

Supplementary Material of:

Molecular characterization of gaseous and particulate oxygenated compounds at a remote site in Cape Corsica in the western Mediterranean basin.

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Supplementary material 1:
Identification and quantification of compounds during ChArMEx campaign.
DMM : Derivatized Molar Mass ; MM : Molar Mass ; MS : Mass Spectra ; RT : Retention Time ; QL : Quantification Limit ; ND : Not Detected

Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification methods	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
Carbonyl Compounds													
EI : 117, 161, 181, 236	253	1	58	Propanal		0.33 10 ^{-0.5}	Standard Rossignol (2012) Müller et al. (2006)	Butanal-d8	Pentanal	181	200 ± 69	181	10 ± 1
EI : 117, 181, 195, 197, 198, 251	251	1	56	Acroleine		0.33 10 ^{-0.7}	Standard Rossignol (2012) Jaoui et al. (2014)	3-Methylbutanal-d2	Methacrolein	181	734 ± 125	DMM	6 ± 1
EI : 43, 181, 239, 250, 267	267	1	72	Methylpropanal		0.25 10 ^{-0.8}	MS/RT Rossignol (2012)	3-Methylbutanal-d2	2-Ethylbutanal	ND	ND	43	1 ± 0,4
EI : 43, 57, 181, 195, 250	267	1	72	2-Butanone (= Methyl Ethyl Ketone)		0.25 10 ^{-0.8}	Standard Müller et al. (2006)	2-Hexanone-d5	2-Hexanone-d5	DMM – 181	230 ± 18	DMM	blank
EI : 41, 69, 181, 265	265	1	75	Methacrolein		0.25 10 ^{-1.0}	Standard Healy et al. (2008)	3-Methylbutanal-d2	Methacrolein	DMM	230 ± 16	DMM	2 ± 1
EI : 42, 56, 69, 99, 117, 181, 195, 264, 265	265	1	75	Methyl Vinyl Ketone (= 3-Buten-2-one)		0.25 10 ^{-1.0}	Standard Healy et al. (2008)	2-Hexanone-d5	3-Buten-2-one	181	539 ± 30	DMM	3 ± 0,5
EI : 41, 56, 131, 181, 195, 235, 264	267	1	72	Butanal		0.25 10 ^{-0.9}	Standard Müller et al. (2006)	Butanal-d8	Pentanal	181	88 ± 75	181	blank
EI : 58, 100, 181, 221, 253, 281 CI : 282, 310, 322	281	1	86	3-Methyl-2-butanone		0.2 10 ^{-1.2}	MS/RT/Nist Rossignol (2012)	2-Hexanone-d5	2-Hexanone-d5	ND	ND	DMM	1 ± 1
EI : 46, 93, 117, 181, 195, 218, 281	281	1	86	3-Pentanone		0.2 10 ^{-1.3}	MS/RT Rossignol (2012)	2-Hexanone-d5	2-Butanone	181	< QL	ND	ND
EI : 43, 71, 167, 181, 195, 252, 264, 281 CI : 282, 310, 322	281	1	86	2-Methylbutanal		0.2 10 ^{-1.3}	MS/RT	Butanal-d8	Pentanal	ND	ND	181	1 ± 1
EI : 41, 55, 69, 161, 181, 222, 239	281	1	86	Pentanal		0.2 10 ^{-1.4}	Standard Müller et al. (2006)	Butanal-d8	Pentanal	181	303 ± 129	DMM - 42	2 ± 0,4
EI : 72, 94, 117, 181, 197, 236, 253, 277	295	1	100	2-Hexanone		0.17 10 ^{-1.7}	Standard Berndt et al. (2003)	2-Hexanone-d5	2-Hexanone	DMM - 42	85 ± 4	72	blank
EI : 43, 181, 278, 293 CI : 294, 322, 334	293	1	98	4-Hexen-3-one		0.17 10 ^{-2.0}	MS/RT/Nist	/	/	ND	ND	181	blank

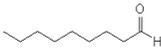
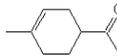
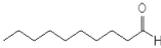
Identification and quantification of compounds during ChArMEx campaign.

DMM : Derivatized Molar Mass ; MM : Molar Mass ; MS : Mass Spectra ; RT : Retention Time ; QL : Quantification Limit ; ND : Not Detected

Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification methods	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 43, 181, 278, 293 CI : 294, 322, 334	293	1	98	5-Hexen-3-one		0.17 10 ^{-1.7}	MS/RT/Nist	/	/	ND	ND	181	blank
EI : 43, 98, 117, 131, 161, 181, 264, 279	279	1	84	3-Methyl-2-butenal		0.2 10 ^{-1.5}	Standard	3-Methylbutanal-d2	3-Methyl-2-butenal	DMM - 15	< QL	181	<QL
EI : 41, 55, 72, 86, 181, 230, 267, 309	309	1	114	3-Heptanone		0.14 10 ^{-2.2}	MS/RT/Nist Rossignol (2012)	/	/	ND	ND	DMM	<QL
EI : 41, 66, 82, 114, 161, 181, 239	295	1	100	Hexanal		0.17 10 ^{-1.8}	MS/RT/Nist Rossignol (2012)	Butanal-d8	Pentanal	181	311 ± 247	181	3 ± 0.5
EI : 41, 99, 161, 181, 222, 239, 252, 295	295	1	100	4-Methylpentanal		0.17 10 ^{-1.7}	MS/RT/Nist	2-Hexanone-d5	2-Ethylbutanal	ND	ND	43	20 ± 1
EI : 128, 181, 253, 309 CI : 310, 338, 350	309	1	114	2-Heptanone		0.14 10 ^{-2.2}	MS/RT/Nist Rossignol (2012)	2-Hexanone-d5	4-Heptanone	ND	ND	DMM	< QL
EI : 62, 110, 181, 248, 291	291	1	96	2-Furaldehyde		0.4 10 ^{-2.1}	MS/RT/Nist	Benzaldehyde-d6	Pentanal	DMM	blank	ND	ND
EI : 41, 67, 82, 112, 161, 181, 263, 276, 293	293	1	98	Cyclohexanone		0.17 10 ^{-2.1}	MS/RT/Nist Rossignol (2012) Hamilton et al. (2004)	Acetophenone-d8	2-Butanone	181	744 ± 109	181	blank
EI : 41, 55, 69, 99, 128, 161, 181, 222, 239	309	1	114	Heptanal		0.14 10 ^{-2.3}	Standard Müller et al. (2006)	Butanal-d8	Pentanal	181	421 ± 122	181	2 ± 0.5
EI : 51, 65, 77, 103, 106, 167, 181, 258, 315	315	1	120	m-Tolualdehyde		0.13 10 ^{-3.3}	MS/RT/Nist	Acetophenone-d8	3-Methyl-2-butenal	DMM	407 ± 47	ND	ND
EI : 41, 55, 69, 82, 99, 124, 142, 169, 181, 222, 239	323	1	128	Octanal		0.13 10 ^{-2.7}	MS/RT/Nist Rossignol (2012) Müller et al. (2006)	Butanal-d8	Pentanal	ND	ND	181	blank
EI : 41, 55, 72, 117, 236, 253, 280, 322 CI : 338, 366, 378	337	1	142	2,6-Dimethyl-4-heptanone		0.11 10 ^{-2.9}	MS/RT	2-Hexanone-d5	4-Heptanone	ND	ND	181	1 ± 1
EI : 39, 51, 65, 77, 89, 181, 271, 301	301	1	106	Benzaldehyde		0.14 10 ^{-2.8}	Standard Müller et al. (2006)	Benzaldehyde-d6	Pentanal	181	586 ± 144	181	blank
EI : 41, 50, 77, 106, 181, 258, 315	315	1	120	Acetophenone		0.13 10 ^{-3.1}	Standard Hamilton et al. (2004)	Acetophenone-d8	2-Butanone	ND	ND	181	blank

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Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification method	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 41, 55, 69, 81, 99, 117, 156, 161, 181, 222, 239	337	1	142	Nonanal		0.11 10 ^{-3.2}	MS/RT/Nist Rossignol (2012) Matsunaga et al. (2003)	Butanal-d8	Pentanal	ND	ND	181	blank
EI : 181, 221, 253, 276, 290	333	1	138	Nopinone		0.11 10 ^{-3.3}	Standard Cahill et al, (2006)	2-Hexanone-d5	Nopinone	DMM - 43	673 ± 44	DMM - 43	3 ± 0,3
EI : 41, 79, 95, 110, 152, 181, 290 CI : 334, 362, 374	333	1	138	Ketolimone		0.11 10 ^{-3.2}	MS/RT Rossignol (2012)	Acetophenone-d8	2-Butanone	181	<QL	ND	ND
EI : 41, 55, 69, 83, 99, 117, 161, 181, 222, 239	351	1	156	Decanal		0.10 10 ^{-3.6}	MS/RT/Nist Rossignol (2012) Matsunaga et al. (2003)	Butanal-d8	Pentanal	181	2809 ± 192	181	1 ± 0,5
EI : 99, 117, 161, 181, 195, 239, 448	448	2	58	Glyoxal		1.0 10 ^{-1.6}	Standard Matsunaga et al. (2004)	2,3-Butanedione-d6	Glyoxal	DMM	3017 ± 184	DMM - 197	1 ± 0,2
EI : 41, 55, 161, 181, 195, 222, 239, 265, 462	462	2	72	Methylglyoxal		0.67 10 ^{-1.2}	Standard Matsunaga et al. (2004)	2,3-Butanedione-d6	Methylglyoxal	DMM - 197	700 ± 69	DMM - 197	13 ± 1
EI : 42, 99, 161, 181, 195, 279, 446, 476	476	2	86	Dimethylglyoxal		0.5 10 ^{-1.6}	Standard Rossignol (2012) Jaoui et al, (2012)	2,3-Butanedione-d6	Dimethylglyoxal	DMM - 197	286 ± 63	181	9 ± 1
EI : 42, 82, 161, 181, 195, 208, 252, 279, 293, 309, 490	490	2	100	4-Oxopentanal		0.4 10 ^{-2.2}	Standard Matsunaga et al. (2004)	2,3-Butanedione-d6	4-Oxopentanal	DMM - 181	3903 ± 182	ND	ND
Hydroxyl compounds and carboxylic acids													
EI : 45, 55, 73, 75, 85, 99, 129, 171	186	1	72	2-Propenoic acid		0.67 10 ^{-2.8}	MS/RT/Nist	Pentanoic-d9 acid	Methacrylic acid	DMM - 57	211 ± 106	ND	ND
EI : 75, 115, 131, 149, 173	188	1	74	Glyoxilic acid		1.5 10 ^{-5.6}	Standard Cahill et al, (2006)	Pentanoic-d9 acid	Methacrylic acid	DMM - 57	1042 ± 225	ND	ND
EI : 45, 75, 115, 131, 149, 173	188	1	74	Propanoic acid		0.67 10 ^{-2.5}	MS/RT/Nist Cahill et al, (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	862 ± 106	ND	ND
EI : 41, 69, 99, 143, 185	200	1	86	Methacrylic acid		0.5 10 ^{-3.2}	Standard	Pentanoic-d9 acid	Methacrylic acid	DMM - 57	128 ± 111	DMM - 57	0,4 ± 1

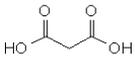
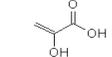
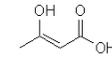
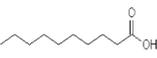
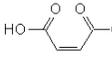
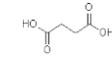
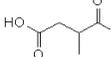
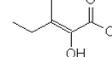
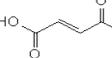
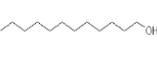
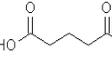
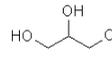
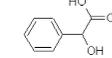
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Identification									Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification method	Substitut	External standard	Gaseous Phase		Particulate phase		
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)	
EI : 43, 73, 75, 103, 115, 145	202	1	88	Pyruvic acid		1 10 ^{-3.6}	Standard Kawamura et Yasui (2005)	Pentanoic-d9 acid	Pyruvic acid	DMM - 57	interferences	DMM - 57	0,3 ± 1	
EI : 41, 75, 99, 143, 185	200	1	86	Crotonic acid		0.5 10 ^{-3.3}	Standard	Pentanoic-d9 acid	Crotonic acid	DMM - 57	<QL	DMM - 57	2 ± 0,5	
EI : 41, 58, 75, 115, 129, 159, 201	216	1	102	Pentanoic acid		0.4 10 ^{-3.5}	Étalon	Heptanoic acid -d13	Heptanoic acid	DMM - 57	483 ± 70	DMM - 57	blank	
EI : 47, 58, 75, 115, 129, 173	230	1	116	3-Ethylbutyrique acid		0.33 10 ^{-3.9}	MS/RT	Pentanoic-d9 acid	2-Ethylbutyric acid	DMM - 57	118 ± 55	ND	ND	
EI : 41, 75, 131, 173, 215	230	1	116	Hexanoic acid		0.33 10 ^{-4.0}	MS/RT/Nist Rossignol (2012)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	722 ± 73	DMM - 57	blank	
EI : 43, 75, 99, 129, 145, 155, 173, 181, 215	230	1	116	Levulinic acid		0.6 10 ^{-4.6}	standard Jaoui et al. (2006)	Heptanoic acid -d13	Levulinic acid	DMM - 85	606 ± 91	DMM - 57	10 ± 1	
EI : 41, 75, 95, 116, 131, 187, 229	244	1	130	Heptanoic acid		0.29 10 ^{-4.5}	Standard Rossignol (2012)	Heptanoic acid -d13	Heptanoic acid	131	399 ± 48	DMM - 57	blank	
EI : 41, 57, 73, 85, 103, 133, 147, 189, 219, 247	304	2	76	Glycolic acid		1.5 10 ^{-4.6}	Standard Cahill et al, (2006)	Heptanoic acid -d13	Glycolic acid	147	201 ± 67	115	19 ± 2	
EI : 41, 57, 73, 115, 133, 147, 189, 217, 247, 275, 317	332	2	104	3,3-dihydroxy-2-butanone		0.75 10 ^{-3.5}	MS/RT	Heptanoic acid -d13	Glycolic acid	ND	ND	DMM - 57	<QL	
EI : 41, 57, 73, 117, 131, 147, 189, 201, 231, , 301	316	2	88	2-Buten-1,4-diol		0.5 10 ^{-4.4}	Standard	Heptanoic acid -d13	Succinic acid	ND	ND	147	<QL	
EI : 41, 57, 73, 115, 147, 189, 261, 303	318	2	90	Oxalic acid		2 10 ^{-5.6}	Standard Cahill et al, (2006)	Heptanoic acid -d13	Succinic acid	DMM - 57	<QL	115	277 ± 17	
EI : 43, 57, 73, 99, 117, 133, 147, 173, 189, 247, 275, 317	332	2	104	2-Hydroxy-2-methylpropanoic acid		0.75 10 ^{-5.3}	Nist/MS/RT Rossignol (2012)	Heptanoic acid -d13	Glycolic acid	147	41 ± 100	DMM - 57	blank	
EI : 41, 57, 73, 75, 115, 133, 147, 189, 218, 303, 318	318	2	90	3-Hydroxypropanoic acid		1 10 ^{-5.1}	Nist/SM/TR Rossignol (2012)	Heptanoic acid -d13	Glycolic acid	DMM - 57	39 ± 62	DMM - 57	<QL	
EI : 41, 75, 117, 129, 131, 171, 215, 257	272	1	158	Nonanoic acid		0.22 10 ^{-5.5}	MS/RT/Nist Rossignol (2012)	Heptanoic acid -d13	Heptanoic acid	131	blank	DMM - 57	blank	

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										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 41, 57, 73, 115, 133, 147, 189, 275, 317	332	2	104	Malonic acid		1.3 10 ^{-6.1}	Nist/MS/RT Cahill et al. (2006)	Heptanoic acid -d13	Succinic acid	ND	ND	73	3 ± 1
EI : 45, 57, 73, 133, 147, 157, 185, 259, 301	316	2	88	2-Hydroxy-2-propenoic acid		1 10 ^{-3.6}	MS/RT	Heptanoic acid -d13	Glycolic acid	ND	ND	DMM - 57	<QL
EI : 41, 57, 73, 133, 147, 199, 273, 315	330	2	102	3-Hydroxy-2-butenic acid		0.75 10 ^{-4.1}	Nist/MS/RT	Heptanoic acid -d13	Glycolic acid	ND	ND	DMM - 57	<QL
EI : 41, 75, 129, 131, 229, 271	286	1	172	Decanoic acid		0.2 10 ^{-6.0}	Nist/MS/RT Cahill et al. (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	blank	DMM - 57	blank
EI : 41, 57, 73, 117, 133, 147, 189, 287, 329	344	2	116	Maleic acid		1 10 ^{-6.9}	Nist/MS/RT Cahill et al. (2006)	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 15	2 ± 1
EI : 41, 57, 73, 115, 129, 147, 189, 243, 289, 331	346	2	118	Succinic acid		1 10 ^{-6.6}	Standard Cahill et al. (2006)	Heptanoic acid -d13	Succinic acid	MMD - 57	blank	DMM - 131	27 ± 2
EI : 41, 73, 115, 147, 189, 229, 303, 345	360	2	132	A2-Methylsuccinic acid		0.8 10 ^{-7.0}	MS/RT Kawamura et Yasui (2005)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	blank
EI : 41, 57, 73, 75, 115, 133, 147, 289, 301, 343	358	2	130	2-Hydroxy-3-Methyl-2-pentenoic acid		0.5 10 ^{-5.0}	MS/RT/Nist	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	4 ± 1
EI : 41, 57, 73, 75, 84, 113, 133, 156, 230, 245, 287, 329	344	2	116	Fumaric acid		1 10 ^{-6.9}	MS/RT/Nist Rossignol (2012) Cahill et al. (2006)	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 15	3 ± 1
EI : 41, 57, 75, 95, 129, 131, 243, 285, 300	300	1	186	Undecanoic acid		0.18 10 ^{-6.5}	Nist/MS/RT Cahill et al. (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	blank	ND	ND
EI : 41, 57, 75, 83, 97, 115, 129, 143, 185, 227, 243, 285	300	1	186	1-Dodecanol		0.08 10 ^{-5.7}	MS/RT/Nist	Heptanoic acid -d13	Heptanoic acid	DMM - 57	blank	ND	ND
EI : 41, 57, 73, 75, 129, 147, 189, 303, 345	360	2	132	Glutaric acid		0.8 10 ^{-7.1}	Standard Cahill et al. (2006)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	16 ± 1
EI : 41, 57, 73, 89, 115, 133, 147, 171, 189, 245, 377, 419	434	3	92	Glycerol		1 10 ^{-6.3}	Standard Jaoui et al. (2014)	Glycerol-d8	Glycerol	DMM - 57	1646 ± 131	DMM - 57	56 ± 4
EI : 73, 75, 147, 189, 221, 257, 295, 323, 365	380	2	152	Mandelic acid		0.38 10 ^{-7.8}	MS/RT	Heptanoic acid -d13	Glycolic acid	DMM - 57	21 ± 1	ND	ND

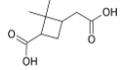
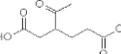
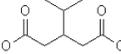
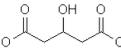
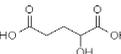
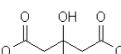
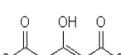
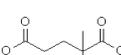
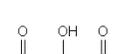
Identification and quantification of compounds during ChArMEx campaign.

DMM : Derivatized Molar Mass ; MM : Molar Mass ; MS : Mass Spectra ; RT : Retention Time ; QL : Quantification Limit ; ND : Not Detected

Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification method	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 39, 75, 89, 129, 131, 257, 299	314	1	200	Dodecanoic acid		0.17 10 ^{-7.1}	MS/RT Rossignol (2012) Cahill et al, (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	blank	DMM - 57	blank
EI : 41, 57, 73, 133, 147, 159, 175, 177, 189, 221, 231, 391, 433	448	3	106	2,3-Dihydroxypropanoic acid		1.3 10 ^{-7.6}	Nist/MS/RT Rossignol (2012) (Kourtchev et al., 2008b)	Pentanoic-d9 acid Glycerol-d8	Glycerol	ND	ND	DMM - 57	20 ± 2
EI : 41, 57, 73, 111, 147, 227, 309, 317, 343, 359	374	2	146	Hexanedioic acid		0.67 10 ^{-7.6}	MS/RT/Nist Rossignol (2012) Cahill et al, (2006)	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 15	1 ± 1
EI : 41, 57, 73, 115, 133, 147, 189, 231, 245, 273, 303, 318, 377, 405, 447	462	3	120	2-Methylglyceric acid (= 2-MGA)		1 10 ^{-7.9}	Standard Claeys et al. (2004)	Pentanoic-d9 acid Glycerol-d8	Glycerol	ND	ND	DMM - 57	9 ± 1
EI : 41, 73, 133, 147, 185, 197, 271, 315, 343	372	2	144	3-Methyl-2-pentenedioic acid		0.67 10 ^{-7.7}	MS/RT/Nist	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	30 ± 2
EI : 41, 57, 73, 115, 133, 147, 189, 207, 221, 263, 271, 377, 405, 447	462	3	120	Erythrose or Erythrulose		1.0 10 ^{-8.0}	MS/RT Jaoui et al. (2014)	Pentanoic-d9 acid	2-MGA	ND	ND	DMM - 57	45 ± 3
EI : 41, 75, 129, 178, 206, 271	328	1	214	Tridecanoic acid		0.15 10 ^{-7.6}	MS/RR Rossignol (2012) Cahill et al, (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	65 ± 68	ND	ND
EI : 41, 57, 73, 115, 133, 147, 175, 185, 189, 213, 287, 317, 345, 391, 419, 461	476	3	134	Methyltartronic acid		1.25 10 ^{-9.2}	MS/RT	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 131	6 ± 1
EI : 41, 57, 73, 75, 111, 147, 185, 317, 345, 387	402	2	174	Ketonorlimonic acid		0.71 10 ^{-9.4}	MS/RT Rossignol (2012) Kleindienst et al. (2007)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	15 ± 1
EI : 41, 69, 96, 75, 129, 207, 285	342	1	228	Tetradecanoic acid		0.14 10 ^{-8.0}	Nist/MS/RT Cahill et al, (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	314 ± 100	DMM - 57	blank
EI : 41, 73, 115, 133, 147, 189, 217, 247, 287, 419, 461	476	3	134	Malic acid		1.25 10 ^{-9.4}	Standard Rossignol (2012) Cahill et al, (2006)	Heptanoic acid -d13	Glycolic acid	ND	ND	DMM - 15	33 ± 3
EI : 41, 73, 115, 147, 189, 217, 273, 301, 331, 405, 433, 475	490	3	148	DHOPA (=4-Oxo-2,3-dihydroxypentanoic acid)		1.0 10 ^{-9.3}	Standard Kleindienst et al. (2004)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	2 ± 0,1
EI : 41, 57, 73, 105, 119, 133, 147, 163, 189, 221, 263, 337, 359, 379	394	2	166	1,2-Benzenedicarboxylic acid		0.5 10 ^{-9.3}	Nist/MS/RT Kleindienst et al. (2012)	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 131	4 ± 1

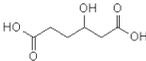
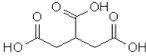
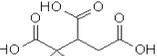
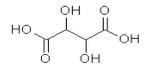
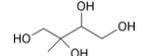
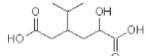
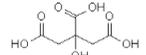
Identification and quantification of compounds during ChArMEx campaign.

DMM : Derivatized Molar Mass ; MM : Molar Mass ; MS : Mass Spectra ; RT : Retention Time ; QL : Quantification Limit ; ND : Not Detected

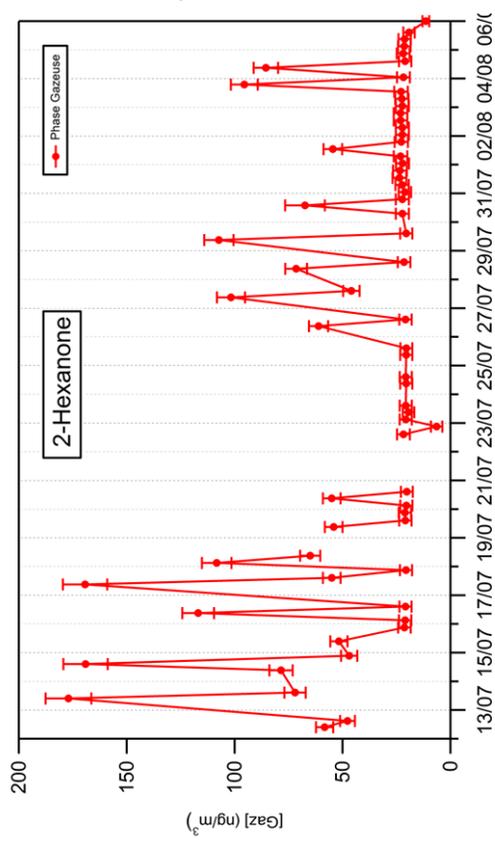
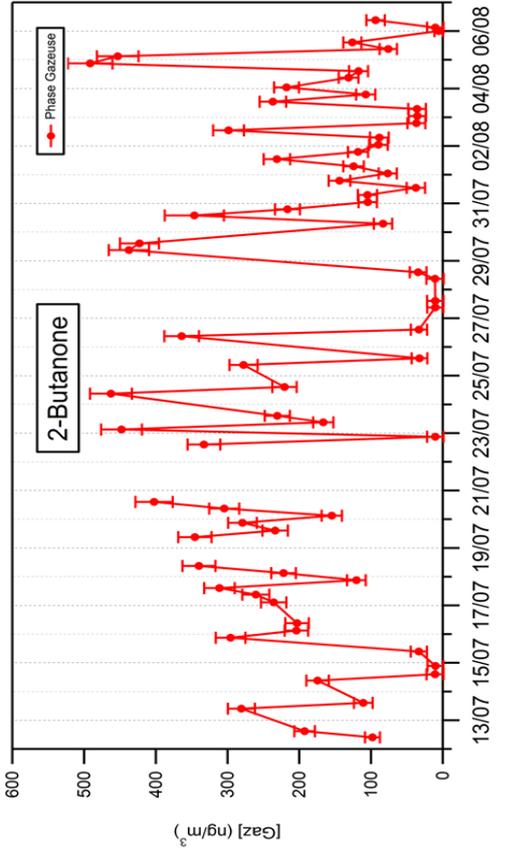
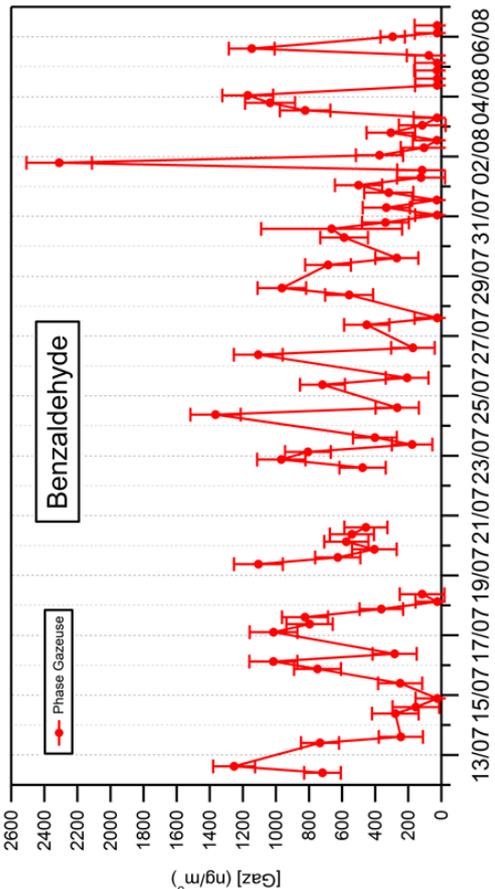
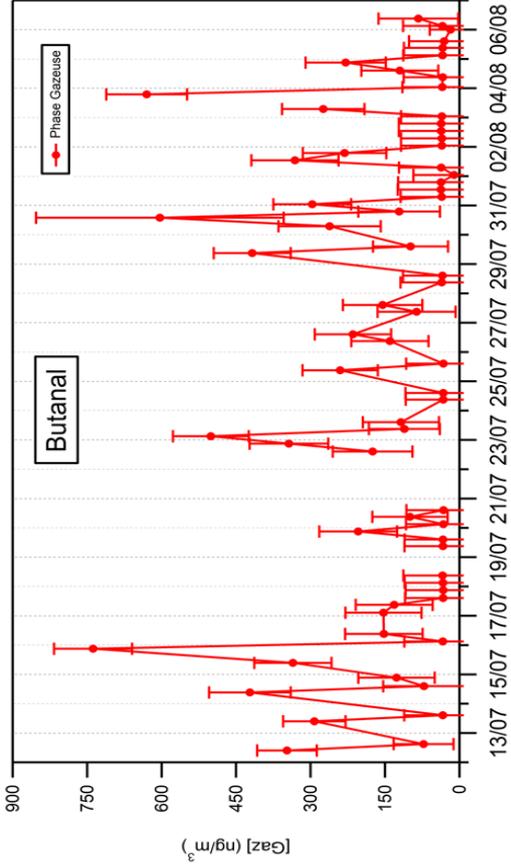
Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification method	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 55, 75, 129, 157, 171, 214, 357, 399	414	2	186	Pinic acid		0.44 10 ^{-8.8}	Standard (Yu et al., 1999a)	Heptanoic acid -d13	Pinic acid	ND	ND	DMM - 57	4 ± 1
EI : 41, 55, 75, 97, 105, 111, 125, 185, 199, 227, 331, 359, 401	416	2	188	Ketolimonic acid		0.63 10 ^{-9.9}	MS/RT Rossignol (2012) Kleindienst et al. (2007)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	6 ± 1
EI : 73, 75, 111, 129, 157, 185, 213, 271, 299, 317, 345, 387	402	2	174	3-Isopropyl-pentanedioic acid		0.5 10 ^{-8.5}	MS/RT Jaoui et al. (2005)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	17 ± 2
EI : 75, 83, 89, 97, 129, 207, 299, 341	356	1	242	Pentadecanoic acid		0.13 10 ^{-8.6}	Nist/MS/RT Cahill et al. (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	335 ± 110	ND	ND
EI : 44, 73, 115, 133, 147, 175, 227, 259, 301, 355, 433, 447, 459, 475	490	3	148	HGA (=3-Hydroxyglutaric acid)		1.0 10 ^{-9.7}	Standard Rossignol (2012) Claeys et al. (2007)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	5 ± 0.3
EI : 41, 57, 73, 115, 133, 147, 149, 171, 189, 245, 261, 273, 303, 331, 359, 405, 433, 475	490	3	148	2-Hydroxyglutaric acid		1.0 10 ^{-9.7}	MS/RT Rossignol (2012) (Kourtchev et al., 2008b)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	3 ± 1
EI : 39, 73, 99, 115, 133, 147, 185, 315, 345, 419, 431, 447, 461, 476, 489	504	3	162	3-Hydroxy-3-methylglutaric acid		0.83 10 ^{-9.9}	MS/RT/Nist	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	4 ± 0.2
EI : 73, 133, 147, 189, 259, 299, 375, 431, 447, 473	488	3	146	3-Hydroxy-2-pentenedioic acid		1.0 10 ^{-8.5}	Nist/MS/RT	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	4 ± 1
EI : 41, 73, 115, 147, 203, 287, 315, 373, 447, 489	504	3	162	2-Hydroxy-2-methylglutaric acid		0.83 10 ^{-9.9}	MM/RT	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	1 ± 0.2
EI : 41, 73, 105, 147, 189, 217, 259, 301, 329, 461, 503	518	3	176	3-Hydroxy-4,4-dimethylglutaric acid		0.71 10 ^{-10.4}	MS/RT Kleindienst et al. (2007)	Heptanoic acid -d13	Succinic acid	ND	ND	DMM - 57	7 ± 0.4
EI : 43, 75, 117, 129, 313, 355	370	1	256	Hexadecanoic acid		0.13 10 ^{-9.2}	MS/RT Rossignol (2012) Cahill et al. (2006)	Heptanoic acid -d13	Heptanoic acid	131	blank	DMM - 57	7 ± 1

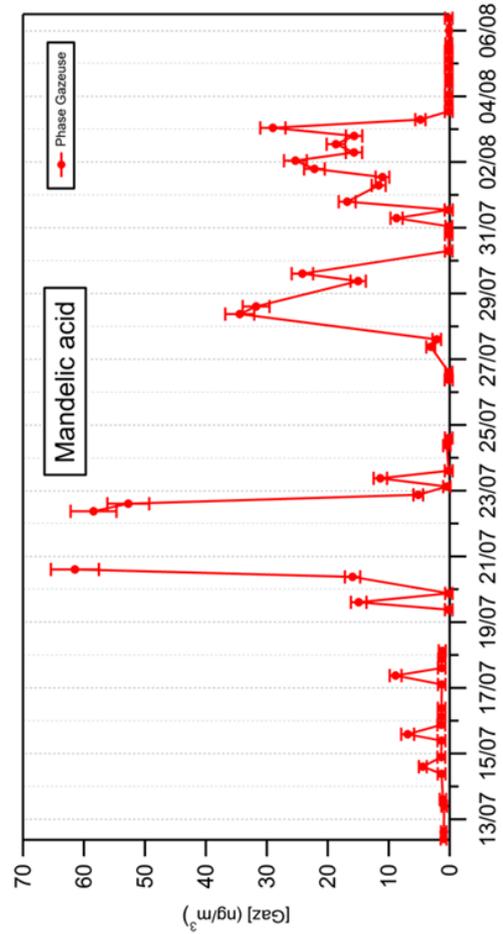
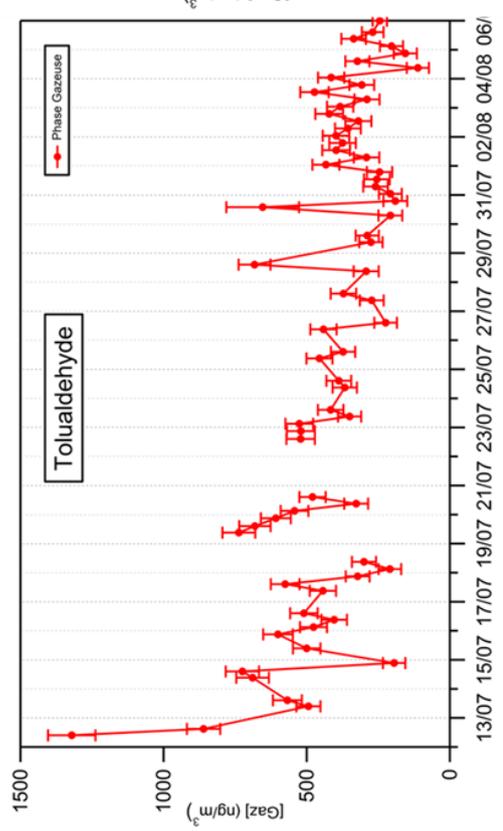
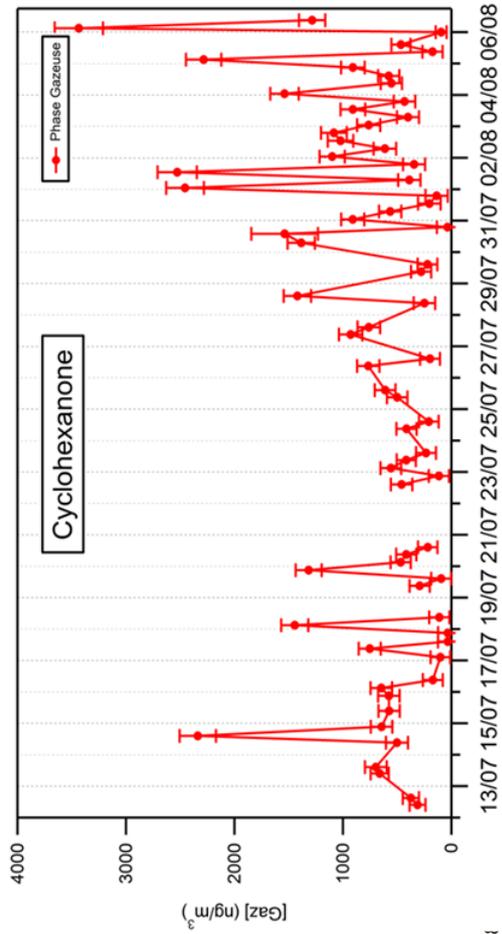
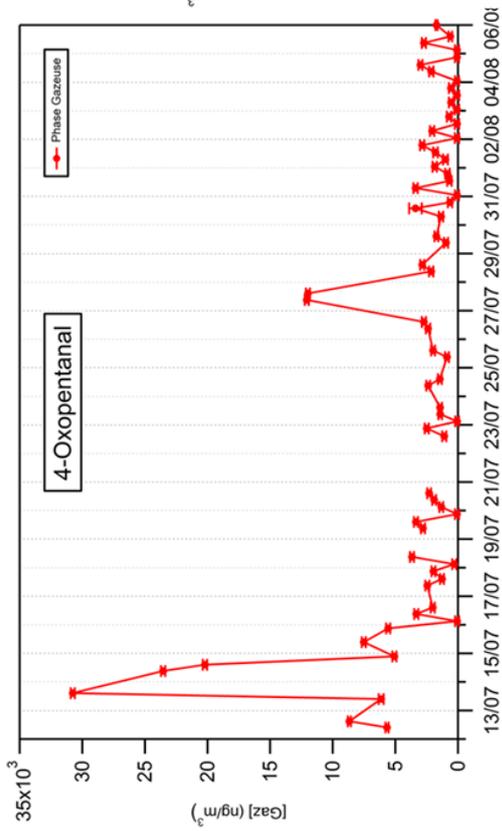
Identification and quantification of compounds during ChArMEx campaign.

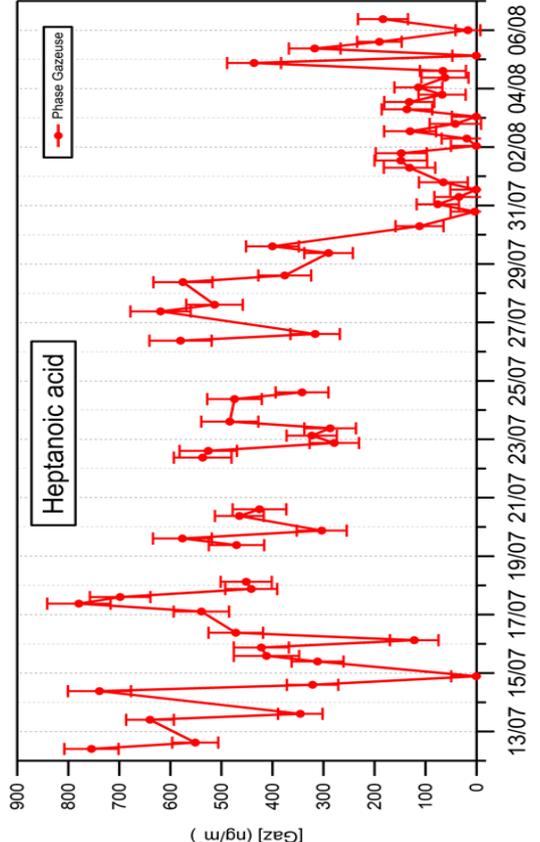
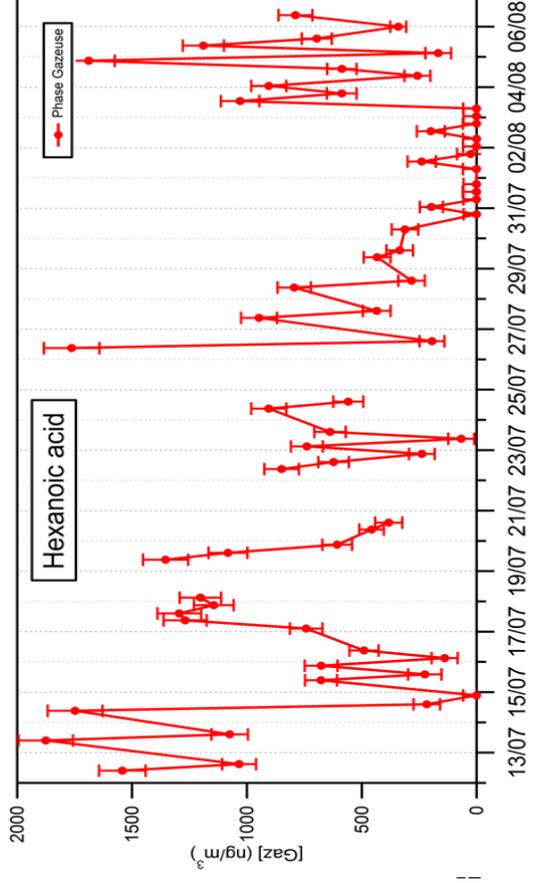
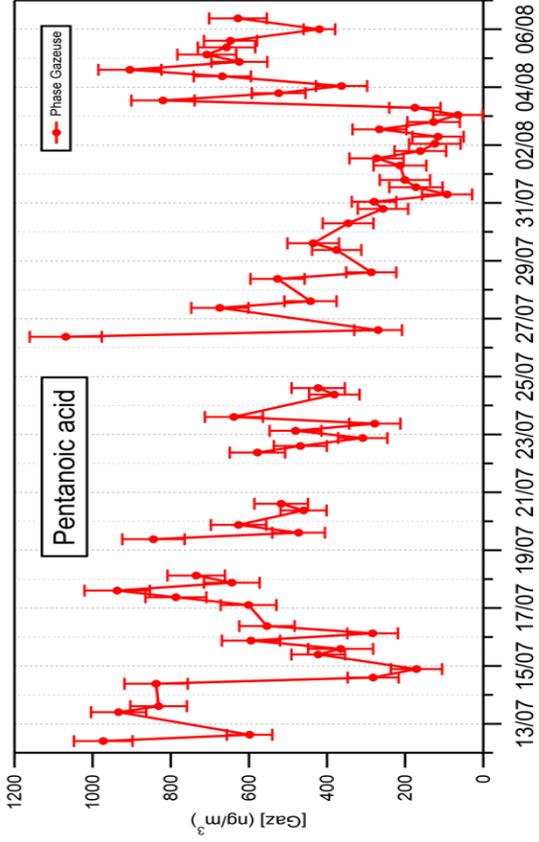
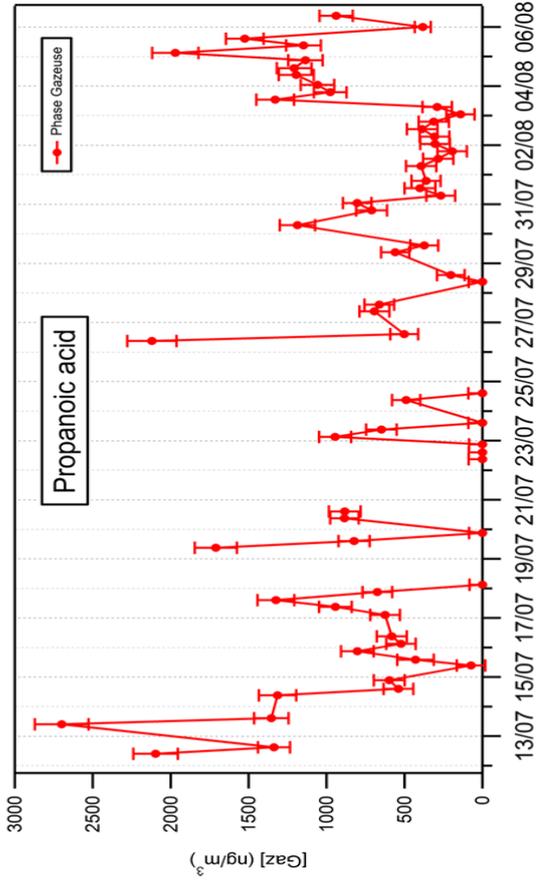
DMM : Derivatized Molar Mass ; MM : Molar Mass ; MS : Mass Spectra ; RT : Retention Time ; QL : Quantification Limit ; ND : Not Detected

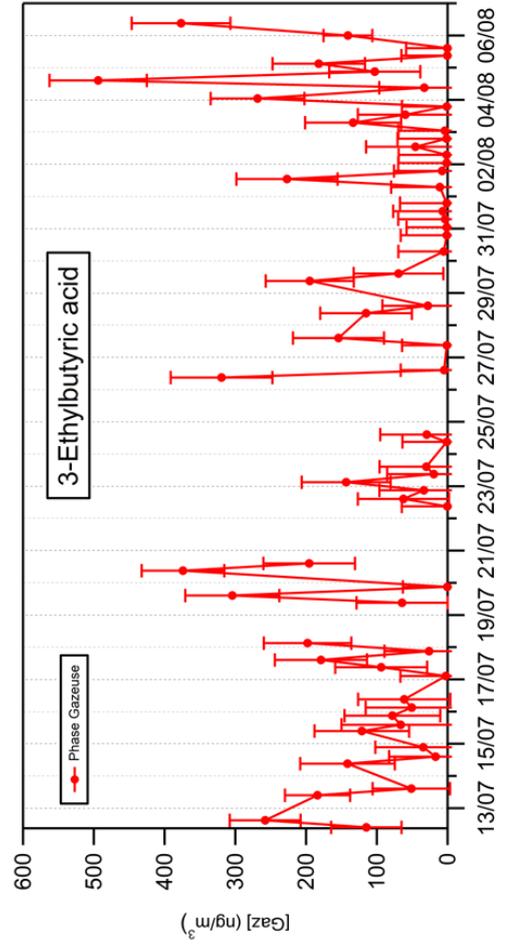
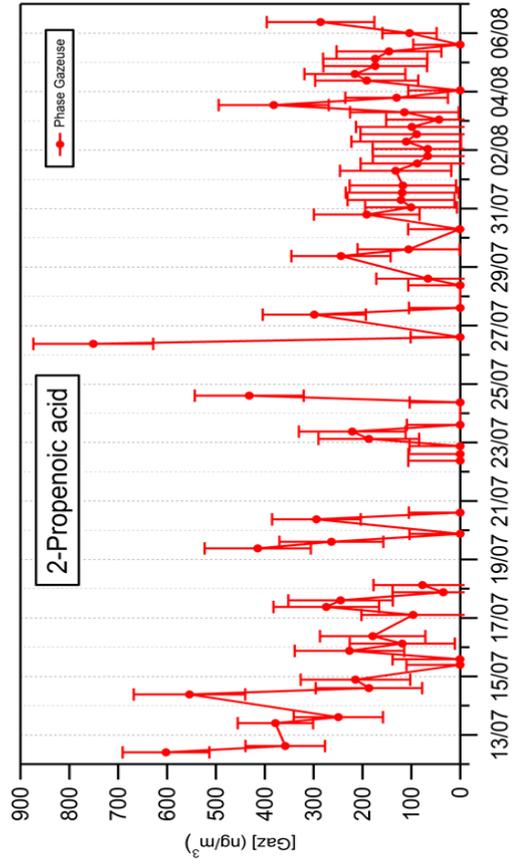
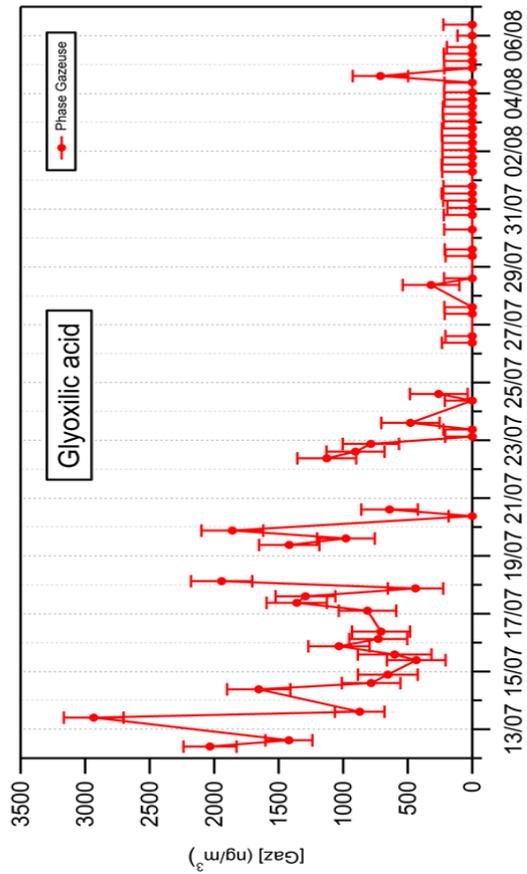
Identification								Quantification					
Main Fragments	DMM	Number of functions	MM	Name	Structure	O/C Log (Saturation Vapor Pressure)	Identification method	Substitut	External standard	Gaseous Phase		Particulate phase	
										m/z integrated	Concentration (ng/m ³)	m/z integrated	Concentration (ng/m ³)
EI : 45, 59, 73, 115, 133, 147, 231, 273, 447, 489	504	3	162	3-Hydroxyhexanedioic acid		0.83 10 ^{-10.2}	MS/RT Rossignol (2012)	Heptanoic acid -d13	Glutaric acid	ND	ND	DMM - 57	7 ± 0,4
EI : 41, 57, 73, 115, 147, 289, 461, 475, 503	518	3	176	Tricarballic acid		1.0 10 ^{-11.7}	Standard Fu et Kawamura (2011)	Heptanoic acid -d13	Tricarballic acid	ND	ND	73	49 ± 3
EI : 73, 99, 115, 147, 189, 255, 287, 317, 329, 489, 531	546	3	204	MBTCA (= 3-Methyl-1,2,3-tricarboxylic acid)		0.75 10 ^{-12.5}	Standard (Szmigielski et al., 2007a)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	7 ± 1
EI : 45, 55, 73, 115, 133, 147, 189, 199, 221, 281, 373, 549, 591	606	4	150	Tartaric acid		1.5 10 ^{-12.1}	Standard Cahill et al, (2006)	Tartric acid-d2	Tartric acid	ND	ND	DMM - 57	4 ± 1
EI : 41, 73, 89, 115, 147, 231, 303, 403, 535,	592	4	136	Methyl-Tetrols (2 spikes) 2-methylerythritol and 2-methylthreitol		0.8 10 ^{-9.0}	MS/RT Claeys et al. (2004)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	0,3 ± 0,02
EI : 41, 57, 73, 115, 147, 191, 241, 317, 357, 431, 489, 531	546	3	204	2-Hydroxy-4-isopropyl-hexanedioic acid		0.56 10 ^{-11.6}	MS/RT Kleindienst et al. (2007)	Tartric acid-d2	Glutaric acid	ND	ND	DMM - 57	1 ± 0,01
EI : 41, 43, 73, 75, 129, 341, 383	398	1	284	Octadecanoic acid		0.11 10 ^{-10.3}	MS/RT Rossignol (2012) Cahill et al, (2006)	Heptanoic acid -d13	Heptanoic acid	DMM - 57	blank	DMM - 57	4 ± 1
EI : 73, 115, 147, 189, 357, 403, 431, 459, 591, 633	648	4	192	Citric acid		1.2 10 ^{-14.3}	Standard Kawamura et Yasui (2005)	Tartric acid-d2	Citric acid	ND	ND	73	15 ± 1

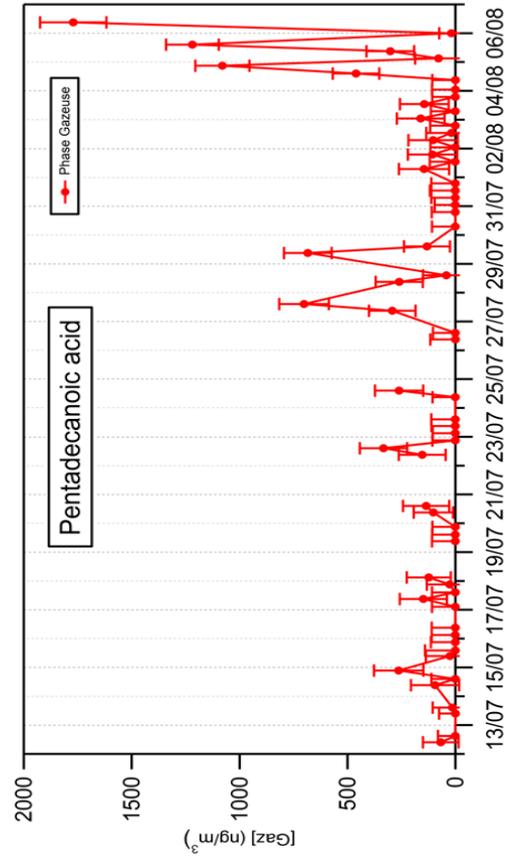
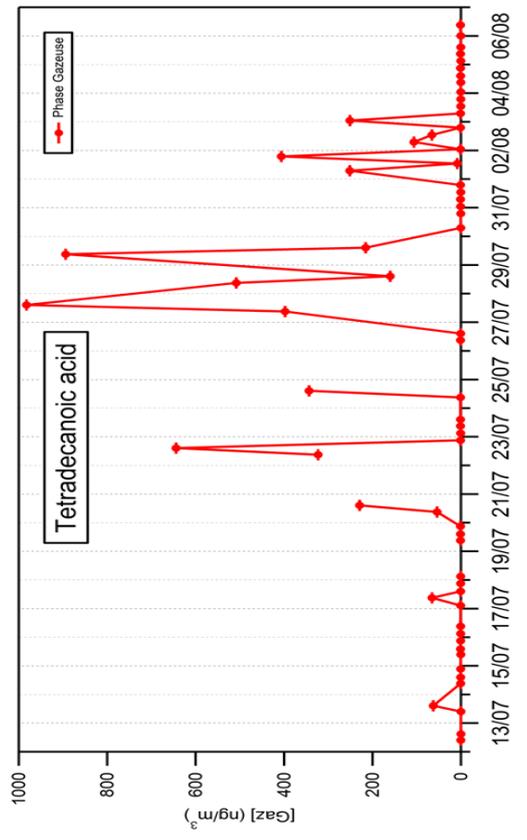
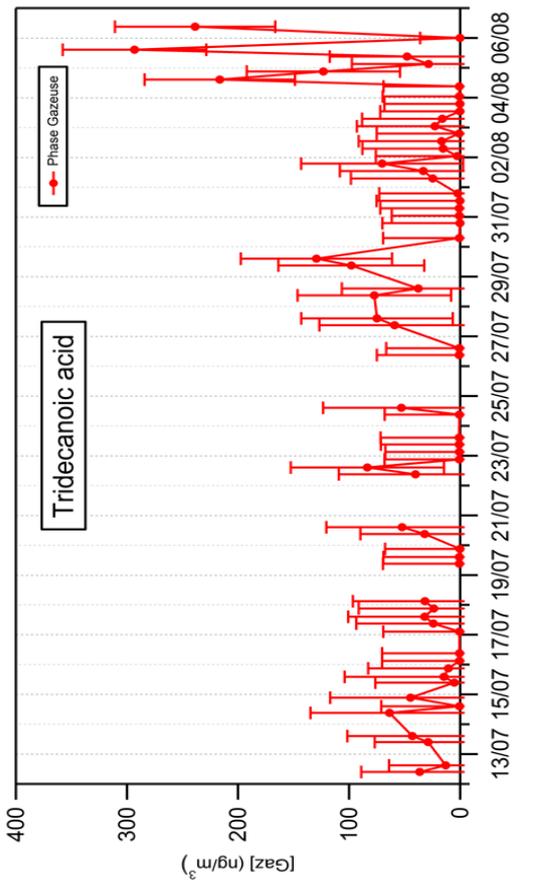
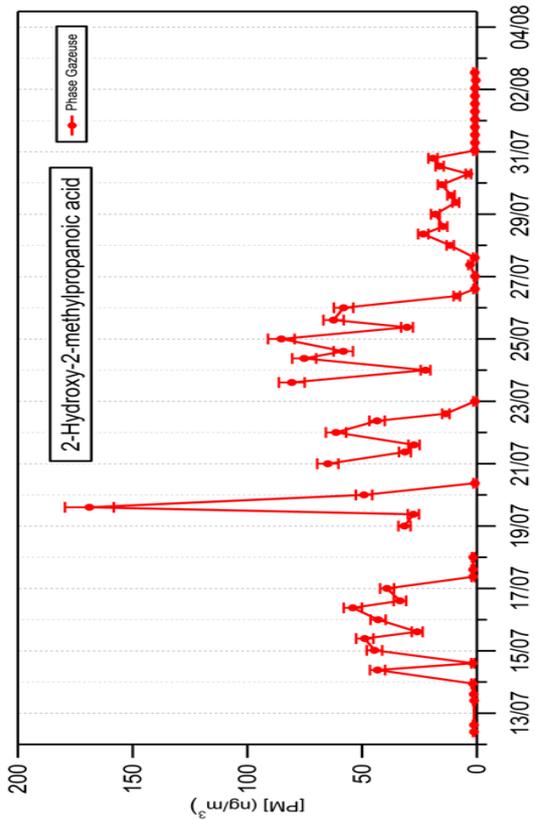
Supplementary material 2: Time series of compounds measured during ChArMEx campaign (in the gas phase in red and in the particulate phase in blue).

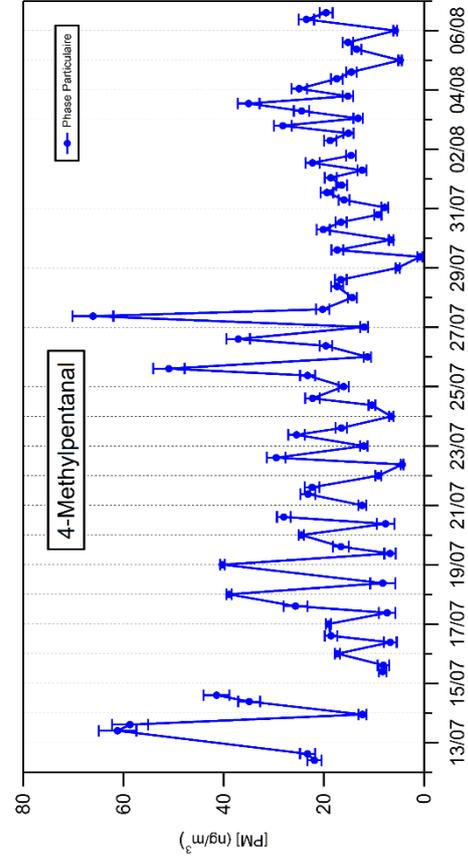
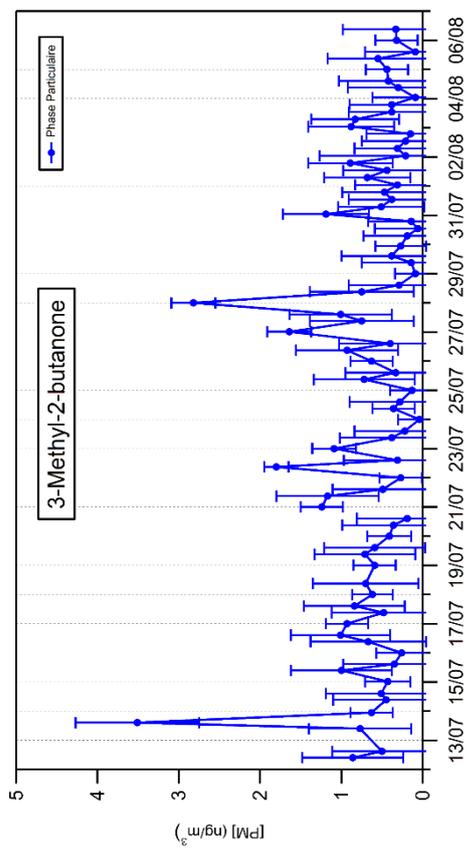
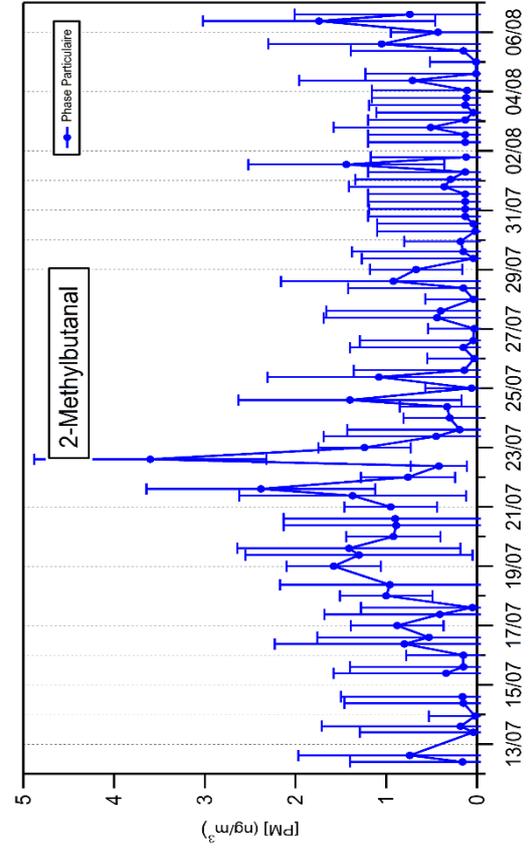
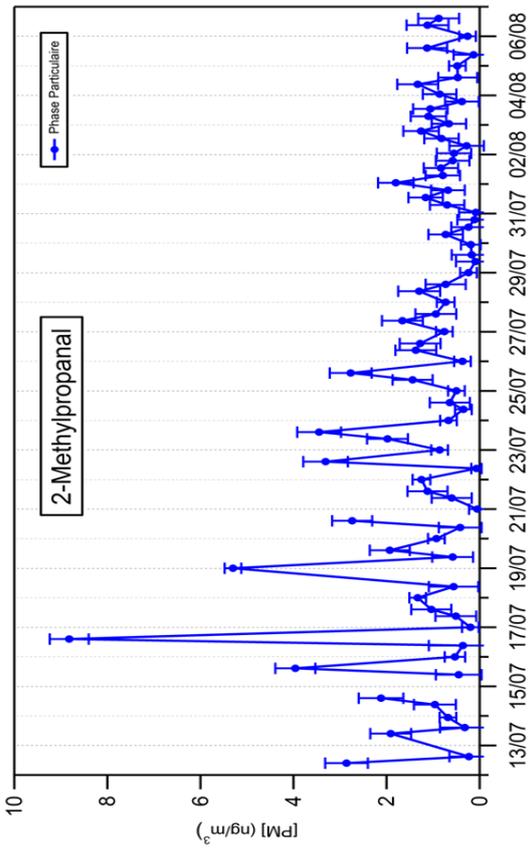


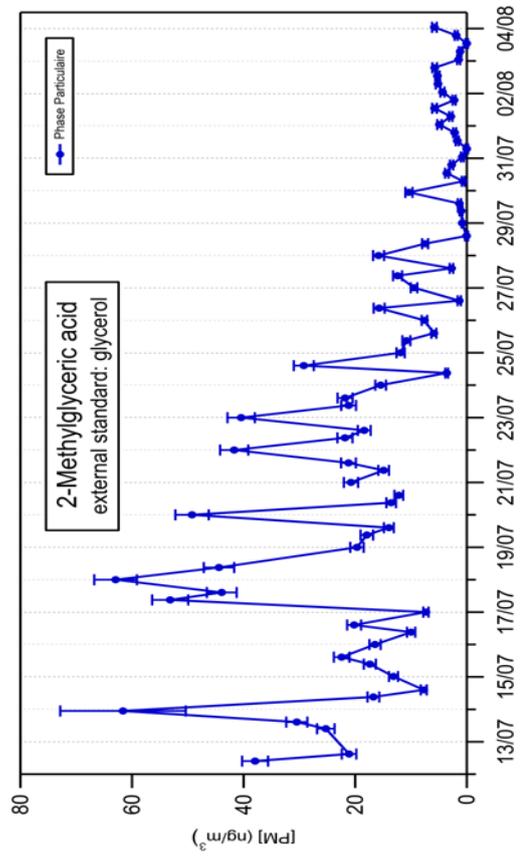
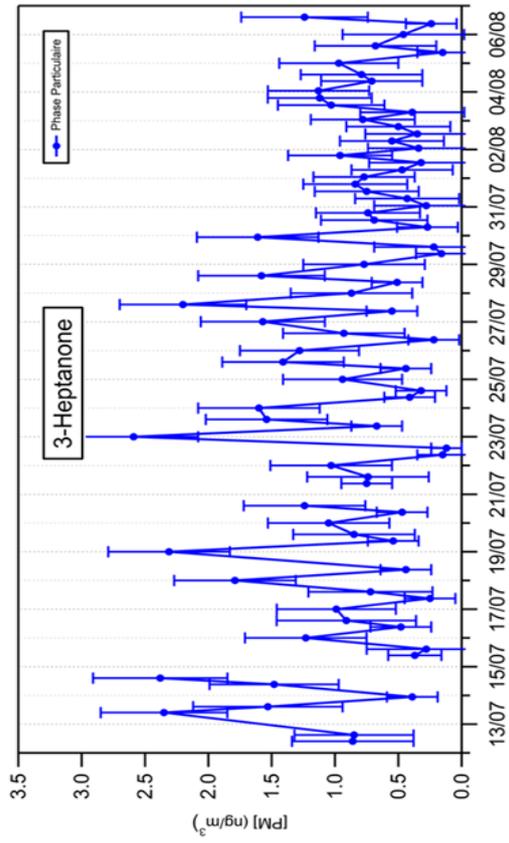
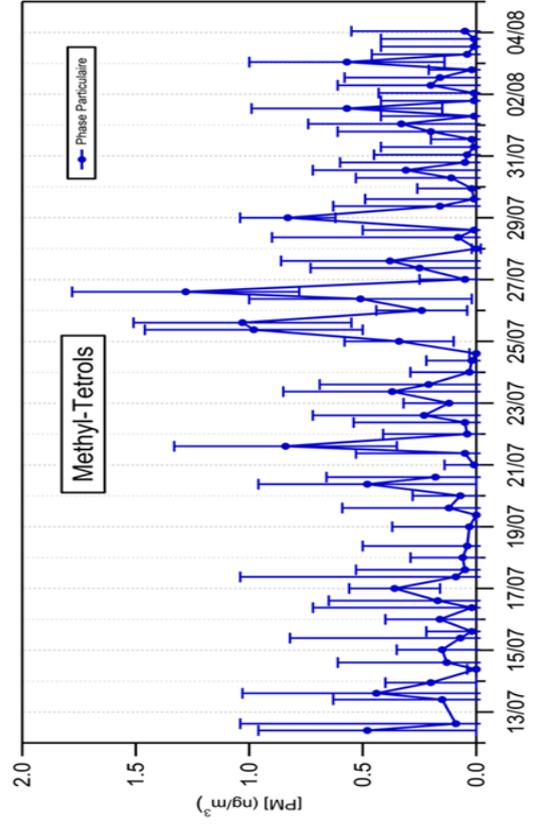
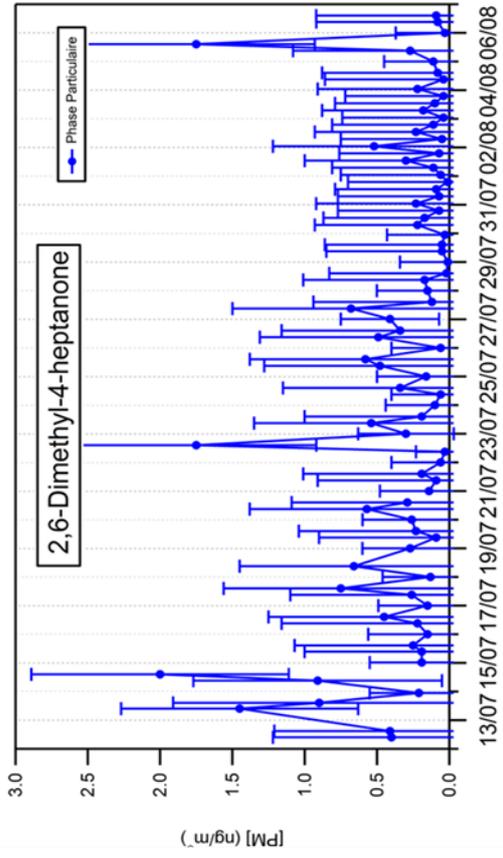


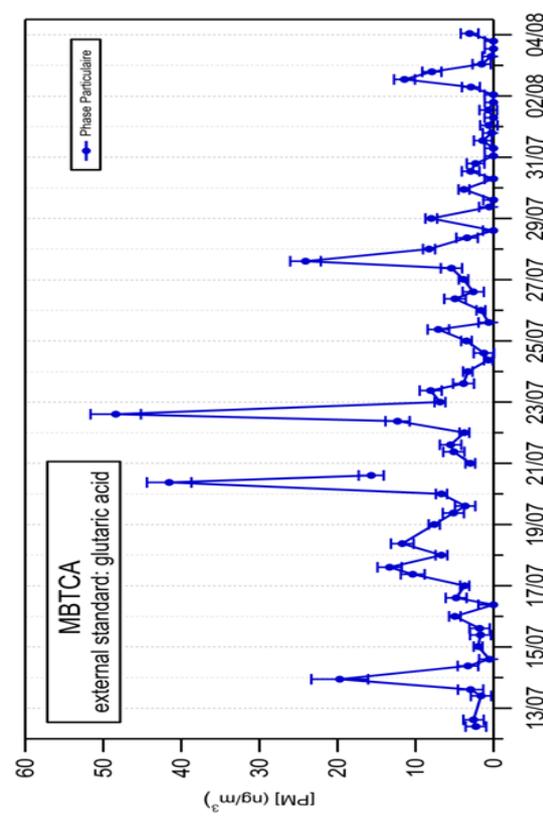
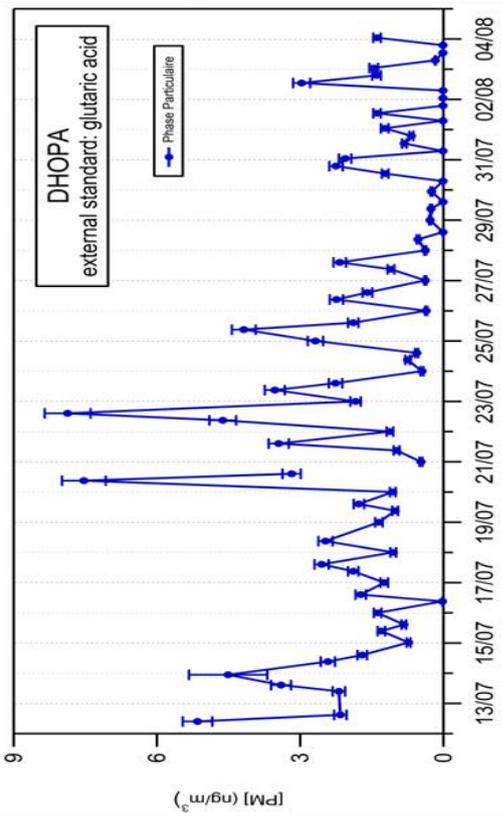
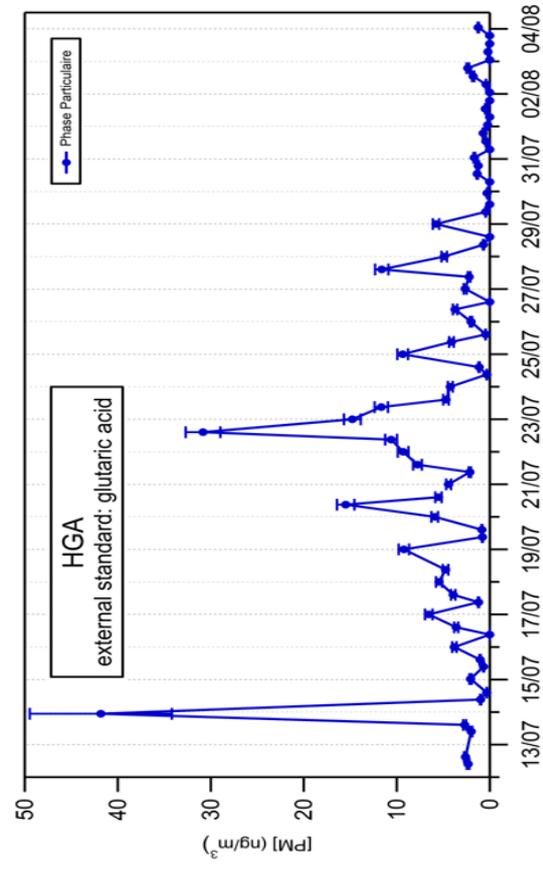
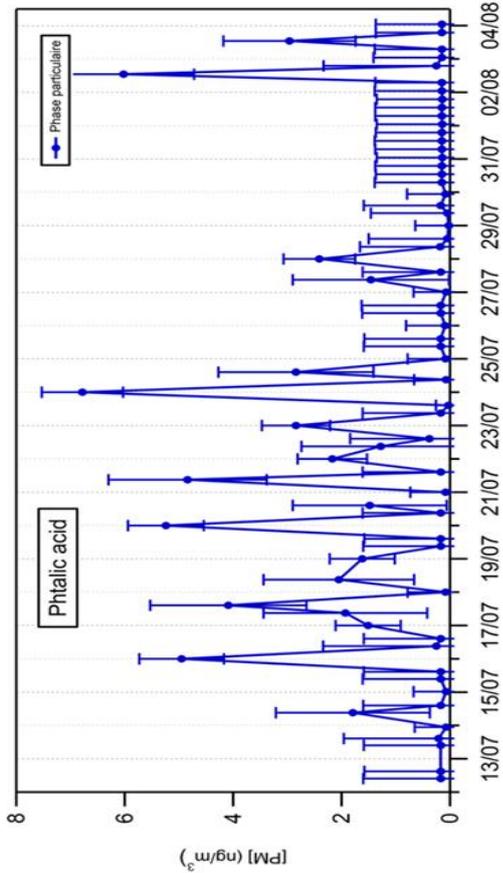


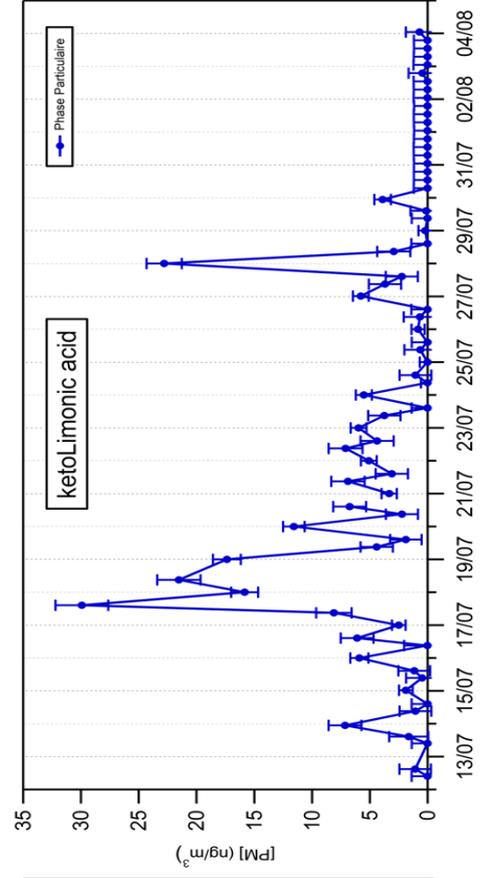
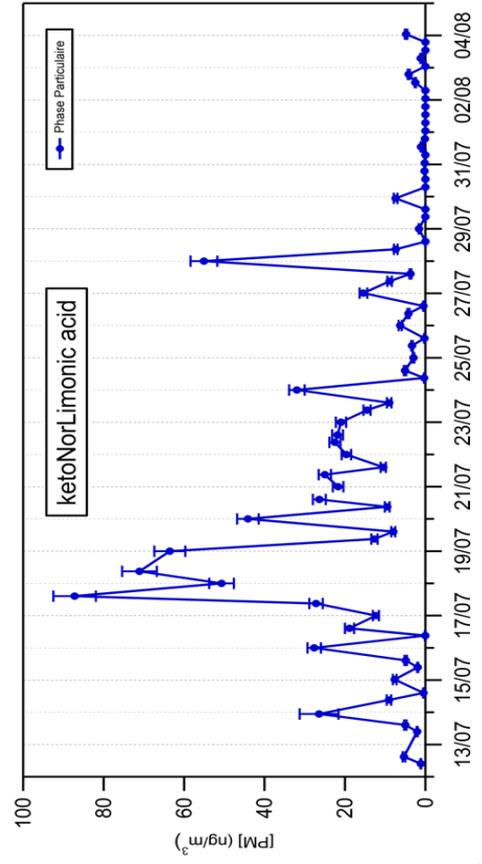
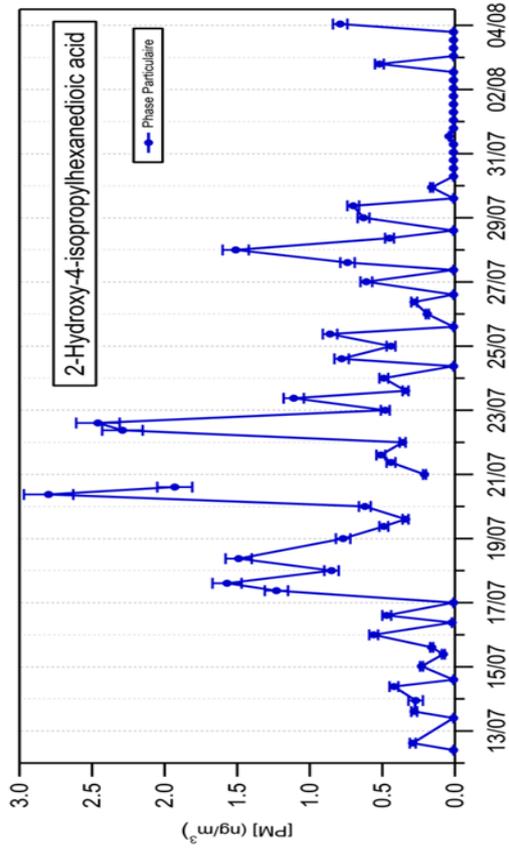
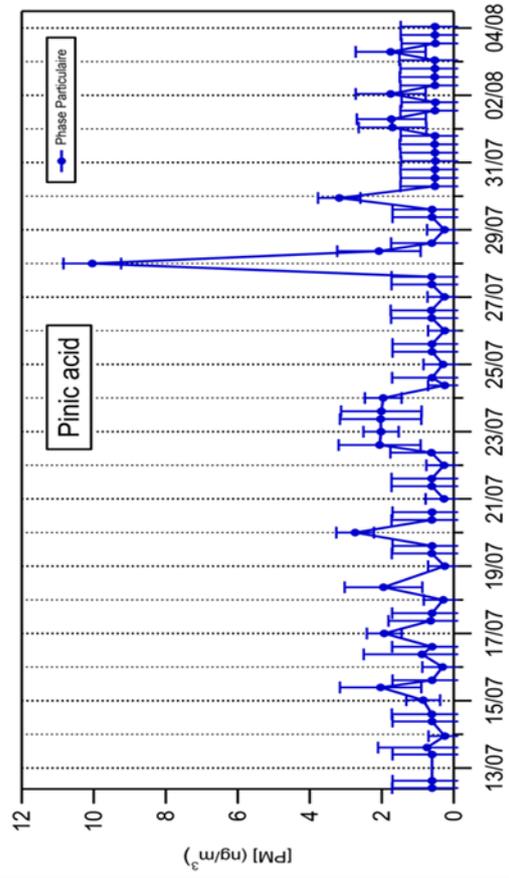


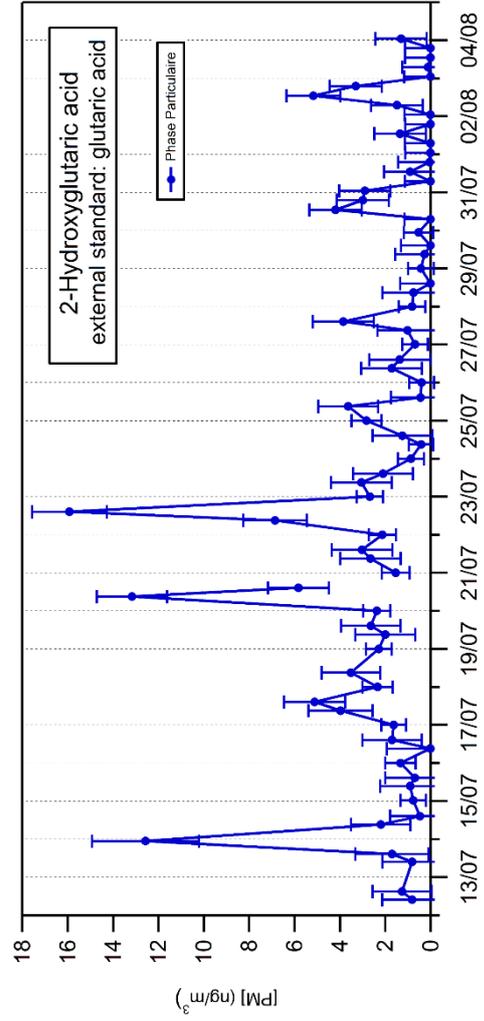
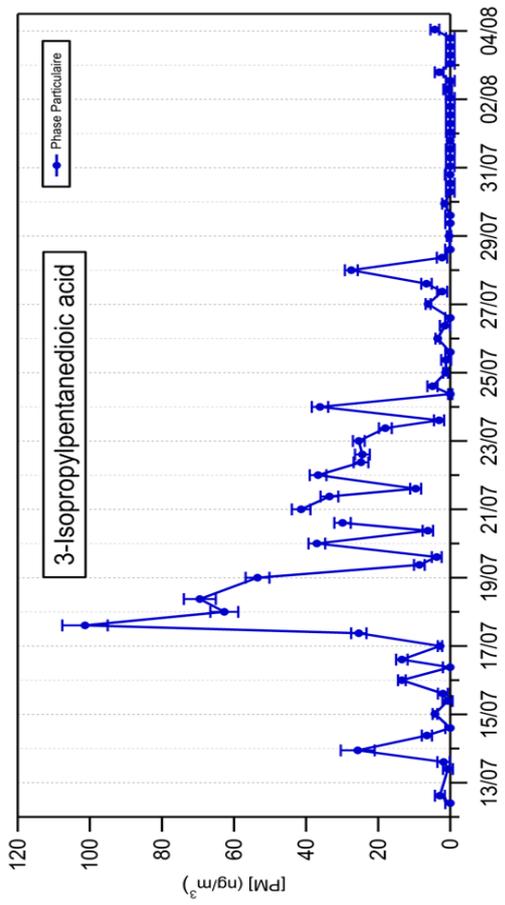
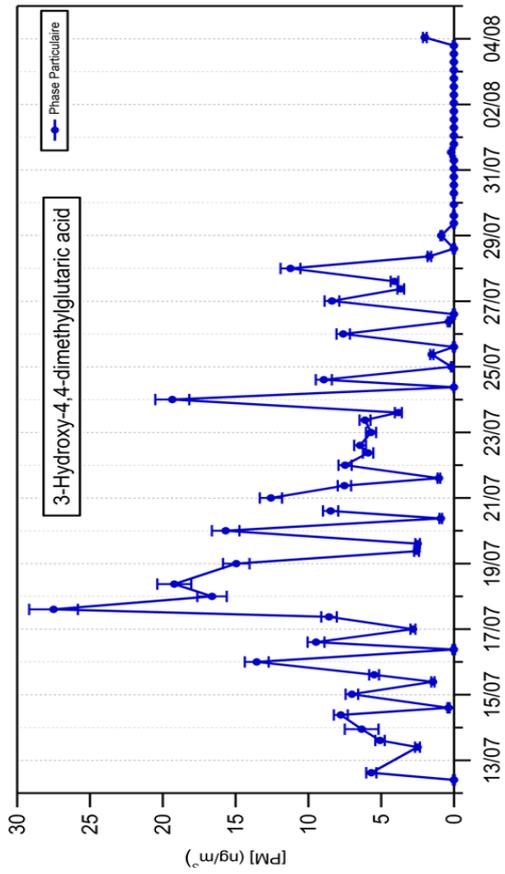


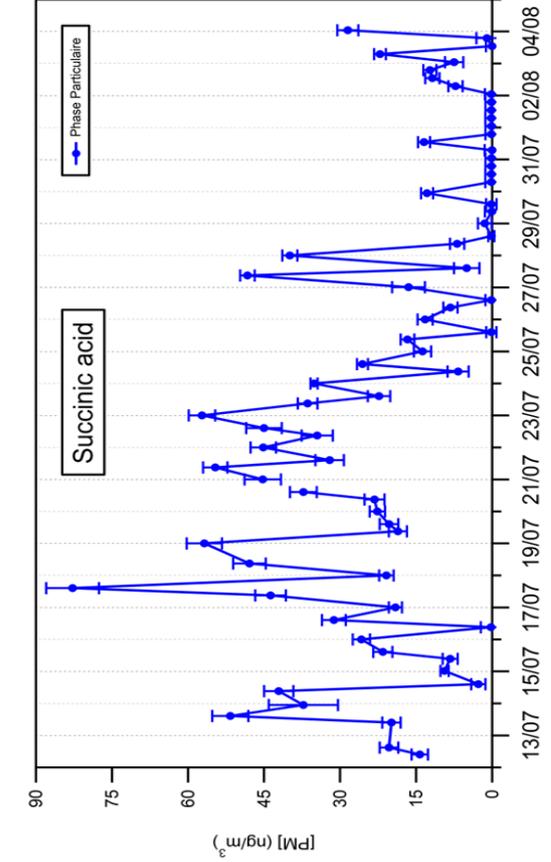
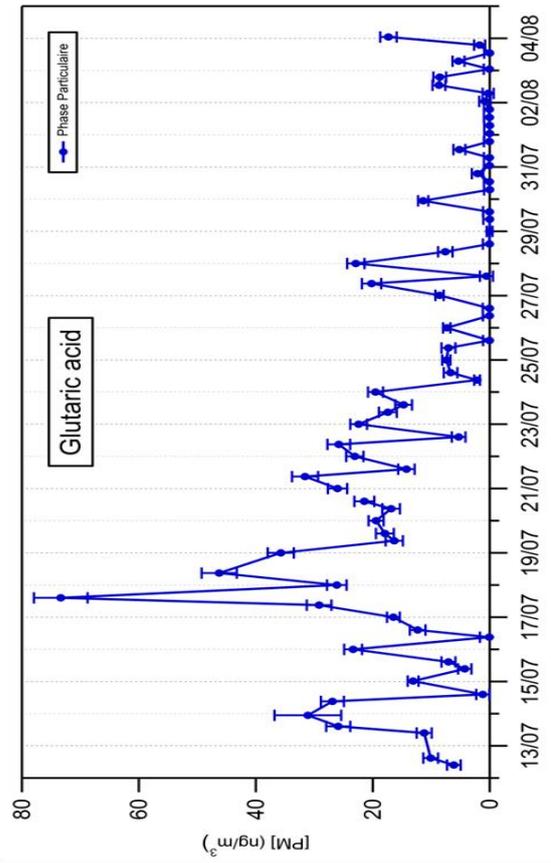
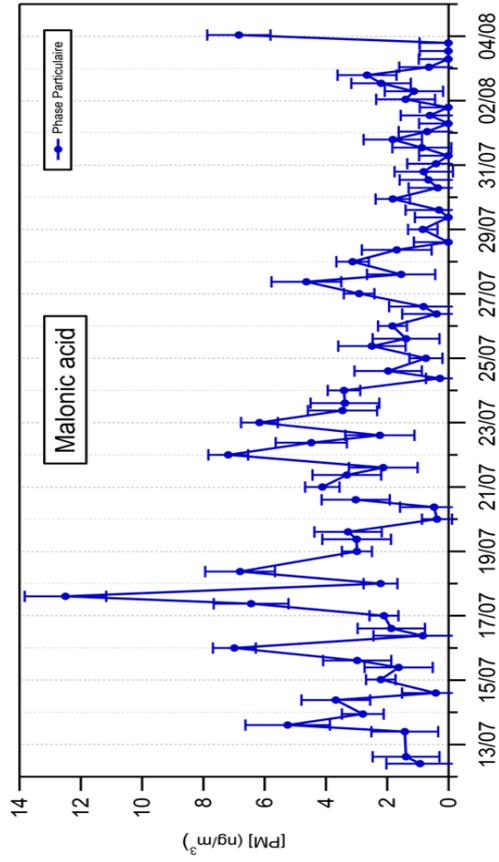
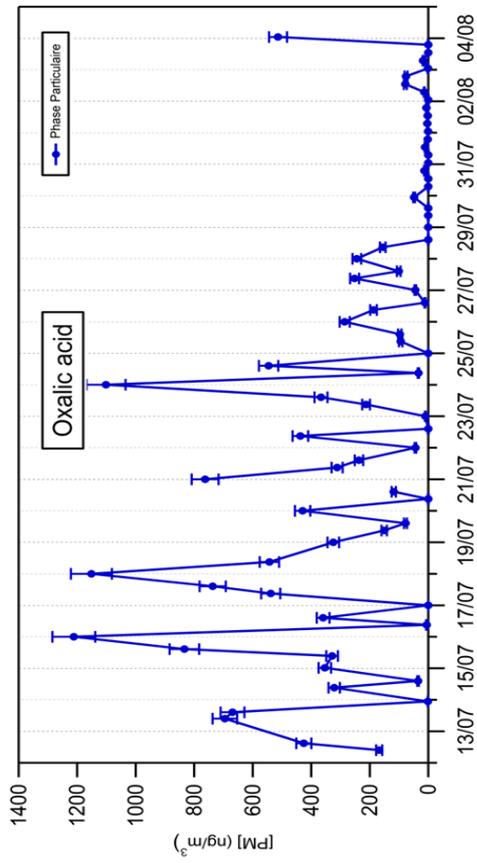


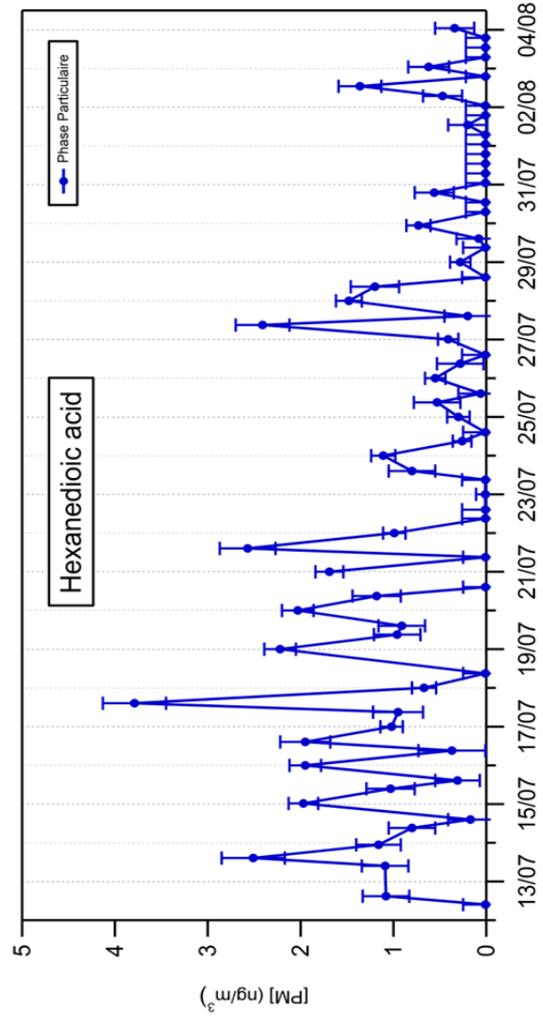
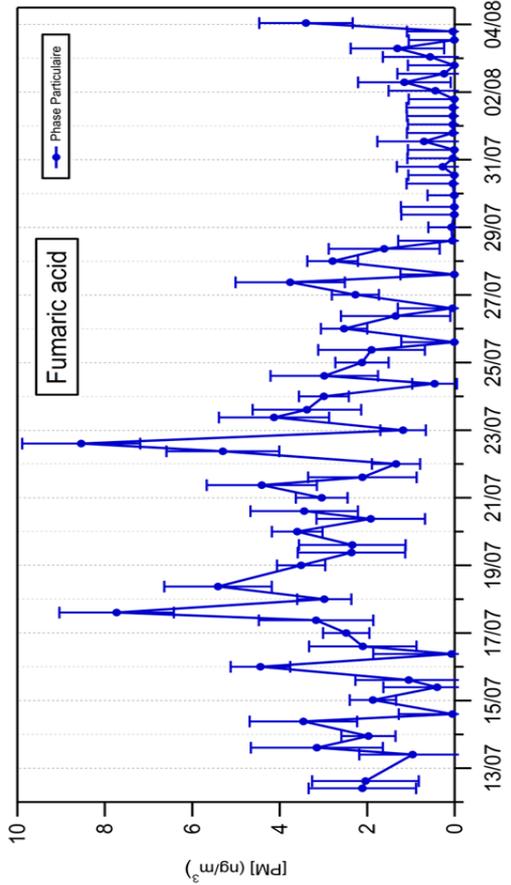
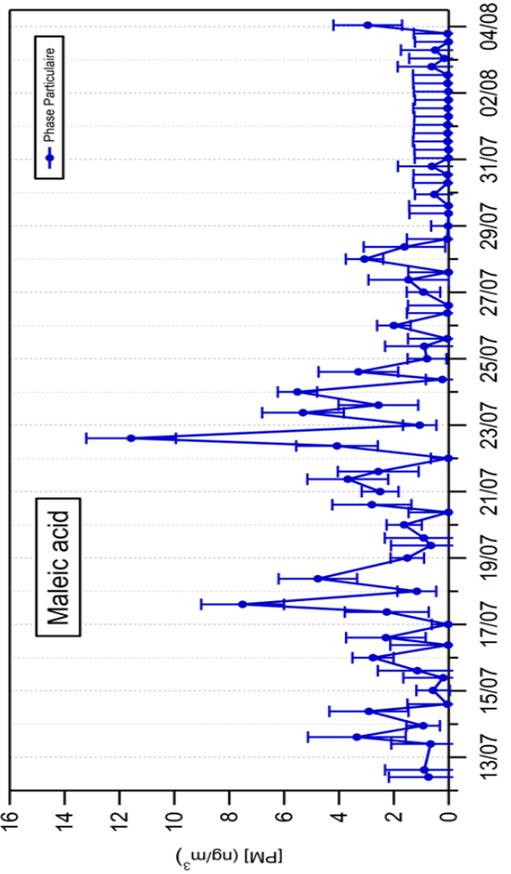


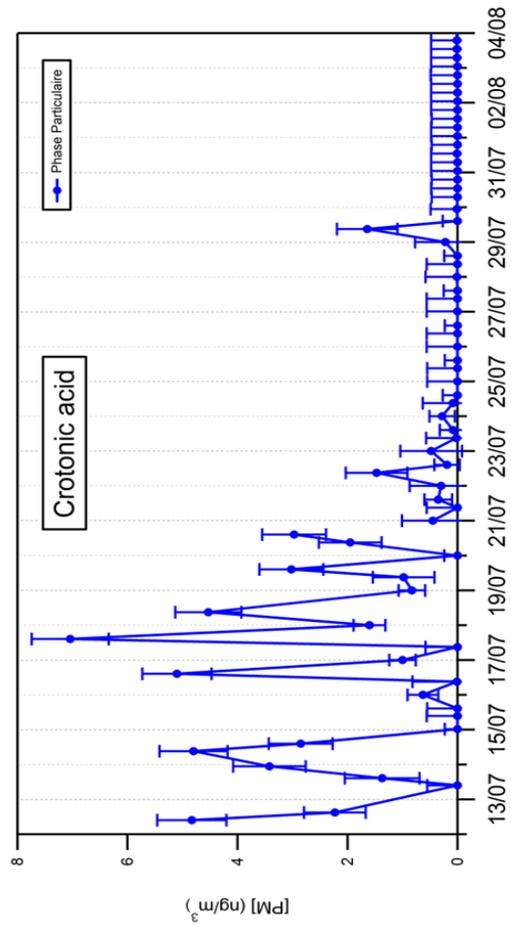
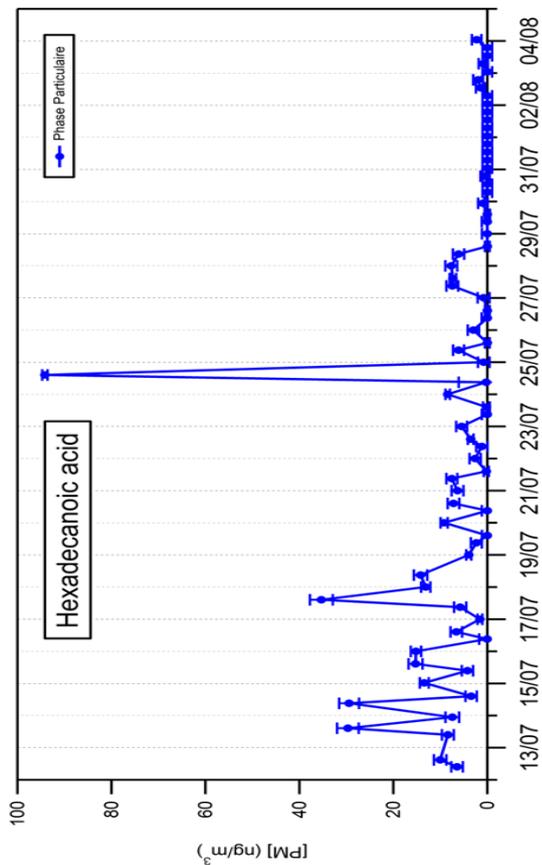
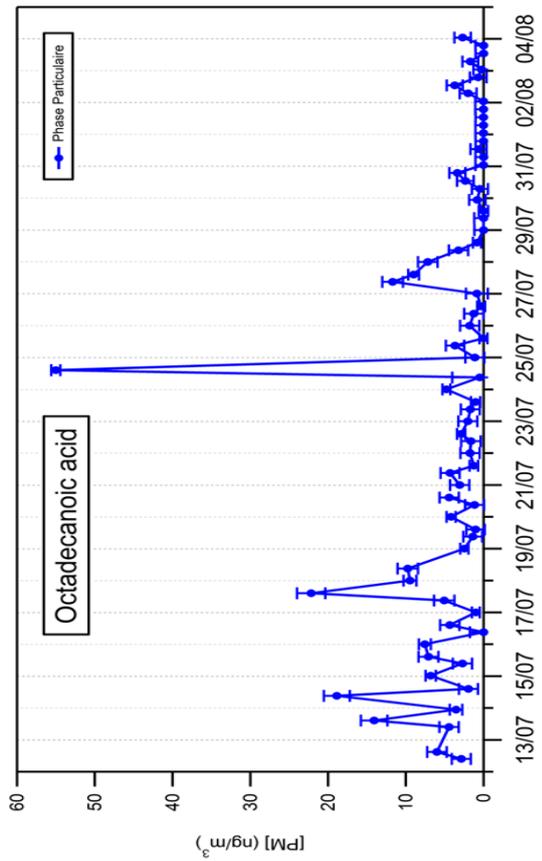


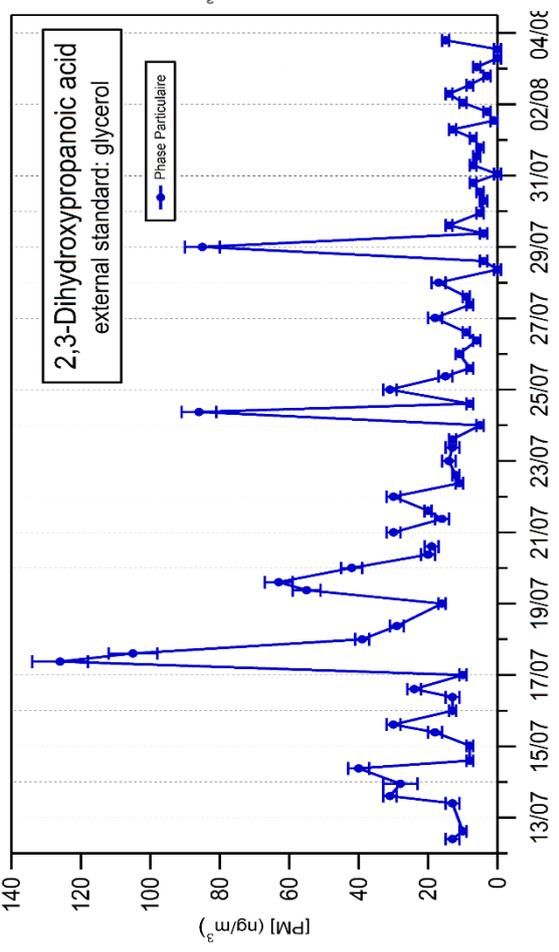
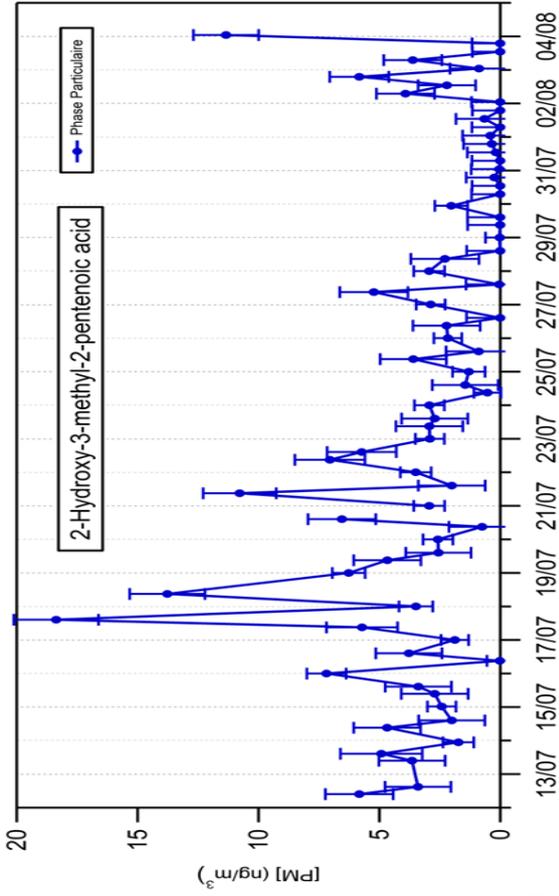


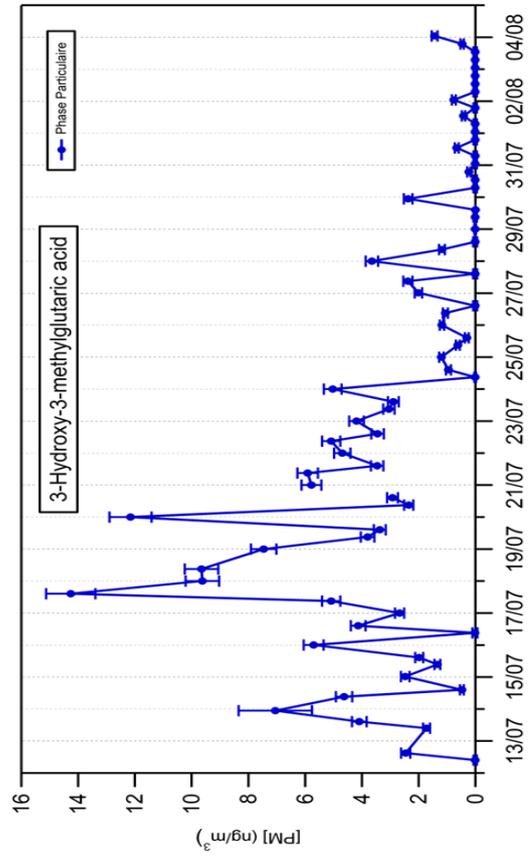
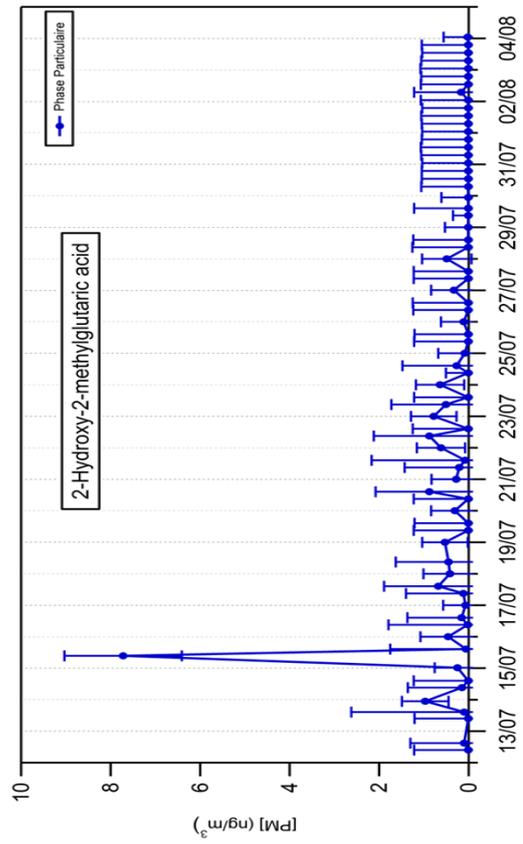
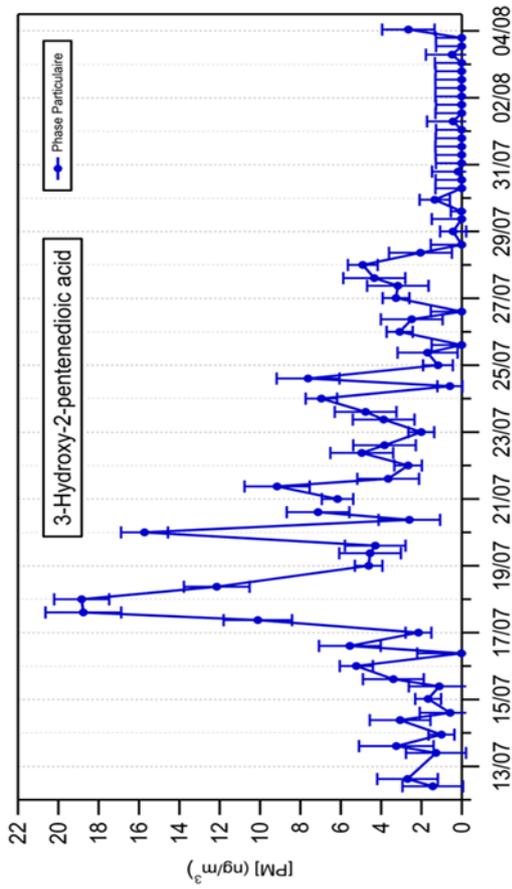
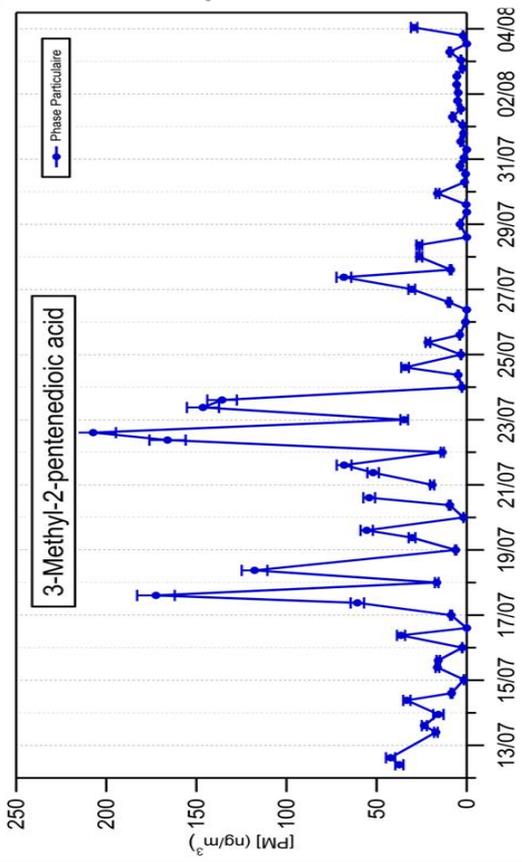


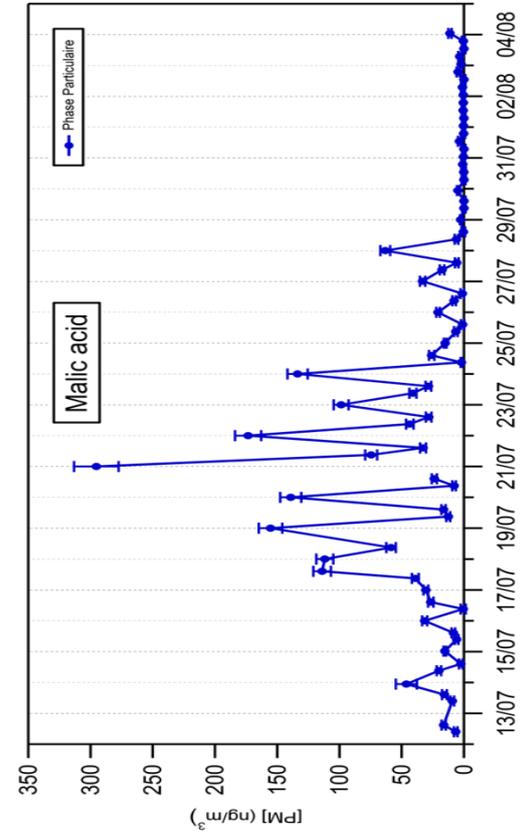
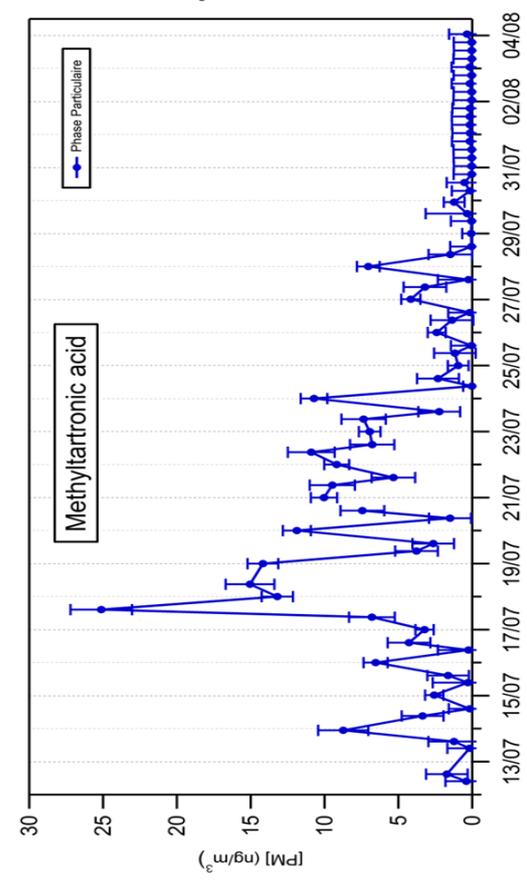
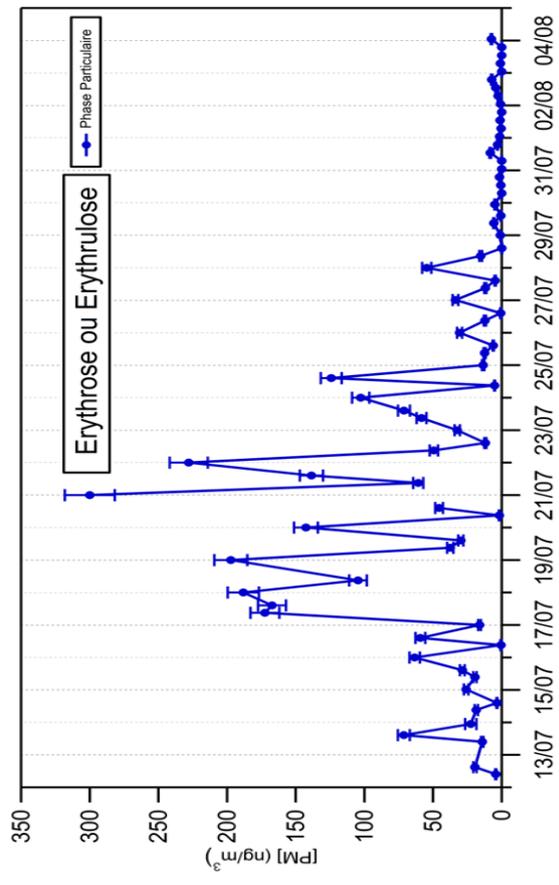


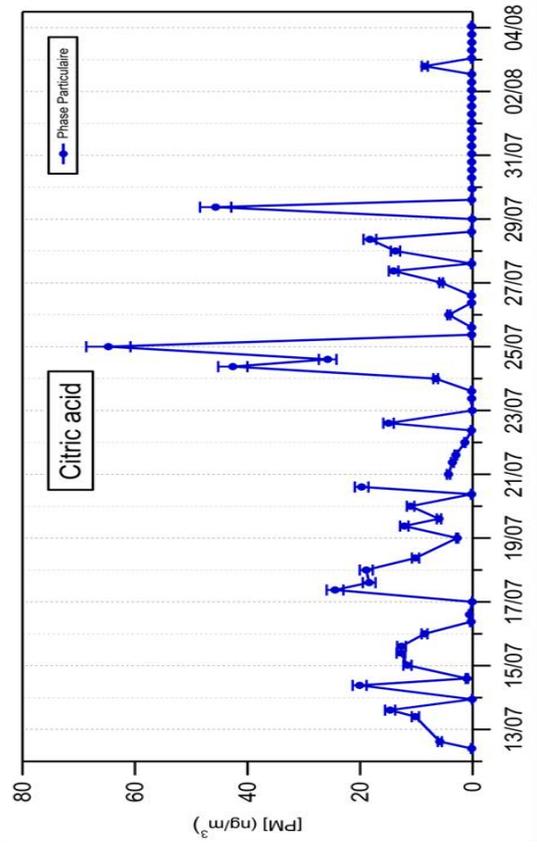
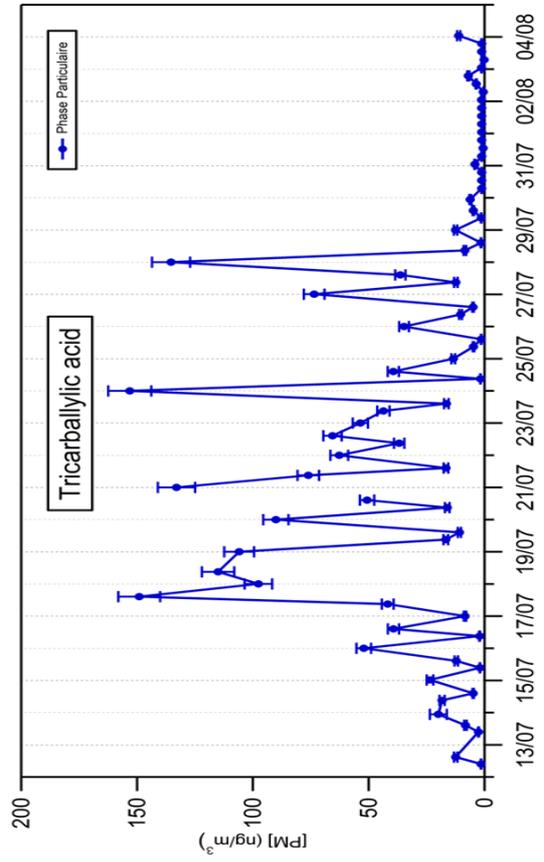
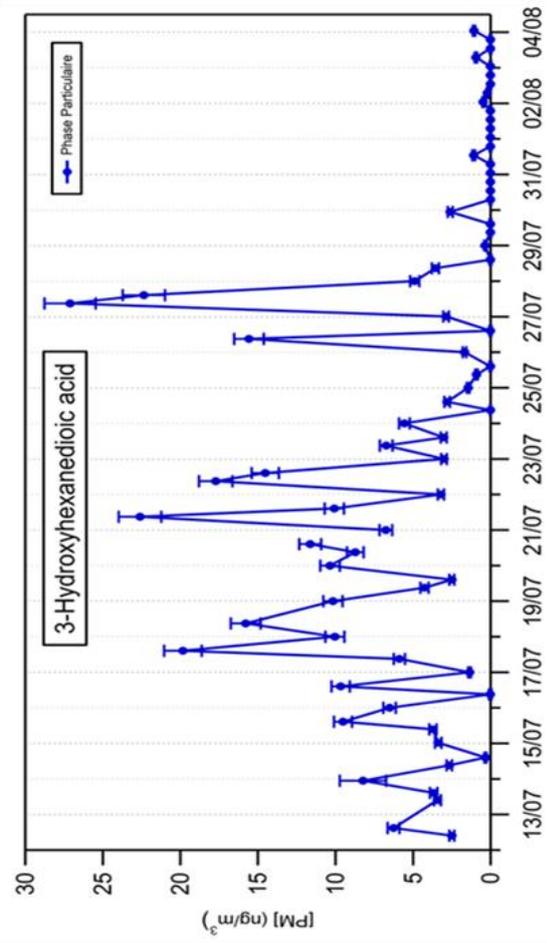


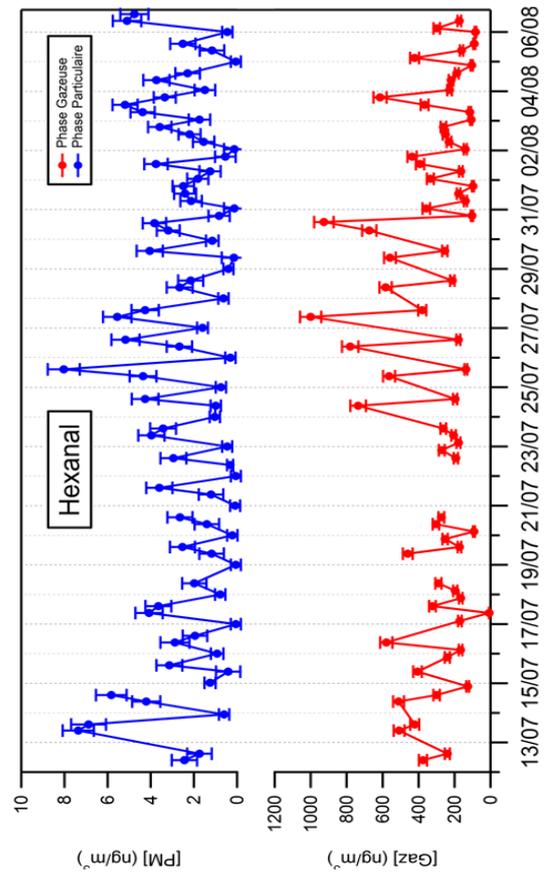
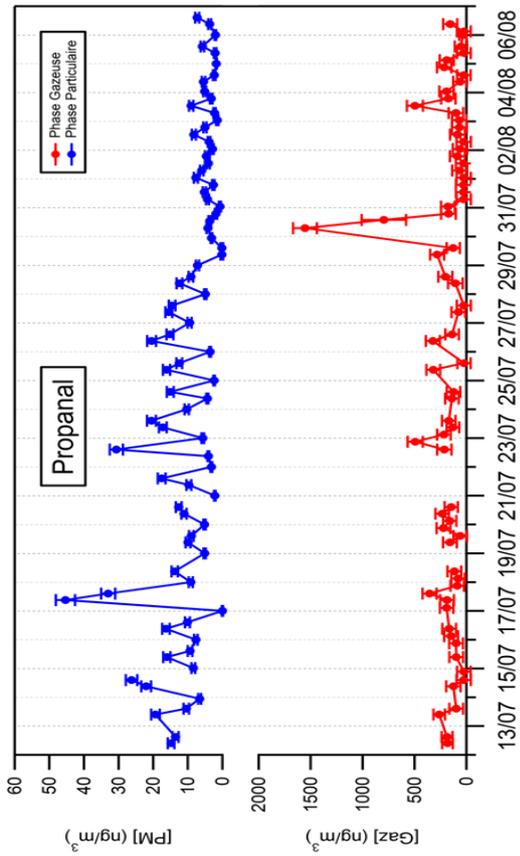
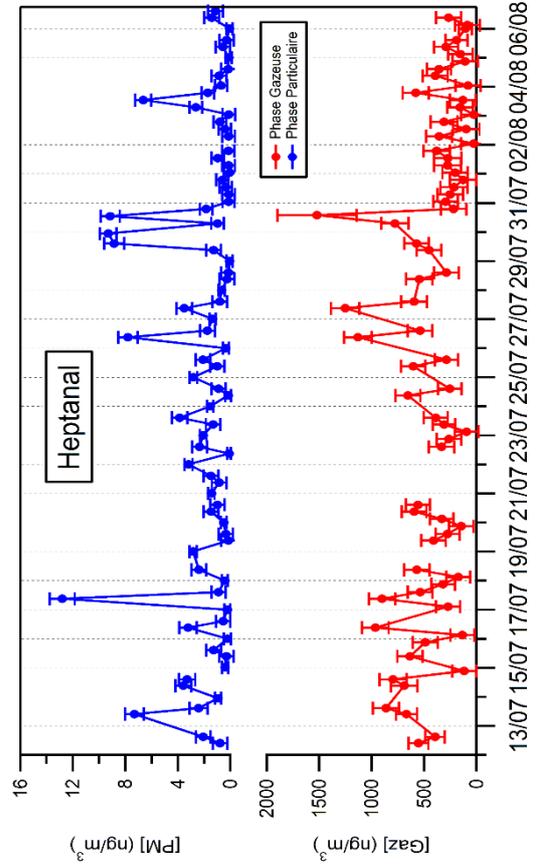
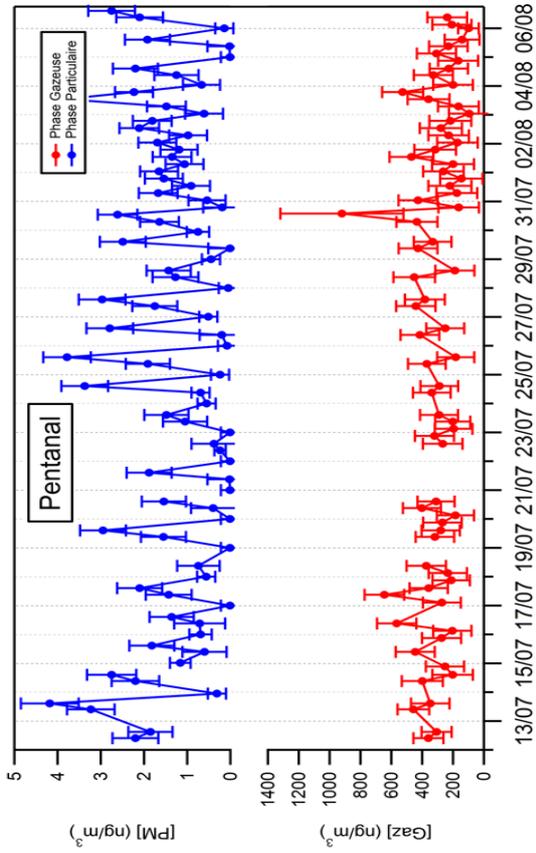


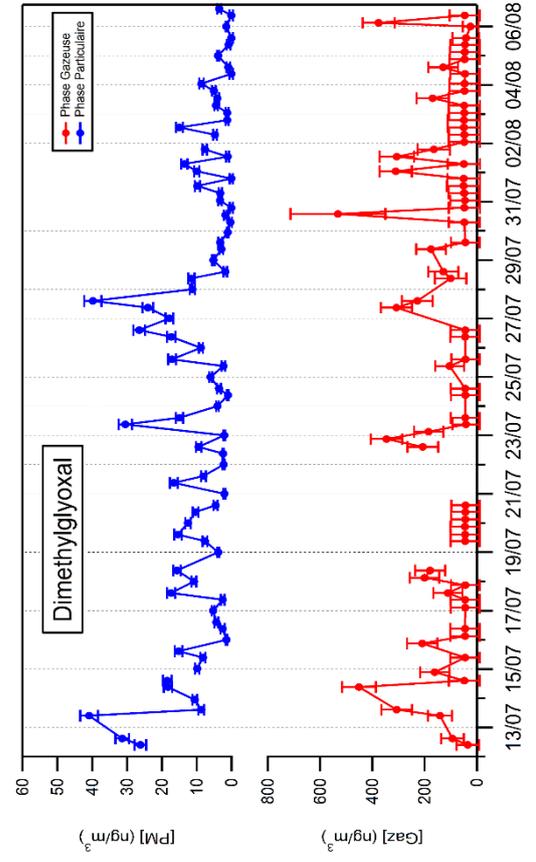
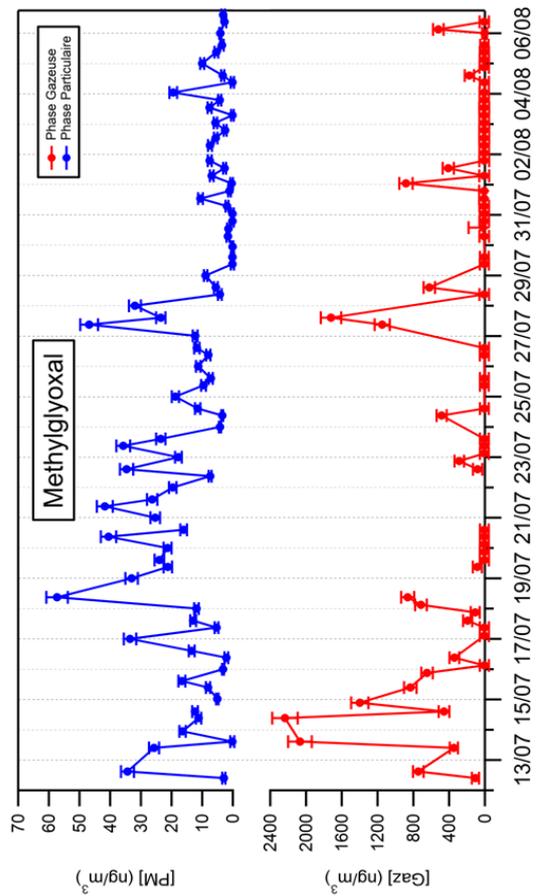
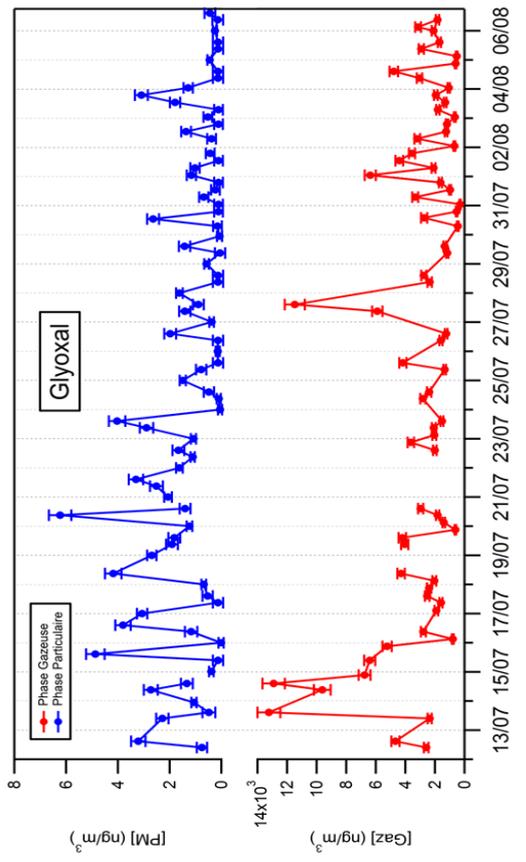
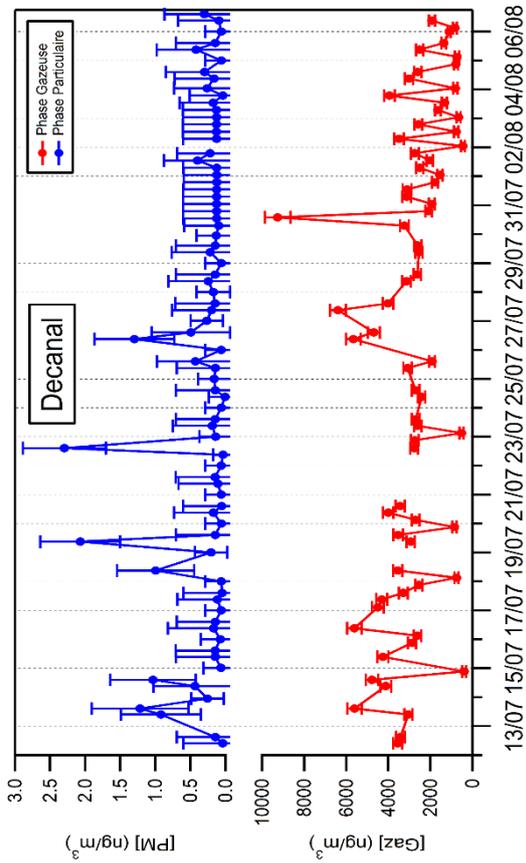


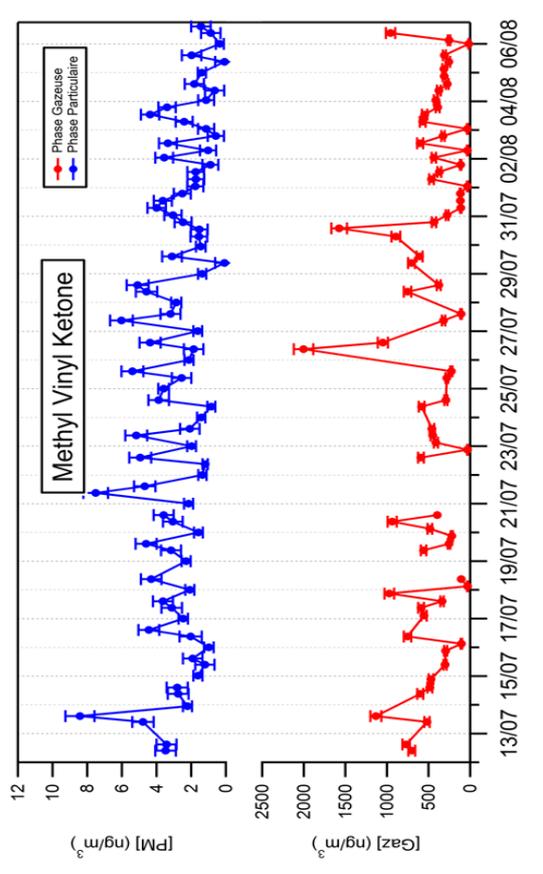
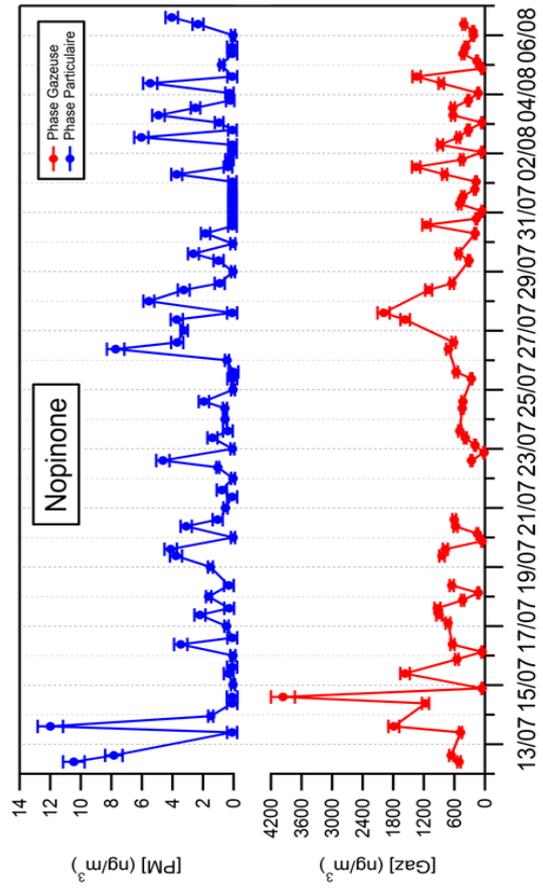
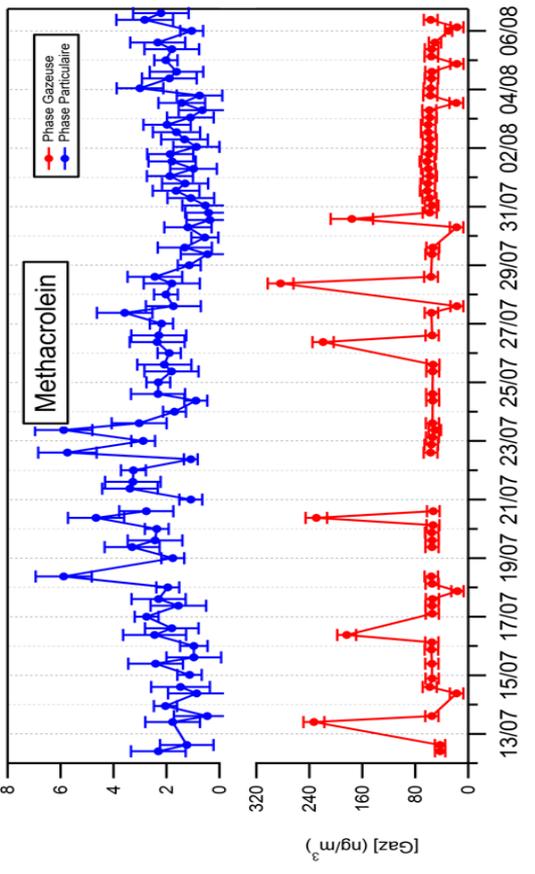
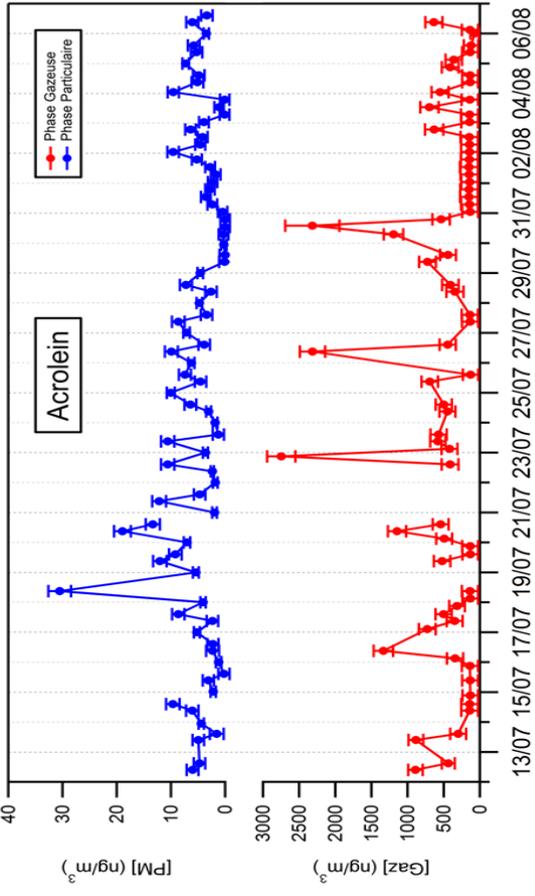


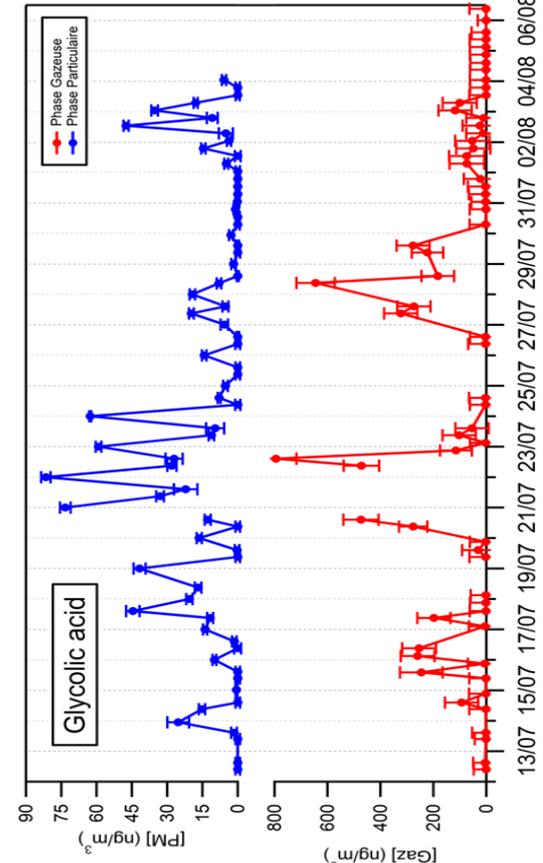
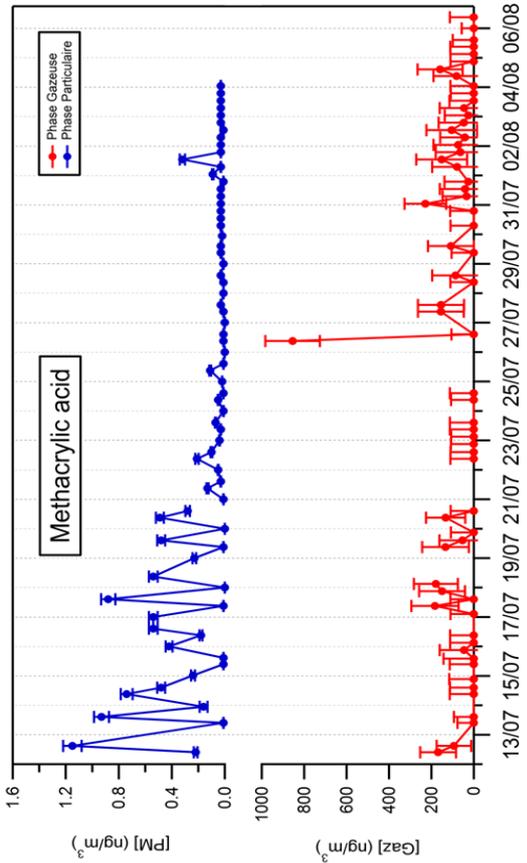
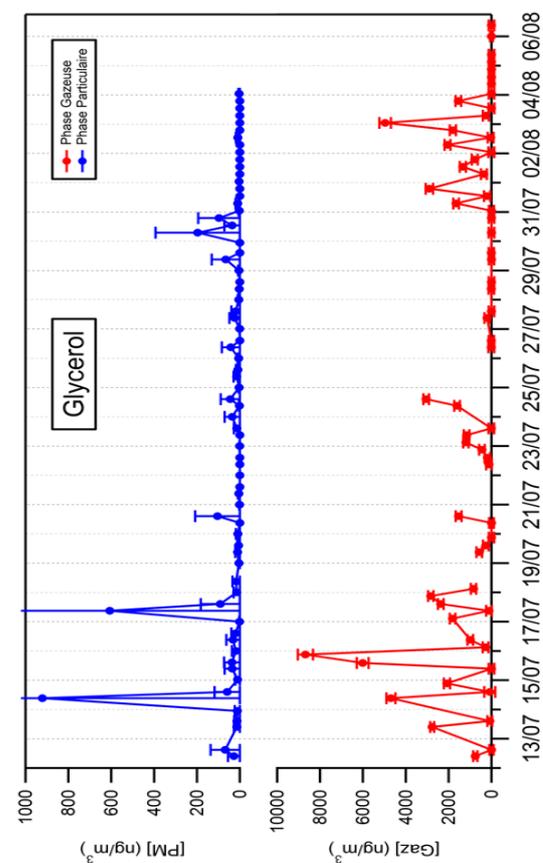
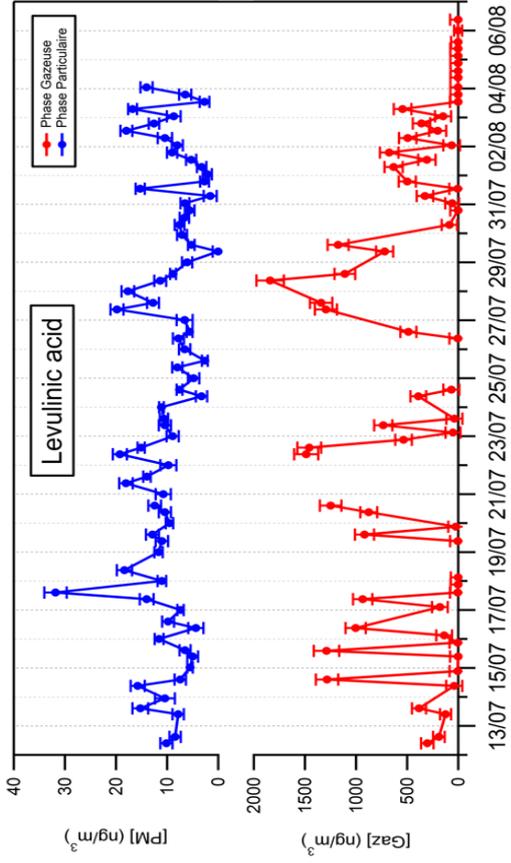












Supplementary material 3: Time series of MSA (methanesulfonic acid, black line) and water soluble HULIS (red line) during ChArMEx campaign.

