Electronic Supplementary Material (ESI) for RSC Advances.

<Supplementary information>

Benzene-Glycol Nucleic Acid (BGNA)-DNA Chimeras: Synthesis, Binding Properties, and Ability to Elicit Human RNase H Activity

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Contents

Fig. S1. UV-melting profiles of duplexes.

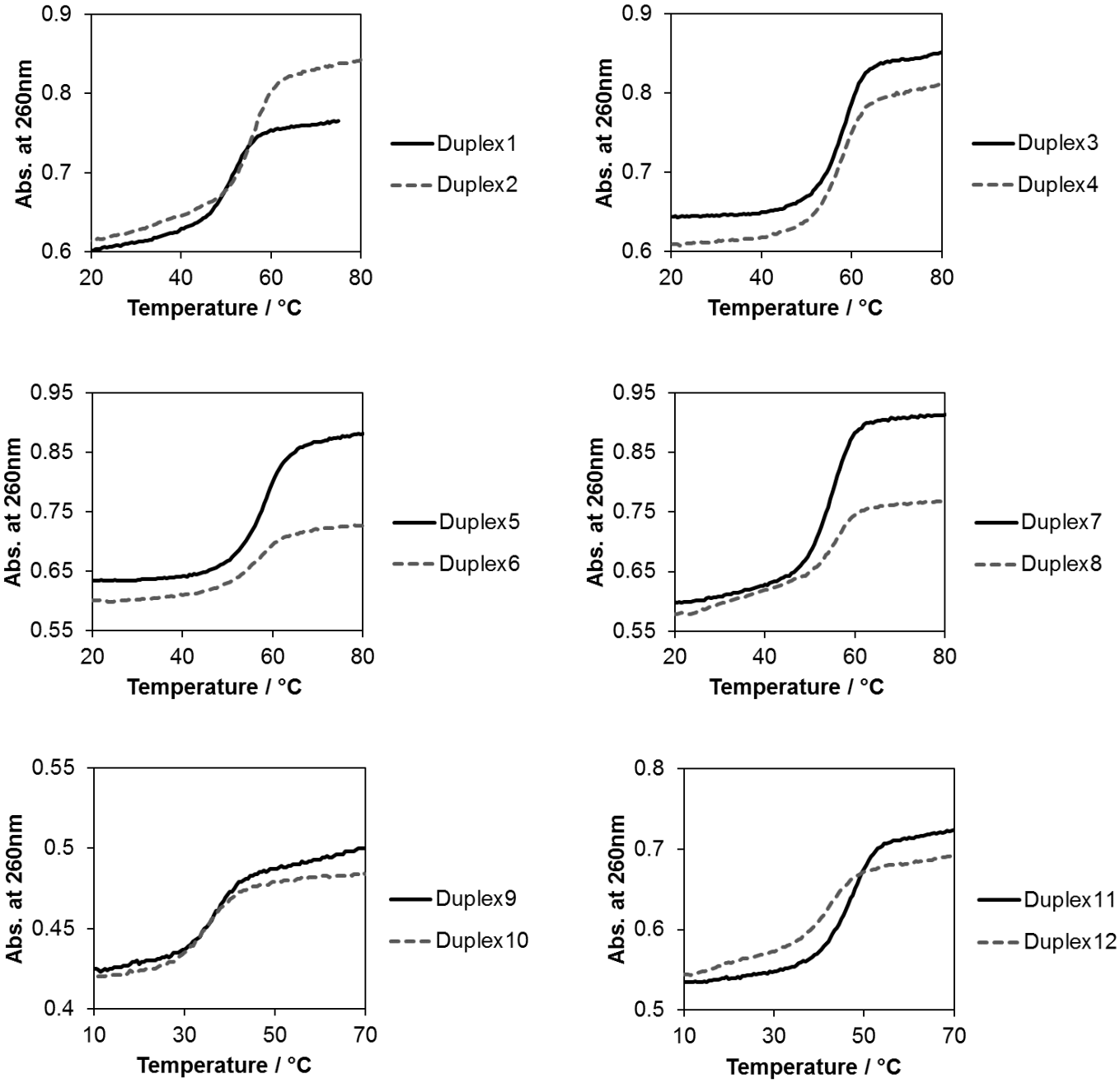


Fig. S2. UV-melting profiles duplexes containing two mismatched base pairs.

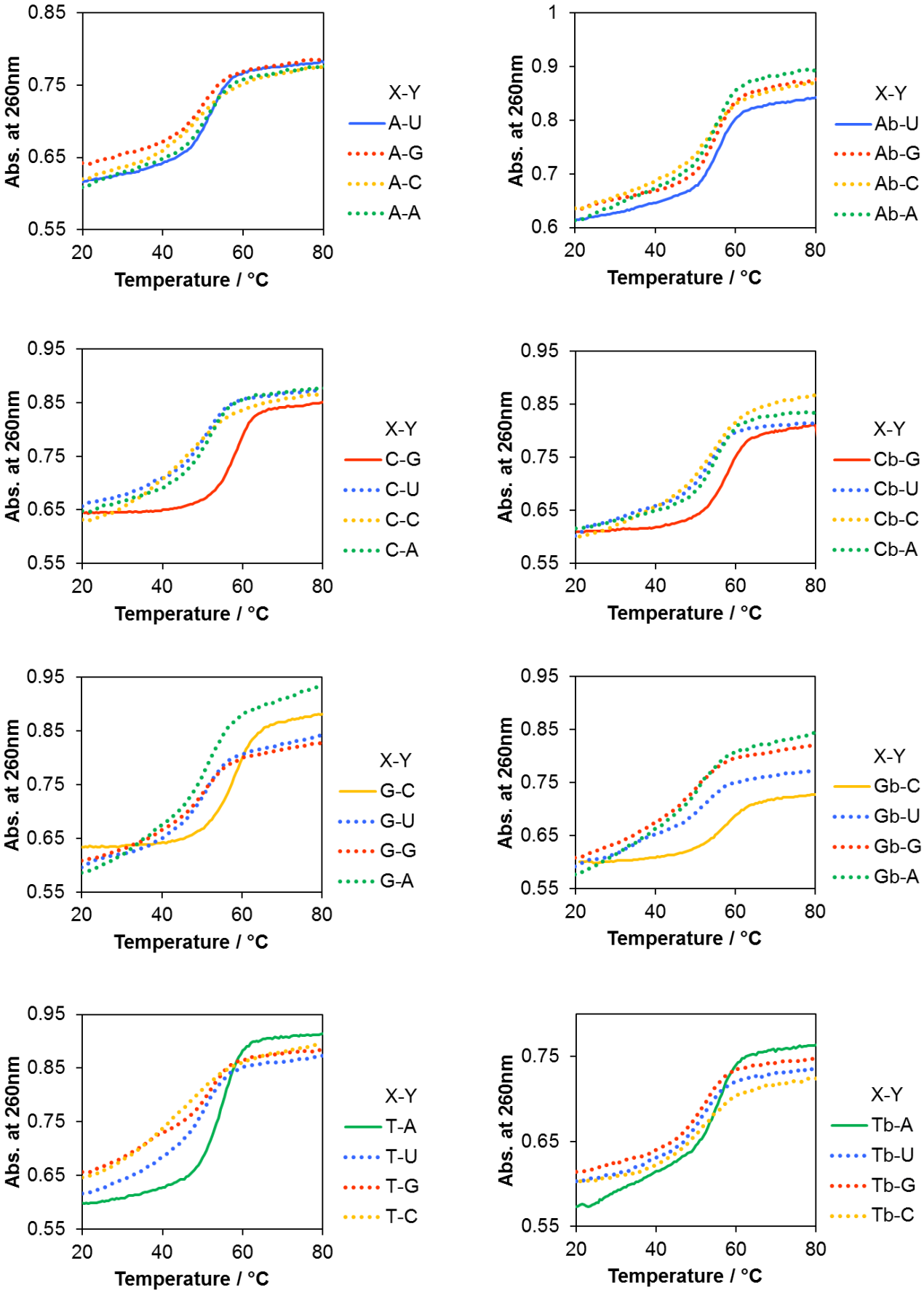
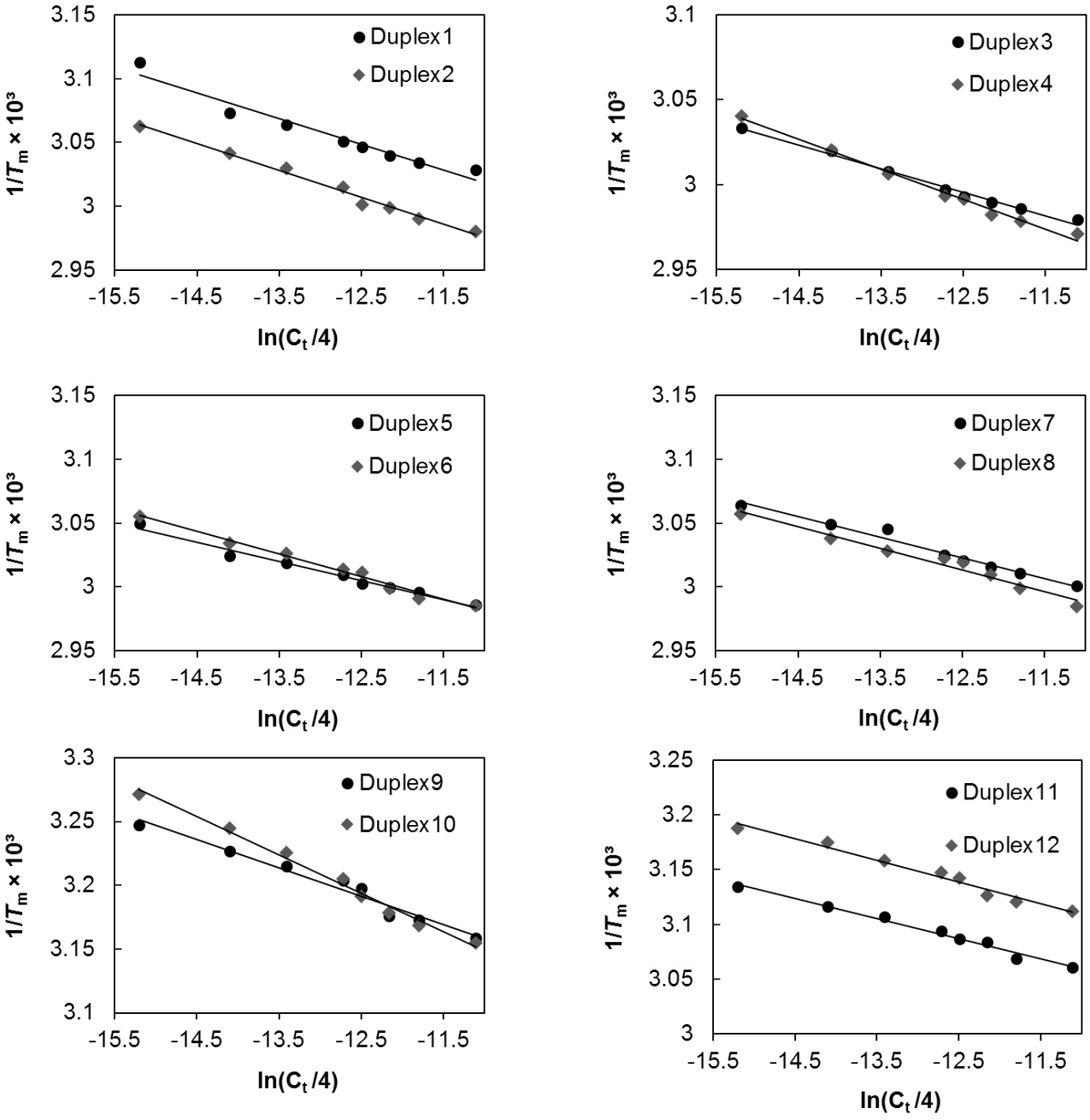


Table S1. T_m values of duplexes.

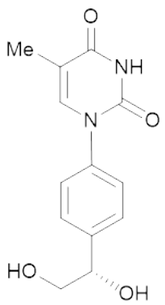
		5'-d(A**X**AGTTCACTACTCA**X**A)-3' 3'-r(U**Y**UCAAGUGAUGAGU**Y**U)-5'			
		Y			
		U	**G**	**C**	**A**
X	**A**	**52.3**	50.6 (-1.7)	50.2 (-2.1)	51.7 (-0.6)
	C	52.3 (-5.7)	**58.0**	45.7 (-12.3)	51.9 (-6.1)
	G	50.3 (-7.2)	51.0 (-6.5)	**57.5**	53.4 (-4.1)
	T	51.6 (-3.2)	53.2 (-1.6)	47.2 (-7.6)	**54.8**

		5'-d(A**X**A^{b}GTTCACTACTC**A**^{b}**X**A^{b})-3' 3'-r(U**Y**UCAAGUGAUGAGU**Y**U)-5'			
		Y			
		U	**G**	**C**	**A**
X	**A**^{b}	**55.6**	54.9 (-0.7)	54.6 (-1.0)	55.3 (-0.3)
	C^{b}	54.5 (-3.4)	**57.9**	55.1 (-2.8)	55.3 (-2.6)
	G^{b}	54.1 (-2.3)	52.6 (-3.8)	**56.4**	55.3 (-1.1)
	T^{b}	52.7 (-2.6)	52.1 (-3.2)	50.8 (-4.5)	**55.3**

Fig. S3. Graphical data of $1/T_m$ versus $\ln(C_T/4)$ plots.



20161006t-monomer-10.jdf



3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Author           = delta
Experiment       = single_pulse.ex2
Sample_id        = S#573373
Solvent          = DMSO-D6
Creation_time    =  6-OCT-2016 15:48:38
Revision_time    =  6-DEC-2016 10:22:09
Current_time     =  6-DEC-2016 10:22:27

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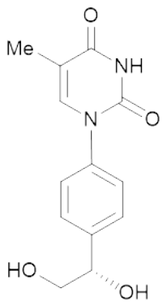
Dim_size         = 13107
Dim_title        = 1H
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 5[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 8
Total_scans      = 8

X_90_width       = 13.5[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 2.2[dB]
X_pulse          = 6.75[us]
Irr_mode         = Off
Tri_mode         = Off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Recvr_gain       = 48
Relaxation_delay = 5[s]
Repetition_time  = 6.4548992[s]
Temp_get         = 24.3[dC]
```

20161006t-monomer13c-6.jdf



3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Filename          = 20161006t-monomer13c-
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#575367
Solvent           = DMSO-D6
Creation_time     =  6-OCT-2016 15:57:27
Revision_time     =  6-DEC-2016 09:57:25
Current_time      =  6-DEC-2016 09:57:53

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Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 110
Total_scans       = 110

X_90_width        = 11.5[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 5.7[dB]
X_pulse           = 3.83333333[us]
Irr_atn_dec       = 22[dB]
Irr_atn_noe       = 22[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Temp_get          = 24.5[dC]
```
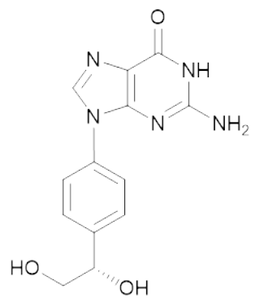

20161031g-monomer-4.jdf



4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Filename          = 20161031g-monomer-4.j
Author            = delta
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Solvent           = DMSO-D6
Creation_time     = 31-OCT-2016 10:19:38
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Current_time      =  6-DEC-2016 10:35:14

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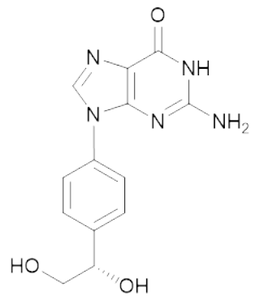
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 2.18365952[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.45794685[Hz]
X_sweep           = 7.5030012[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 11.3275[us]
X_acq_time        = 2.18365952[s]
X_angle           = 45[deg]
X_atn             = 1[dB]
X_pulse           = 5.66375[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 7.18365952[s]
Temp_get          = 22.8[dC]
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 17[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
Sample_action     = LOADED
Sample_state      = LOAD
Sample_status     = LOADED
Changer_sample    = 0
```

20161028g-monomer13C-8.jdf



4

abundance

157.1376
154.0293
151.0450
143.0264
136.4666
133.6730
127.1514
123.4424
117.1401
73.2333
67.2742
39.7098
39.5000
39.2902
13.4897

X : parts per Million : 13C

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Filename          = 20161028g-monomer13C-
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#504219
Solvent           = DMSO-D6
Creation_time     = 28-OCT-2016 14:23:09
Revision_time     =  6-DEC-2016 10:35:59
Current_time      =  6-DEC-2016 10:36:15

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 512
Total_scans       = 512

X_90_width        = 9.4[us]
X_acq_time        = 1.04333312[s]
X_angle           = 30[deg]
X_atn             = 3.2[dB]
X_pulse           = 3.13333333[us]
Irr_atn_dec       = 20.20655[dB]
Irr_atn_noe       = 20.20655[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 23.4[dC]
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 16[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
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Sample_state      = LOAD
Sample_status     = = LOADED
Changer_sample    = 0
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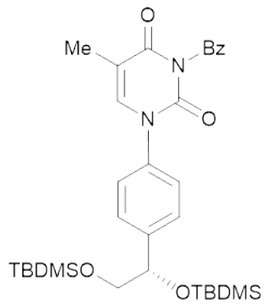
20161006t-coupling-6.jdf



6

abundance

X : parts per Million : 1H

7.9735
7.5005
7.4559
7.4421
7.3345
7.3196
7.2875
7.2600
4.7314
4.7211
4.7119
3.6388
3.6274
3.5152
3.5071
2.0183
2.0161
1.5580
0.8846
0.8800
0.8468
−0.0328
−0.0454
−0.0499

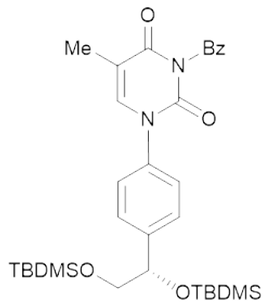
```
Filename         = 20161006t-coupling-6.
Author           = delta
Experiment       = single_pulse.ex2
Sample_id        = S#582732
Solvent          = CHLOROFORM-D
Creation_time    =  6-OCT-2016 16:04:24
Revision_time    =  6-DEC-2016 09:42:29
Current_time     =  6-DEC-2016 09:46:45

Data_format      = 1D COMPLEX
Dim_size         = 13107
Dim_title        = 1H
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 5[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 8
Total_scans      = 8

X_90_width       = 13.5[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 2.2[dB]
X_pulse          = 6.75[us]
Irr_mode         = Off
Tri_mode         = Off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Recvr_gain       = 42
Relaxation_delay = 5[s]
Repetition_time  = 6.4548992[s]
Temp_get         = 24.3[dC]
```

20161006t-coupling13C-8.jdf



6

abundance

X : parts per Million : 13C

168.8508
163.1634
149.2512
143.7936
140.5095
137.1774
134.9465
131.6815
130.4655
129.1059
127.4878
125.6782
111.1054
77.2107
77.0000
76.7894
75.3053
69.7041
25.9282
25.8133
18.3737
18.2397
12.3895
−4.7685
−4.9312
−5.4579

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Filename         = 20161006t-coupling13C
Author           = delta
Experiment       = single_pulse_dec
Sample_id        = S#592577
Solvent          = CHLOROFORM-D
Creation_time    =  6-OCT-2016 16:44:11
Revision_time    =  6-DEC-2016 09:51:31
Current_time     =  6-DEC-2016 09:51:53

Data_format      = 1D COMPLEX
Dim_size         = 26214
Dim_title        = 13C
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 0.69206016[s]
X_domain         = 13C
X_freq           = 150.91343039[MHz]
X_offset         = 100[ppm]
X_points         = 32768
X_prescans       = 4
X_resolution     = 1.44496109[Hz]
X_sweep          = 47.34848485[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 512
Total_scans      = 512

X_90_width       = 11.5[us]
X_acq_time       = 0.69206016[s]
X_angle          = 30[deg]
X_atn            = 5.7[dB]
X_pulse          = 3.83333333[us]
Irr_atn_dec      = 22[dB]
Irr_atn_noe      = 22[dB]
Irr_noise        = WALTZ
Decoupling       = TRUE
Initial_wait     = 1[s]
Noe              = TRUE
Noe_time         = 2[s]
Recvr_gain       = 58
Relaxation_delay = 2[s]
Repetition_time  = 2.69206016[s]
Temp_get         = 24.6[dC]
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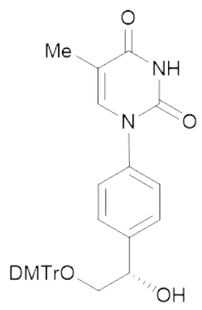
20161020T.trityl-14.jdf



7

abundance

X : parts per Million : 1H

8.6171
8.4590
7.2921
7.2806
7.2772
7.2600
7.2485
6.8294
6.8156
4.8126
4.8046
4.7989
3.7819
3.3513
3.3456
3.3353
3.3296
3.2437
3.2288
2.0343
1.9427
1.9404
1.2487

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Filename         = 20161020T.trityl-14.j
Author           = delta
Experiment       = single_pulse.ex2
Sample_id        = S#625594
Solvent          = CHLOROFORM-D
Creation_time    = 20-OCT-2016 17:15:35
Revision_time    =  6-DEC-2016 10:01:07
Current_time     =  6-DEC-2016 10:02:08

Data_format      = 1D COMPLEX
Dim_size         = 13107
Dim_title        = 1H
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 5[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 8
Total_scans      = 8

X_90_width       = 13.5[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 2.2[dB]
X_pulse          = 6.75[us]
Irr_mode         = Off
Tri_mode         = Off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Recvr_gain       = 44
Relaxation_delay = 5[s]
Repetition_time  = 6.4548992[s]
Temp_get         = 25.7[dC]
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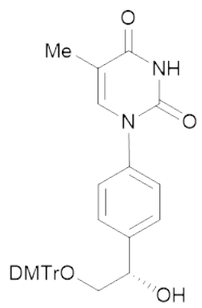
20161020T.trityl13C-7.jdf



7

abundance

X : parts per Million : 13C

163.7474
158.5866
150.0459
144.5787
141.3712
140.5573
137.8285
135.7029
130.0059
128.0431
127.8995
127.3920
126.9324
126.0707
113.2118
111.0958
86.6705
77.2107
77.0000
76.7798
72.7105
68.9955
55.2174
12.2459

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Filename         = 20161020T.trityl13C-7
Author           = delta
Experiment       = single_pulse_dec
Sample_id        = S#627193
Solvent          = CHLOROFORM-D
Creation_time    = 20-OCT-2016 17:29:36
Revision_time    =  6-DEC-2016 10:03:07
Current_time     =  6-DEC-2016 10:04:26

Data_format      = 1D COMPLEX
Dim_size         = 26214
Dim_title        = 13C
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 0.69206016[s]
X_domain         = 13C
X_freq           = 150.91343039[MHz]
X_offset         = 100[ppm]
X_points         = 32768
X_prescans       = 4
X_resolution     = 1.44496109[Hz]
X_sweep          = 47.34848485[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 247
Total_scans      = 247

X_90_width       = 11.5[us]
X_acq_time       = 0.69206016[s]
X_angle          = 30[deg]
X_atn            = 5.7[dB]
X_pulse          = 3.83333333[us]
Irr_atn_dec      = 22[dB]
Irr_atn_noe      = 22[dB]
Irr_noise        = WALTZ
Decoupling       = TRUE
Initial_wait     = 1[s]
Noe              = TRUE
Noe_time         = 2[s]
Recvr_gain       = 58
Relaxation_delay = 2[s]
Repetition_time  = 2.69206016[s]
Temp_get         = 25.9[dC]
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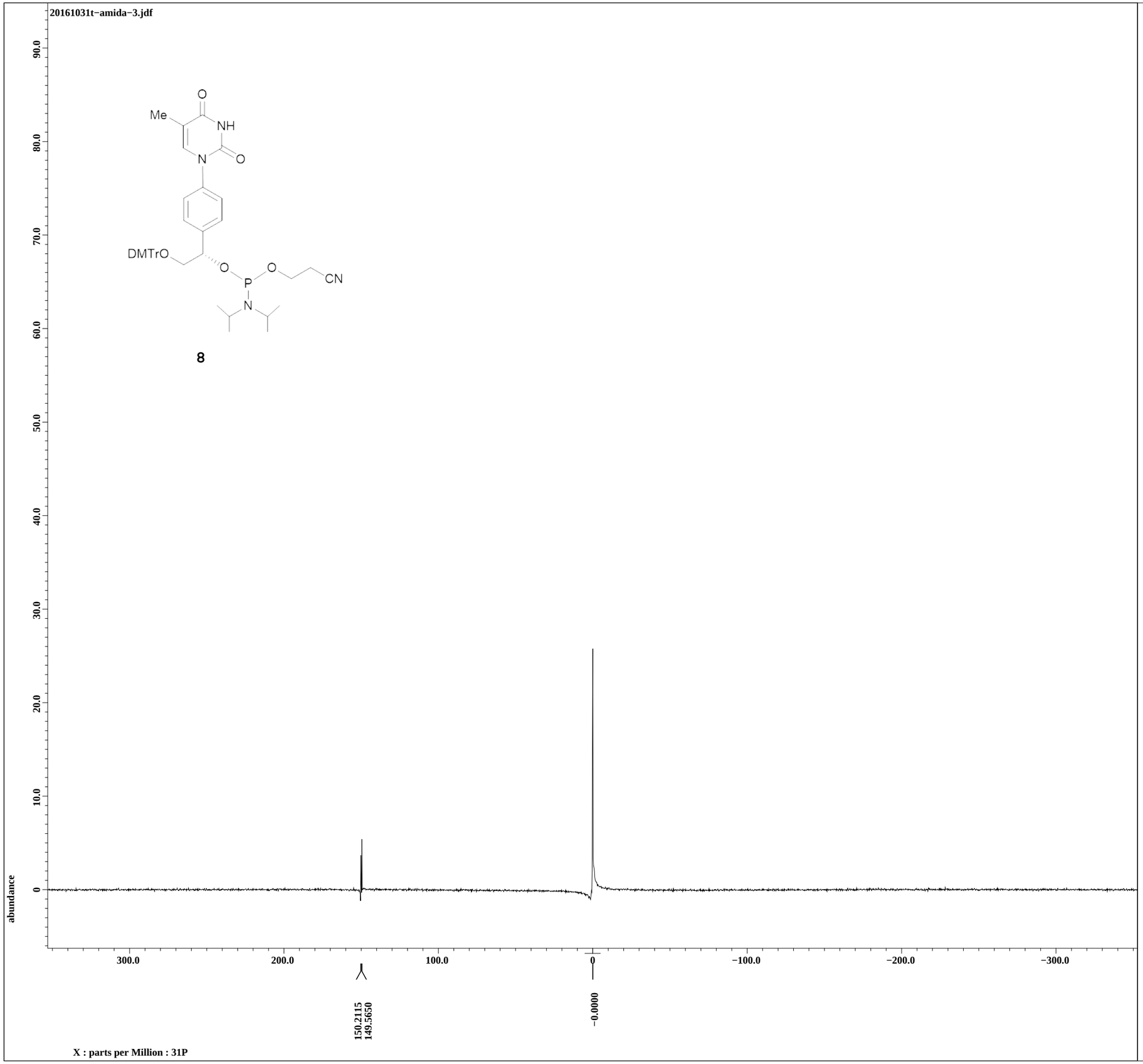


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Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#363785
Solvent           = CHLOROFORM-D
Creation_time     = 31-OCT-2016 10:13:28
Revision_time     =  6-DEC-2016 10:36:37
Current_time      =  6-DEC-2016 10:36:56

Data_format       = 1D COMPLEX
Dim_size          = 3276
Dim_title         = 31P
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 28.672[ms]
X_domain          = 31P
X_freq            = 161.83469309[MHz]
X_offset          = 0[ppm]
X_points          = 4096
X_prescans        = 4
X_resolution      = 34.87723214[Hz]
X_sweep           = 142.85714286[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 394
Total_scans       = 394

X_90_width        = 10.8[us]
X_acq_time        = 28.672[ms]
X_angle           = 30[deg]
X_atn             = 2.5[dB]
X_pulse           = 3.6[us]
Irr_atn_dec       = 20.20655[dB]
Irr_atn_noe       = 20.20655[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.028672[s]
Temp_get          = 22.9[dC]
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 16[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
Sample_action     = LOADED
Sample_state      = LOAD
Sample_status     = LOADED
Changer_sample    = 0
```
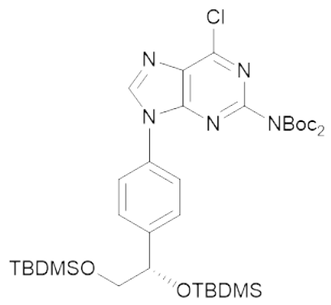

201507302A6ClPcoupling-4.jdf



9

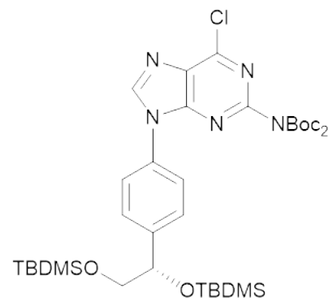
abundance

X : parts per Million : 1H

8.4110	
7.6585	
7.6448	
7.5658	
7.5509	
7.2600	
4.7829	
4.7726	
4.7623	
3.7006	
3.5644	
3.5472	
3.5380	
1.5797	
1.4423	
0.9051	
0.8937	
0.8582	
0.1001	
−0.0087	
−0.0316	
−0.0591	

```
Filename          = 201507302A6ClPcouplin
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#351530
Solvent           = CHLOROFORM-D
Creation_time     = 30-JUL-2015 09:27:19
Revision_time     =  6-DEC-2016 10:05:58
Current_time      =  6-DEC-2016 10:06:23

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 600.1723046[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 600.1723046[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 16
Total_scans       = 16

X_90_width        = 12.8[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 2.2[dB]
X_pulse           = 6.4[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.4548992[s]
Temp_get          = 27.9[dC]
```

201507302A6ClPcoupling13C-4.jdf



9

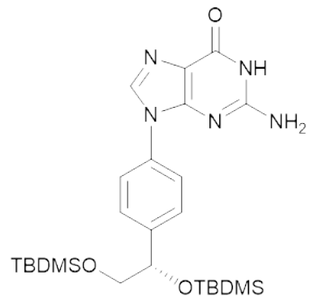
abundance

X : parts per Million : 13C

152.5928
152.0854
151.7024
150.6108
144.6841
144.0425
132.7922
130.4272
127.9665
122.6717
83.6449
77.2107
77.0000
76.7798
75.2478
69.6179
27.8719
25.9186
25.8229
18.3642
18.2588
-4.7015
-5.4196
-5.5249

```
Filename          = 201507302A6ClPcouplin
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#357700
Solvent           = CHLOROFORM-D
Creation_time     = 30-JUL-2015 09:53:33
Revision_time     =  6-DEC-2016 10:07:23
Current_time      =  6-DEC-2016 10:08:29

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 363
Total_scans       = 363

X_90_width        = 11.6[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 6.2[dB]
X_pulse           = 3.86666667[us]
Irr_atn_dec       = 17.67207[dB]
Irr_atn_noe       = 17.67207[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Temp_get          = 29.4[dC]
```

20160920g-6.jdf



10

abundance

X : parts per Million : 1H

12.3150

7.7490
7.5658
7.5521
7.4856
7.4719
7.2600

6.5603

4.7669
4.7566
4.7474

3.6629
3.6503
3.5724
3.5632

2.8841
2.8749
2.7707

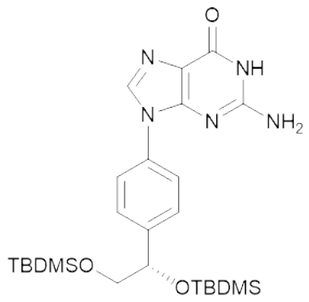
1.5007

1.2533
0.9052
0.8719
0.8468
0.7998
0.7666

0.0955
0.0703
0.0050
−0.0099

```
Filename          = 20160920g-6.jdf
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#356325
Solvent           = CHLOROFORM-D
Creation_time     = 20-SEP-2016 09:48:21
Revision_time     =  6-DEC-2016 10:11:23
Current_time      =  6-DEC-2016 10:11:50

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 600.1723046[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 600.1723046[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 13.5[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 2.2[dB]
X_pulse           = 6.75[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.4548992[s]
Temp_get          = 24.9[dC]
```

20160920g13c-4.jdf



10

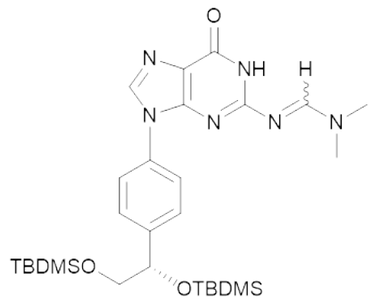
abundance

X : parts per Million : 13C

159.4100
153.9907
151.4438
142.6925
136.7083
133.8358
127.5261
122.9685
117.5779
77.2107
77.0000
76.7894
75.4681
69.8285
25.9761
25.8708
18.4120
18.2780
−4.6536
−5.3334
−5.4866

```
Filename          = 20160920g13c-4.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#357717
Solvent           = CHLOROFORM-D
Creation_time     = 20-SEP-2016 10:01:11
Revision_time     =  6-DEC-2016 10:12:50
Current_time      =  6-DEC-2016 10:13:17

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = TRUE
Mod_return        = 1
Scans             = 225
Total_scans       = 225

X_90_width        = 11.5[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 5.7[dB]
X_pulse           = 3.83333333[us]
Irr_atn_dec       = 20.421[dB]
Irr_atn_noe       = 20.421[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Temp_get          = 25.3[dC]
```

20160920dmf-dma-11.jdf



11

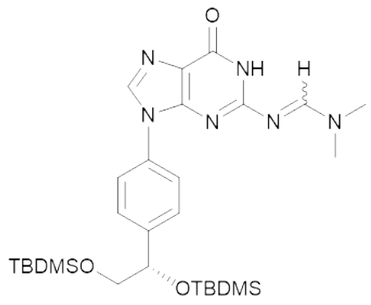
abundance

X : parts per Million : 1H

8.5438	
7.8258	
7.5681	
7.5543	
7.5005	
7.4856	
7.2600	
4.7669	
4.7577	
4.7474	
3.6903	
3.6789	
3.5667	
3.5575	
3.5506	
3.1487	
3.1120	
0.8994	
0.8582	
0.8330	
−0.0099	
−0.0179	
−0.0339	

```
Filename          = 20160920dmf-dma-11.jd
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = S#368217
Solvent           = CHLOROFORM-D
Creation_time     = 20-SEP-2016 10:08:10
Revision_time     =  6-DEC-2016 10:15:29
Current_time      =  6-DEC-2016 10:16:32

Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 1.4548992[s]
X_domain          = 1H
X_freq            = 600.1723046[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.68733284[Hz]
X_sweep           = 11.26126126[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 600.1723046[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 13.5[us]
X_acq_time        = 1.4548992[s]
X_angle           = 45[deg]
X_atn             = 2.2[dB]
X_pulse           = 6.75[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.4548992[s]
Temp_get          = 25[dC]
```

20160920dmf-dma13C-4.jdf



11

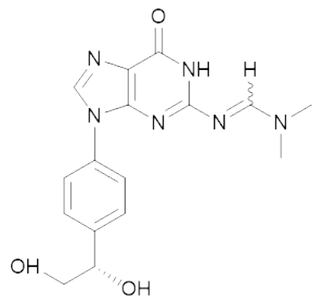
abundance

X : parts per Million : 13C

158.0121
156.8344
150.0076
142.6925
137.4647
134.0465
127.5069
123.1504
121.1493
77.2107
77.0000
76.7894
75.3436
69.7424
41.3436
35.2157
25.9282
25.8229
18.3833
18.2588
−4.6919
−5.4483
−5.4866

```
Filename          = 20160920dmf-dma13C-4.
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#369579
Solvent           = CHLOROFORM-D
Creation_time     = 20-SEP-2016 10:27:22
Revision_time     =  6-DEC-2016 10:18:17
Current_time      =  6-DEC-2016 10:18:35

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 361
Total_scans       = 361

X_90_width        = 11.5[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 5.7[dB]
X_pulse           = 3.83333333[us]
Irr_atn_dec       = 20.421[dB]
Irr_atn_noe       = 20.421[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Temp_get          = 25.4[dC]
```

20160920g-datsusi-4.jdf



12

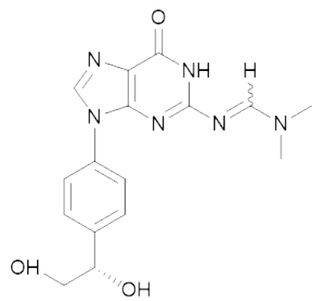
abundance

11.4159
8.4795
8.1600
7.7374
7.7225
7.5129
7.4992
5.3484
5.3416
4.7804
4.7713
4.7609
4.6086
3.4863
3.4760
3.4680
3.3180
3.1256
3.0145
2.4900
1.0561
1.0447
1.0332

X : parts per Million : 1H

```
Filename         = 20160920g-datsusi-4.j
Author           = delta
Experiment       = single_pulse.ex2
Sample_id        = S#401915
Solvent          = DMSO-D6
Creation_time    = 20-SEP-2016 11:04:07
Revision_time    =  6-DEC-2016 10:20:10
Current_time     =  6-DEC-2016 10:21:15

Data_format      = 1D COMPLEX
Dim_size         = 13107
Dim_title        = 1H
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 5[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 8
Total_scans      = 8

X_90_width       = 13.5[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 2.2[dB]
X_pulse          = 6.75[us]
Irr_mode         = Off
Tri_mode         = Off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Recvr_gain       = 46
Relaxation_delay = 5[s]
Repetition_time  = 6.4548992[s]
Temp_get         = 25[dC]
```

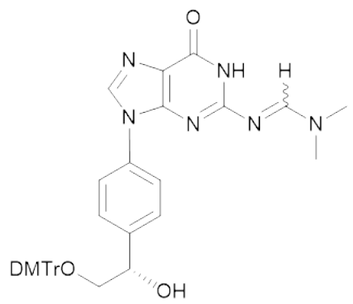
20160920g-datsusi13c-4.jdf



12


```
Filename          = 20160920g-datsusi13c-
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#403086
Solvent           = DMSO-D6
Creation_time     = 20-SEP-2016 11:15:27
Revision_time     =  6-DEC-2016 10:24:13
Current_time      =  6-DEC-2016 10:25:20

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECA 600
Spectrometer      = DELTA2_NMR

Field_strength    = 14.09636928[T] (600[M
X_acq_duration    = 0.69206016[s]
X_domain          = 13C
X_freq            = 150.91343039[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 1.44496109[Hz]
X_sweep           = 47.34848485[kHz]
Irr_domain        = 1H
Irr_freq          = 600.1723046[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 195
Total_scans       = 195

X_90_width        = 11.5[us]
X_acq_time        = 0.69206016[s]
X_angle           = 30[deg]
X_atn             = 5.7[dB]
X_pulse           = 3.83333333[us]
Irr_atn_dec       = 20.421[dB]
Irr_atn_noe       = 20.421[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 58
Relaxation_delay  = 2[s]
Repetition_time   = 2.69206016[s]
Temp_get          = 25.4[dC]
```

20161006g-trityl-7.jdf



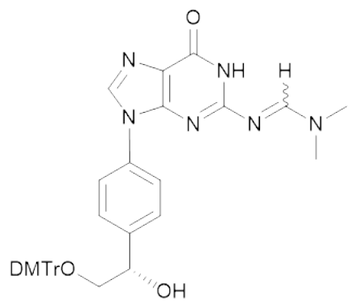
13

```
Filename         = 20161006g-trityl-7.jd
Author           = delta
Experiment       = single_pulse.ex2
Sample_id        = S#586546
Solvent          = CHLOROFORM-D
Creation_time    =  6-OCT-2016 16:11:29
Revision_time    =  6-DEC-2016 10:27:26
Current_time     =  6-DEC-2016 10:28:05

Data_format      = 1D COMPLEX
Dim_size         = 13107
Dim_title        = 1H
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 1.4548992[s]
X_domain         = 1H
X_freq           = 600.1723046[MHz]
X_offset         = 5[ppm]
X_points         = 16384
X_prescans       = 1
X_resolution     = 0.68733284[Hz]
X_sweep          = 11.26126126[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Tri_domain       = 1H
Tri_freq         = 600.1723046[MHz]
Tri_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 16
Total_scans      = 16

X_90_width       = 13.5[us]
X_acq_time       = 1.4548992[s]
X_angle          = 45[deg]
X_atn            = 2.2[dB]
X_pulse          = 6.75[us]
Irr_mode         = Off
Tri_mode         = Off
Dante_presat     = FALSE
Initial_wait     = 1[s]
Recvr_gain       = 54
Relaxation_delay = 5[s]
Repetition_time  = 6.4548992[s]
Temp_get         = 24.3[dC]
```


8.5976 8.4235 7.7834 7.5291 7.4616 7.4478 7.3963 7.2989 7.2840 7.2600 6.8363 6.8214 4.8676 3.7842 3.3720 3.3651 3.2861 3.0479 2.9597 2.8852 2.8807 1.5831

X : parts per Million : 1H

20160920g-tr13C-4.jdf



13

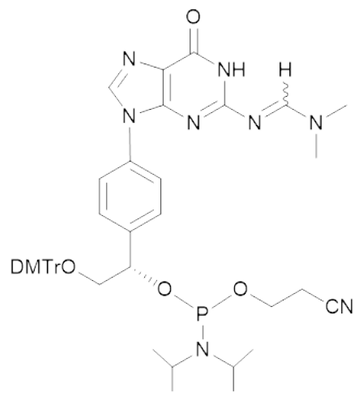
abundance

X : parts per Million : 13C

158.5674
158.0217
157.9164
156.8727
150.1416
144.6745
140.8158
137.3498
135.7604
134.3720
129.9963
128.0335
127.8995
127.4399
126.9037
123.9068
121.0056
113.1926
86.5939
77.4405
77.2107
77.0000
76.7894
72.7680
68.9764
55.2078
41.1425
35.1296

```
Filename         = 20160920g-tr13C-4.jdf
Author           = delta
Experiment       = single_pulse_dec
Sample_id        = S#386536
Solvent          = CHLOROFORM-D
Creation_time    = 20-SEP-2016 10:52:04
Revision_time    =  6-DEC-2016 10:28:51
Current_time     =  6-DEC-2016 10:29:10

Data_format      = 1D COMPLEX
Dim_size         = 26214
Dim_title        = 13C
Dim_units        = [ppm]
Dimensions       = X
Site             = ECA 600
Spectrometer     = DELTA2_NMR

Field_strength   = 14.09636928[T] (600[M
X_acq_duration   = 0.69206016[s]
X_domain         = 13C
X_freq           = 150.91343039[MHz]
X_offset         = 100[ppm]
X_points         = 32768
X_prescans       = 4
X_resolution     = 1.44496109[Hz]
X_sweep          = 47.34848485[kHz]
Irr_domain       = 1H
Irr_freq         = 600.1723046[MHz]
Irr_offset       = 5[ppm]
Clipped          = FALSE
Mod_return       = 1
Scans            = 289
Total_scans      = 289

X_90_width       = 11.5[us]
X_acq_time       = 0.69206016[s]
X_angle          = 30[deg]
X_atn            = 5.7[dB]
X_pulse          = 3.83333333[us]
Irr_atn_dec      = 20.421[dB]
Irr_atn_noe      = 20.421[dB]
Irr_noise        = WALTZ
Decoupling       = TRUE
Initial_wait     = 1[s]
Noe              = TRUE
Noe_time         = 2[s]
Recvr_gain       = 58
Relaxation_delay = 2[s]
Repetition_time  = 2.69206016[s]
Temp_get         = 25.4[dC]
```

20161031g-amida-3.jdf



14


```
Filename          = 20161031g-amida-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = S#352669
Solvent           = CHLOROFORM-D
Creation_time     = 31-OCT-2016 09:53:18
Revision_time     =  6-DEC-2016 10:37:08
Current_time      =  6-DEC-2016 10:37:22

Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 31P
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 400P
Spectrometer      = DELTA2_NMR

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 0.229376[s]
X_domain          = 31P
X_freq            = 161.83469309[MHz]
X_offset          = 0[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 4.35965402[Hz]
X_sweep           = 142.85714286[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 256
Total_scans       = 256

X_90_width        = 10.8[us]
X_acq_time        = 0.229376[s]
X_angle           = 30[deg]
X_atn             = 2.5[dB]
X_pulse           = 3.6[us]
Irr_atn_dec       = 20.20655[dB]
Irr_atn_noe       = 20.20655[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 2.229376[s]
Temp_get          = 22.8[dC]
Spin_action       = SPIN ON
Spin_state        = SPIN ON
Spin_status       = SPIN ON
Spin_get          = 13[Hz]
Spin_set          = 15[Hz]
Spin_gas_source   = AIR
Sample_action     = LOADED
Sample_state      = LOAD
Sample_status     = LOADED
Changer_sample    = 0
```