Improved results handling for the Total Petroleum Hydrocarbon (TPH) testing of soils and leachates by Gas Chromatography using Links for LIMS

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Background

Total Petroleum Hydrocarbons (TPH) in any soil analysis are defined as all of the hydrocarbons extractable by the test method from the sample within the carbon range from circa C_8 to circa C_{40} . This range is appropriate for the determination of contamination caused by products such as diesel, fuel, heating and lubricating oils, paraffin / kerosene and white spirit. In soils the method is used to determine components in the 1 to 1000 mg/kg concentration range where the limit of detection is 1 mg/kg.

A popular choice for this analysis is an Agilent 6890 or 7890 Gas Chromatograph (GC) used with the OpenLab CDS desktop software. Figure 2: Links for LIMS result review screen with sample names and qualifier codes. A set of automated filtering calculations have been applied automatically. Note some columns and/or samples are greyed out as these are not required for LIMS upload.

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	Sample Name	Qual	Dil	C8-C10	C10-C12	C10-C16	C10-C24	C10-C40	C12-C16	C16-C21	C16-C24	C16-C35	C21-C34	C21-C35	C21-C40	C24-C40	C25-C40	C35-C44
43	86206	aro	1	1.54	0.20	0.00	1.32	8.16	0.00	0.73	0.00	7.82	0.00	7.09	7.23	0.00	0.00	0.14
44	86207	ali	1	0.52	0.00	0.00	0,60	10.69	0.00	0.25	0.00	10.24	0.00	9.99	10.44	0.00	0.00	0.45
45	86207	aro	1	1.42	0.18	0.00	1.18	4.86	0.00	0.70	0.00	4.44	0.00	3.74	3.98	0.00	0.00	0.24
46	86208	ali	1	0.50	0.00	0.00	4.23	8.65	0.07	1.76	0.00	8.18	0.00	6.42	6.81	0.00	0.00	0.40
47	86208	aro	1	1.43	0.17	0.00	3.84	7.29	0.00	1.66	0.00	7.01	0,00	5.35	5.45	0.00	0.00	0.10
48	Blank		1	0.87	0.00	0.00	0.02	1,59	0.00	0.02	0.00	0.00	0.00	1.29	1,57	0.00	0.00	0.00
49	AQC		1	1.59	0.49	0.00	139.42	333.33	21.21	62.00	0.00	0.00	0.00	219.76	249.64	0.00	0.00	0.00
50	Check		1	5.31	20,77	0.00	844.84	1345.00	198.67	444.95	0.00	0.00	0.00	857.36	680.41	0.00	0.00	0.00
51	hex		1	0.15	0.19	0.00	5,14	57.03	0.00	1.08	0.00	0.00	0.00	47.62	55.76	0.00	0.00	0.00
52	check		1	5.21	14.72	0.00	853.82	1414.00	196.37	450.04	0.00	0.00	0.00	740.69	752.51	0.00	0.00	0.00
53	86106	ali	1	0.53	0.30	0.00	2.18	7.72	0.31	0.95	0.00	6.92	0.00	5.97	6.15	0.00	0.00	0.18
54	86106	aro	1	1.04	0.00	0.00	2.71	13.83	0.00	1.56	0.00	12,67	0.00	11.11	12.27	0.00	0.00	1.16
55	86107	ali	1	0.30	0.00	0.00	0.40	3.77	0.00	0.10	0.00	3.63	0.00	3.53	3.67	0.00	0.00	0.14
56	86107	aro	1	0.87	0.00	0.00	1,71	7,11	0.00	0.84	0.00	6.93	0.00	6.09	6,27	0.00	0.00	0.18
57	86108	ali	1	0.30	0.00	0.00	0.95	7.12	0.00	0.31	0.00	6.68	0.00	6.38	6,81	0.00	0.00	0.43
58	86108	aro	1	0.93	0.00	0.00	4.06	12.42	0.00	1.59	0.00	11.35	0.00	9.76	10.83	0.00	0.00	1.07
59	86109	ali	1	0.33	0.00	0.00	1.82	6.93	0.00	0.75	0.00	6.74	0.00	5.99	6.19	0.00	0.00	0.19
60	86109	aro	1	0.93	0.00	0.00	4.70	12.35	0.00	1.84	0.00	12,15	0.00	10.31	10.51	0.00	0.00	0.20
61	86116	ali	1	0.35	0.13	0.00	1420.00	>6000.00	8.03	197.95	0.00	21020.00	0.00	20820.00	20930.00	0.00	0.00	109.39
62	86116	aro	1	0.62	1.48	0.00	499.31	7131.00	3.96	71.58	0.00	7104.00	0.00	7032.00	7054.00	0.00	0.00	21.06
63	86141	ali	1	0.30	0.00	0.00	0.00	4.49	0.00	0.00	0.00	4.05	0.00	4.05	4.49	0.00	0.00	0.43
64	86144	ali	1	0.38	0.00	0.00	1.26	8.38	0.00	0.31	0.00	8.18	0.00	7.87	8.07	0.00	0.00	0.21
65	86146	ali	1	0.46	0.00	0.00	0.89	4.85	0.00	0.47	0.00	4.70	0.00	4.23	4,38	0.00	0.00	0.15
66	86166	ali	1	0.64	2.64	0.00	100.50	107.24	76.41	20.74	0.00	28.02	0.00	7.28	7.44	0.00	0.00	0.16
67	86167	ali	1	0.68	5.47	0.00	180.47	188.25	134.74	38.88	0.00	47.89	0.00	9:01	9.17	0.00	0.00	0.16
68	86168	ali	1	0.71	9.39	0.00	236.45	263.73	172.81	50.37	0.00	80.68	0.00	30.31	31,16	0.00	0.00	0.84
69	86169	ali	1	0.63	5.27	0.00	175.73	185.66	129.26	38.96	0.00	50.96	0.00	12.00	12.17	0.00	0.00	0.17
70	86170	ali	1	0.47	0.00	0.00	10.13	20.38	0.00	2.84	0.00	20.20	0.00	17.36	17.55	0.00	0.00	0.18
71	86174	ali	1	0.53	0.00	0.00	0.00	4.30	0.00	0.00	0.00	4.07	0.00	4.07	4,30	0.00	0.00	0.23
72	86174	aro	1	0.89	0.00	0.00	0.41	1.99	0.00	0.41	0.00	1.99	0.00	<mark>1.58</mark>	1,58	0.00	0.00	0.00
73	Blank		1	1,12	0.08	0.00	0.62	3.09	0.10	0.45	0.00	0.00	0.00	2.20	2.47	0.00	0.00	0.00
74	AQC		1	2.20	0.35	0.00	134.02	328.18	19.86	58.68	0.00	0.00	0.00	230,89	249.29	0.00	0.00	0.00
75	Check		1	5.43	15.34	0.00	866.89	1432.00	198.78	457.43	0.00	0.00	0.00	746.05	760.29	0.00	0.00	0.00
76	86209	ali	1	0.33	0.00	0.00	0,48	4.82	0.00	0.18	0.00	4.66	0.00	4,48	4.64	0.00	0.00	0.16
77	86209	aro	1	0.94	0.00	0.00	0.91	4.30	0.00	0.65	0.00	4.13	0.00	3.48	3.65	0.00	0.00	0.17



laboratory systems integration



Challenges

Challenges with this analysis arise as follows:

- Unplanned/unexpected samples containing large concentrations of TPH which can contaminate the instrument and column and render it unusable.
- The handling of results from groups rather than discrete components.
- Dealing with mixtures of sample types in a single run where turnaround time is important.
- Flagging of over range samples and results and the alignment to LIMS test codes.

Improved Result handling

This poster describes how the CSols **Links for LIMS** software application can address these challenges and hence provide a streamlined mechanism for working with the TPH method and OpenLab to maximize the productivity of the instrument.

Instrument loading

Many laboratories work with LIMS worklists. A worklist is typically a batch of samples which have been registered together at the same time (First in, first out - FIFO), assigned the same method and prepared together. Without filtering based on some other biographical criteria, there is a danger that highly concentrated samples can be randomly placed with other samples. This might lead to inadvertent contamination of the instrument. With **Links for LIMS** generating worklists, it's easy to add further criteria when building the lists, to extract additional LIMS data to highlight potential concentrated samples and as a fall back easily remove or move samples in the batch sequence before analysis.

System Messi	ige>																	
4																		F
84	86238	ali	1	0.35	0.00	0.00	0.50	3.37	0.00	0.14	0.00	3.23	0.00	3.09	3.23	0.00	0.00	0.13 💌
83	86236	aro	1	1.15	0.00	0.00	0.73	3.32	0.00	0.68	0.00	3.32	0.00	2.64	2.64	0.00	0.00	0.00
	00200	ali	1	0.37	0.00	0.00	0.00	3.13	0.00	0.00	0.00	2.97	0.00	2.97	3.13	0.00	0.00	0.16
82	86236	- Fi	100															

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Groups not components

When working with the TPH results the **Links for LIMS** instrument 'driver' automatically extracts group data contained in the 'group' report section of the OpenLab rather than component data for each sample in the batch.

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		Summed Peaks Report								
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	Name	Start Time [min]	End Time [min]	[pA*s]	[mg/kg]					
	C8-C10	3,600	5.000	5.15626	1.6793					
	C8-C40	3,600	13,950	5.15626 41.18691 3.68572e-1	13,4138					
	C10-C12	5.000	5.850	3.68572e-1	0.1200					
	C10-C24	5,000	8,660	3,65359	1.1899					
	C10-C40	5.000	13.950	36.03064	11.7345					
	C16-C21	6.960	8.090	2.12548	0.6922					
	C16-C35	6.960	11.050	34.92192	11.3734					
	C21-C35	8.090	11.050	3.65359 36.03064 2.12548 34.92192 32.79644	10.6812					
	C21-C40	8.090	13.950	33.53659 7.40146e-1	10.9222					
	C35-C44	11.050	18.950	7.40146e-1	0.2411					
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		Total Area [pA*s]	[mg/kg]							
		Total Area [pA*s]	[mg/kg]	r						
	 C8-C10	Total Area [pA*s] 	[mg/kg]	I.						
	C8-C10 C8-C40	Total Area [pA*s] 5.15626 41.18691	[mg/kg] 1.6793 13.4138	I.						
	C8-C10 C8-C40 C10-C12	Total Area [pA*s] 	[mg/kg] 1.6793 13.4138 0.1200	I.						
	C8-C10 C8-C40 C10-C12 C10-C24	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359	[mg/kg] 1.6793 13.4138 0.1200 1.1899	L.						
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40	Total Area [pA*s] 	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345	L.						
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734	Ľ						
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C40	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C40 C35-C44	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C35 C21-C40 C35-C44 C8	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567	1						
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C35 C21-C40 C35-C44 C8 C10	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C24 C16-C21 C16-C21 C16-C35 C21-C35 C21-C35 C21-C40 C35-C44 C8 C10 C12	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1 0.00000	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594 0.0000							
	 C8-C10 C8-C40 C10-C12 C10-C24 C10-C21 C16-C21 C16-C35 C21-C35 C21-C35 C21-C40 C35-C44 C8 C10 C12 C16	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1 0.00000 0.00000	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594 0.0000 0.0000							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C40 C35-C44 C8 C10 C12 C16 C21	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1 0.00000 0.00000 6.32814e-1	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594 0.0000 0.0000 0.1778	Γ						
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C35 C21-C40 C35-C24 C8 C10 C12 C16 C21 C24	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1 0.00000 6.32814e-1 3.20680e-1	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594 0.0000 0.0798							
	C8-C10 C8-C40 C10-C12 C10-C24 C10-C40 C16-C21 C16-C35 C21-C35 C21-C40 C35-C44 C8 C10 C12 C16 C21	Total Area [pA*s] 5.15626 41.18691 3.68572e-1 3.65359 36.03064 2.12548 34.92192 32.79644 33.53659 7.40146e-1 2.55302 2.68036e-1 0.00000 0.00000 6.32814e-1	[mg/kg] 1.6793 13.4138 0.1200 1.1899 11.7345 0.6922 11.3734 10.6812 10.9222 0.2411 0.6567 0.0594 0.0000 0.0000 0.1778 0.778 0.798 0.1172							

Mixture of samples

C40 C44 Totals :

Busy laboratories will want to maximize the use of their instruments and will often mix samples of different types

0.00000 0.0000 5.30866 3.1302

Detection limits and over range samples

The qualifier codes further also allow the results to be correctly aligned to the correct respective detection limit settings. This will allow Links for LIMS to automatically report whether a specific result is under or over its detection limit. Results are flagged accordingly and if active the 'Autozap' rule will either set the result and/or sample to 'Zapped'. This does not delete the data but flags to LIMS how to treat the sample and save time for the analyst applying predefined procedures. e.g. the test could be repeated after dilution, simply report the results as high or the entire sample is zapped.

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57	86108	ali	1	0.30	0.00	0.00	0.95	7.12				
58	86108	aro	1	0.93	0.00	0.00	4.06	12.42				
59	86109	ali	1	0.33	0.00	0.00	1.82	6.93				
60	86109	aro	1	0.93	0.00	0.00	4.70	12.35				
61	86116	ali	1	0.35	0.13	0.00	1420.00	>6000.00				
62	86116	aro	1	0.62	1.48	0.00	499.31	7131.00				
63	86141	ali	1	0.30	0 🔄 C	ell Details	to be all	COLUMN TWO IS				
64	86144	ali	1	0.38	0	<u>a</u> l						
65	86146	ali	1	0.46	0							
66	86166	ali	1	0.64	2 SAN	IPLE POS	ITION 61					
67	86167	ali	1	0.68		ie on Scre	en		86116			
68	86168	ali	1	0.71		ie as Run			86116_ali			
69	86169	ali	1	0.63	5 LIMS	_	o ·		86116			
70	86170	ali	1	0.47		s for LIMS	Sample T	ype	LIMS Sample			
71	86174	ali	1	0.53		s for LIMS	Method		ТРН			
72	86174 Black	aro	1	0.89	0							
73	Blank		1	1.12 2.20	0	-C40						
74	AQC Check		1	5.43		ument Iter	n		C10-C40			
75	86209	ali	1	0.33		Value Ierical Val	lue		2.114e4 21140			
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	Sample Name	Qual	C8-C10	C10-C12	C10-C40	C12-C16	C16-C21
1	Rinse	ali					
2	Rinse	aro					
3	Hexane	ali					
4	Hexane	aro					
5	86076	ali					
6	86076	aro					
7	86077	ali					
8	86077	aro					
9	86078	ali					
10	86078	aro					
11	86079	ali					
12	86079	aro					
13	86100	ali					
14	86100	aro					
15	86101	ali					
16	86101	aro					
17	86078	ali					
18	86078	aro					
19	86078	ali					
20	86078	aro					
21	86079	ali					
22	86079	aro					
23	86100	ali					
24	86100	aro					
25	86100	ali					
26	86100	aro					
27	2201548	ali					

Figure 1: Run extracted from LIMS ready for instrument setup

in batch runs. However while the TPH GC analysis method may not vary for different sample types, each type will either require different groups of components to be reported, and/or will have a unique LIMS test (determinand) code. Without the application of some logic at the instrument level, it is often impossible for a LIMS to cope directly with this large matrix of sample type/group/test codes in a result export, and will require results to be input manually. Links for LIMS however uses 'qualifier codes' to label each sample, and logic set into the Links for LIMS TPH

method is able to automatically align types, groups and test codes together, making it simple for the analyst to process results quickly.

Summary

Links for LIMS can be used to automatically apply a complex set of rules tuned to the TPH method running on a set of GC instrument results running OpenLab. This saves valuable analyst time freeing them up to perform further laboratory tasks.

Further Information

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