Short Course on Using
LIMS for Lasers
for H_2O Stable Isotopes

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2014

Isotope Hydrology Laboratory
Water Resources Section

IAEA
International Atomic Energy Agency

Lasers in the Lab

- Laser spectroscopy is fast becoming the *de-facto* method to measure δ^2H and $\delta^{18}O$ in waters.
- LAS instrumentation is relatively easy to install and operate.

- However – routine laboratory operations are made <u>difficult due to substantive offline data manipulation</u> required in Excel to obtain the final results.
- Manufacturer software not suitable for sample and data management.

IAEA

LGR Data Overload!!!!

h2o_20121011_019_LIMS - Microsoft Excel Preview

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW

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I4 | 1000

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC
1	Analysis	Peak Nr	Ignore	Time Code	Line	Identifier 1	Identifier 2	Port	Amount	Amount Unit	Commenas	Configuratio	Is Ref	_Temp_Celsius	stdv_Celsius	H2O_N/cm3	stdv_H2O	HOD/H2O	stdv_HOD/HOH	H2018/H2O	stdH2018/H2O	D/H	stdD/H	O18/O16	std018/O16	delta D/H	stdev delta D/H	delta 18O/16O	stdev delta 18O/16O
2	L-000416	1	-1	11-10-12 15:39	1	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	8.56E-04	3.07E+16	2.06E+13	2.88E-04	1.58E-07	1.98E-03	2.79E-07	1.44E-04	7.89E-08	1.98E-03	2.79E-07	-7.63E+01	0.00E+00	-1.10E+01	0.00E+00
3	L-000416	2	-1	11-10-12 15:40	2	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.14E-03	3.03E+16	2.24E+13	2.87E-04	1.35E-07	1.98E-03	2.36E-07	1.44E-04	6.73E-08	1.98E-03	2.36E-07	-7.79E+01	0.00E+00	-1.11E+01	0.00E+00
4	L-000416	3	0	11-10-12 15:42	3	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.38E-03	3.08E+16	1.80E+13	2.87E-04	1.08E-07	1.98E-03	3.37E-07	1.44E-04	5.40E-08	1.98E-03	3.37E-07	-7.80E+01	0.00E+00	-1.12E+01	0.00E+00
5	L-000416	4	0	11-10-12 15:43	4	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.27E-03	3.03E+16	2.09E+13	2.87E-04	1.54E-07	1.98E-03	2.25E-07	1.44E-04	7.72E-08	1.98E-03	2.25E-07	-7.83E+01	0.00E+00	-1.12E+01	0.00E+00
6	L-000416	5	0	11-10-12 15:44	5	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.41E-03	3.05E+16	2.19E+13	2.87E-04	1.03E-07	1.98E-03	2.17E-07	1.44E-04	5.15E-08	1.98E-03	2.17E-07	-7.83E+01	0.00E+00	-1.12E+01	0.00E+00
7	L-000416	6	0	11-10-12 15:46	6	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.35E-03	3.03E+16	1.80E+13	2.87E-04	1.23E-07	1.98E-03	2.45E-07	1.44E-04	6.17E-08	1.98E-03	2.45E-07	-7.86E+01	0.00E+00	-1.12E+01	0.00E+00
8	L-000416	7	0	11-10-12 15:47	7	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.62E-03	3.07E+16	1.88E+13	2.87E-04	1.54E-07	1.98E-03	2.36E-07	1.44E-04	7.72E-08	1.98E-03	2.36E-07	-7.85E+01	0.00E+00	-1.12E+01	0.00E+00
9	L-000416	8	0	11-10-12 15:48	8	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.76E+01	1.35E-03	3.02E+16	1.84E+13	2.87E-04	1.24E-07	1.98E-03	2.13E-07	1.43E-04	6.20E-08	1.98E-03	2.13E-07	-7.91E+01	0.00E+00	-1.13E+01	0.00E+00
10	L-000416	9	0	11-10-12 15:50	9	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.13E-03	3.02E+16	2.10E+13	2.87E-04	1.30E-07	1.98E-03	1.86E-07	1.44E-04	6.52E-08	1.98E-03	1.86E-07	-7.83E+01	0.00E+00	-1.11E+01	0.00E+00
11	L-000416	10	0	11-10-12 15:51	10	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.60E-03	3.03E+16	1.93E+13	2.87E-04	1.11E-07	1.98E-03	2.45E-07	1.44E-04	5.55E-08	1.98E-03	2.45E-07	-7.86E+01	0.00E+00	-1.12E+01	0.00E+00
12	L-000416	11	0	11-10-12 15:52	11	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.53E-03	3.03E+16	2.13E+13	2.87E-04	1.24E-07	1.98E-03	2.43E-07	1.44E-04	6.19E-08	1.98E-03	2.43E-07	-7.86E+01	0.00E+00	-1.12E+01	0.00E+00
13	L-000416	12	0	11-10-12 15:54	12	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.29E-03	3.02E+16	2.28E+13	2.87E-04	1.31E-07	1.98E-03	2.35E-07	1.43E-04	6.56E-08	1.98E-03	2.35E-07	-7.88E+01	0.00E+00	-1.12E+01	0.00E+00
14	L-000416	13	0	11-10-12 15:55	13	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.27E-03	3.01E+16	1.87E+13	2.87E-04	1.23E-07	1.98E-03	3.45E-07	1.44E-04	6.17E-08	1.98E-03	3.45E-07	-7.87E+01	0.00E+00	-1.12E+01	0.00E+00
15	L-000416	14	0	11-10-12 15:56	14	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.40E-03	3.04E+16	2.25E+13	2.87E-04	1.49E-07	1.98E-03	2.54E-07	1.43E-04	7.46E-08	1.98E-03	2.54E-07	-7.92E+01	0.00E+00	-1.12E+01	0.00E+00
16	L-000416	15	0	11-10-12 15:58	15	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.32E-03	3.07E+16	1.68E+13	2.87E-04	1.24E-07	1.98E-03	3.27E-07	1.44E-04	6.18E-08	1.98E-03	3.27E-07	-7.80E+01	0.00E+00	-1.11E+01	0.00E+00
17	L-000416	16	0	11-10-12 15:59	16	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.37E-03	3.03E+16	1.93E+13	2.87E-04	1.15E-07	1.98E-03	2.63E-07	1.44E-04	5.74E-08	1.98E-03	2.63E-07	-7.83E+01	0.00E+00	-1.12E+01	0.00E+00
18	L-000416	17	0	11-10-12 16:00	17	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.45E-03	3.07E+16	1.93E+13	2.87E-04	1.05E-07	1.98E-03	2.44E-07	1.44E-04	5.24E-08	1.98E-03	2.44E-07	-7.85E+01	0.00E+00	-1.11E+01	0.00E+00
19	L-000416	18	0	11-10-12 16:02	18	W-3 / / 208/808/	DIW Wash	Mar-28	1000	nL		H2O	0	2.75E+01	1.29E-03	3.04E+16	2.14E+13	2.87E-04	1.40E-07	1.98E-03	2.71E-07	1.44E-04	7.00E-08	1.98E-03	2.71E-07	-7.86E+01	0.00E+00	-1.12E+01	0.00E+00
20	L-000417	1	-1	11-10-12 16:03	19	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	1.51E-03	3.10E+16	1.85E+13	3.10E-04	1.31E-07	2.00E-03	1.92E-07	1.55E-04	6.56E-08	2.00E-03	1.92E-07	-3.62E+00	0.00E+00	-2.48E-01	0.00E+00
21	L-000417	2	-1	11-10-12 16:04	20	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	7.20E-04	3.09E+16	1.72E+13	3.11E-04	1.09E-07	2.01E-03	2.48E-07	1.56E-04	5.46E-08	2.01E-03	2.48E-07	-1.09E+00	0.00E+00	7.40E-03	0.00E+00
22	L-000417	3	0	11-10-12 16:06	21	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	1.51E-03	3.06E+16	1.80E+13	3.11E-04	7.73E-08	2.01E-03	3.19E-07	1.56E-04	3.86E-08	2.01E-03	3.19E-07	-9.04E-01	0.00E+00	9.08E-02	0.00E+00
23	L-000417	4	0	11-10-12 16:07	22	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	1.26E-03	3.05E+16	2.12E+13	3.11E-04	1.34E-07	2.01E-03	2.56E-07	1.56E-04	6.69E-08	2.01E-03	2.56E-07	-5.77E-01	0.00E+00	-4.72E-04	0.00E+00
24	L-000417	5	0	11-10-12 16:08	23	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	1.22E-03	3.03E+16	1.54E+13	3.11E-04	1.26E-07	2.01E-03	1.89E-07	1.56E-04	6.31E-08	2.01E-03	1.89E-07	-1.04E+00	0.00E+00	4.31E-02	0.00E+00
25	L-000417	6	0	11-10-12 16:10	24	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.75E+01	7.37E-04	3.06E+16	1.68E+13	3.11E-04	1.32E-07	2.01E-03	3.23E-07	1.56E-04	6.62E-08	2.01E-03	3.23E-07	-3.48E-01	0.00E+00	8.75E-02	0.00E+00
26	L-000417	7	0	11-10-12 16:11	25	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.74E+01	1.31E-03	3.03E+16	1.63E+13	3.11E-04	1.58E-07	2.01E-03	2.31E-07	1.56E-04	7.89E-08	2.01E-03	2.31E-07	-6.12E-01	0.00E+00	6.90E-02	0.00E+00
27	L-000417	8	0	11-10-12 16:12	26	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.74E+01	1.48E-03	3.06E+16	1.94E+13	3.12E-04	1.50E-07	2.01E-03	2.46E-07	1.56E-04	7.49E-08	2.01E-03	2.46E-07	1.57E-01	0.00E+00	1.48E-01	0.00E+00
28	L-000417	9	0	11-10-12 16:14	27	W-31 / / 208/808/	IAEA LabStd 11	03-Oct	1000	nL		H2O	0	2.74E+01	1.97E-03	3.06E+16	1.83E+13	3.11E-04	1.60E-07	2.01E-03	2.43E-07	1.56E-04	7.99E-08	2.01E-03	2.43E-07	-3.12E-01	0.00E+00	6.59E-02	0.00E+00
29	L-000418	1	-1	11-10-12 16:15	28	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.23E-03	3.09E+16	1.84E+13	2.55E-04	2.01E-07	1.96E-03	2.65E-07	1.28E-04	1.01E-07	1.96E-03	2.65E-07	-1.81E+02	0.00E+00	-2.41E+01	0.00E+00
30	L-000418	2	-1	11-10-12 16:16	29	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.06E-03	3.10E+16	1.94E+13	2.53E-04	1.26E-07	1.96E-03	2.82E-07	1.27E-04	6.32E-08	1.96E-03	2.82E-07	-1.87E+02	0.00E+00	-2.46E+01	0.00E+00
31	L-000418	3	0	11-10-12 16:18	30	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.31E-03	3.09E+16	2.00E+13	2.53E-04	1.61E-07	1.96E-03	2.27E-07	1.26E-04	8.04E-08	1.96E-03	2.27E-07	-1.89E+02	0.00E+00	-2.46E+01	0.00E+00
32	L-000418	4	0	11-10-12 16:19	31	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.51E-03	3.10E+16	2.32E+13	2.53E-04	1.38E-07	1.96E-03	2.49E-07	1.26E-04	6.89E-08	1.96E-03	2.49E-07	-1.89E+02	0.00E+00	-2.46E+01	0.00E+00
33	L-000418	5	0	11-10-12 16:20	32	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.39E-03	3.09E+16	1.87E+13	2.53E-04	1.40E-07	1.96E-03	1.76E-07	1.26E-04	7.01E-08	1.96E-03	1.76E-07	-1.89E+02	0.00E+00	-2.48E+01	0.00E+00
34	L-000418	6	0	11-10-12 16:22	33	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.37E-03	3.09E+16	2.12E+13	2.52E-04	1.25E-07	1.96E-03	2.83E-07	1.26E-04	6.25E-08	1.96E-03	2.83E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
35	L-000418	7	0	11-10-12 16:23	34	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.34E-03	3.09E+16	1.85E+13	2.52E-04	1.21E-07	1.96E-03	2.66E-07	1.26E-04	6.07E-08	1.96E-03	2.66E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
36	L-000418	8	0	11-10-12 16:24	35	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.28E-03	3.05E+16	1.75E+13	2.52E-04	1.44E-07	1.96E-03	3.10E-07	1.26E-04	7.20E-08	1.96E-03	3.10E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
37	L-000418	9	0	11-10-12 16:26	36	W-32 / / 208/808/	IAEA LabStd 9	03-Jan	1000	nL		H2O	0	2.74E+01	1.35E-03	3.08E+16	2.04E+13	2.52E-04	1.12E-07	1.96E-03	2.82E-07	1.26E-04	5.62E-08	1.96E-03	2.82E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
38	L-000419	1	-1	11-10-12 16:27	37	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.24E-03	3.10E+16	1.89E+13	2.52E-04	1.26E-07	1.96E-03	2.81E-07	1.26E-04	6.31E-08	1.96E-03	2.81E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
39	L-000419	2	-1	11-10-12 16:28	38	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.21E-03	3.10E+16	2.01E+13	2.52E-04	1.55E-07	1.96E-03	2.59E-07	1.26E-04	7.73E-08	1.96E-03	2.59E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
40	L-000419	3	0	11-10-12 16:30	39	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	8.73E-04	3.10E+16	2.03E+13	2.52E-04	1.14E-07	1.96E-03	3.07E-07	1.26E-04	5.70E-08	1.96E-03	3.07E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
41	L-000419	4	0	11-10-12 16:31	40	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.59E-03	3.10E+16	2.28E+13	2.52E-04	1.22E-07	1.96E-03	2.46E-07	1.26E-04	6.09E-08	1.96E-03	2.46E-07	-1.90E+02	0.00E+00	-2.47E+01	0.00E+00
42	L-000419	5	0	11-10-12 16:32	41	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.56E-03	3.06E+16	2.10E+13	2.52E-04	1.76E-07	1.96E-03	3.10E-07	1.26E-04	8.82E-08	1.96E-03	3.10E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
43	L-000419	6	0	11-10-12 16:34	42	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.49E-03	3.09E+16	2.17E+13	2.52E-04	1.61E-07	1.96E-03	2.85E-07	1.26E-04	8.07E-08	1.96E-03	2.85E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
44	L-000419	7	0	11-10-12 16:35	43	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.32E-03	3.09E+16	2.17E+13	2.52E-04	8.83E-08	1.96E-03	3.03E-07	1.26E-04	4.41E-08	1.96E-03	3.03E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
45	L-000419	8	0	11-10-12 16:36	44	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.47E-03	3.07E+16	2.32E+13	2.52E-04	1.80E-07	1.96E-03	1.69E-07	1.26E-04	9.01E-08	1.96E-03	1.69E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
46	L-000419	9	0	11-10-12 16:38	45	W-32 / / 208/808/	IAEA LabStd 9	03-Feb	1000	nL		H2O	0	2.74E+01	1.42E-03	3.10E+16	2.15E+13	2.52E-04	9.57E-08	1.96E-03	2.49E-07	1.26E-04	4.78E-08	1.96E-03	2.49E-07	-1.90E+02	0.00E+00	-2.48E+01	0.00E+00
47	L-000420	1	-1	11-10-12 16:39	46	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.74E+01	1.50E-03	3.10E+16	2.36E+13	3.09E-04	1.64E-07	2.00E-03	2.74E-07	1.54E-04	8.18E-08	2.00E-03	2.74E-07	-8.62E+00	0.00E+00	-5.32E-01	0.00E+00
48	L-000420	2	-1	11-10-12 16:40	47	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.74E+01	1.39E-03	3.09E+16	1.90E+13	3.11E-04	1.15E-07	2.01E-03	2.38E-07	1.55E-04	5.75E-08	2.01E-03	2.38E-07	-2.51E+00	0.00E+00	-9.56E-02	0.00E+00
49	L-000420	3	0	11-10-12 16:42	48	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.74E+01	1.44E-03	3.08E+16	2.39E+13	3.11E-04	1.15E-07	2.01E-03	2.69E-07	1.56E-04	5.75E-08	2.01E-03	2.69E-07	-1.26E+00	0.00E+00	-3.77E-02	0.00E+00
50	L-000420	4	0	11-10-12 16:43	49	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.74E+01	1.54E-03	3.07E+16	2.14E+13	3.11E-04	1.08E-07	2.01E-03	3.03E-07	1.56E-04	5.40E-08	2.01E-03	3.03E-07	-9.51E-01	0.00E+00	-1.05E-02	0.00E+00
51	L-000420	5	0	11-10-12 16:44	50	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.73E+01	1.09E-03	3.10E+16	2.25E+13	3.11E-04	9.90E-08	2.01E-03	2.97E-07	1.56E-04	4.95E-08	2.01E-03	2.97E-07	-4.52E-01	0.00E+00	7.96E-04	0.00E+00
52	L-000420	6	0	11-10-12 16:46	51	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.73E+01	1.25E-03	3.08E+16	1.86E+13	3.11E-04	9.59E-08	2.01E-03	2.36E-07	1.56E-04	4.79E-08	2.01E-03	2.36E-07	-4.86E-01	0.00E+00	-5.45E-02	0.00E+00
53	L-000420	7	0	11-10-12 16:47	52	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.73E+01	1.38E-03	3.10E+16	1.56E+13	3.11E-04	1.26E-07	2.01E-03	2.47E-07	1.56E-04	6.30E-08	2.01E-03	2.47E-07	-1.71E-01	0.00E+00	2.98E-02	0.00E+00
54	L-000420	8	0	11-10-12 16:48	53	W-31 / / 208/808/	IAEA LabStd 11	03-Nov	1000	nL		H2O	0	2.73E+01	1.14E-03	3.09E+16	2.31E+13	3.12E-04	1.43E-07	2.01E-03	2.34E-07	1.56E-04	7.13E-08	2.01E-03	2.34E-07	-5.00E-02	0.00E+00	1.28E-02	0.00E+00

h2o_20121011_019_LIMS

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IAEA

Picarro Data Overload!!!!

HBDS42_IsoWater_20121011_154644 - Microsoft Excel Preview

FILE HOME INSERT PAGE LAYOUT FORMULAS DATA REVIEW VIEW

Leonard Wassenaar

E2 | 1

	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y
1	Time Code	Port	Inj Nr	d(18_16)Mean	d(D_H)Mean	H2O_Mean	Ignore	Good	Identifier 1	Identifier 2	Gas Configuration	days_Mean	d(18_16)_SD	d(D_H)_SD	H2O_SD	d(18_16)_Sl	d(D_H)_Sl	H2O_Sl	DAS Temp	Tray	Sample	Job	Method
2	2012/10/11 15:34:02	1-01	1	0.071	-5.22	21286	-1	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.62226	0.26	1.689	178	-0.014	0.04	17.44	33.313	MT1-Frnt	1	86	IHL10
3	2012/10/11 15:42:48	1-01	2	0.234	-3.612	20130	-1	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.62833	0.257	1.105	171	-0.021	0.03	16.69	33.125	MT1-Frnt	1	86	IHL10
4	2012/10/11 15:51:35	1-01	3	0.329	-2.829	19462	-1	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.63444	0.278	1.057	165	-0.022	0.031	15.85	33.188	MT1-Frnt	1	86	IHL10
5	2012/10/11 16:00:21	1-01	4	0.466	-2.338	20040	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.64053	0.242	1.221	179	-0.016	0.015	16.89	33.25	MT1-Frnt	1	86	IHL10
6	2012/10/11 16:09:08	1-01	5	0.34	-1.298	22751	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.64662	0.273	0.976	179	-0.019	-0.011	18.5	33.188	MT1-Frnt	1	86	IHL10
7	2012/10/11 16:17:55	1-01	6	0.399	-0.685	22931	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.65271	0.271	1.11	201	-0.014	0.016	19.62	33.125	MT1-Frnt	1	86	IHL10
8	2012/10/11 16:26:42	1-01	7	0.536	-1.605	19919	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.65883	0.227	1.126	169	-0.016	-0.008	16.07	33.125	MT1-Frnt	1	86	IHL10
9	2012/10/11 16:35:29	1-01	8	0.484	-1.122	19839	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.66493	0.228	1.078	165	-0.017	-0.001	15.68	33.125	MT1-Frnt	1	86	IHL10
10	2012/10/11 16:44:15	1-01	9	0.465	-0.7	21349	0	1	W-31 / / 208 / 808	IAEA Lab Std 11	H2O	284.67102	0.3	1.119	174	-0.018	0.019	16.97	33.125	MT1-Frnt	1	86	IHL10
11	2012/10/11 16:53:01	1-02	1	-23.021	-173.052	20445	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.67712	0.202	1.513	177	-0.009	-0.061	16.65	33	MT1-Frnt	2	86	IHL10
12	2012/10/11 17:01:47	1-02	2	-23.175	-177.926	20854	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.68318	0.209	1.137	194	-0.013	0.063	17.86	32.938	MT1-Frnt	2	86	IHL10
13	2012/10/11 17:10:34	1-02	3	-24.377	-188.121	22206	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.68931	0.255	0.927	180	-0.009	0.008	17.3	32.938	MT1-Frnt	2	86	IHL10
14	2012/10/11 17:19:21	1-02	4	-24.632	-190.654	23584	-1	0	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.69543	0.245	1.161	171	-0.012	0.031	17.36	32.938	MT1-Frnt	2	86	IHL10
15	2012/10/11 17:28:08	1-02	5	-24.465	-191.822	19788	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.70146	0.201	0.969	179	-0.014	0.043	16.77	32.875	MT1-Frnt	2	86	IHL10
16	2012/10/11 17:36:54	1-02	6	-24.574	-192.639	19668	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.7076	0.241	1.201	161	-0.014	0.045	15.34	32.875	MT1-Frnt	2	86	IHL10
17	2012/10/11 17:45:41	1-02	7	-24.736	-193.159	22823	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.71369	0.249	0.984	177	-0.017	0.042	17.79	32.875	MT1-Frnt	2	86	IHL10
18	2012/10/11 17:54:28	1-02	8	-24.619	-193.219	19729	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.71983	0.192	1.048	144	-0.007	0.025	14.5	32.875	MT1-Frnt	2	86	IHL10
19	2012/10/11 18:03:15	1-02	9	-24.711	-193.862	21724	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.72589	0.264	1.103	152	-0.018	0.028	15.7	32.813	MT1-Frnt	2	86	IHL10
20	2012/10/11 18:12:02	1-03	1	-24.682	-194.601	19863	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.73196	0.22	0.965	190	-0.011	-0.007	16.96	32.938	MT1-Frnt	3	86	IHL10
21	2012/10/11 18:20:49	1-03	2	-24.648	-194.748	19588	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.73812	0.277	1.154	147	-0.017	0.017	14.19	33	MT1-Frnt	3	86	IHL10
22	2012/10/11 18:29:35	1-03	3	-24.547	-193.58	19977	-1	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.74418	0.296	1.308	175	-0.023	0.066	16.54	33.063	MT1-Frnt	3	86	IHL10
23	2012/10/11 18:38:23	1-03	4	-24.595	-194.639	19269	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.75032	0.264	1.077	147	-0.017	0.015	14.21	33.063	MT1-Frnt	3	86	IHL10
24	2012/10/11 18:47:11	1-03	5	-24.552	-194.25	19745	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.75637	0.226	1.037	177	-0.015	-0.023	16.48	33.063	MT1-Frnt	3	86	IHL10
25	2012/10/11 18:55:57	1-03	6	-24.777	-194.592	20725	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.76254	0.281	1.1	149	-0.015	0.012	14.84	33.063	MT1-Frnt	3	86	IHL10
26	2012/10/11 19:04:44	1-03	7	-24.605	-195.391	19867	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.76855	0.28	1.435	181	-0.019	0.041	16.75	33.063	MT1-Frnt	3	86	IHL10
27	2012/10/11 19:13:31	1-03	8	-24.608	-194.891	19582	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.77469	0.215	1.133	159	-0.014	0.005	15.14	33.063	MT1-Frnt	3	86	IHL10
28	2012/10/11 19:22:19	1-03	9	-24.513	-194.608	19814	0	1	W-32 / / 208 / 808	IAEA LabStd 9	H2O	284.78078	0.241	1.139	185	-0.014	0	16.61	33.063	MT1-Frnt	3	86	IHL10
29	2012/10/11 19:31:05	1-04	1	-2.806	-31.51	19840	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.78693	0.272	1.508	146	-0.02	0.055	14.58	33.063	MT1-Frnt	4	86	IHL10
30	2012/10/11 19:39:54	1-04	2	-1.223	-15.47	19690	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.793	0.284	1.267	183	-0.02	-0.023	16.57	33.063	MT1-Frnt	4	86	IHL10
31	2012/10/11 19:48:40	1-04	3	-1.015	-11.161	19798	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.79911	0.254	1.011	173	-0.017	-0.015	16.27	33.063	MT1-Frnt	4	86	IHL10
32	2012/10/11 19:57:28	1-04	4	-0.99	-9.695	20028	0	1	W-1001 / / 208 / 808	OH13	H2O	284.8052	0.282	1.264	167	-0.017	-0.015	16.28	33.063	MT1-Frnt	4	86	IHL10
33	2012/10/11 20:06:15	1-04	5	-0.638	-7.048	18729	0	1	W-1001 / / 208 / 808	OH13	H2O	284.81131	0.244	1.382	153	-0.018	-0.037	14.64	33.063	MT1-Frnt	4	86	IHL10
34	2012/10/11 20:15:02	1-04	6	-0.759	-7.129	21387	0	1	W-1001 / / 208 / 808	OH13	H2O	284.8174	0.302	0.868	185	-0.022	-0.014	17.66	33.125	MT1-Frnt	4	86	IHL10
35	2012/10/11 20:23:48	1-04	7	-0.644	-6.008	20536	0	1	W-1001 / / 208 / 808	OH13	H2O	284.82354	0.221	1.188	141	-0.015	-0.067	14.51	33.063	MT1-Frnt	4	86	IHL10
36	2012/10/11 20:32:36	1-04	8	-0.598	-6.118	18891	0	1	W-1001 / / 208 / 808	OH13	H2O	284.8296	0.251	0.966	155	-0.016	0.002	14.7	33.063	MT1-Frnt	4	86	IHL10
37	2012/10/11 20:41:24	1-04	9	-0.686	-4.529	23136	-1	0	W-1001 / / 208 / 808	OH13	H2O	284.83568	0.227	0.904	198	-0.017	0.001	19.76	33.063	MT1-Frnt	4	86	IHL10
38	2012/10/11 20:50:11	1-05	1	-0.566	-4.376	19518	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.84183	0.284	1.183	161	-0.021	0.027	15.38	33.125	MT1-Frnt	5	86	IHL10
39	2012/10/11 20:58:59	1-05	2	-0.511	-5.025	19723	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.8479	0.223	1.087	170	-0.014	-0.008	15.93	33.125	MT1-Frnt	5	86	IHL10
40	2012/10/11 21:07:47	1-05	3	-0.517	-4.174	19775	-1	1	W-1001 / / 208 / 808	OH13	H2O	284.85402	0.253	1.435	171	-0.016	0.05	16.6	33.063	MT1-Frnt	5	86	IHL10
41	2012/10/11 21:16:35	1-05	4	-0.486	-3.643	19504	0	1	W-1001 / / 208 / 808	OH13	H2O	284.86015	0.253	1.289	158	-0.016	0.029	15.14	33.125	MT1-Frnt	5	86	IHL10
42	2012/10/11 21:25:23	1-05	5	-0.519	-4.633	19581	0	1	W-1001 / / 208 / 808	OH13	H2O	284.86627	0.238	1.406	150	-0.016	-0.007	14.9	33.125	MT1-Frnt	5	86	IHL10
43	2012/10/11 21:34:12	1-05	6	-0.527	-4.506	19689	0	1	W-1001 / / 208 / 808	OH13	H2O	284.87241	0.278	1.049	155	-0.022	-0.022	14.91	33.125	MT1-Frnt	5	86	IHL10
44	2012/10/11 21:43:00	1-05	7	-0.511	-3.725	19673	0	1	W-1001 / / 208 / 808	OH13	H2O	284.87851	0.219	1.197	154	-0.014	0.023	15.3	33.125	MT1-Frnt	5	86	IHL10
45	2012/10/11 21:51:48	1-05	8	-0.407	-3.555	19734	0	1	W-1001 / / 208 / 808	OH13	H2O	284.88463	0.235	0.979	163	-0.018	0.036	15.61	33.125	MT1-Frnt	5	86	IHL10
46	2012/10/11 22:00:36	1-05	9	-0.524	-4.266	19678	0	1	W-1001 / / 208 / 808	OH13	H2O	284.89071	0.226	1.165	165	-0.016	0.01	15.56	33.125	MT1-Frnt	5	86	IHL10
47	2012/10/11 22:09:23	1-06	1	-4.943	-36.489	19340	-1	1	W-1002 / / 208 / 808	OH14	H2O	284.89683	0.272	1.25	151	-0.018	0.001	14.59	33.125	MT1-Frnt	6	86	IHL10
48	2012/10/11 22:18:12	1-06	2	-4.878	-36.861	19899	-1	1	W-1002 / / 208 / 808	OH14	H2O	284.90295	0.247	1.089	166	-0.016	0.006	15.69	33.125	MT1-Frnt	6	86	IHL10

HBDS42_IsoWater_20121011_154644

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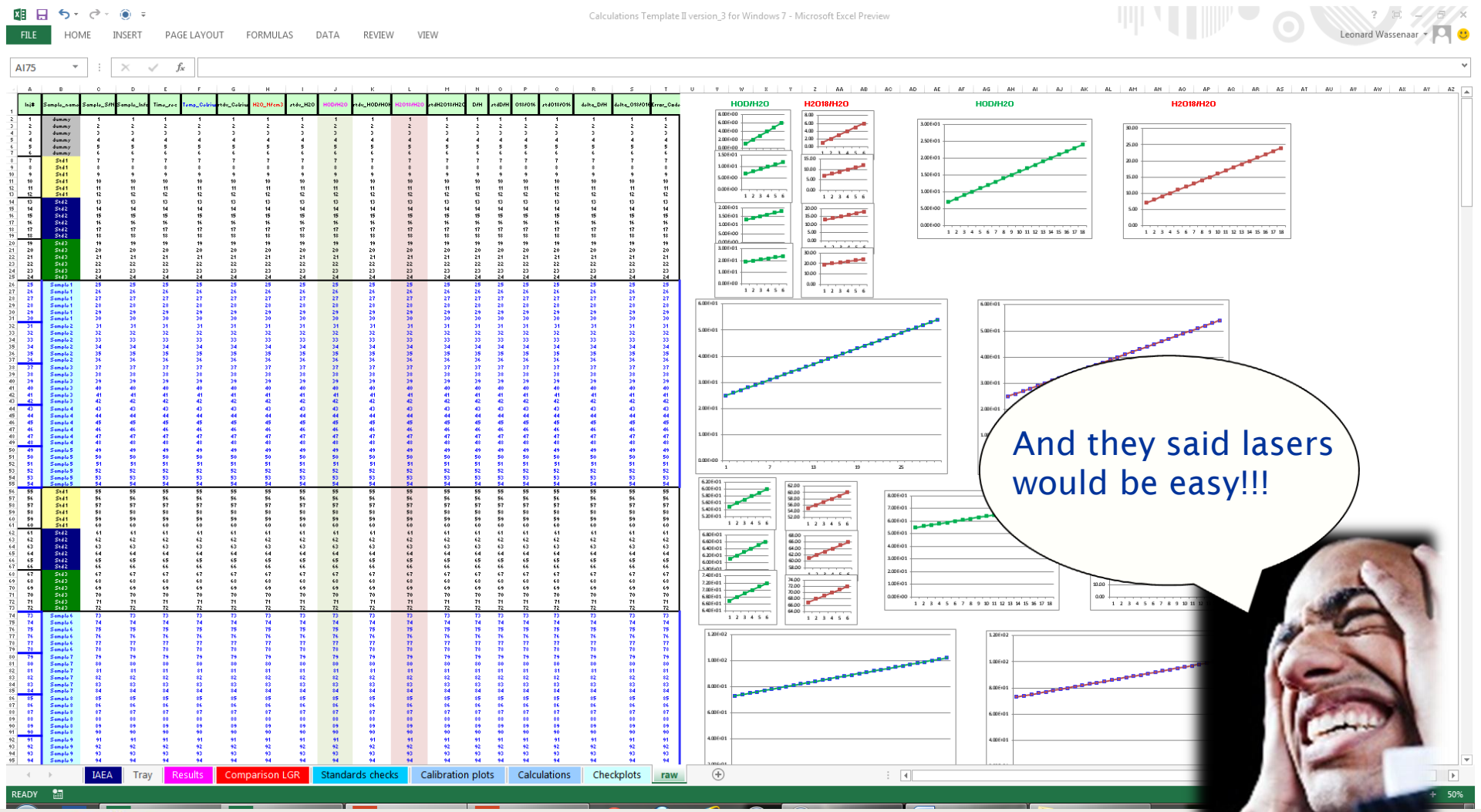
Required Checks / Corrections

1. Locate “bad” samples based on H_2O yield.
2. Determine inter-sample memory / carryover corrections.
3. Correct for linearity (variable water – syringe).
4. Ignore first 2-4 injections to reduce memory.
5. Adjust for instrumental drift (linear or non-linear).
6. Normalization to VSMOW/SLAP Scales.
7. Track lab QA/QC over time.

Can YOU do all of this easily using Excel?

IAEA

Corrections in Excel – IAEA



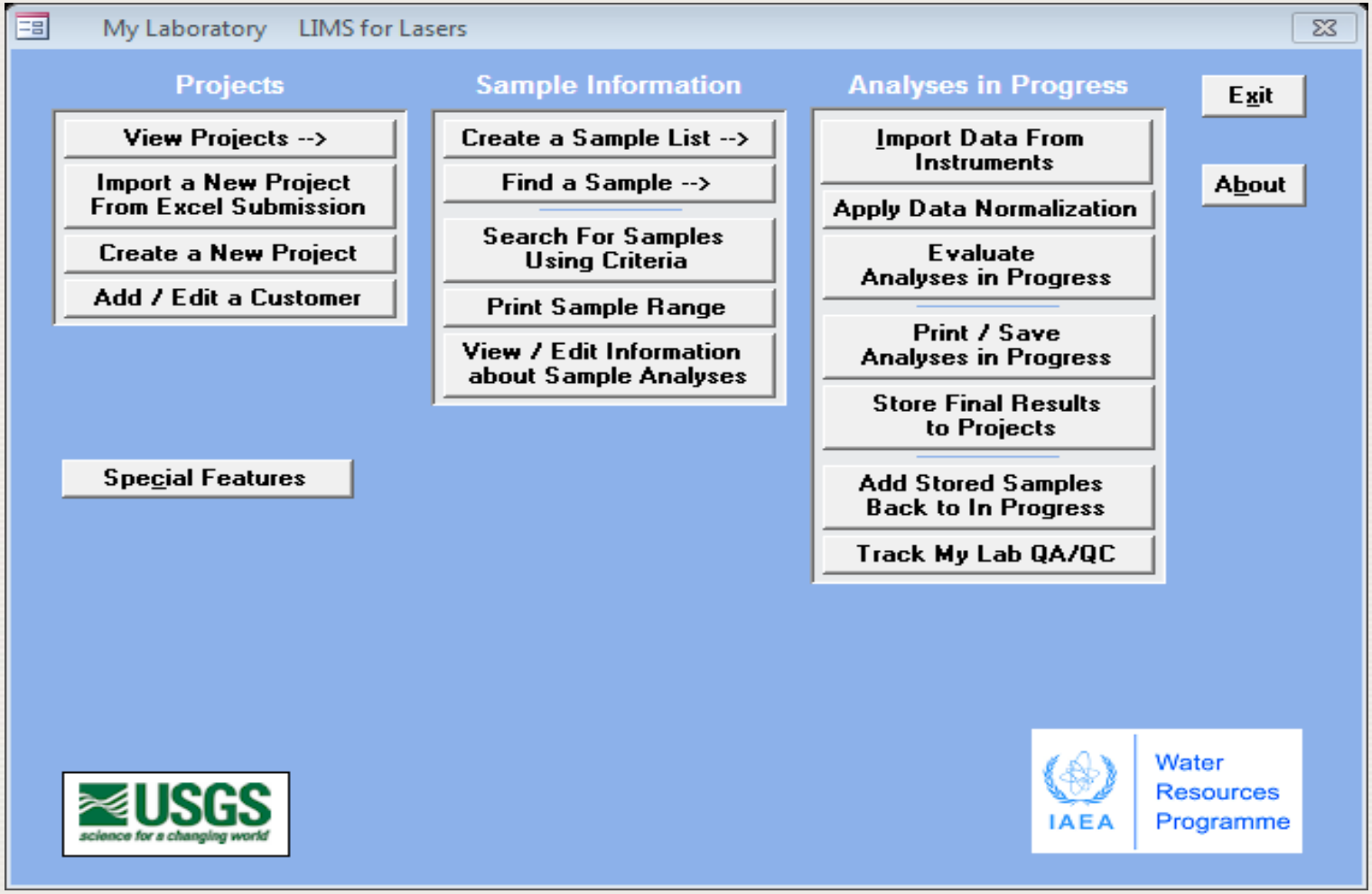
IAEA

LIMS for Lasers

- New software dedicated to laser spectroscopy co-developed by USGS and IAEA in 2012.
- Graphical user interface (Windows/Access).
- LIMS automates all required checks and corrections with a few mouse clicks.
- Uses IT approach with systematic templates.
- Manage multiple instruments (lasers/IRMS v9).
- Complete client, project and sample management package for the long-term.

IAEA

Introducing *LIMS for Lasers*



IAEA

LIMS for Lasers – Outline

- Install *LIMS for Lasers* for laboratory.
- Customize LIMS for your laboratory, install instruments.
- Create a client, projects and test samples.
- Create laboratory and control standards, instrument run-list templates.
- Import LAS data from Picarro and LGR.
- Apply between-sample memory corrections, drift, or check for bad analyses.
- Normalize the data to VSMOW/SLAP scales.
- Evaluate results of samples and control.
- Storing and reporting of client data.
- Tracking QA/QC.

IAEA

Help into the future

LIMS for Lasers & User Manual

Your comments and feedback will be considered to improve the software and manual

IAEA Support

We can troubleshoot your backend database via email or phone.

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