Yasuda-Shedlovsky Result

Sample name:	**cs000092**	Experiment start time:	**19/08/2011 15:28:02**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19013_cs000092_UV-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	3.34	±0.03	22.83	-1368.7619	0.9963	0.180 M	29.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11H-19013 Points 91 to 138	23.78 %	Up	UV-metric pKa	75.8	43.0 M	0.188 M	29.3°C	☑	3.14
11H-19013 Points 45 to 89	31.95 %	Up	UV-metric pKa	75.2	38.7 M	0.183 M	29.7°C	☑	3.05
11H-19013 Points 4 to 43	42.65 %	Up	UV-metric pKa	74.7	33.0 M	0.170 M	28.1°C	☑	2.98

Graphs

Sample name:	**cs000092**	Experiment start time:	**19/08/2011 15:28:02**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19013_cs000092_UV-metric psKa.t3r**		

UV-metric psKa Titration 1 of 3 11H-19013 Points 4 to 43

Graphs

Sample name:	**cs000092**	Experiment start time:	**19/08/2011 15:28:02**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19013_cs000092_UV-metric psKa.t3r**		

UV-metric psKa Titration 2 of 3 11H-19013 Points 45 to 89

Graphs

Sample name:	**cs000092**	Experiment start time:	**19/08/2011 15:28:02**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19013_cs000092_UV-metric psKa.t3r**		

UV-metric psKa Titration 3 of 3 11H-19013 Points 91 to 138

Graphs

Sample name:	**cs000092**	Experiment start time:	**19/08/2011 15:28:02**
Assay name:	**UV-metric psKa**	Analyst:	
Assay ID:	**11H-19013**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1108\11H-19013_cs000092_UV-metric psKa.t3r**		

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000092		
Sample by	Volume		
Sample volume	0.0080 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-mpsKa.t3r
Molecular weight	345.40		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	3.20		
logp (XH +)	-10.00	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-mpsKa.t3r
logP (neutral X)	-10.00	19/08/2011 11:40:08	E:\T3 DATA\1108\11H-15007-1_EX965325003-001_pH-mpsKa.t3r