

Supporting information

Surface Interaction of Ribonucleic Acid Constituents with Spinel Ferrite Nanoparticles: A Prebiotic Chemistry Experiment

Md. Asif Iqubal, Rachana Sharma and Kamaluddin*

Department of Chemistry, IIT Roorkee, Roorkee 247667, Uttarakhand, India

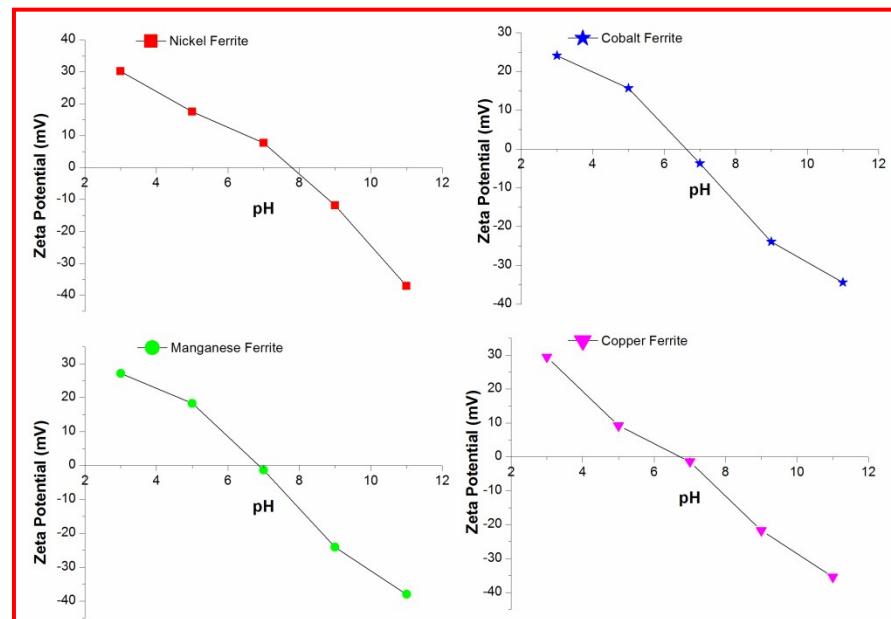


Figure S1: Zero point charge curve of metal ferrites

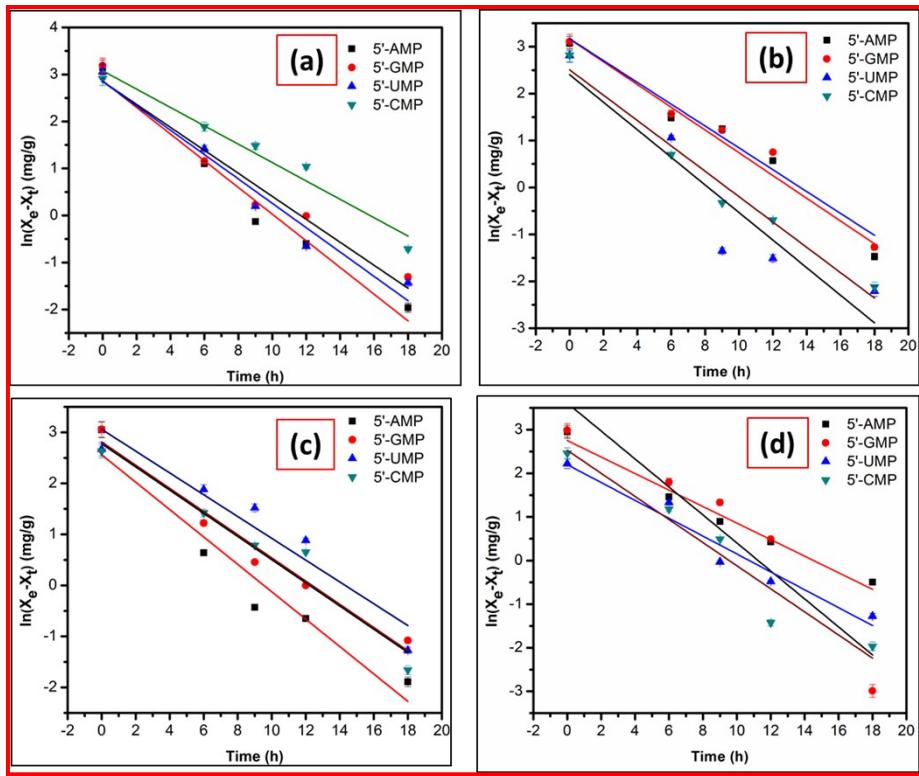


Figure S2: The pseudo first order plots of metal ferrites (a) NiFe_2O_4 (b) CoFe_2O_4 (c) CuFe_2O_4 and (d) MnFe_2O_4

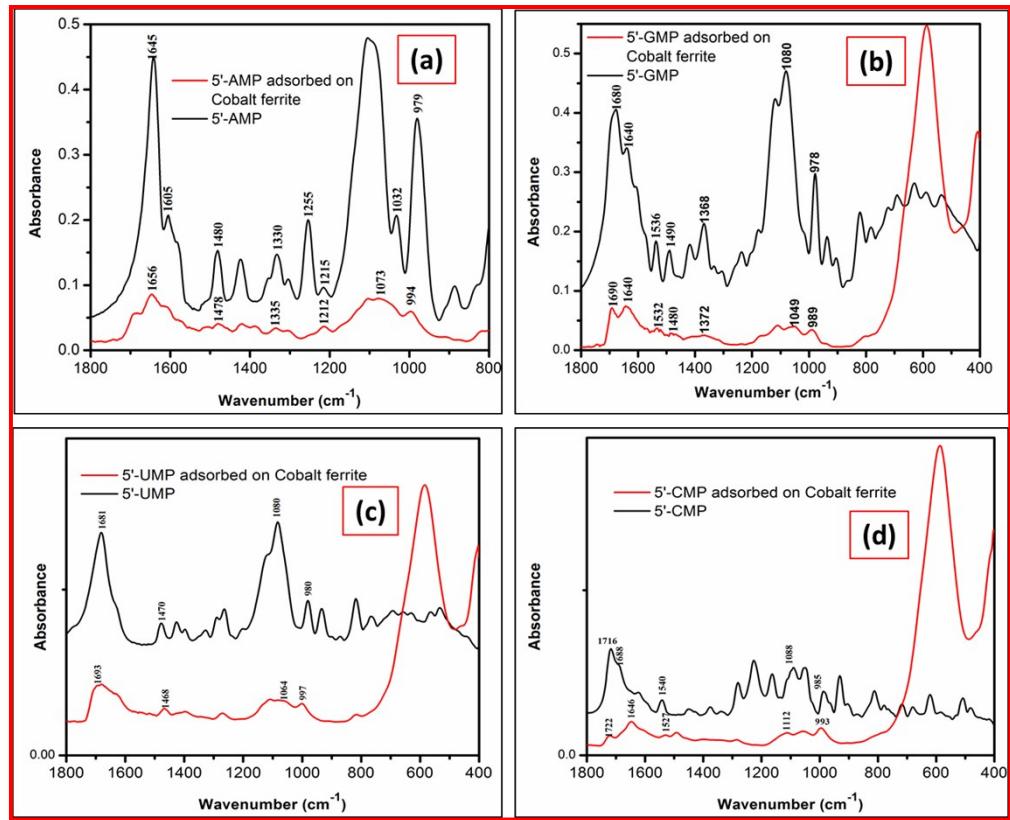


Figure S3: Infra-red spectra of ribonucleotides (a) 5'-AMP, (b) 5'-GMP, (c) 5'-UMP and (d) 5'-CMP before and after interaction with cobalt ferrite

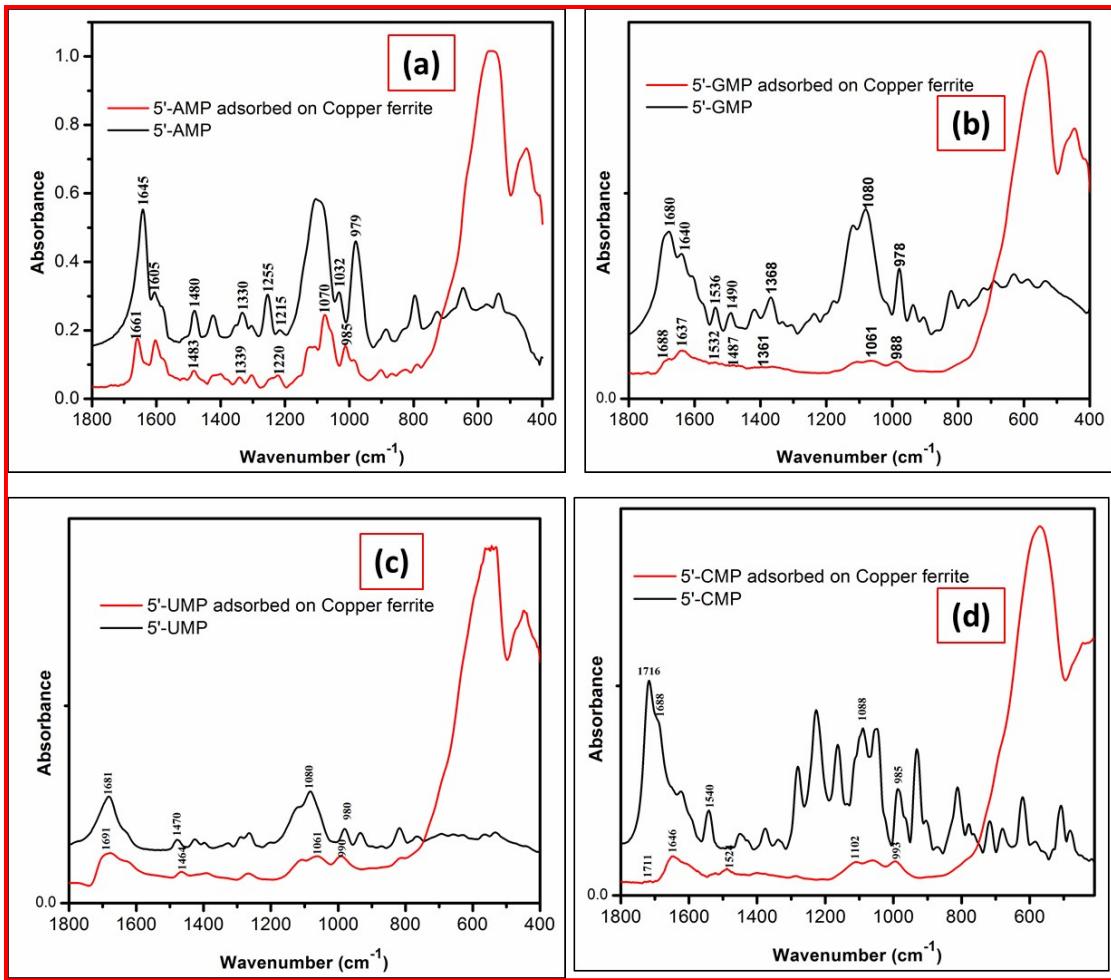


Figure S4: Infra-red spectra of ribonucleotides (a) 5'-AMP, (b) 5'-GMP, (c) 5'-UMP and (d) 5'-CMP before and after interaction with copper ferrite

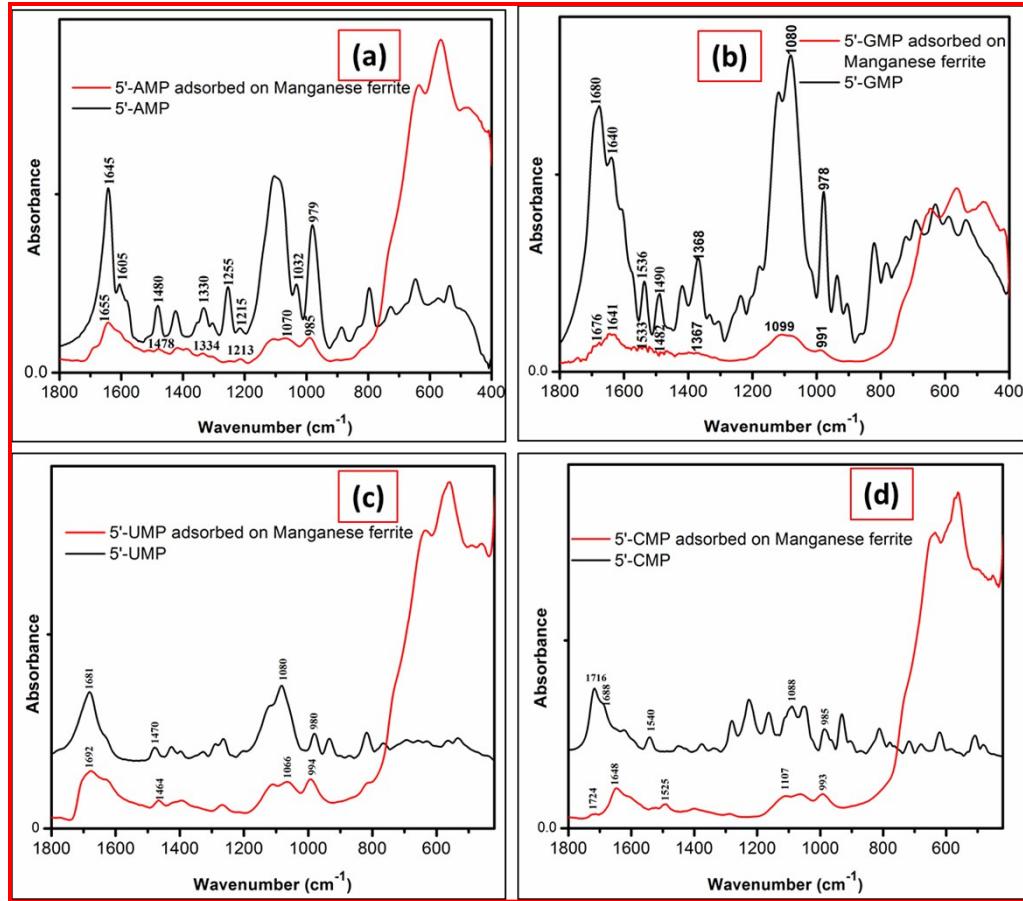


Figure S5: Infra-red spectra of ribonucleotides (a) 5'-AMP, (b) 5'-GMP, (c) 5'-UMP and (d) 5'-CMP before and after interaction with manganese ferrite

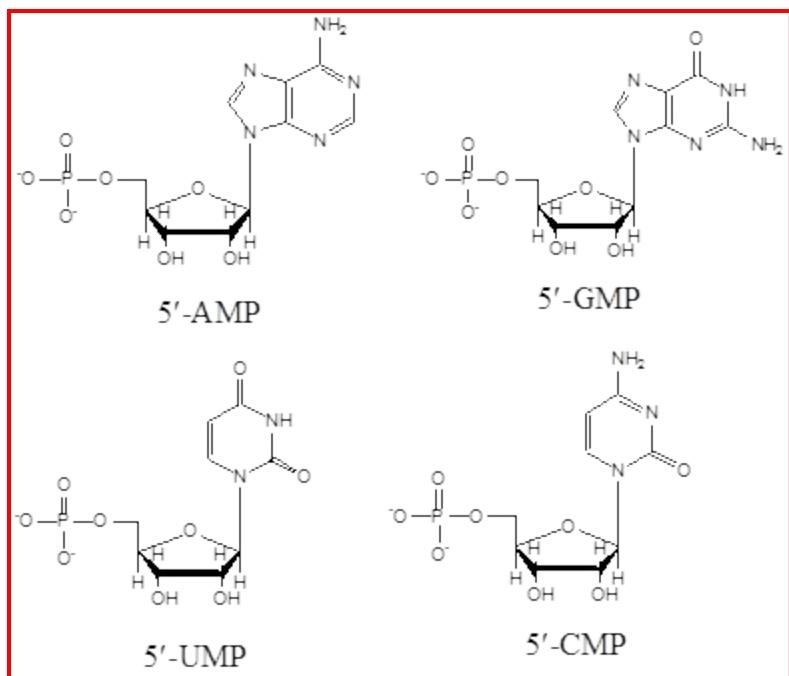


Figure S6: Structure of purine (5'-AMP and 5'-GMP) and pyrimidine (5'-UMP and 5'-CMP) ribonucleotides

Table S1: Langmuir constants for adsorption of ribose nucleotides on metal ferrite at pH~4.00

| Metal ferrite | 5'-AMP | | | 5'-GMP | | | 5'-UMP | | | 5'-CMP | | |
|----------------------------------|----------------|--------------------------|--|----------------|--------------------------|--|----------------|--------------------------|--|----------------|--------------------------|--|
| | R ² | X _m (mg/g) | K _L ×10 ⁴ (L/mol) | R ² | X _m (mg/g) | K _L ×10 ⁴ (L/mol) | R ² | X _m (mg/g) | K _L ×10 ⁴ (L/mol) | R ² | X _m (mg/g) | K _L ×10 ⁴ (L/mol) |
| NiFe ₂ O ₄ | 0.99 | 33.78 | 0.22 | 0.99 | 30.65 | 0.22 | 0.99 | 25.13 | 10.63 | 0.99 | 20.08 | 8.41 |
| CoFe ₂ O ₄ | 0.98 | 30.20 | 3.81 | 0.99 | 23.58 | 4.13 | 0.97 | 21.56 | 1.42 | 0.99 | 17.20 | 3.30 |
| CuFe ₂ O ₄ | 0.99 | 22.57 | 5.00 | 0.99 | 21.21 | 4.59 | 0.98 | 14.10 | 3.02 | 0.99 | 12.98 | 2.21 |
| MnFe ₂ O ₄ | 0.98 | 21.54 | 3.08 | 0.99 | 15.92 | 12.38 | 0.99 | 9.56 | 2.12 | 0.99 | 9.46 | 1.88 |

Table S2: Comparison of rate constants calculated based on first-order and second-order kinetic models for NiFe₂O₄

| Kinetic model | 5'-AMP | 5'-GMP | 5'-UMP | 5'-CMP |
|--------------------------|--------|--------|--------|--------|
| Pseudo first order | | | | |
| R ² | 0.96 | 0.95 | 0.95 | 0.95 |
| k ₁ (L/hr) | 0.28 | 0.29 | 0.26 | 0.20 |
| X _e (mg/g) | 16.94 | 17.32 | 17.27 | 21.73 |
| Pseudo second order | | | | |
| R ² | 0.99 | 0.99 | 0.99 | 0.99 |
| k ₂ (g/mg hr) | 0.09 | 0.07 | 0.06 | 0.02 |
| X _e (mg/g) | 23.75 | 24.78 | 21.88 | 19.71 |

Table S3: Comparison of rate constants calculated based on first-order and second-order kinetic models for CoFe₂O₄

| Kinetic model | 5'-AMP | 5'-GMP | 5'-UMP | 5'-CMP |
|--------------------------|--------|--------|--------|--------|
| Pseudo first order | | | | |
| R ² | 0.96 | 0.96 | 0.83 | 0.96 |
| k ₁ (L/hr) | 0.24 | 0.23 | 0.29 | 0.27 |
| X _e (mg/g) | 23.57 | 23.80 | 11.02 | 12.25 |
| Pseudo second order | | | | |
| R ² | 0.99 | 0.99 | 0.99 | 0.99 |
| k ₂ (g/mg hr) | 0.04 | 0.03 | 0.11 | 0.11 |
| X _e (mg/g) | 22.37 | 23.41 | 17.04 | 17.15 |

Table S4: Comparison of rate constants calculated based on first-order and second-order kinetic models for CuFe₂O₄

| Kinetic model | 5'-AMP | 5'-GMP | 5'-UMP | 5'-CMP |
|--------------------------|--------|--------|--------|--------|
| Pseudo first order | | | | |
| R ² | 0.92 | 0.96 | 0.89 | 0.93 |
| k ₁ (L/hr) | 0.27 | 0.23 | 0.21 | 0.23 |
| X _e (mg/g) | 12.93 | 15.96 | 21.30 | 16.61 |
| Pseudo second order | | | | |
| R ² | 0.99 | 0.99 | 0.96 | 0.99 |
| k ₂ (g/mg hr) | 0.10 | 0.06 | 0.01 | 0.03 |
| X _e (mg/g) | 21.74 | 21.99 | 17.09 | 14.88 |

Table S5: Comparison of rate constants calculated based on first-order and second-order kinetic models for MnFe₂O₄

| Kinetic model | 5'-AMP | 5'-GMP | 5'-UMP | 5'-CMP |
|--------------------------|--------|--------|--------|--------|
| Pseudo first order | | | | |
| R ² | 0.97 | 0.87 | 0.93 | 0.91 |
| k ₁ (L/hr) | 0.19 | 0.32 | 0.20 | 0.26 |
| X _e (mg/g) | 15.64 | 36.96 | 9.00 | 12.54 |
| Pseudo second order | | | | |
| R ² | 0.99 | 0.99 | 0.98 | 0.99 |
| k ₂ (g/mg hr) | 0.04 | 0.03 | 0.04 | 0.06 |
| X _e (mg/g) | 20.00 | 21.09 | 10.30 | 12.42 |

Table S6: Typical infrared spectral frequencies (cm⁻¹) of ribonucleotides before and after absorption on NiFe₂O₄

| Group/Moiet | 5'-AMP | Adsorbed 5'-AMP | 5'-GMP | Adsorbed 5'-GMP | 5'-UMP | Adsorbed 5'-UMP | 5'-CMP | Adsorbed 5'-CMP |
|---|--------|-----------------|--------|-----------------|--------|-----------------|--------|-----------------|
| NH ₂ | 1645 | 1655 | 1640 | 1640 | - | - | 1688 | 1645 |
| > C(6)=O | - | - | 1680 | 1687 | - | - | - | - |
| > C(2)=O | - | - | - | - | 1681 | 1694 | 1716 | 1721 |
| Pyrimidine/ Imidazole vibration | 1330 | 1336 | 1536 | 1533 | - | - | - | - |
| Imidazole | 1215 | 1212 | 1368 | 1364 | - | - | - | - |
| vN-7-C-8 + δC-8-H | 1480 | 1474 | 1490 | 1483 | - | - | - | - |
| PO ₃ ²⁻ antisymmetric stretching | 1032 | 1061 | 1080 | 1056 | 1080 | 1057 | 1088 | 1114 |
| PO ₃ ²⁻ symmetric stretching | 979 | 991 | 978 | 988 | 980 | 997 | 985 | 994 |

Table S7: Typical infrared spectral frequencies (cm^{-1}) of ribonucleotides before and after absorption on CoFe_2O_4

| Group/Moiet | 5'-AMP | Adsorbed 5'-AMP | 5'-GMP | Adsorbed 5'-GMP | 5'-UMP | Adsorbed 5'-UMP | 5'-CMP | Adsorbed 5'-CMP |
|---|--------|-----------------|--------|-----------------|--------|-----------------|--------|-----------------|
| NH ₂ | 1645 | 1656 | 1640 | 1640 | - | - | 1688 | 1646 |
| > C(6)=O | - | - | 1680 | 1690 | - | - | - | - |
| > C(2)=O | - | - | - | - | 1681 | 1693 | 1716 | 1722 |
| Pyrimidine/ Imidazole vibration | 1330 | 1335 | 1536 | 1532 | - | - | - | - |
| Imidazole | 1215 | 1212 | 1368 | 1372 | - | - | - | - |
| vN-7-C-8 + δC-8-H | 1480 | 1478 | 1490 | 1480 | - | - | - | - |
| PO ₃ ²⁻ antisymmetric stretching | 1032 | 1073 | 1080 | 1049 | 1080 | 1064 | 1088 | 1112 |
| PO ₃ ²⁻ symmetric stretching | 979 | 994 | 978 | 989 | 980 | 997 | 985 | 993 |

Table S8: Typical infrared spectral frequencies (cm^{-1}) of ribonucleotides before and after absorption on CuFe_2O_4

| Group/Moiet | 5'-AMP | Adsorbed 5'-AMP | 5'-GMP | Adsorbed 5'-GMP | 5'-UMP | Adsorbed 5'-UMP | 5'-CMP | Adsorbed 5'-CMP |
|---|--------|-----------------|--------|-----------------|--------|-----------------|--------|-----------------|
| NH ₂ | 1645 | 1661 | 1640 | 1637 | - | - | 1688 | 1646 |
| > C(6)=O | - | - | 1680 | 1688 | - | - | - | - |
| > C(2)=O | - | - | - | - | 1681 | 1691 | 1716 | 1711 |
| Pyrimidine/ Imidazole vibration | 1330 | 1339 | 1536 | 1532 | - | - | - | - |
| Imidazole | 1215 | 1220 | 1368 | 1361 | - | - | - | - |
| vN-7-C-8 + δC-8-H | 1480 | 1483 | 1490 | 1487 | - | - | - | - |
| PO ₃ ²⁻ antisymmetric stretching | 1032 | 1070 | 1080 | 1061 | 1080 | 1061 | 1088 | 1102 |
| PO ₃ ²⁻ symmetric stretching | 979 | 985 | 978 | 988 | 980 | 990 | 985 | 993 |

Table S9: Typical infrared spectral frequencies (cm^{-1}) of ribonucleotides before and after absorption on MnFe_2O_4

| Group/Moiet | 5'-AMP | Adsorbed 5'-AMP | 5'-GMP | Adsorbed 5'-GMP | 5'-UMP | Adsorbed 5'-UMP | 5'-CMP | Adsorbed 5'-CMP |
|---|--------|-----------------|--------|-----------------|--------|-----------------|--------|-----------------|
| NH ₂ | 1645 | 1655 | 1640 | 1641 | - | - | 1688 | 1648 |
| > C(6)=O | - | - | 1680 | 1676 | - | - | - | - |
| > C(2)=O | - | - | - | - | 1681 | 1692 | 1716 | 1724 |
| Pyrimidine/ Imidazole vibration | 1330 | 1334 | 1536 | 1533 | - | - | - | - |
| Imidazole | 1215 | 1213 | 1368 | 1367 | - | - | - | - |
| vN-7-C-8 + δC-8-H | 1480 | 1478 | 1490 | 1482 | - | - | - | - |
| PO ₃ ²⁻ antisymmetric stretching | 1032 | 1070 | 1080 | 1099 | 1080 | 1066 | 1088 | 1107 |
| PO ₃ ²⁻ symmetric stretching | 979 | 985 | 978 | 991 | 980 | 994 | 985 | 993 |