

1 **Rapid and portable mid-infrared analysis of wet sediment samples by a novel “filter-press” attenuated total reflectance**
2 **method**

3 Leslie J. Janik^{a,b*}, Stuart L. Simpson^c, Mark Farrell^d, Luke M. Mosley^b

4 ^aCSIRO Land and Water, Kurna Country, Waite Road, Urrbrae, South Australia, Australia

5 ^bSchool of Biological Sciences, University of Adelaide, Kurna Country, Adelaide, South Australia, Australia.

6 ^cCSIRO Environment, Tharawal Country, Lucas Heights, New South Wales, Australia.

7 ^dCSIRO Agriculture and Food, Kurna Country, Waite Road, Urrbrae, South Australia, Australia.

8 * Correspondence to Leslie Janik. Email: les.janik@csiro.au. ORCID: 0000-0003-0259-1097.

9

10

11 **SUPPLEMENTARY INFORMATION**

12 **Site description**

13 The Coorong Lagoon is a long (~100 km), shallow (~1.3 m mean depth) and narrow (~0.5-2 km wide) estuarine-hypersaline lagoon system at the end of
14 Australia's largest river system, the Murray. It is an inverse estuary system, with salinities, nutrient and OC concentrations increasing with distance away from
15 the river mouth (Mosley et al. 2020). The Coorong has a semi-arid climate with mean annual rainfall in the local area of 383 mm, net open water (Morton's
16 Lake) evaporation of approx. 800 mm/year and mean maximum and minimum air temperatures of 20.9 and 11.9°C respectively, although temperature can
17 increase to >40°C in summer (Mosley et al. 2023). External sediment sources include the River Murray, which has dominant illitic and smectitic clay contents
18 (Gingele and De Deckker 2005), minor local contributions from the nearby Salt Creek catchment higher in quartz and dolomite (Merry and Fitzpatrick 2005),
19 and sand blown in from the seaward dune system.

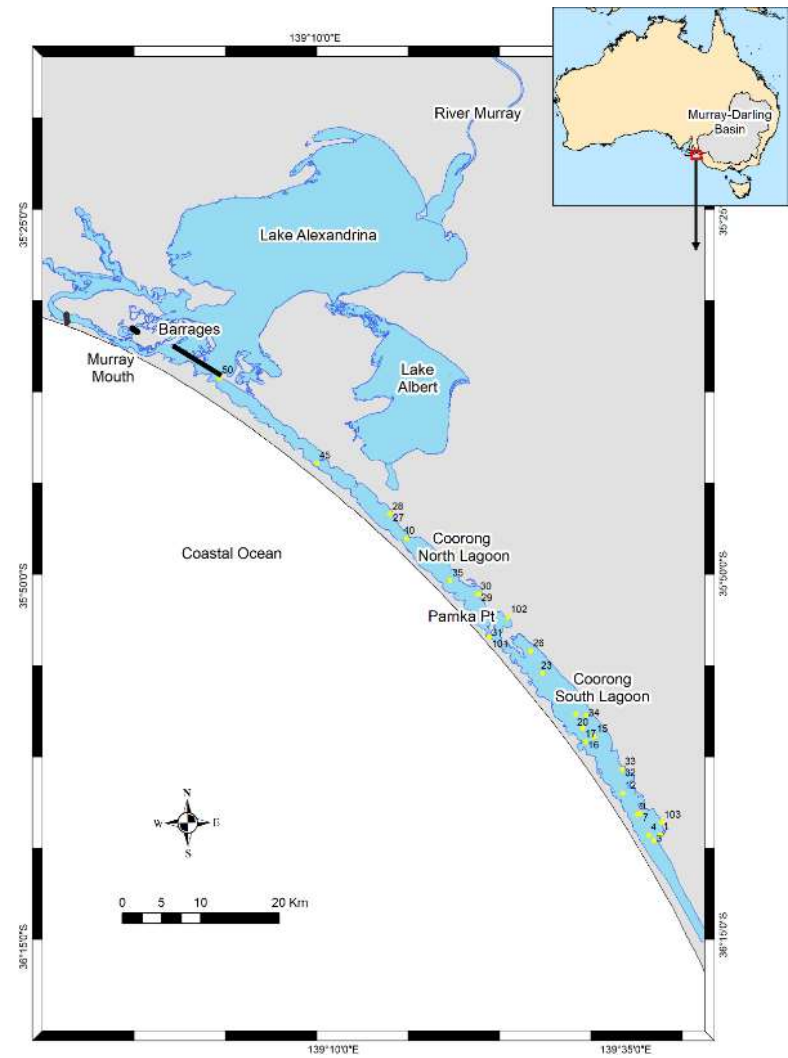
20

21

22 **Fig. S1**

23 *Map of the Coorong Lagoon including location of water and sediment sampling*
24 *sites. Calibration samples (Set-1) are located at site numbers 1-50. For Set-2,*
25 *Parnka Point is located at site number 101 (Sediments T1 and T2), Parnka South*
26 *at 102 (Sediments T3-T6) and Tea Tree at site 103 (Sediments T7-T11)*

27



28 **Fig. S2**



29

30 *Method of collecting core samples with the polycarbonate push tube for analysis*

31



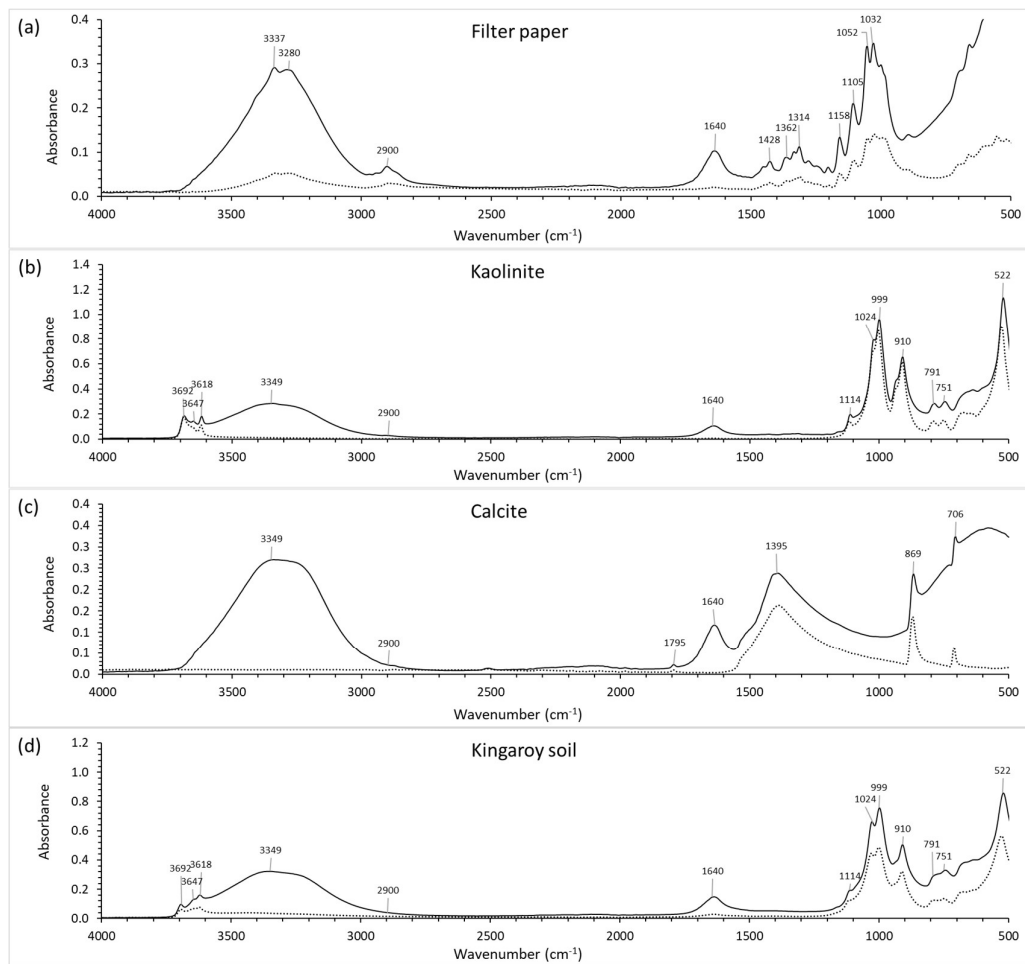
33

34 *Examples of core samples from (a) Tea Tree and (b) Parnka Point taken with the polycarbonate push tube for analysis*

35

36

37 **Fig. S4**



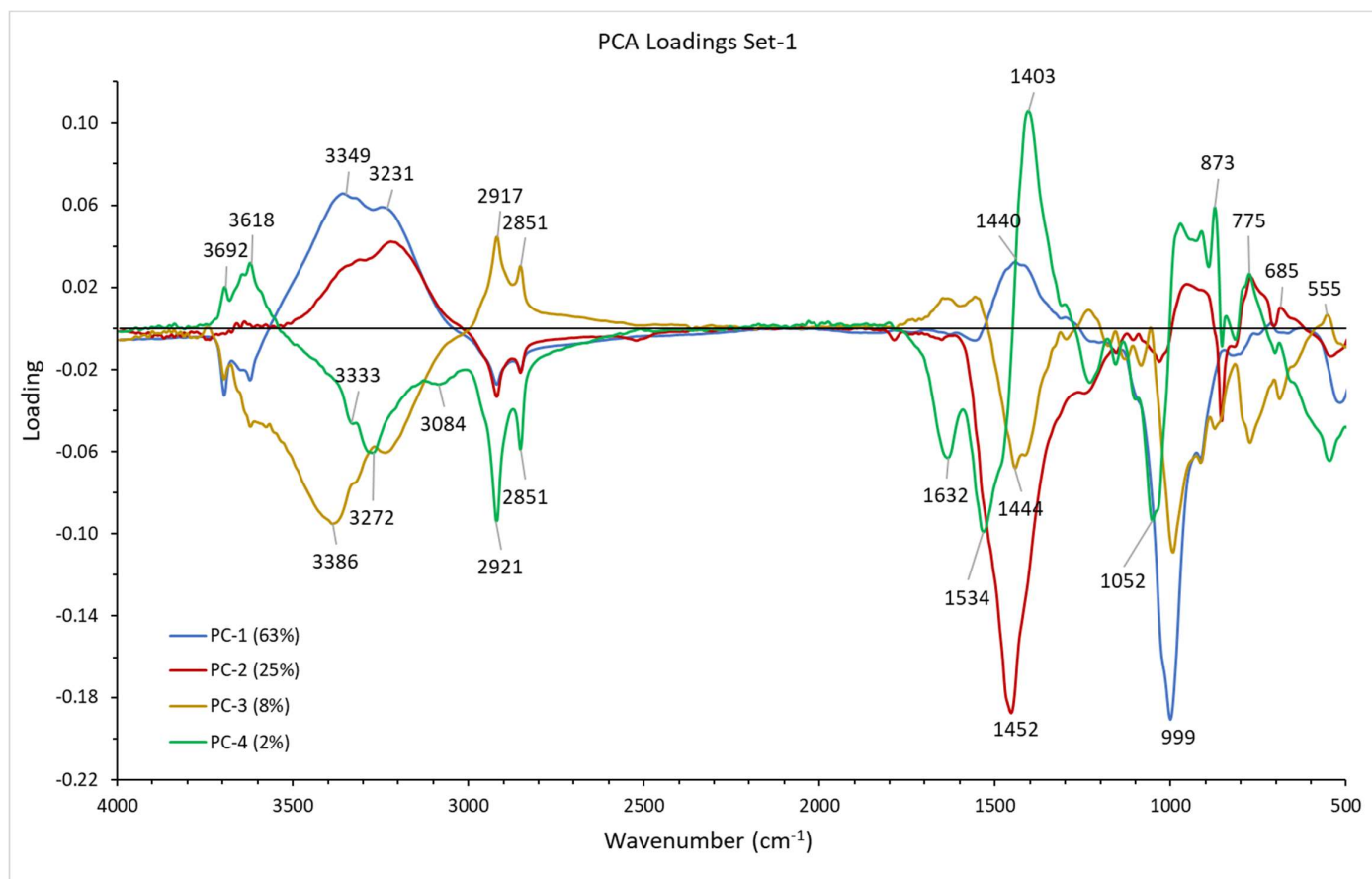
38

39 *ATR spectra of (a) filter paper (Whatman #5), (b) low crystallinity kaolinite (Birdwood, South Australia), (c) calcite (Calcium carbonate, Merck) and (d)*

40 *Kingaroy soil (QLD, Australia), pressed dry (···) and then wet filter-pressed (—) onto the crystal surface.*

41

42 **Fig. S5**

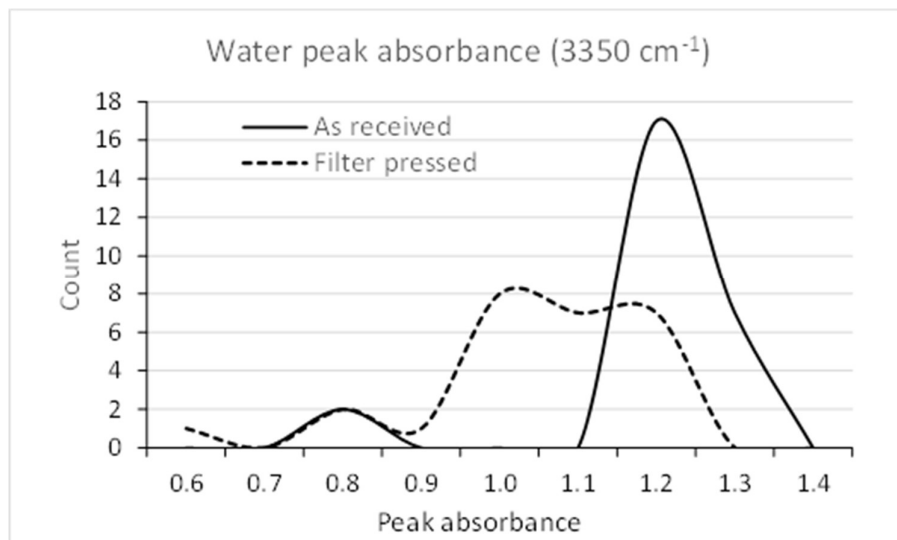


43

44 *PCA loading spectra of the filter-paper pressed Set-1 sediment samples after removal of samples C13, C14 and C17. Frequencies of the major peaks are*
45 *indicated in the figure.*

46

47 **Fig. S6**



48
49 *Absorbance distributions of the 3350 cm⁻¹ water peak for the As-received and Filter pressed calibration spectra*

50 **Table S1** Laboratory data for sediments in the Coorong Set-1

Sediment	ID	ID and Depth (cm)	Easting (GDA Zone54)	Northing (GDA Zone54)	TEXTURE (ISSS)	WATER (%)	TOC (%)	TIC (%)	CLAY (%)	SILT (%)	SAND (%)	pH	EC (dS/m)	TP (mg/kg)	TN (%)	AVS (%)	CRS (%)
C1	1	01 0-5 cm	377352	6000352	Sand	28.8	0.26	8.36	7	1	92	9.3	12	163	0.05	0	0.06
C2	3	03 0-5 cm	376503	5999578	Sand	19.3	0.3	7.1	5	0	95	9.2	9	171	0.04	0	0.05
C3	4	04 0-5 cm	375811	6000267	Clay	80.4	6.36	3.74	57	1	42	8.5	96	547	0.78	0.02	0.21
C4	7	07 0-5 cm	374751	6003071	Clay	79.3	6.31	3.03	70	9	21	8.4	95	504	0.75	0.05	0.26
C5	9	09 0-5 cm	374370	6002924	Clay	80.6	6.64	2.68	79	2	19	8.3	109	688	0.78	0.04	0.23
C6	12	12 0-5 cm	372513	6005638	Sandy Loam	36.8	0.82	5.24	11	1	88	9.2	21	130	0.14	0	0.06
C7	15	15 0-5 cm	368883	6012868	Clay	80.1	5.55	2.28	82	4	15	8.4	100	522	0.72	0.05	0.29
C8	16	16 0-5 cm	367763	6012281	Sandy Clay	66.9	2.97	5.19	35	1	64	8.6	58	422	0.38	0.04	0.18
C9	17	17 0-5 cm	367412	6013992	Clay	71.3	3.9	1.87	51	3	46	8.5	65	371	0.45	0.07	0.26

C10	20	20 0-5 cm	366520	6015827	Clay	80.2	5.94	1.29	92	7	1	8.4	98	580	0.75	0.06	0.29
C11	23	23 0-5 cm	362271	6020991	Clay	80.8	5.16	1.36	90	4	6	8.4	101	685	0.7	0.05	0.27
C12	26	26 0-5 cm	360755	6023844	Clay	74.3	2.58	4.65	82	15	3	8.5	75	373	0.46	0.06	0.27
C13	27.1	27.1 0-2 cm	342792	6041428	Sand	18.4	0.3	0.06	4	1	95	9	8	47	0.05	<0.01	0.01
C14	27.2	27.2 2-5 cm	342792	6041428	Sand	18.6	0.18	0.19	2	1	97	9.1	6	21	0.03	<0.01	0.01
C15	27.3	27.3 5-10 cm	342792	6041428	Sand	25.2	0.13	0.06	3	2	95	9	5	23	0.03	0.01	0.01
C16	28	28 0-5 cm	342726	6041376	Sand	21.1	0.39	0.15	5	0	95	9	5	64	0.05	0.01	0.02
C17	29	29 0-5 cm	354117	6031137	Sandy Loam	29.9	0.82	0.83	15	1	84	8.9	16	79	0.1	0.04	0.08
C18	30	30 0-5 cm	353988	6031130	Sandy Clay Loam	38.6	0.96	2	20	0	80	8.8	19	89	0.09	0.01	0.14
C19	31	31 0-5 cm	355432	6025659	Sandy Clay	58.4	2.63	2.2	39	3	58	8.6	41	331	0.31	0.08	0.24
C20	32	32 0-5 cm	372471	6008708	Sand	26.1	0.71	0.81	7	2	91	8.9	14	73	0.07	0.02	0.03
C21	33	33 0-5 cm	372471	6008709	Sandy Loam	27.7	0.75	0.71	10	0	90	9	14	84	0.08	0.02	0.04
C22	34	34 0-5 cm	367842	6015627	Sand	21.6	0.35	3.18	6	0	94	9.1	11	58	0.06	0.01	0.04
C23	35	35 0-5 cm	350402	6032876	Clay	77.4	5.55	0.41	83	13	4	8.3	73	528	0.68	0.08	0.64
C24	40	40 0-5 cm	344861	6038275	Sandy Loam	42.3	1.26	0.21	16	1	83	8.5	17	166	0.17	0.05	0.17
C25	45	45 0-5 cm	333434	6047916	Clay	64.8	1.67	1.15	50	1	50	8.4	21	281	0.24	0.05	0.65
C26	50	50 0-5 cm	320955	6058852	Sandy Loam	42.3	1.09	0.42	11	1	89	8.6	8	215	0.13	0.04	0.14

ISSS = International Soil Science Society. Particle size: Clay <2 µm Silt = 2-20 µm; Sand >20 µm. . EC on sediment following 1:5 water addition.
 TOC – total organic carbon, TIC – total inorganic carbon. AVS – Acid Volatile Sulfide, CRS – Chromium Reducible Sulfur

51
52
53
54

55 **Table S2** Laboratory data for sediments at Parnka and Tea Tree (Set-2).

Sediment	ID	Site and Depth	Easting (GDA Zone54)	Northing (GDA Zone54)	TEXTURE (ISSS)	WATER (%)	TOC (%)	TIC (%)	CLAY (%)	SILT (%)	SAND (%)	pH	EC (dS/m)	TP (mg/kg)	TN (%)	AVS (%)	CRS (%)
T1	101-1	Parnka Point 0-2cm				Wet	4.91					8.93	42.8	665	0.69	0.068	0.45
T2	101-2	Parnka Point 8-10cm				Wet	2.2					8.97	30.8	337	0.29	0.04	0.2
T3	102-1	Parnka Sth A 0-2cm				Wet	1.14					9.28	17.5	180	0.14	0.006	0.13
T4	102-2	Parnka Sth A 2-4cm				Wet	0.70					9.42	13.5	133	0.08	0.001	0.13
T5	102-3	Parnka Sth B 0-2cm				Wet	2.35					9.18	43.4	288	0.27	0.011	0.18
T6	102-4	Parnka Sth B 2-4cm				Wet	0.75					9.47	13	183	0.09	0.002	0.16
T7	103-1	Tea Tree 0-2cm				Wet	0.83					9.56	12.8	94	0.11	0.001	0.03
T8	103-2	Tea Tree 2-4cm				Wet	0.73					9.55	13.3	98	0.08	0.002	0.03
T9	103-3	Tea Tree 4-6cm				Wet	0.63					9.56	13.2	52	0.07	0.001	0.04
T10	103-4	Tea Tree 6-8cm				Wet	0.59					9.52	12.3	59	0.06	0.001	0.04
T11	103-5	Tea Tree 8-10				Wet	0.89					9.13	12.9	118	0.11	0.003	0.129

ISSS = International Soil Science Society. Particle size: Clay <2 µm Silt = 2-20 µm; Sand >20 µm. . EC on sediment following 1:5 water addition.
 TOC – total organic carbon, TIC – total inorganic carbon. AVS – Acid Volatile Sulfide, CRS – Chromium Reducible Sulfur.

56
57
58
59

