Supporting Information

Demonstration of Arithmetic Calculations by DNA Tile-Based Algorithmic Self-Assembly

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Figure S1. Schematic of the binding domains of rule building blocks (*i.e.*, propagator, connector, and solution tiles) for addition and subtraction.

Table S1. Sticky-end binding domains with specific DNA base sequences in propagator, connector, and solution tiles for addition operation.

Table S2. Sticky-end binding domains with specific DNA base sequences in propagator, connector, and solution tiles for subtraction operation.

Figure S2. A sequence diagram with cartoon representation of the double-crossover (DX) tiles for the propagators used in the addition and subtraction operations.

Table S3. Sequence information of propagators for addition and subtraction.

Figure S3. A sequence diagram with cartoon representation of the connectors for addition.

Table S4. Sequence information of connectors for addition.

Figure S4. A sequence diagram with cartoon representation of the connectors for subtraction.

Table S5. Sequence information of connectors for subtraction.

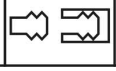
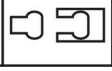
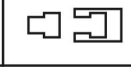
Figure S5. A sequence diagram with cartoon representation of the solutions for addition.

Table S6. Sequence information of solutions for addition.

Figure S6. A sequence diagram with cartoon representation of the solutions for subtraction.

Table S7. Sequence information of solutions for subtraction.

a)

Definition	Dummy (d)	Input (I_L or I_R)	$Carry_{Out}/2$ $\pm(C_O/2)$	Input+($Carry_{In}/2$) ([I_L or I_R]$\pm C_I/2$
Diagram				

b)

d			d′
0			0′
1			1′
0_c			0_c′
$½_c$			$½_c$′
$(0+0_c)$			$(0+0_c)'$
$(1+0_c)$			$(1+0_c)'$
$(0+½_c)$			$(0+½_c)'$
$(1+½_c)$			$(1+½_c)'$

c)

d			d′
0			0′
1			1′
$0_{c,l}$			$0_{c,l}$′
$-½_{c,l}$			$-½_{c,l}$′
$(0+0_{c,l})$			$(0+0_{c,l})'$
$(1+0_{c,l})$			$(1+0_{c,l})'$
$(0-½_{c,l})$			$(0-½_{c,l})'$
$(1-½_{c,l})$			$(1-½_{c,l})'$
$0_{c,r}$			$0_{c,r}$′
$-½_{c,r}$			$-½_{c,r}$′
$(0+0_{c,r})$			$(0+0_{c,r})'$
$(1+0_{c,r})$			$(1+0_{c,r})'$
$(0-½_{c,r})$			$(0-½_{c,r})'$
$(1-½_{c,r})$			$(1-½_{c,r})'$

Figure S1. Schematic of the binding domains of rule building blocks (*i.e.*, propagator, connector, and solution tiles) for addition and subtraction. (a) Binding domains of Dummy, Input, $Carry_{Out}/2$, and Input + ($Carry_{In}/2$) with corresponding geometrical representations. We have considered four types (*i.e.*, Dummy, Input, $Carry_{Out}/2$, and Input + ($Carry_{In}/2$)) of binding domains to demonstrate arithmetic calculation. Geometrical representations of the binding domains are also shown. **(b)** Name and corresponding geometrical representation of the binding domains for addition with specific colour coding. Pairs (d-d**'**), (0-0**'** and 1-1**'**), (0_c-0_c**'** and $½_c$-$½_c$**'**), and [$(0+0_c)$-$(0+0_c)$**'**, $(1+0_c)$-$(1+0_c)$**'**, $(0+½_c)$-$(0+½_c)$**'**, and $(1+½_c)$-$(1+½_c)$**'**] belong to Dummy, Input, $Carry_{Out}/2$, and Input + ($Carry_{In}/2$) binding domains, respectively. Geometrical representation of unprimed and primed specific binding domains with identical colour coding (which were complementary to each other). **(c)** Name and corresponding geometrical representation of the binding domains for subtraction with specific colour coding. Binding domain pairs: (d-d**'**), (0-0**'** and 1-1**'**), ($0_{c,l}$-$0_{c,l}$**'** and $-½_{c,l}$- $-½_{c,l}$**'**), ($0_{c,r}$-$0_{c,r}$**'** and $-½_{c,r}$- $-½_{c,r}$**'**), [$(0+0_{c,l})$-$(0+0_{c,l})$**'**, $(1+0_{c,l})$-$(1+0_{c,l})$**'**, $(0-½_{c,l})$-$(0-½_{c,l})$**'**, and $(1-½_{c,l})$-$(1-½_{c,l})$**'**], and [$(0+0_{c,r})$-$(0+0_{c,r})$**'**, $(1+0_{c,r})$-$(1+0_{c,r})$**'**, $(0-½_{c,r})$-$(0-½_{c,r})$**'**, and $(1-½_{c,r})$-$(1-½_{c,r})$**'**] belong to Dummy, Input, $Carry_{Out}/2$ on left, $Carry_{Out}/2$ on right, Input + ($Carry_{In}/2$) on left, and Input + ($Carry_{In}/2$) on right, respectively

Sticky-end name	5′ to 3′	5′ to 3′	Sticky-end name
d	aactg	cagtt	d′
0	ctagt	actag	0′
1	agcat	atgct	1′
0_c	gcgta	tacgc	0_c′
$½_c$	agtcc	ggact	$½_c$′
$(0+0_c)$	tcgtc	gacga	$(0+0_c)$′
$(1+0_c)$	ctgag	ctcag	$(1+0_c)$′
$(0+½_c)$	gacga	tcgtc	$(0+½_c)$′
$(1+½_c)$	atcgg	ccgat	$(1+½_c)$′

Table S1. Sticky-end binding domains with specific DNA base sequences in propagator, connector, and solution tiles for addition operation. The complementary sticky end pairs are indicated by unprimed and primed symbols (e.g. d and d**′**).

Sticky-end name	5′ to 3′	5′ to 3′	Sticky-end name
d	aactg	cagtt	d′
0	ctagt	actag	0′
1	agcat	atgct	1′
$0_{c,l}$	gcgta	tacgc	$0_{c,l}$′
$-½_{c,l}$	agtcc	ggact	$-½_{c,l}$′
$(0+0_{c,l})$	tcgtc	gacga	$(0+0_{c,l})$′
$(1+0_{c,l})$	ctgag	ctcag	$(1+0_{c,l})$′
$(0-½_{c,l})$	gacga	tcgtc	$(0-½_{c,l})$′
$(1-½_{c,l})$	atcgg	ccgat	$(1-½_{c,l})$′
$0_{c,r}$	tgcca	tggca	$0_{c,r}$′
$-½_{c,r}$	cgtac	gtacg	$-½_{c,r}$′
$(0+0_{c,r})$	ggtct	agacc	$(0+0_{c,r})$′
$(1+0_{c,r})$	aggct	agcct	$(1+0_{c,r})$′
$(0-½_{c,r})$	gtacc	ggtag	$(0-½_{c,r})$′
$(1-½_{c,r})$	taggc	gccta	$(1-½_{c,r})$′

Table S2. Sticky-end binding domains with specific DNA base sequences in propagator, connector, and solution tiles for subtraction operation. The complementary sticky end pairs are indicated by unprimed and primed symbols (e.g. 0 and 0**′**).

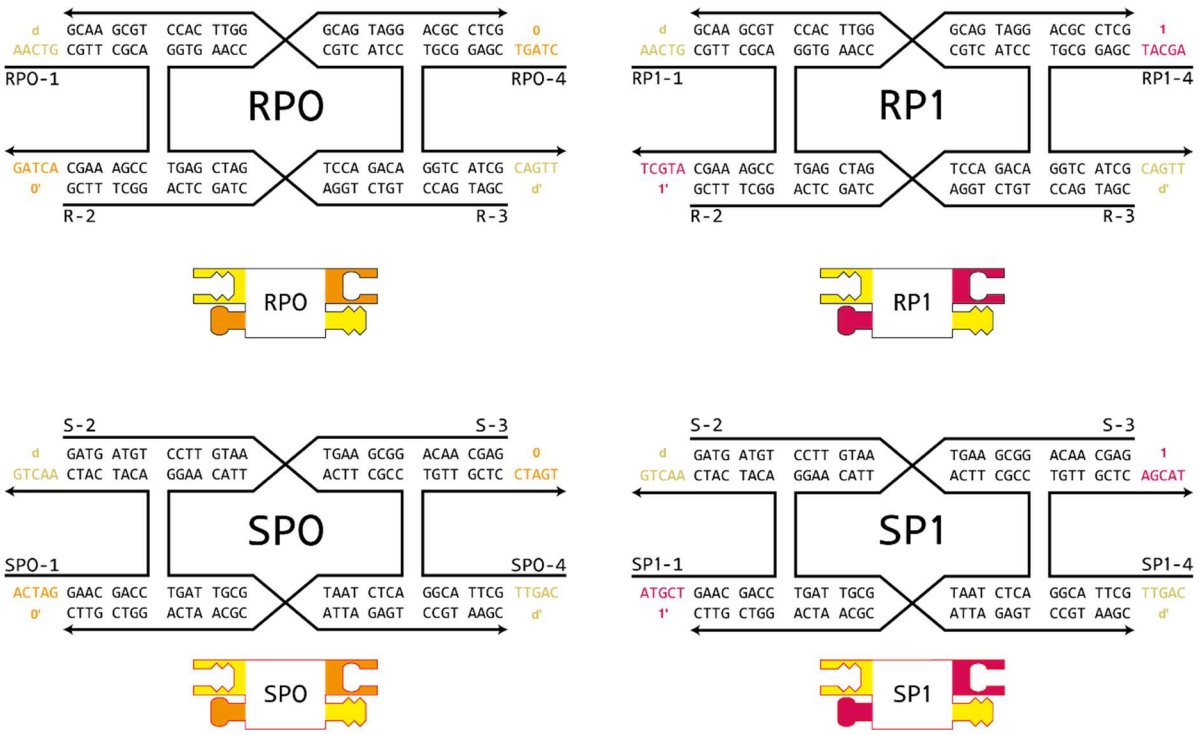


Figure S2. A sequence diagram with cartoon representation of the double-crossover (DX) tiles for the propagators used in the addition and subtraction operations. A propagator (four kinds, *i.e.*, RP0, RP1, SP0, and SP1 are available) delivers the initial input value placed on left side (I_L, which is either 0 or 1) through the next propagator (0′ or 1′) to the connector (0′ or 1′). The propagator can also deliver the initial input value placed on right side (I_R) if it is rotated along the y-axis. Two inputs I_L and I_R are added to get the sum. For subtraction operation, I_R (subtrahend) is subtracted from I_L (minuend).

Tile	Strand	Length	Sequence (5’ to 3’)
RP0	RP0-1	26mers	aactgcgttcgcaccgaaagcactag
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	RP0-4	26mers	ctagtcgaggcgtggtcatcgcagtt
RP1	RP1-1	26mers	aactgcgttcgcaccgaaagcatgct
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	RP1-4	26mers	agcatcgaggcgtggtcatcgcagtt
SP0	SP0-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	SP0-4	26mers	cagttgcttacggtgttgctcctagt
SP1	SP1-1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	SP1-4	26mers	cagttgcttacggtgttgctcagcat

Table S3. Sequence information of propagators for addition and subtraction.

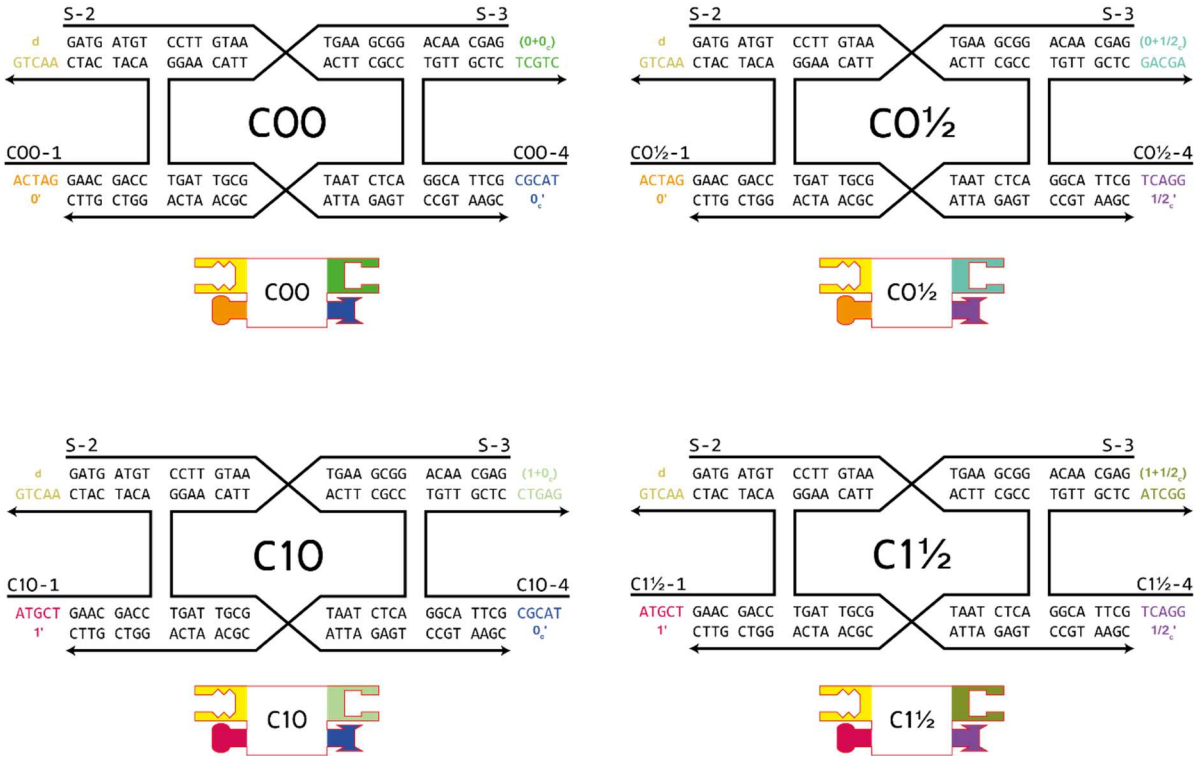


Figure S3. A sequence diagram with cartoon representation of the connectors for addition. A connector (C00, C0, C10½, and C1½), which is placed between propagator and solution tiles, delivers bit information (0 or 1, which is obtained from propagator) to the solution tiles from both left and right sides.

Tile	Strand	Length	Sequence (5' to 3')
C00	C00-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C00-4	26mers	tacgcgcttacggtgttgctctcgtc
C10	C10-1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C10-4	26mers	tacgcgcttacggtgttgctcctgag
C0½	C0½ -1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C0½ -4	26mers	ggactgcttacggtgttgctcgacga
C1½	C1½ -1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C1½ -4	26mers	ggactgcttacggtgttgctcatcgg

Table S4. Sequence information of connectors for addition.

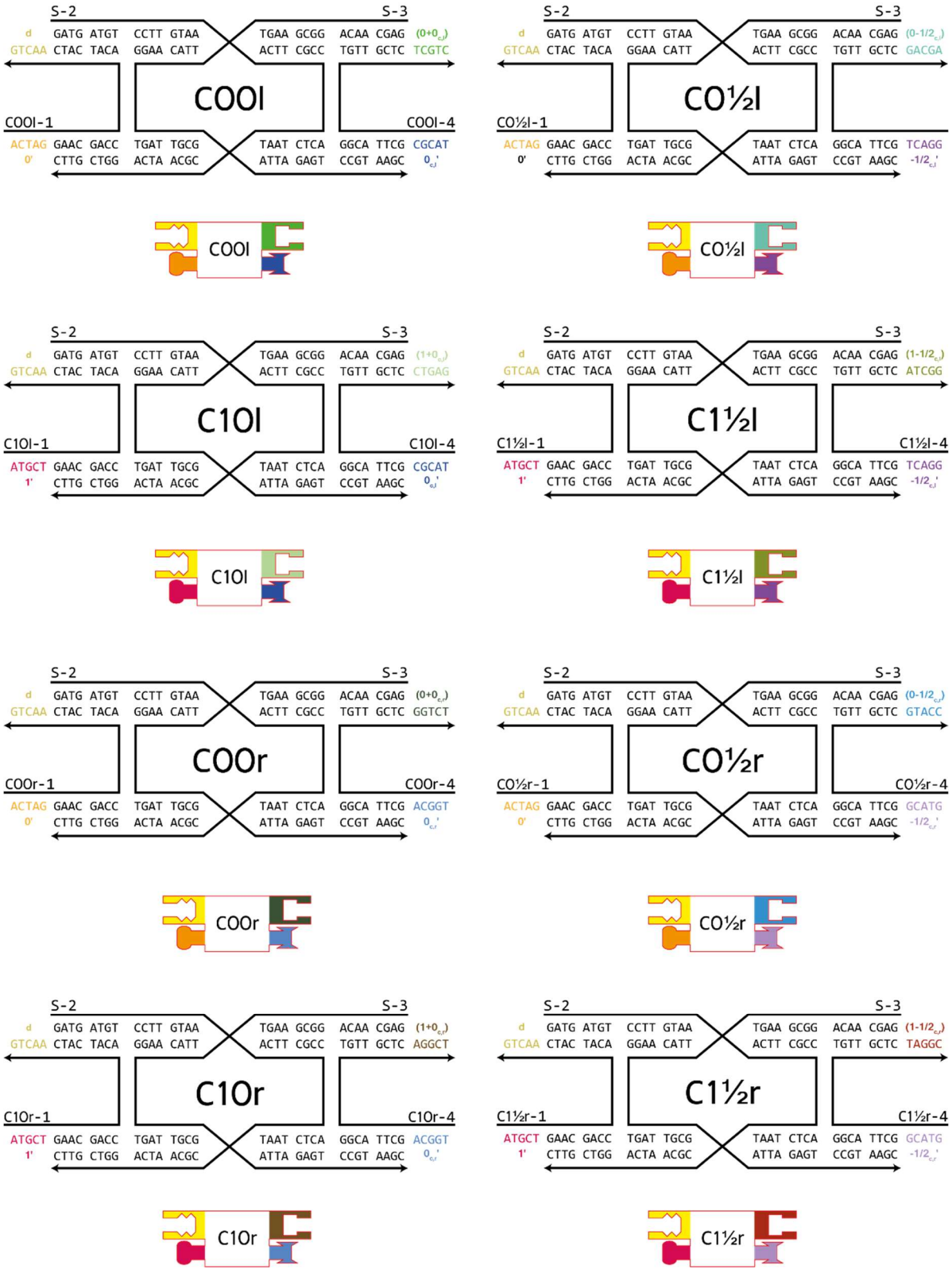


Figure S4. A sequence diagram with cartoon representation of the connectors for subtraction. A connector (C00l, C0½l, C10l, C1½l, C00r, C0½r, C10r, and C1½r), which is placed between propagator and solution tiles, delivers bit information (0 or 1, which is obtained from propagator) to the solution either from left (via C00l, C0½l, C10l, and C1½l) or right (C00r, C0½r, C10r, and C1½r).

Tile	Strand	Length	Sequence (5' to 3')
C00l	C00l-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C00l-4	26mers	tacgcgcttacggtgttgctctcgtc
C10l	C10l-1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C10l-4	26mers	tacgcgcttacggtgttgctcctgag
C0½l	C0½l-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C0½l-4	26mers	ggactgcttacggtgttgctcgacga
C1½l	C1½ -1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C1½l-4	26mers	ggactgcttacggtgttgctcatcgg
C00r	C00r-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C00r-4	26mers	tggcagcttacggtgttgctcggtct
C10r	C10r-1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C10r-4	26mers	tggcagcttacggtgttgctcaggct
C0½r	C0½r-1	26mers	actaggaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C0½r-4	26mers	gtacggcttacggtgttgctcgtacc
C1½r	C1½r-1	26mers	atgctgaacgaccacatcatcaactg
	S-2	48mers	gatgatgtccttgtaaacttcgccactctaatcgcaatcaggtcgttc
	S-3	48mers	gagcaacaggcgaagtttacaaggtgattgcgattagagtccgtaagc
	C1½r-4	26mers	gtacggcttacggtgttgctctaggc

Table S5. Sequence information of connectors for subtraction.

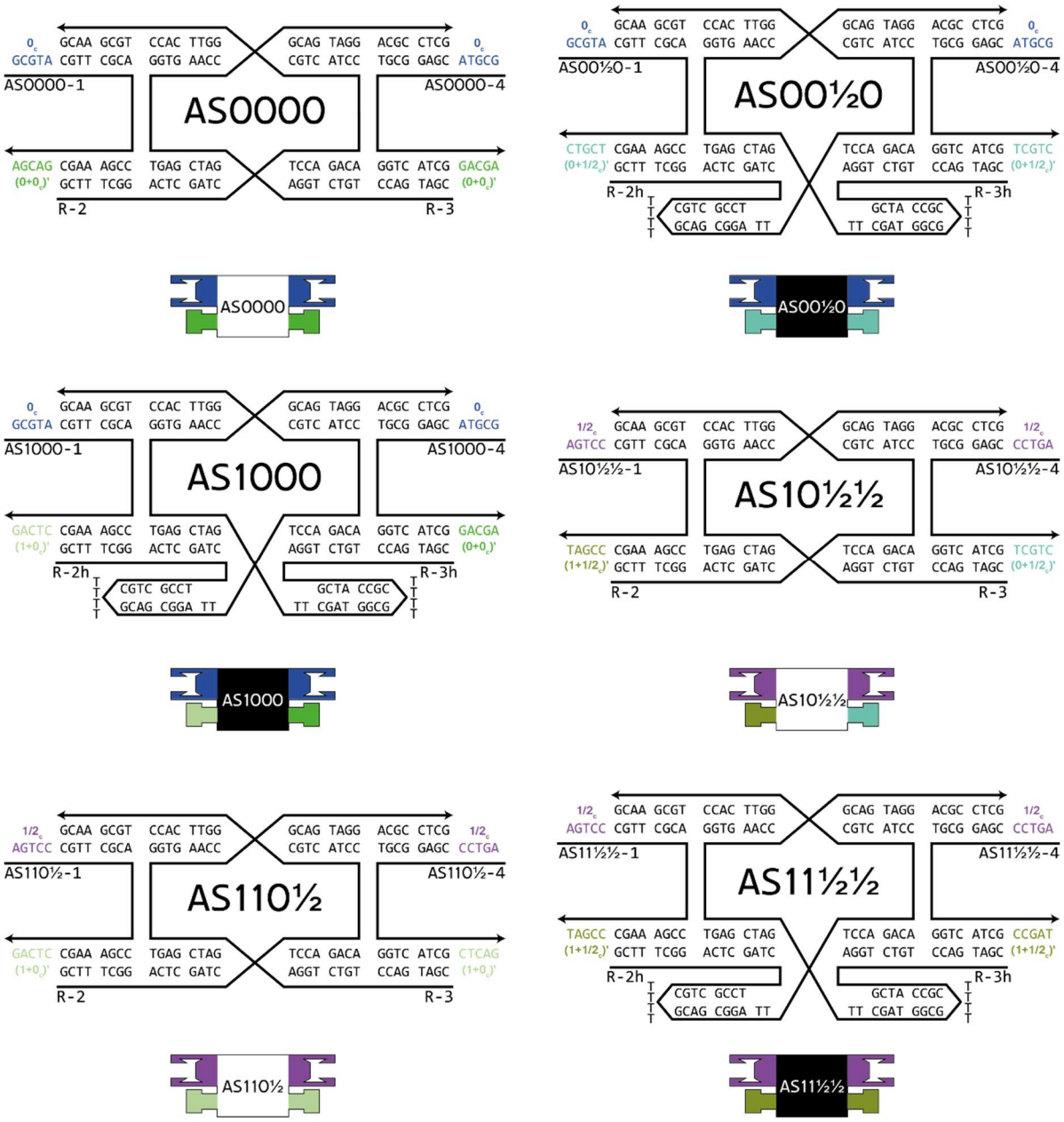


Figure S5. A sequence diagram with cartoon representation of the solutions for addition. A solution, *i.e.*, AS0000, AS00½0, AS1000, AS10½½, AS110½, and AS11½½, which is placed at the centre of crystal, reveals the result of summation based on the information obtained from left and right connectors.

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Tile	Strand	Length	Sequence (5' to 3')
AS0000	AS0000-1	26mers	gcgtacgttcgcaccgaaagcgacga
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	AS0000-4	26mers	gcgtacgaggcgtggtcatcggacga
AS1000	AS1000-1	26mers	gcgtacgttcgcaccgaaagcctcag
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	AS1000-4	26mers	gcgtacgaggcgtggtcatcggacga
AS110½	AS110½ -1	26mers	agtcccgttcgcaccgaaagcctcag
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	AS110½ -4	26mers	agtcccgaggcgtggtcatcgctcag
AS00½0	AS00½0-1	26mers	gcgtacgttcgcaccgaaagctcgtc
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	AS00½0-4	26mers	gcgtacgaggcgtggtcatcgtcgtc
AS10½½	AS10½½ -1	26mers	agtcccgttcgcaccgaaagcccgat
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	AS10½½ -4	26mers	agtcccgaggcgtggtcatcgtcgtc
AS11½½	AS11½½ -1	26mers	agtcccgttcgcaccgaaagcccgat
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	AS11½½ -4	26mers	agtcccgaggcgtggtcatcgccgat

Table S6. Sequence information of solutions for addition.

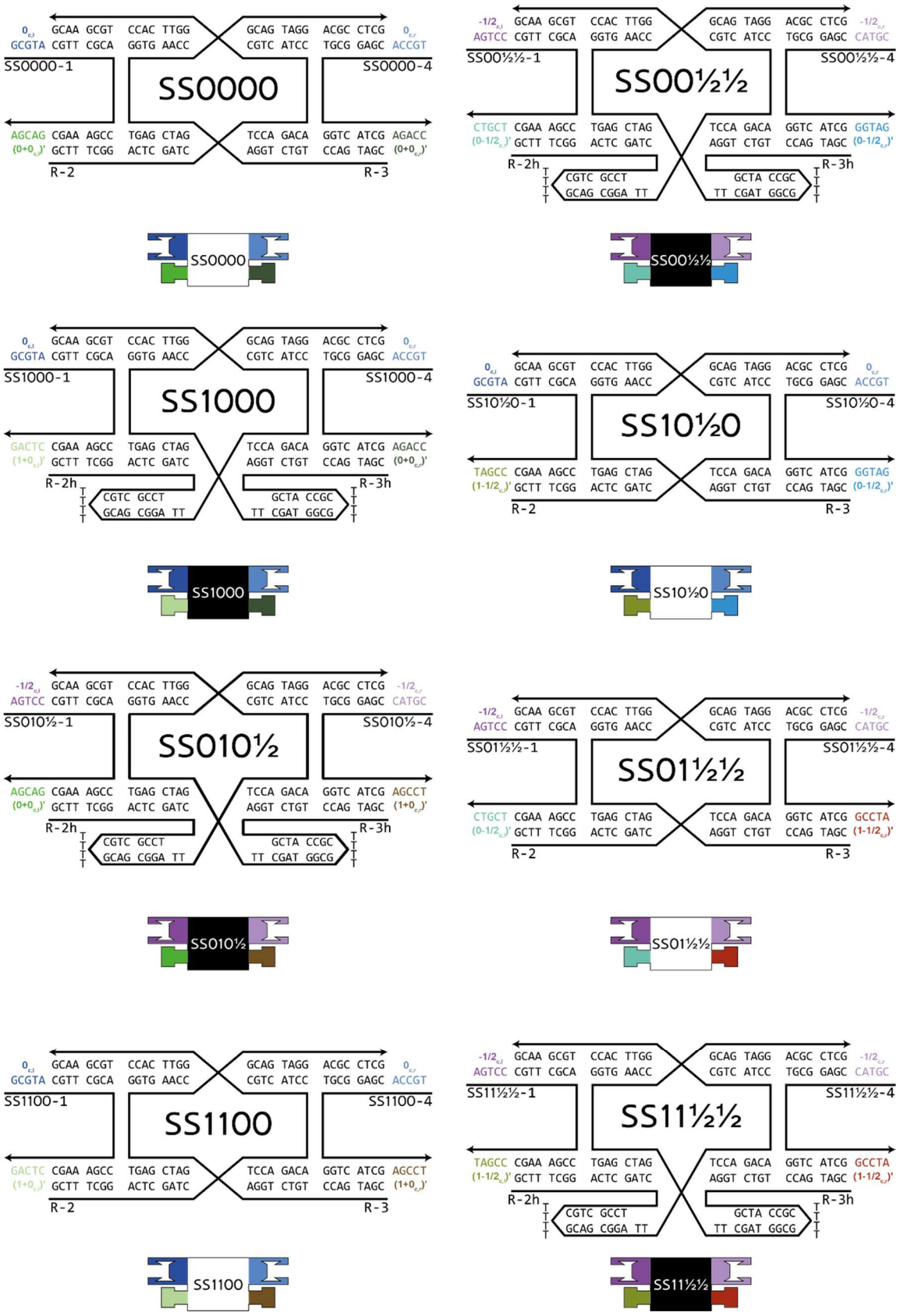

Figure S6. A sequence diagram with cartoon representation of the solutions for subtraction. A solution, *i.e.*, SS0000, SS00½½, SS1000, SS10½0, SS010½, SS01½½, SS1100, or SS11½½, which is placed at the centre of crystal, reveals the result of subtraction based on the information obtained from left and right connectors.

Tile	Strand	Length	Sequence (5' to 3')
SS0000	SS0000-1	26mers	gcgtacgttcgcaccgaaagcgacga
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	SS0000-4	26mers	tgccacgaggcgtggtcatcgagacc
SS010½	SS010½ -1	26mers	agtcccgttcgcaccgaaagcgacga
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	SS010½ -4	26mers	cgtaccgaggcgtggtcatcgagcct
SS1000	SS1000-1	26mers	gcgtacgttcgcaccgaaagcctcag
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	SS1000-4	26mers	tgccacgaggcgtggtcatcgagacc
SS1100	SS1100-1	26mers	gcgtacgttcgcaccgaaagcctcag
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	SS1100-4	26mers	tgccacgaggcgtggtcatcgagcct
SS00½½	SS00½½ -1	26mers	agtcccgttcgcaccgaaagctcgtc
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	S00½½ -4	26mers	cgtaccgaggcgtggtcatcgggtag
SS01½½	SS01½½ -1	26mers	agtcccgttcgcaccgaaagctcgtc
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	SS01½½ -4	26mers	cgtaccgaggcgtggtcatcggccta
SS10½0	SS10½0-1	26mers	gcgtacgttcgcaccgaaagcccgat
	R-2	48mers	gctttcggactcgatctccagacacctactgcggttcacctgcgaacg
	R-3	48mers	cgatgacctgtctggagatcgagtggtgaaccgcagtaggacgcctcg
	SS10½0-4	26mers	tgccacgaggcgtggtcatcgggtag
SS11½½	SS11½½ -1	26mers	agtcccgttcgcaccgaaagcccgat
	R-2h	70mers	gctttcggactcgatctccgctgcttttgcagcggatttccagacacctactgcggttcacctgcgaacg
	R-3h	70mers	cgatgacctgtctggagctaccgcttttgcggtagcttgatcgagtggtgaaccgcagtaggacgcctcg
	SS11½½ -4	26mers	cgtaccgaggcgtggtcatcggccta

Table S7. Sequence information of solutions for subtraction.