

Table S1: List of molecule classes in the vesicle transport model. Each class can contain an arbitrary number of molecule species. Note, that vesicles are also compartments by itself. All molecules that bind to a compartment membrane can also bind to vesicle membranes.

	Coat	<p>Function: Vesicle Budding</p> <ul style="list-style-type: none"> • Polymerization shapes the vesicle • Specific interactions select SNARE, Motor and Cargo molecules to ensure proper sorting 		Motors	<p>Function: Directed Transport</p> <ul style="list-style-type: none"> • Pull vesicles along cytoskeleton filaments <p>States:</p> <ol style="list-style-type: none"> free in cytoplasm bound to membrane of compartment <p>Represents: Kinesins, Dyneins, Myosins</p>
	“Coat Catcher”	<p>Function: Selecting Coat Molecules</p> <ul style="list-style-type: none"> • Specific interactions bind free Coat molecules to the compartment membrane to ensure proper sorting <p>States:</p> <ol style="list-style-type: none"> bound to membrane of compartment <p>Represents: Specific molecules or motifs in the compartment membrane</p>		“Motor Catcher”	<p>Function: Selecting Motor Molecules</p> <ul style="list-style-type: none"> • Specific interactions bind free Motor proteins to the compartment membrane to refill the local pool <p>States:</p> <ol style="list-style-type: none"> bound to membrane of compartment <p>Represents: Specific molecules or motifs in the compartment membrane</p>
	Tethers	<p>Function: Involved in Vesicle Fusion</p> <ul style="list-style-type: none"> • Tethering factors tether vesicles, initiating fusion • Note: not included in the present model, therein their function is taken over by SNAREs <p>States:</p> <ol style="list-style-type: none"> bound to membrane of compartment <p>Represents: (Yeast:) Vps 18, GSG1, Sec34-37, Tip 1, ...</p>		Cargo	<p>Function: ... to be transported and sorted</p> <ul style="list-style-type: none"> • Cargo molecules are just cargo inside the vesicles • The presence of Cargo molecules triggers vesicle budding <p>States:</p> <ol style="list-style-type: none"> free in the lumen of the compartment bound to membrane of compartment <p>Represents: All molecules that have to be sorted and transported in the membrane trafficking system. Note: Coat and Motor Catchers can be treated as Cargo as well in order to transport and sort them.</p>
	SNAREs	<p>Function: Addressing and Vesicle Fusion</p> <ul style="list-style-type: none"> • SNAREs specify the fusion partner =“Addressing” • SNAREs mediate vesicles fusion <p>States:</p> <ol style="list-style-type: none"> bound to membrane of compartment <p>Represents: (Yeast:) Ufe1, Sed5, Tlg2, Pep12, Vam3, Sso1, Sso2, Sec20, Bos1, Gos1, Vti1, Sec9, Spo20, Slt1, Sft1, Bet1, Tlg1, Syn8, Vam7, Sec9, Spo20, Sec22, Ykt6, Nyv1, Snc1, Snc2</p>		Other Species	<p>Function:</p> <ul style="list-style-type: none"> • Other molecules in the cell can interact with the molecules in the compartments <p>States:</p> <ol style="list-style-type: none"> outside of the compartments <p>Represents: All other molecules in the cell, especially signaling molecules that can be activated by membrane bound receptor complexes</p>