Yasuda-Shedlovsky Result

Sample name:	**CS000166**	Experiment start time:	**07/09/2011 17:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07020**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07020_CS000166_Fast UV psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	3.82	±0.03	-5.42	860.5822	0.9840	0.201 M	25.6°C
Yasuda-Shedlovsky	8.87	±0.08	-7.69	1433.4789	0.9612	0.201 M	25.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1	
11I-07020 Points 105 to 157	19.88 %	Up	UV-metric pKa	77.4	45.2 M	0.206 M	25.4°C	☑	4.03	☑
11I-07020 Points 53 to 104	26.73 %	Up	UV-metric pKa	77.1	41.6 M	0.204 M	25.1°C	☑	4.14	☑
11I-07020 Points 3 to 52	35.84 %	Up	UV-metric pKa	76.0	36.7 M	0.194 M	26.3°C	☑	4.33	☑

Graphs

Sample name:	**CS000166**	Experiment start time:	**07/09/2011 17:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07020**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07020_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 1 of 3 11I-07020 Points 3 to 52

Graphs

Sample name:	**CS000166**	Experiment start time:	**07/09/2011 17:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07020**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07020_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 2 of 3 11I-07020 Points 53 to 104

Graphs

Sample name:	**CS000166**	Experiment start time:	**07/09/2011 17:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07020**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07020_CS000166_Fast UV psKa.t3r**		

Fast UV psKa Titration 3 of 3 11I-07020 Points 105 to 157

Graphs

Sample name:	**CS000166**	Experiment start time:	**07/09/2011 17:20:12**
Assay name:	**Fast UV psKa**	Analyst:	
Assay ID:	**11I-07020**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-07020_CS000166_Fast UV psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000166		
Sample by	Volume	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	446.49		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	4.00		
pKa 2	9.50		
logP (XH2 2+)	-10.00	07/09/2011 14:20:39	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logp (XH +)	-10.00		
logP (neutral X)	-10.00		