**Electronic Supplementary Material for**

# Compatibility Study of Peptide and Glycerol Using Chromatographic and Spectroscopic Techniques: Application to a Novel Antimicrobial Peptide Cbf-14 Gel

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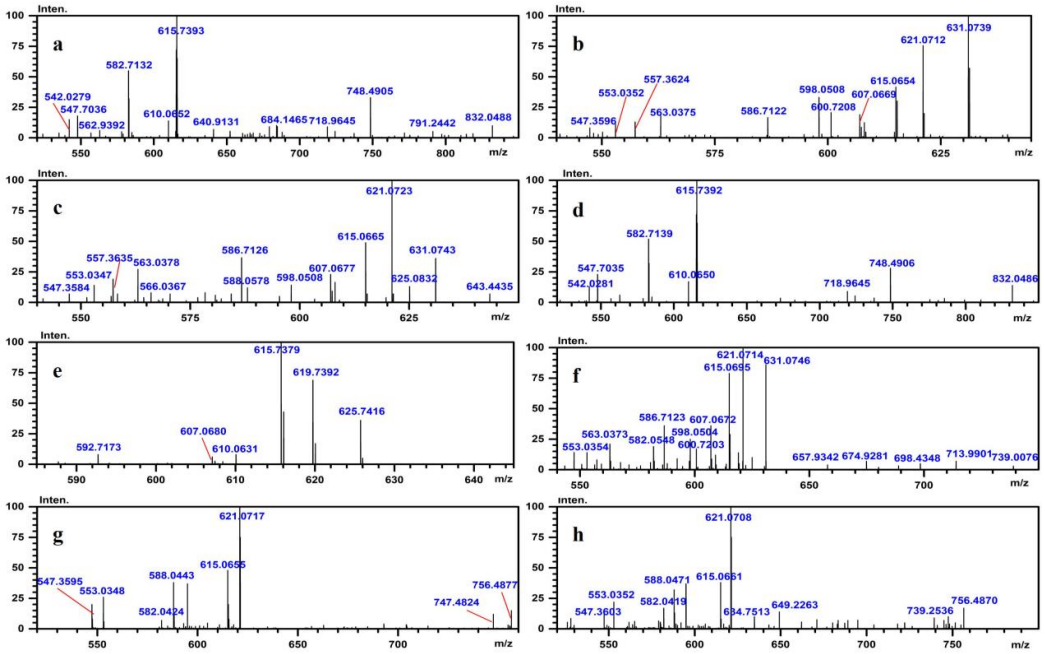
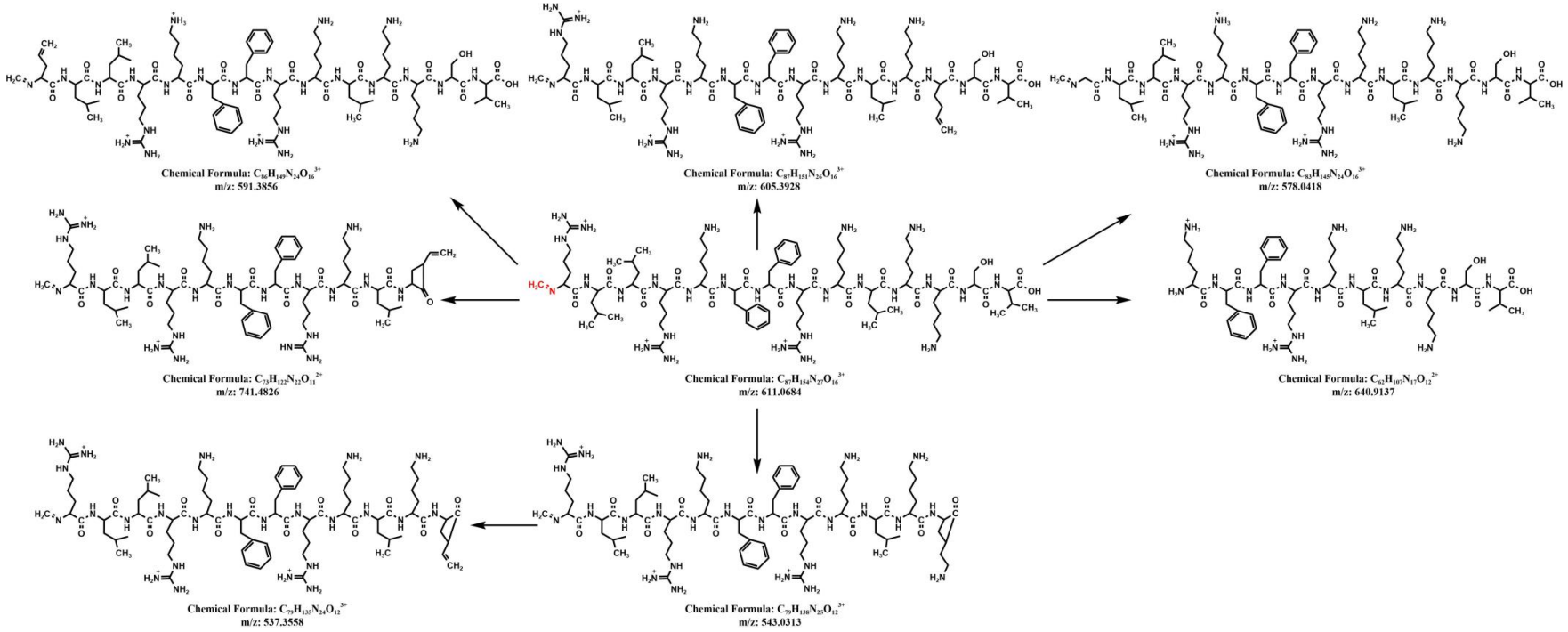



**Figure S1.** The secondary mass spectra of (a) impurity 1, *m/z* 615.7393; (b) impurity 3, *m/z* 631.0739; (c) impurity 5, *m/z* 631.0743; (d) impurity 7, *m/z* 615.7392; (e) impurity 8, *m/z* 625.7416; (f) impurity 9, *m/z* 631.0746; (g) impurity 10, *m/z* 621.0717; (h) impurity 11, *m/z* 621.0708.

**a**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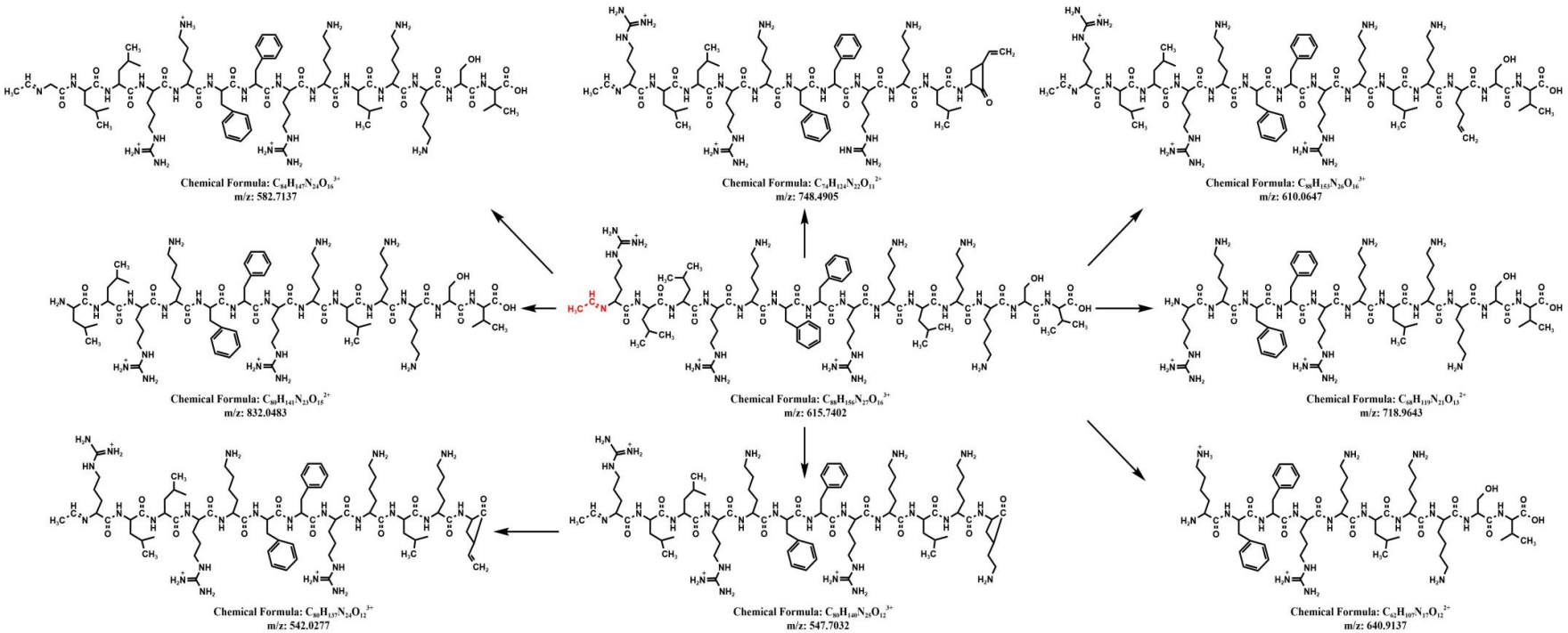
Chemical Formula: C87H151N24O16 3+
m/z: 605.3928
Chemical Formula: C83H145N23O16 3+
m/z: 578.0418
Chemical Formula: C73H122N22O11 2+
m/z: 741.4826
Chemical Formula: C97H154N27O16 3+
m/z: 611.0684
Chemical Formula: C92H107N17O12 2+
m/z: 640.9137
Chemical Formula: C79H136N24O12 3+
m/z: 537.3558
Chemical Formula: C79H138N25O12 3+
m/z: 543.0313

.

**b**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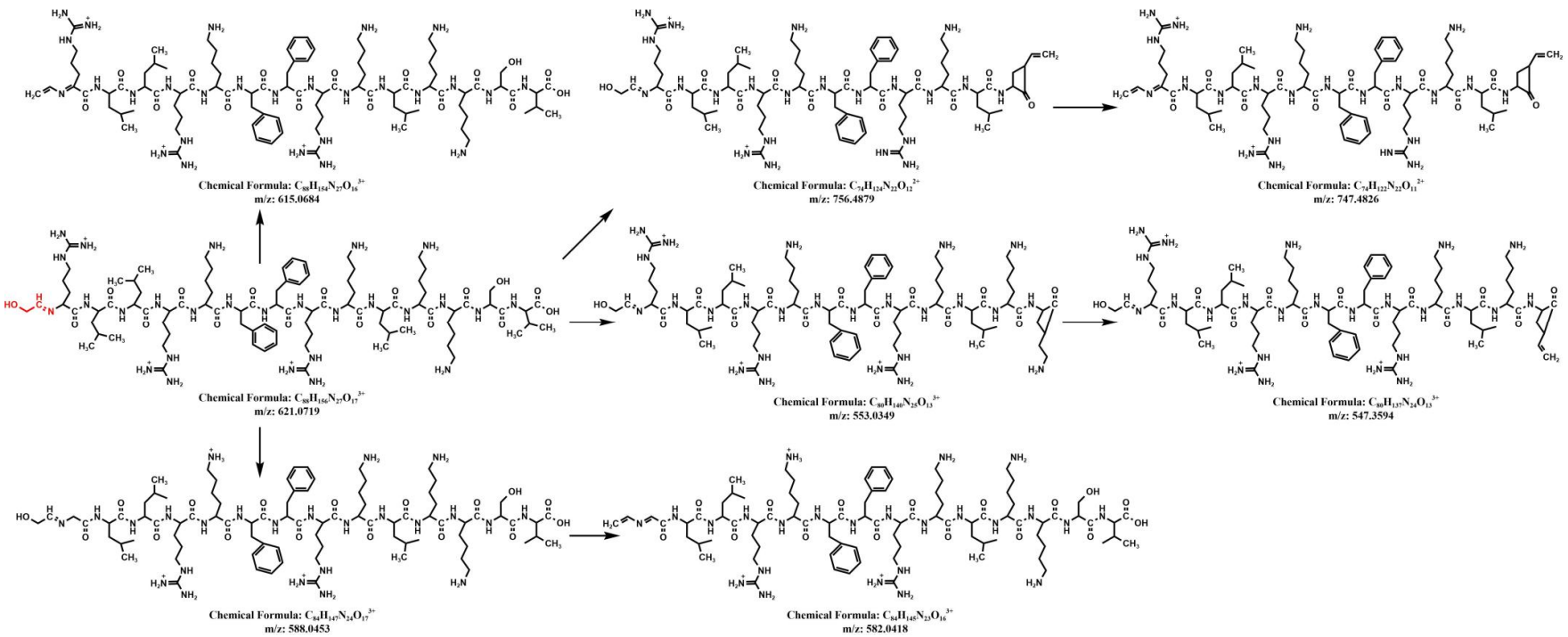
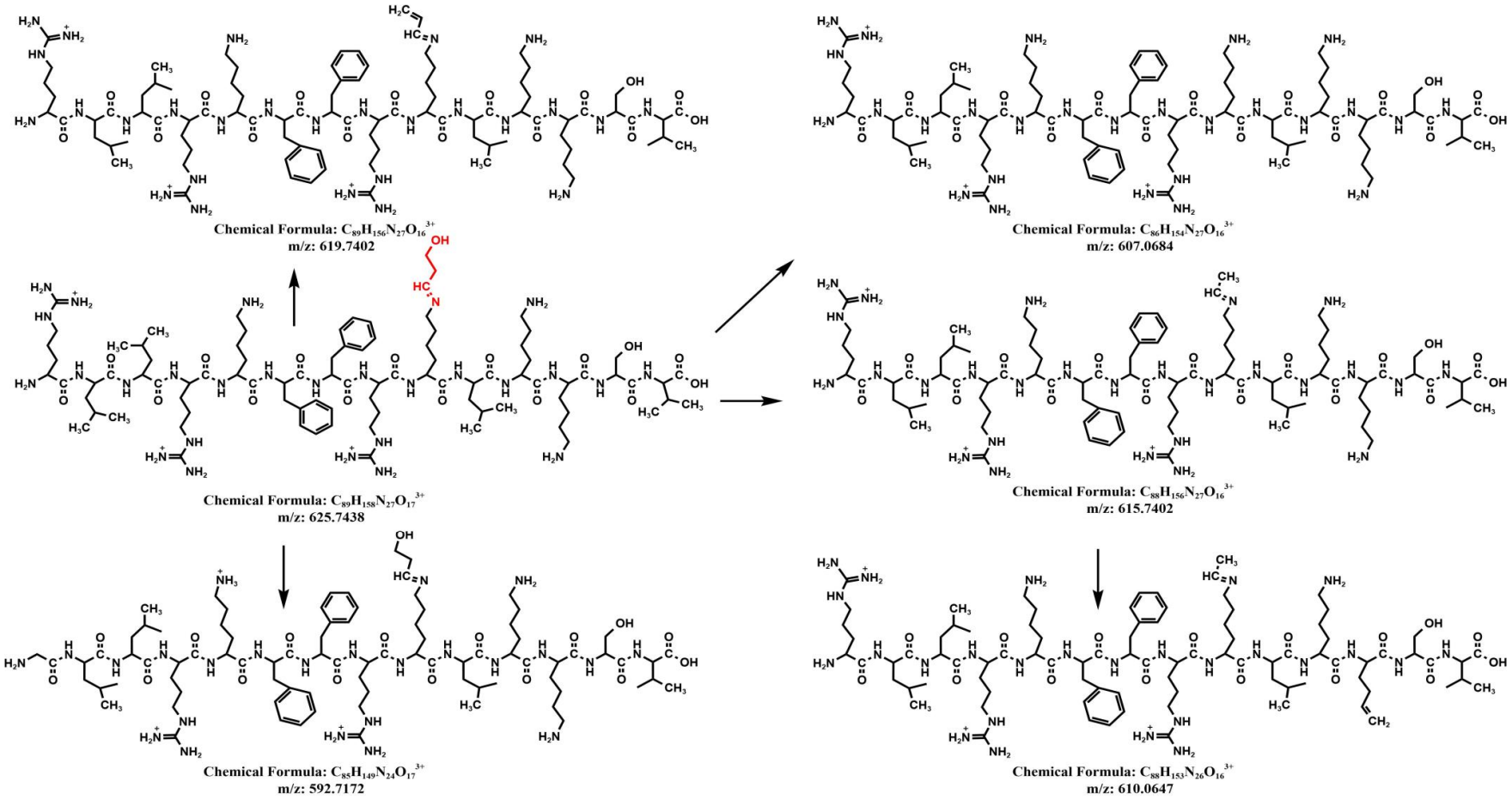
m/z: 582.7137
Chemical Formula: C74H124N22O11 2+
m/z: 748.4905
Chemical Formula: C88H153N28O16 3+
m/z: 610.0647
Chemical Formula: C88H144N23O15 2+
m/z: 832.0483
Chemical Formula: C88H156N27O16 3+
m/z: 615.7402
Chemical Formula: C68H119N21O13 2+
m/z: 718.9643
Chemical Formula: C80H137N24O12 3+
m/z: 542.0277
Chemical Formula: C80H140N28O12 3+
m/z: 547.7032
Chemical Formula: C92H107N17O12 2+
m/z: 640.9137

**c**


Chemical Formula: C86H154N27O16 3+
m/z: 615.0684
Chemical Formula: C74H124N22O12 2+
m/z: 756.4879
Chemical Formula: C74H122N22O11 2+
m/z: 747.4826
Chemical Formula: C86H156N27O17 3+
m/z: 621.0719
Chemical Formula: C80H140N25O13 3+
m/z: 553.0349
Chemical Formula: C80H137N24O13 3+
m/z: 547.3594
Chemical Formula: C86H147N24O17 3+
m/z: 588.0453
Chemical Formula: C86H145N23O16 3+
m/z: 582.0418

**d**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m/z: 619.7402
Chemical Formula: $C_{86}H_{154}N_{27}O_{16}^{3+}$
m/z: 607.0684
Chemical Formula: $C_{89}H_{158}N_{27}O_{17}^{3+}$
m/z: 625.7438
Chemical Formula: $C_{88}H_{156}N_{27}O_{16}^{3+}$
m/z: 615.7402
Chemical Formula: $C_{85}H_{149}N_{24}O_{17}^{3+}$
m/z: 592.7172
Chemical Formula: $C_{88}H_{153}N_{26}O_{16}^{3+}$
m/z: 610.0647

**e**

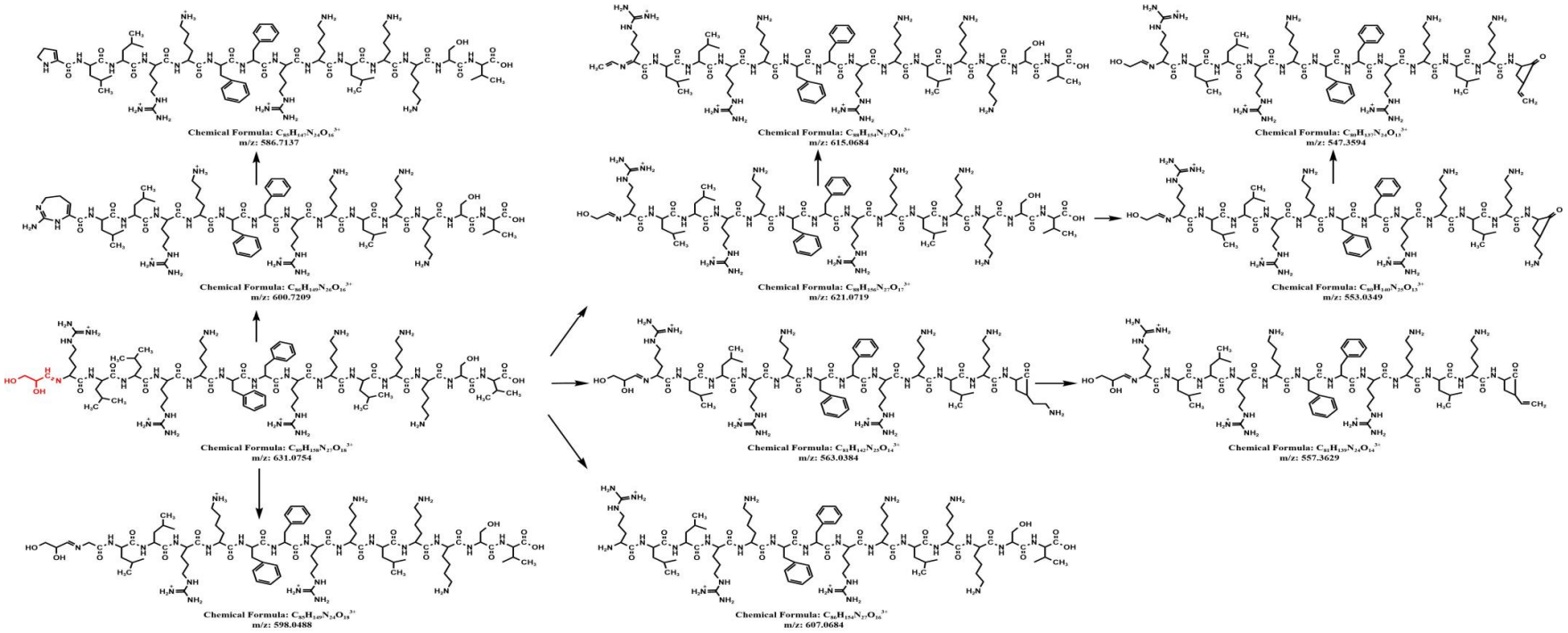
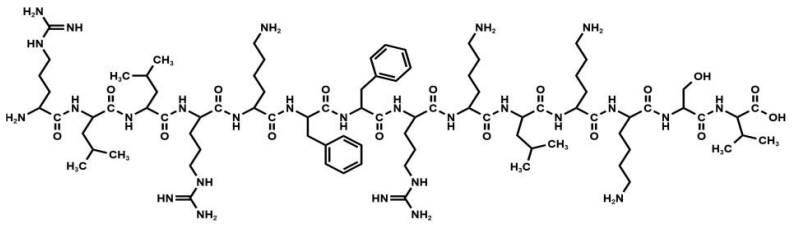


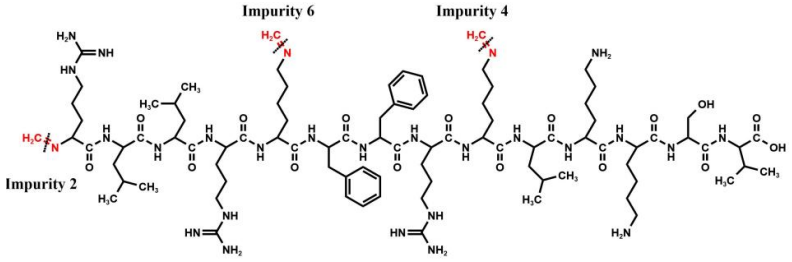

**Figure S2.** Plausible fragmentation pathways of (a) N-methylene-Cbf-14 (represented as impurity 2, and impurity 4, 6 were similar); (b) N-ethylidene-Cbf-14 (represented as impurity 1, and impurity 7 was similar); (c) N-(2-hydroxyethylidene)-Cbf-14 ( represented as impurity 10, and impurity11 was similar); (d) N-(3-hydroxypropylidene)-Cbf-14 (impurity 8); (e) N-(2,3-dihydroxypropylidene)-Cbf-14 (represented as impurity 3, and impurity 5, 9 were similar).

**a**

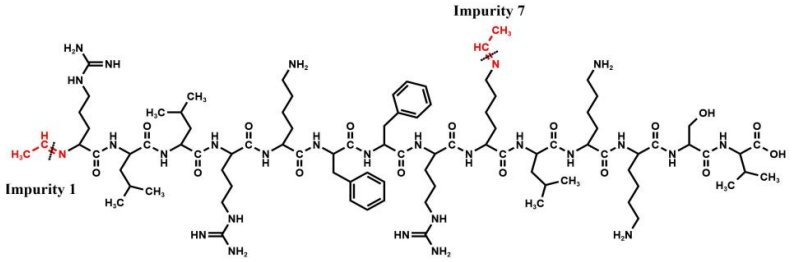


Cbf-14

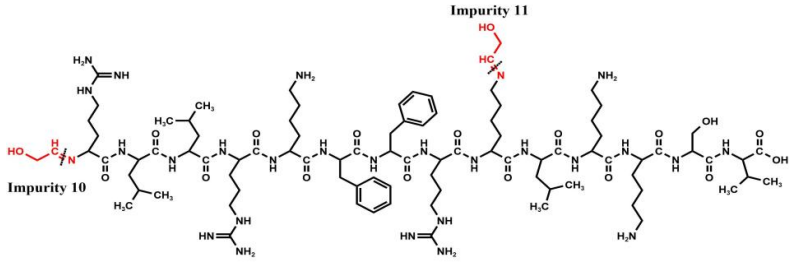
**b**



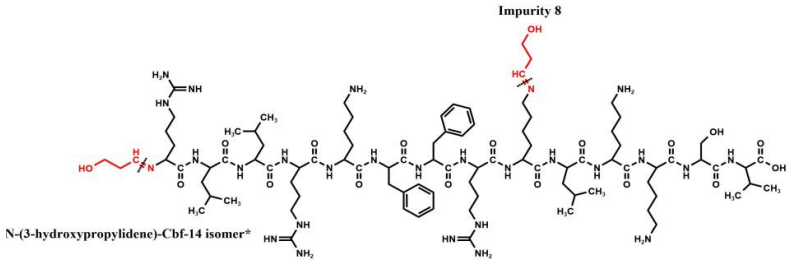

**c**




**d**




**e**




**f**

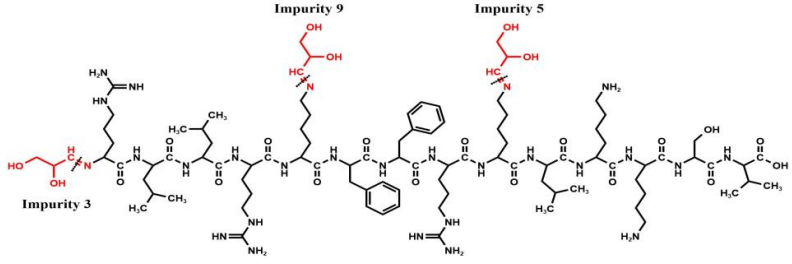


**Figure S3.** Deduced structures of compounds in this study. (a) Cbf-14; (b) N-methylene-Cbf-14 (impurity 2, 4, 6); (c) N-ethylidene-Cbf-14 (impurity 1, 7); (d) N-(2-hydroxyethylidene)-Cbf-14 (impurity 10, 11); (e) N-(3-hydroxypropylidene)--Cbf-14 (impurity 8); (f) N-(2,3-dihydroxypropylidene)-Cbf-14 (impurity 3, 5, 9).
* The impurity formed when Cbf-14 reacted with 3-hydroxypropanal (as shown in Fig 3e at $t_R$ 24.8 min) was not detected in the gel.