Yasuda-Shedlovsky Result

Sample name:	**CS000095**	Experiment start time:	**26/07/2011 16:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26022_CS000095_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.05	±0.05	19.04	-1094.6436	0.9851	0.202 M	29.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11G-26022 Points 119 to 178	24.52 %	Up	UV-metric pKa	75.9	42.7 M	0.209 M	29.0°C	☑	3.01
11G-26022 Points 60 to 118	32.71 %	Up	UV-metric pKa	75.4	38.3 M	0.204 M	28.9°C	☑	2.91
11G-26022 Points 3 to 59	43.84 %	Up	UV-metric pKa	73.5	32.3 M	0.192 M	31.3°C	☑	2.64

Graphs

Sample name:	**CS000095**	Experiment start time:	**26/07/2011 16:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26022_CS000095_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11G-26022 Points 3 to 59 Quality: Good

Graphs

Sample name:	**CS000095**	Experiment start time:	**26/07/2011 16:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26022_CS000095_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11G-26022 Points 60 to 118 Quality: Good

Graphs

Sample name:	**CS000095**	Experiment start time:	**26/07/2011 16:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26022_CS000095_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11G-26022 Points 119 to 178 Quality: Good

Graphs

Sample name:	**CS000095**	Experiment start time:	**26/07/2011 16:50:56**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11G-26022**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1107\11G-26022_CS000095_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000095		
Sample by	Volume		
Sample volume	0.0200 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
Molecular weight	369.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
pKa 1	4.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logp (XH +)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r
logP (neutral X)	-10.00	26/07/2011 12:26:03	E:\T3 DATA\1107\11G-23004_CS000041_pH-metric psKa.t3r