**Joint quantification of PAH and oxy-PAH from standard reference materials (urban dust and diesel particulate matter) and diesel soot surrogate by GC-MS**

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| **SUPPLEMENTARY MATERIAL** |

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1. **Qualitative analysis**

**Table S1.** Results of qualitative analysis of Printex-U, SRM 1649b and 1650b samples by GC-MS SCAN mode, 2 µL of injection volume.

**RT:** Retention Time

**Match:** Can be defined as a factor that indicates correlation between structure of the detected compound and the compound present in the database.

**Table S1.** Results of qualitative analysis of Printex-U, SRM 1649b and 1650b samples by GC-MS SCAN mode, 2 µL of injection volume.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Peak****number** | **RT (min)** | **Compounds** | **CAS number** | **Match** | **Samples** |
| 1 | 10.501 | cis-4,4-Dimethyl-2-pentene | 000762-63-0 | 53 | Printex-U |   |   |
| 2 | 10.664 | 3-Methyl-1-pentene | 000760-20-3 | 59 | Printex-U | SRM 1649b |   |
| 3 | 11.758 | 1,1-Dichloro-2,2-dichloroethane | 000079-34-5 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 4 | 13.993 | Benzaldehyde | 000100-52-7 | 94 | Printex-U |   |   |
| 5 | 14.547 | Dodecane | 000112-40-3 | 93 | Printex-U |   |   |
| 6 | 16.050 | Benzyl alcohol | 000100-51-6 | 96 | Printex-U |   | SRM 1650b |
| 7 | 19.854 | Tetradecane | 000629-59-4 | 96 | Printex-U |   |   |
| 8 | 20.682 | Naphthalene | 000091-20-3 | 93 | Printex-U | SRM 1649b | SRM 1650b |
| 9 | 21.413 | Benzo[c]thiophene | 000270-82-6 | 95 | Printex-U |   |   |
| 10 | 21.432 | 2-Hydroxy-5-chlorobenzaldehyde | 000635-93-8 | 98 |   | SRM 1649b |   |
| 11 | 23.257 | Quinoline | 000091-22-5 | 97 | Printex-U |   |   |
| 12 | 23.541 | 1-Methylnaphthalene | 000090-12-0 | 96 | Printex-U |   |   |
| 13 | 24.318 | 2-Methylnaphthalene | 000091-57-6 | 96 | Printex-U |   |   |
| 14 | 24.770 | Heptadecane | 000629-78-7 | 97 | Printex-U |   |   |
| 15 | 26.096 | Biphenyl | 000092-52-4 | 95 | Printex-U |   |   |
| 16 | 26.171 | 1,6-Dimethylnaphthalene | 000575-43-9 | 94 | Printex-U |   |   |
| 17 | 26.236 | 1,7-Dimethylnaphthalene | 000575-37-1 | 95 | Printex-U |   |   |
| 18 | 26.376 | Phthalic anhydride | 000085-44-9 | 91 | Printex-U |   |   |
| 19 | 26.799 | 2,6-Dimethylnaphthalene | 000581-42-0 | 98 | Printex-U |   |   |
| 20 | 26.967 | 2,7-Dimethylnaphthalene | 000582-16-1  | 97 | Printex-U |   |   |
| 21 | 27.502 | 2,3-Dimethylnaphthalene | 000581-40-8 | 97 | Printex-U |   |   |
| 22 | 27.828 – 27.833 | 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 006846-50-0 | 90 |   | SRM 1649b | SRM 1650b |
| 23 | 28.689 | 3-Methylbiphenyl | 000643-93-6 | 94 | Printex-U |   |   |
| 24 | 29.043 | 4-Methylbiphenyl | 000644-08-6 | 94 | Printex-U |   |   |
| 25 | 29.243 | Acenaphthylene | 000208-96-8 | 90 | Printex-U | SRM 1649b | SRM 1650b |
| 26 | 29.541 | Octadecane | 000593-45-3 | 97 | Printex-U | SRM 1649b | SRM 1650b |
| 27 | 29.974 | Acenaphthene | 000083-32-9 | 83 | Printex-U | SRM 1649b | SRM 1650b |
| 28 | 30.724 | Dibenzofuran | 000132-64-9 | 87 | Printex-U |   |   |
| 29 | 31.487 | 1-Naphthalenecarbonitrile | 000086-53-3 | 97 | Printex-U |   |   |
| 30 | 31.822 | 2-Naphthalenecarboxaldehyde | 000066-99-9 | 98 | Printex-U |   |   |
| 31 | 31.967 | 1,4-Dihydro-methylethylidene-1,4-methanonaphthalene | 007350-72-3  | 76 | Printex-U |   |   |
| 32 | 32.293 | Nonadecane | 000629-92-5 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 33 | 32.493 | 2-Naphthalenecarbonitrile | 000613-46-7 | 97 | Printex-U |   |   |
| 34 | 32.847 – 32.856 | Diethyl Phthalate | 000084-66-2 | 98 | Printex-U | SRM 1649b | SRM 1650b |
| 35 | 33.200 | Fluorene | 000086-73-7 | 97 | Printex-U | SRM 1649b | SRM 1650b |
| 36 | 33.615 | 2-Pentadecanone, 6,10,14-trimethyl | 000502-69-2 | 91 |   | SRM 1649b |   |
| 37 | 33.764 | [1,1'-Biphenyl]-4-carboxaldehyde | 003218-36-8 | 91 | Printex-U |   |   |
| 38 | 34.187 | 4-Methyldibenzofuran | 007320-53-8 | 89 | Printex-U |   |   |
| 39 | 34.271 | 2-phenyl-2,4,6-Cycloheptatrien-1-one | 014562-09-5 | 86 | Printex-U |   |   |
| 40 | 35.118 | Dibenzo[a,e]pyran | 000092-83-1  | 84 | Printex-U |   |   |
| 41 | 35.407 – 35.440 | Eicosane | 000112-95-8 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 42 | 36.250 | 1,2-dimethyl-naphtho[2,1-b]furan | 129812-23-3 | 74 | Printex-U |   |   |
| 43 | 37.097 | Acridine | 000260-94-6  | 65 | Printex-U |   |   |
| 44 | 37.469 | 2-[(ethylamino)methyl]-4-nitro-phenol | 1000400-09-7 | 59 | Printex-U |   |   |
| 45 | 37.688 | 2-[2-Phenylethenyl]phenol | 042224-48-6 | 72 | Printex-U |   |   |
| 46 | 38.098 | 1,2-dimethyl-naphtho[2,1-b]furan | 129812-23-3 | 60 | Printex-U |   |   |
| 47 | 38.661 | 4-Carbomethoxy-3-methoxy-4-methyl-2,5-cyclohexadien-1-one | 120696-19-7 | 90 | Printex-U |   |   |
| 48 | 38.954 – 38.996 | n-Hexadecanoic acid | 000057-10-3 | 98 | Printex-U | SRM 1649b | SRM 1650b |
| 49 | 41.338 – 41.347 | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | 000084-69-5 | 86 |   | SRM 1649b | SRM 1650b |
| 50 | 41.408 | 9-Fluorenone | 000486-25-9 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 51 | 41.566 | Dibenzothiophene | 000132-65-0 | 95 | Printex-U |   |   |
| 52 | 41.952 | Naphtho[1,2-b]thiophene | 000234-41-3 | 97 | Printex-U |   |   |
| 53 | 42.781 – 42.790 | Docosane | 000629-97-0 | 96 |   | SRM 1649b | SRM 1650b |
| 54 | 43.084 | Phenanthrene | 000085-01-8 | 78 | Printex-U | SRM 1649b | SRM 1650b |
| 55 | 43.223 | Anthracene | 000120-12-7 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 56 | 43.633 | Naphtho[2,1-b]thiophene | 000233-02-3 | 96 | Printex-U |   |   |
| 57 | 44.247 | Benzo[h]quinoline | 000230-27-3 | 95 | Printex-U |   |   |
| 58 | 44.811 | Acridine | 000260-94-6 | 95 | Printex-U |   |   |
| 59 | 45.062 | Dibenzothiophene | 000132-65-0 | 93 | Printex-U |   |   |
| 60 | 45.332 | 3-Methyldibenzothiophene | 016587-52-3 | 97 | Printex-U |   |   |
| 61 | 45.630 | 9-Ethenyl anthracene | 002444-68-0 | 96 | Printex-U |   |   |
| 62 | 46.231 – 46.240 | Dibutyl phthalate | 000084-74-2 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 63 | 46.314 | Tetraethyl pyrazine | 038325-19-8 | 64 | Printex-U |   |   |
| 64 | 46.519 | Benzo[f]isoquinoline | 000229-67-4 | 91 | Printex-U |   |   |
| 65 | 46.771 | Anthrone | 000090-44-8 | 93 | Printex-U |   |   |
| 66 | 46.938 | 2,6,10-trimethyl tetradecane | 014905-56-7 | 91 |   | SRM 1649b |   |
| 67 | 46.952 | Octacosane | 000630-02-4 | 91 | Printex-U |   | SRM 1650b |
| 68 | 47.166 | 1-Methylphenanthrene | 000832-69-9 | 96 | Printex-U |   |   |
| 69 | 47.245 – 47.250 | Octadecanoic acid | 000057-11-4 | 99 |   | SRM 1649b | SRM 1650b |
| 70 | 47.450 – 47.501 | Naphthalic anhydride | 000081-84-5 | 96 | Printex-U |   | SRM 1650b |
| 71 | 47.674 – 47.702 | 3-Methylphenanthrene | 000832-71-3 | 94 | Printex-U |   | SRM 1650b |
| 72 | 47.916 | 2-Methylanthracene | 000613-12-7 | 90 | Printex-U |   |   |
| 73 | 48.349 | 1-Phenanthrenol | 002433-56-9 | 90 | Printex-U |   |   |
| 74 | 48.609 | 6-Cyclohexylnonadecane | 1000357-25-3 | 91 |   |   | SRM 1650b |
| 75 | 49.145 | 1a,9b-dihydro-1H-Cyclopropa[l]phenanthrene | 000949-41-7 | 96 | Printex-U |   |   |
| 76 | 49.457 | Naphtho[2,3-b]norbornadiene | 107426-38-0 | 90 | Printex-U |   |   |
| 77 | 51.291 – 51.314 | Tetracosane | 000646-31-1 | 98 |   | SRM 1649b | SRM 1650b |
| 78 | 51.337 | 2-Phenylnaphthalene | 000612-94-2 | 97 | Printex-U |   |   |
| 79 | 51.524 | 1,2-Acenaphthylenedione | 000082-86-0 | 98 | Printex-U |   |   |
| 80 | 52.180 | 1-Docosene | 001599-67-3 | 95 |   | SRM 1649b |   |
| 81 | 52.189 | Cyclotetracosane | 000297-03-0 | 96 |   |   | SRM 1650b |
| 82 | 52.329 | 2,7-dimethylphenanthrene | 001576-69-8 | 95 | Printex-U |   |   |
| 83 | 52.511 – 52.557 | 1H-Phenalen-1-one | 000548-39-0 | 94 | Printex-U |   | SRM 1650b |
| 84 | 53.069 | Anthralin | 001143-38-0 | 59 | Printex-U |   |   |
| 85 | 53.097 | n-Heptadecylcyclohexane | 019781-73-8 | 93 |   |   | SRM 1650b |
| 86 | 53.479 | 4-Hydroxy-9-fluorenone | 001986-00-1 | 93 | Printex-U |   |   |
| 87 | 53.484 | 3,6-Dimethylphenanthrene | 001576-67-6 | 62 |   |   | SRM 1650b |
| 88 | 54.037 | 1,7-Dimethylphenanthrene | 000483-87-4 | 95 | Printex-U |   |   |
| 89 | 54.270 – 54.321 | 9,10-Anthraquinone | 000084-65-1 | 98 | Printex-U | SRM 1649b | SRM 1650b |
| 90 | 55.420 – 55.425 | Pentacosane | 000629-99-2 | 91 |   | SRM 1649b | SRM 1650b |
| 91 | 55.797 | 5,6-Dihydro-4H-benz[de]anthracene | 004389-09-7 | 58 | Printex-U |   |   |
| 92 | 56.212 | 2,4-Diamino-6-[3,4-dichlorophenyl]-5-methylthieno[2,3-d]pyrimidine | 042160-12-3 | 60 |   | SRM 1649b |   |
| 93 | 57.185 – 57.408 | Fluoranthene | 000206-44-0 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 94 | 57.780 | Cyclopenta(def)phenanthrenone | 005737-13-3 | 98 | Printex-U |   |   |
| 95 | 57.990 | 1,2,3,6,7,8-Hexahydropyrene | 001732-13-4 | 70 | Printex-U |   |   |
| 96 | 58.069 | 4-Phenylpyridine | 000939-23-1 | 35 |   | SRM 1649b |   |
| 97 | 58.763 | 1,1'-(1,3-butadiyne-1,4-diyl)bisbenzene | 000886-66-8 | 68 | Printex-U |   |   |
| 98 | 58.842 | Benzo[b]naphtho[2,3-d]furan | 000243-42-5 | 87 | Printex-U |   |   |
| 99 | 59.191 | 9-Anthracenecarbonitrile | 001210-12-4 | 94 | Printex-U |   |   |
| 100 | 59.219 | Hexacosane | 000630-01-3 | 94 |   | SRM 1649b |   |
| 101 | 59.847 | Phenaleno[1,9-bc]thiophene | 079965-99-4 | 90 | Printex-U |   |   |
| 102 | 60.015 – 60.313 | Naphthalic anhydride | 000081-84-5 | 98 | Printex-U |   | SRM 1650b |
| 103 | 60.313 | Valerenic acid | 003569-10-6 | 90 |   | SRM 1649b |   |
| 104 | 60.527 – 60.732 | Pyrene | 000129-00-0 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 106 | 61.011 | 2,10-Dimethyl-2,3,4,5,6,7-hexahydro-1H-2-benzazonine | 077581-13-6 | 86 | Printex-U |   |   |
| 107 | 61.519 | 11H-Benzo[a]fluorene | 000238-84-6 | 93 | Printex-U |   |   |
| 108 | 61.691 | Pyrene, 1-methyl- | 002381-21-7 | 92 | Printex-U |   |   |
| 109 | 61.868 – 61.877 | cis-9,10-Octadecenoamide | 000301-02-0 | 99 | Printex-U | SRM 1649b | SRM 1650b |
| 110 | 62.217 | Benzo[b]naphtho[2,3-d]furan | 000243-42-5 | 91 | Printex-U |   |   |
| 111 | 62.734 | Heptacosane | 000593-49-7 | 85 |   | SRM 1649b |   |
| 112 | 63.241 | 2-Methylpyrene | 003442-78-2 | 89 | Printex-U |   |   |
| 113 | 63.367 | 2-Methylfluoranthene | 033543-31-6 | 83 | Printex-U |   |   |
| 114 | 63.530 – 63.586 | Methyl dehydroabietate | 001235-74-1 | 89 | Printex-U |   | SRM 1650b |
| 115 | 63.855 | Mitotane | 000053-19-0 | 93 | Printex-U |   |   |
| 116 | 64.773 | 4-Methylpyrene | 003353-12-6 | 96 | Printex-U |   |   |
| 117 | 65.992 | Octacosane | 000630-02-4 | 99 |   | SRM 1649b |   |
| 118 | 66.104 | 11H-Benzo[b]fluorene | 000243-17-4 | 70 | Printex-U |   |   |
| 119 | 67.133 – 67.147 | Bis(2-ethylhexyl) phthalate | 000117-81-7 | 99 | Printex-U | SRM 1649b | SRM 1650b |
| 120 | 69.065 | Nonacosane | 000630-03-5 | 94 |   | SRM 1649b |   |
| 121 | 69.121 | 4,4'-Biphenyldicarboxaldehyde | 000066-98-8 | 41 | Printex-U |   |   |
| 122 | 69.414 | 11H-Isoindolo[2,1-a]benzimidazol-11-one | 002717-05-7 | 59 | Printex-U |   |   |
| 123 | 70.317 | 1,2'-Binaphthalene | 004325-74-0 | 96 | Printex-U |   |   |
| 124 | 70.401 | Benzofluorenone | 000479-79-8 | 98 | Printex-U | SRM 1649b | SRM 1650b |
| 125 | 71.085 | Benzo[b]naphtho[2,3-d]thiophene | 000243-46-9 | 98 | Printex-U |   |   |
| 126 | 71.188 | 5,6-Dihydro-6-oxodibenzo(b,f)-1,4-thiazepine | 003159-07-7 | 64 | Printex-U |   |   |
| 127 | 71.732 | Cyclopenta[cd]pyrene | 027208-37-3 | 95 | Printex-U |   |   |
| 128 | 72.719 | 3-Chloro-5H-dibenz[b,f]azepine | 039607-90-4 | 59 | Printex-U |   |   |
| 129 | 72.845 | 7H-Benz[de]anthracen-7-one | 000082-05-3 | 94 | Printex-U |   |   |
| 130 | 73.627 | Benz[a]anthracene | 000056-55-3 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 131 | 74.404 | 3,4-Dihydrocyclopenta(cd)pyrene | 025732-74-5 | 95 | Printex-U |   |   |
| 132 | 74.511 | Chrysene | 000218-01-9 | 89 | Printex-U | SRM 1649b | SRM 1650b |
| 133 | 74.619 | 9,10-o-Benzenoanthracene | 000477-75-8 | 89 | Printex-U |   |   |
| 134 | 74.702 | Hentriacontane | 000630-04-6 | 96 |   | SRM 1649b |   |
| 135 | 74.861 | N-phenylthiazolo[4,5-c]pyridin-2-amine | 1000400-95-0 | 50 | Printex-U |   |   |
| 136 | 75.089 | 9-Phenylanthracene | 000602-55-1 | 95 | Printex-U |   |   |
| 137 | 76.132 | 3,3,5,5-Tetramethyl-2,3,5,6-tetrahydro-S-indacene-1,7-dione | 055591-17-8 | 58 | Printex-U |   |   |
| 138 | 77.370 | Benzanthrone | 000082-05-3 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 139 | 78.701 | 2-phenylphenanthrene | 004325-77-3 | 86 | Printex-U |   |   |
| 140 | 79.656 | 2,2'-Binaphthalene | 000612-78-2 | 95 | Printex-U |   |   |
| 141 | 79.888 | Benz(a)anthracene-7,12-dione | 002498-66-0 | 83 | Printex-U | SRM 1649b | SRM 1650b |
| 142 | 83.748 | Naphthacene-5,12-dione | 001090-13-7 | 83 | Printex-U | SRM 1649b |   |
| 143 | 86.001 | 1,2-Diphenyl-3-chlorocarbonyl-cyclopropene | 006415-58-3 | 53 |   | SRM 1649b |   |
| 144 | 86.033 | Benzo[b]fluoranthene | 000205-99-2 | 99 | Printex-U | SRM 1649b | SRM 1650b |
| 145 | 86.322 | Benzo[k]fluoranthene | 000207-08-9 | 97 | Printex-U | SRM 1649b | SRM 1650b |
| 146 | 86.760 | Perylene | 000198-55-0 | 95 | Printex-U |   |   |
| 147 | 87.044 | Aceanthrenequinone | 006373-11-1 | 42 | Printex-U |   |   |
| 148 | 87.667 | 4,5-Dihydrobenzo[a]pyrene | 57652-66-1  | 78 | Printex-U |   |   |
| 149 | 90.689 | Benzo[a]pyrene | 000050-32-8 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 150 | 91.354 | Benzo[e]pyrene | 000192-97-2 | 98 | Printex-U |   |   |
| 151 | 92.993 | Benzo[j]fluoranthene | 000205-82-3 | 96 | Printex-U |   |   |
| 152 | 93.105 | Benzo[cd]pyrenone | 003074-00-8 | 96 | Printex-U | SRM 1649b | SRM 1650b |
| 153 | 98.700 | Biacenaphthenylidene | 002435-82-7 | 55 | Printex-U |   |   |
| 154 | 104.510 | Indeno[1,2,3-cd]pyrene | 000193-39-5 | 95 | Printex-U | SRM 1649b | SRM 1650b |
| 155 | 105.474 | Dibenz[a,h]anthracene | 000053-70-3 | 38 | Printex-U | SRM 1649b | SRM 1650b |
| 156 | 105.972 | Dibenzo[def,mno]chrysene | 000191-26-4 | 94 | Printex-U |   |   |
| 157 | 110.842 | Benzo[ghi]perylene | 000191-24-2 | 96 | Printex-U | SRM 1649b | SRM 1650b |