

SUPPORTING INFORMATION

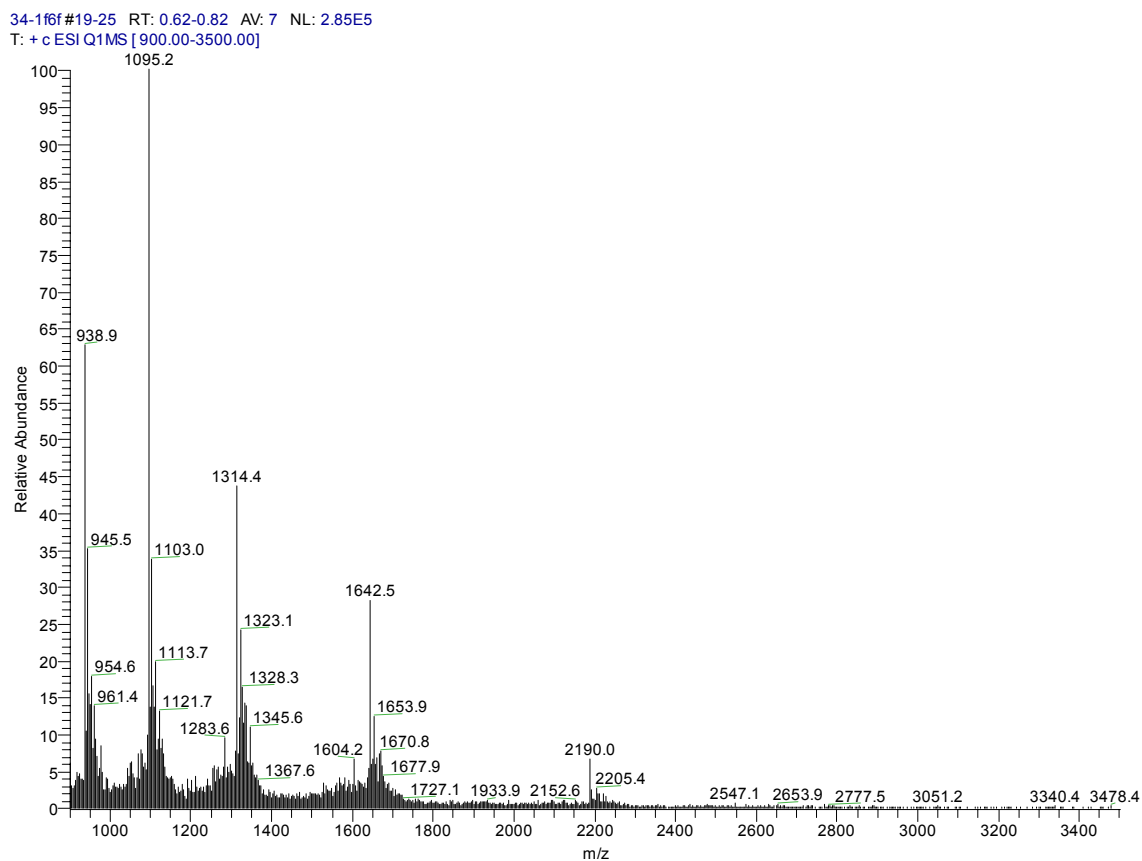
Bioconjugate Chemistry

Synthesis of Radiometal-Labeled and Fluorescent Cell-Permeating Peptide-PNA Conjugates for Targeting the *bcl-2* Proto-Oncogene

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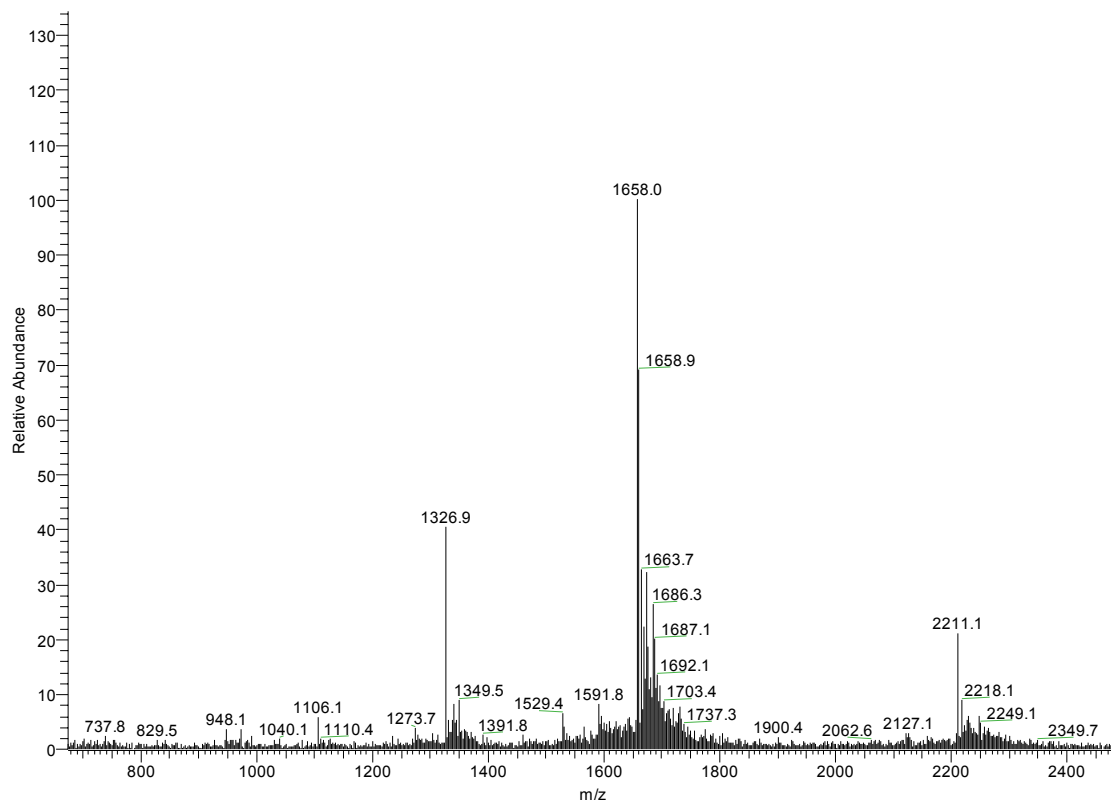
Electrospray ionization (ESI) mass spectra of peptide-PNA conjugates. Lower abundance molecular ions at higher m/z ratios represent adducts of the desired products with sodium, potassium, and counterions (formic acid or trifluoroacetic acid) present in the infusion system.

ESI mass spectrum of conjugate **2**: m/z 2190.0 ($M+3H$)³⁺, 1642.5 ($M+4H$)⁴⁺, 1314.2 ($M+5H$)⁵⁺, 1095.1 ($M+6H$)⁶⁺, 938.9 ($M+7H$)⁷⁺. The observed molecular ions were consistent with the theoretical molecular weight of **2**, calcd ($M+H$)⁺ = 6569.1.



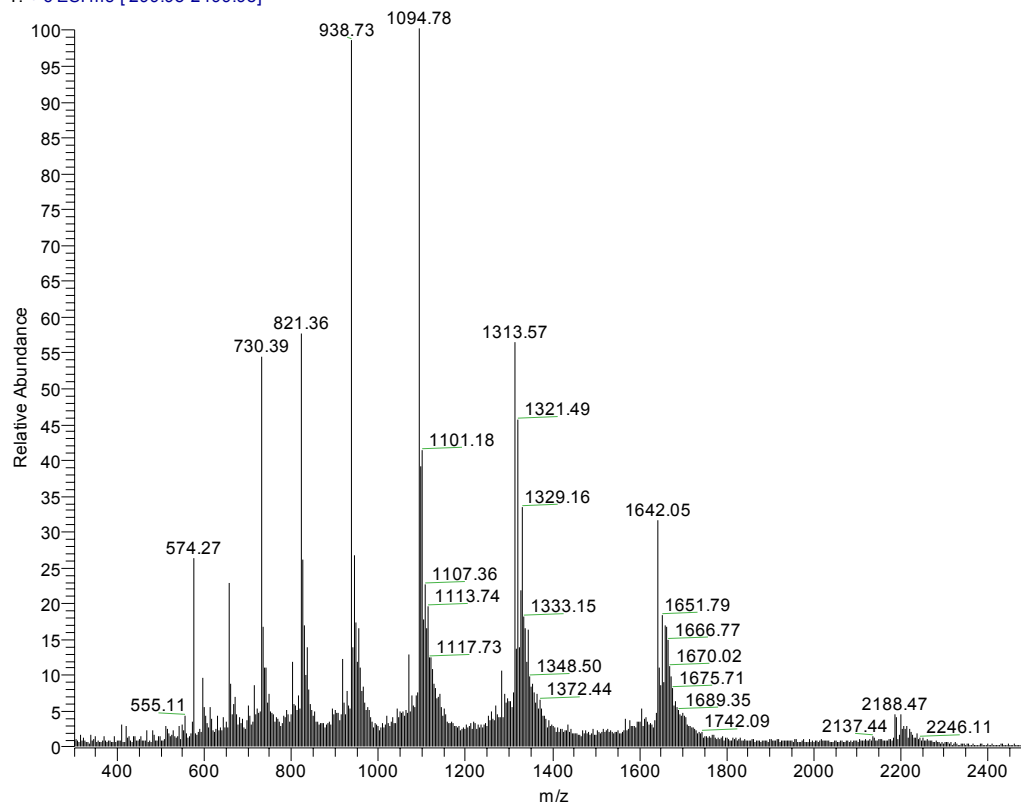
ESI mass spectrum of conjugate **3**: m/z 2211.1 ($M+3H$)³⁺, 1658.0 ($M+4H$)⁴⁺, 1326.9 ($M+5H$)⁵⁺, 1106.1 ($M+6H$)⁶⁺, 948.1 ($M+7H$)⁷⁺. The observed molecular ions were consistent with the theoretical molecular weight of **3**, calcd ($M+H$)⁺ = 6629.2.

PA#35-58 RT: 0.87-1.45 AV: 24 NL: 2.12E4
T: + c ESI Q1MS [300.00-2500.00]



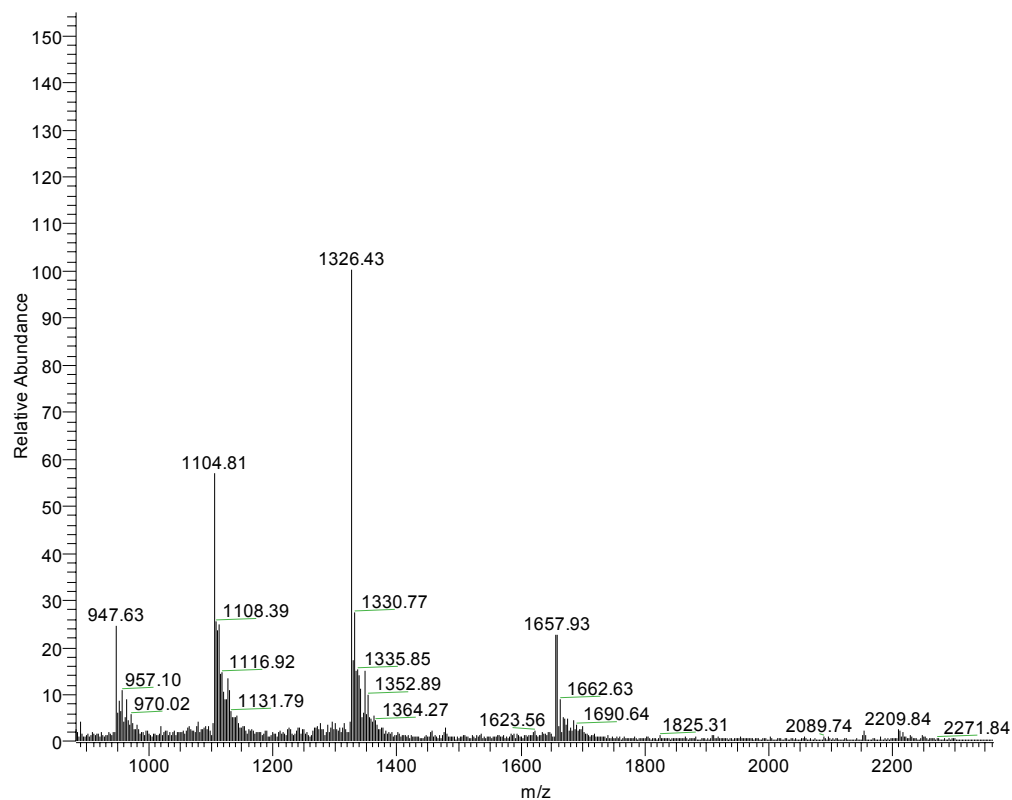
ESI mass spectrum of conjugate **4**: m/z 2188.5 ($M+3H$)³⁺, 1642.1 ($M+4H$)⁴⁺, 1313.6 ($M+5H$)⁵⁺, 1094.8 ($M+6H$)⁶⁺, 938.7 ($M+7H$)⁷⁺, 821.3 ($M+8H$)⁸⁺, 730.4 ($M+9H$)⁹⁺. The observed molecular ions were consistent with the theoretical molecular weight of **4**, calcd ($M+H$)⁺ = 6569.1.

riptd4-k(do)ant#10-15 RT: 0.67-1.00 AV: 6 NL: 1.60E6
T: + c ESI ms [299.98-2499.98]



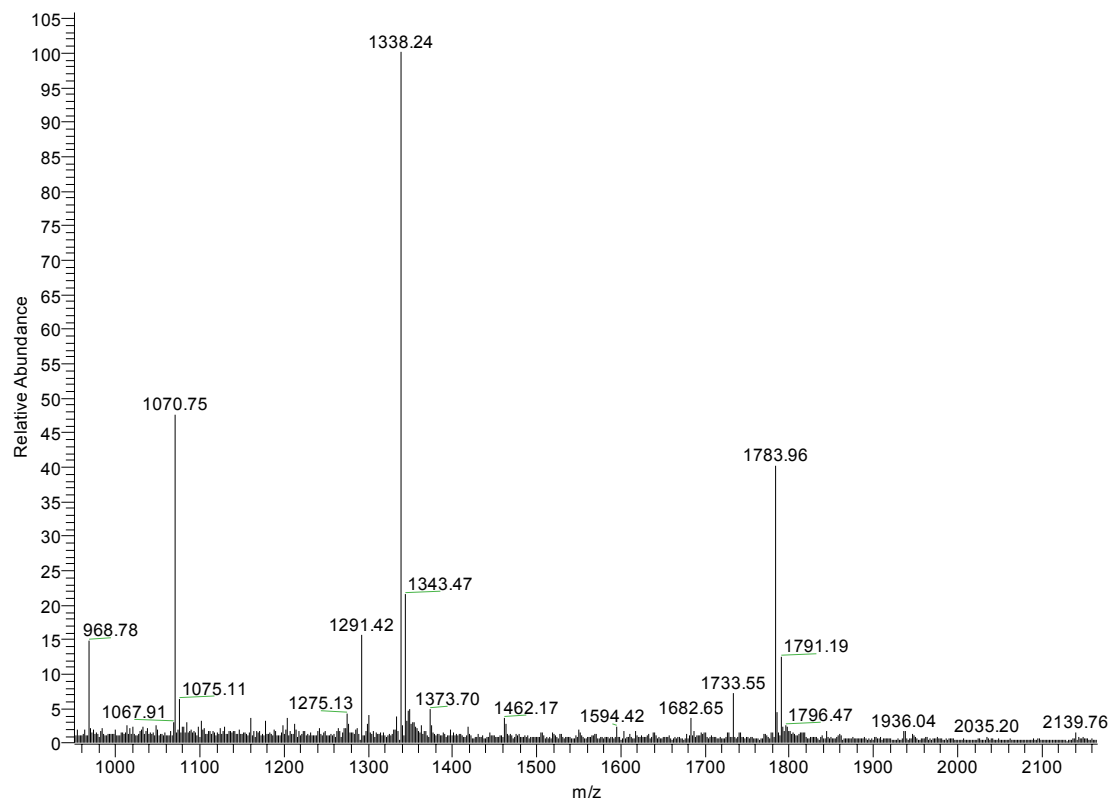
ESI mass spectrum of conjugate **5**: m/z 2209.8 ($M+3H$)³⁺, 1657.9 ($M+4H$)⁴⁺, 1326.4 ($M+5H$)⁵⁺, 1104.8 ($M+6H$)⁶⁺, and 947.6 ($M+7H$)⁷⁺. The observed molecular ions were consistent with the theoretical molecular weight of **5**, calcd ($M+H$)⁺ = 6629.2.

ri-ptd4-kd-n2pna #9-11 RT: 0.41-0.51 AV: 3 NL: 4.07E5
T: + c ESI ms [299.96-2500.02]



ESI mass spectrum of conjugate **6**: m/z 1784.0 ($M+3H$)³⁺, 1338.2 ($M+4H$)⁴⁺, 1070.8 ($M+5H$)⁵⁺. The observed molecular ions were consistent with the theoretical molecular weight of **6**, calcd ($M+H$)⁺ = 5333.1.

k(tmr)ant#1-45 RT: 0.02-2.95 AV: 45 NL: 2.82E6
T: + c ESI ms [299.98-2499.98]



ESI mass spectrum of conjugate **7**: m/z 2197.3 ($M+3H$)³⁺, 1648.4 ($M+4H$)⁴⁺, 1319.4 ($M+5H$)⁵⁺, 1099.1 ($M+6H$)⁶⁺, 942.2 ($M+7H$)⁷⁺, 824.6 ($M+8H$)⁸⁺, 733.3 ($M+9H$)⁹⁺. The observed molecular ions were consistent with the molecular weight of **7**, calcd ($M+H$)⁺ = 6593.5.

riptd4-antpna #1 RT: 0.01 AV: 1 NL: 5.97E5
T: + c ESI ms [299.98-2499.98]

