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SUPPORT INFORMATION

Synthesis and characterization of some novel tetrazol liquid crystals.

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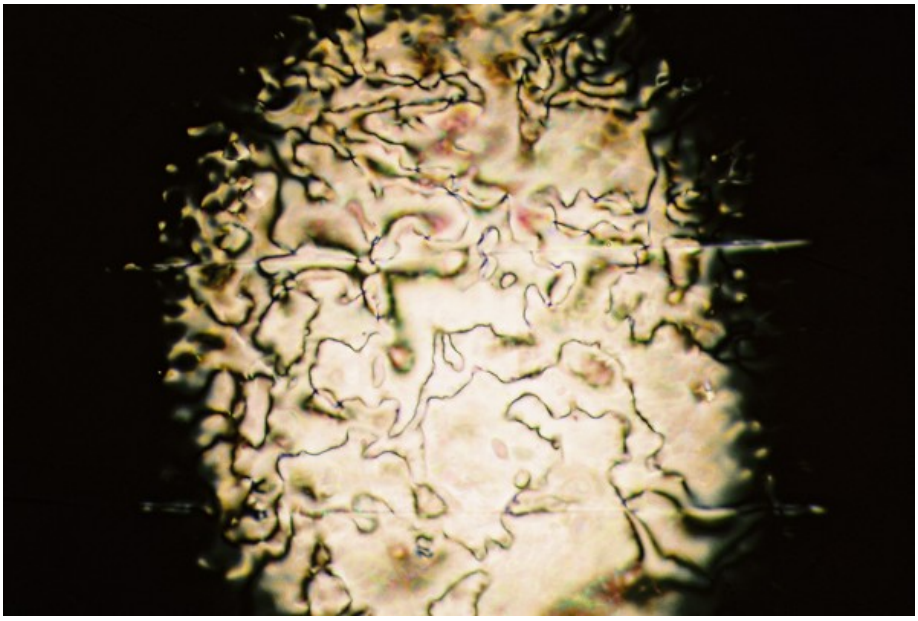

Figure S1. Schlieren texture observed for nematic mesophase upon cooling at 79°C for **5g**.

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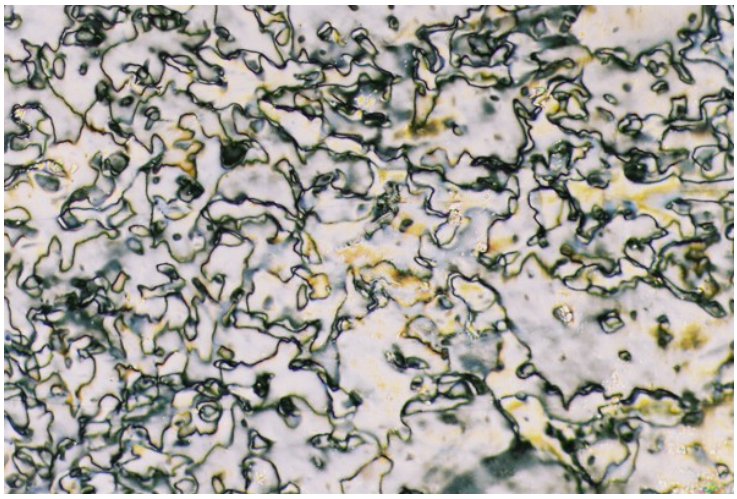
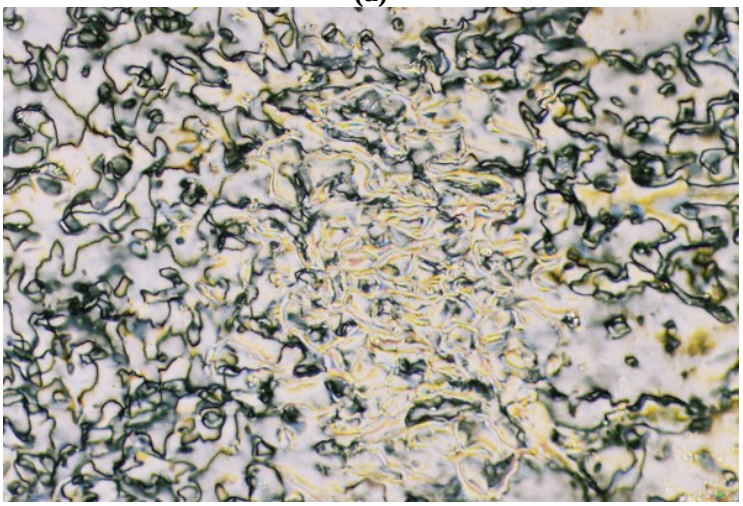
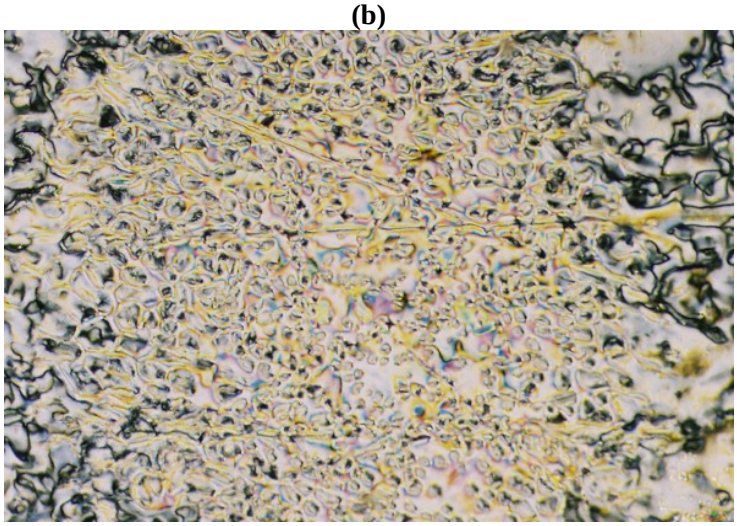


(a)



(b)



(c)

Figure S2. (a), (b) and (c) Schlieren texture observed during the mesophase transition from nematic to smectic mesophase upon cooling at *ca* 71°C for **5g**.

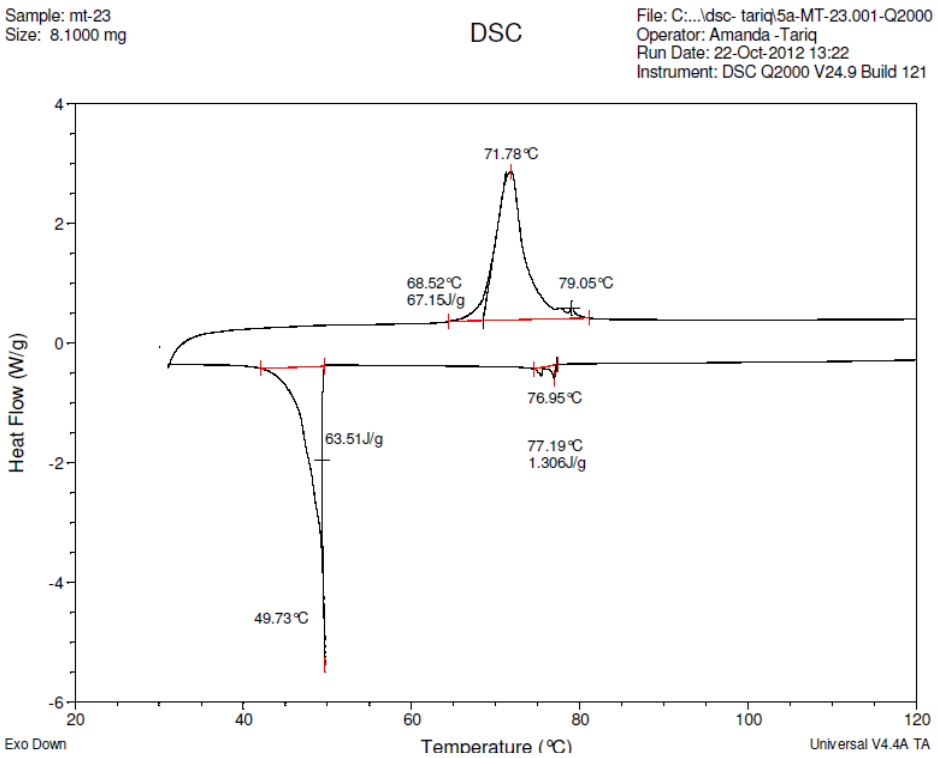


Figure S3. DSC TA Q2000 at 10 °/min for **5a**.

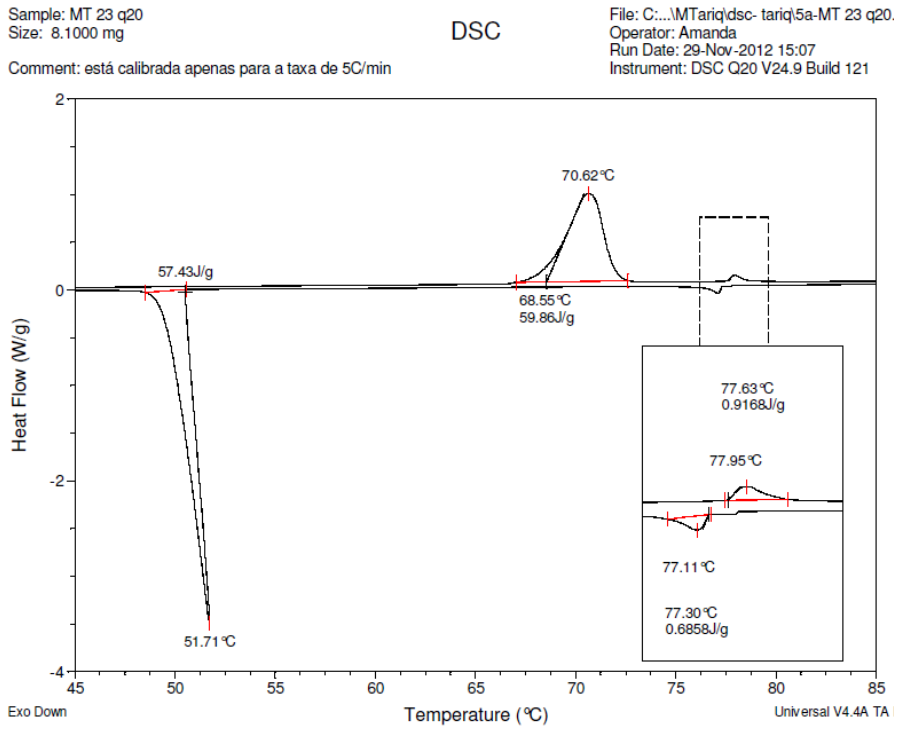


Figure S4. DSC TA Q20 at 5 °/min for **5a**.

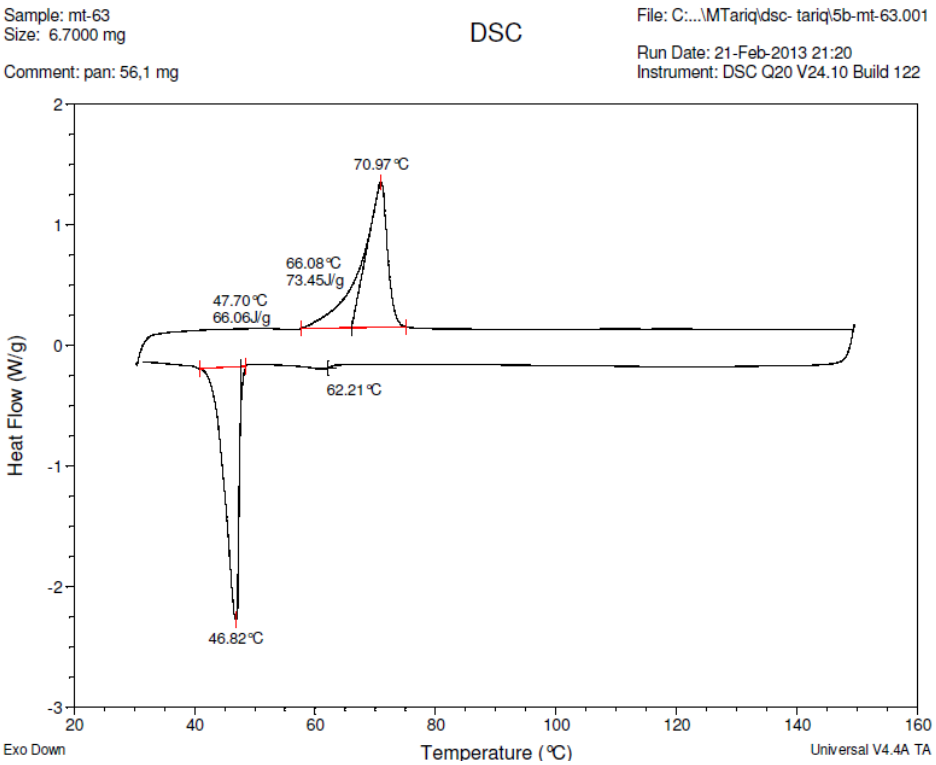


Figure S5. DSC TA Q20 at 5 °/min for **5b**.

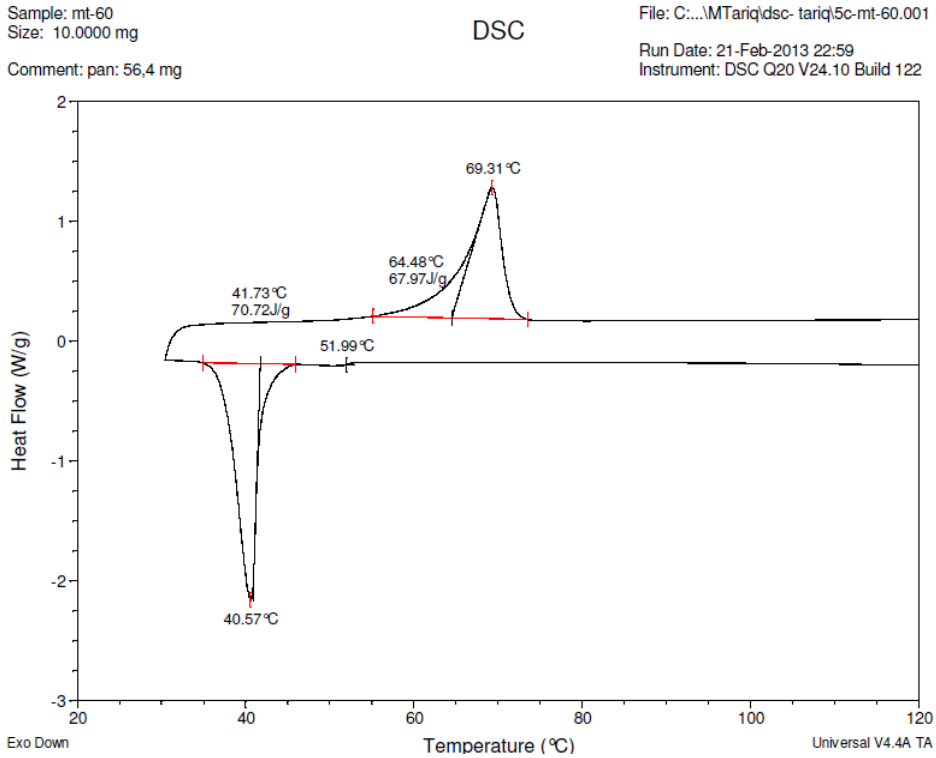


Figure S6. DSC TA Q20 at 5 °/min for **5c**.

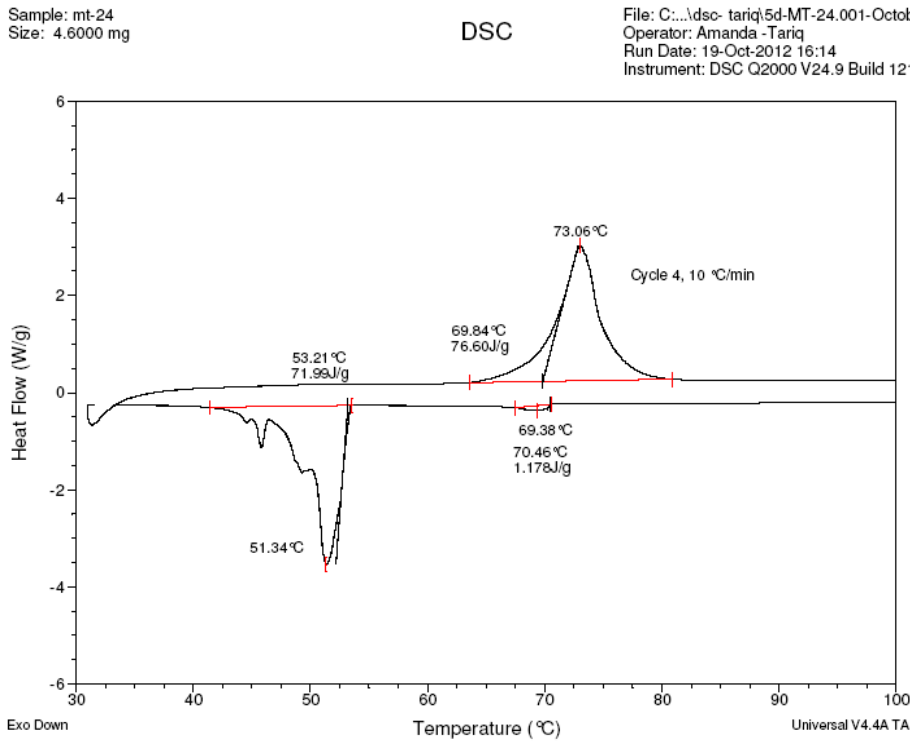


Figure S7. DSC TA Q2000 at 10 °/min for **5d**.

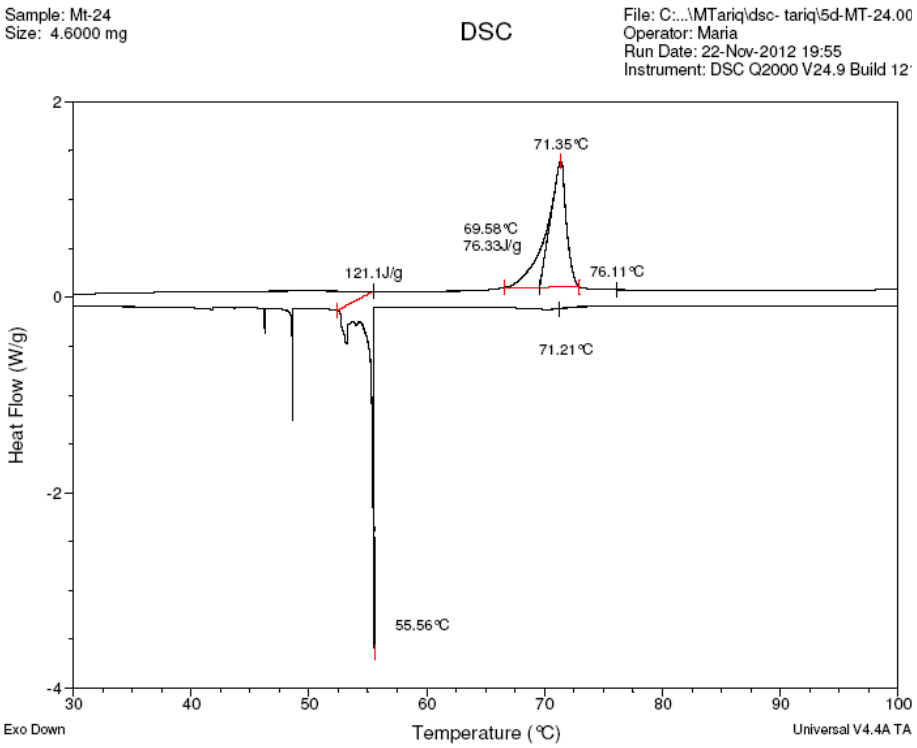


Figure S8. DSC TA Q2000 at 2 °/min for **5d**.

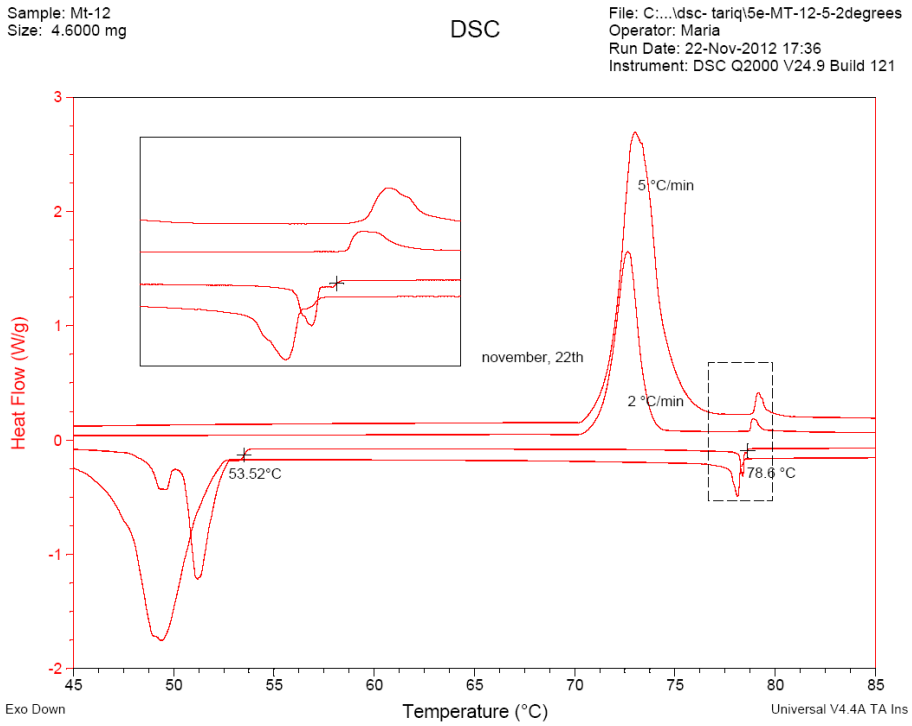


Figure S9. DSC TA Q2000 at 5 C°/min and 2 °C/min for **5e** (on november, 22th).

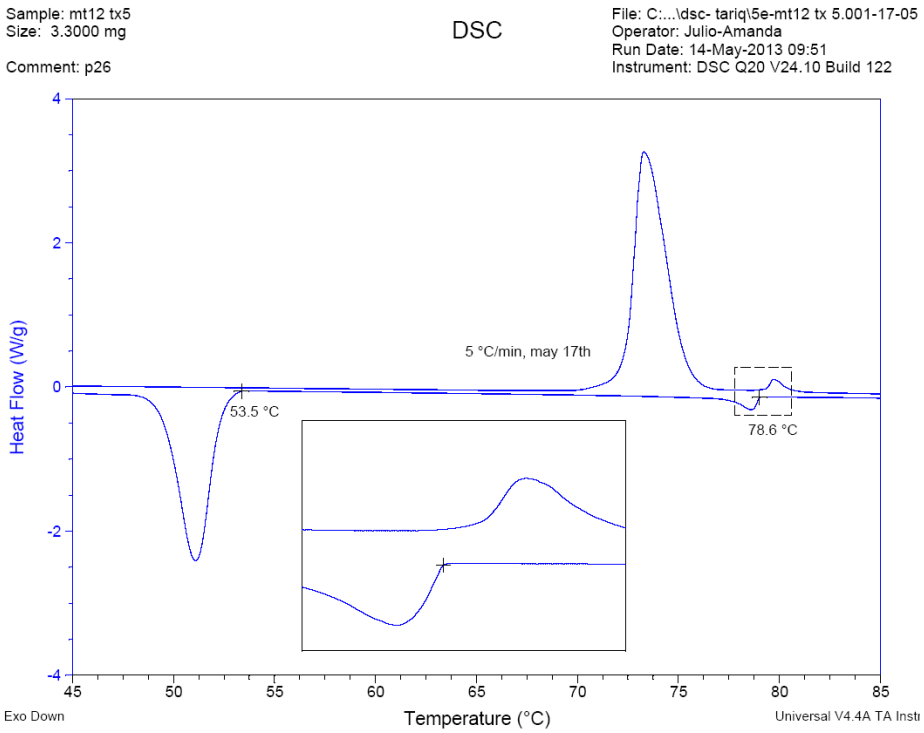


Figure S10. DSC TA Q2000 at 5 °/min for **5e** (on may, 17th)

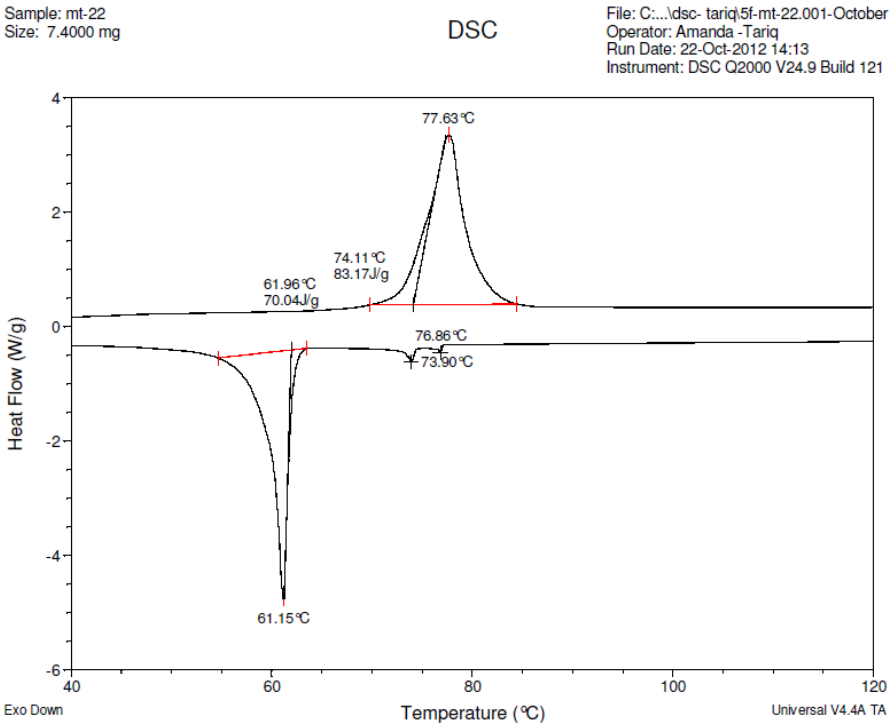


Figure S11. DSC TA Q2000 at 10 °/min for **5f**.

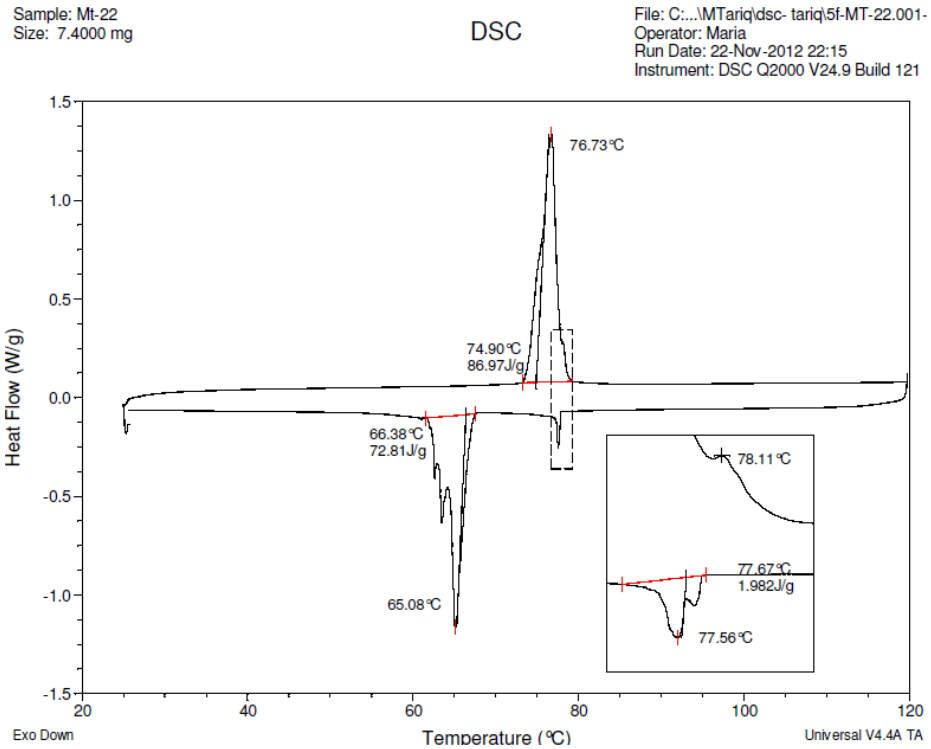


Figure S12. DSC TA Q2000 at 2 °/min for **5f**.

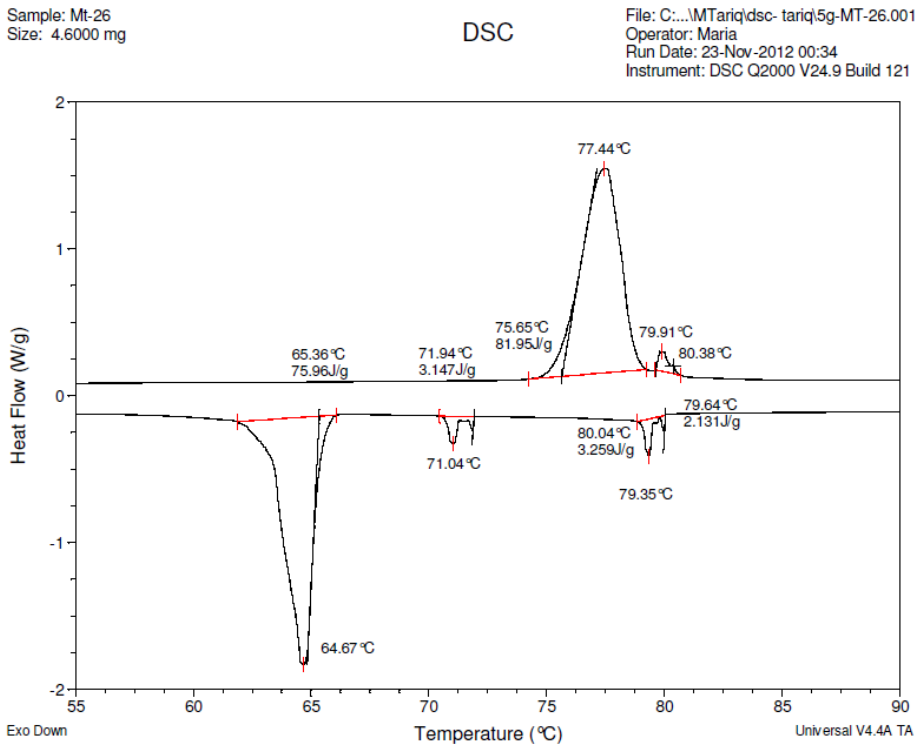


Figure S13. DSC TA Q2000 at 3 °/min for **5g**.

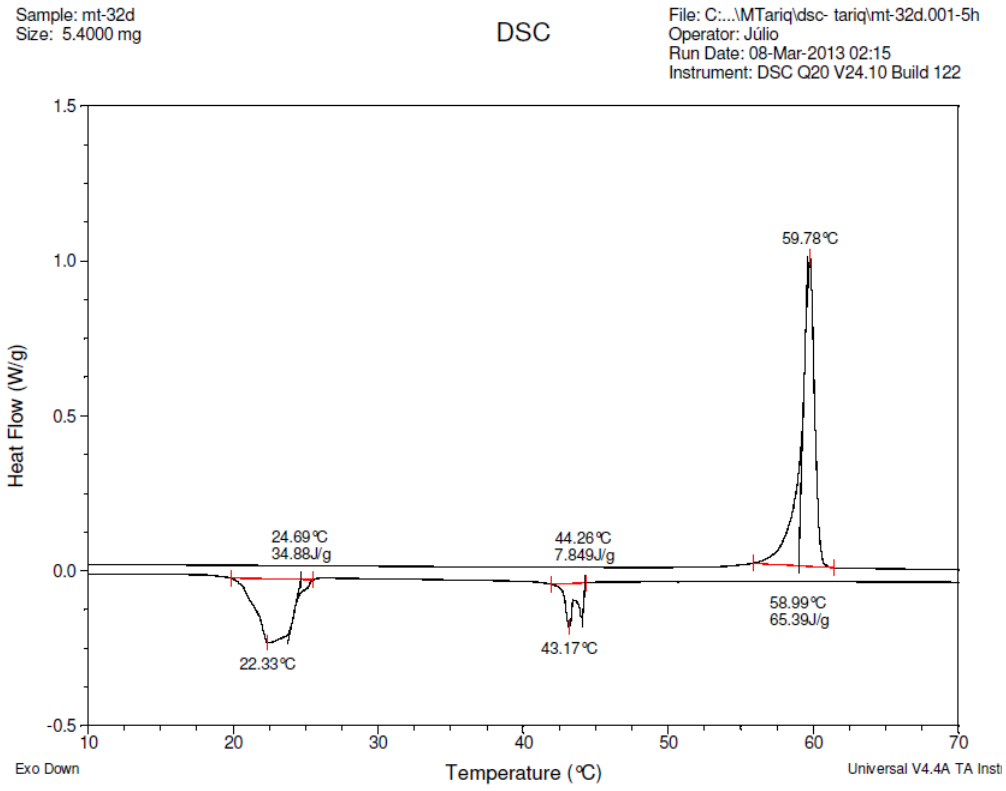


Figure S14. DSC TA Q20 at 1 °/min for **5h**.

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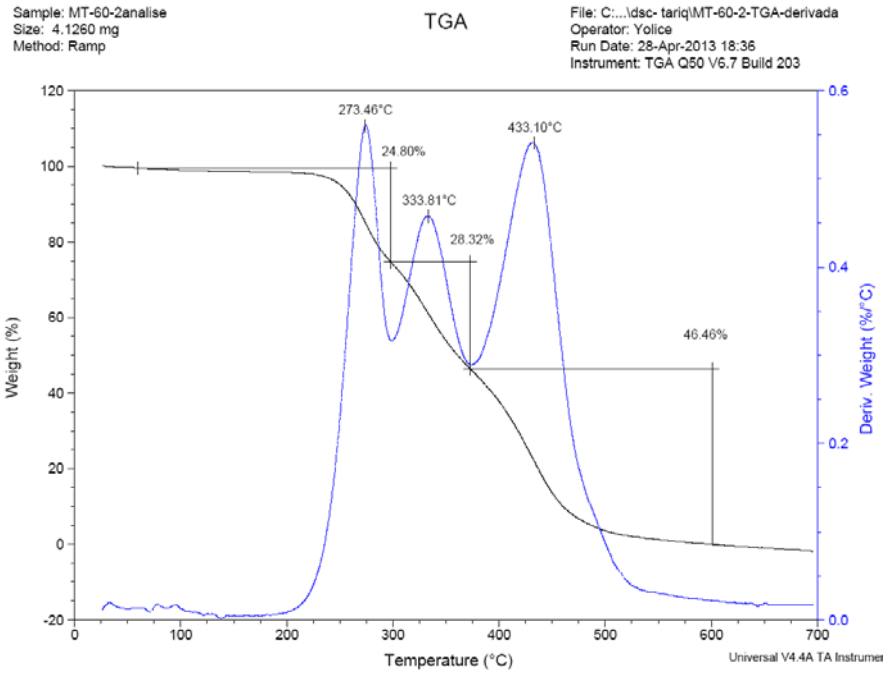

Figure S15. TGA/DTG curve for **5c** in the temperature range 20 – 600 ^{o}C. A derivative weight loss curve has been added to show the point at which weight loss is most apparent.

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SUPPORT INFORMATION

X-Ray data

Synthesis and Characterization of some novel tetrazol Liquid Crystals.

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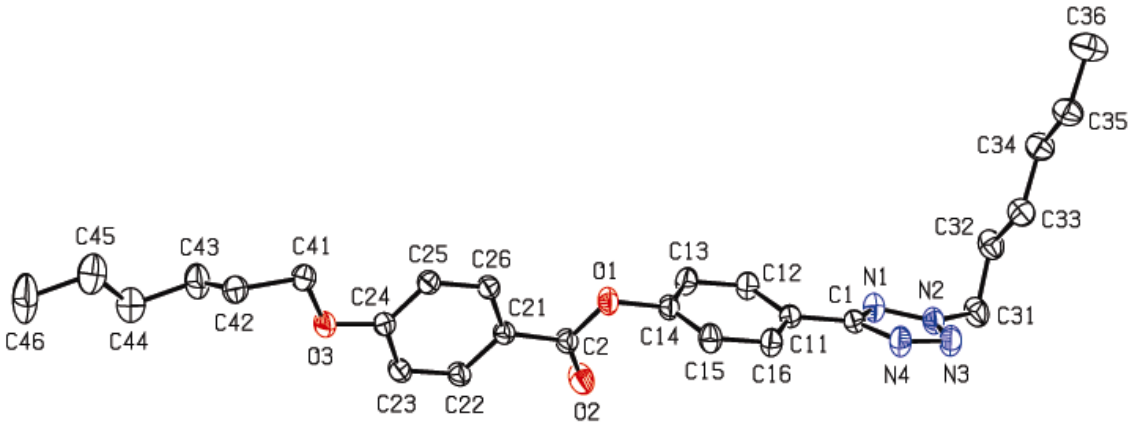
1. Single Crystal X-ray Diffraction

1.1. Compound **5a**



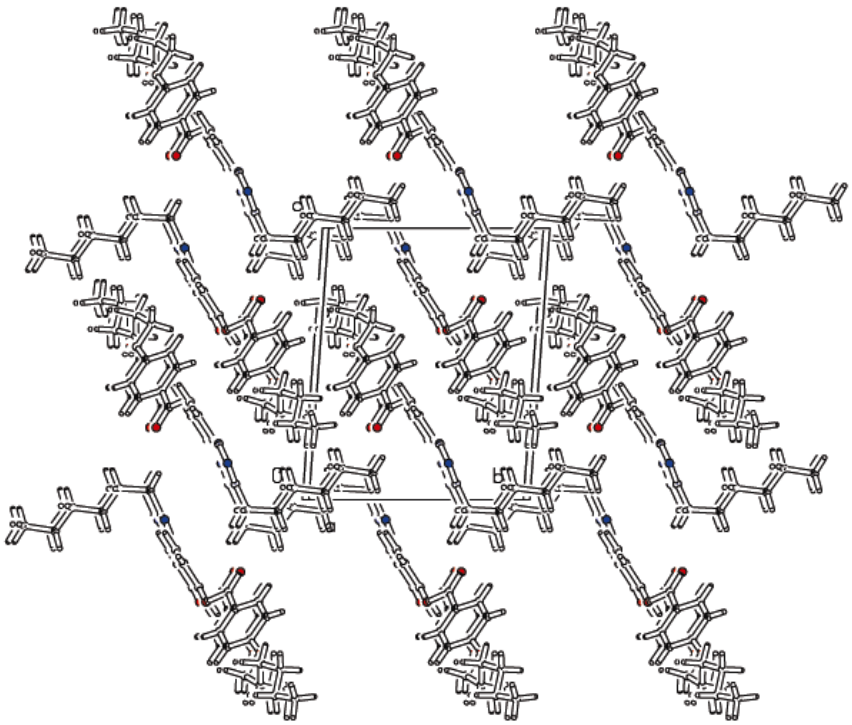


Table 1. Crystal data and structure refinement for **5a**.

Empirical formula	$C_{26}H_{34}N_4O_3$

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Formula weight	450.57	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 8.8808(3) Å	α= 82.731(2)°.
	b = 10.9801(3) Å	β= 72.7700(10)°.
	c = 13.8034(4) Å	γ = 76.798(2)°.
Volume	1249.11(7) $Å^3$	
Z	2	
Density (calculated)	1.198 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	484	
Crystal size	0.40 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.91 to 31.10°.	
Index ranges	$-12 \le h \le 12$, $-15 \le k \le 15$, $-20 \le l \le 20$	
Reflections collected	28779	
Independent reflections	8005 [R(int) = 0.0207]	
Completeness to theta = 31.10°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8005 / 0 / 300	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1824	
R indices (all data)	R1 = 0.0785, wR2 = 0.2006	
Largest diff. peak and hole	1.146 and -0.468 $e.Å^{-3}$	

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Table 2. Bond lengths [Å] and angles [°] for **5a**.

C(1)-N(1)	1.3321(17)	C(32)-H(32B)	0.9900
C(1)-N(4)	1.3515(17)	C(33)-C(34)	1.521(2)
C(1)-C(11)	1.4678(17)	C(33)-H(33A)	0.9900
C(2)-O(2)	1.2016(17)	C(33)-H(33B)	0.9900
C(2)-O(1)	1.3613(16)	C(34)-C(35)	1.518(2)
C(2)-C(21)	1.4746(17)	C(34)-H(34A)	0.9900
C(11)-C(16)	1.3905(19)	C(34)-H(34B)	0.9900
C(11)-C(12)	1.3944(18)	C(35)-C(36)	1.523(3)
C(12)-C(13)	1.3884(18)	C(35)-H(35A)	0.9900
C(12)-H(12)	0.9500	C(35)-H(35B)	0.9900
C(13)-C(14)	1.383(2)	C(36)-H(36A)	0.9800
C(13)-H(13)	0.9500	C(36)-H(36B)	0.9800
C(14)-C(15)	1.3807(19)	C(36)-H(36C)	0.9800
C(14)-O(1)	1.4030(15)	C(41)-O(3)	1.4336(17)
C(15)-C(16)	1.3897(18)	C(41)-C(42)	1.522(2)
C(15)-H(15)	0.9500	C(41)-H(41A)	0.9900
C(16)-H(16)	0.9500	C(41)-H(41B)	0.9900
C(21)-C(26)	1.3883(17)	C(42)-C(43)	1.537(3)
C(21)-C(22)	1.3976(18)	C(42)-H(42A)	0.9900
C(22)-C(23)	1.3793(18)	C(42)-H(42B)	0.9900
C(22)-H(22)	0.9500	C(43)-C(44)	1.536(3)
C(23)-C(24)	1.3960(18)	C(43)-H(43A)	0.9900
C(23)-H(23)	0.9500	C(43)-H(43B)	0.9900
C(24)-O(3)	1.3556(15)	C(44)-C(45)	1.491(3)
C(24)-C(25)	1.3946(18)	C(44)-H(44A)	0.9900
C(25)-C(26)	1.3942(17)	C(44)-H(44B)	0.9900
C(25)-H(25)	0.9500	C(45)-C(46)	1.551(3)
C(26)-H(26)	0.9500	C(45)-H(45A)	0.9900
C(31)-N(2)	1.4637(19)	C(45)-H(45B)	0.9900
C(31)-C(32)	1.517(2)	C(46)-H(46A)	0.9800
C(31)-H(31A)	0.9900	C(46)-H(46B)	0.9800
C(31)-H(31B)	0.9900	C(46)-H(46C)	0.9800
C(32)-C(33)	1.523(2)	N(1)-N(2)	1.3272(16)
C(32)-H(32A)	0.9900	N(2)-N(3)	1.3125(19)

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N(3)-N(4)	1.3234(18)		
N(1)-C(1)-N(4)	112.17(12)	O(3)-C(24)-C(23)	114.70(12)
N(1)-C(1)-C(11)	123.90(11)	C(25)-C(24)-C(23)	120.42(12)
N(4)-C(1)-C(11)	123.92(12)	C(26)-C(25)-C(24)	119.08(12)
O(2)-C(2)-O(1)	122.38(12)	C(26)-C(25)-H(25)	120.5
O(2)-C(2)-C(21)	124.90(12)	C(24)-C(25)-H(25)	120.5
O(1)-C(2)-C(21)	112.71(11)	C(21)-C(26)-C(25)	120.84(12)
C(16)-C(11)-C(12)	119.73(12)	C(21)-C(26)-H(26)	119.6
C(16)-C(11)-C(1)	120.18(11)	C(25)-C(26)-H(26)	119.6
C(12)-C(11)-C(1)	120.08(12)	N(2)-C(31)-C(32)	112.21(12)
C(13)-C(12)-C(11)	120.24(12)	N(2)-C(31)-H(31A)	109.2
C(13)-C(12)-H(12)	119.9	C(32)-C(31)-H(31A)	109.2
C(11)-C(12)-H(12)	119.9	N(2)-C(31)-H(31B)	109.2
C(14)-C(13)-C(12)	118.99(12)	C(32)-C(31)-H(31B)	109.2
C(14)-C(13)-H(13)	120.5	H(31A)-C(31)-H(31B)	107.9
C(12)-C(13)-H(13)	120.5	C(31)-C(32)-C(33)	114.45(14)
C(15)-C(14)-C(13)	121.74(12)	C(31)-C(32)-H(32A)	108.6
C(15)-C(14)-O(1)	118.66(12)	C(33)-C(32)-H(32A)	108.6
C(13)-C(14)-O(1)	119.57(12)	C(31)-C(32)-H(32B)	108.6
C(14)-C(15)-C(16)	119.06(13)	C(33)-C(32)-H(32B)	108.6
C(14)-C(15)-H(15)	120.5	H(32A)-C(32)-H(32B)	107.6
C(16)-C(15)-H(15)	120.5	C(34)-C(33)-C(32)	112.43(13)
C(15)-C(16)-C(11)	120.25(12)	C(34)-C(33)-H(33A)	109.1
C(15)-C(16)-H(16)	119.9	C(32)-C(33)-H(33A)	109.1
C(11)-C(16)-H(16)	119.9	C(34)-C(33)-H(33B)	109.1
C(26)-C(21)-C(22)	119.28(11)	C(32)-C(33)-H(33B)	109.1
C(26)-C(21)-C(2)	123.39(11)	H(33A)-C(33)-H(33B)	107.9
C(22)-C(21)-C(2)	117.33(11)	C(35)-C(34)-C(33)	113.99(13)
C(23)-C(22)-C(21)	120.62(12)	C(35)-C(34)-H(34A)	108.8
C(23)-C(22)-H(22)	119.7	C(33)-C(34)-H(34A)	108.8
C(21)-C(22)-H(22)	119.7	C(35)-C(34)-H(34B)	108.8
C(22)-C(23)-C(24)	119.75(12)	C(33)-C(34)-H(34B)	108.8
C(22)-C(23)-H(23)	120.1	H(34A)-C(34)-H(34B)	107.7
C(24)-C(23)-H(23)	120.1	C(34)-C(35)-C(36)	113.13(15)
O(3)-C(24)-C(25)	124.88(12)	C(34)-C(35)-H(35A)	109.0

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C(36)-C(35)-H(35A)	109.0	H(43A)-C(43)-H(43B)	107.5
C(34)-C(35)-H(35B)	109.0	C(45)-C(44)-C(43)	114.25(18)
C(36)-C(35)-H(35B)	109.0	C(45)-C(44)-H(44A)	108.7
H(35A)-C(35)-H(35B)	107.8	C(43)-C(44)-H(44A)	108.7
C(35)-C(36)-H(36A)	109.5	C(45)-C(44)-H(44B)	108.7
C(35)-C(36)-H(36B)	109.5	C(43)-C(44)-H(44B)	108.7
H(36A)-C(36)-H(36B)	109.5	H(44A)-C(44)-H(44B)	107.6
C(35)-C(36)-H(36C)	109.5	C(44)-C(45)-C(46)	110.7(2)
H(36A)-C(36)-H(36C)	109.5	C(44)-C(45)-H(45A)	109.5
H(36B)-C(36)-H(36C)	109.5	C(46)-C(45)-H(45A)	109.5
O(3)-C(41)-C(42)	106.07(12)	C(44)-C(45)-H(45B)	109.5
O(3)-C(41)-H(41A)	110.5	C(46)-C(45)-H(45B)	109.5
C(42)-C(41)-H(41A)	110.5	H(45A)-C(45)-H(45B)	108.1
O(3)-C(41)-H(41B)	110.5	C(45)-C(46)-H(46A)	109.5
C(42)-C(41)-H(41B)	110.5	C(45)-C(46)-H(46B)	109.5
H(41A)-C(41)-H(41B)	108.7	H(46A)-C(46)-H(46B)	109.5
C(41)-C(42)-C(43)	113.35(13)	C(45)-C(46)-H(46C)	109.5
C(41)-C(42)-H(42A)	108.9	H(46A)-C(46)-H(46C)	109.5
C(43)-C(42)-H(42A)	108.9	H(46B)-C(46)-H(46C)	109.5
C(41)-C(42)-H(42B)	108.9	N(2)-N(1)-C(1)	101.67(11)
C(43)-C(42)-H(42B)	108.9	N(3)-N(2)-N(1)	113.98(12)
H(42A)-C(42)-H(42B)	107.7	N(3)-N(2)-C(31)	123.03(12)
C(44)-C(43)-C(42)	115.40(15)	N(1)-N(2)-C(31)	122.97(13)
C(44)-C(43)-H(43A)	108.4	N(2)-N(3)-N(4)	106.44(11)
C(42)-C(43)-H(43A)	108.4	N(3)-N(4)-C(1)	105.74(12)
C(44)-C(43)-H(43B)	108.4	C(2)-O(1)-C(14)	115.73(10)
C(42)-C(43)-H(43B)	108.4	C(24)-O(3)-C(41)	119.26(11)

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Table 3. Torsion angles [°] for **5a**.

N(1)-C(1)-C(11)-C(16)	167.29(14)	C(24)-C(25)-C(26)-C(21)	0.6(2)
N(4)-C(1)-C(11)-C(16)	-11.5(2)	N(2)-C(31)-C(32)-C(33)	61.06(18)
N(1)-C(1)-C(11)-C(12)	-11.6(2)	C(31)-C(32)-C(33)-C(34)	174.93(13)
N(4)-C(1)-C(11)-C(12)	169.59(14)	C(32)-C(33)-C(34)-C(35)	177.46(13)
C(16)-C(11)-C(12)-C(13)	0.7(2)	C(33)-C(34)-C(35)-C(36)	178.00(15)
C(1)-C(11)-C(12)-C(13)	179.63(13)	O(3)-C(41)-C(42)-C(43)	-64.74(17)
C(11)-C(12)-C(13)-C(14)	-0.3(2)	C(41)-C(42)-C(43)-C(44)	168.18(16)
C(12)-C(13)-C(14)-C(15)	-0.2(2)	C(42)-C(43)-C(44)-C(45)	61.7(2)
C(12)-C(13)-C(14)-O(1)	177.62(12)	C(43)-C(44)-C(45)-C(46)	177.01(18)
C(13)-C(14)-C(15)-C(16)	0.4(2)	N(4)-C(1)-N(1)-N(2)	0.44(16)
O(1)-C(14)-C(15)-C(16)	-177.44(13)	C(11)-C(1)-N(1)-N(2)	-178.45(12)
C(14)-C(15)-C(16)-C(11)	-0.1(2)	C(1)-N(1)-N(2)-N(3)	-0.34(16)
C(12)-C(11)-C(16)-C(15)	-0.5(2)	C(1)-N(1)-N(2)-C(31)	-178.57(13)
C(1)-C(11)-C(16)-C(15)	-179.43(13)	C(32)-C(31)-N(2)-N(3)	-104.58(17)
O(2)-C(2)-C(21)-C(26)	-177.91(15)	C(32)-C(31)-N(2)-N(1)	73.50(18)
O(1)-C(2)-C(21)-C(26)	3.31(19)	N(1)-N(2)-N(3)-N(4)	0.12(18)
O(2)-C(2)-C(21)-C(22)	2.9(2)	C(31)-N(2)-N(3)-N(4)	178.35(13)
O(1)-C(2)-C(21)-C(22)	-175.89(12)	N(2)-N(3)-N(4)-C(1)	0.15(17)
C(26)-C(21)-C(22)-C(23)	-0.3(2)	N(1)-C(1)-N(4)-N(3)	-0.39(17)
C(2)-C(21)-C(22)-C(23)	178.91(13)	C(11)-C(1)-N(4)-N(3)	178.50(13)
C(21)-C(22)-C(23)-C(24)	0.6(2)	O(2)-C(2)-O(1)-C(14)	-0.6(2)
C(22)-C(23)-C(24)-O(3)	179.57(12)	C(21)-C(2)-O(1)-C(14)	178.23(11)
C(22)-C(23)-C(24)-C(25)	-0.3(2)	C(15)-C(14)-O(1)-C(2)	-100.88(15)
O(3)-C(24)-C(25)-C(26)	179.87(12)	C(13)-C(14)-O(1)-C(2)	81.21(16)
C(23)-C(24)-C(25)-C(26)	-0.3(2)	C(25)-C(24)-O(3)-C(41)	1.9(2)
C(22)-C(21)-C(26)-C(25)	-0.3(2)	C(23)-C(24)-O(3)-C(41)	-177.88(13)
C(2)-C(21)-C(26)-C(25)	-179.44(12)	C(42)-C(41)-O(3)-C(24)	178.29(12)

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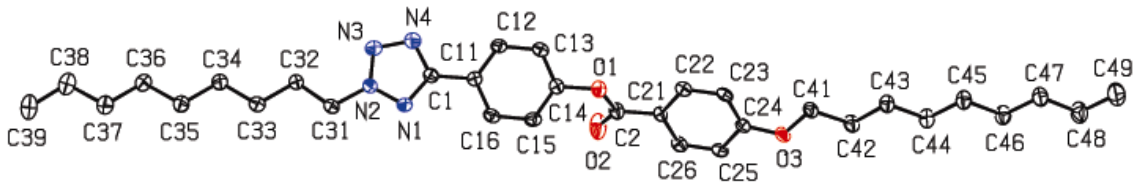
1.2. Compound **5f**



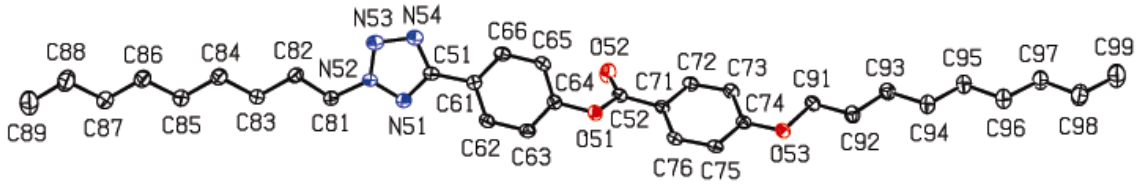


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Table 4. Crystal data and structure refinement for **5f**.

Empirical formula	$C_{32}H_{46}N_4O_3$	
Formula weight	534.73	
Temperature	190(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 6.1964(4) Å	α= 93.630(3)°.
	b = 7.3745(4) Å	β= 94.782(3)°.
	c = 33.1004(18) Å	γ = 95.576(3)°.
Volume	1496.24(15) $Å^3$	
Z	2	
Density (calculated)	1.187 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	580	
Crystal size	0.38 x 0.38 x 0.10 mm^3	
Theta range for data collection	3.32 to 31.85°.	
Index ranges	$-4 \le h \le 9$, $-10 \le k \le 9$, $-48 \le l \le 48$	
Reflections collected	17024	
Independent reflections	10061 [R(int) = 0.0328]	
Completeness to theta = 31.85°	98.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10061 / 3 / 707	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0661, wR2 = 0.1720	
R indices (all data)	R1 = 0.0790, wR2 = 0.1794	
Largest diff. peak and hole	0.431 and -0.301 $e.Å^{-3}$	

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Table 5. Bond lengths [Å] and angles [°] for **5f**.

Molecule 1

N(1)-N(2)	1.342(4)	C(31)-C(32)	1.513(5)
N(2)-N(3)	1.307(4)	C(31)-H(31A)	0.9900
N(3)-N(4)	1.327(4)	C(31)-H(31B)	0.9900
C(1)-N(1)	1.333(4)	C(32)-C(33)	1.530(5)
C(1)-N(4)	1.359(4)	C(32)-H(32A)	0.9900
C(1)-C(11)	1.469(4)	C(32)-H(32B)	0.9900
C(2)-O(2)	1.205(4)	C(33)-C(34)	1.530(5)
C(2)-O(1)	1.359(4)	C(33)-H(33A)	0.9900
C(2)-C(21)	1.475(4)	C(33)-H(33B)	0.9900
C(11)-C(12)	1.378(4)	C(34)-C(35)	1.526(5)
C(11)-C(16)	1.398(4)	C(34)-H(34A)	0.9900
C(12)-C(13)	1.394(5)	C(34)-H(34B)	0.9900
C(12)-H(12)	0.9500	C(35)-C(36)	1.525(5)
C(13)-C(14)	1.366(4)	C(35)-H(35A)	0.9900
C(13)-H(13)	0.9500	C(35)-H(35B)	0.9900
C(14)-C(15)	1.383(4)	C(36)-C(37)	1.529(6)
C(14)-O(1)	1.415(4)	C(36)-H(36A)	0.9900
C(15)-C(16)	1.390(5)	C(36)-H(36B)	0.9900
C(15)-H(15)	0.9500	C(37)-C(38)	1.523(6)
C(16)-H(16)	0.9500	C(37)-H(37A)	0.9900
C(21)-C(26)	1.389(4)	C(37)-H(37B)	0.9900
C(21)-C(22)	1.404(4)	C(38)-C(39)	1.534(7)
C(22)-C(23)	1.389(5)	C(38)-H(38A)	0.9900
C(22)-H(22)	0.9500	C(38)-H(38B)	0.9900
C(23)-C(24)	1.388(4)	C(39)-H(39A)	0.9800
C(23)-H(23)	0.9500	C(39)-H(39B)	0.9800
C(24)-O(3)	1.363(4)	C(39)-H(39C)	0.9800
C(24)-C(25)	1.399(4)	C(41)-O(3)	1.438(4)
C(25)-C(26)	1.378(5)	C(41)-C(42)	1.521(5)
C(25)-H(25)	0.9500	C(41)-H(41A)	0.9900
C(26)-H(26)	0.9500	C(41)-H(41B)	0.9900
C(31)-N(2)	1.468(4)	C(42)-C(43)	1.528(4)

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C(42)-H(42A)	0.9900	C(46)-H(46A)	0.9900
C(42)-H(42B)	0.9900	C(46)-H(46B)	0.9900
C(43)-C(44)	1.528(5)	C(47)-C(48)	1.515(5)
C(43)-H(43A)	0.9900	C(47)-H(47A)	0.9900
C(43)-H(43B)	0.9900	C(47)-H(47B)	0.9900
C(44)-C(45)	1.532(5)	C(48)-C(49)	1.528(6)
C(44)-H(44A)	0.9900	C(48)-H(48A)	0.9900
C(44)-H(44B)	0.9900	C(48)-H(48B)	0.9900
C(45)-C(46)	1.522(5)	C(49)-H(49A)	0.9800
C(45)-H(45A)	0.9900	C(49)-H(49B)	0.9800
C(45)-H(45B)	0.9900	C(49)-H(49C)	0.9800
C(46)-C(47)	1.530(5)		

C(1)-N(1)-N(2)	100.8(3)	C(15)-C(14)-O(1)	120.2(3)
N(3)-N(2)-N(1)	115.0(3)	C(14)-C(15)-C(16)	118.7(3)
N(3)-N(2)-C(31)	124.1(3)	C(14)-C(15)-H(15)	120.6
N(1)-N(2)-C(31)	120.8(3)	C(16)-C(15)-H(15)	120.6
N(2)-N(3)-N(4)	105.7(3)	C(15)-C(16)-C(11)	119.8(3)
N(3)-N(4)-C(1)	106.3(3)	C(15)-C(16)-H(16)	120.1
N(1)-C(1)-N(4)	112.2(3)	C(11)-C(16)-H(16)	120.1
N(1)-C(1)-C(11)	125.5(3)	C(26)-C(21)-C(22)	119.4(3)
N(4)-C(1)-C(11)	122.3(3)	C(26)-C(21)-C(2)	116.2(3)
O(2)-C(2)-O(1)	122.6(3)	C(22)-C(21)-C(2)	124.4(3)
O(2)-C(2)-C(21)	124.2(3)	C(23)-C(22)-C(21)	120.0(3)
O(1)-C(2)-C(21)	113.2(3)	C(23)-C(22)-H(22)	120.0
C(12)-C(11)-C(16)	120.0(3)	C(21)-C(22)-H(22)	120.0
C(12)-C(11)-C(1)	120.5(3)	C(24)-C(23)-C(22)	120.0(3)
C(16)-C(11)-C(1)	119.5(3)	C(24)-C(23)-H(23)	120.0
C(11)-C(12)-C(13)	120.3(3)	C(22)-C(23)-H(23)	120.0
C(11)-C(12)-H(12)	119.9	O(3)-C(24)-C(23)	126.3(3)
C(13)-C(12)-H(12)	119.9	O(3)-C(24)-C(25)	113.8(3)
C(14)-C(13)-C(12)	118.9(3)	C(23)-C(24)-C(25)	120.0(3)
C(14)-C(13)-H(13)	120.5	C(26)-C(25)-C(24)	120.0(3)
C(12)-C(13)-H(13)	120.5	C(26)-C(25)-H(25)	120.0
C(13)-C(14)-C(15)	122.2(3)	C(24)-C(25)-H(25)	120.0
C(13)-C(14)-O(1)	117.5(3)	C(25)-C(26)-C(21)	120.6(3)

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C(25)-C(26)-H(26)	119.7	C(37)-C(36)-H(36B)	109.1
C(21)-C(26)-H(26)	119.7	H(36A)-C(36)-H(36B)	107.8
N(2)-C(31)-C(32)	113.2(3)	C(38)-C(37)-C(36)	113.1(4)
N(2)-C(31)-H(31A)	108.9	C(38)-C(37)-H(37A)	109.0
C(32)-C(31)-H(31A)	108.9	C(36)-C(37)-H(37A)	109.0
N(2)-C(31)-H(31B)	108.9	C(38)-C(37)-H(37B)	109.0
C(32)-C(31)-H(31B)	108.9	C(36)-C(37)-H(37B)	109.0
H(31A)-C(31)-H(31B)	107.8	H(37A)-C(37)-H(37B)	107.8
C(31)-C(32)-C(33)	109.5(3)	C(37)-C(38)-C(39)	112.5(4)
C(31)-C(32)-H(32A)	109.8	C(37)-C(38)-H(38A)	109.1
C(33)-C(32)-H(32A)	109.8	C(39)-C(38)-H(38A)	109.1
C(31)-C(32)-H(32B)	109.8	C(37)-C(38)-H(38B)	109.1
C(33)-C(32)-H(32B)	109.8	C(39)-C(38)-H(38B)	109.1
H(32A)-C(32)-H(32B)	108.2	H(38A)-C(38)-H(38B)	107.8
C(34)-C(33)-C(32)	113.1(3)	C(38)-C(39)-H(39A)	109.5
C(34)-C(33)-H(33A)	109.0	C(38)-C(39)-H(39B)	109.5
C(32)-C(33)-H(33A)	109.0	H(39A)-C(39)-H(39B)	109.5
C(34)-C(33)-H(33B)	109.0	C(38)-C(39)-H(39C)	109.5
C(32)-C(33)-H(33B)	109.0	H(39A)-C(39)-H(39C)	109.5
H(33A)-C(33)-H(33B)	107.8	H(39B)-C(39)-H(39C)	109.5
C(35)-C(34)-C(33)	112.1(3)	O(3)-C(41)-C(42)	104.3(2)
C(35)-C(34)-H(34A)	109.2	O(3)-C(41)-H(41A)	110.9
C(33)-C(34)-H(34A)	109.2	C(42)-C(41)-H(41A)	110.9
C(35)-C(34)-H(34B)	109.2	O(3)-C(41)-H(41B)	110.9
C(33)-C(34)-H(34B)	109.2	C(42)-C(41)-H(41B)	110.9
H(34A)-C(34)-H(34B)	107.9	H(41A)-C(41)-H(41B)	108.9
C(36)-C(35)-C(34)	113.4(3)	C(41)-C(42)-C(43)	114.3(3)
C(36)-C(35)-H(35A)	108.9	C(41)-C(42)-H(42A)	108.7
C(34)-C(35)-H(35A)	108.9	C(43)-C(42)-H(42A)	108.7
C(36)-C(35)-H(35B)	108.9	C(41)-C(42)-H(42B)	108.7
C(34)-C(35)-H(35B)	108.9	C(43)-C(42)-H(42B)	108.7
H(35A)-C(35)-H(35B)	107.7	H(42A)-C(42)-H(42B)	107.6
C(35)-C(36)-C(37)	112.5(3)	C(44)-C(43)-C(42)	110.8(3)
C(35)-C(36)-H(36A)	109.1	C(44)-C(43)-H(43A)	109.5
C(37)-C(36)-H(36A)	109.1	C(42)-C(43)-H(43A)	109.5
C(35)-C(36)-H(36B)	109.1	C(44)-C(43)-H(43B)	109.5

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C(42)-C(43)-H(43B)	109.5	H(46A)-C(46)-H(46B)	107.7
H(43A)-C(43)-H(43B)	108.1	C(48)-C(47)-C(46)	113.5(3)
C(43)-C(44)-C(45)	114.2(3)	C(48)-C(47)-H(47A)	108.9
C(43)-C(44)-H(44A)	108.7	C(46)-C(47)-H(47A)	108.9
C(45)-C(44)-H(44A)	108.7	C(48)-C(47)-H(47B)	108.9
C(43)-C(44)-H(44B)	108.7	C(46)-C(47)-H(47B)	108.9
C(45)-C(44)-H(44B)	108.7	H(47A)-C(47)-H(47B)	107.7
H(44A)-C(44)-H(44B)	107.6	C(47)-C(48)-C(49)	113.5(4)
C(46)-C(45)-C(44)	112.9(3)	C(47)-C(48)-H(48A)	108.9
C(46)-C(45)-H(45A)	109.0	C(49)-C(48)-H(48A)	108.9
C(44)-C(45)-H(45A)	109.0	C(47)-C(48)-H(48B)	108.9
C(46)-C(45)-H(45B)	109.0	C(49)-C(48)-H(48B)	108.9
C(44)-C(45)-H(45B)	109.0	H(48A)-C(48)-H(48B)	107.7
H(45A)-C(45)-H(45B)	107.8	C(48)-C(49)-H(49A)	109.5
C(45)-C(46)-C(47)	113.6(3)	C(48)-C(49)-H(49B)	109.5
C(45)-C(46)-H(46A)	108.8	H(49A)-C(49)-H(49B)	109.5
C(47)-C(46)-H(46A)	108.8	C(48)-C(49)-H(49C)	109.5
C(45)-C(46)-H(46B)	108.8	H(49A)-C(49)-H(49C)	109.5
C(47)-C(46)-H(46B)	108.8	H(49B)-C(49)-H(49C)	109.5

Molecule 2

C(51)-N(51)	1.329(4)	C(65)-C(66)	1.384(5)
C(51)-N(54)	1.360(4)	C(65)-H(65)	0.9500
C(51)-C(61)	1.463(4)	C(66)-H(66)	0.9500
C(52)-O(52)	1.199(4)	C(71)-C(76)	1.386(4)
C(52)-O(51)	1.359(3)	C(71)-C(72)	1.396(4)
C(52)-C(71)	1.483(4)	C(72)-C(73)	1.389(4)
C(61)-C(62)	1.391(4)	C(72)-H(72)	0.9500
C(61)-C(66)	1.402(4)	C(73)-C(74)	1.395(4)
C(62)-C(63)	1.387(5)	C(73)-H(73)	0.9500
C(62)-H(62)	0.9500	C(74)-O(53)	1.367(4)
C(63)-C(64)	1.379(4)	C(74)-C(75)	1.393(4)
C(63)-H(63)	0.9500	C(75)-C(76)	1.386(4)
C(64)-C(65)	1.392(4)	C(75)-H(75)	0.9500
C(64)-O(51)	1.403(4)	C(76)-H(76)	0.9500

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C(81)-N(52)	1.460(4)	C(91)-H(91A)	0.9900
C(81)-C(82)	1.512(5)	C(91)-H(91B)	0.9900
C(81)-H(81A)	0.9900	C(92)-C(93)	1.518(5)
C(81)-H(81B)	0.9900	C(92)-H(92A)	0.9900
C(82)-C(83)	1.527(5)	C(92)-H(92B)	0.9900
C(82)-H(82A)	0.9900	C(93)-C(94)	1.519(5)
C(82)-H(82B)	0.9900	C(93)-H(93A)	0.9900
C(83)-C(84)	1.527(5)	C(93)-H(93B)	0.9900
C(83)-H(83A)	0.9900	C(94)-C(95)	1.524(5)
C(83)-H(83B)	0.9900	C(94)-H(94A)	0.9900
C(84)-C(85)	1.521(5)	C(94)-H(94B)	0.9900
C(84)-H(84A)	0.9900	C(95)-C(96)	1.519(5)
C(84)-H(84B)	0.9900	C(95)-H(95A)	0.9900
C(85)-C(86)	1.518(5)	C(95)-H(95B)	0.9900
C(85)-H(85A)	0.9900	C(96)-C(97)	1.524(5)
C(85)-H(85B)	0.9900	C(96)-H(96A)	0.9900
C(86)-C(87)	1.513(5)	C(96)-H(96B)	0.9900
C(86)-H(86A)	0.9900	C(97)-C(98)	1.514(6)
C(86)-H(86B)	0.9900	C(97)-H(97A)	0.9900
C(87)-C(88)	1.517(6)	C(97)-H(97B)	0.9900
C(87)-H(87A)	0.9900	C(98)-C(99)	1.527(6)
C(87)-H(87B)	0.9900	C(98)-H(98A)	0.9900
C(88)-C(89)	1.517(7)	C(98)-H(98B)	0.9900
C(88)-H(88A)	0.9900	C(99)-H(99A)	0.9800
C(88)-H(88B)	0.9900	C(99)-H(99B)	0.9800
C(89)-H(89A)	0.9800	C(99)-H(99C)	0.9800
C(89)-H(89B)	0.9800	N(51)-N(52)	1.327(4)
C(89)-H(89C)	0.9800	N(52)-N(53)	1.317(4)
C(91)-O(53)	1.433(4)	N(53)-N(54)	1.338(4)
C(91)-C(92)	1.505(5)		

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C(2)-O(1)-C(14)	115.4(2)	C(72)-C(71)-C(52)	116.4(3)
C(24)-O(3)-C(41)	120.3(2)	C(73)-C(72)-C(71)	120.9(3)
C(52)-O(51)-C(64)	115.8(2)	C(73)-C(72)-H(72)	119.6
C(74)-O(53)-C(91)	117.5(2)	C(71)-C(72)-H(72)	119.6
N(52)-N(51)-C(51)	102.4(3)	C(72)-C(73)-C(74)	118.9(3)
N(53)-N(52)-N(51)	114.1(3)	C(72)-C(73)-H(73)	120.5
N(53)-N(52)-C(81)	124.5(3)	C(74)-C(73)-H(73)	120.5
N(51)-N(52)-C(81)	121.3(3)	O(53)-C(74)-C(75)	115.8(3)
N(52)-N(53)-N(54)	105.9(3)	O(53)-C(74)-C(73)	124.0(3)
N(53)-N(54)-C(51)	105.7(3)	C(75)-C(74)-C(73)	120.2(3)
N(51)-C(51)-N(54)	111.9(3)	C(76)-C(75)-C(74)	120.4(3)
N(51)-C(51)-C(61)	123.1(3)	C(76)-C(75)-H(75)	119.8
N(54)-C(51)-C(61)	125.1(3)	C(74)-C(75)-H(75)	119.8
O(52)-C(52)-O(51)	123.4(3)	C(71)-C(76)-C(75)	119.9(3)
O(52)-C(52)-C(71)	124.2(3)	C(71)-C(76)-H(76)	120.1
O(51)-C(52)-C(71)	112.4(2)	C(75)-C(76)-H(76)	120.1
C(62)-C(61)-C(66)	119.5(3)	N(52)-C(81)-C(82)	114.3(3)
C(62)-C(61)-C(51)	118.9(3)	N(52)-C(81)-H(81A)	108.7
C(66)-C(61)-C(51)	121.5(3)	C(82)-C(81)-H(81A)	108.7
C(63)-C(62)-C(61)	120.5(3)	N(52)-C(81)-H(81B)	108.7
C(63)-C(62)-H(62)	119.7	C(82)-C(81)-H(81B)	108.7
C(61)-C(62)-H(62)	119.7	H(81A)-C(81)-H(81B)	107.6
C(64)-C(63)-C(62)	118.9(3)	C(81)-C(82)-C(83)	109.2(3)
C(64)-C(63)-H(63)	120.6	C(81)-C(82)-H(82A)	109.8
C(62)-C(63)-H(63)	120.6	C(83)-C(82)-H(82A)	109.8
C(63)-C(64)-C(65)	122.0(3)	C(81)-C(82)-H(82B)	109.8
C(63)-C(64)-O(51)	118.2(3)	C(83)-C(82)-H(82B)	109.8
C(65)-C(64)-O(51)	119.8(3)	H(82A)-C(82)-H(82B)	108.3
C(66)-C(65)-C(64)	118.6(3)	C(82)-C(83)-C(84)	113.8(3)
C(66)-C(65)-H(65)	120.7	C(82)-C(83)-H(83A)	108.8
C(64)-C(65)-H(65)	120.7	C(84)-C(83)-H(83A)	108.8
C(65)-C(66)-C(61)	120.4(3)	C(82)-C(83)-H(83B)	108.8
C(65)-C(66)-H(66)	119.8	C(84)-C(83)-H(83B)	108.8
C(61)-C(66)-H(66)	119.8	H(83A)-C(83)-H(83B)	107.7
C(76)-C(71)-C(72)	119.7(3)	C(85)-C(84)-C(83)	112.6(3)
C(76)-C(71)-C(52)	123.9(3)	C(85)-C(84)-H(84A)	109.1

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C(83)-C(84)-H(84A)	109.1	C(92)-C(91)-H(91A)	110.1
C(85)-C(84)-H(84B)	109.1	O(53)-C(91)-H(91B)	110.1
C(83)-C(84)-H(84B)	109.1	C(92)-C(91)-H(91B)	110.1
H(84A)-C(84)-H(84B)	107.8	H(91A)-C(91)-H(91B)	108.4
C(86)-C(85)-C(84)	114.4(3)	C(91)-C(92)-C(93)	113.6(3)
C(86)-C(85)-H(85A)	108.6	C(91)-C(92)-H(92A)	108.8
C(84)-C(85)-H(85A)	108.6	C(93)-C(92)-H(92A)	108.8
C(86)-C(85)-H(85B)	108.6	C(91)-C(92)-H(92B)	108.8
C(84)-C(85)-H(85B)	108.6	C(93)-C(92)-H(92B)	108.8
H(85A)-C(85)-H(85B)	107.6	H(92A)-C(92)-H(92B)	107.7
C(87)-C(86)-C(85)	113.6(3)	C(92)-C(93)-C(94)	113.2(3)
C(87)-C(86)-H(86A)	108.9	C(92)-C(93)-H(93A)	108.9
C(85)-C(86)-H(86A)	108.9	C(94)-C(93)-H(93A)	108.9
C(87)-C(86)-H(86B)	108.9	C(92)-C(93)-H(93B)	108.9
C(85)-C(86)-H(86B)	108.9	C(94)-C(93)-H(93B)	108.9
H(86A)-C(86)-H(86B)	107.7	H(93A)-C(93)-H(93B)	107.8
C(86)-C(87)-C(88)	114.2(3)	C(93)-C(94)-C(95)	114.6(3)
C(86)-C(87)-H(87A)	108.7	C(93)-C(94)-H(94A)	108.6
C(88)-C(87)-H(87A)	108.7	C(95)-C(94)-H(94A)	108.6
C(86)-C(87)-H(87B)	108.7	C(93)-C(94)-H(94B)	108.6
C(88)-C(87)-H(87B)	108.7	C(95)-C(94)-H(94B)	108.6
H(87A)-C(87)-H(87B)	107.6	H(94A)-C(94)-H(94B)	107.6
C(89)-C(88)-C(87)	113.4(4)	C(96)-C(95)-C(94)	113.4(3)
C(89)-C(88)-H(88A)	108.9	C(96)-C(95)-H(95A)	108.9
C(87)-C(88)-H(88A)	108.9	C(94)-C(95)-H(95A)	108.9
C(89)-C(88)-H(88B)	108.9	C(96)-C(95)-H(95B)	108.9
C(87)-C(88)-H(88B)	108.9	C(94)-C(95)-H(95B)	108.9
H(88A)-C(88)-H(88B)	107.7	H(95A)-C(95)-H(95B)	107.7
C(88)-C(89)-H(89A)	109.5	C(95)-C(96)-C(97)	114.5(3)
C(88)-C(89)-H(89B)	109.5	C(95)-C(96)-H(96A)	108.6
H(89A)-C(89)-H(89B)	109.5	C(97)-C(96)-H(96A)	108.6
C(88)-C(89)-H(89C)	109.5	C(95)-C(96)-H(96B)	108.6
H(89A)-C(89)-H(89C)	109.5	C(97)-C(96)-H(96B)	108.6
H(89B)-C(89)-H(89C)	109.5	H(96A)-C(96)-H(96B)	107.6
O(53)-C(91)-C(92)	108.2(3)	C(98)-C(97)-C(96)	113.6(3)
O(53)-C(91)-H(91A)	110.1	C(98)-C(97)-H(97A)	108.9

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C(96)-C(97)-H(97A)	108.9	C(99)-C(98)-H(98B)	108.9
C(98)-C(97)-H(97B)	108.9	H(98A)-C(98)-H(98B)	107.7
C(96)-C(97)-H(97B)	108.9	C(98)-C(99)-H(99A)	109.5
H(97A)-C(97)-H(97B)	107.7	C(98)-C(99)-H(99B)	109.5
C(97)-C(98)-C(99)	113.3(4)	H(99A)-C(99)-H(99B)	109.5
C(97)-C(98)-H(98A)	108.9	C(98)-C(99)-H(99C)	109.5
C(99)-C(98)-H(98A)	108.9	H(99A)-C(99)-H(99C)	109.5
C(97)-C(98)-H(98B)	108.9	H(99B)-C(99)-H(99C)	109.5

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Table 6. Torsion angles [°] for **5f**.

O(2)-C(2)-O(1)-C(14)	1.4(5)	O(2)-C(2)-C(21)-C(22)	164.4(4)
C(21)-C(2)-O(1)-C(14)	-177.9(3)	O(1)-C(2)-C(21)-C(22)	-16.4(5)
C(13)-C(14)-O(1)-C(2)	-110.7(3)	C(26)-C(21)-C(22)-C(23)	-0.2(5)
C(15)-C(14)-O(1)-C(2)	72.2(4)	C(2)-C(21)-C(22)-C(23)	179.2(3)
C(23)-C(24)-O(3)-C(41)	-3.2(5)	C(21)-C(22)-C(23)-C(24)	-1.0(5)
C(25)-C(24)-O(3)-C(41)	175.9(3)	C(22)-C(23)-C(24)-O(3)	-179.7(3)
C(42)-C(41)-O(3)-C(24)	-167.6(3)	C(22)-C(23)-C(24)-C(25)	1.2(4)
N(4)-C(1)-N(1)-N(2)	0.3(4)	O(3)-C(24)-C(25)-C(26)	-179.5(3)
C(11)-C(1)-N(1)-N(2)	179.8(3)	C(23)-C(24)-C(25)-C(26)	-0.3(4)
C(1)-N(1)-N(2)-N(3)	-0.4(4)	C(24)-C(25)-C(26)-C(21)	-0.9(5)
C(1)-N(1)-N(2)-C(31)	-177.0(3)	C(22)-C(21)-C(26)-C(25)	1.1(5)
C(32)-C(31)-N(2)-N(3)	10.4(5)	C(2)-C(21)-C(26)-C(25)	-178.3(3)
C(32)-C(31)-N(2)-N(1)	-173.3(3)	N(2)-C(31)-C(32)-C(33)	-175.7(3)
N(1)-N(2)-N(3)-N(4)	0.4(4)	C(31)-C(32)-C(33)-C(34)	-178.9(3)
C(31)-N(2)-N(3)-N(4)	176.8(3)	C(32)-C(33)-C(34)-C(35)	-178.1(3)
N(2)-N(3)-N(4)-C(1)	-0.2(4)	C(33)-C(34)-C(35)-C(36)	-179.9(3)
N(1)-C(1)-N(4)-N(3)	-0.1(4)	C(34)-C(35)-C(36)-C(37)	-179.2(3)
C(11)-C(1)-N(4)-N(3)	-179.6(3)	C(35)-C(36)-C(37)-C(38)	179.9(4)
N(1)-C(1)-C(11)-C(12)	-178.6(3)	C(36)-C(37)-C(38)-C(39)	178.7(4)
N(4)-C(1)-C(11)-C(12)	0.8(5)	O(3)-C(41)-C(42)-C(43)	-175.6(3)
N(1)-C(1)-C(11)-C(16)	2.0(5)	C(41)-C(42)-C(43)-C(44)	-178.6(3)
N(4)-C(1)-C(11)-C(16)	-178.6(3)	C(42)-C(43)-C(44)-C(45)	179.8(3)
C(16)-C(11)-C(12)-C(13)	1.8(5)	C(43)-C(44)-C(45)-C(46)	179.9(3)
C(1)-C(11)-C(12)-C(13)	-177.5(3)	C(44)-C(45)-C(46)-C(47)	179.9(3)
C(11)-C(12)-C(13)-C(14)	0.2(5)	C(45)-C(46)-C(47)-C(48)	178.8(3)
C(12)-C(13)-C(14)-C(15)	-2.6(5)	C(46)-C(47)-C(48)-C(49)	179.9(4)
C(12)-C(13)-C(14)-O(1)	-179.6(3)	N(54)-C(51)-N(51)-N(52)	-0.3(4)
C(13)-C(14)-C(15)-C(16)	2.8(5)	C(61)-C(51)-N(51)-N(52)	178.0(3)
O(1)-C(14)-C(15)-C(16)	179.8(3)	C(51)-N(51)-N(52)-N(53)	0.3(4)
C(14)-C(15)-C(16)-C(11)	-0.7(5)	C(51)-N(51)-N(52)-C(81)	178.5(3)
C(12)-C(11)-C(16)-C(15)	-1.5(5)	C(82)-C(81)-N(52)-N(53)	-17.6(5)
C(1)-C(11)-C(16)-C(15)	177.8(3)	C(82)-C(81)-N(52)-N(51)	164.4(3)
O(2)-C(2)-C(21)-C(26)	-16.2(5)	N(51)-N(52)-N(53)-N(54)	-0.2(4)
O(1)-C(2)-C(21)-C(26)	163.0(3)	C(81)-N(52)-N(53)-N(54)	-178.3(3)

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N(52)-N(53)-N(54)-C(51)	0.0(4)	C(72)-C(71)-C(76)-C(75)	1.1(4)
N(51)-C(51)-C(61)-C(62)	0.9(5)	C(52)-C(71)-C(76)-C(75)	-177.7(3)
N(54)-C(51)-C(61)-C(62)	179.0(3)	C(74)-C(75)-C(76)-C(71)	1.1(4)
N(51)-C(51)-C(61)-C(66)	-177.1(3)	N(52)-C(81)-C(82)-C(83)	179.2(3)
N(54)-C(51)-C(61)-C(66)	1.0(5)	C(81)-C(82)-C(83)-C(84)	179.0(3)
C(66)-C(61)-C(62)-C(63)	-0.6(5)	C(82)-C(83)-C(84)-C(85)	178.0(3)
C(51)-C(61)-C(62)-C(63)	-178.7(3)	C(83)-C(84)-C(85)-C(86)	-179.3(3)
C(61)-C(62)-C(63)-C(64)	1.2(5)	C(84)-C(85)-C(86)-C(87)	179.5(3)
C(62)-C(63)-C(64)-C(65)	-0.6(5)	C(85)-C(86)-C(87)-C(88)	-178.8(4)
C(62)-C(63)-C(64)-O(51)	178.5(3)	C(86)-C(87)-C(88)-C(89)	-179.5(4)
C(63)-C(64)-C(65)-C(66)	-0.6(5)	O(53)-C(91)-C(92)-C(93)	172.0(3)
O(51)-C(64)-C(65)-C(66)	-179.7(3)	C(91)-C(92)-C(93)-C(94)	-177.1(3)
C(64)-C(65)-C(66)-C(61)	1.2(5)	C(92)-C(93)-C(94)-C(95)	175.5(3)
C(62)-C(61)-C(66)-C(65)	-0.6(5)	C(93)-C(94)-C(95)-C(96)	-178.1(3)
C(51)-C(61)-C(66)-C(65)	177.4(3)	C(94)-C(95)-C(96)-C(97)	178.3(3)
O(52)-C(52)-C(71)-C(76)	-166.7(3)	C(95)-C(96)-C(97)-C(98)	180.0(3)
O(51)-C(52)-C(71)-C(76)	13.5(4)	C(96)-C(97)-C(98)-C(99)	-179.4(4)
O(52)-C(52)-C(71)-C(72)	14.4(5)	N(51)-C(51)-N(54)-N(53)	0.2(4)
O(51)-C(52)-C(71)-C(72)	-165.4(2)	C(61)-C(51)-N(54)-N(53)	-178.1(3)
C(76)-C(71)-C(72)-C(73)	-1.8(4)	O(52)-C(52)-O(51)-C(64)	-2.2(4)
C(52)-C(71)-C(72)-C(73)	177.1(3)	C(71)-C(52)-O(51)-C(64)	177.6(2)
C(71)-C(72)-C(73)-C(74)	0.2(4)	C(63)-C(64)-O(51)-C(52)	110.8(3)
C(72)-C(73)-C(74)-O(53)	-176.2(3)	C(65)-C(64)-O(51)-C(52)	-70.1(4)
C(72)-C(73)-C(74)-C(75)	2.1(4)	C(75)-C(74)-O(53)-C(91)	-171.8(3)
O(53)-C(74)-C(75)-C(76)	175.7(2)	C(73)-C(74)-O(53)-C(91)	6.6(4)
C(73)-C(74)-C(75)-C(76)	-2.8(4)	C(92)-C(91)-O(53)-C(74)	170.5(2)