**Table S2**. Online database matching of the most abundant molecular formulae for each biomolecule group carried out from FT-ICR MS data.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |
| **Lignin** |   |   |   |   |   |
| Formula | compound |   |   |   |   |
| C17H12O6 | 5-(3-phenylprop-2-enoyloxy)benzene-1,3-dicarboxylic acidFujikinetin |
| C20H14O5 | diphenyl 2-hydroxybenzene-1,3-dicarboxylateSophoracoumestan A |
| C17H12O5 | phenyl 7-methoxy-2-oxochromene-3-carboxylateHaloquinone |
| C20H14O4 | 1,4-di(benzofuran-2-yl)butane-1,4-dione2-(4-phenoxybenzoyl)benzoic acid |
| C17H12O7 | 5-(4-methylbenzoyl)benzene-1,2,4-tricarboxylic acidDalspinin |
| C20H14O7 | 2-(3,4,5,6-tetrahydroxy-9H-xanthen-9-yl)benzoic acidAscochytatin |
| C19H14O4 | 1-(2-methoxybenzoyl)naphthalene-2-carboxylic acid3,5-Diphenoxybenzoic acid |
| C17H12O4 | 2-[(2-oxochromen-3-yl)methoxy]benzaldehyde3-Methylflavone-8-carboxylic acid |
| C19H14O5 | 3-(6-acetyloxynaphthalen-2-yl)oxybenzoic acidVulpinic acid |
| C16H12O5 | 2-(9-oxoxanthen-2-yl)oxypropanoic acidPrunetin |  |
|  |  |  |  |  |  |
| C21H15O5N1 | Dibenzoylmononitrosoorcin4-(1,3-Dioxo-1,3-dihydro-isoindol-2-ylmethyl)-3-hydroxy-naphthalene-2-carboxylic acid methyl ester |
| C20H15O5N1 | 2-nitro-4-(3-phenylmethoxyphenyl)benzoic acid |  |
| C18H13O3N1 | 2,6-diphenyl-3-nitrophenol |  |  |  |
| C21H15O3N1 | cis-4-(p-nitrostyryl)benzophenone |  |  |
| C20H15O3N1 | phenyl 3-benzamidobenzoate3-benzoylamino-4-hydroxybenzophenone |
| C20H15O6N1 | 7-amino-6-benzoyl-4,9-dimethoxyfuro[3,2-g]chromen-5-oneOxophoebine |
| C17H13O5N1 | Phthalimidomethyl 3-methoxybenzoate1-((Ethoxycarbonyl)amino)-4-hydroxyanthraquinone |
| C17H13O4N1 | aristolamideN-Phthaloyl-L-phenylalanine |  |  |
| C15H11O4N1 | 2-(benzoylamino)-α-oxo-Benzeneacetic acid4'-Nitroflavanone |
| C15H11O5N1 | 2-(4-acetylphenyl)-4-nitrobenzoic acidBostrycoidin |  |
|  |  |  |  |  |  |
| C8H8O3S1 | 3-(methylsulfinyl)-Benzoic acid |  |  |
| C15H12O6S2 | methyl 2-oxo-2-(4,6,6-trioxo-3,5-dihydro-2H-thiopyrano[3,2-c]thiochromen-3-yl)acetate |
| C16H12O4S1 | 2-Phenylthiomethyl-3-carboxy-5-hydroxybenzofuran |  |
| C16H12O3S1 | 5-methoxy-3-phenyl-1-benzothiophene-2-carboxylic acid |
| C15H12O4S1 | 2-benzylsulfanylbenzene-1,3-dicarboxylic acid |  |
|  |  |  |  |  |  |
| **Lipid** |   |   |   |   |   |
| C28H56O2 | Octacosanoic acid. Montanic acid |  |  |
| C20H32O2 | Arachidonic acid |  |  |  |
| C26H52O2 | Hexacosanoic acid |  |  |  |
| C28H56O3 | 2-Hydroxyoctacosanoic acid |  |  |
| C18H36O2 | Stearic acid |  |  |  |  |
| C30H60O2 | Melissic acid |  |  |  |  |
| C28H54O4 | Octacosanedioic acid |  |  |  |
| C27H54O2 | Heptacosanoic acid |  |  |  |
| C26H52O3 | 2-Hydroxyhexacosanoic acid |  |  |
| C25H50O2 | Pentacosanoic acid |  |  |  |
|  |  |  |  |  |  |
| C18H30O3S1 | Dodecylbenzenesulfonic acid |  |  |
| C16H26O3S1 | 3-(Ethylsulfanyl)-2-[4-(tetrahydro-2-furanyloxy)butylidene]cyclohexanone |
| C16H26O3S1 | Benzenesulfonic acid, decyl- |  |  |
| C12H18O4S2 | 2-[2-(2-methylprop-2-enoyloxy)ethyldisulfanyl]ethyl 2-methylprop-2-enoate |
| C13H20O4S2 | dipropan-2-yl 2-(1,3-dithian-2-ylidene)propanedioate |  |
|  |  |  |  |  |  |
| **CAS** |   |   |   |   |   |
| C20H10O6 | Bilawsone |  |  |  |  |
| C20H10O5 | Bulgarein  |  |  |  |  |
| C21H10O7 | Chembl4163702 |  |  |  |
| C19H10O5 | Haemodordioxolane |  |  |  |
| C18H10O5 | Kinobscurinone |  |  |  |
| C22H12O7 | 4-(9,10-dioxoanthracen-2-yl)oxyphthalic acid |  |
| C22H12O7 | spiroxin C |  |  |  |  |
| C19H10O6 | Dehydrodolineone |  |  |  |
| C21H10O6 | Eucapsitrione |  |  |  |
| C21H12O5 | balsaminone A |  |  |  |
|  |  |  |  |  |  |
| C19H9O5N1 | 3-(1,3-BENZOXAZOL-2-YL) PYRANO[3,2-C]CHROMENE-2,5-DIONE |
| C18H9O4N1 | Nitrobenzanthracenedione |  |  |  |
| C17H9O6N1 | 4,11-dihydroxy-5,10-dioxo-1H-naphtho[2,3-f]indole-3-carboxylic acid |
| C19H11O6N1 | Hypecoumine |  |  |  |
| C20H11O4N1 | Anthraquinone, 1-(m-nitrophenyl) |  |  |
| C17H9O5N1 | 2-Furancarboxylic acid 3-oxo-3H-phenoxazine-7-yl ester |  |
| C20H11O5N1 | Chembl4127273 |  |  |  |
| C16H9O4N1 | Kalbretorine |  |  |  |  |
| C18H11O4N1 | Atherospermidine |  |  |  |
| C18H9O6N1 | 6-(2-Nitrophenoxy)-1H,3H-benzo[de]isochromene-1,3-dione |
|  |  |  |  |  |  |
| C18H8O4S1 | Name:6-hydroxy-4-oxa-11-thia-benzo[def]chrysene-5,12-dione |
| C17H8O6S1 | 4-Hydroxy-3-(2-thienylcarbonyl)-5H-spiro[furan-2,2'-indene]-1',3',5-trione |
| C16H8O4S1 | 5,10-Dihydroxyanthra[2,3-b]thiophene-4,11-dione |  |
| C16H8O5S1 | 1-Hydroxypyrene sulfate |  |  |  |
| C15H10O4S1 | 2-acetyl-8-methoxybenzo[f][1]benzothiole-4,9-dione |  |
| C17H10O4S1 | 7-Oxobenzo[a]phenalene-8-sulfonic acid |  |  |
| C18H10O5S1 | 4-(benzenesulfonyl)benzo[f][2]benzofuran-1,3-dione |  |
| C15H10O5S1 | Sulfoflavone |  |  |  |  |
| C16H8O6S1 | 5-hydroxy-7-(3-hydroxy-2-oxochromen-4-yl)-1,3-benzoxathiol-2-one |
| C20H10O4S1 | Benzo[a]pyrenesulfate |  |  |  |
|  |  |  |  |  |  |
| C15H7O5N1S1 | 6-Oxo-6H-anthra(9,1-cd)isothiazole-3-carboxylic acid |  |
| C18H9O4N1S1 | bis-6H-1-benzopyrano[4,3-b][1,4]thiazine |  |  |
| C16H9O4N1S1 | 4-o-nitrophenylthio-1,2-naphthoquinone |  |  |
| C17H9O5N1S1 | 3-(Benzenesulfonyl)benzo[f][1,2]benzoxazole-4,9-dione |  |
| C16H9O3N1S1 | 3-(benzo[d]thiazol-2-yl)-8-hydroxy-2H-chromen-2-one |  |
| C14H7O3N1S1 | 9,10,10-trioxothioxanthene-3-carbonitrile |  |
| C16H9O5N1S1 | 1-(benzenesulfonyl)indole-2,3-dicarboxylic anhydride |  |
| C13H7O5N1S1 | 5-Hydroxy-7-(4-nitrophenyl)-1,3-benzoxathiol-2-one |  |
|  |  |  |  |  |  |
| **Protein** |   |   |   |   |   |
| C19H19O4N1 | Nandinine |  |  |  |  |
| C17H17O6N1 | Maculosine |  |  |  |  |
| C17H17O5N1 | Hippeastrine |  |  |  |  |
| C15H15O5N1 | Actiketal |  |  |  |  |
| C15H15O6N1 | Ascorbigen |  |  |  |  |
| C21H21O4N1 | Zindoxifene |  |  |  |  |
| C17H17O4N1 | Carbobenzoxyphenylalanine |  |  |
| C21H21O6N1 | Corynoline |  |  |  |  |
| C21H21O5N1 | Corlumine |  |  |  |  |
| C18H19O5N1 | Melicopicine |  |  |  |  |
|  |  |  |  |  |  |
| **UHC** |   |   |   |   |   |
| C20H28O2 | Retinoic acid |  |  |  |  |
| C20H14O2 | 1,2-Dibenzoylbenzene |  |  |  |
| C20H16O2 | Triphenylacetic acid |  |  |  |
| C21H16O2 | Diphenylmethyl benzoate |  |  |  |
| C22H16O2 | 1,12-Dimethoxyperylene |  |  |  |
|  |  |  |  |  |  |
| C21H13O2N1 | 4-PHENYLBENZOFURO[3,2-g]QUINOLIN-2(1H)-ONE |  |
| C20H11O2N1 | Anthrachinolinchinon |  |  |  |
| C20H12O2N2 | 6-(3-Pyridinyl)-5H-indeno(1,2-c)isoquinoline-5,11(6H)-dione |
| C20H10O2N2 | Dibenzophenazinedione |  |  |  |
| C20H13O2N1 | Styrylnaphthalimide |  |  |  |