Supporting Information for:

3D Small molecule microarray with enhanced sensitivity and immobilization capacity monitored by surface plasmon resonance imaging

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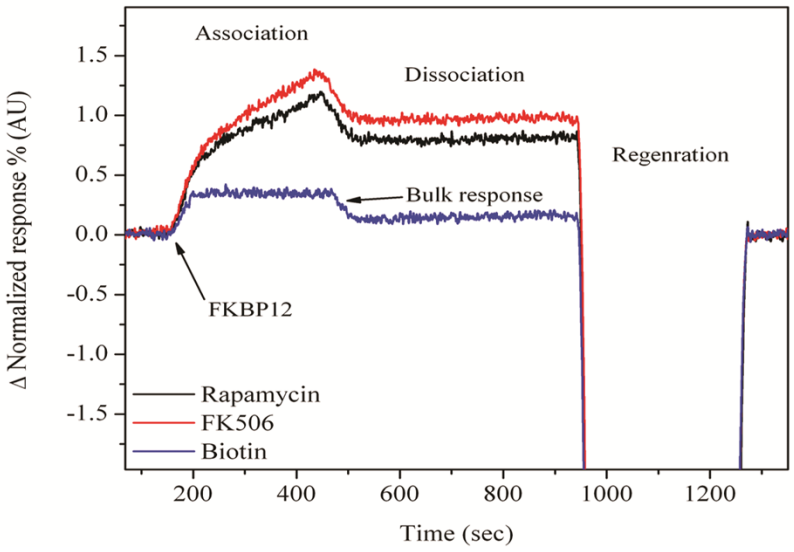
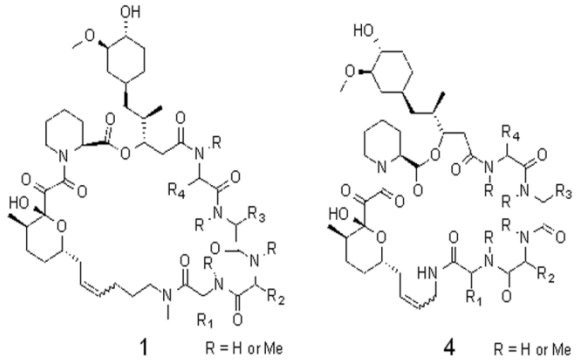


Figure S-1: SPR imaging graph showing a complete cycle of FKBP12 protein (100nM) including association, dissociation and regeneration step. Data here is without substraction of negative control.



	Building blocks			
Compound	R_1	R_2	R_3	R_4
1A	Sar	Phe	Val	Ala
1B	Leu	D-Phe	Pro	N-Me-Val
1C	D-Val	N-Me-Ile	Gly	N-Me-Ala
4A	Sar	Phe	Val	Ala
4B	Leu	D-Phe	Pro	N-Me-Val
4C	D-Val	N-Me-Ile	Gly	N-Me-Ala

Figure S-2: Structures of six rapafucin compounds

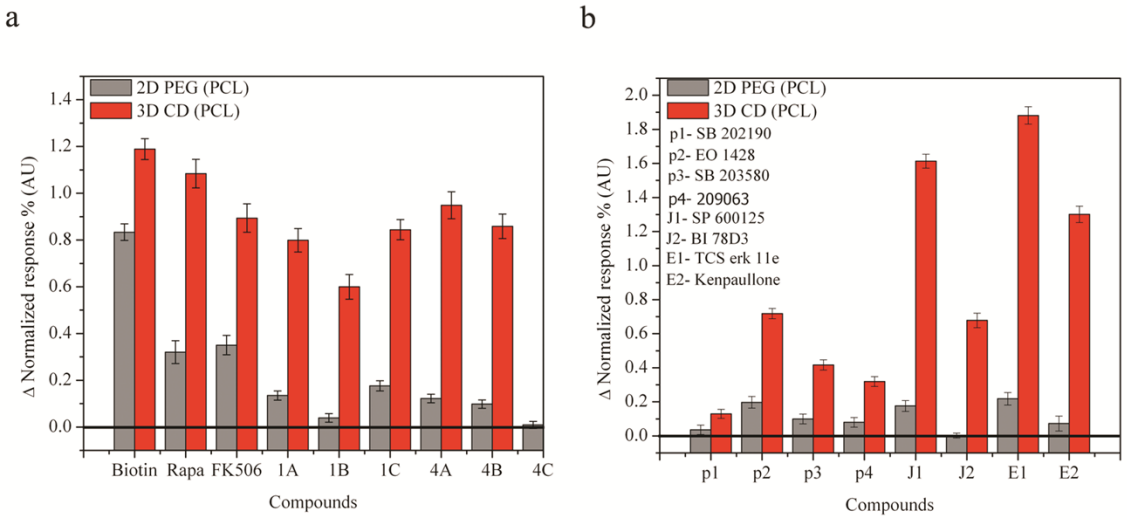


Figure S-3: Comparison of all compounds interaction on 2D and 3D photo-cross-linked surface by SPRi (a) response with standard deviation from 3 different slides of FKBP binding ligands and (b) all kinase inhibitors used in this study.

Surface	C%	O%	S%	N%	F%
2D PEG (PCL)	61.898	29.325	3.087	2.702	2.989
3D CD (PCL)	60.008	24.753	4.523	6.717	3.999

Table S-1: Table representing atomic concentration characterized by X-ray photoelectron spectroscopy

Compounds	Ka(1/Ms)	Kd(1/s)	KA(1/M)	KD(M)
Rapamycin	6.65×10^{4}	1.16×10^{-3}	5.73×10^{7}	1.75×10^{-8}
FK506	7.59×10^{4}	2.02×10^{-3}	3.77×10^{7}	2.66×10^{-8}
1A	1.25×10^{4}	0.024	5.2×10^{5}	1.92×10^{-6}
1B	7.52×10^{3}	0.0291	2.59×10^{5}	3.87×10^{-6}
1C	8.16×10^{3}	0.0177	4.6×10^{5}	2.17×10^{-6}
4A	1.87×10^{3}	0.0147	1.27×10^{5}	7.85×10^{-6}
4B	6.4×10^{3}	0.0149	4.31×10^{5}	2.32×10^{-6}
4C	-	-	-	-

Table S-2: Table showing kinetic parameters of FKBP12 binding ligands produced from 2D PCL slides.

Compounds	Ka(1/Ms)	Kd(1/s)	KA(1/M)	KD(M)
Rapamycin	6.09×10^{4}	2.22×10^{-4}	2.74×10^{8}	3.65×10^{-9}
FK506	5.21×10^{4}	3.87×10^{-4}	1.35×10^{8}	7.42×10^{-9}
1A	4.95×10^{4}	2.72×10^{-3}	1.82×10^{7}	5.51×10^{-8}
1B	6.93×10^{4}	4.32×10^{-3}	1.61×10^{7}	6.23×10^{-8}
1C	5.87×10^{4}	4.71×10^{-3}	1.25×10^{7}	8.03×10^{-8}
4A	5.41×10^{4}	4.95×10^{-3}	1.09×10^{7}	9.16×10^{-8}
4B	$3.54e\times10^{4}$	8.49×10^{-3}	4.17×10^{6}	2.4×10^{-7}
4C	5.4×10^{4}	5.1×10^{-3}	1.06×10^{7}	9.45×10^{-8}

Table S-3: Table showing kinetic parameters of FKBP12 binding ligands produced from 3D PCL slides.

Compounds	Ka	Kd	KA	KD
SB 239063	6.65×10^{3}	1.76×10^{-4}	3.78×10^{7}	2.65×10^{-8}
SB 202190	7.49×10^{3}	2.41×10^{-4}	3.1×10^{7}	3.22×10^{-8}
SB 203580	2.9×10^{3}	4.23×10^{-4}	6.85×10^{6}	1.46×10^{-7}
EO 1428	2.9×10^{3}	2.3×10^{-4}	1.26×10^{7}	7.92×10^{-8}
SP600125	6.96×10^{3}	8.18×10^{-4}	8.51×10^{6}	1.18×10^{-7}
BI 78D3	5.15×10^{3}	5.49×10^{-4}	9.37×10^{6}	1.07×10^{-7}
TCS erk 11e	1.4×10^{4}	1.01×10^{-3}	1.38×10^{7}	7.23×10^{-8}
Kenpaullone	9.94×10^{3}	7.35×10^{-4}	1.35×10^{7}	7.4×10^{-8}

Table S-4: Table showing kinetic parameters of kinase inhibitors against their relative targets ligands produced from 2D PCL slides.