

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

C. D. O'Connell-Cooper<sup>1\*</sup>, L. M. Thompson<sup>1</sup>, J. G. Spray<sup>1</sup>, J. A. Berger<sup>2</sup>, R. Gellert<sup>3</sup>, M.  
McCraig<sup>3</sup>, S. J. VanBommel<sup>4</sup>, A. Yen<sup>5</sup>

<sup>1</sup>Planetary and Space Science Centre, University of New Brunswick, Fredericton, Canada

<sup>2</sup>NASA Johnson Space Center, Houston, TX, USA

<sup>3</sup>University of Guelph, Ontario, Canada

<sup>4</sup>Washington University, St Louis, MO, USA

<sup>5</sup>Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA

Corresponding author: Catherine O'Connell-Cooper [oconnell.cooper@unb.ca](mailto:oconnell.cooper@unb.ca)

**Key points:**

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

2. Multiple episodes of alteration and diagenesis identified

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

## Abstract

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

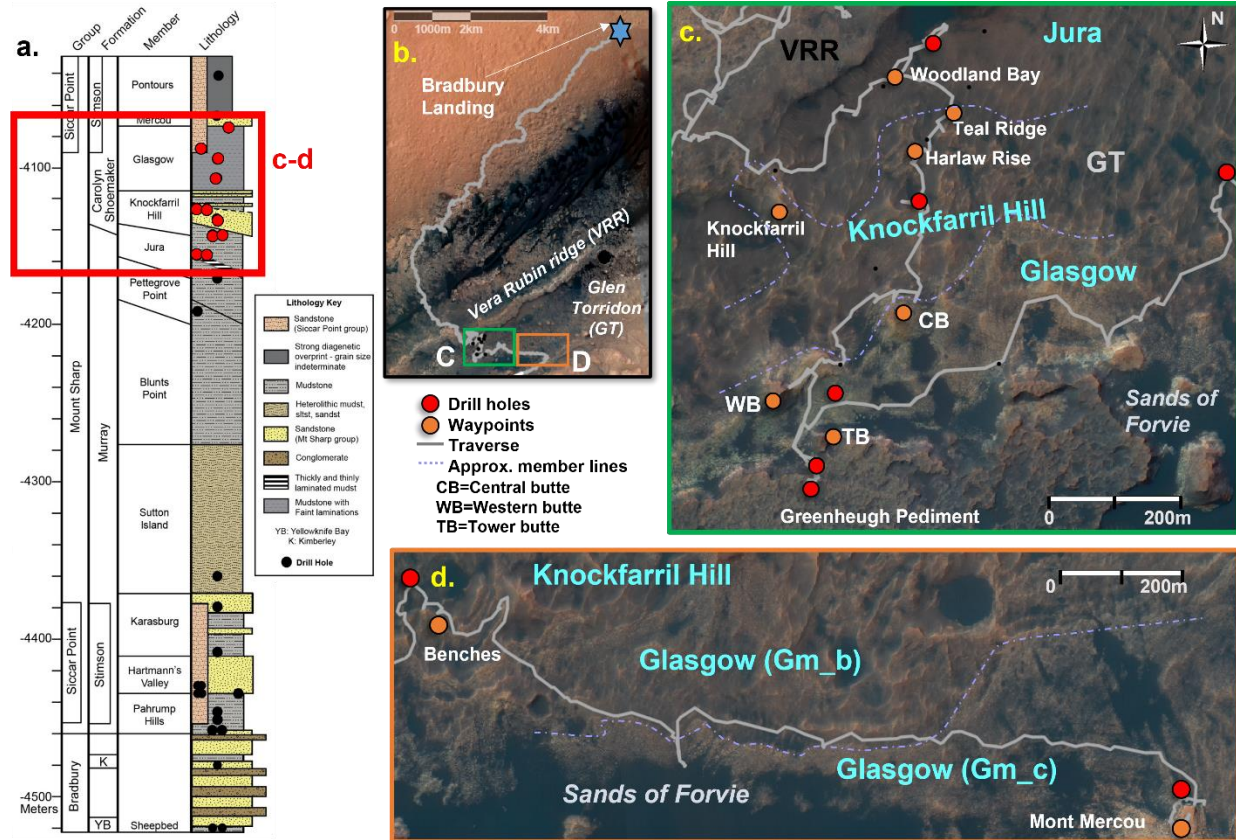
## Plain Language Summary

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

## 1. Introduction

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

Since descending from the erosion-resistant Vera Rubin ridge (VRR) [e.g., Fraeman et al., 2020] in January 2019, *Curiosity* has been exploring the phyllosilicate unit or trough [Anderson and Bell, 2010; Fraeman et al., 2016], skirting along the edge of VRR in a topographical low (informally called “Glen Torridon”) (Figure 1) below the layered sulfate units identified from orbit [e.g., Milliken et al., 2010]. Glen Torridon comprises a series of units with an Fe/Mg smectite clay-rich spectral signature (orbitally defined, pre landing) [e.g., Fraeman et al., 2016; Milliken et al., 2010], a major objective of MSL’s primary mission, as clay minerals record fluid conditions and can enhance organic matter preservation [Summons et al., 2011]. The change from clay- to sulfate-rich conditions with increasing elevation indicates a fundamental shift in 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 <sup>10</sup>	Description	Drill targets	Location Notes	Other names	
Mount Sharp Group <sup>1</sup>	Murray (Mf) <sup>1,3,4</sup>	Jura <sup>9</sup> (Jura in study area = Jm_Gt) <sup>10</sup>	High-K facies	dominant morphology; mudstones; pebbles, some larger boulders and "rubble"	-	main clay-rich trough, lower most Glen Torridon	Phyllosilicate trough <sup>15</sup> phyllosilicate layers <sup>16</sup> phyllosilicate unit <sup>2</sup> Clay-bearing unit <sup>19, 20</sup>	Smooth claybearing unit (sCBU) <sup>17,18</sup>
			High-Mg facies	fine sandstone; "coherent" beds, in situ	Aberlady (AL)			
					Kilmarie (KM)			
	Carolyn Shoemaker (CSf) <sup>5,6</sup>	Knockfarril Hill (KHm) <sup>5,6</sup>	High-K facies	finer sandstones, layers within coarser bedrock	Glen Etive 1 (GE1) Glen Etive 2 (GE2)	overlying Jm_Gt, to Central butte, and edge of Western butte		Fractured claybearing unit (fU) <sup>17,18</sup>
			High-Mg facies	dominant morphology: cross-stratified sandstone ridges and hills	Mary Anning 1 (MA1) Mary Anning 3 (MA3) Groken (GR)			
		KHm to Gm	Benches <sup>5,6</sup>	series of resistant benches, with fine-grained pebbles, boulders etc	-	transition KHm to Gm		-
		Glasgow <sup>5,6</sup>	Gm_a, including buttes zone	finely laminated mudstones, abundant diagenetic features (veins, nodules)	Glasgow (GG)	Central, Western, Tower buttes & traverse to Mary Anning (MA)		Intermediate fractured claybearing unit (fIU) <sup>17,18</sup>
			Gm_b		-	post-MA, to base of Mont Mercou		
			Gm_c		Nontron (NT)			
			Gm_HT	"Hutton interval" - Zone of intense alteration, in contact with overlying Basal Siccar Point unconformity	Hutton (HT)	Top of Tower butte, in contact with overlying Basal Siccar Point unconformity <sup>12,13</sup>		
Siccar Point Group <sup>2</sup>	Stimson (Sf) <sup>7,8</sup>	Stimson @ Greenheugh Pediment <sup>12</sup>	Capping rock <sup>11,13,14</sup> , above Basal Siccar Point unconformity	Edinburgh (EB)	Capping rock on Greenheugh Pediment			

**Table 1. Summary of units within Glen Torridon.**

<sup>1</sup>Grotzinger et al., 2015. <sup>2</sup>Fraeman et al., 2016. <sup>3</sup>Fedo et al., 2019. <sup>4</sup>Stack et al., 2019. <sup>5</sup>Bennet et al., this issue. <sup>6</sup>Fedo et al., this issue. <sup>7</sup>Banham et al., 2018. <sup>8</sup>Banham et al., 2021. <sup>9</sup>Edgar et al., 2020. <sup>10</sup>As defined herein. <sup>11</sup>Thompson et al., this issue. <sup>12</sup>Banham et al., this issue. <sup>13</sup>Bryk et al., 2019, 2020. <sup>14</sup>Malin & Edgett, 2000. <sup>15</sup>Anderson & Bell, 2010. <sup>16</sup>Milliken et al., 2010. <sup>17</sup>Stack et al., 2017. <sup>18</sup>Cofield et al., 2017. <sup>19</sup>Bennet et al., 2018. <sup>20</sup>Fox et al., 2018.

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

## 2. Context – orbital mapping and definition of units

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

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

The **Jura member (Jm; Murray formation)** within Glen Torridon (hereafter **Jm\_GT**) (Section 4.1) is stratigraphically equivalent to the lacustrine Jura member on VRR (Jm\_VRR) [Edgar et al., 2020; Fedo et al., 2020, this issue]. The Jm\_GT is dominated by pebbly regolith, larger boulders, and rare flat lying patches of finely laminated mudstones (Figures S2a-d), 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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### 3. Instrumentation, data sets and statistical methodology

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

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

#### 3.2 APXS Sample sets

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



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

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

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

(2b) Recommended drill fines and associated host bedrock targets. Targets assessed on FWHM (i.e., Full Width Half Maximum, measure of data quality), lifetime length, distance from target and target coverage (for fines).

<sup>2</sup>Target type: R=Rock; F-DT=tailings fines; F-DBA=fines.

Table 2a.																		
Target <sup>1</sup>	Soi <sup>2</sup>	Type <sup>3</sup>	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Cr <sub>2</sub> O <sub>3</sub>	MnO	FeO	MgO	CaO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>	SO <sub>3</sub>	Cl	Ni	Zn	Br
Mean Mf+CSf (n=488) <sup>4</sup>	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) <sup>5</sup>		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
Arbuthnott_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
Smooorg	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	0.75	628	639	88
Almond_raster2	2437	RT	42.80	1.15	9.14	0.69	0.40	21.80	8.97	6.56	2.57	0.54	0.80	3.83	0.61	542	432	45
Iapetus	2437	R	48.53	1.13	9.07	0.36	0.14	22.52	5.51	3.04	2.59	1.01	0.73	4.15	0.91	854	1172	462
Urr	2441	R	48.83	1.14	9.39	0.34	0.10	22.66	5.01	2.80	2.61	1.36	0.67	3.68	1.12	883	1217	38
Tolsta	2449	R	50.77	1.14	9.25	0.30	0.08	22.48	4.49	2.51	2.41	1.24	0.69	3.22	1.05	692	1063	719

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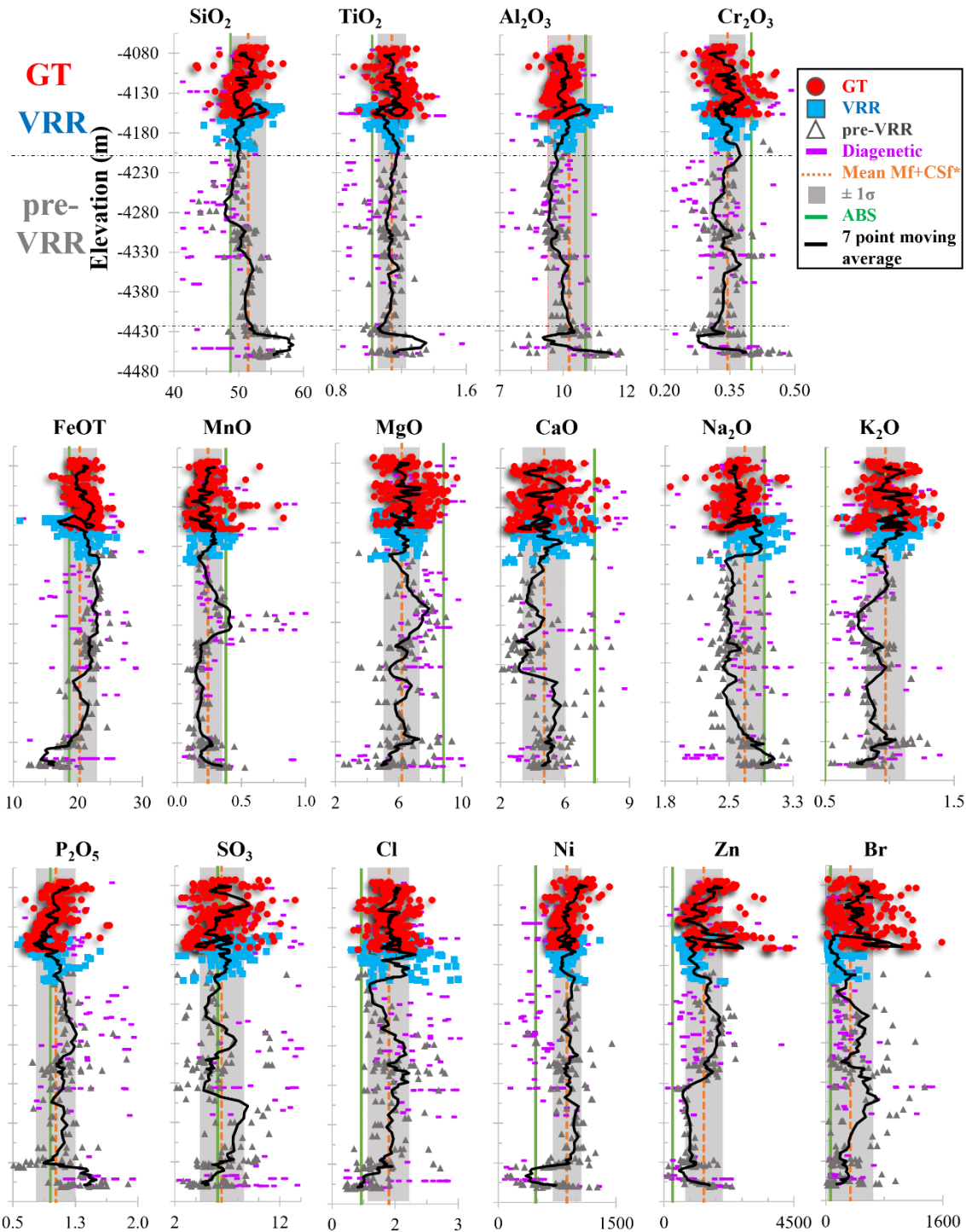
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Target	Sol	Type <sup>2</sup>	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Cr <sub>2</sub> O <sub>3</sub>	MnO	FeO	MgO	CaO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>	SO <sub>3</sub>	Cl	Ni	Zn	Br
<b>Carolyn Shoemaker formation: Knockfarril Hill member (KHM)</b>																		
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
Beauld_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
Buckley_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_Shettland_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	43.68	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		

Target	Sol	Type <sup>2</sup>	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Cr <sub>2</sub> O <sub>3</sub>	MnO	FeO	MgO	CaO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>	SO <sub>2</sub>	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	0.35	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	0.30	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	1013	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	0.32	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	1448	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	1780	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	8.95	0.32	0.14	21.17	5.07	3.81	2.41	0.95	0.88	5.67	1.17	861	1580	135
Dordogne_DRT	3031	R	46.17	1.02	8.73	0.27	0.19	18.20	5.10	5.53	2.34	0.93	1.21	8.57	1.31	1067	1915	241
Dordogne_offset	3031	R	46.89	0.97	8.83	0.29	0.19	18.02	5.17	5.26	2.33	0.93	1.03	8.39	1.29	1052	1910	210
Limeyrat_DRT	3034	R	48.26	1.01	8.92	0.30	0.23	19.38	4.83	4.32	2.43	0.97	0.92	6.43	1.38	1219	2454	532
Limeyrat_offset	3034	R	44.41	0.99	8.26	0.28	0.21	18.37	5.16	5.92	2.30	0.84	1.10	10.24	1.35	1136	2445	623
Fleurac	3035	RT	45.20	0.89	8.79	0.40	0.33	21.00	8.95	5.79	2.43	0.58	0.80	3.77	0.79	936	1103	231
Fleurac_offset	3035	RT	42.86	0.94	8.76	0.46	0.43	21.46	10.54	6.76	2.44	0.44	0.78	3.36	0.59	805	445	83
Chalus_DRT	3037	R	45.15	1.														

Target	Sol	Type <sup>2</sup>	SiO <sub>2</sub>	TiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	Cr <sub>2</sub> O <sub>3</sub>	MnO	FeO	MgO	CaO	Na <sub>2</sub> O	K <sub>2</sub> O	P <sub>2</sub> O <sub>5</sub>	SO <sub>3</sub>	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
Balliekin	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
Glasgow1_dump_corrected	2775	F-DBA	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
Nontron_offset	3054	R	46.6	0.97	8.45	0.28	0.23	17.03	4.95	5.75								



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

### 3.3. Statistical treatment of APXS data

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

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

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

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

### **4.1 Murray formation – Jura member**

#### **4.1.1. Jura member within Glen Torridon (herein Jm\_GT)**

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

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



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

#### 4.1.2. Jm\_GT Agglomerative Hierarchical Clustering Analysis (AHCA)

AHCA was performed on Jm\_GT bedrock ( $n=40$ ), using model parameters described previously (Section 3.3; Supplementary Text S2b). For all three models, at cluster size  $K=6$  ( $K_6$ ), two groups are formed, falling along previously defined facies lines: high-K facies targets dominate Group A, whilst Group B consists of high-Mg facies and intermediate-facies targets (Table S5a; Figures S8a-d). Models are very similar, with 90% ( $n=36$ ) of targets falling into the same group, and the majority falling into the same cluster. For all models, the target “Haddington” (sol\_2408; AL+KM drill locale) which is high-K but also has very high Mn and Zn, falls into Group B. For Models A+B, Group A contains only high-K targets, but gains four intermediate-Mg targets (with moderate Mn, P, Zn) for Model C. The high-K target *Hill of Skares* clusters within Group A for Models A+C, but Group B for Model B only.

#### 4.1.3. Jm\_GT Multivariate Principal Component Analysis (PCA)

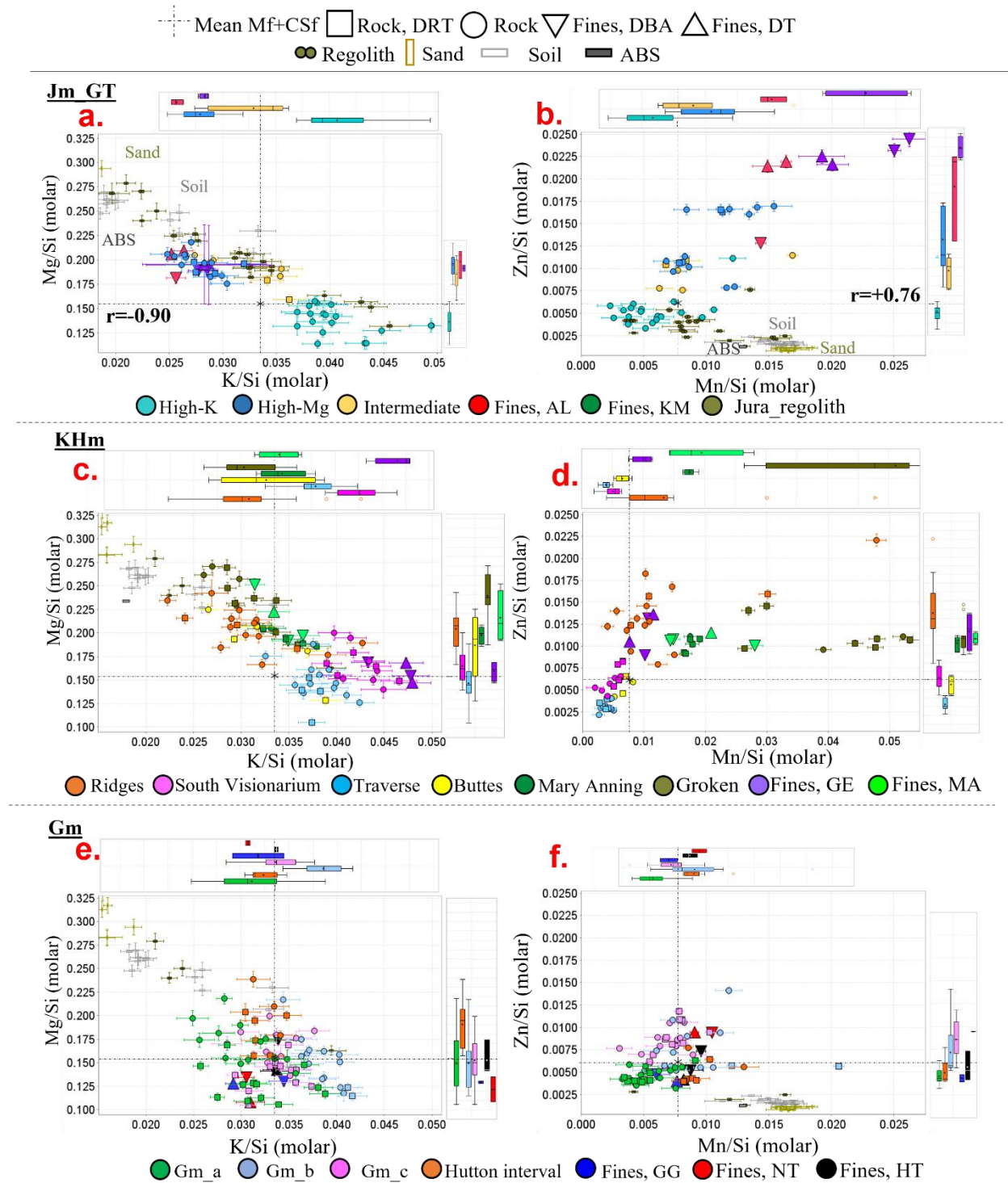
PCA analysis was applied to the AHCA Model A results to identify major trends (Figure S9a). Group A ( $C_1$ - $C_3$ , primarily high-K-facies,  $n=18$ ) is characterized by a trend to higher K, Si, Ni, Fe and Group B ( $C_4$ - $C_5$ , primarily high-Mg targets,  $n=22$ ) to higher values for all other

elements. Calculating percentage change in means, relative to mean Mf+CSf (Figure S9b), Group A trends to depleted Mn, Mg, Ca, P, S, Cl, Zn. Group A is relatively homogenous, but with enrichment Ni in C<sub>1</sub>, Al, Cr, Na in C<sub>2</sub> ( $r=+0.87$  for Al+Cr), Cl in C<sub>3</sub> and a marked Br depletion in C<sub>2</sub> but enrichment in C<sub>3</sub>. Group B shows strong differences between clusters, with some evidence for geographical clustering. C<sub>5</sub> (targets from Woodland Bay area) are enriched in Mn, Mg, Na, S, Cl, Zn, Br. C<sub>6</sub> (predominantly intermediate targets, plus *Haddington*) is depleted in Ca, S, P but very enriched in Br. C<sub>4</sub> (primarily located in the Aberlady and Kilmarie drill locale) is enriched in both Mn and Zn, with highest Zn values for Jm\_GT in this cluster.

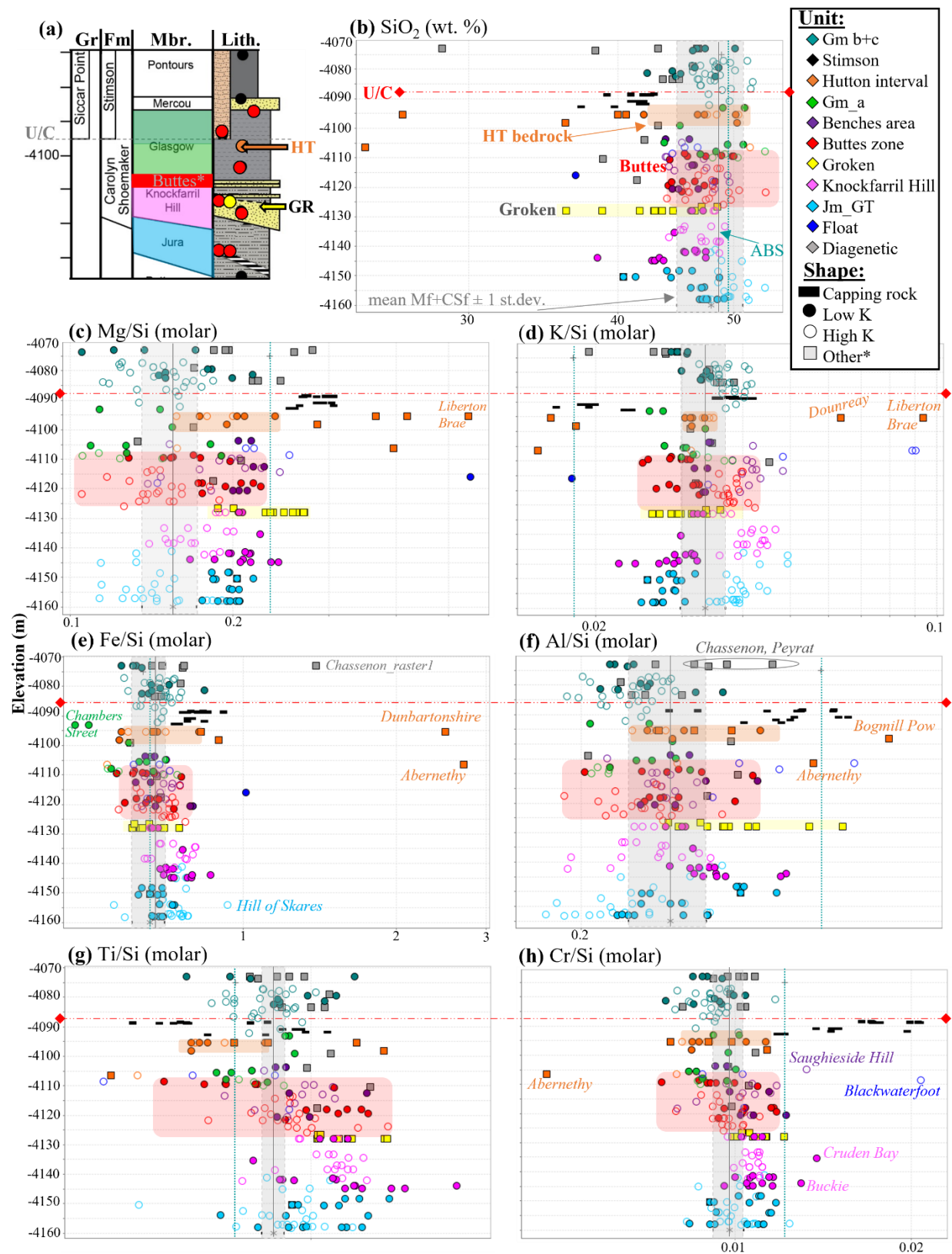
## **4.2 Carolyn Shoemaker formation – Knockfarril Hill member**

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

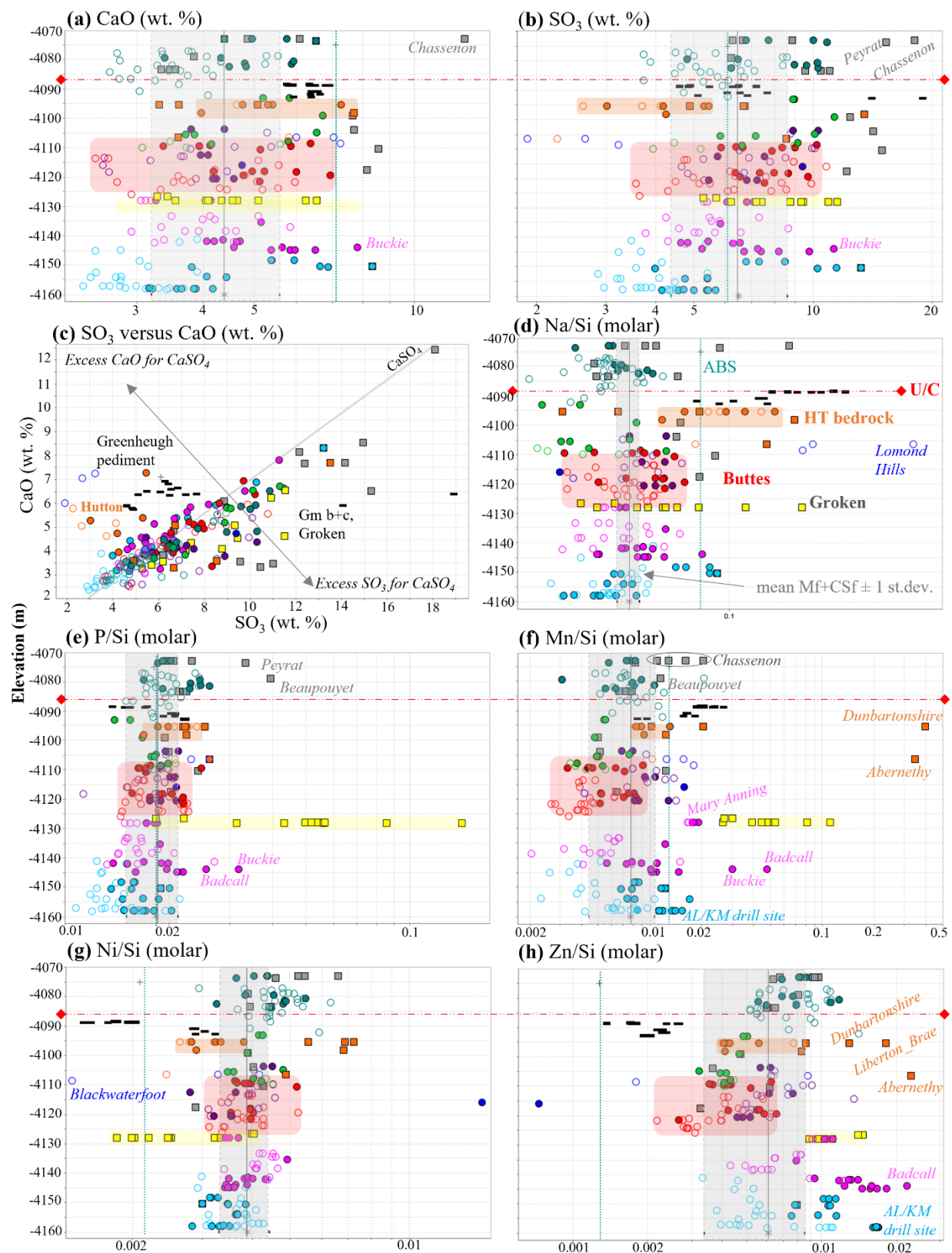
APXS analyses of KHm targets show that fine-grained targets are enriched in K (defined as:  $K/Si > \text{mean Mf+CSf} > Mg/Si$ ); whilst coarser targets are enriched in Mg (defined as:  $K/Si < \text{mean Mf+CSf} < Mg/Si$ ) (Tables S1, S6a). The paired *Glen Etive* drill holes (GE1 and GE2; sols 2486 and 2527, respectively) are co-located at the southern end of the Visionarium (an area of scarps and ridges, Bennett et al., this issue) in a layer of slightly finer-grained [Rivera-Hernandez et al., 2020a; Minitti et al., 2021] high K, moderate Mg material (Figures 1, 3c-d, S1). The paired *Mary Anning* drill holes (MA1 and MA3; sols 2838 and 2870, respectively), located in coarser grained Mg-rich sandstones, mark a brief detour from the MSAR (once the main KHm campaign had finished) to facilitate a TMAH SAM experiment [Williams et al., 2021] (Figures 1, S1). The nodular MnO-P<sub>2</sub>O<sub>5</sub> rich target *Groken* (GR; sol 2910), co-located with MA, was the focus of an opportunistic drill campaign (Figures 1, S1, S3e).



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



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



**Figure 5.** Mobile element concentrations within Glen Torridon (Legend as per Figure 4). **5a-b.** CaO and SO<sub>3</sub> weight percent versus elevation (metres); logarithmic x-axis. **5c.** SO<sub>3</sub> versus CaO (weight percent). **5d-h.** Concentrations (X/Si molar) versus elevation (metres); logarithmic x-axis.

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

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



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

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

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

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

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

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

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



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

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

APXS analyses also reveal geochemical differences between the pre- and post-MA Gm units (Gm\_a, Gm\_b) and subtle trends of change across the lateral extent of Gm (from the buttes to Mont Mercou) (Figures 3-5, 6b). Post\_MA Gm targets trend to higher Fe, K, plus mobile (Mn, P, Zn, Ni) and volatile elements (Cl, Br), than pre\_MA targets, with lower concentrations for all other elements (Tables S1-2). Statistically significant variances are identified between Gm\_a and 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,

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

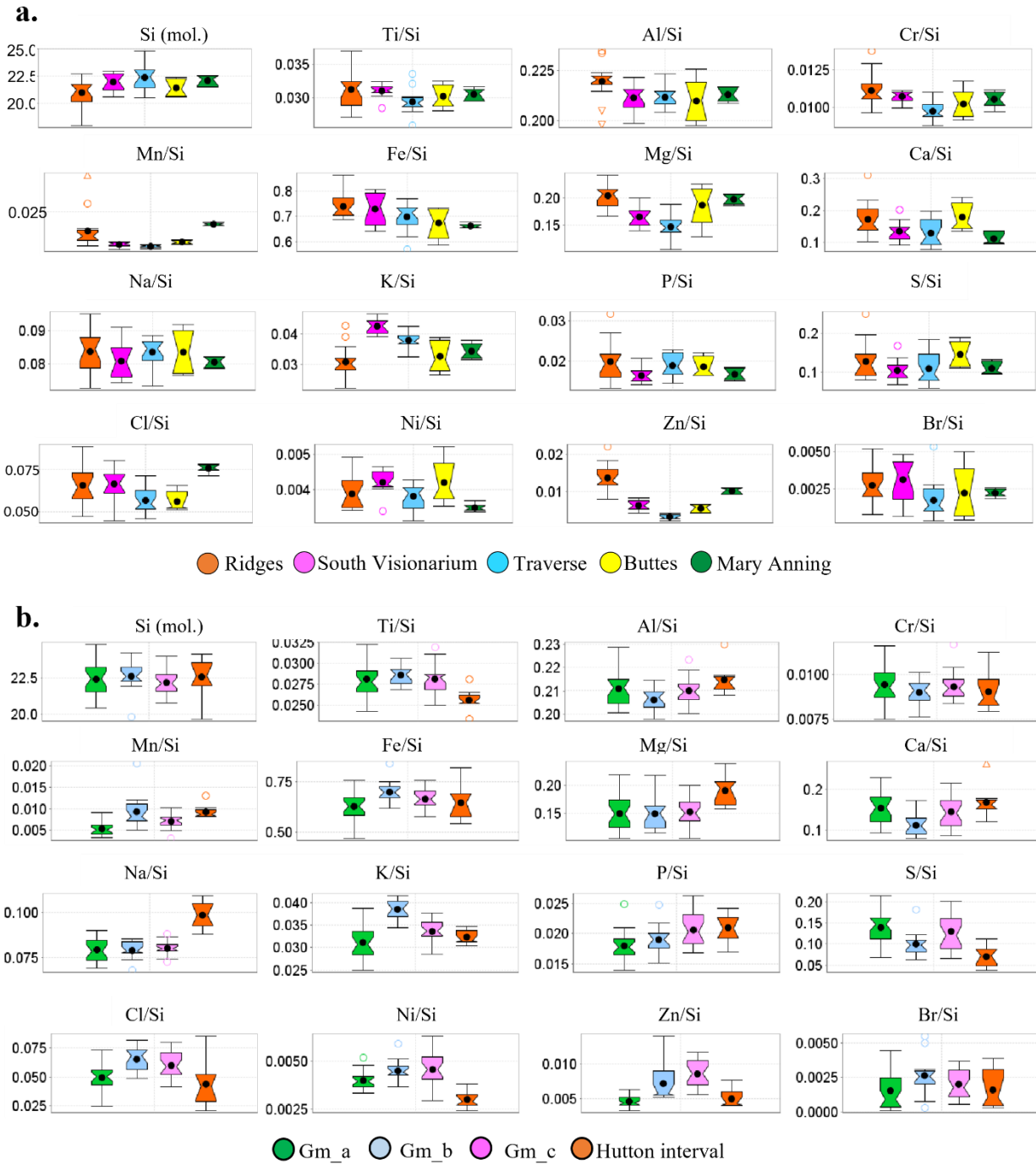
### 4.3.3. Hutton interval

The Hutton interval (*Gm-HT*) (sols-2660-2691) (Tables 2, S1) is a layer of Gm bedrock and complex vein networks that occurs at the top of Tower Butte (Figures 1c, S5) below the Siccar point unconformity and in contact with the overlying Greenheugh pediment (GP) [see also Thompson et al., this issue for further discussion]. Although this interval contains the characteristic thin laminations that mark it as part of the Gm, a unique geochemical and mineralogical signature was documented here by APXS [this paper; Thompson et al., this issue], ChemCam [Dehouck, et al., this issue; Gasda et al., this issue] and CheMin [Thorpe et al., this issue]. Relative to mean underlying Gm\_a bedrock, Hutton bedrock trends to enriched Mg, Na, Mn, and depleted S, Ni (Tables 2, S1; Figures 4c, 5b, 5d, 5f-g, 6b). Although S is depleted, Ca is not, indicating that a decoupling of Ca and S (Figure 5c). Additionally, some samples trend to low Ti, and high Al, P, Zn, (Figures 4g, 4f, 5e, 5h, 6b). A similar geochemical composition is identified at the highest point achieved by *Curiosity* on Western Butte in the bedrock target *Buchan Haven* (sol\_2640) and vein target *Abernethy* (sol\_2642) (Tables 2, S1). The correlations between K, Mn, Mg and Zn identified in other GT units are completely absent from the Hutton interval. Evidence for more alteration with increased proximity to GP is manifest in the form of more abundant nodules and veins. Complex FeO-MnO-rich (*Dunbartonshire* (sol\_2691),

*Abernethy*: FeO 40 wt.%, MnO 5-6%) and MgO-K<sub>2</sub>O-rich (*Liberton Brae* (sol\_2666): MgO 17 wt. %, K<sub>2</sub>O 2 w%) vein networks are identified at both at Hutton and Western Butte (Figure S5).

#### 4.4. Benches

The “benches” unit represents a second transition between KHm and Gm (Figure 1d), through a series of resistant topographic “benches” with rubbly bedrock in between benches [Bennet et al., this issue]. However, unlike the clear facies transition identified at Central Butte, the “Benches” transition zone is not well defined stratigraphically, resulting in some ambiguity about whether this unit is more correctly placed with KHm or Gm. Targets are in family with other Glen Torridon bedrock (Tables 2, S1), but there are some distinctions (Figures 4-5). Coherent targets (e.g., *Muckle Minn*, sol\_2935) which comprise the bulk of APXS targets here, have higher Mg/Si than mean Mf+CSf, whilst rubbly targets (e.g., *Mail Beach*, sol\_2933) have high K/Si (i.e., > mean Mf+CSf). However, moderate targets (high K *plus* high Mg) are more common in the Bench unit than previously described units, comprising >50% of bench targets. The target *Hart Fell* (sol\_2938) has both high Mg and K, but also very high Zn (2808 ppm). There are also examples of a “chaotic” texture, in the high-Mg *Garth Ness* target (sol\_2928), which is not reflected in the composition; the benches exhibit the highest mean Mg/Si, K/Si, Na/Si, S/Si and Cl/Si for any GT bedrock facies or subunit (excluding the Hutton interval, Groken and other diagenetic targets). Similar to the KHm-Gm transition zone at the buttes, mean Zn/Si trends low, however Mn/Si trends high.



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

#### 4.5. Unconsolidated sediments in Glen Torridon

Twelve unconsolidated sediment targets were analyzed during the traverse to Mont Mercou (Table 2, S1). All but two samples were active sands, using S, Cl, Zn abundances as a proxy for dust cover and, by implication, activity levels. All sand targets are in family with active sands analyzed prior to the ridge. Offcrest samples show enrichment in T-Cr, a trend previously identified in the second phase of the Bagnold Dunes campaign and onwards [O’Connell-Cooper et al., 2018]. Crest samples typically show enrichment in Mg-Ni. Grain size and depositional settings of samples are discussed in Weitz et al. [this issue]. In contrast, *Balliekin* (sol\_2706) and *Auld Reekie* (sol\_2731), both overlying Stimson formation substrate on the Greenheugh pediment, plot with soil measurements, such as *Portage* and other soil targets analyzed prior to the Bagnold Dunes campaign, which are in family with average basaltic soil (ABS) from the MSL and MER missions [O’Connell-Cooper et al., 2017].

#### 4.6. APXS Drill fines analysis – comparison to host bedrock

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

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

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

## **5. Discussion and implications**

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

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

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

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

### **5.1. Relationship to Jura member on VRR (herein Jm\_VRR)**

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

Thompson et al. [2020] subdivide the Jm\_VRR (on the basis of spectral signature, via orbital mapping) into *Jm\_VRR\_tan* (targets from areas mapped orbitally as tan coloured; the dominant lithology) and *Jm\_VRR\_blue* (targets from more discrete areas, mapped orbitally as



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

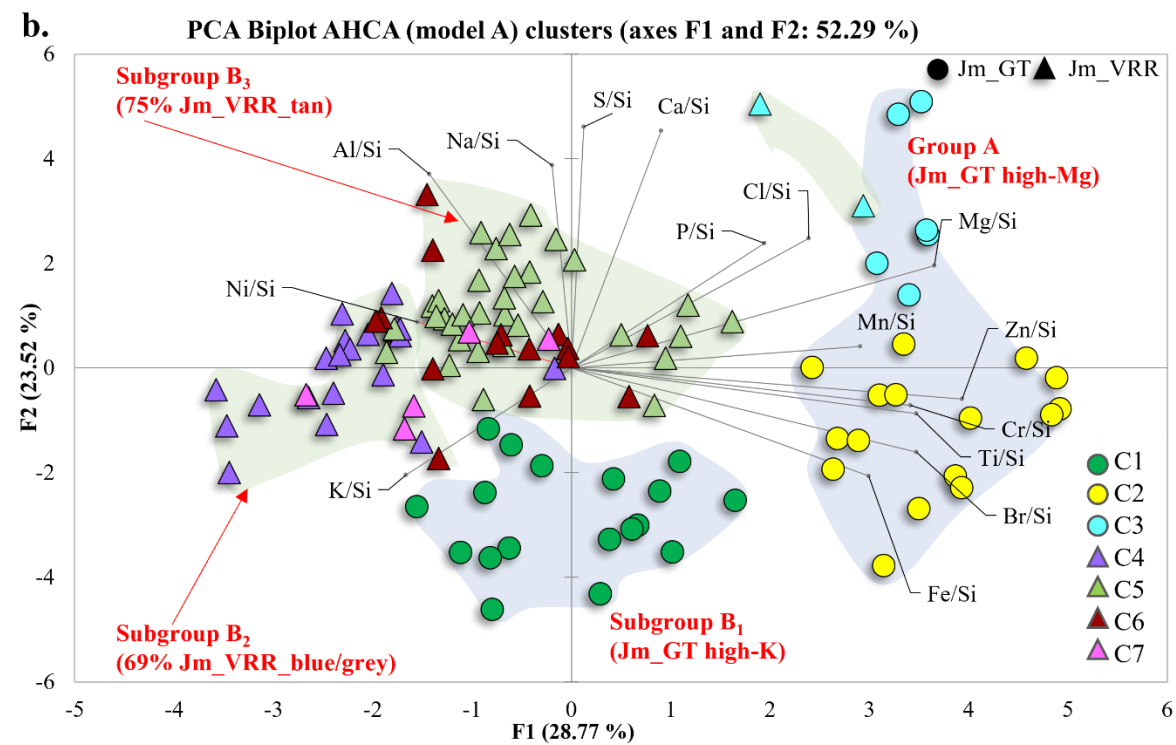
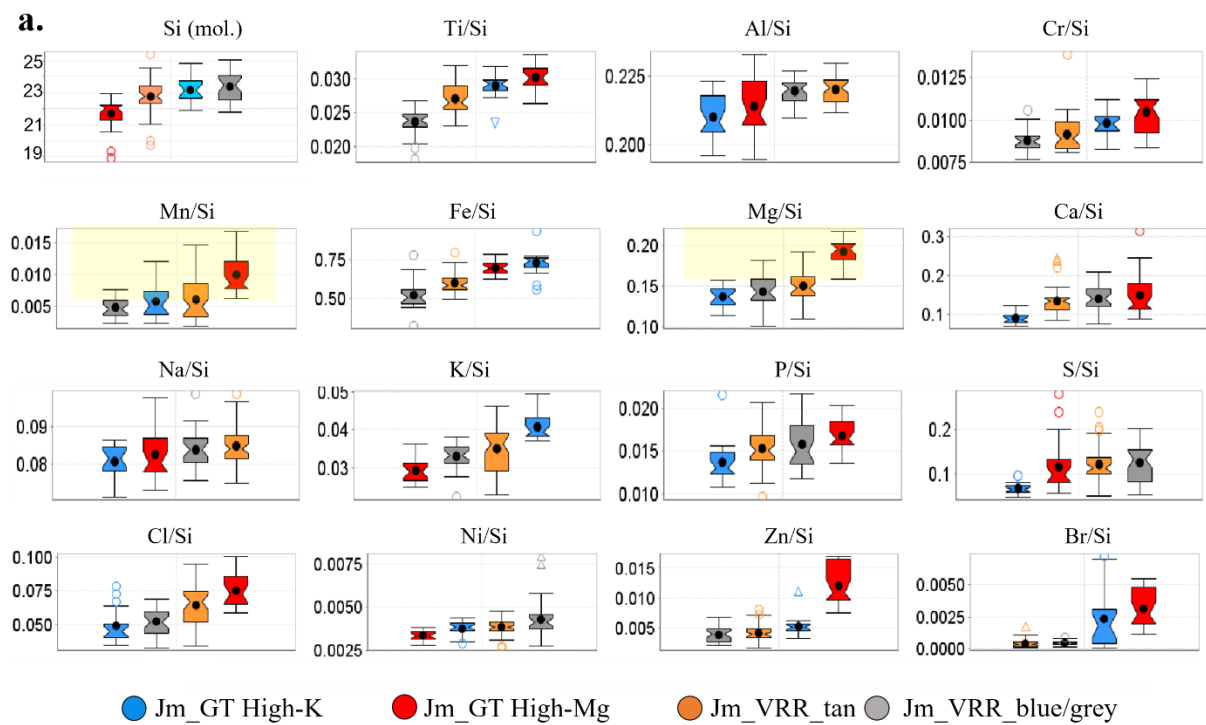
AHCA and PCA were undertaken for all Jura targets to investigate compositional differences or similarities, regardless of location (Tables S5a; Figure 7b). Ideal cluster size ( $K_4$ ) places all Jm\_VRR targets in a single unit or cluster, whilst splitting Jm\_GT into three clusters along (high K or high Mg) facies lines, thus confirming the homogeneity of Jm\_VRR when compared to Jm\_GT. Forcing  $K_7$  to facilitate more detailed analysis splits targets into two groups A and B. Group A consists of Jm\_GT intermediate to high Mg facies targets, plus two Jm\_VRR\_tan targets (from the *Rockhall* drill locale). All other targets are found in Group B, which is split into three subgroups: B<sub>1</sub> Jm\_GT high-K targets only; B<sub>2</sub> dominated by Jm\_VRR\_blue/grey, no Jm\_GT; B<sub>3</sub> dominated by Jm\_VRR\_tan, no Jm\_GT. The key observation from this AHCA and PCA analysis is the confirmation of the unusual nature of the Jm\_GT high-Mg targets (Figure 7b).

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

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

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

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

## 5.2 Relationship between Jm\_GT and the Knockfarril Hill member (KHm)

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

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

This result is in agreement with CheMin results from across Glen Torridon, which indicate 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 sites on/in contact with the overlying pediment (6-8%) [Thorpe et al., this issue]. However,

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

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

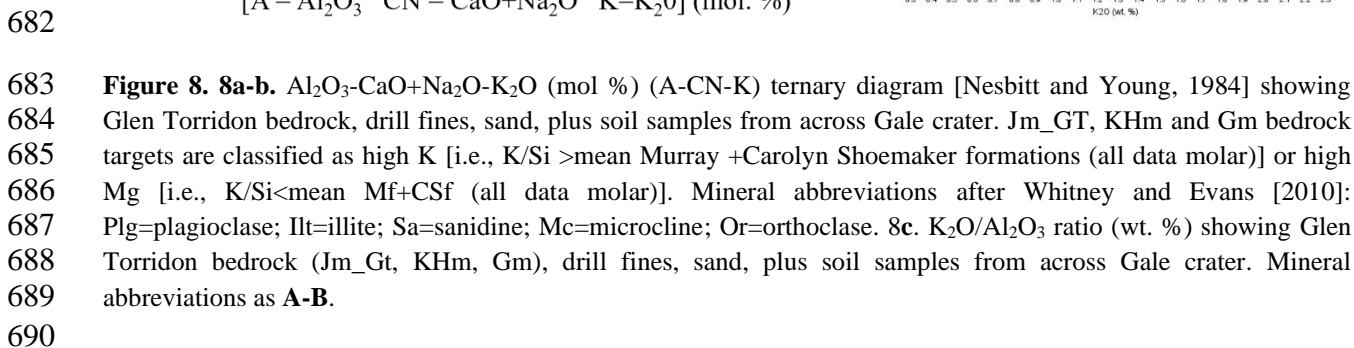
Alternatively, Fox et al. [2019a, 2021] suggest dust cover, related to morphology, as a potential source of the differences in CRISM spectra intensity, with dust plausibly masking an equivalent absorption from KHm. The relatively larger surface area of coherent bedrock slabs (such as the sandstones that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

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

### 5.3 The K-Mg relationship

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

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



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

However, the evidence for mineral segregation is limited and not definitive. Plotting all 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 Nesbitt and Young, 2010] to identify trends of enrichment in K-bearing mineral phases, enrichment in alkali feldspars is not identified. A tentative trend of increasing illitization is 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 CheMin results indicate highest phyllosilicate content in the high-K facies drill targets (GE1), drill targets from all three GT members (Jm\_GT, KHm, Gm) are enriched in phyllosilicates (23-34 wt. %) (Section 5.2) [Thorpe et al., this issue]. The alkali feldspar sanidine is detected in all samples but highest in the high-Mg target MA1. Pyroxene is also highest in MA1, but almost equivalent in GE2 (high-K target), whilst olivine is not detected in any sample.

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

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



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

## 5.5. Element mobilization and alteration

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

**5.5.1. Ca+S:** In general, CaO+SO<sub>3</sub> show a strong correlation ( $r \geq +0.90$ ), indicating addition of CaSO<sub>4</sub> rich fluids (Table S3, Figure 5c). A trend of lower mean CaO+SO<sub>3</sub> (relative to mean Mf+CSf) in high-K targets is identified in GT bedrock (Jm\_GT, KHm, Gm) (Figures 5a-c), with higher values in high-Mg targets. As high K is typically found in finer grained targets (e.g., Jm\_GT mudstones), we can infer that higher CaO+SO<sub>3</sub> are found in coarser targets (e.g., KHm sandstones from Harlaw rise). This suggests that Ca+S rich fluids were utilizing the greater permeability of the coarser sandstones, resulting in higher concentrations in these targets.

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

This suggests a concentration of CaSO<sub>4</sub>-rich fluids in the Glen Torridon area, potentially capped by the overlying Stimson formation, moving outwards, weakening with distance from this zone. This fits with the model proposed for the VRR [e.g., Thompson et al., 2020; Bristow et al., 2019; Frydenvang et al., 2020; Rampe et al., 2020; Turner et al., 2021] (Section 5.1), whereby an overlying relatively impermeable caprock acts as a control on diagenetic activity.

CaSO<sub>4</sub> veins are present both parallel to bedding and cross-cutting bedding, the latter indicating later diagenetic activity (e.g., Figures S2c-d, S3a, S6a, S6d). Whilst many vein targets are primarily CaSO<sub>4</sub>, some targets also show evidence for other fluid activity e.g., the *Chassenon* vein target (sol\_3069-3071), at the base of Mont Mercou, exhibits a CaSO<sub>4</sub>-rich rim, but a Fe-rich core, which also showed some Na+Mn enrichment, but low Zn and Ni (Figure S6f).

Although Ca concentrations are high in the Hutton interval on Tower butte just below the unconformity, S is depleted, indicating a decoupling and an increase in Ca not related to CaSO<sub>4</sub>. This is also noted at the highest elevation attained on Western butte in the bedrock target *Buchan\_Haven* (sol\_2640). Conversely, there is evidence for increasing S, relative to Ca, across the CSf - in KHm targets (most notably at the Groken locale, but also the ridges and in the benches area), and in Gm\_b+c bedrock. A number of Gm\_c nodular targets (*An\_Dun*, sol\_2967; *Peyrat*, sol\_3051) show evidence for enriched S+Mg relative to bedrock.

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

depleted, relative to mean Mf+CSf (Figure 5d). Statistically significant variance is not identified for Na between Jm\_GT, KHm or “typical” Gm bedrock units (Table S3a-c). However, both the Hutton interval (plus *Buchan\_Haven* on Western butte) and capping rock show a significant enrichment in Na, as do a number of float rock targets (*Lomond Hills*, *Heinrich Waenke*, *Blackwaterfoot*), speculated to be related to the capping unit [e.g., Thompson et al., this issue]. Statistically significant variance for Na is identified between HT, capping rock and all other units within GT. The Groken targets also show a significant enrichment in Na. A number of Hutton samples with high Na also trend to high Cl. Slight enrichment in Na (+S±Ca) is identified in some vein (*Chassenon\_raster1*, sol\_3071) and nodular (*Peyrat*) Gm\_c targets.

### 5.5.3. Mn, P, Zn, Ni:

Strong positive correlation relationships are present between Mg, Mn, Zn within Jm\_GT 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 all three elements enriched (i.e., >1 standard deviation from mean Mf+CSf) in coarser grained targets, but not observed in Gm (Section 4.3; Table S3c; Figures 3e-g, 4c, 5f, 5h). Strong local enrichments in all three are identified in the Groken, Mary Anning, Aberlady and Kilmarie drill locales, and at Teal ridge and Harlaw rise (e.g., *Badcall + Buckie*). Within the buttes zone, higher Mg is identified in “coherent” outcrops (relatively resistant to erosion) but both Mn and Zn concentrations are typically less than mean Mf+CSf, with neither element showing signs of enrichment and lowest values in the fine-grained KHm targets on the traverse to the buttes. Zn does not increase with increasing elevation up into the pre\_MA Glasgow member (Gm\_a) or into the Hutton interval, with values remaining similar to those in the buttes. However, Hutton vein targets such as *Dunbartonshire* (sol\_2691) and *Abernethy* (sol\_2642) (Figure S5) show both highly enriched Zn and Mn. Post\_MA Glasgow member (Gm\_b+Gm\_c) shows a trend of

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

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

P is depleted at lower elevations (Figure 5e) but steadily increases with elevation, with highest mean (other than GR) in the Hutton interval. As with Ca+S, P concentrations are lower in K-rich targets than Mg-rich targets for Jm\_GT, KHm and Gm. sandstones. Highest P concentrations are associated with nodular Gm\_c targets (*Beaupouyet*, sol\_3015 (Figure S6d); *Peyrat*). Nodules in the Groken samples are significantly enriched in both Mn and P, with a near perfect correlation ( $r=+0.99$ ) (Table S3c; Figs. 5e-f, S3e). This is not identified in the co-located Mn-rich MA samples, where P is below mean Mf+CSf, but is seen in Jm\_GT high-Mg targets ( $+0.61$ ), suggesting localized enrichment via Mn-P rich fluids. Below the VRR, strong P-Mn correlations were identified in BPm nodular targets (e.g., *Jones Marsh*, sol\_1727) [Thompson et al., 2020].

## 6. Conclusion

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

leading to higher levels of Ca, S, P, Mn, Zn in coarser targets within Jm\_GT and KHm.

Ca, S, P concentrations in Jm\_GT and KHm also decrease with distance from the Basal

Siccar Point unconformity on the Greenheugh pediment, suggesting that the capping rock

may have acted as a conduit for fluids and/or a system cap.

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

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

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

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