**Supplementary Material**

**Machine learning models for fast selection of amino acids as green thermodynamic inhibitors for natural gas hydrate**

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**Table S1** Properties of amino acids and hydrate phase equilibrium data [1-7]

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Amino Acid | No. | MW | pI | hI | conc | C1% | C2% | C3% | P | T |
| Glycine | 1 | 75.07 | 6.06 | -0.40 | 2.05 | 100.00 | 0.00 | 0.00 | 2.94 | 274.45 |
| Glycine | 2 | 75.07 | 6.06 | -0.40 | 2.05 | 100.00 | 0.00 | 0.00 | 4.43 | 278.35 |
| Glycine | 3 | 75.07 | 6.06 | -0.40 | 2.05 | 100.00 | 0.00 | 0.00 | 5.93 | 281.15 |
| Glycine | 4 | 75.07 | 6.06 | -0.40 | 2.05 | 100.00 | 0.00 | 0.00 | 7.43 | 283.25 |
| Glycine | 5 | 75.07 | 6.06 | -0.40 | 2.05 | 100.00 | 0.00 | 0.00 | 8.97 | 284.85 |
| Glycine | 6 | 75.07 | 6.06 | -0.40 | 5.21 | 100.00 | 0.00 | 0.00 | 2.95 | 273.95 |
| Glycine | 7 | 75.07 | 6.06 | -0.40 | 5.21 | 100.00 | 0.00 | 0.00 | 4.41 | 277.65 |
| Glycine | 8 | 75.07 | 6.06 | -0.40 | 5.21 | 100.00 | 0.00 | 0.00 | 5.91 | 280.45 |
| Glycine | 9 | 75.07 | 6.06 | -0.40 | 5.21 | 100.00 | 0.00 | 0.00 | 7.40 | 282.45 |
| Glycine | 10 | 75.07 | 6.06 | -0.40 | 5.21 | 100.00 | 0.00 | 0.00 | 8.93 | 284.30 |
| Glycine | 11 | 75.07 | 6.06 | -0.40 | 8.58 | 100.00 | 0.00 | 0.00 | 2.94 | 273.35 |
| Glycine | 12 | 75.07 | 6.06 | -0.40 | 8.58 | 100.00 | 0.00 | 0.00 | 4.42 | 277.25 |
| Glycine | 13 | 75.07 | 6.06 | -0.40 | 8.58 | 100.00 | 0.00 | 0.00 | 5.90 | 279.95 |
| Glycine | 14 | 75.07 | 6.06 | -0.40 | 8.58 | 100.00 | 0.00 | 0.00 | 7.40 | 282.05 |
| Glycine | 15 | 75.07 | 6.06 | -0.40 | 8.58 | 100.00 | 0.00 | 0.00 | 8.92 | 283.75 |
| Glycine | 16 | 75.07 | 6.06 | -0.40 | 11.42 | 100.00 | 0.00 | 0.00 | 2.92 | 272.85 |
| Glycine | 17 | 75.07 | 6.06 | -0.40 | 11.42 | 100.00 | 0.00 | 0.00 | 4.40 | 276.75 |
| Glycine | 18 | 75.07 | 6.06 | -0.40 | 11.42 | 100.00 | 0.00 | 0.00 | 5.88 | 279.45 |
| Glycine | 19 | 75.07 | 6.06 | -0.40 | 11.42 | 100.00 | 0.00 | 0.00 | 7.35 | 281.40 |
| Glycine | 20 | 75.07 | 6.06 | -0.40 | 11.42 | 100.00 | 0.00 | 0.00 | 8.87 | 283.05 |
| Glycine | 21 | 75.07 | 6.06 | -0.40 | 2.05 | 93.00 | 5.00 | 2.00 | 1.25 | 276.25 |
| Glycine | 22 | 75.07 | 6.06 | -0.40 | 2.05 | 93.00 | 5.00 | 2.00 | 1.95 | 280.45 |
| Glycine | 23 | 75.07 | 6.06 | -0.40 | 2.05 | 93.00 | 5.00 | 2.00 | 2.66 | 283.05 |
| Glycine | 24 | 75.07 | 6.06 | -0.40 | 2.05 | 93.00 | 5.00 | 2.00 | 3.37 | 285.05 |
| Glycine | 25 | 75.07 | 6.06 | -0.40 | 2.05 | 93.00 | 5.00 | 2.00 | 4.09 | 286.75 |
| Glycine | 26 | 75.07 | 6.06 | -0.40 | 5.21 | 93.00 | 5.00 | 2.00 | 1.24 | 275.85 |
| Glycine | 27 | 75.07 | 6.06 | -0.40 | 5.21 | 93.00 | 5.00 | 2.00 | 1.95 | 280.15 |
| Glycine | 28 | 75.07 | 6.06 | -0.40 | 5.21 | 93.00 | 5.00 | 2.00 | 2.65 | 282.65 |
| Glycine | 29 | 75.07 | 6.06 | -0.40 | 5.21 | 93.00 | 5.00 | 2.00 | 3.36 | 284.75 |
| Glycine | 30 | 75.07 | 6.06 | -0.40 | 5.21 | 93.00 | 5.00 | 2.00 | 4.10 | 286.45 |
| Glycine | 31 | 75.07 | 6.06 | -0.40 | 8.58 | 93.00 | 5.00 | 2.00 | 1.25 | 275.45 |
| Glycine | 32 | 75.07 | 6.06 | -0.40 | 8.58 | 93.00 | 5.00 | 2.00 | 1.95 | 279.75 |
| Glycine | 33 | 75.07 | 6.06 | -0.40 | 8.58 | 93.00 | 5.00 | 2.00 | 2.64 | 282.25 |
| Glycine | 34 | 75.07 | 6.06 | -0.40 | 8.58 | 93.00 | 5.00 | 2.00 | 3.36 | 284.35 |
| Glycine | 35 | 75.07 | 6.06 | -0.40 | 8.58 | 93.00 | 5.00 | 2.00 | 4.09 | 285.95 |
| Glycine | 36 | 75.07 | 6.06 | -0.40 | 11.42 | 93.00 | 5.00 | 2.00 | 1.25 | 274.85 |
| Glycine | 37 | 75.07 | 6.06 | -0.40 | 11.42 | 93.00 | 5.00 | 2.00 | 1.94 | 279.15 |
| Glycine | 38 | 75.07 | 6.06 | -0.40 | 11.42 | 93.00 | 5.00 | 2.00 | 2.65 | 281.75 |
| Glycine | 39 | 75.07 | 6.06 | -0.40 | 11.42 | 93.00 | 5.00 | 2.00 | 3.36 | 283.85 |
| Glycine | 40 | 75.07 | 6.06 | -0.40 | 11.42 | 93.00 | 5.00 | 2.00 | 4.07 | 285.35 |
| Alanine | 41 | 89.09 | 6.11 | 1.80 | 2.43 | 100.00 | 0.00 | 0.00 | 2.95 | 274.25 |
| Alanine | 42 | 89.09 | 6.11 | 1.80 | 2.43 | 100.00 | 0.00 | 0.00 | 4.41 | 278.25 |
| Alanine | 43 | 89.09 | 6.11 | 1.80 | 2.43 | 100.00 | 0.00 | 0.00 | 5.92 | 281.05 |
| Alanine | 44 | 89.09 | 6.11 | 1.80 | 2.43 | 100.00 | 0.00 | 0.00 | 7.43 | 283.25 |
| Alanine | 45 | 89.09 | 6.11 | 1.80 | 2.43 | 100.00 | 0.00 | 0.00 | 8.95 | 284.85 |
| Alanine | 46 | 89.09 | 6.11 | 1.80 | 6.12 | 100.00 | 0.00 | 0.00 | 2.95 | 273.95 |
| Alanine | 47 | 89.09 | 6.11 | 1.80 | 6.12 | 100.00 | 0.00 | 0.00 | 4.41 | 277.65 |
| Alanine | 48 | 89.09 | 6.11 | 1.80 | 6.12 | 100.00 | 0.00 | 0.00 | 5.91 | 280.35 |
| Alanine | 49 | 89.09 | 6.11 | 1.80 | 6.12 | 100.00 | 0.00 | 0.00 | 7.36 | 282.35 |
| Alanine | 50 | 89.09 | 6.11 | 1.80 | 6.12 | 100.00 | 0.00 | 0.00 | 8.93 | 284.15 |
| Alanine | 51 | 89.09 | 6.11 | 1.80 | 10.02 | 100.00 | 0.00 | 0.00 | 2.93 | 273.05 |
| Alanine | 52 | 89.09 | 6.11 | 1.80 | 10.02 | 100.00 | 0.00 | 0.00 | 4.40 | 276.95 |
| Alanine | 53 | 89.09 | 6.11 | 1.80 | 10.02 | 100.00 | 0.00 | 0.00 | 5.90 | 279.85 |
| Alanine | 54 | 89.09 | 6.11 | 1.80 | 10.02 | 100.00 | 0.00 | 0.00 | 7.39 | 281.92 |
| Alanine | 55 | 89.09 | 6.11 | 1.80 | 10.02 | 100.00 | 0.00 | 0.00 | 8.91 | 283.58 |
| Alanine | 56 | 89.09 | 6.11 | 1.80 | 2.43 | 93.00 | 5.00 | 2.00 | 1.25 | 276.15 |
| Alanine | 57 | 89.09 | 6.11 | 1.80 | 2.43 | 93.00 | 5.00 | 2.00 | 1.95 | 280.15 |
| Alanine | 58 | 89.09 | 6.11 | 1.80 | 2.43 | 93.00 | 5.00 | 2.00 | 2.66 | 282.95 |
| Alanine | 59 | 89.09 | 6.11 | 1.80 | 2.43 | 93.00 | 5.00 | 2.00 | 3.37 | 284.85 |
| Alanine | 60 | 89.09 | 6.11 | 1.80 | 2.43 | 93.00 | 5.00 | 2.00 | 4.10 | 286.65 |
| Alanine | 61 | 89.09 | 6.11 | 1.80 | 6.12 | 93.00 | 5.00 | 2.00 | 1.25 | 275.75 |
| Alanine | 62 | 89.09 | 6.11 | 1.80 | 6.12 | 93.00 | 5.00 | 2.00 | 1.95 | 279.95 |
| Alanine | 63 | 89.09 | 6.11 | 1.80 | 6.12 | 93.00 | 5.00 | 2.00 | 2.66 | 282.55 |
| Alanine | 64 | 89.09 | 6.11 | 1.80 | 6.12 | 93.00 | 5.00 | 2.00 | 3.36 | 284.55 |
| Alanine | 65 | 89.09 | 6.11 | 1.80 | 6.12 | 93.00 | 5.00 | 2.00 | 4.11 | 286.35 |
| Alanine | 66 | 89.09 | 6.11 | 1.80 | 10.02 | 93.00 | 5.00 | 2.00 | 1.24 | 275.15 |
| Alanine | 67 | 89.09 | 6.11 | 1.80 | 10.02 | 93.00 | 5.00 | 2.00 | 1.95 | 279.45 |
| Alanine | 68 | 89.09 | 6.11 | 1.80 | 10.02 | 93.00 | 5.00 | 2.00 | 2.66 | 282.05 |
| Alanine | 69 | 89.09 | 6.11 | 1.80 | 10.02 | 93.00 | 5.00 | 2.00 | 3.36 | 284.15 |
| Alanine | 70 | 89.09 | 6.11 | 1.80 | 10.02 | 93.00 | 5.00 | 2.00 | 4.09 | 285.75 |
| Serine | 71 | 105.09 | 5.70 | -0.80 | 7.14 | 100.00 | 0.00 | 0.00 | 2.94 | 273.75 |
| Serine | 72 | 105.09 | 5.70 | -0.80 | 7.14 | 100.00 | 0.00 | 0.00 | 4.42 | 277.45 |
| Serine | 73 | 105.09 | 5.70 | -0.80 | 7.14 | 100.00 | 0.00 | 0.00 | 5.92 | 280.25 |
| Serine | 74 | 105.09 | 5.70 | -0.80 | 7.14 | 100.00 | 0.00 | 0.00 | 7.43 | 282.25 |
| Serine | 75 | 105.09 | 5.70 | -0.80 | 7.14 | 100.00 | 0.00 | 0.00 | 8.94 | 284.05 |
| Serine | 76 | 105.09 | 5.70 | -0.80 | 15.29 | 100.00 | 0.00 | 0.00 | 2.94 | 272.65 |
| Serine | 77 | 105.09 | 5.70 | -0.80 | 15.29 | 100.00 | 0.00 | 0.00 | 4.40 | 276.50 |
| Serine | 78 | 105.09 | 5.70 | -0.80 | 15.29 | 100.00 | 0.00 | 0.00 | 5.89 | 279.15 |
| Serine | 79 | 105.09 | 5.70 | -0.80 | 15.29 | 100.00 | 0.00 | 0.00 | 7.38 | 281.20 |
| Serine | 80 | 105.09 | 5.70 | -0.80 | 15.29 | 100.00 | 0.00 | 0.00 | 8.89 | 282.85 |
| Serine | 81 | 105.09 | 5.70 | -0.80 | 7.14 | 93.00 | 5.00 | 2.00 | 1.24 | 275.45 |
| Serine | 82 | 105.09 | 5.70 | -0.80 | 7.14 | 93.00 | 5.00 | 2.00 | 1.95 | 279.75 |
| Serine | 83 | 105.09 | 5.70 | -0.80 | 7.14 | 93.00 | 5.00 | 2.00 | 2.66 | 282.55 |
| Serine | 84 | 105.09 | 5.70 | -0.80 | 7.14 | 93.00 | 5.00 | 2.00 | 3.37 | 284.45 |
| Serine | 85 | 105.09 | 5.70 | -0.80 | 7.14 | 93.00 | 5.00 | 2.00 | 4.07 | 286.15 |
| Serine | 86 | 105.09 | 5.70 | -0.80 | 15.29 | 93.00 | 5.00 | 2.00 | 1.24 | 274.05 |
| Serine | 87 | 105.09 | 5.70 | -0.80 | 15.29 | 93.00 | 5.00 | 2.00 | 1.94 | 278.35 |
| Serine | 88 | 105.09 | 5.70 | -0.80 | 15.29 | 93.00 | 5.00 | 2.00 | 2.64 | 281.45 |
| Serine | 89 | 105.09 | 5.70 | -0.80 | 15.29 | 93.00 | 5.00 | 2.00 | 3.35 | 283.45 |
| Serine | 90 | 105.09 | 5.70 | -0.80 | 15.29 | 93.00 | 5.00 | 2.00 | 4.05 | 284.75 |
| Proline | 91 | 115.13 | 6.30 | -1.60 | 7.77 | 100.00 | 0.00 | 0.00 | 2.94 | 273.65 |
| Proline | 92 | 115.13 | 6.30 | -1.60 | 7.77 | 100.00 | 0.00 | 0.00 | 4.42 | 277.35 |
| Proline | 93 | 115.13 | 6.30 | -1.60 | 7.77 | 100.00 | 0.00 | 0.00 | 5.91 | 280.05 |
| Proline | 94 | 115.13 | 6.30 | -1.60 | 7.77 | 100.00 | 0.00 | 0.00 | 7.42 | 282.25 |
| Proline | 95 | 115.13 | 6.30 | -1.60 | 7.77 | 100.00 | 0.00 | 0.00 | 8.93 | 283.85 |
| Proline | 96 | 115.13 | 6.30 | -1.60 | 16.51 | 100.00 | 0.00 | 0.00 | 2.93 | 272.30 |
| Proline | 97 | 115.13 | 6.30 | -1.60 | 16.51 | 100.00 | 0.00 | 0.00 | 4.41 | 276.15 |
| Proline | 98 | 115.13 | 6.30 | -1.60 | 16.51 | 100.00 | 0.00 | 0.00 | 5.87 | 278.85 |
| Proline | 99 | 115.13 | 6.30 | -1.60 | 16.51 | 100.00 | 0.00 | 0.00 | 7.38 | 280.95 |
| Proline | 100 | 115.13 | 6.30 | -1.60 | 16.51 | 100.00 | 0.00 | 0.00 | 8.87 | 282.50 |
| Proline | 101 | 115.13 | 6.30 | -1.60 | 28.99 | 100.00 | 0.00 | 0.00 | 2.89 | 268.40 |
| Proline | 102 | 115.13 | 6.30 | -1.60 | 28.99 | 100.00 | 0.00 | 0.00 | 4.33 | 272.49 |
| Proline | 103 | 115.13 | 6.30 | -1.60 | 28.99 | 100.00 | 0.00 | 0.00 | 5.78 | 275.05 |
| Proline | 104 | 115.13 | 6.30 | -1.60 | 28.99 | 100.00 | 0.00 | 0.00 | 7.23 | 277.00 |
| Proline | 105 | 115.13 | 6.30 | -1.60 | 28.99 | 100.00 | 0.00 | 0.00 | 8.70 | 278.65 |
| Proline | 106 | 115.13 | 6.30 | -1.60 | 38.75 | 100.00 | 0.00 | 0.00 | 2.84 | 264.90 |
| Proline | 107 | 115.13 | 6.30 | -1.60 | 38.75 | 100.00 | 0.00 | 0.00 | 4.24 | 268.10 |
| Proline | 108 | 115.13 | 6.30 | -1.60 | 38.75 | 100.00 | 0.00 | 0.00 | 5.66 | 270.65 |
| Proline | 109 | 115.13 | 6.30 | -1.60 | 38.75 | 100.00 | 0.00 | 0.00 | 7.07 | 272.65 |
| Proline | 110 | 115.13 | 6.30 | -1.60 | 38.75 | 100.00 | 0.00 | 0.00 | 8.47 | 274.00 |
| Proline | 111 | 115.13 | 6.30 | -1.60 | 7.77 | 93.00 | 5.00 | 2.00 | 1.24 | 274.85 |
| Proline | 112 | 115.13 | 6.30 | -1.60 | 7.77 | 93.00 | 5.00 | 2.00 | 1.95 | 279.35 |
| Proline | 113 | 115.13 | 6.30 | -1.60 | 7.77 | 93.00 | 5.00 | 2.00 | 2.65 | 282.05 |
| Proline | 114 | 115.13 | 6.30 | -1.60 | 7.77 | 93.00 | 5.00 | 2.00 | 3.36 | 283.95 |
| Proline | 115 | 115.13 | 6.30 | -1.60 | 7.77 | 93.00 | 5.00 | 2.00 | 4.07 | 285.45 |
| Proline | 116 | 115.13 | 6.30 | -1.60 | 16.51 | 93.00 | 5.00 | 2.00 | 1.23 | 273.65 |
| Proline | 117 | 115.13 | 6.30 | -1.60 | 16.51 | 93.00 | 5.00 | 2.00 | 1.93 | 277.65 |
| Proline | 118 | 115.13 | 6.30 | -1.60 | 16.51 | 93.00 | 5.00 | 2.00 | 2.63 | 280.45 |
| Proline | 119 | 115.13 | 6.30 | -1.60 | 16.51 | 93.00 | 5.00 | 2.00 | 3.34 | 282.45 |
| Proline | 120 | 115.13 | 6.30 | -1.60 | 16.51 | 93.00 | 5.00 | 2.00 | 4.06 | 283.75 |
| Proline | 121 | 115.13 | 6.30 | -1.60 | 28.99 | 93.00 | 5.00 | 2.00 | 1.24 | 270.75 |
| Proline | 122 | 115.13 | 6.30 | -1.60 | 28.99 | 93.00 | 5.00 | 2.00 | 1.90 | 274.50 |
| Proline | 123 | 115.13 | 6.30 | -1.60 | 28.99 | 93.00 | 5.00 | 2.00 | 2.60 | 277.10 |
| Proline | 124 | 115.13 | 6.30 | -1.60 | 28.99 | 93.00 | 5.00 | 2.00 | 3.29 | 279.20 |
| Proline | 125 | 115.13 | 6.30 | -1.60 | 28.99 | 93.00 | 5.00 | 2.00 | 4.00 | 280.65 |
| Proline | 126 | 115.13 | 6.30 | -1.60 | 38.75 | 93.00 | 5.00 | 2.00 | 1.21 | 267.65 |
| Proline | 127 | 115.13 | 6.30 | -1.60 | 38.75 | 93.00 | 5.00 | 2.00 | 1.89 | 271.25 |
| Proline | 128 | 115.13 | 6.30 | -1.60 | 38.75 | 93.00 | 5.00 | 2.00 | 2.57 | 274.00 |
| Proline | 129 | 115.13 | 6.30 | -1.60 | 38.75 | 93.00 | 5.00 | 2.00 | 3.26 | 275.70 |
| Proline | 130 | 115.13 | 6.30 | -1.60 | 38.75 | 93.00 | 5.00 | 2.00 | 3.93 | 276.75 |
| Glycine | 131 | 75.07 | 6.06 | -0.40 | 5.00 | 100.00 | 0.00 | 0.00 | 4.55 | 277.90 |
| Glycine | 132 | 75.07 | 6.06 | -0.40 | 5.00 | 100.00 | 0.00 | 0.00 | 6.15 | 280.90 |
| Glycine | 133 | 75.07 | 6.06 | -0.40 | 5.00 | 100.00 | 0.00 | 0.00 | 7.50 | 282.75 |
| Glycine | 134 | 75.07 | 6.06 | -0.40 | 5.00 | 100.00 | 0.00 | 0.00 | 9.84 | 285.20 |
| Glycine | 135 | 75.07 | 6.06 | -0.40 | 10.00 | 100.00 | 0.00 | 0.00 | 4.65 | 277.25 |
| Glycine | 136 | 75.07 | 6.06 | -0.40 | 10.00 | 100.00 | 0.00 | 0.00 | 6.10 | 280.00 |
| Glycine | 137 | 75.07 | 6.06 | -0.40 | 10.00 | 100.00 | 0.00 | 0.00 | 7.62 | 282.10 |
| Glycine | 138 | 75.07 | 6.06 | -0.40 | 10.00 | 100.00 | 0.00 | 0.00 | 9.98 | 284.50 |
| Glycine | 139 | 75.07 | 6.06 | -0.40 | 15.00 | 100.00 | 0.00 | 0.00 | 4.60 | 276.80 |
| Glycine | 140 | 75.07 | 6.06 | -0.40 | 15.00 | 100.00 | 0.00 | 0.00 | 6.20 | 279.70 |
| Glycine | 141 | 75.07 | 6.06 | -0.40 | 15.00 | 100.00 | 0.00 | 0.00 | 7.58 | 281.55 |
| Glycine | 142 | 75.07 | 6.06 | -0.40 | 15.00 | 100.00 | 0.00 | 0.00 | 9.65 | 283.73 |
| Glycine | 143 | 75.07 | 6.06 | -0.40 | 20.00 | 100.00 | 0.00 | 0.00 | 4.80 | 276.50 |
| Glycine | 144 | 75.07 | 6.06 | -0.40 | 20.00 | 100.00 | 0.00 | 0.00 | 6.45 | 279.40 |
| Glycine | 145 | 75.07 | 6.06 | -0.40 | 20.00 | 100.00 | 0.00 | 0.00 | 7.53 | 280.80 |
| Glycine | 146 | 75.07 | 6.06 | -0.40 | 20.00 | 100.00 | 0.00 | 0.00 | 9.77 | 283.10 |
| Alanine | 147 | 89.09 | 6.11 | 1.80 | 10.00 | 100.00 | 0.00 | 0.00 | 4.61 | 277.55 |
| Alanine | 148 | 89.09 | 6.11 | 1.80 | 10.00 | 100.00 | 0.00 | 0.00 | 6.10 | 280.15 |
| Alanine | 149 | 89.09 | 6.11 | 1.80 | 10.00 | 100.00 | 0.00 | 0.00 | 7.52 | 282.20 |
| Alanine | 150 | 89.09 | 6.11 | 1.80 | 10.00 | 100.00 | 0.00 | 0.00 | 9.55 | 284.30 |
| Proline | 151 | 115.13 | 6.30 | -1.60 | 10.00 | 100.00 | 0.00 | 0.00 | 4.55 | 277.60 |
| Proline | 152 | 115.13 | 6.30 | -1.60 | 10.00 | 100.00 | 0.00 | 0.00 | 6.15 | 280.30 |
| Proline | 153 | 115.13 | 6.30 | -1.60 | 10.00 | 100.00 | 0.00 | 0.00 | 7.59 | 282.40 |
| Proline | 154 | 115.13 | 6.30 | -1.60 | 10.00 | 100.00 | 0.00 | 0.00 | 9.82 | 284.85 |
| Serine | 155 | 105.09 | 5.70 | -0.80 | 10.00 | 100.00 | 0.00 | 0.00 | 4.56 | 277.70 |
| Serine | 156 | 105.09 | 5.70 | -0.80 | 10.00 | 100.00 | 0.00 | 0.00 | 6.10 | 280.55 |
| Serine | 157 | 105.09 | 5.70 | -0.80 | 10.00 | 100.00 | 0.00 | 0.00 | 7.57 | 282.50 |
| Serine | 158 | 105.09 | 5.70 | -0.80 | 10.00 | 100.00 | 0.00 | 0.00 | 9.80 | 285.00 |
| Arginine | 159 | 174.20 | 10.76 | -4.50 | 10.00 | 100.00 | 0.00 | 0.00 | 4.70 | 278.55 |
| Arginine | 160 | 174.20 | 10.76 | -4.50 | 10.00 | 100.00 | 0.00 | 0.00 | 6.10 | 281.05 |
| Arginine | 161 | 174.20 | 10.76 | -4.50 | 10.00 | 100.00 | 0.00 | 0.00 | 7.56 | 282.90 |
| Arginine | 162 | 174.20 | 10.76 | -4.50 | 10.00 | 100.00 | 0.00 | 0.00 | 9.65 | 285.40 |
| Lysine | 163 | 146.19 | 9.47 | -3.90 | 5.00 | 100.00 | 0.00 | 0.00 | 4.60 | 278.15 |
| Lysine | 164 | 146.19 | 9.47 | -3.90 | 5.00 | 100.00 | 0.00 | 0.00 | 6.30 | 281.25 |
| Lysine | 165 | 146.19 | 9.47 | -3.90 | 5.00 | 100.00 | 0.00 | 0.00 | 8.20 | 283.70 |
| Lysine | 166 | 146.19 | 9.47 | -3.90 | 5.00 | 100.00 | 0.00 | 0.00 | 10.01 | 285.62 |
| Lysine | 167 | 146.19 | 9.47 | -3.90 | 10.00 | 100.00 | 0.00 | 0.00 | 4.90 | 278.05 |
| Lysine | 168 | 146.19 | 9.47 | -3.90 | 10.00 | 100.00 | 0.00 | 0.00 | 6.19 | 280.30 |
| Lysine | 169 | 146.19 | 9.47 | -3.90 | 10.00 | 100.00 | 0.00 | 0.00 | 8.03 | 283.00 |
| Lysine | 170 | 146.19 | 9.47 | -3.90 | 10.00 | 100.00 | 0.00 | 0.00 | 10.40 | 285.20 |
| L-valine | 171 | 117.15 | 6.02 | 4.20 | 1.00 | 100.00 | 0.00 | 0.00 | 3.60 | 276.20 |
| L-valine | 172 | 117.15 | 6.02 | 4.20 | 1.00 | 100.00 | 0.00 | 0.00 | 5.10 | 279.40 |
| L-valine | 173 | 117.15 | 6.02 | 4.20 | 1.00 | 100.00 | 0.00 | 0.00 | 6.60 | 282.10 |
| L-valine | 174 | 117.15 | 6.02 | 4.20 | 1.00 | 100.00 | 0.00 | 0.00 | 8.10 | 284.10 |
| L-threonine | 175 | 119.12 | 5.60 | -0.70 | 1.00 | 100.00 | 0.00 | 0.00 | 4.60 | 278.60 |
| L-threonine | 176 | 119.12 | 5.60 | -0.70 | 1.00 | 100.00 | 0.00 | 0.00 | 6.30 | 281.50 |
| L-threonine | 177 | 119.12 | 5.60 | -0.70 | 1.00 | 100.00 | 0.00 | 0.00 | 8.20 | 284.00 |
| L-threonine | 178 | 119.12 | 5.60 | -0.70 | 1.00 | 100.00 | 0.00 | 0.00 | 10.10 | 286.00 |
| L-asparagine | 179 | 132.12 | 5.43 | -3.50 | 1.00 | 100.00 | 0.00 | 0.00 | 4.30 | 277.90 |
| L-asparagine | 180 | 132.12 | 5.43 | -3.50 | 1.00 | 100.00 | 0.00 | 0.00 | 6.10 | 281.50 |
| L-asparagine | 181 | 132.12 | 5.43 | -3.50 | 1.00 | 100.00 | 0.00 | 0.00 | 7.60 | 283.30 |
| L-asparagine | 182 | 132.12 | 5.43 | -3.50 | 1.00 | 100.00 | 0.00 | 0.00 | 10.30 | 286.10 |
| L-phenylalanine | 183 | 165.19 | 5.76 | 2.80 | 1.00 | 100.00 | 0.00 | 0.00 | 3.60 | 276.20 |
| L-phenylalanine | 184 | 165.19 | 5.76 | 2.80 | 1.00 | 100.00 | 0.00 | 0.00 | 5.10 | 279.80 |
| L-phenylalanine | 185 | 165.19 | 5.76 | 2.80 | 1.00 | 100.00 | 0.00 | 0.00 | 6.60 | 282.20 |
| L-phenylalanine | 186 | 165.19 | 5.76 | 2.80 | 1.00 | 100.00 | 0.00 | 0.00 | 8.20 | 284.00 |
| L-valine | 187 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 3.50 | 275.70 |
| L-valine | 188 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 5.20 | 279.40 |
| L-valine | 189 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 6.60 | 281.70 |
| L-valine | 190 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 8.00 | 283.50 |
| L-threonine | 191 | 119.12 | 5.60 | -0.70 | 5.00 | 100.00 | 0.00 | 0.00 | 4.00 | 277.00 |
| L-threonine | 192 | 119.12 | 5.60 | -0.70 | 5.00 | 100.00 | 0.00 | 0.00 | 6.30 | 281.50 |
| L-threonine | 193 | 119.12 | 5.60 | -0.70 | 5.00 | 100.00 | 0.00 | 0.00 | 8.30 | 283.90 |
| L-threonine | 194 | 119.12 | 5.60 | -0.70 | 5.00 | 100.00 | 0.00 | 0.00 | 10.20 | 285.70 |
| L-asparagine | 195 | 132.12 | 5.43 | -3.50 | 5.00 | 100.00 | 0.00 | 0.00 | 3.50 | 275.80 |
| L-asparagine | 196 | 132.12 | 5.43 | -3.50 | 5.00 | 100.00 | 0.00 | 0.00 | 5.10 | 279.30 |
| L-asparagine | 197 | 132.12 | 5.43 | -3.50 | 5.00 | 100.00 | 0.00 | 0.00 | 6.60 | 281.90 |
| L-asparagine | 198 | 132.12 | 5.43 | -3.50 | 5.00 | 100.00 | 0.00 | 0.00 | 8.10 | 283.70 |
| L-phenylalanine | 199 | 165.19 | 5.76 | 2.80 | 5.00 | 100.00 | 0.00 | 0.00 | 3.60 | 275.90 |
| L-phenylalanine | 200 | 165.19 | 5.76 | 2.80 | 5.00 | 100.00 | 0.00 | 0.00 | 5.10 | 279.40 |
| L-phenylalanine | 201 | 165.19 | 5.76 | 2.80 | 5.00 | 100.00 | 0.00 | 0.00 | 6.50 | 281.90 |
| L-phenylalanine | 202 | 165.19 | 5.76 | 2.80 | 5.00 | 100.00 | 0.00 | 0.00 | 8.00 | 283.90 |
| Arginine | 203 | 174.20 | 10.76 | -4.50 | 5.00 | 100.00 | 0.00 | 0.00 | 4.55 | 278.80 |
| Arginine | 204 | 174.20 | 10.76 | -4.50 | 5.00 | 100.00 | 0.00 | 0.00 | 6.15 | 281.30 |
| Arginine | 205 | 174.20 | 10.76 | -4.50 | 5.00 | 100.00 | 0.00 | 0.00 | 7.50 | 283.30 |
| Arginine | 206 | 174.20 | 10.76 | -4.50 | 5.00 | 100.00 | 0.00 | 0.00 | 9.84 | 285.90 |
| Valine | 207 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 4.60 | 278.60 |
| Valine | 208 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 6.20 | 281.40 |
| Valine | 209 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 7.58 | 283.00 |
| Valine | 210 | 117.15 | 6.02 | 4.20 | 5.00 | 100.00 | 0.00 | 0.00 | 9.65 | 285.80 |

Abbreviations: molecular weight (MW, g mol-1), isoelectric point (pI), hydropathy index (hI), mass concentration (conc, wt%), CH4 in the natural gas (C1%), C2H6 in the natural gas (C2%), C3H8 in the natural gas (C3%), pressure (P, MPa), temperature (T, K).

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