Yasuda-Shedlovsky Result

Sample name:	**CS000150**	Experiment start time:	**29/08/2011 14:29:54**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29015_CS000150_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	7.60	±0.01	4.49	376.4980	0.9929	0.208 M	27.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-29015 Points 106 to 157	23.26 %	Up	UV-metric pKa	76.3	43.3 M	0.211 M	28.0°C	☑	7.78
11H-29015 Points 54 to 105	32.15 %	Up	UV-metric pKa	75.9	38.6 M	0.211 M	27.6°C	☑	7.87
11H-29015 Points 3 to 53	43.15 %	Up	UV-metric pKa	74.8	32.7 M	0.201 M	27.8°C	☑	8.01

Graphs

Sample name:	**CS000150**	Experiment start time:	**29/08/2011 14:29:54**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29015_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11H-29015 Points 3 to 53

Graphs

Sample name:	**CS000150**	Experiment start time:	**29/08/2011 14:29:54**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29015_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11H-29015 Points 54 to 105

Graphs

Sample name:	**CS000150**	Experiment start time:	**29/08/2011 14:29:54**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29015_CS000150_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11H-29015 Points 106 to 157

Graphs

Sample name:	**CS000150**	Experiment start time:	**29/08/2011 14:29:54**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11H-29015**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-29015_CS000150_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000150		
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	385.40		
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