Supporting information

A Hydroxylated – HMPA Enhances Both Reduction Potential and Proton Donation in SmI_2 Reactions.

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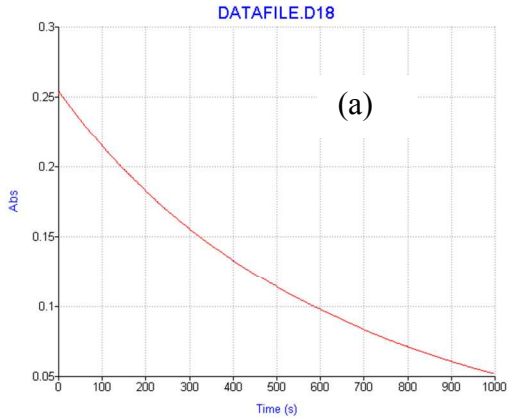
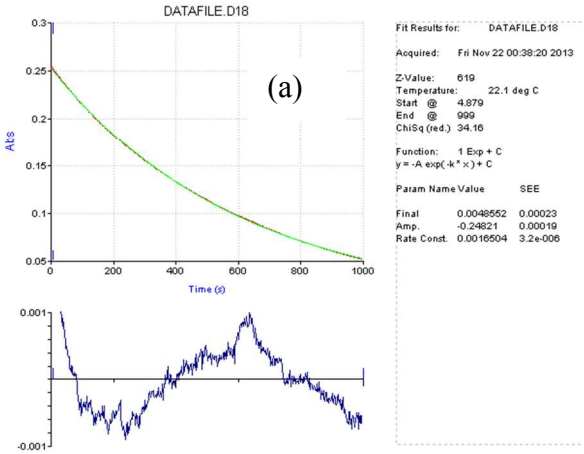
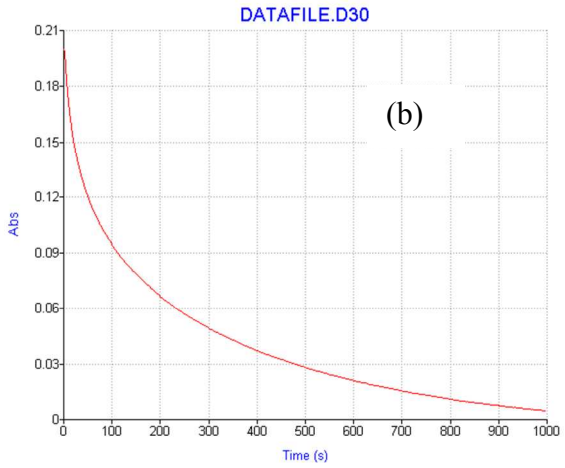
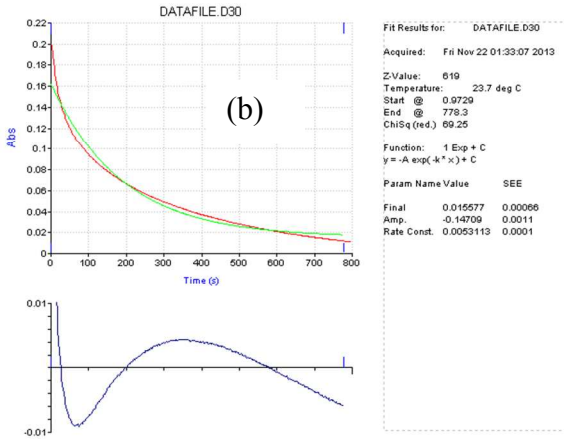
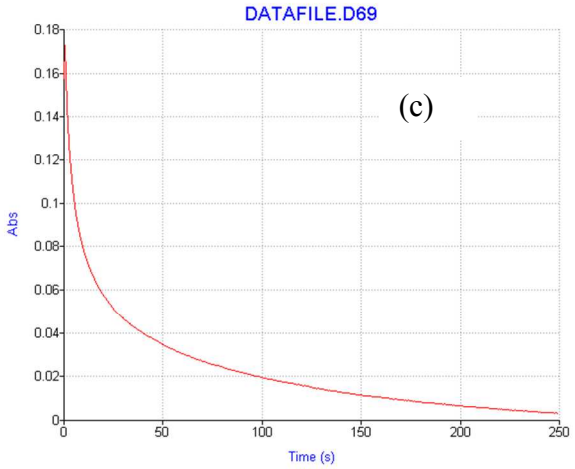
Figure S1: Kinetic trace and fit to a first-order analysis in the reaction of benzyl chloride (25mM), SmI_2 (2.5 mM) in the presence of; (a) 0 mM additive; (b) 5mM HOMPA; (c) 5mM HMPA; (d) 10mM HOMPA; (e) 10mM HMPA; (f) 15mM HOMPA; (g) 15mM HMPA; (h) 20mM HOMPA; (i) 20mM HMPA.







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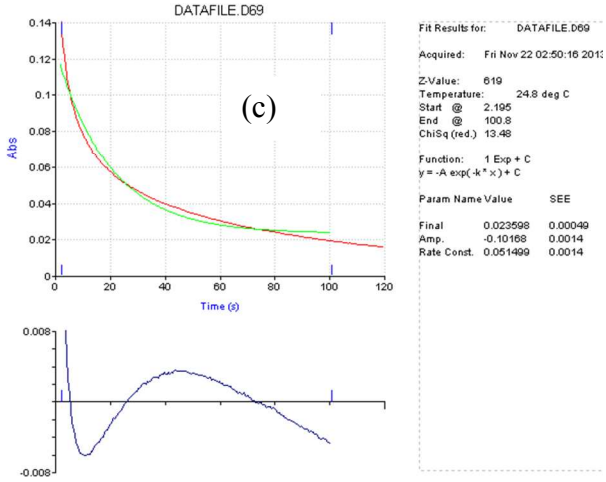
Abs
Time (s)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(c)
Abs
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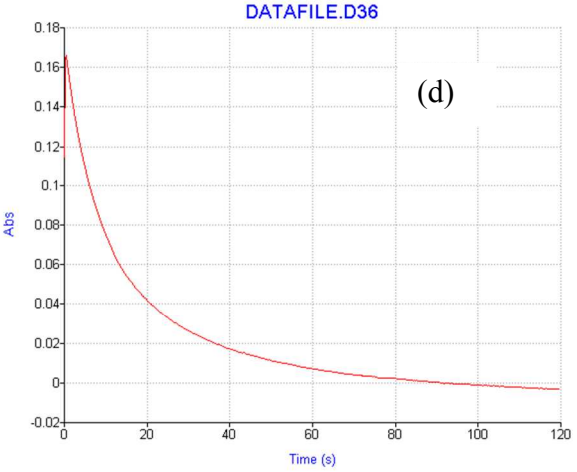
Start @ 2.195
End @ 100.8
ChiSq (red.) 13.48
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final 0.023598 0.00049
Amp. -0.10168 0.0014
Rate Const. 0.051499 0.0014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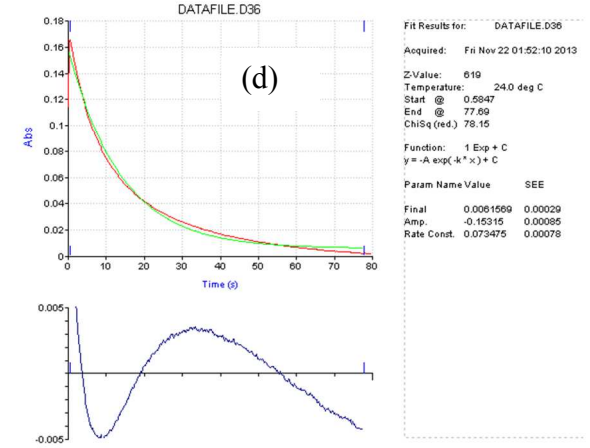
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(d)
Abs
Time (s)
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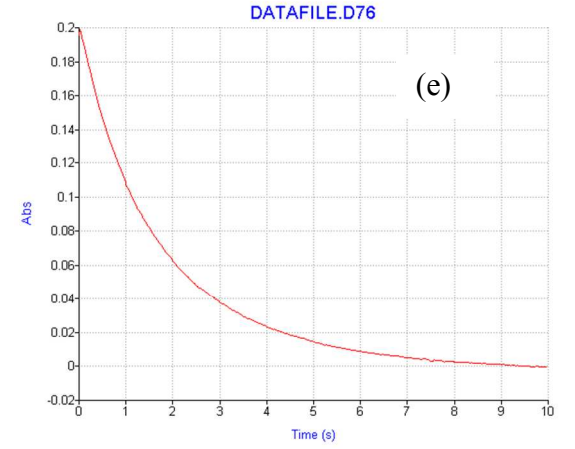
Z-Value: 619
Temperature: 24.0 deg C
Start @ 0.5847
End @ 77.69
ChiSq (red.) 78.15
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final 0.0061569 0.00029
Amp. -0.15315 0.00085
Rate Const. 0.073475 0.00078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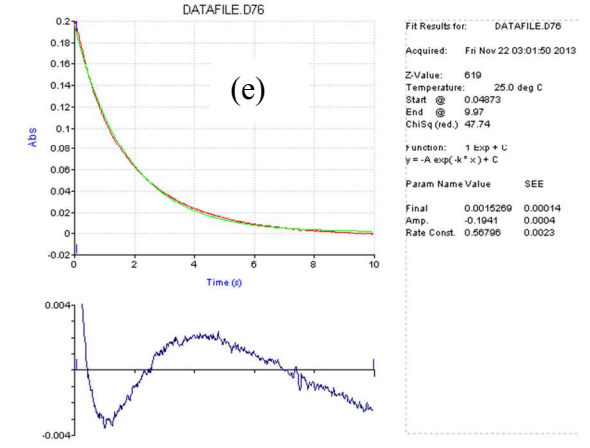
(e)
Abs
Time (s)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(e)
Abs
Time (s)
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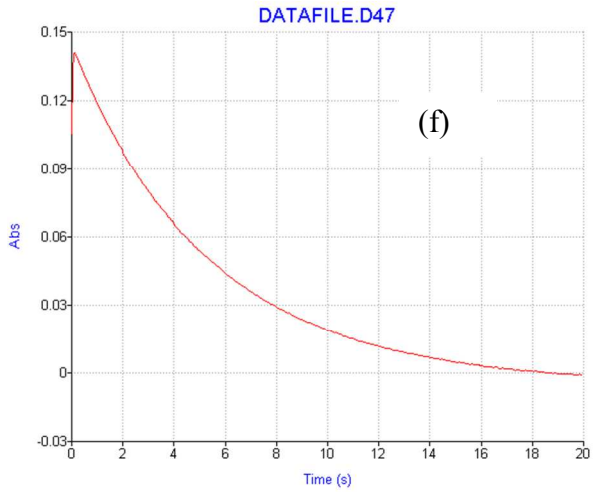
Z-Value: 619
Temperature: 25.0 deg C
Start @ 0.04873
End @ 9.97
ChiSq (red.) 47.74
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final 0.0015269 0.00014
Amp. -0.1941 0.0004
Rate Const. 0.56796 0.0023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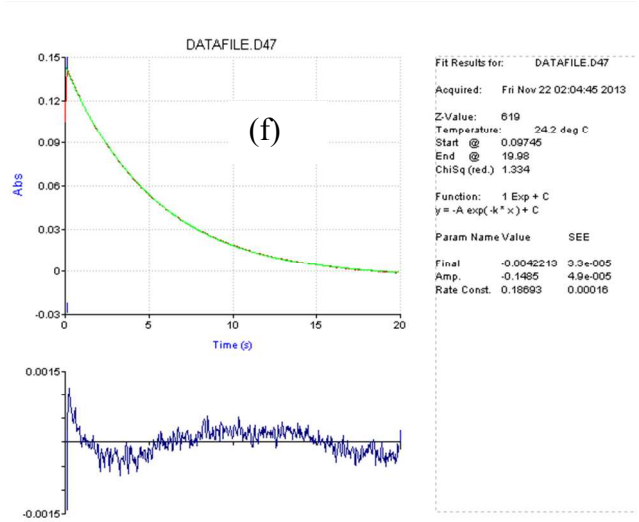
Time (s)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(f)
Abs
Time (s)
Fit Results for: DATAFILE.D47
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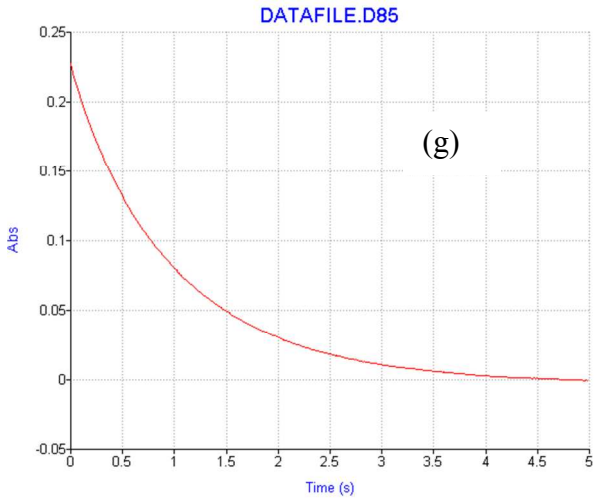
Z-Value: 619
Temperature: 24.2 deg C
Start @ 0.09745
End @ 19.98
ChiSq (red.) 1.334
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final -0.0042213 3.3e-005
Amp. -0.1485 4.9e-005
Rate Const. 0.18693 0.00016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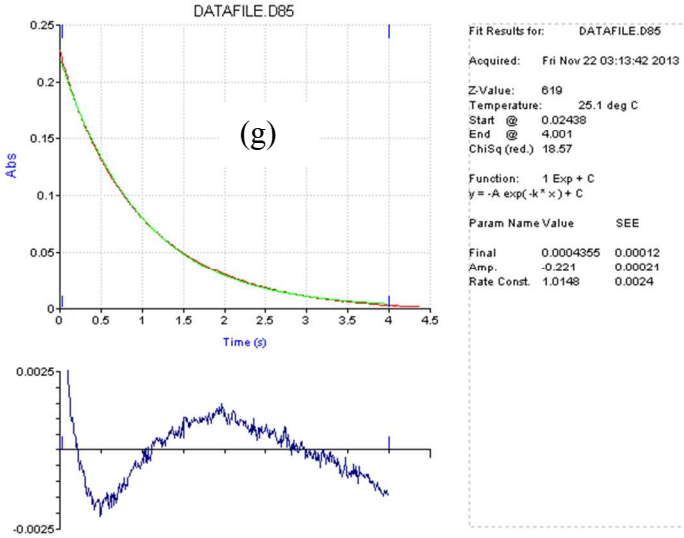
(g)
Abs
Time (s)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(g)
Abs
Time (s)
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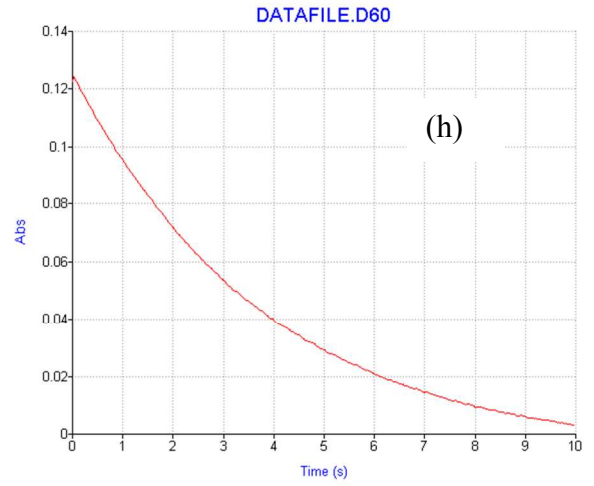
Temperature: 25.1 deg C
Start @ 0.02438
End @ 4.001
ChiSq (red.) 18.57
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final 0.0004355 0.00012
Amp. -0.221 0.00021
Rate Const. 1.0148 0.0024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(h)
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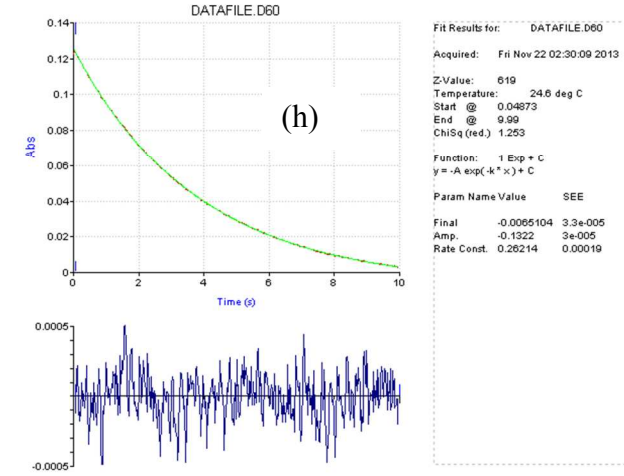
Time (s)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(h)
Abs
Time (s)
Fit Results for: DATAFILE.D60
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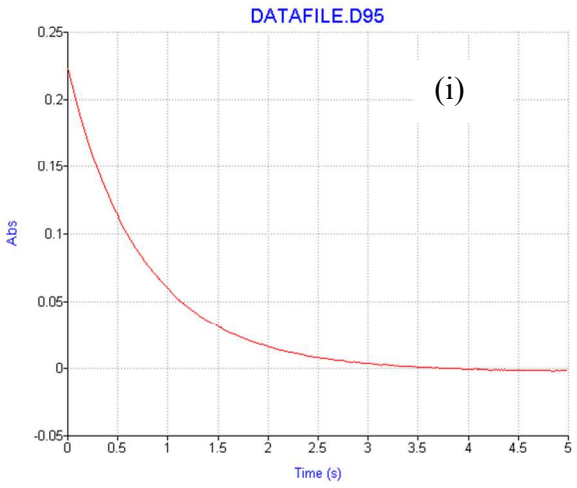
Z-Value: 619
Temperature: 24.6 deg C
Start @ 0.04873
End @ 9.99
ChiSq (red.) 1.253
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final -0.0065104 3.3e-005
Amp. -0.1322 3e-005
Rate Const. 0.26214 0.00019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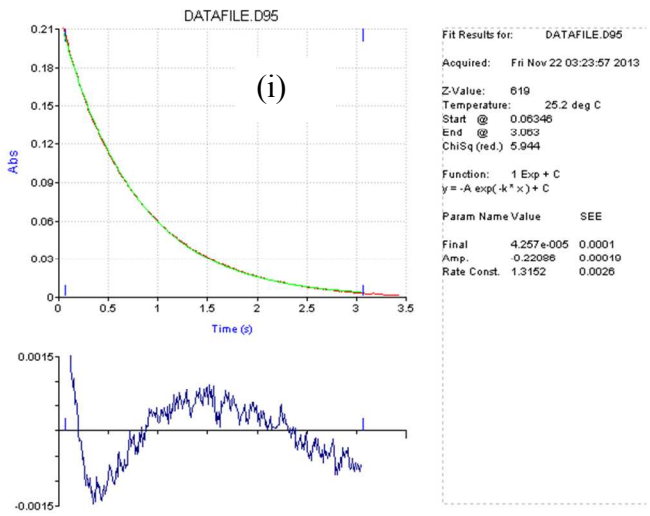
(i)
Abs
Time (s)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(i)
Abs
Time (s)
Fit Results for: DATAFILE.D95
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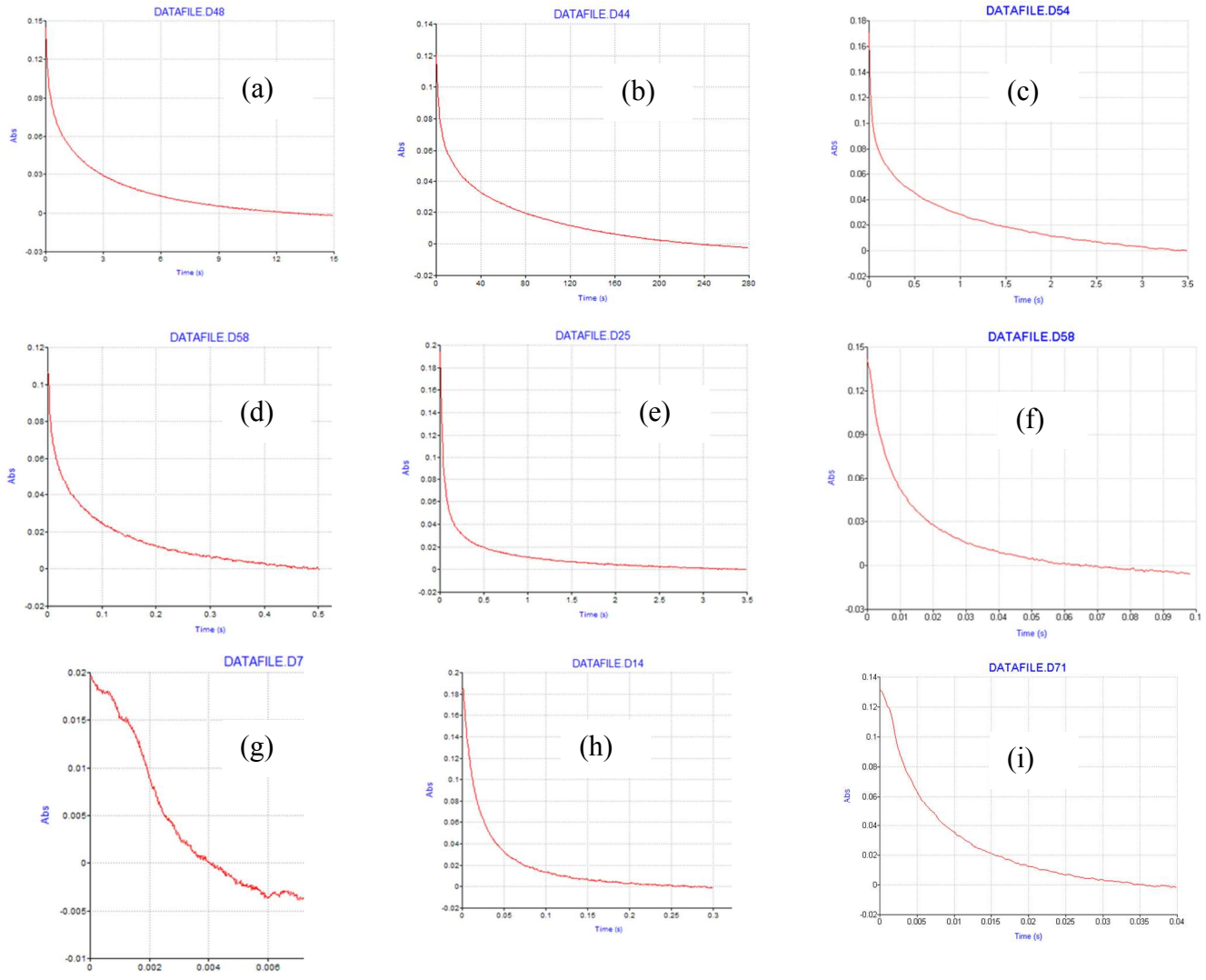
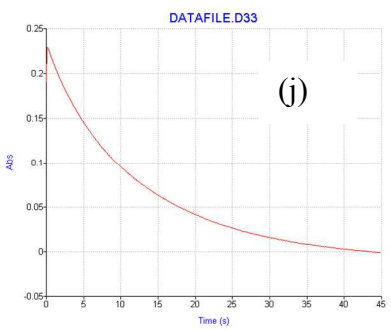
Temperature: 25.2 deg C
Start @ 0.06346
End @ 3.053
ChiSq (red.) 5.944
Function: 1 Exp + C
y = -A exp(-k * x) + C
Param Name Value SEE
Final 4.257e-005 0.0001
Amp. -0.22086 0.00010
Rate Const. 1.3152 0.0026

Figure S2: Kinetic trace in the reaction of methyl cinnamate (25 mM), SmI_2 (2.5 mM) in the presence of; (a) 2.5 mM HOMPA; (b) 2.5 mM HMPA; (c) 2.5 mM HMPA + 0.5 M MeOH; (d) 5 mM HOMPA; (e) 5 mM HMPA; (f) 5 mM HMPA + 0.5 M MeOH; (g) 10 mMHOMPA; (h) 10 mM HMPA; (i) 10mM HMPA + 0.5 M MeOH; (j) 0.25 M MeOH; (k) 0.5 M MeOH; (l) 1.0 M MeOH ; (m) 2.0 M MeOH.

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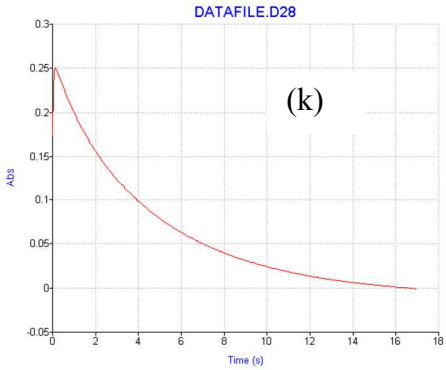
(j)
Abs
Time (s)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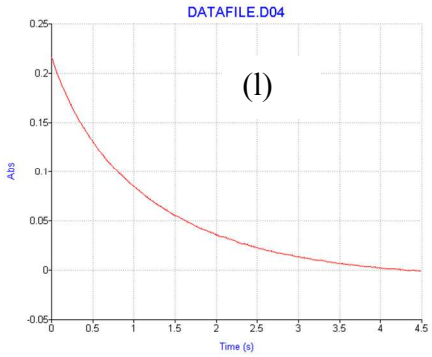
Time (s)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Abs
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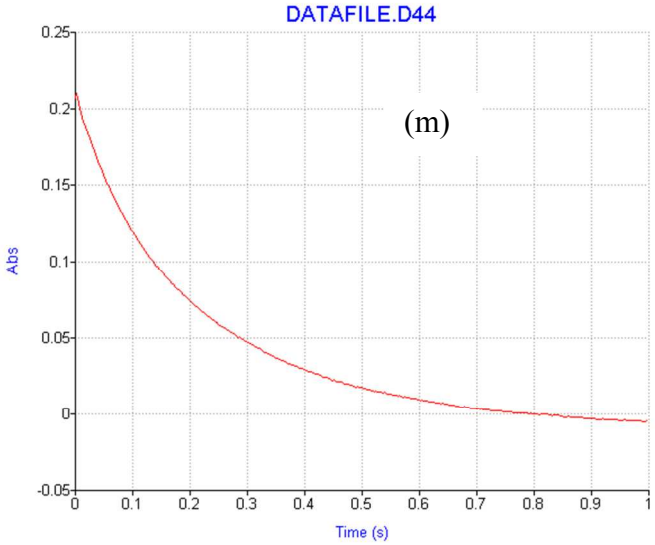
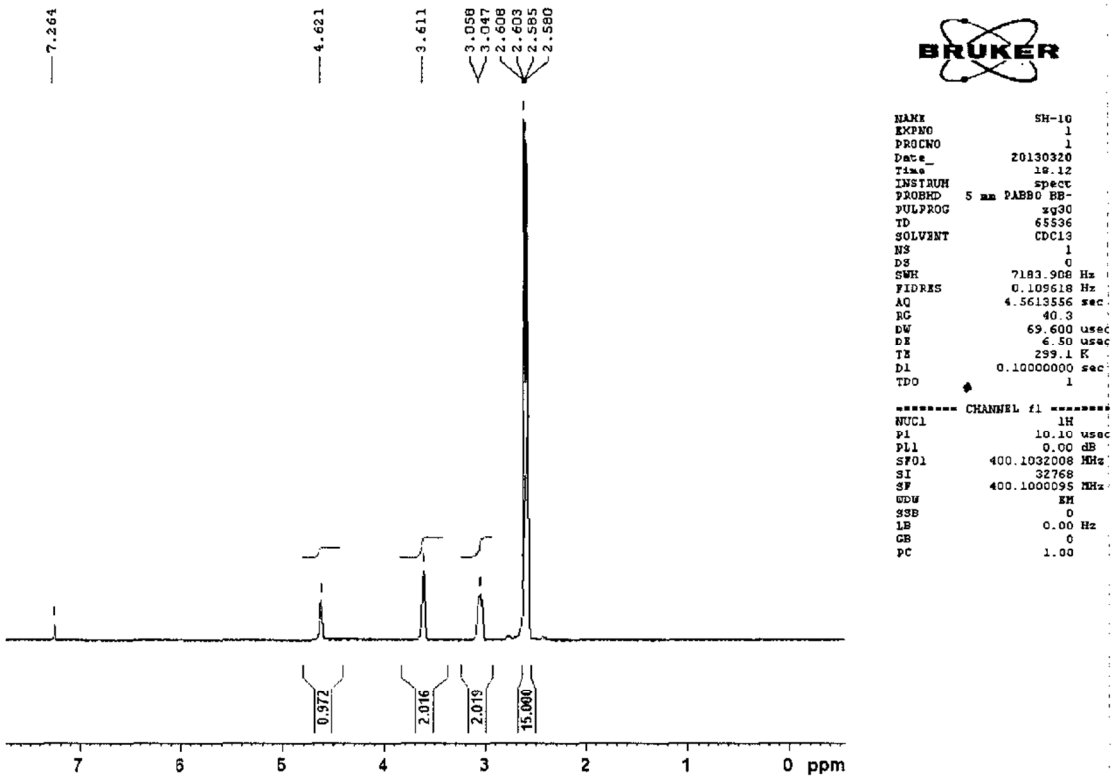
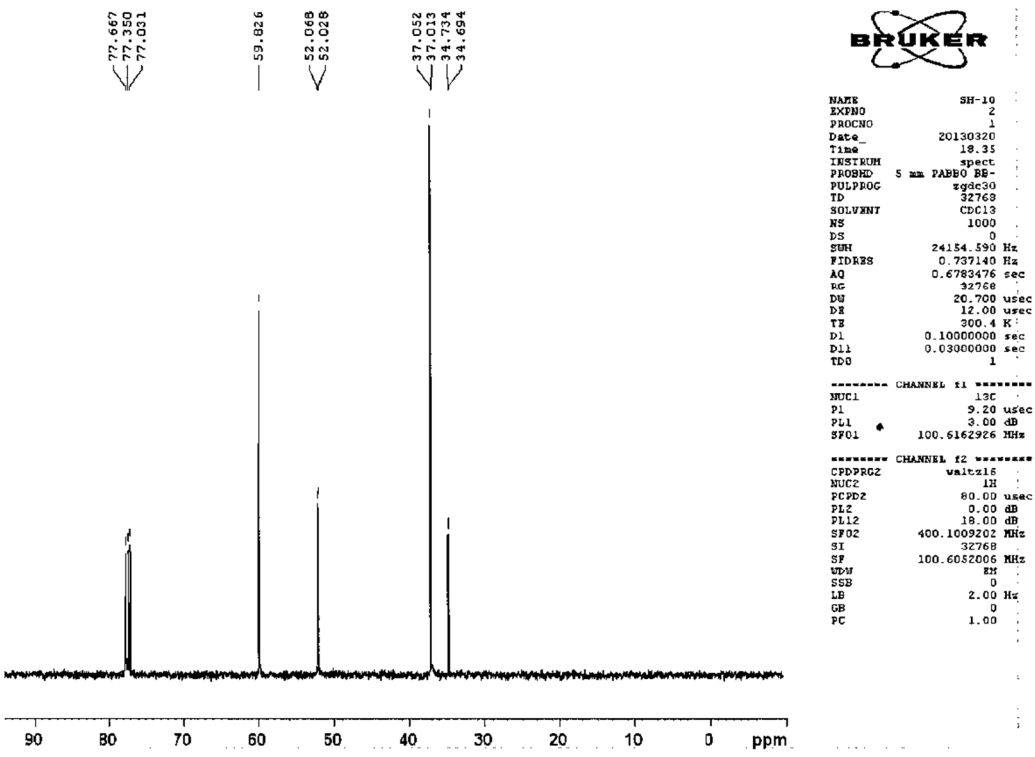

DATAFILE.D44
(m)
Abs
Time (s)

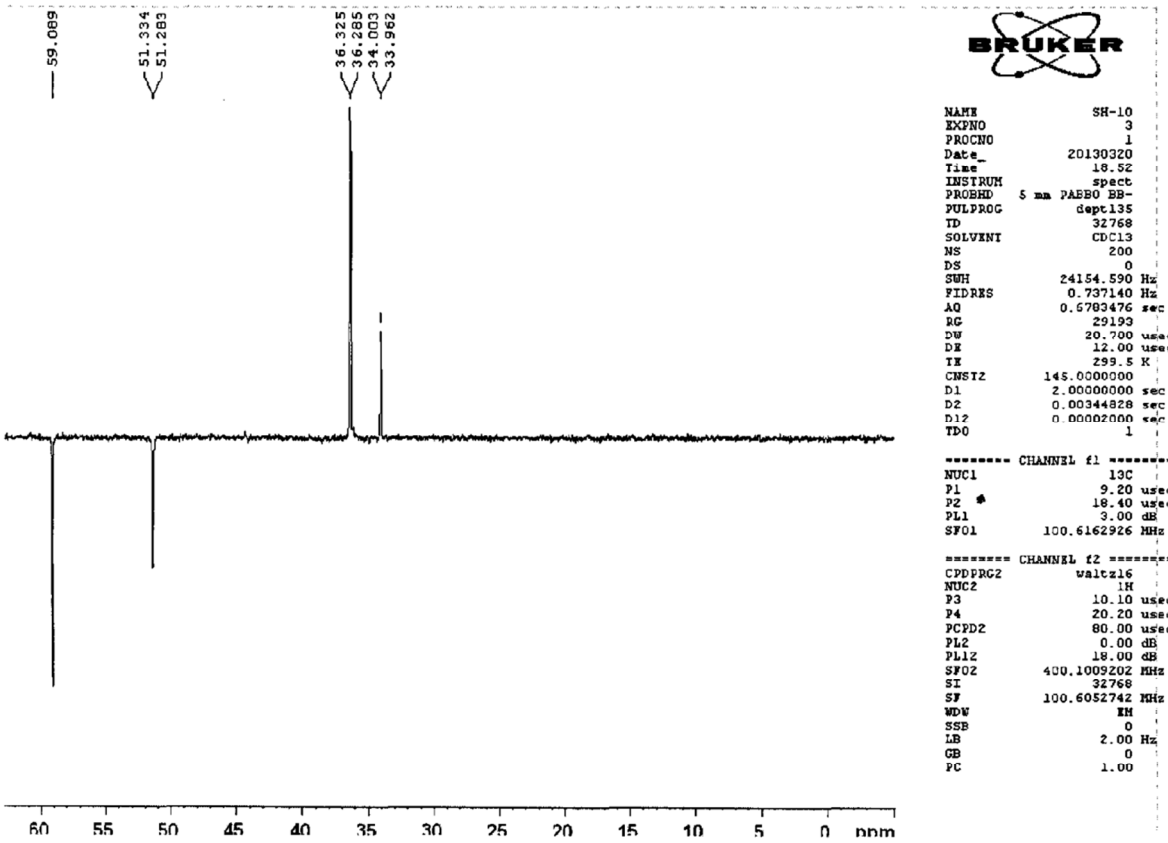
Spectra of HOMPA



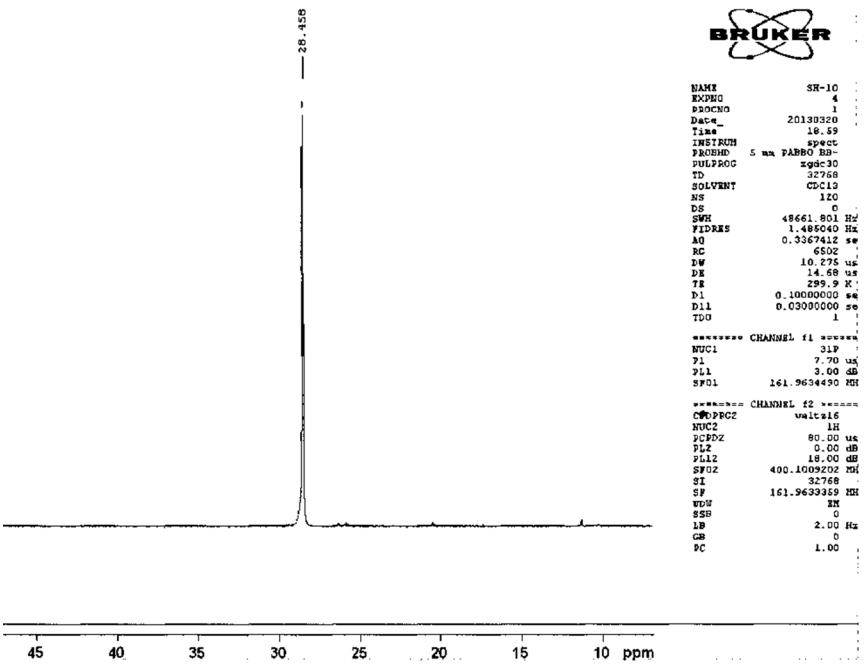
^{1}H NMR spectrum of HOMPA



^{13}C NMR spectrum of HOMPA



DEPT 135 NMR spectrum of HOMPA



^{31}P NMR spectrum of HOMPA