Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting information

Screening of efficient polymers for siRNA delivery in a library of hydrophobically modified polyethyleneimines

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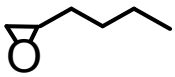
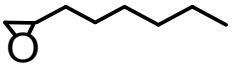
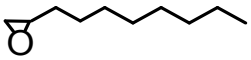
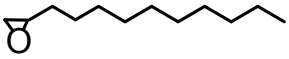
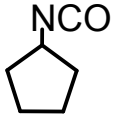
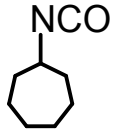
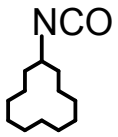
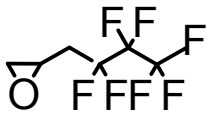
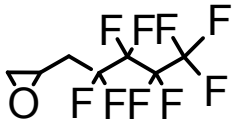
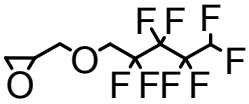
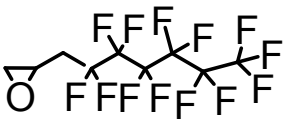
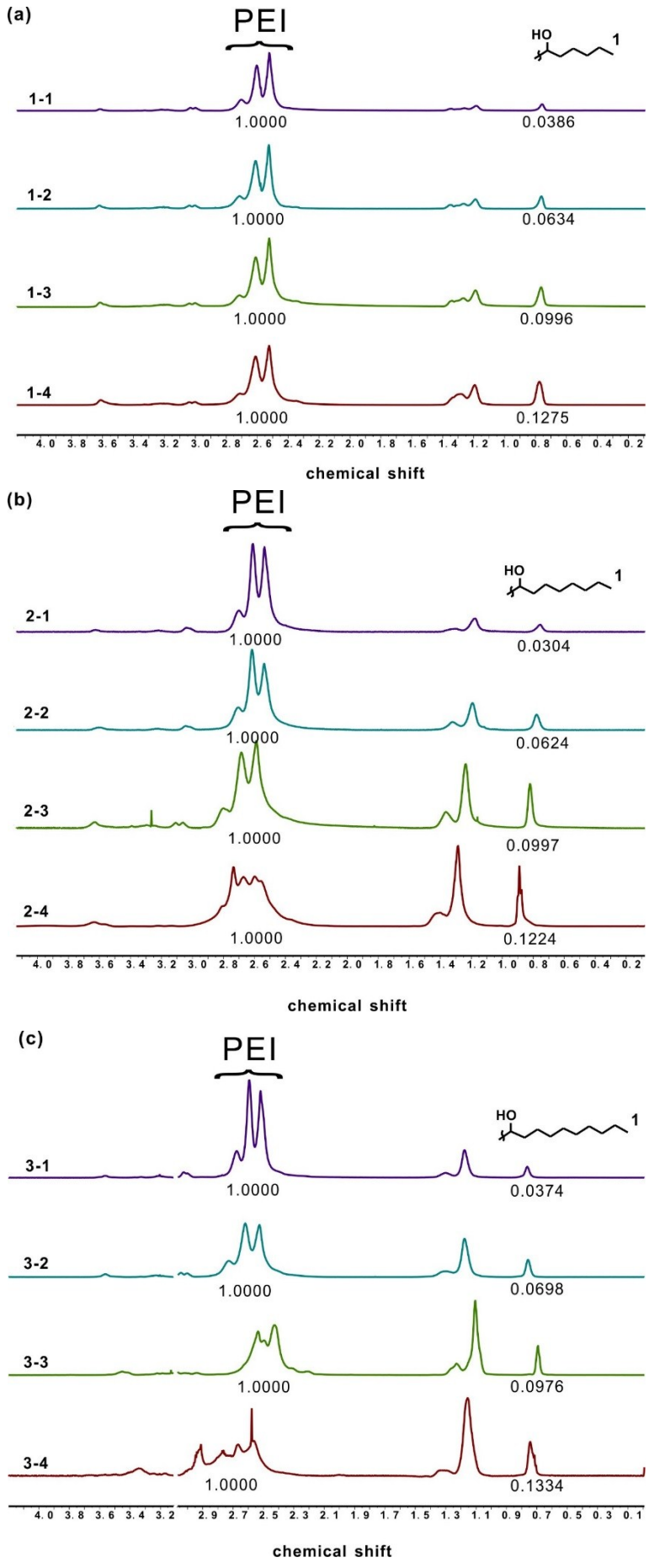
Table S1. Feeding ratios of the ligand and bPEI during synthesis and characterizations of the synthesized materials.

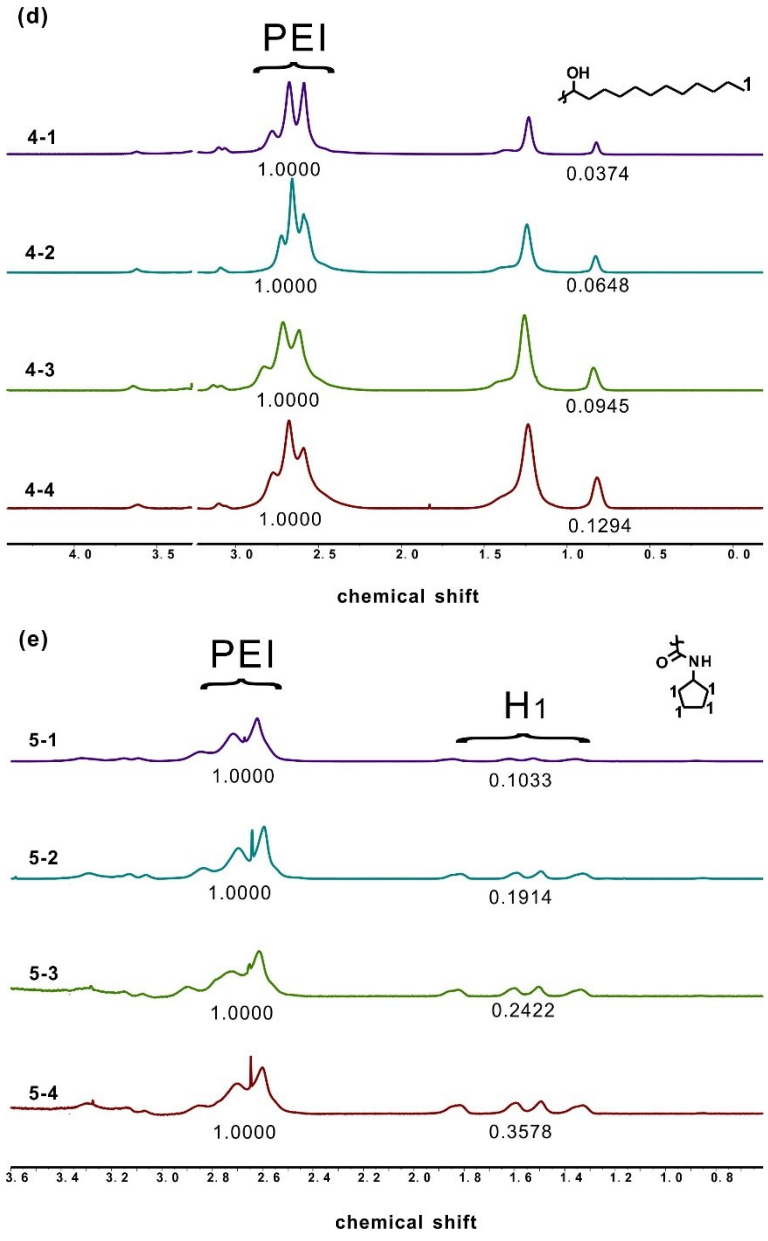
Ligand	Chemical Structure	Feeding molar ratio [a]	n [b]	Polymer
1		36	30	1-1
		72	49	1-2
		108	77	1-3
		143	99	1-4
2		72	24	2-1
		143	48	2-2
		172	77	2-3
		286	95	2-4
3		36	29	3-1
		72	54	3-2
		86	76	3-3
		108	103	3-4
4		36	29	4-1
		72	50	4-2
		143	73	4-3
		172	100	4-4
5		36	30	5-1
		72	56	5-2
		100	70	5-3
		125	104	5-4
6		36	25	6-1
		72	57	6-2
		100	79	6-3
		125	108	6-4
7		25	23	7-1
		50	42	7-2
		75	73	7-3
		100	100	7-4

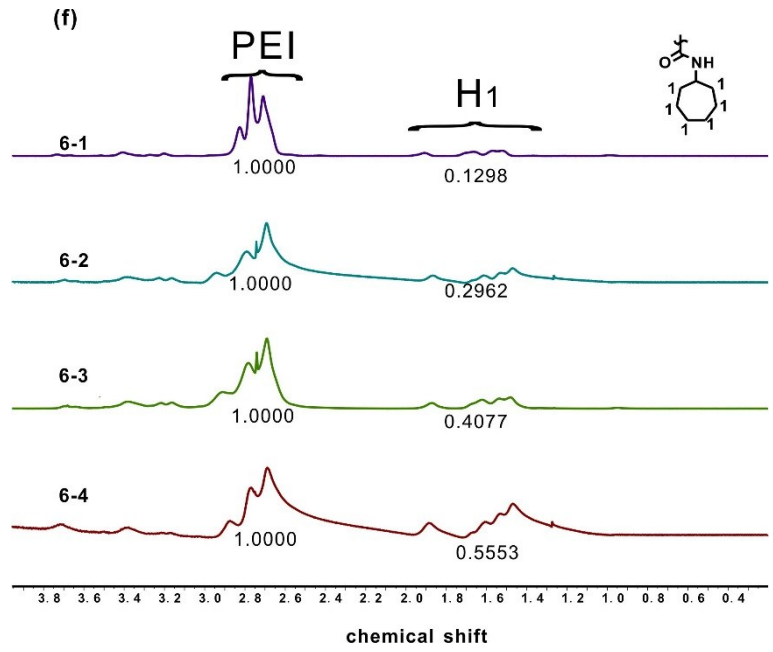
8		25	23	8-1
		50	49	8-2
		75	75	8-3
		100	100	8-4
9		72	27	9-1
		108	52	9-2
		143	68	9-3
		215	98	9-4
10		36	28	10-1
		72	54	10-2
		108	76	10-3
		143	102	10-4
11		25	21	11-1
		50	46	11-2
		72	71	11-3
		108	105	11-4
12		36	30	12-1
		72	51	12-2
		108	76	12-3
		143	112	12-4

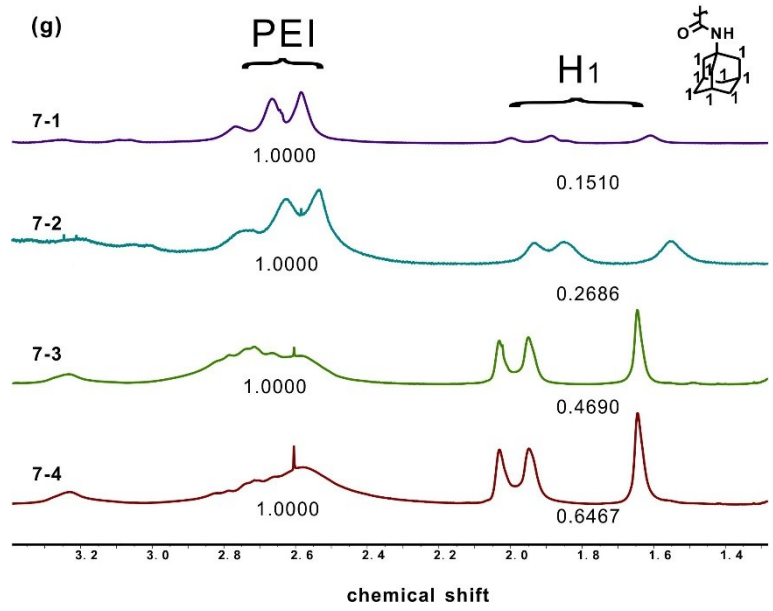
[a] Feeding ratio is the molar ratio of the hydrophobic ligands to bPEI during synthesis.

[b] n is the average number of modified ligands on each bPEI calculated by ^{1}H NMR or elemental analysis.


(a)
PEI
HO
1
1-1
1.0000
0.0386
1-2
1.0000
0.0634
1-3
1.0000
0.0996
1-4
1.0000
0.1275
4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2
chemical shift
(b)
PEI
HO
1
2-1
1.0000
0.0304
2-2
1.0000
0.0624
2-3
1.0000
0.0997
2-4
1.0000
0.1224
4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2
chemical shift
(c)
PEI
HO
1
3-1
1.0000
0.0374
3-2
1.0000
0.0698
3-3
1.0000
0.0976
3-4
1.0000
0.1334
4.0 3.8 3.6 3.4 3.2
2.9 2.7 2.5 2.3 2.1 1.9 1.7 1.5 1.3 1.1 0.9 0.7 0.5 0.3 0.1
chemical shift


(d)
PEI
OH
1
4-1
1.0000
0.0374
4-2
1.0000
0.0648
4-3
1.0000
0.0945
4-4
1.0000
0.1294
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
chemical shift
(e)
PEI
H1
NH
1
1
1
5-1
1.0000
0.1033
5-2
1.0000
0.1914
5-3
1.0000
0.2422
5-4
1.0000
0.3578
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
chemical shift


(f)
PEI
H1
NH
6-1
1.0000
0.1298
6-2
1.0000
0.2962
6-3
1.0000
0.4077
6-4
1.0000
0.5553
3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4
chemical shift


(g)
PEI
H1
NH
7-1
1.0000
0.1510
7-2
1.0000
0.2686
7-3
1.0000
0.4690
7-4
1.0000
0.6467
3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4
chemical shift

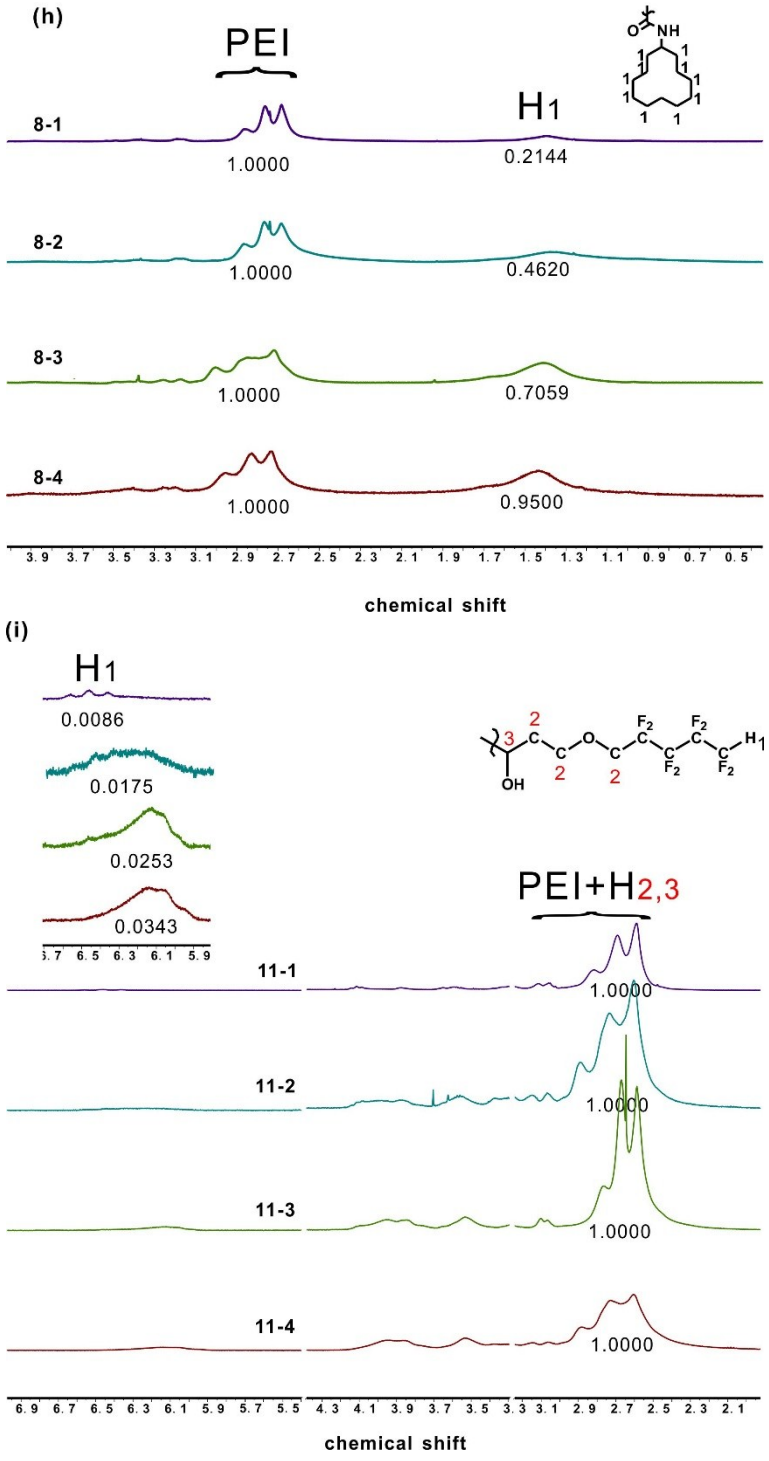
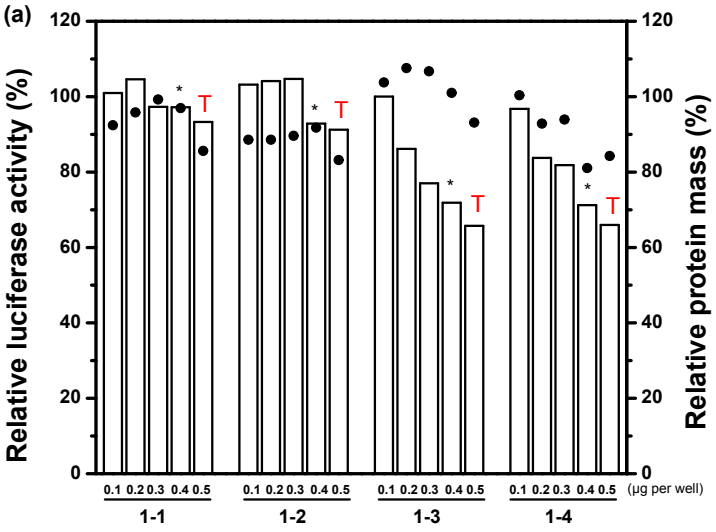
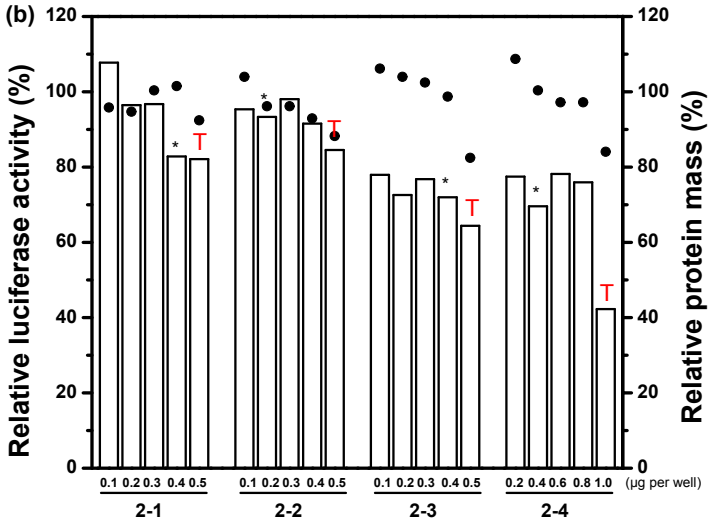
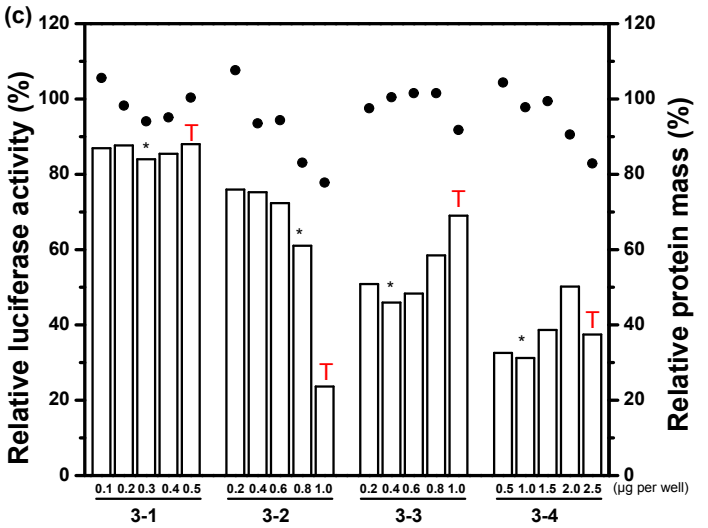
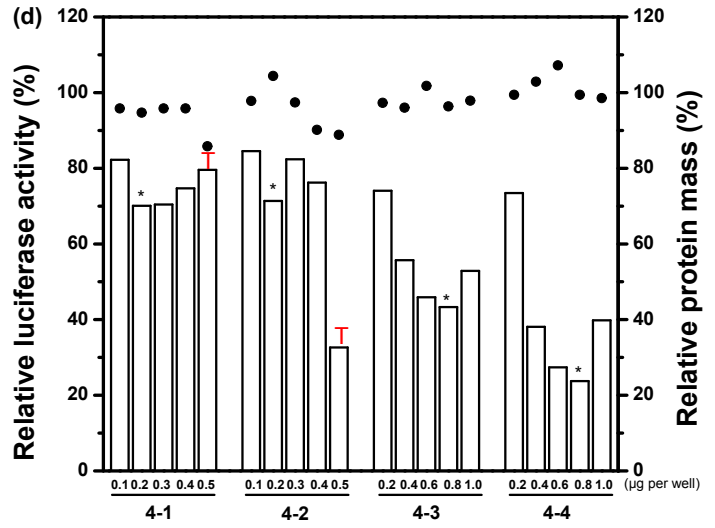


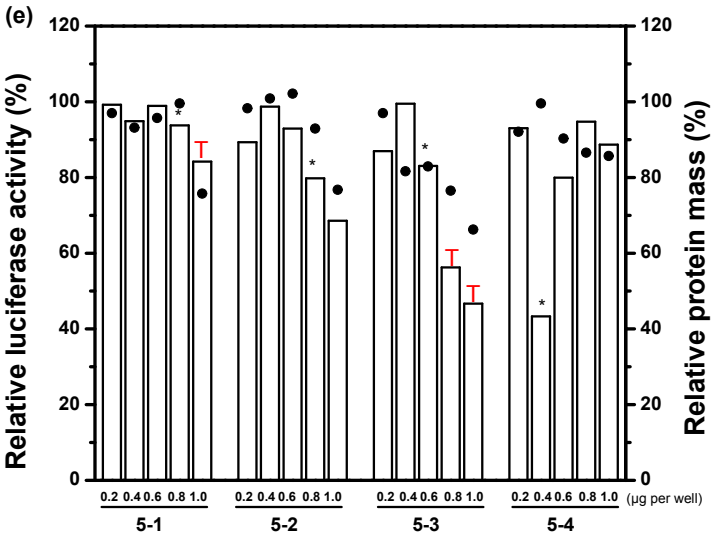
Fig. S1 ^{1}H-NMR spectra of the synthesized materials in D_2O (a - i).

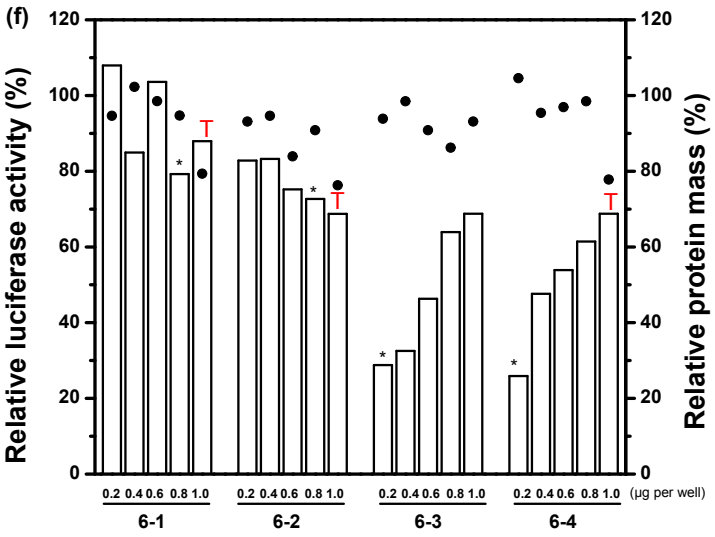

(a)
Relative luciferase activity (%)
Relative protein mass (%)
0 20 40 60 80 100 120
0.1 0.2 0.3 0.4 0.5
1-1
0.1 0.2 0.3 0.4 0.5
1-2
0.1 0.2 0.3 0.4 0.5
1-3
0.1 0.2 0.3 0.4 0.5
1-4
(μg per well)

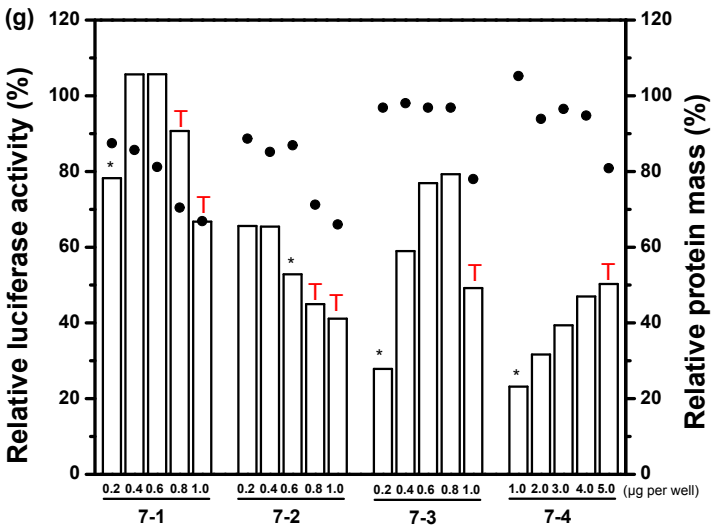

(b)
Relative luciferase activity (%)
Relative protein mass (%)
0 20 40 60 80 100 120
0.1 0.2 0.3 0.4 0.5
2-1
0.1 0.2 0.3 0.4 0.5
2-2
0.1 0.2 0.3 0.4 0.5
2-3
0.2 0.4 0.6 0.8 1.0
2-4
(μg per well)

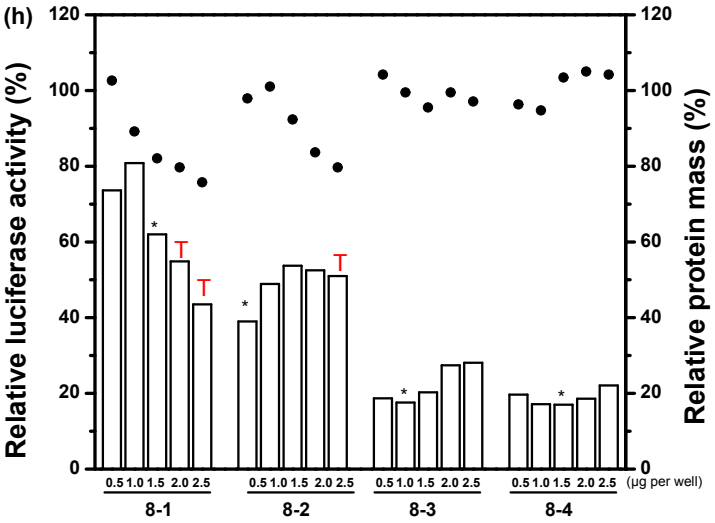

(c)
Relative luciferase activity (%)
Relative protein mass (%)
0 20 40 60 80 100 120
0.1 0.2 0.3 0.4 0.5
3-1
0.2 0.4 0.6 0.8 1.0
3-2
0.2 0.4 0.6 0.8 1.0
3-3
0.5 1.0 1.5 2.0 2.5
3-4
(μg per well)

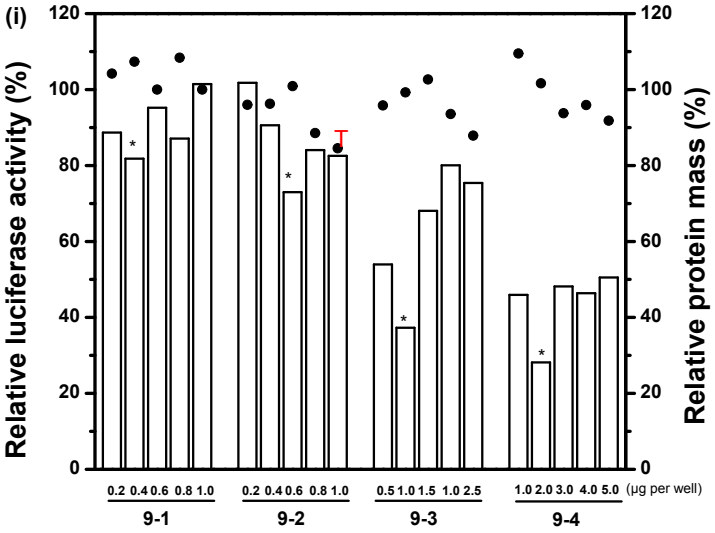

(d)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.1 0.2 0.3 0.4 0.5
0.1 0.2 0.3 0.4 0.5
0.2 0.4 0.6 0.8 1.0
0.2 0.4 0.6 0.8 1.0
(μg per well)
4-1
4-2
4-3
4-4

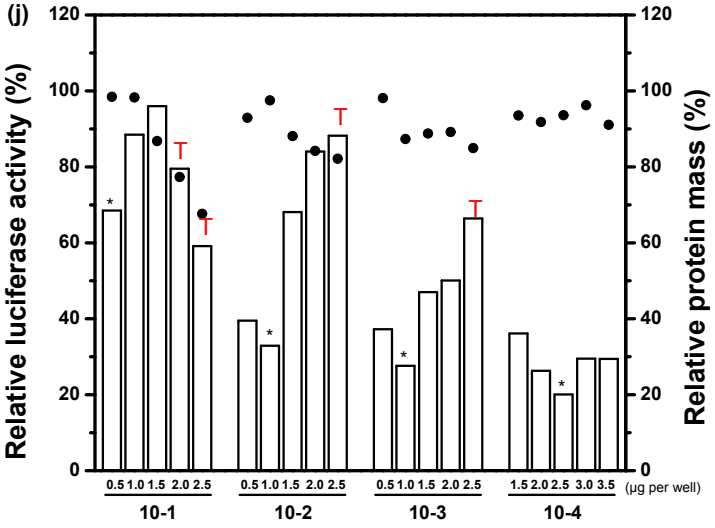

(e)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.2 0.4 0.6 0.8 1.0
0.2 0.4 0.6 0.8 1.0
0.2 0.4 0.6 0.8 1.0
0.2 0.4 0.6 0.8 1.0
(μg per well)
5-1
5-2
5-3
5-4

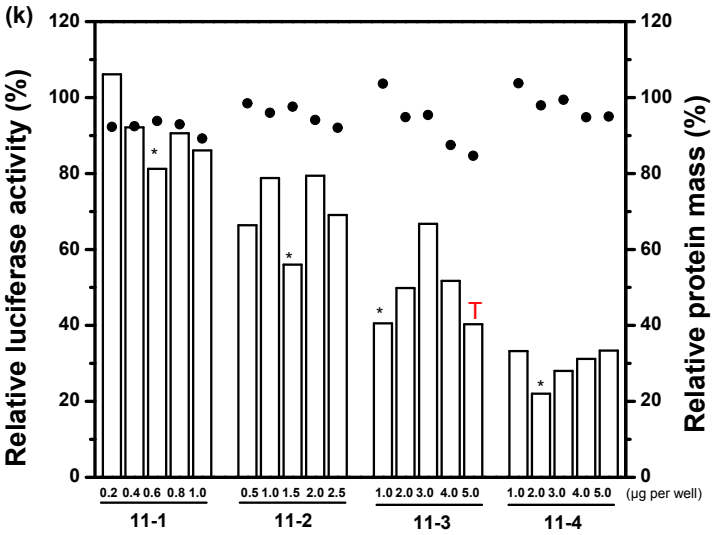

(f)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.2 0.4 0.6 0.8 1.0
(μg per well)
6-1
6-2
6-3
6-4


(g)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.2 0.4 0.6 0.8 1.0
1.0 2.0 3.0 4.0 5.0
(μg per well)
7-1
7-2
7-3
7-4


(h)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.5 1.0 1.5 2.0 2.5
0.5 1.0 1.5 2.0 2.5
0.5 1.0 1.5 2.0 2.5
0.5 1.0 1.5 2.0 2.5
(μg per well)
8-1
8-2
8-3
8-4


(i)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.2 0.4 0.6 0.8 1.0
0.2 0.4 0.6 0.8 1.0
0.5 1.0 1.5 1.0 2.5
1.0 2.0 3.0 4.0 5.0
(μg per well)
9-1
9-2
9-3
9-4


(j)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.5 1.0 1.5 2.0 2.5
0.5 1.0 1.5 2.0 2.5
0.5 1.0 1.5 2.0 2.5
1.5 2.0 2.5 3.0 3.5
(μg per well)
10-1
10-2
10-3
10-4


(k)
Relative luciferase activity (%)
Relative protein mass (%)
0
20
40
60
80
100
120
0.2 0.4 0.6 0.8 1.0
0.5 1.0 1.5 2.0 2.5
1.0 2.0 3.0 4.0 5.0
1.0 2.0 3.0 4.0 5.0
(μg per well)
11-1
11-2
11-3
11-4

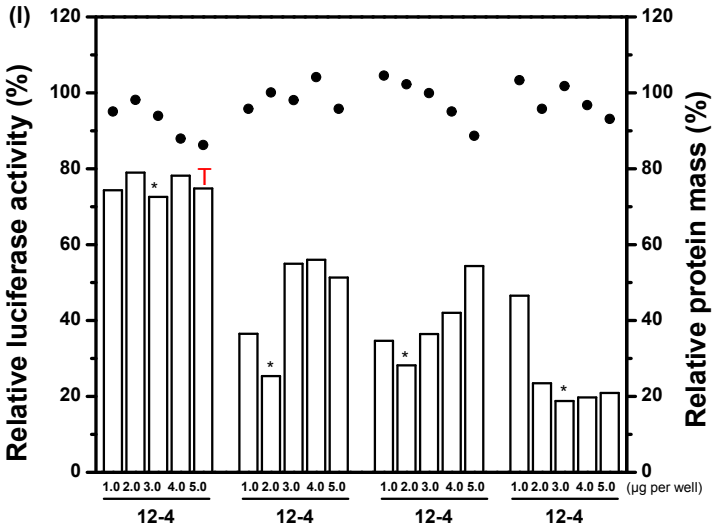


Fig. S2 Gene silencing efficacies of modified PEIs on HeLa-Luc cells for 24 h (a-l). The siRNA dose was 10 nM (0.133 μg/mL). "*" Represents the optimal weight for each material in gene silencing. "T" indicates toxicity on the transfected cells.

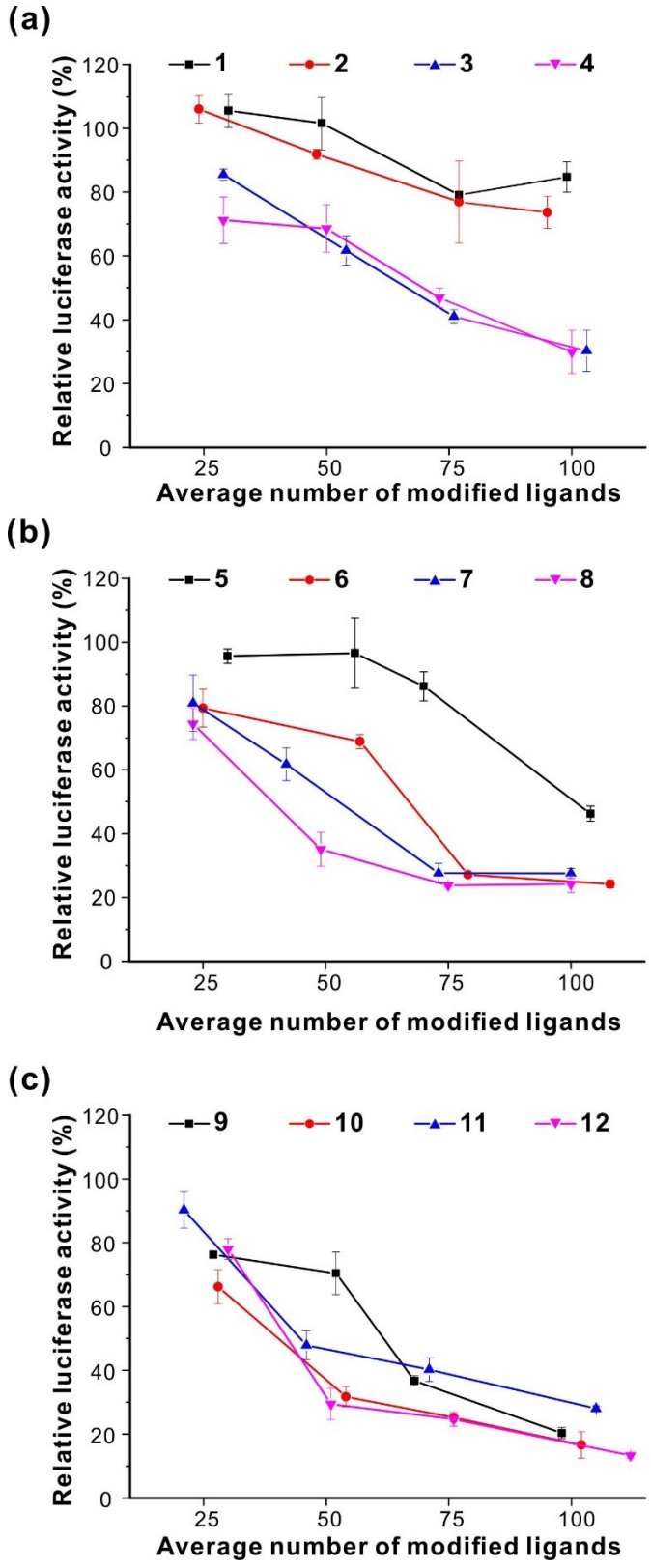


Fig. S3 Gene silencing efficacies of alkane- (a), cycloalkane- (b) and fluoroalkane- (c) modified bPEI on HeLa-Luc cells. The optimal transfection condition for each material was chosen according to the screening results in Fig. S2. The siRNA dose was 10 nM (0.133 μg/mL).

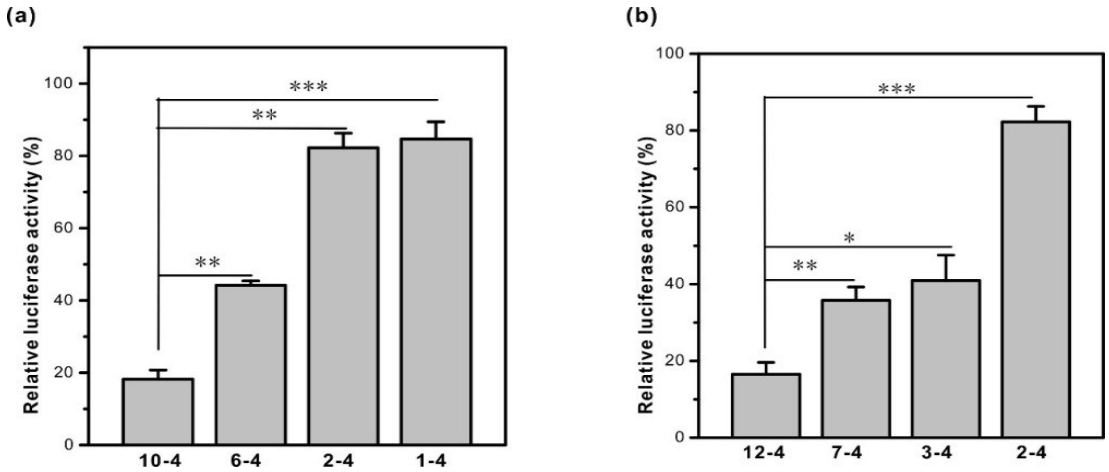


Fig. S4 Gene silencing efficacies of 10-4 (a) and 12-4(b) with their aliphatic analogues in MDA-MB231-Luc cells. The siRNA dose was 10 nM (0.133 μg/mL). *$p < 0.05$, **$p < 0.01$, and ***$p < 0.001$ analyzed by Student's t-test.

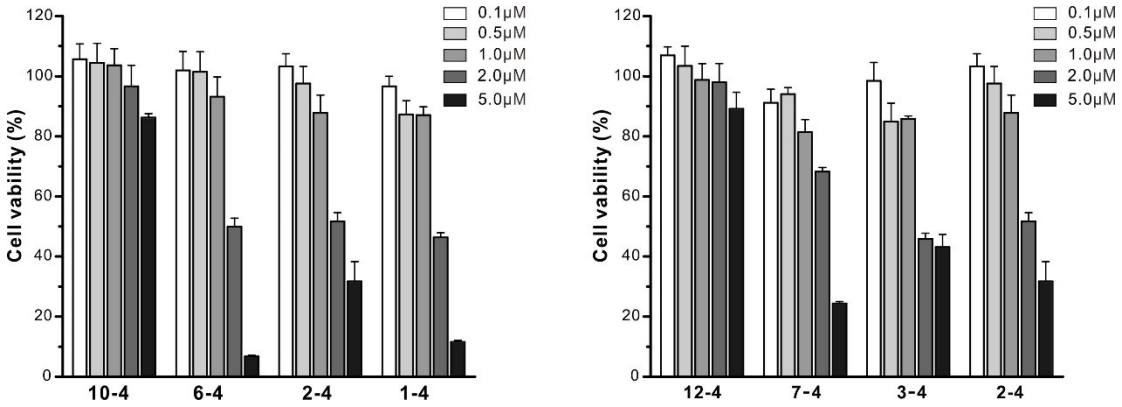


Fig. S5 Comparison of the cell viabilities of 10-4 and 12-4 with their respective alkylated and cycloalkylated analogues in HeLa-Luc cells.