Supporting Information

Base Metal Iron Catalyzed Sustainable Oxidation of Vanillyl Alcohol to Vanillic Acid in Deep Eutectic Solvent and Implementation of Vanillic Acid for Fine-Chemical Synthesis

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Syntheses of ligand and corresponding iron complex

General experimental. Syntheses of ligand and iron complex were carried out in air. All solvents (acetonitrile, dichloromethane, diethyl ether, hexanes, ethyl acetate, ethanol, methanol) and chemicals were purchased from commercial suppliers and used without further purification. For recording NMR spectra, CDCl₃ and DMSO-d₆ was purchased from Sigma-Aldrich and used without further purification. ¹H and ¹³C NMR spectra were recorded at Bruker AV-400 and JEOL-400 (¹H at 400 MHz and ¹³C at 101 MHz). ¹H NMR chemical shifts are referenced in parts per million (ppm) with respect to tetramethylsilane (δ 0.00 ppm) and ¹³C (¹H) NMR chemical shifts are referenced in parts per million (ppm) with respect to CDCl₃ (δ 77.16 ppm). The coupling constants (*J*) are reported in hertz (Hz). The following abbreviations are used to describe multiplicity: s = singlet, bs = broad signal, d = doublet, t = triplet, q = quadtrate, m = multiplate. High resolution mass spectra were recorded on a Bruker micrOTOF-Q II Spectrometer. Elemental analysis was carried out on a EuroEA Elemental Analyser. Infrared (IR) spectra were recorded on a Perkin-Elmer FT-IR spectrophotometer. Crystal data were collected with Rigaku Oxford diffractometer and with INCOATEC micro source (Mo-Kα radiation, λ = 0.71073 Å, multilayer optics) at 293 K.

Synthesis of (E)-N-(2-morpholinoethyl)-1-(pyridin-2-yl)methanimine. In a pressure tube, picolinaldehyde (1.07 g, 10.0 mmol) in ethanol (5mL) was added dropwise to a solution of 2-morpholinoethan-1-amine (1.30 g,10.0 mmol) in ethanol (15mL). The reaction mixture was allowed to stirred for 24 h at 65 °C. Then the reaction mixture was cooled down to room temperature and solvent was removed under reduced pressure to obtained the pure product as reddish liquid (2.12 g, 97%). ¹H NMR (CDCl₃): δ 7.16 (t, *J*=6 Hz, 1H), 6.90 (d, *J* = 6.0 Hz, 1H), 6.85 (t, *J* = 8.0 Hz, 1H), 6.73 (t, *J*=7 Hz, 1H), 5.85 (s, 1H), 5.54 (s, 1H), 3.43 (t, *J*=4 Hz, 4H), 2.80 (t, *J*= 3 Hz, 2H), 2.66 (t, *J*=3 Hz, 2H), 2.45 (t, *J*=3 Hz, 4H), ¹³C{¹H} NMR (CDCl₃): 155.26, 125.34, 1123.69, 118.37, 114.56, 56.76, 44.68, 48.56, 44.27.

Synthesis of L1. To a solution of (E)-N-(2-morpholinoethyl)-1-(pyridin-2-yl)methanimine (2.19 g, 10.0 mmol) in methanol, NaBH₄ (1.11 g, 30 mmol) was added slowly at 0 °C and the resultant reaction mixture was stirred at r.t. for 24 hours. After completion of the reaction, all the volatiles were removed under high vacuum. The product was extracted with dichloromethane (20 mL) to give a reddish liquid as pure compound (1.98 g, 90%). ¹H NMR (CDCl₃): δ 7.19 (t, *J* = 6 Hz, 1H), 6.98 (d, *J* = 6.0 Hz, 1H), 6.87 (t, *J* = 8.0 Hz, 1H), 6.77 (t, *J*=7 Hz, 1H), 3.98 (s, 1H), 3.76 (t, *J* = 4 Hz, 4H), 2.73 (t, *J* = 3 Hz, 2H), 2.50 (t, *J* = 3 Hz, 2H),

2.43 (t, *J* = 3 Hz, 4H), ¹³C{¹H} NMR (CDCl₃): 158.29, 128.66, 128.34, 122.62, 118.94, 116.34, 66.93, 57.42, 53.61, 52.41, 44.57.

Following are the ¹H and ¹³C{¹H} NMR spectra of L_1 :



Figure S1. ¹H NMR (400 MHz) spectrum of L₁ in CDCl₃ at r.t.



Figure S2. ¹³C{¹H} NMR (400 MHz) spectrum of L_1 in CDCl₃ at r.t.



Figure S3. Mass spectrum of 1.



Figure S4. IR spectrum of L₁.



Figure S5. IR spectrum of 1.

General procedure for oxidations (reaction optimization and). Vanillyl alcohol (0.038 g, 0.25 mmol) and complex 1 (5/ 3/ 2/ 1 mol %) and TBHP (75 µL, 0.50 mmol) were taken in deep eutectic solvent (ChCl/glycerol (1:2 molar ratio): 2 mL) and was transferred into a seal tube fitted with a magnetic stir-bar. The reaction mixture was heated at appropriate temperature (r.t./ 100 °C) in an oil bath for appropriate time (1 to 12 h). Thereafter, the reaction mixture was cooled down to r.t. (in case of heating) and was extracted using ethyl acetate (3 X 5 mL). All volatiles were removed under reduced pressure to give white solid as pure product. The product was analysed by ¹H NMR spectroscopy using 1,3,5-trimethoxybenzene as standard.

Note: 20 mg complex **1** was dissolved in 4 mL of DES to prepare a stock solution. Required amounts of solutions were taken for oxidations using micropipette.

General procedure for gram-scale oxidation of vanillyl alcohol. Vanillyl alcohol (1.54 g, 10 mmol) and complex 1 (0.079 g, 0.20 mmol) and TBHP (2.8 mL) were taken in deep eutectic solvent (ChCl/glycerol (1:2 molar ratio): 20 mL) and was transferred into a seal tube fitted with a magnetic stir-bar. The reaction mixture was allowed to run for 1 hours at room temperature. Thereafter, the reaction mixture was extracted with ethyl acetate (3 X 15 mL) and all the volatiles were removed under reduced pressure to obtained white solid as pure product. The purity of product was analysed by ¹H NMR spectroscopy.

General procedure for the esterification of vanillyl alcohol. Vanillic acid (0.084 g, 0.50 mmol) and different alcohols (1.2 equivalent, 0.60 mmol) and *p*-toluenesulfonic acid (0.258 g, 1.5 mmol) were taken in dry toluene (3 mL) and transferred in a pressure tube. The reaction mixture was allowed to run for 24 h at reflux condition. After completion of the reaction the excess solvent and alcohol was removed using reduced pressure and solid was obtained. The solid was dissolved in ethyl acetate (5 mL). Then, the organic solution was washed with aqueous NaHCO₃ solutions and dried by anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure to obtain oily liquid as crude product. The crude was further characterised by ¹H NMR spectroscopy and no further purification was needed.

General procedure for the recycling of media and calculation of *E*-factor and TON:

Method A: Vanillyl alcohol (1.54 g, 10 mmol), complex **1** (0.079 g, 0.20 mmol) and TBHP (2.8 mL, 20 mmol) were taken into a round bottom flask with a magnetic stir-bar. Thereafter, deep eutectic solvent (10 ml, (ChCl/glycerol (1:2 molar ratio)) was added into the mixture. The resultant reaction mixture was allowed to run for 1 h at r.t. After completion of the reaction, the reaction mixture was extracted using ethyl acetate (2 X 10 mL) and remaining mixture of

catalyst in DES was used for next reaction run. The ethyl acetate solution was dried under high vacuum to give pure vanillic acid (1.66 g, 99%). For the second run, vanillyl alcohol (1.52 g, 10 mmol) and TBHP (1.8 ml) were added to recovered mixture of reaction media and catalyst. The resultant reaction mixture was allowed to run for 1 h at r.t. Thereafter, entire process was repeated for five times. The yields of vanillic acid in the next five runs are the following: 2^{nd} run (1.63 g, 97%), 3^{rd} run (1.63 g, 97%), 4^{th} run (1.62 g, 96%) 5^{th} run (1.62 g, 96%) and 6^{th} run (1.62 g, 96%). No significant change in catalytic activity was observed. Finally, used ethyl acetate was further recovered using solvent distillation technique (~80% recovered) and reused. The amount of media recovered is as follows: 1^{st} run: 11.90 g; 2^{nd} cycle: 11.75 g; 3^{rd} cycle: 11.64 g; 4^{th} cycle: 11.57 g; 5^{th} cycle: 11.49 g; 6^{th} cycle 11.37 g.

Overall E-factor for six consecutive reaction runs

Method A:	2 mol% of catalyst loading, r.t., 2 h in C	hCl/glycerol (1:2)
Substrate:	Vanillyl alcohol (10 mmol)	= 1.54 g
	TBHP (20 mmol)	= 2.57 g
Catalyst:	Complex 1 (2 mol %)	= 0.079 g
Solvent:	ChCl/glycerol (10 mL) x 1.190	= 11.90 g
	Ethyl acetate (20 ml) x 0.90	= 18.00 g
E factor -	mass (waste)	
E-factor –	mass (product)	
_	15.42 g (TBHP) + 0.079 g (Iron cata medium) + 18.00 g (EtOAc to e	alyst) + 11.90 g (reaction extract Vanillic acid)
_	1.64 g + 1.63 g + 1.63 g + 1.62 g +	1.62 +1.62 g (product)

= 4.65 kg waste / 1 kg of product

$$TON (1st run) = \frac{9.9 \text{ mmol (yield of vanillic acid)}}{0.2 \text{ mmol (amount of catalyst)}} = 49$$
$$TON (all 6 runs) = \frac{(9.9 + 9.7 + 9.7 + 9.6 + 9.6 + 9.6) \text{ mmol (yield of vanillic acid)}}{0.2 \text{ mmol (amount of catalyst)}} = 290$$

General procedure for the recycling of media and calculation of *E*-factor and TON: Method B: Vanillyl alcohol (1.52 g, 10 mmol), complex 1 (0.079 g, 0.20 mmol) and H_2O_2 (2.4 mL, 20 mmol) were taken into a round bottom flask with a magnetic stir-bar. Thereafter, deep eutectic solvent (10 ml, (ChCl/glycerol (1:2 molar ratio)) was added into the mixture. The resultant reaction mixture was allowed to run for 3 h at r.t. After completion of the reaction, the reaction mixture was extracted using ethyl acetate (2 X 10 mL) and remaining mixture of catalyst in DES was used for next reaction run. The ethyl acetate solution was dried under high vacuum to give pure vanillic acid (1.66 g, 99%). For the second run, vanillyl alcohol (1.52 g, 10 mmol) and H₂O₂ (0.68 mL) were added to recovered mixture of reaction media and catalyst. The resultant reaction mixture was allowed to run for 3 h at r.t. Thereafter, entire process was repeated for five times. The yields of vanillic acid in the next five runs are the following: 2nd run (1.62 g, 96%), 3rd run (1.63 g, 97%), 4th run (1.62 g, 96%) 5th run (1.62 g, 96%) and 6th run (1.61 g, 96%). No significant change in catalytic activity was observed. Finally, used ethyl acetate was further recovered using solvent distillation technique (~80% recovered) and reused. The amount of media recovered is as follows: 1st run: 11.90 g; 2nd cycle: 11.79 g; 3rd cycle: 11.65 g; 4th cycle: 11.55 g; 5th cycle: 11.50 g; 6th cycle 11.45 g.

Overall E-factor for six consecutive reaction runs

Method B: 2 mol% of catalyst loading, r.t., 3 h in ChCl/glycerol (1:2)

Substrate:	Vanillyl alcohol (10 mmol)	= 1.540 g
	H ₂ O ₂ (20 mmol)	= 2.67 g
Catalyst:	Complex 1 (2 mol %)	= 0.079 g
Solvent:	ChCl/glycerol (10 mL) x 1.190	= 11.90 g
	Ethyl acetate (20 ml) x 0.902	= 18.00 g
E-factor = -	mass (waste)	
	mass (product)	
	15.42 g (H ₂ O ₂) + 0.079 g (Iron catalys + 18.00 g (EtOAc to extra	t) + 11.9 g (reaction medium) act Vanillic acid)
=	1.66 g + 1.62 g + 1.63 g + 1.62 g +	- 1.62 +1.61 g (product)

= 4.65 kg waste / 1 kg of product

$$TON (1st run) = \frac{9.9 \text{ mmol (yield of vanillic acid)}}{0.2 \text{ mmol (amount of catalyst)}} = 49$$
$$TON (all 6 runs) = \frac{(9.9 + 9.6 + 9.7 + 9.6 + 9.6 + 9.6) \text{ mmol (yield of vanillic acid)}}{0.2 \text{ mmol (amount of catalyst)}} = 290$$

General procedure for the synthesis of vanillic diester: butyl 4-hydroxy-3-methoxybenzoate (0.112 g, 0.5 mmol) and triethylamine (104 μ L, 1.5 mmol) were dissolved in dry DCM (5 mL) in a Schlenk tube under inert condition. The mixture was stirred in an ice bath and under a N₂

atmosphere, acetyl chlorides (1.2 equivalent, 0.60 mmol) was dropped into the reaction mixture slowly for 10 min. Then, the temperature was warmed to room temperature and the mixture was reacted for 6 h. The reaction mixture was washed three times with distilled water (15 mL) and dried over with Na₂SO₄. The solution was filtered and organic solvent was removed under reduced pressure to give colourless oil as pure product. The product was further dried for 1 h under reduced pressure.

Following are the representative ¹H NMR spectra of the crude product:



Figure S6. ¹H NMR (DMSO-d₆, 400 MHz) spectrum of crude product obtained from the oxidation of vanillyl alcohol (0.25 mmol) performed at r.t. for 1 h with 2 mol% of **1** in DES. (NMR standard 1,3,5 trimethoxy benzene (0.25 mmol) is indicated with * and OCH₃ of vanillyl alcohol is indicated with *).



Figure S7. 1H NMR (DMSO-d₆ 400 MHz) spectrum of crude product obtained from the oxidation of vanillyl alcohol (0.25 mmol) performed at r.t. for 2 h with 2 mol% of **1** in DES. (NMR standard 1,3,5 trimethoxy benzene (0.25 mmol) is indicated with * and OCH₃ of vanillyl alcohol is indicated with *).

NMR data of products



Vanillic acid. Vanillic acid as white solid (42 mg, 98%) was synthesized according to the general procedure. 1H NMR (400 MHz, DMSO-d₆) δ 12.51 (bs, 1H), 9.86 (br, 1H), 7.54 – 7.33 (m, 2H), 6.84 (d, J = 8.4 Hz, 1H), 3.81 (s, 3H), ¹³C NMR (101 MHz, DMSO) δ 167.68, 151.54, 147.67, 123.93, 122.04, 115.47, 113.12, 55.97.



Methyl 4-hydroxy-3-methoxybenzoate(**E**_{1a}) methyl 4-hydroxy-3-methoxybenzoateas as colourless liquid (87 mg, 97%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl₃) δ 7.52 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.43 (d, *J* = 2.0 Hz, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.24 (bs, 1H), 3.78 (s, 3H), 3.77 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 167.12, 150.21, 146.33, 124.17, 122.02, 114.26, 111.86, 55.99, 52.01.



Ethyl 4-hydroxy-3-methoxybenzoate (**E**_{1b}). ethyl 4-hydroxy-3-methoxybenzoate as light brown liquid (94 mg, 96%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl₃) δ 7.64 (dd, J = 8.3, 1.5 Hz, 1H), 7.55 (d, J = 2.0 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 5.98 (br, 1H), 4.35 (q, J = 7.0 Hz, 2H), 3.91 (s, 3H), 1.38 (t, J = 7.0 Hz, 3H) ¹³C NMR (101 MHz, CDCl₃) δ 166.59, 150.06, 146.26, 124.09, 122.47, 114.14, 111.78, 60.86, 56.03, 14.37.



Butyl 4-hydroxy-3-methoxybenzoate (E_{1c}). butyl 4-hydroxy-3-methoxybenzoate as colourless liquid (108 mg, 97%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl3) δ 7.64 (dd, J = 8.3, 1.8 Hz, 1H), 7.56 (d, J = 2.0 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 6.38 (br, 1H), 4.30 (t, J = 6.0 Hz, 2H), 3.91 (s, 3H), 1.75 (m, 2H), 1.47 (m, 2H), 0.98 (t, J = 7.5 Hz, 3H)⁻¹³C NMR (101 MHz, CDCl3) δ 166.64, 150.05, 146.27, 124.07, 122.52, 114.13, 111.79, 64.75, 56.03, 30.82, 19.29, 13.78.



Hexyl 4-hydroxy-3-methoxybenzoate (E_{1d}). hexyl 4-hydroxy-3-methoxybenzoate as colourless liquid (118 mg, 94%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl3) δ 7.65 (dd, J = 8.3, 1.8 Hz, 1H), 7.56 (d, J = 1.8 Hz, 1H), 6.95 (d, J = 8.3 Hz, 1H), 6.31 (br, 1H), 4.30 (t, J = 6.7 Hz, 2H), 3.93 (s, 3H), 1.82 – 1.67 (m, 2H), 1.38 (m, 6H), 0.91 (t, J = 7.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl3) δ 166.61, 150.02, 146.24, 124.07, 122.56, 114.11, 111.77, 65.04, 56.04, 31.48, 28.72, 25.72, 22.56, 14.01.



Pentyl 4-hydroxy-3-methoxybenzoate (E_{1e}). Pentyl 4-hydroxy-3-methoxybenzoate as colourless liquid (117 mg, 99%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl3) δ 7.64 (dd, J = 8.3, 1.5 Hz, 1H), 7.56 (d, J = 2.0 Hz, 1H), 6.94 (d, J = 8.0 Hz, 1H), 6.37 (br, 1H), 4.29 (t, J = 7.0 Hz, 2H), 3.91 (s, 3H), 1.83 – 1.71 (m, 2H), 1.46 – 1.32 (m, 4H), 0.93 (t, J = 7.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl3) δ 166.63, 150.05, 146.27, 124.06, 122.53, 114.13, 111.79, 65.03, 56.03, 28.46, 28.21, 22.37, 13.99.



Butyl 4-acetoxy-3-methoxybenzoate (E_{2a}). butyl 4-acetoxy-3-methoxybenzoate as colourless liquid (126 mg, 95%) was synthesized according to the general procedure. 1H NMR (400 MHz, CDCl3) δ 7.71 – 7.64 (m, 2H), 7.11 (d, *J* = 8.0 Hz, 1H), 4.34 (t, *J* = 6.5 Hz, 2H), 3.90 (s, 3H), 2.34 (s, 3H), 1.84 – 1.68 (m, 2H), 1.48 (dd, *J* = 15.0, 7.5 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H). 13C NMR (101 MHz, CDCl3) δ 168.50, 165.94, 151.03, 143.52, 129.23, 122.72, 122.51, 113.40, 65.06, 56.05, 30.76, 20.63, 19.25, 13.75.



Butyl 3-methoxy-4-(propionyloxy) benzoate (E_{2b}). butyl 3-methoxy-4-(propionyloxy) benzoate as colourless liquid (151 mg, 98%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl₃) δ 7.70 – 7.63 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 4.33 (t, *J* = 6.0 Hz, 2H), 3.88 (s, 3H), 2.60 (t, *J* = 7.0 Hz, 2H), 1.81 – 1.71 (m, 4H), 1.47 (m, 4H), 0.98 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 171.35, 165.97, 151.07, 143.67, 129.07, 122.72, 122.50, 113.35, 65.02, 56.00, 33.69, 30.76, 26.98, 22.15, 19.25, 13.71,13.74.



Butyl 3-methoxy-4-(octanoyloxy)- benzoate (E_{2c}). butyl 3-methoxy-4-(octanoyloxy)benzoate as colourless liquid (173 mg, 99%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl₃) δ 7.70 – 7.63 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 1H), 4.33 (t, *J* = 6.0 Hz, 2H), 3.88 (s, 3H), 2.59 (t, *J* = 8.0 Hz, 2H), 1.76 (m, 4H), 1.42 – 1.27 (m, 10H), 0.99 (t, *J* = 7.4 Hz, 3H), 0.90 (t, *J* = 6.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 171.35, 165.96, 151.07, 143.68, 129.07, 122.72, 122.50, 113.35, 65.02, 55.98, 33.99, 31.69, 30.76, 28.95, 24.96, 22.60, 19.25, 14.06, 13.74.



Butyl 4-(dodecanoyloxy)-3-methoxybenzoat(E_{2d}). Butyl 3-methoxy-4-(octanoyloxy)benzoate as colourless liquid (197 mg, 97%) was synthesized according to the general procedure. ¹H NMR (400 MHz, CDCl₃) δ 7.69 – 7.64 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 1H), 4.33 (t, *J* = 6.0 Hz, 2H), 3.88 (s, 3H), 2.59 (t, *J* = 7.0 Hz, 2H), 1.76 (m, 4H), 1.52 – 1.41 (m, 4H), 1.28 (s, 14H), 0.98 (t, *J* = 8.0 Hz, 3H), 0.90 (t, *J* = 6.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 171.32, 165.94, 151.07, 143.68, 129.06, 122.71, 122.49, 113.34, 65.00, 55.96, 33.99, 31.91, 30.77, 29.72, 28.89, 24.96, 22.69, 19.25, 14.10, 13.74.



Figure S8. ¹H NMR (400 MHz) spectrum of **vanillic acid** in DMSO-d₆ at r.t. (* marks as water peak)



Figure S9.¹³C {¹H} NMR (101 MHz) spectrum of vanillic acid in DMSO-d₆ at r.t.



Figure S10. ¹H NMR (400 MHz) spectrum of **methyl 4-hydroxy-3-methoxybenzoate**in CDCl₃ at r.t.



Figure S11.¹³C{¹H} NMR (101MHz) spectrum of **methyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S12. ¹H NMR (400 MHz) spectrum of **ethyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S13.¹³C {¹H} NMR (101 MHz) spectrum of **ethyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.

80	3	3	លួស	66
22	r.	5	2.2	φġ



Figure S14.¹H NMR (400 MHz) spectrum of **butyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S15.¹³C {¹H} NMR (101 MHz) spectrum of **butyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S16. ¹H NMR (400 MHz) spectrum of **hexyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S17. ¹³C {¹H} NMR (101 MHz) spectrum of **hexyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.





Figure S18. ¹H NMR (400 MHz) spectrum of **pentyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S19. ¹³C{¹H} NMR (101 MHz) spectrum of **pentyl 4-hydroxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S20. ¹H NMR (400 MHz) spectrum of **butyl 4-acetoxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S21. ¹³C {¹H} NMR (101 MHz) spectrum of **butyl 4-acetoxy-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S22. ¹H NMR (400 MHz) spectrum of **butyl 3-methoxy-4-(propionyloxy) benzoate** in CDCl₃ at r.t.



Figure S23. ¹³C {¹H} NMR (101 MHz) spectrum of **butyl 3-methoxy-4-(propionyloxy) benzoate** in CDCl₃ at r.t.





Figure S24. ¹H NMR (400 MHz) spectrum of **butyl 3-methoxy-4-(octanoyloxy)benzoate** in CDCl₃ at r.t.



Figure S25. ^{13}C {¹H} NMR (101 MHz) spectrum of butyl 3-methoxy-4-(octanoyloxy)-benzoate in CDCl₃ at r.t.

-3.88 -3.89 -3.89 -3.88 -3.89 -3.88 -3.89 -3.88 -3.88 -3.88 -3.88 -3.88 -3.88 -3.88 -3.89 -3.99 -3.89 -3.99 -3 -3.99 -3.



7.07

7.68 7.68 7.68

Figure S26. ¹H NMR (400 MHz) spectrum of **butyl 4-(dodecanoyloxy)-3-methoxybenzoate** in CDCl₃ at r.t.



Figure S27. ¹³C {¹H} NMR (101 MHz) spectrum of **butyl 4-(dodecanoyloxy)-3-methoxybenzoate** in CDCl₃ at r.t.

X-ray structure determination

Crystallographic data and structure determinations details are compiled in Table S1. The crystals were obtained by slow diffusion of diethyl ether into a solution of **1** in DCM at r.t. The crystals were coated with silicon oil on a glass slide and a suitable single crystal was mounted on a glass fibre. Crystal data were collected with a Rigaku Oxford diffractometer and with an INCOATEC micro source (Mo-K α radiation, $\lambda = 0.71073$ Å, multilayer optics) at 100 K. The structure was determined using direct methods employed in ShelXT,^{S4} OleX,^{S5} and refinement was carried out using least-square minimization implemented in ShelXL.^{S6} All nonhydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atom positions were fixed geometrically in idealized positions and were refined using a riding model. CCDC 2243929 (for complex **1**) contains the supplementary crystallographic data.

Empirical formula	$C_{16}H_{25}FeN_3O_5$
CCDC	2243929
Formula weight (g mol ⁻¹)	395.24
Temperature (K)	100.00(10)
Wavelength	0.71073
Crystal system	orthorhombic
Space group	Pna2 ₁
<i>a</i> (Å)	12.6355(3)
<i>b</i> (Å)	12.7504(4)
<i>c</i> (Å)	11.0033(3)
α (deg)	90
β (deg)	90
γ (deg)	90
volume (Å ³)	1772.72(8)
Ζ	4
D_{calc} (g cm ⁻³)	1.4811
$\mu (\mathrm{mm}^{-1})$	0.882
<i>F</i> (000)	832
Crystal Size	$0.2 imes 0.2 imes 0.1 \text{mm}^3$
θ Range (deg)	7.16 to 63.74
Index Ranges	$-16 \le h \le 18, -18 \le k \le 18, -15 \le l \le$
	15
Reflections collected	18716
Independent reflections (R _{int})	$4611 [R_{int} = 0.0440, R_{sigma} = 0.0395]$
Completeness to theta = 25.07°	99.60
Refinement method	Full-matrix least-squares on F ²
Data/Restraints/parameters	4611/1/228
Goodness-of-fit on F2	0.761
Final <i>R</i> indices $[I>2\sigma(I)]$	$R_1 = 0.0315,$
	$wR_2 = 00.0913$
<i>R</i> indices (all data)	$\mathbf{R}_1 = 0.0363, \mathbf{wR}_2 = 0.0976$
Largest diff. peak/hole (e Å ⁻³)	1.39/-1.06

Table S1. Crystallographic Data and Refinement Parameters for complex 1



Figure S28. Molecular Structure of complex **1** showing 30% Ellipsoids [Hydrogen atoms are omitted for clarity. Selected bond distances (Å) and angles (deg): Fe-N1 2.207(3), Fe-N2 2.171(3); Fe-N3 2.378(3), and N1-Fe-N2 74.48(9), N1-Fe-N3 153.46(8), N2-Fe-N3 79.12(9).

Table S2.	(DES (ChC	l/glycerol (1:2)), [Fe] 2 mol%	, r.t., 1 h): Zero Pass	CHEM21 green met	rics toolkit (METHOD A)
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	Supplementary Information	ation: Ap	pendix 2		Summary o	f Zero Pas	ss Metrics Toolk	sit										
	x7' 1 1 · · · 1																	
	Yield, conversion, selec	cuvity, Al	L, KME		G (] (D (¥7.1	D 1/				*** 1 1 /	X7 1	D 1/	
	Reactant (Limiting	Mass	MW	Mol	Catalyst	Mass (g)	Reagent	Mass	Reaction solvent	Volume	Density	Mass (g)	Work up chemical	Mass	Workup solvent	Volume	Density	Mass (g)
	Reactant First)	(g)						(g)		(cm ³)	(g ml ⁻¹)			(g)		(cm3)	(g ml ⁻¹)	
	Vanillyl alcohol	1.541	154.150	0.010	[Fe]	0.790			DES	10.000	1.190	11.900			Ethyl acetate	20.000	0.902	18.040
	TBHP	1.800	90.120	0.020														
	Total	3.341	244.270			0.790						11.900		0.000				18.040
									Flag									
	molecular	weight (of product				Yield	99.1	99.1									
	$AE = \frac{1}{total molecua}$	lr weigh	t of reacto	$\frac{1}{nts} \times 10$	0		Conversion	100.0	100.0									
		Ŭ					Selectivity		99.1					mass	mw	mol		
	mass of iso	lated pro	oduct				AE	68.9					Product	1.667	168.340	0.0099026		
	$RME = \frac{1}{total mass}$	of react	ants × 10	0			RME	49.9						mass				
													Unreacted limiting					
	Solvents (Zero Pass)												reactant	0.000				
	Highly hazardous solve	nts (Red	flag for any	of the foll	owing)			L	ist Highly Hazardo	us Solvents	Below							
	Et ₂ O, Be	enzene, CO	Cl ₄ , chlorofo	m, DCE, ni	tromethane, C	CS ₂ , HMPA	1		Non	e								
	2 /	, 	*		,							_						
	Health and Safety (Zer	o Pass)																
	Health & safety (Red fl	ag for an	v of the follo	wing)			L	ist substa	nces plus the red fl	agged H-co	des below							
	Highly ex	plosive		H200,	H201, H202,	H203			None	88								
	Explosive them	nal runaw	ay		H240				None									
	Fatally	toxic		H3	00, H310, H3	30			None									
	Mutag	enic			H350				None									
Repro-toxic H360							None											
Serious environmental implications H420							None											
							1						,					

Supplementary Informa	tion: Append	lix 2		Summary	of First Pa	s Metrics Too	olkit											
Yield, AE, RME, MI/PM	MI and OE																	
Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (g)	Reagent	Mass	(g)	Reaction solvent	Volume (cm ³)	Density (g ml ⁻¹)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density (g ml ⁻¹)	Mass (g)
Vanillyl alcohol	1.541	154.150	0.010	[Fe]	0.079				DES	10.000	1.190	11.900			Ethyl acetate	20.000	0.902	18.040
TBHP	1.800	90.120	0.020									0.000						0.000
Total	3.341	244.270			0.079		0.00)				11.900		0.000				18.040
							X7: 1.1		00.1	Flag								
							Conversion	,	99.1 100.0	99.1								
							Selectivity	1	99.1	99.1					Mass	MW	Mol	
$RME = \frac{mass of isolat}{mass of isolat}$	ted product ×	100					AE		68.9				Prod	uct	1.667	168.340	0.010	
total mass of	reactants						RME		49.9	OE	72.4				mass			
molecular	weight of m	oduct											Unreacted	limiting				
$AE = \frac{motectular}{total molecular}$	weight of pi	reactants ×1	100				PMI total		20.0				react	ant	0.00			
ioiui motecuu	ir weight of	reactants					PMI Reacti	on	9.2									
ta	otal mass in	a process or	process st	tep			PMI reacta	nts,										
mass intensity = -	m	ass of produ	ct	<u> </u>			reagents, ca	atlyst	2.1									
							PMI reaction	on										
$OE = \frac{RME}{4E} \times 100$							solvents		7.1									
AL																		
							PMI Worku	ıp	10.8									
							PMI Worku	ıp										
							chemical		0.0									
							PMI worku	р										
							solvents		10.8									_
Solvents (First Pass)							Liet	colvon	te below									
Preferred solve	ents	water, EtC tBuOH, BnO	DH, nBuOH H, ethylene	, AcOipr, Ac glycol, aceto sulfolane	OnBu, PhO one, MEK, N	Me, MeOH, AIBK, AcOEt,	choline cl	loride:	glycerol (1:2)									
Problematic solvents: only if substitution doe advantages)	(acceptable es not offer	DMSO, cyc AcOMe, T MTBE, cycl o	clohexanone FHF, heptan ohexane, ch	e, DMPU, Ac ne, Me-cyclol llorobenzene, THF	OH, Ac2O, hexane, tolu formic acic	Acetonitrile, ene, xylene, I, pyridine, Me	-	NON	Æ									
Hazardous solvents: The have significant health a concerns.	nese solvents ind/or safety	dioxane, pent	tane, TEA, DMA, NMI	diisopropyl e P, methoxyet	ether, DME hanol, hexar	, DCM, DMF, æ		NON	IE.									
Highly hazardous solvents which are agre used, even in scre	vents: The ed not to be eening	Et ₂ O, Benz	æne, CCl ₄ , o	chloroform, I HMPA	OCE, nitrom	ethane, CS ₂ ,		NON	Æ									
					_													
Catalyst/enzyme (First I	Pass)		0	Tick							Tick							
Catalyst or enzyme use without any ca	d, or reaction atalyst/reager	i takes place its.	Green Flag	Х		Facile n	ecovery of a	catalyst	/enzyme	Green Flag	Х							
Use of stoichiometric	c quantities o	f reagents	Amber Flag			cataly	st/enzyme i	not reco	overed	Amber Flag								
Use of reagents in excess Red Flag																		

Table S3. (ChCl/glycerol (1:2)), [Fe] 1 mol%, r.t., 1 h): First Pass CHEM21 green metrics toolkit

Critical elements											-						
Supply remaining	Flag colour	Note	1 H]	Remaining years until depletion of	s If					2 He						
 5-50 years	Red Flag	element	1.00794 3	4 Be	known reserves (based on current rate o extraction)	of		5 6 B	c 7 N	* 9 0 F	4.002602 10 Ne						
50-500 years	Amber Flag		6.941 11	9,012182	5-50 years 50-100 years			10.811 12 13 14	0107 14.00674	15.9994 18.99840 16 17	20.1797						
+500 years	Green Flag	Fe	22.58977 19	7 24.3050 20 21	22 23 24	25 26	27 28 29	26.98153 28 30 31 32	51 P 0855 39.97376 23	32.066 35.4527 34 35	Ar 39.948 36						
			39.0983 37	Ca Sc 40.078 44.95591 58 39	Ti V Cr 47,867 50,9415 51,9961 40 41 42	Mn Fe 54.93804 55.845 43 44	Co Ni Cu 58.93320 58.0934 63.546 45 46 47	Zn Ga 6 65.39 69.723 72 48 69 50	Ge As 61 74.52160 51	Se Br 78.96 79.904 52 53	Kr 83.80 54						
			Rb 85.4678	Sr Y 87.62 88.9085	Zr Nb Mo 91.224 92.99638 95.94	Tc Ru (58) 101.07	Rh Pd Ag 102.5055 106.42 107.5082	Cd In	Sn Sb 121.760	Te l 127.60 126.9044	Xe 131.29						
			55 Cs	56 57 Ba La*	Hf Ta W	Re Os	77 78 79 Ir Pt Au 101.011 100.018 100.018	Hg TI	Pb Bi	84 85 Po At	Rn						
			87 Fr	Ra Ac ‡	104 105 106 Rf Db Sg	107 108 Bh Hs	109 110 111 Mt Ds Rq	112 113 11 Uub Uut U	115 luq Uup	116 117 Lv Uus	118 Uuo						
			(223)	226.025 (227)	(257) (260) (263)	(262) (265)	(266) (271) (272)	(285) (284) (28	9) (288)	(292)							
				Lanthanid	ss * Ce Pr I	Nd Pm	Sm Eu Gd	65 66 67 Tb Dv H	o Er	Tm Yb	⁷¹ Lu						
				cantina	140.9077 144.24 (14 50 91 00	145) 150.36 93	151.964 157.25 158.9253 94 55 95	158.9253 162.50 164. 97 98 99	100 167.26	168.9342 173.04 101 102	174.967						
				Actinide	s‡ Th Pa	U Np	Pu Am Cm	Bk Cf E	s Fm	Md No	Lr -						
					232.0381 231.0289 23	(217)	(244) (243) (247)	(247) (251) (252	(257)	(254) (259)	(262)						
Energy (First Pass)			Tick							Tick	1						
Reaction run between	0 to 70°C	Green Flag	х		React	tion run at	reflux	Red Flag									
Reaction run between -2	20 to 0 or 70	Amber Flag															
 Reaction run below -2	0 or above				Reaction run 5°C	C or more l boiling poir	below the solvent nt	Green Flag		х							
140°C		Red Flag															
Datah /Aara			Tt.L.	1	XVl- TT				-	T :4	1						
 Batch/How Flow	Greet	n Flag	Пск		work Up	quenching	7			List							
Batch	Ambe	r Flag	х			filtration	>										
					c	centrifugation	on	Green Elag	F	iltration,							
					CI	rystallisati	on	Green Thag	Ev	aporation							
					Low temperatur	ire distillati	ion/evaporation/										
					solvent exchang	ige, quenchi	ing into aqueous	Amber Flag									
					chromato	ography/ion	n exchange										
					hig	igh tempera	ture	Red Flag									
					multipl	le recrystal	llisation										
Health & safety							List substances	and H-codes	List s	substances a	nd H-codes	List su	bstances and	H-codes			
account of suffry	Red	Flag	Amb	er Flag	Green Fla	lag									1		
Highly explosive	H200, H201,	, H202, H203	g Amber Flag 02, H203 H205, H220, H224		If no red or a flagged H codes	amber es present											
Explosive thermal runaway	H230, H2	240, H250	н	241	then green f	flag						chloride	Choline	1335 11303			
Toxic	H300, H3	310, H330	H301, H	311, H331,								Glycer	ol:H319, Ethy	Acetate:			
Long Term toxicity	H340, H350, H3	H360, H370, 372	H341, H H371	351, H361, , H373								1	H225,H319,H3	36			
Environmental implications	H400, H410	, H411, H420	H401	, H412													
Use of chemica	ls of environr	mental concer	n		List substanc	ces of very	high concern										
Chemical identified as Substances of Very High Concern by Chemical identified as Substances of Very High Concern by			Red Flag														
Cilcinis																	

C 1 4 T C				6	67. D.		•.										
Supplementary Informa	penaix 2		Summary o	oi Lero Pa	ss Metrics Toolk	at											
Yield, conversion, selec	tivity, AF	, RME															
Reactant (Limiting	Mass	MW	Mol	Catalyst	Mass (g)	Reagent	Mass	Reaction solvent	Volume	Density	Mass (g)	Work up chemical	Mass	Workup solvent	Volume	Density	Mass (g)
Reactant First)	(g)			-	_	_	(g)	(g)		$(g ml^{-1})$	_	_	(g)	_	(cm3)	$(g ml^{-1})$	_
										· •						, e,	
Vanillyl alcohol	1.541	154,150	0.010	[Fe]	0.079			DES	10.000	1.190	11.900			Ethyl acetate	20.000	0.902	18,040
H2O2	0.680	34,130	0.020		0.017												
Total	0.056	188.280			0.079						11.900		0.000				18.040
								Flag									
molecular	weight d	of product		_		Yield	98.8	98.8									
$AE = \frac{1}{total molecua}$	lr wei ah	t of reacta	$\frac{1}{mts} \times 10$	0		Conversion	100.0	100.0									
		,				Selectivity	98.8	98.8					mass	mw	mol		
mass of iso	lated pro	oduct				AE	89.4					Product	1.662	168.340	0.0098729		
$RML = \frac{1}{total mass}$	of react	ants × 10	0			RME	2967.9						mass				
												Unreacted limiting					
Solvents (Zero Pass)												reactant	0.000				
Highly hazardous solve	nts (Red	flag for any	of the foll	owing)			L	ist Highly Hazardo	us Solvents	Below							
Et ₂ O, Be	enzene, CC	l ₄ , chlorofor	m, DCE, ni	tromethane, C	CS ₂ , HMPA	A		Non	e								
2 ,	,		, ,	,	2/	1											
Health and Safety (Zero	Pass)																
Health & safety (Red fl	ag for any	y of the follo	wing)			L	ist substa	nces plus the red fl	agged H-co	des below	3						
Highly ex	plosive		H200,	H201, H202,	H203			None	00								
Explosive them	nal runawa	av	,	H240				None									
Fatally	toxic	-	H3	00. H310. H3	30			None									
Mutag	enic			H350				None									
Repro-t	oxic			H360				None									
Serious environme	ntal implic	ations		H420				None									
a contra do entra onimien	in inpite					1		110110									

Table S4. (DES (ChCl/glycerol (1:2)), [Fe] 2 mol%, r.t., 3 h): Zero Pass CHEM21 green metrics toolkit (METHOD B)

Supplementary morna	anom append			Summing		b litetiteb 10													
Yield, AE, RME, MI/P	MI and OE																		
Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (g)	Reagent	Mass	(g)	Reaction solvent	Volume	(cm ³)	Density (g ml ⁻¹)	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm3)	Density (g ml ⁻¹)	Mass (g)
Vanillyl alcohol	1.541	154,150	0.010	[Fe]	0.079				DES	10.00	0	1.190	11.900			Ethyl acetate	20.000	0.902	18.040
H2O2	0.680	34.130	0.020	[10]	0.077				DLD	10.00		1.1.70	0.000			Engraceate	20.000	0.702	0.000
Total	2.221	188.280			0.079		0.00)					11.900		0.000				18.040
										Flag									
							Yield		99.0		99.0								
							Conversion	1	100.0		100.0								_
mass of isola	ted product						Selectivity		99.0	•	99.0					Mass	MW	Mol	
RME = total mass of	f reactants ×	100					AE		89.4	OF		02.0		Prod	uct	1.666	168.340	0.010	-
							KIVIE		73.0	OE		63.9		Unnegated	lineitin o	mass			
ME molecular	weight of pr	oduct	100				PMI total		10 /					reacted	ant	0.00			
total molecua	l <mark>r weight of</mark>	reactants 🔨	100				PMI React	on	8.5					react	ant	0.00			
							DMI roacto	nto											
$massintensity = \frac{t}{2}$	otal mass in	a process or	process s	tep			reagents c	nts, atlvet	1.4										
nices inconsity	m	ass of produ	ct				neugenis, ei	atiyst	1.4										
DMF							PMI reaction	on	7.1										
$OE = \frac{RML}{AE} \times 100$							solvents		7.1										
									10.0										
							PMI Worki	ıp	10.8										
							PMI Work	ıp	0.0										
							chemical		0.0										
							PMI worku	р	10.0										
							solvents		10.8	•									
Solvente (First Pass)							List	aalman	ta halam										
Preferred solv	ents	water Ft(OH nBuOH	AcOipr Ac	OnBu PhO	Me MeOH	List	sorven	ts below										
Treeffed Solv	cito	tBuOH, BnO	H, ethylene	glycol, aceto sulfolane	one, MEK, M	AIBK, AcOEt	, choline cl	nloride:	glycerol (1:2)										
Problematic solvents: only if substitution do advantages	(acceptable es not offer)	DMSO, cyc AcOMe, 1 MTBE, cycle	clohexanone THF, heptar ohexane, ch	e, DMPU, Ac ne, Me-cyclol nlorobenzene,	OH, Ac2O, nexane, tolu formic acio	Acetonitrile, ene, xylene, l, pyridine, Me	÷												
				THF				NON	IE										
Hazardous solvents: T have significant health concerns.	hese solvents and/or safety	dioxane, pen	itane, TEA, DMA, NM	diisopropyl e P, methoxyetl	ther, DME hanol, hexar	, DCM, DMF, ne		NON	Æ										
Highly hazardous so solvents which are agree used, even in scr	lvents: The eed not to be eening	Et ₂ O, Benz	zene, CCl ₄ ,	chloroform, I HMPA	OCE, nitrom	ethane, CS ₂ ,		NO											
								NON	(E										
Catalyst/enzyme (First	Pass)			Tick								Tick							
Catalyst or enzyme use without any of	ed, or reaction	takes place	Green Flag	X		Facile	recovery of o	catalyst	/enzyme	Green F	lag	X							
Use of stoichiometri	c quantities of	f reagents	Amber Flag			catal	yst/enzyme	not reco	overed	Amber F	Flag								
Use of rea	gents in excess	ŝ	Red Flag																

Table S5. (DES (ChCl/glycerol (1:2)), [Fe] 2 mol%, r.t., 3 h): Zero Pass CHEM21 green metrics toolkit (METHOD B) Supplementary Information: Appendix 2 Summary of First Pass Metrics Toolkit

Critical elements														
Supply remaining	Flag colour	Note	1 H]	Remaining years until depletion of				2 He					
 5-50 years	Red Flag	element	1.00794 3	Be	known reserves (based on current rate of extraction)		5 6 B	7 8 9 N O F	4,002602 10 Ne					
50-500 years	Amber Flag		6.941 11	9.012182	5-50 years 50-100 years		10.811 12.0 13 14	14.00674 15.9994 18.99840 15 16 17	20.1797					
+500 years	Green Flag	Fe	22.58977 19	7 24.3050 20 21	22 23 24 25	26 27 28 29	26.98153 28.9	Image: Non-Section (1) Image: Non-Section (1)<	39.948 36					
			39.0983 37	Ca Sc 40.078 44.95591 18 39	Ti V Cr Mr 47.867 50.9415 51.9961 54.533 40 41 42 43	Fe Co Ni Cu 55.845 58.93320 58.6934 63.546 44 45 46 47	Zn Ga G 65.39 69.723 72.6 48 49 50	As Se Br 1 78.92160 78.96 79.904 51 52 53	Kr 83.80 54					
			Rb 85.4678	Sr Y 87.62 88.9085	Zr Nb Mo Tc 91.224 92.99638 95.94 (98)	Ru Rh Pd Ag 101.07 102.9055 106.42 507.8482	Cd In S	n Sb Te l 121.760 127.60 126.904	Xe 131.29					
			55 Cs	Ba La*	72 73 74 75 Hf Ta W Re 100.0470 100.0470 100.0470 100.0470	76 77 78 79 Os Ir Pt Au 100.11 100.11 100.010 100.000	Hg TI P	b Bi Po At	Rn					
			87 Fr	88 89 Ra Ac ‡	101 100,000 101 100,000 104 105 106 107 Rf Db Sg Bh	108 109 130 111 Hs Mt Ds Rq	112 113 114 Uub Uut U	115 116 117 Uuq Uup Lv Uus	118 Uuo					
			(223)	226.025 (227)	(257) (260) (263) (262)	(265) (266) (271) (272)	(285) (284) (289	(288) (292)						
				Lanthanid	es* Ce Pr Nd	61 62 63 64 Pm Sm Eu Gd	65 66 67 Tb Dy He	68 69 70 Er Tm Yb	n Lu					
					140.9077 144.24 (145) 50 91 92	150.36 151.964 157.25 158.9253 93 94 95 96	158.9253 162.50 164.9 97 98 99	03 167.26 168.9342 173.04 100 101 102	174.967					
				Actinide	es‡ Th Pa U	Np Pu Am Cm	Bk Cf E	Fm Md No	Lr					
					232.0381 231.0289 238.0289	(237) (244) (243) (247)	(247) (251) (252)	(257) (258) (259)	(262)					
Energy (First Pass)			Tick					Tick						
Reaction run between	0 to 70°C	Green Flag	х		Reaction	run at reflux	Red Flag							
Reaction run between -2	20 to 0 or 70	Amber Flag			0-									
 Reaction run below -?	0 or above		<u></u>		boiling point G			х						
140°C		Red Flag				51								
Datah /Aara			Tt.L.		XX anda Tim			T :	_					
Flow	Greet	n Flag	TICK		work Up	enching		List						
Batch	Ambe	r Flag	х		fil	tration								
					centr	ifugation	Green Flag	Filtration,						
					cryst	allisation	Green Plag	Evaporation						
					Low temperature d	istillation/evaporation/								
					sublimation (< 1) solvent exchange, o	40 C at atmospheric quenching into aqueous	Amber Flag							
					chromatogra	nhv/ion exchange								
					high to	emperature	Red Flag							
					multiple re	crystallisation								
Health & asfaty						List substances	and H-codes	List substances	and H-codes	List su	bstances and	H-codes		
rieanth & safety	Red	Flag	Amb	er Flag	Green Flag									
Highly explosive	H200, H201,	, H202, H203	H205, H	220, H224	If no red or amb flagged H codes pr	er								
Explosive thermal	H230, H2	240, H250	н	241	then green flag					chloride	Choline H315,H319,H	335,H303		
Toxic	H300, H3	310, H330	H301, H	311, H331,						Glycero	ol:H319, Ethyl	Acetate:		
Long Term toxicity	H340, H350, H3	H360, H370, 372	H341, H3 H371	351, H361, , H373						H225,H319	9,H336, Hydro H0904	gen perxode		
Environmental	H372 H371, H373 H400, H410, H411, H420 H401, H412		, H412											
impications														
Use of chemica	ls of environr	mental concer	n		List substances	of very high concern								
Chemical identified as Substances of Very High Concern by Red Fla				Red Flag										
Criems	ce which are t	uniscu												

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