

Supplementary Information

Preparation, Characterisation and Evaluation of Brazilian Clay-Based Catalysts for use in Esterification Reactions

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Data for calculation of the response factors of acids and esters standards

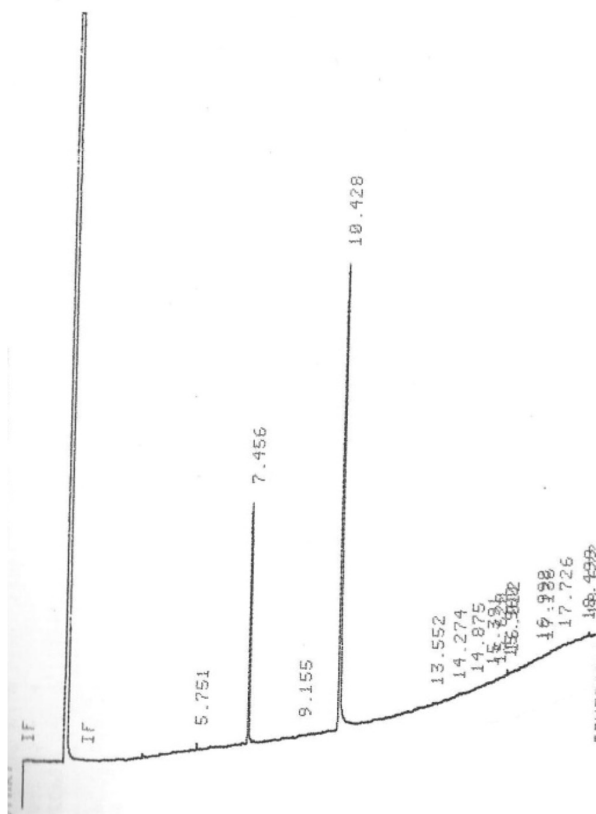


Figure S1. Chromatogram of lauric acid (t_R 10.4 min) and internal standard (t_R 7.5 min).

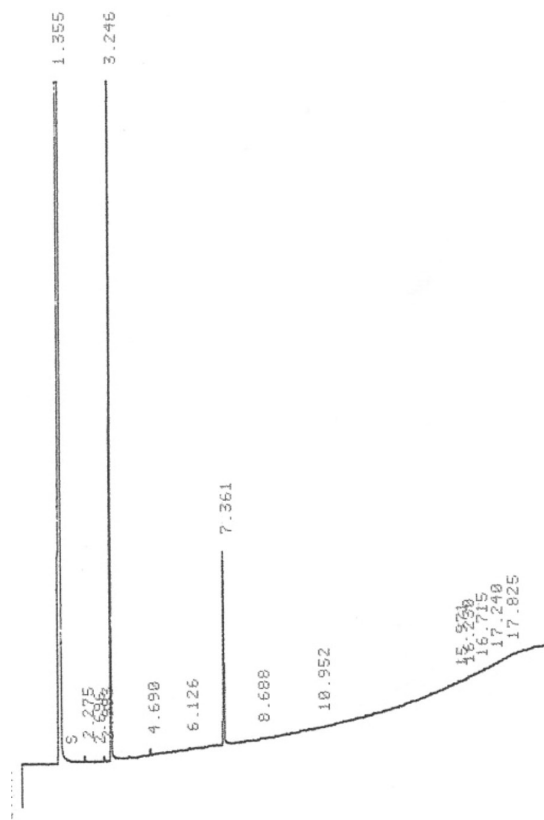


Figure S2. Chromatogram of methyl laurate (t_R 3.2 min) and internal standard (t_R 7.4 min).

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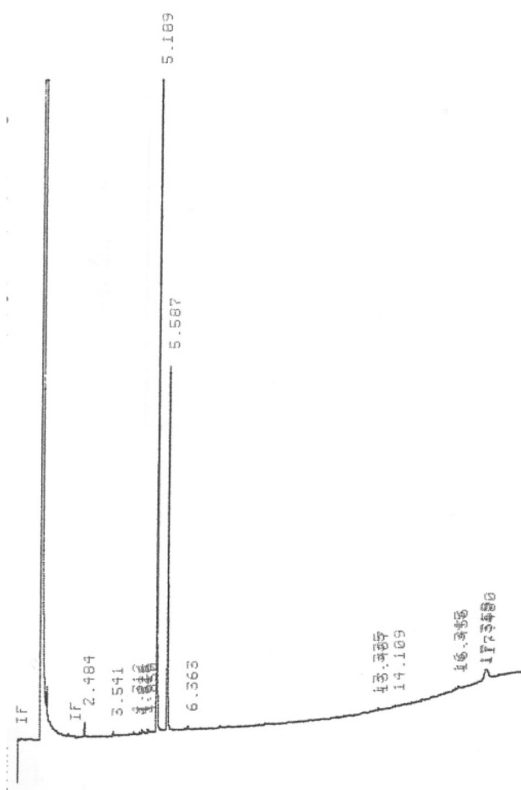


Figure S3. Chromatogram of hexyl laurate (t_R 5.2 min) and internal standard (t_R 5.6 min).

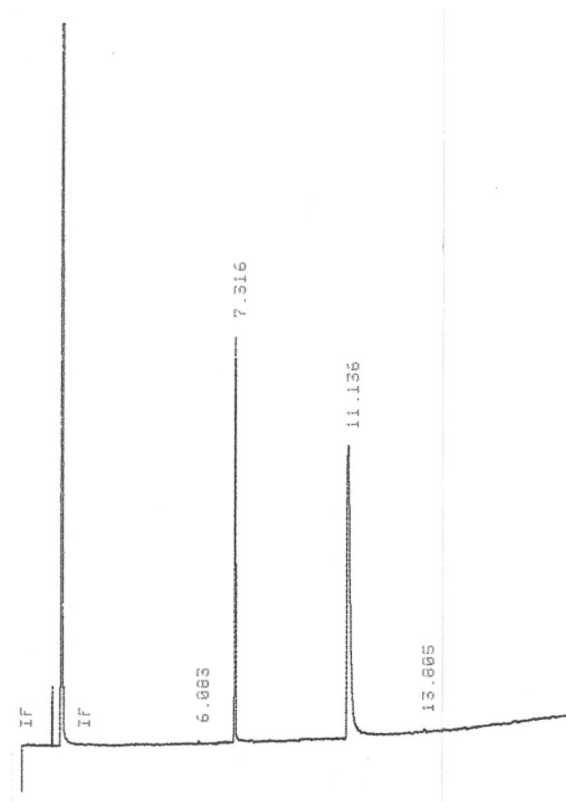


Figure S5. Chromatogram of phenylacetic acid (t_R 11.1 min) and internal standard (t_R 7.3 min).

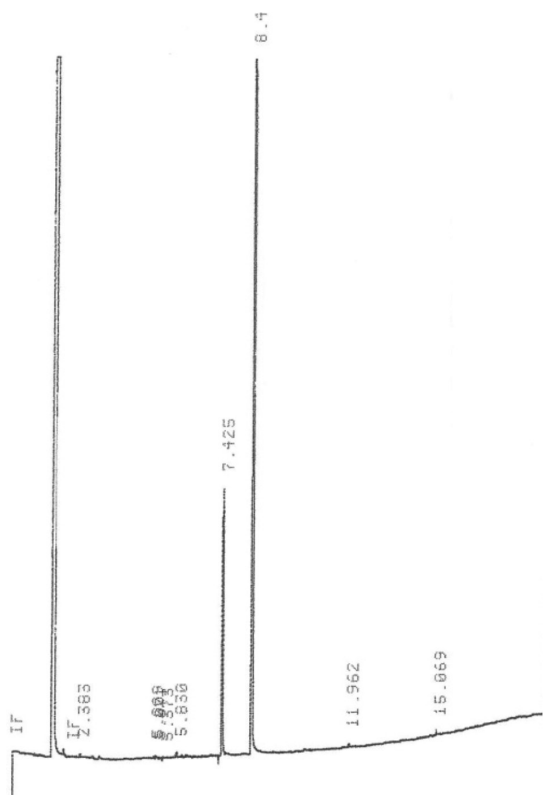


Figure S4. Chromatogram of cyclohexyl laurate (t_R 8.4 min) and internal standard (t_R 7.4 min).

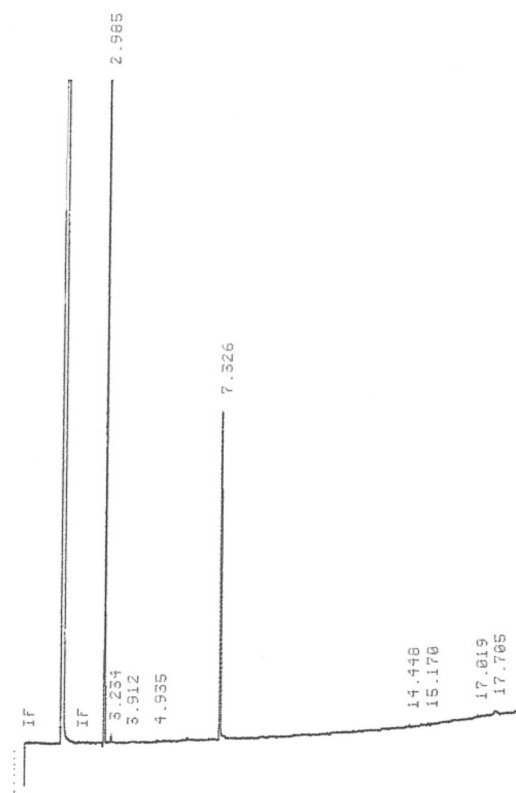


Figure S6. Chromatogram of methyl phenylacetate (t_R 3.0 min) and internal standard (t_R 7.3 min).

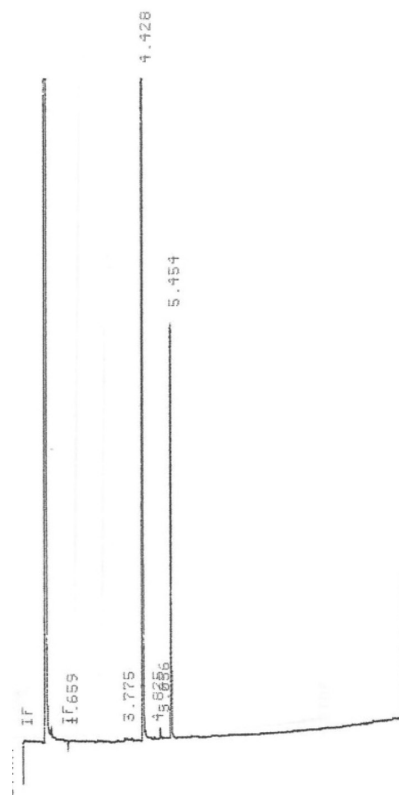


Figure S7. Chromatogram of hexyl phenylacetate (t_R 4.4 min) and internal standard (t_R 5.4 min).

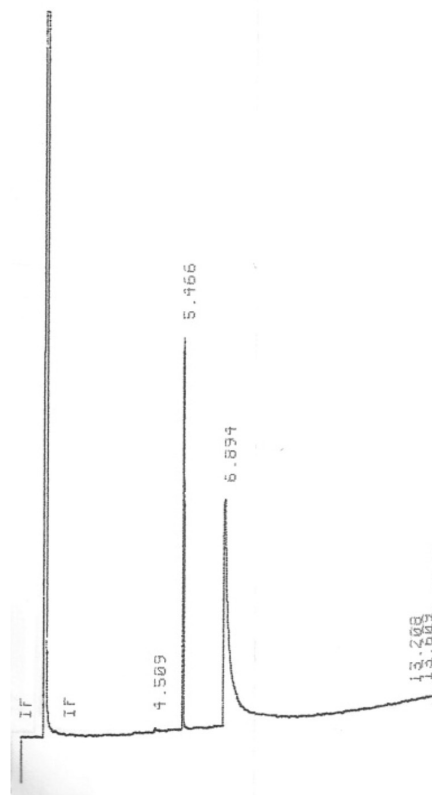


Figure S9. Chromatogram of benzoic acid (t_R 6.9 min) and internal standard (t_R 5.5 min).

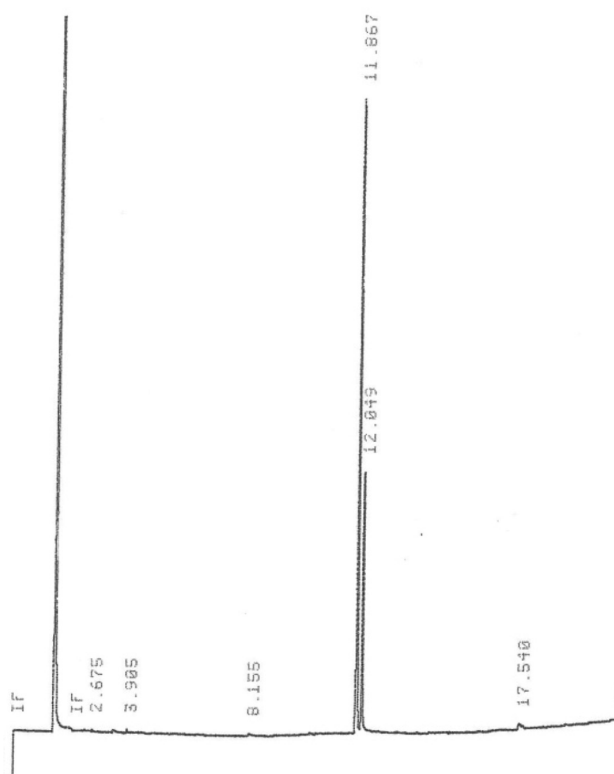


Figure S8. Chromatogram of cyclohexyl phenylacetate (t_R 11.9 min) and internal standard (t_R 12.0 min).

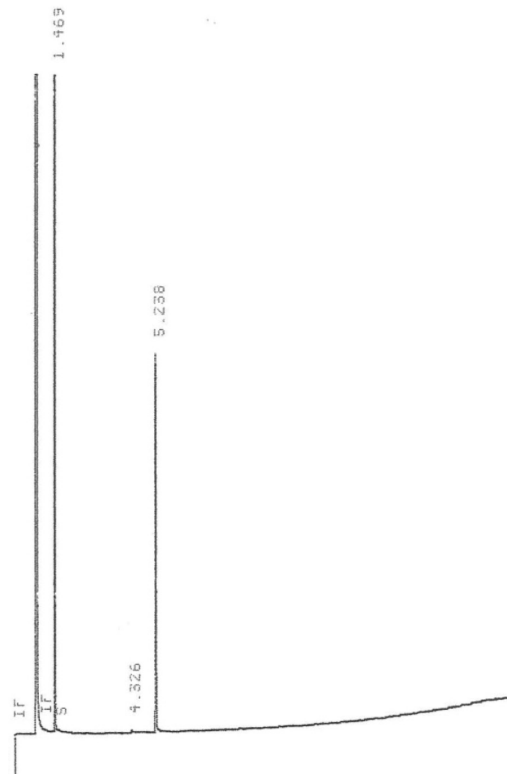


Figure S10. Chromatogram of methyl benzoate (t_R 1.5 min) and internal standard (t_R 5.2 min).

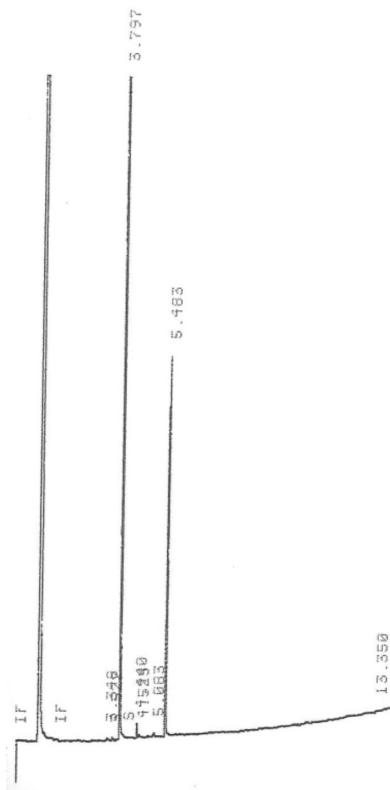


Figure S11. Chromatogram of hexyl benzoate (t_R 3.8 min) and internal standard (t_R 5.5 min).

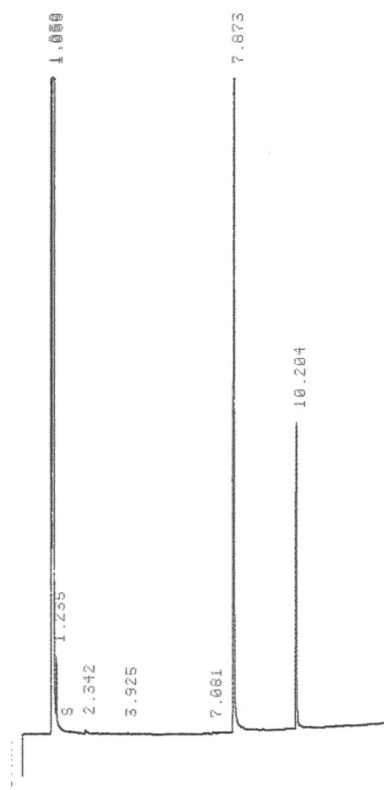


Figure S13. Chromatogram of cyclohexanoic acid (t_R 7.9 min) and internal standard (t_R 10.2 min).

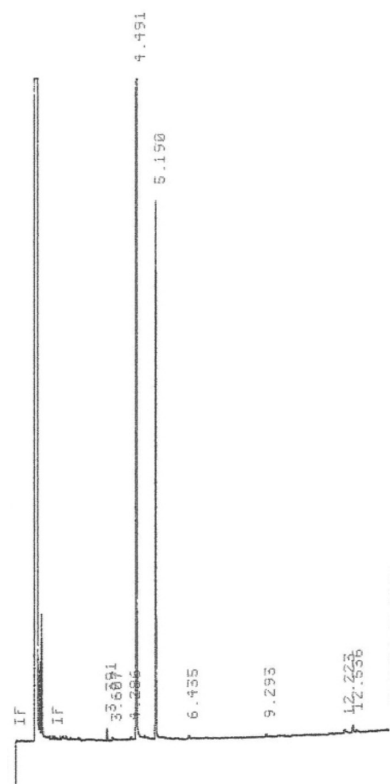


Figure S12. Chromatogram of cyclohexyl benzoate (t_R 4.5 min) and internal standard (t_R 5.2 min).

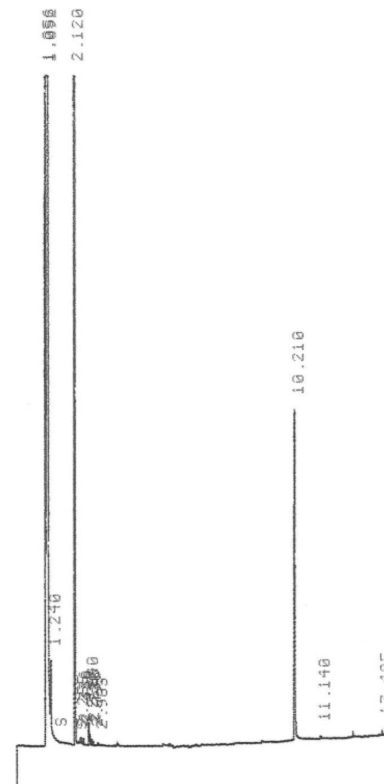


Figure S14. Chromatogram of methyl cyclohexanoate (t_R 2.1 min) and internal standard (t_R 10.2 min).

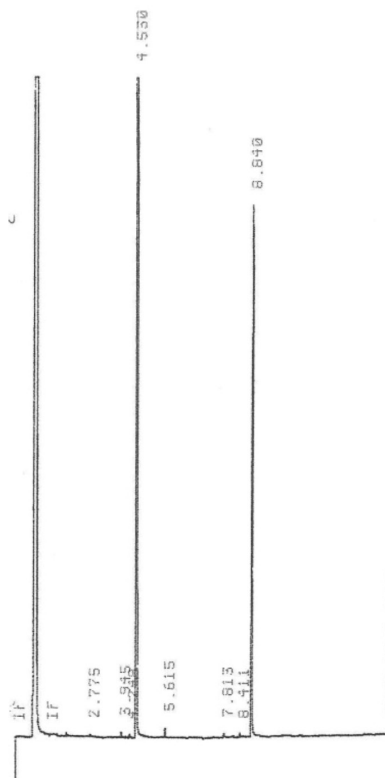


Figure S15. Chromatogram of hexyl cyclohexanoate (t_R 4.5 min) and internal standard (t_R 8.8 min).

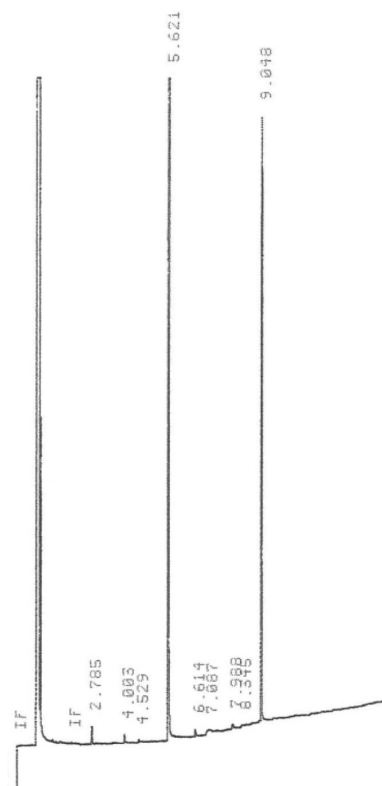


Figure S16. Chromatogram of cyclohexyl cyclohexanoate (t_R 5.6 min) and internal standard (t_R 9.0 min).

Table S1. Data for calculation of the response factors of acids and esters standards

Standard	S _{Area}	S _{Conc}	IS _{Area}	IS _{Conc}	F _R	F _R
lauric acid	218841	1020	83333	268	0.690	0.684
lauric acid	216720	1020	83928	268	0.678	
methyl laurate	492794	1040	71675	268	1.772	1.758
methyl laurate	539675	1040	79744	268	1.744	
cyclohexyl laurate	412109	1630	77671	268	0.872	0.876
cyclohexyl laurate	506955	1630	94774	268	0.879	
hexyl laurate	323411	1330	107778	238.5	0.538	0.534
hexyl laurate	368092	1330	124750	238.5	0.529	
phenylacetic acid	384842	1620	136902	248	0.430	0.421
phenylacetic acid	378276	1620	140893	248	0.411	
methyl phenylacetate	438196	1410	156421	248	0.493	0.509
methyl phenylacetate	366980	1410	122895	248	0.525	
cyclohexyl phenylacetate	1366540	1710	144943	248	1.367	1.375
cyclohexyl phenylacetate	1394862	1710	146311	248	1.383	
hexyl phenylacetate	904087	1670	122677	239	1.055	1.054
hexyl phenylacetate	927589	1670	126073	239	1.053	
cyclohexanoic acid	412674	1340	108036	265.5	0.757	0.727
cyclohexanoic acid	372292	1340	105803	265.5	0.697	
methyl cyclohexanoate	728707	1940	112690	265.5	0.885	0.913
methyl cyclohexanoate	596780	1940	86712	265.5	0.942	
cyclohexyl cyclohexanoate	891191	1630	159304	238.5	0.818	0.827
cyclohexyl cyclohexanoate	1070347	1630	187300	238.5	0.836	
hexyl cyclohexanoate	2038730	2870	167994	241	1.019	1.021
hexyl cyclohexanoate	1993908	2870	163741	241	1.022	
benzoic acid	262536	960	98661	265.5	0.736	0.756
benzoic acid	249880	960	89095	265.5	0.776	
methyl benzoate	263392	940	92042	265.5	0.808	0.806
methyl benzoate	279626	940	98359	265.5	0.803	
cyclohexyl benzoate	640039	1850	104871	238.5	0.787	0.785
cyclohexyl benzoate	568059	1850	93466	238.5	0.783	
hexyl benzoate	874892	1630	116861	239	1.098	1.101
hexyl benzoate	863688	1630	114751	239	1.104	

S_{Area} = standard area; S_{Conc} = standard concentration at mg L⁻¹; IS_{Area} = internal standard area; IS_{Conc} = internal standard concentration at mg L⁻¹; F_R = response factor; F_R = (S_{Area}/S_{Conc})/(IS_{Area}/IS_{Conc}).

Table S2. Oven temperature program used on GC-FID analyses

Product	Oven temperature program	tR / min		
		acid	ester	IS
methyl phenylacetate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	8.7	3.0	5.4
hexyl phenylacetate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	8.7	4.4	5.4
cyclohexyl phenylacetate	5 min at 140 °C followed to 180 °C at 8 °C min ⁻¹ . After 3 min at 180 °C followed to 220 °C at 3 °C min ⁻¹	17.6	11.9	12.0
methyl laurate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	8.1	1.4	5.5
hexyl laurate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	8.1	5.1	5.5
cyclohexyl laurate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	8.1	8.4	5.5
methyl benzoate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	6.9	1.5	5.2
hexyl benzoate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	6.9	3.8	5.5
cyclohexyl benzoate	140 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 220 °C at 3 °C min ⁻¹	6.9	4.5	5.2
methyl cyclohexanoate	100 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 200 °C at 3 °C min ⁻¹	6.9	1.5	9.0
hexyl cyclohexanoate	100 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 200 °C at 3 °C min ⁻¹	6.8	4.5	8.8
cyclohexyl cyclohexanoate	100 °C to 180 °C at 10 °C min ⁻¹ followed by 180 °C to 200 °C at 3 °C min ⁻¹	6.9	5.6	9.0