Generating skeleton reaction network for reactions of large-scale ReaxFF MD pyrolysis simulations based on machine learning predicted reaction class

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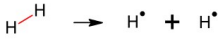
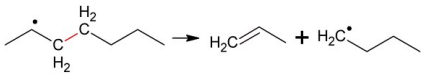
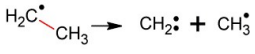
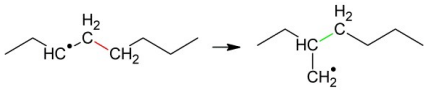
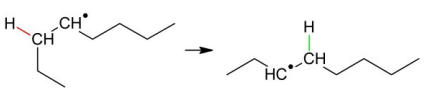
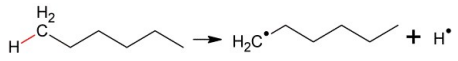
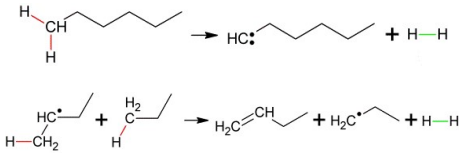
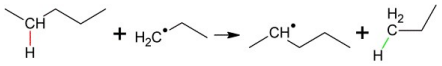
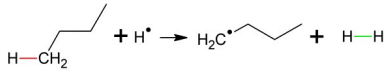
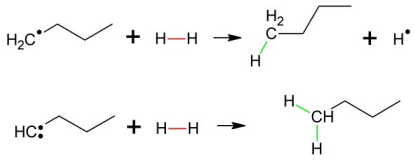
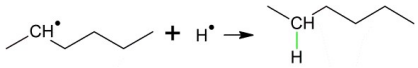
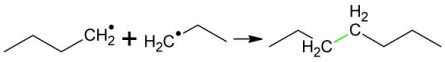
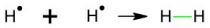
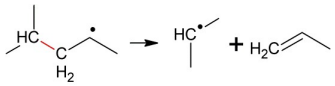
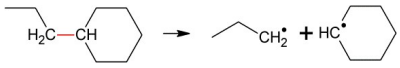
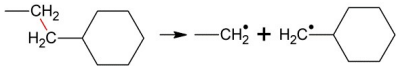
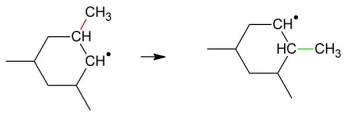
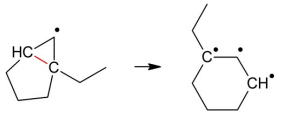
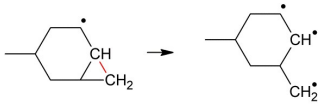
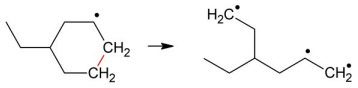
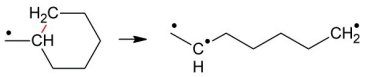
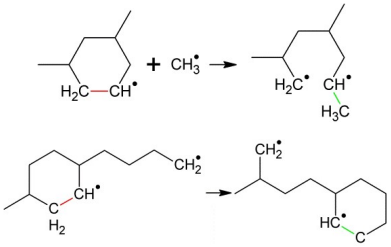
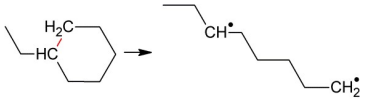
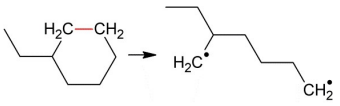
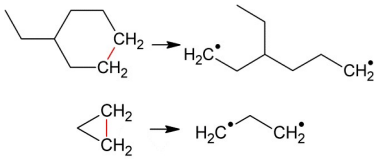
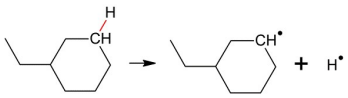
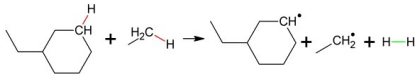
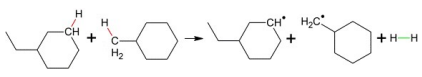
SUPPORTING INFORMATION

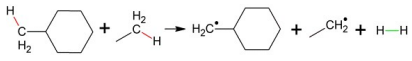
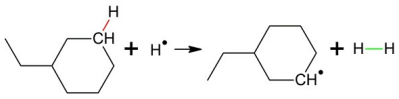
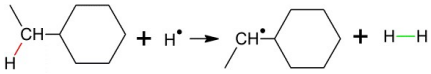
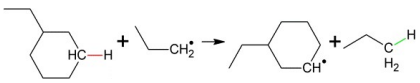
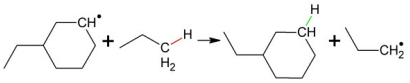
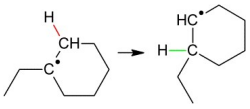
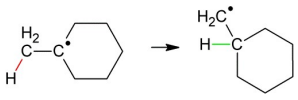
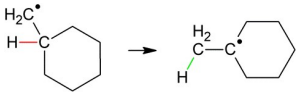
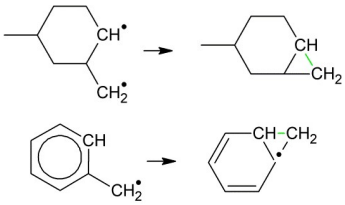
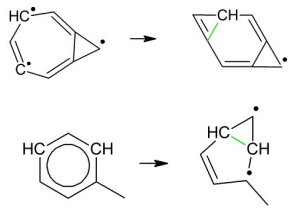
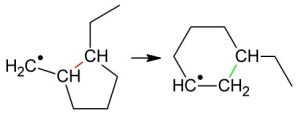
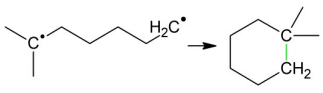
Supplementary materials S1

Table S1.1 Reactions classes (RxC) of hydrocarbon pyrolysis defined for the classification of ReaxFF MD simulated reactions in SRG-Reax

RxC	RxC name	Reaction instances	Reaction depiction & Classification priority note	Reaction class group
1	C-C bond homolysis		Homolysis of C-C at varied positions	I. Homolysis
2	H-H bond homolysis		H_2 formed at high temperatures is unstable, which may cleavage into H	
3	*β*-scission		*β*-scission of radicals at varied positions	II. Carbon chain breaks induced by radicals, including chain branching
4	*α*-scission		Infrequent reaction at high temperature	
5	Intra-molecular chain isomerization		Intra-molecular isomerization may lead to branching	
6	Intra-molecular H-shift		H-shift may occur to its neighbor C atom or other C atoms	III. Intra-molecular H-shift on a

				carbon chain
7	H detachment			IV. Dehydrogenation of a carbon chain
8	H_2 formation via dehydrogenation			
9	Inter-molecular H-abstraction by C			V. H-abstraction of a carbon chain
10	H-abstraction by H			
11	H-abstraction of H_2 by C		High-temperature reaction due to H_2 unstableness, where H_2 is considered as C_0	
12	H radical addition to C			VI. Radical consumption
13	Recombination of C radicals			
14	Combination of H radicals			
15	Isopropyl detachment		Isopropyl detachment induced by C chain radical Isopropyl detachment induced by isopropyl radical	VII. Branch detachment relevant to propene formation
16	Detachment of isopropyl radical			
17	α-branched bond scission of C ring			VIII. Neighboring branch bond scission of α- and β- for carbon cyclics
18	β-branched bond scission of C ring			
19	Branch shift of C ring		Reconnection of the dropped side chain to other C of same ring	
20	Polycyclic bridge cleavage into a large ring		The type of polycyclic bridge cleavage has higher priority than ring opening	IX. Ring-opening: relevant to the bridge bond of polycyclics
21	Adjacent C-C ring bond cleavage of			

	polycyclic bridge bond			
22	*β*-ring opening of ring carbon radical			
23	*β*-ring opening of branched carbon radical			X. Ring-opening: induced by radical
24	*α*-ring opening of ring carbon radical		Infrequent reaction (*α*-ring opening of ring carbon radical tends to its recombination with other C radical)	
25	*α*-ring bond scission of ring branch		Ring-opening at ring C neighboring to branching C	XI. Ring-opening: relative to the position of the branched chain, its priority is lower than the reaction types of Groups IX and X.
26	*β*-ring bond scission of ring branch			
27	Ring bond scission except for *α* and *β* ring bond of ring branch		Ring bond scission except for Type 25 and Type 26	
28	Ring dehydrogenation		Dehydrogenation of C-H on a ring	XII. Cyclic-relevant dehydrogenation
29	H_2 formation via dehydrogenation of ring and acyclic fragment		H_2 formation of ring H with H from acyclic dehydrogenation	
30	H_2 formation via dehydrogenation of ring and α-C of ring branch		This type focuses on ring branch dehydrogenation of *α*-C, which tends to consequent ring opening. Ring branch dehydrogenation of *β*/γ-C will be classified into Type 29.	

31	H_2 formation via dehydrogenation of α-C of ring branch and acyclic fragment			
32	Cyclic H-abstraction by H			XIII. Cyclic-relevant H-abstraction
33	H-abstraction of α-C on ring branch by H			
34	Cyclic H-abstraction by acyclic radical			
35	Acyclic H-abstraction by ring radical			
36	Intra-ring H-shift			XIV. Cyclic-relevant H-shift
37	Ring branch H-shift to ring			
38	Ring H-shift to ring branch			
39	Ring increment via branch linked to host ring			XV. Formation and isomerization of ring structures, a possible pathway for aryl ring opening
40	Ring increment via intra-ring carbons connecting			
41	Ring opening and recombination		Similar to chain isomerization	
42	Chain cyclization		Chain isomerization into a ring via connecting of intra-chain carbon	

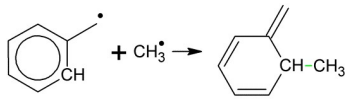
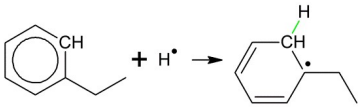
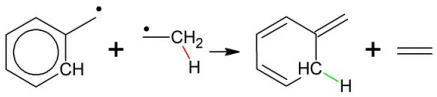
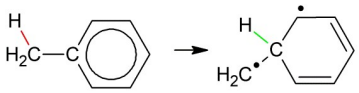
43	Combination of aromatic carbon and C radical fragment		XVI. Aromatic ring π structure broken by aromatic carbon joining other structural fragments or atoms, a possible pathway for aryl ring opening
44	Combination of aromatic carbon and H		
45	H-abstraction by aromatic carbon		
46	H-shift from branched-chain to host aromatic ring		

Table S1.2 Fuel models, ReaxFF MD pyrolysis simulation conditions covered, and reaction analysis parameters of VARxMD for preparing reaction data set

Fuel model	Simulation condition (Isothermal simulation using NVT ensemble, simulation time-step = 0.1 fs)		
	Simulation temperature (K)	Reaction duration time (ps)	Sampling interval of ReaxFF MD simulation / Output frame interval for VARxMD analysis (ps)
n-dodecane	2000	250	0.25
	2500	250	0.25
	3000	250	0.25
3-component surrogate model of RP-3	2800	270	1
4-component surrogate model of RP-3	2800	270	1
45-component baseline model of RP-3	2800	270	1
24-component baseline model of RP-1	2800	250	0.1

Supplementary materials S2

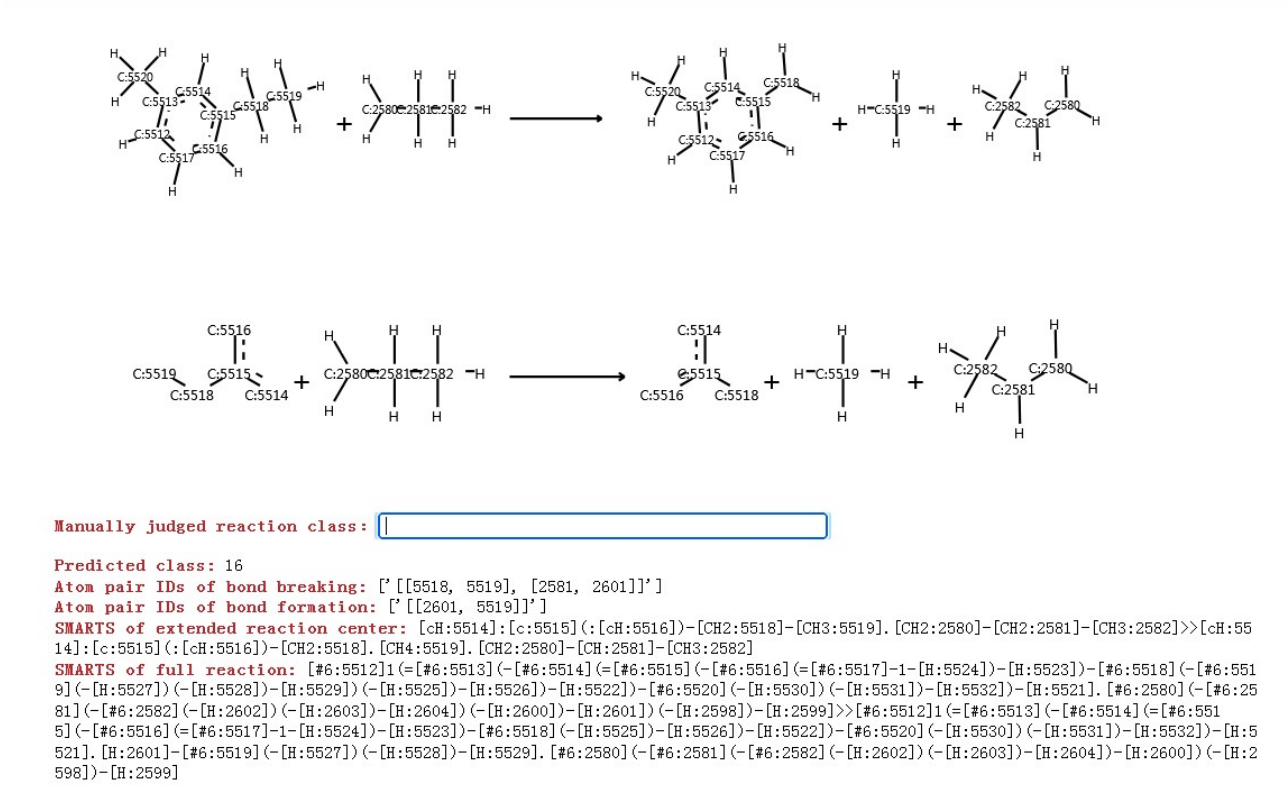


Fig. S2 Manual check and labeling of high uncertainty predicted reactions in the active learning of SRG-Reax.

Supplementary materials S3

Table S3.1 The reaction features in Input 1 of the tri-training classifier

Reaction feature name	Feature description
Features of broken or formed bond (Level 1)	
BondType	The type of broken or formed bond
IsAromatic	Whether the broken or formed bond is an aromatic bond
NumBridgedRings	How many rings does the broken or formed bond belong to
BondOrderReaxFF	The bond order of broken or formed bond
FunctionalGroups	The functional group types that the formed or broken bond belongs to
Atom features of reaction site (Level 2)	
Mass	Relative atomic mass of a reaction site
NumRadicalElectrons	The number of radical electrons a reaction site has
Degree	The number of atoms connected to a reaction site (excluding those connected to H atoms)
TotalValence	Total valence of a reaction site
IsAromatic	Whether the reaction site is an aromatic atom

NumBridgedRings	The number of rings a reaction site belongs to
TotalNumHs	Number of H atoms connected to the reaction site
GasteigerCharges	Gasteiger charges of a reaction site
CrippenContribs	The relative contributions of a reaction site in a molecule calculated by considering the chemical environment surrounding the reaction site and the interactions between neighboring atoms.
LabuteASAContribs	The solvent-accessible surface area (SASA) contributions of the reaction site in a molecule
TPSAContribs	The contribution of a reaction site to the topological polar surface area (TPSA) of a molecule
NumPiElectrons	The number of π electrons of a reaction site
NumLonePairElectronsReaxFF	The number of lone pair electrons in a reaction site
NetChargeReaxFF	The net charge of a reaction site
TotalBondOrderReaxFF	The total bond order of all covalent bonds associated with the reaction site
Features of all neighbor structures of broken/formed bond (Level 3)	
NumRadicalElectrons	The total number of radical electrons that all neighbor atoms of a broken/formed bond have
NumPiElectrons	The total number of π electrons of all neighbor atoms of a broken/formed bond
NumRingAtoms	The total number of rings that all neighbor atoms of a broken/formed bond belong to
NumNonRingRadicals	The total number of radical electrons that all non-cyclic neighbor atoms of a broken/formed bond have
FunctionalGroups	The functional group types that all neighbor atoms of a broken/formed bond belong to
Features of full reaction (Level 4)	
NumBrokenBonds	Number of broken bonds
NumFormedBonds	Number of formed bonds
NumReactiveAtomsInReactants	Number of non-H reaction sites in reactants
NumReactiveAtomsInProducts	Number of non-H reaction sites in products
NumReactantFragments	Number of reactant fragments
NumProductFragments	Number of product fragments

Table S3.2 The definations of the 18 full reaction features in Input 3 of the tri-training classifier

Reaction feature name	Feature description
NumReactantFragments	Number of reactant fragments
NumProductFragments	Number of product fragments
NumBrokenBonds	Number of broken bonds
NumGenerateBonds	Number of formed bonds
NumReactAtomsInReactants	Number of reaction site in reactants (Non-implicit H atom)
NumReactAtomsInProducts	Number of reaction site in products (Non-implicit H atom)

NumAromaticBrokenBonds	Number of aromatic broken bonds
NumAromaticFormedBonds	Number of aromatic formed bonds
NumBrokenRingBonds	Number of broken bonds of ring structures
NumFormedRingBonds	Number of formed bonds of ring structures
NumRadicalElectronsOfRxnSitesInReact	The total number of radical electrons of reaction site in reactants
NumRadicalElectronsOfRxnSitesInProd	The total number of radical electrons of reaction site in products
NumAromaticAtomsOfRxnSitesInReact	The total number of aromatic reaction site in reactants
NumAromaticAtomsOfRxnSitesInProd	The total number of aromatic reaction site in products
NumRingAtomsOfRxnSitesInReact	Number of reaction site of ring structures in reactants
NumRingAtomsOfRxnSitesInProd	Number of reaction site of ring structures in products
NumPiElectronsOfRxnSitesInReact	The total number of π electrons of reaction sites in reactants
NumPiElectronsOfRxnSitesInProd	The total number of π electrons of reaction sites in products

Table S3.3 Details of 196 reaction features in vector of Input 1 highlighted in Fig. 4

 # 0–5 full reaction features of Level 4

'NumReactantFragments','NumProductFragments','NumBrokenBonds','NumFormedBonds','NumReactiveAtomsInReactants','NumReactiveAtomsInProducts'

 # Bond breaking

 # 6–17 1st broken bond (BB1)

 # bond (B) features of Level 1

,'BB1_B_BondType','BB1_B_IsAromatic','BB1_B_NumBridgedRings','BB1_B_BondOrderReaxFF','BB1_B_FunctionalGroup'

its environment (E) structure features of Level 3

,'BB1_E_NumRadicalElectrons','BB1_E_NumPiElectrons','BB1_E_NumRingAtoms','BB1_E_NumNonRingRadicals','BB1_E_FunctionalGroupType1','BB1_E_FunctionalGroupType2','BB1_E_FunctionalGroupType3'

 # 18–29 2nd broken bond (BB2)

 # bond (B) features of Level 1

,'BB2_B_BondType','BB2_B_IsAromatic','BB2_B_NumBridgedRings','BB2_B_BondOrderReaxFF','BB2_B_FunctionalGroup'

its environment (E) structure features of Level 3

,'BB2_E_NumRadicalElectrons','BB2_E_NumPiElectrons','BB2_E_NumRingAtoms','BB2_E_NumNonRingRadicals','BB2_E_FunctionalGroupType1','BB2_E_FunctionalGroupType2','BB2_E_FunctionalGroupType3'

 # Bond formation

 # 30–37 1st formed bond (FB1)

 # bond (B) features of Level 1

,'FB1_B_BondType','FB1_B_IsAromatic','FB1_B_NumBondRings','FB1_B_BondOrder'

its environment (E) structure features of Level 3

,'FB1_E_NumRadicalElectrons','FB1_E_NumPiElectrons','FB1_E_NumAtomRings','FB1_E_NumNonRingRadicals'

 # 38–45 2nd formed bond (FB2)

 # bond (B) features of Level 1

,'FB2_B_BondType','FB2_B_IsAromatic','FB2_B_NumBondRings','FB2_B_BondOrder'

its environment (E) structure features of Level 3

,'FB2_E_NumRadicalElectrons','FB2_E_NumPiElectrons','FB2_E_NumAtomRings','FB2_E_NumNonRingRadicals'

 # Atoms of reaction sites in reactants

 # 46–60 atom features of the 1st reaction site (BA1) in reactants of Level 2

,'BA1_Mass','BA1_NumRadicalElectrons','BA1_Degree','BA1_TotalValence','BA1_IsAromatic','BA1_NumBridgedRings','BA1_TotalNumHs','BA1_GasteigerCharges','BA1_CrippenContribs','BA1_LabuteASAContribs','BA1_TPSAContribs','BA1_NumPiElectrons','BA1_NumLonePairElectronsReaxFF','BA1_NetChargeReaxFF','BA1_TotalBondOrderReaxFF'

 # 61–75 atom features of the 2nd reaction site (BA2) in reactants of Level 2

,'BA2_Mass','BA2_NumRadicalElectrons','BA2_Degree','BA2_TotalValence','BA2_IsAromatic','BA2_NumBridgedRings','BA2_TotalNumHs','BA2_GasteigerCharges','BA2_CrippenContribs','BA2_LabuteASAContribs','BA2_TPSAContribs','BA2_NumPiElectrons','BA2_NumLonePairElectronsReaxFF','BA2_NetChargeReaxFF','BA2_TotalBondOrderReaxFF'

 # 76–90 atom features of the 3rd reaction site (BA3) in reactants of Level 2

,'BA3_Mass','BA3_NumRadicalElectrons','BA3_Degree','BA3_TotalValence','BA3_IsAromatic','BA3_NumBridgedRings','BA3_TotalNumHs','BA3_GasteigerCharges','BA3_CrippenContribs','BA3_LabuteASAContribs','BA3_TPSAContribs','BA3_NumPiElectrons','BA3_NumLonePairElectronsReaxFF','BA3_NetChargeReaxFF','BA3_TotalBondOrderReaxFF'

 # 91–105 atom features of the 4th reaction site (BA4) in reactants of Level 2

,'BA4_Mass','BA4_NumRadicalElectrons','BA4_Degree','BA4_TotalValence','BA4_IsAromatic','BA4_NumBridgedRings','BA4_TotalNumHs','BA4_GasteigerCharges','BA4_CrippenContribs','BA4_LabuteASAContribs','BA4_TPSAContribs','BA4_NumPiElectrons','BA4_NumLonePairElectronsReaxFF','BA4_NetChargeReaxFF','BA4_TotalBondOrderReaxFF'

 # 106–120 atom features of the 5th reaction site (BA5) in reactants of Level 2

,'BA5_Mass','BA5_NumRadicalElectrons','BA5_Degree','BA5_TotalValence','BA5_IsAromatic','BA5_NumBridgedRings','BA5_TotalNumHs','BA5_GasteigerCharges','BA5_CrippenContribs','BA5_LabuteASAContribs','BA5_TPSAContribs','BA5_NumPiElectrons','BA5_NumLonePairElectronsReaxFF','BA5_NetChargeReaxFF','BA5_TotalBondOrderReaxFF'

 # Atoms of reaction sites in products

 # 121–135 atom features of the 1st reaction site (FA1) in products of Level 2

,'FA1_Mass','FA1_NumRadicalElectrons','FA1_Degree','FA1_TotalValence','FA1_IsAromatic','FA1_NumBridgedRings','FA1_TotalNumHs','FA1_GasteigerCharges','FA1_CrippenContribs','FA1_LabuteASAContribs','FA1_TPSAContribs','FA1_NumPiElectrons','FA1_NumLonePairElectronsReaxFF','FA1_NetChargeReaxFF','FA1_TotalBondOrderReaxFF'

 # 136–150 atom features of the 2nd reaction site (FA2) in products of Level 2

,'FA2_Mass','FA2_NumRadicalElectrons','FA2_Degree','FA2_TotalValence','FA2_IsAromatic','FA2_NumBridgedRings','FA2_TotalNumHs','FA2_GasteigerCharges','FA2_CrippenContribs','FA2_LabuteASAContribs','FA2_TPSAContribs','FA2_NumPiElectrons','FA2_NumLonePairElectronsReaxFF','FA2_NetChargeReaxFF','FA2_TotalBondOrderReaxFF'

 # 151–165 atom features of the 3rd reaction site (FA3) in products of Level 2

,'FA3_Mass','FA3_NumRadicalElectrons','FA3_Degree','FA3_TotalValence','FA3_IsAromatic','FA3_NumBridgedRings','FA3_TotalNumHs','FA3_GasteigerCharges','FA3_CrippenContribs','FA3_LabuteASAContribs','FA3_TPSAContribs','FA3_NumPiElectrons','FA3_NumLonePairElectronsReaxFF','FA3_NetChargeReaxFF','FA3_TotalBondOrderReaxFF'

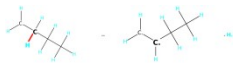
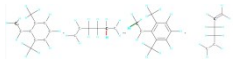
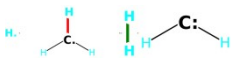
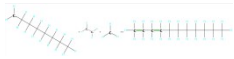
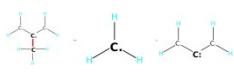
 # 166–180 atom features of the 4th reaction site (FA4) in products of Level 2

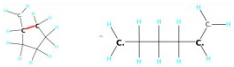
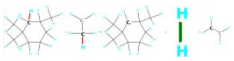
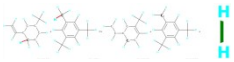
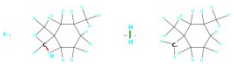
,'FA4_Mass','FA4_NumRadicalElectrons','FA4_Degree','FA4_TotalValence','FA4_IsAromatic','FA4_NumBridgedRings','FA4_TotalNumHs','FA4_GasteigerCharges','FA4_CrippenContribs','FA4_LabuteASAContribs','FA4_TPSAContribs','FA4_NumPiElectrons','FA4_NumLonePairElectronsReaxFF','FA4_NetChargeReaxFF','FA4_TotalBondOrderReaxFF'

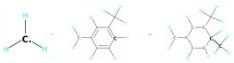
 # 181–195 atom features of the 5th reaction site (FA5) in products of Level 2

,'FA5_Mass','FA5_NumRadicalElectrons','FA5_Degree','FA5_TotalValence','FA5_IsAromatic','FA5_NumBridgedRings','FA5_TotalNumHs','FA5_GasteigerCharges','FA5_CrippenContribs','FA5_LabuteASAContribs','FA5_TPSAContribs','FA5_NumPiElectrons','FA5_NumLonePairElectronsReaxFF','FA5_NetChargeReaxFF','FA5_TotalBondOrderReaxFF'

Table S3.4 Sample data of the 18 types of reaction descriptors

RxC	Sample reactions	18 reaction features of Input 3																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1		1	2	1	0	2	2	0	0	0	0	0	2	0	0	0	0	0	0
2		1	2	1	0	2	2	0	0	0	0	0	2	0	0	0	0	0	0
3		1	2	1	0	2	2	0	0	0	0	0	2	0	0	0	0	0	0
5		1	1	1	1	3	3	0	0	0	0	1	1	0	0	0	0	0	0
5		1	1	1	1	3	3	0	0	0	0	4	4	0	0	0	0	0	0
6		1	1	1	1	2	2	0	0	0	0	1	1	0	0	0	0	0	0
7		1	2	1	0	1	2	0	0	0	0	0	2	0	0	0	0	0	0
8		2	3	2	1	2	4	0	0	0	0	0	2	0	0	1	1	0	0
9		2	2	1	1	2	2	0	0	0	0	1	0	0	0	0	0	0	1
10		2	2	1	1	2	3	0	0	0	0	2	2	0	0	0	0	0	0
11		2	2	1	1	3	2	0	0	0	0	1	1	0	0	0	0	0	0
12		2	1	0	1	2	1	0	0	0	1	1	0	0	0	1	1	1	0
13		2	1	0	1	2	2	0	0	0	0	2	0	0	0	0	0	0	0
14		2	1	0	1	2	2	0	0	0	0	2	0	0	0	0	0	0	0
15		1	2	1	0	2	2	0	0	0	0	0	2	0	0	0	0	0	0
16		1	2	1	0	2	2	0	0	0	0	1	3	0	0	0	0	0	0
17		1	2	1	0	2	2	0	0	0	0	0	2	0	0	1	1	0	0

18		1	2	1	0	2	2	0	0	0	0	0	2	0	0	0	0	0	0
19		1	1	1	1	3	3	0	0	1	1	1	0	0	0	2	2	2	3
20		1	1	1	0	2	2	0	0	1	0	0	0	0	0	4	2	2	4
21		1	1	1	0	2	2	0	0	0	0	0	2	0	0	3	1	0	0
22		1	1	1	0	2	2	0	0	1	0	0	2	0	0	2	0	0	0
23		1	1	1	0	2	2	0	0	1	0	0	2	0	0	2	0	0	0
25		1	1	1	0	2	2	0	0	0	0	0	2	0	0	2	0	0	0
26		1	1	1	0	2	2	0	0	0	0	0	2	0	0	2	0	0	0
27		1	1	1	0	2	2	0	0	1	0	0	2	0	0	2	0	0	0
28		1	2	1	0	1	2	0	0	0	0	0	2	0	0	1	1	0	0
29		2	3	2	1	2	4	0	0	0	0	0	2	0	0	1	1	0	0
30		2	3	2	1	2	4	0	0	1	0	0	2	0	0	1	1	0	0
31		2	3	2	2	3	5	0	0	0	0	1	1	0	0	0	2	0	0
33		2	2	1	1	2	3	0	0	0	0	1	1	0	0	0	0	0	0
34		2	2	1	1	2	2	0	0	0	0	1	1	0	0	1	1	0	0
35		2	2	1	1	2	2	0	0	0	1	0	2	0	0	1	1	2	0
36		1	1	1	1	2	2	0	0	1	1	0	3	0	0	2	2	3	0
37		1	1	1	1	2	2	0	0	1	0	1	1	0	0	1	1	0	0
39		1	1	0	1	2	2	0	0	0	0	2	0	0	0	1	3	0	0
40		1	1	0	1	2	2	0	0	0	0	2	0	0	0	2	4	0	0
41		1	1	1	1	3	3	0	0	1	0	1	1	0	0	2	3	0	0

42		1	1	0	1	2	2	0	0	0	0	2	0	0	0	0	2	0	0
43		2	1	0	1	2	2	0	0	0	0	1	0	1	0	1	1	1	0
44		2	1	0	1	2	1	0	0	0	1	1	0	1	0	1	1	1	0
44		2	1	0	1	2	1	0	0	0	1	1	0	1	0	1	1	1	0
45		2	2	1	1	2	2	0	0	0	1	0	1	1	0	1	1	1	0
46		1	1	1	1	2	2	0	0	1	0	0	1	1	0	1	1	1	0

Supplementary materials S4

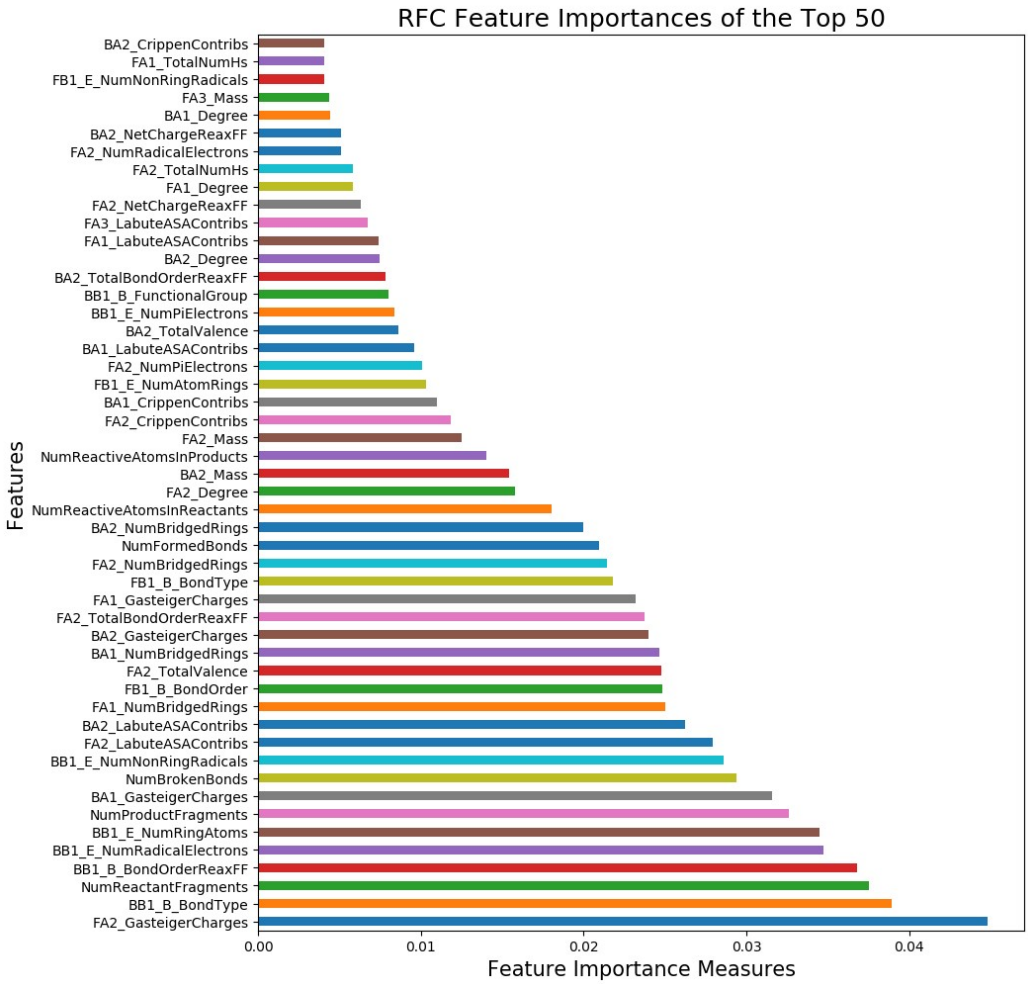


Fig. S4 Feature importance of the top 50 among the 196 features of Input 1 of the single random forest classifier (RFC) adopted in the tri-training classifier.

Table S4 Evaluation results of reaction fingerprint (FP) candidates for single classifier of tri-training based on random forest

Reaction descriptions		Micro-F1 score with different FP bit size					
Input type	**FP type**	**128**	**256**	**512**	**1024**	**2048**	**4096**
Input 2	AtomPairs	0.918	0.913	0.916	0.920	0.917	0.916
∑ FP of products	Morgan2	0.951	0.955	0.957	0.959	0.957	0.958
- ∑ FP of reactants	TopologicalTorsions	0.662	0.664	0.662	0.665	0.663	0.659
Input 3	AtomPairs	0.932	0.932	0.933	0.931	0.932	0.932
(∑ ERC FP of products	Morgan2	0.951	0.952	0.953	0.952	0.952	0.953
- ∑ ERC FP of reactants)	TopologicalTorsions	0.928	0.927	0.928	0.928	0.927	0.928
+ 18 reaction features							
Input 3 without reaction features	AtomPairs	0.779	0.778	0.780	0.781	0.782	0.782
(∑ ERC FP of products	Morgan2	0.910	0.915	0.915	0.916	0.915	0.915
- ∑ ERC FP of reactants)	TopologicalTorsions	0.474	0.476	0.475	0.475	0.475	0.475

Supplementary materials S5

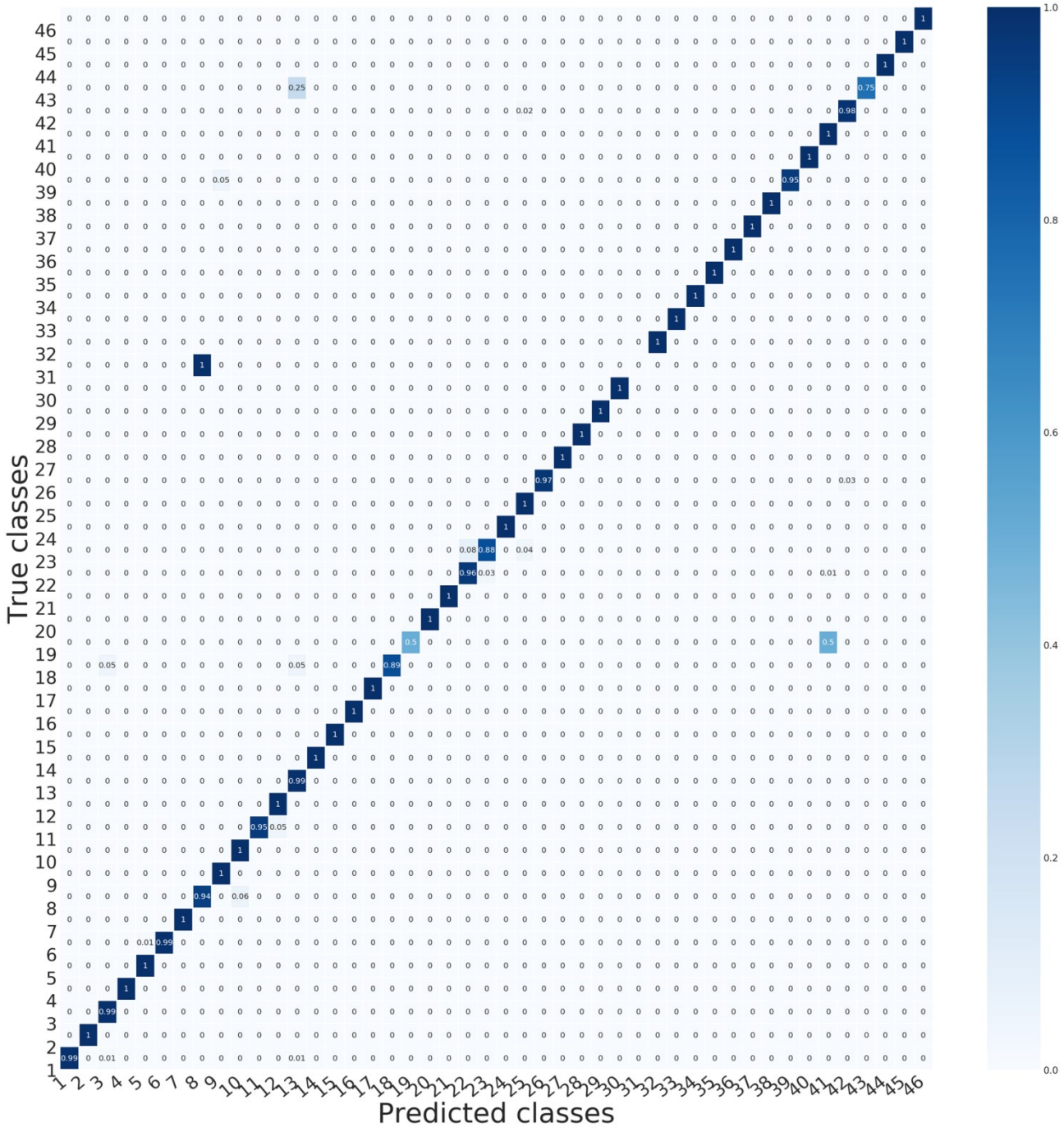


Fig. S5 Confusion matrix of all 46 classes after reaction classifier refinement.