

1 **Statistical analysis of APXS-derived chemistry of the clay-bearing Glen Torridon region**
2 **and Mount Sharp group, Gale crater, Mars**

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19 Key points:

20 1. Alpha Particle X-ray Spectrometer data for Glen Torridon, Gale crater documents subtle
21 compositional changes

22 2. Multiple episodes of alteration and diagenesis identified

23 3. Compositional similarities between Glen Torridon members confirms the highly localized
24 nature of the Vera Rubin ridge alteration

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29 Abstract

30 The Glen Torridon stratigraphic sequence marks the transition from the low energy
31 lacustrine-dominated Murray formation (Mf) (Jura member: Jm) to the more diverse Carolyn
32 Shoemaker formation (CSf) (Knockfarril Hill member: KHm; Glasgow member: Gm), indicating
33 a change in overall depositional setting. Alpha Particle X-ray Spectrometer (APXS) results and
34 statistical analysis reveals that the bulk primary geochemistry of Mf targets are broadly in family
35 with CSf targets, but with subtle compositional and diagenetic trends with increasing elevation.
36 APXS results reveal significant compositional differences between Jm_GT and the
37 stratigraphically equivalent Jura on Vera Rubin ridge (Jm_VRR). APXS data defines two
38 geochemical facies (high-K or high-Mg) with a strong bimodal grain distribution in Jm_GT and
39 KHm. The contact between KHm to Gm is marked by abrupt sedimentological changes but a
40 similar composition for both. Away from the contact, the KHm and Gm plot discretely,
41 suggesting a zone of common alteration at the transition and/or a gradual transition in
42 provenance with increasing elevation in the Gm. APXS results point to a complex history of
43 diagenesis within Glen Torridon, with increasing diagenesis close to the Basal Siccar Point
44 unconformity on the Greenheugh pediment, and with proximity to the beginning of the clay
45 sulfate transition. Elemental mobility is evident in localized enrichments or depletions of Ca, S,
46 Mn, P, Zn, Ni. The highly altered Hutton interval, in contact with the unconformity on Tower
47 butte, is also identified on Western Butte, indicating that the “interval” was once laterally
48 extensive.

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50 **Plain Language Summary**

51 The MSL Curiosity rover traversed the Glen Torridon locale in Gale crater, Mars, finding
52 evidence in the rocks of a change from a lake setting to a river setting, with increasing elevation
53 through the rock record. Geochemical results from the Alpha Particle X-ray Spectrometer
54 (APXS) confirm a slow change in composition over time as the sediments that formed the rock
55 were laid down. Fluids percolated through the sediments, altering the composition, with
56 localized enrichments of calcium, sulfur, manganese, phosphorus, sodium, zinc, nickel, which
57 are now present as veins or small rectangular nodules and concentrations.

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61 **1. Introduction**

62 The Mars Science Laboratory (MSL) rover *Curiosity* has been exploring Gale crater, Mars,
63 since August 2012, with the primary mission to seek and characterize past habitable
64 environments [Grotzinger et al., 2012]. Gale crater is a ~155km diameter impact crater, with a 5
65 km high central mound, Aeolis Mons, (informally known as Mount Sharp) [Milliken et al., 2010;
66 Grotzinger et al., 2012; Golombek et al., 2012], forming close to the Noachian-Hesperian
67 transition, c. 3.7 ± 0.1 Ga [Le Deit et al., 2013; Thomson et al., 2011]. The Mount Sharp Group
68 encompasses a series of sedimentary siliciclastic rocks, deposited under predominantly fluvial
69 and lacustrine conditions (Bradbury, Murray and Carolyn Shoemaker formations) [e.g.,
70 Grotzinger et al., 2014, 2015; Rice et al., 2017; Stack et al., 2019; Edgar et al., 2020; Fedo et al.,
71 2020, this issue]. These deposits are overlain unconformably (along the Basal Siccar Point
72 unconformity) by aeolian deposits of the Siccar Point Group [Stimson formation] [e.g., Banham
73 et al., 2018, this issue; Bryk et al., 2019, 2020].

74 Since descending from the erosion-resistant Vera Rubin ridge (VRR) [e.g., Fraeman et al.,
75 2020] in January 2019, *Curiosity* has been exploring the phyllosilicate unit or trough [Anderson
76 and Bell, 2010; Fraeman et al., 2016], skirting along the edge of VRR in a topographical low
77 (informally called “Glen Torridon”) (Figure 1) below the layered sulfate units identified from
78 orbit [e.g., Milliken et al., 2010]. Glen Torridon comprises a series of units with an Fe/Mg
79 smectite clay-rich spectral signature (orbitally defined, pre landing) [e.g., Fraeman et al., 2016;
80 Milliken et al., 2010], a major objective of MSL’s primary mission, as clay minerals record fluid
81 conditions and can enhance organic matter preservation [Summons et al., 2011]. The change
82 from clay- to sulfate-rich conditions with increasing elevation indicates a fundamental shift in
83 environmental and depositional across the boundary [Bibring et al., 2006; Milliken et al., 2010].

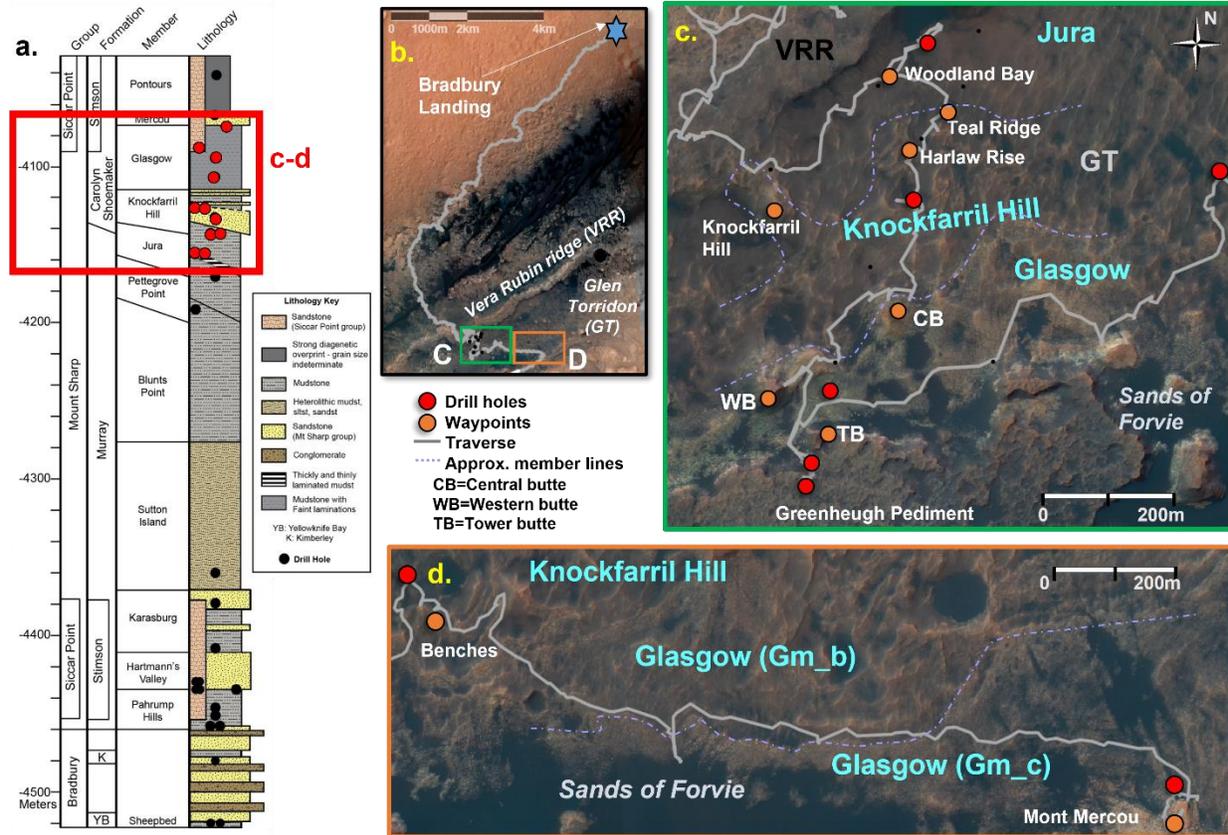


Figure 1. Stratigraphic column for Curiosity's traverse in Gale crater, Mars and localization maps. Stratigraphic column after Fedo et al., 2021, this issue. Base maps for images 1b-1d: High Resolution Stereo Camera (HiRise; on board the European Space Agency (ESA) Mars Express orbiter) orbital images of Gale crater, Mars. Image credit: NASA/JPL-Caltech.

(1a) Stratigraphic column for Gale crater highlighting in red the area covered by this study. Drill holes for the campaign (red circles) are (in sol order): Aberlady (AL); Kilmarie (KM); Glen Etive 1+2 (GE1+GE2); Hutton (HT); Edinburgh (EB); Glasgow (GG); Mary Anning 1+3 (MA1+MA3); Groken (GR); Nontron (NT). (1b). Map of Gale crater, with rover traverse shown in grey, highlighting the study area in Glen Torridon, showing approximate member boundaries (purple dashed lines) between Jura, Knockfarril Hill and Glasgow members. (Fedo et al., this issue for detailed stratigraphic maps). (1c) Sols 2300-2921 comprises the descent from VRR to the MA and GR drill locales. (1d) Sols 2925-3072 comprises the post-MA traverse to the NT drill at the base of Mont Mercou. Glasgow member is subdivided into Gm_a, Gm_b and Gm_c, based on compositional variations defined herein (Section 4.3.1); subunit boundary (purple dashed line) in 1d. after Hughes et al., this issue, 2021.

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	Formation	Member	Subunits ¹⁰	Description	Drill targets	Location Notes	Other names	
Mount Sharp Group ¹	Murray (Mf) ^{1,3,4}	Jura ⁹ (Jura in study area = Jm_Gt) ¹⁰	High-K facies	dominant morphology; mudstones; pebbles, some larger boulders and "rubble"	-	main clay-rich trough, lower most Glen Torridon	Phyllosilicate trough ¹⁵ phyllosilicate layers ¹⁶ phyllosilicate unit ² Clay-bearing unit ^{19,20}	Smooth claybearing unit (sCBU) ^{17,18}
			High-Mg facies	fine sandstone; "coherent" beds, in situ	<i>Aberlady</i> (AL) <i>Kilmarie</i> (KM)			
	Knockfarril Hill (KHm) ^{5,6}	High-K facies	High-Mg facies	finer sandstones, layers within coarser bedrock	<i>Glen Etive 1</i> (GE1) <i>Glen Etive 2</i> (GE2)	overlying Jm_Gt, to Central butte, and edge of Western butte		Fractured claybearing unit (fU) ^{17,18}
				dominant morphology: cross-stratified sandstone ridges and hills	<i>Mary Anning 1</i> (MA1) <i>Mary Anning 3</i> (MA3) <i>Groken</i> (GR)			
		KHm to Gm	Benches ^{5,6}	series of resistant benches, with fine-grained pebbles, boulders etc	-	transition KHm to Gm		
	Carolyn Shoemaker (CSf) ^{5,6}	Glasgow ^{5,6}	Gm_a, including buttes zone	finely laminated mudstones, abundant diagenetic features (veins, nodules)	<i>Glasgow</i> (GG)	Central, Western, Tower buttes & traverse to Mary Anning (MA)		Intermediate fractured claybearing unit (fIU) ^{17,18}
					-	post-MA, to base of Mont Mercou		
					<i>Nontron</i> (NT)			
			Gm_HT	"Hutton interval" - Zone of intense alteration, in contact with overlying Basal Siccar Point unconformity	<i>Hutton</i> (HT)	Top of Tower butte, in contact with overlying Basal Siccar Point unconformity ^{12,13}		
	Siccar Point Group ²	Stimson (Sf) ^{7,8}	Stimson @ Greenheugh Pediment ¹²		Capping rock ^{11,13,14} , above Basal Siccar Point unconformity	<i>Edinburgh</i> (EB)		Capping rock on Greenheugh Pediment

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Table 1. Summary of units within Glen Torridon.

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¹Grotzinger et al., 2015. ²Fraeman et al., 2016. ³Fedo et al., 2019. ⁴Stack et al., 2019. ⁵Bennet et al., this issue. ⁶Fedo et al., this issue. ⁷Banham et al., 2018.

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⁸Banham et al., 2021. ⁹Edgar et al., 2020. ¹⁰As defined herein. ¹¹Thompson et al., this issue. ¹²Banham et al., this issue. ¹³Bryk et al., 2019, 2020. ¹⁴Malin &

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Edgett, 2000. ¹⁵Anderson & Bell, 2010. ¹⁶Milliken et al., 2010. ¹⁷Stack et al., 2017. ¹⁸Cofield et al., 2017. ¹⁹Bennet et al., 2018. ²⁰Fox et al., 2018.

108 In this work, we present Alpha Particle X-ray Spectrometer (APXS) results for the Glen
109 Torridon region. Section 2 places the Glen Torridon traverse in context with orbitally identified
110 units and with in situ stratigraphically defined units. Section 3 gives details of the instrument, the
111 data sets analyzed by APXS, and the statistical methodology used. Section 4 presents the
112 analytical results across the traverse, which are discussed in section 5.

113 **2. Context – orbital mapping and definition of units**

114 The Glen Torridon region has been extensively mapped using orbital data, combining both
115 morphology and spectral signature to define units [e.g., Fraeman et al., 2016; Hughes et al.,
116 2021, this issue]. As part of the Glen Torridon campaign, unit definitions have been refined via
117 in situ mapping and sedimentological analysis [e.g., Fedo et al., 2020, this issue; Bennet et al.,
118 2018, this issue]. Table 1 relates the orbitally defined units to those defined by in situ
119 (formations, members), and the geochemical sub-units as defined herein, based on APXS data.

120 The Glen Torridon campaign started with descent from the Vera Rubin ridge (VRR) (sol
121 2302) (Figure 1c) and ends (for the purposes herein) at the *Nontron* drill site, at the base of Mont
122 Mercou (sol 3072) (Figure 1d). It encompasses three sedimentary members (Jura, Knockfarril
123 and Glasgow) and marks the transition from the fluvio-lacustrine Murray formation (Mf) [e.g.,
124 Grotzinger et al., 2015; Fedo et al., 2019] to the more diverse Carolyn Shoemaker formation
125 (CSf) [Bennet et al., this issue; Fedo et al., this issue].

126 The **Jura member (Jm; Murray formation)** within Glen Torridon (hereafter **Jm_GT**)
127 (Section 4.1) is stratigraphically equivalent to the lacustrine Jura member on VRR (Jm_VRR)
128 [Edgar et al., 2020; Fedo et al., 2020, this issue]. The Jm_GT is dominated by pebbly regolith,
129 larger boulders, and rare flat lying patches of finely laminated mudstones (Figures S2a-d),
130 interpreted to represent low energy lacustrine environments [Edgar et al., 2020; Caravaca et al.,

131 this issue]. Less commonly, there are coarser grained, continuous bedrock targets (Figure S10e),
132 up to sandstone grain size [Rivera Hernandez et al., 2020a, 2020b; Minitti et al., 2020, 2021].
133 These are interpreted to have been deposited under higher energy conditions, such as a fluvial
134 environment or a fluvially influenced lakeshore [Caravaca et al., this issue].

135 The base of the **Knockfarril Hill** mbr (**KHm**; Carolyn Shoemaker formation) marks the
136 beginning of the Carolyn Shoemaker formation (CSf) [Bennet et al., this issue; Fedo et al., this
137 issue] (Section 4.2). The KHm is dominated by hills, ridges and mesas (e.g., Knockfarril Hill,
138 Teal ridge, Harlaw rise) (Figures S3a-b), extending (within the study area) to the lower
139 elevations of Central and Western buttes (Figure 1c). Both finer-grained and coarser-grained
140 facies are identified within KHm [Caravaca et al., this issue; Rivera Hernandez et al., 2020a,
141 2020b; Minitti et al., 2020, 2021]. Finer-grained targets are fine-grained mudstones to sandstone
142 grain size, manifesting as rubble, pebbles and coherent layers within coarser beds (e.g., the Glen
143 Etive drill locale) (Figures S3c-d). Cross stratification is identified in the coarser sandstones,
144 indicating a change in depositional setting to a fluvial-dominated environment [Caravaca et al.,
145 this issue].

146 The **Glasgow** mbr (**Gm**; Carolyn Shoemaker formation) is characterized by thinly
147 laminated sandstones, typically light-toned (Figures S4a-b, S6a-f) and with an abundance of
148 diagenetic features, such as fracturing and nodules (rare to absent in the underlying KHm and
149 Jm_GT) [Bryk et al., 2020; Fedo et al., 2019, this issue] (Section 4.3). The Gm stretches laterally
150 from the buttes (Central, Western, Tower) to Mont Mercou (Figures 1c-d) lying stratigraphically
151 above Knockfarril Hill (KHm) but below the layered sulfate unit [e.g., Milliken et al., 2020].

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154 **3. Instrumentation, data sets and statistical methodology**

155 **3.1. MSL Alpha Particle X-ray Spectrometer (APXS) instrumentation**

156 The Canadian-built APXS instrument onboard MSL *Curiosity*, the third generation APXS on
157 martian rovers, is used to determine elemental chemistry of both rock and unconsolidated
158 materials (sand and soil), through a combination of X-ray fluorescence (XRF) and particle-
159 induced X-ray emission (PIXE) [e.g., Gellert et al., 2006, 2015; Campbell et al., 2012;
160 Grotzinger et al., 2012; VanBommel et al., 2016, 2017] [Supporting Information Text (S1)]. Six
161 curium-244 (^{244}Cm) radionuclide sources located on the sensor head irradiate a given sample
162 with alpha particles and X-ray radiation, resulting in characteristic X-rays from the target, which
163 are used to derive a spectrum or histogram of detected energies [Gellert et al., 2006]. Peaks in the
164 spectrum primarily correspond to element(s) present in the target, including major and minor
165 elements with atomic number Z 11-26 (from sodium to iron), and select trace elements
166 (including Ni, Zn, Br). Data are presented as elemental concentrations (in wt% oxide, wt%
167 element, or $\mu\text{g/g}$), with 2σ statistical precision error [Gellert et al., 2006] [Supporting
168 Information Text (S1)].

169 **3.2 APXS Sample sets**

170 This study presents compositional data from bedrock targets, diagenetic features, and Glen
171 Torridon drill fines, as analyzed by APXS (Tables 2a-b; Supplementary data file Table S1).
172 Bedrock samples include “as-is” unbrushed targets and targets largely cleared of dust, via
173 brushing with the arm-mounted Dust Removal Tool (DRT). Features such as veins and nodules
174 are analyzed routinely to monitor potential changes in diagenetic conditions. These features are
175 listed in Tables 2a-b, S1, but not included in bedrock averages. Where individual targets are
176 discussed in the text below, the name is given in italics followed by the sol of acquisition.

177 Ten targets were drilled in Murray and Carolyn Shoemaker formation bedrock during the
178 Glen Torridon campaign (Section 4.6) (Figs. 1a, S1; Table 2a-b). Drill fines include “tailings”
179 samples (generated by the drilling process) and “DBA” (dumped) samples, the latter of which
180 are equivalent to material analyzed by the MSL CheMin X-ray diffraction (XRD) system used to
181 determine phase crystallography and mineralogy [Blake et al., 2013]. Table 2b lists the highest
182 quality drill fines for each target, based on standoff from (i.e., distance above) fines, length of
183 integration, percentage of fines in APXS FOV (field of view), and the highest quality host
184 bedrock measurement [see Berger et al., 2020 for more discussion on drill fine evaluation].

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201 **Table 2.** APXS compositional data for Glen Torridon, sol 2304 to sol 3072. All data reported as wt. % except Ni,
202 Zn, Br (ppm). Errors, elevation, location data are compiled in Table S1 (Supplementary Data). Stimson formation,
203 Greenheugh pediment (sols 2694-2733) in Thompson et al., this issue.

204 (2a) All targets, grouped by formation, member and date. ¹Target names correspond to PDS names. ²Sol = a martian
205 solar day has a mean period of 24 h, 39 min, and 35.244 s and is referred to as a sol. ³Target type: R=Rock;
206 RT=regolithic pebble-sand mix; F=(drill) fines; V=vein; N=nodule; Ft=float; SL=soil; SD=Sand. ⁴Mean
207 Mf+CSf=mean Murray and Carolyn Shoemaker formation, average based on 488 targets (Supplementary Text S2
208 for discussion). ⁵Average basaltic soil (ABS), average based on 90 APXS soil analyses from Gale crater (MSL),
209 Gusev Crater (Spirit Rover, Mars Exploration Rover-A) (MER-A) and Meridiani Planum (Opportunity Rover,
210 MER-B) [O’Connell-Cooper et al., 2017].

211 (2b) Recommended drill fines and associated host bedrock targets. Targets assessed on FWHM (i.e., Full Width
212 Half Maximum, measure of data quality), lifetime length, distance from target and target coverage (for fines).
213 ²Target type: R=Rock; F-DT=tailings fines; F-DBA=fines.

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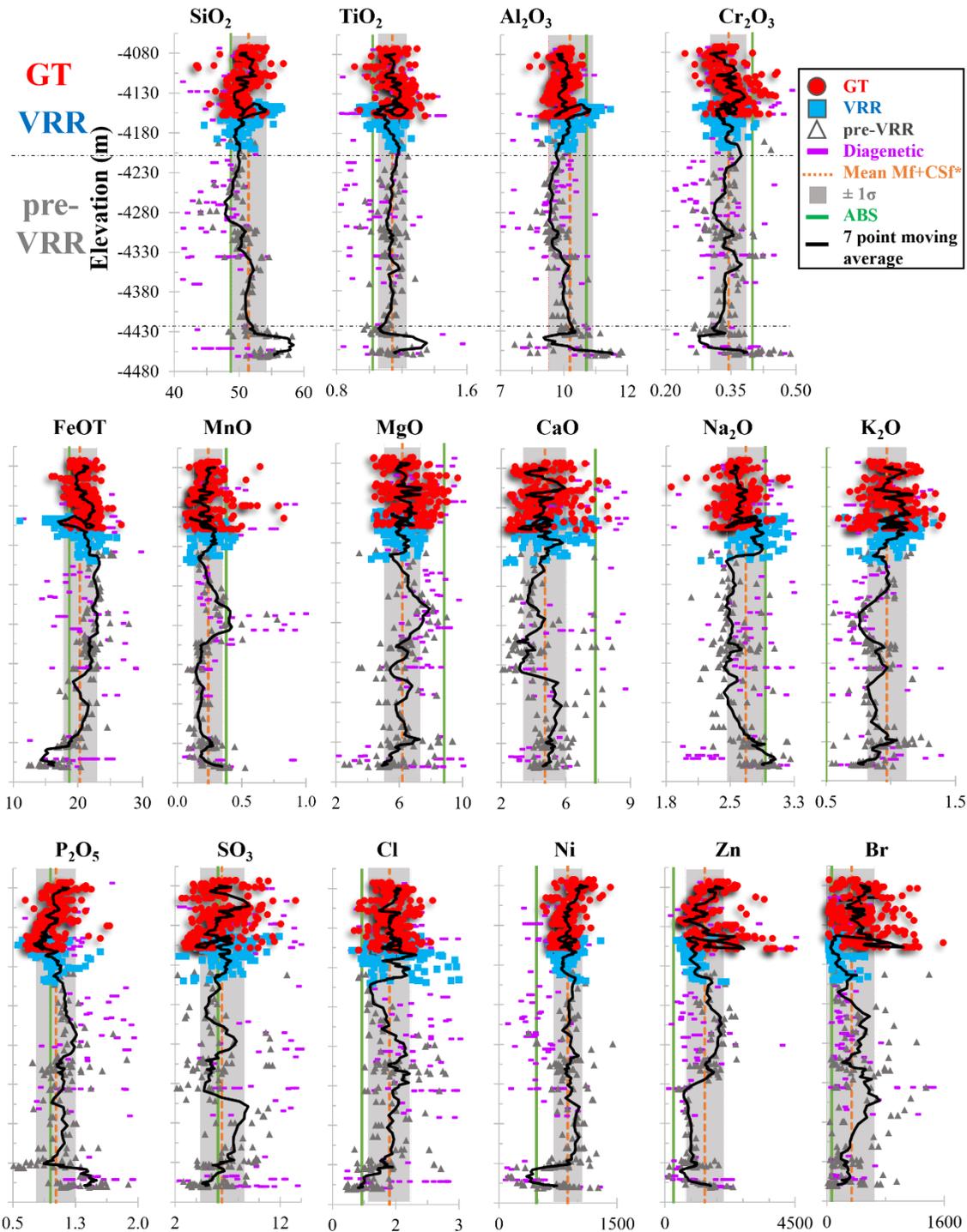
Table 2a.

Target ¹	SoI ²	Type ³	SiO ₂	TiO ₂	Al ₂ O ₃	Cr ₂ O ₃	MnO	FeO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	Cl	Ni	Zn	Br	
Mean Mf+CSf (n=488) ⁴	720-3072		47.88	1.06	9.07	0.32	0.22	18.88	5.74	4.39	2.49	0.90	0.94	6.48	1.26	873	1370	334	
Average basaltic soil (ABS) ⁵		SL	45.44	0.95	9.68	0.38	0.35	17.39	8.23	6.62	2.71	0.46	0.88	6.09	0.69	476	293	62	
Murray formation: Jura (Glen Torridon) member (Jm Gt)																			
St. Fergus	2304	R	47.83	1.15	9.27	0.33	0.11	21.42	4.91	3.61	2.46	1.33	0.77	5.37	1.13	981	1031	27	
Brent_1	2308	RT	48.27	1.06	9.52	0.37	0.15	22.01	5.76	3.90	2.63	1.09	0.64	3.48	0.77	674	749	26	
Brent_raster2	2308	RT	47.37	1.10	9.36	0.42	0.23	21.50	6.68	4.55	2.61	0.87	0.72	3.62	0.75	678	690	35	
Brent_raster3	2308	RT	47.04	1.09	9.52	0.47	0.24	21.10	6.98	4.98	2.67	0.86	0.73	3.46	0.68	612	512	12	
Isbister	2311	RT	45.75	0.94	8.77	0.44	0.22	21.87	7.02	4.51	2.71	0.87	0.64	4.75	1.10	723	756	513	
Emerald_centre	2315	RT	48.27	1.13	9.32	0.35	0.12	20.03	5.66	3.96	2.57	1.19	0.72	4.98	1.39	767	948	342	
Emerald_raster1	2315	RT	48.04	1.12	9.30	0.36	0.12	20.03	5.83	4.02	2.60	1.16	0.72	5.04	1.37	780	926	371	
Emerald_raster2	2315	RT	50.30	1.13	9.50	0.33	0.11	20.38	5.14	3.16	2.68	1.29	0.65	3.87	1.17	798	981	295	
Curlew_DRT	2318	R	45.01	1.13	9.03	0.34	0.22	17.94	6.83	5.38	2.73	0.81	0.76	7.29	2.12	660	2245	375	
Gannet	2318	R	43.94	1.08	8.78	0.33	0.22	18.34	6.70	5.94	2.50	0.70	0.75	8.50	1.82	674	2333	231	
Ladder_Hills	2320	R	46.18	1.21	9.21	0.32	0.24	17.57	6.53	5.39	2.68	0.75	0.72	6.77	1.95	682	2196	319	
Alloa	2333	R	41.36	0.95	8.51	0.26	0.29	17.28	6.99	6.64	2.51	0.63	0.89	11.47	1.80	672	1514	287	
Auchterarder	2333	R	40.43	0.92	8.09	0.25	0.30	15.93	6.37	8.33	2.49	0.58	0.82	13.21	1.80	568	1503	505	
Fife	2347	R	48.66	1.16	9.07	0.39	0.20	19.86	6.92	3.81	2.46	0.82	0.71	3.99	1.47	878	2466	387	
Arbutnott_DRT	2349	R	44.33	1.08	8.21	0.32	0.21	16.59	6.39	6.88	2.27	0.73	0.74	10.26	1.52	723	2202	578	
Caledonia_centre	2349	RT	46.82	1.12	8.94	0.45	0.22	21.56	6.86	4.38	2.56	0.91	0.75	3.93	1.18	725	875	901	
Caledonia_left	2349	RT	44.94	1.23	8.62	0.53	0.30	21.59	7.64	5.41	2.44	0.70	0.79	4.61	0.95	696	633	649	
Caledonia_right	2349	RT	44.30	1.02	8.82	0.58	0.41	20.73	9.21	6.78	2.54	0.49	0.59	3.72	0.63	658	476	118	
Crieff	2352	R	49.89	0.91	9.16	0.33	0.12	19.93	6.02	3.16	2.61	1.09	0.66	3.57	1.82	869	1310	1209	
Snorre	2356	R	48.49	1.12	8.70	0.33	0.11	20.30	5.39	3.90	2.52	1.08	0.77	5.41	1.45	829	859	1587	
Stonebriggs_centre	2356	RT	46.74	1.14	8.76	0.37	0.26	21.54	6.99	4.41	2.70	0.91	0.78	4.03	1.08	880	894	441	
Stonebriggs_left	2356	RT	46.86	0.90	9.14	0.45	0.20	21.68	6.99	4.04	2.45	0.86	0.81	4.11	1.05	751	1180	479	
Stonebriggs_right	2356	RT	46.19	0.98	8.74	0.41	0.24	21.84	7.23	4.61	2.58	0.81	0.85	4.08	0.99	703	881	414	
Rutherglen	2359	R	47.26	0.97	9.03	0.30	0.21	19.45	7.21	4.06	2.36	0.77	0.85	5.40	1.55	810	2139	774	
Ardmillan	2361	R	49.07	1.14	8.87	0.33	0.19	22.04	5.39	2.80	2.50	1.12	0.75	4.48	0.97	893	1065	581	
Ardnamurchan	2363	R	49.53	1.12	9.05	0.33	0.24	22.37	5.23	2.79	2.48	1.07	0.74	3.59	1.11	963	1179	416	
Maud	2363	R	51.21	1.15	9.54	0.33	0.19	21.96	4.50	2.38	2.63	1.12	0.70	2.97	1.01	964	1123	211	
Longannet	2365	R	49.07	1.14	8.95	0.28	0.25	19.56	6.67	3.17	2.30	0.84	0.78	4.71	1.66	777	3799	728	
Aberlady_DRT	2367	R	48.44	1.12	9.44	0.30	0.33	19.49	7.03	3.21	2.46	0.75	0.82	4.16	1.88	640	3699	486	
Aberlady_offset	2367	R	47.42	1.16	9.07	0.34	0.32	19.79	7.26	3.65	2.18	0.73	0.81	4.99	1.63	734	3678	521	
Aberlady_triage	2367	R	47.54	1.03	9.27	0.30	0.34	19.51	7.18	3.57	2.51	0.70	0.92	4.58	1.80	747	3690	472	
Seil	2377	R	47.25	1.07	8.70	0.36	0.44	18.95	7.53	3.88	2.30	0.66	1.03	5.38	1.70	775	3745	825	
Aberlady_drill_tailings_pale	2380	F	42.46	1.20	8.34	0.35	0.42	21.38	6.89	6.07	2.24	0.63	0.77	8.00	0.55	756	4351	529	
Aberlady_drill_tailings_red	2380	F	42.28	1.18	7.79	0.36	0.38	20.74	6.74	6.56	2.24	0.60	0.75	9.17	0.55	701	4229	644	
Aberlady_dump_corrected	2380	F	41.55	1.08	8.24	0.38	0.36	20.59	5.84	7.03	2.21	0.60	0.81	9.89	0.95	818	2494	211	
Kilmarie	2382	R	46.83	1.18	8.51	0.35	0.38	19.59	7.35	4.17	2.30	0.70	0.86	5.68	1.46	694	3511	1086	
Kilmarie_offset	2382	R	47.09	1.16	8.63	0.36	0.40	19.69	7.49	3.84	2.32	0.70	0.85	5.43	1.40	730	3706	1060	
Kilmarie_dump_centre	2402	F	38.56	1.10	7.34	0.36	0.61	19.86	5.66	9.23	1.78	0.62	0.97	12.96	0.32	662	4411	129	
Kilmarie_dump_offset	2402	F	38.41	1.15	7.19	0.38	0.58	20.09	5.62	9.41	1.78	0.60	0.94	12.92	0.32	775	4164	107	
Kilmarie_drill_tailings_pale	2404	F	37.04	1.12	6.26	0.28	0.43	19.41	5.60	9.98	1.35	0.59	0.64	16.19	0.46	592	3894	669	
Kilmarie_drill_tailings_red	2404	F	39.59	1.16	6.91	0.34	0.48	20.32	5.97	8.12	1.50	0.64	0.81	12.81	0.63	714	3996	806	
Haddington	2408	R	47.87	1.19	8.51	0.35	0.35	21.85	5.84	3.12	2.36	1.04	0.76	4.52	1.62	859	2490	1609	
Galashiels	2413	R	51.46	1.17	8.97	0.36	0.13	18.13	5.76	3.42	2.36	1.14	0.66	4.37	1.61	876	1456	1124	
Grampian_Mountains	2414	R	47.60	1.00	8.87	0.35	0.18	20.70	7.04	3.68	2.33	0.95	0.83	4.49	1.55	778	1729	1053	
Broad_Cairn_DRT	2415	R	49.05	1.15	8.43	0.35	0.20	22.40	6.04	2.86	2.31	1.00	0.87	3.30	1.51	763	2389	1256	
Broad_Cairn_offset	2415	R	47.34	1.13	8.49	0.35	0.24	22.15	6.56	3.30	2.37	0.91	0.99	4.27	1.30	680	2404	1170	
Broad_Cairn_triage	2415	R	47.22	1.10	8.30	0.40	0.22	22.13	6.70	3.46	2.37	0.94	0.83	4.35	1.45	811	2160	1185	
Hillhead	2419	R	49.50	1.13	9.65	0.28	0.18	22.38	5.05	2.67	2.49	1.03	0.57	3.77	0.87	963	992	76	
Kinghorn	2419	R	49.66	1.15	8.99	0.33	0.29	22.76	4.82	2.59	2.46	1.10	0.83	3.67	1.04	995	1055	230	
Kintore	2419	R	49.34	1.10	9.64	0.35	0.17	21.37	5.52	2.99	2.65	1.06	0.69	3.92	0.90	722	908	96	
Crakaig	2422	R	49.98	1.09	8.66	0.32	0.07	21.59	5.91	2.81	2.24	1.07	0.66	4.08	1.13	896	1363	721	
Morningside_raster1	2424	RT	38.86	0.90	7.60	0.27	0.20	16.92	6.82	9.64	2.34	0.60	0.76	13.84	1.02	606	837	309	
Morningside_raster2	2424	RT	45.02	1.06	8.66	0.38	0.26	21.72	7.23	4.85	2.56	0.80	0.85	5.32	1.00	888	905	566	
Morningside_raster3	2424	RT	45.39	1.07	8.60	0.42	0.37	20.36	7.90	5.12	2.42	0.65	0.92	5.24	1.17	818	1621	469	
Mons_Graupius	2427	R	46.05	1.17	8.72	0.36	0.47	20.29	7.31	4.43	2.37	0.71	0.92	5.40	1.35	785	2464	541	
Tobermory	2427	R	46.99	1.06	8.70	0.37	0.23	20.50	7.26	4.43	2.46	0.77	0.74	4.75	1.38	811	1666	489	
Gullane	2431	R	53.10	1.17	10.17	0.34	0.34	17.79	5.22	2.74	2.58	1.34	0.75	3.27	0.87	771	1338	321	
Hill_of_Skares	2431	R	46.88	1.10	8.62	0.31	0.21	26.24	4.92	2.46	2.53	1.06	1.08	3.20	1.05	849	1384	382	
Smoogro	2434	R	51.38	1.09	9.67	0.32	0.15	21.42	4.56	2.52	2.72	1.25	0.65	2.86	1.07	985	1311	448	
Almond_raster1	2437	RT	46.20	1.11	9.09	0.46	0.23	21.66	7.36	4.86	2.57	0.84	0.86	3.75	0.7				

Target	Sol	Type ²	SiO ₂	TiO ₂	Al ₂ O ₃	Cr ₂ O ₃	MnO	FeO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	Cl	Ni	Zn	Br	
Carolyn Shoemaker formation: Knockfarril Hill member (KHM)																			
Calgary_Bay	2442	R	42.99	1.13	8.50	0.31	0.38	20.11	7.82	5.83	2.32	0.54	1.01	7.38	1.16	707	3362	426	
Balnakettle	2443	R	42.92	1.15	8.86	0.34	0.27	20.45	8.06	5.37	2.39	0.65	0.97	6.70	1.27	725	2922	450	
Beauloy_DRT	2443	R	42.73	1.05	8.30	0.28	0.28	18.55	7.14	6.51	2.26	0.58	0.97	9.77	1.09	684	3122	406	
Stack_of_Glencoul	2446	R	43.65	1.10	8.57	0.32	0.27	19.17	6.98	5.96	2.34	0.71	0.75	8.19	1.41	712	3720	492	
Badcall	2450	R	43.31	1.08	8.50	0.31	1.25	20.69	6.20	5.64	2.13	0.68	1.19	7.25	0.96	697	4465	159	
Buckie_DRT	2450	R	38.44	1.11	7.97	0.34	0.70	19.96	6.22	7.81	2.30	0.64	1.31	11.27	1.43	655	2861	602	
Magnus_Bay	2452	R	47.38	1.18	9.14	0.36	0.29	19.87	6.12	4.57	2.32	0.86	1.00	5.25	1.18	861	2743	272	
Perth	2454	R	48.63	1.03	8.50	0.35	0.12	20.63	6.67	3.24	2.23	1.07	0.69	4.77	1.49	997	2778	1184	
Newtonhill	2458	R	45.54	1.04	8.76	0.33	0.20	19.50	7.55	4.62	2.48	0.81	0.74	6.28	1.50	922	2506	544	
Oykel_DRT	2458	R	46.53	1.18	8.41	0.35	0.22	19.97	6.62	4.57	2.26	0.94	0.81	6.26	1.34	837	2690	1056	
Sligachan	2461	R	46.57	1.13	9.09	0.37	0.25	19.72	7.77	4.20	2.46	0.76	0.95	4.83	1.38	761	2861	779	
Feshie	2462	R	45.43	1.02	8.80	0.31	0.30	19.87	6.97	4.70	2.35	0.78	0.97	6.55	1.43	815	2723	418	
Tay	2463	R	47.38	1.06	9.29	0.37	0.16	19.59	7.22	4.07	2.43	0.85	0.70	4.63	1.68	891	3097	591	
Ecclefechan	2465	R	46.39	1.12	8.78	0.34	0.22	19.61	7.56	4.36	2.48	0.82	0.84	5.44	1.60	848	2034	793	
Kirbuster	2465	R	46.54	1.14	9.09	0.35	0.42	20.49	6.83	3.38	2.59	1.12	1.35	4.30	1.92	964	1953	754	
Paible	2468	R	48.61	1.08	9.50	0.33	0.06	22.61	5.27	2.93	2.53	1.23	0.74	3.78	1.02	773	1196	141	
Nith	2470	R	48.41	1.16	9.25	0.35	0.13	18.84	5.69	4.41	2.30	1.11	0.74	5.64	1.64	924	1297	322	
Solway_Firth_DRT	2471	R	47.39	1.17	8.64	0.36	0.17	18.80	6.16	4.61	2.35	1.04	1.05	6.56	1.31	907	1348	831	
East_Shetland_DRT	2472	R	48.72	1.18	9.14	0.37	0.15	18.75	5.86	3.92	2.51	1.10	0.93	5.13	1.82	939	1223	967	
Essendy	2472	R	47.03	1.17	8.24	0.34	0.15	21.79	6.19	3.70	2.22	1.15	0.82	5.02	1.71	1023	1391	1064	
Mither_Tap	2474	R	46.93	1.14	8.82	0.33	0.09	22.48	5.81	3.34	2.54	1.17	0.81	4.59	1.53	882	1086	1024	
Moine	2474	R	44.14	1.08	8.55	0.33	0.11	19.91	5.13	5.83	2.53	1.09	0.88	8.67	1.47	851	886	144	
Cruden_Bay	2477	R	44.61	0.96	8.60	0.42	0.33	20.42	7.76	5.15	2.49	0.75	0.90	5.82	1.22	1026	1650	343	
Fetterangus	2478	R	45.36	1.12	8.56	0.34	0.17	21.91	6.85	3.99	2.44	1.06	0.81	5.55	1.43	974	1382	679	
Fetterangus_offset	2478	R	45.14	1.14	8.49	0.33	0.17	21.88	7.00	4.21	2.35	1.01	0.72	5.80	1.37	949	1364	633	
Glen_Etive_1_DRT	2482	R	49.19	1.16	9.07	0.35	0.17	20.37	5.69	3.49	2.31	1.29	0.79	4.25	1.45	961	1819	685	
Glen_Etive_1_offset	2482	R	47.88	1.15	8.75	0.36	0.19	19.71	6.12	4.12	2.35	1.19	0.78	5.47	1.47	955	1837	832	
Glen_Etive_2_DRT	2483	R	45.51	1.10	8.30	0.34	0.18	19.93	6.32	5.09	2.28	1.07	0.81	7.30	1.29	963	1759	922	
Glen_Etive_1_dump_centre	2523	F	43.87	1.21	8.41	0.39	0.27	23.46	5.74	5.03	2.18	1.07	0.81	6.37	0.78	1042	1834	281	
Glen_Etive_1_tailings	2524	F	47.38	1.30	8.59	0.40	0.22	23.57	5.41	3.85	2.14	1.28	0.77	4.13	0.49	1168	2327	153	
Glen_Etive_2_dump_corrected	2552	F	38.64	1.14	7.30	0.36	0.25	20.16	4.63	9.66	1.81	1.04	0.69	13.17	0.71	1006	2372	82	
Glen_Etive_2_tailings	2553	F	41.68	1.22	7.68	0.39	0.29	22.23	5.44	6.71	2.04	1.11	0.84	9.32	0.55	1056	2651	240	
High_Plains	2557	RT	47.27	1.10	9.09	0.33	0.12	22.68	5.97	3.47	2.56	1.05	0.75	4.47	0.91	840	626	88	
Skipness	2558	RT	43.26	1.02	9.34	0.47	0.31	20.56	8.39	6.34	2.70	0.58	0.85	5.19	0.80	645	392	121	
Orkney	2563	RT	44.53	1.03	9.07	0.42	0.25	21.84	7.42	4.93	2.73	0.67	0.82	5.05	0.98	727	587	119	
Shetland	2564	R	49.01	1.14	9.23	0.32	0.10	22.67	4.78	2.93	2.64	1.17	0.76	3.65	1.34	770	709	254	
South_Ronaldsay_DRT	2567	R	47.71	1.08	8.71	0.31	0.11	20.09	5.11	4.30	2.43	1.03	1.13	6.30	1.39	949	622	617	
White_Craig	2567	R	43.97	1.15	8.67	0.31	0.10	19.45	6.42	5.53	2.40	0.93	0.88	8.56	1.38	882	651	202	
Ben_Hope	2570	R	48.00	1.06	8.86	0.34	0.13	20.64	5.99	3.59	2.50	1.06	0.93	4.98	1.60	826	887	597	
Glen_Mark	2572	R	44.34	1.03	8.33	0.29	0.14	18.20	7.11	6.00	2.46	0.79	0.97	8.66	1.21	820	874	428	
Stonehive	2574	R	41.51	0.98	8.09	0.28	0.16	17.22	5.91	8.14	2.47	0.75	0.90	12.15	1.24	560	632	183	
Upperhill_DRT	2574	R	47.96	1.05	8.36	0.30	0.19	20.91	4.78	4.21	2.31	1.05	0.85	6.17	1.47	960	1037	1125	
Pobie_Bank	2577	R	50.55	1.19	9.29	0.38	0.14	18.83	5.71	3.67	2.51	1.06	0.81	4.50	1.09	898	694	92	
Gleneagles	2579	R	45.65	1.05	8.17	0.32	0.17	20.15	6.40	4.79	2.40	0.95	0.80	7.61	1.10	1115	1340	573	
Conachair_DRT	2581	R	47.26	1.15	8.77	0.38	0.20	18.27	7.09	4.76	2.32	0.78	0.89	6.54	1.16	892	1452	209	
Conachair_offset	2581	R	44.08	1.12	8.78	0.31	0.22	15.52	7.68	6.95	2.55	0.66	1.04	9.72	1.09	729	1210	84	
Blawhorn	2587	R	45.24	1.02	8.60	0.29	0.14	19.89	6.15	5.12	2.52	0.83	1.07	7.53	1.23	841	566	534	
Gorgie	2587	R	45.81	1.05	8.61	0.30	0.13	19.72	5.13	5.06	2.44	0.92	1.11	8.32	1.15	917	595	75	
Nedd	2590	R	49.57	1.00	9.20	0.31	0.08	19.85	5.24	3.52	2.56	1.02	0.88	5.15	1.19	900	505	256	
Ard_Neakie	2591	R	49.73	1.14	9.34	0.33	0.09	20.71	5.16	3.33	2.58	1.15	0.78	4.30	1.09	727	675	348	
Glen_Doll	2591	R	45.52	1.14	8.63	0.32	0.12	19.81	5.48	5.17	2.48	0.98	1.11	7.85	1.16	723	609	157	
Muckie_Flugga_DRT	2591	R	47.37	1.11	8.53	0.32	0.12	20.42	5.60	4.44	2.52	0.99	0.97	6.08	1.17	757	644	1184	
Everbay_DRT	2598	R	53.17	1.16	9.64	0.34	0.09	18.21	4.34	2.76	2.46	1.12	1.25	3.58	1.56	915	877	604	
Inverurie_DRT	2601	R	45.90	1.04	8.50	0.30	0.11	17.58	4.95	5.95	2.32	0.94	1.06	9.90	1.18	855	848	218	
Latherton	2601	R	47.98	1.07	9.15	0.32	0.12	19.65	5.98	3.80	2.65	1.01	0.96	5.49	1.52	918	885	285	
Kintyre_Way_offset	2819	R	48.45	1.10	9.07	0.29	0.14	21.90	5.50	2.65	2.64	1.09	0.88	4.80	1.19	905	917	451	
Kintyre_Way	2820	R	48.73	1.11	9.13	0.31	0.12	21.99	5.35	2.51	2.66	1.09	0.88	4.73	1.09	899	961	349	
Breamish_DRT	2826	R	46.98	1.11	9.11	0.33	0.85	18.48	7.30	3.43	2.38	0.89	1.11	5.70	1.77	878	3204	311	
Breamish_offset	2826	R	48.45	1.15	9.16	0.35	0.79	17.80	7.04	3.28	2.30	0.98	0.95	5.28	1.96	916	3177	292	
Mary_Anning_DRT	2833	R	48.07	1.17	8.91	0.36	0.51	18.96	7.21	3.06	2.38	0.94	0.83	5.39	1.75	760	2415	558	
Mary_Anning_offset	2833	R	47.14	1.14	9.01	0.33	0.50	18.81	7.49	3.26	2.41	0.88	0.87	6.06	1.66	774	2444	567	
Mary_Anning_dump_1	2851	F	43.71	1.10	8.01	0.37	0.39	20.44	6.50	5.83	2.15	0.86	0.70	8.59	0.93	906	2192	239	
Mary_Anning_dump_2	2851	F	42.85	1.11	8.05	0.32	0.37	19.77	6.55	6.32	2.16	0.88	0.73	9.60	0.91	867	2124	56	
Mary_Anning_tailings	2853	F	45.14	1.15	8.09	0.37	0.57	19.64	7.79	4.32	2.12	0.85	0.85	7.90	0.77	784	2430	478	
Ayton_raster1	2857	R	44.46	1.05	8.78	0.33	1.40	16.97	7.90	4.05	2.40	0.74	2.67	7.20	1.66	457	2296	369	
Ayton_raster2	2857	R	38.79	1.01	8.19	0.30	1.91	16.26	7.86	6.25	2.52	0.57	3.56	10.93	1.53	367	1967	263	
Ayton_raster3	2857	R	36.19	0.88	7.84	0.25	2.44	16.27	7.59	6.54	2.62	0.55	5.49	11.52	1.49	309	1505	232	
Mary_Anning_2_DRT	2858	R	48.18	1.11	9.01	0.32	0.48	18.98	7.05	3.12	2.44	0.99	0.77	5.40	1.75	776	2089	475	
Mary_Anning_2_offset	2858	R	48.28	1.11	8.89	0.34	0.49	19.08	6.96	3.19	2.40	1.03	0.80	5.31	1.71	793	2065	473	
Falkirk_Wheel	2862	R	43.49	1.08	8.58	0.36	1.03	18.32	8.68	4.34	2.13	0.73	2.01	7.41	1.47	656</			

Target	Sol	Type ²	SiO ₂	TiO ₂	Al ₂ O ₃	Cr ₂ O ₃	MnO	FeO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₂	Cl	Ni	Zn	Br	
Carolyn Shoemaker formation: Glasgow member (Gm)																			
Sourhope	2583	R	46.37	1.11	8.84	0.33	0.21	18.26	6.30	4.95	2.40	0.85	0.93	7.98	1.20	857	1191	78	
Foggy_Moss	2585	Ft	48.06	1.09	9.41	0.34	0.12	18.72	5.40	4.44	2.25	0.92	0.94	6.69	1.31	935	1175	128	
Kirkcudbrightshire	2585	R	45.29	1.14	8.53	0.36	0.22	18.42	7.65	5.22	2.52	0.72	0.93	7.32	1.32	840	1187	747	
Well_Run	2604	R	47.98	1.03	9.10	0.26	0.18	19.38	5.73	4.19	2.38	0.94	1.03	6.37	1.11	890	1147	165	
Staxigoe	2606	R	48.25	1.19	8.99	0.38	0.15	17.87	6.45	4.19	2.64	0.87	0.81	6.37	1.46	895	1274	435	
Gretna_Green	2608	Ft	36.84	0.44	5.08	0.68	0.35	22.42	15.63	4.74	1.68	0.37	0.83	9.40	1.22	2623	126	66	
Scotnish_DRT	2608	R	46.69	1.06	8.47	0.30	0.11	17.64	4.23	5.55	2.16	1.02	0.76	10.78	0.94	732	894	213	
Renfrewshire	2611	R	47.28	1.05	8.89	0.33	0.11	17.53	5.09	5.08	2.31	0.95	0.81	8.94	1.27	783	1287	19	
Glenmard_Wood	2613	R	44.21	1.07	8.93	0.33	0.19	20.12	6.76	5.13	2.51	0.62	0.81	7.88	1.14	1073	1074	122	
North_Esk	2616	R	45.74	0.99	8.64	0.28	0.12	17.75	6.17	5.85	2.51	0.66	0.80	8.99	1.05	848	781	189	
Ben_Arnaboll_DRT	2631	R	45.48	0.86	8.67	0.27	0.25	16.69	5.95	6.37	2.42	0.73	0.86	10.22	0.72	772	1332	178	
Blackwaterfoot	2631	Ft	44.42	0.77	9.16	0.63	0.48	19.13	8.74	7.25	3.22	1.21	0.90	3.23	0.74	293	373	57	
Buchan_Haven_DRT	2640	R	51.62	0.94	9.83	0.28	0.32	16.76	6.30	5.80	3.05	0.91	1.15	2.26	0.50	587	1547	89	
Heinrich_Waenke	2641	Ft	45.49	1.01	9.09	0.32	0.43	18.72	7.44	7.05	3.36	2.28	1.13	2.66	0.66	889	1876	38	
Abernethy	2642	V	24.55	0.43	5.20	0.08	5.11	40.12	7.53	3.59	1.66	0.21	0.69	8.55	1.81	560	2630	519	
Lomond_Hills	2642	Ft	46.64	0.92	10.20	0.28	0.25	17.06	7.89	6.00	4.17	2.37	1.31	1.90	0.58	716	1367	74	
Kennedys Pass	2645	R	48.86	1.01	9.05	0.25	0.13	18.61	5.87	4.12	2.38	0.78	0.98	6.39	1.30	838	810	356	
Arbroath	2647	R	49.86	1.00	9.42	0.34	0.10	16.93	5.75	3.94	2.61	0.84	0.88	6.63	1.25	910	984	54	
Moffat_Hills	2653	R	47.36	0.98	9.19	0.30	0.18	19.03	5.63	3.37	2.18	0.82	1.26	8.34	0.95	878	960	65	
Trossachs_DRT	2653	R	50.02	1.08	8.86	0.31	0.14	18.27	4.98	3.93	2.68	0.88	0.92	5.86	1.71	898	946	1040	
Rannoch_Moor	2656	R	46.90	1.03	9.02	0.31	0.15	18.79	6.91	4.15	2.62	0.79	0.95	6.62	1.22	926	890	540	
Sauchiehall_DRT	2656	R	49.18	1.06	8.88	0.29	0.11	16.84	4.02	5.59	2.19	0.94	0.91	8.95	0.77	845	907	75	
Marchmont	2658	R	43.75	0.94	8.32	0.30	0.20	18.52	6.16	6.55	2.28	0.68	0.86	10.11	0.86	981	659	42	
Beefstand_Hill_DRT	2744	R	50.95	1.04	9.51	0.29	0.15	19.14	4.31	3.71	2.37	0.88	0.99	5.82	0.58	828	935	74	
Beefstand_Hill_offset	2744	R	49.41	1.03	9.11	0.29	0.15	19.20	4.86	3.85	2.26	0.84	0.94	7.16	0.65	830	956	82	
Glasgow_1_DRT	2749	R	53.11	1.12	9.50	0.32	0.11	17.28	4.65	3.47	2.32	0.96	1.19	4.46	1.15	1080	1103	607	
Glasgow_1_offset	2749	R	48.32	1.00	8.73	0.29	0.11	15.98	4.76	5.79	2.33	0.86	1.03	9.16	1.27	913	972	494	
Glasgow1_dump_corrected	2775	F	46.87	1.08	8.74	0.38	0.17	18.82	4.74	6.11	2.23	0.91	1.03	7.48	1.12	964	1039	200	
Glasgow1_tailings	2776	F	47.51	1.10	8.69	0.41	0.22	19.02	4.71	6.22	2.11	0.78	1.05	6.99	0.91	916	876	29	
Heather_Island_DRT	2785	R	42.12	0.98	7.48	0.28	0.13	16.75	4.35	7.69	2.40	0.82	0.90	14.16	1.65	794	720	568	
Hedgeley_Moor_DRT	2792	R	50.37	1.10	8.97	0.30	0.13	21.17	4.83	3.07	2.40	1.08	1.08	3.94	1.18	992	951	936	
Hedgeley_Moor_offset	2792	R	48.00	1.08	8.66	0.32	0.16	21.39	5.50	3.72	2.45	0.99	0.93	5.21	1.24	1015	921	799	
Chambers_Street_DRT	2801	R	51.04	1.15	9.08	0.37	0.17	14.34	4.49	5.19	2.25	0.79	0.76	8.89	1.13	1018	1159	1029	
Chambers_Street_offset	2801	R	48.96	1.11	9.12	0.34	0.16	14.65	5.56	5.82	2.32	0.71	0.81	8.98	1.15	954	1155	310	
Capercaille	2803	R	45.08	1.03	8.55	0.30	0.13	16.14	5.39	6.73	2.38	0.85	0.81	11.30	1.01	821	983	95	
Capercaille_offset	2803	R	43.21	1.04	8.58	0.32	0.13	15.60	5.65	7.66	2.48	0.76	0.90	12.40	1.01	791	952	95	
Edinburrie	2959	R	47.68	1.02	8.72	0.33	0.34	19.46	5.90	4.09	2.22	0.99	0.92	6.09	1.55	1318	3143	687	
Achnasheen	2965	R	49.59	1.11	9.18	0.29	0.18	20.62	5.15	3.04	2.37	1.08	0.95	4.71	1.33	918	1713	438	
Dun_Eideann	2967	R	47.61	1.10	8.85	0.30	0.32	19.95	5.85	3.60	2.35	1.08	1.02	5.90	1.52	991	2090	443	
Auchnafree_Hill	2969	R	51.66	1.11	9.47	0.32	0.23	19.17	5.32	2.78	2.57	1.12	0.87	3.73	1.22	1073	1735	517	
Coupar_Angus	2969	R	49.72	1.04	8.92	0.30	0.20	18.80	5.80	2.92	2.50	1.13	0.80	6.12	1.31	911	1329	689	
Torness	2972	R	51.85	1.13	9.14	0.28	0.16	19.71	4.74	2.67	2.23	1.19	0.95	4.47	1.17	893	1252	71	
Carn_Mor	2974	R	46.67	1.04	8.50	0.31	0.19	19.83	6.65	3.01	2.59	0.99	1.02	7.11	1.70	946	1204	725	
Cod_Baa_DRT	2975	R	46.76	1.07	8.62	0.31	0.29	19.69	6.13	4.05	2.37	0.92	1.11	6.57	1.60	1177	2067	699	
An_Dun_raster1	2976	N	45.01	1.01	8.36	0.25	0.18	18.14	7.58	3.55	2.57	0.92	1.06	9.56	1.46	832	1266	560	
An_Dun_raster2	2976	N	43.59	1.02	8.33	0.31	0.19	18.02	8.26	3.47	2.18	0.87	1.00	11.02	1.38	910	1307	504	
An_Dun_raster3	2976	N	44.40	1.06	8.16	0.31	0.21	18.43	7.65	3.34	2.17	0.96	1.07	10.44	1.45	922	1347	524	
Ronas_Hill	2989	R	50.13	1.09	9.22	0.31	0.24	20.36	6.03	2.79	2.41	0.95	0.98	3.89	1.21	1008	2066	126	
Tomb_of_the_Eagles	3004	R	48.89	1.06	8.81	0.31	0.25	19.68	5.94	3.25	2.41	1.00	0.99	5.29	1.67	998	2059	623	
Easthouses	3007	R	46.93	1.06	8.67	0.31	0.27	20.42	6.36	3.74	2.48	0.96	1.09	5.73	1.60	1046	1208	576	
Easthouses_offset	3007	R	46.86	1.01	8.75	0.30	0.23	19.58	5.90	4.17	2.51	1.02	0.98	6.69	1.64	972	1203	536	
Gageac_et_Rouillac	3010	R	47.84	1.08	8.59	0.31	0.22	20.63	6.06	3.45	2.55	1.00	0.99	5.21	1.60	1005	1157	1232	
La_Roque_Gageac_DRT	3011	R	48.19	1.10	8.42	0.30	0.35	21.69	4.29	3.62	2.39	1.13	1.05	5.49	1.45	994	1286	1127	
Champagnac	3013	R	42.34	1.01	7.59	0.22	0.27	21.38	7.12	4.79	2.28	0.82	1.12	8.98	1.62	959	1099	504	
Beaupouyet	3015	N	46.21	1.11	8.42	0.31	0.32	20.92	6.07	3.84	2.25	0.89	1.95	6.20	1.15	844	1746	152	
Neuvic	3018	R	48.29	1.09	8.59	0.30	0.60	19.83	4.64	4.06	2.38	1.12	0.91	6.34	1.46	1153	1271	675	
Lunas	3020	R	48.36	1.14	8.95	0.32	0.21	20.63	5.58	3.36	2.37	1.01	1.03	5.00	1.67	966	1275	566	
Tamnies	3022	R	49.66	1.11	9.41	0.27	0.22	21.73	4.75	2.76	2.48	1.13	1.01	3.73	1.19	1043	2505	176	
Biron	3024	R	49.02	1.07	9.18	0.33	0.21	20.16	6.15	3.35	2.44	0.90	0.88	4.50	1.21	1096	2409	405	
Coutures_DRT	3024	R	51.36	1.17	9.08	0.33	0.17	18.02	4.97	3.75	2.43	1.08	1.31	4.85	1.13	706	1488	667	
Labouquerie	3026	R	48.61	1.18	9.06	0.33	0.09	19.29	6.88	3.39	2.46	0.82	1.28	4.81	1.37	875	1740	572	
Brantôme	3027	R	46.37	1.08	8.58	0.33	0.25	19.94	6.45	4.32	2.38	0.88	0.84	6.46	1.53	985	1504	471	
Firbeix	3028	R	48.07	1.05</															

Target	Sol	Type ²	SiO ₂	TiO ₂	Al ₂ O ₃	Cr ₂ O ₃	MnO	FeO	MgO	CaO	Na ₂ O	K ₂ O	P ₂ O ₅	SO ₃	Cl	Ni	Zn	Br	
Carolyn Shoemaker formation: Glasgow member, Hutton interval																			
Bogmill_Pow	2660	R	36.15	0.94	8.12	0.28	0.27	19.49	8.01	7.70	2.58	0.37	0.87	13.49	1.34	1153	1403	397	
Cullivoe_DRT	2660	R	50.33	0.99	9.55	0.29	0.28	17.26	7.60	3.97	2.79	0.89	0.91	4.26	0.62	683	963	68	
Cairnbulg	2662	R	47.27	0.93	9.05	0.28	0.24	19.19	7.69	4.75	2.96	0.89	1.14	4.18	1.11	716	907	107	
Berwickshire_DRT	2663	R	47.50	0.94	8.73	0.29	0.24	20.10	7.36	4.62	2.94	0.93	1.16	3.71	1.19	712	946	506	
Hutton_DRT_offset	2665	R	50.21	1.00	9.34	0.29	0.25	17.41	6.75	5.29	3.26	0.89	1.07	3.02	0.98	661	947	248	
Hutton_triage	2665	R	46.66	0.94	8.74	0.36	0.25	19.02	7.36	5.40	2.70	0.80	0.93	5.30	1.01	727	935	236	
Hutton_DRT_centre	2666	R	50.50	1.00	9.53	0.28	0.25	18.03	6.16	5.05	3.38	0.94	1.12	2.63	0.88	658	938	219	
Liberton_Brae	2666	V	40.60	0.85	7.62	0.25	0.25	16.25	17.11	3.31	1.86	2.14	0.97	6.67	1.42	1052	3433	486	
Moorfoot_Hills	2666	R	42.04	0.92	8.54	0.30	0.33	20.69	7.78	7.27	2.89	0.74	1.00	5.46	1.68	749	1097	765	
Traprain_Law	2667	R	48.42	1.00	9.03	0.30	0.25	18.74	6.72	5.18	2.93	0.93	1.25	4.12	0.71	597	1746	883	
Hutton_dump_centre	2684	F	49.29	1.07	9.27	0.28	0.26	18.68	5.39	6.10	3.51	0.93	1.04	2.99	0.91	716	1191	70	
Hutton_dump_corrected	2684	F	46.64	1.07	9.29	0.31	0.27	19.94	6.29	5.88	3.39	0.89	1.09	3.71	0.91	739	1598	131	
Hutton_tailings	2686	F	50.55	1.06	9.46	0.31	0.25	19.23	5.58	5.28	3.68	0.96	1.12	1.43	0.84	698	988	21	
Downreay	2690	V	40.01	1.00	7.95	0.27	0.49	19.88	11.36	5.07	2.04	1.43	1.09	6.73	2.18	1283	1613	822	
Dunbartonshire_refined	2691	V	26.38	0.58	5.09	0.14	6.33	39.65	8.57	3.60	1.57	0.24	0.62	4.89	1.97	893	1593	750	
Carolyn Shoemaker formation: Benches unit - KHM-Gm transition																			
Bablin	2925	R	48.20	1.09	9.29	0.35	0.41	18.34	6.80	3.88	2.56	1.07	0.96	5.30	1.36	709	1397	558	
Bablin_offset	2925	R	46.70	1.04	8.88	0.39	0.36	18.88	7.69	4.57	2.64	0.88	0.88	5.46	1.33	701	1129	429	
Garth_Ness	2928	R	44.96	1.05	8.41	0.33	0.22	21.28	6.97	4.18	2.46	0.84	0.91	6.79	1.27	744	965	740	
Garth_Ness_offset	2928	R	44.44	0.99	8.22	0.31	0.23	21.31	7.06	4.24	2.38	0.83	1.00	7.23	1.32	739	1000	910	
Rachan	2931	R	49.63	1.07	9.37	0.27	0.24	21.03	5.35	2.66	2.55	1.15	0.60	4.82	1.02	723	1118	80	
Mail_Beach	2933	R	49.45	1.13	9.40	0.29	0.22	20.40	5.63	2.59	2.72	1.21	0.80	4.66	1.07	806	1150	370	
Hunt_Hill_DRT	2935	R	46.13	1.17	8.98	0.36	0.26	17.05	7.79	4.09	2.46	0.88	1.03	7.53	1.91	602	1654	366	
Muckle_Minn	2935	R	46.32	1.05	9.39	0.31	0.30	18.31	8.19	3.96	2.58	0.83	1.00	5.73	1.63	790	1329	316	
Hart_Fell	2938	R	44.60	1.08	8.39	0.31	0.26	19.39	8.44	3.18	2.30	1.00	0.93	7.77	1.81	955	2808	901	
West Loch	2940	R	47.45	0.98	8.83	0.35	0.35	21.43	6.37	2.61	2.55	1.29	0.83	5.28	1.17	867	1273	216	
Geesa_Water	2942	R	45.86	1.06	8.57	0.36	0.38	19.22	7.48	3.63	2.42	1.08	0.91	6.88	1.72	857	1576	618	
St_Ninian	2943	R	44.11	1.05	8.53	0.31	0.25	19.23	7.71	3.68	2.54	1.06	0.97	8.53	1.67	813	1135	575	
Ingliston	2945	R	47.21	1.14	8.94	0.38	0.31	18.16	6.89	3.79	2.57	1.11	0.88	6.52	1.66	910	1619	815	
Lasswade_DRT	2945	R	38.83	0.99	7.75	0.28	0.29	15.79	6.22	8.55	2.38	0.99	1.01	14.93	1.66	776	1121	850	
Giova_DRT	2949	R	43.98	1.02	8.21	0.29	0.21	18.39	7.00	4.59	2.28	1.01	0.89	9.95	1.74	931	1878	611	
Giova_offset	2949	R	43.86	1.03	8.22	0.32	0.21	17.81	6.76	5.38	2.32	0.94	0.93	10.09	1.75	871	1725	557	
Saughieside_Hill	2951	R	45.28	0.99	8.16	0.41	0.26	19.25	5.36	5.28	2.33	1.07	0.95	8.75	1.42	859	1367	832	
Rest_and_Be_Thankful_DRT	2955	R	43.86	0.99	8.43	0.29	0.21	17.65	7.34	4.39	2.45	0.85	1.00	10.30	1.88	925	1280	375	
Rest_and_Be_Thankful_offset	2955	R	45.89	1.02	8.69	0.29	0.19	17.71	7.28	3.80	2.39	0.88	0.96	8.90	1.67	918	1220	408	
Unconsolidated sediments																			
Auld_Reekie	2731	SL	44.23	0.96	9.23	0.53	0.42	19.62	9.00	7.07	2.64	0.44	0.81	4.31	0.61	478	238	29	
Ballieikine	2706	SL	43.44	1.02	9.30	0.48	0.40	18.83	9.08	7.24	2.55	0.52	0.80	5.47	0.72	480	324	40	
Airor	2993	SD	43.03	0.92	8.12	0.38	0.43	22.03	11.43	6.95	2.25	0.33	0.82	2.69	0.43	1231	144	39	
Alba	2313	SD	43.53	1.20	8.92	0.73	0.45	20.88	9.56	7.05	2.42	0.39	0.72	3.52	0.52	443	236	29	
Braewick_Beach	2989	SD	42.49	0.93	8.63	0.54	0.42	21.77	10.90	7.05	2.49	0.37	0.76	2.97	0.53	823	219	44	
Burrowgate	2558	SD	40.62	1.14	8.67	0.56	0.40	22.10	8.78	6.71	2.58	0.48	0.86	6.20	0.72	727	467	168	
Clackmannanshire	2564	SD	42.72	0.99	9.10	0.53	0.44	20.63	9.73	7.22	2.62	0.45	0.77	4.08	0.58	570	213	22	
Dunoon	2409	SD	42.58	0.86	8.72	0.40	0.41	21.35	11.39	7.02	2.52	0.42	0.74	2.93	0.48	1036	156	59	
Ellon	2410	SD	44.25	0.88	10.03	0.31	0.35	18.16	8.23	7.37	2.79	0.56	0.94	5.27	0.68	862	269	96	
Gairsay	2409	SD	44.59	0.90	9.06	0.48	0.42	20.13	9.76	7.25	2.53	0.40	0.75	3.12	0.48	529	210	38	
Nairn	2410	SD	43.67	0.85	8.57	0.50	0.45	21.13	10.90	6.92	2.45	0.35	0.70	2.87	0.44	744	194	57	
Ratharsair	2992	SD	42.19	1.11	8.74	0.72	0.47	21.94	10.36	7.15	2.44	0.38	0.75	3.12	0.48	562	228	32	
Traquair	2995	SD	43.81	0.94	8.54	0.52	0.44	21.18	10.62	7.11	2.36	0.38	0.73	2.76	0.45	740	182	41	
Table 2b.																			
Carolyn Shoemaker formation: Knockfarril Hill member (KHM)																			
Glen_Etive_1_DRT	2482	R	49.19	1.16	9.07	0.35	0.17	20.37	5.69	3.49	2.31	1.29	0.79	4.25	1.45	961	1819	685	
Glen_Etive_2_DRT	2483	R	45.51	1.1	8.3	0.34	0.18	19.93	6.32	5.09	2.28	1.07	0.81	7.3	1.29	963	1759	922	
Glen_Etive_1_tailings	2524	F-DT	47.38	1.3	8.59	0.4	0.22	23.57	5.41	3.85	2.14	1.28	0.77	4.13	0.49	1168	2327	153	
Glen_Etive_2_dump_corrected	2552	F-DBA	38.64	1.14	7.3	0.36	0.25	20.16	4.63	9.66	1.81	1.04	0.69	13.17	0.71	1006	2372	82	
Mary_Anning_DRT	2833	R	48.07	1.17	8.91	0.36	0.51	18.96	7.21	3.06	2.38	0.94	0.83	5.39	1.75	760	2415	558	
Mary_Anning_dump_2	2851	F-DBA	42.85	1.11	8.05	0.32	0.37	19.77	6.55	6.32	2.16	0.88	0.73	9.6	0.91	867	2124	56	
Mary_Anning_3_DRT	2867	R	46.01	1.09	8.68	0.35	0.53	18.83	7.42	4.14	2.38	0.82	0.91	6.79	1.53	737	2321	472	
Mary_Anning_3_dump_2	2890	F-DBA	38.96	1.06	7.83	0.36	0.66	18.22	7.59	7.77	2.21	0.69	1.37	12.06	0.89	674	1826	58	
Groken_DRT	2906	R	43.56	1.03	8.49	0.3	1.4	16.43	8	4.09	2.43	0.77	2.64	8.76	1.73	500	2175	329	
Groken_offset	2906	R	41.73	1.03	8.45	0.29	1.2	15.18	8.72	4.64	2.48	0.67	2.22	11.5	1.57	388	1924	249	
Groken_tailings	2921	F-DT	37.32	1.1	7.59	0.42	1.07	19.66	9.35	6.15	2.33	0.6	2.13	11.33	0.5	630	2118	254	
Carolyn Shoemaker formation: Glasgow member (Gm)																			
Hutton_DRT_centre	2666	R	50.5	1	9.53	0.28	0.25	18.03	6.16	5.05	3.38	0.94	1.12	2.63	0.88	658	938	219	
Hutton_dump_corrected	2684	F-DBA	46.64	1.07	9.29	0.31	0.27	19.94	6.29	5.88	3.39	0.89	1.09	3.71	0.91	739	1598	131	
Glasgow_1_DRT	2749	R	53.11	1.12	9.5	0.32	0.11	17.28	4.65	3.47	2.32	0.96	1.19	4.46	1.15	1080	1103	607	
Glasgow_1_dump_corrected	2775	F-DBA	46.87	1.08	8.74	0.38	0.17	18.82											



224

225 **Figure 2.** Major and trace element data versus elevation; all data weight percent, except Ni, Zn, Br (ppm). Data
 226 includes all data from Murray (Mf) and Carolyn Shoemaker (CSf) formation targets, divided into pre-Vera Rubin
 227 ridge targets (VRR) (grey symbols) (Table S1d), VRR targets (blue symbols) (Table 1c) and Glen Torridon targets
 228 (red symbols) (Table S1a). Diagenetic features are denoted by pink rectangles. Mean Mf+CSf is denoted by the
 229 dashed orange line, with ± 1 standard deviation shaded in grey. A seven point moving average (black solid line) was
 230 calculated to show the broad compositional trend with respect to increasing elevation (and increasing sol). Average
 231 basaltic soil [ABS; O'Connell-Cooper et al., 2017] is denoted by green solid line

232 **3.3. Statistical treatment of APXS data**

233 Standard univariate analysis results (mean, standard error, z-scores and % change from mean
234 Murray and Carolyn Shoemaker formations concentrations [“Mf+CSf”] (number of targets = 488
235 bedrock and fines targets; Supplemental Text S2a) are given in Table S1. Unless otherwise
236 stated, all data discussed in this paper are in the form of element/Si molar ratios. Si was assessed
237 to be a suitable denominator, as >95% of bedrock targets fall within the normal range ($\leq \pm 1.96$)
238 when assessing via z-scores (Table S1). However, values for drill fines and diagenetic features
239 typically fall outside the normal range. Differences in concentrations between members/subunits
240 for a given element identified were analyzed for statistical significance. Distribution was
241 determined to be non-normal for most populations (Shapiro-Wilk test), with unequal variances
242 (Levene’s test). Kruskal-Wallis tests were used to determine if any statistically significant
243 differences existed within the dataset for a given element. Games-Howell post-hoc tests
244 determined which pairings showed differences (Tables S5-7). Pearson correlation coefficient
245 analysis (r) results were calculated to identify compositional trends (Table S3). Principal
246 Component analysis (PCA) was conducted, using transformed molar/Si ratio data to identify
247 major elemental trends.

248 Agglomerative Hierarchical Clustering analysis (AHCA) was run to investigate similarities
249 within members and to identify, if possible, alteration trends (Supplemental Text S2c for
250 discussion; Tables S5-7; Figures S8, S10-11). All data was in the form of $\text{Log}_{10}[\text{element/Si}]$
251 mole ratios. For each data set, three model parameters were run. Model A includes all elements
252 routinely reported on by APXS. Following Mittlefehldt et al. [2018, 2021], Model B excludes the
253 volatile elements S, Cl, Br, to minimize the effect of such variable elements on the bedrock

254 clustering. Model C excludes S, Cl, Br and the mobile elements Mn, P, Zn, Ni to examine the
255 extent of alteration [e.g., Mittlefehldt et al. 2018, 2021].

256 **4. APXS compositional results and statistical analysis**

257 **4.1 Murray formation – Jura member**

258 **4.1.1. Jura member within Glen Torridon (herein Jm_GT)**

259 The Jm_GT was previously subdivided, based on morphological expression, into the
260 “rubbly_Jura” and “coherent_Jura” respectively [e.g., O’Connell-Cooper et al., 2021]. A strong
261 inverse relationship between potassium and grain size is identified throughout Jm_GT. The
262 dominant “rubbly” morphology primarily comprises finely laminated K-rich mudstones and
263 angular to rounded pebbles (Figures S2a-d). The compositional similarity between the loose
264 pebble regolith and the flat lying patches suggests that the pebbles are locally derived (Figures
265 3a-b). The less abundant “coherent Jura” comprises coarser grained, magnesium-rich targets.
266 Although high-K targets are the dominant morphology, both Jm_GT drill targets, Aberlady (AL;
267 sol 2370) and Kilmarie (KM; sol 2384), are co-located on adjacent high-Mg blocks (Figures 1,
268 S1, S2e), due to the difficulty in finding a suitable, drillable target within the rubbly high-K
269 material.

270 The K-Mg relationship within Jm_GT targets is of particular interest, with 93% of
271 samples falling into compositional endmembers, defined by “ $K/Si > \text{mean } Mf+CSf > Mg/Si$ ” (high-
272 K-facies) *or* “ $K/Si < \text{mean } Mf+CSf < Mg/Si$ ” (high-Mg-facies) (Tables S1, S5a). A small subset of
273 targets (n=6) show intermediate K and Mg, falling outside of the compositional endmembers
274 defined above – these are grouped herein with the high-Mg facies. There is no overlap in either
275 K or Mg concentrations between high-K and high-Mg facies (Figure 3a), and limited overlap for
276 Zn and Mn (depleted in high-K-facies, enriched in high-Mg-facies) (relative to mean Mf+CSf)

277 (Figure 3b). Univariate correlation analysis identifies strong negative Pearson correlation
278 coefficients (r) between K-Mg (r : -0.90), K-Mn (r : -0.68) and K-Zn (r : -0.63), and positive
279 correlations between Mg, Mn and Zn (r : +0.58 to +0.65) (Figures 3a-b; Table S3a). These
280 relationships (K, Mg, Mn, Zn) are not identified for the Mf+CSf in general, except in the Blunts
281 Point (BPm): K-Mg r =-0.80; Mg-Zn-Mn r =+0.47 to +0.59) and Sutton Island (SI_m) members
282 (Mg-Zn-Mn r =0.56 to 0.62) (Table S3f). Statistically significant variance is identified between
283 the two facies for all elements, except Ti, Al, Cr, Fe, Na, Br, which have broad in compositional
284 ranges for both types (Table S5d; Figure 7a).

285 **4.1.2. Jm_GT Agglomerative Hierarchical Clustering Analysis (AHCA)**

286 AHCA was performed on Jm_GT bedrock (n =40), using model parameters described
287 previously (Section 3.3; Supplementary Text S2b). For all three models, at cluster size K =6 (K_6),
288 two groups are formed, falling along previously defined facies lines: high-K facies targets
289 dominate Group A, whilst Group B consists of high-Mg facies and intermediate-facies targets
290 (Table S5a; Figures S8a-d). Models are very similar, with 90% (n =36) of targets falling into the
291 same group, and the majority falling into the same cluster. For all models, the target
292 “*Haddington*” (sol_2408; AL+KM drill locale) which is high-K but also has very high Mn and
293 Zn, falls into Group B. For Models A+B, Group A contains only high-K targets, but gains four
294 intermediate-Mg targets (with moderate Mn, P, Zn) for Model C. The high-K target *Hill of*
295 *Skares* clusters within Group A for Models A+C, but Group B for Model B only.

296 **4.1.3. Jm_GT Multivariate Principal Component Analysis (PCA)**

297 PCA analysis was applied to the AHCA Model A results to identify major trends (Figure
298 S9a). Group A (C₁-C₃, primarily high-K-facies, n =18) is characterized by a trend to higher K, Si,
299 Ni, Fe and Group B (C₄-C₅, primarily high-Mg targets, n =22) to higher values for all other

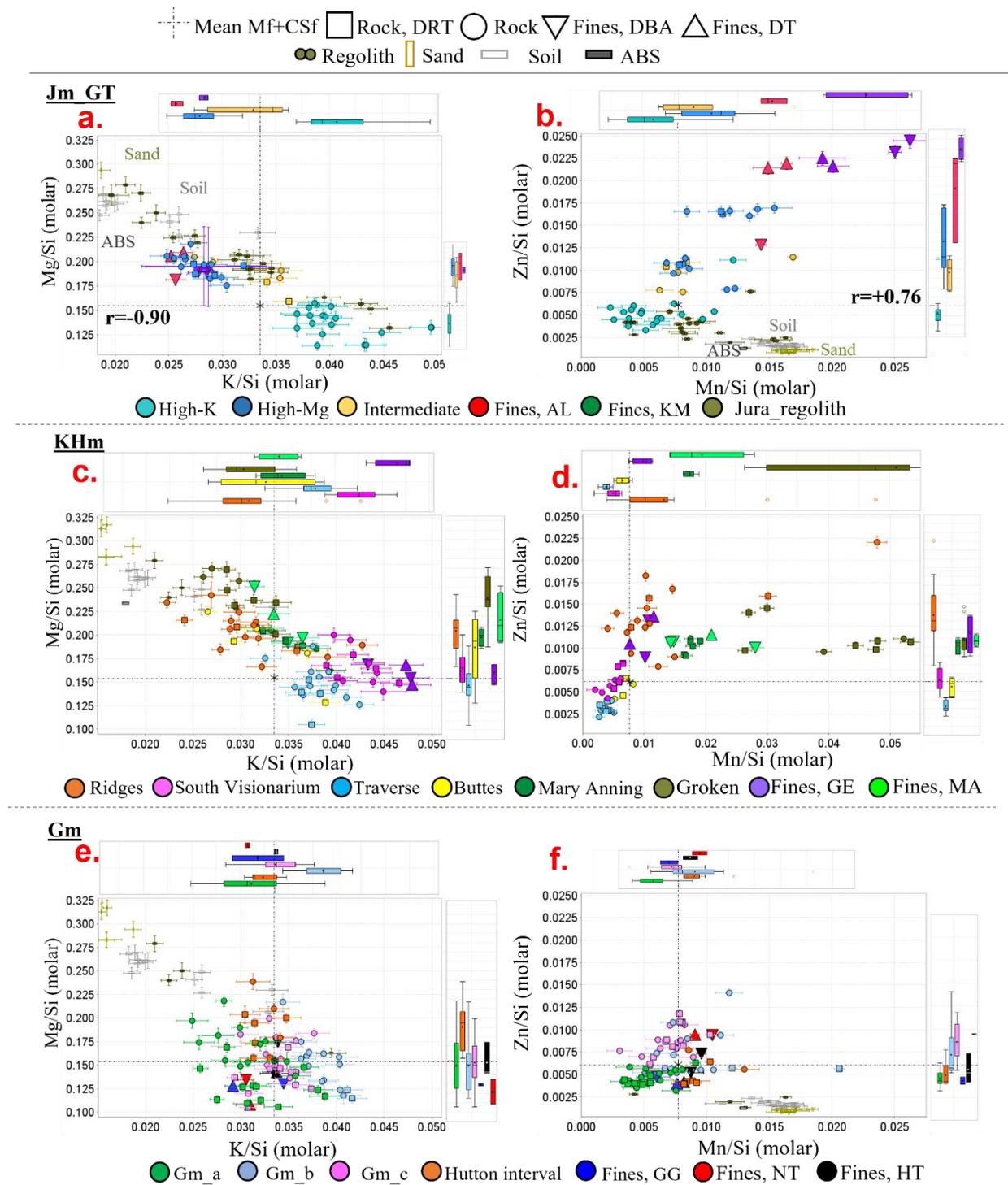
300 elements. Calculating percentage change in means, relative to mean Mf+CSf (Figure S9b),
301 Group A trends to depleted Mn, Mg, Ca, P, S, Cl, Zn. Group A is relatively homogenous, but
302 with enrichment Ni in C₁, Al, Cr, Na in C₂ ($r=+0.87$ for Al+Cr), Cl in C₃ and a marked Br
303 depletion in C₂ but enrichment in C₃. Group B shows strong differences between clusters, with
304 some evidence for geographical clustering. C₅ (targets from Woodland Bay area) are enriched in
305 Mn, Mg, Na, S, Cl, Zn, Br. C₆ (predominantly intermediate targets, plus *Haddington*) is depleted
306 in Ca, S, P but very enriched in Br. C₄ (primarily located in the Aberlady and Kilmorie drill
307 locale) is enriched in both Mn and Zn, with highest Zn values for Jm_GT in this cluster.

308 **4.2 Carolyn Shoemaker formation – Knockfarril Hill member**

309 **4.2.1. Knockfarril Hill member (KHm)**

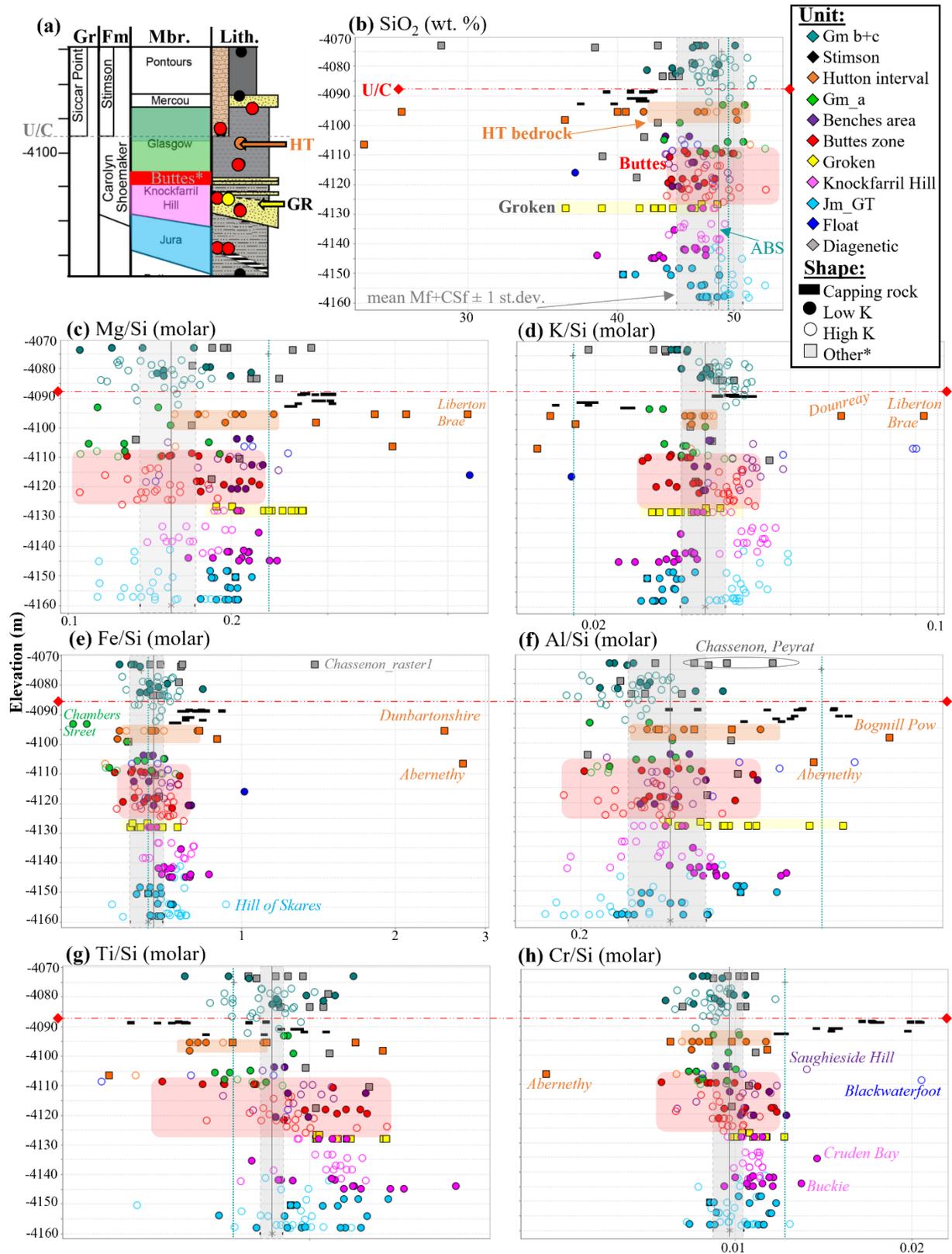
310 APXS analyses of KHm targets show that fine-grained targets are enriched in K (defined as:
311 $K/Si > \text{mean Mf+CSf} > Mg/Si$); whilst coarser targets are enriched in Mg (defined as: $K/Si < \text{mean}$
312 $Mf+CSf < Mg/Si$) (Tables S1, S6a). The paired *Glen Etive* drill holes (GE1 and GE2; sols 2486
313 and 2527, respectively) are co-located at the southern end of the Visionarium (an area of scarps
314 and ridges, Bennett et al., this issue) in a layer of slightly finer-grained [Rivera-Hernandez et al.,
315 2020a; Minitti et al., 2021] high K, moderate Mg material (Figures 1, 3c-d, S1). The paired *Mary*
316 *Anning* drill holes (MA1 and MA3; sols 2838 and 2870, respectively), located in coarser grained
317 Mg-rich sandstones, mark a brief detour from the MSAR (once the main KHm campaign had
318 finished) to facilitate a TMAH SAM experiment [Williams et al., 2021] (Figures 1, S1). The
319 nodular MnO-P₂O₅ rich target *Groken* (GR; sol 2910), co-located with MA, was the focus of an
320 opportunistic drill campaign (Figures 1, S1, S3e).

321



322

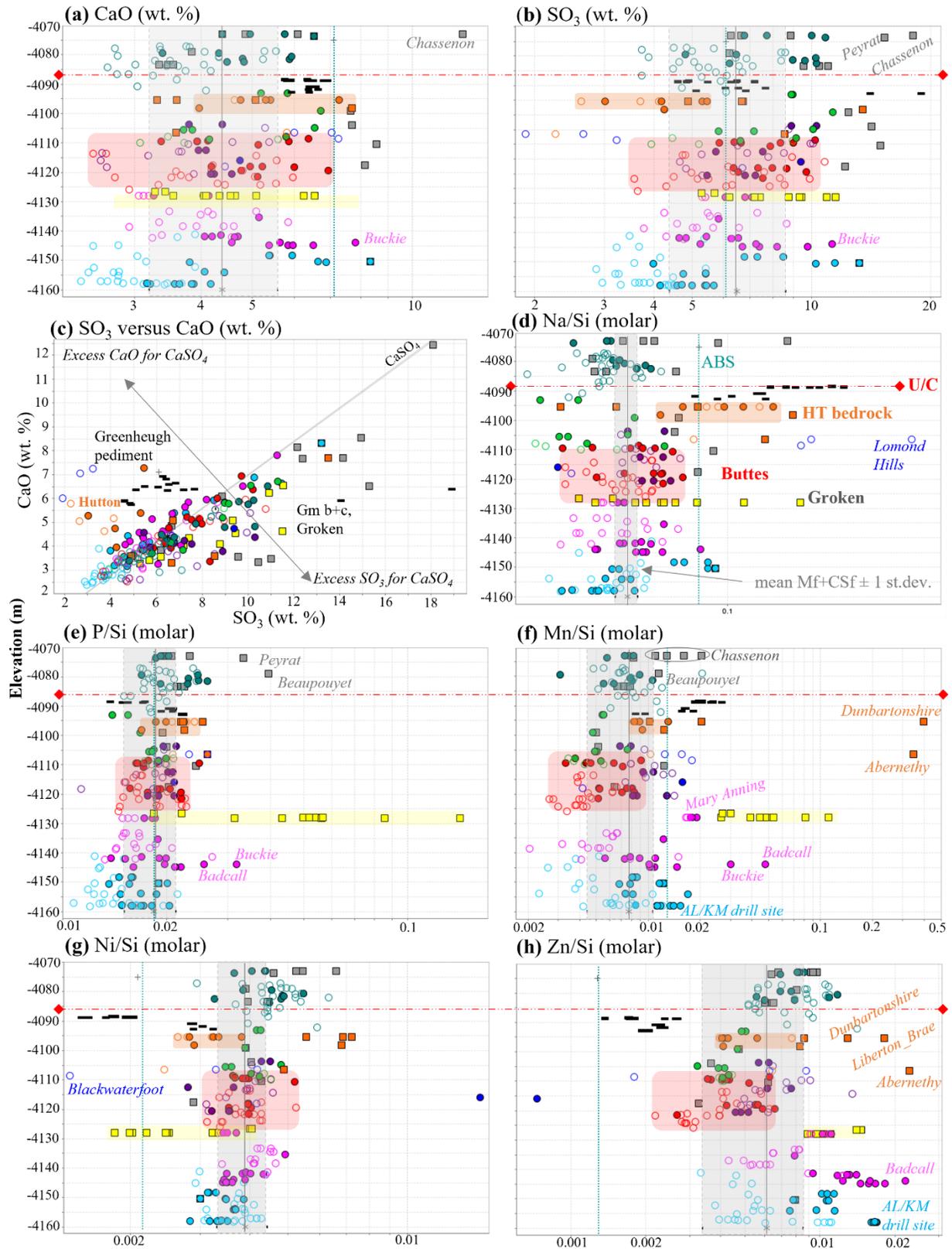
323 **Figure 3.** K-Mg and Mn-Zn compositional data (x-y graphs with Tukey outlier plots), for bedrock and fines targets
 324 (no diagenetic features). All data is in X/Si molar form. Members are subdivided into facies or subunits (see text for
 325 details). Tukeys: central box is mid 50% of data (Q1-Q3). Outliers (circles) are $> 1.5 * (Q3-Q1)$ from the central box;
 326 far outliers (triangles) are $> 3.0 * (Q3-Q1)$. Mean Mf+CSf = mean Murray and Carolyn Shoemaker formations
 327 (Tables S1, S2; Supplementary Text S2a). ABS = Average Basaltic Soil [O'Connell-Cooper et al., 2017]. **3a-b.** Jura
 328 member, Glen Torridon (Jm_GT). **3c-d.** Knockfarril Hill member (KHm). **3e-f.** Glasgow member (Gm).



330 **Figure 4.** Major oxide concentrations within Glen Torridon. **4a.** Stratigraphic column after Fedo et al., this issue,
331 with study area in colour. **4b-h.** All data (X/Si) molar (except **4b**, in weight percent) versus elevation (metres);
332 logarithmic x-axis for all plots (**b-h**). The red dashed line represents the Siccar Point Basal unconformity, the dark
333 grey line mean Mf+CSf, the grey shaded areas ± 1 standard deviation, and the green dashed line Average Basaltic
334 soil (ABS) [O'Connell-Cooper et al., 2017]. The buttes transition zone is shaded in red for each plot.
335

336

337



339 **Figure 5.** Mobile element concentrations within Glen Torridon (Legend as per Figure 4). **5a-b.** CaO and SO₃ weight
340 percent versus elevation (metres); logarithmic x-axis. **5c.** SO₃ versus CaO (weight percent). **5d-h.** Concentrations
341 (X/Si molar) versus elevation (metres); logarithmic x-axis.
342

343 Compositional endmembers are less well developed within KHm than Jm_GT, with 35% of
344 samples exhibiting both Mg and K higher than mean Mf+CSf. However, targets with highest K
345 concentrations continue to trend to lower Mg, Mn, Zn, whilst highest Mg targets exhibit lower K,
346 and higher Mg, Mn, Zn (Figures 3c-d; Tables S3, S6a). The KHm shows compositional variation
347 with location and can be subdivided into five broad units, with statistically significant differences
348 identified between units (Table S6d; Figures 3c-d, 7A).

349 (1) **Ridge** targets (dominated by high-Mg/low K targets, number of targets (n) =16),
350 encompassing Teal ridge and Harlaw rise, are characterized by depletion in K, but trend high for
351 other elements, with highest mean Ti, Al, Cr, Fe, Mg, Na, P, Zn concentrations. (2) Post-ridge
352 targets at the southern end of the Visionarium (**South_Vis**) (dominated by high K/moderate Mg
353 targets, n=12), including the Glen Etive (GE) drill sites. (3) **Traverse** targets (dominated by high-
354 K/low Mg targets, n=16) are a broad group of post-GE targets, incorporating five targets from
355 the traverse to the buttes, and eleven along the base of the buttes, to the edge of Western butte.
356 South_Vis targets are enriched in Cr, Cl, Ni, Br but depleted in P, whilst traverse targets exhibit
357 the opposite pattern. (4) **Butte** targets (a mix of high-K + high-Mg targets, n=5), along the
358 contact with the overlying Glasgow member (Gm), have the highest mean Ca, S, but lowest Al,
359 Cl, with Fe concentrations amongst the lowest identified in KHm. (5) Mary Anning (**MA**) drill
360 site (high-Mg/low to moderate K targets, n=6) targets exhibit the highest mean Mn (excluding
361 the Groken locale and other outliers) and differ from the ridge targets (also high-Mg-facies) in
362 that they have low mean Fe, Ca, P. Although the Groken (GR) drill target is co-located with MA,
363 they exhibit an anomalous composition, with very high z-scores (Table S1) – targets have very

364 high mean Al, Mn, Mg, Na, P, S, Cl but very low Ni. In particular, MnO is very high, with
365 concentrations up to 2.44 wt. % observed, compared to the 0.35 ± 0.04 wt% found in average
366 basaltic (MER and MSL) soils (ABS) [O’Connell-Cooper et al., 2017]. Accordingly, they are
367 treated separately from other KHm targets, and are not included in the AHC analysis below.

368 **4.2.2. KHm Agglomerative Hierarchical Clustering Analysis (AHCA)**

369 AHCA confirms the validity of the KHm geographical and facies divisions. Three AHC
370 models (Section 3.3) were run using $\text{Log}_{10}[\text{X/Si}]$ (molar) data for bedrock targets only (n=55) (no
371 fines). Ideal cluster size was identified using the “elbow method” as $K=6$ (K_6).

372 All models result in two major groupings (Table S6a; Figures S10a-d). Models B (no S, Cl,
373 Br) and C (also excludes Mn, P, Zn, Ni) resulted in very similar cluster organizations with two
374 broad groupings, each dominated by either high-K or high-Mg targets. 84% of targets remain in
375 the same group regardless of model, with Group A dominated by high-K (variable Mg, typically
376 low to moderate) South Vis and traverse targets (18% ridges, buttes; *no* MA targets) and Group
377 B comprising high-Mg targets (ridges, buttes, MA) only. Model A shows the strong effect of S
378 enrichment in the ridge targets, with these targets in a separate group to all other targets (Figure
379 S10b). For model B, distance between class centroids (Table S6b) confirms the similarity
380 between Group A clusters (distances ≤ 0.427) and between Group B clusters (0.356). For model
381 C, distances are slightly higher: Group A ≤ 0.234 ; Group B s ≤ 0.279 .

382 **4.3 Carolyn Shoemaker formation – Glasgow member**

383 **4.3.1. Glasgow member (Gm)**

384 The traverse across the Glasgow member (Gm) was bisected by a detour into Knockfarril
385 Hill (KHm) (sols 2826-2921) to facilitate drilling at MA (Figure 1) in support of the SAM
386 TMAH experiment [Williams et al., 2021]. Gm is split herein into pre_MA (*Gm_a*) and

387 post_MA (**Gm_b**) (Tables S1, S7a; Figures 1b-d, S4). The post_MA unit is further subdivided,
388 with the identification of a sub-unit (**Gm_c**) which skirts along the Sands of Forvie, and up to the
389 base of Mont Mercou (Figure 1c-d, S4). The boundaries of this subunit are based on recent
390 CRISM mapping by Hughes et al. [2021, this issue], who identified a rougher “rubbly” or
391 fractured texture in this area. Three targets were drilled in Gm. Drill target *Glasgow* (GG; sol
392 2754) was drilled in the buttes area (Gm_a), whilst *Nontron* (NT; sol 3056) was drilled in Gm_c
393 bedrock at the base of Mont Mercou. An additional target *Hutton* (HT; sol 2668) was drilled
394 within the “**Hutton interval**”, a zone of Gm rocks just below the Basal Siccar Point
395 unconformity and in contact with the overlying Greenheugh pediment, which are treated herein
396 as a separate but related unit.

397 The abrupt change at Central butte from cross-stratification structures to thin laminations,
398 coupled with a sharp increase in diagenetic features (Figure S6), delineates a sharp
399 sedimentological contact between KHm and Gm [Bennet et al., this issue; Fedo et al., this issue].
400 However, APXS analyses indicate a subtle geochemical transition between KHm and Gm in the
401 area of the buttes (Section 5.4), marked by a trend to lower means, especially for Mg, Ca, Mn,
402 Ni, Zn, Br (Figures 4c, 5a, 5f-h). Statistically significant variance was not identified for any
403 element (except K/Si), indicating a degree of similarity.

404 APXS analyses also reveal geochemical differences between the pre- and post-MA Gm units
405 (Gm_a, Gm_b) and subtle trends of change across the lateral extent of Gm (from the buttes to
406 Mont Mercou) (Figures 3-5, 6b). Post_MA Gm targets trend to higher Fe, K, plus mobile (Mn, P,
407 Zn, Ni) and volatile elements (Cl, Br), than pre_MA targets, with lower concentrations for all
408 other elements (Tables S1-2). Statistically significant variances are identified between Gm_a and
409 both post_MA units (Mn, K, Cl, Zn, Ni), between Gm_a & Gm_b only (Al, Fe, Ca, S) and Gm_a

410 & Gm_c only (P) (Table S7d). Minor compositional differences are also identified in the
411 post_MA eastward traverse, from Gm_b to Gm_c, with decreases in Ti, Fe, Mn, K, Cl, and
412 increases for all other elements; K, S, Ca show statistically significant variance (Table S7d).

413 The strong correlation relationships (K, Mn, Mg, Zn), key to defining the lower GT units, are
414 weakly developed or absent in Gm as a whole (Table S3c). A negative K-Mg correlation is
415 identified in Gm_b ($r=-0.83$), and a positive Mg-Mn correlation in Gm_a ($r=+0.67$); positive
416 correlations between Zn and Mg+Mn are absent. However, a moderate positive correlation
417 between Ni and Zn is identified in both Gm_b ($r=+0.54$) and Gm_c ($r=+0.63$) – this correlation
418 is not identified in any GT unit.

419 **4.3.2. Gm Agglomerative Hierarchical Clustering Analysis (AHCA)**

420 Three AHCA models (Section 3.3; Supplementary Text S1) were run on the Glasgow member
421 data, using $\text{Log}_{10}[\text{X/Si}]$ (molar) data for bedrock targets only ($n=63$), for an ideal cluster size of
422 $K=7$ (K_7) (Tables S7a-c; Supp. Figs. S11a-d). All models resulted in two major groupings, with
423 51% of targets remaining in the same group regardless of model. For Models A (all elements
424 included) and B (excluding volatiles S, Cl, Br), 68-84% of all Gm_a targets fall in Group A,
425 whilst 93-100% of Gm_b targets and 70-78% of all Gm_c targets fall into Group B (Table S7c),
426 suggesting a compositional divide between the pre_MA (Gm_a) and the post_MA
427 (Gm_b+Gm_c) units. This divide is not as striking for Model C (no volatiles, *plus* no Mn, Zn,
428 Ni, P), where Gm_a and Gm_b targets are divided equally between Groups A and B, but Gm_c
429 is found predominantly in Group B.

430 Comparing Models A and B, overlap targets (i.e., in the same group for both models) are
431 roughly split evenly between the three Gm units, suggesting the contribution of volatile elements
432 is relatively uniform across the Glasgow member. However, comparing Model B to Model C,

433 overlap targets are 67% Gm_a, 7% Gm_b and 27% Gm_c, indicating that mobile elements (Mn,
434 P, Zn, Ni) have a larger effect on composition (Table 7c). This can be attributed to the much
435 lower levels of all four mobile elements in Gm_a. Zn and Mn are depleted in the transition zone
436 from KHm to Gm at the buttes (Section 5.4), whilst both P and Ni are enriched in the post-MA
437 units, with concentrations increasing with distance from the buttes and proximity to Mont
438 Mercou.

439 **4.3.3. Hutton interval**

440 The Hutton interval (*Gm-HT*) (sols-2660-2691) (Tables 2, S1) is a layer of Gm bedrock
441 and complex vein networks that occurs at the top of Tower Butte (Figures 1c, S5) below the
442 Siccar point unconformity and in contact with the overlying Greenheugh pediment (GP) [see also
443 Thompson et al., this issue for further discussion]. Although this interval contains the
444 characteristic thin laminations that mark it as part of the Gm, a unique geochemical and
445 mineralogical signature was documented here by APXS [this paper; Thompson et al., this issue],
446 ChemCam [Dehouck, et al., this issue; Gasda et al., this issue] and CheMin [Thorpe et al., this
447 issue]. Relative to mean underlying Gm_a bedrock, Hutton bedrock trends to enriched Mg, Na,
448 Mn, and depleted S, Ni (Tables 2, S1; Figures 4c, 5b, 5d, 5f-g, 6b). Although S is depleted, Ca is
449 not, indicating that a decoupling of Ca and S (Figure 5c). Additionally, some samples trend to
450 low Ti, and high Al, P, Zn, (Figures 4g, 4f, 5e, 5h, 6b). A similar geochemical composition is
451 identified at the highest point achieved by *Curiosity* on Western Butte in the bedrock target
452 *Buchan Haven* (sol_2640) and vein target *Abernethy* (sol_2642) (Tables 2, S1). The correlations
453 between K, Mn, Mg and Zn identified in other GT units are completely absent from the Hutton
454 interval. Evidence for more alteration with increased proximity to GP is manifest in the form of
455 more abundant nodules and veins. Complex FeO-MnO-rich (*Dunbartonshire* (sol_2691),

456 *Abernethy*: FeO 40 wt.%, MnO 5-6%) and MgO-K₂O-rich (*Liberton Brae* (sol_2666): MgO 17
457 wt. %, K₂O 2 w%) vein networks are identified at both at Hutton and Western Butte (Figure S5).

458 **4.4. Benches**

459 The “benches” unit represents a second transition between KHm and Gm (Figure 1d),
460 through a series of resistant topographic “benches” with rubbly bedrock in between benches
461 [Bennet et al., this issue]. However, unlike the clear facies transition identified at Central Butte,
462 the “Benches” transition zone is not well defined stratigraphically, resulting in some ambiguity
463 about whether this unit is more correctly placed with KHm or Gm. Targets are in family with
464 other Glen Torridon bedrock (Tables 2, S1), but there are some distinctions (Figures 4-5).
465 Coherent targets (e.g., *Muckle Minn*, sol_2935) which comprise the bulk of APXS targets here,
466 have higher Mg/Si than mean Mf+CSf, whilst rubbly targets (e.g., *Mail Beach*, sol_2933) have
467 high K/Si (i.e., > mean Mf+CSf). However, moderate targets (high K *plus* high Mg) are more
468 common in the Bench unit than previously described units, comprising >50% of bench targets.
469 The target *Hart Fell* (sol_2938) has both high Mg and K, but also very high Zn (2808 ppm).
470 There are also examples of a “chaotic” texture, in the high-Mg *Garth Ness* target (sol_2928),
471 which is not reflected in the composition; the benches exhibit the highest mean Mg/Si, K/Si,
472 Na/Si, S/Si and Cl/Si for any GT bedrock facies or subunit (excluding the Hutton interval,
473 Groken and other diagenetic targets). Similar to the KHm-Gm transition zone at the buttes, mean
474 Zn/Si trends low, however Mn/Si trends high.



475

476 **Figure 6. Tukey plots, showing compositional trends for Knockfarril Hill and Glasgow**
 477 **member subunits. 6a.** Knockfarril Hill (KHm) subunits, defined by geographical location (Table S1-S2, S6).
 478 **6b.** Glasgow (Gm) subunits and Hutton interval (Table S1-S2, S7). Tukey plot interpretation: Black circle is mean
 479 value for a given unit. The central box represents the mid 50% of data (Q1-Q3). Outliers (circles) are > 1.5* (Q3-
 480 Q1) from the central box; far outliers (triangles) are > 3.0 * (Q3-Q1). All data is in element/Si (molar) form except
 481 first plot (Si molar) for both 6a and 6b.
 482

483 **4.5. Unconsolidated sediments in Glen Torridon**

484 Twelve unconsolidated sediment targets were analyzed during the traverse to Mont
485 Mercou (Table 2, S1). All but two samples were active sands, using S, Cl, Zn abundances as a
486 proxy for dust cover and, by implication, activity levels. All sand targets are in family with
487 active sands analyzed prior to the ridge. Offcrest samples show enrichment in T-Cr, a trend
488 previously identified in the second phase of the Bagnold Dunes campaign and onwards
489 [O’Connell-Cooper et al., 2018]. Crest samples typically show enrichment in Mg-Ni. Grain size
490 and depositional settings of samples are discussed in Weitz et al. [this issue]. In contrast,
491 *Balliekine* (sol_2706) and *Auld Reekie* (sol_2731), both overlying Stimson formation substrate
492 on the Greenheugh pediment, plot with soil measurements, such as *Portage* and other soil targets
493 analyzed prior to the Bagnold Dunes campaign, which are in family with average basaltic soil
494 (ABS) from the MSL and MER missions [O’Connell-Cooper et al., 2017].

495 **4.6. APXS Drill fines analysis – comparison to host bedrock**

496 Ten holes were drilled in Murray and Carolyn Shoemaker bedrock targets during the
497 Glen Torridon campaign [Jm_GT, n=2; KHm, n=5; Gm, n=3] (Figs. 1, 3a-f, S1; Tables 2a-b,
498 S1), with an additional target in the Stimson formation (Sf) (*Edinburgh* (EB), on the Greenheugh
499 pediment (discussed in detail in Thompson et al., this issue). Targets represent a variety of
500 bedrock, as defined by K and Mg: (1) low K, high Mg: *Aberlady* (AL), *Kilmarie* (KM); (2) high
501 K, moderate Mg: *Glen Etive* 1+2 (GE1, GE2); (3) moderate K, high Mg: *Mary Anning* 1+3
502 (MA1, MA3), *Groken* (GR); (4) moderate K, low Mg: *Glasgow* (GG), *Nontron* (NT), *Hutton*
503 (HT) (Table 2b; Figure S1). Drill fines typically follow the trend of host bedrock, but there are
504 some variations, both relative to host bedrock, and between DBA and tailings samples.

505 Cl trends to lower for drill fines than bedrock, with lower concentrations for all tailings
506 than DBA samples, except KM DBA. Br concentrations in fines are typically \leq host bedrock for
507 all samples, but AL, KM, and MA1 tailings are enriched, relative to bedrock. Ti and Cr are
508 enriched in Jura and Knockfarril Hill member drill fines relative to host bedrock. Fe is enriched
509 in fines for all samples, relative to a given host bedrock, with the enrichment less pronounced in
510 the Glasgow samples (GG, NT, HT). Both GR fines and the nodular rich host bedrock are
511 enriched in both P and Mn, with a near perfect correlation between these elements ($r=+0.99$). Ca
512 and S are typically enriched in fines relative to bedrock for all samples.

513 The KM samples show the most differences to the GT bedrock. The DBA samples are
514 enriched in Mn and P (also seen in MA and GR), up to 20-26% wt. Ca+S, and an enrichment in
515 Zn in both DBA and tailings (also seen in AL tailings). Na and Al concentrations are similar to
516 host bedrock for the majority of fines samples; however, the KM tailings are significantly
517 depleted in both.

518 **5. Discussion and implications**

519 The Glen Torridon clay unit was proposed as an important MSL traverse waypoint prior to
520 landing; it was interpreted as a lithological unit that could help inform planetary processes that
521 influence habitability [Grotzinger et al., 2012]. The local enrichment in phyllosilicates in Glen
522 Torridon (Fe/Mg smectites), inferred from orbital spectroscopy [e.g., Fraeman et al., 2016;
523 Milliken et al., 2010; Fox et al., 2018; Stack et al., 2017] was of high interest, as smectites are
524 considered to be favorable indicators of ancient habitable environments and to aid in the
525 preservation of organic molecules [e.g., Summons et al., 2011].

526 Additionally, orbital mapping revealed spatial variations in the smectite signature, with
527 highest signatures closest to VRR, decreasing to a smectite-sulfate mix with distance from VRR

528 and into the transition to the overlying sulfate unit. The transition to a more sulfate-enriched
529 lithology was considered to be indicative of changing environmental and depositional conditions,
530 with broad implications for our understanding of both Gale crater [e.g., Milliken et al., 2010]
531 and, at a more global scale, across Mars [e.g., Bibring et al., 2006].

532 APXS results from the exploration of Gale crater will therefore be assessed from two
533 perspectives (1) the significance of the clay-rich material within the trough and (2) variations as
534 *Curiosity* moved from the trough towards the clay-sulfate transition.

535 **5.1. Relationship to Jura member on VRR (herein Jm_VRR)**

536 Although orbital mapping placed the trough above VRR in terms of stratigraphy
537 [Fraeman et al., 2016], in situ analysis shows that the Jura within Glen Torridon (Jm_GT) is
538 stratigraphically equivalent to that on the ridge (Jm_VRR) (Section 2; Table 1) [Fedo et al.,
539 2020, this issue]. Similarities in facies, and the absence of a clear tectonic or depositional break
540 between the two suggest comparable depositional environments (low energy, lacustrine) [Fox et
541 al., 2019b; Edgar et al., 2020; Caravaca et al., this issue], despite the difference in morphological
542 expression. However, APXS identifies geochemical differences between the Jm_GT and
543 Jm_VRR. Jm_GT exhibits lower mean Si, Al Ca, Na, P, S, Ni than mean Jm_VRR. Statistically
544 significant variance is identified for 10 of the 16 reported elements (Table S4), a higher
545 proportion than with any other Mf or CSf member (except Pahrump Hills, PHm). Notably, the
546 strong correlation relationships (K, Mg, Mn, Zn) observed in Jm_GT are not identified in
547 Jm_VRR.

548 Thompson et al. [2020] subdivide the Jm_VRR (on the basis of spectral signature, via
549 orbital mapping) into *Jm_VRR_tan* (targets from areas mapped orbitally as tan coloured; the
550 dominant lithology) and *Jm_VRR_blue* (targets from more discrete areas, mapped orbitally as

551 blue or grey). Comparing these subunits with the Jm_GT high-K and high-Mg facies allows a
552 more detailed analysis, identifying statistically significant variance for all elements reported on:
553 Al, Ca, Na, S, (high-K targets: $VRR_{tan} \pm VRR_{blue}$); Si, Mn, Ni (high-Mg targets: VRR_{blue}
554 + VRR_{tan}); all other elements (both high-K & high-Mg facies: VRR_{blue} *and/or* VRR_{tan})
555 (Table 5e; Figure 7a).

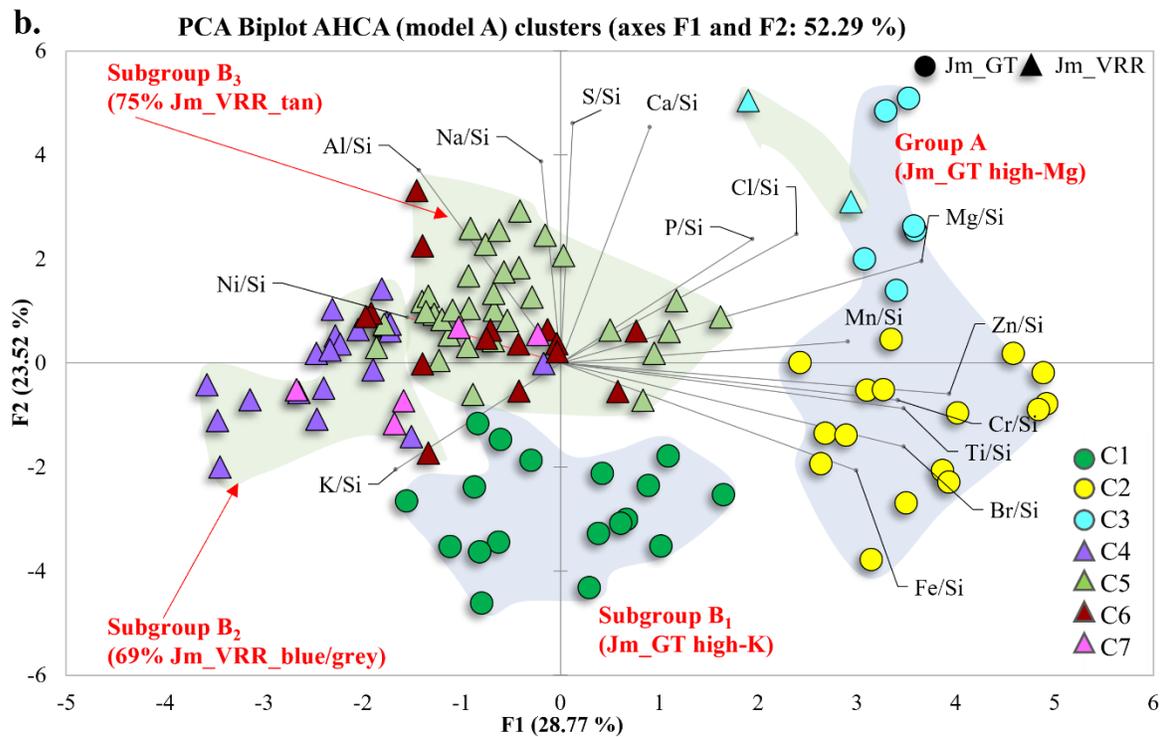
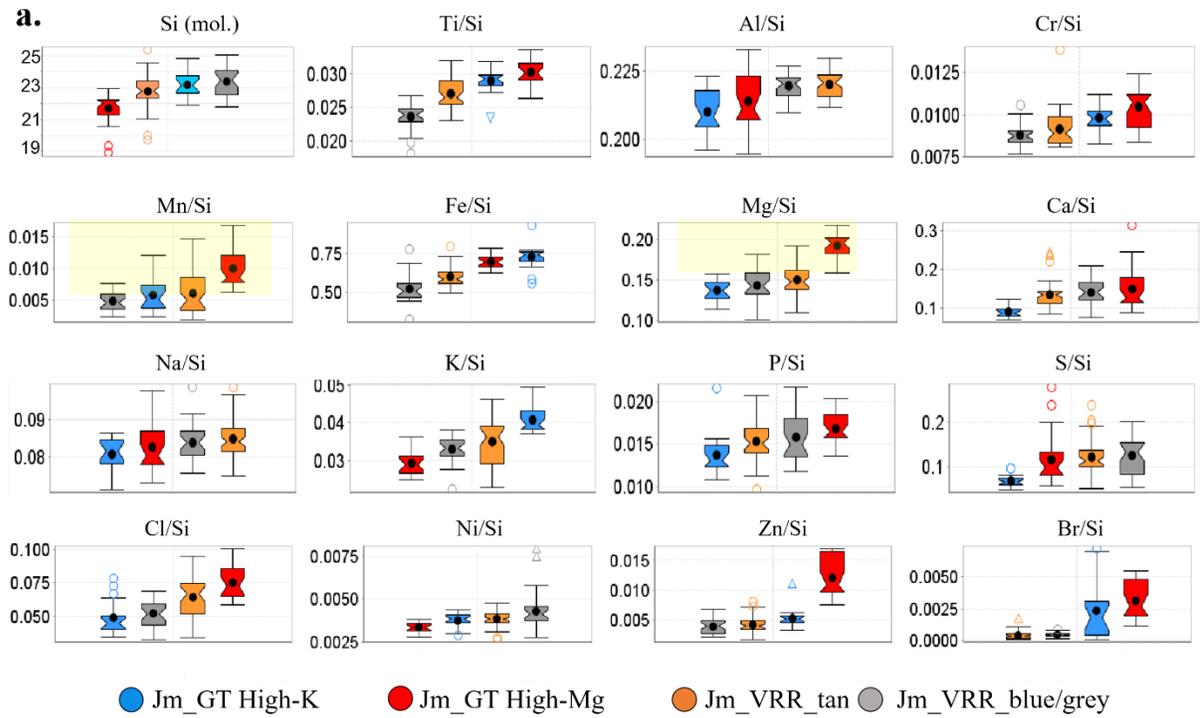
556 AHCA and PCA were undertaken for all Jura targets to investigate compositional
557 differences or similarities, regardless of location (Tables S5a; Figure 7b). Ideal cluster size (K_4)
558 places all Jm_VRR targets in a single unit or cluster, whilst splitting Jm_GT into three clusters
559 along (high K or high Mg) facies lines, thus confirming the homogeneity of Jm_VRR when
560 compared to Jm_GT. Forcing K_7 to facilitate more detailed analysis splits targets into two groups
561 A and B. Group A consists of Jm_GT intermediate to high Mg facies targets, plus two
562 Jm_VRR_tan targets (from the *Rockhall* drill locale). All other targets are found in Group B,
563 which is split into three subgroups: B₁ Jm_GT high-K targets only; B₂ dominated by
564 Jm_VRR_blue/grey, *no* Jm_GT; B₃ dominated by Jm_VRR_tan, *no* Jm_GT. The key
565 observation from this AHCA and PCA analysis is the confirmation of the unusual nature of the
566 Jm_GT high-Mg targets (Figure 7b).

567 CheMin also identified mineralogical differences between Jm_GT [Thorpe et al., this
568 issue] and JM_VRR drill targets [Rampe et al., 2020]. Jm_GT is enriched in phyllosilicates (28
569 wt. %) relative to Jm_VRR (5-13%). Plagioclase is half that identified in Jm_VRR (Jm_GT: 9-
570 10%; Jm_VRR: 20-22%). Hematite in Jm_GT ranges from 1.06% to 1.71%, and magnetite was
571 not identified. In contrast, iron oxides are enriched in Jm_VRR: hematite ranges from 2.90% to
572 9.30%, and magnetite is present (0.60%). Minor akageneite and jarosite are also identified on the
573 ridge [Rampe et al., 2020].

574 The compositional and morphological ridge expression led previous work [e.g., Bristow et al.,
575 2019; Fraeman et al., 2020; Frydenvang et al., 2020; Rampe et al., 2020; Turner et al., 2021] to
576 infer the presence of a diagenetic front, along the ridge, overlain by a relatively impermeable
577 caprock. Bristow et al. [2021] suggest silica-poor brines as a means to convert clays along the
578 ridge into iron oxides and oxyhydroxides, with recrystallization of ferric iron oxides enhancing
579 cementation and thus preventing erosion. APXS compositional data from Jm_VRR broadly
580 supports this model [Thompson et al., 2020]. An assessment of the relative bedrock strength,
581 inferred by the level of drill intensity required [Peters et al., 2018], confirm the inherent strength
582 of Jm_VRR compared to Jm_GT [Stack et al., this issue]. Targets within Glen Torridon range
583 from <8 MPa (targets: AL, GE1, GR) to 8.5 MPa (KM, GE2, MA1, MA3, GG, HT), in contrast
584 to the Jm_VRR drill target (*Rockhall*, RH), which had an assessed strength of 8-12.5 MPa.

585 APXS data supports the theory that the Jura sediments within Glen Torridon represent the
586 original composition of the Jura member, in contrast to the altered Jura along the ridge. In
587 contrast to the Jm_VRR, the Jm_GT shows little evidence of alteration, with very low levels of
588 Ca+S, few veins or diagenetic features, which otherwise increase slowly upwards in the KHm,
589 indicating low levels of post-depositional alteration. The compositional continuity observed by
590 APXS from Jm_GT to the overlying Knockfarril Hill (KHm) (Section 5.2), which then grades
591 upwards into Glasgow (Section 5.3) supports the idea that the Jm_GT is a primary composition.
592 This interpretation is consistent with the suggestion by Rudolph et al. [this issue] that the clays in
593 Glen Torridon were authigenic, forming in the Jura's lacustrine depositional environment.
594 Without recrystallization of ferric iron oxides (as suggested for the VRR by Bristow et al., 2021)
595 the softer, less resistant GT deposits were also susceptible to erosion than their altered
596 counterparts on VRR, resulting in the current day trough expression.

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602 **Figure 7.** Comparison of Jura member targets, from VRR and Glen Torridon. **A.** Tukey plot comparisons of the
603 Jm_GT (high-K and high-Mg) and Jm_VRR (tan and blue/grey) subunits (see text for details). All data in element/Si
604 (molar) form except first plot (Si molar) (Table S1). Yellow shaded area highlights high values for Mn, Mg, K, Zn
605 values in Jm_GT. Black circle is mean value for a given unit. Units within a given plot shown in order of increasing
606 mean value, left to right. Tukey plot interpretation: the central box represents the mid 50% of data (Q1-Q3). Outliers
607 (circles) are $> 1.5 * (Q3-Q1)$ from the central box; far outliers (triangles) are $> 3.0 * (Q3-Q1)$. **B.** Multivariate PCA
608 biplot showing compositional distinctions, both between Jm_VRR and Jm_GT, and between Jm_VRR and Jm_GT
609 subunits (Table S5a, S5e).
610

611 **5.2 Relationship between Jm_GT and the Knockfarril Hill member (KHm)**

612 The main phyllosilicate trough was mapped orbitally as two distinct units based on
613 morphology (smooth and polygonally fractured) with a smectite signal identified in both, but
614 stronger in Jm_GT (Section 2), leading to an expectation of compositional variations between the
615 two units. However, on the basis of APXS data, we see no evidence for substantial compositional
616 differences between Jm_GT and KHm. In situ analysis reveals that both K-rich mudstones
617 (dominant in Jm_GT; Section 4.1) and Mg-rich sandstones (dominant in KHm; Section 4.2) are
618 present in both members. The interfingering of these lithologies suggests a gradual change in
619 overall energy regimes, rather than an abrupt transition, moving from predominantly low energy
620 lacustrine, to higher energy fluvial environment or lakeshore with fluvial input environment in
621 KHm, but with episodic changes [Edgar et al., 2020; Caravaca et al., this issue].

622 APXS analysis reveals a high degree of similarity between the two members, with broad
623 overlap for the majority of elements (Figures 4, 5) and limited statistically significant differences
624 (Ni, P – Table S4). In contrast, both members show statistically significant variance from
625 Jm_VRR, and with the overlying Gm (Table S4).

626 This result is in agreement with CheMin results from across Glen Torridon, which indicate
627 that all three GT members (Jm_GT, KHm, Gm) are enriched in phyllosilicates (23-34 wt. %) [Thorpe et al., this issue] relative to VRR drill sites (5-13%) [Rampe et al., 2020] or GT drill
628 sites on/in contact with the overlying pediment (6-8%) [Thorpe et al., this issue]. However,
629

630 pre_VRR drill sites (*Marimba, Quela, Sebina*) also contain high levels of phyllosilicates (15-
631 28%) [Bristow et al., 2018]. Within GT, phyllosilicate abundances are highest in GE1 (34%) and
632 lowest in GG (23%) but concentrations are comparable (26-30%) for other targets, whether
633 drilled in high-K facies bedrock (GE2) or high-Mg (AL, KM, MA1, MA3) facies bedrock
634 targets. Although the CRISM signature predicted higher smectite abundances in Jm_GT,
635 CheMin report highest phyllosilicate abundances in KHm (GE1: 34 wt.%). However,
636 morphology constraints precluded drilling in Jm_GT high-K targets (present as rubble and
637 pebbles), and both Jm_GT drill targets are in Mg-rich coherent bedrock, whilst the GE drill
638 samples (KHm) were drilled in a K-rich finer grained layer, within a more coherent Mg-rich
639 sandstone.

640 This suggests that the difference in spectral intensity noted by orbital mappers was driven by
641 factors other than geochemical composition. Cofield et al. [2017] suggested that weathering out
642 of clay minerals from one (clay-rich) unit could provide a mantle or cover on a second (clay-
643 poor) unit, giving the illusion of smectites in both. However, given the compositional similarity
644 between Jm_GT and KHm, as reported by both APXS and CheMin, this scenario seems unlikely.

645 Alternatively, Fox et al. [2019a, 2021] suggest dust cover, related to morphology, as a
646 potential source of the differences in CRISM spectra intensity, with dust plausibly masking an
647 equivalent absorption from KHm. The relatively larger surface area of coherent bedrock slabs
648 (such as the sandstones that make up the KHm ridges) (Section 4.2.1) (Figures S3a-b) gather
649 more dust than the (typically smaller) pebbles and rubble that constitute much of the Jm_GT
650 (Section 4.1.1) (Figures S2a-d). Because the Mg content of dust [Berger et al., 2016] is higher
651 than that of Mf bedrock, unbrushed dusty targets tend to have higher Mg concentrations than
652 brushed rocks and drilled fines [Berger et al., 2020]. Comparing Mg concentrations in brushed

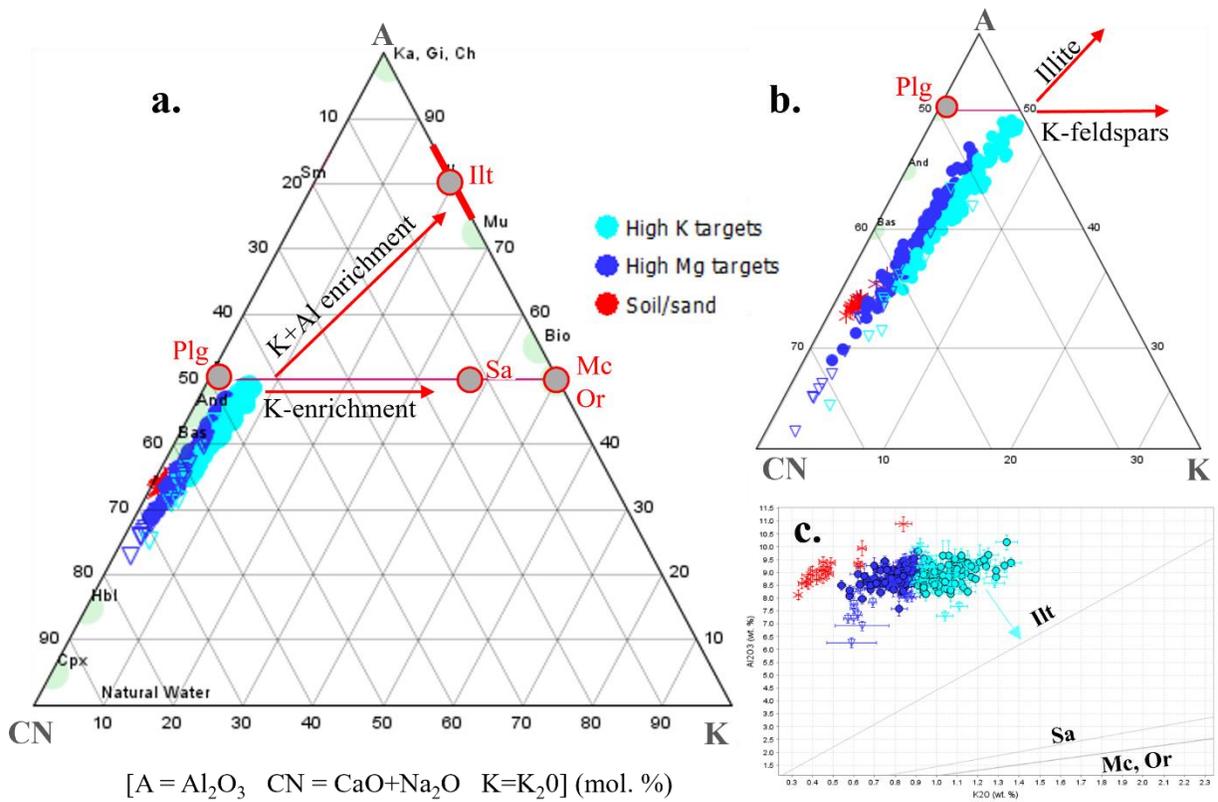
653 and unbrushed targets can be helpful in assessing the degree to which dust is present, although
654 caution should be taken with interpreting results, as the brushing of smaller, fragmented samples
655 was precluded (due to risk to the brush), leading to an inherent target selection bias. For both
656 KHm and Gm, unbrushed targets (60-65% of targets) have slightly higher mean Mg (Gm:
657 0.131135; KHm: 0.179379) than brushed targets (Gm: 0.16335; KHm: 0.171687). In contrast,
658 mean Mg is higher for Jm_GT brushed targets (15% of targets) (0.184017) than unbrushed
659 (0.163336), providing evidence that dust build up is limited on the rubbly targets. As the Jm_GT
660 landscape is dominated by rubbly material, it follows that less dust will be present across the
661 unit, compared to the KHm, where the phyllosilicate signal is hindered by dust buildup. This
662 seems the most plausible explanation for the intensity differential.

663 **5.3 The K-Mg relationship**

664 Two key compositional characteristics of the lower Glen Torridon units (Jm_GT and
665 KHm) are (1) the very well-developed anti-correlation relationship between K and Mg (Sections
666 4.1, 4.2; Table S3a-b; Figures 3a, 3c), and (2) the inverse relationship between K and grain size.
667 The anti-correlation between K and Mg is not identified on VRR, in the bulk of the underlying
668 Murray formation (Mf) or overlying Carolyn Shoemaker formation (CSf). However, it is
669 identified in the Blunts Point member (BPm), below the ridge (BPm: K-Mg $r=-0.80$) (Table S3f),
670 and within the Glasgow member subunit Gm_b (K-Mg $r=-0.83$) (Section 4.3.1; Table S3c).

671 The bimodal grain distribution within the Jm_GT and KHm has a significant correlation
672 with the composition of each facies. Fine-grained targets are typically K-rich [defined as
673 $K/Si > \text{mean Mf+CSf}$], with high Si, Fe, Ni, but low concentrations of mobile elements such as
674 Ca, S, P, Mn, Zn. Coarse grained targets are typically Mg-rich [defined $K/Si < \text{mean Mf+CSf}$],
675 with moderate to very high concentrations of Ca, S, P, Mn, Zn, Ni. The higher permeability of

676 the coarser grained targets, allowing more extensive post-depositional percolation of fluids, may
 677 explain the higher concentrations of mobile elements in the GT coarse grained targets. This
 678 suggests that the inverse relationship between K and grain size reflects a primary sorting process,
 679 such as the segregation of less dense, felsic [K-rich, Al-rich etc.] minerals (alkali feldspars, illites
 680 etc) from denser, mafic [Mg-rich, Fe-rich, Ni-rich etc.] minerals (e.g., pyroxene, olivine) [e.g.,
 681 Fedo et al., 2015], with finer-grained less dense minerals concentrating in lower energy



682

683 **Figure 8. 8a-b.** Al_2O_3 - $CaO+Na_2O$ - K_2O (mol %) (A-CN-K) ternary diagram [Nesbitt and Young, 1984] showing
 684 Glen Torridon bedrock, drill fines, sand, plus soil samples from across Gale crater. Jm_GT, KHm and Gm bedrock
 685 targets are classified as high K [i.e., $K/Si > \text{mean Murray +Carolyn Shoemaker formations}$ (all data molar)] or high
 686 Mg [i.e., $K/Si < \text{mean Mf+CSf}$ (all data molar)]. Mineral abbreviations after Whitney and Evans [2010]:
 687 Plg=plagioclase; Ilt=illite; Sa=sanidine; Mc=microcline; Or=orthoclase. 8c. K_2O/Al_2O_3 ratio (wt. %) showing Glen
 688 Torridon bedrock (Jm_Gt, KHm, Gm), drill fines, sand, plus soil samples from across Gale crater. Mineral
 689 abbreviations as A-B.

690

691 lacustrine sediments, and coarser, denser minerals in the higher energy fluvial sediments.
692 Compositional endmembers are less well developed within KHm than Jm_GT (30% of samples
693 falling outside endmembers), indicating more overlap between high-K and high-Mg facies
694 depositional settings, or a greater degree of mixing.

695 However, the evidence for mineral segregation is limited and not definitive. Plotting all
696 bedrock data on a $\text{Al}_2\text{O}_3\text{-CaO+Na}_2\text{O-K}_2\text{O}$ (A-CN-K) ternary diagram (Figures 8a-b) [after
697 Nesbitt and Young, 2010] to identify trends of enrichment in K-bearing mineral phases,
698 enrichment in alkali feldspars is not identified. A tentative trend of increasing illitization is
699 identified on the A-CN-K plot (Figures 8a-b), and on $\text{K}_2\text{O/Al}_2\text{O}_3$ ratio plots (Figure 8c). Whilst
700 CheMin results indicate highest phyllosilicate content in the high-K facies drill targets (GE1),
701 drill targets from all three GT members (Jm_GT, KHm, Gm) are enriched in phyllosilicates (23-
702 34 wt. %) (Section 5.2) [Thorpe et al., this issue]. The alkali feldspar sanidine is detected in all
703 samples but highest in the high-Mg target MA1. Pyroxene is also highest in MA1, but almost
704 equivalent in GE2 (high-K target), whilst olivine is not detected in any sample.

705 **5.4. Relationship between KHm and Glasgow member (Gm)**

706 Although the sedimentological boundary between KHm and Gm was well defined by a
707 change from cross stratified sandstones to finely laminated sandstones [Fedo et al., 2020, this
708 issue], with an abrupt increase in diagenetic features at the transition, APXS did not detect a
709 significant change in composition at the buttes (Section 4.3.1). Variance analysis for *bulk* KHm
710 and Gm reveals some elements with statistically significant variance (Ti, Cr, Fe, Mg, Si, K)
711 (Table S4) between the members; however, variance analysis using KHm and Gm
712 geographically defined units finds no statistically significant variance between KHm and Gm
713 targets at the buttes.

714 The majority of elements have a relatively similar profile for both KHm and Gm targets along
715 the buttes (Figure S7). In particular, both units (plus other Gm_a targets) show a marked
716 depletion (relative to mean Mf+CSf) in Mn and Zn. The lack of a strong geochemical change
717 from KHm to overlying Gm in the area of the buttes could suggest a transitional period, with a
718 common source of material for the end of the KHm and beginning of Gm. However,
719 compositional variations are identified within Gm, from pre-MA to post MA and additionally,
720 moving eastward towards Mont Mercou with an increasing abundance of diagenetic features
721 identified (Section 4.3.1; Figure S6). This suggests a change in (a) provenance with increasing
722 elevation through Gm and/or (b) alteration processes from KHm to Gm.

723 **5.5. Element mobilization and alteration**

724 Evidence for the mobilization of Mn, Zn, P, Ca, S and Ni has been previously identified
725 in Gale crater (pre Glen Torridon) [e.g., Thompson et al., 2020; Berger et al., 2017; Kronyak et
726 al., 2019; Sun et al., Nachon et al.,]. APXS identifies evidence for fluid mobilization and
727 multiple episodes of alteration across Glen Torridon. Patterns change with grain size of host
728 rock, elevation, proximity to the capping rock, and the clay-sulfate transition zone, lying above
729 Mont Mercou and just beyond the study area.

730 **5.5.1. Ca+S:** In general, CaO+SO₃ show a strong correlation ($r \geq +0.90$), indicating
731 addition of CaSO₄ rich fluids (Table S3, Figure 5c). A trend of lower mean CaO+SO₃ (relative to
732 mean Mf+CSf) in high-K targets is identified in GT bedrock (Jm_GT, KHm, Gm) (Figures 5a-c),
733 with higher values in high-Mg targets. As high K is typically found in finer grained targets (e.g.,
734 Jm_GT mudstones), we can infer that higher CaO+SO₃ are found in coarser targets (e.g., KHm
735 sandstones from Harlaw rise). This suggests that Ca+S rich fluids were utilizing the greater
736 permeability of the coarser sandstones, resulting in higher concentrations in these targets.

737 Coarser Jm_GT targets are enriched in Ca+S but to a lesser extent than KHm sandstones,
738 pointing to a trend of increasing Ca+S with elevation. Values increase with increasing elevation
739 in the CSf to the Hutton interval, with mean values decreasing slightly in post-buttes Gm targets
740 (Tables 2, S1; Figures 5a-b) – however, S is depleted in the Hutton interval itself.

741 This suggests a concentration of CaSO₄-rich fluids in the Glen Torridon area, potentially
742 capped by the overlying Stimson formation, moving outwards, weakening with distance from
743 this zone. This fits with the model proposed for the VRR [e.g., Thompson et al., 2020; Bristow et
744 al., 2019; Frydenvang et al., 2020; Rampe et al., 2020; Turner et al., 2021] (Section 5.1),
745 whereby an overlying relatively impermeable caprock acts as a control on diagenetic activity.

746 CaSO₄ veins are present both parallel to bedding and cross-cutting bedding, the latter
747 indicating later diagenetic activity (e.g., Figures S2c-d, S3a, S6a, S6d). Whilst many vein targets
748 are primarily CaSO₄, some targets also show evidence for other fluid activity e.g., the
749 *Chassenon* vein target (sol_3069-3071), at the base of Mont Mercou, exhibits a CaSO₄-rich rim,
750 but a Fe-rich core, which also showed some Na+Mn enrichment, but low Zn and Ni (Figure S6f).

751 Although Ca concentrations are high in the Hutton interval on Tower butte just below the
752 unconformity, S is depleted, indicating a decoupling and an increase in Ca not related to CaSO₄.
753 This is also noted at the highest elevation attained on Western butte in the bedrock target
754 *Buchan_Haven* (sol_2640). Conversely, there is evidence for increasing S, relative to Ca, across
755 the CSf - in KHm targets (most notably at the Groken locale, but also the ridges and in the
756 benches area), and in Gm_b+c bedrock. A number of Gm_c nodular targets (*An_Dun*, sol_2967;
757 *Peyrat*, sol_3051) show evidence for enriched S+Mg relative to bedrock.

758 **5.5.2. Na:** Na shows little change in Jm_GT or KHm, or the buttes area, with respect to elevation
759 (or grain size), with mean values very close to mean Mf+CSf, whilst the post-buttes Gm units are

760 depleted, relative to mean Mf+CSf (Figure 5d). Statistically significant variance is not identified
761 for Na between Jm_GT, KHm or “typical” Gm bedrock units (Table S3a-c). However, both the
762 Hutton interval (plus *Buchan_Haven* on Western butte) and capping rock show a significant
763 enrichment in Na, as do a number of float rock targets (*Lomond Hills*, *Heinrich Waenke*,
764 *Blackwaterfoot*), speculated to be related to the capping unit [e.g., Thompson et al., this issue].
765 Statistically significant variance for Na is identified between HT, capping rock and all other units
766 within GT. The Groken targets also show a significant enrichment in Na. A number of Hutton
767 samples with high Na also trend to high Cl. Slight enrichment in Na (+S±Ca) is identified in
768 some vein (*Chassenon_raster1*, sol_3071) and nodular (*Peyrat*) Gm_c targets.

769 **5.5.3. Mn, P, Zn, Ni:**

770 Strong positive correlation relationships are present between Mg, Mn, Zn within Jm_GT
771 and KHm ($r=+0.53$ to $+0.86$) (Sections 4.1, 4.2; 5.3; Table S3a-b; Figures 3a-d, 4c, 5f, 5h), with
772 all three elements enriched (i.e., >1 standard deviation from mean Mf+CSf) in coarser grained
773 targets, but not observed in Gm (Section 4.3; Table S3c; Figures 3e-g, 4c, 5f, 5h). Strong local
774 enrichments in all three are identified in the Groken, Mary Anning, Aberlady and Kilmarie drill
775 locales, and at Teal ridge and Harlaw rise (e.g., *Badcall + Buckie*). Within the buttes zone, higher
776 Mg is identified in “coherent” outcrops (relatively resistant to erosion) but both Mn and Zn
777 concentrations are typically less than mean Mf+CSf, with neither element showing signs of
778 enrichment and lowest values in the fine-grained KHm targets on the traverse to the buttes. Zn
779 does not increase with increasing elevation up into the pre_MA Glasgow member (Gm_a) or into
780 the Hutton interval, with values remaining similar to those in the buttes. However, Hutton vein
781 targets such as *Dunbartonshire* (sol_2691) and *Abernethy* (sol_2642) (Figure S5) show both
782 highly enriched Zn and Mn. Post_MA Glasgow member (Gm_b+Gm_c) shows a trend of

783 increasing Zn with proximity to Mont Mercou, identified in both low-K and high-K targets,
784 suggesting a change in alteration processes. Mn is slightly enriched in Hutton interval bedrock
785 (typically $>$ mean but $<$ 1 stdeva). The Mn enrichment in K-poor and depletion in K-rich targets
786 is not identified in the Glasgow member. Post_MA Gm_b targets closest to the benches area
787 have the highest Mn, which decreases slightly with elevation and increasing proximity to Mont
788 Mercou.

789 The majority of GT bedrock targets (other than Gm_b+c) have Ni concentrations within 1
790 standard deviation of mean Mf+CSf, with slightly higher values in K-rich targets (e.g., Glen
791 Etive drill locale) and lower values in the Aberlady/Kilmarie drill locale and the Hutton interval
792 (Figure 5g). The Groken targets are depleted, as are the capping rock targets. In contrast,
793 Gm_b+c trend to high Ni, with highest values again in K-rich targets, and a positive correlation
794 identified between Zn-Ni ($r=+0.54$ to $+0.63$; Table S3c) not identified in any other unit.

795 P is depleted at lower elevations (Figure 5e) but steadily increases with elevation, with
796 highest mean (other than GR) in the Hutton interval. As with Ca+S, P concentrations are lower in
797 K-rich targets than Mg-rich targets for Jm_GT, KHm and Gm. sandstones. Highest P
798 concentrations are associated with nodular Gm_c targets (*Beaupouyet*, sol_3015 (Figure S6d);
799 *Peyrat*). Nodules in the Groken samples are significantly enriched in both Mn and P, with a near
800 perfect correlation ($r=+0.99$) (Table S3c; Figs. 5e-f, S3e). This is not identified in the co-located
801 Mn-rich MA samples, where P is below mean Mf+CSf, but is seen in Jm_GT high-Mg targets
802 ($+0.61$), suggesting localized enrichment via Mn-P rich fluids. Below the VRR, strong P-Mn
803 correlations were identified in BPm nodular targets (e.g., *Jones Marsh*, sol_1727) [Thompson et
804 al., 2020].

805

806 **6. Conclusion**

- 807 ○ The Glen Torridon campaign marks the transition from the low energy lacustrine-
- 808 dominated environment of the Murray formation (Jura) to the more diverse Carolyn
- 809 Shoemaker formation (Knockfarril Hill and Glasgow), indicating a change in overall
- 810 depositional settings. However, APXS results and statistical analysis reveals that the bulk
- 811 primary geochemistry within Glen Torridon does not show a significant shift in overall
- 812 composition. Targets within the Carolyn Shoemaker formation are broadly in family with
- 813 those in the underlying Murray formation but do show some subtle geochemical trends
- 814 with increasing elevation.
- 815 ○ APXS data identifies compositional differences between the Jura member within Glen
- 816 Torridon (Jm_GT) and the stratigraphically equivalent Jura member on Vera Rubin ridge
- 817 (Jm_VRR). The characteristic alteration on the ridge is absent from the Jm_GT, which
- 818 shows instead a strong similarity to the overlying Knockfarril Hill member (KHm).
- 819 Interpretation of the distinctive VRR morphology and composition, absent from the
- 820 Jm_GT or overlying Knockfarril Hill member, as resulting from highly localized
- 821 alteration processes is confirmed.
- 822 ○ Within Jm_GT and KHm, APXS data defines two geochemical endmembers (high-K or
- 823 high-Mg) that correlate with a strong bimodal grain distribution (inverse relationship
- 824 between grain size and K concentrations. APXS data highlights the very strong intra-
- 825 facies similarity for the two members, indicating a common source and a continuation of
- 826 processes (e.g., K enrichment in fine grained sediments) over time.
- 827 ○ The bimodal nature of the grain distribution had a strong effect on alteration patterns,
- 828 with greater permeability in coarser grained targets facilitating movement of fluids,

829 leading to higher levels of Ca, S, P, Mn, Zn in coarser targets within Jm_GT and KHm.
830 Ca, S, P concentrations in Jm_GT and KHm also decrease with distance from the Basal
831 Siccar Point unconformity on the Greenheugh pediment, suggesting that the capping rock
832 may have acted as a conduit for fluids and/or a system cap.

833 ○ APXS identifies a transition zone from KHm to the overlying Glasgow member (Gm) in
834 the buttes zone, with similar composition in both members in the transition zone.
835 However, clustering and variance analysis shows that, outside of the buttes, the KHm and
836 Gm plot discretely. APXS results suggest a zone of common alteration at the buttes
837 and/or a gradual transition in provenance with increasing elevation in the Gm.

838 ○ APXS results point to a complex history of alteration, with multiple episodes, including
839 multiple generations of Ca-S rich fluids, multi-generation veins and localized
840 enrichments or depletions of Mn, P, Zn, Ni, Na, and in Ca (relative to S) and S (relative
841 to Ca). The anomalous Hutton interval on Tower butte provides evidence for increasing
842 alteration with proximity to the unconformity, with abundant nodules and complex vein
843 networks.

844

845

846 **Acknowledgements:** MSL APXS is managed & financed by the Canadian Space Agency
847 (CSA). We appreciate & acknowledge the support of engineers at JPL and the MSL science team
848 during operations. We thank F. Calef for the drill location map and drill hole images (Figure S1).
849 Mastcam mosaics were processed by the Mastcam team at Malin Space Science Systems
850 (NASA/JPL-Caltech/MSSS). Mars Hand Lens Imager (MAHLI) images were acquired by the
851 MAHLI team at Malin Space Science Systems (NASA/JPL-Caltech/MSSS).

852 All data used in this article are listed in the references, tables, and supplements. [Data tables S1
853 through S7 will be hosted in a data repository. We are currently seeking a host for the data.]. All
854 raw and reduced APXS data are available at the Planetary Data System, [http://pds-
855 geosciences.wustl.edu/missions/msl/apxs.htm](http://pds-geosciences.wustl.edu/missions/msl/apxs.htm).

856 Science team member funding for O’Connell-Cooper, Thompson, Spray, Boyd, Gellert, and
857 McCraig is provided by the CSA. Berger was funded by a NASA Postdoctoral Program
858 fellowship administered by USRA. VanBommel was supported by NASA/Caltech/JPL Contract
859 1549716 to Washington University in St. Louis for participation in the Mars Science
860 Laboratory Science Team.

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864 **being submitted.**

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