Electronic Supplementary Material (ESI) for Green Chemistry.

SUPPORTING INFORMATION

Identification and Expression of a CHMO from *Pseudomonas aeruginosa* strain Pa1242: Application to the Bioconversion of Cyrene™ into Key Precursor (*S*)-γ-Hydroxymethyl-Butyrolactone

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Contents

DNA sequence of the cyclohexanone monooxygenase (CHMO) from *Pseudomonas aeruginosa* strain Pa1242

gtggtagcaactaaagatttcgacgccatcgtcgttggcgcagggtttggcggtctgtatatgctgaaaaaactg
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Protein sequence of the cyclohexanone monooxygenase (CHMO) from *Pseudomonas aeruginosa* strain Pa1242

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QGFQFSK

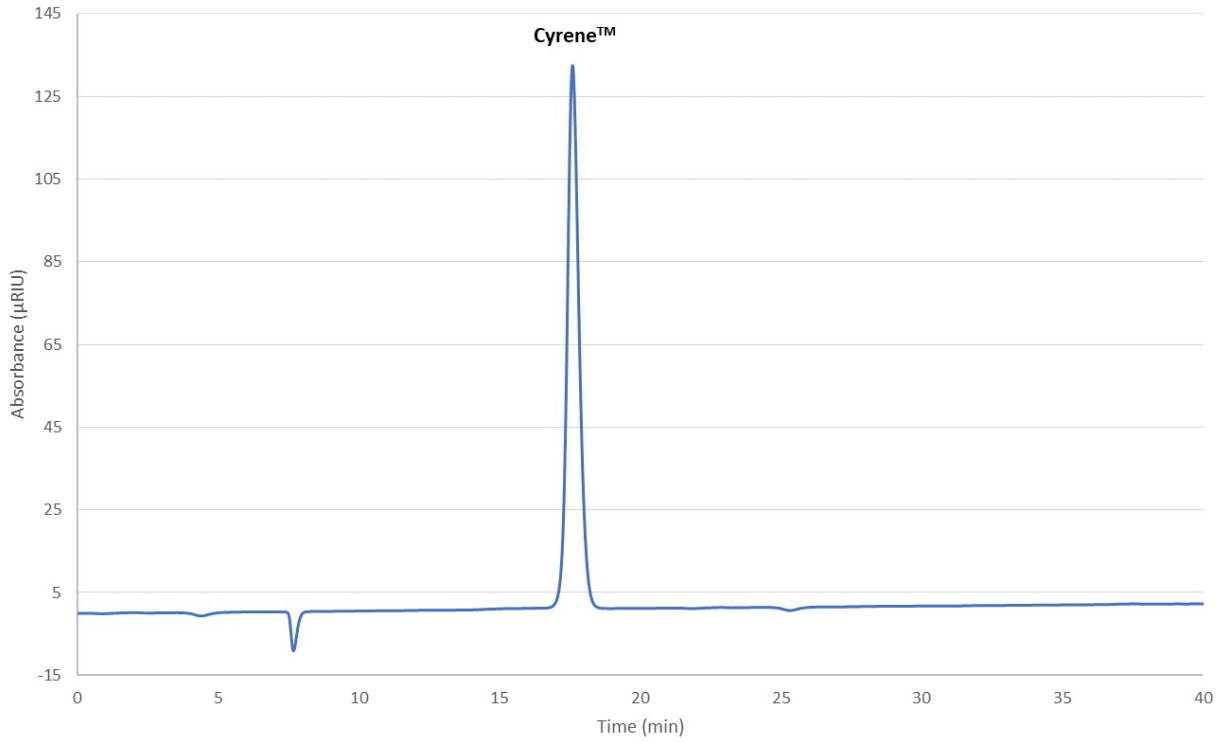
Box Behnken design for optimization of the conversion rate (experimental values calculated accordingly the consumption of Cyrene™, analyzed by HPLC)

Experimental number	Factors			Cyrene™ consumption (%)
	Glucose (g/L)	IPTG (mM)	OD_{600}	
1	4	0.1	2	44
2	40	0.1	2	72
3	4	0.5	2	44
4	4	0.5	2	72
5	40	0.3	1	44
6	4	0.3	1	57
7	40	0.3	3	34
8	4	0.3	3	74
9	40	0.1	1	60
10	22	0.5	1	53
11	22	0.1	3	75
12	22	0.5	3	77
13	22	0.3	2	73
14	22	0.3	2	74
15	22	0.3	2	75

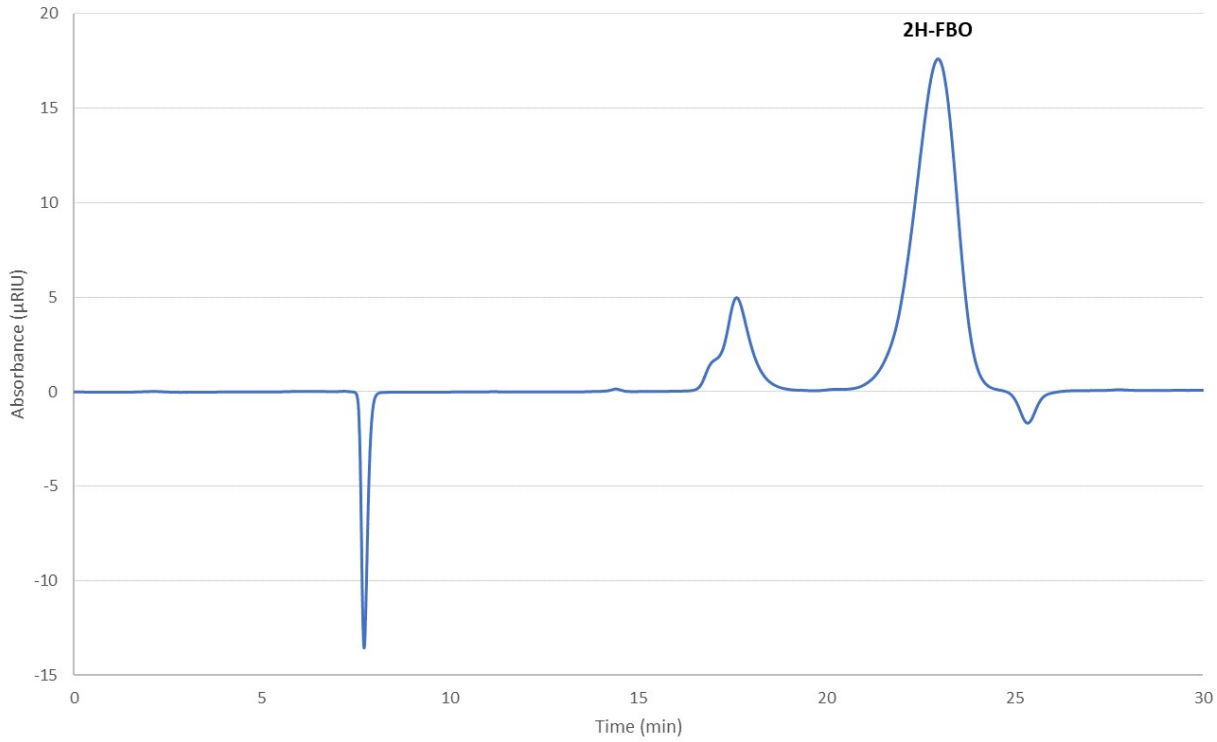
Experimental design for the influence of C/N ratio on the conversion rate (experimental values calculated accordingly the consumption of Cyrene™, analyzed by HPLC)

Experimental number	Factors			Cyrene™ consumption (%)
	Glucose (g/L)	NH_4Cl (g/L)	OD_{600}	
1	20	1	2	77
2	20	3.25	2	75
3	20	5.5	2	76
4	20	7.75	2	73
5	20	10	2	73
6	20	5.5	2	73
7	20	5.5	2	74
8	20	5.5	2	78

HPLC of standard Cyrene™



HPLC of Standard 2H-FBO



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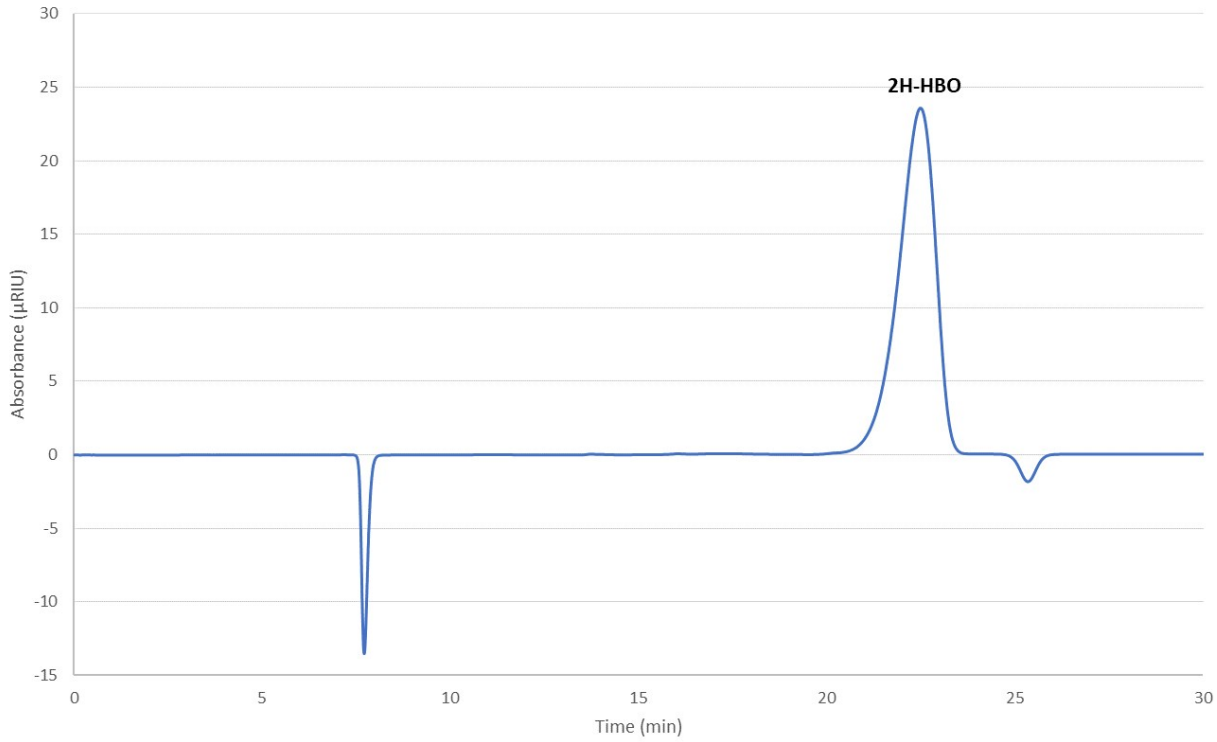
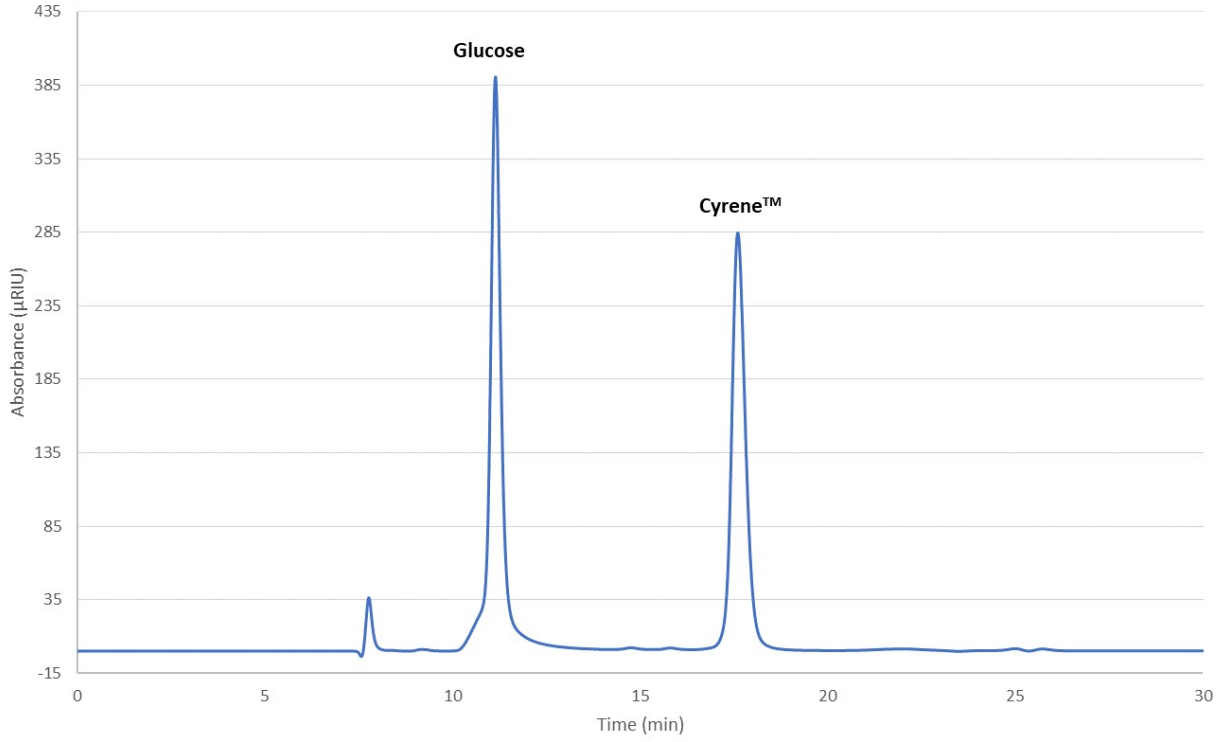
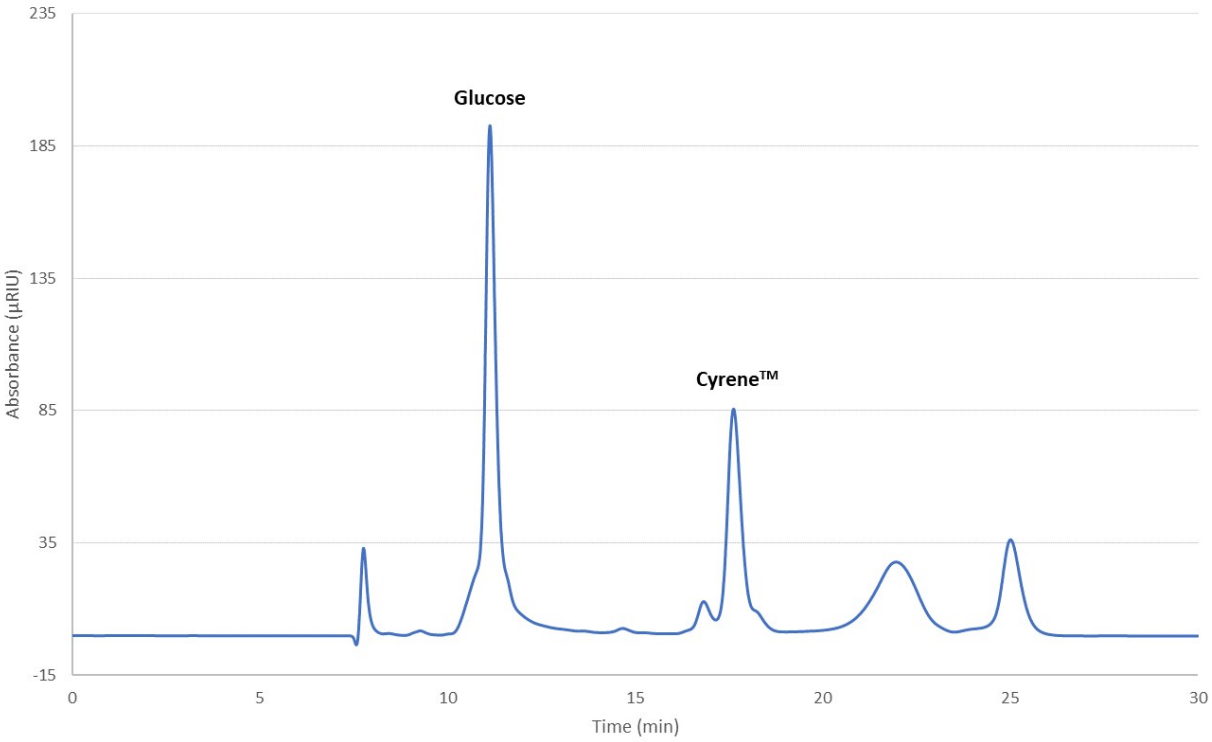


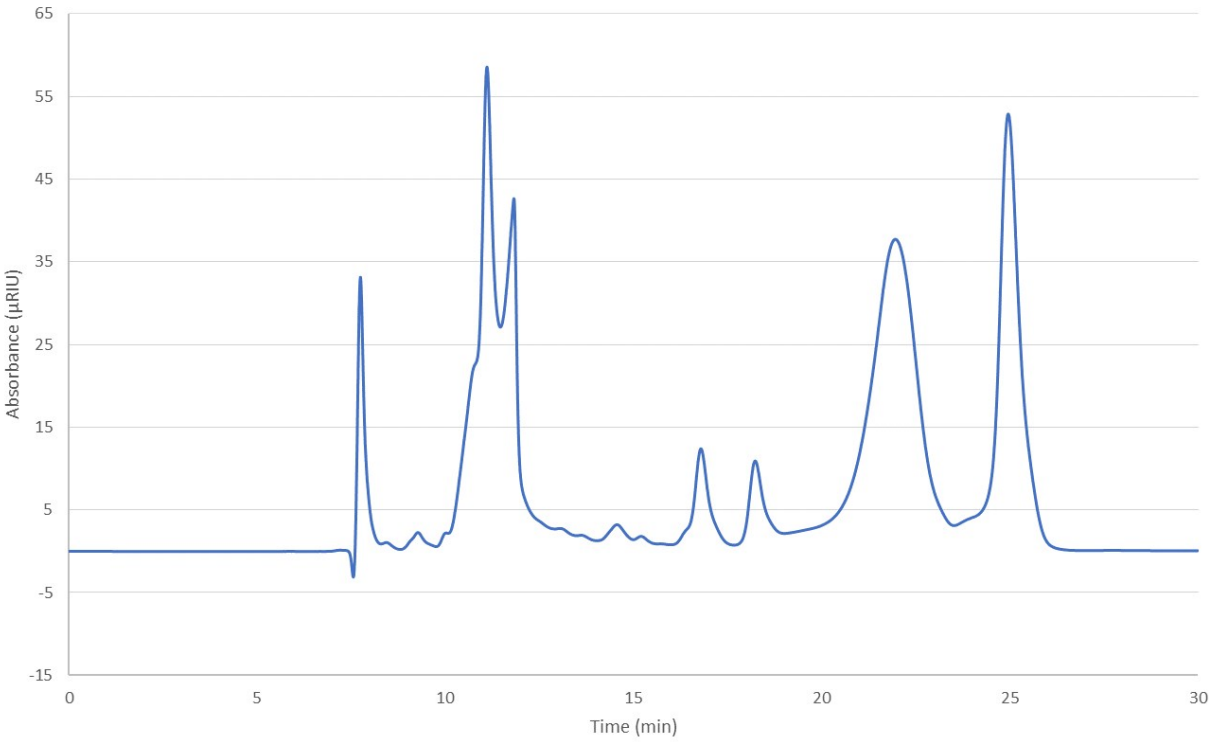
Representative HPLC of the culture media at the initial time



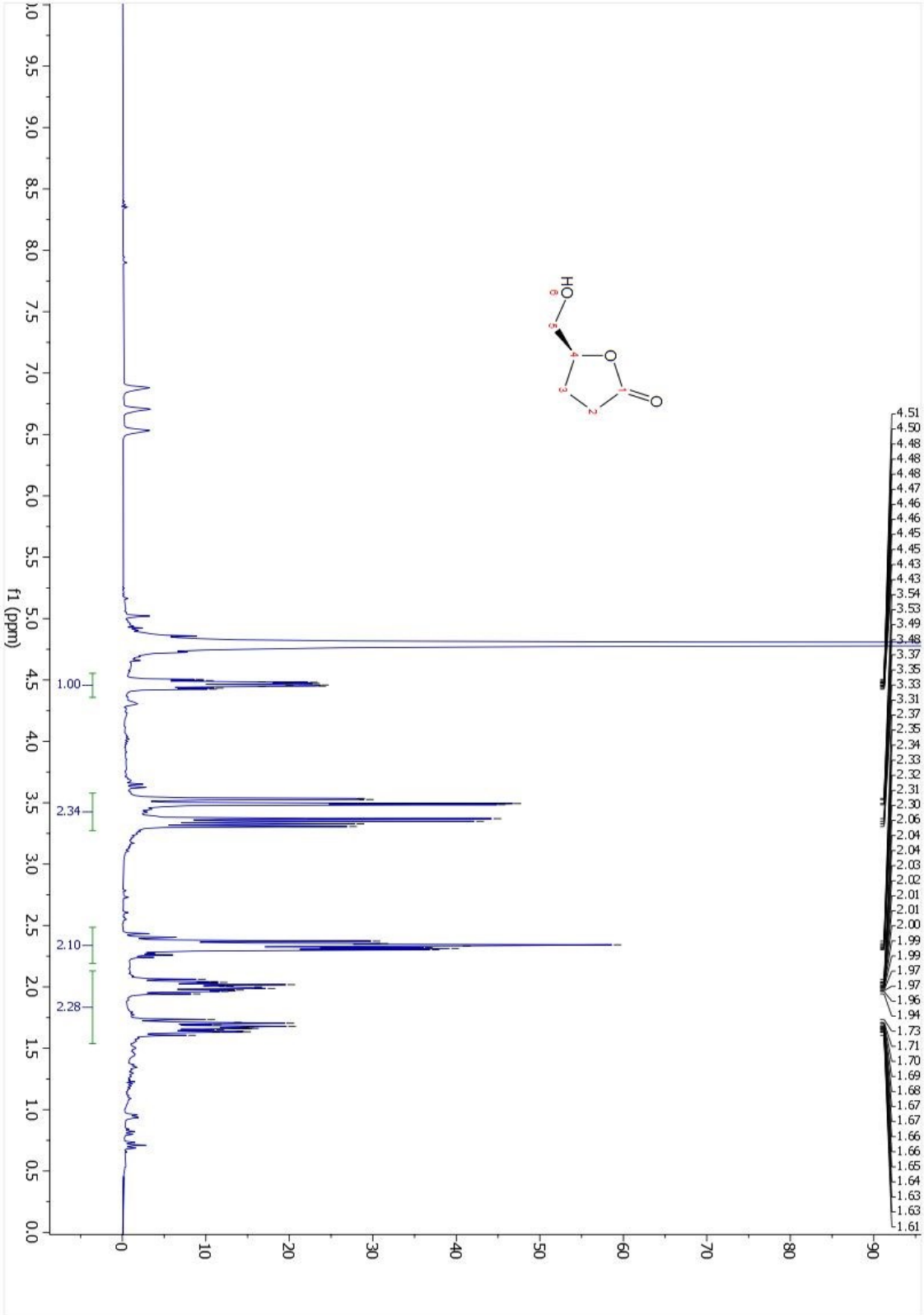
Representative HPLC of the culture media at an intermediate time



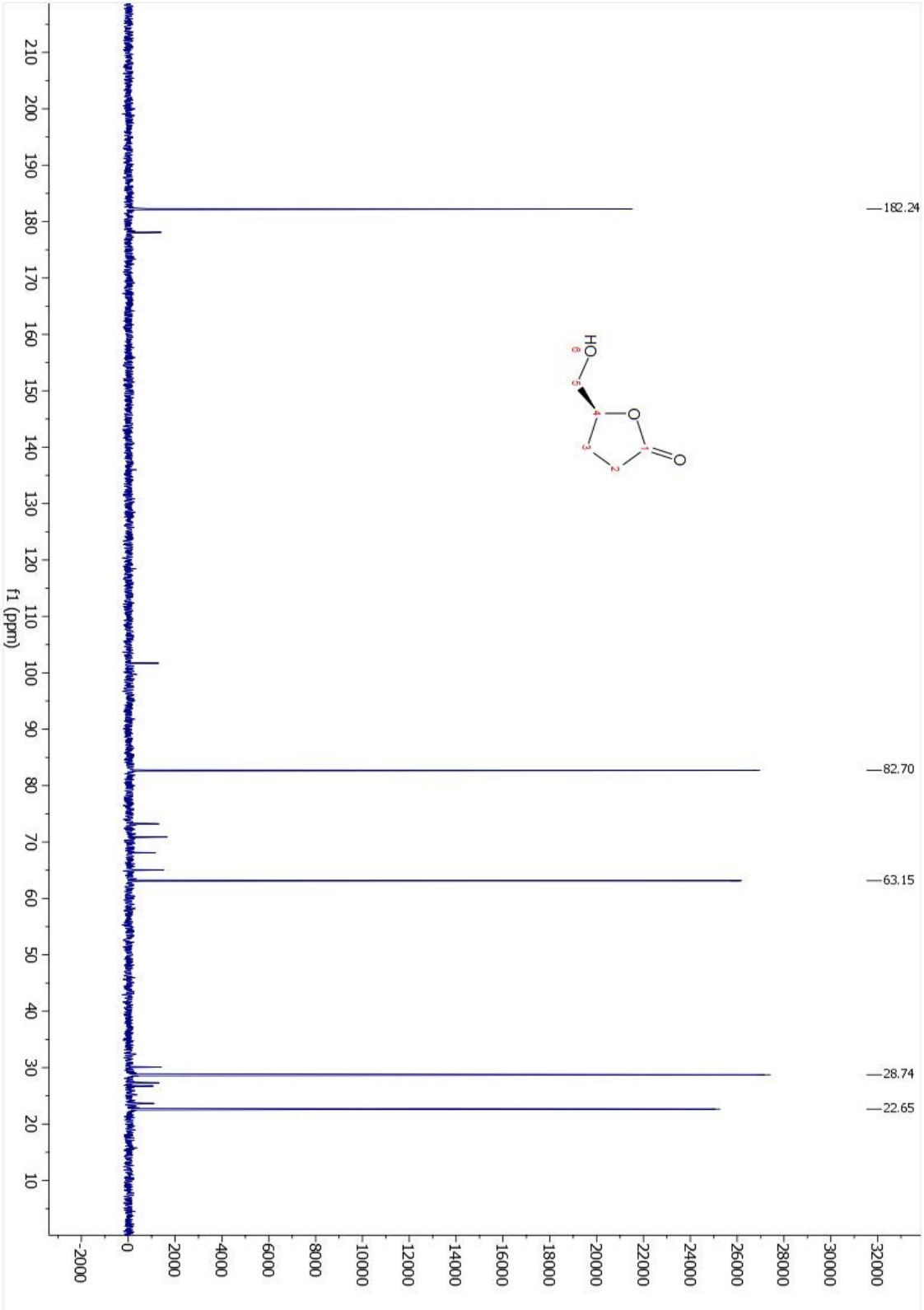
Representative HPLC of the culture media at the end of the bioconversion



^{1}H-NMR spectrum



^{13}C-NMR spectrun



Calculation of the E-factor, sEF and AE for the different processes

		Compounds		MW (g/mol)	masse (g)	n (mol)	Output compound	masse (g)	MW (g/mol)	Yield (%)	AE (%)	E factor	sEF
Koseki *et al.* *Heterocycles* 1990	Entry 1	Reagents	Cyrene	128.13	5	0.04	2H-HBO	3.94	116.05	87	41.11	18.07	1.57
			peracetic acid	76.05	3.65	0.05							
			DMSO	78.13	1.48	0.02							
		Solvent	Acetic acid	60.05	65	1.08							
			Methanol	32.04	39.5	1.23							
Flourat *et al.* *Green Chem.* 2015	Entry 2	Reagents	Cyrene	128.13	5	0.04	2H-HBO	3.4	116.05	75	58.42	26.65	10.47
			30% aq. H_2O_2	34.01	25	0.563							
			Cal-B	-	cat.	-							
			HCl	36.5	9	0.48							
		Solvent	Ethyl acetate	88.11	55	0.62							
			HEPES	238.3	2.12	0.01							
			Methanol	32.04	320	9.99							
Bonneau *et al.* *Green Chem.* 2018	Entry 3	Reagents	Cyrene	128.13	8.44	0.07	2H-HBO	5.5	116.05	72	71.57	3.83	2.01
			30% aq. H_2O_2	34.01	8.1	0.07							
		Solvent	Water	18	10	0.56							
Mouterde *et al.* 2021	Entry 4	Reagents	Cyrene	128.13	5	0.04	2H-HBO	4.07	116.05	90	90.57	63.95	1.46
			IPTG	238.31	0.0092	0.00							
			Glucose	180.15	5	0.03							
		Solvent	Na_2HPO_4	141.96	3.2	0.02							
			KH_2PO_4	136.08	0.75	0.01							
			NaCl	58.44	0.125	0.00							
			NH_4Cl	53.49	0.25	0.00							
			Water	18	250	13.89							