

Figure S1. Inhibition effects of T90A on ZIKV infection

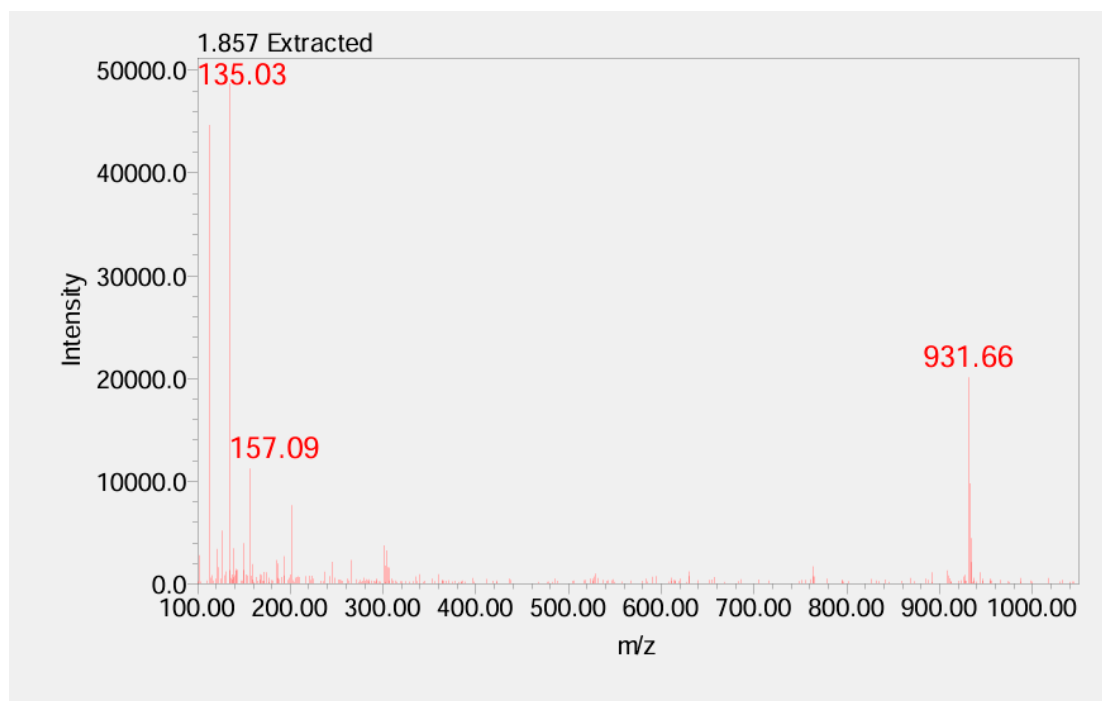


Figure S2. Mass spectrum of T90A-F3-a'

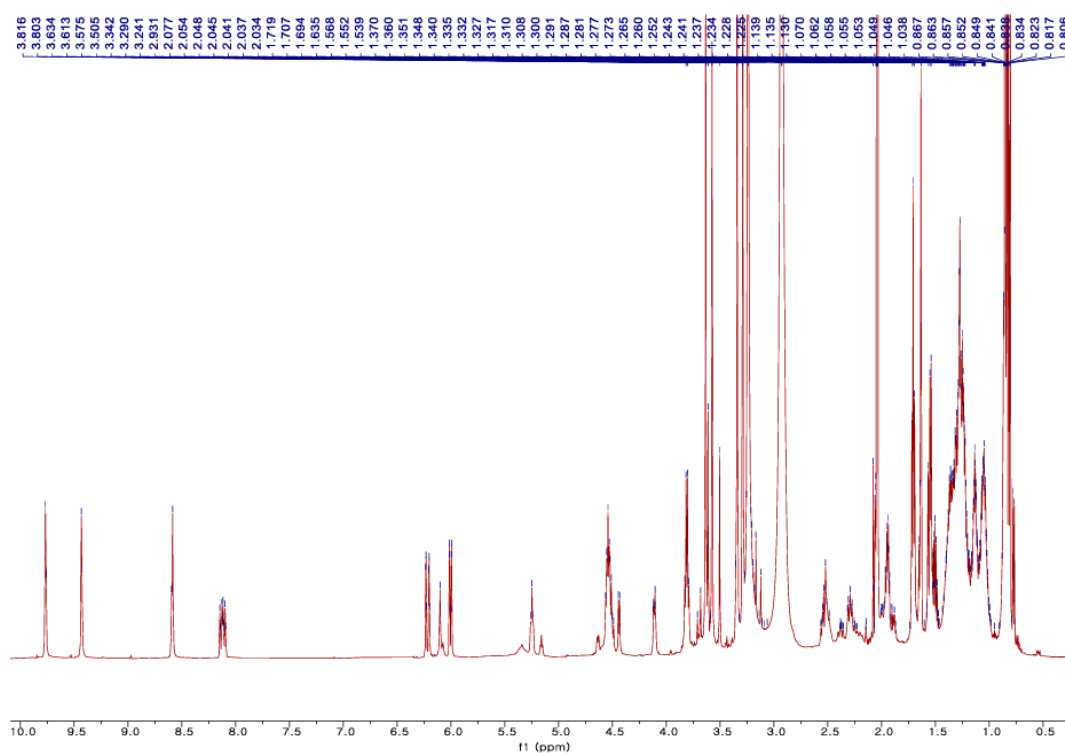


Figure S3. ¹H-NMR spectrum of T90A-F3-a'

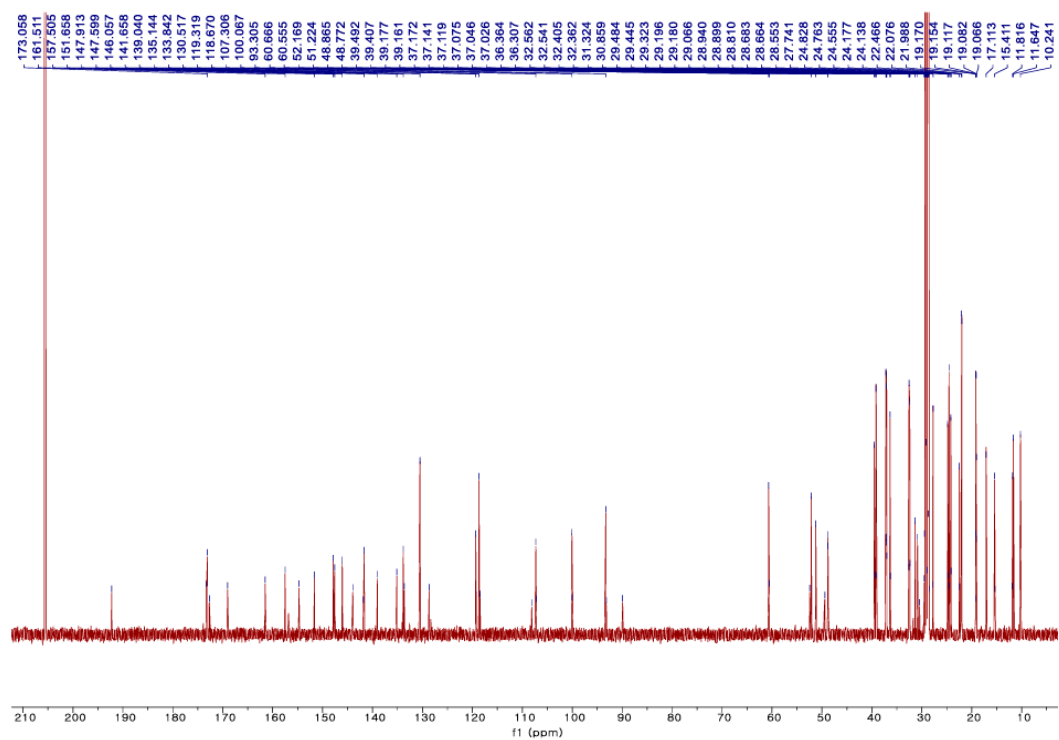


Figure S4. ¹³C-NMR spectrum of T90A-F3-a'

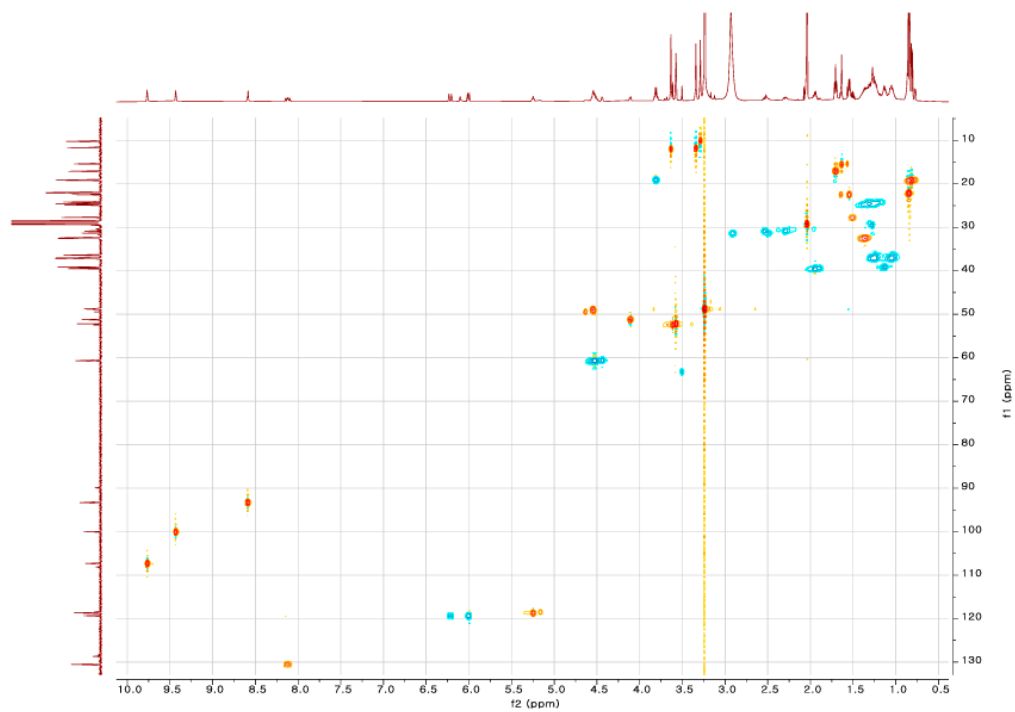


Figure S5. HSQC spectrum of T90A-F3-a'

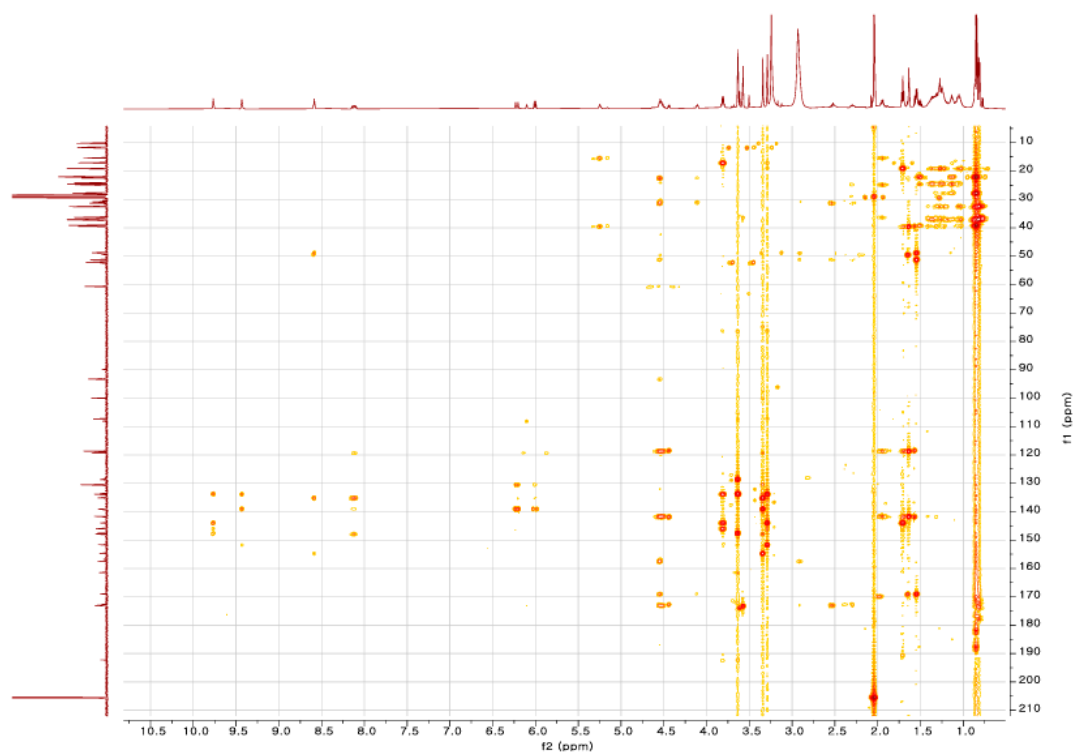


Figure S6. HMBC spectrum of T90A-F3-a'

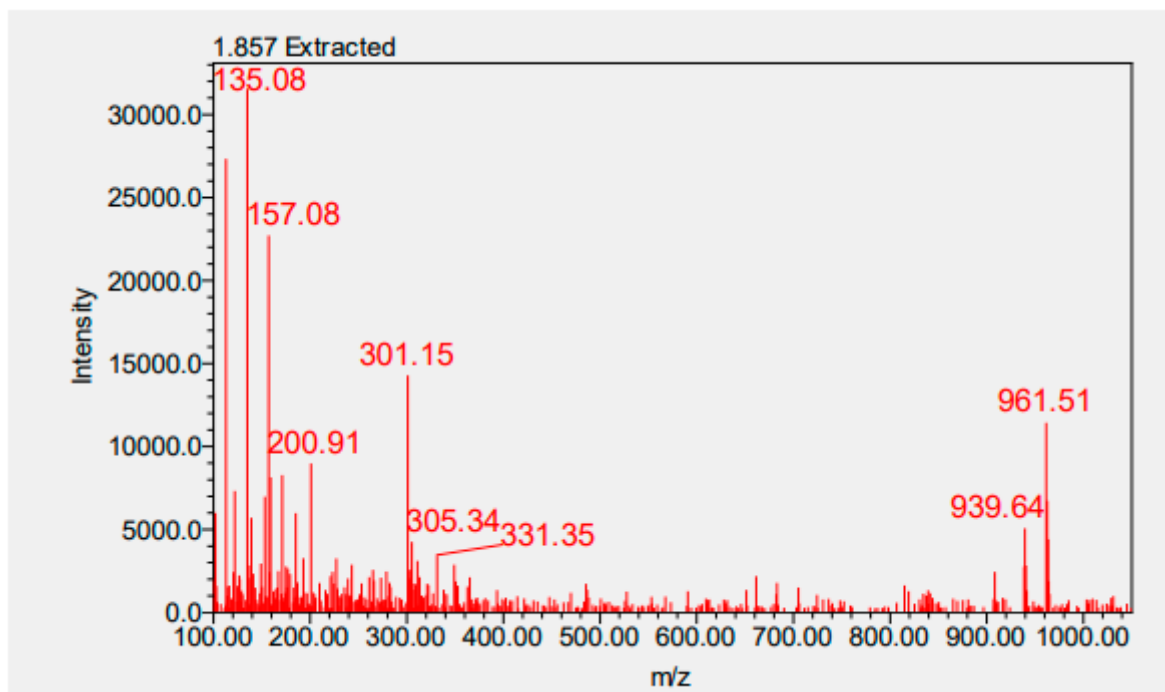


Figure S7. Mass spectrum of T90A-F3-b'

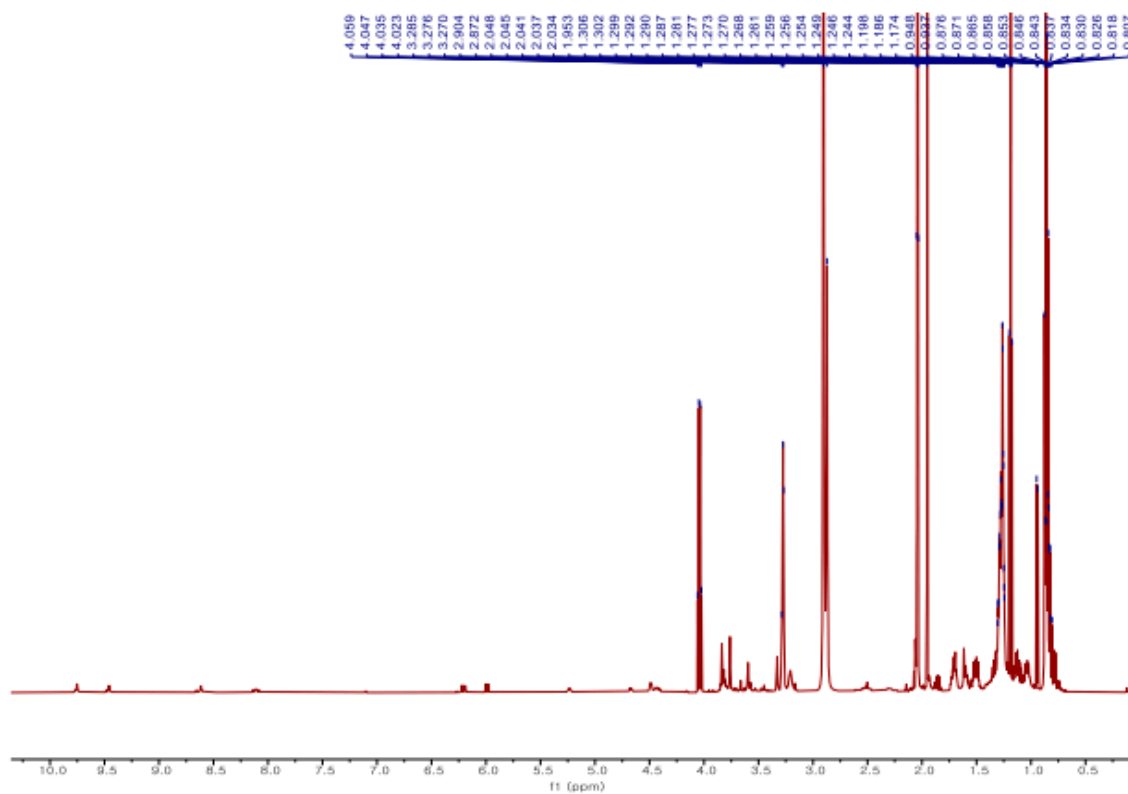


Figure S8. ¹H-NMR spectrum of T90A-F3-b'

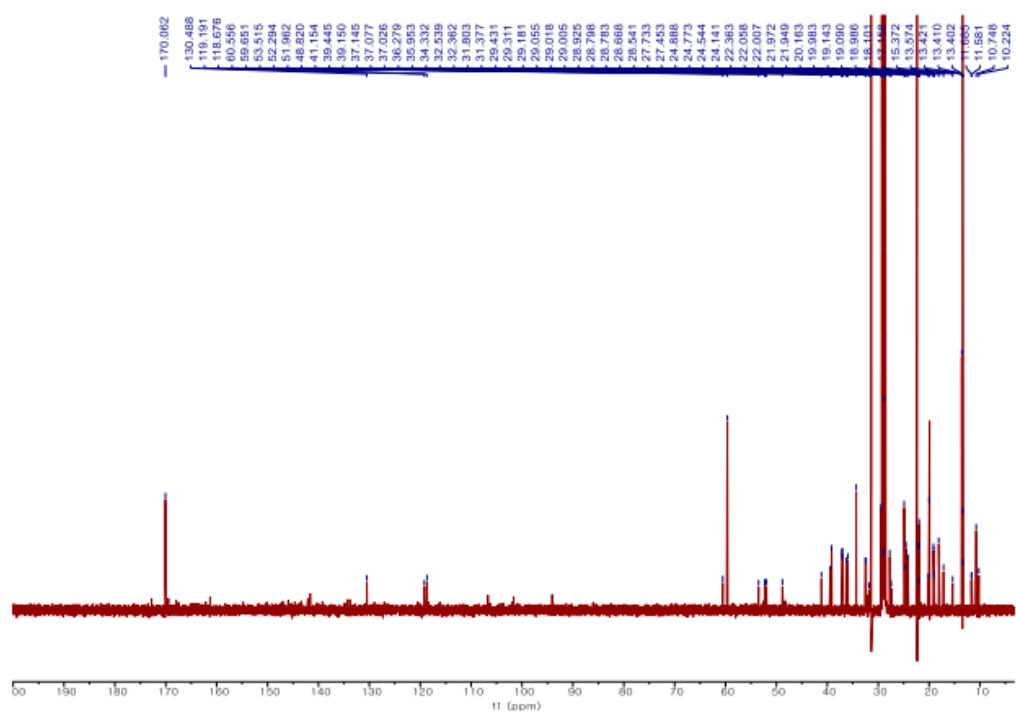


Figure S9. ¹³C-NMR spectrum of T90A-F3-b'

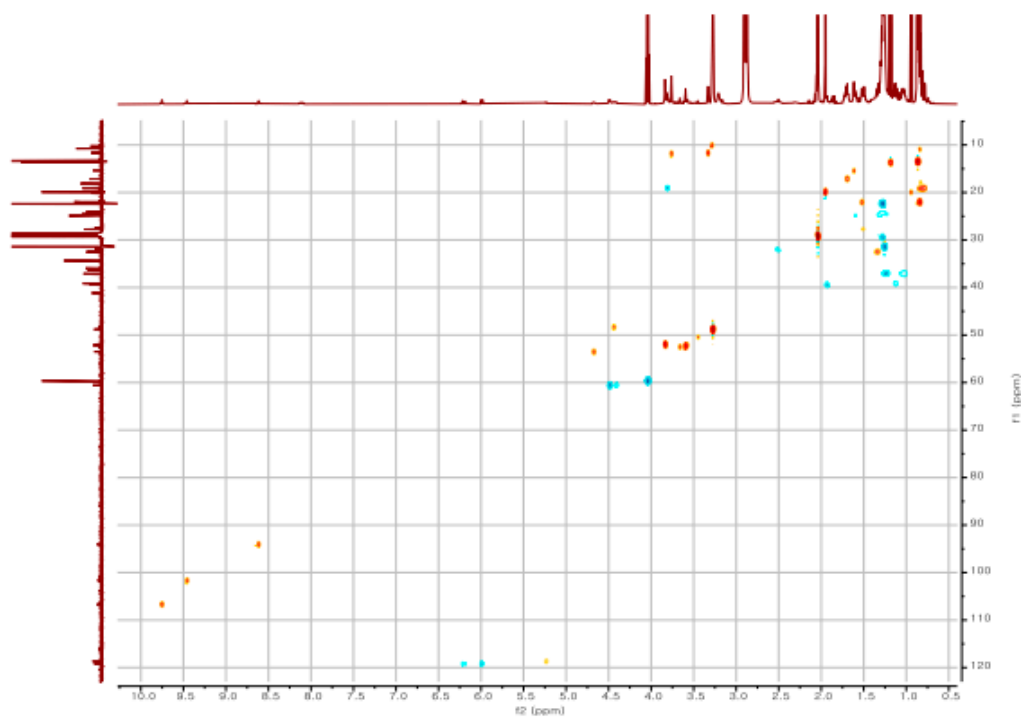


Figure S10. HSQC spectrum of T90A-F3-b'

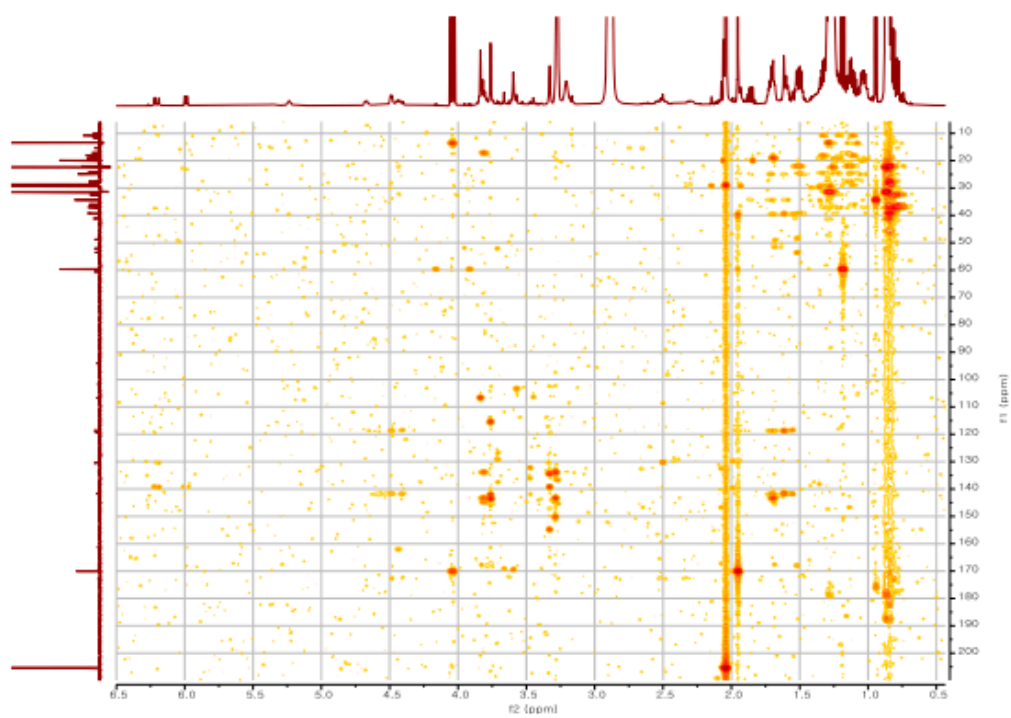


Figure S11. HMBC spectrum of T90A-F3-b'

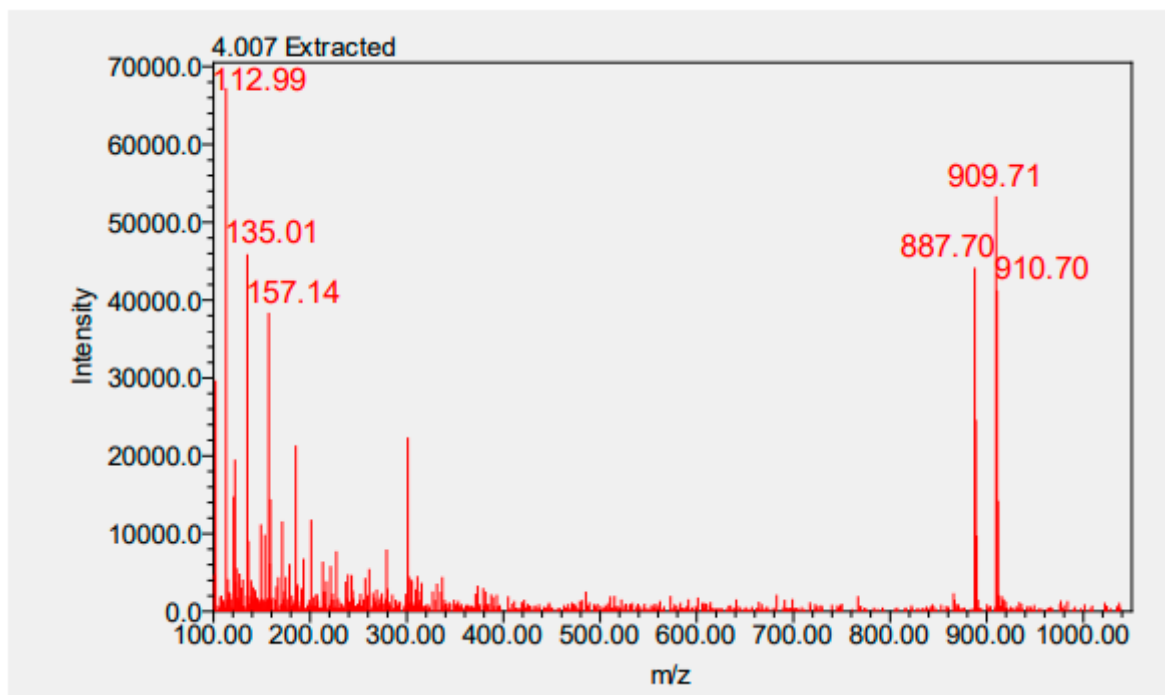


Figure S12. Mass spectrum of T90A-F3-c'

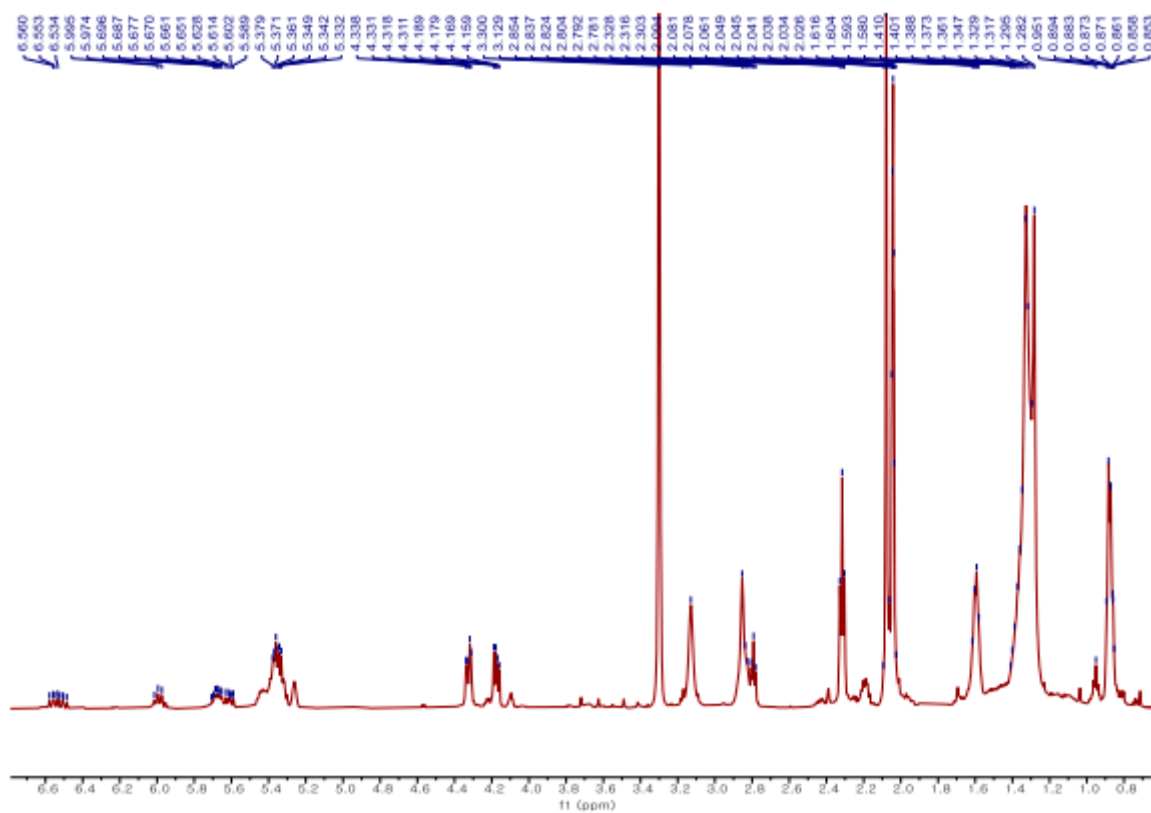


Figure S13. ¹H-NMR spectrum of T90A-F3-c'

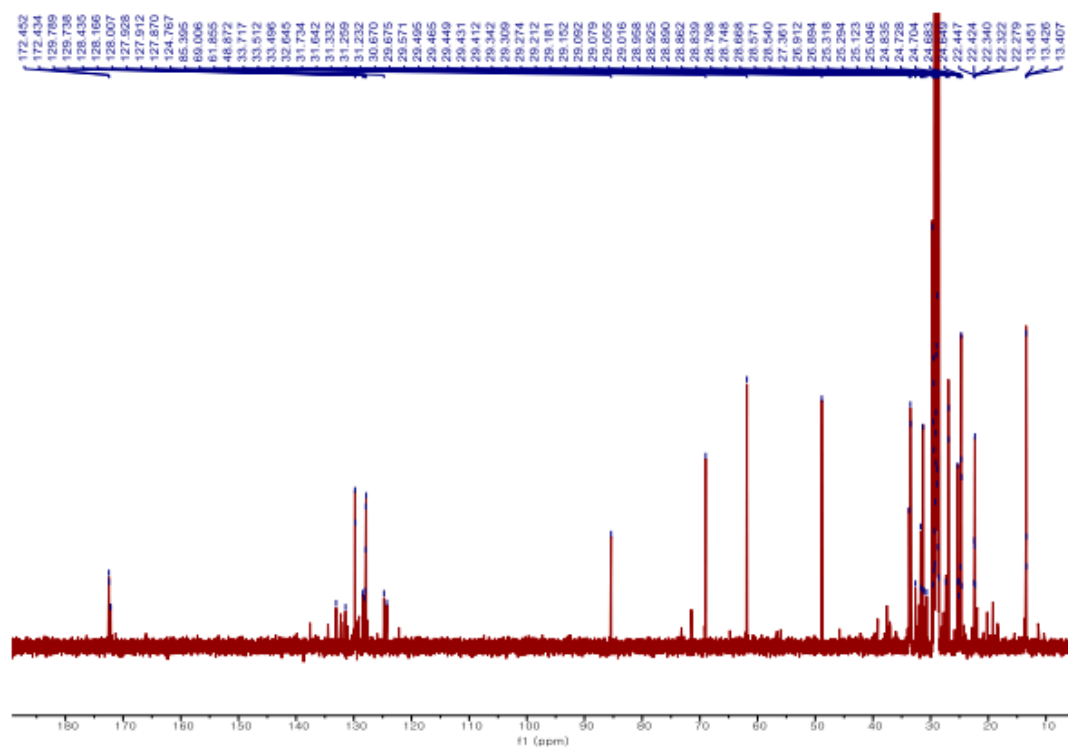


Figure S14. ¹³C-NMR spectrum of T90A-F3-c'

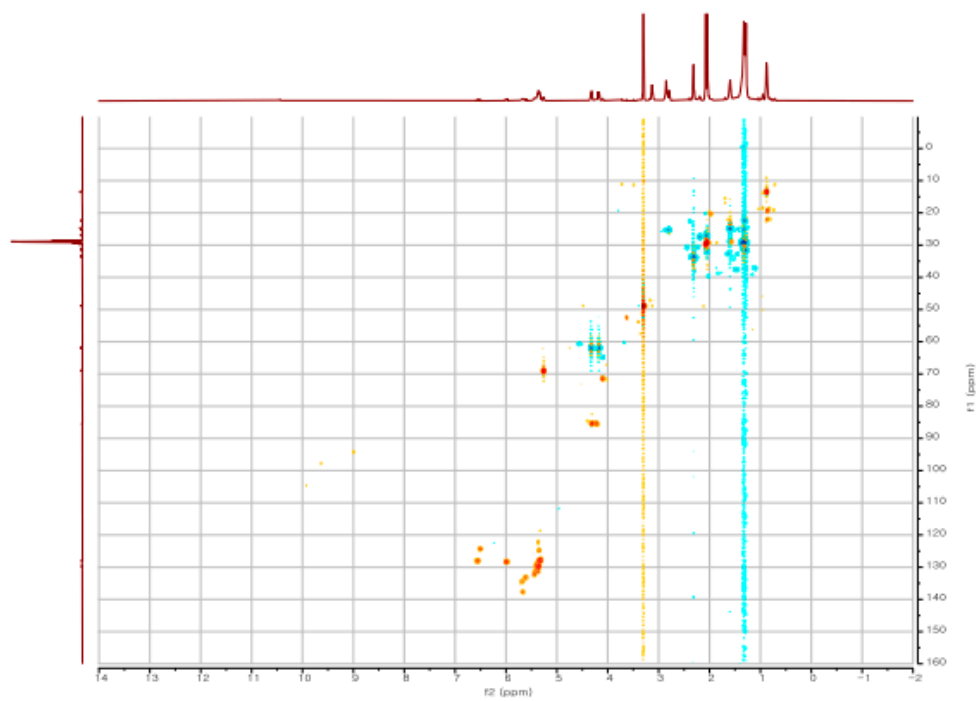


Figure S15. HSQC spectrum of T90A-F3-c'

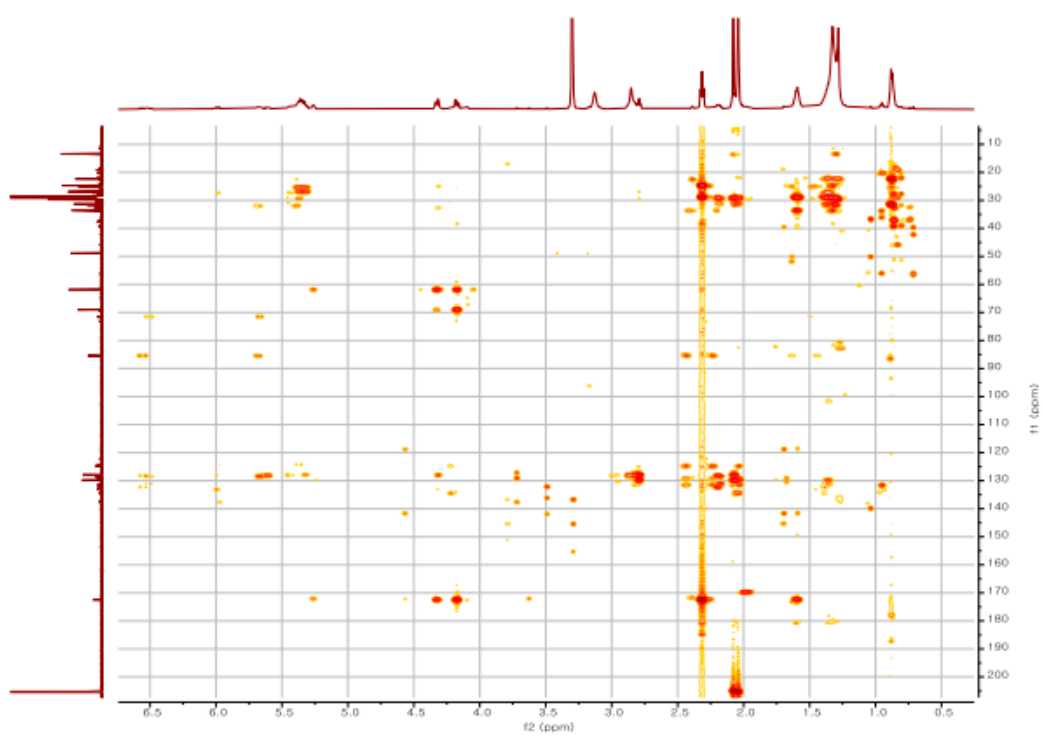


Figure S16. HMBC spectrum of T90A-F3-c'

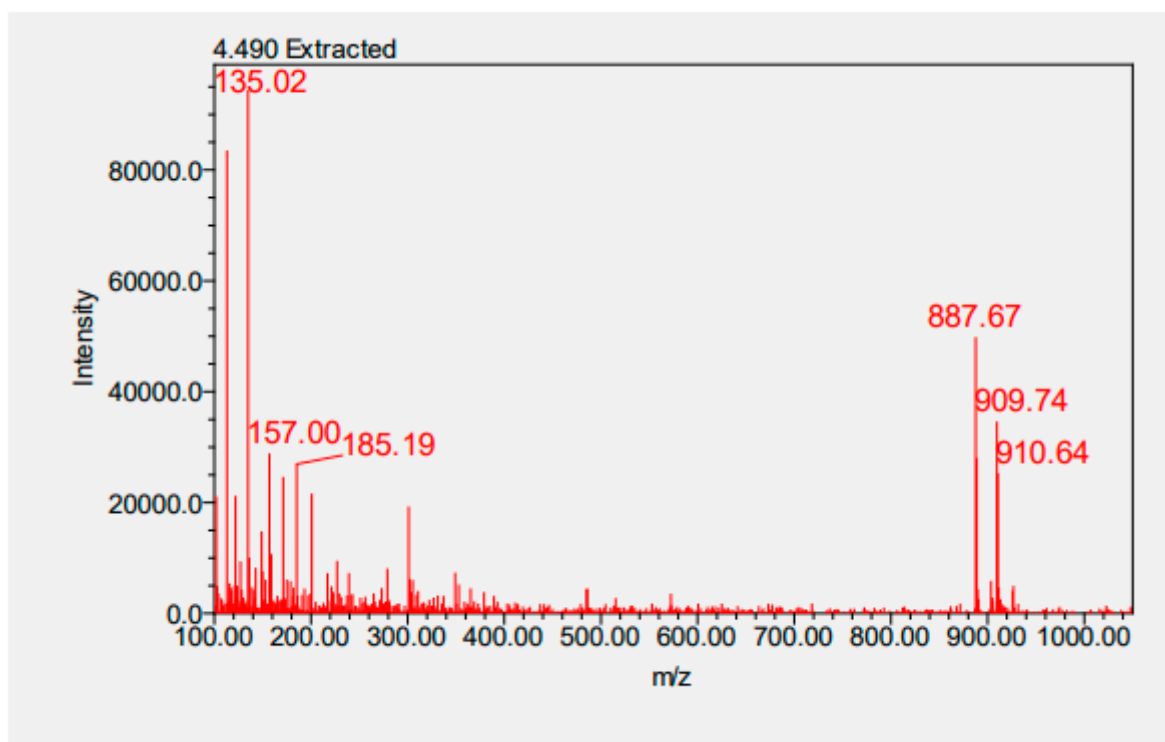


Figure S17. Mass spectrum of T90A-F3-d'

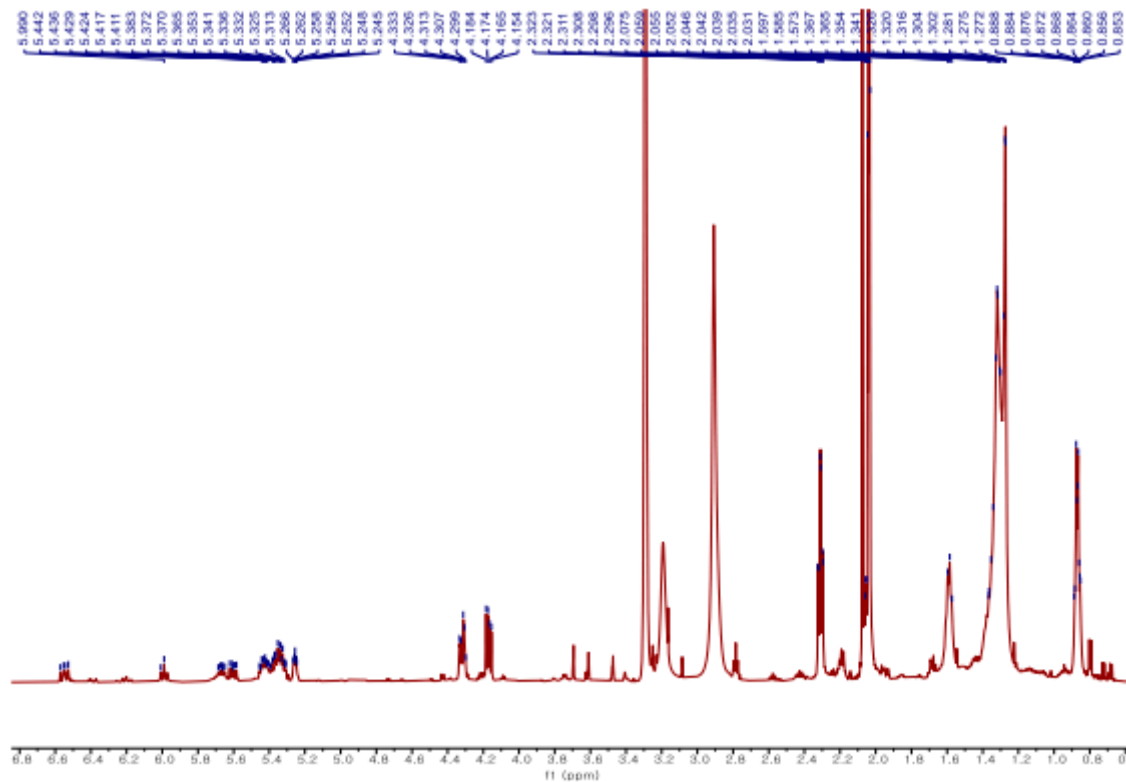


Figure S18. ¹H-NMR spectrum of T90A-F3-d'

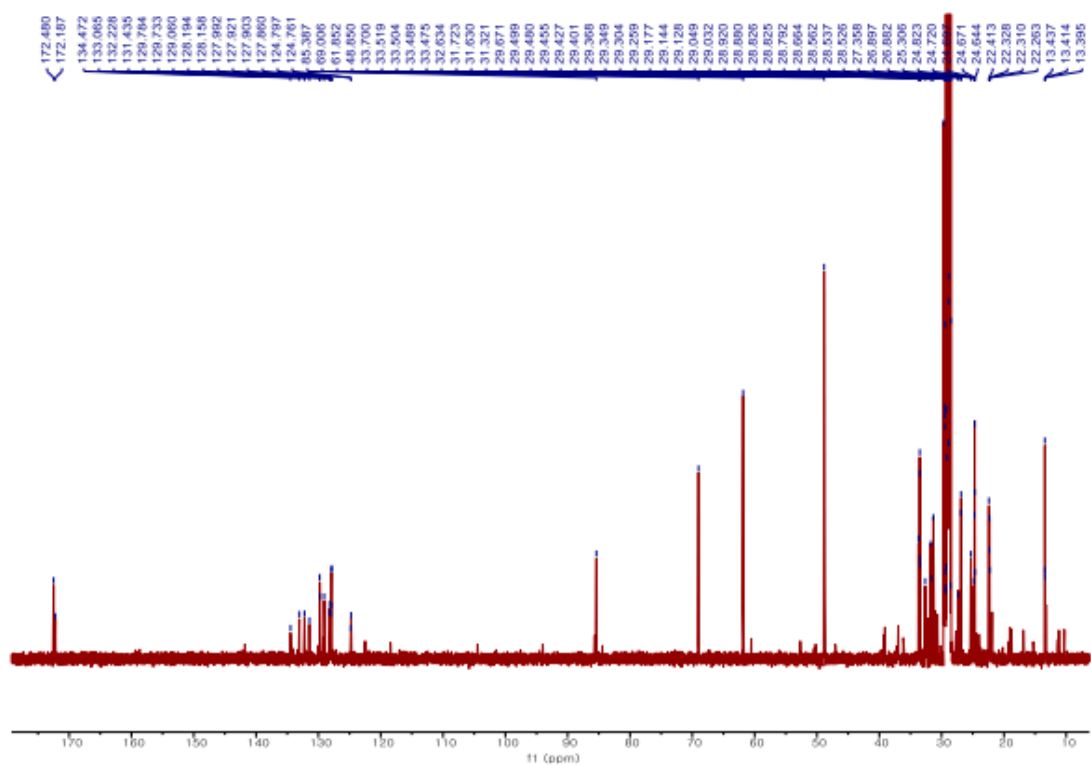


Figure S19. ^{13}C -NMR spectrum of T90A-F3-d'

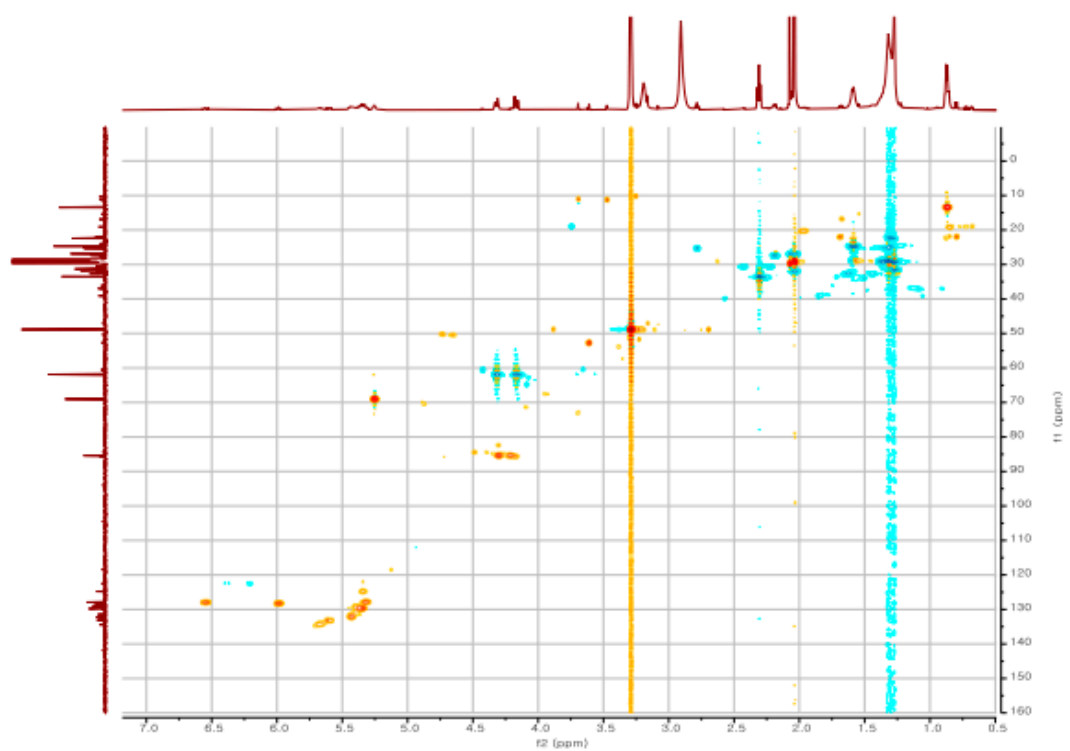


Figure S20. HSQC spectrum of T90A-F3-d'

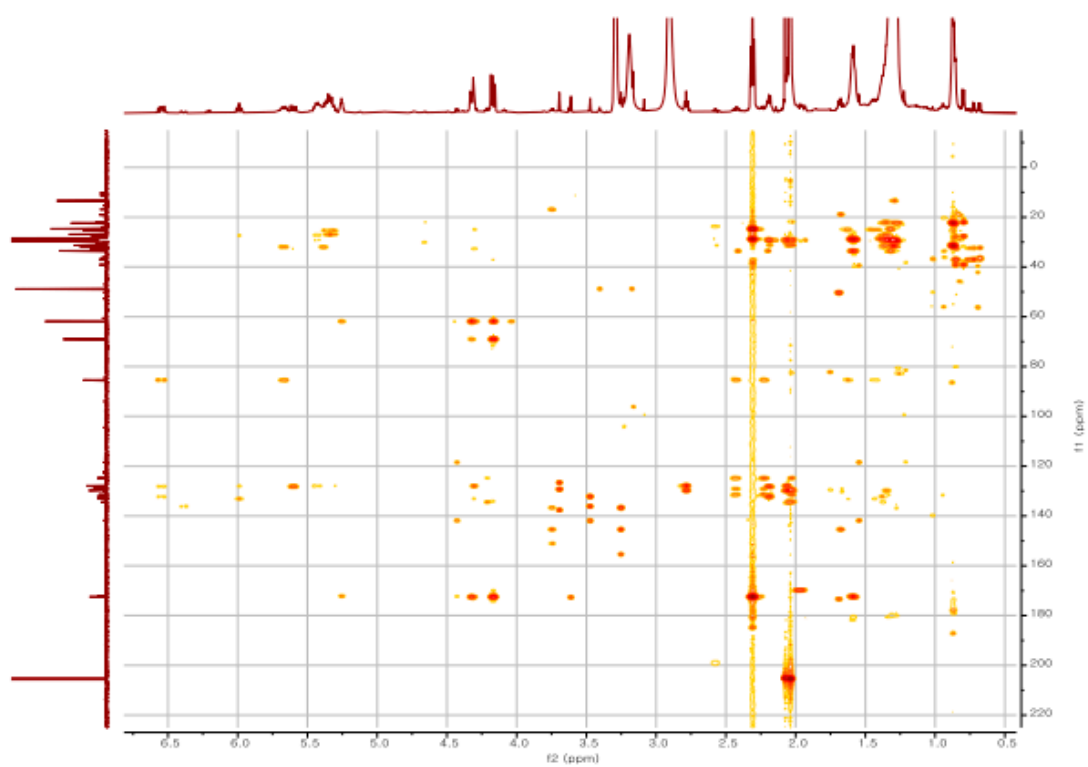


Figure S21. HMBC spectrum of T90A-F3-d'

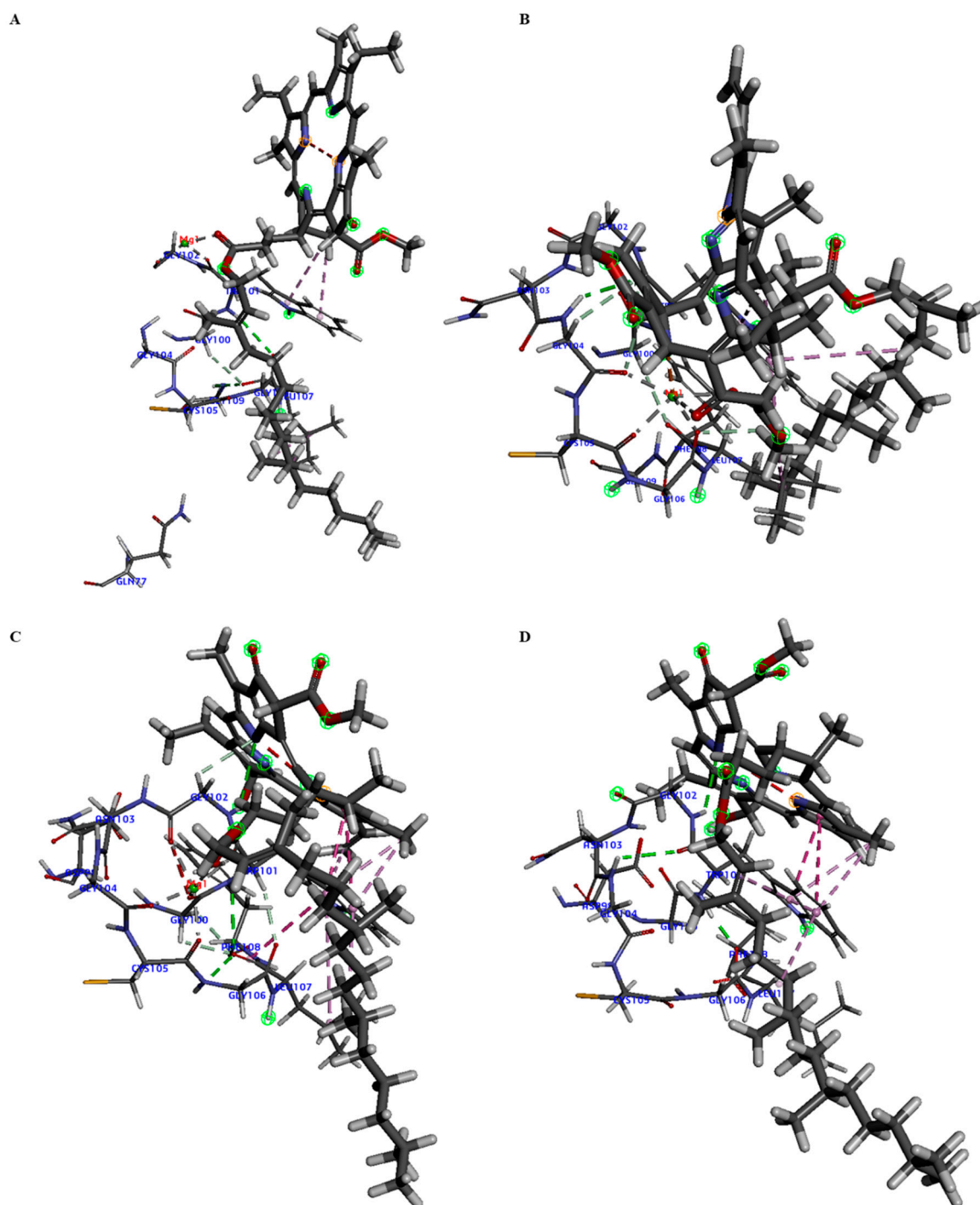


Figure S22. The docking poses of chlorophylls to zika virus envelop protein (5JHM). Chlorophyll A (A), chlorin e6-131-152-dimethyl-173-phytyl ester (B), hydroxychlorophyll A (C), and hydroxypheophytin A (D).

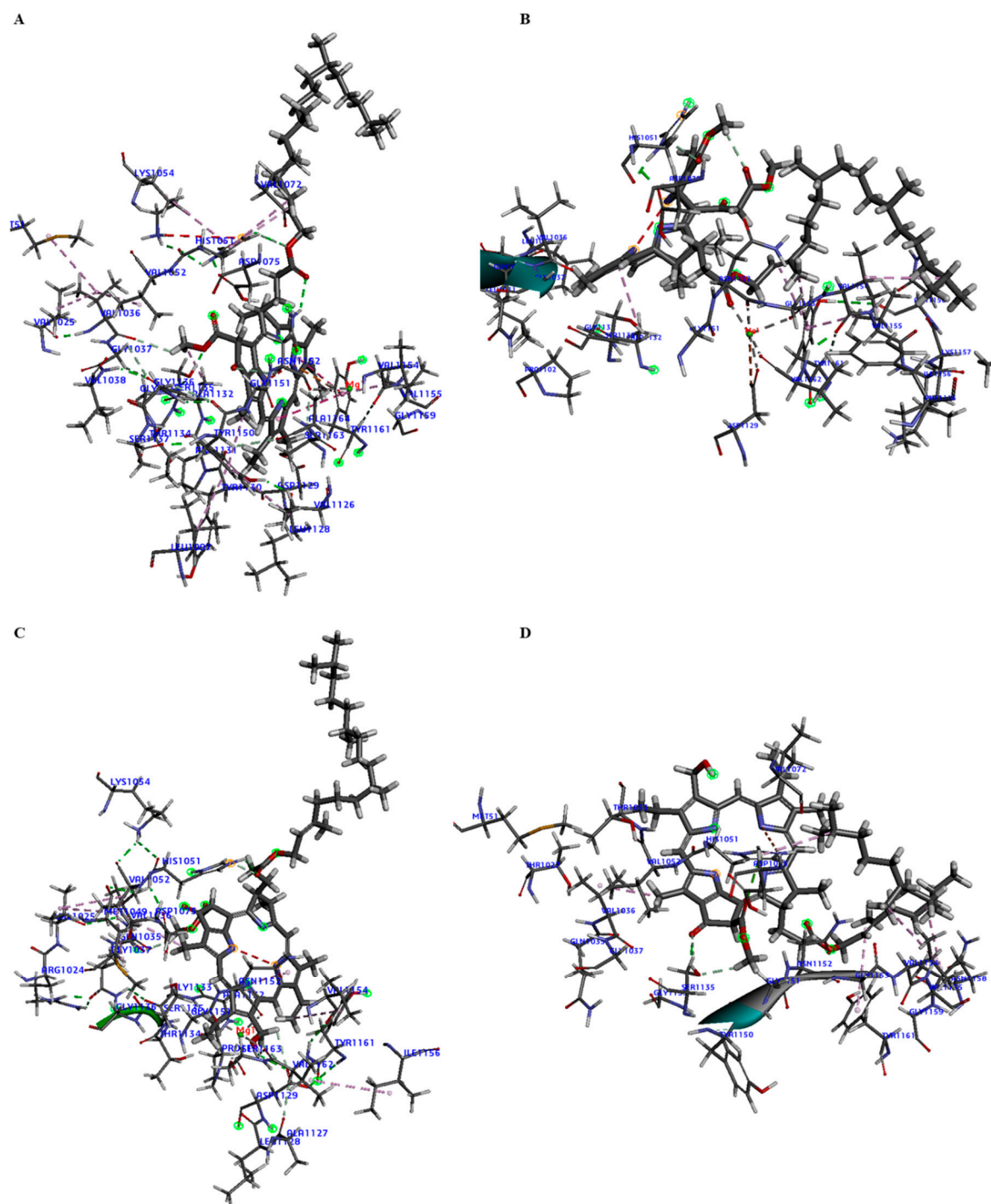


Figure S23. The docking poses of chlorophylls to zika virus NS2B/NS3 (5LC0).

Chlorophyll A (A), chlorin e6-131-152-dimethyl-173-phytyl ester (B), hydroxychlorophyll A (C), and hydroxypheophytin A (D).

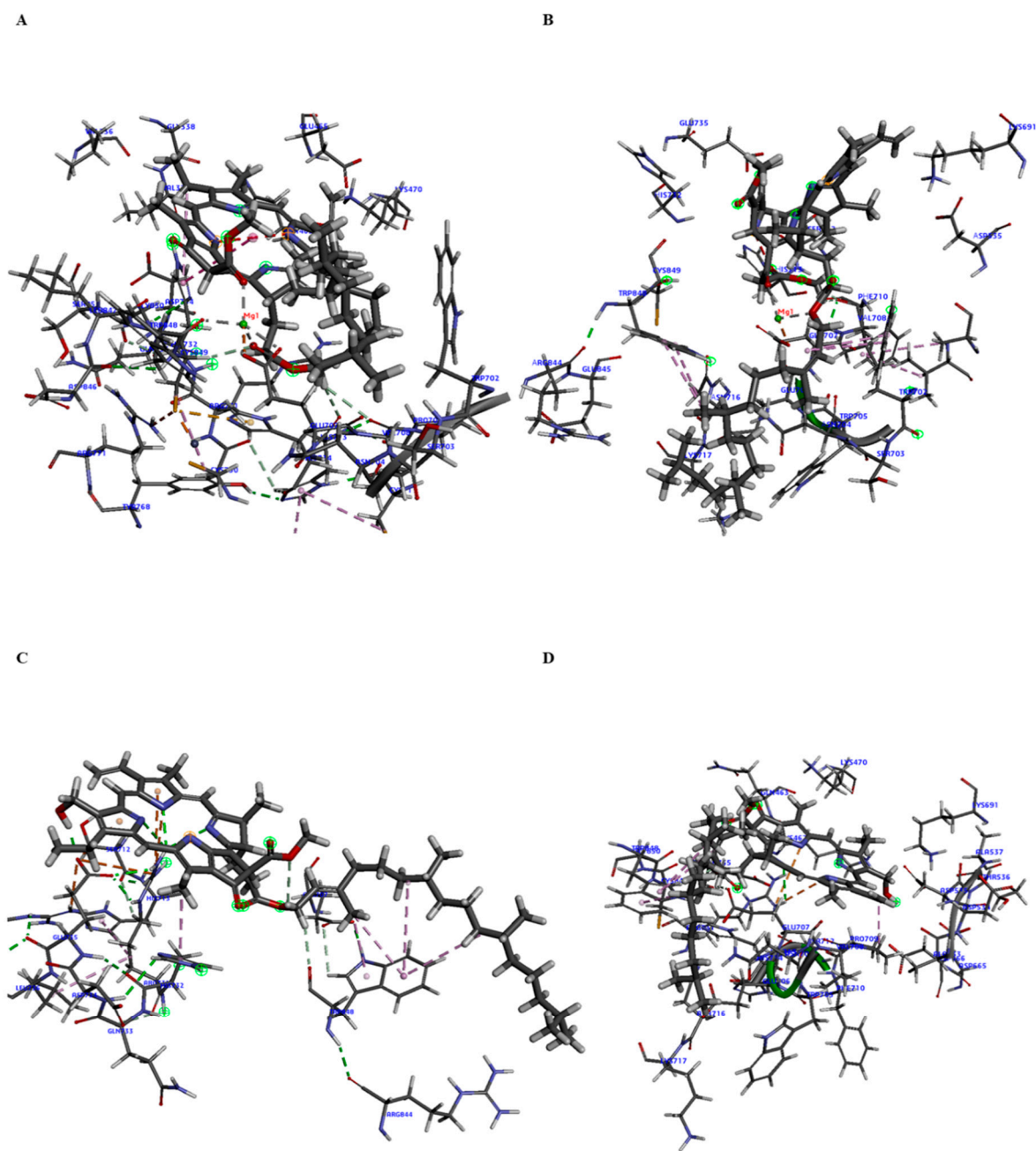


Figure S24. The docking poses of chlorophylls to zika virus RdRp (5TFR). Chlorophyll A (A), chlorin e6-131-152-dimethyl-173-phytyl ester (B), hydroxychlorophyll A (C), and hydroxypheophytin A (D).

Table S1. The chromatogram signal values of T90A-F3-a'.

| No. | RT | Area | % Area | Height | Denotation | Purity |
|------------|-----------|-------------|---------------|---------------|-------------------|---------------|
| 1 | 7.185 | 563,223 | 1.13 | 66,421 | | |
| 2 | 7.509 | 2,710,245 | 5.43 | 79,377 | | |
| 3 | 9.403 | 2,059,629 | 4.13 | 182,586 | | |
| 4 | 9.742 | 4,970,304 | 9.97 | 201,985 | | |
| 5 | 10.311 | 13,685,517 | 27.44 | 324,309 | | |
| 6 | 14.374 | 1,847,745 | 3.70 | 39,916 | | |
| 7 | 15.204 | 24,036,018 | 48.19 | 2,026,402 | T90A-F3-a' | 99.08% |

Table S2. The chromatogram signal values of T90A-F3-b'.

| No. | RT | Area | % Area | Height | Denotation | Purity |
|------------|-----------|-------------|---------------|---------------|-------------------|---------------|
| 1 | 7.134 | 7,419 | 0.01 | 620 | | |
| 2 | 7.390 | 17,752 | 0.03 | 3,602 | | |
| 3 | 12.188 | 13,931 | 0.03 | 1,109 | | |
| 4 | 13.078 | 44,326,154 | 80.99 | 2,009,474 | T90A-F3-b' | 98.05% |
| 5 | 23.040 | 10,364,223 | 18.94 | 224,979 | | |

Table S3. The chromatogram signal values of T90A-F3-c' and T90A-F3-d'.

| No. | RT | Area | % Area | Height | Denotation | Purity |
|------------|-----------|-------------|---------------|---------------|-------------------|---------------|
| 1 | 6.267 | 105,061 | 0.23 | 1,426 | | |
| 2 | 8.433 | 24,234 | 0.05 | 1,187 | | |
| 3 | 8.883 | 93,888 | 0.21 | 1,896 | | |
| 4 | 10.041 | 157,505 | 0.35 | 3,307 | | |
| 5 | 29.233 | 228,021 | 0.50 | 6,582 | | |
| 6 | 31.817 | 10,955,148 | 24.25 | 124,283 | T90A-F3-c' | 94.68% |
| 7 | 34.914 | 27,951,798 | 61.88 | 307,649 | T90A-F3-d' | 99.61% |

Table S4. The calculated binding energies between chlorophylls (hydroxychlorophyll a and hydroxypheophytin a) and zika virus proteins.

| Chlorophyll | Protein | Binding energy (kcal/mol) |
|----------------------|------------------|----------------------------------|
| Hydroxychlorophyll A | Envelope protein | -511.311 |
| | NS2B/NS3 | -751.503 |
| | RdRp | -899.910 |
| Hydroxypheophytin A | Envelope protein | -122.571 |
| | NS2B/NS3 | -286.441 |
| | RdRp | -337.940 |

Table S5. The non-bond interaction between chlorophylls chlorophylls (hydroxychlorophyll a and hydroxypheophytin a) and Zika virus proteins.

| Chlorophyll | Protein | Non-bond interaction in active site |
|-------------------------|---------------------|--|
| Hydroxychlorophyll A | Envelope protein | Mg ²⁺ -GLY100, Mg ²⁺ -TRP101, Mg ²⁺ -GLY102, Mg ²⁺ -GLY104, Mg ²⁺ -CYS105, C3-TRP101 (6), C3-GLY102 (2), C3-LEU107 |
| | NS2B/NS3 | Mg ²⁺ -GLY1151, Mg ²⁺ -ASN1152, Mg ²⁺ -VAL1162, Mg ²⁺ -SER1163, C3-GLN1035, C3-VAL1036, C3-HIS1051 (2), C3-VAL1052, C3-ASP1129 (3), C3-ALA1132, C3-TYR1161, C3-VAL1162 |
| | RdRp | C3-ARG731 (5), C3-HIS732, C3-GLU735 (2), C3-TRP848 (5) |
| Hydroxypheophytin A | Envelope protein | C4-TRP101 (5), C4-GLY102 |
| | NS2B/NS3 | C4-VAL1036, C4-HIS1051 (4), C4-SER1135 (3), C4-VAL1154, C4-VAL1155, C4-TYR1161 |
| | RdRp | C4-GLU707, C4-PRO709, C4-ARG731 (3), C4-TRP848 (3), C4-CYS849 |

The number in parentheses indicates the number of the non-bond interactions.