

Appendix B

Clumped isotope and bulk trace metal data
for modern, Ordovician and Cambrian fossil
materials

Sample ID	Age	Fossil	Minerology	Call#	Replicate #	d13C	d13C SD	d18Omin
NBIB_4_12_250	0.0	IB	Calcite	MOD	1	1.96	0.00	2.01
NBIB_4_12_90	0.0	IB	Calcite	MOD	1	1.82	0.00	1.21
PIB_24_12_12_POW	0.0	IB	Calcite	MOD	1	-4.37	0.00	-1.52
PIB_24_12_POW	0.0	IB	Calcite	MOD	1	-3.86	0.00	-1.76
PIB_4_12_250	0.0	IB	Calcite	MOD	1	-4.47	0.00	-0.45
PIB_4_12_90	0.0	IB	Calcite	MOD	2	-4.58	0.30	-0.44
PIB_NaOH_H2O2	0.0	IB	Calcite	MOD	1	-3.89	0.01	-0.93
PIB_none	0.0	IB	Calcite	MOD	3	-3.51	0.10	-0.86
SPB	0.0	B	Calcite	MOD	5	1.86	0.03	-0.32
TBIB_NaOH_H2O2	0.0	IB	Calcite	MOD	1	-1.79	0.01	0.36
TIIB_24_12_POW	0.0	IB	Calcite	MOD	1	1.18	0.00	0.29
TIIB_24BHP_12_POW	0.0	IB	Calcite	MOD	1	1.69	1.28	0.03
WAIB_NaOH_H2O2	0.0	IB	Calcite	MOD	1	-0.01	0.00	1.29
A 551 alt	437.0	B	Calcite	PREV	1	0.74		-3.46
A-958	437.0	B	Calcite	PREV	1	1.71		-5.10
A-958-2	437.0	B	Calcite	PREV	1	2.43		-3.46
A-958-3	437.0	B	Calcite	PREV	1	1.82		-5.63
A-958-4	437.0	B	Calcite	PREV	2	-0.28		-4.67
A1356a-07	437.0	B	Calcite	PREV	1	1.71		-5.12
A1356a-07	437.0	B	Calcite	PREV	1	1.94		-5.34
A1356a-37	437.0	B	Calcite	PREV	1	1.78		-5.11
A1380b-30	437.0	B	Calcite	PREV	1	2.08		-5.00
A1391b-06	437.0	B	Calcite	PREV	1	1.49		-4.67
A1391b-06	437.0	B	Calcite	PREV	1	2.03		-4.94
A1391b-31	437.0	B	Calcite	PREV	2	0.43		-4.87
A1391b-31	437.0	B	Calcite	PREV	2	-0.14		-4.22
922_F_RC	438.0	RC	Calcite	ORD	1	1.52	0.01	-3.25
916_B_S1	440.0	B	Calcite	ORD	1	0.87	0.02	-4.75
916_Bc_RC	440.0	RC	Calcite	ORD	1	1.49	0.01	-4.47
916_MF_1_B	440.0	B	Calcite	ORD	1	1.32	0.02	-4.05
916_MF_B_4	440.0	B	Calcite	ORD	1	1.32	0.02	-4.13
916_MF_RC2	440.0	RC	Calcite	ORD	1	1.04	0.02	-4.31
916_MF3_RC	440.0	RC	Calcite	ORD	2	1.88	0.01	-4.03
916MF_2_B	440.0	B	Calcite	ORD	1	1.14	0.01	-4.45
911_2.1_RC	443.5	RC	Calcite	ORD	1	2.20	0.02	-2.72
912.98_1_B	443.5	B	Calcite	ORD	3	2.12	0.02	-3.46
912.98_2_B	443.5	B	Calcite	ORD	1	2.43	0.02	-3.25
912.98_2_RC	443.5	RC	Calcite	ORD	2	2.07	0.01	-3.51
Lbec_F_B	443.5	B	Calcite	ORD	1	1.80	0.01	-3.58
901_12_RC_1	444.5	RC	Calcite	ORD	2	4.47	0.12	0.04
901_12_RC_2	444.5	RC	Calcite	ORD	2	4.08	0.03	-0.60
901_19_RC	444.5	RC	Calcite	ORD	2	0.89	0.08	-3.32

Table B.1: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	Age	Fossil	Minerology	Call#	Replicate #	d13C	d13C SD	d18Omin
901_19_RC_2	444.5	RC	Calcite	ORD	2	1.07	0.01	-3.09
901_10_RC_1	445.0	RC	Calcite	ORD	2	4.18	0.01	-0.78
901_10_RC_2	445.0	RC	Calcite	ORD	2	4.86	0.00	-1.23
901_8.5_B	445.5	B	Calcite	ORD	1	2.26	0.01	-2.38
901_8.5_Mud	445.5	M	Calcite	ORD	1	2.36	0.02	-3.22
908_1_T	445.7	T	Calcite	ORD	3	0.05	0.02	-3.13
908_LF_1_RC	445.7	RC	Calcite	ORD	1	-0.72	0.01	-3.67
908_LF_2_M	445.7	M	Calcite	ORD	1	-0.75	0.02	-4.89
912.8_1_B	445.7	B	Calcite	ORD	4	0.85	0.02	-2.97
912.8_2_T	445.7	T	Calcite	ORD	3	0.14	0.02	-3.30
912.8_B_2	445.7	B	Calcite	ORD	1	0.74	0.02	-3.25
904.25_1_B	446.0	B	Calcite	ORD	1	1.06	0.02	-4.18
904.4_1_B	446.0	B	Calcite	ORD	1	1.78	0.02	-3.42
ElkR1	446.5	RC	Calcite	PREV	1	1.04		-4.18
ElkR2	446.7	RC	Calcite	PREV	3	2.16		-2.92
WWR1	446.8	RC	Calcite	PREV	3	-0.6		-4.63
WWR2	446.8	RC	Calcite	PREV	1	-0.18		-4.84
906_1_T	447.0	T	Calcite	ORD	3	-0.24	0.02	-4.04
906_2_T	447.0	T	Calcite	ORD	1	-0.29	0.01	-4.01
906_23_30_1_B	447.0	B	Calcite	ORD	1	-0.19	0.01	-4.05
906_23_30_T_1	447.0	T	Calcite	ORD	1	-0.36	0.01	-3.90
907.23F_1_B	447.0	B	Calcite	ORD	1	-0.29	0.01	-3.85
918_52_2_B	447.0	B	Calcite	ORD	1	0.31	0.02	-3.11
918_43.2_1_B	447.0	B	Calcite	ORD	2	0.51	0.01	-3.25
918_43.2_B2	447.0	B	Calcite	ORD	2	0.30	0.02	-3.50
918_52_1_B	447.0	B	Calcite	ORD	1	0.40	0.01	-3.14
SGH-W 43 T1	447.0	T	Calcite	PREV	1	-1.37		-4.44
SGH-W-42.2 R1	447.0	RC	Calcite	PREV	1	0.09		-4.05
SGH-W-43.0-B1	447.0	B	Calcite	PREV	1	0.41		-4.88
Wayne Bb	447.0	B	Calcite	PREV	1	-1.02		-4.47
MOS_B	447.5	B	Calcite	ORD	2	0.12	0.00	-5.01
MOS_B	447.5	B	Calcite	PREV	2	0.12		-5.01
MOS_T	447.5	T	Calcite	ORD	2	-0.77	0.01	-4.79
MOS_T	447.5	T	Calcite	PREV	2	-0.77		-4.79
KY127B1	448.0	B	Calcite	PREV	1	0.21		-4.88
HC-K T1	449.0	T	Calcite	PREV	1	-0.08		-4.27
HC-K-18-B1	449.0	B	Calcite	PREV	1	0.86		-4.88
MM1-Bb	449.0	B	Calcite	PREV	1	1.73		-5.07
Mol Isotelus b	449.0	T	Calcite	PREV	1	0.18		-5.12
DPL_B	452.0	B	Calcite	ORD	2	0.51	0.01	-5.42
DB_RC	453.0	RC	Calcite	ORD	1	-0.12	0.00	-4.60
DB_SE_B_1	453.0	B	Calcite	ORD	2	1.08	0.01	-4.30

Table B.2: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	Age	Fossil	Minerology	Call#	Replicate #	d13C	d13C SD	d18Omin
DB_SE_C1	453.0	M	Calcite	ORD	2	-0.46	0.05	-5.02
DB_SE_M	453.0	M	Calcite	ORD	3	-0.99	0.02	-4.98
DB_SE_R_1	453.0	RC	Calcite	ORD	2	-0.40	0.05	-5.38
DB_SE_R2	453.0	RC	Calcite	ORD	1	-0.08	0.00	-4.70
DB_SE_S1	453.0	B	Calcite	ORD	4	0.58	0.01	-5.39
DB_SE_S2	453.0	B	Calcite	ORD	3	0.66	0.01	-5.80
DB_SE_S3	453.0	B	Calcite	ORD	2	0.84	0.02	-4.68
DB_SE_S4	453.0	B	Calcite	ORD	1	0.59	0.00	-5.30
DB_SE_S5	453.0	B	Calcite	ORD	3	0.36	0.00	-5.80
DB_SE_S6	453.0	B	Calcite	ORD	3	0.15	0.04	-5.46
DB_SE_T1	453.0	T	Calcite	ORD	2	-0.86	0.03	-5.45
DIB_24BHP_12_POW	453.0	IB	Calcite	ORD	2	-1.49	0.01	-5.30
DIB_NaOH_H2O2	453.0	IB	Calcite	ORD	3	-1.62	0.11	-5.47
DIB_SE_2_NaOH_H2O2	453.0	IB	Calcite	ORD	2	-1.53	0.08	-5.16
Dec_B_1	455.0	B	Calcite	ORD	2	0.43	0.01	-4.76
Dec_B_spar	455.0	B	Calcite	ORD	1	-0.27	0.02	-4.48
Dec_T_2	455.0	T	Calcite	ORD	2	-0.53	0.01	-5.03
DB_D_4.05_B	455.5	B	Calcite	ORD	1	1.34	0.00	-4.39
DB_D_4.65_B	455.5	B	Calcite	ORD	1	1.38	0.00	-5.06
DRO_D_4.0-4.5_B	455.5	B	Calcite	ORD	1	0.05	0.00	-6.04
DCQ_-0.15	456.0	B	Calcite	ORD	2	-0.52	0.03	-4.80
DRSQ_8_B	456.0	B	Calcite	ORD	1	-0.86	0.00	-5.19
DRSQ_2.1_B	456.0	B	Calcite	ORD	1	-0.36	0.00	-4.60
Asery_M	465.0	M	Calcite	ORD	4	0.54	0.04	-5.91
Asery_T1	465.0	T	Calcite	ORD	3	0.69	0.01	-5.60
Kunda_M	467.0	M	Calcite	ORD	3	0.51	0.01	-4.92
Kunda_T	467.0	T	Calcite	ORD	3	0.04	0.01	-5.97
VkB11	468.0	B	Calcite	ORD	1	-0.30	0.00	-5.26
VkB12	468.0	B	Calcite	ORD	2	0.04	0.01	-5.23
VkB13	468.0	B	Calcite	ORD	3	-0.07	0.00	-5.34
VkB14	468.0	B	Calcite	ORD	2	-0.56	0.00	-5.32
VkB15	468.0	B	Calcite	ORD	1	-0.59	0.00	-5.91
VkB16	468.0	B	Calcite	ORD	3	-0.01	0.00	-5.34
VkB17	468.0	B	Calcite	ORD	1	-0.37	0.00	-5.34
VkB18	468.0	B	Calcite	ORD	3	0.34	0.01	-5.19
VkB2	468.0	B	Calcite	ORD	1	0.50	0.00	-5.12
VkB3	468.0	B	Calcite	ORD	1	-0.04	0.00	-5.63
VkB4	468.0	B	Calcite	ORD	4	-0.08	0.00	-5.33
VkB7	468.0	B	Calcite	ORD	1	0.30	0.00	-5.22
VkB8	468.0	B	Calcite	ORD	2	-0.60	0.01	-5.24
VkB5	472.0	B	Calcite	ORD	1	-0.24	0.00	-5.87
CIB_NaOH_H2O2	492.0	IB	Calcite	CAM	3	-4.55	0.05	-7.28

Table B.3: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	Age	Fossil	Minerology	Call#	Replicate #	d13C	d13C SD	d18Omin
EC_M	492.0	M	Calcite	CAM	1	-1.40	0.00	-5.12
ECIB1	492.0	IB	Calcite	CAM	1	-4.51	0.02	-7.06
ECIB2	492.0	IB	Calcite	CAM	1	-5.02	0.00	-7.05
ECIB5	492.0	IB	Calcite	CAM	2	-5.55	0.00	-7.07

Table B.4: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	d18O SD	T IL	T SEM	T ARF	T SEM	W ARF	W SD
NBIB_4_12_250	0.01	57.54	5.64	51.61	3.69	9.35	0.64
NBIB_4_12_90	0.01	58.26	7.49	52.30	5.20	8.66	0.91
PIB_24_12_12_POW	0.01	26.50	3.38	19.40	4.32	-0.34	0.92
PIB_24_12_POW	0.01	33.80	3.83	26.94	3.94	0.97	0.80
PIB_4_12_250	0.01	39.82	3.58	34.29	3.23	3.73	0.63
PIB_4_12_90	0.26	35.48	0.33	29.92	1.02	2.89	0.20
PIB_NaOH_H2O2	0.02	41.15	3.05	34.40	2.63	3.26	0.51
PIB_none	0.15	58.74	3.18	52.75	1.71	6.65	0.29
SPB	0.02	17.37	1.34	11.26	1.47	-0.90	0.33
TBIB_NaOH_H2O2	0.01	16.80	1.35	9.16	1.45	-0.69	0.33
TIIB_24_12_POW	0.01	30.12	0.55	23.15	1.59	2.25	0.33
TIIB_24BHP_12_POW	2.22	48.93	20.13	42.19	16.31	5.68	3.13
WAIB_NaOH_H2O2	0.01	22.26	0.22	14.92	1.76	1.51	0.39
A 551 alt		48.20	4.30			3.26	0.78
A-958		43.90	0.00			0.83	0.00
A-958-2		45.10	2.90			2.70	0.52
A-958-3		35.80	0.00			-1.19	0.00
A-958-4		36.60	3.20			-0.07	0.62
A1356a-07		34.20	0.00			-0.98	0.00
A1356a-07		33.70	0.00			-1.30	0.00
A1356a-37		35.70	0.00			-0.69	0.00
A1380b-30		34.80	0.00			-0.75	0.00
A1391b-06		44.60	2.50			1.39	0.46
A1391b-06		35.30	0.00			-0.59	0.00
A1391b-31		35.70	4.30			-0.45	0.83
A1391b-31		37.30	3.10			0.51	0.59
922_F_RC	0.02	53.56	4.38	50.50	2.84	3.86	0.49
916_B_S1	0.03	40.88	3.57	44.97	3.42	1.38	0.62
916_Bc_RC	0.02	44.55	3.47	48.88	2.97	2.35	0.52
916_MF_1_B	0.04	52.03	5.41	48.99	3.86	2.79	0.68
916_MF_B_4	0.03	38.17	3.28	42.08	3.42	1.48	0.63
916_MF_RC2	0.04	36.32	3.88	40.09	4.21	0.93	0.78
916_MF3_RC	0.13	39.56	3.16	41.68	1.31	1.50	0.24
916MF_2_B	0.03	49.99	3.57	50.49	2.47	2.65	0.43
911_2.1_RC	0.03	34.99	1.71	38.66	2.23	2.26	0.42
912.98_1_B	0.03	41.21	3.24	42.90	1.97	2.30	0.36
912.98_2_B	0.03	45.46	4.00	49.83	3.40	3.74	0.60
912.98_2_RC	0.00	43.30	6.23	45.62	3.63	2.74	0.65
Lbec_F_B	0.01	43.86	4.44	40.75	3.65	1.79	0.68
901_12_RC_1	0.36	28.88	0.08	32.01	1.35	3.78	0.26
901_12_RC_2	0.02	24.18	0.73	26.86	2.57	2.12	0.52
901_19_RC	0.24	28.73	6.91	30.17	6.03	0.05	1.20

Table B.5: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	d18O SD	T IL	T SEM	T ARF	T SEM	W ARF	W SD
901_19_RC_2	0.03	34.52	0.86	38.15	1.45	1.80	0.27
901_10_RC_1	0.03	29.29	0.69	32.46	1.89	3.04	0.37
901_10_RC_2	0.02	27.88	3.12	30.92	4.42	2.29	0.88
901_8.5_B	0.02	39.41	3.55	43.41	3.55	3.48	0.65
901_8.5_Mud	0.04	52.36	6.46	57.08	5.22	5.00	0.88
908_1_T	0.05	33.58	3.09	35.95	2.57	1.35	0.49
908_LF_1_RC	0.02	41.91	4.26	42.24	3.82	1.97	0.70
908_LF_2_M	0.04	59.68	4.93	56.52	2.95	3.22	0.49
912.8_1_B	0.03	43.47	5.40	45.01	3.12	3.18	0.56
912.8_2_T	0.05	44.06	1.60	44.52	2.79	2.76	0.50
912.8_B_2	0.04	49.01	6.12	53.58	5.15	4.38	0.89
904.25_1_B	0.03	62.68	4.11	59.44	2.07	4.43	0.34
904.4_1_B	0.05	41.05	4.30	45.15	4.12	2.75	0.74
ElkR1		62.1	2.9			4.85	0.48
ElkR2		35.7	2			1.52	0.39
WWR1		39.5	2.5			0.5	0.46
WWR2		40.9	3.6			0.54	0.68
906_1_T	0.06	42.22	2.41	43.81	3.18	1.88	0.58
906_2_T	0.03	41.21	3.51	45.33	3.34	2.18	0.60
906_23_30_1_B	0.01	52.91	5.09	49.86	3.51	2.94	0.61
906_23_30_T_1	0.03	38.57	4.60	42.50	4.67	1.78	0.86
907.23F_1_B	0.02	55.14	6.60	52.06	4.70	3.52	0.81
918_52_2_B	0.05	38.68	2.60	42.63	2.70	2.61	0.49
918_43.2_1_B	0.03	42.52	5.52	43.08	1.40	2.55	0.25
918_43.2_B2	0.04	33.96	0.40	37.54	1.07	1.28	0.20
918_52_1_B	0.01	50.64	4.37	47.60	3.04	3.46	0.54
SGH-W 43 T1		43.6	4			1.44	0.75
SGH-W-42.2 R1		35.6	4.4			0.36	0.85
SGH-W-43.0-B1		39.7	2.7			0.3	0.51
Wayne Bb		34.2	3.3			-0.34	0.65
MOS_B	0.01	36.11	0.92	30.45	1.50	-1.60	0.30
MOS_B		31.1	0.94			-1.47	0.18
MOS_T	0.02	34.61	4.32	28.91	4.51	-1.68	0.90
MOS_T		29.44	5.67			-1.57	1.13
KY127B1		56.7	0			3.27	0
HC-K T1		39.4	6.1			0.86	1.18
HC-K-18-B1		53	0			2.64	0
MM1-Bb		42.9	0			0.68	0
Mol Isotelus b		62.4	0			3.96	0
DPL_B	0.04	40.96	2.57	35.37	2.32	-1.06	0.44
DB_RC	0.00	41.64	5.89	36.17	5.04	-0.08	0.97
DB_SE_B_1	0.05	41.71	8.97	36.17	8.00	0.21	1.55

Table B.6: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	d18O SD	T IL	T SEM	T ARF	T SEM	W ARF	W SD
DB_SE_C1	0.11	48.97	8.28	43.89	6.87	0.91	1.26
DB_SE_M	0.04	41.82	3.43	36.46	3.23	-0.41	0.61
DB_SE_R_1	0.05	47.62	1.22	42.02	0.90	0.21	0.16
DB_SE_R2	0.01	45.36	3.55	40.29	2.77	0.58	0.51
DB_SE_S1	0.07	41.09	2.13	34.77	1.69	-1.14	0.32
DB_SE_S2	0.04	48.49	3.21	42.28	2.82	-0.16	0.52
DB_SE_S3	0.02	40.30	1.57	33.55	1.61	-0.67	0.31
DB_SE_S4	0.01	44.29	4.28	37.56	3.40	-0.53	0.64
DB_SE_S5	0.08	49.65	3.86	43.43	3.38	0.04	0.61
DB_SE_S6	0.18	46.07	3.31	39.88	2.81	-0.26	0.52
DB_SE_T1	0.23	45.86	6.28	40.80	5.31	-0.08	0.99
DIB_24BHP_12_POW	0.04	47.77	1.87	41.04	1.30	0.12	0.24
DIB_NaOH_H2O2	0.08	45.92	3.76	40.29	3.15	-0.20	0.58
DIB_SE_2_NaOH_H2O2	0.30	45.16	1.84	38.43	1.45	-0.23	0.27
Dec_B_1	0.03	40.88	3.21	43.07	1.23	1.02	0.22
Dec_B_spar	0.03	35.20	2.20	38.88	2.69	0.54	0.50
Dec_T_2	0.00	42.53	4.85	44.81	2.46	1.07	0.44
DB_D_4.05_B	0.00	31.76	1.43	25.91	2.17	-1.87	0.44
DB_D_4.65_B	0.01	41.92	5.63	42.95	5.19	0.70	0.95
DRO_D_4.0-4.5_B	0.00	48.43	4.32	42.74	3.16	-0.33	0.58
DCQ_-0.15	0.03	41.71	2.24	36.14	2.15	-0.29	0.41
DRSQ_8_B	0.00	36.12	1.53	37.18	2.01	-0.49	0.38
DRSQ_2.1_B	0.01	48.44	5.03	42.75	3.75	1.13	0.69
Asery_M	0.06	39.37	3.29	34.52	2.59	-1.71	0.50
Asery_T1	0.02	39.41	2.08	35.64	1.42	-1.19	0.27
Kunda_M	0.08	35.73	1.95	30.99	1.85	-1.40	0.36
Kunda_T	0.02	40.25	1.51	36.47	2.36	-1.41	0.45
VkB11	0.00	35.10	2.53	31.97	2.86	-1.56	0.56
VkB12	0.01	36.24	2.36	33.16	2.70	-1.29	0.52
VkB13	0.01	40.29	0.93	36.62	0.77	-0.75	0.15
VkB14	0.03	36.49	1.02	33.42	1.51	-1.33	0.29
VkB15	0.00	40.24	4.39	37.28	4.01	-1.19	0.76
VkB16	0.02	42.77	2.95	39.88	2.63	-0.14	0.49
VkB17	0.01	34.38	2.35	31.22	2.78	-1.77	0.54
VkB18	0.08	37.90	1.33	34.88	1.64	-0.92	0.31
VkB2	0.01	39.15	3.74	36.17	3.53	-0.61	0.67
VkB3	0.01	42.71	5.44	37.34	4.57	-0.90	0.87
VkB4	0.03	34.42	2.05	30.69	2.67	-1.87	0.53
VkB7	0.01	45.32	5.92	39.95	4.76	-0.01	0.89
VkB8	0.03	40.10	0.74	35.92	2.07	-0.77	0.39
VkB5	0.01	37.18	4.95	31.77	4.65	-2.20	0.91
CIB_NaOH_H2O2	0.03	46.45	1.12	39.72	0.89	-2.12	0.16

Table B.7: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	d18O SD	T IL	T SEM	T ARF	T SEM	W ARF	W SD
EC_M	0.01	49.56	7.73	46.77	6.17	1.32	1.11
ECIB1	0.03	31.24	1.16	25.51	2.00	-4.63	0.41
ECIB2	0.01	39.04	6.66	33.34	5.92	-3.09	1.16
ECIB5	0.07	32.06	2.76	28.89	3.42	-3.97	0.68

Table B.8: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	D47	D47 ARF	D47 SD	D47 SEM	Fe	Mn	Sr	PC1	taxon PC1
NBIB_4_12_250	0.540	0.605	0.028	0.010					
NBIB_4_12_90	0.539	0.603	0.039	0.014					
PIB_24_12_12_POW	0.641	0.716	0.049	0.017					
PIB_24_12_POW	0.613	0.686	0.041	0.015					
PIB_4_12_250	0.592	0.659	0.030	0.011					
PIB_4_12_90	0.607	0.675	0.004	0.004					
PIB_NaOH_H2O2	0.588	0.659	0.024	0.009					
PIB_none	0.537	0.602	0.007	0.005					
SPB	0.681	0.752	0.014	0.007					
TBIB_NaOH_H2O2	0.683	0.761	0.018	0.007					
TIIB_24_12_POW	0.627	0.701	0.016	0.006					
TIIB_24BHP_12_POW	0.564	0.633	0.132	0.047					
WAIB_NaOH_H2O2	0.659	0.735	0.021	0.008					
A 551 alt					0	0	0	0.00	0.00
A-958					0	0	0	0.00	0.00
A-958-2					162	61	980	0.60	0.60
A-958-3					0	0	0	0.00	0.00
A-958-4					91	36	902	-0.14	-0.37
A1356a-07					0	0	0	0.00	0.00
A1356a-07					0	0	0	0.00	0.00
A1356a-37					0	0	0	0.00	0.00
A1380b-30					0	0	0	0.00	0.00
A1391b-06					168	58	846	0.61	1.33
A1391b-06					0	0	0	0.00	0.00
A1391b-31					38	47	997	-0.54	-1.10
A1391b-31					37	17	1252	-1.32	-1.96
922_F_RC	0.551	0.608	0.021	0.008	137	69	759	0.62	0.60
916_B_S1	0.589	0.625	0.028	0.010	98	18	477	-0.49	0.28
916_Bc_RC	0.577	0.613	0.023	0.008	32	14	880	-1.50	-1.07
916_MF_1_B	0.555	0.613	0.030	0.011	0	0	0	0.00	0.00
916_MF_B_4	0.598	0.634	0.029	0.011	112	20	784	-0.40	-0.12
916_MF_RC2	0.604	0.640	0.037	0.013	0	0	0	0.00	0.00
916_MF3_RC	0.593	0.635	0.005	0.004	198	41	814	0.48	0.56
916MF_2_B	0.561	0.608	0.021	0.007	159	45	990	0.37	0.35
911_2.1_RC	0.609	0.645	0.019	0.007	267	76	418	1.22	0.00
912.98_1_B	0.588	0.631	0.010	0.006	40	14	1100	-1.39	-1.99
912.98_2_B	0.574	0.610	0.026	0.010	51	21	900	-0.91	-0.74
912.98_2_RC	0.581	0.623	0.015	0.011	101	80	780	0.52	0.39
lbec_F_B	0.579	0.638	0.031	0.011	186	55	746	0.66	0.75
901_12_RC_1	0.631	0.667	0.006	0.005	0	0	0	0.00	0.00
901_12_RC_2	0.650	0.686	0.013	0.010	205	49	772	0.64	0.75
901_19_RC	0.632	0.674	0.030	0.021	0	0	0	0.00	0.00

Table B.9: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	D47	D47 ARF	D47 SD	D47 SEM	Fe	Mn	Sr	PC1	taxon PC1
901_19_RC_2	0.610	0.646	0.006	0.005	541	365	329	2.84	0.00
901_10_RC_1	0.630	0.666	0.009	0.007	98	18	477	-0.49	0.28
901_10_RC_2	0.635	0.671	0.022	0.015	64	22	704	-0.69	-0.45
901_8.5_B	0.593	0.630	0.030	0.011	69	19	672	-0.73	-0.53
901_8.5_Mud	0.554	0.590	0.037	0.013	0	0	0	0.00	0.00
908_1_T	0.614	0.654	0.014	0.009	0	0	0	0.00	0.00
908_LF_1_RC	0.585	0.633	0.036	0.012	0	0	0	0.00	0.00
908_LF_2_M	0.535	0.592	0.021	0.008	0	0	0	0.00	0.00
912.8_1_B	0.580	0.625	0.018	0.009	0	0	0	0.00	0.00
912.8_2_T	0.579	0.626	0.014	0.008	90	29	640	-0.25	0.46
912.8_B_2	0.564	0.600	0.038	0.014	54	12	704	-1.23	-1.24
904.25_1_B	0.528	0.584	0.013	0.005	0	0	0	0.00	0.00
904.4_1_B	0.588	0.624	0.034	0.012	0	0	0	0.00	0.00
ElkR1					403	203	461	2.17	0
ElkR2					54	28	680	-0.62	-0.31
WWR1					71	22	1160	-0.7	-1.07
WWR2					0	0	0	0	0
906_1_T	0.584	0.628	0.016	0.010	51	36	762	-0.50	-0.12
906_2_T	0.588	0.624	0.027	0.010	59	20	742	-0.82	-0.63
906_23_30_1_B	0.553	0.610	0.027	0.010	0	0	0	0.00	0.00
906_23_30_T_1	0.596	0.632	0.040	0.014	63	17	684	-0.88	-0.73
907.23F_1_B	0.547	0.604	0.036	0.013	34	10	878	-1.70	-1.23
918_52_2_B	0.596	0.632	0.022	0.008	120	45	580	0.27	0.88
918_43.2_1_B	0.583	0.631	0.005	0.004	219	160	467	1.60	2.78
918_43.2_B2	0.612	0.648	0.004	0.004	0	0	0	0.00	0.00
918_52_1_B	0.559	0.617	0.024	0.009	0	0	0	0.00	0.00
SGH-W 43 T1					0	0	0	0	0
SGH-W-42.2 R1					0	0	0	0	0
SGH-W-43.0-B1					0	0	0	0	0
Wayne Bb					52	31	584	-0.55	-0.2
MOS_B	0.605	0.673	0.007	0.005	0	0	0	0.00	0.00
MOS_B					0	0	0	0	0
MOS_T	0.610	0.679	0.023	0.016	0	0	0	0.00	0.00
MOS_T					0	0	0	0	0
KY127B1					0	0	0	0	0
HC-K T1					0	0	0	0	0
HC-K-18-B1					0	0	0	0	0
MM1-Bb					0	0	0	0	0
Mol Isotelus b					0	0	0	0	0
DPL_B	0.588	0.656	0.010	0.008	862	162	918	0.00	0.00
DB_RC	0.586	0.653	0.046	0.016	0	0	0	0.00	0.00
DB_SE_B_1	0.586	0.653	0.036	0.026	535	100	933	0.00	0.00

Table B.10: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	D47	D47 ARF	D47 SD	D47 SEM	Fe	Mn	Sr	PC1	taxon PC1
DB_SE_C1	0.564	0.628	0.028	0.020	847	353	138	0.00	0.00
DB_SE_M	0.586	0.652	0.018	0.011	1125	268	77	0.00	0.00
DB_SE_R_1	0.568	0.634	0.002	0.003	0	0	0	0.00	0.00
DB_SE_R2	0.574	0.639	0.024	0.009	23	219	140	0.00	0.00
DB_SE_S1	0.588	0.658	0.010	0.006	157	115	865	0.00	0.00
DB_SE_S2	0.565	0.633	0.014	0.009	288	115	929	0.00	0.00
DB_SE_S3	0.591	0.662	0.007	0.006	836	133	824	0.00	0.00
DB_SE_S4	0.578	0.648	0.030	0.011	1365	118	905	0.00	0.00
DB_SE_S5	0.562	0.629	0.017	0.010	1046	271	606	0.00	0.00
DB_SE_S6	0.572	0.641	0.015	0.009	489	185	760	0.00	0.00
DB_SE_T1	0.573	0.638	0.023	0.016	1148	570	235	0.00	0.00
DIB_24BHP_12_POW	0.567	0.637	0.005	0.004	0	0	0	0.00	0.00
DIB_NaOH_H2O2	0.573	0.639	0.017	0.010	0	0	0	0.00	0.00
DIB_SE_2_NaOH_H2O2	0.575	0.645	0.006	0.005	0	0	0	0.00	0.00
Dec_B_1	0.589	0.631	0.004	0.004	39	15	763	-1.30	-0.81
Dec_B_spar	0.608	0.644	0.024	0.009	166	46	308	0.60	1.31
Dec_T_2	0.583	0.625	0.010	0.007	77	28	566	-0.36	0.30
DB_D_4.05_B	0.620	0.690	0.022	0.008	0	0	0	0.00	0.00
DB_D_4.65_B	0.585	0.631	0.044	0.016	0	0	0	0.00	0.00
DRO_D_4.0-4.5_B	0.565	0.632	0.026	0.010	987	504	675	0.00	0.00
DCQ_-0.15	0.586	0.653	0.010	0.007	0	0	0	0.00	0.00
DRSQ_8_B	0.605	0.649	0.017	0.007	0	0	0	0.00	0.00
DRSQ_2.1_B	0.565	0.632	0.032	0.011	0	0	0	0.00	0.00
Asery_M	0.594	0.659	0.017	0.009	2744	377	84	0.00	0.00
Asery_T1	0.593	0.655	0.007	0.005	1794	472	115	0.00	0.00
Kunda_M	0.606	0.671	0.011	0.007	2214	639	126	0.00	0.00
Kunda_T	0.591	0.652	0.013	0.008	3064	954	137	0.00	0.00
VkB11	0.608	0.667	0.027	0.010	1108	459	736	0.00	0.00
VkB12	0.604	0.663	0.013	0.009	1051	439	573	0.00	0.00
VkB13	0.591	0.651	0.002	0.003	258	287	957	0.00	0.00
VkB14	0.603	0.662	0.007	0.005	0	0	0	0.00	0.00
VkB15	0.591	0.649	0.036	0.013	0	0	0	0.00	0.00
VkB16	0.583	0.641	0.014	0.008	1032	279	856	0.00	0.00
VkB17	0.611	0.670	0.027	0.010	0	0	0	0.00	0.00
VkB18	0.599	0.657	0.009	0.006	511	359	562	0.00	0.00
VkB2	0.594	0.653	0.032	0.012	0	0	0	0.00	0.00
VkB3	0.583	0.649	0.041	0.015	110	277	1164	0.00	0.00
VkB4	0.611	0.672	0.018	0.009	178	204	870	0.00	0.00
VkB7	0.575	0.640	0.042	0.015	365	312	430	0.00	0.00
VkB8	0.591	0.654	0.009	0.007	1840	567	617	0.00	0.00
VkB5	0.601	0.668	0.045	0.016	219	189	1089	0.00	0.00
CIB_NaOH_H2O2	0.571	0.641	0.003	0.003	0	0	0	0.00	0.00

Table B.11: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	D47	D47 ARF	D47 SD	D47 SEM	Fe	Mn	Sr	PC1	taxon PC1
EC_M	0.562	0.619	0.050	0.018	0	0	0	0.00	0.00
ECIB1	0.622	0.691	0.020	0.008	0	0	0	0.00	0.00
ECIB2	0.595	0.663	0.056	0.020	0	0	0	0.00	0.00
ECIB5	0.619	0.679	0.017	0.012	0	0	0	0.00	0.00

Table B.12: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	logFe	logMn	logSr	PCA1	PCA1_Norm	PCA1_NormR	textural alt
NBIB_4_12_250							
NBIB_4_12_90							
PIB_24_12_12_POW							
PIB_24_12_POW							
PIB_4_12_250							
PIB_4_12_90							
PIB_NaOH_H2O2							
PIB_none							
SPB							
TBIB_NaOH_H2O2							
TIIB_24_12_POW							
TIIB_24BHP_12_POW							
WAIB_NaOH_H2O2							
A 551 alt	0.00	0.00	0.00	0.00	0.0000		no
A-958	0.00	0.00	0.00	0.00	0.0000		no
A-958-2	2.21	1.79	2.99	2.15	0.0119	0.9881	no
A-958-3	0.00	0.00	0.00	0.00	0.0000		no
A-958-4	1.96	1.56	2.96	1.83	0.0101	0.9899	no
A1356a-07	0.00	0.00	0.00	0.00	0.0000		no
A1356a-07	0.00	0.00	0.00	0.00	0.0000		no
A1356a-37	0.00	0.00	0.00	0.00	0.0000		no
A1380b-30	0.00	0.00	0.00	0.00	0.0000		no
A1391b-06	2.23	1.76	2.93	2.16	0.0120	0.9880	yes
A1391b-06	0.00	0.00	0.00	0.00	0.0000		no
A1391b-31	1.58	1.67	3.00	1.63	0.0090	0.9910	no
A1391b-31	1.57	1.23	3.10	1.30	0.0072	0.9928	no
922_F_RC	2.14	1.84	2.88	2.16	0.0120	0.9880	no
916_B_S1	1.99	1.26	2.68	1.70	0.0095	0.9905	no
916_Bc_RC	1.51	1.15	2.94	1.23	0.0068	0.9932	no
916_MF_1_B	0.00	0.00	0.00	0.00	0.0000		no
916_MF_B_4	2.05	1.30	2.89	1.73	0.0096	0.9904	no
916_MF_RC2	0.00	0.00	0.00	0.00	0.0000		no
916_MF3_RC	2.30	1.61	2.91	2.11	0.0117	0.9883	no
916MF_2_B	2.20	1.65	3.00	2.05	0.0114	0.9886	no
911_2.1_RC	2.43	1.88	2.62	2.44	0.0136	0.9864	yes
912.98_1_B	1.60	1.15	3.04	1.28	0.0071	0.9929	no
912.98_2_B	1.71	1.32	2.95	1.49	0.0083	0.9917	no
912.98_2_RC	2.00	1.90	2.89	2.11	0.0117	0.9883	no
Lbec_F_B	2.27	1.74	2.87	2.19	0.0121	0.9879	no
901_12_RC_1	0.00	0.00	0.00	0.00	0.0000		no
901_12_RC_2	2.31	1.69	2.89	2.18	0.0121	0.9879	yes
901_19_RC	0.00	0.00	0.00	0.00	0.0000		no

Table B.13: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	logFe	logMn	logSr	PCA1	PCA1_Norm	PCA1_NormR	textural alt
901_19_RC_2	2.73	2.56	2.52	3.14	0.0175	0.9825	yes
901_10_RC_1	1.99	1.26	2.68	1.70	0.0095	0.9905	no
901_10_RC_2	1.81	1.34	2.85	1.59	0.0089	0.9911	no
901_8.5_B	1.84	1.28	2.83	1.58	0.0088	0.9912	no
901_8.5_Mud	0.00	0.00	0.00	0.00	0.0000		no
908_1_T	0.00	0.00	0.00	0.00	0.0000		yes
908_LF_1_RC	0.00	0.00	0.00	0.00	0.0000		yes
908_LF_2_M	0.00	0.00	0.00	0.00	0.0000		yes
912.8_1_B	0.00	0.00	0.00	0.00	0.0000		no
912.8_2_T	1.95	1.46	2.81	1.79	0.0099	0.9901	no
912.8_B_2	1.73	1.08	2.85	1.36	0.0076	0.9924	no
904.25_1_B	0.00	0.00	0.00	0.00	0.0000		yes
904.4_1_B	0.00	0.00	0.00	0.00	0.0000		no
ElkR1	2.61	2.31	2.66	2.85	0.0200	0.9842	yes
ElkR2	1.73	1.45	2.83	1.62	0.0100	0.9910	no
WWR1	1.85	1.34	3.06	1.58	0.0100	0.9912	no
WWR2	0	0	0	0	0.0000		no
906_1_T	1.71	1.56	2.88	1.66	0.0092	0.9908	no
906_2_T	1.77	1.30	2.87	1.54	0.0085	0.9915	no
906_23_30_1_B	0.00	0.00	0.00	0.00	0.0000		no
906_23_30_T_1	1.80	1.23	2.84	1.52	0.0084	0.9916	no
907.23F_1_B	1.53	1.00	2.94	1.15	0.0064	0.9936	no
918_52_2_B	2.08	1.65	2.76	2.02	0.0112	0.9888	no
918_43.2_1_B	2.34	2.20	2.67	2.59	0.0144	0.9856	no
918_43.2_B2	0.00	0.00	0.00	0.00	0.0000		yes
918_52_1_B	0.00	0.00	0.00	0.00	0.0000		no
SGH-W 43 T1	0	0	0	0	0.0000		no
SGH-W-42.2 R1	0	0	0	0	0.0000		no
SGH-W-43.0-B1	0	0	0	0	0.0000		no
Wayne Bb	1.72	1.49	2.77	1.65	0.0100	0.9908	no
MOS_B	0.00	0.00	0.00	0.00	0.0000		no
MOS_B	0	0	0	0	0.0000		no
MOS_T	0.00	0.00	0.00	0.00	0.0000		no
MOS_T	0	0	0	0	0.0000		no
KY127B1	0	0	0	0	0.0000		yes
HC-K T1	0	0	0	0	0.0000		no
HC-K-18-B1	0	0	0	0	0.0000		yes
MM1-Bb	0	0	0	0	0.0000		no
Mol Isotelus b	0	0	0	0	0.0000		yes
DPL_B	2.94	2.21	2.96	2.96	0.0164	0.9836	no
DB_RC	0.00	0.00	0.00	0.00	0.0000		no
DB_SE_B_1	2.73	2.00	2.97	2.67	0.0148	0.9852	no

Table B.14: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	logFe	logMn	logSr	PCA1	PCA1_Norm	PCA1_NormR	textural alt
DB_SE_C1	2.93	2.55	2.14	3.35	0.0186	0.9814	no
DB_SE_M	3.05	2.43	1.89	3.41	0.0189	0.9811	no
DB_SE_R_1	0.00	0.00	0.00	0.00	0.0000		no
DB_SE_R2	1.36	2.34	2.15	2.10	0.0117	0.9883	no
DB_SE_S1	2.20	2.06	2.94	2.34	0.0130	0.9870	no
DB_SE_S2	2.46	2.06	2.97	2.52	0.0140	0.9860	no
DB_SE_S3	2.92	2.12	2.92	2.90	0.0161	0.9839	no
DB_SE_S4	3.14	2.07	2.96	3.00	0.0167	0.9833	no
DB_SE_S5	3.02	2.43	2.78	3.20	0.0178	0.9822	no
DB_SE_S6	2.69	2.27	2.88	2.84	0.0158	0.9842	no
DB_SE_T1	3.06	2.76	2.37	3.54	0.0197	0.9803	no
DIB_24BHP_12_POW	0.00	0.00	0.00	0.00	0.0000		no
DIB_NaOH_H2O2	0.00	0.00	0.00	0.00	0.0000		no
DIB_SE_2_NaOH_H2O2	0.00	0.00	0.00	0.00	0.0000		no
Dec_B_1	1.59	1.18	2.88	1.32	0.0074	0.9926	no
Dec_B_spar	2.22	1.66	2.49	2.18	0.0121	0.9879	no
Dec_T_2	1.89	1.45	2.75	1.74	0.0097	0.9903	no
DB_D_4.05_B	0.00	0.00	0.00	0.00	0.0000		no
DB_D_4.65_B	0.00	0.00	0.00	0.00	0.0000		no
DRO_D 4.0-4.5_B	2.99	2.70	2.83	3.36	0.0187	0.9813	no
DCQ_-0.15	0.00	0.00	0.00	0.00	0.0000		no
DRSQ_8_B	0.00	0.00	0.00	0.00	0.0000		no
DRSQ_2.1_B	0.00	0.00	0.00	0.00	0.0000		no
Asery_M	3.44	2.58	1.92	3.77	0.0210	0.9790	no
Asery_T1	3.25	2.67	2.06	3.68	0.0205	0.9795	no
Kunda_M	3.35	2.81	2.10	3.83	0.0213	0.9787	no
Kunda_T	3.49	2.98	2.14	4.04	0.0224	0.9776	no
VkB11	3.04	2.66	2.87	3.36	0.0187	0.9813	no
VkB12	3.02	2.64	2.76	3.35	0.0186	0.9814	no
VkB13	2.41	2.46	2.98	2.75	0.0153	0.9847	no
VkB14	0.00	0.00	0.00	0.00	0.0000		no
VkB15	0.00	0.00	0.00	0.00	0.0000		no
VkB16	3.01	2.45	2.93	3.18	0.0177	0.9823	no
VkB17	0.00	0.00	0.00	0.00	0.0000		no
VkB18	2.71	2.55	2.75	3.07	0.0171	0.9829	no
VkB2	0.00	0.00	0.00	0.00	0.0000		no
VkB3	2.04	2.44	3.07	2.46	0.0137	0.9863	no
VkB4	2.25	2.31	2.94	2.55	0.0141	0.9859	no
VkB7	2.56	2.49	2.63	2.95	0.0164	0.9836	no
VkB8	3.26	2.75	2.79	3.59	0.0200	0.9800	no
VkB5	2.34	2.28	3.04	2.57	0.0143	0.9857	no
CIB_NaOH_H2O2	0.00	0.00	0.00	0.00	0.0000		no

Table B.15: Clumped isotopic data from the Modern, Ordovician and Cambrian

Sample ID	logFe	logMn	logSr	PCA1	PCA1_Norm	PCA1_NormR	textural alt
EC_M	0.00	0.00	0.00	0.00	0.0000		no
ECIB1	0.00	0.00	0.00	0.00	0.0000		no
ECIB2	0.00	0.00	0.00	0.00	0.0000		no
ECIB5	0.00	0.00	0.00	0.00	0.0000		no

Table B.16: Clumped isotopic data from the Modern, Ordovician and Cambrian