

# 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<sub>8</sub> to circa C<sub>40</sub>. 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.

## 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.

Sample Name	Qual	C8-C10	C10-C12	C10-C40	C12-C16	C16-C21
1. Rinse	all					
2. Rinse	aro					
3. Hexane	all					
4. Hexane	aro					
5. 86076	all					
6. 86076	aro					
7. 86077	all					
8. 86077	aro					
9. 86078	all					
10. 86078	aro					
11. 86079	all					
12. 86079	aro					
13. 86100	all					
14. 86100	aro					
15. 86101	all					
16. 86101	aro					
17. 86078	all					
18. 86078	aro					
19. 86078	all					
20. 86078	aro					
21. 86079	all					
22. 86079	aro					
23. 86100	all					
24. 86100	aro					
25. 86100	all					
26. 86100	aro					
27. 2261548	all					

Figure 1: Run extracted from LIMS ready for instrument setup

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.

Sample Name	Qual	Df	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	1.30	0.16	0.00	0.73	0.00	7.80	0.00	7.09	7.23	0.00	0.00	0.14	
44. 86207	all	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	1.16	0.00	0.00	0.70	0.00	1.81	0.00	3.74	3.88	0.00	0.00	0.24	
46. 86208	all	1	0.50	0.00	0.00	4.23	8.65	0.07	1.76	0.00	8.18	0.00	4.42	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	7.51	0.00	5.35	5.45	0.00	0.00	0.10	
48. Blank																		
49. AQC																		
50. Check																		
51. hex																		
52. Check																		
53. 86106	all	1	0.53	0.30	0.00	2.10	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	13.85	0.00	1.56	0.00	12.67	0.00	11.11	12.27	0.00	0.00	1.18	
55. 86107	all	1	0.30	0.00	0.00	0.40	3.77	0.00	0.10	0.00	3.63	0.00	3.55	3.67	0.00	0.00	0.14	
56. 86107	aro	1	0.27	0.00	0.00	0.71	7.11	0.00	0.84	0.00	7.52	0.00	6.09	6.27	0.00	0.00	0.16	
57. 86108	all	1	0.30	0.00	0.00	0.95	7.12	0.00	0.31	0.00	6.68	0.00	6.09	6.27	0.00	0.00	0.43	
58. 86108	aro	1	0.93	0.00	0.00	4.00	12.42	0.00	1.59	0.00	11.35	0.00	9.76	10.83	0.00	0.00	1.07	
59. 86109	all	1	0.33	0.00	0.00	1.62	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	12.20	0.00	1.84	0.00	12.25	0.00	10.31	10.51	0.00	0.00	0.20	
61. 86116	all	1	0.35	0.13	0.00	1420.00	>6000.00	0.00	0.00	0.00	21020.00	0.00	2000.00	2000.00	0.00	0.00	109.39	
62. 86116	aro	1	0.62	1.48	0.00	499.31	7111.00	0.00	3.96	71.58	0.00	7111.00	0.00	7322.00	7354.00	0.00	0.00	21.06
63. 86141	all	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	all	1	0.38	0.00	0.00	1.38	8.38	0.00	0.31	0.00	8.18	0.00	7.87	8.07	0.00	0.00	0.21	
65. 86146	all	1	0.46	0.00	0.00	0.69	4.85	0.00	0.47	0.00	4.70	0.00	4.23	4.38	0.00	0.00	0.15	
66. 86166	all	1	0.64	2.64	0.00	1100.50	107.24	76.41	20.74	0.00	28.62	0.00	7.28	7.44	0.00	0.00	0.16	
67. 86167	all	1	0.68	5.47	0.00	180.67	188.25	134.74	38.89	0.00	47.89	0.00	9.81	9.17	0.00	0.00	0.16	
68. 86168	all	1	0.71	9.39	0.00	230.45	263.73	172.81	50.37	0.00	30.68	0.00	30.31	31.16	0.00	0.00	0.84	
69. 86169	all	1	0.63	5.27	0.00	175.73	185.66	129.26	38.96	0.00	50.98	0.00	12.00	12.17	0.00	0.00	0.17	
70. 86170	all	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	all	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	1.30	0.00	0.41	0.00	1.30	0.00	1.58	1.58	0.00	0.00	0.00	
73. Blank																		
74. AQC																		
75. Check																		
76. 86209	all	1	0.33	0.00	0.00	0.40	4.82	0.00	0.18	0.00	4.66	0.00	4.45	4.64	0.00	0.00	0.16	
77. 86209	aro	1	0.94	0.00	0.00	0.91	4.31	0.00	0.65	0.00	4.11	0.00	3.48	3.65	0.00	0.00	0.17	
78. 86217	all	1	0.33	0.00	0.00	0.31	4.29	0.00	0.09	0.00	4.07	0.00	3.95	4.15	0.00	0.00	0.22	
79. 86218	all	1	0.34	0.00	0.00	0.54	4.72	0.00	0.16	0.00	4.55	0.00	4.30	4.56	0.00	0.00	0.17	
80. 86233	all	1	0.36	0.00	0.00	0.13	3.59	0.00	0.13	0.00	3.39	0.00	3.28	3.45	0.00	0.00	0.19	
81. 86233	aro	1	1.30	0.00	0.00	0.69	3.50	0.00	0.69	0.00	3.50	0.00	2.91	2.91	0.00	0.00	0.00	
82. 86236	all	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	
83. 86236	aro	1	1.15	0.00	0.00	0.73	8.01	0.00	0.68	0.00	7.13	0.00	2.54	2.84	0.00	0.00	0.00	
84. 86236	all	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	

## 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.

Summed Peaks Report

Signal	Start Time (min)	End Time (min)	Total Area (µA*s)	Amount (mg/kg)
CB-C10	3.600	8.000	5.15626	1.4793
CB-C40	13.950	41.18691	13.4138	1.12891
C10-C12	9.000	3.48372e+1	3.4200	0.95359
C10-C24	5.000	3.45359	1.1899	36.03064
C10-C40	5.000	13.950	36.03064	11.7945
C16-C21	6.960	11.050	2.12548	0.6922
C16-C35	6.960	11.050	34.92192	11.3734
C21-C35	8.090	11.050	32.79444	10.4812
C21-C40	8.090	13.950	33.53659	10.9222
C35-C44	11.050	16.950	7.40146e-1	0.2411
Totals				62.0477

Figure 3: Example OpenLab group sample report file

## 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.

Sample Name	Qual	Df	C8-C10	C10-C12	C10-C40	C12-C16	C16-C21
57. 86108	all	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	all	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	all	1	0.35	0.13	0.00	1420.00	>6000.00
62. 86116	aro	1	0.62	1.48	0.00	499.31	7111.00
63. 86141	all	1	0.30	0.00	0.00	0.00	4.49
64. 86144	all	1	0.38	0.00	0.00	1.38	8.38
65. 86146	all	1	0.46	0.00	0.00	0.69	4.85
66. 86166	all	1	0.64	2.64	0.00	1100.50	107.24
67. 86167	all	1	0.68	5.47	0.00	180.67	188.25
68. 86168	all	1	0.71	9.39	0.00	230.45	263.73
69. 86169	all	1	0.63	5.27	0.00	175.73	185.66
70. 86170	all	1	0.47	0.00	0.00	10.13	20.38
71. 86174	all	1	0.53	0.00	0.00	0.41	1.30
72. 86174	aro	1	0.89	0.00	0.00	0.41	1.30
73. Blank							
74. AQC							
75. Check							
76. 86209	all	1	0.33	0.00	0.00	0.40	4.82

Figure 4: Result detail for the over range sample showing rule applied.

## Mixture of samples

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