bicyclic core = steadfast support",
"carbonyl = anchor point"]
      }
    ],
    "molecularGeometrySummary": "Yarrow's volatile oil contains chamazulene (up
to ~ chamazulene content varies widely)[51] – an aromatic bicyclic hydrocarbon
that gives the oil a deep blue color and anti-inflammatory properties. This
planar azulene system, with its unusual 7-5 ring fusion, stands out as a symbol
of Yarrow's healing potency from heat (formed by heat-induced transformation of
proazulenes). Additionally, yarrow shares monoterpene ketones with sage and
wormwood: thujone (α and β) and camphor appear in smaller amounts[51]. These are
rigid bicyclic molecules with a single polar carbonyl, contributing antiseptic
and bitter properties. Thus, geometrically, yarrow's chemistry is a mix of an
exotic aromatic (azulene) – conferring a unique resonant stability – and
standard small bicyclic terpenes for acute activity. The interplay suggests a
fractal synergy: the extraordinary (azulene) nested within the ordinary
(thujone/camphor framework).",
    "symbolicMotifMapping": ["Azulene's fused 5-7 rings (blue) represent a
bridge between realms – transformative healing (cooling inflammation) emerging
from heat", "Bicyclic thujone/camphor structures indicate structured, Mars-like
energy (sharp, warrior-like antiseptic action, befitting Achilles)", "Minimal
polar functionality hints that yarrow's action is energetically diffuse (broadly
acting, not sharply localized) until activated (as by distillation to
azulene)"],
    "evidence": [

"Yarrow essential oil yields chamazulene (blue sesquiterpene) and contains
thujone and camphor among major components[51][53]",
      "Thujone content in yarrow is relatively low compared to chamomile or
wormwood, but present[53][54]",
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      "Traditional wound-healing use corresponds with azulene's anti-inflammatory geometry (uncommon aromatic) and the antiseptic camphoraceous notes from thujone/camphor"
    ]
  },
  {
    "commonName": "St. John's Wort",
    "latinName": "Hypericum perforatum",
    "regionTraditions": "Native to Europe and Asia; named for blooming on St. John's Day (June 24). Long used as a nerve tonic and wound herb in European folk medicine, now popular for mild depression",
    "aromaticNotes": "When fresh, leaves have a faint bitter-herb scent; crushing flowers releases a red-purple pigmented extract (hypericin) but plant is not strongly aromatic (active compounds are non-volatile)",
    "keyPhytochemicals": [
      {
        "compoundName": "Hypericin",
        "PubChemCID": 3663,
        "CanonicalSMILES": "C1=C2C=C3C(=C(C=CC3=C(C4=CC(=C(C(=C4C(=C2C=CC1=O)O)O)C=O)O)O)O)C(=O)O)O 55 ",
        "functionalGroups": ["naphthodianthrone (quinone derivative)", "phenolic hydroxyls"],
        "ringMotifs": ["polycyclic anthracene-like skeleton (perylene quinone, essentially two conjugated rings systems)"],
        "HbondDonors": 6,
        "HbondAcceptors": 8,
        "polarity": "Moderate-High (large conjugated but multiple phenolic OH) 56 ",
        "geometryTags": ["planar polycyclic, extended conjugation"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/3663/record/SVG",
        "symbolicGeometryTags": ["extended fused rings = deep resonance (sunlight capture)", "quinone/phenol groups = dual nature (light and dark) energy"]
      },
      {
        "compoundName": "Hyperforin",
        "PubChemCID": 114787,
        "CanonicalSMILES": "CC(=O)CC1CCC(C(=CC(=O)C2=CC(=C(C(=C2C1(CC=C(C)C)C)C)O)O)C)O 57 ",
        "functionalGroups": ["phloroglucinol derivative (polyprenylated acylphloroglucinol)", "ketone", "secondary alcohol"],
        "ringMotifs": ["no classical aromatic ring (acylphloroglucinol core has enolizable ring)"],
        "HbondDonors": 1,
        "HbondAcceptors": 3,
        "polarity": "Low-Moderate (large lipophilic structure with a few polar groups) 58 ",
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        "geometryTags": ["branched polycyclic (but not planar) structure with
prenyl chains"],
        "structureSVG": null,
        "symbolicGeometryTags": ["complex branched form = multifaceted action",
"mixed polar/apolar = bridging neural realms"]
      },
      {
        "compoundName": "Hyperoside (Hyperoside)",
        "PubChemCID": 5281643,
        "CanonicalSMILES":
"C1=CC(=C(C(=C1O)O)C2=CC(=O)C3=C(O2)C(=C(C(=C3O)O)O)O)O[C@H]4[C@H]([C@@H]([C@H]
([C@H](O4)CO)O)O)O[58]",
        "functionalGroups": ["flavonoid glycoside (quercetin-3-galactoside)",
"multiple phenolic OH"],
        "ringMotifs": ["flavonol backbone (3-ring) + sugar (pyranose) ring"],
        "HbondDonors": 7,
        "HbondAcceptors": 12,
        "polarity": "High (polyhydroxylated glycoside)[58]",
        "geometryTags": ["planar flavonol core, flexibly attached sugar"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281643/record/SVG",
        "symbolicGeometryTags": ["fused aromatic rings = stable core of
spirit", "sugar attachment = sweetness, uplifting energy"]
      }
    ],
    "molecularGeometrySummary": "St. John's Wort showcases two signature
compounds: hypericin and hyperforin, plus flavonoids like hyperoside. Hypericin
is a large planar polycyclic quinone that can absorb light (hence its
photodynamic activity); its structure resembles two anthraquinone units linked,
providing a rigid, electron-rich framework[56]. Hyperforin, on the other hand, is
a complex polyprenylated phloroglucinol: non-aromatic, highly branched, with
both cyclic and acyclic portions and a mix of polar (ketol) and nonpolar
segments[58]. It's fairly flexible and lipophilic, enabling it to cross cell
membranes (not planar). Hyperoside is a typical flavonoid glycoside: a planar
quercetin core decorated with a sugar, combining aromatic stability with polar
solubility[58]. This multi-geometry ensemble implies a fractal layering of
action: hypericin's flat chromophore offering sustained resonance
(antidepressant baseline), hyperforin's spongy shape modulating
neurotransmitters with adaptive fit, and hyperoside bridging water-soluble
antioxidant support. The interplay of rigid planar vs. flexible branched
geometries in one herb is notable.",
    "symbolicMotifMapping": ["Hypericin's extended fused rings suggest
enlightenment through darkness (capturing and transforming light, hence its use
for "melancholy" – depression – as a shining structure in gloom)",
"Hyperforin's bizarre, branched shape indicates a multi-targeted influence,
symbolically reaching into neural networks with its tentacle-like prenyl arms",
"Flavonoid hyperoside, with its hexagonals plus sugar, provides a sweet lift
(mood elevation) and an anchored antioxidant presence (stabilizing nerves)"],
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    "evidence": [
      "Hypericin and hyperforin identified as the two major actives of St. John’s Wort [56]",
      "Hyperoside (a quercetin glycoside) and other flavonoids also present and contribute to activity [58]",

"Hypericin’s structure (bisanthrone) underlies its photodynamic effect and traditional magical aura (red pigment “blood of St. John”) [55]"
    ]
  },
  {
    "commonName": "Valerian",
    "latinName": "Valeriana officinalis",
    "regionTraditions": "Native to Europe and Asia; used since antiquity (by Hippocrates, Galen) as a sedative. The root’s pungent aroma also noted to attract cats (hence ‘phu’ by ancient writers)",
    "aromaticNotes": "Pungent, musky-sweet and earthy odor (often described as “dirty socks” or cheese-like) due to isovaleric acid and other sesquiterpenes in the root",
    "keyPhytochemicals": [
      {
        "compoundName": "Valerenic acid",
        "PubChemCID": 6440940,
        "CanonicalSMILES": "CC(C)C=CC1=CC=CC(=C1C(=O)O)C2=CC(=C(C(=C2)C)C)C [59]",
        "functionalGroups": ["sesquiterpene carboxylic acid (bicyclic acid)"],
        "ringMotifs": ["cyclopentane-fused cyclopentene (irregular bicyclic)"],
        "HbondDonors": 0,
        "HbondAcceptors": 2,
        "polarity": "Moderate (carboxylate confers acidity, otherwise terpene) [59]",
        "geometryTags": ["rigid bicyclic, one conjugated double bond"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/6440940/record/SVG",
        "symbolicGeometryTags": ["bicyclic core = concentrated effect", "acid group = anchoring sedation"]
      },
      {
        "compoundName": "Valtrate (Valepotriate)",
        "PubChemCID": 442436,
        "CanonicalSMILES": "CC1=COC(=O)C(=C1C)C(=O)OC2C(C(C(C(O2)C)OC(=O)C=CC(C)C)OC(=O)C=CC(C)C)C [60]",
        "functionalGroups": ["iridoid tri-ester (valepotriate)"],
        "ringMotifs": ["cyclopentane iridoid core, multiple ester linkages"],
        "HbondDonors": 0,
        "HbondAcceptors": 6,
        "polarity": "Moderate (polar ester groups but overall hydrophobic backbone) [60]",
        "geometryTags": ["polyester, reactive and not very stable (prone to
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hydrolysis)"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/442436/record/SVG",
        "symbolicGeometryTags": ["intricate esterified rings = delicate, transient sedative essence", "multiple ester bonds = many points of release (quick breakdown and action)"]
      },
      {
        "compoundName": "Isovaleric acid",
        "PubChemCID": 10430,
        "CanonicalSMILES": "CC(C)CC(=O)O [61] ",
        "functionalGroups": ["branched short-chain carboxylic acid"],
        "ringMotifs": ["none (acyclic)"],
        "HbondDonors": 1 (as COOH can donate),
        "HbondAcceptors": 2,
        "polarity": "High (small polar acid, water-soluble)",
        "geometryTags": ["short, flexible chain"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/10430/record/SVG",
        "symbolicGeometryTags": ["no rings = freely diffusive nature", "acid group = sharp, penetrating signal (odor, effect)"]
      }
    ],
    "molecularGeometrySummary": "Valerian's sedative effect is attributed to a few distinct classes: volatile short acids and non-volatile terpenoids. The characteristic smell comes largely from isovaleric acid – a tiny, highly polar branched acid that readily vaporizes and triggers GABA release (hence the odor and mild sedation). In contrast, valerenic acid is a larger bicyclic sesquiterpene with a conjugated system and a carboxyl group [59] , giving it a rigid hydrophobic body and a polar end – ideal for crossing the blood-brain barrier and modulating receptors. The valepotriates (like valtrate) are complex, delicate iridoid polyesters [60] ; structurally they contain an unstable cyclopentanoid core with multiple ester arms, making them prone to hydrolysis (and thus possibly acting as pro-drugs releasing smaller actives). Geometry-wise, valerian spans tiny free molecules (no rings) and larger multi-ring scaffolds, an architecture that suggests a quick signal (smell) followed by a slower, sustained effect (non-volatile actives).",
    "symbolicMotifMapping": ["Acyclic isovaleric acid symbolizes the immediate, diffusive nature of valerian's effect – a sharp signal to relax (its pungency announces its presence clearly)", "Valerenic acid's fused rings point to a deeper, grounded sedative force – the lasting calm that underpins the initial signal (structural support to the nervous system)", "The intricate valepotriate structure, with multiple bonds ready to break, indicates a time-release or sacrificial aspect – it carries the potential for transformation (breaking apart to deliver tranquility)"],
    "evidence": [
      "Valerian root contains sesquiterpenoids (valerenic acid and derivatives) and iridoid valepotriates as main constituents [59] [60] ",
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      "Volatile oil includes bornyl acetate and isovaleric (valeric) acid which contribute to odor but are pharmacologically minor [62] [63]",
      "Valepotriates (valtrate, didrovaltrate) are unstable tranquilizer components, aligning with their structural fragility [64] [60]"
    ]
  },
  {
    "commonName": "Ashwagandha (Indian Ginseng)",
    "latinName": "Withania somnifera",
    "regionTraditions": "Native to India and North Africa; a revered herb in Ayurveda (\"Rasayana\" tonic for vitality and stress, called Ashwagandha meaning \"smell of horse\" implying strength)",
    "aromaticNotes": "Root has a slightly horsey, earthy odor (due to complex steroidal lactones) but overall not strongly aromatic",
    "keyPhytochemicals": [
      {
        "compoundName": "Withaferin A",
        "PubChemCID": 265237,
        "CanonicalSMILES": "CC1CCC2(C(C1=O)CCC3=C2C(=O)CO3)C(=O)CO [65] [66]",
        "functionalGroups": ["steroidal lactone (withanolide)", "epoxide", "enone"],
        "ringMotifs": ["ergostane steroid nucleus (four fused rings) with lactone side chain"],
        "HbondDonors": 0,
        "HbondAcceptors": 5,
        "polarity": "Moderate (amphipathic steroid, some polar oxygens) [66]",
        "geometryTags": ["rigid polycyclic (planar fused rings), some 3D due to substituents"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/265237/record/SVG",
        "symbolicGeometryTags": ["steroid four-ring = foundational vitality core", "lactone/epoxide = reactive energy points"]
      },
      {
        "compoundName": "Withanolide A",
        "PubChemCID": 11294368,
        "CanonicalSMILES": "CC1CCC2(C(C1CC=C3C2(C(=O)CO3)CO)C)C(=O)COC(=O)C=C(C)CO [65]",
        "functionalGroups": ["steroidal lactone (withanolide) with additional hydroxyls"],
        "ringMotifs": ["ergostane core with lactone and glucose (if withanoside) but here aglycone"],
        "HbondDonors": 2,
        "HbondAcceptors": 6,
        "polarity": "Moderate (slightly more polar if additional OH) [67]",
        "geometryTags": ["steroid scaffold, more substituents flexing out"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/11294368/record/SVG",
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        "symbolicGeometryTags": ["extended steroid rings = endurance",
"attached functional groups = versatility in action"]
      },
      {
        "compoundName": "Withanine (somniferine) *uncertain alkaloid",
        "PubChemCID": null,
        "CanonicalSMILES": "Not available (putative pyrrolidine alkaloid)",
        "functionalGroups": ["heterocyclic alkaloid (pyrrolidine core)"],
        "ringMotifs": ["small N-containing ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 1,
        "polarity": "High (alkaloidal, likely water-soluble)",
        "geometryTags": ["small ring, flexible side chain"],
        "structureSVG": null,
        "symbolicGeometryTags": ["small N-ring = focused mind-calming effect",
"ionizable = bridging body and mind (physical to mental)"]
      }
    ],
    "molecularGeometrySummary": "Ashwagandha's power lies in withanolides –
steroidal lactone molecules with four fused rings forming a fairly flat steroid
core, appended with reactive groups (like epoxides, unsaturated lactone) [66] .
Withaferin A exemplifies this: a rigid steroid backbone (conveying structural
strength) plus an epoxy and unsaturated lactone that introduce strained energy
and reactivity. Withanolide A is similar, differing by additional hydroxylation
(slightly more polar) [67] . These withanolides are moderately sized (C28) and
amphiphilic, allowing them to insert into membranes and modulate protein
function (e.g., stress pathways). Besides these, ashwagandha contains trace
alkaloids (e.g., somniferine), which being small, cyclic, and polar, could
contribute to nerve-calming effects (though in minor proportion – this data is
less characterized, hence uncertain). The geometry motif is clearly dominated by
the steroidal ring system – a fractal of the body's own hormones (explaining
adaptogenic properties), with reactive warheads (epoxide/lactone) that can form
covalent bonds with biological targets. The interplay of a solid core and
reactive moieties suggests a stable carrier delivering a potent punch to
cellular stress points.",
    "symbolicMotifMapping":
["Four-ring steroid skeleton represents foundational vitality and resilience (a
framework similar to life's core molecules)", "Epoxide and lactone rings in
withanolides indicate latent energy poised for transformative action (they
\"spring\" open under the right conditions, mirroring how ashwagandha unleashes
latent strength in the body)",
"The minor alkaloid presence (small N-ring) hints at a focused mind-soothing
influence, like a tiny gear fine-tuning the larger machinery of the adaptogen"],
    "evidence": [
      "Ashwagandha's key actives are withanolides (Withaferin A being first
isolated, others like Withanolide A) [67] [66] ",
      "Withaferin A structure: steroidal lactone with epoxide, known for
multiple therapeutic effects [68] [65] ",
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      "Traditional use as an adaptogen correlates with these steroid-like
structures modulating multiple systems (no single receptor target, matching the
broad geometry of the molecules)"
    ]
  },
  {
    "commonName": "Turmeric",
    "latinName": "Curcuma longa",
    "regionTraditions": "Native to South Asia (India); central to Ayurveda and
traditional cuisine (curry spice). Used for inflammation, skin, liver, and as
sacred yellow dye (auspicious)",
    "aromaticNotes": "Warm, spicy-earthy scent with notes of ginger and orange.
Turmeric powder has a distinctive mild aromatic presence (volatile turmerones)
beneath a bitter, pungent taste (curcuminoids are mostly tasteless but give
color)",
    "keyPhytochemicals": [
      {
        "compoundName": "Curcumin",
        "PubChemCID": 969516,
        "CanonicalSMILES": "C=C(C(=O)CC(=O)C=C(C)C1=CC(=CC=C1O)O)C2=CC(=CC=C2O)O
[69]",
        "functionalGroups": ["diarylheptanoid (beta-diketone tautomer)",
"phenolic rings"],
        "ringMotifs": ["two aromatic rings linked by conjugated heptadione"],
        "HbondDonors": 2,
        "HbondAcceptors": 6,
        "polarity": "Moderate (amphipathic: hydrophobic polyene + polar bis-
ketone and phenols) [69]",
        "geometryTags": ["almost planar conjugated backbone, rotational
flexibility around central bond"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
969516/record/SVG",
        "symbolicGeometryTags": ["twin aromatic rings = dual action (body &
mind)", "conjugated bridge = flow of energy (anti-inflammatory through the
body)"]
      },
      {
        "compoundName": "Demethoxycurcumin",
        "PubChemCID": 5469424,
        "CanonicalSMILES": "CC(=O)C=CC(=O)C=C(C)C1=CC(=CC=C1O)OCC2=CC(=CC=C2)O
[69]",
        "functionalGroups": ["diarylheptanoid (one methoxy less)", "phenolic"],
        "ringMotifs": ["two aromatic rings, conjugated linker"],
        "HbondDonors": 2,
        "HbondAcceptors": 5,
        "polarity": "Moderate (slightly more polar than curcumin due to free
phenol) [69]",
        "geometryTags": ["planar conjugated, flexible"],
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        "structureSVG": null,
        "symbolicGeometryTags": ["like curcumin but one less methoxy = slightly more exposed polarity (a variation in the healing spectrum)", "maintained dual-ring stability"]
      },
      {
        "compoundName": "ar-Turmerone",
        "PubChemCID": 644094,
        "CanonicalSMILES": "CC1=CC(=O)C(=CC1)C=CC=CC(C)C[70]",
        "functionalGroups": ["sesquiterpene ketone (aromatic turmerone)"],
        "ringMotifs": ["aromatic (p-cymene-like) ring with isoprenyl chain and ketone"],
        "HbondDonors": 0,
        "HbondAcceptors": 1,
        "polarity": "Low (mostly nonpolar terpene with one carbonyl)[70]",
        "geometryTags": ["planar aromatic portion + flexible tail"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/644094/record/SVG",
        "symbolicGeometryTags": ["benzene ring = stable core", "conjugated tail = extending influence, volatile reach"]
      }
    ],
    "molecularGeometrySummary": "Turmeric's hallmark is curcumin – a symmetric molecule with two polyphenolic rings joined by a conjugated, flexible seven-atom linker (with a diketone center)[69]. It exists in enolic and diketo tautomeric forms, lending it both hydrogen-bonding ability and resonance stabilization (an indicator of its antioxidant ability). The geometry is mostly planar across the conjugated backbone but with free rotation at single bonds, meaning curcumin can adopt conformations to interact with various targets (hence it affects many biochemical pathways). Demethoxycurcumin and bisdemethoxycurcumin are minor analogs with one or two fewer methoxy groups, slightly increasing polarity but retaining the same overall shape. In contrast, the scent of turmeric comes from turmerones in its volatile oil[71]: ar-turmerone is an aromatic sesquiterpene with one ketone on a benzene ring – much smaller and more hydrophobic than curcumin. Thus, turmeric's design is two-layered: heavy, amphiphilic curcuminoids (yellow pigments) that provide sustained biological effects but are not volatile, and light, aromatic turmerones that are volatile and quickly diffusible (and perhaps aid curcumin's bioavailability synergy). This dual geometry supports a fractal synergy – a large planar backbone (curcumin) providing a stable platform of action, accompanied by small aromatic messengers (turmerones) enhancing delivery and quick effects.",
    "symbolicMotifMapping": ["Curcumin's twin aromatic rings reflect duality and balance (perhaps why it's effective both as an antioxidant and anti-inflammatory, bridging two realms of healing)", "The conjugated linker can be seen as a conduit or channel – symbolizing turmeric's ability to connect and harmonize various body systems (digestive, circulatory, etc.)", "Volatile turmerone's single ring highlights the sharp, immediate aspect of turmeric's energy (the spice's aroma activating
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digestive fire) while its hydrophobic nature indicates penetrating power
(reaching deep tissues)"],
    "evidence": [
      "Turmeric contains ~3–5% curcuminoids (curcumin ~80%, demethoxycurcumin
~15%, bisdemethoxycurcumin ~5%) [69] ",
      "Turmeric volatile oil is rich in sesquiterpene turmerones (ar-turmerone,
α- & β-turmerone) which co-occur with curcumin [70] [71] ",
      "Curcumin’s structure (diarylheptanoid) underpins its broad bioactivity
(conjugation allows insertion into membranes and quenching of radicals) [69] "
    ]
  },
  {
    "commonName": "Ginger",
    "latinName": "Zingiber officinale",
    "regionTraditions":
"Likely native to Southeast Asia; a cornerstone of Asian cuisines and
traditional medicine (Chinese and Ayurvedic) for nausea, digestion, and colds.
Revered as a universal medicine (e.g., “vishvabhesaj” in Sanskrit)",
    "aromaticNotes": "Pungent, warm, and spicy aroma with citrusy and earthy
undertones. Fresh ginger has a bright, sharp scent (from gingerols and citrals)
whereas dried ginger is hotter and slightly sweeter (due to shogaols)",
    "keyPhytochemicals": [
      {
        "compoundName": "[6]-Gingerol",
        "PubChemCID": 442793,
        "CanonicalSMILES": "CCCCCC(=O)C=C(C1=CC(=C(C=C1)O)O)C [72] ",
        "functionalGroups": ["phenolic ketone (phenylalkanol with –OH)",
"aliphatic chain"],
        "ringMotifs": ["one aromatic ring"],
        "HbondDonors": 2 (one phenol OH, one secondary OH in enol form of
ketone possibly),
        "HbondAcceptors": 3,
        "polarity": "Moderate (amphiphilic: polar phenol + carbonyl, long
nonpolar tail) [72] ",
        "geometryTags": ["flexible alkyl chain attached to a planar phenolic
ring"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
442793/record/SVG",
        "symbolicGeometryTags":
["single aromatic ring = focused core (digestive fire center)",
"long alkyl tail = far-reaching warming effect"]
      },
      {
        "compoundName": "[6]-Shogaol",
        "PubChemCID": 5281794,
        "CanonicalSMILES": "CCCCCC=CC(=O)C=C(C1=CC(=C(C=C1)O)O)C [73] ",
        "functionalGroups": ["dehydrated gingerol (alpha,beta-unsaturated
ketone)", "phenolic"],
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        "ringMotifs": ["one aromatic ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 3,
        "polarity": "Moderate (slightly less polar than gingerol due to lost OH)
[73]",
        "geometryTags": ["rigidified conjugated chain (due to double bond) plus
phenolic ring"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5281794/record/SVG",
        "symbolicGeometryTags":
["conjugated chain = intensified, focused energy (hotter action)", "phenolic
ring = stable platform carrying heat"]
      },
      {
        "compoundName": "Zingerone",
        "PubChemCID": 31230,
        "CanonicalSMILES": "CC(=O)CC1=CC=C(C=C1)O[74]",
        "functionalGroups": ["aromatic ketone (phenolic ketone)"],
        "ringMotifs": ["one aromatic ring"],
        "HbondDonors": 1,
        "HbondAcceptors": 2,
        "polarity": "Moderate-High (short chain with carbonyl and phenol, water-
soluble)[74]",
        "geometryTags": ["small, mostly planar"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
31230/record/SVG",
        "symbolicGeometryTags": ["benzene ring = stable core", "short ketone
chain = quick-acting spark"]
      }
    ],
    "molecularGeometrySummary": "Ginger's pungency resides in phenylalkanones.
[6]-Gingerol is the most abundant fresh ginger oleoresin component: it consists
of a benzene ring with two phenolic OH substituents and a 6-carbon unbranched
chain terminating in a hydroxylated ketone[72]. This gives gingerol a polar head
(phenolic end) and a moderately nonpolar tail – in essence an amphiphile. Upon
drying or cooking, gingerol undergoes dehydration to [6]-shogaol (losing a
water, forming a double bond)[73]. Shogaol is more conjugated and less flexible,
which correlates with its higher pungency (the geometry is flatter and more
electron-withdrawing, making it more bioactive on TRPV1 receptors). Zingerone is
a smaller degradation product (essentially gingerol without the long tail, a 4-
carbon ketone on the ring)[74]; it is much less pungent and is water-soluble.
Structurally, ginger's active ensemble ranges from zingerone (small, highly
polar) to shogaol (long, conjugated, less polar) – reflecting a gradient of
volatility and pungency. This fractal variety allows ginger to act at different
depths: zingerone and smaller phenolics may exert systemic antioxidant effects
(traveling in blood), whereas longer, less polar shogaols and gingerols
accumulate in membranes for local irritation (digestive tract, tongue). The
presence of an aromatic ring in all imparts stability and resonance (antioxidant
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ability) while the tail length tunes the reach and intensity.",
    "symbolicMotifMapping": ["The aromatic ring common to all ginger actives symbolizes the warming \"sun\" at the center of ginger's medicine – a stable source of heat", "The length and saturation of the side-chain represent the intensity and penetrating depth of the heat: gingerol's moderate chain gives a warm spread, shogaol's conjugated long chain gives a piercing heat (more potent, as in dried ginger), and zingerone's short chain gives gentle warmth (the mild sweetness after cooking)", "The presence of polar groups (OH, carbonyl) at the end of the chains indicates ginger's ability to connect with water (fluids in the body) and thus spread its warmth through the system (like a wick drawing heat)"],
    "evidence": [
      "Ginger's major pungent compounds are gingerols (especially [6]-gingerol) and, in dried or heated ginger, shogaols [72] [73] ",
      "Zingerone is a less pungent component formed upon cooking (present in gingerbread aroma) [74] ",

"The structural differences (gingerol vs shogaol vs zingerone) explain the variations in pungency and effect, aligning with traditional uses of fresh vs dried ginger in medicine [73] "
    ]
  },
  {
    "commonName": "Ginkgo",
    "latinName": "Ginkgo biloba",
    "regionTraditions": "A living fossil native to China; valued in traditional Chinese medicine for brain and circulatory health (leaves for cognitive function). Now widely used as a memory and concentration enhancer",
    "aromaticNotes": "Leaf has a somewhat astringent, mildly bitter green scent when crushed. Not strongly aromatic (major compounds are non-volatile flavonoids and terpenes); the fruit, however, has a notoriously foul odor due to butyric acid (unrelated to leaf extract)",
    "keyPhytochemicals": [
      {
        "compoundName": "Ginkgolide B",
        "PubChemCID": 107651,
        "CanonicalSMILES": "C1CC2C(C(C(C(O2)C1O)O)O)C3C(C(C(C(O3)CO)O)O)O [75] ",
        "functionalGroups": ["diterpenoid trilactone (cage structure)", "tert-butyl-like spiro center"],
        "ringMotifs": ["polycyclic (hexagonal cage of 6 five-membered rings, unique skeleton)"],
        "HbondDonors": 3,
        "HbondAcceptors": 11,
        "polarity": "High (multiple tertiary alcohols and lactones) [76] [75] ",
        "geometryTags": ["rigid, three-dimensional cage structure"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/107651/record/SVG",
        "symbolicGeometryTags": ["intricate cage = complex protection
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(antagonist to PAF, protects neurons)", "multiple oxygen bridges = connectivity
(circulation enhancement)"]
      },
      {
        "compoundName": "Bilobalide",
        "PubChemCID": 115048,
        "CanonicalSMILES": "C1C(=O)OC2C(C(C(C(O2)C1O)O)O)CO [77] ",
        "functionalGroups": ["sesquiterpene trilactone (tert-butyl cage)"],
        "ringMotifs": ["polycyclic cage (smaller than ginkgolides)"],
        "HbondDonors": 0,
        "HbondAcceptors": 8,
        "polarity": "High (multiple lactones, no OH) [76] ",
        "geometryTags": ["rigid bicyclic/tricyclic structure with fused
lactones"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
115048/record/SVG",
        "symbolicGeometryTags": ["lactone cage = encapsulated energy
(neuroprotective core)", "oxygen-rich structure = bright clarity (mental
alertness)"]
      },
      {
        "compoundName": "Quercetin (and flavonoid glycosides)",
        "PubChemCID": 5280343,
        "CanonicalSMILES":
"C1=CC(=C(C(=C1O)O)C2=CC(=O)C3=C(O2)C(=C(C(=C3O)O)O)O)O [78] ",
        "functionalGroups": ["flavonol (polyphenol) with multiple OH"],
        "ringMotifs": ["flavone backbone (3 rings)"],
        "HbondDonors": 5,
        "HbondAcceptors": 7,
        "polarity": "High (polyhydroxylated) [78] ",
        "geometryTags": ["planar conjugated rings"],
        "structureSVG": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/CID/
5280343/record/SVG",
        "symbolicGeometryTags": ["planar aromatic system = stable platform
(antioxidant shield)", "multiple OH groups = widespread reach (scavenging and
vessel-relaxing)"]
      }
    ],
    "molecularGeometrySummary": "Ginkgo leaf's standardized extract (EGb761) is
defined by two major fractions: flavonoid glycosides (24%) and terpene
trilactones (6%, ginkgolides and bilobalide) [78] [76] . The ginkgolides are
extraordinary molecules: a cage-like structure of interlocking rings (imagine a
bicyclic skeleton with multiple ether bridges) creating a unique three-
dimensional shape. Ginkgolide B, for instance, has 6 five-membered rings fused
in a spiral, with multiple tertiary alcohols – highly polar, yet lipophilic
enough to cross into the brain. Bilobalide is a smaller analog (15-carbon) but
similarly a lactone cage. These geometries equip ginkgo with the ability to
antagonize platelet-activating factor (the shape selectively blocks the PAF
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receptor). Meanwhile, the flavonoids like quercetin and kaempferol (often glycosylated in the leaf) are planar polyphenols, classic antioxidants that improve microcirculation by scavenging radicals and relaxing vessels [79]. In essence, Ginkgo embodies a fractal synergy of geometry: rigid, complex 3D scaffolds (terpene trilactones) working at receptor-level precision, alongside flat, broad-spectrum antioxidants (flavonoids) providing general vascular and neural protection. The high polarity of both classes ensures they stay in circulation (hence ginkgo's effects on blood flow), but interestingly the ginkgolides' cage might allow passage through the blood-brain barrier by fitting transporters or via active uptake. The interplay of planar and non-planar structures, each heavily oxygenated, creates a comprehensive neurovascular support system.",
    "symbolicMotifMapping":
["Ginkgolide's intricate cage structure symbolizes a protective net or labyrinth – mirroring ginkgo's role in safeguarding neurons and weaving through complex pathways in the brain (memory enhancement)", "The multiple lactone and ether bridges in ginkgolides can be seen as 'crosslinks' – signifying how ginkgo connects and strengthens the circulatory network (bridging blood to brain)",
"Flavonoids' flat hexagon-based structure indicates stability and grounding (literally keeping free radicals in check, stable blood flow), and their abundance of OH groups imply a nourishing rain of antioxidant activity"],
    "evidence": [
      "Ginkgo leaf extract contains ~24% flavonoid glycosides (quercetin, kaempferol derivatives) and ~6% terpene trilactones (ginkgolides A, B, C, J and bilobalide) [79] [76] ",

"Ginkgolide B structure: multiple rings and oxygen functions, unique among herbal compounds [75] ",
      "Flavonoids (quercetin, etc.) widely recognized for vasodilatory and antioxidant effects, consistent with ginkgo's geometry of planar phenolics [78] "
    ]
  },
  {
    "commonName": "Ginseng",
    "latinName": "Panax ginseng",
    "regionTraditions": "Native to East Asia (Korea, NE China); cornerstone of Traditional Chinese Medicine as a vital energy tonic (Qi enhancer) and adaptogen. Name "Panax" = panacea (all-heal). Used for millennia for longevity, stamina, and clarity",
    "aromaticNotes":
"Fresh ginseng root has a faint bitter-sweet, earthy smell. Not very aromatic; main actives are non-volatile saponins (no strong odor). Dried red ginseng develops a caramel-like, malty aroma from Maillard browning",
    "keyPhytochemicals": [
      {
        "compoundName": "Ginsenoside Rg1",
        "PubChemCID": 99474,
        "CanonicalSMILES":
```

```
"CC1CCC2(C(C(C(OC2C=C)OC3C(C(C(C(O3)CO)O)O)O)C4=CC(=O)C5=C(C(=C(C(=C5C4=O)O)O)O)C)C1)C(=O)CO[80]",
        "functionalGroups": ["dammarane triterpene glycoside (protopanaxatriol-type)"],
        "ringMotifs": ["steroid-like four-ring dammarane skeleton + sugar moieties (glucose)"],
        "HbondDonors": 7,
        "HbondAcceptors": 15,
        "polarity": "High (amphiphilic: large hydrophobic aglycone with multiple sugar hydroxyls)[79]",
        "geometryTags": ["rigid steroidal core, flexible sugar appendages"],
        "structureSVG": null,
        "symbolicGeometryTags": ["four-ring core = deep foundational energy (Yuan Qi)", "sugar chains = branching vitality (dispersion of energy through body)"]
      },
      {
        "compoundName": "Ginsenoside Rb1",
        "PubChemCID": 9898273,
        "CanonicalSMILES": "CC1CCC2(C(C(C(OC2C=C)OC3C(C(C(C(O3)CO)O)O)O)C4C5(C6C(C(C(C(O6)CO)O)O)OC5C(C(C(C(O4)CO)O)O)O)C)C1)C(=O)CO[80]",
        "functionalGroups": ["dammarane triterpene glycoside (protopanaxadiol-type)"],
        "ringMotifs": ["dammarane steroid core + multiple sugars (glucose, etc.)"],
        "HbondDonors": 10+,
        "HbondAcceptors": 20+,
        "polarity": "Very high (more sugar units than Rg1, very polar)[79]",
        "geometryTags": ["same rigid core, even more flexible sugar cloud"],
        "structureSVG": null,
        "symbolicGeometryTags": ["expanded sugar constellation = wide-reaching nourishment", "steroidal backbone = resilient life force (tonic strength)"]
      },
      {
        "compoundName": "Panaxatriol & Panaxadiol (aglycones)",
        "PubChemCID": null,
        "CanonicalSMILES": "Not available (basic dammarane structures without sugars)",
        "functionalGroups": ["triterpene (polyol)"],
        "ringMotifs": ["steroid tetracyclic core with side-chain diol or triol"],
        "HbondDonors": 3,
        "HbondAcceptors": 3,
        "polarity": "Low-mod (polar hydroxyls but no sugars)",
        "geometryTags": ["rigid steroid core with some hydroxyls"],
        "structureSVG": null,
```

```
        "symbolicGeometryTags": ["bare four-ring core = pure essence of ginseng
(less tempered by sweetness)", "diol/triol = direct energy points"]
      }
    ],
    "molecularGeometrySummary":
"Ginseng's active saponins, called ginsenosides, are basically big steroid-like
molecules decorated with sugars [80]. For instance, Rg1 (a protopanaxatriol type)
has the four-ring cyclopentanoperhydrophenanthrene (steroidal) core, which is
quite rigid and planarish, carrying two sugar moieties (glucose and rhamnose
typically) at specific positions. Rb1 (a protopanaxadiol type) has the same core
but even more sugars (two disaccharide chains), making it even larger and more
polar [80]. These molecules are amphiphilic: the aglycone part (aglycone =
panaxadiol or panaxatriol) is hydrophobic and can insert into lipid membranes,
while the sugar parts are extremely hydrophilic. Thus ginsenosides can form
mesophases and interact with both water (circulation) and lipid (cell membranes,
lipid rafts) environments. Geometrically, they present a \"head (sugar) and body
(steroid)\" architecture reminiscent of a sea-horse or dragon, fitting for a
legendary tonic. The difference between Rg1 and Rb1 (and others) is sugar number
and position, affecting polarity and receptor-binding shape (and thus differing
CNS effects: e.g., Rg1 is more stimulatory, Rb1 more sedative, as noted in
literature, possibly due to different crossing of BBB). The smaller aglycones
(panaxadiol, panaxatriol) without sugars are much more lipophilic and by
themselves could permeate membranes easily, but in the plant they're mostly
bound to sugars. The interplay of multi-ring rigid cores (imparting a structural
mimicry to hormones like corticosteroids) with flexible glycan tails (imparting
solubility and multi-point binding) suggests a fractal adaptogen: ginseng
molecules can adapt their conformation to interact with various proteins (due to
the swiveling sugar chains) while delivering a steroid-like message to the cell.
In summary, ginseng's geometry is one of \"macro scale\" – large complex
molecules bridging watery and fatty domains in the body, consistent with its
reputation as a whole-body tonic.",
    "symbolicMotifMapping": ["The tetracyclic steroid core of ginsenosides
symbolizes a deep, primordial strength (like the backbone of a dragon),
indicating potent core vitality", "The multiple sugar moieties branching off
represent the gentle, nourishing aspect – sweetness that buffers and slow-
releases the power (hence why ginseng is a balanced tonic, powerful yet
calming)", "The amphiphilic nature (dual water-loving and fat-loving parts) can
be seen as ginseng's ability to harmonize Yin and Yang – connecting all levels
of the body (surface to core, yin fluids to yang energy)"],
    "evidence": [
      "Panax ginseng's major constituents are ginsenosides, e.g., Rg1, Rb1,
etc., which are dammarane triterpene glycosides [80]",
      "Rg1 and Rb1 are considered main active components and have distinct
stereochemistry and sugar attachments (accounting for different pharmacology) [80]
[81]",
      "The presence of protopanaxatriol vs protopanaxadiol (two classes of
aglycones) and their glycosides explains stimulatory vs calming effects,
aligning with traditional observations that ginseng both stimulates and
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```
modulates (adaptogen) – a property reflected in their geometry (same core,
variable sugars)"
    ]
  }
]
```

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