Yasuda-Shedlovsky Result

Sample name:	**CS000031**	Experiment start time:	**29/08/2011 10:16:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.72	±0.01	11.70	-408.8448	0.9952	0.204 M	26.5°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29005 Points 105 to 156	19.23 %	Up	UV-metric pKa	77.0	45.5 M	0.209 M	26.6°C	☑	4.73
11H-29005 Points 53 to 104	26.12 %	Up	UV-metric pKa	76.7	41.9 M	0.205 M	26.4°C	☑	4.75
11H-29005 Points 3 to 52	35.43 %	Up	UV-metric pKa	76.0	36.9 M	0.197 M	26.5°C	☑	4.76

Graphs

Sample name:	**CS000031**	Experiment start time:	**29/08/2011 10:16:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29005 Points 3 to 52

Graphs

Sample name:	**CS000031**	Experiment start time:	**29/08/2011 10:16:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29005 Points 53 to 104

Graphs

Sample name:	**CS000031**	Experiment start time:	**29/08/2011 10:16:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29005 Points 105 to 156

Graphs

Sample name:	**CS000031**	Experiment start time:	**29/08/2011 10:16:07**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29005**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000031		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	406.46		
Individual pKa ionic environments	No		
Number of pKas	1	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	29/08/2011 10:14:12	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r