Methionine and its hydroxy analogues: the paths toward their sustainable chemical synthesis †

Sergio Calderon-Ardila, [a] Didier Morvan, [b] Olivier Péruch, [b] Virginie Bellière-Baca, [b] Michiel Dusselier *[a] and Bert F. Sels *[a]

SUPPORTING INFORMATION

***Table S1**: Detailed quantitative sustainability metrics for the synthesis of D,L-Met and HMTBA produced by industrial (1-3) and renewable (4-6) synthetic routes.*

Metric		Yield (%)	AE (%)	RME (%)	OE (%)	PMI (g ·g^{-1})	PMI RRC (g ·g^{-1})	PMI Solv (g ·g^{-1})	PMI WU (g ·g^{-1})	RI (g ·g^{-1})	RP (%)
Process	Step										
(1) Propene to D,L-Met (through hydantoin)		**81.0**	**40.7**	**17.9**	**43.9**	**31.0**	**6.7**	**20.7**	**3.6**	**28.3**	**91.1**
	1	90.0	75.7	60.0	79.2	9.9	1.8	3.2	5.0		
	2	91.1	100	90.9	90.9	3.7	2.6	1.1	0		
	3	99.8	90.6	58.5	64.6	5.5	1.7	3.8	0		
	4	99.1	60.0	30.9	51.6	15.7	3.2	11.2	1.2		
	5	100	72.7	62.4	85.8	1.6	1.6	0	0		
(2) Propene to D,L-Met (through cyanohydrin)		**67.7**	**60.8**	**16.6**	**27.3**	**31.4**	**7.2**	**19.9**	**4.3**	**28.8**	**91.8**
	1	90.0	75.7	60.0	79.2	9.9	1.8	3.2	5.0		
	2	97.9	100	92.1	92.1	3.6	2.6	1.0	0		
	3	98.1	100	79.5	79.5	1.8	1.3	0.6	0		
	4	77.0	65.6	18.7	28.5	24.1	5.3	17.0	1.8		
(3) Propene to D,L-HMTBA		**71.8**	**50.0**	**37.2**	**74.4**	**11.1**	**3.9**	**3.3**	**3.9**	**7.3**	**66.0**
	1	90.0	75.7	60.0	79.2	9.9	1.8	3.2	5.0		
	2	91.1	100	90.9	90.9	3.7	2.6	1.1	0		
	3	93.2	100	90.3	90.3	2.1	1.1	1.0	0		
	4	94.0	53.2	45.3	85.2	3.7	2.2	0	1.5		
(4) DHA to D,L-HMTBA (through 2-HBL)		**68.0**	**66.3**	**38.3**	**57.7**	**144.8**	**3.5**	**122.1**	**19.1**	**45.7**	**92.5**
	1	68.0	85.0	38.5	45.3	53.8	3.9	49.8	0		
	2	100	72.0	65.4	90.8	108.9	1.5	88.2	19.1		
(5) Tetrose to D,L-HMTBA (through MVG)		**38.1**	**42.7**	**19.0**	**44.4**	**68.0**	**6.9**	**59.6**	**1.5**	**65.2**	**95.9**
	1	50.0	76.3	29.0	58.4	4.8	53.5	0	0		
	2	81.0	100	78.1	78.1	5.0	1.5	3.6	0		
	3	94.0	47.6	40.8	85.6	4.0	2.5	0	1.5		
(6) GA dimer to D,L-HMTBA		**35.2**	**42.7**	**12.7**	**29.6**	**650.5**	**14.5**	**634.5**	**1.5**	**641**	**98.5**
	1	37.5	82.0	17.6	21.5	556.7	11.4	545.3	0		
	2	94.0	47.6	40.8	85.6	4.0	2.5	0	1.5		

AE: Atom economy. RME: Reaction mass efficiency. OE: Optimum efficiency. PMI: process mass intensity. PMI RRC: PMI for reactants, reagents and catalysts. PMI Solv: PMI of solvents. PMI WU: PMI of species used in reaction work-ups. RI: Renewables intensity. RP: Renewables percentage.