



ChemAxon
discovery informatics

JChem Web Services

The New Story

Gabor Guta

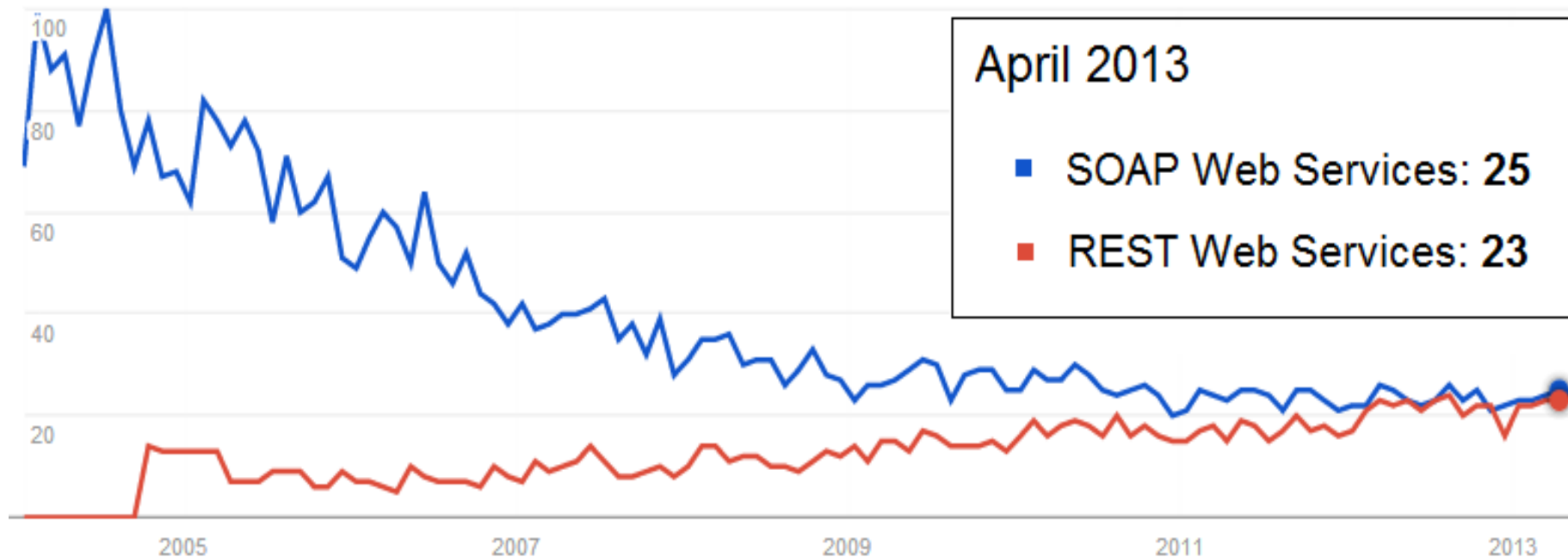
Jonathan Lee



Agenda

- The birth of the new **REST API**
- The **Cloud** experiment
- Explaining the **Web Services products**
- **Advantages** of the Web Services

Trends in Web Services Technology



Source: Google Trends

The background of the image is a dark, black space filled with numerous thin, silver-colored wires. These wires are arranged in a grid-like pattern, with some wires being straight and others curving. Small, reflective spheres are attached to the wires, creating a shimmering, metallic effect. The overall aesthetic is futuristic and technical.

Thin Clients

Python

PHP

JavaScript

Easy to Learn



Ready for Integration



The JavaScript Experiment

Plexus – JavaScript Application

Marvin for JS

Backend – REST web services

Caching/
Meta-data/
Monitoring

JChem
Base

Calculators

Markush
Enum.

Etc.

Functionality

Connection
Management

Meta-data
Handling

ChemAxon JChem

Caching

Progress
Monitoring

The Cloud Experiment

Simple to deploy

Stateless functions

Distributed JChem Search

No Built-in Split & Merge Currently

Available Products

JChem „Classic” Web Services

This is **our existing SOAP** Web Service platform – 5.x

JChem Web Services

Our brand **new REST** Web Services product – 6.0



Provided Services

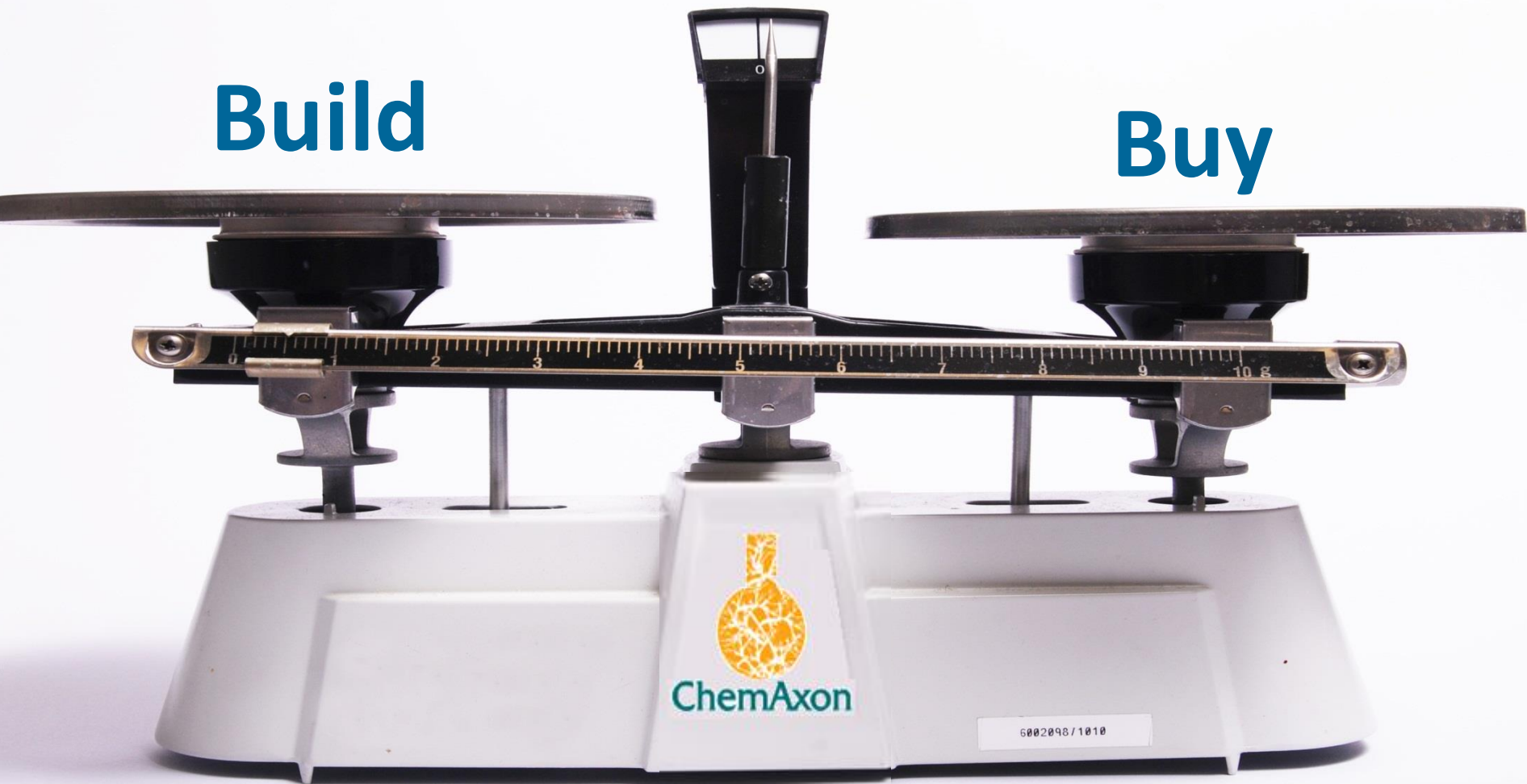
Service Category	SOAP	REST
Database	Yes	6.0
Molecular Conversion	Yes	6.0
Chemical Terms	Yes	6.0
Markush Enumeration	Yes	6.0
Standardization	Yes	6.1
Reactor	Yes	6.1
Admin Functions	No	6.0
Authentication / ACL	No	6.1

Service APIs

- SOAP API
 - <http://www.chemaxon.com/webservices/developers/Guide.html>
 - Chemical Terms Expressions
- REST API
 - <http://restdemo.chemaxon.com/>
 - Simple Format Conversion

Build

Buy



Why in-house development is hard?

”It is **three times** as **difficult to build reusable** components as single use components...”

”...a reusable component **should be tried out** in **three different applications** before it will be sufficiently general to accept into a reuse library.”

“Biggerstaff's Rules of Three.”

Road Map

- **Integration** with Registration System and IJC Web Client
- **Expose all** of the existing **features**
- **Authentication/Access Control**
- Built in **distributed** functionality

Summary

- New **REST API**
- Experiments in the **Cloud**
- **Maintenance strategy** of the products
- **Advantages** of the Web Services