

Supplementary Materials: GC×GC-TOFMS for the Analysis of Metabolites Produced by Termites (*Reticulitermes flavipes*) Bred on Different Carbon Sources

Catherine Brasseur, Julien Bauwens, Cédric Tarayre, Catherine Millet, Christel Mattéotti, Philippe Thonart, Jacqueline Destain, Frédéric Francis, Eric Haubruge, Daniel Portetelle, Micheline Vandenberg, Edwin De Pauw and Jean-François Focant

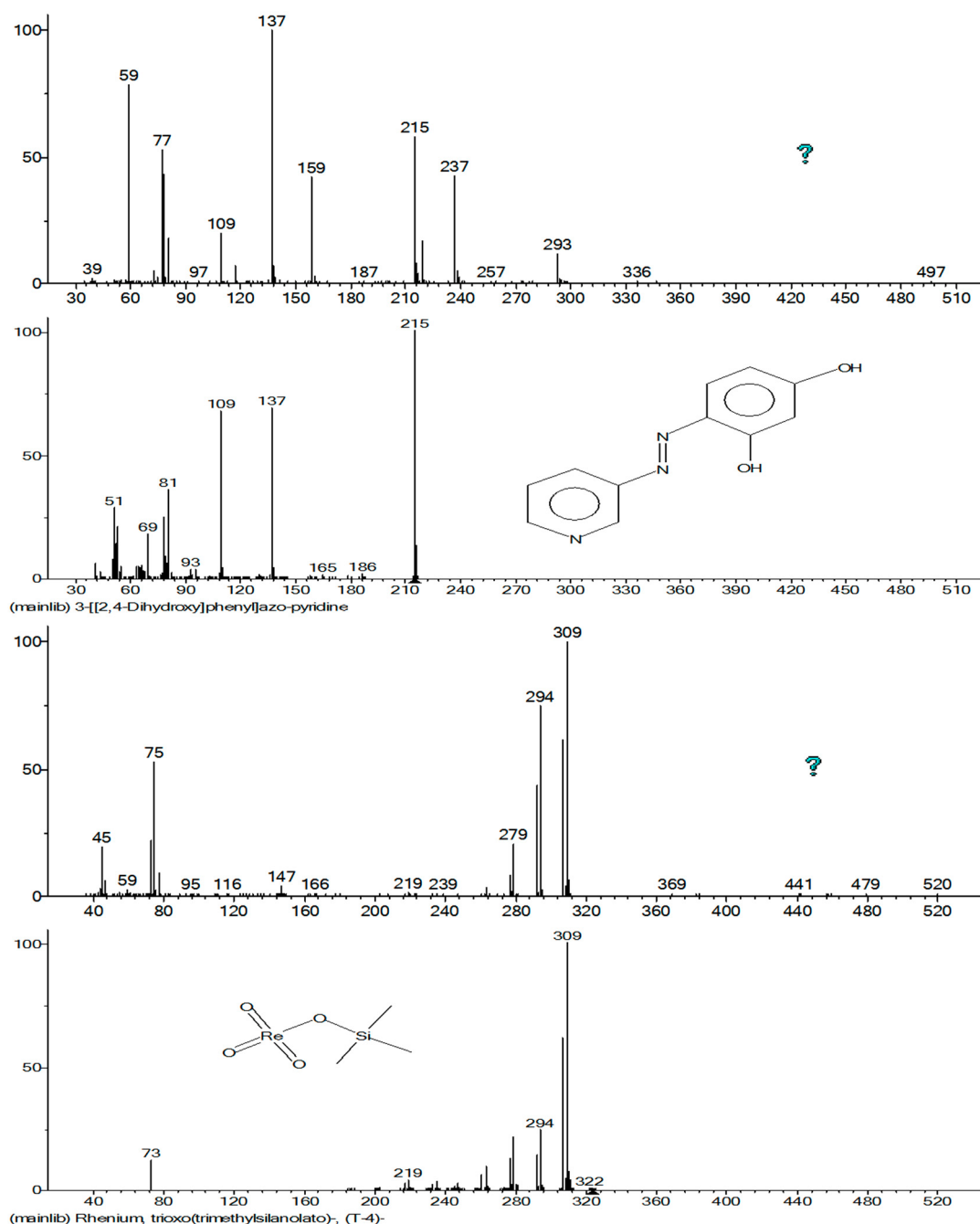


Figure S1. Mass spectra of unwanted peaks detected during two-dimensional gas chromatography-time-of-flight mass spectrometry (GC×GC-TOFMS) analysis of derivatized termite gut samples.

Table S1. Retention Times of metabolites identified in the termite guts.

Compound Name	Retention 1D (min)		Retention 2D (s)	
	Mean	Stdev	Mean	Stdev
Lactic acid	11.73	0.05	0.66	0.02
Caproic acid	11.96	0.07	0.71	0.02
Alanine	12.16	0.06	0.77	0.02
Valine	13.61	0.04	1.15	0.05
<i>N</i> -Methylvaleramide	14.04	0.05	0.66	0.01
Leucine	14.45	0.09	1.25	0.03
Asparagine	14.47	0.05	0.83	0.02
1,2,4-butanetriol	14.71	0.05	1.66	0.02
Isoleucine	14.74	0.04	1.32	0.04
Glycine	14.98	0.09	1.42	0.03
Benzoic acid	15.04	0.03	1.17	0.03
Glyceric acid	15.32	0.04	1.36	0.05
Serine	15.90	0.09	1.48	0.03
Phenylacetic acid	16.04	0.07	1.27	0.03
Phosphite	16.21	0.09	0.80	0.03
Threonine	16.22	0.07	1.62	0.03
2-Ketovaline	16.64	0.06	0.84	0.04
Succinic Acid	16.67	0.08	1.18	0.02
Meso-Erythritol	16.86	0.09	2.12	0.06
Phosphate	17.37	0.11	1.00	0.03
<i>N</i> -acetyl-lysine	17.42	0.07	1.95	0.03
Beta-Alanine	17.69	0.07	1.62	0.02
Fumaric acid	17.76	0.08	1.20	0.03
Phenylpropanoic acid	18.16	0.08	1.60	0.02
2-Piperidone	18.20	0.03	1.75	0.04
Pentose isomer	18.56	0.08	1.64	0.04
Malic acid	19.38	0.07	1.61	0.03
Erythrose	19.57	0.07	1.30	0.02
Xylose	19.68	0.06	2.72	0.06
Aspartic acid	20.01	0.06	1.75	0.06
Ornithine	20.62	0.03	2.31	0.07
Arabitol	21.02	0.06	2.81	0.06
Hexopyranosiduronic acid	21.07	0.06	2.45	0.08
2-Ketoglutaric acid	21.19	0.05	1.80	0.03
Phenylalanine	21.53	0.08	2.17	0.07
Putrescine	21.92	0.04	2.97	0.05
Glutamic acid	22.14	0.04	1.95	0.06
Nicotinamide	22.61	0.04	1.41	0.03
5-oxoproline	23.30	0.04	1.52	0.07
Fructose	23.70	0.07	3.00	0.11
Galactose	24.06	0.06	2.85	0.12
Citric acid	25.44	0.04	2.14	0.06
Pipecolic acid	25.61	0.04	1.59	0.10
Fructopyranose-P	26.14	0.04	2.09	0.06
Glutamine	26.64	0.09	2.11	0.07
Inositol isomer	27.08	0.03	3.33	0.04
Tyrosine	27.18	0.07	2.84	0.04
Inositol myo-	28.52	0.06	3.35	0.07
Uric acid	29.24	0.27	3.05	0.09

Table S2. Peak volume of metabolites identified in the termite guts.

Compound Name	Volume					
	Mean (Avicel)	Mean (Wood)	Mean (Xylan)	Stdev (Avicel)	Stdev (Wood)	Stdev (Xylan)
Lactic acid	7,966,770	6,500,200	7,328,819	2,531,798	3,404,378	1,516,848
Caproic acid	1,443,527	779,050	1,462,738	758,764	435,781	78,775
Alanine	6,157,507	7,119,423	4,452,419	2,914,036	3,352,259	321,798
Valine	12,842,712	15,594,834	15,468,511	4,227,079	10,178,527	1,737,128
N-Methylvaleramide	14,134,738	9,081,414	12,289,882	4,607,522	4,640,259	235,706
Leucine	9,481,363	8,177,785	6,184,592	3,256,629	4,684,283	1,611,280
Asparagine	1,106,653	1,028,114	1,066,256	56,253	542,383	120,583
1,2,4-butanetriol	558,560	744,904	2,014,048	232,461	601,644	111,880
Isoleucine	9,157,640	7,156,224	5,527,126	2,252,799	4,133,871	1,360,223
Glycine	18,484,615	16,394,324	16,044,483	2,052,782	8,164,320	2,915,100
Benzoic acid	1,269,645	1,995,883	1,246,058	264,493	966,069	73,180
Glyceric acid	9,358,802	6,263,126	4,735,452	2,578,346	3,122,969	422,216
Serine	9,219,931	9,420,392	10,531,554	3,430,868	5,013,039	1,377,227
Phenylacetic acid	439,896	327,472	852,336	55,607	198,891	93,260
Phosphite	21,336,770	17,472,915	17,695,657	7,885,749	8,608,444	1,474,419
Threonine	1,1154,304	10,442,844	9,523,935	5,259,316	5,589,448	1,249,982
2-Ketovaline	643,610	335,033	424,001	459,923	167,957	22,280
Succinic Acid	4,384,527	4,511,203	5,297,680	1,186,606	2,119,314	2,273,916
Meso-Erythritol	2,605,120	3,097,940	11,468,811	789,616	1,627,251	2,607,774
Phosphate	16,129,522	11,807,699	14,767,078	2,952,783	4,668,995	841,521
N-acetyl-lysine	1,800,173	1,281,210	1,732,478	278,526	547,449	150,855
Beta-Alanine	2,831,937	2,270,661	5,167,730	324,988	1,106,423	2,118,531
Fumaric acid	850,746	878,332	863,000	72,654	451,097	68,488
Phenylpropanoic acid	242,173	454,438	209,213	10,802	233,745	30,821
2-Piperidone	7,274,717	3,936,497	5,368,777	806,391	1,822,893	1,062,102
Pentose isomer	1,432,518	1,126,171	1,465,597	79,972	551,158	78,797
Malic acid	3,368,639	3,313,371	4,141,091	350,491	2,000,101	157,945
Erythrose	421,199	447,117	994,950	56,605	233,535	354,354
Xylose	1,871,902	3,334,081	3,585,588	286,698	2,147,230	851,462
Aspartic acid	12,085,511	10,018,994	7,504,551	1,862,150	5,184,443	598,325
Ornithine	9,241,322	7,134,426	8,784,488	1,270,020	3,766,047	311,726
Arabitol	882,309	1,177,997	2,792,054	164,513	511,550	914,427
Hexopyranosiduronic acid	935,148	1,086,185	1,571,457	78,339	490,242	364,769
2-Ketoglutaric acid	1,540,141	817,570	2,473,778	550,814	418,598	1,025,053
Phenylalanine	6,283,158	4,182,455	5,579,822	1,928,412	2,173,422	787,021
Putrescine	14,204,309	8,125,982	9,748,637	1,467,078	4,429,097	1,747,980
Glutamic acid	12,443,635	7,963,943	8,040,707	2,724,438	4,199,323	796,168
Nicotinamide	3,719,044	2,688,559	2,874,446	806,357	1,411,716	195,741
5-oxoproline	30,155,892	18,740,275	17,059,053	5,833,850	10,067,767	1,545,885
Fructose	4,061,666	3,296,394	2,891,539	338,166	1,621,817	557,004
Galactose	3,026,816	2,994,672	1,901,408	694,037	2,159,068	229,834
Citric acid	34,568,660	22,994,282	18,058,545	4,452,942	13,743,164	1,569,831
Pipecolic acid	5,872,385	3,872,976	4,347,298	470,840	1,962,292	693,751
Fructopyranose-P	10,895,044	5,488,584	3,028,676	2,551,501	2,856,835	331,498
Glutamine	3,035,765	1,669,050	1,520,446	1,343,521	907,838	176,329
Inositol isomer	24,410,558	11,216,122	15,974,510	10,336,922	5,862,506	1,484,465
Tyrosine	21,096,572	10,934,314	5,671,344	8,267,746	6,514,885	617,348
Inositol myo-	17,083,578	15,544,552	7,234,282	6,022,485	7,790,154	1,296,088
Uric acid	348,593,151	44,607,685	235,417,671	51,349,956	39,708,151	97,109,424

Table S3. Percent Response of metabolites identified in the termite guts.

Compound Name	Percent Response					
	Mean (Avicel)	Mean (Wood)	Mean (Xylan)	Stdev (Avicel)	Stdev (Wood)	Stdev (Xylan)
Lactic acid	0.169	0.190	0.179	0.044	0.032	0.034
Caproic acid	0.030	0.022	0.036	0.014	0.004	0.005
Alanine	0.134	0.210	0.108	0.068	0.007	0.006
Valine	0.277	0.429	0.376	0.094	0.147	0.016

<i>N</i> -Methylvaleramide	0.301	0.266	0.301	0.085	0.038	0.029
Leucine	0.206	0.229	0.149	0.081	0.049	0.028
Asparagine	0.024	0.030	0.026	0.000	0.004	0.004
1,2,4-butanetriol	0.012	0.021	0.049	0.005	0.011	0.004
Isoleucine	0.198	0.200	0.133	0.057	0.045	0.024
Glycine	0.398	0.477	0.388	0.063	0.041	0.035
Benzoic acid	0.027	0.059	0.031	0.005	0.005	0.004
Glyceric acid	0.199	0.182	0.115	0.044	0.015	0.004
Serine	0.200	0.270	0.258	0.082	0.038	0.041
Phenylacetic acid	0.009	0.009	0.021	0.001	0.002	0.005
Phosphite	0.463	0.514	0.430	0.186	0.055	0.006
Threonine	0.243	0.298	0.232	0.123	0.045	0.029
2-Ketovaline	0.014	0.010	0.010	0.009	0.001	0.001
Succinic Acid	0.094	0.133	0.128	0.026	0.006	0.049
Meso-Erythritol	0.056	0.090	0.280	0.018	0.013	0.065
Phosphate	0.345	0.362	0.362	0.060	0.033	0.054
<i>N</i> -acetyl-lysine	0.039	0.039	0.042	0.006	0.003	0.001
Beta-Alanine	0.061	0.067	0.125	0.007	0.005	0.044
Fumaric acid	0.018	0.025	0.021	0.002	0.003	0.002
Phenylpropanoic acid	0.005	0.013	0.005	0.0001	0.002	0.0003
2-Piperidone	0.156	0.117	0.132	0.019	0.011	0.033
Pentose isomer	0.031	0.033	0.036	0.002	0.004	0.004
Malic acid	0.072	0.093	0.101	0.010	0.025	0.009
Erythrose	0.009	0.013	0.024	0.001	0.003	0.008
Xylose	0.040	0.091	0.089	0.007	0.031	0.028
Aspartic acid	0.260	0.293	0.183	0.044	0.043	0.017
Ornithine	0.199	0.205	0.215	0.036	0.028	0.030
Arabitol	0.019	0.036	0.069	0.004	0.007	0.028
Hexopyranosiduronic acid	0.020	0.032	0.038	0.003	0.001	0.007
2-Ketoglutaric acid	0.033	0.024	0.061	0.012	0.003	0.026
Phenylalanine	0.136	0.121	0.137	0.045	0.016	0.025
Putrescine	0.305	0.231	0.239	0.034	0.039	0.050
Glutamic acid	0.269	0.232	0.197	0.069	0.038	0.027
Nicotinamide	0.080	0.077	0.070	0.019	0.010	0.005
5-oxoproline	0.648	0.535	0.415	0.131	0.080	0.027
Fructose	0.087	0.096	0.071	0.004	0.007	0.013
Galactose	0.065	0.080	0.047	0.017	0.037	0.009
Citric acid	0.745	0.635	0.440	0.131	0.168	0.027
Pipecolic acid	0.126	0.112	0.107	0.016	0.011	0.023
Fructopyranose-P	0.233	0.159	0.074	0.053	0.022	0.001
Glutamine	0.066	0.050	0.037	0.033	0.012	0.001
Inositol isomer	0.521	0.327	0.392	0.212	0.049	0.066
Tyrosine	0.457	0.307	0.138	0.190	0.080	0.002
Inositol myo-	0.365	0.452	0.177	0.124	0.040	0.031
Uric acid	7.50	1.18	5.65	1.40	0.83	2.20