Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

Supplemental Information for

Auto-QChem: an automated workflow for the generation and storage of DFT calculations for organic molecules

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Table S1: Features extracted from Gaussian log file and stored in qchem_descriptors collection in the DB for fast access.

Molecular Features	Atom Features	Vibrational Modes	Excited State Transitions
charge	APT_charge	Frequencies	ES_transition
multiplicity	Mulliken_charge	Red masses	ES_osc_strength
number_of_atoms	ES_root_Mulliken_charge	Frc consts	ES_<S**2>
molar_mass	NPA_charge	IR Inten	
molar_volume	ES_root_NPA_charge	Dip str	
ES_root_molar_volume	NPA_core	Rot str	
electronic_spatial_extent	ES_root_NPA_core	E-M angle	
ES_root_electronic_spatial_extent	NPA_valence	X	
dipole	ES_root_NPA_valence	Y	
ES_root_dipole	NPA_Rydberg	Z	
G	ES_root_NPA_Rydberg		
G_thermal_correction	NMR_shift		
H	NMR_anisotropy		
H_thermal_correction	Vbur		
E	X		
E_thermal_correction	Y		
E_scf	Z		
E_zpe			
zero_point_correction			
homo_energy			
lumo_energy			
electronegativity			
hardness			