**Supplementary Material**

**Network pharmacology of *Dracaena* sp. in Guangxi and its related species leaf secondary metabolites possess antioxidant properties**

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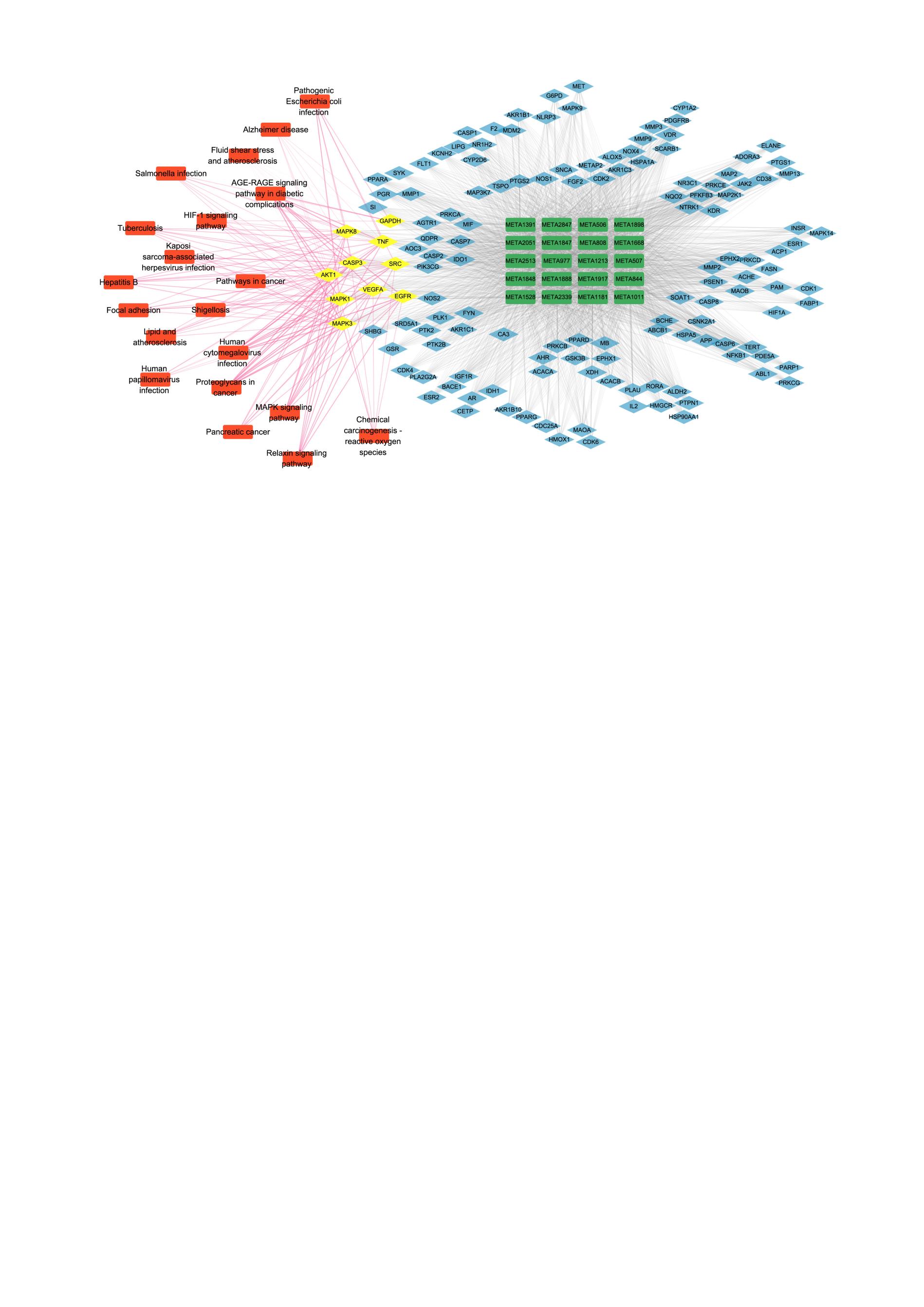
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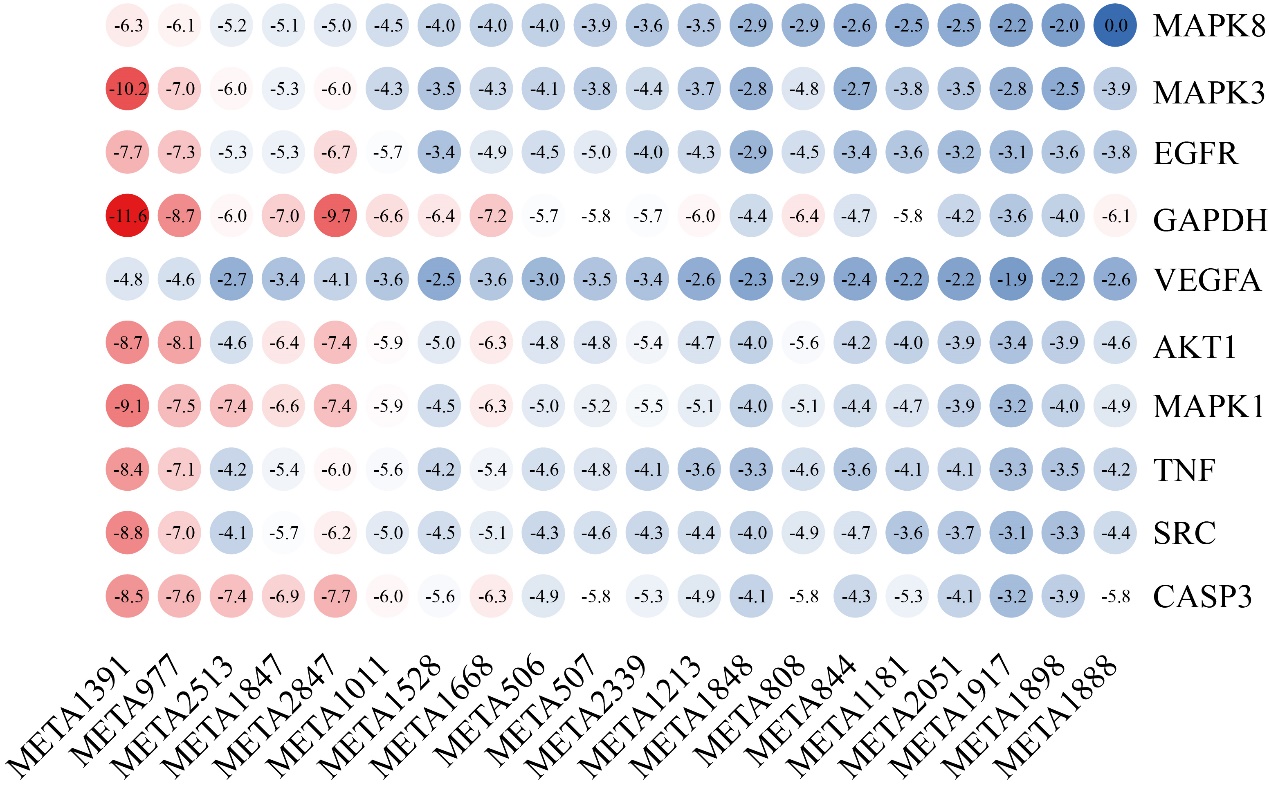
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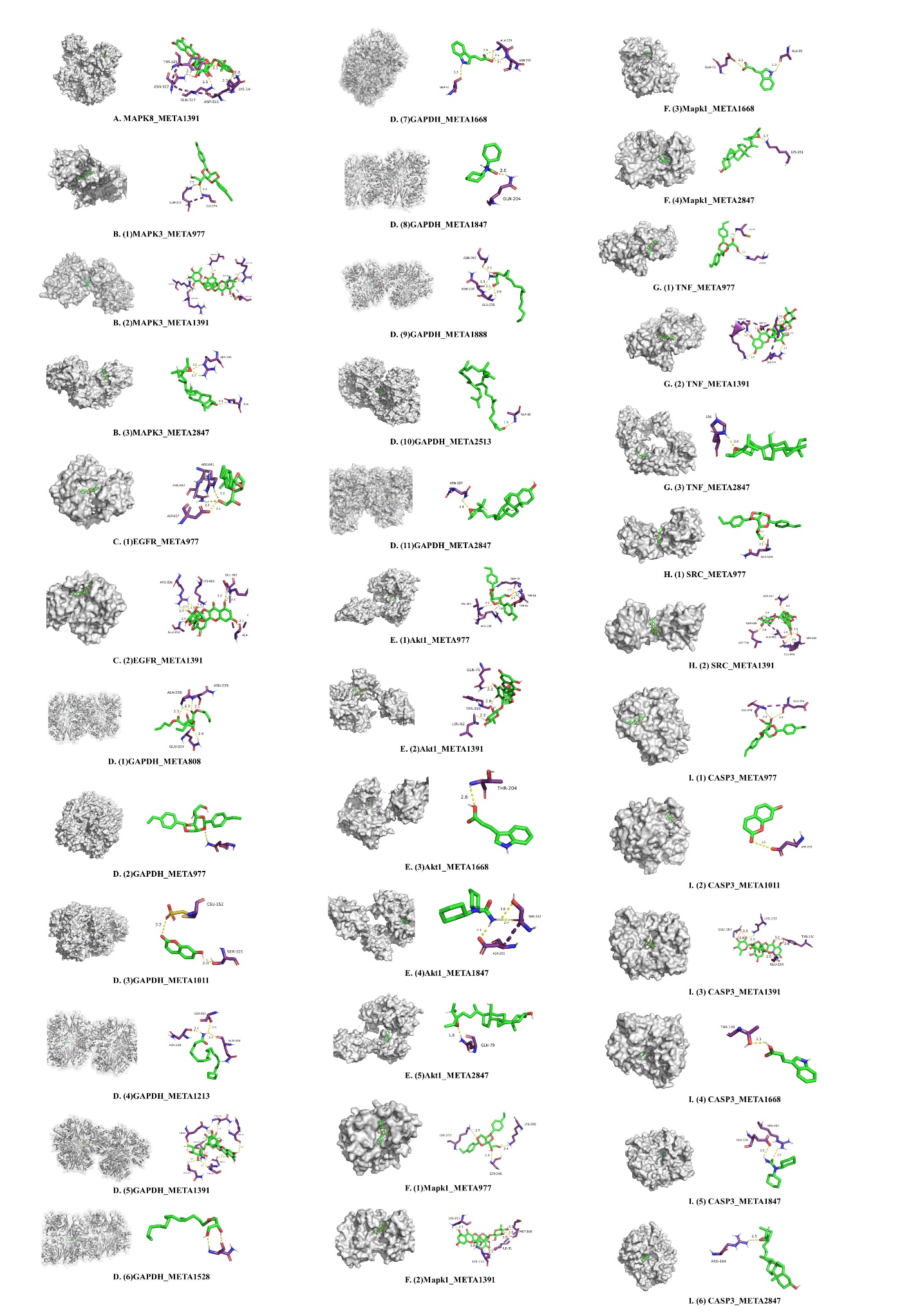
1These authors have contributed equally to this work



**Figure S1.** Compound-target-pathway network. The 138 potential targets most associated with antioxidant activity and the top 10 targets with the highest degree value were associated with metabolic pathways



**Figure S2.** Heat map of binding energies between potential active ingredients and core targets.



**Figure S3.** A-I, molecular docking diagrams of different targets and compounds.

**Table S1.** The information of sampling sites of *Dracaena*

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Species** | **Sample code** | **Localities** | **Longitude(E)** | **Latitude**  **(N)** | **Altitude**  **(m)** |
| *Dracaena* sp. in Guangxi | JX2 | Jingxi City, Guangxi,China | 106°33′ | 23°01′ | 792 |
| CZ4 | Jiangzhou Distric, Guangxi,China | 107°45′ | 22°72′ | 301 |
| C6 | Daxin County, Guangxi,China | 107°08′ | 22°57′ | 371 |
| C13 | Daxin County, Guangxi,China | 106°85′ | 22°37′ | 235 |
| RM1 | Nanning City, Guangxi regions,China | 108°33′ | 22°82′ | 112 |
| BM3 | Bama county, Guangxi,China | 107°25′ | 24°14′ | 291 |
| *Dracaena angustifolia* | CH | Nanning City, Guangxi regions,China | 108°17′ | 22°50′ | 101 |
| *Dracaena cambodiana* | HN | Nanning City, Guangxi regions,China | 108°17′ | 22°50′ | 101 |
| *Dracaena cochinchinensis* | CB | Jinghong City, Yunnan Province, China | 101°27′ | 21°92′ | 500 |
| *Dracaena marginata* | HB | Nanning City, Guangxi regions,China | 108°17′ | 22°50′ | 101 |
| *Dracaena elliptica* | XZ | Fangchenggang City, Guangxi,China | 107°65′ | 21°35′ | 206 |
| *Yucca schidigera* | SL | Nanning City, Guangxi regions,China | 108°23′ | 22°47′ | 280 |

**Table S2.** Abundant compounds common to *Dracaena* sp. in Guangxi

|  |  |  |
| --- | --- | --- |
| **Metabolites name** | **Formula** | **Mass spectrum** |
| 19-Hydroxyurs-12-en-3-yl acetate | C32H52O3 |  |
| Naronapride | C27H41ClN4O5 |  |
| difenoconazole | C19H17Cl2N3O3 |  |
| Usnic acid | C18H16O7 |  |
| 7-Dechlorogriseofulvin | C17H18O6 |  |
| 8-Hydroxy-4-methoxy-7-methyl-7,8-dihydro-5H-furo[2,3-g]isochromen-5-one | C13H12O5 |  |
| 1,7-Dihydroxy-3-methoxy-2-prenylxanthone | C19H18O5 |  |
| Leucylasparagine | C10H19N3O4 |  |
| 4-tert-Butylphenyl Salicylate | C17H18O3 |  |
| 4-Chloro-N-{[(2R,3S,4R,5S)-3,4-dihydroxy-5-{2-oxo-2-[4-(2-pyridinyl)-1-piperazinyl]ethyl}tetrahydro-2-furanyl]methyl}benzenesulfonamide | C22H27ClO6S |  |
| 3-Hydroxy-1-phenyl-1-icosanone | C26H44O2 |  |
| 3-[(2,6-Dimethylheptanoyl)oxy]-4-(trimethylammonio)butanoate | C16H31NO4 |  |
| Chrysin | C15H10O4 |  |
| 7-hydroxy-5-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one | C16H14O4 |  |
| N6-Methyladenine | C6H7N5 |  |
| Daidzein | C15H10O4 |  |
| Yangonin | C15H14O4 |  |
| N-[(1R,9S)-11-(1-Acetyl-4-piperidinyl)-6-oxo-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-5-yl]-4-chlorobenzenesulfonamide | C24H29ClN4O4S |  |
| (3S,4R)-3,4,5-Trihydroxy-4'-oxo-3',4,4',5-tetrahydro-2'H,3H-spiro[furan-2,1'-naphthalene]-6'-carboxylic acid | C14H14O7 |  |
| Vitamin A | C20H30O |  |
| (9cis)-Retinal | C20H28O |  |
| 1,4,5,6-tetrahydro-6-oxonicotinic acid | C6H7NO3 |  |
| Androstanolone | C19H30O2 |  |
| Pterostilbene | C16H16O3 |  |
| (1R,2R,5S,8S,9S,10R,12S)-5,12-Dihydroxy-11-methyl-6-methylene-16-oxo-15-oxapentacyclo[9.3.2.1-5,8-.0-1,10-.0-2,8-]heptadecane-9-carboxylic acid | C19H24O6 |  |

**Table S3.** Flavonoids unique to *Dracaen*a sp. in Guangxi

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **NO.** | **Metabolites name** | **Formula** | **BM3** | **C6** | **C13** | **CZ4** | **JX2** | **RM1** |
| **Area** | | | | | |
| 1 | 3-hydroxyflavanone | C15 H12 O3 | 2695062.111 | 0 | 0 | 0 | 0 | 0 |
| 2 | 2-{3-[6-(3,5-Dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methyl-2-cyclohexen-1-yl]-2,4-dihydroxyphenyl}-5,7-dihydroxy-2,3-dihydro-4H-chromen-4-one | C35 H30 O11 | 0 | 8306121.511 | 0 | 0 | 0 | 21789563.57 |
| 3 | 2-[(2R,6R)-6-Hydroxy-8,9-dimethoxy-1,2,6,6a,12,12a-hexahydrochromeno[3,4-b]furo[2,3-h]chromen-2-yl]-2-propen-1-yl beta-D-glucopyranoside | C29 H34 O12 | 0 | 0 | 0 | 3042679.286 | 0 | 0 |
| 4 | 2-Hydroxy-3-(5-hydroxy-7,8-dimethoxy-4-oxo-4H-chromen-2-yl)phenyl β-D-glucopyranoside | C23 H24 O12 | 0 | 0 | 0 | 0 | 0 | 10523645.49 |
| 5 | 2-{4-[(3-{[3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy]phenyl}-7-hydroxy-3,4-dihydro-2H-1-benzopyran-4-one | C26 H30 O13 | 9442446.512 | 0 | 0 | 10505424.34 | 0 | 0 |
| 6 | 3,5,7-trihydroxy-2-phenyl-4H-chromen-4-one | C15 H10 O5 | 0 | 0 | 0 | 0 | 8628171.198 | 0 |
| 7 | 5-hydroxy-2-phenyl-4H-chromen-4-one | C15 H10 O3 | 19554179.46 | 0 | 0 | 0 | 0 | 0 |
| 8 | 5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-6-methoxy-7-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one | C23 H24 O12 | 0 | 0 | 0 | 0 | 0 | 14982550.04 |
| 9 | 7-(beta-D-Glucopyranosyloxy)-5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-O-[(2E)-3-(3,4-dihydroxyphenyl)-2-propenoyl]-2-O-beta-D-glucopyranosyl-alpha-D-glucopyranoside | C42 H46 O24 | 0 | 0 | 0 | 8.546 | 0 | 0 |
| 10 | 5,7-DIHYDROXY-3',4',5'-TRIMETHOXYFLAVANONE | C18 H18 O7 | 0 | 0 | 0 | 0 | 11571372.81 | 8753584.275 |
| 11 | 5,7-dihydroxy-6-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one | C16 H14 O5 | 0 | 0 | 22346275.6 | 0 | 0 | 0 |
| 12 | Dracorubin | C32 H24 O5 | 0 | 0 | 0 | 4834974.748 | 0 | 0 |
| 13 | Diosmetin | C16 H12 O6 | 0 | 21211785.42 | 0 | 9917034.285 | 7747079.242 | 0 |
| 14 | 7-hydroxy-5-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one | C16 H14 O4 | 0 | 13935065.52 | 9814292.395 | 14560848.3 | 30311060.82 | 0 |
| 15 | 7-Chloro-2-(3,4-dimethoxyphenyl)-3,5,8-trihydroxy-6-methoxy-4H-chromen-4-one | C18 H15 Cl O8 | 7640870.785 | 0 | 0 | 0 | 0 | 0 |
| 16 | Chrysin | C15 H10 O4 | 26148980.01 | 38956374.31 | 0 | 14126740.53 | 129713525.7 | 67000900.02 |
| 17 | Isorhamnetin | C16 H12 O7 | 0 | 0 | 0 | 3852536.715 | 0 | 0 |
| 18 | Kaempferol | C42 H46 O23 | 0 | 0 | 0 | 2826848 | 0 | 2845155.632 |
| 19 | Pinocembrin 7-rhamnosylglucoside | C27 H32 O13 | 0 | 0 | 0 | 0 | 0 | 45890255.87 |
| 20 | Poncirin | C28 H34 O14 | 0 | 5752132.146 | 0 | 0 | 0 | 0 |
| 21 | Phloridzin | C21 H24 O10 | 0 | 2191239.178 | 0 | 0 | 0 | 0 |
| 22 | Naringin dihydrochalcone | C27 H34 O14 | 0 | 0 | 0 | 0 | 15205435.41 | 0 |
| 23 | Quercitrin | C21 H20 O11 | 0 | 28611546.36 | 7524189.09 | 0 | 0 | 0 |
| 24 | Tricin | C17 H14 O7 | 0 | 0 | 0 | 5622488.57 | 3574711.078 | 0 |
| 25 | (+/-)-Hesperetin | C16 H14 O6 | 0 | 0 | 42830311.69 | 0 | 0 | 0 |
| 26 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-{[(2S,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl]oxy}-4H-chromen-4-one | C20 H18 O11 | 0 | 0 | 0 | 10104100.39 | 0 | 6182190.025 |
| 27 | 2-(3,4-Dihydroxyphenyl)-5-hydroxy-6,7-dimethoxy-4-oxo-4H-chromen-3-yl beta-D-glucopyranoside | C23 H24 O13 | 0 | 0 | 0 | 0 | 11903080.83 | 0 |
| 28 | dalpatein | C18 H14 O7 | 22008103.07 | 0 | 0 | 15272943.66 | 0 | 0 |
| 29 | 7-hydroxy-3-phenyl-4H-chromen-4-one | C15 H10 O3 | 9571273.755 | 0 | 0 | 0 | 0 | 0 |
| 30 | Daidzein | C15 H10 O4 | 57942131.56 | 23675868.36 | 0 | 10.013 | 70266331.07 | 37775440.83 |
| 31 | ACETYLGLYCITIN | C24 H24 O11 | 0 | 0 | 0 | 0 | 5518454.121 | 0 |
| 32 | 4-Ethyl-7-hydroxy-3-(p-methoxyphenyl)coumarin | C18 H16 O4 | 0 | 7078142.529 | 0 | 0 | 0 | 0 |
| 33 | 3-(2-Hydroxy-4-methoxyphenyl)-8,8-dimethyl-2H,8H-pyrano[2,3-f]chromen-2-one | C21 H18 O5 | 0 | 0 | 6893890.999 | 0 | 0 | 7043057.133 |
|
|
|
| 34 | Medicarpin 3-O-glucoside-6'-malonate | C25 H26 O12 | 0 | 3167059.858 | 0 | 0 | 0 | 0 |

**Table S4.** Secondary metabolites in WGCNA modules.

|  |  |  |
| --- | --- | --- |
| **Modules** | **META ID** | **Metabolites name** |
| black | META12 | PEG n6 |
| black | META39 | NP-005474 |
| black | META64 | Bacancosin |
| black | META71 | 3,3â€²-Dithiobis[4,5-dihydro-2-methylfuran] |
| black | META77 | 2,3-Dinor-6-keto-PGF1 |
| black | META242 | Terodiline |
| black | META252 | Salicylic acid |
| black | META269 | Phenylglyoxylic acid |
| black | META285 | Norcapillene |
| black | META419 | 2-Hydroxy-3,4,5-trimethoxybenzoic acid |
| black | META449 | Dabigatran |
| black | META525 | Z-Gly-Pro |
| black | META556 | Tauropine |
| black | META583 | Phenylacetylglycine dimethylamide |
| black | META625 | N-Acetylleucylleucyltyrosinamide |
| black | META666 | Melagatran |
| black | META690 | Lombricine |
| black | META693 | L-Methionine sulfoxide |
| black | META700 | L-Glutamic acid |
| black | META710 | Leucyltryptophan |
| black | META724 | L-(-)-methionine |
| black | META725 | L-(-)-Asparagine |
| black | META748 | Glycyl-L-leucine |
| black | META753 | Glu-Glu |
| black | META754 | Glucosylgalactosyl hydroxylysine |
| black | META788 | DL-Arginine |
| black | META860 | 4-Carboxy-2-[(5-oxidanidyl-5-oxidanylidenenorvalyl)amino]butanoate |
| black | META878 | 2-amino-2,3,7-trideoxy-D-lyxo-hept-6-ulosonic acid |
| black | META947 | Cinnamic acid |
| black | META1038 | Oxagrelate |
| black | META1096 | 3-Methylsulfolene |
| black | META1171 | MFCD00045988 |
| black | META1198 | Hexadecanamide |
| black | META1231 | DG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/0:0) |
| black | META1317 | 16-Heptadecyne-1,2,4-triol |
| black | META1445 | Apigenin |
| black | META1590 | 1-Linoleoyl-2-Hydroxy-sn-glycero-3-PC |
| black | META1628 | 2,2-Bis(hydroxymethyl)propionic acid |
| black | META1669 | Sumatriptan |
| black | META1684 | 5-Methoxy-3-indoleaceate |
| black | META1824 | 2-Methoxynaphthalene |
| black | META1865 | Methyl mesylate |
| black | META1882 | Methylarsonic acid |
| black | META1898 | N,N-Diisopropylethylamine (DIPEA) |
| black | META1941 | Valerophenone |
| black | META1967 | PEG-4 |
| black | META1969 | PEG n7 |
| black | META2013 | intercept |
| black | META2037 | Furfural |
| black | META2063 | Deidaclin |
| black | META2066 | Damascenone |
| black | META2110 | 6-O-Phosphonohex-2-ulofuranose |
| black | META2114 | 5-methylthioribose |
| black | META2135 | 4,6,9-Trimethyl-3,5,8,10-tetraoxadodecane |
| black | META2168 | 1-Thio-beta-D-glucopyranose |
| black | META2255 | 4-Iodoanisole |
| black | META2277 | Hydroquinone |
| black | META2432 | Friedelin |
| black | META2438 | EN0350000 |
| black | META2446 | Diosgenin |
| black | META2448 | dehydroretinaldehyde |
| black | META2471 | all-trans-phytofluene |
| black | META2498 | 3-decaprenyl-4-hydroxy-5-methoxybenzoic acid |
| black | META2523 | 15-cis-4,4'-diapophytoene |
| black | META2559 | (+/-)-Camphor |
| black | META2560 | (+)-Nootkatone |
| black | META2617 | Nitrendipine |
| black | META2636 | Uridine |
| black | META2655 | Ethosuximide |
| black | META2797 | Campesterol |
| black | META2799 | Calcitriol |
| black | META2855 | (17beta)-4,4-Difluoro-17-hydroxy-17-methylandrost-5-en-3-one |
| black | META2881 | lymecycline |
| black | META2887 | EPTAZOCINE |
| black | META2888 | Acetyl hexamethyl tetralin |
| black | META2896 | 3,3',3''-[3,8,13,17-Tetrakis(carboxymethyl)-18-(3-hydroperoxy-3-oxopropyl)-2,7,12-porphyrintriyl]tripropanoic acid |
| black | META2900 | Vernolate |
| black | META2971 | (1R,2R,3S,6S,7R,9S,10S,11S,13R,14R)-11-(1-Hydroxy-2-propanyl)-3,7,10-trimethyl-15-oxapentacyclo[7.5.1.0-1,6-.0-7,13-.0-10,14-]pentadecane-2,6,9,11,13,14-hexol |
| blue | META03 | tp |
| blue | META16 | ON1225000 |
| blue | META22 | NP-019722 |
| blue | META55 | Meperidine-d5 |
| blue | META115 | NP-015559 |
| blue | META192 | Mitoxantrone |
| blue | META234 | Viminol |
| blue | META236 | Tyramine |
| blue | META321 | Hostmaniane |
| blue | META333 | Fenipentol |
| blue | META371 | BZ7175000 |
| blue | META386 | Benzaldehyde |
| blue | META422 | 2,6-di-tert-butylhydroquinone |
| blue | META494 | (-)-citrinin |
| blue | META510 | cis-1,2-dihydroxy-1,2-dihydrodibenzothiophene |
| blue | META520 | Amide C18 |
| blue | META577 | Piracetam |
| blue | META594 | Oxaceprol |
| blue | META624 | N-Acetyl-L-glutamic acid |
| blue | META630 | N6,N6,N6-Trimethyl-L-lysine |
| blue | META631 | N5-Dinitrophenyl-L-ornithine methyl ester |
| blue | META672 | Lysylvaline |
| blue | META685 | L-Pyroglutamic acid |
| blue | META704 | Leu-Val |
| blue | META707 | Leu-Leu |
| blue | META722 | L-(-)-Threonine |
| blue | META835 | anticapsin |
| blue | META858 | 4-Guanidinobutyric acid |
| blue | META862 | 4-[Amino(carboxy)methyl]-5-oxoproline |
| blue | META883 | 2,3,4,5-tetrahydrodipicolinic acid |
| blue | META889 | 1-Oxo-1,2,4-butanetricarboxylic acid |
| blue | META920 | (2R,5R,8S,13R,16S,19R)-19-{[(2R,3R,4R,5S,6R)-3-Acetamido-5-{[(2S,3R,4R,5S,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]oxy}-2-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4- yl]oxy}-8-(4-aminobutyl)-13-carboxy-2,5,16-trimethyl-4,7,10,15,18-pentaoxo-3,6,9,14,17-pentaazaicosan-1-oic acid |
| blue | META933 | Sinapinic acid |
| blue | META974 | (2E)-3-(3,4-Dimethoxyphenyl)acrylic acid |
| blue | META977 | Bis(4-ethylbenzylidene)sorbitol |
| blue | META997 | Heliettin |
| blue | META1040 | N'-[4-(trifluoromethyl)benzoyl]-6-quinoxalinecarbohydrazide |
| blue | META1095 | 2,5-Dimethyl-4-ethoxy-3(2H)-furanone |
| blue | META1108 | α-Linolenic acid |
| blue | META1109 | α-Eleostearic acid |
| blue | META1113 | VS1180000 |
| blue | META1117 | Undecanedioic acid |
| blue | META1130 | RI2735000 |
| blue | META1140 | PGF1? |
| blue | META1154 | O-beta-D-glucosyl-trans-zeatin |
| blue | META1181 | Linolenic acid ethyl ester |
| blue | META1185 | Linoelaidic Acid |
| blue | META1202 | glycidyl oleate |
| blue | META1249 | Bis(2-ethylhexyl)adipate |
| blue | META1259 | acetic acid geranyl ester |
| blue | META1291 | 3-[(15Z,19Z)-11,12-Dihydroxy-15,19-dotriacontadien-1-yl]-5-methyl-2(5H)-furanone |
| blue | META1314 | 1-Octadecyl (2Z)-2-butenedioate |
| blue | META1331 | 11-Aminoundecanoic acid |
| blue | META1333 | 10-Undecenoic acid |
| blue | META1344 | (all-Z)-20-hydroxy-5,8,11,14-Eicosatetraenoic acid |
| blue | META1411 | myricetin 3-O-beta-D-galactopyranoside |
| blue | META1432 | Eriodictyol |
| blue | META1482 | 3-{[(2S,3R,4S,5R,6R)-3,5-dihydroxy-6-(hydroxymethyl)-4-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}oxan-2-yl]oxy}-5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one |
| blue | META1528 | L-α-PALMITIN |
| blue | META1545 | 1,3-Dihydroxy-2-propanyl (7Z,10Z,13Z,16Z)-7,10,13,16-docosatetraenoate |
| blue | META1570 | DL-Dipalmitoylphosphatidylcholine |
| blue | META1587 | 1-Myristoyl-2-hydroxy-sn-glycero-3-PE |
| blue | META1594 | 1-heptadecanoyl-sn-glycero-3-phosphate |
| blue | META1599 | 1-(sn-glycero-3-phospho)-1D-myo-inositol |
| blue | META1607 | (2R)-1-{[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-3-hydroxy-2-propanyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate |
| blue | META1627 | 3-Hydroxysebacic acid |
| blue | META1651 | Adenine |
| blue | META1668 | trans-3-Indoleacrylic acid |
| blue | META1674 | Methyl 2,3-dihydro-3-hydroxy-2-oxo-1H-indole-3-acetate |
| blue | META1680 | DL-Tryptophan |
| blue | META1693 | Elaeokanine C |
| blue | META1739 | alpha-Ketoglutaric acid |
| blue | META1774 | Lariciresinol 4-O-glucoside |
| blue | META1788 | (-)-Lupinine |
| blue | META1897 | N,N-Dimethyldecylamine N-oxide |
| blue | META1904 | Hydrolyzed fumonisin B1 |
| blue | META1931 | (8E)-2-Amino-8-octadecene-1,3,4-triol |
| blue | META1981 | N-Acetyl-D-quinovosamine |
| blue | META2018 | Hexitol |
| blue | META2019 | Hexaric acid |
| blue | META2036 | Gamithromycin |
| blue | META2040 | Ethylvanillin isobutyrate |
| blue | META2115 | 5-Hydroxymethyl-2-furaldehyde |
| blue | META2142 | 3-Deoxy-D-manno-octulosonic acid |
| blue | META2157 | 2-Deoxyhexopyranose |
| blue | META2162 | 2,4-OCTADIENAL |
| blue | META2175 | 1-Deoxy-L-mannitol |
| blue | META2188 | (E,E)-2,4-Dodecadienal |
| blue | META2199 | (-)-Shikimic acid |
| blue | META2201 | 8561 |
| blue | META2206 | Phenmetrazine |
| blue | META2221 | Beauvericin |
| blue | META2253 | 8,9-Dimethoxy-2-(2-phenyldiazenyl)-3-(2-thienyl)-5,6-dihydropyrrolo[2,1-a]isoquinoline-1-carbonitrile |
| blue | META2307 | piscidic acid |
| blue | META2403 | Lupeol |
| blue | META2404 | Lupenone |
| blue | META2405 | loganate |
| blue | META2426 | Geranylacetone |
| blue | META2437 | ent-cassa-12,15-diene |
| blue | META2475 | adonirubin |
| blue | META2483 | 5-[5-(methoxycarbonyl)-5,8a-dimethyl-2-methylidene-decahydronaphthalen-1-yl]-3-methylpentanoic acid |
| blue | META2529 | (R)-tetraprenyl-beta-curcumene |
| blue | META2632 | 1-Piperideine |
| blue | META2694 | N-dodecanoylsphinganine |
| blue | META2756 | Medrogestone |
| blue | META2830 | 25-Azacholesterol |
| blue | META2833 | 20-alfa-Dhydrodydrogesterone |
| blue | META2930 | 1,3,5-Heptatriene |
| brown | META06 | PPG n8 |
| brown | META219 | ethylene thiourea |
| brown | META224 | 2-Methylthiazolidine |
| brown | META271 | Phenethylamine |
| brown | META286 | N-Desmethyl-loperamide |
| brown | META292 | N4-{4-[1-cyano-2-(2-pyridyl)vinyl]phenyl}-5-methyl-3-phenylisoxazole-4-carboxamide |
| brown | META394 | Acetanilide |
| brown | META414 | 3-(tert-Butyl)-N-[4-(2,3-dihydroimidazo[2,1-b][1,3]thiazol-6-yl)phenyl]-1-methyl-1H-pyrazole-5-carboxamide |
| brown | META493 | (3R)-8-hydroxy-3-(4-methoxyphenyl)-3,4-dihydro-1H-2-benzopyran-1-one |
| brown | META514 | DIMBOA |
| brown | META527 | VIRILON |
| brown | META528 | Vigabatrin |
| brown | META593 | oxiracetam |
| brown | META609 | nicotianamine |
| brown | META613 | N-feruloylglycine |
| brown | META660 | MFCD00025555 |
| brown | META669 | Mavik |
| brown | META673 | Lys-Pro |
| brown | META692 | L-Norleucine |
| brown | META703 | Levetiracetam |
| brown | META709 | leu-gln |
| brown | META726 | Isoleucine |
| brown | META783 | DL-Phenylalanine |
| brown | META785 | DL-Lysine |
| brown | META809 | Citric acid |
| brown | META831 | Arg-pro |
| brown | META836 | AMPA |
| brown | META844 | Acetylcadaverine |
| brown | META927 | Hexyl cinnamaldehyde |
| brown | META955 | 3-Methyl-2-butenyl caffeate |
| brown | META979 | Tasimelteon |
| brown | META993 | Maraniol |
| brown | META1052 | Eptapirone |
| brown | META1131 | RG5925700 |
| brown | META1132 | RG3715000 |
| brown | META1173 | Methyl linoleate |
| brown | META1175 | Methyl 15-cyanopentadecanoate |
| brown | META1208 | Falcarindiol |
| brown | META1223 | DL-Mevalonic acid |
| brown | META1270 | 5,6-DHET |
| brown | META1284 | 3-[(3-Hydroxyundecanoyl)oxy]-4-(trimethylammonio)butanoate |
| brown | META1303 | 2-Hydroxy-22-methyltetracosanoic acid |
| brown | META1322 | 13S-hydroxyoctadecadienoic acid |
| brown | META1364 | (12Z)-9,10,11-trihydroxyoctadec-12-enoic acid |
| brown | META1475 | 4',5,7-TRIMETHOXYFLAVONE |
| brown | META1500 | (2R)-5-hydroxy-7-methoxy-2-phenyl-3,4-dihydro-2H-1-benzopyran-4-one |
| brown | META1518 | Hexyl 2-furoate |
| brown | META1519 | Furaspor |
| brown | META1521 | 5-Formyl-2-furoic acid |
| brown | META1526 | Monoolein |
| brown | META1564 | MFCD00133435 |
| brown | META1567 | LysoPC(18:3(9Z,12Z,15Z)) |
| brown | META1577 | 1-Stearoyl-2-hydroxy-sn-glycero-3-PE |
| brown | META1620 | 2-(12-Tridecyn-1-yl)furan |
| brown | META1662 | Methyl 1-[(1S)-2,2-dimethyl-2,3-dihydro-1H-inden-1-yl]-1H-imidazole-5-carboxylate |
| brown | META1678 | haplophytine |
| brown | META1745 | 4-Methylene-2-oxoglutarate |
| brown | META1806 | NPPB |
| brown | META1827 | 2,6-Di-iso-propylnaphthalene |
| brown | META1856 | Triisobutyl phosphate |
| brown | META1861 | Dibutyl phosphate |
| brown | META1903 | Linoleoyl Ethanolamide |
| brown | META1913 | Diethanolamine |
| brown | META1955 | shrimp shell |
| brown | META1971 | o-Succinylbenzoate |
| brown | META1994 | MFCD00057515 |
| brown | META2008 | Kynurenine |
| brown | META2030 | glycerin |
| brown | META2048 | D-ribosylnicotinate |
| brown | META2085 | Bevenopran |
| brown | META2106 | Alanylclavam |
| brown | META2160 | 2-[(5Z)-5-tetradecenyl]cyclobutanone |
| brown | META2184 | 1-(6-Nonyl-3-pyridinyl)-1-decanone |
| brown | META2200 | (-)-3-dehydroshikimic acid |
| brown | META2251 | Ancymidol |
| brown | META2256 | 2444643WXK |
| brown | META2268 | p-Cresol |
| brown | META2282 | Eugenol |
| brown | META2283 | dopamine |
| brown | META2335 | Carfentanil |
| brown | META2385 | Phenol, 2-(3,7-dimethylocta-2,6-dienyl)- |
| brown | META2387 | p-cymene |
| brown | META2451 | Curcumene |
| brown | META2539 | (3S,5R,6S)-5,6-epoxy-3-hydroxy-5,6-dihydro-12'-apo-beta-caroten-12'-al |
| brown | META2548 | (2E,4E,6E,8E,10E,12E,14E)-15-(4-Hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl)-4,9,13-trimethyl-2,4,6,8,10,12,14-pentadecaheptaenal |
| brown | META2558 | (+/-)-Methoprene |
| brown | META2576 | 6,7-Dihydropteridine |
| brown | META2581 | (+)-Riboflavin |
| brown | META2601 | 6-(1-Hydroxyethyl)-3-(hydroxymethyl)-2,7-dioxabicyclo[4.1.0]hept-3-en-5-one |
| brown | META2623 | MA4000000 |
| brown | META2644 | 5,6-Dihydrothymidine |
| brown | META2680 | amquinate |
| brown | META2717 | Terminaline |
| brown | META2755 | Megestrol |
| brown | META2778 | Estra-1,3,5(10)-trien-3-ol |
| brown | META2789 | Desoxycorticosterone acetate |
| brown | META2803 | Androsterone glucuronide |
| brown | META2820 | 3-Methoxyestra-1,3,5(10),16-tetraene |
| brown | META2839 | 17,21-Dihydroxypregnenolone |
| brown | META2842 | .beta.-Estradiol |
| brown | META2851 | (25R)-3-Oxocholest-4-en-26-al |
| brown | META2966 | (1R,7R,10R)-4,10,11,11-Tetramethyl-3-methylenetricyclo[5.3.1.0-1,5-]undec-4-ene |
| cyan | META79 | 15,23-Dihydroxyspirost-5-en-3-yl hexopyranosyl-(1->2)hexopyranosyl-(1->4)hexopyranoside |
| cyan | META116 | NP-014789 |
| cyan | META229 | Perlapine |
| cyan | META309 | Mesalazine |
| cyan | META421 | 2-{3-[2-(1H-Imidazol-2-ylmethyl)-6-methoxyphenoxy]benzyl}-1H-imidazole |
| cyan | META512 | 202-791 |
| cyan | META534 | Valine |
| cyan | META540 | Tritace |
| cyan | META566 | saccharopine |
| cyan | META573 | pretyrosine |
| cyan | META578 | Piperacillin |
| cyan | META579 | Pipecolic acid |
| cyan | META677 | lys-gln |
| cyan | META678 | lys-asn |
| cyan | META711 | Leucylproline |
| cyan | META713 | L-dihydroanticapsin |
| cyan | META728 | Indoleacetylaspartate |
| cyan | META729 | Indole-3-acryloylglycine |
| cyan | META734 | Homo-L-arginine |
| cyan | META741 | H3HP-DO3A |
| cyan | META759 | gamma-Glutamyl-gamma-glutamylglutamic acid |
| cyan | META764 | Gabapentin |
| cyan | META771 | etifenin |
| cyan | META797 | D-(+)-Proline |
| cyan | META801 | CYCLO(-SER-TYR) |
| cyan | META850 | Aceglutamide |
| cyan | META876 | 2-Amino-4-[(3-aminopropyl)amino]butanoic acid |
| cyan | META945 | Ethyl cinnamate |
| cyan | META1030 | MFCD18783096 |
| cyan | META1118 | Traumatin |
| cyan | META1145 | Palmitoyl Serinol |
| cyan | META1150 | Palmitamide |
| cyan | META1158 | N,N-Bis(2-hydroxyethyl)dodecanamide |
| cyan | META1244 | Carboprost |
| cyan | META1273 | 4-(Trimethylammonio)-3-(undecanoyloxy)butanoate |
| cyan | META1324 | 13,14-dihydro Prostaglandin F1α |
| cyan | META1381 | Wogonin |
| cyan | META1388 | Scrophulein |
| cyan | META1433 | Efloxate |
| cyan | META1435 | DJ3013000 |
| cyan | META1455 | 5-hydroxy-6,7-dimethoxy-2-phenyl-4H-chromen-4-one |
| cyan | META1541 | 1-Stearoylglycerol |
| cyan | META1574 | 2-Hydroxy-3-(phosphonooxy)propyl (15Z)-15-tetracosenoate |
| cyan | META1582 | 1-Oleoyl-lysophosphatidic acid |
| cyan | META1713 | Formononetin |
| cyan | META1738 | Levulinic acid |
| cyan | META1750 | 2-Keto-glutaramic acid |
| cyan | META1896 | N-Methyldioctylamine |
| cyan | META1905 | histidinol |
| cyan | META1906 | galegine |
| cyan | META1911 | DL-Carnitine |
| cyan | META2113 | 5-O-methyl embelin |
| cyan | META2144 | 3-{[(2S,3R,4S,5S,6R)-6-({[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}methyl)-3,4,5-trihydroxyoxan-2-yl]oxy}-2-methyl-4H-pyran-4-one |
| cyan | META2217 | N-[(1S)-4-Carbamimidamido-1-carboxybutyl]asparaginylaspartic acid |
| cyan | META2478 | abietatriene |
| cyan | META2615 | Picolinic acid |
| cyan | META2627 | Ciclopirox |
| cyan | META2654 | Prolinamide |
| cyan | META2679 | arborinine |
| cyan | META2742 | Norethindrone |
| cyan | META2761 | Hydroxyprogesterone |
| cyan | META2763 | Hydrocortisone caproate |
| cyan | META2809 | Allopregnanolone |
| cyan | META2858 | Resveratrol-4'-O-Glucuronide |
| cyan | META2884 | benzquinamide |
| cyan | META2929 | 3-Allylcyclohexene |
| green | META40 | NP-005196 |
| green | META62 | Decarbamoyl-neosaxitoxin |
| green | META74 | 2-Methyl-4-oxo-3-[(2E)-2-penten-1-yl]-2-cyclopenten-1-yl hexopyranoside |
| green | META107 | NP-020139 |
| green | META174 | 5'-S-Methyl-5'-thioadenosine |
| green | META186 | kamassin |
| green | META202 | Megastachine |
| green | META208 | NI3400000 |
| green | META257 | p-Xylene |
| green | META262 | Propofol |
| green | META289 | n-Amylbenzene |
| green | META318 | imazamethabenz-methyl |
| green | META361 | Cumene |
| green | META398 | 5-carboxyvanillic acid |
| green | META425 | 2,4-Dimethylbenzaldehyde |
| green | META463 | bendiocarb |
| green | META474 | Stigmatellin Y |
| green | META480 | Flindersiachromone |
| green | META498 | prochlorperazine |
| green | META516 | Valpromide |
| green | META517 | Stearamide |
| green | META570 | Propamocarb |
| green | META626 | N-Acetylleucylleucylleucylleucyltyrosinamide |
| green | META655 | MFCD00672375 |
| green | META698 | L-Glutaminyl-L-proline |
| green | META723 | L-(-)-Serine |
| green | META751 | Glutaric acid |
| green | META814 | CAPTOPRIL-L-CYSTEINE |
| green | META815 | Capsi-amide |
| green | META895 | 1-(4-Amino-4-carboxybutanoyl)-2-piperidinecarboxylic acid |
| green | META938 | Paprazine |
| green | META972 | (2E)-3-(4-Hydroxyphenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide |
| green | META1089 | Vitamin C |
| green | META1111 | YQ2978400 |
| green | META1153 | Oleamide |
| green | META1182 | Linolenelaidic acid |
| green | META1240 | cis-5-Tetradecenoylcarnitine |
| green | META1263 | 9-Oxo-10(E),12(E)-octadecadienoic acid |
| green | META1269 | 8-[(Aminomethyl)sulfanyl]-6-sulfanyloctanoic acid |
| green | META1272 | 4-Hydroxynonenal |
| green | META1309 | 2,3-Bis(octanoyloxy)propanimidic acid |
| green | META1350 | (4S)-4-[(9Z,12Z,15Z)-9,12,15-Octadecatrienoyloxy]-4-(trimethylammonio)butanoate |
| green | META1352 | (3R)-4,4-Dimethyl-2-oxotetrahydro-3-furanyl beta-D-glucopyranoside |
| green | META1373 | (−)-trans-Methyl dihydrojasmonate |
| green | META1412 | Myricetin |
| green | META1458 | 5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-7-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one |
| green | META1473 | 5,7-dihydroxy-2-(3-hydroxy-4-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phenyl)-4H-chromen-4-one |
| green | META1498 | 1-(2,4-dihydroxyphenyl)-2-(3,5-dimethoxyphenyl)propan-1-one |
| green | META1598 | 1,2-Dioleoyl-sn-glycero-3-PE |
| green | META1641 | Propentofylline |
| green | META1656 | 4-Oxo-4-(1H-purin-6-ylamino)butanoic acid |
| green | META1712 | Genistein |
| green | META1736 | OI1695000 |
| green | META1749 | 2-Oxobutyric acid |
| green | META1787 | 3-{(1R,9S)-6-Oxo-11-[4-(2-pyridinyl)benzyl]-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-5-yl}benzonitrile |
| green | META1831 | 1,1,6-Trimethyl-1,2-dihydronaphthalene |
| green | META1847 | N,N'-Dicyclohexylurea |
| green | META1885 | THREO-SPHINGOSINE, (-)- |
| green | META1887 | Stearoylethanolamide |
| green | META1935 | ZMP |
| green | META1958 | S-(-)-Cathinone |
| green | META2148 | 3,5-di-tert-Butyl-4-hydroxybenzaldehyde |
| green | META2205 | Tridemorph |
| green | META2218 | Homoanserine |
| green | META2241 | kresoxim-methyl |
| green | META2270 | Paracetamol |
| green | META2275 | Mesitol |
| green | META2311 | Ibuprofen |
| green | META2349 | EUPATORIOCHROMENE |
| green | META2386 | Phaseic acid |
| green | META2424 | gibberellin A53 |
| green | META2439 | Echinenone |
| green | META2440 | ecabet |
| green | META2443 | D-α-Tocopherol |
| green | META2454 | Crocetin |
| green | META2489 | 4-[(2-Isopropyl-5-methylcyclohexyl)oxy]-4-oxobutanoic acid |
| green | META2495 | 4-(1,2-Dihydroxy-2-propanyl)-1-methyl-1,2-cyclohexanediol |
| green | META2526 | 10'-apo-beta-carotenal |
| green | META2561 | (+)-Gibberellic acid |
| green | META2595 | 2-Aminoadenosine |
| green | META2629 | 5'-O-beta-D-Glucosylpyridoxine |
| green | META2659 | 1-(14-methylhexadecanoyl)pyrrolidine |
| green | META2685 | (+)-2,7-Dideoxypancratistatin |
| green | META2723 | Quingestanol acetate |
| green | META2749 | MFCD00057815 |
| green | META2750 | MFCD00010474 |
| green | META2777 | Estra-1,3,5(10)-trien-3-yl hydrogen sulfate |
| greenyellow | META49 | MFCD00870472 |
| greenyellow | META84 | 1,2-Dideoxy-3-C-methyl-1-(2,5,5,8a-tetramethyl-1,4,4a,5,6,7,8,8a-octahydro-1-naphthalenyl)pentitol |
| greenyellow | META111 | NP-018660 |
| greenyellow | META147 | Methyl 1-(hexopyranosyloxy)-5-hydroxy-7-(hydroxymethyl)-1,4a,5,7a-tetrahydrocyclopenta[c]pyran-4-carboxylate |
| greenyellow | META167 | 1-Stearoyl lysophosphatidic acid |
| greenyellow | META213 | 2-Ethyl-4,5-dimethylthiazole |
| greenyellow | META232 | XT2570000 |
| greenyellow | META240 | TI1100000 |
| greenyellow | META282 | Octyl hydrogen phthalate |
| greenyellow | META376 | Bis(2-ethylhexyl) phthalate |
| greenyellow | META435 | 1,4-Di-tert-butylbenzene |
| greenyellow | META740 | hercynine |
| greenyellow | META832 | arg-leu |
| greenyellow | META996 | hymecromone |
| greenyellow | META1053 | CP-642931 |
| greenyellow | META1061 | Uracil |
| greenyellow | META1066 | primidone |
| greenyellow | META1076 | Cytosine |
| greenyellow | META1094 | 2-O-ETHYL ASCORBIC ACID |
| greenyellow | META1116 | UNII:74D1OHC38H |
| greenyellow | META1124 | Stearidonic acid |
| greenyellow | META1148 | Palmitelaidic acid methyl ester |
| greenyellow | META1178 | Maleamic acid |
| greenyellow | META1179 | MACAMIDE 1 |
| greenyellow | META1201 | Glycidyl Stearate |
| greenyellow | META1255 | Amide C22 |
| greenyellow | META1261 | 9S,13R-12-Oxophytodienoic acid |
| greenyellow | META1294 | 3-(acetamidomethylidene)-2-(hydroxymethyl)succinic acid |
| greenyellow | META1299 | 2-Hydroxyethyl 12-hydroxyoctadecanoate |
| greenyellow | META1312 | 2-(2-Carboxyethyl)-4-methyl-5-pentyl-3-furoic acid |
| greenyellow | META1316 | 1-Linoleoyl glycerol |
| greenyellow | META1326 | 13(S)-HpOTrE |
| greenyellow | META1353 | (3aR,4R,5R,6aS)-5-Hydroxy-4-[(1E,3S)-3-hydroxy-1-octen-1-yl]hexahydro-2H-cyclopenta[b]furan-2-one |
| greenyellow | META1394 | Rhamnetin |
| greenyellow | META1397 | Quercetin-3β-D-glucoside |
| greenyellow | META1470 | 5,7-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one |
| greenyellow | META1503 | (±)-Naringenin |
| greenyellow | META1523 | 2,5-Furandicarboxylic acid |
| greenyellow | META1562 | O-{[(2R)-2-[(7Z,10Z,13Z,16Z)-7,10,13,16-Docosatetraenoyloxy]-3-(pentadecanoyloxy)propoxy](hydroxy)phosphoryl}-L-serine |
| greenyellow | META1646 | Hypoxanthin |
| greenyellow | META1773 | (+/-)-C75 |
| greenyellow | META1855 | Tris(2-chloroethyl) phosphate |
| greenyellow | META1910 | D-Sphingosine |
| greenyellow | META1917 | Choline |
| greenyellow | META2111 | 6-O-Phosphono-D-gluconic acid |
| greenyellow | META2134 | 4,6-Henicosanedione |
| greenyellow | META2226 | Noroxycodone-d3 |
| greenyellow | META2334 | lamtidine |
| greenyellow | META2350 | DL-TYROSINE |
| greenyellow | META2423 | gibberellin A7 |
| greenyellow | META2441 | Ebelactone B |
| greenyellow | META2482 | 5-[5-hydroxy-3-(hydroxymethyl)pentyl]-8a-(hydroxymethyl)-5,6-dimethyl-3,4,4a,5,6,7,8,8a-octahydronaphthalene-1-carboxylic acid |
| greenyellow | META2491 | 4,8,12-trimethyltrideca 1,3,7,11-tetraene |
| greenyellow | META2513 | 2,6,10,14,18,22,26,30-Dotriacontaoctaen-1-ol, 3,7,11,15,19,23,27,31-octamethyl-, (all-E)- |
| greenyellow | META2562 | (+)-geniposide |
| greenyellow | META2565 | (.+-.)-Limonene |
| greenyellow | META2592 | 8-hydroxy-deoxyguanosine |
| greenyellow | META2594 | 2'-Deoxyadenosine |
| greenyellow | META2648 | Uridine 5'-diphosphogalactose |
| greenyellow | META2677 | Cinchophen |
| greenyellow | META2696 | CERAMIDE 3 |
| greenyellow | META2698 | C16-Dihydroceramide |
| greenyellow | META2699 | C14-Dihydroceramide |
| greenyellow | META2710 | Tetrahydrodeoxycorticosterone |
| greenyellow | META2774 | Estrane |
| greenyellow | META2787 | doxercalciferol |
| greenyellow | META2819 | 4,6-CHOLESTADIEN-3-ONE |
| greenyellow | META2847 | (3beta,24R,24'R)-fucosterol epoxide |
| greenyellow | META2852 | (22S)-22-hydroxycampest-4-en-3-one |
| greenyellow | META2853 | (22R,23R,24S)-22,23-Dihydroxyergost-4-en-3-one |
| greenyellow | META2885 | Tetralin |
| greenyellow | META2893 | Pheophorbide A |
| greenyellow | META2931 | 1,2,3,4-Tetramethyl-1,3-cyclopentadiene |
| grey | META124 | NP-000924 |
| grey | META168 | LU3453000 |
| grey | META227 | oxazolidinone |
| grey | META358 | Cyclopentynafil |
| grey | META404 | 4-Methoxybenzaldehyde |
| grey | META490 | 2,2-Dimethyl-8-prenylchromene 6-carboxylic acid |
| grey | META533 | Val-Ser |
| grey | META576 | Pivagabine |
| grey | META622 | N-Acetyl-L-leucine |
| grey | META627 | N-Acetyl-L-aspartic acid |
| grey | META636 | N-[(1-{[(3E,9E)-5-Isopropyl-2,7-dioxo-1,6-diazacyclododeca-3,9-dien-8-yl]amino}-3-methyl-1-oxo-2-butanyl)carbamoyl]valine |
| grey | META643 | N(6)-[(indol-3-yl)acetyl]-L-lysine |
| grey | META682 | L-threo-3-Phenylserine |
| grey | META702 | L-gamma-Glutamyl-L-leucine |
| grey | META745 | Gly-Leu |
| grey | META765 | fructosylglycine |
| grey | META777 | epsilon-(gamma-Glutamyl)-lysine |
| grey | META786 | DL-Glutamic acid |
| grey | META799 | Cystathionine ketimine |
| grey | META882 | 2-[(2-Amino-2-carboxyethyl)thio]butanedioic acid |
| grey | META911 | (2S,4R,9a'S)-1'-Hydroxy-4-{2-[(1S)-1-hydroxyethyl]-4-oxo-3(4H)-quinazolinyl}-2',2'-dimethyl-1',9a'-dihydro-3H-spiro[furan-2,9'-imidazo[1,2-a]indole]-3',5(2'H,4H)-dione |
| grey | META985 | Phenprocoumon |
| grey | META1010 | 8-[(3,3-Dimethyl-2-oxiranyl)methyl]-7-methoxy-2H-chromen-2-one |
| grey | META1063 | Thymine |
| grey | META1112 | YD4593000 |
| grey | META1174 | Methyl Jasmonate |
| grey | META1258 | Acetylcarnitine |
| grey | META1319 | 15S-hydroxyeicosatrienoic acid |
| grey | META1430 | Hispidulin |
| grey | META1543 | 1-Oleoyl-rac-glycerol |
| grey | META1556 | Platelet-activating factor |
| grey | META1560 | PC(18:3(9Z,12Z,15Z)/18:2(9Z,12Z)) |
| grey | META1600 | (2R)-3-{[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl pentadecanoate |
| grey | META1623 | MFCD00070502 |
| grey | META1624 | Ethyl malate |
| grey | META1657 | 3-Methyladenine |
| grey | META1835 | 8WWZ0E633P |
| grey | META1842 | diethyl oxalpropionate |
| grey | META1891 | porphobilinogen |
| grey | META2083 | bis-beta-D-fructofuranose 1,2':2,3'-dianhydride |
| grey | META2186 | .alpha.-Glucoheptitol |
| grey | META2298 | 3,4-Dihydroxyphenylglycol |
| grey | META2317 | Camostat |
| grey | META2331 | Nipecotic acid |
| grey | META2392 | MM0335000 |
| grey | META2528 | 1,1',2,2',7',8'-Hexahydro-psi,psi-carotene-1,1'-diol |
| grey | META2541 | (3S)-5-[(4aR,8aS)-2,5,5,8a-Tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid |
| grey | META2640 | Edoxudine |
| grey | META2785 | Drostanolone propionate |
| grey | META2823 | 3b-Hydroxy-5-cholenoic acid |
| grey | META2925 | Allylcyclohexane |
| grey60 | META41 | NP-003294 |
| grey60 | META92 | (3beta,8xi,9xi,17xi,20S,22E,24R)-24-Methyl-9,19-cyclolanosta-22,25-dien-3-ol |
| grey60 | META135 | Phenethyl Î²-primeveroside |
| grey60 | META230 | Desipramine |
| grey60 | META301 | Mibampator |
| grey60 | META675 | lys-leu |
| grey60 | META780 | EDDA |
| grey60 | META834 | APM |
| grey60 | META879 | 2-Acetamido-2-deoxy-D-gluconolactone |
| grey60 | META910 | (2S,4S)-4-Amino-2-hydroxy-2-methylpentanedioic acid |
| grey60 | META1060 | Veronal |
| grey60 | META1219 | Docosatetraenoic acid |
| grey60 | META1224 | Dimethyl sebacate |
| grey60 | META1230 | Dihomo-gamma-linolenic acid |
| grey60 | META1256 | Adipic acid |
| grey60 | META1339 | 1,3-dilinolenoylglycerol |
| grey60 | META1361 | (2E)-3-Phenyl-2-propen-1-yl 6-O-beta-D-arabinofuranosyl-beta-D-glucopyranoside |
| grey60 | META1405 | Pectolinarigenin |
| grey60 | META1450 | 7-{[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}oxan-2-yl]oxy}-5-hydroxy-2-(4-hydroxyphenyl)-3-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-({[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}methyl)oxan-2-yl]oxy}-4H-chromen-4-one |
| grey60 | META1477 | 3-Methoxy-5,7,3',4'-tetrahydroxy-flavone |
| grey60 | META1517 | LV1850000 |
| grey60 | META1536 | 3-O-beta-D-galactosyl-sn-glycerol |
| grey60 | META1610 | (2R)-1-(Pentadecanoyloxy)-3-(phosphonooxy)-2-propanyl docosanoate |
| grey60 | META1663 | Indane |
| grey60 | META1695 | (+)-castanospermine |
| grey60 | META1704 | olmelin |
| grey60 | META1707 | IN00295 |
| grey60 | META1784 | Isoliquiritigenin |
| grey60 | META1800 | 3-O-(alpha-L-oleandrosyl)oleandolide |
| grey60 | META1875 | 2-methoxyacetaminophen sulfate |
| grey60 | META1932 | (3Z,6E)-N-Hydroxy-2,4,4,7-tetramethyl-6,8-nonadien-3-imine |
| grey60 | META2035 | Gentiopicrin |
| grey60 | META2068 | D-(+)-Maltose |
| grey60 | META2107 | AF4878000 |
| grey60 | META2161 | 2,6-Dideoxy-3-O-methyl-L-arabino-hexopyranose |
| grey60 | META2185 | [(3S,3aR,5aR,7Z,11E,14aR,14bR)-3-Isopropenyl-5a,12,14b-trimethyl-1,2,3,3a,4,5,5a,6,9,10,13,14,14a,14b-tetradecahydrocycloundeca[e]inden-8-yl]methanol |
| grey60 | META2234 | trans-Anethole |
| grey60 | META2262 | Vanillyl mandelic acid |
| grey60 | META2276 | Kukoamine A |
| grey60 | META2415 | Hecogenin |
| grey60 | META2477 | Abietic acid |
| grey60 | META2479 | 7-Isopropyl-4a-methyl-1-methylene-1,2,3,4,4a,9,10,10a-octahydrophenanthrene |
| grey60 | META2493 | 4-(4-hydroxy-2,6,6-trimethyl-3-{[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}cyclohex-1-en-1-yl)butan-2-one |
| grey60 | META2578 | 1-Hydroxy-1-[(6R)-4-hydroxy-2-imino-1,2,5,6,7,8-hexahydro-6-pteridinyl]-2-propanyl beta-D-glucopyranoside |
| grey60 | META2625 | Isoniazid |
| grey60 | META2646 | 1-Pentofuranosyl-2,4(1H,3H)-pyrimidinedione |
| grey60 | META2705 | Typhasterol |
| grey60 | META2719 | Sitosterol |
| grey60 | META2726 | Progesterone |
| grey60 | META2808 | allylestrenol |
| grey60 | META2837 | 17beta-Methylestra-1,3,5(10)-trien-3-ol |
| lightcyan | META14 | PC |
| lightcyan | META119 | NP-005013 |
| lightcyan | META141 | NP-013285 |
| lightcyan | META290 | Nafenopin |
| lightcyan | META596 | ophthalmic acid |
| lightcyan | META602 | N-Pentacosanoylglycine |
| lightcyan | META718 | L-Alanyl-3-{[(3-carbamoyl-2-oxiranyl)carbonyl]amino}-L-alanine |
| lightcyan | META822 | Boc-Asn-Oh |
| lightcyan | META847 | ACETYL PROLINE |
| lightcyan | META881 | 2-[3-carboxylato-3-(methylammonio)propyl]-L-histidine dizwitterion |
| lightcyan | META926 | Flavokawain A |
| lightcyan | META1006 | Byakangelicol |
| lightcyan | META1009 | Aesculin |
| lightcyan | META1092 | 4-Hydroxy-5-methylfuran-3(2H)-one |
| lightcyan | META1121 | Thapsic acid |
| lightcyan | META1172 | Methyl undec-10-enoate |
| lightcyan | META1190 | Lauramide |
| lightcyan | META1213 | Erucamide |
| lightcyan | META1215 | Eicosapentanoic acid |
| lightcyan | META1246 | C10-Carnitine |
| lightcyan | META1359 | (2E,4Z)-N-Isobutyl-2,4-octadecadienamide |
| lightcyan | META1360 | (2E,4E,12Z)-N-Isobutyl-2,4,12-octadecatrienamide |
| lightcyan | META1362 | (2E)-2-Tridecene-4,6,8-triyn-1-ol |
| lightcyan | META1392 | Robinetin |
| lightcyan | META1409 | Naringin |
| lightcyan | META1422 | Kaempferitrin |
| lightcyan | META1566 | Lysophosphatidylinositol |
| lightcyan | META1636 | Tonapofylline |
| lightcyan | META1730 | 1-Isothiocyanato-7-(methylthio)heptane |
| lightcyan | META1761 | Cefepime |
| lightcyan | META1783 | 1-(2,4-Dihydroxy-6-methoxy-3,5-dimethylphenyl)-3-phenyl-1-propanone |
| lightcyan | META1912 | dinotefuran |
| lightcyan | META1968 | PEG n8 |
| lightcyan | META2012 | Isophorone |
| lightcyan | META2054 | Dihydrojasmone |
| lightcyan | META2064 | dehypoxanthine futalosine |
| lightcyan | META2289 | adrenaline |
| lightcyan | META2410 | Î¾-Carotene |
| lightcyan | META2452 | Cuminaldehyde |
| lightcyan | META2453 | Cuauhtemone |
| lightcyan | META2470 | all-trans-retinal |
| lightcyan | META2593 | 5'-O-Carboxyinosine |
| lightcyan | META2720 | samandarone |
| lightcyan | META2821 | 3-dehydro-6-deoxoteasterone |
| lightcyan | META2824 | 3beta-hydroxy-4beta-methyl-5alpha-cholest-7-ene-4alpha-carboxylic acid |
| lightcyan | META2831 | 24-methylenecycloartanol |
| lightcyan | META2843 | (6beta,8xi,11beta,14xi,16alpha)-9-Fluoro-6,11,17,21-tetrahydroxy-16-methylpregna-1,4-diene-3,20-dione |
| lightcyan | META2911 | melamine |
| lightcyan | META2913 | Cyromazine |
| lightcyan | META2924 | BIISOCROTYL |
| lightcyan | META2939 | N-2--(Carboxymethyl)arginine |
| lightgreen | META101 | (11cis,13cis,13'cis)-1,2,7,7',8,8',11',12'-Octahydro-1,2-epoxy-psi,psi-carotene |
| lightgreen | META120 | NP-004549 |
| lightgreen | META122 | NP-001216 |
| lightgreen | META283 | n-Propyl GalIate |
| lightgreen | META402 | 4-Nitroaniline |
| lightgreen | META433 | 2-((4-Nitrophenoxy)methyl)oxirane |
| lightgreen | META437 | 1-(4-benzhydrylpiperazino)-3-[4-(1,2,3-thiadiazol-4-yl)phenoxy]-2-propanol |
| lightgreen | META507 | 2-Hydroxybenzothiazole |
| lightgreen | META608 | nitrilotriacetic acid |
| lightgreen | META654 | MFCD01320532 |
| lightgreen | META816 | Capryloylglycine |
| lightgreen | META820 | Brivaracetam |
| lightgreen | META872 | 2JXY218SZI |
| lightgreen | META877 | 2-amino-3-carboxymuconic acid semialdehyde |
| lightgreen | META886 | 2-(3-Hydroxy-3,4,5,6-tetrahydro-1H-cyclopenta[c]furan-4-yl)-3-methoxy-3-oxopropanoic acid |
| lightgreen | META887 | 2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid |
| lightgreen | META948 | Caffeic acid phenethyl ester |
| lightgreen | META995 | Imperatorin |
| lightgreen | META1164 | MFCD03411993 |
| lightgreen | META1200 | Glycol stearate |
| lightgreen | META1320 | 15,16-DiHODE |
| lightgreen | META1357 | (2R,3R,4S,5S,6R)-2-{[4-(4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-yl]oxy}-6-(hydroxymethyl)oxane-3,4,5-triol |
| lightgreen | META1513 | 2(3H)-Furanone, dihydro-3,4-divanillyl- |
| lightgreen | META1520 | 5-Hydroxy-2-furoic acid |
| lightgreen | META1647 | Guanine |
| lightgreen | META1744 | 5-guanidino-2-oxopentanoic acid |
| lightgreen | META1748 | 3,5-Dioxooctanedioic acid |
| lightgreen | META1805 | (5E,7E,10R,12R,13E,16R,17R,18S,22S)-22-Ethyl-10,12,16,18-tetrahydroxy-17-methyloxacyclodocosa-3,5,7,13-tetraen-2-one |
| lightgreen | META1838 | Phosphoric acid |
| lightgreen | META1843 | Dibutyl malate |
| lightgreen | META1929 | 1,1-Diethyl-3-oxo-2-triazanolate |
| lightgreen | META1959 | RV0540000 |
| lightgreen | META1989 | MJ9700000 |
| lightgreen | META2042 | Ethanal tetramer |
| lightgreen | META2047 | D-Saccharic acid |
| lightgreen | META2051 | Dipropylene glycol dimethyl ether |
| lightgreen | META2055 | Diethylene glycol |
| lightgreen | META2092 | benzoquinone |
| lightgreen | META2121 | 4-Oxocyclohexanecarboxylic acid |
| lightgreen | META2300 | 2-Methoxy-phloroglucinol |
| lightgreen | META2319 | (+)-dihydromethysticin |
| lightgreen | META2366 | UD3357700 |
| lightgreen | META2378 | Reduced Vitamin K |
| lightgreen | META2588 | Guanosine |
| lightgreen | META2602 | 2,6-Dimethyl-γ-pyrone |
| lightgreen | META2642 | Cytarabine |
| lightgreen | META2657 | 1-Vinyl-2-pyrrolidone |
| lightgreen | META2672 | Kynurenic acid |
| lightyellow | META56 | KG7967000 |
| lightyellow | META210 | doramapimod |
| lightyellow | META362 | CU8460000 |
| lightyellow | META440 | (Z)-Hex-3-enyl benzoate |
| lightyellow | META515 | Irinotecan |
| lightyellow | META543 | Tricine |
| lightyellow | META545 | tranexamic acid |
| lightyellow | META650 | Mimosine |
| lightyellow | META793 | dihydroxyphenylalanine |
| lightyellow | META936 | Phaseolic acid |
| lightyellow | META1163 | MFCD05863969 |
| lightyellow | META1205 | g-Butyrobetaine |
| lightyellow | META1234 | delta-guanidinovaleric acid |
| lightyellow | META1236 | Daminozide |
| lightyellow | META1241 | cis-12-Octadecenoic acid methyl ester |
| lightyellow | META1387 | Tangeritin |
| lightyellow | META1427 | IN00488 |
| lightyellow | META1428 | IN00150 |
| lightyellow | META1442 | Casticin |
| lightyellow | META1462 | 5,8-dihydroxy-2-(4-hydroxyphenyl)-7-methoxy-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}-4H-chromen-4-one |
| lightyellow | META1511 | 4,4'-(3,4-Dimethyltetrahydrofuran-2,5-diyl)bis(2-methoxyphenol) |
| lightyellow | META1515 | Payzone |
| lightyellow | META1532 | DIBEHENIN |
| lightyellow | META1539 | 2-Hydroxyfelbamate |
| lightyellow | META1568 | L-alpha-lysophosphatidylcholine |
| lightyellow | META1583 | 1-oleoyl-2-linoleyl-sn-glycero-3-phosphoethanolamine |
| lightyellow | META1659 | Temozolomide |
| lightyellow | META1819 | lawsone |
| lightyellow | META1826 | 2,6-DIMETHYLNAPHTHALENE |
| lightyellow | META1934 | α-Lactose |
| lightyellow | META2000 | Melonal |
| lightyellow | META2091 | Benzoyl glucuronide |
| lightyellow | META2140 | 3-O-feruloyl-D-quinic acid |
| lightyellow | META2244 | guaietolin |
| lightyellow | META2257 | 2-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol |
| lightyellow | META2266 | Shogaol |
| lightyellow | META2374 | RG5927903 |
| lightyellow | META2381 | p-menth-3-ene |
| lightyellow | META2393 | Militarinone A |
| lightyellow | META2480 | 7-deoxyloganin |
| lightyellow | META2487 | 4beta-methylzymosterol-4-carbaldehyde |
| lightyellow | META2609 | streptonigrin |
| lightyellow | META2656 | 2-Pyrrolidone |
| lightyellow | META2716 | Testosterone |
| lightyellow | META2772 | ethylestrenol |
| lightyellow | META2773 | Estriol |
| lightyellow | META2825 | 3a,7a-Dihydroxycholanoic acid |
| magenta | META21 | NP-019725 |
| magenta | META125 | NP-000587 |
| magenta | META158 | 3Î±,7Î±-Dihydroxy-5Î²-cholestanoic acid |
| magenta | META217 | trimethadione |
| magenta | META279 | ortho-Phthalaldehyde |
| magenta | META293 | N'2-[3-(trifluoromethyl)benzoyl]-5-(trifluoromethyl)pyridine-2-carbohydrazonamide |
| magenta | META350 | Dieugenol |
| magenta | META357 | DA9185000 |
| magenta | META379 | Benzyl succinate |
| magenta | META380 | Benzyl isobutyl ketone |
| magenta | META382 | Benzyl butyl phthalate |
| magenta | META406 | 4-Dodecylbenzenesulfonic acid |
| magenta | META408 | 4-Aminophenol |
| magenta | META475 | Precocene II |
| magenta | META481 | Eugenitin |
| magenta | META535 | val-arg |
| magenta | META634 | N2-Succinyl-L-glutamic acid 5-semialdehyde |
| magenta | META774 | Ethyl acetate |
| magenta | META792 | dilauroyl peroxide |
| magenta | META842 | Actinonin |
| magenta | META863 | 4-[(E)-2-{[2-(4-Hydroxyphenyl)ethyl]amino}vinyl]-2,3-dihydro-2,6-pyridinedicarboxylic acid |
| magenta | META871 | 2-methylcitric acid |
| magenta | META902 | (E)-2-[(2S)-2-Amino-2-carboxyethoxy]-2-hydroxyethenediazonium |
| magenta | META949 | Caffeic acid |
| magenta | META986 | phellopterin |
| magenta | META987 | Oxypeucedanin |
| magenta | META1000 | Esculetin |
| magenta | META1004 | Coumarin |
| magenta | META1013 | 7-Hydroxy-6-methoxy-2-oxo-2H-chromen-8-yl beta-D-allopyranoside |
| magenta | META1028 | Tetrahydrocurcumin |
| magenta | META1031 | Curcumin |
| magenta | META1075 | Dihydrothymine |
| magenta | META1078 | cis-Cycothiamine |
| magenta | META1098 | lactide |
| magenta | META1114 | VS1150000 |
| magenta | META1165 | MFCD00209536 |
| magenta | META1209 | Ethyl oleate |
| magenta | META1277 | 3-Hydroxytridecanoic acid |
| magenta | META1341 | 1,2-Dilinoleoyl-sn-glycerol |
| magenta | META1358 | (2E,6Z)-N-Ethyl-2,6-nonadienamide |
| magenta | META1479 | 3-{[4,5-dihydroxy-6-(hydroxymethyl)-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}oxan-2-yl]oxy}-5-hydroxy-2-(4-hydroxyphenyl)-7-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}-4H-chromen-4-one |
| magenta | META1490 | 2-(4-Hydroxyphenyl)-5,6,7,8-tetramethoxy-2,3-dihydro-4H-chromen-4-one |
| magenta | META1709 | Glycitein |
| magenta | META1734 | Succinylacetone |
| magenta | META1822 | Acetylshikonin |
| magenta | META1864 | 1-(1H-Imidazol-5-yl)-3-(phosphonooxy)-2-propanone |
| magenta | META1888 | sphinganine |
| magenta | META1976 | Neochlorogenic acid |
| magenta | META1991 | MFCD08277028 |
| magenta | META1992 | MFCD00801046 |
| magenta | META2006 | Linamarin |
| magenta | META2058 | diacetylphloroglucinol |
| magenta | META2070 | D-(-)-Quinic acid |
| magenta | META2077 | Chlorogenic acid |
| magenta | META2100 | Apocynin |
| magenta | META2118 | 5-[(E)-2-Carboxyvinyl]-2-hydroxyphenyl beta-D-glucopyranosiduronic acid |
| magenta | META2124 | 4'-Methoxyacetophenone |
| magenta | META2187 | (Z)-desulfoglucotropeolin |
| magenta | META2189 | (3R,5R)-1,3,5-Trihydroxy-4-{[(2E)-3-(4-hydroxy-3-methoxyphenyl)-2-propenoyl]oxy}cyclohexanecarboxylic acid |
| magenta | META2195 | (1S,3R,4R,5R)-1,3,4-trihydroxy-5-{[(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxy}cyclohexane-1-carboxylic acid |
| magenta | META2197 | (1r,3R,4s,5S)-4-{[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy}-1,3,5-trihydroxycyclohexane-1-carboxylic acid |
| magenta | META2230 | 1â€²-Acetoxyeugenol acetate |
| magenta | META2239 | methocarbamol |
| magenta | META2346 | MUD |
| magenta | META2356 | ARECOLINE |
| magenta | META2420 | gitogenin |
| magenta | META2473 | Allamandin |
| magenta | META2531 | (all-E)-Phytoene |
| magenta | META2600 | Butopyronoxyl |
| magenta | META2661 | Ulodesine |
| magenta | META2734 | Petromyzonol |
| magenta | META2739 | Norgestrel |
| magenta | META2745 | Nandrolone phenpropionate |
| magenta | META2926 | 5-Ethyl-3,8-dimethyl-1,7-dihydroazulene |
| midnightblue | META10 | p-Isopropyl-α-methylstyrene |
| midnightblue | META75 | 2-Hydroxy-4-[(1R)-1-hydroxy-2-(methylamino)ethyl]phenyl Î²-D-glucopyranosiduronic acid |
| midnightblue | META87 | [3-(Hydroxymethyl)-3-methyl-2-oxobicyclo[2.2.1]hept-1-yl]methyl hexopyranoside |
| midnightblue | META109 | NP-019483 |
| midnightblue | META129 | 3-[14-Ethyl-13-formyl-21-(methoxycarbonyl)-4,8,18-trimethyl-20-oxo-9-vinyl-3-phorbinyl]propanoic acid |
| midnightblue | META159 | 3-[2-(β-D-Glucopyranosyloxy)-4-methoxyphenyl]propanoic acid |
| midnightblue | META218 | imicyafos |
| midnightblue | META320 | Hydroxy vardenafil |
| midnightblue | META323 | Hexylbenzene |
| midnightblue | META336 | Ethopabate |
| midnightblue | META347 | Diisodecyl phthalate |
| midnightblue | META417 | 2-Phenyl-4-pentenal |
| midnightblue | META420 | 2-beta-D-glucosyle anthranilate |
| midnightblue | META445 | (2E)-5-methyl-2-phenylhex-2-enal |
| midnightblue | META468 | Butylphthalide |
| midnightblue | META542 | Triethyl citrate |
| midnightblue | META565 | SECONAL |
| midnightblue | META587 | Perindoprilat |
| midnightblue | META606 | N-Nitrosoproline |
| midnightblue | META607 | N-lauroylglycine |
| midnightblue | META640 | N,N-Dihydroxy-L-valine |
| midnightblue | META813 | carisoprodol |
| midnightblue | META818 | Butyryl-L-homoserine lactone |
| midnightblue | META830 | asn-pro |
| midnightblue | META870 | 2-morpholinoacetic acid |
| midnightblue | META890 | 1-Cyclohexenecarboxylic Acid |
| midnightblue | META893 | 1-{[(3S,4S,5R)-2,3,4-Trihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]methyl}-2-pyrrolidinecarboxylic acid |
| midnightblue | META921 | (+/-)-pantetheine |
| midnightblue | META931 | sinapoylglucose |
| midnightblue | META952 | 4-Methoxycinnamic acid |
| midnightblue | META965 | (2Z)-N-(3-Aminopropyl)-N-{4-[(3-aminopropyl)amino]butyl}-3-(4-hydroxy-3,5-dimethoxyphenyl)acrylamide |
| midnightblue | META976 | Cinnamyl alcohol |
| midnightblue | META1059 | 1-[3-(Methylsulfanyl)phenyl]-3-({(2R,4S,5S)-5-[(4-phenyl-1-piperazinyl)methyl]-1-azabicyclo[2.2.2]oct-2-yl}methyl)urea |
| midnightblue | META1106 | DL-Cerulenin |
| midnightblue | META1184 | Linoleamide |
| midnightblue | META1235 | Decyl beta-D-threo-hexopyranoside |
| midnightblue | META1274 | 3-Oxotetradecanoic acid |
| midnightblue | META1296 | 2S-Amino-tridecanoic acid |
| midnightblue | META1313 | 1-oleoyl-2-linoleoyl-sn-glycerol |
| midnightblue | META1416 | Luteolin |
| midnightblue | META1454 | 6-(5-Hydroxy-3,7-dimethoxy-4-oxo-4H-chromen-2-yl)-2,3-dimethoxyphenyl beta-D-glucopyranoside |
| midnightblue | META1533 | DIACETIN MONOPROPANOATE |
| midnightblue | META1615 | Furfuranol |
| midnightblue | META1622 | 5,7-dihydroxy-3-[(4-methoxyphenyl)methyl]-3,4-dihydro-2H-1-benzopyran-4-one |
| midnightblue | META1777 | trilobine |
| midnightblue | META1811 | β,β-dimethylacrylshikonin |
| midnightblue | META1921 | 3,4-dehydrothiomorpholine-3-carboxylic acid |
| midnightblue | META2056 | Dibenzo-18-crown-6 |
| midnightblue | META2279 | Hexylresorcinol |
| midnightblue | META2309 | Methyldopa |
| midnightblue | META2315 | 3-(3,5-Dimethoxyphenyl)propanoic acid |
| midnightblue | META2328 | Pseudopelletierine |
| midnightblue | META2343 | (2,7-Dimethyloctahydro-1H-cyclopenta[c]pyridin-4-yl)methanol |
| midnightblue | META2368 | trans-geranic acid |
| midnightblue | META2428 | Geniposidic acid |
| midnightblue | META2468 | Artemisinin |
| midnightblue | META2472 | all-trans-4,4'-diapophytofluene |
| midnightblue | META2474 | All E-Teprenone |
| midnightblue | META2577 | 4a,5-dihydroriboflavin |
| midnightblue | META2676 | citibrasine |
| midnightblue | META2760 | hydroxyprogesterone caproate |
| midnightblue | META2832 | 24-methylenecholesterol |
| pink | META57 | Jasmonal |
| pink | META102 | (11cis,13cis,13'cis)-1,1',2,2',7,7',8,8',11',12'-Decahydro-1',2'-epoxy-psi,psi-carotene |
| pink | META110 | NP-018716 |
| pink | META126 | Methyl (3S,4S,21R)-14-ethyl-13-formyl-4,8,18-trimethyl-20-oxo-3-(3-oxo-3-{[(2E,7R,11R)-3,7,11,15-tetramethyl-2-hexadecen-1-yl]oxy}propyl)-9-vinyl-21-phorbinecarboxylate |
| pink | META127 | LT9970000 |
| pink | META130 | 1-O-Arsonopentofuranose |
| pink | META222 | 5-Hydantoinpropionic acid |
| pink | META264 | prenoxdiazine |
| pink | META280 | Orphenadrine |
| pink | META335 | Ethylparaben |
| pink | META360 | cyclandelate |
| pink | META384 | Benzoic acid |
| pink | META401 | 4-Phenylbutyric acid |
| pink | META424 | 2,5-di-tert-Butylhydroquinone |
| pink | META427 | 2,4-Dichlorotoluene |
| pink | META430 | 2,2'-Methylenebis(4-methyl-6-tert-butylphenol) |
| pink | META439 | [1,1'-biphenyl]-2,2'-dicarboxylic acid |
| pink | META568 | Quwenzhi |
| pink | META574 | Pregabalin |
| pink | META616 | N-CAFFEOYL-L-ASPARTIC ACID |
| pink | META621 | N-Acetyl-L-phenylalanine |
| pink | META856 | 4-Methyleneglutamic acid |
| pink | META905 | (3S,9S,14aR)-3,6-Dimethyl-9-{6-[(2S)-2-oxiranyl]-6-oxohexyl}decahydropyrrolo[1,2-a][1,4,7,10]tetraazacyclododecine-1,4,7,10-tetrone |
| pink | META942 | Methyl cinnamate |
| pink | META960 | (E)-p-coumaric acid |
| pink | META964 | (E)-3,4,5-Trimethoxycinnamic acid |
| pink | META983 | Scoparone |
| pink | META1084 | 5-Methylcytosine |
| pink | META1110 | α,α-Trehalose |
| pink | META1125 | Stearic acid |
| pink | META1136 | Prostaglandin G2 |
| pink | META1144 | Panthenol |
| pink | META1169 | MFCD00083370 |
| pink | META1183 | Linoleic acid |
| pink | META1193 | Juniperic acid |
| pink | META1217 | Dodecanedioic acid |
| pink | META1239 | Corchorifatty acid F |
| pink | META1260 | A-12(13)-EpODE |
| pink | META1304 | 2-hydroxy Lignoceric Acid |
| pink | META1328 | 12-oxo Phytodienoic Acid |
| pink | META1329 | 12-HSA |
| pink | META1363 | (15Z)-9,12,13-Trihydroxy-15-octadecenoic acid |
| pink | META1366 | (±)9-HpODE |
| pink | META1525 | Triacetin |
| pink | META1579 | 1-Palmitoyl-2-hydroxy-sn-glycero-3-PE |
| pink | META1731 | IBERVERIN |
| pink | META1741 | 6-Hydroxy-5-methyl-4,11-dioxoundecanoic acid |
| pink | META1769 | epsilon-Caprolactone |
| pink | META1772 | 2-Isocapryloyl-3R-hydroxymethyl-gamma-butyrolactone |
| pink | META1798 | oleandolide |
| pink | META1845 | Tetramethylurea |
| pink | META1872 | Dodecyl sulfate |
| pink | META1873 | 4-(3-Oxopentyl)phenyl hydrogen sulfate |
| pink | META2020 | Hexanal |
| pink | META2021 | Hex-2-ulose |
| pink | META2027 | Hept-2-ulose |
| pink | META2049 | D-PANTOTHENIC ACID |
| pink | META2119 | 5-(3',5'-Dihydroxyphenyl)-gamma-valerolactone 3-O-glucuronide |
| pink | META2147 | 3,6,9,12-tetraoxatridecan-1-ol |
| pink | META2213 | (4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one |
| pink | META2326 | TO0127900 |
| pink | META2329 | Pipercitine |
| pink | META2336 | Benzylfentanyl |
| pink | META2363 | Violaxanthin |
| pink | META2367 | Tretinoin |
| pink | META2396 | MFCD06656300 |
| pink | META2517 | 2,3-Dimethoxy-5-methyl-6-(3-methyl-2-buten-1-yl)-1,4-benzenediol |
| pink | META2586 | N6-threonylcarbamoyladenosine |
| pink | META2599 | Kojic acid |
| pink | META2626 | Deferiprone |
| pink | META2663 | Xanthurenic acid |
| pink | META2729 | Pregnanediol-3-glucuronide |
| pink | META2814 | 7alpha,25-Dihydroxycholesterol |
| pink | META2874 | NSC 622050 |
| pink | META2938 | N-6--(5-Oxo-D-isoleucyl)-L-lysine |
| purple | META09 | PPG n5 |
| purple | META37 | NP-007694 |
| purple | META60 | HMBA |
| purple | META65 | ACPC |
| purple | META178 | Guvacine |
| purple | META180 | Cinchonan-9-ol |
| purple | META189 | 11-Nitro-1-undecene |
| purple | META214 | 2,4,5-Trimethyl-1,3-thiazole |
| purple | META244 | Sulfapyridine |
| purple | META291 | N5-phenyl-4-methyl-1,2,3-thiadiazole-5-carboxamide |
| purple | META303 | MFCD00276655 |
| purple | META355 | DH2207000 |
| purple | META363 | CU5774000 |
| purple | META503 | Benzothiazole |
| purple | META506 | 2-Mercaptobenzothiazole |
| purple | META544 | trans-4-Hydroxy-L-proline |
| purple | META552 | TEP |
| purple | META600 | N-Phenylacetylglutamic acid |
| purple | META638 | N,N-dimethylarginine |
| purple | META648 | MPTP |
| purple | META680 | L-Tyrosine |
| purple | META683 | L-Theanine |
| purple | META750 | glu-thr |
| purple | META769 | FF-MAS |
| purple | META789 | DL-2,6-Diaminopimelic acid |
| purple | META802 | Cyclo(leucylprolyl) |
| purple | META817 | C8-HSL |
| purple | META845 | Acetylarginine |
| purple | META848 | ACETYL ARGININE |
| purple | META884 | 2-(acetylamino)-3-(1H-indol-3-yl)propanoic acid |
| purple | META891 | 1-Aminocyclohexanecarboxylic acid |
| purple | META897 | .alpha.-Aminoadipic acid |
| purple | META918 | (2S)-2-Piperazinecarboxamide |
| purple | META1003 | Decursin |
| purple | META1011 | 7-Hydroxycoumarine |
| purple | META1064 | Pyrantel |
| purple | META1065 | pydanon |
| purple | META1147 | Palmitic acid |
| purple | META1149 | Palmitelaidic acid |
| purple | META1160 | myristic acid |
| purple | META1210 | Ethyl myristate |
| purple | META1253 | Arachidonic acid |
| purple | META1429 | Hyperoside |
| purple | META1448 | 7-hydroxy-2-(4-hydroxyphenyl)-5-methoxy-3,4-dihydro-2H-1-benzopyran-4-one |
| purple | META1614 | Harmine |
| purple | META1634 | (+/-)-2-Hydroxyglutaric acid |
| purple | META1671 | SB236057A |
| purple | META1694 | (1S,6S)-6-Aminooctahydro-1-indolizinyl acetate |
| purple | META1737 | MFCD20640990 |
| purple | META1812 | Shikalkin |
| purple | META1817 | Naphthalene |
| purple | META1886 | Thiram |
| purple | META1895 | Oleoylethanolamide |
| purple | META1925 | 2-Amino-1,3,4-octadecanetriol |
| purple | META1930 | (E)-5-(methylsulfanyl)pentanal oxime |
| purple | META2034 | Glucoheptonic Acid |
| purple | META2069 | D-(−)-Salicin |
| purple | META2075 | cyclo-Dopa 5-O-glucoside |
| purple | META2165 | 2-(4-Hydroxyphenyl)ethyl 6-O-[(2R,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside |
| purple | META2220 | Enalkiren |
| purple | META2233 | Troxipide |
| purple | META2249 | Atomoxetine |
| purple | META2269 | Paradol |
| purple | META2280 | Guaiacol |
| purple | META2299 | 3,4-dihydroxyphenylacetic acid |
| purple | META2324 | Mirtazapine |
| purple | META2330 | Pethidine |
| purple | META2370 | steviol |
| purple | META2637 | Thymidine |
| purple | META2647 | 1-(beta-D-Ribofuranosyl)-1,2-dihydropyrimidine |
| purple | META2725 | Promegestone |
| purple | META2740 | Norethisterone enanthate |
| purple | META2746 | Nandrolone |
| purple | META2916 | Leucomalachite green |
| red | META04 | TF5775000 |
| red | META13 | PEG n5 |
| red | META91 | (3S,3'S,5R,5'R,8'R,9'cis)-3'-Methyl-6,7-didehydro-5,5',6,8'-tetrahydro-5',8'-epoxy-beta,beta-carotene-3,5-diol |
| red | META267 | Phenylmethylsulfonyl fluoride |
| red | META302 | MFCD01748352 |
| red | META324 | Heptylbenzene |
| red | META346 | Dimethyl phthalate |
| red | META351 | Diethyl phthalate |
| red | META352 | Dibutyl phthalate |
| red | META359 | Cyclopentolate |
| red | META368 | CETYL BENZOATE |
| red | META370 | cannabidiolic acid |
| red | META372 | Butylparaben |
| red | META447 | 1228222 |
| red | META476 | MOLLICELLIN B |
| red | META597 | N-Undecanoylglycine |
| red | META598 | N-Tridecanoylglycine |
| red | META651 | MHPG |
| red | META656 | MFCD00153469 |
| red | META727 | Iprofenin |
| red | META743 | Gly-Lys |
| red | META744 | Gly-l-pro |
| red | META808 | Citroflex 4 |
| red | META810 | cis-trihomoaconitic acid |
| red | META846 | Acetylagmatine |
| red | META957 | 2-Acetoxy-3-[3-(4-hydroxy-phenyl)-acryloyloxy]-succinic acid |
| red | META961 | (E)-Ferulic acid |
| red | META1019 | 5,6,7-Trimethoxy-2H-chromen-2-one |
| red | META1069 | pentobarbital |
| red | META1070 | metharbital |
| red | META1085 | 2-Methoxy-3-methylpyrazine |
| red | META1099 | Acmimycin |
| red | META1119 | Traumatic Acid |
| red | META1133 | RG1300000 |
| red | META1152 | Oleic acid |
| red | META1176 | Methyl (9E)-9-octadecenoate |
| red | META1188 | Leukotriene B4 |
| red | META1194 | Itaconic acid |
| red | META1247 | butoctamide |
| red | META1248 | Brassylic acid |
| red | META1254 | Arachidic acid |
| red | META1265 | 9,10-Dihydroxystearic acid |
| red | META1321 | 14,18-Dihydroxy-12-oxo-9,13,15-octadecatrienoic acid |
| red | META1338 | 1,4-Anhydro-6-O-dodecanoyl-2,3-bis-O-(2-hydroxyethyl)-D-glucitol |
| red | META1377 | (-)-pinellic acid |
| red | META1400 | Quercetin |
| red | META1469 | 5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-O-(6-deoxyhexopyranosyl)hexopyranoside |
| red | META1531 | DOG |
| red | META1551 | (2S)-1-Hydroxy-3-(pentadecanoyloxy)-2-propanyl (8Z,11Z,14Z)-8,11,14-icosatrienoate |
| red | META1565 | MFCD00036904 |
| red | META1589 | 1-linoleoyl-sn-glycero-3-phosphoethanolamine |
| red | META1619 | 2-(Diethoxymethyl)furan |
| red | META1649 | Epiguanine |
| red | META1740 | alpha-ketoadipic acid |
| red | META1752 | 2-(3-CARBOXYPROPIONYL)-6-HYDROXY-CYCLOHEXA-2,4-DIENE CARBOXYLIC ACID |
| red | META1832 | .beta.-Naphthol ethyl ether |
| red | META1836 | (−)-nabilone |
| red | META1846 | neptamustine |
| red | META1927 | 1-Tetradecylamine |
| red | META1965 | Picein |
| red | META2045 | Embelin |
| red | META2052 | Diprogulic Acid |
| red | META2061 | D-Glucono-delta-lactone |
| red | META2086 | beta-Syringin |
| red | META2089 | beta-D-Ethyl glucuronide |
| red | META2211 | UNII:V9Q7UUZ15U |
| red | META2254 | 4-Methoxyaniline |
| red | META2264 | Vanillin |
| red | META2290 | AC 45594 |
| red | META2308 | Metirosine |
| red | META2340 | 2-(Hydroxymethyl)-1-methyl-3,4,5-piperidinetriol |
| red | META2344 | (1S,4aS)-1,4a-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalene |
| red | META2427 | Geranyl glucoside |
| red | META2430 | Genipin |
| red | META2435 | Etretinate |
| red | META2488 | 4-[(3E,5E,7E,9E,11E)-15-Hydroxy-3,7,12-trimethyl-3,5,7,9,11-pentadecapentaen-1-yn-1-yl]-3,5,5-trimethyl-3-cyclohexen-1-ol |
| red | META2589 | dihydrozeatin riboside |
| red | META2591 | Adenosine |
| red | META2724 | Quinestrol |
| red | META2757 | Levonorgestrel |
| red | META2800 | Boldione |
| red | META2818 | 5b-Cholestane-3a,7a,12a,26-tetrol |
| red | META2886 | ionene |
| red | META2897 | 3,3'-(3,8,13,17-Tetramethyl-7,12-divinyl-2,3,6,7,8,11,12,13,14,17,22,24-dodecahydroporphyrin-2,18-diyl)dipropanoic acid |
| red | META2919 | 3-Tropanol |
| royalblue | META07 | PPG n7 |
| royalblue | META226 | thiamazole |
| royalblue | META237 | Triphenylphosphine oxide |
| royalblue | META308 | mesityl (4-methylphenyl) sulfone |
| royalblue | META373 | Butylated hydroxytoluene |
| royalblue | META383 | Benzophenone |
| royalblue | META505 | 2-Methyl-S-benzothiazole |
| royalblue | META519 | Decanamide |
| royalblue | META541 | Trimecaine |
| royalblue | META559 | Succinic anhydride |
| royalblue | META635 | N-{[3-Ethyl-11,15-dihydroxy-7-isopropyl-3-methyl-10-(methylamino)-6,9-dioxo-2-oxa-5,8-diazabicyclo[10.3.1]hexadeca-1(16),12,14-trien-4-yl]carbonyl}glycine |
| royalblue | META714 | L-coprine |
| royalblue | META732 | Hypusine |
| royalblue | META928 | Cinnamaldehyde |
| royalblue | META962 | (E)-4-Methoxycinnamic acid |
| royalblue | META1005 | Coumafuryl |
| royalblue | META1138 | prohydrojasmon |
| royalblue | META1250 | behenic acid |
| royalblue | META1355 | (2S)-1-Hydroxy-3-(pentadecanoyloxy)-2-propanyl (9Z,12Z,15Z)-9,12,15-octadecatrienoate |
| royalblue | META1410 | Naringenin |
| royalblue | META1421 | Kaempferol |
| royalblue | META1461 | 5-Demethylnobiletin |
| royalblue | META1494 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}-4H-chromen-4-one |
| royalblue | META1690 | 1-(1,3,3-Trimethyl-2,3-dihydro-1H-indol-2-yliden)acetone |
| royalblue | META1726 | N-2-Ethylhexyl bicycloheptenedicarboximide |
| royalblue | META1900 | MFCD00674434 |
| royalblue | META1923 | 2-Hydroxy-N-(2-hydroxyethyl)propionamide |
| royalblue | META1948 | Tiaprofenic acid |
| royalblue | META2005 | Malondialdehyde |
| royalblue | META2025 | heptaminol |
| royalblue | META2102 | Amfepramone |
| royalblue | META2126 | 4-Hydroxybenzaldehyde |
| royalblue | META2182 | 1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid |
| royalblue | META2320 | nylon cyclic dimer |
| royalblue | META2450 | Decylubiquinone |
| royalblue | META2494 | 4-(4-hydroxy-2,2,6-trimethyl-6-{[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}cyclohexylidene)but-3-en-2-one |
| royalblue | META2510 | 235BBF3K97 |
| royalblue | META2522 | 2-(3-Hydroxy-3,7,11,15-tetramethylhexadecyl)-3,5,6-trimethyl-1,4-benzoquinone |
| royalblue | META2622 | navenone A |
| royalblue | META2779 | Ergosterol |
| royalblue | META2864 | Combretastatin A-4 |
| salmon | META113 | NP-016455 |
| salmon | META114 | NP-015948 |
| salmon | META128 | APC |
| salmon | META206 | Secnidazole |
| salmon | META209 | fenamole |
| salmon | META223 | 3-Nitrosothiazolidine |
| salmon | META225 | XJ6642800 |
| salmon | META243 | TBHQ |
| salmon | META338 | DQ6125000 |
| salmon | META344 | Dinocton 6 |
| salmon | META345 | Di-n-Amyl phthalate |
| salmon | META387 | bentiamine |
| salmon | META399 | 4-Undecylbenzenesulfonic acid |
| salmon | META462 | N-(4-Heptanyl)-1,3-benzodioxole-5-carboxamide |
| salmon | META489 | 2-Acetamido-4-(5-amino-2,2-dimethyl-4-oxo-3,4-dihydro-2H-chromen-6-yl)-4-oxobutyl 16-methylheptadecanoate |
| salmon | META532 | Valyl-4-hydroxyproline |
| salmon | META550 | tetrahomomethionine |
| salmon | META585 | phe-asn |
| salmon | META592 | PALGLY |
| salmon | META652 | MFCD09953737 |
| salmon | META662 | Methyl alpha-aspartylphenylalaninate |
| salmon | META667 | mebutamate |
| salmon | META668 | MDMA |
| salmon | META676 | LYSINOALANINE, (S,R)- |
| salmon | META746 | Gly-DL-Phe |
| salmon | META779 | Eglumetad |
| salmon | META825 | Benserazide |
| salmon | META839 | Ala-Tyr |
| salmon | META840 | ALA-PRO |
| salmon | META978 | (Z)- -amylcinnamyl alcohol |
| salmon | META1062 | Toxopyrimidine |
| salmon | META1101 | 2-arachidonoylglycerol |
| salmon | META1122 | tert-Butyl 3-amino-1-methyl-2,3-dioxopropylcarbamate |
| salmon | META1159 | Myristoleic acid |
| salmon | META1162 | Misoprostol |
| salmon | META1177 | Margaric acid |
| salmon | META1268 | 8-{3-Oxo-2-[(2E)-2-penten-1-yl]-1-cyclopenten-1-yl}octanoic acid |
| salmon | META1516 | NP-003827 |
| salmon | META1547 | 1,3-Dihydroxy-2-propanyl (13Z)-13-docosenoate |
| salmon | META1549 | (2S)-3-Hydroxy-1,2-propanediyl dibutanoate |
| salmon | META1584 | 1-Oleoyl-2-hydroxy-sn-glycero-3-PE |
| salmon | META1689 | 1,2-Dimethoxy-2'-(methylsulfanyl)-1,2-dihydro-4'H-spiro[indole-3,5'-[1,3]thiazole] |
| salmon | META1735 | Pyruvic acid |
| salmon | META1751 | 2-hydroxy-6-ketononadienedioic acid |
| salmon | META1770 | DEHYDROASCORBIC ACID |
| salmon | META1785 | N-[(1R,9S)-11-(4-Fluorobenzyl)-6-oxo-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-5-yl]isonicotinamide |
| salmon | META1869 | N-[2-Hydroxy-4-(sulfooxy)phenyl]acetamide |
| salmon | META2104 | alpha-L-Glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-D-glucopyranos yl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-D-glucopyranose |
| salmon | META2105 | alpha-L-Glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-L-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranos yl-(1->4)-alpha-D-glucopyranosyl-(1->4)-D-glucopyranose |
| salmon | META2108 | Acetophenone |
| salmon | META2180 | 1,4-D-xylobiose |
| salmon | META2242 | hexamidine |
| salmon | META2278 | Homovanillic acid |
| salmon | META2291 | 6-Gingerol |
| salmon | META2433 | frescolat ML |
| salmon | META2461 | Betulin |
| salmon | META2485 | 4-Ketomyxol |
| salmon | META2525 | 10-Hydroxyligustroside |
| salmon | META2619 | Nicotinic acid |
| salmon | META2658 | 1-Hexadecanoylpyrrolidine |
| salmon | META2662 | Ruxolitinib |
| salmon | META2673 | Huperzine |
| salmon | META2675 | FG7175000 |
| salmon | META2741 | Norethisterone acetate |
| salmon | META2804 | androstenol |
| salmon | META2845 | (3beta,9xi,14xi,22S,25S)-26-Hydroxy-22,25-epoxyfurost-5-en-3-yl 6-deoxy-alpha-L-mannopyranosyl-(1-4)-[beta-D-glucopyranosyl-(1-2)]-beta-D-glucopyranoside |
| salmon | META2901 | thiodiglycol |
| tan | META58 | Î³-Oxo-3-pyridinebutanal |
| tan | META105 | NP-021797 |
| tan | META117 | NP-014604 |
| tan | META154 | 5-Methoxy-1H-indol-6-yl Î²-D-glucopyranosiduronic acid |
| tan | META238 | Tolycaine |
| tan | META245 | Styrene |
| tan | META259 | Propylparaben |
| tan | META277 | Oryzalin |
| tan | META339 | DO0750000 |
| tan | META381 | Benzyl butyrate |
| tan | META443 | (2Z)-4-Methyl-2-phenyl-2-pentenal |
| tan | META644 | N-(3-Carboxypropanoyl)-5-hydroxynorvaline |
| tan | META688 | L-Phenylalanine |
| tan | META736 | H-Met(O)-OH |
| tan | META851 | a Jasmonoyl-glutamine |
| tan | META913 | (2S)-4-Methyl-2-({[(3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]methyl}amino)pentanoic acid |
| tan | META924 | (-)-threo-isodihomocitric acid |
| tan | META939 | octinoxate |
| tan | META966 | (2Z)-3-Phenyl-1-(1-pyrrolidinyl)-2-propen-1-one |
| tan | META994 | Khellactone, Cis-(-)- |
| tan | META1104 | Etoglucid |
| tan | META1137 | propionylcarnitine |
| tan | META1161 | Myristamide |
| tan | META1195 | isopropylmalic acid |
| tan | META1211 | Ethyl Linoleate |
| tan | META1237 | Cyprodenate |
| tan | META1276 | 3-Methyl-5-pentyl-2-furanpentadecanoic acid |
| tan | META1278 | 3-Hydroxytetradecanedioic acid |
| tan | META1305 | 2-Acetamido-2-deoxy-3-O-(6-deoxy-alpha-L-galactopyranosyl)-D-glucose |
| tan | META1311 | 2-(alpha-D-mannosyl)-D-glyceric acid |
| tan | META1337 | 1,4-Bis(2-ethylhexyl) sulfosuccinate |
| tan | META1342 | 1-(9Z-hexadecenoyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycerol |
| tan | META1349 | (4S)-4-hydroxy-3,5,5-trimethyl-4-[(1E)-3-{[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}but-1-en-1-yl]cyclohex-2-en-1-one |
| tan | META1385 | Tetramethylscutellarein |
| tan | META1440 | Cianidanol |
| tan | META1510 | yatein |
| tan | META1542 | 1-Palmitoleoyl-2-oleoyl-sn-glycerol |
| tan | META1597 | 1,2-Dipalmitoleoyl-sn-glycero-3-phosphocholine |
| tan | META1686 | 5-Hydroxy-DL-tryptophan |
| tan | META1754 | (2-Carboxy-2-oxoethyl)(hydroxy)oxophosphonium |
| tan | META1807 | Heroin-d3 |
| tan | META1942 | undecenal |
| tan | META1984 | N-(2-Phenylethyl)-beta-D-glucopyranuronosylamine |
| tan | META1990 | MFCD24849370 |
| tan | META2002 | Megalomicin C1 |
| tan | META2029 | GW7340000 |
| tan | META2065 | Dambonitol |
| tan | META2103 | AM9627000 |
| tan | META2222 | b-Ala-Lys |
| tan | META2243 | Guaifenesin |
| tan | META2293 | 5-Chloro-3-fluoro-1,2-benzenediol |
| tan | META2297 | 3-BHA |
| tan | META2342 | (2E,4E,16Z)-1-(1-Piperidinyl)-2,4,16-icosatrien-1-one |
| tan | META2359 | alpha-D-Glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranos yl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose |
| tan | META2375 | RG5927200 |
| tan | META2377 | Rehmaionoside C |
| tan | META2434 | Farnesylacetone |
| tan | META2501 | 3,4-Dihydrocadalene |
| tan | META2505 | 2-Methoxy-6-[(2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-octamethyl-2,6,10,14,18,22,26,30-dotriacontaoctaen-1-yl]phenol |
| tan | META2553 | (1S,2R,5S)-2-Isopropyl-5-methylcyclohexyl 3-oxobutanoate |
| tan | META2613 | Pyridoxal |
| tan | META2736 | oxandrolone |
| tan | META2748 | MFCD00133847 |
| tan | META2766 | Gonan-3-ol |
| tan | META2768 | FZ7700000 |
| tan | META2812 | 7-ketodeoxycholic acid |
| tan | META2826 | 3?,5?,6?-trihydroxycholestane |
| tan | META2889 | 2-(1-benzothiophen-3-ylmethylene)-3,4-dihydronaphthalen-1(2H)-one |
| turquoise | META88 | (7Z)-Ophiobola-3(24),7,19-triene |
| turquoise | META170 | Camelinin |
| turquoise | META203 | molinate |
| turquoise | META231 | zinniol |
| turquoise | META251 | Sibrafiban |
| turquoise | META258 | Protocatechuic acid |
| turquoise | META270 | Phenylethyl alcohol |
| turquoise | META287 | N-benzyl-N-methyl-N'-phenylurea |
| turquoise | META311 | LQ5400000 |
| turquoise | META312 | Lidocaine |
| turquoise | META348 | Diisobutylphthalate |
| turquoise | META366 | cis-3-Hexenyl phenylacetate |
| turquoise | META389 | Aspirin |
| turquoise | META395 | 6-phenylundecane |
| turquoise | META403 | 4-Methylbenzophenone |
| turquoise | META444 | (2-methylcyclopentyl)(phenyl)methanone oxime |
| turquoise | META508 | 2,2-Dithiobis(benzothiazole) |
| turquoise | META569 | Pyridinoline |
| turquoise | META595 | Oseltamivir |
| turquoise | META610 | N-Heptadecanoylglycine |
| turquoise | META611 | N-glycoloyl-D-mannosaminolactone |
| turquoise | META618 | N-Acetylvanilalanine |
| turquoise | META628 | N-acetyl-L-2-aminoadipic acid |
| turquoise | META665 | meprobamate |
| turquoise | META695 | L-Isoleucyl-L-alanyl-D-arginine |
| turquoise | META795 | DEET |
| turquoise | META804 | clavulanic acid |
| turquoise | META807 | Citroflex A-4 |
| turquoise | META885 | 2-(4-Isopropyl-4-methyl-5-oxo-4,5-dihydro-1H-imidazol-2-yl)-4-methylbenzoic acid |
| turquoise | META940 | N-trans-sinapoyltyramine |
| turquoise | META982 | Scopoletin |
| turquoise | META989 | MUGlcU |
| turquoise | META999 | Esculin |
| turquoise | META1039 | nifurquinazol |
| turquoise | META1073 | Eterobarb |
| turquoise | META1115 | Valproic acid |
| turquoise | META1127 | Sorbic acid |
| turquoise | META1128 | Sebacic acid |
| turquoise | META1155 | N-Methylhexanamide |
| turquoise | META1167 | MFCD00130070 |
| turquoise | META1267 | 9-(3-Methyl-5-pentyl-2-furyl)nonanoic acid |
| turquoise | META1283 | 3-[(6-Oxodecanoyl)oxy]-4-(trimethylammonio)butanoate |
| turquoise | META1286 | 3-[(3-Hydroxydecanoyl)oxy]-4-(trimethylammonio)butanoate |
| turquoise | META1289 | 3-[(19Z)-15,16-Dihydroxy-19-dotriaconten-1-yl]-5-methyl-2(5H)-furanone |
| turquoise | META1293 | 3,4-Dimethyl-5-pentyl-2-furanpentadecanoic acid |
| turquoise | META1298 | 2-Hydroxypropyl stearate |
| turquoise | META1327 | 13(S)-HOTrE |
| turquoise | META1351 | (3Z,6E,8E,12Z,15Z,18Z)-3,6,8,12,15,18-Docosahexaen-10-ol |
| turquoise | META1374 | (-)-Rhododendrin |
| turquoise | META1403 | Pinocembrin |
| turquoise | META1476 | 4',5,6,7-Tetramethoxyflavanone |
| turquoise | META1505 | (-)-8-Prenylnaringenin |
| turquoise | META1508 | 9H-Fluoren-9-one |
| turquoise | META1514 | (+)-syringaresinol |
| turquoise | META1561 | O-{Hydroxy[(2R)-2-(palmitoyloxy)-3-(pentadecanoyloxy)propoxy]phosphoryl}-L-serine |
| turquoise | META1575 | 2-[(11Z,14Z)-icosadienoyl]-sn-glycero-3-phosphoethanolamine |
| turquoise | META1593 | 1-heptadecanoyl-sn-glycero-3-phosphocholine |
| turquoise | META1609 | (2R)-1-{[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-3-hydroxy-2-propanyl (11Z)-11-icosenoate |
| turquoise | META1617 | 2-Decylfuran |
| turquoise | META1631 | 12-Hydroxylauric acid |
| turquoise | META1661 | Ninhydrin |
| turquoise | META1667 | 3-oxoindane-1-carboxylic acid |
| turquoise | META1675 | Methoxybrassinin |
| turquoise | META1679 | edotecarin |
| turquoise | META1719 | 7-{[(2S,3R,4S,5S,6R)-6-({[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy}methyl)-3,4,5-trihydroxyoxan-2-yl]oxy}-5-hydroxy-3-(4-hydroxyphenyl)-6-methoxy-4H-chromen-4-one |
| turquoise | META1808 | Dextromethorphan |
| turquoise | META1908 | EJ4025000 |
| turquoise | META1918 | Butenylcarnitine |
| turquoise | META1949 | Tetraacetylethylenediamine |
| turquoise | META1997 | Methyl 9-oxononanoate |
| turquoise | META2026 | Heptaethylene Glycol |
| turquoise | META2031 | glutaral |
| turquoise | META2084 | Bis(2-butoxyethyl) ether |
| turquoise | META2098 | Arbutin |
| turquoise | META2146 | 3-[3-(beta-D-Glucopyranosyloxy)-2-hydroxyphenyl]propanoic acid |
| turquoise | META2181 | 1,3,5-trihydroxy-4-{[(2E)-3-(3-hydroxy-4-methoxyphenyl)prop-2-enoyl]oxy}cyclohexane-1-carboxylic acid |
| turquoise | META2193 | (2S)-3-Hydroxy-2-({[(3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]methyl}amino)butanoic acid |
| turquoise | META2202 | ATEE |
| turquoise | META2203 | (+/-)-Eucalyptol |
| turquoise | META2232 | Venlafaxine |
| turquoise | META2235 | Ro 20-1724 |
| turquoise | META2246 | exalamide |
| turquoise | META2263 | Vanillyl alcohol |
| turquoise | META2271 | noradrenaline |
| turquoise | META2287 | Benzenol |
| turquoise | META2292 | 5-Henicosyl-1,3-benzenediol |
| turquoise | META2339 | 2,2,6,6-Tetramethyl-1-piperidinol (TEMPO) |
| turquoise | META2355 | CYCLURON |
| turquoise | META2365 | UNII:6S7S02945H |
| turquoise | META2376 | Retinyl acetate |
| turquoise | META2406 | LINALYL BUTYRATE |
| turquoise | META2408 | Lamioside |
| turquoise | META2417 | guaiazulene |
| turquoise | META2543 | (3E)-4,8-Dimethyl-1,3,7-nonatriene |
| turquoise | META2547 | (2E,6E)-Farnesol |
| turquoise | META2557 | (±)-(2E)-Abscisic acid |
| turquoise | META2584 | Succinyladenosine |
| turquoise | META2620 | Nicotinamide |
| turquoise | META2674 | Graveoline |
| turquoise | META2686 | Cernuine |
| turquoise | META2721 | Samandarin |
| turquoise | META2822 | 3-Dehydro-2-deoxyecdysone |
| turquoise | META2850 | (25S)-5beta-spirostan-3beta-yl beta-D-glucoside |
| turquoise | META2854 | (22E)-Ergosta-5,7,22,24(28)-tetraen-3-ol |
| turquoise | META2857 | (+)-Estrone |
| turquoise | META2871 | (-)-akuammicine |
| turquoise | META2883 | Drotaverine |
| turquoise | META2903 | S-[(1Z)-N-Hydroxy-8-(methylsulfanyl)octanimidoyl]cysteine |
| turquoise | META2908 | 5-nitrothiophene-3-carbaldehyde 3-(2-pyridyl)hydrazone |
| turquoise | META2918 | 8-Methyl-8-azabicyclo[3.2.1]oct-3-yl (2E)-2-methyl-2-butenoate |
| yellow | META17 | NP-022531 |
| yellow | META53 | Methyl {2-[(2E)-5-(hexopyranosyloxy)-2-penten-1-yl]-3-oxocyclopentyl}acetate |
| yellow | META108 | NP-019498 |
| yellow | META118 | NP-005128 |
| yellow | META121 | NP-003191 |
| yellow | META166 | 7440 |
| yellow | META176 | Trigonelline |
| yellow | META177 | Nitrosoguvacoline |
| yellow | META284 | Norfentanyl |
| yellow | META343 | Diphenolic acid |
| yellow | META410 | 4-(Heptyloxy)benzoic acid |
| yellow | META461 | Safrole |
| yellow | META467 | Coumarone |
| yellow | META473 | Trolox |
| yellow | META553 | Tentoxin |
| yellow | META558 | Succinyl proline |
| yellow | META561 | Stachydrine |
| yellow | META571 | Prolylleucine |
| yellow | META601 | N-Pentadecanoylglycine |
| yellow | META619 | N-Acetylvaline |
| yellow | META701 | L-gamma-Glutamyl-L-valine |
| yellow | META731 | ilomastat |
| yellow | META766 | Fructoselysine |
| yellow | META904 | (5E)-2,10-Diamino-5-{[(5-amino-5-carboxypentyl)amino]methyl}-5-undecenedioic acid |
| yellow | META909 | (2S,4S)-4-hydroxy-2,3,4,5-tetrahydrodipicolinic acid |
| yellow | META914 | (2S)-3-Phenyl-2-({[(3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)tetrahydro-2-furanyl]methyl}amino)propanoic acid |
| yellow | META919 | (2S)-2-Amino-8-hydroxyoctanoic acid |
| yellow | META922 | (+/-)-Camphoric acid |
| yellow | META953 | 4-coumaroylshikimic acid |
| yellow | META954 | 4-Coumaric acid |
| yellow | META1047 | 2-(4-chlorophenyl)-3-phenylquinoxaline |
| yellow | META1056 | Aderbasib |
| yellow | META1068 | pentoxyl |
| yellow | META1081 | aspergillic acid |
| yellow | META1090 | Furaneol |
| yellow | META1126 | Sorbitan, monododecanoate |
| yellow | META1157 | Nervonic acid |
| yellow | META1214 | epi-jasmonic acid |
| yellow | META1226 | Dihydro-PGF1? |
| yellow | META1232 | Desthiobiotin |
| yellow | META1238 | Cxa-10 |
| yellow | META1279 | 3-Hydroxypentadecanoic acid |
| yellow | META1300 | 2-Hydroxy-4-oxohenicosyl acetate |
| yellow | META1365 | (10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid |
| yellow | META1372 | (+)-Fluprostenol |
| yellow | META1379 | 5,7-Dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-3-yl 6-deoxy-alpha-L-mannopyranosyl-(1-2)-[6-deoxy-alpha-L-mannopyranosyl-(1-6)]hexopyranoside |
| yellow | META1380 | Xanthorhamnin |
| yellow | META1382 | Trifolin |
| yellow | META1391 | Rutin |
| yellow | META1407 | NICTOFLORIN |
| yellow | META1414 | Mauritianin |
| yellow | META1446 | Afzelin |
| yellow | META1480 | 3-{[(2S,3R,4S,5S,6R)-4,5-dihydroxy-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}-6-({[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}methyl)oxan-2-yl]oxy}-5,7-dihydroxy-2-(4-hydroxyphenyl)-6-methoxy-4H-chromen-4-one |
| yellow | META1481 | 3-{[(2S,3R,4S,5R,6R)-4,5-dihydroxy-3-{[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}-6-({[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy}methyl)oxan-2-yl]oxy}-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4H-chromen-4-one |
| yellow | META1580 | 1-palmitoyl-2-[(9Z,12Z,15Z)-octadecatrienoyl]-sn-glycero-3-phosphocholine |
| yellow | META1677 | Indole |
| yellow | META1766 | UQ1355000 |
| yellow | META1809 | Dexylosylpradimicin C |
| yellow | META1814 | PharmaGSID 47337 |
| yellow | META1821 | Deoxyshikonin |
| yellow | META1823 | 2-Methylnaphthalene |
| yellow | META1848 | Diethylpyrocarbonate |
| yellow | META1867 | paracetamol sulfate |
| yellow | META1884 | α-Linolenoyl Ethanolamide |
| yellow | META1892 | Phytosphingosine |
| yellow | META1894 | Oryzalin metabolite |
| yellow | META1953 | Spiroxamine |
| yellow | META1964 | Poly THF n5 |
| yellow | META1974 | N-Ethyl-N-methylcathinone |
| yellow | META1988 | MM3670000 |
| yellow | META1996 | Methyl vinyl ketone |
| yellow | META2011 | Isopropyl beta-D-galactopyranoside |
| yellow | META2071 | D-(−)-Erythrose |
| yellow | META2076 | Cyclododecanone |
| yellow | META2116 | 5-Formylfurfural |
| yellow | META2192 | (2S,3S)-2,3-dihydro-3-hydroxyanthranilic acid zwitterion |
| yellow | META2231 | Viloxazine |
| yellow | META2245 | Gemfibrozil |
| yellow | META2261 | (2Z)-3-(3,4,5-Trimethoxyphenyl)-2-propen-1-yl acetate |
| yellow | META2274 | MFCD00004231 |
| yellow | META2313 | 3-Phenylpropanoic acid |
| yellow | META2332 | miglustat |
| yellow | META2371 | Squalene |
| yellow | META2436 | Epifriedelanol |
| yellow | META2464 | Asiaticoside |
| yellow | META2467 | Artemotil |
| yellow | META2486 | 4-hydroxy-3-octaprenylbenzoic acid |
| yellow | META2514 | 2,5-Dihydroxy-3-[(2E,6E,10E)-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraen-1-yl]-1,4-benzoquinone |
| yellow | META2530 | (E,E)-alpha-Farnesene |
| yellow | META2533 | (6R,10S)-13-[(2S)-6-Hydroxy-2,5,7,8-tetramethyl-3,4-dihydro-2H-chromen-2-yl]-2,6,10-trimethyltridecanoic acid |
| yellow | META2580 | 1,5,6,7-tetrahydropteridin |
| yellow | META2618 | Nifedipine |
| yellow | META2697 | Cedefingol |
| yellow | META2731 | Pregnane-3,20-dione |
| yellow | META2807 | Androst-4-en-3-one |
| yellow | META2834 | 1Î²-Hydroxycholic acid |
| yellow | META2849 | (2beta,3alpha,5alpha,16beta,17beta)-3,17-Diacetoxy-2,16-bis(1-methyl-1-piperidiniumyl)androstane |
| yellow | META2882 | N-Methylanhalonine |
| yellow | META2927 | 4-Vinylcyclohexene |

**Table S5**. Relative total secondary metabolites content in *Dracaena* sp. in Guangxi and related species

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **META ID** | **Metabolites name** | **BM3** | **C6** | **C13** | **CZ4** | **JX2** | **RM1** | **SL** | **XZ** | **CB** | **CH** | **HB** | **HN** |
| META1917 | Choline | 5292757912 | 10667452540 | 8044778762 | 7706301889 | 7841747820 | 8353674015 | 3237653121 | 5999350070 | 8307438376 | 8260494641 | 9701349374 | 6570952154 |
| META2513 | 2,6,10,14,18,22,26,30-Dotriacontaoctaen-1-ol, 3,7,11,15,19,23,27,31-octamethyl-, (all-E)- | 8010998674 | 6103634256 | 7778709135 | 6285084249 | 6833170616 | 6095453762 | 12041553952 | 6285917036 | 6051776122 | 6384132431 | 6232354306 | 6152003334 |
| META1847 | N,N'-Dicyclohexylurea | 4671474900 | 4812329150 | 4810185335 | 4811480125 | 4825275485 | 4659791520 | 4817939182 | 4822868039 | 4815237928 | 4815338415 | 4811636322 | 4823238747 |
| META506 | 2-Mercaptobenzothiazole | 4693238190 | 4700667175 | 4696644216 | 4707493298 | 4710641528 | 4699497272 | 4703425100 | 4700363163 | 4706688890 | 4679421464 | 4686284897 | 4688771674 |
| META2051 | Dipropylene glycol dimethyl ether | 4165119338 | 4176986381 | 4172413162 | 4186978238 | 4169214923 | 4176823132 | 4188436284 | 4178320076 | 4188482208 | 4172804850 | 4168464902 | 4178953979 |
| META1898 | N,N-Diisopropylethylamine (DIPEA) | 3341291830 | 3268891150 | 3263413915 | 3277738439 | 3232397060 | 3268469145 | 3260320091 | 3236436750 | 3255654570 | 3252261099 | 3260060427 | 3257003310 |
| META1011 | 7-Hydroxycoumarine | 2429936320 | 3931817805 | 4227362675 | 2441493808 | 5218591844 | 10401124187 | 1225605132 | 1224420732 | 1226372293 | 1218699546 | 1220056906 | 1221612188 |
| META2339 | 2,2,6,6-Tetramethyl-1-piperidinol (TEMPO) | 2450397758 | 2448827940 | 2448003944 | 2449106881 | 2452782336 | 2452025141 | 2445161195 | 2451079524 | 2448487900 | 2455933440 | 2450611571 | 2451802673 |
| META1181 | Linolenic acid ethyl ester | 187776730.5 | 61548204.59 | 38249501.72 | 60700801.49 | 499442168.9 | 82710127.23 | 26703429.2 | 4907692134 | 17911194532 | 430578055.8 | 1761578985 | 175638869.5 |
| META1213 | Erucamide | 1360727309 | 1997395431 | 1647647398 | 1948824979 | 2017562874 | 2209896236 | 1696806518 | 3977407127 | 3523098075 | 1696138734 | 1492930566 | 2470405088 |
| META1528 | L-α-PALMITIN | 705864895.1 | 1045014876 | 1026268263 | 1617069875 | 1131473787 | 1156548657 | 732721479.9 | 1969265944 | 6450588496 | 3532158047 | 3670252829 | 1311517649 |
| META808 | Citroflex 4 | 1653792840 | 1638485880 | 1658766756 | 1664413957 | 1716862484 | 1674822205 | 1653973710 | 1661770772 | 1734518149 | 1663340009 | 1754098439 | 1811585603 |
| META1668 | trans-3-Indoleacrylic acid | 1126751159 | 7325220501 | 728715889.5 | 2039633688 | 1615306450 | 636191749.5 | 241314377.6 | 466806334.2 | 2233344109 | 543527849.5 | 1363539019 | 1041234915 |
| META507 | 2-Hydroxybenzothiazole | 1539202918 | 1543511165 | 1541330537 | 1546624596 | 1544120379 | 1542771586 | 1546411354 | 1543875535 | 1547072436 | 1538055130 | 1538430871 | 1541673535 |
| META1391 | Rutin | 986562393.2 | 554126936.7 | 499566342.5 | 1780396543 | 644854881.8 | 3483394639 | 42588818.41 | 348703829.1 | 3040533607 | 36361593.72 | 3217210182 | 1375863660 |
| META844 | Acetylcadaverine | 1057287535 | 1051891424 | 1417104412 | 1416303370 | 1417791024 | 1416495730 | 1053419738 | 1415128836 | 1411245327 | 1421831457 | 1426546326 | 1418829750 |
| META2847 | (3beta,24R,24'R)-fucosterol epoxide | 591516582.6 | 1551508836 | 1200160852 | 2066311552 | 1232000953 | 778007957.6 | 246072205.3 | 1929682294 | 555308572.5 | 1609398999 | 433252459.6 | 1048324343 |
| META977 | Bis(4-ethylbenzylidene)sorbitol | 872297327.1 | 871150119.2 | 872398323 | 875484225.7 | 869163748.2 | 1081691453 | 1327294156 | 1015844842 | 1277796750 | 869461985.5 | 871054643.1 | 935251659.4 |
| META1888 | sphinganine | 883341668.3 | 883030970.3 | 884394664.1 | 884711570.4 | 887757078.6 | 880060489.1 | 1009968455 | 882113153.2 | 914249903.7 | 881562750.4 | 1022863567 | 1024454465 |
| META1848 | Diethylpyrocarbonate | 639845495.2 | 49139714.11 | 910825635.6 | 902422707.4 | 641019199.3 | 446884106.5 | 2087949895 | 267985602.7 | 2713424268 | 16624973.79 | 924836195.2 | 628963357.8 |