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ELECTRONIC SUPPLEMENTARY INFORMATION

Title: The conjugate of jasmonic acid and tetrapeptide as a novel promising biologically active compound

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Journal: New Journal of Chemistry

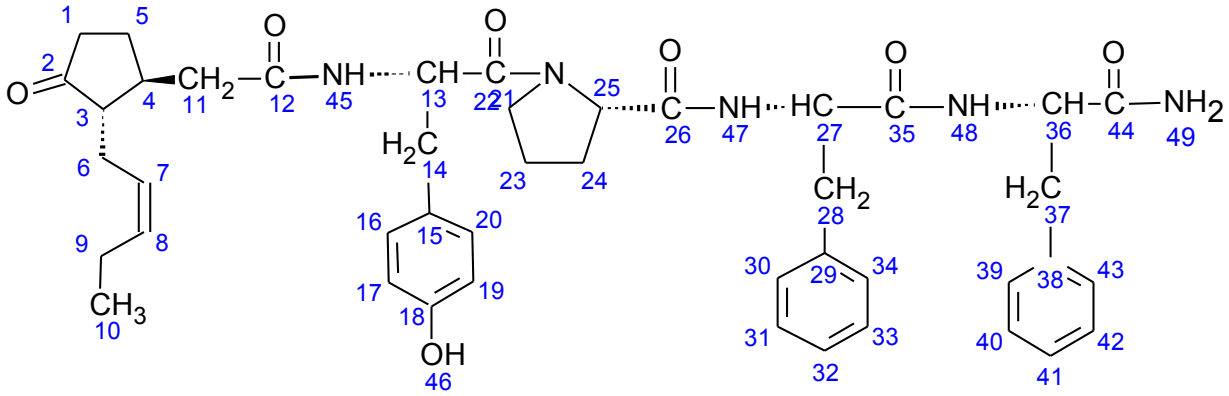
^{1}H NMR

Stereoisomer 1:

JA-YPFF-NH_2: ^{1}H NMR ($CDCl_3$, 600 MHz): δ_H 0.90 (3H, t, H-10), 1.29 (2H,m, H-5), 1.62 (2H,br, H-23), 1.70-1.78 (1H,m,H-3), 1.85 (2H,br, H-24), 1.98 (2H, quint, H-9), 2.01-2.06 (2H, m, H-11), 2.24 (2H, br, H-6), 2.27 (1H, br, H-4), 2.32 (2H, br, H-5), 2.47 (2H, br, H-1), 2.89 (2H, br, H-28), 2.96 (2H, br, H-37), 3.19 (2H, br, H-14), 3.67 (2H, br, H-22), 4.37 (1H, br, H-25), 4.70 (1H, br, H-27), 4.78 (1H, br, H-36), 4.88 (1H, br, H-13), 5.14-5.20 (1H, m, H-7), 5.33-5.48 (1H, m, H-8), 6.61-6.83 (2H, m, H-16, H-20), 6.94 (2H, br, H-17,H-19), 7.03-7.26 (10H, m, H-30-H-34 and H-39-H-43), 7.31 (1H, s, H-45), 7.53 (1H, s, H-48), 7.93 (1H, s, H47).

Stereoisomer 2:

JA-YPFF-NH_2: ^{1}H NMR ($CDCl_3$, 600 MHz): δ_H 0.86 (3H, t, H-10), 1.29 (2H,m, H-5), 1.62 (2H,br, H-23), 1.70-1.78 (1H,m,H-3), 1.85 (2H,br, H-24), 1.98 (2H, quint, H-9), 2.01-2.06 (2H, m, H-11), 2.24 (2H, br, H-6), 2.27 (1H, br, H-4), 2.32 (2H, br, H-5), 2.47 (2H, br, H-1), 2.89 (2H, br, H-28), 2.96 (2H, br, H-37), 3.19 (2H, br, H-14), 3.52 (2H, br, H-22), 4.37 (1H, br, H-25), 4.70 (1H, br, H-27), 4.78 (1H, br, H-36), 4.88 (1H, br, H-13), 5.23-5.30 (1H, m, H-7), 5.33-5.48 (1H, m, H-8), 6.61-6.83 (2H, m, H-16, H-20), 6.94 (2H, br, H-17,H-19), 7.03-7.26 (10H, m, H-30-H-34 and H-39-H-43), 7.31 (1H, s, H-45), 7.53 (1H, s, H-48), 7.93 (1H, s, H47).



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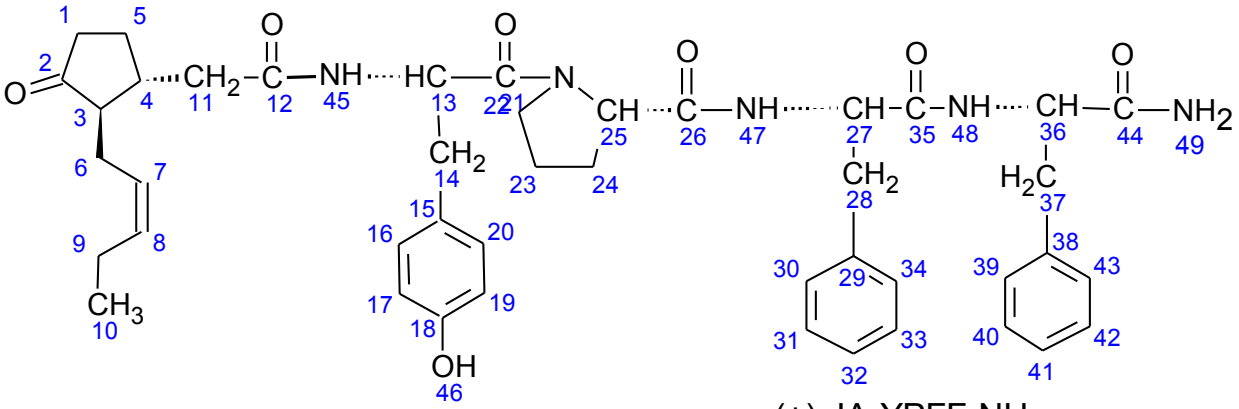
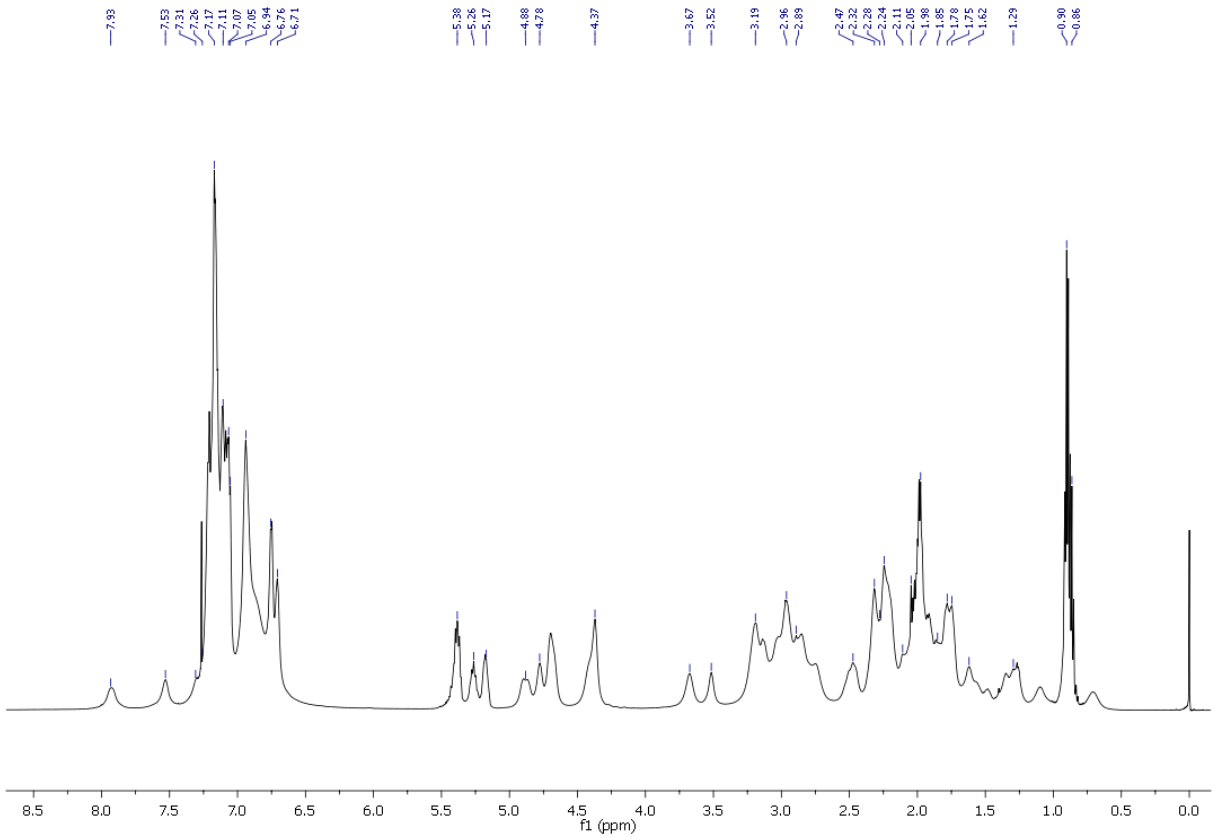


(+)-JA-YPFF-NH_2


7.93
7.53
7.31
7.26
7.17
7.11
7.07
7.05
6.94
6.76
6.71
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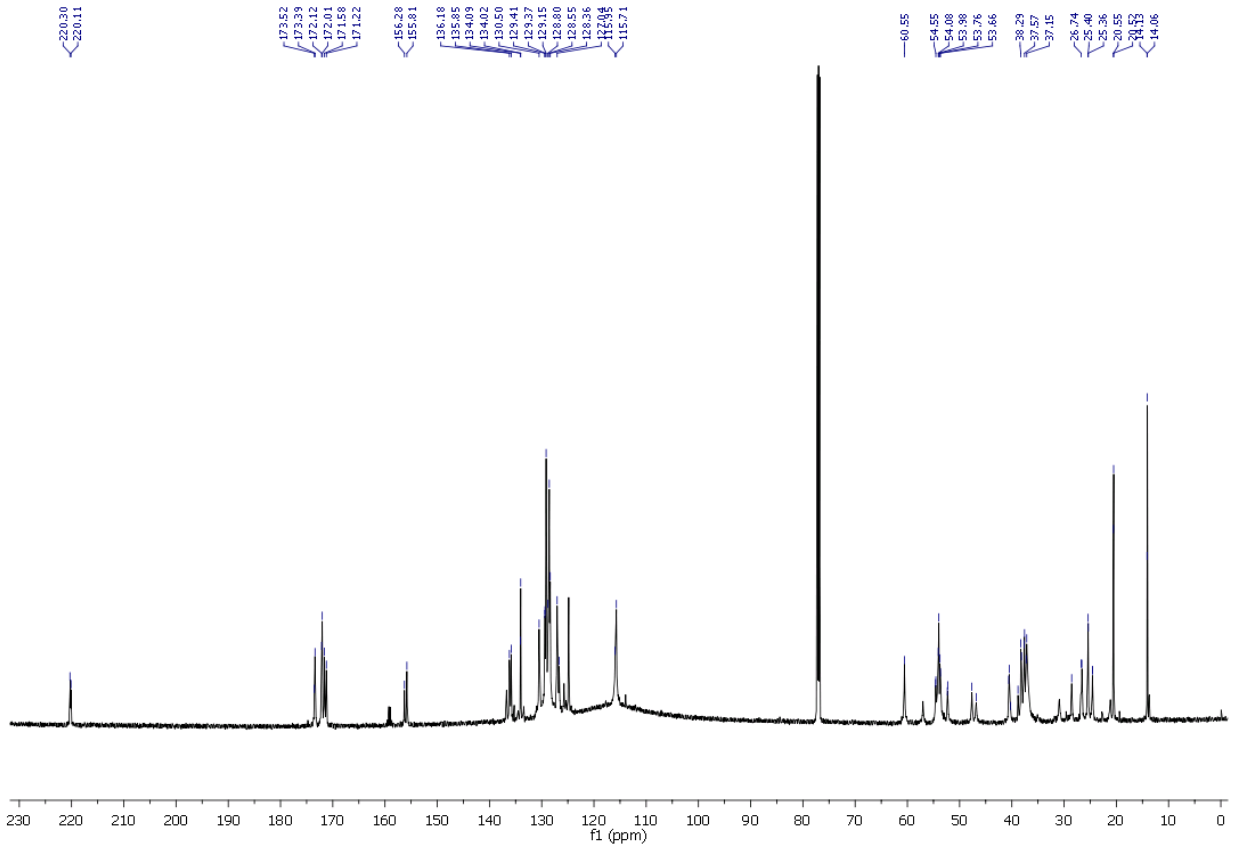
5.26
5.17
4.88
4.78
4.37
3.67
3.52
3.19
2.96
2.89
2.47
2.32
2.28
2.24
2.11
2.05
1.98
1.85
1.78
1.75
1.62
1.29
0.90
0.86
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

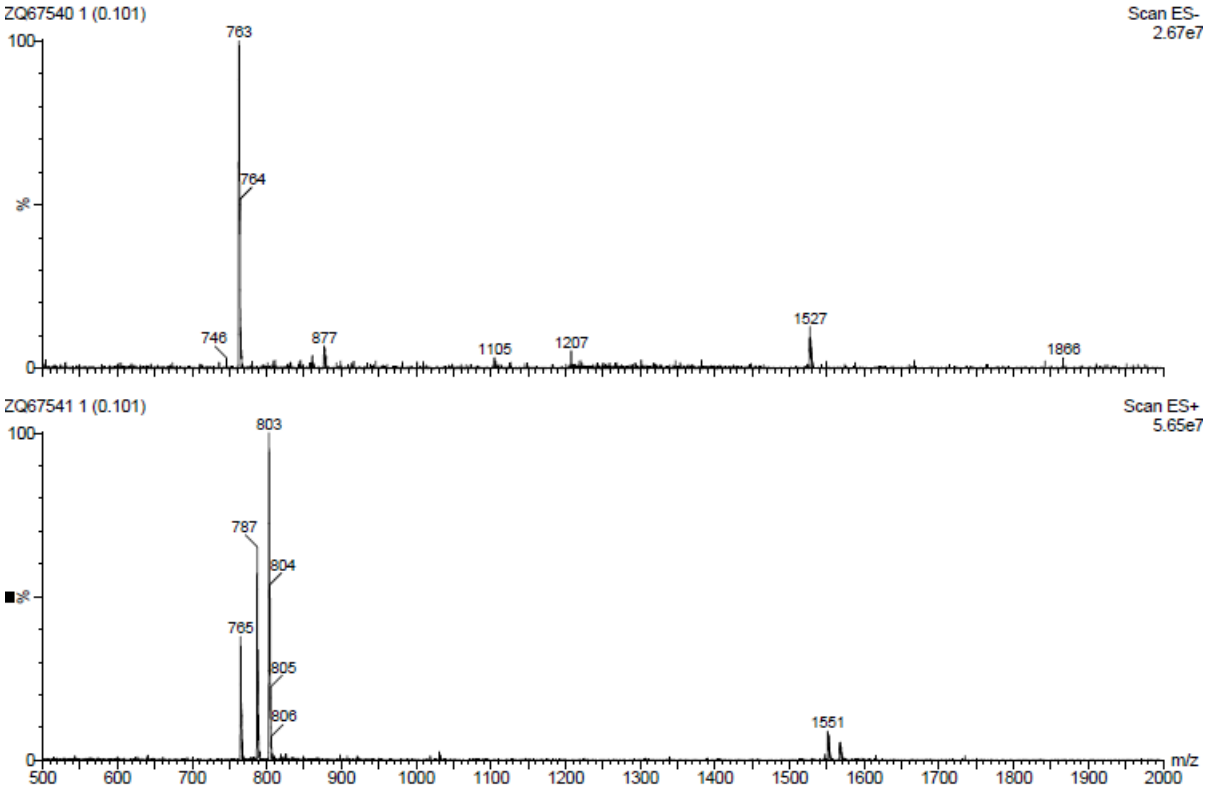
^{13}C NMR

Stereoisomer 1:
JA-YPFF-NH_2: ^{13}C NMR ($CDCl_3$, 600 MHz): δ_C 14.06 (C-10), 20.52 (C-9), 24.55 (C-23), 25.36 (C-6), 26.60 (C-5), 28.55 (C-24), 37.15 (C-14), 37.57 (C-11), 38.16 (C-37), 38.29 (C-28), 38.82 (C-4), 40.2 (C-11), 40.50 (C-1), 47.66 (C-22), 52.29 (C-13), 53.98 (C-36), 53.76 (C-3), 54.55 (C-27), 60.55 (C-25), 115.7 (C-17, C-19), 124.79 (C-7), 125.72-129.15 (C-30-C-34, C-39-C-43), 129.37 (C-15), 130.50 (C-16, C-20), 134.02 (C-8), 135.85 (C-29, C-37), 155.81 (C-18), 171.22 (C-26), 171.58 (C-35), 172.01 (C-21), 172.12 (C-44), 173.39 (C-12), 220.30 (C-2).

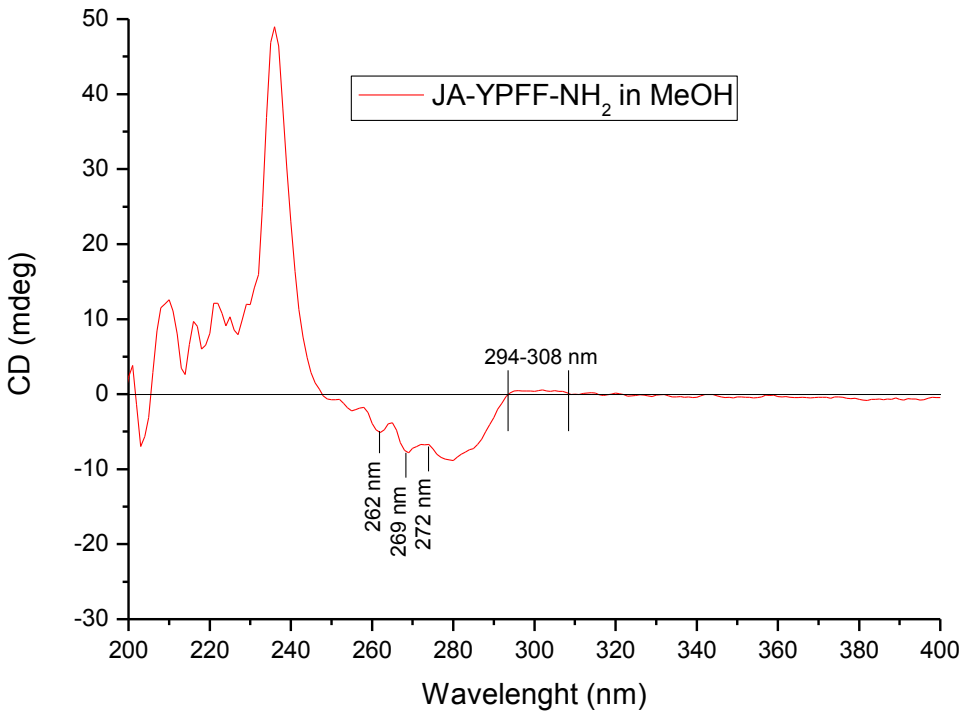
Stereoisomer 2:
JA-YPFF-NH_2: ^{13}C NMR ($CDCl_3$, 600 MHz): δ_C 14.13 (C-10), 20.52 (C-9), 24.57 (C-23), 25.39 (C-6), 26.76 (C-5), 28.55 (C-24), 37.26 (C-14), 37.66 (C-11), 38.16 (C-37), 38.29 (C-28), 38.82 (C-4), 40.2 (C-11), 40.60 (C-1), 46.83 (C-22), 52.34 (C-13), 54.08 (C-36), 53.66 (C-3), 54.60 (C-27), 60.55 (C-25), 115.95 (C-17, C-19), 124.94 (C-7) 125.72-129.15 (C-30-C-34, C-39-C-43), 129.41 (C-15), 130.38 (C-16, C-20), 134.09 (C-8), 136.18 (C-29, C-37), 156.28(C-18), 171.22 (C-26), 171.58 (C-35), 172.01 (C-21), 172.12 (C-44), 173.52 (C-12), 220.1 (C-2)

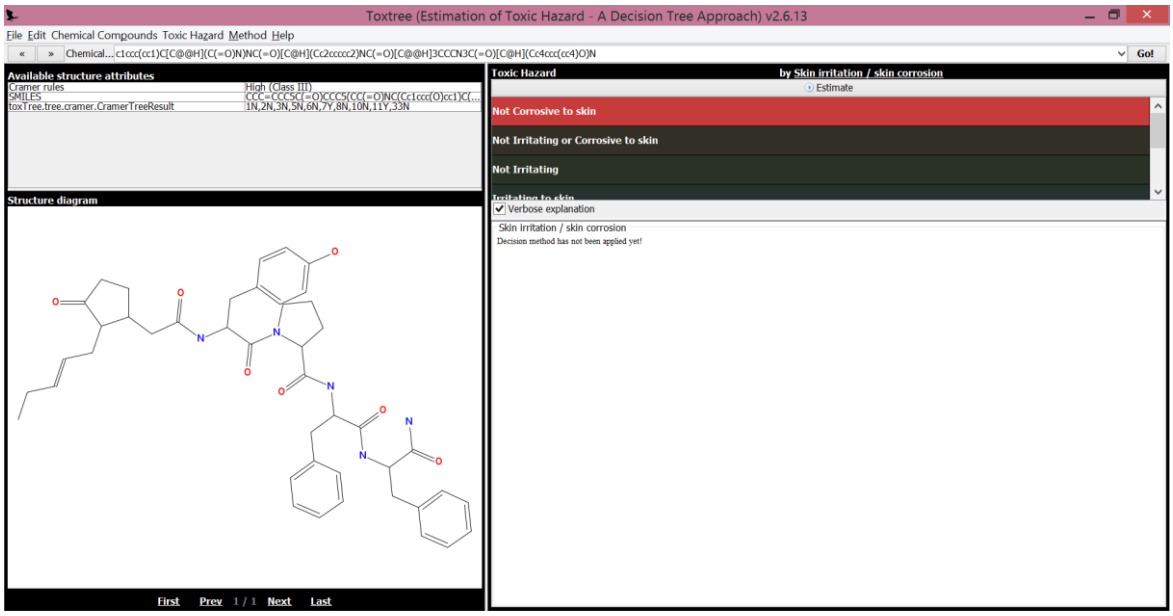


ESI-MS spectrum of JA-YPFF-NH_2 conjugate.



CD spectrum of JA-YPFF-NH_2 conjugate.



The CD spectra of the conjugate were analyzed in the near-UV. Near-UV CD band is very broad in the region 250–310 nm. According to the literature (S.M. Kelly, N.C. Price, *Curr Protein Pept. Sci.* 2000, **1**(4), 349-384; S.R. Martin, P.M. Bayley, Absorption and Circular Dichroism Spectroscopy *in* Calcium-binding protocols from Methods and Techniques Biology 2001. pp. 43-56, Humana Press. Totowa, NK), two negative CD signals may be characterized as L-Proline (262 nm) and L- Phenylalanine (269 nm). The CD band in the region 272 nm-294 nm includes broad and not well-resolved signal, probably from L-Tyrosine (that usually gives signal in the range 270-290 nm) and from (-)-JA. Furthermore, there is also a broad signal in the region 294-308 nm, which may be characterized as (+)-JA. However, it is difficult to clearly characterize partial enantiomers of jasmonic acid without having high quality standards of each possible stereoisomeric form of JA.

The results of Toxtree estimation of JA-YPFF-NH_2 properties