

**Supporting Information for**  
**Toward the Rational Design of Sustainable Hair Dyes**  
**Using Cheminformatics Approaches:**  
**Step 1. Database Development and Analysis**

Tova N. Williams,<sup>\*,1</sup> Melaine A. Kuenemann,<sup>2</sup> George A. Van Den Driessche,<sup>2</sup>

Antony J. Williams,<sup>3</sup> Denis Fourches,<sup>2</sup> and Harold S. Freeman<sup>\*,1</sup>

1. *Fiber and Polymer Science Program, North Carolina State University, 1020 Main Campus Drive, Raleigh, North Carolina, 27606, United States.*
2. *Department of Chemistry, Bioinformatics Research Center, North Carolina State University, 1 Lampe Drive, Raleigh, North Carolina, 27607, United States.*
3. *National Center for Computational Toxicology, United States Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Park, North Carolina, 27711, United States.*

**No. of Pages – 84**

**No. of Figures – 1**

**No. of Tables – 7**

## 1. Hair Dye Substance Database (HDSD)

**Table S1.** Hair Dye Substance Database (HDSD) contents.

Full HDSD Excel sheet and SDF available at: <https://doi.org/10.6084/m9.figshare.5505856>

| HDSD_ID | Substance Name                        | CASRNs                            | DTXIDs                                   | Cluster | Substance Type | Dye Type  | Dye Color | Dye Chromophore |
|---------|---------------------------------------|-----------------------------------|------------------------------------------|---------|----------------|-----------|-----------|-----------------|
| 1       | 1,2,3,4-Tetrahydro-6-nitroquinoxaline | 41959-35-7,<br>158006-54-3 (Salt) | DTXSID70436630,<br>DTXSID70436630 (Salt) | 1       | Dye            | Semiperm. | Yellow    | Nitro           |
| 2       | 1,2,3-Trihydroxybenzene               | 87-66-1                           | DTXSID6025983                            | 2       | Precursor      |           |           |                 |
| 3       | 1,2,4-Benzenetriacetate               | 613-03-6                          | DTXSID60873914                           | 1       | Not Assigned   |           |           |                 |
| 4       | 1,2,4-Trihydroxybenzene               | 533-73-3                          | DTXSID3040930                            | 2       | Precursor      |           |           |                 |
| 5       | 1,3,5-Trihydroxybenzene               | 108-73-6                          | DTXSID9048354                            | 2       | Precursor      |           |           |                 |
| 6       | 1,3-Bis-(2,4-diaminophenoxy)-propane  | 81892-72-0,<br>74918-21-1 (Salt)  | DTXSID80868327,<br>DTXSID40225891 (Salt) | 1       | Precursor      |           |           |                 |

|    |                                        |                                    |                                          |   |           |  |  |  |
|----|----------------------------------------|------------------------------------|------------------------------------------|---|-----------|--|--|--|
| 7  | 1,5-Naphthalenediol                    | 83-56-7                            | DTXSID2052574                            | 2 | Precursor |  |  |  |
| 8  | 1,7-Naphthalenediol                    | 575-38-2                           | DTXSID0060359                            | 2 | Precursor |  |  |  |
| 9  | 1-Acetoxy-2-methoxynaphthalene         | 27581-07-3                         | DTXSID80873456                           | 2 | Precursor |  |  |  |
| 10 | 1-Acetoxy-2-methylnaphthalene          | 5697-02-9                          | DTXSID30205546                           | 2 | Precursor |  |  |  |
| 11 | 1-Hydroxyethyl-4,5-diaminopyrazole     | 155601-17-5,<br>155601-30-2 (Salt) | DTXSID60437818,<br>DTXSID20165928 (Salt) | 3 | Precursor |  |  |  |
| 12 | 1-Naphthol                             | 90-15-3                            | DTXSID6021793                            | 2 | Precursor |  |  |  |
| 13 | 1-Beta-Hydroxyethyl-2,4-diaminobenzene | 14572-93-1                         | DTXSID10436215                           | 2 | Precursor |  |  |  |
| 14 | 2,2'-Methylenebis-4-aminophenol        | 63969-46-0,<br>27311-52-0 (Salt)   | DTXSID30213808,<br>DTXSID10181758 (Salt) | 2 | Precursor |  |  |  |

|    |                                         |                                                                            |                                                                                            |   |           |  |  |  |
|----|-----------------------------------------|----------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|---|-----------|--|--|--|
| 15 | 2,3-Diaminodihydroxy-pyrazolopyrazolone | 857035-94-0,<br>857035-95-1 (Salt)                                         | DTXSID30235005,<br>DTXSID90235006 (Salt)                                                   | 3 | Precursor |  |  |  |
| 16 | 2,3-Indolinedione                       | 91-56-5                                                                    | DTXSID3038694                                                                              | 4 | Precursor |  |  |  |
| 17 | 2,3-Naphthalenediol                     | 92-44-4                                                                    | DTXSID2043903                                                                              | 2 | Precursor |  |  |  |
| 18 | 2,4,5,6-Tetraaminopyrimidine            | 1004-74-6,<br>49647-58-7 (Salt),<br>5392-28-9 (Salt),<br>39944-62-2 (Salt) | DTXSID9043807,<br>DTXSID20892469 (Salt),<br>DTXSID0037023 (Salt),<br>DTXSID90494393 (Salt) | 3 | Precursor |  |  |  |
| 19 | 2,4,5-Trihydroxytoluene                 | 1124-09-0                                                                  | DTXSID70150026                                                                             | 2 | Precursor |  |  |  |
| 20 | 2,4-Diamino-5-methylphenetol            | 141614-04-2,<br>113715-25-6 (Salt)                                         | DTXSID60578432,<br>DTXSID30150542 (Salt)                                                   | 2 | Precursor |  |  |  |
| 21 | 2,4-Diamino-5-methylphenoxyethanol      | 141614-05-3,<br>113715-27-8 (Salt)                                         | DTXSID30621727,<br>DTXSID90150543 (Salt)                                                   | 2 | Precursor |  |  |  |
| 22 | 2,4-Diaminoanisole                      | 615-05-4,<br>39156-41-7 (Salt)                                             | DTXSID5041358,<br>DTXSID7020398 (Salt)                                                     | 2 | Precursor |  |  |  |

|    |                                                |                                                        |                                                                  |   |           |           |        |     |
|----|------------------------------------------------|--------------------------------------------------------|------------------------------------------------------------------|---|-----------|-----------|--------|-----|
| 23 | 2,4-Diaminodiphenylamine                       | 136-17-4                                               | DTXSID10159619                                                   | 2 | Precursor |           |        |     |
| 24 | 2,4-Diaminophenol                              | 95-86-3,<br>137-09-7 (Salt)                            | DTXSID7043748,<br>DTXSID9020401 (Salt)                           | 2 | Precursor |           |        |     |
| 25 | 2,4-Diaminophenoxyethanol                      | 70643-19-5,<br>66422-95-5 (Salt),<br>70643-20-8 (Salt) | DTXSID0073619,<br>DTXSID3070462 (Salt),<br>DTXSID70892454 (Salt) | 2 | Precursor |           |        |     |
| 26 | 2,4-Diaminotoluene                             | 95-80-7                                                | DTXSID4020402                                                    | 2 | Precursor |           |        |     |
| 27 | 2,5,6-Triamino-4-pyrimidinol                   | 1004-75-7,<br>35011-47-3 (Salt)                        | DTXSID3061396,<br>DTXSID80192518 (Salt)                          | 3 | Precursor |           |        |     |
| 28 | 2,5-Diaminoanisole                             | 5307-02-8                                              | DTXSID7063766                                                    | 2 | Precursor |           |        |     |
| 29 | 2,6-Bis(2-hydroxyethoxy)-3,5-pyridinediamine   | 117907-42-3,<br>85679-72-7 (Salt)                      | DTXSID90698192,<br>DTXSID70234956 (Salt)                         | 3 | Precursor |           |        |     |
| 30 | 2,6-Diamino-3-<br>((pyridine-3-yl)azo)pyridine | 28365-08-4                                             | DTXSID90182607                                                   | 3 | Dye       | Semiperm. | Yellow | Azo |

|    |                                               |                               |                                       |   |              |  |  |  |
|----|-----------------------------------------------|-------------------------------|---------------------------------------|---|--------------|--|--|--|
| 31 | 2,6-Diaminopyridine                           | 141-86-6                      | DTXSID0040127                         | 3 | Precursor    |  |  |  |
| 32 | 2,6-Diaminotoluene                            | 823-40-5                      | DTXSID4027319                         | 2 | Not Assigned |  |  |  |
| 33 | 2,6-Dihydroxy-3,4-dimethylpyridine            | 84540-47-6                    | DTXSID50233528                        | 3 | Precursor    |  |  |  |
| 34 | 2,6-Dihydroxy-4-methylpyridine                | 4664-16-8                     | DTXSID60196892                        | 3 | Precursor    |  |  |  |
| 35 | 2,6-Dihydroxyethylaminotoluene (HC Violet AS) | 149330-25-6                   | DTXSID30164225                        | 2 | Not Assigned |  |  |  |
| 36 | 2,6-Dimethoxy-3,5-pyridinediamine             | 85679-78-3, 56216-28-5 (Salt) | DTXSID10388503, DTXSID10388503 (Salt) | 3 | Precursor    |  |  |  |
| 37 | 2,6-Dinitrotoluene                            | 606-20-2                      | DTXSID5020528                         | 1 | Not Assigned |  |  |  |
| 38 | 2,7-Naphthalenediol                           | 582-17-2                      | DTXSID2060387                         | 2 | Precursor    |  |  |  |

|    |                                    |                                    |                                        |   |           |           |              |       |
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| 39 | 2-Amino-3-hydroxypyridine          | 16867-03-1                         | DTXSID50168588                         | 3 | Precursor |           |              |       |
| 40 | 2-Amino-3-nitrophenol              | 603-85-0                           | DTXSID70209063                         | 1 | Dye       | Semiperm. | Orange       | Nitro |
| 41 | 2-Amino-4,6-dinitrophenol          | 96-91-3,<br>831-52-7 (Salt)        | DTXSID5024479                          | 1 | Dye       | Semiperm. | Red          | Nitro |
| 42 | 2-Amino-4-hydroxyethylaminoanisole | 83763-47-7,<br>83763-48-8 (Salt)   | DTXSID50232617                         | 2 | Precursor |           |              |       |
| 43 | 2-Amino-4-nitrophenol              | 99-57-0                            | DTXSID6020062                          | 1 | Dye       | Semiperm. | Yellow       | Nitro |
| 44 | 2-Amino-5-ethylphenol              | 182499-90-7,<br>149861-22-3 (Salt) | DTXSID40405691                         | 2 | Precursor |           |              |       |
| 45 | 2-Amino-5-nitrophenol              | 121-88-0                           | DTXSID1020063                          | 1 | Dye       | Semiperm. | Not Assigned | Nitro |
| 46 | 2-Amino-6-chloro-4-nitrophenol     | 6358-08-3,<br>62625-14-3 (Salt)    | DTXSID3074868,<br>DTXSID0024472 (Salt) | 1 | Dye       | Semiperm. | Orange       | Nitro |

|    |                                                                      |                                                    |                                                                 |   |           |           |              |                |
|----|----------------------------------------------------------------------|----------------------------------------------------|-----------------------------------------------------------------|---|-----------|-----------|--------------|----------------|
| 47 | 2-Amino-methyl- <i>p</i> -aminophenol                                | 79352-72-0,<br>135043-64-0 (Salt)                  | DTXSID80420186,<br>DTXSID80159227 (Salt)                        | 2 | Precursor |           |              |                |
| 48 | 2-Chloro-5-nitro- <i>N</i> -hydroxyethyl- <i>p</i> -phenylenediamine | 50610-28-1                                         | DTXSID90866157                                                  | 1 | Dye       | Semiperm. | Red          | Nitro          |
| 49 | 2-Chloro-6-ethylamino-4-nitrophenol                                  | 131657-78-8                                        | DTXSID00157169                                                  | 1 | Dye       | Semiperm. | Orange       | Nitro          |
| 50 | 2-Chloro- <i>p</i> -phenylenediamine                                 | 615-66-7,<br>61702-44-1 (Salt),<br>615-46-3 (Salt) | DTXSID3043944,<br>DTXSID0020284 (Salt),<br>DTXSID9060651 (Salt) | 2 | Precursor |           |              |                |
| 51 | 2-Hydroxyethyl picramic acid                                         | 99610-72-7                                         | DTXSID40244163                                                  | 1 | Dye       | Semiperm. | Red          | Nitro          |
| 52 | 2-Hydroxyethylamino-5-nitroanisole                                   | 66095-81-6                                         | DTXSID50867206                                                  | 1 | Dye       | Semiperm. | Not Assigned | Nitro          |
| 53 | 2-Hydroxynaphthoquinone                                              | 83-72-7                                            | DTXSID2025428                                                   | 5 | Dye       | Semiperm. | Orange       | Naphthoquinone |
| 54 | 2-methoxy-4-nitrophenol                                              | 3251-56-7                                          | DTXSID4062935                                                   | 1 | Dye       | Semiperm. | Not Assigned | Nitro          |

|    |                                                      |                                    |                                          |   |           |           |                 |       |
|----|------------------------------------------------------|------------------------------------|------------------------------------------|---|-----------|-----------|-----------------|-------|
| 55 | 2-Methoxymethyl- <i>p</i> -phenylenediamine          | 337906-36-2,<br>337906-37-3 (Salt) | DTXSID50187451,<br>DTXSID10187452 (Salt) | 2 | Precursor |           |                 |       |
| 56 | 2-Methyl-1-naphthol                                  | 7469-77-4                          | DTXSID50225665                           | 2 | Precursor |           |                 |       |
| 57 | 2-Methyl-4-nitroaniline                              | 99-52-5                            | DTXSID3025629                            | 1 | Precursor |           |                 |       |
| 58 | 2-Methyl-5-aminophenol                               | 2835-95-2                          | DTXSID9024489                            | 2 | Precursor |           |                 |       |
| 59 | 2-Methylresorcinol                                   | 608-25-3                           | DTXSID0025571                            | 2 | Precursor |           |                 |       |
| 60 | 2-Nitro-5-glyceryl methylaniline                     | 80062-31-3                         | DTXSID50868556                           | 1 | Dye       | Semiperm. | Not<br>Assigned | Nitro |
| 61 | 2-Nitro- <i>N</i> -hydroxyethyl- <i>p</i> -anisidine | 57524-53-5                         | DTXSID70206133                           | 1 | Dye       | Semiperm. | Not<br>Assigned | Nitro |
| 62 | 2-Nitro- <i>p</i> -phenylenediamine                  | 5307-14-2                          | DTXSID4020957                            | 1 | Dye       | Semiperm. | Red             | Nitro |

|    |                             |                                  |                                          |   |           |  |  |  |
|----|-----------------------------|----------------------------------|------------------------------------------|---|-----------|--|--|--|
| 63 | 3,3'-Dihydroxydiphenylamine | 65461-91-8                       | DTXSID30215786                           | 2 | Precursor |  |  |  |
| 64 | 3,4-Diaminobenzoic acid     | 619-05-6                         | DTXSID00210920                           | 2 | Precursor |  |  |  |
| 65 | 3,4-Diaminotoluene          | 496-72-0                         | DTXSID9024930                            | 2 | Precursor |  |  |  |
| 66 | 3,4-Dihydroxyaniline        | 13047-04-6                       | DTXSID30156569                           | 2 | Precursor |  |  |  |
| 67 | 3,4-Methylenedioxyaniline   | 14268-66-7                       | DTXSID8065743                            | 2 | Precursor |  |  |  |
| 68 | 3,4-Methylenedioxyphenol    | 533-31-3                         | DTXSID9021267                            | 2 | Precursor |  |  |  |
| 69 | 3-Amino-2,4-dichlorophenol  | 61693-42-3,<br>61693-43-4 (Salt) | DTXSID20210684,<br>DTXSID80210685 (Salt) | 2 | Precursor |  |  |  |
| 70 | 3-Chloro-4-aminophenol      | 17609-80-2                       | DTXSID30170083                           | 2 | Precursor |  |  |  |

|    |                                                           |                                    |                                          |   |              |           |              |       |
|----|-----------------------------------------------------------|------------------------------------|------------------------------------------|---|--------------|-----------|--------------|-------|
| 71 | 3-Methylamino-4-nitrophenoxyethanol                       | 59820-63-2                         | DTXSID30208552                           | 1 | Dye          | Semiperm. | Yellow       | Nitro |
| 72 | 3-Nitro-4-aminophenoxyethanol                             | 50982-74-6                         | DTXSID70198983                           | 1 | Dye          | Semiperm. | Not Assigned | Nitro |
| 73 | 3-Nitro- <i>p</i> -cresol                                 | 2042-14-0                          | DTXSID90879085                           | 1 | Not Assigned |           |              |       |
| 74 | 3-Nitro- <i>p</i> -hydroxyethylaminophenol<br>(HC Red 54) | 65235-31-6                         | DTXSID00215536                           | 1 | Dye          | Semiperm. | Red          | Nitro |
| 75 | 4-(Methylamino)-2,6-dinitrophenol                         | 20291-98-9                         | DTXSID90174168                           | 1 | Dye          | Semiperm. | Violet       | Nitro |
| 76 | 4,4'-Diaminodiphenylamine                                 | 537-65-5                           | DTXSID1060217                            | 2 | Precursor    |           |              |       |
| 77 | 4,5-Diamino-1-((4-chlorophenyl)methyl)-1H-pyrazole        | 157469-55-1,<br>163183-00-4 (Salt) | DTXSID20873915,<br>DTXSID90892456 (Salt) | 3 | Precursor    |           |              |       |
| 78 | 4,5-Diamino-1-methylpyrazole                              | 45514-38-3,<br>21616-59-1 (Salt)   | DTXSID30437805,<br>DTXSID30437805 (Salt) | 3 | Precursor    |           |              |       |

|    |                                                      |                                  |                                          |   |           |           |              |       |
|----|------------------------------------------------------|----------------------------------|------------------------------------------|---|-----------|-----------|--------------|-------|
| 79 | 4,6-Bis(2-hydroxyethoxy)- <i>m</i> -phenylenediamine | 94082-77-6,<br>94082-85-6 (Salt) | DTXSID00578431,<br>DTXSID20240380 (Salt) | 1 | Precursor |           |              |       |
| 80 | 4-Amino-2-nitrodiphenylamine-2'-carboxylic acid      | 117907-43-4                      | DTXSID70151952                           | 1 | Dye       | Semiperm. | Red          | Nitro |
| 81 | 4-Amino-2-nitrophenol                                | 119-34-6                         | DTXSID6020064                            | 1 | Dye       | Semiperm. | Not Assigned | Nitro |
| 82 | 4-Amino-3-fluorophenol                               | 399-95-1                         | DTXSID60192950                           | 2 | Precursor |           |              |       |
| 83 | 4-Amino-3-nitrophenol                                | 610-81-1                         | DTXSID50209864                           | 1 | Dye       | Semiperm. | Orange       | Nitro |
| 84 | 4-Aminobenzenesulfonic acid                          | 121-57-3                         | DTXSID6024464                            | 2 | Precursor |           |              |       |
| 85 | 4-Amino- <i>m</i> -cresol                            | 2835-99-6                        | DTXSID2049262                            | 2 | Precursor |           |              |       |
| 86 | 4-Amino- <i>o</i> -cresol                            | 2835-96-3                        | DTXSID2062662                            | 2 | Precursor |           |              |       |

|    |                                                |                                 |                                          |   |              |           |              |       |
|----|------------------------------------------------|---------------------------------|------------------------------------------|---|--------------|-----------|--------------|-------|
| 87 | 4-Chloro-2-aminophenol                         | 95-85-2                         | DTXSID5024473                            | 2 | Precursor    |           |              |       |
| 88 | 4-Chlororesorcinol                             | 95-88-5                         | DTXSID8052643                            | 2 | Precursor    |           |              |       |
| 89 | 4-Ethoxy- <i>m</i> -phenylenediamine           | 5862-77-1                       | DTXSID80207333                           | 2 | Precursor    |           |              |       |
| 90 | 4-Ethylamino-3-nitrobenzoic acid               | 2788-74-1                       | DTXSID00182178                           | 1 | Dye          | Semiperm. | Not Assigned | Nitro |
| 91 | 4-Hydroxyindole                                | 2380-94-1                       | DTXSID3057696                            | 3 | Precursor    |           |              |       |
| 92 | 4-Hydroxypropylamino-3-nitrophenol (HC Red BN) | 92952-81-3                      | DTXSID70239209                           | 1 | Dye          | Semiperm. | Red          | Nitro |
| 93 | 4-Methoxy-3-aminophenol                        | 29644-12-0                      | DTXSID80605714                           | 2 | Precursor    |           |              |       |
| 94 | 4-Methoxytoluene-2,5-diamine                   | 5307-00-6,<br>56496-88-9 (Salt) | DTXSID90201145,<br>DTXSID20205035 (Salt) | 2 | Not Assigned |           |              |       |

|     |                                             |                                                    |                                                                  |   |           |           |              |       |
|-----|---------------------------------------------|----------------------------------------------------|------------------------------------------------------------------|---|-----------|-----------|--------------|-------|
| 95  | 4-Nitro- <i>m</i> -phenylenediamine         | 5131-58-8                                          | DTXSID1025770                                                    | 1 | Dye       | Semiperm. | Not Assigned | Nitro |
| 96  | 4-Nitro- <i>o</i> -phenylenediamine         | 99-56-9,<br>68239-82-7 (Salt),<br>6219-77-8 (Salt) | DTXSID9020958,<br>DTXSID50887308 (Salt),<br>DTXSID8064141 (Salt) | 1 | Dye       | Semiperm. | Yellow       | Nitro |
| 97  | 4-Nitrophenyl aminoethylurea                | 27080-42-8                                         | DTXSID80873916                                                   | 1 | Dye       | Semiperm. | Not Assigned | Nitro |
| 98  | 5-((2-Hydroxyethyl)amino)- <i>o</i> -cresol | 55302-96-0                                         | DTXSID70203849                                                   | 2 | Precursor |           |              |       |
| 99  | 5,6-Dihydroxyindoline                       | 3131-52-0                                          | DTXSID20185242                                                   | 3 | Precursor |           |              |       |
| 100 | 5-Amino-2,6-dimethoxy-3-hydroxypyridine     | 104333-03-1                                        | DTXSID00146396                                                   | 3 | Precursor |           |              |       |
| 101 | 5-Amino-4-chloro- <i>o</i> -cresol          | 110102-86-8,<br>110102-85-7 (Salt)                 | DTXSID00149145,<br>DTXSID00149145 (Salt)                         | 2 | Precursor |           |              |       |
| 102 | 5-Amino-4-fluoro-2-methylphenol             | 122455-85-0,<br>163183-01-5 (Salt)                 | DTXSID40436208,<br>DTXSID90892456 (Salt)                         | 2 | Precursor |           |              |       |

|     |                                    |                                  |                                          |   |           |  |  |  |
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| 103 | 5-Amino-6-chloro- <i>o</i> -cresol | 84540-50-1,<br>80419-48-3 (Salt) | DTXSID80233531,<br>DTXSID20230307 (Salt) | 2 | Precursor |  |  |  |
| 104 | 5-Chloro-2-aminophenol             | 28443-50-7                       | DTXSID6067385                            | 2 | Precursor |  |  |  |
| 105 | 5-Hydroxy-1,4-benzodioxane         | 10288-36-5                       | DTXSID10145557                           | 2 | Precursor |  |  |  |
| 106 | 5-Methylresorcinol                 | 504-15-4                         | DTXSID2060123                            | 2 | Precursor |  |  |  |
| 107 | 6-Amino- <i>m</i> -cresol          | 2835-98-5                        | DTXSID20182594                           | 2 | Precursor |  |  |  |
| 108 | 6-Amino- <i>o</i> -cresol          | 17672-22-9                       | DTXSID80170179                           | 2 | Precursor |  |  |  |
| 109 | 6-Hydroxybenzomorpholine           | 26021-57-8                       | DTXSID20180671                           | 2 | Precursor |  |  |  |
| 110 | 6-Hydroxyindole                    | 2380-86-1                        | DTXSID20178497                           | 3 | Precursor |  |  |  |

|     |                               |                                  |                                          |   |           |                      |                 |                |
|-----|-------------------------------|----------------------------------|------------------------------------------|---|-----------|----------------------|-----------------|----------------|
| 111 | 6-Methoxy-2,3-pyridinediamine | 28020-38-4,<br>94166-62-8 (Salt) | DTXSID80388570,<br>DTXSID30240917 (Salt) | 3 | Precursor |                      |                 |                |
| 112 | 6-Nitro-2,5-pyridinediamine   | 69825-83-8                       | DTXSID30220113                           | 3 | Dye       | Semiperm.            | Not<br>Assigned | Nitro          |
| 113 | 6-Nitro- <i>o</i> -toluidine  | 570-24-1                         | DTXSID7025631                            | 1 | Dye       | Semiperm.            | Not<br>Assigned | Nitro          |
| 114 | C.I. Acid Black 1             | 1064-48-8                        | DTXSID1024415                            | 5 | Dye       | Semiperm.            | Black           | Azo            |
| 115 | C.I. Acid Blue 1              | 129-17-9                         | DTXSID3026065                            | 6 | Dye       | Semiperm.            | Blue            | Triarylmethane |
| 116 | C.I. Acid Blue 3              | 3536-49-0                        | DTXSID00873918                           | 6 | Dye       | Semiperm.            | Blue            | Triarylmethane |
| 117 | C.I. Acid Blue 62             | 4368-56-3                        | DTXSID3044673                            | 5 | Dye       | Temp./Semi-<br>perm. | Blue            | Anthraquinone  |
| 118 | C.I. Acid Blue 74             | 860-22-0                         | DTXSID1020190                            | 4 | Dye       | Semiperm.            | Blue            | Indigoid       |

|     |                     |           |                |   |     |                  |        |                |
|-----|---------------------|-----------|----------------|---|-----|------------------|--------|----------------|
| 119 | C.I. Acid Blue 9    | 2650-18-2 | DTXSID4034310  | 6 | Dye | Temp./Semi-perm. | Blue   | Triarylmethane |
| 120 | C.I. Acid Brown 13  | 6373-79-1 | DTXSID10873924 | 7 | Dye | Semiperm.        | Brown  | Nitro          |
| 121 | C.I. Acid Green 25  | 4403-90-1 | DTXSID2024903  | 5 | Dye | Temp./Semi-perm. | Green  | Anthraquinone  |
| 122 | C.I. Acid Green 50  | 3087-16-9 | DTXSID4046577  | 6 | Dye | Semiperm.        | Green  | Triarylmethane |
| 123 | C.I. Acid Orange 10 | 1936-15-8 | DTXSID6021082  | 5 | Dye | Semiperm.        | Orange | Azo            |
| 124 | C.I. Acid Orange 24 | 1320-07-6 | DTXSID7041708  | 8 | Dye | Temp./Semi-perm. | Orange | Azo            |
| 125 | C.I. Acid Orange 3  | 6373-74-6 | DTXSID1021081  | 1 | Dye | Temp./Semi-perm. | Orange | Nitro          |
| 126 | C.I. Acid Orange 6  | 547-57-9  | DTXSID70873925 | 8 | Dye | Semiperm.        | Orange | Azo            |

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| 127 | C.I. Acid Orange 7 | 633-96-5   | DTXSID0038881 | 5 | Dye | Temp./Semi-perm. | Orange | Azo      |
| 128 | C.I. Acid Red 14   | 3567-69-9  | DTXSID3021225 | 8 | Dye | Semiperm.        | Red    | Azo      |
| 129 | C.I. Acid Red 18   | 2611-82-7  | DTXSID9021213 | 5 | Dye | Temp./Semi-perm. | Red    | Azo      |
| 130 | C.I. Acid Red 27   | 915-67-3   | DTXSID2021232 | 5 | Dye | Semiperm.        | Red    | Azo      |
| 131 | C.I. Acid Red 33   | 3567-66-6  | DTXSID1044562 | 5 | Dye | Temp./Semi-perm. | Red    | Azo      |
| 132 | C.I. Acid Red 35   | 6441-93-6  | DTXSID7064360 | 5 | Dye | Semiperm.        | Red    | Azo      |
| 133 | C.I. Acid Red 51   | 16423-68-0 | DTXSID7021233 | 4 | Dye | Semiperm.        | Red    | Xanthene |
| 134 | C.I. Acid Red 52   | 3520-42-1  | DTXSID7021235 | 4 | Dye | Temp./Semi-perm. | Red    | Xanthene |

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| 135 | C.I. Acid Red 73    | 5413-75-2  | DTXSID1041712 | 8 | Dye | Semiperm.        | Red    | Azo            |
| 136 | C.I. Acid Red 87    | 17372-87-1 | DTXSID0025234 | 9 | Dye | Temp./Semi-perm. | Red    | Xanthene       |
| 137 | C.I. Acid Red 92    | 18472-87-2 | DTXSID1031090 | 9 | Dye | Semiperm.        | Red    | Xanthene       |
| 138 | C.I. Acid Red 95    | 33239-19-9 | DTXSID6091552 | 4 | Dye | Semiperm.        | Red    | Xanthene       |
| 139 | C.I. Acid Violet 43 | 4430-18-6  | DTXSID6041717 | 5 | Dye | Temp./Semi-perm. | Violet | Anthraquinone  |
| 140 | C.I. Acid Violet 49 | 1694-09-3  | DTXSID7021441 | 6 | Dye | Temp.            | Violet | Triarylmethane |
| 141 | C.I. Acid Violet 9  | 6252-76-2  | DTXSID3044968 | 8 | Dye | Semiperm.        | Violet | Xanthene       |
| 142 | C.I. Acid Yellow 1  | 846-70-8   | DTXSID1041718 | 1 | Dye | Semiperm.        | Yellow | Nitro          |

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| 143 | C.I. Acid Yellow 23 | 1934-21-0  | DTXSID1021455  | 3 | Dye | Temp./Semi-perm. | Yellow | Azo            |
| 144 | C.I. Acid Yellow 36 | 587-98-4   | DTXSID5041722  | 2 | Dye | Semiperm.        | Yellow | Azo            |
| 145 | C.I. Acid Yellow 73 | 518-47-8   | DTXSID9025328  | 4 | Dye | Semiperm.        | Yellow | Xanthene       |
| 146 | C.I. Basic Blue 26  | 2580-56-5  | DTXSID0038889  | 6 | Dye | Semiperm.        | Blue   | Triarylmethane |
| 147 | C.I. Basic Blue 3   | 55840-82-9 | DTXSID8051384  | 4 | Dye | Semiperm.        | Blue   | Oxazine        |
| 148 | C.I. Basic Blue 41  | 12270-13-2 | DTXSID3051624  | 3 | Dye | Semiperm.        | Blue   | Azo            |
| 149 | C.I. Basic Blue 47  | 12217-43-5 | DTXSID10153531 | 5 | Dye | Semiperm.        | Blue   | Anthraquinone  |
| 150 | C.I. Basic Blue 54  | 15000-59-6 | DTXSID30879827 | 3 | Dye | Semiperm.        | Blue   | Azo            |

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| 151 | C.I. Basic Blue 6   | 966-62-1    | DTXSID40874040 | 4 | Dye | Semiperm.            | Blue  | Oxazine            |
| 152 | C.I. Basic Blue 7   | 2390-60-5   | DTXSID5038888  | 6 | Dye | Semiperm.            | Blue  | Triarylmethane     |
| 153 | C.I. Basic Blue 9   | 61-73-4     | DTXSID0023296  | 4 | Dye | Semiperm.            | Blue  | Thiazine           |
| 154 | C.I. Basic Blue 99  | 68123-13-7  | DTXSID60874042 | 5 | Dye | Temp./Semi-<br>perm. | Blue  | Iminonapthoquinone |
| 155 | C.I. Basic Brown 1  | 10114-58-6  | DTXSID5024558  | 8 | Dye | Semiperm.            | Brown | Azo                |
| 156 | C.I. Basic Brown 16 | 26381-41-9  | DTXSID20874043 | 8 | Dye | Temp./Semi-<br>perm. | Brown | Azo                |
| 157 | C.I. Basic Brown 17 | 176742-32-8 | DTXSID50879829 | 8 | Dye | Temp./Semi-<br>perm. | Brown | Azo                |
| 158 | C.I. Basic Brown 4  | 8005-78-5   | DTXSID60892281 | 8 | Dye | Semiperm.            | Brown | Azo                |

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| 159 | C.I. Basic Green 1   | 633-03-4    | DTXSID1048700  | 6 | Dye | Semiperm. | Green  | Triarylmethane |
| 160 | C.I. Basic Green 4   | 569-64-2    | DTXSID1025512  | 6 | Dye | Semiperm. | Green  | Triarylmethane |
| 161 | C.I. Basic Orange 1  | 4438-16-8   | DTXSID3063467  | 2 | Dye | Semiperm. | Orange | Azo            |
| 162 | C.I. Basic Orange 2  | 532-82-1    | DTXSID0024559  | 2 | Dye | Semiperm. | Orange | Azo            |
| 163 | C.I. Basic Orange 31 | 97404-02-9  | DTXSID40874045 | 3 | Dye | Semiperm. | Orange | Azo            |
| 164 | C.I. Basic Orange 69 | 226940-14-3 | DTXSID20879811 | 8 | Dye | Semiperm. | Orange | Azo            |
| 165 | C.I. Basic Red 1     | 989-38-8    | DTXSID1021243  | 6 | Dye | Semiperm. | Red    | Xanthene       |
| 166 | C.I. Basic Red 14    | 12217-48-0  | DTXSID0041723  | 4 | Dye | Semiperm. | Red    | Methine        |

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| 167 | C.I. Basic Red 2     | 477-73-6   | DTXSID60874047 | 3 | Dye | Semiperm.            | Red    | Azine          |
| 168 | C.I. Basic Red 22    | 12221-52-2 | DTXSID20874048 | 3 | Dye | Semiperm.            | Red    | Azo            |
| 169 | C.I. Basic Red 46    | 12221-69-1 | DTXSID30879822 | 3 | Dye | Semiperm.            | Red    | Azo            |
| 170 | C.I. Basic Red 51    | 77061-58-6 | DTXSID80874049 | 3 | Dye | Semiperm.            | Red    | Azo            |
| 171 | C.I. Basic Red 76    | 68391-30-0 | DTXSID10879784 | 8 | Dye | Temp./Semi-<br>perm. | Red    | Azo            |
| 172 | C.I. Basic Red 9     | 569-61-9   | DTXSID1021247  | 5 | Dye | Not<br>Assigned      | Red    | Triarylmethane |
| 173 | C.I. Basic Violet 1  | 8004-87-3  | DTXSID8046666  | 6 | Dye | Semiperm.            | Violet | Triarylmethane |
| 174 | C.I. Basic Violet 10 | 81-88-9    | DTXSID6042369  | 4 | Dye | Semiperm.            | Violet | Xanthene       |

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| 175 | C.I. Basic Violet 11 | 2390-63-8  | DTXSID5051737  | 4 | Dye | Semiperm. | Violet | Xanthene        |
| 176 | C.I. Basic Violet 14 | 632-99-5   | DTXSID6021246  | 5 | Dye | Semiperm. | Violet | Triarylmethane  |
| 177 | C.I. Basic Violet 16 | 6359-45-1  | DTXSID6052320  | 4 | Dye | Semiperm. | Violet | Methine         |
| 178 | C.I. Basic Violet 2  | 3248-91-7  | DTXSID80879817 | 5 | Dye | Semiperm. | Violet | Triarylmethane  |
| 179 | C.I. Basic Violet 3  | 548-62-9   | DTXSID5020653  | 6 | Dye | Semiperm. | Violet | Triarylmethane  |
| 180 | C.I. Basic Violet 4  | 2390-59-2  | DTXSID5038913  | 6 | Dye | Semiperm. | Violet | Triarylmethane  |
| 181 | C.I. Basic Yellow 11 | 4208-80-4  | DTXSID5052092  | 4 | Dye | Semiperm. | Yellow | Azacyanobenzene |
| 182 | C.I. Basic Yellow 13 | 12217-50-4 | DTXSID40879818 | 4 | Dye | Semiperm. | Yellow | Azacyanobenzene |

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| 183 | C.I. Basic Yellow 2  | 2465-27-2  | DTXSID9020114  | 5 | Dye | Semiperm.            | Yellow | Diphenylmethane  |
| 184 | C.I. Basic Yellow 28 | 54060-92-3 | DTXSID20879816 | 4 | Dye | Semiperm.            | Yellow | Dizacarbocyanine |
| 185 | C.I. Basic Yellow 29 | 68134-38-3 | DTXSID00887196 | 4 | Dye | Semiperm.            | Yellow | Dizacarbocyanine |
| 186 | C.I. Basic Yellow 3  | 2151-60-2  | DTXSID60175849 | 5 | Dye | Semiperm.            | Yellow | Diphenylmethane  |
| 187 | C.I. Basic Yellow 40 | 12221-86-2 | DTXSID30892450 | 3 | Dye | Semiperm.            | Yellow | Coumarin         |
| 188 | C.I. Basic Yellow 57 | 68391-31-1 | DTXSID50275928 | 4 | Dye | Temp./Semi-<br>perm. | Yellow | Azo              |
| 189 | C.I. Basic Yellow 87 | 68259-00-7 | DTXSID9071349  | 3 | Dye | Semiperm.            | Yellow | Dizacarbocyanine |
| 190 | C.I. Direct Black 51 | 3442-21-5  | DTXSID30879786 | 8 | Dye | Temp.                | Black  | Azo              |

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| 191 | C.I. Direct Red 23    | 3441-14-3  | DTXSID90879787 | 7 | Dye | Semiperm.            | Red    | Azo           |
| 192 | C.I. Direct Red 80    | 25188-41-4 | DTXSID0045044  | 7 | Dye | Temp./Semi-<br>perm. | Red    | Azo           |
| 193 | C.I. Direct Red 81    | 3441-14-3  | DTXSID90879787 | 8 | Dye | Semiperm.            | Red    | Azo           |
| 194 | C.I. Direct Violet 48 | 37279-54-2 | DTXSID20879790 | 7 | Dye | Semiperm.            | Violet | Azo           |
| 195 | C.I. Direct Yellow 12 | 2870-32-8  | DTXSID5041728  | 8 | Dye | Semiperm.            | Yellow | Azo           |
| 196 | C.I. Disperse Black 9 | 20721-50-0 | DTXSID7066645  | 1 | Dye | Semiperm.            | Orange | Azo           |
| 197 | C.I. Disperse Blue 1  | 2475-45-8  | DTXSID7020188  | 5 | Dye | Semiperm.            | Blue   | Anthraquinone |
| 198 | C.I. Disperse Blue 3  | 2475-46-9  | DTXSID9041730  | 5 | Dye | Semiperm.            | Blue   | Anthraquinone |

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| 199 | C.I. Disperse Blue 377 | 67674-26-4 | DTXSID2070550  | 5 | Dye | Semiperm. | Blue   | Anthraquinone |
| 200 | C.I. Disperse Blue 7   | 3179-90-6  | DTXSID8025208  | 1 | Dye | Semiperm. | Blue   | Anthraquinone |
| 201 | C.I. Disperse Brown 1  | 23355-64-8 | DTXSID9066883  | 5 | Dye | Semiperm. | Brown  | Azo           |
| 202 | C.I. Disperse Orange 3 | 730-40-5   | DTXSID7061061  | 1 | Dye | Semiperm. | Orange | Azo           |
| 203 | C.I. Disperse Red 11   | 2872-48-2  | DTXSID1062677  | 5 | Dye | Semiperm. | Red    | Anthraquinone |
| 204 | C.I. Disperse Red 15   | 116-85-8   | DTXSID1059440  | 5 | Dye | Semiperm. | Red    | Anthraquinone |
| 205 | C.I. Disperse Red 17   | 3179-89-3  | DTXSID80879791 | 1 | Dye | Semiperm. | Red    | Azo           |
| 206 | C.I. Disperse Violet 1 | 128-95-0   | DTXSID2041252  | 5 | Dye | Semiperm. | Violet | Anthraquinone |

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| 207 | C.I. Disperse Violet 4 | 1220-94-6  | DTXSID8051621  | 5 | Dye | Semiperm.       | Violet | Anthraquinone |
| 208 | C.I. Disperse Yellow 3 | 2832-40-8  | DTXSID6021450  | 8 | Dye | Not<br>Assigned | Yellow | Azo           |
| 209 | C.I. Food Black 1      | 2519-30-4  | DTXSID2020183  | 7 | Dye | Semiperm.       | Black  | Azo           |
| 210 | C.I. Food Black 2      | 2118-39-0  | DTXSID40879792 | 7 | Dye | Not<br>Assigned | Black  | Azo           |
| 211 | C.I. Mordant Black 1   | 16279-54-2 | DTXSID5066031  | 8 | Dye | Not<br>Assigned | Black  | Azo           |
| 212 | C.I. Mordant Red 11    | 72-48-0    | DTXSID5045960  | 5 | Dye | Not<br>Assigned | Red    | Anthraquinone |
| 213 | C.I. Solvent Black 3   | 4197-25-5  | DTXSID0052091  | 8 | Dye | Not<br>Assigned | Black  | Azo           |
| 214 | C.I. Solvent Black 5   | 11099-03-9 | DTXSID0026040  | 3 | Dye | Not<br>Assigned | Black  | Azine         |

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| 215 | C.I. Solvent Blue 35  | 17354-14-2 | DTXSID5044605 | 5 | Dye | Not Assigned | Blue   | Anthraquinone |
| 216 | C.I. Solvent Green 3  | 128-80-3   | DTXSID9044376 | 5 | Dye | Semiperm.    | Green  | Anthraquinone |
| 217 | C.I. Solvent Green 7  | 6358-69-6  | DTXSID4041739 | 8 | Dye | Semiperm.    | Green  | Pyrene        |
| 218 | C.I. Solvent Orange 1 | 2051-85-6  | DTXSID9062146 | 8 | Dye | Not Assigned | Orange | Azo           |
| 219 | C.I. Solvent Red 1    | 1229-55-6  | DTXSID3061635 | 8 | Dye | Not Assigned | Red    | Azo           |
| 220 | C.I. Solvent Red 23   | 85-86-9    | DTXSID3041742 | 8 | Dye | Semiperm.    | Red    | Azo           |
| 221 | C.I. Solvent Red 3    | 6535-42-8  | DTXSID6064402 | 8 | Dye | Not Assigned | Red    | Azo           |
| 222 | C.I. Solvent Red 72   | 596-03-2   | DTXSID7024904 | 4 | Dye | Semiperm.    | Red    | Phthalein     |

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| 223 | C.I. Solvent Violet 13 | 81-48-1    | DTXSID1026293  | 5 | Dye | Semiperm.    | Violet | Anthraquinone  |
| 224 | C.I. Solvent Yellow 29 | 6706-82-7  | DTXSID50879809 | 6 | Dye | Not Assigned | Yellow | Azo            |
| 225 | C.I. Solvent Yellow 33 | 8003-22-3  | DTXSID7024906  | 5 | Dye | Not Assigned | Yellow | Quinoline      |
| 226 | C.I. Solvent Yellow 44 | 2478-20-8  | DTXSID7062453  | 4 | Dye | Not Assigned | Yellow | Naphthalimide  |
| 227 | C.I. Vat Red 1         | 2379-74-0  | DTXSID9058735  | 4 | Dye | Temp.        | Red    | Thioindigoid   |
| 228 | FD&C Green 3           | 2353-45-9  | DTXSID3020673  | 6 | Dye | Temp.        | Green  | Triarylmethane |
| 229 | FD&C Red 4             | 4548-53-2  | DTXSID2021234  | 8 | Dye | Temp.        | Red    | Azo            |
| 230 | FD&C Red 40            | 25956-17-6 | DTXSID4024436  | 8 | Dye | Temp.        | Red    | Azo            |

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| 231 | FD&C Yellow 6 | 2783-94-0                          | DTXSID6021456                            | 8 | Dye | Temp./Semi-<br>perm. | Yellow | Azo            |
| 232 | HC Blue 1     | 2784-94-3                          | DTXSID6020191                            | 1 | Dye | Semiperm.            | Blue   | Nitro          |
| 233 | HC Blue 10    | 102767-27-1,<br>173994-75-7 (Salt) | DTXSID00879793,<br>DTXSID50892457 (Salt) | 1 | Dye | Semiperm.            | Blue   | Nitro          |
| 234 | HC Blue 11    | 3920-15-2, 910463-<br>51-3 (Salt)  | DTXSID60879794,<br>DTXSID30238394 (Salt) | 1 | Dye | Semiperm.            | Blue   | Nitro          |
| 235 | HC Blue 12    | 104516-93-0,<br>132885-85-9 (Salt) | DTXSID70456717,<br>DTXSID10892458 (Salt) | 1 | Dye | Semiperm.            | Blue   | Nitro          |
| 236 | HC Blue 14    | 99788-75-7                         | DTXSID40879813                           | 1 | Dye | Semiperm.            | Blue   | Anthraquinone  |
| 237 | HC Blue 15    | 74578-10-2                         | DTXSID3072793                            | 5 | Dye | Temp./Semi-<br>perm. | Blue   | Triarylmethane |
| 238 | HC Blue 2     | 33229-34-4                         | DTXSID6020193                            | 1 | Dye | Semiperm.            | Blue   | Nitro          |

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| 239 | HC Blue 6   | 93633-79-5,<br>93633-78-4 (Salt)   | DTXSID10420179,<br>DTXSID90892451 (Salt) | 1 | Dye | Semiperm. | Blue   | Nitro         |
| 240 | HC Blue 7   | 90817-34-8, 83732-<br>72-3 (Salt)  | DTXSID80420888,<br>DTXSID80879796 (Salt) | 3 | Dye | Semiperm. | Blue   | Aminopyridine |
| 241 | HC Blue 8   | 22366-99-0,<br>166377-62-4 (Salt)  | DTXSID50176901,<br>DTXSID20168095 (Salt) | 5 | Dye | Semiperm. | Blue   | Anthraquinone |
| 242 | HC Blue 9   | 114087-41-1,<br>209323-30-8 (Salt) | DTXSID70892292,<br>DTXSID00879814 (Salt) | 1 | Dye | Semiperm. | Blue   | Nitro         |
| 243 | HC Brown 1  | 767241-32-7,<br>83803-98-9 (Salt)  | DTXSID40892466,<br>DTXSID40879797 (Salt) | 8 | Dye | Semiperm. | Brown  | Azo           |
| 244 | HC Brown 2  | 774492-40-9,<br>83803-99-0 (Salt)  | DTXSID80892465,<br>DTXSID00879798 (Salt) | 8 | Dye | Semiperm. | Brown  | Azo           |
| 245 | HC Green 1  | 52136-25-1                         | DTXSID60200145                           | 1 | Dye | Semiperm. | Green  | Benzoquinone  |
| 246 | HC Orange 1 | 54381-08-7                         | DTXSID0068949                            | 1 | Dye | Semiperm. | Orange | Nitro         |

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| 247 | HC Orange 2 | 85765-48-6                       | DTXSID30235065                           | 1 | Dye | Semiperm. | Orange | Nitro             |
| 248 | HC Orange 3 | 81612-54-6                       | DTXSID60879799                           | 1 | Dye | Semiperm. | Orange | Nitro             |
| 249 | HC Red 1    | 2784-89-6                        | DTXSID4062640                            | 1 | Dye | Semiperm. | Red    | Nitro             |
| 250 | HC Red 10   | 95576-89-9                       | DTXSID10879800                           | 5 | Dye | Semiperm. | Red    | Iminobenzoquinone |
| 251 | HC Red 11   | 95576-92-4                       | DTXSID70879801                           | 1 | Dye | Semiperm. | Red    | Nitro             |
| 252 | HC Red 13   | 29705-39-3,<br>94158-13-1 (Salt) | DTXSID10183853,<br>DTXSID60240824 (Salt) | 1 | Dye | Semiperm. | Red    | Nitro             |
| 253 | HC Red 16   | 160219-76-1                      | DTXSID70634533                           | 1 | Dye | Semiperm. | Red    | Nitro             |
| 254 | HC Red 3    | 2871-01-4                        | DTXSID2021236                            | 1 | Dye | Semiperm. | Red    | Nitro             |

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| 255 | HC Red 7     | 24905-87-1                       | DTXSID90179613                           | 1 | Dye | Semiperm. | Red    | Nitro             |
| 256 | HC Red 8     | 13556-29-1,<br>97404-14-3 (Salt) | DTXSID40892461,<br>DTXSID00242948 (Salt) | 5 | Dye | Semiperm. | Red    | Anthraquinone     |
| 257 | HC Red 9     | 56330-88-2                       | DTXSID30879802                           | 5 | Dye | Semiperm. | Red    | Iminobenzoquinone |
| 258 | HC Violet 1  | 82576-75-8                       | DTXSID50231887                           | 1 | Dye | Semiperm. | Violet | Nitro             |
| 259 | HC Violet 2  | 104226-19-9                      | DTXSID60146352                           | 1 | Dye | Semiperm. | Violet | Nitro             |
| 260 | HC Yellow 10 | 109023-83-8                      | DTXSID40148798                           | 1 | Dye | Semiperm. | Yellow | Nitro             |
| 261 | HC Yellow 11 | 73388-54-2                       | DTXSID30223629                           | 1 | Dye | Semiperm. | Yellow | Nitro             |
| 262 | HC Yellow 12 | 59320-13-7                       | DTXSID50208059                           | 1 | Dye | Semiperm. | Yellow | Nitro             |

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| 263 | HC Yellow 13 | 10442-83-8  | DTXSID10146483 | 1 | Dye | Semiperm. | Yellow | Nitro |
| 264 | HC Yellow 14 | 90349-40-9  | DTXSID90879803 | 5 | Dye | Semiperm. | Yellow | Nitro |
| 265 | HC Yellow 15 | 138377-66-9 | DTXSID70160645 | 1 | Dye | Semiperm. | Yellow | Nitro |
| 266 | HC Yellow 2  | 4926-55-0   | DTXSID0063650  | 1 | Dye | Semiperm. | Yellow | Nitro |
| 267 | HC Yellow 3  | 56932-45-7  | DTXSID20205479 | 1 | Dye | Semiperm. | Yellow | Nitro |
| 268 | HC Yellow 4  | 59820-43-8  | DTXSID6021458  | 1 | Dye | Semiperm. | Yellow | Nitro |
| 269 | HC Yellow 5  | 56932-44-6  | DTXSID4043939  | 1 | Dye | Semiperm. | Yellow | Nitro |
| 270 | HC Yellow 6  | 104333-00-8 | DTXSID50879804 | 1 | Dye | Semiperm. | Yellow | Nitro |

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|-----|-------------------------------------------------------------|-----------------------------------|------------------------------------------|---|-----------------|-----------|-----------------|-------------------|
| 271 | HC Yellow 7                                                 | 104226-21-3                       | DTXSID10879805                           | 1 | Dye             | Semiperm. | Yellow          | Azo               |
| 272 | HC Yellow 8                                                 | 66612-11-1                        | DTXSID70879806                           | 5 | Dye             | Semiperm. | Yellow          | Iminobenzoquinone |
| 273 | HC Yellow 9                                                 | 141973-33-3,<br>86419-69-4 (Salt) | DTXSID90892294,<br>DTXSID40235536 (Salt) | 1 | Dye             | Semiperm. | Yellow          | Nitro             |
| 274 | Hydroquinone                                                | 123-31-9                          | DTXSID7020716                            | 2 | Precursor       |           |                 |                   |
| 275 | Hydroquinonesulfonic acid                                   | 88-46-0                           | DTXSID8045014                            | 2 | Not<br>Assigned |           |                 |                   |
| 276 | Hydroxyanthraquinone-<br>aminopropyl methyl<br>morpholinium | 47569-30-2,<br>38866-20-5 (Salt)  | DTXSID20865931,<br>DTXSID80192119 (Salt) | 5 | Dye             | Semiperm. | Not<br>Assigned | Anthraquinone     |
| 277 | Hydroxyethyl-2,6-dinitro- <i>p</i> -<br>anisidine           | 122252-11-3                       | DTXSID70153552                           | 1 | Dye             | Semiperm. | Yellow          | Nitro             |
| 278 | Hydroxyethyl-2-nitro- <i>p</i> -<br>toluidine               | 100418-33-5                       | DTXSID20143261                           | 1 | Dye             | Semiperm. | Not<br>Assigned | Nitro             |

|     |                                                                         |                                                                         |                                                                                            |   |                 |           |        |       |
|-----|-------------------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|---|-----------------|-----------|--------|-------|
| 279 | Hydroxyethyl-3,4-methylenedioxyaniline                                  | 81329-90-0,<br>94158-14-2 (Salt)                                        | DTXSID00869199,<br>DTXSID20240825 (Salt)                                                   | 2 | Precursor       |           |        |       |
| 280 | Hydroxyethylaminomethyl- <i>p</i> -aminophenol                          | 110952-46-0,<br>135043-63-9 (Salt)                                      | DTXSID30879807,<br>DTXSID20159226 (Salt)                                                   | 2 | Precursor       |           |        |       |
| 281 | Hydroxyethyl- <i>p</i> -phenylenediamine                                | 93841-24-8,<br>93841-25-9 (Salt)                                        | DTXSID80869132,<br>DTXSID90879808 (Salt)                                                   | 2 | Precursor       |           |        |       |
| 282 | Hydroxypropyl-bis-( <i>N</i> -hydroxyethyl- <i>p</i> -phenylenediamine) | 128729-30-6,<br>128729-28-2 (Salt)                                      | DTXSID90879823,<br>DTXSID30155976 (Salt)                                                   | 1 | Precursor       |           |        |       |
| 283 | Hydroxypyridinone                                                       | 822-89-9                                                                | DTXSID70231622                                                                             | 3 | Not<br>Assigned |           |        |       |
| 284 | <i>m</i> -Aminophenol                                                   | 591-27-5,<br>51-81-0 (Salt),<br>68239-81-6 (Salt),<br>38171-54-9 (Salt) | DTXSID3024497,<br>DTXSID10892453 (Salt),<br>DTXSID4071340 (Salt),<br>DTXSID50191558 (Salt) | 2 | Precursor       |           |        |       |
| 285 | <i>m</i> -Phenylenediamine                                              | 108-45-2                                                                | DTXSID4021137                                                                              | 2 | Precursor       |           |        |       |
| 286 | <i>N,N'</i> -Bis-(2-hydroxyethyl)-2-nitro- <i>p</i> -phenylenediamine   | 84041-77-0                                                              | DTXSID90232939                                                                             | 1 | Dye             | Semiperm. | Violet | Nitro |

|     |                                                                                   |                                 |                                        |   |                 |  |  |  |
|-----|-----------------------------------------------------------------------------------|---------------------------------|----------------------------------------|---|-----------------|--|--|--|
|     | (HC Violet BS)                                                                    |                                 |                                        |   |                 |  |  |  |
| 287 | <i>N,N</i> -Bis(2-hydroxyethyl)- <i>p</i> -phenylenediamine                       | 7575-35-1,<br>54381-16-7 (Salt) | DTXSID9043805,<br>DTXSID5020075 (Salt) | 2 | Precursor       |  |  |  |
| 288 | <i>N,N</i> -Diethyl- <i>m</i> -aminophenol                                        | 91-68-9,<br>68239-84-9 (Salt)   | DTXSID9025037,<br>DTXSID4071342 (Salt) | 2 | Precursor       |  |  |  |
| 289 | <i>N,N</i> -Diethyl- <i>p</i> -phenylenediamine                                   | 93-05-0                         | DTXSID2025058                          | 2 | Precursor       |  |  |  |
| 290 | <i>N,N</i> -Diethyltoluene-2,5-diamine                                            | 148-71-0                        | DTXSID7043879                          | 2 | Not<br>Assigned |  |  |  |
| 291 | <i>N,N</i> -Dimethyl-2,6-pyridinediamine                                          | 63763-86-0                      | DTXSID50879824                         | 3 | Precursor       |  |  |  |
| 292 | <i>N,N</i> -Dimethyl- <i>m</i> -aminophenol                                       | 99-07-0                         | DTXSID0025101                          | 2 | Precursor       |  |  |  |
| 293 | <i>N,N'</i> -Dimethyl- <i>N</i> -hydroxyethyl-3-nitro- <i>p</i> -phenylenediamine | 10228-03-2                      | DTXSID20144854                         | 1 | Precursor       |  |  |  |

|     |                                                      |                                                    |                                                                  |   |           |           |     |       |
|-----|------------------------------------------------------|----------------------------------------------------|------------------------------------------------------------------|---|-----------|-----------|-----|-------|
| 294 | <i>N,N</i> -Dimethyl- <i>p</i> -phenylenediamine     | 99-98-9                                            | DTXSID6025149                                                    | 2 | Precursor |           |     |       |
| 295 | <i>N</i> -Cyclopentyl- <i>m</i> -aminophenol         | 104903-49-3                                        | DTXSID90146820                                                   | 2 | Precursor |           |     |       |
| 296 | <i>N</i> -Methoxyethyl- <i>p</i> -phenylenediamine   | 66566-48-1,<br>72584-59-9 (Salt)                   | DTXSID00388517,<br>DTXSID70892459 (Salt)                         | 2 | Precursor |           |     |       |
| 297 | <i>N</i> -Methyl-3-nitro- <i>p</i> -phenylenediamine | 2973-21-9                                          | DTXSID50863066                                                   | 1 | Dye       | Semiperm. | Red | Nitro |
| 298 | <i>N</i> -Methyl- <i>p</i> -aminophenol              | 150-75-4,<br>1936-57-8 (Salt)                      | DTXSID8043783,<br>DTXSID20892464 (Salt)                          | 2 | Precursor |           |     |       |
| 299 | <i>N</i> -Phenyl- <i>p</i> -phenylenediamine         | 101-54-2,<br>2198-59-6 (Salt),<br>4698-29-7 (Salt) | DTXSID7025895,<br>DTXSID9021132 (Salt),<br>DTXSID20884102 (Salt) | 2 | Precursor |           |     |       |
| 300 | <i>o</i> -Aminophenol                                | 95-55-6,<br>67845-79-8 (Salt)                      | DTXSID8024498,<br>DTXSID80892460 (Salt)                          | 2 | Precursor |           |     |       |
| 301 | <i>o</i> -Hydroxyphenol                              | 120-80-9                                           | DTXSID3020257                                                    | 2 | Precursor |           |     |       |

|     |                                   |                                                    |                                                                  |   |           |  |  |  |
|-----|-----------------------------------|----------------------------------------------------|------------------------------------------------------------------|---|-----------|--|--|--|
| 302 | o-Phenylenediamine                | 95-54-5                                            | DTXSID3025881                                                    | 2 | Precursor |  |  |  |
| 303 | p-Aminophenol                     | 123-30-8,<br>51-78-5 (Salt)                        | DTXSID3024499,<br>DTXSID6058760 (Salt)                           | 2 | Precursor |  |  |  |
| 304 | PEG-3,2',2'-di-p-phenylenediamine | 159661-45-7,<br>144644-13-3 (Salt)                 | DTXSID50892295,<br>DTXSID20892449 (Salt)                         | 1 | Precursor |  |  |  |
| 305 | Phenyl methyl pyrazolone          | 89-25-8                                            | DTXSID9021130                                                    | 4 | Precursor |  |  |  |
| 306 | p-Phenylenediamine                | 106-50-3,<br>624-18-0 (Salt),<br>50994-40-6 (Salt) | DTXSID9021138,<br>DTXSID8021141 (Salt),<br>DTXSID00892462 (Salt) | 2 | Precursor |  |  |  |
| 307 | p-Toluenediamine                  | 95-70-5,<br>615-50-9 (Salt)                        | DTXSID6029123,<br>DTXSID50872532 (Salt)                          | 2 | Precursor |  |  |  |
| 308 | Pyridine                          | 110-86-1                                           | DTXSID9021924                                                    | 3 | Precursor |  |  |  |
| 309 | Pyrimidine                        | 289-95-2                                           | DTXSID1051228                                                    | 3 | Precursor |  |  |  |

|     |                       |           |               |   |           |       |      |                |
|-----|-----------------------|-----------|---------------|---|-----------|-------|------|----------------|
| 310 | Quinolinium           | 91-22-5   | DTXSID1021798 | 3 | Precursor |       |      |                |
| 311 | Resorcinol            | 108-46-3  | DTXSID2021238 | 2 | Precursor |       |      |                |
| 312 | Tetrabromophenol blue | 4430-25-5 | DTXSID9063451 | 9 | Dye       | Temp. | Blue | Triarylmethane |
| 313 | Thymol                | 89-83-8   | DTXSID6034972 | 2 | Precursor |       |      |                |

**Table S2.** Sources used for the development of the HDSD.

| Source Type  | Reference                                                                                                                                                                                                                                                                                                                                              | Information Used                             |
|--------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|
| Article      | Corbett, J. F. An historical review of the use of dye precursors in the formulation of commercial oxidation hair dyes. <i>Dyes Pigm.</i> <b>1999</b> , <i>41</i> , 127-136.<br>DOI: <a href="https://doi.org/10.1016/S0143-7208(98)00075-8">10.1016/S0143-7208(98)00075-8</a> .                                                                        | Substance Names, Structures, Classifications |
| Article      | Corbett, J. Chemistry of hair colorant processes - Science as an aid to formulation and development. <i>J. Soc. Cosmet. Chem.</i> <b>1984</b> , <i>35</i> , 297-310.                                                                                                                                                                                   | Substance Names, Classifications             |
| Book Chapter | Chisvert, A.; Cháfer, A.; Salvador, A. Hair Dyes in Cosmetics. Regulatory Aspects and Analytical Methods. In <i>Analysis of Cosmetic Products</i> ; Salvador, A., Chisvert, A., Eds.; Elsevier: Amsterdam, London, 2007; Vol. 1, pp 190-209.<br>DOI: <a href="https://doi.org/10.1016/B978-044452260-3/50033-4">10.1016/B978-044452260-3/50033-4</a> . | Substance Structures, Classifications        |
| Book Chapter | Christie, R. M. Colour in Cosmetics, with Special Emphasis on Hair Coloration. In <i>Colour Chemistry</i> ; Royal Society of Chemistry: Cambridge, United Kingdom, 2015; Vol. 2, pp 250-265.                                                                                                                                                           | Substance Names, Structures, Classifications |
| Book Chapter | Christie, R. M.; Morel, O. J. X. The Coloration of Human Hair. In <i>The Coloration of Wool and other Keratin Fibers</i> ; Lewis, D. M., Rippon, J. A., Eds.; John Wiley & Sons: United Kingdom, 2013; Vol. 1, pp 357-391. DOI:                                                                                                                        | Substance Names, Structures, Classifications |

|                                       |                                                                                                                                                                                                                                                       |                                              |
|---------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|
|                                       | <a href="https://doi.org/10.1002/9781118625118.ch11">10.1002/9781118625118.ch11</a> .                                                                                                                                                                 |                                              |
| Book Chapter                          | Corbett, J. F. 10 Synthetic Dyes for Human Hair. In <i>Colorants for Non-Textile Applications</i> ; Freeman, H. S., Peters, A. T., Eds.; Elsevier: The Netherlands, 2000; Vol. 1, pp 456-477.                                                         | Substance Names, Structures, Classifications |
| Book Chapter                          | Gray, J. Hair colour products. In <i>The World of Hair Colour</i> ; Thomson Learning: Bedford Row, London, 2005; Vol. 1, pp 51-80.                                                                                                                    | Substance Names, Structures, Classifications |
| Book Chapter                          | Robbins, C. R. Dyeing Human Hair. In <i>Chemical and Physical Behavior of Human Hair</i> ; Springer-Verlag: Berlin Heidelberg, 2012; Vol. 5, pp 445-488. DOI: <a href="https://doi.org/10.1007/978-3-642-25611-0_7">10.1007/978-3-642-25611-0_7</a> . | Substance Names, Structures, Classifications |
| Chemical Database - ChemACX           | <a href="http://www.cambridgesoft.com/Ensemble_for_Chemistry/ChemACX/Default.aspx">http://www.cambridgesoft.com/Ensemble for Chemistry/ChemACX/Default.aspx</a>                                                                                       | Substance Structures <sup>1</sup>            |
| Chemical Database - Chemexper         | <a href="https://www.chemexper.com/">https://www.chemexper.com/</a>                                                                                                                                                                                   | Substance Structures                         |
| Chemical Database - Chemical Book     | <a href="https://www.chemicalbook.com/">https://www.chemicalbook.com/</a>                                                                                                                                                                             | Substance Structures <sup>1</sup>            |
| Chemical Database - Chemical Register | <a href="https://www.chemicalregister.com/">https://www.chemicalregister.com/</a>                                                                                                                                                                     | Substance Structures                         |
| Chemical Database - ChemIDPlus        | <a href="https://chem.nlm.nih.gov/chemidplus/">https://chem.nlm.nih.gov/chemidplus/</a>                                                                                                                                                               | Substance Structures <sup>1</sup>            |
| Chemical Database - Chemnet           | <a href="http://www.chemnet.com">http://www.chemnet.com</a>                                                                                                                                                                                           | Substance Structures                         |

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|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|------------------------------------------|
| Chemnet                                                                          |                                                                                                                                   |                                          |
| Chemical Database -<br>ChemSpider                                                | <a href="http://www.chemspider.com/">http://www.chemspider.com/</a>                                                               | Substance Structures                     |
| Chemical Database -<br>Colour Index                                              | <a href="https://colour-index.com/">https://colour-index.com/</a>                                                                 | Substance Structures                     |
| Chemical Database -<br>Cosmetic<br>Ingredients                                   | <a href="http://www.cosmeticsinfo.org/">http://www.cosmeticsinfo.org/</a>                                                         | Structure Classifications                |
| Chemical Database -<br>European<br>Commission<br>Cosmetic Ingredient<br>(CosIng) | <a href="https://ec.europa.eu/growth/sectors/cosmetics/cosining_en">https://ec.europa.eu/growth/sectors/cosmetics/cosining_en</a> | Substance Names, Structures              |
| Chemical Database -<br>Lookchem                                                  | <a href="http://www.lookchem.com/">http://www.lookchem.com/</a>                                                                   | Substance Structures                     |
| Chemical Database -<br>Molbase                                                   | <a href="https://www.molbase.com/">https://www.molbase.com/</a>                                                                   | Substance Structures                     |
| Chemical Database -<br>Pubchem                                                   | <a href="https://pubchem.ncbi.nlm.nih.gov/">https://pubchem.ncbi.nlm.nih.gov/</a>                                                 | Substance Structures,<br>Classifications |
| Chemical Database -<br>SciFinder                                                 | <a href="https://scifinder.cas.org">https://scifinder.cas.org</a>                                                                 | Substance Structures                     |
| Chemical Database -<br>World Dye Variety                                         | <a href="http://www.worlddyevariety.com/">http://www.worlddyevariety.com/</a>                                                     | Substance Structures                     |

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|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|
| Journal Article | Becker, L. C. Final report on the safety assessment of 3-methylamino-4-nitrophenoxyethanol as used in hair dyes. <i>Int J Toxicol.</i> <b>2008</b> , 27, 41-51. DOI: <a href="https://doi.org/10.1080/10915810802244488">10.1080/10915810802244488</a> .                                                                                                        | Substance Classifications                    |
| Journal Article | Fiume, M.; Yamarik, T. A. Final report on the safety assessment of 6-Amino-m-Cresol, 6-Amino-o-Cresol, 4-Amino-m-Cresol, 5-Amino-4-Chloro-o-Cresol, 5-Amino-6-Chloro-o-Cresol, and 4-Chloro-2-Aminophenol. <i>Int. J. Toxicol.</i> <b>2004</b> , 23, 1-22. DOI: <a href="https://doi.org/10.1080/10915810490499037">10.1080/10915810490499037</a> .             | Substance Classifications                    |
| Journal Article | Holman, C. D. J.; Armstrong, B. K. Hutchinson's melanotic freckle melanoma associated with non-permanent hair dyes. <i>Br. J. Cancer</i> <b>1983</b> , 48, 599-601.                                                                                                                                                                                             | Substance Classifications                    |
| Journal Article | Morel, O. J. X.; Christie, R. M. Current trends in the chemistry of permanent hair dyeing. <i>Chem. Rev.</i> <b>2011</b> , 111, 2537-2561. DOI: <a href="https://doi.org/10.1021/cr1000145">10.1021/cr1000145</a> .                                                                                                                                             | Substance Names, Structures, Classifications |
| Journal Article | Søsted, H.; Basketter, D. A.; Estrada, E.; Johansen, J. D.; Patlewicz, G. Y. Ranking of hair dye substances according to predicted sensitization potency: quantitative structure-activity relationships. <i>Contact Derm.</i> <b>2004</b> , 51, 241-254. DOI: <a href="https://doi.org/10.1111/j.0105-1873.2004.00440.x">10.1111/j.0105-1873.2004.00440.x</a> . | Substance Names                              |

|                                                                                          |                                                                                                                                                                                                                                    |                                                 |
|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| Manufacturer<br>Website -<br>ClearSynth, Canada                                          | <a href="https://www.clearsynth.com/en/home.asp">https://www.clearsynth.com/en/home.asp</a>                                                                                                                                        | Substance Classifications                       |
| Manufacturer<br>Website - IRO<br>Group, Inc., China                                      | <a href="http://www.irochemical.com/product/Dying-Intermediates.htm">http://www.irochemical.com/product/Dying-Intermediates.htm</a>                                                                                                | Substance Structures,<br>Classifications        |
| Manufacturer<br>Website - Pylam<br>Products Company,<br>Inc., USA                        | <a href="http://www.pylamdyes.com/products/hair.html">http://www.pylamdyes.com/products/hair.html</a>                                                                                                                              | Substance Names, Classifications                |
| Manufacturer<br>Website - Sigma<br>Aldrich, USA                                          | <a href="https://www.sigmaaldrich.com/united-states.html">https://www.sigmaaldrich.com/united-states.html</a>                                                                                                                      | Substance Structures,<br>Classifications        |
| Manufacturer<br>Website - Yick-Vick<br>Chemicals &<br>Pharmaceuticals<br>(HK) Ltd, China | <a href="http://www.yickvic.com/Catalog/Cosmetic_Hair_Dyeing_Agents.pdf">http://www.yickvic.com/Catalog/Cosmetic_Hair_Dyeing_Agents.pdf</a>                                                                                        | Substance Names                                 |
| Monograph                                                                                | IARC. Some Aromatic Amines, Organic Dyes, and Related Exposures: Occupational exposures of hairdressers and barbers and personal use of hair colourants. <i>IARC Monogr. Eval. Carcinog. Risks Hum.</i> <b>2010</b> , 99, 499-658. | Substance Names, Structures,<br>Classifications |

|       |                                                                                                                                                                                                                                                           |                                              |
|-------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------|
| Other | <a href="http://ec.europa.eu/consumers/sectors/cosmetics/files/doc/hd_updated_safety_file_submitted_117_en.pdf">http://ec.europa.eu/consumers/sectors/cosmetics/files/doc/hd_updated_safety_file_submitted_117_en.pdf</a>                                 | Substance Names                              |
| Other | <a href="http://ec.europa.eu/consumers/sectors/cosmetics/files/pdf/76_substances_en.pdf">http://ec.europa.eu/consumers/sectors/cosmetics/files/pdf/76_substances_en.pdf</a>                                                                               | Substance Names                              |
| Other | <a href="http://ec.europa.eu/DocsRoom/documents/13209/attachments/1/translations/en/renditions/pdf">http://ec.europa.eu/DocsRoom/documents/13209/attachments/1/translations/en/renditions/pdf</a>                                                         | Substance Names                              |
| Other | <a href="http://ec.europa.eu/health/ph_risk/committees/sccp/documents/out267_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sccp/documents/out267_en.pdf</a>                                                                                       | Substance Names                              |
| Other | <a href="https://ec.europa.eu/health/scientific_committees/all_opinions_en">https://ec.europa.eu/health/scientific_committees/all_opinions_en</a>                                                                                                         | Substance Names, Structures, Classifications |
| Other | <a href="https://ec.europa.eu/health/scientific_committees/consumer_safety/docs/sccs_o_037.pdf">https://ec.europa.eu/health/scientific_committees/consumer_safety/docs/sccs_o_037.pdf</a>                                                                 | Substance Names, Classifications             |
| Other | <a href="https://korea.in-cosmetics.com/RXUK/RXUK_InCosmeticsKorea/documents/Patricia.Vesque_Chang-up.pdf?v=636041756936840262">https://korea.in-cosmetics.com/RXUK/RXUK_InCosmeticsKorea/documents/Patricia.Vesque_Chang-up.pdf?v=636041756936840262</a> | Substance Classifications                    |

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|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
| Other  | <a href="http://chemicaland21.com/info/HAIR%20DYE%20SUBSTANCES.htm">http://chemicaland21.com/info/HAIR%20DYE%20SUBSTANCES.htm</a>                                                                                                     | Substance Names                                 |
| Other  | <a href="http://www.cir-safety.org/ingredients">http://www.cir-safety.org/ingredients</a>                                                                                                                                             | Substance Structures,<br>Classifications        |
| Other  | <a href="http://www.compoundchem.com/wp-content/uploads/2015/05/The-Chemistry-of-Permanent-Hair-Dyes.pdf">http://www.compoundchem.com/wp-content/uploads/2015/05/The-Chemistry-of-Permanent-Hair-Dyes.pdf</a>                         | Substance Names, Structures,<br>Classifications |
| Other  | <a href="http://www.unionchemical.com.tw/mana_php/news/file/File/archive/cosmetics/Vivimed/Jarocol%20Hair%20Dyes.pdf">http://www.unionchemical.com.tw/mana_php/news/file/File/archive/cosmetics/Vivimed/Jarocol%20Hair%20Dyes.pdf</a> | Substance Names, Classifications                |
| Patent | Anderson, J. S. United States Patent US5961664 A, 1999.                                                                                                                                                                               | Substance Classifications                       |
| Patent | Birault, V.; Leduc, M.; Terranova, E. United States Patent US 6730789 B1, 2004.                                                                                                                                                       | Substance Classifications                       |
| Patent | Bugaut, A.; Alain Genet, A. United States Patent US4888025 A, 1989.                                                                                                                                                                   | Substance Classifications                       |
| Patent | Chassot, L.; Braun, H. United States Patent US 6602302 B1, 2003.                                                                                                                                                                      | Substance Classifications                       |
| Patent | Gast, A.; Braun, P.; Balzer, W. R.; Deutz, H. United States Patent US 6146429 A, 2000.                                                                                                                                                | Substance Classifications                       |
| Patent | Geibel, W.; Weber, I.; Osan, A.; Speckbacher, M. United States Patent US 20130212810 A1, 2013.                                                                                                                                        | Substance Classifications                       |

|        |                                                                                                         |                           |
|--------|---------------------------------------------------------------------------------------------------------|---------------------------|
| Patent | Kawai, T.; Itou, T. United States Patent US 6746492 B2, 2004.                                           | Substance Classifications |
| Patent | Lange, F. United States Patent US3200040 A, 1965.                                                       | Substance Classifications |
| Patent | Lim, M.; Pan, Y.; Stasaitis, L. R. United States Patent US 6074438 A, 2000.                             | Substance Classifications |
| Patent | Lowe, I.; Gerstung, S.; Balzer, W. R. United States Patent US5766576, 1998.                             | Substance Classifications |
| Patent | Narasimhan, S.; Vena, L. C.; Singh, S.; Dolores Cross, D. United States Patent US 20070169285 A1, 2007. | Substance Classifications |
| Patent | Moeller, H.; Hoeffkes, H. United States Patent US 6371993 B1, 2002.                                     | Substance Classifications |
| Patent | Robert, L.; Charle Roger, C. United States Patent US 3167478 A, 1965.                                   | Substance Classifications |
| Patent | Rose, D.; Hoeffkes, H.; Meinigke, B. United States Patent 2000, US6165230 A.                            | Substance Classifications |
| Patent | Trigg, D. L.; Jones, J. L. United States Patent US 20080189876 A1, 2008.                                | Substance Classifications |
| Patent | Wenke, G.; Wong, Y. M. M. Canada Patent CA 2422690 A1, 2002.                                            | Substance Classifications |

<sup>1</sup>Downloaded chemical structures into PerkinElmer's ChemDraw Professional 15.0 software

## 2. Hierarchical Clustering Stability and Purity

Hierarchical clustering was performed on 313 HDSD compounds using 53 uncorrelated descriptors with distances between HDSD dyes determined with Euclidean distances and cluster groupings with the Ward linkage. Cluster assignments were determined using visual inspection as described by James and coworkers and the ‘*factoextra*’ R-package.<sup>1,2</sup> Next, the clustering reliability was analyzed by measuring cluster stability and purity. Cluster stability measures consider how susceptible the data is to noise from the descriptor matrix. This was performed using the R-package ‘*clValid*’ which computes three stability measures: Average Proportion of Non-Overlap (APN), Average Distance Between Means (ADM), and Figure of Merit (FOM).<sup>3</sup> All three measures should be minimized (scores of 0 indicate ‘good’ clustering stability), but APN has an upper-bound of 1, while the other three measures do not have an upper-bound. These scores were also calculated for average, single, and complete linkages. Cluster purity was also calculated for the average, single, and complete linkages using the Ward linkage cluster results as a reference for comparison. Purity is a measure of how accurate a clustering assignment is between two clustered datasets, and a score of 1 indicates a perfect clustering assignment.<sup>4</sup>

Stability and purity scores for Hierarchical clustering analysis is provided in **Table S3**. Interestingly, the APN scores for all four linkages are considered to be excellent as they are close to zero. The other two stability scores (ADM and FOM) do not have an upper-bound value, so scores that are >1 can still indicate a stable cluster as occurs for ADM (range of 0 to 2) and FOM (range of 0.8 to 0.9). Using the Ward linkage clustering results as a reference, it was possible to measure a purity score for average, single, and complete linkages. Notably, both average and complete linkages had purity scores of 0.62 and 0.72, respectively. Clustering with the single linkage resulted in the lowest purity score of 0.34. Varying the linkage method served as an external validation to determine the reliability of HDSD hierarchical clustering.

Next, cluster stability was tested under conditions of plausible data variation in the dataset using bootstrap sampling. Cluster bootstrap sampling was implemented using the ‘*fpc*’ R-package.<sup>5</sup> First, normal clustering is performed on the original dataset, then a new dataset is developed using random sampling that duplicates some data points and removes other entries.<sup>6</sup> This new dataset is then clustered and a purity score is measured between the clustered datasets. Unlike the previous purity score used to compare clustering results between different linkages, the

purity score generated from the clusterboot() function is by cluster. This enables the individual clusters to be analyzed.

Individual cluster purity scores measured by cluster bootstrap sampling with Ward, average, single, and complete linkages are provided in **Table S4**. For each sampling, 100 clustering iterations were performed. A purity score  $<0.5$  indicates a dissolved or unstable cluster, and purity scores  $>0.6$  indicate that an observable pattern is present in the data. Highly stable clusters will have scores greater than 0.8.<sup>6,7</sup> Using the Ward linkage clusters 1 and 2 are considered highly stable with scores  $>0.7$  (**Table S4**). Notably, clusters 3, 4, and 6 all had scores  $>0.5$ , but  $<0.6$ ; this means that these clusters may be unstable. Clusters 7 and 9 are considered stable with measured purity scores of 0.66 and 0.69, respectively. The only cluster determined to be fully unstable was cluster 8 with a score of 0.49. The large variation in individual cluster purity scores may be a result of differing sizes between clusters. Future HDSD studies will use a more stringent clustering assignment procedure that fully utilizes the validity measures of ADM, FOM, and APN.

Additionally, our initial clustering analysis was performed after removing 10% of the HDSD compounds. This resulted in the clustering of 282 HDSD compounds over 10 iterations. The average purity score from this analysis was 0.87 which indicates that the observed clusters are highly stable when the row dimensionality (*i.e.*, noise introduced by compound entries) is decreased.

Due to the favorable APN, ADM, and FOM stability scores, and high purity scores when row dimensionality and linkage method were varied, it was determined that the observed HDSD clusters is not occurring from noise within the data. The clustered results from the Ward linkage were selected for further analysis because previous studies have analyzed organic-synthetic dyes using the same methodology.<sup>8</sup>

**Table S3.** Stability and purity measures for Hierarchical clustering results using Ward, average, single, complete, and centroid linkages. The purity measure for Ward linkage is not provided, because this was used as the clustering reference.

|                 | APN    | AD   | ADM  | FOM  | Purity |
|-----------------|--------|------|------|------|--------|
| <b>Ward</b>     | 0.15   | 7.09 | 1.24 | 0.79 | Ref.   |
| <b>Average</b>  | 0.01   | 8.59 | 0.16 | 0.91 | 0.62   |
| <b>Single</b>   | 0.0026 | 8.84 | 0.04 | 0.93 | 0.34   |
| <b>Complete</b> | 0.32   | 8.38 | 1.97 | 0.86 | 0.72   |

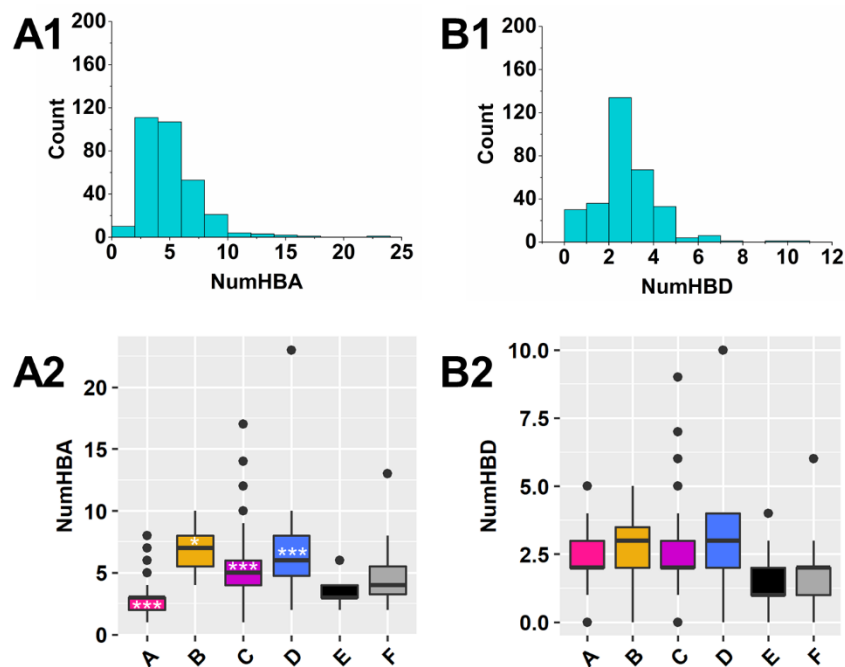
**Table S4.** Individual cluster purity scores determined by bootstrap resampling of clustered data.

|                 | CI1  | CI2  | CI3  | CI4  | CI5  | CI6  | CI7  | CI8  | CI9  |
|-----------------|------|------|------|------|------|------|------|------|------|
| <b>Ward</b>     | 0.70 | 0.84 | 0.55 | 0.62 | 0.56 | 0.56 | 0.66 | 0.47 | 0.69 |
| <b>Average</b>  | 0.95 | 0.83 | 0.58 | 0.72 | 0.66 | 0.47 | 0.70 | 0.62 | 0.57 |
| <b>Single</b>   | 0.98 | 0.64 | 0.69 | 0.49 | 0.67 | 0.67 | 0.62 | 0.63 | 0.64 |
| <b>Complete</b> | 0.65 | 0.36 | 0.40 | 0.59 | 0.70 | 0.40 | 0.68 | 0.69 | 0.38 |

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### 3. Computed Physicochemical Properties – HBA and HBD



**Figure S1.** Distribution of the database according to HBA/hydrogen bond acceptors (A1) and HBD/hydrogen bond donors (B1). Boxplots of the HBA (A2) and HBD (B2) are shown for substance and dye types. Stars on each boxplot represent the level of significance resulting from a pairwise comparison of the particular type (average value) versus all other types (average values) from \*moderately significant ( $0.01 < P\text{-value} < 0.05$ ), \*\*significant ( $0.001 < P\text{-value} < 0.01$ ), to \*\*\*very significant ( $P\text{-value} < 0.001$ ). A, Precursor; B, temporary dye; C, semipermanent dye; D, temporary/semipermanent dye; E, substance type not assigned; F, dye type not assigned.

#### 4. Predictions

**Table S5.** The 22 substances in the HDSD predicted to be mutagens (binary Ames data)<sup>1</sup> with confidence thresholds >90% and their Opinions.

| Substance Name <sup>2</sup>          | Opinion <sup>3</sup>                                                                                                                                                                                                      | Reference <sup>4</sup>        |
|--------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|
| 2,6-Dinitrotoluene                   | Opinion not found.                                                                                                                                                                                                        | -                             |
| 1,2,3-Trihydroxybenzene              | Opinion not found.                                                                                                                                                                                                        | -                             |
| 2-Amino-4,6-dinitrophenol            | Induced frameshift mutations in bacteria in the presence of metabolic activation but did not induce gene mutations or chromosomal aberrations in mammalian cells <i>in vitro</i> ; no <i>in vivo</i> genotoxic potential. | <a href="#">COLIPA N° B28</a> |
| 2-Amino-4-nitrophenol                | Opinion not found.                                                                                                                                                                                                        | -                             |
| 2-Amino-5-nitrophenol                | Opinion not found.                                                                                                                                                                                                        | -                             |
| 2-Amino-6-chloro-4-nitrophenol*      | Negative in Ames test; future studies on genotoxicity/mutagenicity in finished hair dye formulations recommended.                                                                                                         | <a href="#">COLIPA N° B99</a> |
| 2-Methyl-4-nitroaniline              | Opinion not found.                                                                                                                                                                                                        | -                             |
| 2-Nitro- <i>p</i> -phenylenediamine* | Opinion not found.                                                                                                                                                                                                        | -                             |
| 4-Amino-2-nitrophenol                | Opinion not found.                                                                                                                                                                                                        | -                             |
| 4-Amino-3-nitrophenol                | Weakly mutagenic in bacteria (Strain TA98), but considered to have no relevant potential to induce gene mutations; future studies on genotoxicity/mutagenicity in finished hair dye formulations recommended.             | <a href="#">COLIPA N° B51</a> |
| 4-Nitro- <i>m</i> -phenylenediamine* | Opinion not found.                                                                                                                                                                                                        | -                             |
| 4-Nitro- <i>o</i> -phenylenediamine* | Compound itself not considered genotoxic <i>in vivo</i> , however future studies on                                                                                                                                       | <a href="#">COLIPA N° B24</a> |

|                                   |                                                                                                                                                            |                               |
|-----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------|
|                                   | genotoxicity/mutagenicity in finished hair dye formulations recommended.                                                                                   |                               |
| C.I. Basic Orange 1               | Opinion not found.                                                                                                                                         | -                             |
| C.I. Basic Orange 2               | Opinion not found.                                                                                                                                         | -                             |
| C.I. Basic Yellow 2               | Opinion not found.                                                                                                                                         | -                             |
| C.I. Disperse Red 15 <sup>5</sup> | Opinion not found.                                                                                                                                         | -                             |
| C.I. Disperse Violet 1*           | No <i>in vivo</i> genotoxic potential.                                                                                                                     | <a href="#">COLIPA N° C64</a> |
| C.I. Disperse Violet 4            | Opinion not found.                                                                                                                                         | -                             |
| C.I. Mordant Red 11               | Opinion not found.                                                                                                                                         | -                             |
| HC Blue 1                         | Opinion not found.                                                                                                                                         | -                             |
| <i>o</i> -Phenylenediamine*       | Opinion not found.                                                                                                                                         | -                             |
| <i>p</i> -Phenylenediamine*       | Not considered genotoxic, but <i>in vivo</i> genotoxicity and/or carcinogenicity of PPD in combination with hydrogen peroxide and couplers is recommended. | <a href="#">COLIPA N° A7</a>  |

<sup>1</sup>Sushko, I.; Novotarskyi, S.; Körner, R.; Pandey, A. K.; Cherkasov, A.; Li, J.; Gramatica, P.; Hansen, K.; Schroeter, T.; Müller, K. R.; Xi, L.; Liu, H.; Yao, X.; Öberg, T. H.,F.; Dao, P.; Sahinalp, C.; Todeschini, R.; Polishchuk, P.; Artemenko, A.; Kuz'min, V.; Martin, T. M.; Young, D. M.; Fourches, D.; Muratov, E.; Tropsha, A.; Baskin, I.; Horvath, D.; Marcou, G.; Muller, C.; Varnek, A.; Prokopenko, V. V.; Tetko, I. V. Applicability domains for classification problems: Benchmarking of distance to models for Ames mutagenicity set. *J. Chem. Inf. Model.* **2010**, 50, 2094-2111. DOI: [10.1021/ci100253r](https://doi.org/10.1021/ci100253r).

<sup>2</sup>Substances banned for use in European Union are designated with **RED** boxes.

<sup>3</sup>Substances in **GREEN** identified by Opinions as mutagenic/genotoxic; substances in **YELLOW** identified by Opinions as having mutagenic/genotoxic potential; substances in **RED** not identified by Opinions as mutagenic/genotoxic or having mutagenic/genotoxic potential.

<sup>4</sup>References denoted with “COLIPA” refer to Opinions.

<sup>5</sup>C.I. Disperse Red 15 permitted as an impurity of C.I. Disperse Violet 1.

**Table S6.** The 37 substances in the HDSD predicted to be skin sensitizers (binary LLNA data)<sup>1,2</sup> with confidence thresholds >90% and their Opinions.

| Substance Name <sup>3</sup>                                 | Opinion <sup>4</sup>                                                                                     | Reference <sup>5</sup>        |
|-------------------------------------------------------------|----------------------------------------------------------------------------------------------------------|-------------------------------|
| 2,4-Diaminophenoxyethanol                                   | <b>Moderate</b> sensitizer in LLNA.                                                                      | <a href="#">COLIPA N° A42</a> |
| 2,4-Diaminotoluene                                          | Opinion not found.                                                                                       | -                             |
| 2,6-Diaminotoluene                                          | Opinion not found.                                                                                       | -                             |
| 2-Amino-6-chloro-4-nitrophenol*                             | Sensitizer in LLNA.                                                                                      | <a href="#">COLIPA N° B99</a> |
| 2-Chloro-5-nitro-N-hydroxyethyl- <i>p</i> -phenylenediamine | Opinion not found.                                                                                       | -                             |
| 2-Methyl-5-aminophenol                                      | <b>Moderate or strong</b> sensitizer in LLNA.                                                            | <a href="#">COLIPA N° A27</a> |
| 2-Methylresorcinol                                          | <b>Moderate</b> sensitizer in LLNA.                                                                      | <a href="#">COLIPA N° A44</a> |
| 2-Nitro- <i>p</i> -phenylenediamine*                        | Opinion not found.                                                                                       | -                             |
| 3,4-Diaminotoluene                                          | Opinion not found.                                                                                       | -                             |
| 4-(Methylamino)-2,6-dinitrophenol                           | Opinion not found.                                                                                       | -                             |
| 4-Amino- <i>m</i> -cresol                                   | <b>Moderate</b> sensitizer in LLNA.                                                                      | <a href="#">COLIPA N° A74</a> |
| 4-Amino- <i>o</i> -cresol                                   | Opinion not found.                                                                                       | -                             |
| 4-Nitro- <i>m</i> -phenylenediamine*                        | Opinion not found.                                                                                       | -                             |
| 4-Nitro- <i>o</i> -phenylenediamine*                        | Found to be an <b>extreme</b> sensitizer in one LLNA study; and not to be a sensitizer in another study. | <a href="#">COLIPA N° B24</a> |
| 5-Methylresorcinol                                          | Opinion not found.                                                                                       | -                             |
| 6-Amino- <i>m</i> -cresol                                   | Opinion not found.                                                                                       | -                             |
| 6-Amino- <i>o</i> -cresol                                   | Opinion not found.                                                                                       | -                             |
| C.I. Disperse Violet 1*                                     | <b>Moderate</b> sensitizer in LLNA.                                                                      | <a href="#">COLIPA N° C64</a> |
| HC Red 3                                                    | <b>Strong</b> sensitizer in LLNA.                                                                        | <a href="#">COLIPA N° B50</a> |
| HC Red 7                                                    | <b>Moderate or strong</b> sensitizer in LLNA.                                                            | <a href="#">COLIPA N° B36</a> |
| HC Violet 1                                                 | <b>Strong</b> sensitizer in LLNA.                                                                        | <a href="#">COLIPA N° B66</a> |
| HC Yellow 15                                                | Opinion not found.                                                                                       | -                             |
| HC Yellow 5                                                 | Opinion not found.                                                                                       | -                             |

|                                                  |                                                                         |                               |
|--------------------------------------------------|-------------------------------------------------------------------------|-------------------------------|
| HC Yellow 9                                      | Has skin sensitization potential.                                       | <a href="#">COLIPA N° B69</a> |
| Hydroquinone                                     | LLNA data not reported.                                                 | <a href="#">COLIPA N° A21</a> |
| <i>m</i> -Aminophenol                            | <b>Strong</b> sensitizer in LLNA.                                       | <a href="#">COLIPA N° A15</a> |
| <i>m</i> -Phenylenediamine                       | Opinion not found.                                                      | -                             |
| <i>N,N</i> -Dimethyl- <i>p</i> -phenylenediamine | Opinion not found.                                                      | -                             |
| <i>N</i> -Methyl- <i>p</i> -aminophenol          | Opinion not found.                                                      | -                             |
| <i>o</i> -Aminophenol                            | Sensitizer in LLNA.                                                     | <a href="#">COLIPA N° A14</a> |
| <i>o</i> -Hydroxyphenol                          | Opinion not found.                                                      | -                             |
| <i>o</i> -Phenylenediamine*                      | Opinion not found.                                                      | -                             |
| <i>p</i> -Aminophenol                            | LLNA data not reported, although recognized as a human skin sensitizer. | <a href="#">COLIPA N° A16</a> |
| <i>p</i> -Phenylenediamine*                      | <b>Extreme</b> sensitizer in LLNA.                                      | <a href="#">COLIPA N° A7</a>  |
| <i>p</i> -Toluenediamine                         | LLNA data irrelevant. <sup>6</sup>                                      | <a href="#">COLIPA N° A5</a>  |
| Resorcinol                                       | <b>Strong</b> sensitizer in LLNA.                                       | <a href="#">COLIPA N° A11</a> |
| Thymol                                           | Opinion not found.                                                      | -                             |

<sup>1</sup>Alves, V. M.; Muratov, E.; Fourches, D.; Strickland, J.; Kleinstreuer, N.; Andrade, C. H.; Tropsha, A. Predicting chemically-induced skin reactions. Part I: QSAR models of skin sensitization and their application to identify potentially hazardous compounds. *Toxicol Appl Pharmacol.* **2016**, 284, 262-272. DOI: [10.1016/j.taap.2014.12.014](https://doi.org/10.1016/j.taap.2014.12.014).

<sup>2</sup>LLNA, Local Lymph Node Assay

<sup>3</sup>Substances banned for use in European Union are designated with **RED** boxes.

<sup>4</sup>Substances in **GREEN** identified by Opinions as a skin sensitizer; substances in **YELLOW** identified by Opinions as having skin sensitization potential; substances in **RED** not identified by Opinions as a sensitizer or having skin sensitization potential.

<sup>5</sup>References denoted with “COLIPA” refer to Opinions.

<sup>6</sup>Concentrations of test species too high.

**Table S7.** The 269 substances in the HDSD predicted by [Pred-Skin](#)<sup>1</sup> to be sensitizers (human binary data) and their Opinions.

| Substance Name <sup>2</sup>           | Probability | AD <sup>3</sup> | Opinion <sup>4</sup>                                                                               | Reference <sup>5</sup>         |
|---------------------------------------|-------------|-----------------|----------------------------------------------------------------------------------------------------|--------------------------------|
| 1,2,3,4-Tetrahydro-6-nitroquinoxaline | 0.68        | Yes             | Human skin sensitization potential not reported, although potent allergen in GPMT. <sup>6</sup>    | <a href="#">COLIPA N° B104</a> |
| 1,2,3-Trihydroxybenzene               | 0.77        | Yes             | Opinion not found.                                                                                 | -                              |
| 1,2,4-Trihydroxybenzene               | 0.75        | Yes             | Human skin sensitizer.                                                                             | <a href="#">COLIPA N° A33</a>  |
| 1,3,5-Trihydroxybenzene               | 0.80        | Yes             | Opinion not found.                                                                                 | -                              |
| 1,3-Bis-(2,4-diaminophenoxy)-propane  | 0.74        | Yes             | Has skin sensitization potential.                                                                  | <a href="#">COLIPA N° A79</a>  |
| 1,5-Naphthalenediol                   | 0.72        | Yes             | Has skin sensitization potential, and identified as moderate skin sensitizer in LLNA. <sup>7</sup> | <a href="#">COLIPA N° A18</a>  |
| 1,7-Naphthalenediol                   | 0.68        | Yes             | Has skin sensitization potential.                                                                  | <a href="#">COLIPA N° A1</a>   |
| 1-Hydroxyethyl-4,5-diaminopyrazole    | 0.64        | Yes             | Has skin sensitization potential. <sup>8</sup>                                                     | <a href="#">COLIPA N° A154</a> |
| 1-Naphthol                            | 0.70        | Yes             | <b>Strong</b> human skin sensitizer.                                                               | <a href="#">COLIPA N° A17</a>  |

|                                        |      |     |                                                               |                                |
|----------------------------------------|------|-----|---------------------------------------------------------------|--------------------------------|
| 1-Beta-Hydroxyethyl-2,4-diaminobenzene | 0.75 | Yes | Opinion not found.                                            | -                              |
| 2,2'-Methylenebis-4-aminophenol        | 0.75 | Yes | Human skin sensitization potential not reported. <sup>8</sup> | <a href="#">COLIPA N° A155</a> |
| 2,3-Diaminodihydroxypyrazolopyrazolone | 0.63 | Yes | Has skin sensitization potential. <sup>8</sup>                | <a href="#">COLIPA N° A159</a> |
| 2,3-Indolinedione                      | 0.65 | Yes | Human skin sensitizer.                                        | <a href="#">COLIPA N° A129</a> |
| 2,3-Naphthalenediol                    | 0.71 | Yes | Opinion not found.                                            | -                              |
| 2,4,5,6-Tetraaminopyrimidine           | 0.70 | Yes | Has skin sensitization potential. <sup>8</sup>                | <a href="#">COLIPA N° A53</a>  |
| 2,4,5-Trihydroxytoluene                | 0.76 | Yes | Opinion not found.                                            | -                              |
| 2,4-Diamino-5-methylphenetol           | 0.69 | Yes | Has skin sensitization potential. <sup>8</sup>                | <a href="#">COLIPA N° A113</a> |
| 2,4-Diamino-5-methylphenoxyethanol     | 0.62 | No  | Has skin sensitization potential. <sup>8</sup>                | <a href="#">COLIPA N° A116</a> |
| 2,4-Diaminoanisole                     | 0.70 | Yes | Opinion not found.                                            | -                              |

|                                              |      |     |                                                |                                |
|----------------------------------------------|------|-----|------------------------------------------------|--------------------------------|
| 2,4-Diaminodiphenylamine                     | 0.73 | Yes | Opinion not found.                             | -                              |
| 2,4-Diaminophenol                            | 0.76 | Yes | Opinion not found.                             | -                              |
| 2,4-Diaminophenoxyethanol                    | 0.66 | Yes | Has skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A42</a>  |
| 2,4-Diaminotoluene                           | 0.72 | Yes | Opinion not found.                             | -                              |
| 2,5,6-Triamino-4-pyrimidinol                 | 0.68 | Yes | Has skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A143</a> |
| 2,5-Diaminoanisole                           | 0.70 | Yes | Opinion not found.                             | -                              |
| 2,6-Bis(2-hydroxyethoxy)-3,5-pyridinediamine | 0.66 | Yes | Opinion not found.                             | -                              |
| 2,6-Diamino-3-((pyridine-3-yl)azo)pyridine   | 0.70 | Yes | Not recognized as a human skin sensitizer.     | <a href="#">COLIPA N° B111</a> |
| 2,6-Diaminotoluene                           | 0.67 | Yes | Opinion not found.                             | -                              |
| 2,6-Dihydroxy-3,4-dimethylpyridine           | 0.71 | Yes | Has skin sensitization potential.              | <a href="#">COLIPA N° A99</a>  |

|                                               |      |     |                                                         |                                |
|-----------------------------------------------|------|-----|---------------------------------------------------------|--------------------------------|
| 2,6-Dihydroxy-4-methylpyridine                | 0.67 | Yes | Opinion not found.                                      | -                              |
| 2,6-Dihydroxyethylaminotoluene (HC Violet AS) | 0.66 | Yes | Not recognized as a human skin sensitizer.              | <a href="#">COLIPA N° A138</a> |
| 2,6-Dimethoxy-3,5-pyridinediamine             | 0.66 | Yes | Has skin sensitization potential. <sup>8</sup>          | <a href="#">COLIPA N° A101</a> |
| 2,6-Dinitrotoluene                            | 0.67 | Yes | Opinion not found.                                      | -                              |
| 2,7-Naphthalenediol                           | 0.76 | Yes | <b>Moderate</b> human skin sensitizer.                  | <a href="#">COLIPA N° A19</a>  |
| 2-Amino-3-hydroxypyridine                     | 0.58 | Yes | Not recognized as a human skin sensitizer.              | <a href="#">COLIPA N° A132</a> |
| 2-Amino-3-nitrophenol                         | 0.59 | Yes | Has skin sensitization potential.                       | <a href="#">COLIPA N° B55</a>  |
| 2-Amino-4,6-dinitrophenol                     | 0.83 | Yes | Not recognized as a human skin sensitizer. <sup>8</sup> | <a href="#">COLIPA N° B28</a>  |
| 2-Amino-4-hydroxyethylaminoanisol             | 0.66 | Yes | Has skin sensitization potential. <sup>8</sup>          | <a href="#">COLIPA N° A84</a>  |
| 2-Amino-4-nitrophenol                         | 0.71 | Yes | Opinion not found.                                      | -                              |

|                                                                      |      |     |                                                |                                |
|----------------------------------------------------------------------|------|-----|------------------------------------------------|--------------------------------|
| 2-Amino-5-ethylphenol                                                | 0.71 | Yes | Has skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A158</a> |
| 2-Amino-5-nitrophenol                                                | 0.71 | Yes | Opinion not found.                             | -                              |
| 2-Amino-6-chloro-4-nitrophenol                                       | 0.85 | Yes | Human skin sensitizer.                         | <a href="#">COLIPA N° B99</a>  |
| 2-Amino-methyl- <i>p</i> -aminophenol                                | 0.80 | Yes | Opinion not found.                             | -                              |
| 2-Chloro-5-nitro- <i>N</i> -hydroxyethyl- <i>p</i> -phenylenediamine | 0.73 | Yes | Opinion not found.                             | -                              |
| 2-Chloro-6-ethylamino-4-nitrophenol                                  | 0.86 | Yes | Has skin sensitization potential.              | <a href="#">COLIPA N° B89</a>  |
| 2-Chloro- <i>p</i> -phenylenediamine                                 | 0.78 | Yes | <b>Strong</b> human skin sensitizer.           | <a href="#">COLIPA N° A8</a>   |
| 2-Hydroxyethyl picramic acid                                         | 0.85 | Yes | Not recognized as a human skin sensitizer.     | <a href="#">COLIPA N° B72</a>  |
| 2-Hydroxyethylamino-5-nitroanisole                                   | 0.70 | No  | Not recognized as a human skin sensitizer.     | <a href="#">COLIPA N° B52</a>  |
| 2-Hydroxynaphthoquinone                                              | 0.72 | Yes | Human sensitization potential not reported.    | <a href="#">COLIPA N° C146</a> |

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| 2-methoxy-4-nitrophenol                              | 0.70 | Yes | Opinion not found.                             | -                              |
| 2-Methoxymethyl- <i>p</i> -phenylenediamine          | 0.74 | Yes | Has skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A160</a> |
| 2-Methyl-1-naphthol                                  | 0.74 | Yes | <b>Strong</b> human skin sensitizer.           | <a href="#">COLIPA N° A156</a> |
| 2-Methyl-4-nitroaniline                              | 0.70 | Yes | Opinion not found.                             | -                              |
| 2-Methyl-5-aminophenol                               | 0.70 | Yes | Has skin sensitization potential.              | <a href="#">COLIPA N° A27</a>  |
| 2-Methylresorcinol                                   | 0.69 | Yes | Has skin sensitization potential.              | <a href="#">COLIPA N° A44</a>  |
| 2-Nitro- <i>N</i> -hydroxyethyl- <i>p</i> -anisidine | 0.66 | No  | Opinion not found.                             | -                              |
| 2-Nitro- <i>p</i> -phenylenediamine                  | 0.71 | Yes | Opinion not found.                             | -                              |
| 3,3'-Dihydroxydiphenylamine                          | 0.74 | Yes | Opinion not found.                             | -                              |
| 3,4-Diaminotoluene                                   | 0.66 | Yes | Opinion not found.                             | -                              |

|                                                           |      |     |                                                |                               |
|-----------------------------------------------------------|------|-----|------------------------------------------------|-------------------------------|
| 3,4-Dihydroxyaniline                                      | 0.75 | Yes | Opinion not found.                             | -                             |
| 3,4-Methylenedioxyaniline                                 | 0.78 | Yes | Opinion not found.                             | -                             |
| 3,4-Methylenedioxyphenol                                  | 0.80 | Yes | Opinion not found.                             | -                             |
| 3-Amino-2,4-dichlorophenol                                | 0.75 | Yes | Has skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A43</a> |
| 3-Chloro-4-aminophenol                                    | 0.77 | Yes | Opinion not found.                             | -                             |
| 3-Methylamino-4-nitrophenoxyethanol                       | 0.64 | No  | Not recognized as a human skin sensitizer.     | <a href="#">COLIPA N° B58</a> |
| 3-Nitro-4-aminophenoxyethanol                             | 0.60 | No  | Opinion not found.                             | -                             |
| 3-Nitro- <i>p</i> -cresol                                 | 0.69 | Yes | Opinion not found.                             | -                             |
| 3-Nitro- <i>p</i> -hydroxyethylaminophenol<br>(HC Red 54) | 0.72 | Yes | Has skin sensitization potential.              | <a href="#">COLIPA N° B54</a> |
| 4-(Methylamino)-2,6-dinitrophenol                         | 0.82 | Yes | Opinion not found.                             | -                             |

|                                                      |      |     |                                   |                               |
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| 4,4'-Diaminodiphenylamine                            | 0.75 | Yes | Opinion not found.                | -                             |
| 4,5-Diamino-1-((4-chlorophenyl)methyl)-1H-pyrazole   | 0.67 | Yes | Opinion not found.                | -                             |
| 4,5-Diamino-1-methylpyrazole                         | 0.70 | Yes | Opinion not found.                | -                             |
| 4,6-Bis(2-hydroxyethoxy)- <i>m</i> -phenylenediamine | 0.67 | Yes | Opinion not found.                | -                             |
| 4-Amino-2-nitrophenol                                | 0.67 | Yes | Opinion not found.                | -                             |
| 4-Amino-3-fluorophenol                               | 0.76 | Yes | Opinion not found.                | -                             |
| 4-Amino-3-nitrophenol                                | 0.69 | Yes | Extreme human skin sensitizer.    | <a href="#">COLIPA N° B51</a> |
| 4-Aminobenzenesulfonic acid                          | 0.60 | Yes | Opinion not found.                | -                             |
| 4-Amino- <i>m</i> -cresol                            | 0.70 | Yes | Has skin sensitization potential. | <a href="#">COLIPA N° A74</a> |
| 4-Amino- <i>o</i> -cresol                            | 0.70 | Yes | Opinion not found.                | -                             |

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| 4-Chloro-2-aminophenol                            | 0.71 | Yes | Opinion not found.                         | -                              |
| 4-Chlororesorcinol                                | 0.77 | Yes | Has skin sensitization potential.          | <a href="#">COLIPA N° A12</a>  |
| 4-Ethoxy- <i>m</i> -phenylenediamine              | 0.67 | Yes | Opinion not found.                         | -                              |
| 4-Hydroxypropylamino-3-nitrophenol<br>(HC Red BN) | 0.71 | No  | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° B100</a> |
| 4-Methoxy-3-aminophenol                           | 0.68 | Yes | Opinion not found.                         | -                              |
| 4-Methoxytoluene-2,5-diamine                      | 0.71 | Yes | Opinion not found.                         | -                              |
| 4-Nitro- <i>m</i> -phenylenediamine               | 0.71 | Yes | Opinion not found.                         | -                              |
| 4-Nitro- <i>o</i> -phenylenediamine               | 0.74 | Yes | Has skin sensitization potential.          | <a href="#">COLIPA N° B24</a>  |
| 4-Nitrophenyl aminoethylurea                      | 0.76 | No  | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° B70</a>  |
| 5-((2-Hydroxyethyl)amino)- <i>o</i> -cresol       | 0.73 | Yes | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° A31</a>  |

|                                         |      |     |                                                         |                                |
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| 5-Amino-2,6-dimethoxy-3-hydroxypyridine | 0.70 | Yes | Opinion not found.                                      | -                              |
| 5-Amino-4-chloro- <i>o</i> -cresol      | 0.74 | Yes | Not recognized as a human skin sensitizer. <sup>8</sup> | <a href="#">COLIPA N° A117</a> |
| 5-Amino-4-fluoro-2-methylphenol         | 0.73 | Yes | Opinion not found.                                      | -                              |
| 5-Amino-6-chloro- <i>o</i> -cresol      | 0.80 | Yes | Not recognized as a human skin sensitizer.              | <a href="#">COLIPA N° A94</a>  |
| 5-Chloro-2-aminophenol                  | 0.71 | Yes | Opinion not found.                                      | -                              |
| 5-Hydroxy-1,4-benzodioxane              | 0.72 | Yes | Opinion not found.                                      | -                              |
| 5-Methylresorcinol                      | 0.72 | Yes | Opinion not found.                                      | -                              |
| 6-Amino- <i>m</i> -cresol               | 0.65 | Yes | Human sensitization potential not reported.             | <a href="#">COLIPA N° A75</a>  |
| 6-Amino- <i>o</i> -cresol               | 0.73 | Yes | Opinion not found.                                      | -                              |
| 6-Hydroxybenzomorpholine                | 0.69 | Yes | Not recognized as a human skin sensitizer.              | <a href="#">COLIPA N° A25</a>  |

|                               |      |     |                                             |                                |
|-------------------------------|------|-----|---------------------------------------------|--------------------------------|
| 6-Hydroxyindole               | 0.55 | Yes | Has skin sensitization potential.           | <a href="#">COLIPA N° A128</a> |
| 6-Methoxy-2,3-pyridinediamine | 0.66 | Yes | Opinion not found.                          | -                              |
| 6-Nitro- <i>o</i> -toluidine  | 0.59 | Yes | Human sensitization potential not reported. | <a href="#">COLIPA N° B56</a>  |
| C.I. Acid Black 1             | 0.57 | No  | Not recognized as a human skin sensitizer.  | <a href="#">COLIPA N° B15</a>  |
| C.I. Acid Blue 74             | 0.65 | Yes | Opinion not found.                          | -                              |
| C.I. Acid Brown 13            | 0.56 | No  | Opinion not found.                          | -                              |
| C.I. Acid Green 50            | 0.68 | No  | Opinion not found.                          | -                              |
| C.I. Acid Orange 10           | 0.63 | No  | Opinion not found.                          | -                              |
| C.I. Acid Orange 24           | 0.73 | No  | Opinion not found.                          | -                              |
| C.I. Acid Orange 3            | 0.62 | Yes | Opinion not found.                          | -                              |

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| C.I. Acid Orange 6  | 0.70 | Yes | Opinion not found.                          | -                              |
| C.I. Acid Orange 7  | 0.68 | No  | Not recognized as a human skin sensitizer.  | <a href="#">COLIPA N° C15</a>  |
| C.I. Acid Red 14    | 0.74 | Yes | Opinion not found.                          | -                              |
| C.I. Acid Red 18    | 0.63 | No  | Human sensitization potential not reported. | <a href="#">COLIPA N° C175</a> |
| C.I. Acid Red 27    | 0.66 | No  | Opinion not found.                          | -                              |
| C.I. Acid Red 33    | 0.57 | No  | Not recognized as a human skin sensitizer.  | <a href="#">COLIPA N° C22</a>  |
| C.I. Acid Red 51    | 0.60 | No  | Opinion not found.                          | -                              |
| C.I. Acid Red 73    | 0.58 | Yes | Opinion not found.                          | -                              |
| C.I. Acid Red 92    | 0.68 | No  | Not recognized as a human skin sensitizer.  | <a href="#">COLIPA N° C53</a>  |
| C.I. Acid Violet 49 | 0.60 | No  | Opinion not found.                          | -                              |

|                     |      |     |                                             |                                |
|---------------------|------|-----|---------------------------------------------|--------------------------------|
| C.I. Acid Yellow 1  | 0.74 | Yes | Human skin sensitizer.                      | <a href="#">COLIPA N° B1</a>   |
| C.I. Acid Yellow 36 | 0.64 | Yes | Opinion not found.                          | -                              |
| C.I. Basic Blue 26  | 0.65 | No  | Opinion not found.                          | -                              |
| C.I. Basic Blue 41  | 0.70 | No  | Opinion not found.                          | -                              |
| C.I. Basic Blue 47  | 0.67 | No  | Opinion not found.                          | -                              |
| C.I. Basic Blue 54  | 0.80 | No  | Opinion not found.                          | -                              |
| C.I. Basic Blue 7   | 0.61 | No  | Has skin sensitization potential.           | <a href="#">COLIPA N° C46</a>  |
| C.I. Basic Blue 9   | 0.67 | No  | Opinion not found.                          | -                              |
| C.I. Basic Blue 99  | 0.72 | No  | Human sensitization potential not reported. | <a href="#">COLIPA N° C059</a> |
| C.I. Basic Brown 1  | 0.77 | Yes | Opinion not found.                          | -                              |

|                      |      |     |                                   |                                            |
|----------------------|------|-----|-----------------------------------|--------------------------------------------|
| C.I. Basic Brown 16  | 0.71 | No  | Human skin sensitizer.            | <a href="#">COLIPA N° C9</a>               |
| C.I. Basic Brown 17  | 0.66 | No  | Has skin sensitization potential. | <a href="#">COLIPA N° B007</a>             |
| C.I. Basic Brown 4   | 0.75 | Yes | Opinion not found.                | -                                          |
| C.I. Basic Green 1   | 0.66 | No  | Opinion not found.                | -                                          |
| C.I. Basic Green 4   | 0.72 | No  | Opinion not found.                | -                                          |
| C.I. Basic Orange 1  | 0.71 | Yes | Opinion not found.                | -                                          |
| C.I. Basic Orange 2  | 0.77 | Yes | Opinion not found.                | -                                          |
| C.I. Basic Orange 31 | 0.68 | Yes | Has skin sensitization potential. | <a href="#">COLIPA N° B118</a>             |
| C.I. Basic Orange 69 | 0.68 | No  | Has skin sensitization potential. | <a href="#">No COLIPA Reference Number</a> |
| C.I. Basic Red 14    | 0.60 | No  | Opinion not found.                | -                                          |

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| C.I. Basic Red 22    | 0.73 | No  | Opinion not found.                         | -                              |
| C.I. Basic Red 46    | 0.66 | No  | Opinion not found.                         | -                              |
| C.I. Basic Red 51    | 0.76 | No  | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° B116</a> |
| C.I. Basic Red 76    | 0.70 | Yes | Has skin sensitization potential.          | <a href="#">COLIPA N° C8</a>   |
| C.I. Basic Red 9     | 0.71 | Yes | Opinion not found.                         | -                              |
| C.I. Basic Violet 1  | 0.80 | No  | Opinion not found.                         | -                              |
| C.I. Basic Violet 14 | 0.67 | Yes | Opinion not found.                         | -                              |
| C.I. Basic Violet 16 | 0.78 | No  | Opinion not found.                         | -                              |
| C.I. Basic Violet 2  | 0.64 | No  | Has skin sensitization potential.          | <a href="#">COLIPA N° B115</a> |
| C.I. Basic Violet 3  | 0.70 | Yes | Opinion not found.                         | -                              |

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| C.I. Basic Violet 4  | 0.71 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 11 | 0.74 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 13 | 0.76 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 2  | 0.79 | Yes | Opinion not found.                         | -                              |
| C.I. Basic Yellow 28 | 0.76 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 29 | 0.75 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 3  | 0.78 | Yes | Opinion not found.                         | -                              |
| C.I. Basic Yellow 40 | 0.67 | No  | Opinion not found.                         | -                              |
| C.I. Basic Yellow 57 | 0.59 | No  | Has skin sensitization potential.          | <a href="#">COLIPA N° C10</a>  |
| C.I. Basic Yellow 87 | 0.65 | No  | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° B117</a> |

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| C.I. Direct Red 23     | 0.58 | No  | Opinion not found.                | -                              |
| C.I. Direct Red 80     | 0.73 | No  | Opinion not found.                | -                              |
| C.I. Direct Red 81     | 0.66 | No  | Opinion not found.                | -                              |
| C.I. Direct Violet 48  | 0.58 | No  | Opinion not found.                | -                              |
| C.I. Direct Yellow 12  | 0.71 | No  | Opinion not found.                | -                              |
| C.I. Disperse Black 9  | 0.73 | Yes | Has skin sensitization potential. | <a href="#">COLIPA N° C106</a> |
| C.I. Disperse Blue 1   | 0.68 | Yes | Opinion not found.                | -                              |
| C.I. Disperse Blue 3   | 0.64 | No  | Opinion not found.                | -                              |
| C.I. Disperse Blue 377 | 0.64 | Yes | Has skin sensitization potential. | <a href="#">COLIPA N° C179</a> |
| C.I. Disperse Blue 7   | 0.70 | Yes | Opinion not found.                | -                              |

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|-----------------------------------|------|-----|----------------------------------------|-------------------------------|
| C.I. Disperse Brown 1             | 0.83 | Yes | Opinion not found.                     | -                             |
| C.I. Disperse Orange 3            | 0.75 | Yes | Opinion not found.                     | -                             |
| C.I. Disperse Red 11              | 0.57 | Yes | Opinion not found.                     | -                             |
| C.I. Disperse Red 15 <sup>9</sup> | 0.63 | Yes | Opinion not found.                     | -                             |
| C.I. Disperse Red 17              | 0.77 | No  | Has skin sensitization potential.      | <a href="#">COLIPA N° B5</a>  |
| C.I. Disperse Violet 1            | 0.65 | Yes | <b>Moderate</b> human skin sensitizer. | <a href="#">COLIPA N° C64</a> |
| C.I. Disperse Violet 4            | 0.64 | Yes | Opinion not found.                     | -                             |
| C.I. Disperse Yellow 3            | 0.62 | No  | Opinion not found.                     | -                             |
| C.I. Food Black 1                 | 0.64 | No  | Opinion not found.                     | -                             |
| C.I. Food Black 2                 | 0.71 | No  | Opinion not found.                     | -                             |

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| C.I. Mordant Black 1  | 0.63 | No  | Opinion not found.                         | -                                          |
| C.I. Mordant Red 11   | 0.73 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Black 3  | 0.73 | No  | Opinion not found.                         | -                                          |
| C.I. Solvent Black 5  | 0.61 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Blue 35  | 0.70 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Green 3  | 0.60 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Green 7  | 0.63 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Orange 1 | 0.75 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Red 1    | 0.70 | Yes | Opinion not found.                         | -                                          |
| C.I. Solvent Red 23   | 0.73 | Yes | Not recognized as a human skin sensitizer. | <a href="#">No COLIPA Reference Number</a> |

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| C.I. Solvent Red 3     | 0.66 | Yes | Opinion not found.                         | -                              |
| C.I. Solvent Violet 13 | 0.57 | Yes | Opinion not found.                         | -                              |
| C.I. Solvent Yellow 29 | 0.71 | No  | Opinion not found.                         | -                              |
| C.I. Solvent Yellow 33 | 0.61 | Yes | Opinion not found.                         | -                              |
| C.I. Solvent Yellow 44 | 0.60 | Yes | Opinion not found.                         | -                              |
| C.I. Vat Red 1         | 0.74 | No  | Opinion not found.                         | -                              |
| FD&C Red 4             | 0.68 | No  | Opinion not found.                         | -                              |
| FD&C Red 40            | 0.60 | No  | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° C174</a> |
| FD&C Yellow 6          | 0.68 | Yes | Opinion not found.                         | -                              |
| HC Blue 1              | 0.72 | No  | Opinion not found.                         | -                              |

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| HC Blue 11  | 0.77 | No  | Opinion not found.                                  | -                              |
| HC Blue 12  | 0.70 | No  | <b>Moderate</b> human skin sensitizer.              | <a href="#">COLIPA N° B73</a>  |
| HC Blue 2   | 0.77 | No  | Has skin sensitization potential.                   | <a href="#">COLIPA N° B37</a>  |
| HC Blue 7   | 0.66 | Yes | <b>Moderate</b> human skin sensitizer. <sup>8</sup> | <a href="#">COLIPA N° A130</a> |
| HC Blue 8   | 0.74 | No  | Opinion not found.                                  | -                              |
| HC Brown 1  | 0.73 | No  | Opinion not found.                                  | -                              |
| HC Brown 2  | 0.74 | Yes | Opinion not found.                                  | -                              |
| HC Green 1  | 0.79 | No  | Has skin sensitization potential.                   | <a href="#">COLIPA N° C129</a> |
| HC Orange 1 | 0.67 | Yes | Not recognized as a human skin sensitizer.          | <a href="#">COLIPA N° B47</a>  |
| HC Orange 2 | 0.72 | No  | <b>Strong</b> human skin sensitizer.                | <a href="#">COLIPA N° B67</a>  |

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| HC Red 1    | 0.65 | Yes | Human skin sensitizer.                                                                                                                                | <a href="#">COLIPA N° B48</a>  |
| HC Red 10   | 0.75 | No  | Has skin sensitization potential.                                                                                                                     | <a href="#">COLIPA N° B71</a>  |
| HC Red 13   | 0.68 | No  | <b>Moderate</b> human skin sensitizer.                                                                                                                | <a href="#">COLIPA N° B31</a>  |
| HC Red 16   | 0.72 | No  | Human skin sensitization potential not reported.                                                                                                      | <a href="#">COLIPA N° B114</a> |
| HC Red 3    | 0.67 | No  | Has human skin sensitization potential, and identified as extreme contact sensitizer in GPMT <sup>6</sup> and strong sensitizer in LLNA. <sup>7</sup> | <a href="#">COLIPA N° B50</a>  |
| HC Red 7    | 0.68 | No  | Has <b>strong</b> sensitization potential.                                                                                                            | <a href="#">COLIPA N° B36</a>  |
| HC Red 8    | 0.76 | Yes | Human skin sensitization not reported.                                                                                                                | <a href="#">COLIPA N° C119</a> |
| HC Red 9    | 0.77 | No  | Opinion not found.                                                                                                                                    | -                              |
| HC Violet 1 | 0.66 | No  | Has skin sensitization potential.                                                                                                                     | <a href="#">COLIPA N° B66</a>  |
| HC Violet 2 | 0.76 | No  | Has <b>moderate</b> sensitization potential.                                                                                                          | <a href="#">COLIPA N° B98</a>  |

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| HC Yellow 10 | 0.77 | Yes | Not recognized as a human skin sensitizer. | <a href="#">COLIPA N° B81</a>  |
| HC Yellow 11 | 0.75 | Yes | Human skin sensitization not reported.     | <a href="#">COLIPA N° B63</a>  |
| HC Yellow 12 | 0.70 | Yes | Opinion not found.                         | -                              |
| HC Yellow 13 | 0.68 | No  | Has skin sensitization potential.          | <a href="#">COLIPA N° B102</a> |
| HC Yellow 14 | 0.60 | No  | Opinion not found.                         | -                              |
| HC Yellow 15 | 0.64 | No  | Opinion not found.                         | -                              |
| HC Yellow 2  | 0.65 | Yes | Has skin sensitization potential.          | <a href="#">COLIPA N° B41</a>  |
| HC Yellow 3  | 0.58 | No  | Opinion not found.                         | -                              |
| HC Yellow 4  | 0.73 | No  | Has skin sensitization potential.          | <a href="#">COLIPA N° B38</a>  |
| HC Yellow 5  | 0.72 | No  | Opinion not found.                         | -                              |

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| HC Yellow 7                                          | 0.73 | No  | Not recognized as a human skin sensitizer.                         | <a href="#">COLIPA N° B80</a>  |
| HC Yellow 8                                          | 0.71 | No  | Opinion not found.                                                 | -                              |
| HC Yellow 9                                          | 0.76 | No  | Has skin sensitization potential.                                  | <a href="#">COLIPA N° B69</a>  |
| Hydroquinone                                         | 0.77 | Yes | Human skin sensitization not reported.                             | <a href="#">COLIPA N° A21</a>  |
| Hydroquinonesulfonic acid                            | 0.62 | Yes | Opinion not found.                                                 | -                              |
| Hydroxyanthraquinone-aminopropyl methyl morpholinium | 0.62 | No  | Has skin sensitization potential. <sup>8</sup>                     | <a href="#">COLIPA N° C117</a> |
| Hydroxyethyl-2,6-dinitro- <i>p</i> -anisidine        | 0.71 | No  | Has skin sensitization potential.                                  | <a href="#">COLIPA N° B90</a>  |
| Hydroxyethyl-2-nitro- <i>p</i> -toluidine            | 0.62 | No  | Has skin sensitization potential.                                  | <a href="#">COLIPA N° B75</a>  |
| Hydroxyethyl-3,4-methylenedioxyaniline               | 0.78 | Yes | Has <b>strong</b> human skin sensitization potential. <sup>8</sup> | <a href="#">COLIPA N° A98</a>  |
| Hydroxyethylaminomethyl- <i>p</i> -aminophenol       | 0.74 | Yes | Opinion not found.                                                 | -                              |

|                                                                                      |      |     |                                                   |                               |
|--------------------------------------------------------------------------------------|------|-----|---------------------------------------------------|-------------------------------|
| Hydroxyethyl- <i>p</i> -phenylenediamine                                             | 0.75 | Yes | <b>Strong</b> human skin sensitizer. <sup>8</sup> | <a href="#">COLIPA N° A80</a> |
| Hydroxypyridinone                                                                    | 0.67 | Yes | Opinion not found.                                | -                             |
| <i>m</i> -Aminophenol                                                                | 0.72 | Yes | Has skin sensitization potential.                 | <a href="#">COLIPA N° A15</a> |
| <i>m</i> -Phenylenediamine                                                           | 0.72 | Yes | Opinion not found.                                | -                             |
| <i>N,N'</i> -Bis-(2-hydroxyethyl)-2-nitro- <i>p</i> -phenylenediamine (HC Violet BS) | 0.72 | Yes | Not recognized as a human skin sensitizer.        | <a href="#">COLIPA N° B34</a> |
| <i>N,N</i> -Bis(2-hydroxyethyl)- <i>p</i> -phenylenediamine                          | 0.72 | Yes | Has skin sensitization potential. <sup>8</sup>    | <a href="#">COLIPA N° A50</a> |
| <i>N,N</i> -Diethyl- <i>m</i> -aminophenol                                           | 0.69 | Yes | Opinion not found.                                | -                             |
| <i>N,N</i> -Diethyl- <i>p</i> -phenylenediamine                                      | 0.72 | Yes | Opinion not found.                                | -                             |
| <i>N,N</i> -Diethyltoluene-2,5-diamine                                               | 0.72 | Yes | Opinion not found.                                | -                             |
| <i>N,N</i> -Dimethyl-2,6-pyridinediamine                                             | 0.56 | Yes | Opinion not found.                                | -                             |

|                                                                                   |      |     |                                        |                               |
|-----------------------------------------------------------------------------------|------|-----|----------------------------------------|-------------------------------|
| <i>N,N</i> -Dimethyl- <i>m</i> -aminophenol                                       | 0.74 | Yes | Opinion not found.                     | -                             |
| <i>N,N'</i> -Dimethyl- <i>N</i> -hydroxyethyl-3-nitro- <i>p</i> -phenylenediamine | 0.70 | No  | Opinion not found.                     | -                             |
| <i>N,N</i> -Dimethyl- <i>p</i> -phenylenediamine                                  | 0.76 | Yes | Opinion not found.                     | -                             |
| <i>N</i> -Cyclopentyl- <i>m</i> -aminophenol                                      | 0.65 | Yes | Opinion not found.                     | -                             |
| <i>N</i> -Methoxyethyl- <i>p</i> -phenylenediamine                                | 0.81 | Yes | Opinion not found.                     | -                             |
| <i>N</i> -Methyl-3-nitro- <i>p</i> -phenylenediamine                              | 0.69 | Yes | Opinion not found.                     | -                             |
| <i>N</i> -Methyl- <i>p</i> -aminophenol                                           | 0.77 | Yes | Opinion not found.                     | -                             |
| <i>N</i> -Phenyl- <i>p</i> -phenylenediamine                                      | 0.71 | Yes | <b>Extreme</b> human skin sensitizer.  | <a href="#">COLIPA N° A9</a>  |
| <i>o</i> -Aminophenol                                                             | 0.69 | Yes | Human skin sensitization not reported. | <a href="#">COLIPA N° A14</a> |
| <i>o</i> -Hydroxyphenol                                                           | 0.72 | Yes | Opinion not found.                     | -                             |

|                                            |      |     |                                                    |                                            |
|--------------------------------------------|------|-----|----------------------------------------------------|--------------------------------------------|
| <i>o</i> -Phenylenediamine                 | 0.70 | Yes | Opinion not found.                                 | -                                          |
| <i>p</i> -Aminophenol                      | 0.74 | Yes | Has skin sensitization potential.                  | <a href="#">COLIPA N° A16</a>              |
| PEG-3,2',2'-di- <i>p</i> -phenylenediamine | 0.75 | Yes | Not recognized as a human skin sensitizer.         | <a href="#">COLIPA N° A146</a>             |
| <i>p</i> -Phenylenediamine                 | 0.75 | Yes | <b>Extreme</b> human skin sensitizer.              | <a href="#">COLIPA N° A7</a>               |
| <i>p</i> -Toluenediamine                   | 0.72 | Yes | <b>Extreme</b> human skin sensitizer. <sup>8</sup> | <a href="#">COLIPA N° A5</a>               |
| Pyridine                                   | 0.73 | Yes | Opinion not found.                                 | -                                          |
| Pyrimidine                                 | 0.75 | Yes | Opinion not found.                                 | -                                          |
| Resorcinol                                 | 0.74 | Yes | <b>Strong</b> human skin sensitizer.               | <a href="#">COLIPA N° A11</a>              |
| Tetrabromophenol blue                      | 0.57 | No  | Not recognized as a human skin sensitizer.         | <a href="#">No COLIPA Reference Number</a> |
| Thymol                                     | 0.67 | Yes | Opinion not found.                                 | -                                          |

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<sup>1</sup>Braga, R. C.; Alves, V. M.; Muratov, E. N.; Strickland, J.; Kleinstreuer, N.; Trospsha, A.; Andrade, C. H. Pred-Skin: A Fast and Reliable Web Application to Assess Skin Sensitization Effect of Chemicals. *J. Chem. Inf. Model.* **2017**, 57, 1013-1017. DOI: [10.1021/acs.jcim.7b00194](https://doi.org/10.1021/acs.jcim.7b00194).

<sup>2</sup>Substances banned for use in European Union are designated with **RED** boxes.

<sup>3</sup>AD, applicability domain

<sup>4</sup>Substances in **GREEN** identified by Opinions as a skin sensitizer; substances in **YELLOW** identified by Opinions as having skin sensitization potential; substances in **RED** not identified by Opinions as a sensitizer or having skin sensitization potential.

<sup>5</sup>References denoted with “COLIPA” refer to Opinions.

<sup>6</sup>GPMT, Guinea Pig Maximization Test

<sup>7</sup>LLNA, Local Lymph Node Assay

<sup>8</sup>Opinion name references salt.

<sup>9</sup>C.I. Disperse Red 15 permitted as an impurity of C.I. Disperse Violet 1.