

Supplementary data

Compound Name	Affinity (kcal/mol)
F3408-0076	-14.6
F0382-0033	-13.1
F1430-0130	-12.9
F0808-0153	-12.5
F0808-0131	-12.5
F0808-0151	-12.4
F0808-1181	-12.4
F0808-1175	-12.4
F1269-0120	-12.3
F0808-0152	-12.2
F3408-0031	-12.2
F1430-0134	-12
F1430-0138	-12

Table S1 13 compounds were chosen based on binding energy <-12.0 kcal/mol.

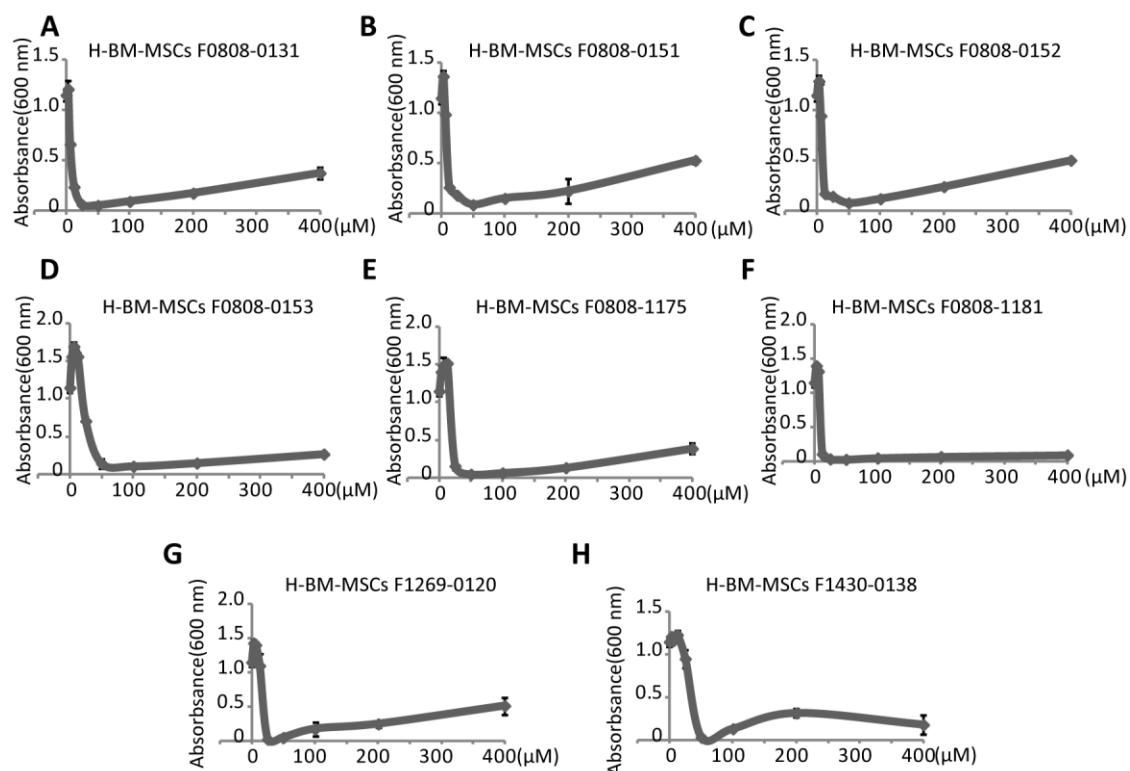


Figure S1 The toxic effects of compounds on H –BM-MSCs.

A tetrazolium salt (WST-8) assay was carried out to study the toxic effects of compounds on H –BM-MSCs.

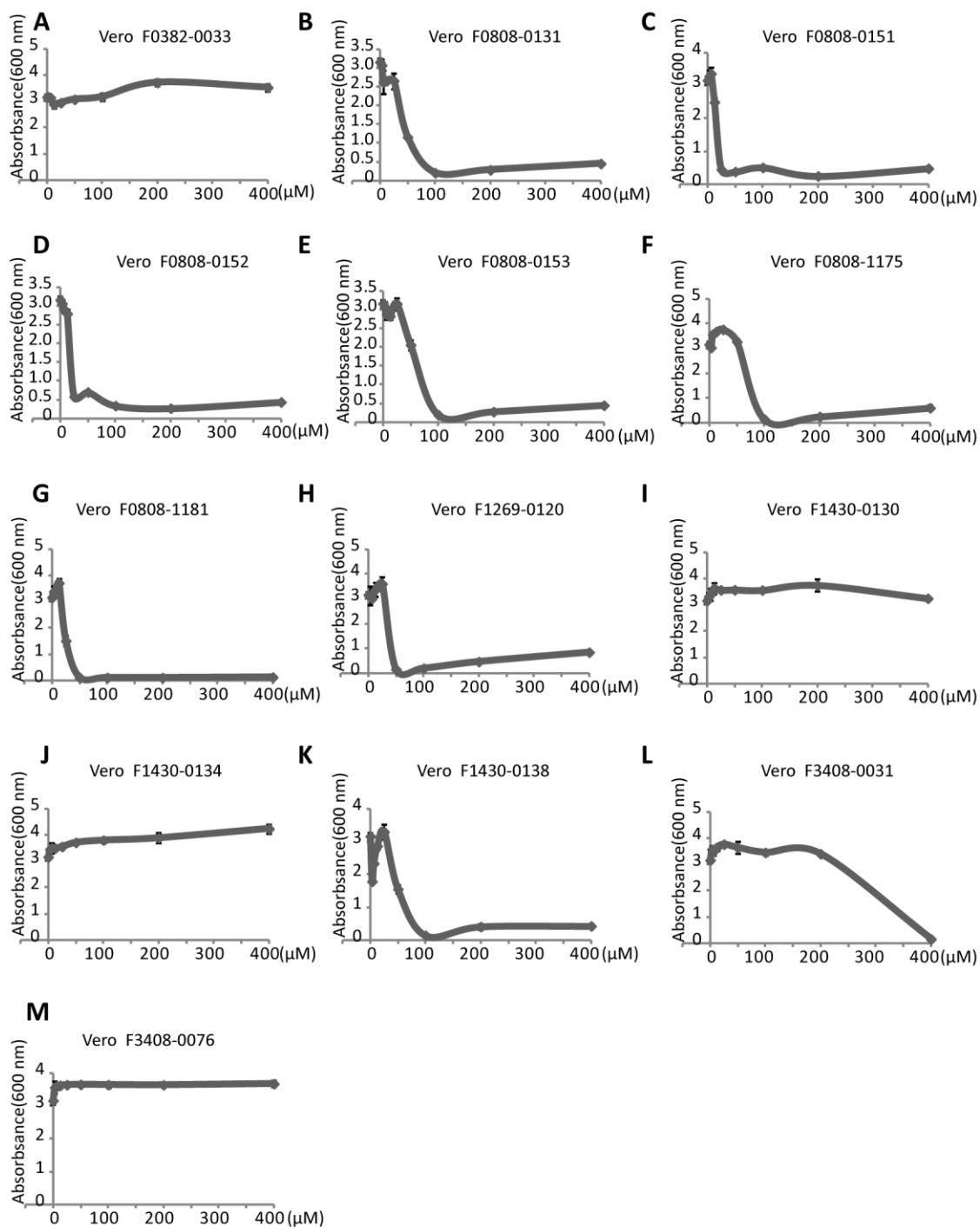


Figure S2 The toxic effects of compounds on Vero cells.

A tetrazolium salt (WST-8) assay was carried out to study the toxic effects of compounds on Vero cells.

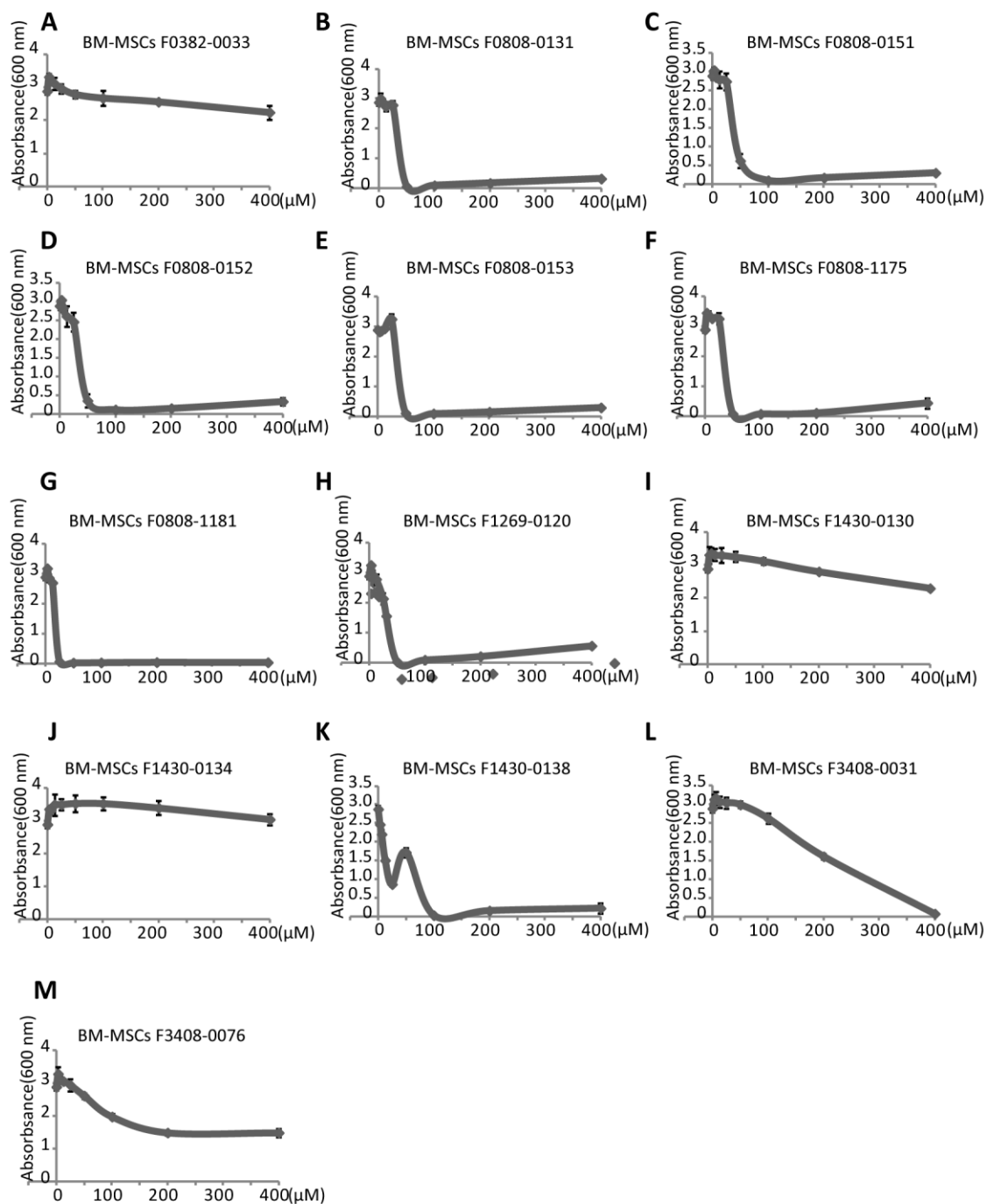


Figure S3 The toxic effects of compounds on mouse BM-MSCs.

A tetrazolium salt (WST-8) assay was carried out to study the toxic effects of compounds on mouse BM-MSCs.