**Electronic Supplementary Information** 

Exergetic life cycle analysis for the selection of chromatographic separation processes in

the pharmaceutical industry: Preparative HPLC versus Preparative SFC.

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Figure S2: P&ID of the Prep-SFC separation in the  $\alpha$  system boundary (energy streams are not shown to reduce complexity)

## Tables:

Table S1: Mass and energy balance in the  $\alpha$  system boundary for the Prep-HPLC separation of 500 g racemic mixture. This table is linked with the annotations in Fig. S1

Tabel S2: Mass and energy balance in the  $\alpha$  system boundary for the Prep-SFC separation of 500 g racemic mixture. This table is linked with the annotations in Fig. S2

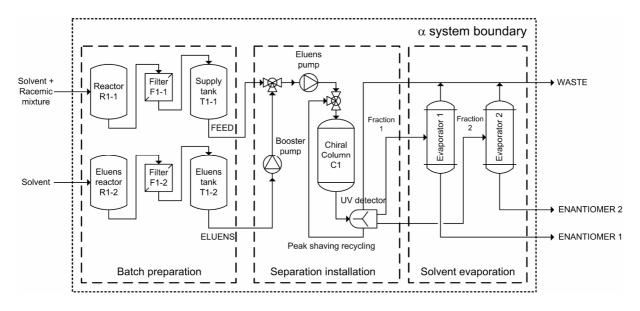


Figure S1: P&ID of the Prep-HPLC separation in the  $\alpha$  system boundary (energy streams are not shown to reduce complexity)

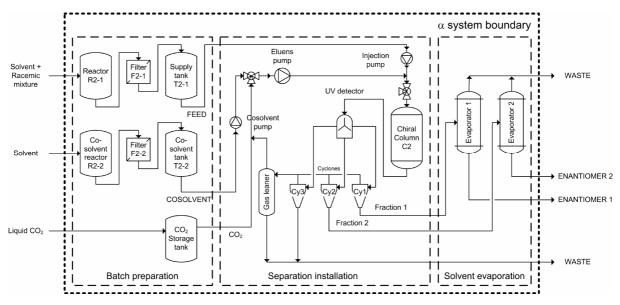


Figure S2: P&ID of the Prep-SFC separation in the  $\alpha$  system boundary (energy streams are not shown to reduce complexity)

Table S1: Mass and energy balance in the  $\alpha$  system boundary for the Prep-HPLC separation of 500 g racemic mixture. This table is linked with the annotations in Fig. S1

Equipment				
BASIC OPERATIONS	INPUT		OUTPUT	
Reactor R1-1				
Inerting	68.75 kJ	Electricity for setting vacuum		
	0.20 kg	N <sub>2</sub> gas at 8 bar		
Pumping in solvents + racemic mixture	57.29 kJ	Electricity for pumping solvents	0.20 kg	N <sub>2</sub>
	0.50 kg	Racemic mixture		2
	26.03 kg	Methanol		
	63.69 kg	Ethanol		
	0.07 kg	N <sub>2</sub> gas at 8 bar		
Stirring	511.50 kJ	Electricity for stirring		
Emptying reactor	0.00 kJ	Gravimetrically	90.22 kg	Solvents + racemic mixture to F1-1
			0.07 kg	N <sub>2</sub>
Cleaning reactor	1.67 kg	Water	1.67 kg	Water
	1.23 kg	Methanol	1.23 kg	Methanol
	10.66 kJ 495.00 kJ	Electricity for pumping solvents Electricity for stirring		
	747.48 kJ	Heat from shellsol (175°C, 6 bar)		
	190.12 kJ	Electricity for pumping heating medium		
	747.48 kJ	Cooling with cold shellsol (4°C, 6 bar)		
ilter F1-1				
Inerting	495.00 kJ	Electricity for setting vacuum		
	0.34 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	90.22 kg	Solvents + racemic mixture from R1-1	0.13 kg	N <sub>2</sub>
Filtration under pressure	0.63 kg	N <sub>2</sub> gas at 8 bar	90.22 kg	Solvent + racemic mixture to T1-1
Emptying filter	0.00 kJ	Manually	0.85 kg	N <sub>2</sub>
Cleaning filter	4.00 kg	Water	4.00 kg	Water
	3.95 kg	Methanol	3.95 kg	Methanol
	29.70 kJ	Electricity for pumping solvents		
	1350.00 kJ	Electricity for stirring		
	4755.62 kJ	Heat from shellsol (175°C, 6 bar)		
	675.00 kJ	Electricity for pumping heating medium		
Supply tank T1-1	4755.62 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Inerting	68.75 kJ	Electricity for setting vacuum		
merting	0.20 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	90.22 kg	Filtered solvents + racemic mixture from F1-1	0.13 kg	N <sub>2</sub>
Emptying tank	0.00 kJ	Gravimetrically	90.22 kg	Solvents + racemic mixture to C1
Lingtying tank	0.00 13	Gravimetricany	0.07 kg	N <sub>2</sub>
Cleaning tank	1.67 kg	Water	1.67 kg	Water
eleaning talin	0.99 kg	Methanol	0.99 kg	Methanol
	0.07 kg	Acetone	0.07 kg	Acetone
	28.65 kJ	Electricity for pumping solvents		
Eluens reactor R1-2				
Inerting	330.00 kJ	Electricity for setting vacuum		
-	0.97 kg	N <sub>2</sub> gas at 8 bar		
Pumping in solvents	419.63 kg	Methanol	0.97 kg	N <sub>2</sub>
	33.69 kg	Acetonitrile		
	0.20 kg	Trifluoroacetic acid		
	0.13 kg	Water		
	275.00 kJ	Electricity for pumping solvents		
	0.32 kg	N <sub>2</sub> gas at 8 bar		
Stirring	5160.00 kJ	Electricity for stirring	452.54.1	Calcada to F1 2
Emptying reactor	0.00 kJ	Gravimetrically	453.64 kg	Solvents to F1-2
Cleaning reactor	8.00 kg	Water	0.32 kg 8.00 kg	N <sub>2</sub> Water
Cleaning reactor	5.93 kg	Methanol	5.93 kg	Methanol
	51.15 kJ	Electricity for pumping solvents	3.33 Kg	chanor
	1620.00 kJ	Electricity for parriping solvents  Electricity for stirring		
	3587.91 kJ	Heat from shellsol (175°C, 6 bar)		
	402.30 kJ	Electricity for pumping heating medium		
	3587.91 kJ	Cooling with cold shellsol (4°C, 6 bar)		

Filter F1-2				
Inerting	990.00 kJ	Electricity for setting vacuum		
	0.69 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	453.64 kg	Solvents from R1-2	0.66 kg	N <sub>2</sub>
Filtration under pressure	1.67 kg	N <sub>2</sub> gas at 8 bar	453.64 kg	Solvent to T1-2
Emptying filter	0.00 kJ	Manually	1.70 kg	N <sub>2</sub>
Cleaning filter	8.00 kg	Water	8.00 kg	Water
<b>0</b>	7.90 kg	Methanol	7.90 kg	Methanol
	59.40 kJ	Electricity for pumping solvents		
	2700.00 kJ	Electricity for stirring		
	9511.24 kJ	Heat from shellsol (175°C, 6 bar)		
	1350.00 kJ	Electricity for pumping heating medium		
	9511.24 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Eluens tank T1-2				
Inerting	330.00 kJ	Electricity for setting vacuum		
	0.97 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	453.64 kg	Filtered solvents F1-2	0.66 kg	N <sub>2</sub>
Emptying tank	0.00 kJ	Gravimetrically	453.64 kg	Eluens to C1
., .		,	0.32 kg	N <sub>2</sub>
Cleaning tank	8.00 kg	Water	8.00 kg	Water
	4.74 kg	Methanol	4.74 kg	Methanol
	0.32 kg	Acetone	0.32 kg	Acetone
	137.52 kJ	Electricity for pumping solvents		
Column C1				
Conditioning	9900.00 kJ	Electricity for pumping		
	8532.00 kJ	Heating with steam (175°C, 9 bar)		
Separation	1392405.06 kJ	Electricity for pumping	47.51 kg	Waste fraction
	543.86 kg	Solution	of which 0.05	kg racemic mixture
	of which 0.5	50 kg racemic mixture	and 47.46	kg solvent mixture
	and 543.3	36 kg solvent mixture	198.75 kg	Fraction 1 to E1-1
	1200000.00 kJ	Heating with steam (175°C, 9 bar)	of which 0.225	kg enantiomer 1
				kg solvent mixture
			297.61 kg	Fraction 2 to E1-2
			of which 0.225	
				kg solvent mixture
Cleaning	9900.00 kJ	Electricity for pumping	67.10 kg	Ethanol
	67.10 kg	Ethanol		
F	8532.00 kJ	Heating with steam (175°C, 9 bar)		
Evaporator E1-1				
Inerting	67.50 kJ	Electricity for setting vacuum		
	0.01 kg	N₂ gas at 8 bar		
Inserting fraction 1	198.75 kg	Fraction 1	0.01 kg	N <sub>2</sub>
	of which 0.2	23 kg enantiomer 1		
		52 kg solvent mixture		
Heating up from 30 °C to 55 °C	220679.46 kJ	Heat from warm water (60°C)		
	5575.32 kJ	Electricity for pumping warm water		
Creating vacuüm	316.46 kJ	Electricity for pumping	198.52 kg	Solvent mixture
Commission	220679.46 kJ	Cooling with cooling water (4°C)		
Scraping	13924.05 kJ	Electricity for the scraper	0.225 l	Frantisman 1
Emtying evaporator	0.00 kJ 0.90 kg	Manually Ethylacetate	0.225 kg 0.90 kg	Enantiomer 1 Ethylacetate
Cleaning evaporator	1.99 kg	Dichloromethane / methanol	1.99 kg	Dichloromethane / methanol
	0.79 kg	Ethanol	0.79 kg	Ethanol
	2591.45 kJ	Heat from warm water (60°C)	U./3 Ng	Edialioi
	103.18 kJ	Electricity for pumping warm water		
	206.35 kJ	Electricity for the scraper		
	2591.45 kJ	Cooling with cooling water (4°C)		
Evaporator E2-2		3 (		
Inerting	67.50 kJ	Electricity for setting vacuum		
	07.30 NJ	vacaum		

Filtration under pressure	1.67 kg	N <sub>2</sub> gas at 8 bar	453.64 kg	Solvent to T1-2
Emptying filter	0.00 kJ	Manually	1.70 kg	N <sub>2</sub>
Cleaning filter	8.00 kg	Water	8.00 kg	Water
	7.90 kg	Methanol	7.90 kg	Methanol
	59.40 kJ	Electricity for pumping solvents		
	2700.00 kJ	Electricity for stirring		
	9511.24 kJ 1350.00 kJ	Heat from shellsol (175°C, 6 bar) Electricity for pumping heating medium		
	9511.24 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Luens tank T1-2	3311.27 N	TTT IN THE COLO STICISON (T. C., O Dail)		
Inerting	330.00 kJ	Electricity for setting vacuum		
	0.97 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	453.64 kg	Filtered solvents F1-2	0.66 kg	N <sub>2</sub>
Emptying tank	0.00 kJ	Gravimetrically	453.64 kg	Eluens to C1
Lingtying tank	0.00 10	Gravinicalically	0.32 kg	N <sub>2</sub>
Cleaning tank	8.00 kg	Water	8.00 kg	Water
Cicarini, Garini	4.74 kg	Methanol	4.74 kg	Methanol
	0.32 kg	Acetone	0.32 kg	Acetone
	137.52 kJ	Electricity for pumping solvents		
Column C1				
Conditioning	9900.00 kJ	Electricity for pumping		
	8532.00 kJ	Heating with steam (175°C, 9 bar)		
Separation	1392405.06 kJ	Electricity for pumping	47.51 kg	Waste fraction
	543.86 kg	Solution		kg racemic mixture
		kg racemic mixture		kg solvent mixture
		kg solvent mixture	198.75 kg	Fraction 1 to E1-1
	1200000.00 kJ	Heating with steam (175°C, 9 bar)	of which 0.225 and 198 52	kg enantiomer 1 kg solvent mixture
			297.61 kg	Fraction 2 to E1-2
			of which 0.225	
				kg solvent mixture
Cleaning	9900.00 kJ	Electricity for pumping	67.10 kg	Ethanol
	67.10 kg	Ethanol		
	8532.00 kJ	Heating with steam (175°C, 9 bar)		
Evaporator E1-1				
Inerting	67.50 kJ	Electricity for setting vacuum		
	0.01 kg	N <sub>2</sub> gas at 8 bar		
Inserting fraction 1	198.75 kg	Fraction 1	0.01 kg	N <sub>2</sub>
		kg enantiomer 1		
		kg solvent mixture		
Heating up from 30 °C to 55 °C	220679.46 kJ	Heat from warm water (60°C)		
Creating vacuim	5575.32 kJ 316.46 kJ	Electricity for pumping warm water	100 52 kg	Calvant mixtura
Creating vacuüm	220679.46 kJ	Electricity for pumping Cooling with cooling water (4°C)	198.52 kg	Solvent mixture
Scraping	13924.05 kJ	Electricity for the scraper		
Emtying evaporator	0.00 kJ	Manually	0.225 kg	Enantiomer 1
Cleaning evaporator	0.90 kg	Ethylacetate	0.90 kg	Ethylacetate
	1.99 kg	Dichloromethane / methanol	1.99 kg	Dichloromethane / methanol
	0.79 kg	Ethanol	0.79 kg	Ethanol
	2591.45 kJ	Heat from warm water (60°C)		
	103.18 kJ	Electricity for pumping warm water		
	206.35 kJ 2591.45 kJ	Electricity for the scraper Cooling with cooling water (4°C)		
Evaporator E2-2	2391.45 KJ	cooming with cooling water (4 C)		
•	67 FO I	Electricity for cotting very		
Inerting	67.50 kJ	Electricity for setting vacuum		
Incorting fraction 2	0.01 kg	N <sub>2</sub> gas at 8 bar Fraction 2	0.01 1	N2
Inserting fraction 2	297.61 kg of which 0.23	kg enantiomer 2	0.01 kg	NZ
		kg solvent mixture		
Heating up from 30 °C to 55 °C	330572.69 kJ	Heat from warm water (60°C)		
	8348.73 kJ	Electricity for pumping warm water		
Creating vacuüm	316.46 kJ	Electricity for pumping	297.39 kg	Solvent mixture
	330572.69 kJ	Cooling with cooling water (4°C)		
Scraping	13924.05 kJ	Electricity for the scraper		
Emtying evaporator	0.00 kJ	Manually	0.225 kg	Enantiomer 2
Cleaning evaporator	0.90 kg	Ethylacetate	0.90 kg	Ethylacetate
	1.99 kg	Dichloromethane / methanol	1.99 kg	Dichloromethane / methanol
	0.79 kg	Ethanol	0.79 kg	Ethanol
	2591.45 kJ 103.18 kJ	Heat from warm water (60°C) Electricity for pumping warm water		
	103.18 kJ 206.35 kJ	Electricity for pumping warm water Electricity for the scraper		
	2591.45 kJ	Cooling with cooling water (4°C)		
	2JJ1.4J NJ	Cooming with Cooming water (4 C)		

Tabel S2: Mass and energy balance in the  $\alpha$  system boundary for the Prep-SFC separation of 500 g racemic mixture. This table is linked with the annotations in Fig. S2

Equipment  BASIC OPERATIONS	INPUT		OUTPUT	
BASIC OPERATIONS	INPOT		001701	
Reactor R2-1				
Inerting	68.75 kJ	Electricity for setting vacuum		
	0.20 kg	N <sub>2</sub> gas at 8 bar		
Pumping in solvents + racemic mixture	57.29 kJ	Electricity for pumping solvents	0.20 kg	N <sub>2</sub>
	0.50 kg	Racemic mixture		
	4.58 kg	Methanol		
	11.21 kg	Ethanol		
	0.18 kg	N <sub>2</sub> gas at 8 bar		
Stirring	90.00 kJ	Electricity for stirring		
Emptying reactor	0.00 kJ	Gravimetrically	16.29 kg	Solvents + racemic mixture to F2-1
			0.18 kg	N <sub>2</sub>
Cleaning reactor	1.67 kg	Water	1.67 kg	Water
	1.23 kg	Methanol	1.23 kg	Methanol
	10.66 kJ	Electricity for pumping solvents		
	495.00 kJ 747.48 kJ	Electricity for stirring Heat from shellsol (175°C, 6 bar)		
	190.12 kJ	Electricity for pumping heating medium		
	747.48 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Filter F2-1				
Inerting	495.00 kJ	Electricity for setting vacuum		
	0.34 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	16.29 kg	Solvents + racemic mixture from R2-1	0.02 kg	N <sub>2</sub>
Filtration under pressure	0.53 kg	N <sub>2</sub> gas at 8 bar	16.29 kg	Solvent + racemic mixture to T2-1
Emptying filter	0.00 kJ	Manually	0.85 kg	N <sub>2</sub>
Cleaning filter	4.00 kg	Water	4.00 kg	Water
Cleaning inter	3.95 kg	Methanol	4.00 kg 3.95 kg	Methanol
	29.70 kJ	Electricity for pumping solvents	3.33 kg	Wethand
	1350.00 kJ	Electricity for stirring		
	4755.62 kJ	Heat from shellsol (175°C, 6 bar)		
	675.00 kJ	Electricity for pumping heating medium		
	4755.62 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Supply tank T2-1				
Inerting	68.75 kJ	Electricity for setting vacuum		
	0.20 kg	N <sub>2</sub> gas at 8 bar		
Pumping in mixture	16.29 kg	Filtered solvents + racemic mixture from F2-1	0.02 kg	N <sub>2</sub>
Emptying tank	0.00 kJ	Gravimetrically	16.29 kg	Solvents + racemic mixture to C2
			0.18 kg	N <sub>2</sub>
Cleaning tank	1.67 kg	Water	1.67 kg	Water
	0.99 kg	Methanol	0.99 kg	Methanol
	0.07 kg	Acetone	0.07 kg	Acetone
	23.40 kJ	Electricity for pumping solvents		
Cosolvent reactor R2-2				
Inerting	165.00 kJ	Electricity for setting vacuum		
	0.49 kg	N <sub>2</sub> gas at 8 bar		
Pumping in solvents	199.89 kg	Ethanol	0.49 kg	N <sub>2</sub>
	137.50 kJ	Electricity for pumping solvents		
	0.20 kg	N <sub>2</sub> gas at 8 bar		
Stirring	1140.00 kJ	Electricity for stirring		
Emptying reactor	0.00 kJ	Gravimetrically	199.89 kg 0.20 kg	Solvents to F2-2 N <sub>2</sub>
Cleaning reactor	4.00 kg	Water	4.00 kg	Water
2	2.96 kg	Methanol	2.96 kg	Methanol
	25.58 kJ	Electricity for pumping solvents	3	
	810.00 kJ	Electricity for stirring		
	1793.96 kJ	Heat from shellsol (175°C, 6 bar)		
	201.15 kJ	Electricity for pumping heating medium		
	1793.96 kJ	Cooling with cold shellsol (4°C, 6 bar)		

Filter F2-2				
Inerting	495.00 kJ	Electricity for setting vacuum		
Description in white	0.34 kg	N <sub>2</sub> gas at 8 bar	0.20 l	N
Pumping in mixture	199.89 kg	Solvents from R2-2	0.29 kg	N <sub>2</sub>
Filtration under pressure	0.79 kg	N <sub>2</sub> gas at 8 bar	199.89 kg	Solvent to T2-2
Emptying filter	0.00 kJ	Manually	0.85 kg	N <sub>2</sub>
Cleaning filter	4.00 kg 3.95 kg	Water Methanol	4.00 kg 3.95 kg	Water Methanol
	29.70 kJ	Electricity for pumping solvents	3.33 Kg	Wethanor
	1350.00 kJ	Electricity for stirring		
	4755.62 kJ	Heat from shellsol (175°C, 6 bar)		
	675.00 kJ	Electricity for pumping heating medium		
	4755.62 kJ	Cooling with cold shellsol (4°C, 6 bar)		
Cosolvent tank T2-2	455.00.11			
Inerting	165.00 kJ	Electricity for setting vacuum		
	0.49 kg	N <sub>2</sub> gas at 8 bar	0.001	
Pumping in mixture	199.89 kg	Filtered solvents F2-2	0.29 kg	N <sub>2</sub>
Emptying tank	0.00 kJ	Gravimetrically	199.89 kg	Eluens to C2 N <sub>2</sub>
Cleaning tank	4.00 kg	Water	0.20 kg 4.00 kg	Water
Cleaning tank	2.37 kg	Methanol	2.37 kg	Methanol
	0.16 kg	Acetone	0.16 kg	Acetone
	65.46 kJ	Electricity for pumping solvents		
Column C2				
Conditioning	19962.00 kJ	Electricity for pumping		
	34200.00 kJ	Electricity for heating		
	25200.00 kJ	Electricity for cooling	100.10.1	Mark for the
Separation	1651575.00 kJ 216.19 kg	Electricity for pumping Solution + modifier	100.40 kg of which 0.03	Waste fraction  kg racemic mixture
	-	50 kg racemic mixture		kg solvent mixture
		69 kg organic solvent	44.27 kg	Fraction 1
	950.00 kg	CO <sub>2</sub> (60 bar, liquid)	of which 0.225	kg enantiomer 1
	2850000.00 kJ	Electricity for heating	and 44.04	kg solvent mixture
	2100000.00 kJ	Electricity for cooling	69.34 kg	Fraction 2
				kg enantiomer 1
				kg solvent mixture
-			950.00 kg	CO <sub>2</sub> (1 atm)
Cleaning	19800.00 kJ	Electricity for pumping	9.60 kg	Ethanol
	9.60 kg	Ethanol	9.60 kg	CO <sub>2</sub> (1 atm)
	9.60 kg	CO <sub>2</sub> (60 bar, liquid)		
	34200.00 kJ 25200.00 kJ	Electricity for heating Electricity for cooling		
Evaporator E2-1	23200.00 KJ	Electricity for cooling		
Inerting	67.50 kJ	Electricity for setting vacuum		
	0.01 kg	N <sub>2</sub> gas at 8 bar		
Inserting fraction 1	44.27 kg	Fraction 1	0.01 kg	N <sub>2</sub>
	<del>-</del>	23 kg enantiomer 1		2
		04 kg solvent mixture		
Heating up from 30 °C to 55 °C	39810.54 kJ	Heat from warm water (60°C)		
	3214.77 kJ	Electricity for pumping warm water		
Creating vacuüm	187.50 kJ	Electricity for setting vacuum	44.04 kg	Solvent mixture
Coroning	39810.54 kJ	Cooling with cooling water (4°C)  Electricity for the scraper		
Scraping Emtying evaporator	8250.00 kJ 0.00 kJ	Manually	0.225 kg	Enantiomer 1
Cleaning evaporator	0.90 kg	Ethylacetate	0.90 kg	Ethylacetate
cicum, getaporator	1.99 kg	Dichloromethane / methanol	1.99 kg	Dichloromethane / methanol
	0.79 kg	Ethanol	0.79 kg	Ethanol
	2591.45 kJ	Heat from warm water (60°C)		
	103.18 kJ	Electricity for pumping warm water		
	206.35 kJ 2591.45 kJ	Electricity for the scraper Cooling with cooling water (4°C)		
Evaporator E2-2	2551.45 N	Training water (4 C)		
Inerting	67.50 kJ	Electricity for setting vacuum		
··· •····•	0.01 kg	N <sub>2</sub> gas at 8 bar		
Inserting fraction 2	69.34 kg	Fraction 2	0.01 kg	N <sub>2</sub>
	-	23 kg enantiomer 2	0.01 kg	4
		11 kg solvent mixture		
Heating up from 30 °C to 55 °C	62461.92 kJ	Heat from warm water (60°C)		
	5035.23 kJ	Electricity for pumping warm water		
Creating vacuüm	187.50 kJ	Electricity for pumping	69.11 kg	Solvent mixture
	62461.92 kJ	Cooling with cooling water (4°C)		

187.50 kJ Electricity for pumping 69.11 kg Solvent mixture 62461.92 kJ Cooling with cooling water (4°C) 8250.00 kJ Electricity for the scraper Emtying evaporator
Cleaning evaporator 0.00 kJ Manually 0.225 kg Enantiomer 2 0.90 kg Ethylacetate 0.90 kg Ethylacetate 1.99 kg Dichloromethane / methanol 1.99 kg Dichloromethane / methanol 0.79 kg 0.79 kg Ethanol Ethanol 2591.45 kJ Heat from warm water (60°C) 103.18 kJ Electricity for pumping warm water 206.35 kJ Electricity for the scraper 2591.45 kJ Cooling with cooling water (4°C) 7

Scraping