

GBsolb: GenB で計算される 蛋白脱溶媒和エネルギー

結果として、1t63 構造において 2120 化合物の予測結合値の計算に成功した(表 1)。さらに 1t63 構造で安定構造が計算されなかった化合物のうち 12 化合物について 2pnu 構造において結合予測値の計算に成功した(表 2)。

#### D. 考察

昨年度構築した 2 ステップの AR 予測モデルを用いて約 3000 化合物の予測計算を実施し 2132 化合物について結合予測値が計算された。これらの結果は、他の *in vitro* 系との比較により *in silico* 予測系の信頼性や適応性の検討に用いられるとともに、次のステップとしての *in vitro* スクリーニングにおける化合物優先順位付けにおける指標として用いられる。

種々の工夫により AR 結合性予測システムの精度は大幅に向上したが、残された課題も多い。標的蛋白-リガンドの結合自由エネルギー推算に関する根本的な難しさ(物理化学における基礎的課題)、水分子の扱いの問題、蛋白構造の動き(induced fit)の問題などである。この中で特に、蛋白構造の動きが、予測の成否を左右する重大なファクターの 1 つとなっている。AR 構造については最近になって知見が増えたとはいえ、様々な化学物質

の構造活性相関データから考えると、未だ解明されていない大きな induced fit の動きがあることは間違いない。現在解析されている複合体構造は全てアゴニスト結合型であり、アンタゴニストが結合した時の蛋白コンフォメーション変化の情報はなく、またアゴニスト結合時にも、もっと大きな構造変化がもたらされるケースがあるのではないかと推測される。自動ドッキングの手法は、蛋白構造の動きまで考慮に入れようとする、探索すべき可能性の数が途方もなく膨大なものになってしまうため、限定的にしか考慮することができない。このような現状では、まず標的蛋白の動きの範囲やパターンを事前に研究しておく、それをうまく *in silico* スクリーニングに組み込んでいくスキームの開発を最重要の課題として捉えている。

#### E. 結論

この新たな AR 結合強度予測システムを用いて、約 3,000 個の化学物質について予測計算を実施し、2132 化合物について AR に対する logRBA 予測値を算出した。*In silico* スクリーニングは、膨大な数の化学物質の評価を非常に高速かつ安価に行うことが可能であり、内分泌かく乱の問題解決に非常に有用なツールである。今回得られた予測計算値は、化合物優先順位付けにおける指標のひとつとして用いられる。

表1 1t63構造により計算されたAR結合予測値

| CAS.No     | cal_logRBA |            |       |            |       |
|------------|------------|------------|-------|------------|-------|
| 100-00-5   | -3.64      | 100-74-3   | -3.44 | 102-16-9   | -2.47 |
| 100-01-6   | -3.23      | 100-79-8   | -2.55 | 102-17-0   | -2.45 |
| 100-02-7   | -3.69      | 100-86-7   | -2.91 | 102-19-2   | -2.49 |
| 100-06-1   | -3.27      | 1008-72-6  | -3.17 | 102-20-5   | -2.27 |
| 100-07-2   | -3.65      | 100-88-9   | -3.56 | 10222-01-2 | -4.46 |
| 100-09-4   | -3.61      | 100-97-0   | -3.77 | 102-27-2   | -2.89 |
| 100-14-1   | -3.5       | 101-02-0   | -2.47 | 102-36-3   | -3.82 |
| 100-18-5   | -2.82      | 101-05-3   | -3.02 | 10238-21-8 | -1.14 |
| 100-20-9   | -3.85      | 101-11-1   | -2.25 | 102-47-6   | -3.5  |
| 100-21-0   | -3.38      | 101-14-4   | -2.38 | 1025-15-6  | -3.63 |
| 100-29-8   | -2.99      | 101-20-2   | -2.43 | 102-60-3   | -0.3  |
| 10031-71-7 | -1.98      | 101-25-7   | -2.63 | 10265-92-6 | -2.83 |
| 10031-82-0 | -2.79      | 101-27-9   | -2.38 | 102-71-6   | -2.59 |
| 10031-93-3 | -2.47      | 101-37-1   | -1.98 | 102-77-2   | -2.41 |
| 10034-93-2 | -5.14      | 101-39-3   | -3.49 | 103-01-5   | -3.53 |
| 100-37-8   | -2.9       | 101-41-7   | -3.15 | 103-05-9   | -1.96 |
| 10039-54-0 | -5.14      | 101-48-4   | -2.8  | 103-07-1   | -2.25 |
| 100-41-4   | -3.21      | 101-49-5   | -3.12 | 103-13-9   | -2.77 |
| 100-42-5   | -3.43      | 101-54-2   | -2.25 | 103-25-3   | -2.98 |
| 10042-59-8 | -1.24      | 10161-34-9 | 0.04  | 103-26-4   | -3.15 |
| 100-43-6   | -3.49      | 101-63-3   | -2.55 | 103-28-6   | -2.72 |
| 100-44-7   | -3.67      | 101-68-8   | -2.39 | 103-29-7   | -2.47 |
| 100-47-0   | -3.79      | 101-77-9   | -1.96 | 103-36-6   | -3.37 |
| 100-48-1   | -3.83      | 101-80-4   | -3.06 | 103-37-7   | -3.19 |
| 100-50-5   | -3.03      | 101-81-5   | -2.72 | 103-38-8   | -2.79 |
| 100-51-6   | -2.95      | 101-83-7   | -2.36 | 1034-01-1  | -2.39 |
| 100-52-7   | -3.52      | 101-84-8   | -2.87 | 103-41-3   | -2.74 |
| 100-53-8   | -3.58      | 101-85-9   | -1.94 | 103-45-7   | -2.73 |
| 100-54-9   | -4         | 101-86-0   | -2.5  | 103-49-1   | -2.75 |
| 10058-43-2 | -2.82      | 10191-18-1 | -3.46 | 103-50-4   | -2.69 |
| 100-63-0   | -3.69      | 10191-41-0 | -0.44 | 103-52-6   | -2.47 |
| 100-64-1   | -3.75      | 101-96-2   | -2.99 | 103-54-8   | -3.14 |
| 100-66-3   | -3.47      | 101-97-3   | -3.16 | 103-56-0   | -2.59 |
| 100-68-5   | -3.64      | 102-01-2   | -2.8  | 103-58-2   | -2.32 |
| 100-69-6   | -3.69      | 102-04-5   | -2.58 | 103-59-3   | -2.66 |
| 1006-99-1  | -3.52      | 102-06-7   | -2.72 | 103-60-6   | -2.53 |
| 100-70-9   | -3.76      | 102-09-0   | -2.63 | 10361-39-4 | -2.45 |
| 10072-05-6 | -2.7       | 102-13-6   | -2.71 | 103-61-7   | -2.22 |

| CAS_No     | cal_logRBA |            |       |           |       |
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| 103-63-9   | -3.58      | 104-94-9   | -3.24 | 107-35-7  | -5.12 |
| 103-64-0   | -3.72      | 105-05-5   | -2.65 | 107-41-5  | -2.67 |
| 103-69-5   | -3.53      | 105-08-8   | -2.65 | 107-45-9  | -3.15 |
| 103-70-8   | -3.67      | 105-12-4   | -3.27 | 1075-38-3 | -2.61 |
| 103-71-9   | -3.56      | 105-13-5   | -2.92 | 107-58-4  | -3.07 |
| 103-73-1   | -3.36      | 10519-11-6 | -1.87 | 107-66-4  | -1.59 |
| 103-76-4   | -3.5       | 10519-12-7 | -1.67 | 1076-97-7 | -3.07 |
| 103-82-2   | -2.31      | 10521-91-2 | -2.51 | 107-74-4  | -1.83 |
| 103-84-4   | -3.61      | 105-30-6   | -3.42 | 107-75-5  | -1.81 |
| 103-85-5   | -3.05      | 105-59-9   | -3.42 | 107-85-7  | -3.74 |
| 103-90-2   | -2.99      | 105-60-2   | -3.3  | 107-88-0  | -3.73 |
| 103-93-5   | -3.09      | 105-67-9   | -3.03 | 1079-01-2 | -2.4  |
| 103-95-7   | -2.08      | 10595-06-9 | -2.44 | 107-95-9  | -4.78 |
| 10402-33-2 | -2.06      | 106-22-9   | -1.7  | 107-98-2  | -3.16 |
| 10402-52-5 | -2.69      | 106-24-1   | -3.13 | 108-01-0  | -3.47 |
| 104-09-6   | -2.8       | 106-25-2   | -2.16 | 1080-12-2 | -2.32 |
| 104-15-4   | -2.54      | 106-37-6   | -4.19 | 108-11-2  | -2.87 |
| 10415-87-9 | -2.34      | 106-38-7   | -3.88 | 108-18-9  | -3.71 |
| 10415-88-0 | -2.24      | 106-40-1   | -3.48 | 108-19-0  | -4.28 |
| 104-20-1   | -2.69      | 106-42-3   | -3.33 | 108-26-9  | -4.4  |
| 104-21-2   | -3         | 106-43-4   | -3.5  | 108-38-3  | -3.53 |
| 104-38-1   | -1.2       | 106-44-5   | -3.06 | 108-39-4  | -3.09 |
| 104-49-4   | -3.58      | 106-47-8   | -3.76 | 108-44-1  | -3.28 |
| 104-53-0   | -3.21      | 106-48-9   | -3.3  | 108-45-2  | -3.79 |
| 104-54-1   | -3.33      | 106-49-0   | -3.66 | 108-46-3  | -3.33 |
| 104-57-4   | -3.3       | 106-50-3   | -3.94 | 108-48-5  | -3.53 |
| 104-62-1   | -3.4       | 106-51-4   | -3.63 | 108-50-9  | -3.51 |
| 104-65-4   | -2.49      | 106-54-7   | -3.98 | 1085-98-9 | -2.97 |
| 104-66-5   | -2.47      | 1066-33-7  | -5.52 | 108-67-8  | -3.24 |
| 1047-16-1  | -2.92      | 107-07-3   | -3.96 | 108-68-9  | -2.67 |
| 104-75-6   | -3.06      | 107-15-3   | -4.38 | 108-77-0  | -4.39 |
| 104-76-7   | -1.94      | 107-16-4   | -4.19 | 108-78-1  | -4.08 |
| 10482-56-1 | -2.83      | 1071-83-6  | -2.62 | 108-80-5  | -3.83 |
| 104-83-6   | -3.71      | 107-18-6   | -4.21 | 108-82-7  | -2.99 |
| 10484-56-7 | -2.51      | 1071-93-8  | -3.08 | 108-86-1  | -3.97 |
| 104-87-0   | -2.95      | 107-19-7   | -4.15 | 108-88-3  | -3.63 |
| 104-88-1   | -3.04      | 107-21-1   | -3.99 | 108-89-4  | -3.58 |
| 104-90-5   | -3.13      | 1072-83-9  | -3.31 | 108-90-7  | -3.97 |
| 104-91-6   | -3.04      | 107-29-9   | -3.96 | 108-91-8  | -3.77 |
| 104-93-8   | -3.48      | 1073-29-6  | -3.56 | 108-93-0  | -3.15 |

| CAS No     | cal_logRBA |           |       |             |       |
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| 108-94-1   | -3.09      | 111-40-0  | -3.95 | 1134-23-2   | -2.68 |
| 108-95-2   | -3.38      | 111-41-1  | -3.81 | 1141-38-4   | -2.66 |
| 108-98-5   | -3.85      | 111-42-2  | -4.11 | 1142-19-4   | -3.07 |
| 108-99-6   | -3.74      | 111-46-6  | -3.71 | 114-26-1    | -2.49 |
| 109-02-4   | -3.81      | 111-48-8  | -3.37 | 114651-37-5 | -2.97 |
| 109-06-8   | -3.82      | 111-49-9  | -3.54 | 114-83-0    | -3.34 |
| 109-08-0   | -3.81      | 1115-20-4 | -2.97 | 115-18-4    | -3    |
| 109-09-1   | -3.9       | 111-70-6  | -2.45 | 115-19-5    | -3.44 |
| 109-55-7   | -3.56      | 111-75-1  | -3.72 | 1152-61-0   | -3.29 |
| 109-56-8   | -2.72      | 111-76-2  | -2.9  | 1156-19-0   | -1.72 |
| 109-59-1   | -3.26      | 111-77-3  | -3.2  | 115-70-8    | -3.24 |
| 109-73-9   | -3.88      | 111-86-4  | -2.81 | 115-77-5    | -2.76 |
| 109-78-4   | -3.8       | 111-87-5  | -2.06 | 115-90-2    | -1.95 |
| 109-83-1   | -4.52      | 111-90-0  | -2.74 | 116-02-9    | -2.63 |
| 109-86-4   | -3.67      | 111-92-2  | -2.85 | 116-06-3    | -2.76 |
| 109-89-7   | -4.09      | 112-24-3  | -3.53 | 116-26-7    | -2.87 |
| 109-97-7   | -4.03      | 112-25-4  | -2.9  | 116-29-0    | -2.93 |
| 110-00-9   | -4.35      | 1122-62-9 | -3.32 | 1163-19-5   | -4.54 |
| 110-02-1   | -4.4       | 112-27-6  | -2.94 | 1166-52-5   | -1.63 |
| 110-03-2   | -2.73      | 1122-91-4 | -3.03 | 116-66-5    | -2.36 |
| 110-21-4   | -3.68      | 112-30-1  | -2.17 | 117-08-8    | -3.4  |
| 110-26-9   | -3.95      | 112-34-5  | -2.34 | 117-34-0    | -3.16 |
| 11031-45-1 | -1.28      | 112-35-6  | -2.82 | 117-79-3    | -2.99 |
| 110-63-4   | -3.52      | 1123-85-9 | -3.05 | 117-80-6    | -3.95 |
| 110-64-5   | -3.31      | 1124-11-4 | -3.33 | 117-98-6    | -0.85 |
| 110-65-6   | -3.49      | 112-42-5  | -1.92 | 118-29-6    | -3.39 |
| 110-72-5   | -4.46      | 112-43-6  | -2.1  | 118-33-2    | -3.65 |
| 110-77-0   | -3.58      | 112-50-5  | -2.38 | 118-48-9    | -2.27 |
| 110-80-5   | -3.45      | 1125-21-9 | -2.61 | 118-55-8    | -2.91 |
| 110-85-0   | -3.84      | 112-53-8  | -1.87 | 118-60-5    | -2.05 |
| 110-86-1   | -3.85      | 112-57-2  | -3.38 | 118-61-6    | -3.22 |
| 110-89-4   | -3.75      | 1125-88-8 | -3.48 | 118-69-4    | -3.59 |
| 110-91-8   | -3.96      | 112-59-4  | -1.92 | 118-71-8    | -3.91 |
| 110-96-3   | -3.18      | 112-60-7  | -1.85 | 118-72-9    | -3.44 |
| 110-97-4   | -2.22      | 1126-34-7 | -3.24 | 118-74-1    | -4.08 |
| 110-98-5   | -3.5       | 112-70-9  | -2.25 | 118-75-2    | -4.14 |
| 1111-78-0  | -5.78      | 112-72-1  | -1.56 | 118-79-6    | -4.05 |
| 111-26-2   | -3.77      | 1129-47-1 | -2.83 | 118-90-1    | -2.81 |
| 111-27-3   | -3.31      | 1131-18-6 | -3.05 | 118-91-2    | -3.39 |
| 111-29-5   | -3.03      | 1131-62-0 | -3.54 | 118-93-4    | -3.38 |

| CAS No    | cal_logRBA |            |       |            |       |
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| 118-96-7  | -3.26      | 1212-29-9  | -2.5  | 122-95-2   | -3.44 |
| 119-10-8  | -2.96      | 121-30-2   | -2.37 | 1229-55-6  | -1.73 |
| 1193-02-8 | -3.69      | 121-32-4   | -2.66 | 122-96-3   | -2.96 |
| 1193-18-6 | -2.93      | 121-33-5   | -3.24 | 122-97-4   | -3.05 |
| 119-33-5  | -3.05      | 121-34-6   | -3.31 | 122-99-6   | -3.46 |
| 119-36-8  | -3.46      | 121-39-1   | -2.58 | 123-00-2   | -3.08 |
| 1194-02-1 | -3.73      | 121-57-3   | -3.58 | 123-01-3   | -1.72 |
| 1194-65-6 | -3.77      | 121-60-8   | -2.5  | 123-07-9   | -2.82 |
| 119-47-1  | -1.81      | 121-69-7   | -3.27 | 123-08-0   | -3    |
| 1195-32-0 | -3.17      | 121-73-3   | -3.66 | 123-11-5   | -3.16 |
| 1196-01-6 | -3.23      | 121-79-9   | -2.93 | 123-17-1   | -1.01 |
| 119-64-2  | -2.89      | 121-82-4   | -3.43 | 123-30-8   | -3.3  |
| 119-65-3  | -3.1       | 121-86-8   | -3.26 | 123-31-9   | -3.24 |
| 1197-01-9 | -2.27      | 121-87-9   | -3.19 | 123-32-0   | -3.67 |
| 119-84-6  | -2.44      | 121-91-5   | -3.16 | 123-39-7   | -4.21 |
| 119-90-4  | -2.04      | 121-98-2   | -3.15 | 123-42-2   | -3.01 |
| 120-11-6  | -2.04      | 122-00-9   | -3.5  | 123-51-3   | -3.24 |
| 120-12-7  | -2.73      | 122-01-0   | -3.91 | 123-75-1   | -4.26 |
| 120-14-9  | -3.34      | 122-03-2   | -2.61 | 123-77-3   | -4.38 |
| 120-18-3  | -2.47      | 122-04-3   | -3.56 | 123-96-6   | -2.03 |
| 120-24-1  | -2.15      | 122-11-2   | -2.35 | 124-02-7   | -3.51 |
| 120-36-5  | -3.49      | 122-14-5   | -2.41 | 124-09-4   | -3.71 |
| 120-45-6  | -3.04      | 122-20-3   | -1.72 | 124-22-1   | -1.75 |
| 120-46-7  | -2.7       | 122-34-9   | -3.55 | 124-40-3   | -4.62 |
| 120-50-3  | -3.05      | 122-39-4   | -2.97 | 124-42-5   | -3.13 |
| 1205-17-0 | -2.44      | 122-42-9   | -3.07 | 124-68-5   | -3.32 |
| 120-55-8  | -2.28      | 122-43-0   | -2.78 | 124-76-5   | -2.5  |
| 120-57-0  | -3.15      | 122-45-2   | -1.76 | 126-00-1   | -2.65 |
| 120-58-1  | -2.92      | 122-59-8   | -2.94 | 126-11-4   | -2.83 |
| 120-61-6  | -3.67      | 122-63-4   | -3.39 | 126-30-7   | -3.56 |
| 120-71-8  | -3.44      | 122-67-8   | -2.51 | 12645-31-7 | -0.05 |
| 120-72-9  | -3.43      | 122-69-0   | -2.83 | 126-58-9   | -2.53 |
| 120-75-2  | -3.56      | 12270-13-2 | -1.46 | 126-86-3   | -1.43 |
| 120-78-5  | -2.46      | 122-70-3   | -2.96 | 127-06-0   | -3.6  |
| 120-80-9  | -3.67      | 122-72-5   | -3.11 | 127-41-3   | -2.6  |
| 120-82-1  | -3.98      | 122-73-6   | -2.33 | 127-47-9   | -4.36 |
| 120-93-4  | -4.19      | 122-74-7   | -2.58 | 127-51-5   | -2.48 |
| 120-95-6  | -1.6       | 122-78-1   | -3.2  | 127-68-4   | -3.24 |
| 121-03-9  | -2.97      | 122-79-2   | -3.78 | 128-37-0   | -2.05 |
| 121-14-2  | -2.6       | 122-84-9   | -3.01 | 128-39-2   | -2.21 |

| CAS_No      | cal_logRBA |            |       |            |       |
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| 128-51-8    | -2.18      | 134-20-3   | -3    | 13925-00-3 | -3.5  |
| 129-73-7    | -2.24      | 134-32-7   | -2.86 | 13925-06-9 | -3.06 |
| 1300-72-7   | -3.07      | 134-62-3   | -2.25 | 13925-08-1 | -3.63 |
| 1300-73-8   | -3.29      | 134-81-6   | -2.85 | 139-40-2   | -3.23 |
| 13014-18-1  | -3.8       | 13491-79-7 | -2.65 | 139-66-2   | -2.93 |
| 13014-24-9  | -3.6       | 134-96-3   | -3.28 | 139-70-8   | -1.88 |
| 13019-22-2  | -2.12      | 135-02-4   | -2.83 | 139-85-5   | -2.71 |
| 13036-41-4  | -3.56      | 135-19-3   | -2.54 | 139-89-9   | -2.99 |
| 130-40-5    | -0.4       | 135-20-6   | -1.69 | 140-07-8   | -2.19 |
| 13078-80-3  | -3.71      | 135-57-9   | -2.93 | 140-10-3   | -3.56 |
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| 13092-66-5  | -3.15      | 135-79-5   | -2.76 | 140-25-0   | -1.18 |
| 131-09-9    | -2.87      | 13598-36-2 | -4.13 | 140-26-1   | -2.43 |
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| 131-17-9    | -3.07      | 136-60-7   | -2.89 | 140-31-8   | -3.48 |
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| 2243-62-1  | -2.86      | 2475-45-8  | -2.39 | 2642-71-9  | -2.09 |
| 2244-16-8  | -2.55      | 2475-46-9  | -3.13 | 26544-23-0 | -1.46 |
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| 2403-88-5  | -2.65      | 25524-95-2 | -1.99 | 280-57-9   | -3.4  |
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| 28588-75-2 | -2.63      | 3101-60-8  | -2.22 | 33509-43-2 | -3.14 |
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| 2873-97-4  | -3.32      | 3132-99-8  | -3.52 | 3399-22-2  | -2.63 |
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| 29036-02-0 | -1.08      | 3149-68-6  | -2.88 | 34375-28-5 | -3.56 |
| 290-37-9   | -4.16      | 31499-72-6 | -1.98 | 34413-35-9 | -3.02 |
| 2905-62-6  | -3.95      | 31502-14-4 | -2.65 | 3446-89-7  | -3.17 |
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| 2919-66-6  | -0.64      | 3173-72-6  | -2.25 | 3487-99-8  | -2.56 |
| 29232-93-7 | -2.93      | 3179-80-4  | -0.74 | 34893-92-0 | -3.94 |
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| 29895-73-6 | -1.93      | 326-61-4   | -2.83 | 3549-23-3  | -2.21 |
| 29911-28-2 | -1.21      | 32737-14-7 | -3.36 | 35541-81-2 | -2.47 |
| 299-27-4   | -3.56      | 327-98-0   | -3.06 | 35554-44-0 | -1.94 |
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| 299-84-3   | -3.33      | 328-74-5   | -3.5  | 355-80-6   | -2.72 |
| 299-86-5   | -2.07      | 328-84-7   | -3.75 | 3558-60-9  | -3.11 |
| 3008-43-3  | -3.17      | 3289-28-9  | -2.93 | 3567-69-9  | -3.44 |
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| 3047-32-3  | -3.57      | 330-54-1   | -2.97 | 3615-41-6  | -2.74 |
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| 6632-68-4  | -2.7        | 6881-94-3  | -2.74 | 7212-44-4  | -0.85 |
| 66346-01-8 | -2.27       | 68855-56-1 | -0.8  | 72-14-0    | -2.57 |
| 66841-25-6 | -0.97       | 68-89-3    | -2.18 | 72-17-3    | -4.44 |
| 66-84-2    | -2.21       | 689-11-2   | -3.07 | 7217-59-6  | -3.59 |
| 67028-40-4 | -2.8        | 68959-28-4 | -1.36 | 72-18-4    | -4.22 |
| 670-96-2   | -3.6        | 69045-78-9 | -3.86 | 72-19-5    | -4.15 |

| CAS_No     | cal_logRBA |            |       |            |       |
|------------|------------|------------|-------|------------|-------|
| 72-54-8    | -2.56      | 7681-76-7  | -2.52 | 78-59-1    | -2.34 |
| 72-56-0    | -1.88      | 76-83-5    | -2.21 | 786-19-6   | -1.59 |
| 72987-62-3 | -3.4       | 768-52-5   | -3.22 | 78-69-3    | -2.29 |
| 730-40-5   | -2.55      | 7695-91-2  | -0.26 | 78-70-6    | -2.03 |
| 732-11-6   | -3.02      | 770-35-4   | -3.27 | 78-83-1    | -3.47 |
| 73-22-3    | -2.99      | 7722-76-1  | -3.84 | 78-90-0    | -4.01 |
| 732-26-3   | -1.65      | 7722-84-1  | -4.7  | 78-92-2    | -3.18 |
| 73250-68-7 | -1.97      | 773-64-8   | -2.83 | 78-96-6    | -3.82 |
| 73-32-5    | -4         | 77-53-2    | -1.98 | 79-14-1    | -4.78 |
| 738-70-5   | -2.31      | 77-54-3    | -2.06 | 79-21-0    | -4.07 |
| 7397-62-8  | -2.71      | 7756-96-9  | -2.86 | 792-74-5   | -2.95 |
| 7400-27-3  | -3.76      | 7757-86-0  | -3.15 | 79-33-4    | -4.07 |
| 7402-29-1  | -2.29      | 7757-93-9  | -3.15 | 79-39-0    | -3.66 |
| 74070-46-5 | -2.02      | 7758/11/04 | -3.15 | 79-50-5    | -3.03 |
| 741-58-2   | -1.81      | 7758-23-8  | -4.16 | 79622-59-6 | -3.42 |
| 7460-74-4  | -2.74      | 7764-50-3  | -2.91 | 79-69-6    | -1.51 |
| 74-79-3    | -1.77      | 77-71-4    | -4.03 | 79-74-3    | -2.32 |
| 74-89-5    | -4.83      | 7773-06-0  | -5.2  | 79-78-7    | -1.93 |
| 7493-57-4  | -1.81      | 7774-44-9  | -2.56 | 80-15-9    | -3.47 |
| 7493-74-5  | -3.1       | 7774-65-4  | -1.78 | 80-27-3    | -2.12 |
| 7493-78-9  | -1.49      | 7774-74-5  | -4.21 | 80-33-1    | -3    |
| 7529-22-8  | -3.32      | 7775-39-5  | -2.57 | 80-35-3    | -2.88 |
| 75-31-0    | -4.05      | 7778-77-0  | -4.16 | 80-38-6    | -2.93 |
| 7540-51-4  | -2.55      | 7778-83-8  | -3.09 | 80-54-6    | -1.81 |
| 7549-33-9  | -2.8       | 7779-77-3  | -2.86 | 80-68-2    | -4.03 |
| 7558-63-6  | -4.51      | 7779-78-4  | -2.59 | 81-13-0    | -2.39 |
| 7558-79-4  | -3.15      | 7779-94-4  | -0.8  | 81-15-2    | -1.76 |
| 7558-80-7  | -4.16      | 7783-20-2  | -5.14 | 81-16-3    | -4.75 |
| 75-64-9    | -3.97      | 7783-28-0  | -3.84 | 81-24-3    | -1.55 |
| 75-65-0    | -3.48      | 77-83-8    | -2.29 | 81-25-4    | -2.13 |
| 7580-85-0  | -2.6       | 7784-67-0  | -2.76 | 81-33-4    | -1.67 |
| 75-86-5    | -3.49      | 77-85-0    | -3.61 | 81-81-2    | -1.41 |
| 75-89-8    | -3.79      | 77-86-1    | -3.94 | 81-83-4    | -2.53 |
| 75-91-2    | -3.54      | 7786-61-0  | -2.91 | 81-84-5    | -2.4  |
| 763-32-6   | -3.28      | 77-93-0    | -1.72 | 818-61-1   | -3.26 |
| 76-39-1    | -3.7       | 77-99-6    | -3.49 | 822-36-6   | -3.81 |
| 765-30-0   | -4.22      | 7803-63-6  | -5.14 | 82-28-0    | -2.05 |
| 7664-38-2  | -3.84      | 781-35-1   | -2.34 | 823-22-3   | -2.81 |
| 766-92-7   | -3.49      | 78-37-5    | -1.99 | 823-40-5   | -3.46 |
| 767-00-0   | -3.15      | 78491-02-8 | -2.8  | 82419-36-1 | -2.08 |

| CAS_No     | cal_logRBA |          |       |          |       |
|------------|------------|----------|-------|----------|-------|
| 82-45-1    | -3.09      | 85-42-7  | -2.75 | 87-90-1  | -4.66 |
| 824-78-2   | -2.22      | 85-44-9  | -3.17 | 87-91-2  | -2.78 |
| 825-51-4   | -1.96      | 85-56-3  | -3.04 | 87-99-0  | -1.94 |
| 82560-54-1 | -1.31      | 85-60-9  | -1.35 | 881-68-5 | -2.61 |
| 825-90-1   | -3         | 85-70-1  | -3.26 | 88-18-6  | -2.69 |
| 826-36-8   | -3.2       | 85-91-6  | -3.12 | 88-19-7  | -3.43 |
| 82654-98-6 | -2.81      | 86-26-0  | -2.87 | 88-21-1  | -5.34 |
| 82-68-8    | -3.73      | 86-30-6  | -2.78 | 882-33-7 | -2.62 |
| 828-00-2   | -2.86      | 86-50-0  | -3.68 | 88-24-4  | -3.11 |
| 830-09-1   | -3.47      | 86-57-7  | -2.82 | 88-26-6  | -2.01 |
| 83130-01-2 | -2.07      | 866-84-2 | -4.72 | 88-27-7  | -1.33 |
| 83-32-9    | -2.66      | 86-73-7  | -2.81 | 88-41-5  | -2.58 |
| 83-34-1    | -3.26      | 86-74-8  | -2.87 | 88-44-8  | -4.99 |
| 83-40-9    | -4.15      | 867-56-1 | -4.07 | 88-51-7  | -4.54 |
| 83-41-0    | -3         | 867-81-2 | -3.44 | 88-53-9  | -4.8  |
| 834-12-8   | -2.59      | 868-14-4 | -4.46 | 88-58-4  | -2.51 |
| 83-44-3    | -0.97      | 868-18-8 | -4.46 | 88-60-8  | -2.51 |
| 83-56-7    | -2.65      | 86-87-3  | -1.99 | 886-50-0 | -2.88 |
| 83-62-5    | -4.06      | 868-77-9 | -3.25 | 88-68-6  | -3.91 |
| 836-30-6   | -2.35      | 870-72-4 | -4.28 | 88-69-7  | -3.14 |
| 83-66-9    | -2.28      | 87-19-4  | -2.9  | 88-72-2  | -3.43 |
| 83-67-0    | -2.77      | 87-20-7  | -2.23 | 88-73-3  | -3.81 |
| 838-88-0   | -2.3       | 87-22-9  | -2.3  | 88-74-4  | -3.89 |
| 839-90-7   | -2.53      | 87-25-2  | -3.73 | 88-75-5  | -3.71 |
| 840-65-3   | -2.81      | 872-55-9 | -3.66 | 887-76-3 | -3.1  |
| 841-06-5   | -2.66      | 87-29-6  | -2.89 | 88-85-7  | -2.45 |
| 84-15-1    | -2.51      | 873-32-5 | -3.57 | 88-89-1  | -2.84 |
| 842-18-2   | -4.46      | 87-41-2  | -2.91 | 88-99-3  | -3.25 |
| 84-51-5    | -2.68      | 874-42-0 | -3.25 | 89-00-9  | -3.54 |
| 84-61-7    | -1.11      | 875-74-1 | -2.52 | 89-25-8  | -3.48 |
| 84-65-1    | -2.94      | 87-60-5  | -3.3  | 89-32-7  | -4.04 |
| 84-66-2    | -2.41      | 87-61-6  | -3.94 | 89-43-0  | -1.15 |
| 846-70-8   | -3.65      | 87-62-7  | -3.42 | 89-46-3  | -1.1  |
| 84-72-0    | -3.19      | 87-67-2  | -3.84 | 89-61-2  | -3.41 |
| 85-00-7    | -1.86      | 87-69-4  | -4.46 | 89-62-3  | -3.56 |
| 85-29-0    | -2.85      | 87-79-6  | -2.77 | 89-63-4  | -3.43 |
| 85-32-5    | -0.57      | 87-82-1  | -4.51 | 89-65-6  | -2.1  |
| 85-34-7    | -3.98      | 87-83-2  | -3.91 | 89-71-4  | -3.63 |
| 85-40-5    | -2.64      | 87-86-5  | -3.88 | 89-74-7  | -3.19 |
| 85-41-6    | -3.14      | 87-89-8  | -2.93 | 89-75-8  | -3.95 |

| CAS_No   | cal_logRBA |          |       |          |       |
|----------|------------|----------|-------|----------|-------|
| 89-78-1  | -2.39      | 920-66-1 | -3.26 | 939-48-0 | -3.25 |
| 89-79-2  | -2.77      | 921-53-9 | -4.46 | 93-97-0  | -3.08 |
| 89-81-6  | -2.88      | 92-15-9  | -2.13 | 93-99-2  | -2.75 |
| 89-82-7  | -2.78      | 923-02-4 | -3.51 | 939-97-9 | -2.02 |
| 89-83-8  | -3.04      | 923-26-2 | -2.64 | 94-02-0  | -2.9  |
| 89-84-9  | -2.74      | 923-32-0 | -2.77 | 940-71-6 | -4.15 |
| 89-86-1  | -3.79      | 924-42-5 | -4.21 | 941-69-5 | -3.53 |
| 89-87-2  | -3.05      | 92-48-8  | -2.36 | 941-98-0 | -2.54 |
| 89-88-3  | -0.71      | 92-59-1  | -2.34 | 94-30-4  | -3.42 |
| 89-97-4  | -2.99      | 92-67-1  | -2.67 | 94-36-0  | -3.35 |
| 89-98-5  | -3.28      | 92-70-6  | -3.44 | 944-22-9 | -2.52 |
| 90-00-6  | -2.87      | 927-20-8 | -2.9  | 94-46-2  | -2.78 |
| 90-04-0  | -3.68      | 92-77-3  | -2.41 | 94-47-3  | -2.46 |
| 90-12-0  | -2.92      | 92-84-2  | -3.11 | 94-48-4  | -2.66 |
| 90-15-3  | -2.95      | 928-72-3 | -4.86 | 94-58-6  | -2.96 |
| 90-17-5  | -3.3       | 92-87-5  | -2.7  | 94-59-7  | -2.93 |
| 90-30-2  | -2.18      | 928-92-7 | -3.56 | 94-60-0  | -2.58 |
| 903-19-5 | -1.76      | 928-94-9 | -3.39 | 94-62-2  | -2.11 |
| 90-41-5  | -3.19      | 928-95-0 | -3.5  | 94-68-8  | -3.06 |
| 90-42-6  | -2.62      | 928-96-1 | -3.52 | 947-04-6 | -1.68 |
| 90-43-7  | -3.16      | 929-06-6 | -3.59 | 94-74-6  | -3.57 |
| 90-66-4  | -2.12      | 92-94-4  | -2.01 | 94-75-7  | -3.1  |
| 90-87-9  | -2.68      | 931-19-1 | -2.96 | 94-81-5  | -3.13 |
| 90-98-2  | -2.79      | 931-36-2 | -3.26 | 94-82-6  | -3.16 |
| 91-01-0  | -2.72      | 93-15-2  | -3.21 | 94-86-0  | -3.11 |
| 91-15-6  | -3.46      | 93-16-3  | -3.27 | 94-96-2  | -1.67 |
| 91-16-7  | -3.49      | 93-18-5  | -2.74 | 94-99-5  | -3.57 |
| 91-20-3  | -3.19      | 93-28-7  | -2.44 | 95-14-7  | -3.24 |
| 91-22-5  | -3.29      | 93-51-6  | -3.32 | 95-15-8  | -3.43 |
| 91-23-6  | -3.49      | 93-54-9  | -2.59 | 95-16-9  | -3.42 |
| 91-53-2  | -2.17      | 93-55-0  | -3.55 | 95-29-4  | -2.52 |
| 915-67-3 | -5.51      | 93-58-3  | -3.8  | 953-17-3 | -2.6  |
| 91-57-6  | -2.92      | 935-92-2 | -3.02 | 95-31-8  | -2.9  |
| 91-59-8  | -3.1       | 93-60-7  | -3.49 | 95-32-9  | -2.21 |
| 91-64-5  | -2.62      | 93-68-5  | -2.53 | 95-33-0  | -2.31 |
| 91-66-7  | -2.72      | 937-14-4 | -3.17 | 95-47-6  | -3.32 |
| 91-68-9  | -2.55      | 93-72-1  | -3.16 | 95-48-7  | -3.34 |
| 91-76-9  | -2.79      | 93-84-5  | -3.17 | 95-49-8  | -3.62 |
| 91-99-6  | -2.45      | 93-89-0  | -3.46 | 95-50-1  | -3.75 |
| 92-00-2  | -2.7       | 93-92-5  | -3.03 | 95-51-2  | -3.84 |

| CAS_No   | cal_logRBA |          |       |         |       |
|----------|------------|----------|-------|---------|-------|
| 95-53-4  | -3.74      | 97-56-3  | -2.36 | 99-91-2 | -3.72 |
| 95-54-5  | -3.64      | 97-64-3  | -3.01 | 99-93-4 | -2.91 |
| 95-55-6  | -3.52      | 97-67-6  | -4.84 | 99-94-5 | -3.23 |
| 95-57-8  | -3.71      | 97-99-4  | -3.03 | 99-96-7 | -3.12 |
| 95-63-6  | -3.1       | 98-00-0  | -3.47 | 99-97-8 | -3.24 |
| 95-65-8  | -2.82      | 98-16-8  | -3.53 | 99-99-0 | -3.23 |
| 95-68-1  | -3.5       | 98-29-3  | -2.55 |         |       |
| 95-69-2  | -3.58      | 98-46-4  | -3.36 |         |       |
| 95-70-5  | -3.56      | 98-51-1  | -2.74 |         |       |
| 95-71-6  | -3.26      | 98-52-2  | -2.18 |         |       |
| 95-72-7  | -3.45      | 98-53-3  | -1.92 |         |       |
| 95-73-8  | -3.84      | 98-55-5  | -2.77 |         |       |
| 95-74-9  | -3.56      | 98-56-6  | -3.89 |         |       |
| 95-75-0  | -3.57      | 98-59-9  | -2.98 |         |       |
| 957-51-7 | -2.15      | 98-73-7  | -2.58 |         |       |
| 95-76-1  | -3.64      | 98-82-8  | -3.1  |         |       |
| 95-80-7  | -3.44      | 98-83-9  | -3.03 |         |       |
| 95-87-4  | -3.09      | 98-86-2  | -3.22 |         |       |
| 959-24-0 | -0.97      | 98-87-3  | -3.93 |         |       |
| 95-93-2  | -2.69      | 98-88-4  | -3.44 |         |       |
| 95-94-3  | -4.12      | 98-89-5  | -2.77 |         |       |
| 961-69-3 | -2.17      | 98-91-9  | -3.42 |         |       |
| 96-23-1  | -3.57      | 98-92-0  | -3.4  |         |       |
| 96-24-2  | -3.19      | 98-94-2  | -2.94 |         |       |
| 96-26-4  | -3.63      | 98-95-3  | -3.63 |         |       |
| 96-27-5  | -3.45      | 98-98-6  | -3.48 |         |       |
| 96-31-1  | -3.62      | 99-30-9  | -3.7  |         |       |
| 96-45-7  | -4.12      | 99-48-9  | -2.34 |         |       |
| 96-53-7  | -3.98      | 99-50-3  | -3.56 |         |       |
| 96-76-4  | -2.15      | 99-51-4  | -3.09 |         |       |
| 97-00-7  | -3.27      | 99-54-7  | -3.81 |         |       |
| 97-17-6  | -2.9       | 99-55-8  | -3.35 |         |       |
| 97-18-7  | -2.76      | 99-62-7  | -2.49 |         |       |
| 97-30-3  | -2.92      | 996-31-6 | -4.44 |         |       |
| 973-21-7 | -1.57      | 99-63-8  | -3.19 |         |       |
| 97-36-9  | -2.02      | 99-65-0  | -3.4  |         |       |
| 97-42-7  | -2.16      | 99-75-2  | -3.35 |         |       |
| 97-45-0  | -2.32      | 99-87-6  | -2.8  |         |       |
| 97-52-9  | -3.08      | 99-88-7  | -3.63 |         |       |
| 97-53-0  | -3         | 99-89-8  | -2.38 |         |       |

表2 2pnu構造により計算されたAR結合予測値

| CAS.No     | cal.logRBA |
|------------|------------|
| 10081-67-1 | -1.39      |
| 120-40-1   | -2.3       |
| 13676-54-5 | -1.75      |
| 145-42-6   | -2.51      |
| 153-18-4   | -1.98      |
| 1934-21-0  | -0.87      |
| 21850-44-2 | -5.07      |
| 52829-07-9 | -1.76      |
| 54395-52-7 | 1.73       |
| 57808-65-8 | -5.49      |
| 70321-86-7 | -0.41      |
| 860-22-0   | -3.18      |