**Appendix A:** Summarized Analytical (Method II) and Predicted MI Information for HBPS Used to Develop the Model to Predict MI Values from Method II data.

 **HPV**  **CASRN5** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Aromatic Extracts 64742-04-7 86141 28 27.7 GE 1 0 0.2 7.6 7.6 1.9 0.2 0

 86187 26.8 26.8 GE 1 0 0 4.1 8.1 6.1 2 0.4

 86303 4 3.4 GE 1 0 0 0.3 2.9 5.8 4.4 1

 89130 54 54.3 GE 1 0 0.1 5.6 8.3 0 0.6 0

 64742-10-5 85255 3.5 3.5 GE 1 0 0.2 1.5 1.5 0.7 0 0

 87336 6.4 6.4 GE 1 0.9 0.5 3.2 0 0 0 0

 Unidentified 85097 4.6 4.6 GE 1 0 0.1 0.3 1 1 1.5 1

 85102 6.8 6.7 GE 1 0 0 0.1 1.2 1.2 0.8 0.4

 85106 10.7 10.7 GE 1 0 0.2 0.9 2.7 1.8 1.8 0.9

 85109 17 17 GE 1 0.2 0.2 0.6 5.6 7.5 3.8 0.8

 85113 9.7 9.7 GE 1 0.1 0.1 0.9 2.8 1.9 1.9 0.9

 Aromatic Extracts/ 85256 2.6 2.6 GE 1 0 0.1 1.9 1 0.3 0 0

 Lubricating Oil Basestock

 Mixture

 Asphalts 64742-93-4 91123 0 0 LT 1 0 0.1 0.1 0.1 0 0 0

 Asphalts (fume) 64642-93-4 89606 6.3 6.3 GE 1 0 0.3 1.4 0.7 0.7 0.3 0

 89607 3.7 3.7 GE 1 0 0.1 0.3 0.3 0.3 0.3 0.3

 89608 8 8.3 GE 1 0 0.3 0.6 0.3 0.2 0.1 0

 8052-42-4 94435 3 4.2 GE 1 0 1.1 1.4 0.7 0.3 0 0.1

 94436 28 4.1 GE 1 0 0.6 1.9 7.6 5.7 3.8 0.4

 94437 20 25.3 GE 1 0 6 9 6 6 6 0.9

 Gas Oils 64741-43-1 85288 5.2 5.2 GE 1 0 2.6 5.3 0.2 0.3 0.4 0.3

 64741-44-2 87523 1 1 GE 1 0.4 2.5 1.3 0 0 0 0

 88773 0 0 LT 1 0 0.7 0.2 0 0 0 0 Yes

 64741-49-7 85242 5.2 5.2 GE 1 0.2 1.8 2.4 0.6 0.4 0.1 0.1

 86175 6.8 6.8 GE 1 0 2 3.4 1.3 0.4 0.1 0.1

 86178 11 10.6 GE 1 0 0.8 4 1.6 0.8 0.3 0.2

**CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

HPV **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Gas Oils 64741-49-7 86186 6.6 6.7 GE 1 0.1 2.7 6.2 0.3 0.1 0.1 0.3 Yes

 86270 6.7 6.7 GE 1 0.9 2.6 3.5 0.9 0.4 0 0.4

 86279 4.6 4.6 GE 1 0.8 4.8 1.6 0.1 0 0 0

 64741-59-9 8281 28.3 28.3 GE 1 2 29.5 14.7 0 0.5 0.5 0

 86182 58 57.9 GE 1 0 17.4 11.6 0 0 0 0

 86191 25 25.1 GE 1 0 13.2 8.8 0 0 0 0

 86195 40 34.6 GE 1 0.4 25.3 10.9 0 0 0 0

 86273 19 19.8 GE 1 0.4 10.9 5.4 0.2 0 0.2 0

 86280 20 20.1 GE 1 0.3 18.1 9 0 0 0.3 0

 87524 14 13.8 GE 1 2 16.8 8.4 0 0 0 0

 87526 7.9 7.9 GE 1 1.1 9.6 6.4 0.2 0 0 0

 87527 1.2 1.2 GE 1 0.8 2 0.8 0.1 0 0 0 Yes

 89295 0 0 LT 1 0.4 42.2 0 0 0 0 0

 89297 0 0 LT 1 0.2 15.2 0 0 0 0 0

 64741-82-8 87213 13 13.3 GE 1 0.1 4.2 6.3 0.3 0 0 0 Yes

 64741-86-2 87088 1.1 1.1 LT 1 0 2.4 0.3 0 0 0 0 Yes

 87467 0 0 LT 1 0 2.3 0.6 0 0 0 0 Yes

 68334-30-5 85202 3.8 3.8 GE 1 0.7 4.1 2 0.3 0 0 0

 85203 3.8 3.9 GE 1 0.7 4.2 2.1 0.1 0 0 0

 68476-30-2 89165 1 1 GE 1 0.1 1.4 1.1 0.1 0 0 0

 89166 1.3 1.2 GE 1 0 3.2 0.8 0 0 0 0

 89167 0.7 0.7 LT 1 0.1 0.8 0.6 0.1 0 0 0

 89169 4.1 4.1 GE 1 0 1.7 2.1 0.1 0 0 0

 89170 3.8 3.8 GE 1 0.2 1.6 1.3 0.2 0 0 0 Yes

 89175 9 9 GE 1 0.1 4.5 5.7 1.1 0 0 0

 89180 2.1 2.1 GE 1 0.4 1.6 2 0.1 0 0 0

 89181 2.8 2.8 GE 1 0.3 1.3 0.8 0 0 0 0

 89182 4 4 GE 1 0.4 1.6 1.6 0.2 0 0 0

**HPV**  **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Gas Oils 68476-30-2 91673 13 12.6 GE 1 0.3 9.6 4.8 0 0.2 0.5 1

 91675 17 17.5 GE 1 0.3 6.1 4.6 1.5 0.8 1.5 0.9

 92200 8.2 8.2 GE 1 0 5.5 5.5 0 0 0 0

 68915-97-9 86174 6.1 6.1 GE 1 0 0.3 4.6 0.6 0.1 0.1 0.1

 86183 9.9 9.9 GE 1 0 0.4 4.3 1.2 0.2 0.1 0.1 Yes

 86190 2 2 GE 1 0.3 3.6 1 0.1 0.2 0 0 Yes

 86271 18 18.3 GE 1 0.1 0.8 5.3 3.2 0.4 0.2 0.1 Yes

 Unidentified 89164 0.8 0.8 LT 1 0 1.1 0.7 0.1 0 0 0 Yes

 89168 3.1 3.1 GE 1 0 1.5 1.9 0.4 0 0 0

 89171 1.4 1.4 GE 1 0.2 3.3 0.9 0 0 0 0

 89172 7.6 7.6 GE 1 0.2 1.6 2.7 0.5 0 0 0

 89173 8.6 8.4 GE 1 0.4 2.1 2.1 0.5 0 0 0 Yes

 89174 2 2 GE 1 0.3 1.6 0.8 0.1 0 0 0

 89176 6.5 6.5 GE 1 0.4 2.4 2.4 0.6 0 0 0

 89177 2.3 2.3 LT 1 0.5 1.4 0.5 0 0 0 0

 89178 2.7 2.7 GE 1 0.4 2.6 1.3 0.2 0 0 0

 89179 1.7 0 LT 1 0.5 1.9 0.5 0 0 0 0

 89183 9.3 9.3 GE 1 0.8 2.5 4.2 1.7 0.1 0 0

 89184 4 4 GE 1 0.4 1.5 1.5 0.2 0 0 0

 89185 0.7 0.7 LT 1 0.1 0.7 0.1 0 0 0 0

 89187 3.9 4.2 LT 1 0.4 0.8 0.6 0.2 0 0 0 Yes

 89296 0 0 LT 1 0 0.5 0.5 1 0.2 0 0

 Heavy Fuel Oils 64741-57-7 85244 5.6 5.6 GE 1 0 0.1 2.5 1.9 1.2 0.5 0

 85289 7.5 7.4 GE 1 0 0 1.4 1.4 1.4 2.1 0.7 Yes

 86107 .8 7.8 GE 1 0 0.1 1.3 1.9 1.9 1.3 0

 86176 5.3 5.3 GE 1 0 0.6 0.9 2.6 1.7 0.9 1.7 es

 86179 7 7 GE 1 0 0.5 1 3.1 2.1 1 2.1

 86189 3.2 3.2 GE 1 0 0.1 0.2 0.6 1.2 2.5 1.2

**HPV**  **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Heavy Fuel Oils 64741-57-7 86269 13.4 13.4 GE 1 0 0.6 5 3.8 2.5 0.9 0 Yes

 86281 11.2 11.2 GE 1 0 0.6 3.6 2.7 1.8 0.7 0.1

 64741-62-4 86001 739 739 GE 1 0 2.6 25.7 19.3 6.4 3.2 0.6

 86002 717 726.2 GE 1 0 1.9 12.3 24.7 12.3 6.2 1.2 Yes

 86015 466 466.4 GE 1 0 0.3 6.2 12.5 9.4 6.2 1.2

 86066 555 555.4 GE 1 0 0.5 10.5 21 10.5 5.3 1.6

 86123 34 33.7 GE 1 0.1 4 4 2.7 2.7 1.2 0.3 Yes

 86180 699 688.1 GE 1 0 1.3 12.7 25.4 12.7 6.4 1.3

 86185 775 774.8 GE 1 0 1.9 25.5 19.1 12.7 5.1 0.6

 86196 873 860.9 GE 1 0 1.5 22.5 30 15 7.5 1.5 Yes

 86484 435 437.8 GE 1 0 1 9.8 19.5 9.8 4.9 1

 87277 142 141.8 GE 1 0 0.4 3.8 5.7 5.7 3.8 0.8 Yes

 87278 168 167.7 GE 1 0 0.9 9.1 9.1 6.1 3 0.9

 87279 170 168.7 GE 1 0 0.8 6.1 6.1 4 2 0.6

 64741-81-7 83366 89 89.1 GE 1 0.1 2.5 5.1 2.5 1.3 0.9 0.1 Yes

 86161 123 122.6 GE 1 0 0.7 6 4.5 3 1.5 0.3

 86181 143 142.7 GE 1 0.2 2.5 12.4 7.4 2.5 0.5 0

 86193 0.7 0.7 LT 1 0.8 2.9 0.4 0 0 0 0

 86194 76 76.2 GE 1 0 0.5 3.2 4.8 4.8 1.6 0.5 Yes

 86198 0 0 LT 1 5.5 2.8 0.6 0.1 0 0 0

 86230 3.5 3.5 GE 1 0.3 2 2.7 1.4 0.4 0.1 0

 86272 112 111.7 GE 1 0.3 4.9 8.1 1.6 0.3 0.2 0

 68476-33-5 86104 85 84.8 GE 1 0 1.5 7.3 2.9 1.3 0.6 0.1

 86108 22 21.9 GE 1 0.3 2.7 2.7 0.9 0.9 0.7 0.3

 86119 8 8 GE 1 0 2.6 2.6 1.8 0.9 0.6 0.2

 68512-62-9 92009 3.9 3.9 GE 1 0 0 0.7 0.7 0.7 1 0.7

 68553-00-4 91674 24 23.1 GE 1 0.1 2.6 5.2 1.3 1.3 1.3 0.9

 Lubricating Oil Basestocks 64741-53-3 84053 4.8 4.8 GE 1 0 0 0 1.1 1.4 0 0 Yes

**HPV**  **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Lubricating Oil Basestocks 64741-53-3 87479 0.9 0 LT 1 0 0 0 0.2 0.6 0.4 0

 92008 5.2 5.2 GE 1 0 0.1 1 1.5 1.5 0.5 0.3

 64741-53-3/64742-70-7 8238 2.1 2.1 GE 1 0 0.2 1.1 1.1 0.3 0.2 0

 64741-96-4 85141 1.8 1.8 GE 1 0 0.5 1.2 0.7 0 0 0

 85142 1 1 LT 1 0 0.5 0.9 0.2 0.1 0 0

 85386 1.2 1.2 GE 1 0 0.5 1.1 0.2 0.1 0 0 Yes

 87584 3.6 3.6 GE 1 0 1.1 3.9 0.6 0.2 0 0 Yes

 87585 0 0 LT 1 0 0.1 0.7 0.4 0.1 0 0 Yes

 87597 0 0 LT 1 0 0 0.1 0.2 0.2 0.1 0

 88484 0 0 LT 1 0.1 0.5 0 0.4 0.1 0.1 0

 88489 0 0 LT 1 0 0.1 0.1 0.1 0.2 0.1 0.1

 88573 0 0 LT 1 0 0.1 0.4 0.1 0 0 0

 88575 0 0 LT 1 0 0 0.1 0.3 0.1 0 0

 64742-17-2 88571 0.8 0.8 LT 1 0 0 0.1 0 0.1 0.1 0.1

 64742-44-5 85105 9.1 9.2 GE 1 0 0.9 7.8 2.2 0.3 0.3 0.2 Yes

 64742-52-5 85108 3.9 3.9 GE 1 0 0.9 2.8 0.5 0.2 0.3 0.1

 86154 0 0 LT 1 0 0 0.2 0 0 0 0

 86155 0 0 LT 1 0 0 0.1 0 0 0 0 Yes

 86156 0.5 0.5 LT 1 0 0 0 0.1 0.1 0 0 Yes

 86461 0 0 LT 1 0 0 0.2 0.2 0.2 0.1 0

 86462 0 0 LT 1 0 0 0 0.1 0.3 0.2 0

 86489 3.9 3.9 GE 1 0 0.8 2.8 0.4 0 0 0

 86514 2.3 2.4 GE 1 0 0.6 1.6 0.3 0.2 0 0

 87116 0.5 0.5 LT 1 0 0.1 1.4 0.2 0 0 0

 87117 0 0.6 LT 1 0 0 0.5 0.4 0.3 0 0

 87399 1 1 LT 1 0 0.6 1.5 0.1 0 0 0

 87453 1.7 1.7 GE 1 0 0.2 0.8 0.5 0.5 0.3 0

 87478 2.2 2.3 GE 1 0 0.5 1.6 0.3 0.1 0 0

**HPV** **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Lubricating Oil Basestocks 64742-52-5 87545 0 0 LT 1 0 0.1 1.5 0.1 0.1 0.1 0

 87598 0 0 LT 1 0 0.8 0.5 0 0 0 0

 87599 0 0 LT 1 0 0 0.5 0.5 0.5 0.2 0

 87600 0 0 LT 1 0 0.1 0.6 0.1 0 0 0 Yes

 87601 0 0 LT 1 0 0 0.8 0.6 0.4 0.2 0

 88056 2 2 LT 1 0 0.5 1.7 0.1 0 0 0 Yes

 88406 0 0 LT 1 0 0.1 0.4 0 0 0 0

 88407 3.7 3.7 GE 1 0 0.6 4.5 1.3 0.4 0 0

 88412 1 1 GE 1 0 0.2 1 0.7 0.7 0.7 0.3

 88488 1.7 1.7 GE 1 0 0.4 0.9 0.4 0.1 0 0

 88506 0.8 0.8 LT 1 0 0.3 1.4 0.1 0 0 0

 88570 0.7 0.7 LT 1 0 0 0.3 0.2 0.2 0 0

 88572 0.4 0.4 LT 1 0 0.5 0.9 0.1 0 0 0

 88574 1 1 LT 1 0 0.1 1 0.1 0 0 0

 88651 0 0 LT 1 0 0.1 0.4 0 0 0 0

 88652 0 0 LT 1 0 0.2 0.6 0.1 0 0 0

 88653 0 0 LT 1 0 0 0.2 0.1 0 0 0

 89299 2 0 LT 1 0 0.3 1.3 0.2 0 0 0

 64742-52-5/64742-53-6 84007 0.9 1.1 GE 1 0 0.5 1.2 0.5 0.1 0 0

 88408 0 0 LT 1 0 0.1 0.6 0 0 0 0

 88409 0.4 0.4 LT 1 0 0 1 0.2 0.1 0 0

 88410 0 0 LT 1 0.1 0.2 0.5 0.2 0 0 0

 64742-53-6 86459 0 0 LT 1 0 0.5 0.4 0 0 0 0

 86460 0 0 LT 1 0 0.1 0.7 0.3 0.1 0.1 0 Yes

 87490 0 0 LT 1 0 1.3 0.6 0 0 0 0

 87492 1.1 1.1 GE 1 0 2.5 1.1 0 0 0 0

 88136 0 0 LT 1 0 0.1 1.3 0.1 0 0 0

 88258 0 0 LT 1 0 0.2 0.7 0.1 0 0 0

**HPV**  **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Lubricating Oil Basestocks 64742-53-6 88487 1.2 1.2 GE 1 0 0.8 1.6 0.2 0.1 0 0

 64742-53-6/64742-52-5 86153 1 1 GE 1 0 0.7 1.3 0.2 0 0 0

 64742-54-7 86148 0 0 LT 1 0 0 0.1 0.1 0.2 0.3 0.3 Yes

 92103 0 0 LT 1 0 0 0 0.1 0.2 0.1 0

 64742-56-9 88088 0 0 LT 1 0 0.1 0.5 0.2 0.1 0 0

 64742-62-7 85158 0 0 LT 1 0 0 0.1 0.3 0.6 0.5 0.1

 90563 0 0 LT 1 0 0 0 0 0 0 0

 64742-65-0 82191 0 0 LT 1 0 0.1 0.4 0.2 0.1 0.1 0

 85098 2.4 2.4 GE 1 0 0.1 1.6 1.3 0.2 0.1 0 Yes

 86133 0 0 LT 1 0 0 0 0 0.1 0.5 0.5

 86142 0 0 LT 1 0 0 0 0 0.1 0.1 0 Yes

 86143 0 0 LT 1 0 0 0.4 0.3 0.1 0 0

 86145 0 0 LT 1 0 0 0 0.2 0.3 0.2 0

 86147 0 0 LT 1 0 0 0.1 0.1 0.2 0.1 0.2

 86149 0 0 LT 1 0 0 0.2 0.1 0 0 0

 87463 1.1 1.1 GE 1 0 0.1 0.3 0.3 0.3 0.3 0.1

 87508 0 0 LT 1 0 0 0.3 0.2 0 0 0

 88089 0 0 LT 1 0 0 0.2 0.2 0.2 0.1 0

 88090 0 0 LT 1 0 0 0 0 0 0.2 0.1

 88091 0 0 LT 1 0 0.3 0 0 0.1 0 0

 88743 0 0 LT 1 0 0 0 0 0 0 0.1

 88744 0 0 LT 1 0 0 0 0 0 0.1 0.3

 90562 0 0 LT 1 0 0 0 0.1 0 0 0

 90564 0 0 LT 1 0 0.2 0.2 0 0 0 0 Yes

 90565 0 0 LT 1 0 0 0 0 0.1 0 0

 91656 0 0 LT 1 0 0 0 0.4 0.1 0 0 Yes

 92099 0.2 0 LT 1 0 0 0.2 0.1 0 0 0

 92102 0.4 0 LT 1 0 0 0 0.2 0.2 0.1 0

**HPV** **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Lubricating Oil Basestocks 64742-65-0 92173 0 0 LT 1 0 0 0.1 0.1 0 0 0

 92174 0 0 LT 1 0 0 0.1 0.2 0.2 0.1 0.1 Yes

 64742-70-7 88638 0 0 LT 1 0 0 0.4 0.1 0.1 0 0

 88639 0 0 LT 1 0 0 0.4 0.2 0.1 0 0

 8042-47-5 90404 0 0 LT 1 0 0 0 0 0.2 0 0

 92062-09-4 90603 0 0 LT 1 0 0 0 0.2 0.2 0.1 0 Yes

 Unidentified 83123 4.1 4.1 GE 1 0 0.6 1.9 0.2 0.1 0.1 0.1

 84063 51.2 32.1 GE 1 6.9 19.2 2.7 0.9 0 0 0

 84064 54.7 53.8 GE 1 12.3 24 10.1 5.9 0 0.5 0

 84071 1.9 1.7 GE 1 0 0.2 0.7 1.6 0.5 0 0 Yes

 84072 1.5 1 GE 1 0 0.3 1.2 1.1 0 0 0

 84073 2.1 1.4 GE 1 0 0.1 0.3 1.1 0.5 0 0

 85104 3.6 3.6 GE 1 0 0.5 3.8 1.1 0.1 0.1 0.1 Yes

 85107 6.5 6.5 GE 1 0 0.6 3.5 1.2 0.2 0.1 0

 85110 4 4 GE 1 0 0.8 2.4 0.4 0.1 0.1 0.1

 85112 9.2 9.2 GE 1 0 0.8 4.2 2.5 0.6 0.1 0

 85373 0 0 LT 1 0 0.3 0.6 0.1 0 0 0

 86127 0 0 LT 1 0 0 0.2 0.1 0 0 0

 86128 0 0 LT 1 0 0 0 0.1 0.2 0.2 0

 86129 0 0 LT 1 0 0.1 0 0 0.1 0.1 0.1

 86132 0 0 LT 1 0 0 0.1 0.2 0.2 0.2 0 Yes

 86157 0.4 0.4 LT 1 0 0.1 0.5 0.4 0.3 0 0

 86162 0 0 LT 1 0 0.1 0.5 0.1 0 0 0

 86163 0 0 LT 1 0 0.1 0.2 0.1 0 0 0

 86164 0 0 LT 1 0 0 0.1 0.1 0.1 0 0

 86165 0 0 LT 1 0 0.1 0.1 0.1 0.1 0.1 0

 86166 0 0 LT 1 0 0.1 0 0 0.1 0.2 0.2

 86220 0 0 LT 1 0 0.1 0 0.1 0.2 0.2 0

**HPV**  **CASRN** **Sample** **Lab**  **Meyers**  **Current**  **1-Ring** **2-Ring 3-Ring** **4-Ring 5-Ring** **6-Ring**  **7-Ring** **Holdout**

 **Category** **Reported**  **Method**  **Model**  **Wt %**  **Wt%** **Wt %** **Wt %** **Wt %** **Wt %** **Wt %** **Sample4**

 **MI1** **MI2 MI3**

 Lubricating Oil Basestocks Unidentified 87360 0 0 LT 1 0 0.6 0.8 0.1 0 0 0

 87366 1.8 1.8 GE 1 0 0.8 2.8 0.2 0 0 0 Yes

 87462 0 0 LT 1 0 0 0.1 0.2 0.2 0.2 0.1 Yes

 87586 0 0 LT 1 0 0 0.2 0.2 0.1 0 0 Yes

 88054 0.7 0 LT 1 0 0.2 1.5 0.1 0 0 0

 89214 0 0 LT 1 0 0.1 0.1 0 0 0 0

 90601 0 0 LT 1 0 0 0 0.1 0.2 0 0

 90602 0 0 LT 1 0 0 0 0.1 0.1 0 0.1

 90604 0 0 LT 1 0 0 0.1 0 0.1 0.1 0

 92158 2.8 2.9 GE 1 0 0 0.3 0.6 0.7 0.7 0.4 Yes

 92159 2.5 2.6 GE 1 0 0.6 2 0.3 0.1 0 0

 92517 1.7 3.8 GE 1 0 1.5 3 0.3 0 0 0

 92518 0.7 0 LT 1 0 0.5 1.8 0.1 0 0 0

 92519 2.3 4.4 GE 1 0 0.8 2.1 0.8 0.3 0.2 0

 92520 0.6 0 LT 1 0 0.1 0.4 0.4 0.3 0.1 0 Yes

 92521 0.6 0 LT 1 0 0.1 0.4 0.5 0.1 0.1 0

 92522 0 0 LT 1 0 0.1 0.2 0.1 0.2 0 0

 92523 0 0 LT 1 0 0.1 0.1 0.1 0 0 0

 950220 0.2 0 LT 1 0 0.1 0.3 0.1 0.1 0 0

 Unidentified 87502 0 0 LT 1 0 0.1 0.1 0.1 0.1 0.1 0.1 Yes

 88098 1.4 1.4 GE 1 0 1.1 2.7 0.2 0 0 0 Yes

1 MI reported in original lab reports, method of determination varied.

2 MI calculated from original data using Myers Method equation 2.2 (Myers, et al. 1981).

3 MI predicted from current model. LT 1 indicates predicted MI is less than 1.0, GE 1 indicates predicted MI is greater than or equal to 1.0.

4 “Holdout samples” indicates the 49 samples used for model testing and validation.

5 When CAS numbers were not provided for samples, they were assigned based on the information provided.