Supporting Information for:

Native-like RNA tertiary structures using a sequence-encoded cleavage agent and refinement by discrete molecular dynamics

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Supporting Figure 1. **SHAPE reactivity profiles for the M4 mutant construct in the presence and absence of MPE.** SHAPE profiles for the M4 RNA in the presence and absence of MPE are shown in solid and open symbols, respectively. The site of the bulged A nucleotide, introduced as part of the MPE binding site, is labeled.

Supporting Figure 2. **Site-directed MPE cleavage.** MPE cleavage data are illustrated for the native sequence tRNA (open bars) and for the M4 mutant that binds MPE (closed bars). The MPE insertion site in the M4 construct is emphasized with a triangle. Net MPE cleavage is calculated by subtracting cleavage intensity for the native sequence from the M4 mutant (see Figure 3 in the main text).

Supporting Dataset S1. A tab-delimited text file reporting the MPE cleavage data shown in Figure 3.

Supporting Figure 1

Supporting Figure 2
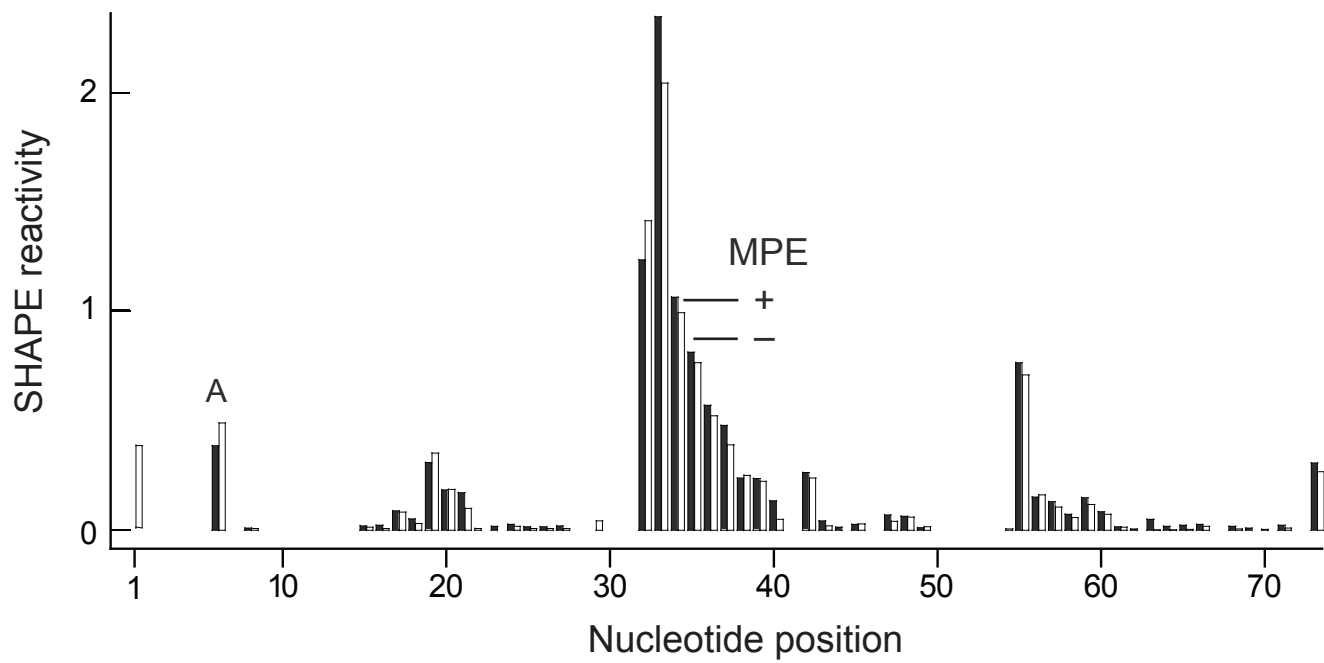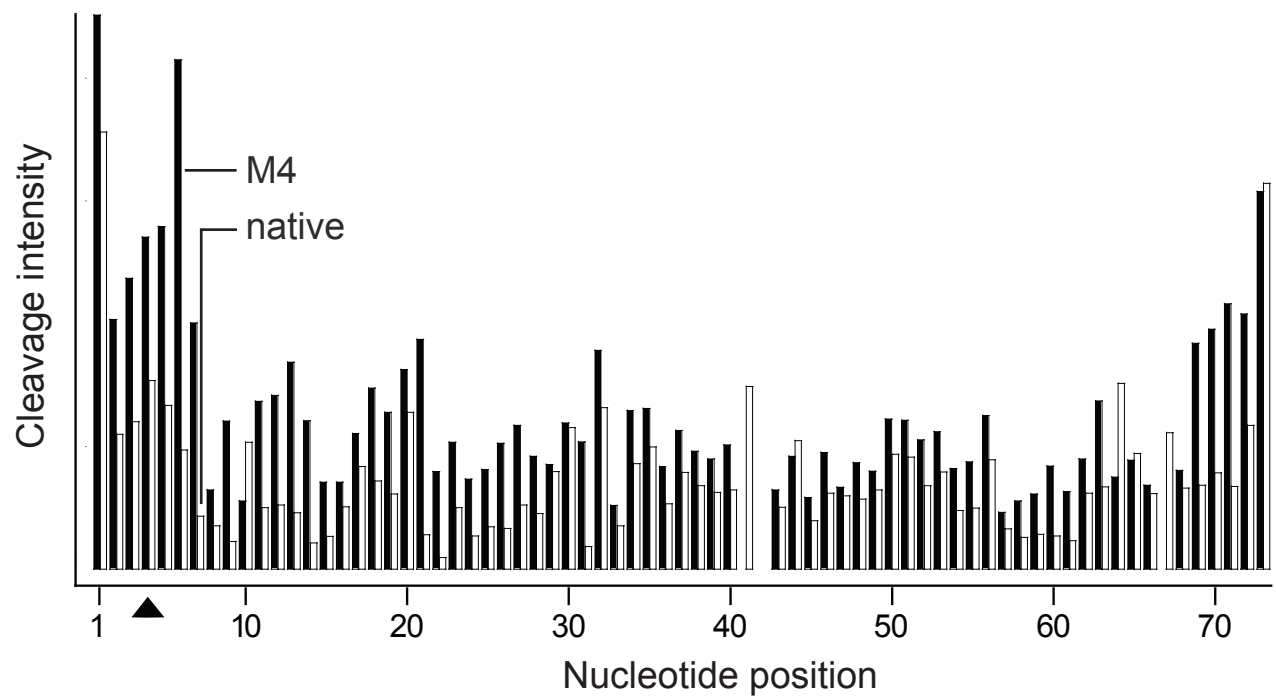
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                 I/<I>
sequence  position  M4    M49   M67

G     1      1.79 3.39 1.32
C     2      1.75 2.81 1.36
C     3      2.18 2.18 2.86
G     4      2.18 0.83 0
U     5      2.73 2.08 1.26
G     6      5.95 1.74 2.29
A     7      2.94 2.3  1.83
U     8      0.55 0.52 0.94
A     9      1.83 0.76 0.9
G     10     0    0    0
U     11     1.62 1.26 2.92
U     12     1.67 1.42 1.69
U     13     2.29 1.08 2.42
A     14     1.87 1.3  1.31
A     15     0.83 0.58 0.46
U     16     0.37 0.44 0.37
G     17     0.5  0.72 0.2
G     18     1.42 1.61 0.81
U     19     1.25 1.72 0.62
C     20     0.65 1.63 0.08
A     21     2.98 1.96 1.59
G     22     1.31 1.73 0.84
A     23     0.99 1.8  0.66
A     24     0.87 0.89 0.62
U     25     0.87 0.61 0.76
G     26     1.3  0.79 1.06
G     27     1.21 0.81 0.9
G     28     0.87 0.47 0.9
C     29     0.11 0.22 0.2
G     30     0.07 0    0
C     31     1.6  0.84 0.98
U     32     0.87 0    0.37
U     33     0.31 0.05 0.16
G     34     0.8  0.11 0.53
U     35     0.59 0.29 0.41
C     36     0.57 0.21 0.51
G     37     0.64 0.12 0.68
C     38     0.53 0.32 0.58
G     39     0.51 0.08 0.3
U     40     0.68 0.1  0.27
G     41     0    0    0.19
C     42     0    0    0
C     43     0.27 0.49 0
A     44     0    0.38 0.22
G     45     0.36 0.2  0.65
A     46     0.62 0.91 0.82
U     47     0.13 1.16 0.47
C     48     0.56 0.48 0.83
G     49     0.28 0.96 1.8
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G	50	0.54	1.53	2.49
G	51	0.57	2.61	1.17
G	52	0.7	2.33	0.79
U	53	0.61	0	0.62
U	54	0.64	5.8	0.37
C	55	0.7	1.74	0.42
A	56	0.67	1.09	0.49
A	57	0.25	0.45	0.29
U	58	0.55	0.72	0.36
U	59	0.61	0.8	0.5
C	60	1.07	1.11	0.61
C	61	0.74	1.68	0.45
C	62	0.53	0	0.28
C	63	1.31	0.77	0.48
G	64	0	0.94	1
U	65	0	1.35	1.83
C	66	0.12	1.09	2.58
G	67	0	0.94	2.09
C	68	0.27	0.56	6.1
G	69	2.16	0.21	3.84
G	70	2.18	0.4	3.28
C	71	2.79	0.43	1.62
G	72	1.7	0.62	0.39
C	73	0	1.42	0
A	74			
A	75			