**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.