

Overview of important SDA input parameters

parameter	description	nnons number of nonspecific constraints	dind distance independ.	ncec number of contacts to form encounter contacts, only used for recording, not for calculation	docking yes/no	Rate calculation yes/no	reaction file	layout of rxnfile	complexes' output Ncmx specifies the max. number of complexes to write	trajectories' output
icommrxn=1	RMS average of all pairwise distances between pairs of atoms given in files rxna12f.	not used	not used	Ncec>=0	no	yes	ignored	specific or nonspecific not considered	validated complex, depends on ncmx (maximum number) and ncec	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)
icommrxn=2	minimal pairwise distance between pair of atoms given in files rxna12f, simultaneous occurrence is monitored for any 1, 2, 3 or 4 pairs.	not used	Dind not used, equivalent to dind=0 and icommrxn=3	Ncec>=0	no	yes	required	specific or nonspecific not considered	Validated complex, depends on ncec and iwrec	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)
icommrxn=3	minimal pairwise distance between a pair of atoms given in files rxna12f, for independent pairs (defined by dind), simultaneous occurrence is monitored for any 1, 2, 3 or 4 pairs	not used	distance of pairs, dind>0 default dind=6	Ncec>=0	no	yes	required	specific or nonspecific not considered	Validated complex, depends on ncec and iwrec,ncmx	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)
icommrxn=4	electron transfer rate constant will be calculated. Files rxna12f (defining the reaction atom pairs) should contain pairs of atoms that may take part in an electron transfer path together with their coupling to the donor or acceptor site.	not used	according to the reaction file	not considered	no	yes (modified for electron transfer)	separate files defined in rxna1f and rxna2f required.	specific or nonspecific not considered	Not used	Not used
icommrxn=5	for docking (no association rate calc.). By using this criteria the energetically best complexes will be present in the fort.55 file (independent of constraints). Any nnons, equivalent to dind=0 (but no independence checked - faster)	not used	not used	not considered	yes	no	save everything	file is not needed	always writes complexes (up to ncmx)	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)
icommrxn=6	for docking (no association rate calc.). Former icommrxn 3 in sdac. Checks all reaction pairs considering nnons. nnons no of independent constraints depending on dind.	n>=0	Dind>0, default 6 Å	not considered	yes	no	specific contact pairs plus ambiguous contacts	first column (specific, nonspecific) is used, coordinates of reacting atoms, no apriori complex,	Up to ncmx	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)

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Icommrxn=7	for docking (no association rate calc.). Alternative to icommrxn=2 in sdac. Do not Check independent reaction pairs.	n>=0	not considered (equivalent to icommrxn=6 with dind=0)	not considered	yes	no	specific contact pairs plus independence of ambiguous contacts	first column (specific, nonspecific) is used, coordinates of reacting atoms, no apriori complex,	Up to ncmx	Nrec!=0, nrec>0 (records specific trajectory, nrec<0 record all trajectories)
Icommrxn=8	Like 6, checks the distance along the z-axis, only	n>=0	Dind>0, default 6		yes	no		only reads coordinates of first protein, and calculates distance in z direction	Up to ncmx	
Icommrxn=9	Like 7, z-axis only	n>=0	Not considered	not considered	yes	no			Up to ncmx	
ibox can be 0, 1 or 2										