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$^1\text{H}$  NMR spectral data for compounds **3**, **11**, **23**, **24**, **26-30**, **32-34**, **37**, **39-41**, **45**, **47-53**, **55-56**, **58**, **60-64**, **67**, **69**, **73**.

$^{13}\text{C}$  NMR spectral data for compounds **3**, **11**, **23-24**, **26-30**, **32-34**, **37**, **39-41**, **45**, **47-53**, **55-56**, **58**, **60-64**, **67**, **69**, **73**.

**X-ray Crystallography.** Single crystals of **49** crystallized from acetonitrile and those of **51** from methanol. The intensity data were collected on a STOE/AED2 diffractometer with  $\omega$ - $2\theta$  scan technique. The cell dimensions were refined against 30 reflections with  $18^\circ < 2\theta < 25^\circ$  for **49** and 44 reflections with  $15^\circ < 2\theta < 35^\circ$  for **51**. Data reduction included corrections for background, Lorentz, polarisation and absorption effects. The absorption corrections were based on numerical integration<sup>1</sup> (transmission factor range, 0.94 to 0.97 for **49** and 0.96 to 0.98 for **51**). The structure was solved by application of direct methods (SHELXS-86<sup>2</sup>) and refined with full-matrix least-squares techniques based on  $F^2$  (SHELXL-93<sup>3</sup>). The non-hydrogen atoms were refined as vibrating anisotropic. The hydrogen atoms were located in a difference electron density map and their positions were refined. Isotropic vibration parameters,  $U_{\text{iso}}$ , for the hydrogen atoms were set to  $1.2 \cdot U_{\text{eq}}$  of the parent non-hydrogen atom. The geometric calculations were performed using the programs SHELXL-93<sup>3</sup> and PLATON.<sup>4</sup> Crystal data and selected details of the refinement calculations of **49** and **51** are listed in Table 2.

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**Table 1.** Selected Bond Lengths (Å) and Torsion Angles (Deg) with e.s.d.'s in Parentheses for the two Independent Molecules in the Crystal Structure of **49**, **a** and **b**.

	<b>49a</b>	<b>49b</b>	<b>50</b>
bond lengths			
C2-C3	1.327(2)	1.325(2)	1.326(3)
C3-C2'	1.451(2)	1.450(2)	1.438(3)
C2'-C3'	1.372(2)	1.368(2)	1.359(3)
C3'-C6'	1.479(2)	1.476(2)	
C5'-C6'			1.466(3)
C6'-C11'	1.397(2)	1.399(2)	1.399(3)
torsion angles			
C2-C3-C2'-C3'	17.6(3)	21.0(3)	175.0(3)
C2'-C3'-C6'-C11'	39.1(2)	40.5(2)	
C4'-C5'-C6'-C11'			175.2(3)

**Table 2.** Crystal Data and Selected Details of the Final Structure Refinements of **49** and **51**.

Compound	<b>49</b>	<b>51</b>
Formula	C <sub>19</sub> H <sub>19</sub> NO <sub>5</sub>	C <sub>21</sub> H <sub>21</sub> NO <sub>5</sub>
Formula weight	341.35	367.39
Space group	<i>P</i> -1	<i>P</i> 2 <sub>1</sub> / <i>a</i>
Radiation; $\lambda$	MoK $\alpha$ ; 0.71073 Å	MoK $\alpha$ ; 0.71073 Å
<i>a</i> , Å	9.985(2)	12.317(2)
<i>b</i> , Å	11.174(3)	10.804(2)
<i>c</i> , Å	15.039(3)	14.961(3)
$\alpha$ , °	93.68(3)	90
$\beta$ , °	94.83(3)	110.073(14)
$\gamma$ , °	91.16(2)	90
<i>V<sub>C</sub></i> , Å <sup>3</sup>	1668.1(7)	1869.8(6)
<i>Z</i>	4	4
<i>D<sub>C</sub></i> , g·cm <sup>-3</sup>	1.359(1)	1.305(1)
<i>T</i> , K	150(2)	150(2)
$\mu_{\text{Mo K}\alpha}$ , cm <sup>-1</sup>	1.0	0.9
Crystal size	0.15 x 0.53 x 0.57 mm	0.30 x 0.42 x 0.50 mm
<i>N</i> <sub>measured</sub>	8527	6028
<i>N</i> <sub>unique</sub>	7648	5452
<i>N</i> [ <i>F</i> <sub>o</sub> > 4σ( <i>F</i> <sub>o</sub> )]	5506	2134
no. of parameters	565	307
<i>R</i> [ <i>F</i> <sub>o</sub> > 4σ( <i>F</i> <sub>o</sub> )]	0.035	0.050
<i>wR</i> ( <i>F</i> <sup>2</sup> ) for all unique data	0.096	0.125
Goof for all unique data	1.04	0.78
Largest diff. peak and hole, e·Å <sup>-3</sup>	-0.2 and 0.3	-0.3 and 0.3

Table 3. Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for 49.

$$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

Atom	x	y	z	$U_{eq}$
N1	-0.3716(1)	-0.2530(1)	0.4652(1)	0.022(1)
C2	-0.2395(1)	-0.2299(1)	0.4334(1)	0.023(1)
C3	-0.1373(1)	-0.2472(1)	0.4932(1)	0.021(1)
C4	-0.1818(1)	-0.2932(1)	0.5789(1)	0.022(1)
C5	-0.2736(1)	-0.1991(1)	0.6192(1)	0.025(1)
C6	-0.3869(1)	-0.1724(1)	0.5489(1)	0.025(1)
C7	-0.3854(1)	-0.3825(1)	0.4878(1)	0.024(1)
C8	-0.2658(2)	-0.4096(1)	0.5535(1)	0.026(1)
O1'	0.0900(1)	-0.2841(1)	0.5387(1)	0.027(1)
C2'	0.0036(1)	-0.2250(1)	0.4816(1)	0.022(1)
C3'	0.0761(1)	-0.1615(1)	0.4260(1)	0.021(1)
C4'	0.2145(1)	-0.1831(1)	0.4516(1)	0.028(1)
C5'	0.2170(1)	-0.2563(1)	0.5192(1)	0.030(1)
C6'	0.0304(1)	-0.0827(1)	0.3548(1)	0.022(1)
C7'	0.1006(1)	-0.0802(1)	0.2783(1)	0.026(1)
C8'	0.0656(2)	-0.0012(1)	0.2132(1)	0.031(1)
C9'	-0.0400(2)	0.0750(1)	0.2231(1)	0.034(1)
C10'	-0.1115(2)	0.0727(1)	0.2980(1)	0.032(1)
C11'	-0.0760(1)	-0.0048(1)	0.3639(1)	0.026(1)
O2	-0.5135(1)	-0.1247(1)	0.3522(1)	0.027(1)
O3	-0.5434(1)	-0.2152(1)	0.2147(1)	0.035(1)
O4	-0.4636(1)	0.0801(1)	0.2697(1)	0.030(1)
O5	-0.6171(1)	0.0086(1)	0.1629(1)	0.048(1)
O15	-0.5308(1)	-0.1259(1)	0.2695(1)	0.020(1)
C16	-0.5414(1)	-0.0037(1)	0.2278(1)	0.021(1)
N1A	0.3597(1)	0.2678(1)	0.0318(1)	0.024(1)
C2A	0.2243(1)	0.2746(1)	0.0621(1)	0.025(1)
C3A	0.1263(1)	0.2567(1)	-0.0030(1)	0.024(1)
C4A	0.1778(1)	0.2233(1)	-0.0930(1)	0.024(1)
C5A	0.2689(1)	0.3275(1)	-0.1160(1)	0.027(1)
C6A	0.3748(2)	0.3581(1)	-0.0377(1)	0.029(1)
C7A	0.3823(2)	0.1445(1)	-0.0118(1)	0.029(1)
C8A	0.2648(2)	0.1124(1)	-0.0821(1)	0.029(1)
O1'A	-0.0998(1)	0.2075(1)	-0.0580(1)	0.036(1)
C2'A	-0.0159(1)	0.2692(1)	0.0074(1)	0.025(1)
C3'A	-0.0911(1)	0.3273(1)	0.0680(1)	0.024(1)
C4'A	-0.2284(2)	0.2976(2)	0.0383(1)	0.036(1)
C5'A	-0.2284(2)	0.2272(2)	-0.0374(1)	0.043(1)
C6'A	-0.0469(1)	0.4079(1)	0.1470(1)	0.024(1)
C7'A	-0.1140(2)	0.4034(1)	0.2244(1)	0.032(1)
C8'A	-0.0774(2)	0.4815(2)	0.2980(1)	0.045(1)
C9'A	0.0273(2)	0.5632(2)	0.2957(1)	0.052(1)
C9'A	0.0943(2)	0.5696(2)	0.2194(1)	0.045(1)
C9'A	0.0570(2)	0.4932(1)	0.1446(1)	0.032(1)
O2A	0.5095(1)	0.2826(1)	0.1982(1)	0.026(1)
O3A	0.5673(1)	0.3684(1)	0.3353(1)	0.026(1)
O4A	0.4974(1)	0.5830(1)	0.2795(1)	0.032(1)
O5A	0.4295(1)	0.4969(1)	0.1452(1)	0.042(1)
C15A	0.5238(1)	0.3706(1)	0.2567(1)	0.019(1)
C16A	0.4784(1)	0.4915(1)	0.2206(1)	0.022(1)

Table 4. Bond lengths [Å] and angles [°] for 49.

N1-C2	1.465(2)
N1-C7	1.514(2)
N1-C6	1.520(2)
C2-C3	1.328(2)
C3-C2'	1.450(2)
C3-C4	1.515(2)
C4-C5	1.538(2)
C4-C8	1.543(2)
C5-C6	1.529(2)
C7-C8	1.532(2)
O1'-C5'	1.360(2)
O1'-C2'	1.375(2)
C2'-C3'	1.373(2)
C3'-C4'	1.433(2)
C3'-C6'	1.478(2)
C4'-C5'	1.344(2)
C6'-C11'	1.397(2)
C6'-C7'	1.398(2)
C7'-C8'	1.387(2)
C8'-C9'	1.380(2)
C9'-C10'	1.385(2)
C10'-C11'	1.386(2)
O2-O15	1.240(2)
O3-O15	1.249(2)
O4-C16	1.300(2)
O5-C16	1.200(2)
O15-C16	1.541(2)
N1A-C2A	1.464(2)
N1A-C6A	1.514(2)
N1A-C7A	1.517(2)
C2A-C3A	1.327(2)
C3A-C2'A	1.451(2)
C3A-C4A	1.515(2)
C4A-C8A	1.537(2)
C4A-C5A	1.538(2)
C5A-C6A	1.531(2)
C7A-C8A	1.532(2)
O1'A-C5'A	1.365(2)
O1'A-C2'A	1.377(2)
C2'A-C3'A	1.368(2)
C3'A-C4'A	1.432(2)
C3'A-C6'A	1.476(2)
C4'A-C5'A	1.342(2)
C6'A-C7'A	1.394(2)
C6'A-C9'A	1.399(2)
C7'A-C8'A	1.384(2)
C8'A-C9'A	1.378(3)
C9'A-C9'A	1.382(3)
C9'A-C9'A	1.387(2)
O2A-C15A	1.275(2)
O3A-C15A	1.226(2)
O4A-C16A	1.308(2)
O5A-C16A	1.202(2)
C15A-C16A	1.550(2)
C2-N1-C7	110.34(11)
C2-N1-C6	109.27(10)
C7-N1-C6	108.81(10)
C3-C2-N1	113.84(12)
C2-C3-C2'	125.68(12)
C2-C3-C4	112.87(12)
C2'-C3-C4	121.44(11)
C3-C4-C5	107.55(11)
C3-C4-C8	107.45(11)

C5-C4-C8	108.35(11)
C6-C5-C4	109.30(11)
N1-C6-C5	108.12(11)
N1-C7-C8	108.08(10)
C7-C8-C4	109.15(11)
C5'-O1'-C2'	107.02(11)
C3'-C2'-O1'	109.53(11)
C3'-C2'-C3	136.65(12)
O1'-C2'-C3	113.80(11)
C2'-C3'-C4'	105.78(12)
C2'-C3'-C6'	130.30(12)
C4'-C3'-C6'	123.89(12)
C5'-C4'-C3'	107.00(13)
C4'-C5'-O1'	110.66(12)
C11'-C6'-C7'	118.64(13)
C11'-C6'-C3'	121.96(12)
C7'-C6'-C3'	119.27(12)
C8'-C7'-C6'	120.50(14)
C9'-C8'-C7'	120.16(14)
C8'-C9'-C10'	120.05(14)
C9'-C10'-C11'	120.1(2)
C10'-C11'-C6'	120.50(14)
O2-O15-O3	127.83(12)
O2-O15-C16	117.21(11)
O3-O15-C16	114.95(11)
O5-C16-O4	125.43(12)
O5-C16-O15	120.70(12)
O4-C16-O15	113.87(11)
C2A-N1A-C6A	109.08(11)
C2A-N1A-C7A	110.78(11)
C6A-N1A-C7A	107.50(11)
C3A-C2A-N1A	114.16(12)
C2A-C3A-C2'A	125.28(12)
C2A-C3A-C4A	112.87(12)
C2'A-C3A-C4A	121.84(12)
C3A-C4A-C8A	107.33(11)
C3A-C4A-C5A	107.71(11)
C8A-C4A-C5A	108.09(11)
C6A-C5A-C4A	109.36(11)
N1A-C6A-C5A	108.23(11)
N1A-C7A-C8A	108.52(11)
C7A-C8A-C4A	108.78(11)
C5'A-O1'A-C2'A	106.93(11)
C3'A-C2'A-O1'A	109.59(12)
C3'A-C2'A-C3A	135.85(12)
O1'A-C2'A-C3A	114.56(11)
C2'A-C3'A-C4'A	105.85(12)
C2'A-C3'A-C6'A	129.46(12)
C4'A-C3'A-C6'A	124.66(13)
C5'A-C4'A-C3'A	107.23(14)
C4'A-C5'A-O1'A	110.39(14)
C7'A-C6'A-C9'A	119.05(13)
C7'A-C6'A-C3'A	119.56(13)
C9'A-C6'A-C3'A	121.31(13)
C8'A-C7'A-C6'A	120.4(2)
C9'A-C8'A-C7'A	120.1(2)
C8'A-C9'A-C9'A	120.3(2)
C9'A-C9'A-C9'A	120.1(2)
C9'A-C9'A-C6'A	120.0(2)
O3A-C15A-O2A	127.40(12)
O3A-C15A-C16A	119.04(11)
O2A-C15A-C16A	113.56(11)
O5A-C16A-O4A	124.89(12)
O5A-C16A-C15A	121.25(11)
O4A-C16A-C15A	113.86(11)

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for 49.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{21}$	$U_{13}$	$U_{12}$
N1	0.021(1)	0.023(1)	0.020(1)	0.004(1)	-0.002(1)	-0.003(1)
C2	0.024(1)	0.025(1)	0.021(1)	0.004(1)	0.001(1)	-0.004(1)
C3	0.023(1)	0.020(1)	0.020(1)	0.000(1)	0.002(1)	-0.002(1)
C4	0.022(1)	0.026(1)	0.019(1)	0.003(1)	-0.001(1)	-0.002(1)
C5	0.026(1)	0.027(1)	0.022(1)	-0.003(1)	0.002(1)	-0.005(1)
C6	0.025(1)	0.022(1)	0.028(1)	-0.003(1)	0.002(1)	-0.001(1)
C7	0.028(1)	0.020(1)	0.025(1)	0.000(1)	0.000(1)	-0.007(1)
C8	0.031(1)	0.021(1)	0.027(1)	0.005(1)	0.001(1)	-0.003(1)
O1'	0.022(1)	0.030(1)	0.028(1)	0.007(1)	0.000(1)	0.002(1)
C2'	0.022(1)	0.022(1)	0.021(1)	0.000(1)	-0.001(1)	0.001(1)
C3'	0.022(1)	0.019(1)	0.023(1)	-0.003(1)	0.002(1)	0.000(1)
C4'	0.020(1)	0.031(1)	0.032(1)	0.001(1)	0.003(1)	0.000(1)
C5'	0.020(1)	0.035(1)	0.036(1)	0.004(1)	0.000(1)	0.003(1)
C6'	0.023(1)	0.018(1)	0.023(1)	-0.001(1)	-0.001(1)	-0.005(1)
C7'	0.029(1)	0.022(1)	0.025(1)	-0.004(1)	0.003(1)	-0.004(1)
C8'	0.042(1)	0.028(1)	0.022(1)	-0.002(1)	0.001(1)	-0.011(1)
C9'	0.047(1)	0.023(1)	0.028(1)	0.003(1)	-0.008(1)	-0.006(1)
C10'	0.035(1)	0.022(1)	0.036(1)	-0.001(1)	-0.005(1)	0.001(1)
C11'	0.028(1)	0.021(1)	0.027(1)	-0.002(1)	0.002(1)	-0.002(1)
O2	0.035(1)	0.024(1)	0.022(1)	0.006(1)	0.001(1)	0.002(1)
O3	0.056(1)	0.019(1)	0.028(1)	-0.001(1)	-0.003(1)	0.005(1)
O4	0.040(1)	0.016(1)	0.033(1)	0.005(1)	-0.010(1)	-0.001(1)
O5	0.060(1)	0.036(1)	0.044(1)	0.019(1)	-0.027(1)	-0.015(1)
O15	0.018(1)	0.019(1)	0.023(1)	0.003(1)	0.002(1)	0.002(1)
C16	0.022(1)	0.019(1)	0.020(1)	0.003(1)	0.002(1)	0.002(1)
N1A	0.022(1)	0.031(1)	0.020(1)	0.000(1)	-0.002(1)	0.000(1)
C2A	0.024(1)	0.031(1)	0.019(1)	-0.002(1)	0.001(1)	0.002(1)
C3A	0.025(1)	0.026(1)	0.021(1)	-0.002(1)	0.002(1)	0.000(1)
C4A	0.022(1)	0.031(1)	0.019(1)	-0.004(1)	-0.001(1)	0.001(1)
C5A	0.028(1)	0.031(1)	0.022(1)	0.005(1)	0.001(1)	0.004(1)
C6A	0.031(1)	0.029(1)	0.028(1)	0.004(1)	0.000(1)	-0.005(1)
C7A	0.031(1)	0.030(1)	0.027(1)	0.002(1)	0.002(1)	0.008(1)
C8A	0.030(1)	0.026(1)	0.029(1)	-0.005(1)	0.003(1)	0.001(1)
O1'A	0.023(1)	0.053(1)	0.030(1)	-0.016(1)	-0.001(1)	-0.004(1)
C2'A	0.023(1)	0.032(1)	0.020(1)	-0.003(1)	-0.001(1)	-0.002(1)
C3'A	0.023(1)	0.028(1)	0.022(1)	0.002(1)	0.002(1)	0.001(1)
C4'A	0.023(1)	0.050(1)	0.034(1)	-0.004(1)	0.003(1)	0.000(1)
C5'A	0.021(1)	0.065(1)	0.039(1)	-0.014(1)	-0.001(1)	-0.006(1)
C6'A	0.028(1)	0.023(1)	0.022(1)	0.001(1)	0.000(1)	0.008(1)
C7'A	0.044(1)	0.027(1)	0.027(1)	0.005(1)	0.008(1)	0.012(1)
C8'A	0.078(1)	0.036(1)	0.024(1)	0.001(1)	0.007(1)	0.023(1)
C9'A	0.080(1)	0.034(1)	0.037(1)	-0.015(1)	-0.011(1)	0.017(1)
C9'A	0.049(1)	0.026(1)	0.056(1)	-0.011(1)	-0.009(1)	0.004(1)
C9'A	0.032(1)	0.026(1)	0.036(1)	-0.002(1)	0.002(1)	0.005(1)
O2A	0.035(1)	0.016(1)	0.024(1)	0.000(1)	-0.004(1)	0.001(1)
O3A	0.034(1)	0.023(1)	0.021(1)	0.003(1)	-0.004(1)	0.001(1)
O4A	0.052(1)	0.016(1)	0.025(1)	-0.001(1)	-0.007(1)	0.003(1)
O5A	0.077(1)	0.020(1)	0.026(1)	0.003(1)	-0.016(1)	0.000(1)
C15A	0.019(1)	0.017(1)	0.021(1)	0.002(1)	0.002(1)	-0.002(1)
C16A	0.028(1)	0.017(1)	0.020(1)	0.002(1)	0.001(1)	-0.002(1)



Table 6. Hydrogen coordinates and isotropic displacement parameters ( $\text{\AA}^2$ ) for **49**.

Atom	x	y	z	$U_{eq}$
H1	-0.4351(16)	-0.2335(14)	0.4223(11)	0.026
H2A	-0.2402(16)	-0.2033(14)	0.3742(11)	0.028
H4	-0.1070(16)	-0.3062(14)	0.6212(10)	0.027
H5A	-0.3096(16)	-0.2297(14)	0.6729(11)	0.030
H5B	-0.2221(16)	-0.1254(15)	0.6390(11)	0.030
H6A	-0.4747(17)	-0.1908(14)	0.5672(11)	0.030
H6B	-0.3835(16)	-0.0902(15)	0.5316(11)	0.030
H7A	-0.3888(16)	-0.4281(14)	0.4321(11)	0.029
H7B	-0.4703(17)	-0.3901(14)	0.5136(11)	0.029
H8A	-0.2987(16)	-0.4405(14)	0.6089(11)	0.031
H8B	-0.2086(16)	-0.4708(15)	0.5253(11)	0.031
H4'	0.2905(17)	-0.1527(15)	0.4266(11)	0.033
H5'	0.2897(17)	-0.2901(15)	0.5564(11)	0.036
H7'	0.1725(17)	-0.1360(15)	0.2691(11)	0.031
H8'	0.1155(17)	0.0014(15)	0.1619(12)	0.037
H9'	-0.0618(17)	0.1307(16)	0.1787(12)	0.040
H10'	-0.1867(18)	0.1264(16)	0.3053(11)	0.038
H11'	-0.1240(16)	-0.0038(14)	0.4171(11)	0.031
H4	-0.4753(17)	0.1511(16)	0.2426(11)	0.036
H1A	0.4208(16)	0.2839(14)	0.0811(11)	0.029
H2AA	0.2193(16)	0.2948(14)	0.1220(11)	0.030
H4A	0.1069(16)	0.2083(14)	-0.1389(11)	0.029
H5AA	0.3106(16)	0.3032(14)	-0.1707(11)	0.032
H5BA	0.2158(16)	0.3992(15)	-0.1284(11)	0.032
H6AA	0.3610(17)	0.4365(16)	-0.0076(11)	0.035
H6BA	0.4655(18)	0.3513(15)	-0.0536(11)	0.035
H7AA	0.3895(17)	0.0922(15)	0.0376(12)	0.035
H7BA	0.4684(18)	0.1528(15)	-0.0391(11)	0.035
H8AA	0.2095(17)	0.0453(15)	-0.0627(11)	0.034
H8BA	0.2981(16)	0.0864(15)	-0.1402(12)	0.034
H4'A	-0.3044(19)	0.3270(16)	0.0661(12)	0.043
H5'A	-0.2960(20)	0.1896(18)	-0.0795(13)	0.052
H7'A	-0.1890(18)	0.3441(16)	0.2252(11)	0.039
H8'A	-0.1229(20)	0.4791(18)	0.3511(14)	0.054
H9'A	0.0522(21)	0.6167(19)	0.3476(15)	0.062
H10A	0.1676(20)	0.6279(19)	0.2160(13)	0.054
H11A	0.1022(17)	0.4991(15)	0.0900(12)	0.038
H4A	0.4762(17)	0.6541(17)	0.2545(11)	0.038

Table 7. Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for 51.

$$U_{eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_j^* \cdot a_i \cdot a_j$$

Atom	x	y	z	$U_{eq}$
N1	0.0402(1)	0.1261(2)	0.1900(1)	0.023(1)
O1'	0.3058(1)	0.0808(1)	0.4611(1)	0.023(1)
C2	0.1382(2)	0.1166(2)	0.2791(1)	0.025(1)
C3	0.1226(2)	0.0372(2)	0.3412(1)	0.024(1)
C4	0.0064(2)	-0.0257(2)	0.3054(2)	0.031(1)
C5	-0.0054(2)	-0.0917(2)	0.2109(2)	0.036(1)
C6	0.0171(2)	0.0016(2)	0.1423(2)	0.030(1)
C7	-0.0662(2)	0.1675(2)	0.2116(2)	0.029(1)
C8	-0.0857(2)	0.0769(2)	0.2842(2)	0.034(1)
C2'	0.2033(2)	0.0156(2)	0.4354(1)	0.023(1)
C3'	0.2006(2)	-0.0540(2)	0.5104(1)	0.027(1)
C4'	0.3058(2)	-0.0316(2)	0.5868(1)	0.027(1)
C5'	0.3666(2)	0.0507(2)	0.5539(1)	0.022(1)
C6'	0.4800(2)	0.1097(2)	0.5960(1)	0.022(1)
C7'	0.5426(2)	0.0948(2)	0.6926(2)	0.031(1)
C8'	0.6501(2)	0.1510(2)	0.7323(2)	0.037(1)
C9'	0.6941(2)	0.2243(2)	0.6770(2)	0.038(1)
C10'	0.6331(2)	0.2385(2)	0.5809(2)	0.033(1)
C11'	0.5268(2)	0.1811(2)	0.5401(2)	0.026(1)
O2	0.5668(1)	0.0781(1)	0.1756(1)	0.039(1)
O3	0.6175(1)	0.2190(1)	0.0897(1)	0.031(1)
O4	0.6721(1)	-0.3131(1)	0.0285(1)	0.031(1)
O5	0.7699(1)	-0.1561(2)	-0.0062(1)	0.034(1)
C12	0.6095(2)	0.1073(2)	0.1148(1)	0.023(1)
C13	0.6579(2)	0.0105(2)	0.0676(1)	0.023(1)
C14	0.6446(2)	-0.1085(2)	0.0757(1)	0.024(1)
C15	0.6947(2)	-0.2043(2)	0.0303(1)	0.023(1)

Table 8. Bond lengths [Å] and angles [°] for 51.

N1-C2	1.463(3)
N1-C6	1.503(3)
N1-C7	1.522(2)
O1'-C5'	1.371(2)
O1'-C2'	1.380(2)
C2-C3	1.326(3)
C3-C2'	1.438(3)
C3-C4	1.507(3)
C4-C8	1.539(3)
C4-C5	1.545(3)
C5-C6	1.531(3)
C7-C8	1.540(3)
C2'-C3'	1.359(3)
C3'-C4'	1.424(3)
C4'-C5'	1.360(3)
C5'-C6'	1.466(3)
C6'-C7'	1.394(3)
C6'-C11'	1.399(3)
C7'-C8'	1.391(3)
C8'-C9'	1.383(3)
C9'-C10'	1.384(3)
C10'-C11'	1.387(3)
O2-C12	1.238(2)
O3-C12	1.278(2)
O4-C15	1.206(2)
O5-C15	1.332(2)
C12-C13	1.495(3)
C13-C14	1.307(3)
C14-C15	1.483(3)
C2-N1-C6	109.4(2)
C2-N1-C7	109.1(2)
C6-N1-C7	109.1(2)
C5'-O1'-C2'	106.87(14)
C3-C2-N1	114.3(2)
C2-C3-C2'	125.1(2)
C2-C3-C4	113.0(2)
C2'-C3-C4	121.8(2)
C3-C4-C8	106.9(2)
C3-C4-C5	108.2(2)
C8-C4-C5	108.2(2)
C6-C5-C4	109.2(2)
N1-C6-C5	108.6(2)
N1-C7-C8	108.5(2)
C4-C8-C7	108.8(2)
C3'-C2'-O1'	109.4(2)
C3'-C2'-C3	134.0(2)
O1'-C2'-C3	116.6(2)
C2'-C3'-C4'	107.2(2)
C5'-C4'-C3'	106.4(2)
C4'-C5'-O1'	110.1(2)
C4'-C5'-C6'	133.7(2)
O1'-C5'-C6'	116.2(2)
C7'-C6'-C11'	119.2(2)
C7'-C6'-C5'	120.1(2)
C11'-C6'-C5'	120.6(2)
C8'-C7'-C6'	119.9(2)
C9'-C8'-C7'	120.3(2)
C8'-C9'-C10'	120.1(2)
C9'-C10'-C11'	120.1(2)
C10'-C11'-C6'	120.3(2)
O2-C12-O3	123.4(2)
O2-C12-C13	120.5(2)
O3-C12-C13	116.0(2)
C14-C13-C12	124.2(2)
C13-C14-C15	124.0(2)
O4-C15-O5	124.0(2)
O4-C15-C14	124.1(2)
O5-C15-C14	111.9(2)

Table 9. Anisotropic displacement parameters ( $\text{\AA}^2$ ) for **51**.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
N(1)	0.018(1)	0.029(1)	0.024(1)	0.005(1)	0.011(1)	-0.001(1)
O(1')	0.015(1)	0.033(1)	0.023(1)	0.002(1)	0.007(1)	-0.003(1)
C(2)	0.018(1)	0.031(1)	0.029(1)	-0.001(1)	0.011(1)	-0.004(1)
C(3)	0.018(1)	0.030(1)	0.025(1)	0.000(1)	0.010(1)	-0.003(1)
C(4)	0.021(1)	0.042(1)	0.028(1)	0.012(1)	0.006(1)	-0.010(1)
C(5)	0.037(1)	0.032(1)	0.031(1)	0.005(1)	0.002(1)	0.010(1)
C(6)	0.029(1)	0.031(1)	0.030(1)	0.001(1)	0.009(1)	0.000(1)
C(7)	0.019(1)	0.041(1)	0.032(1)	0.005(1)	0.015(1)	0.006(1)
C(8)	0.019(1)	0.059(2)	0.028(1)	0.008(1)	0.011(1)	-0.003(1)
C(2')	0.019(1)	0.028(1)	0.025(1)	-0.003(1)	0.011(1)	-0.003(1)
C(3')	0.023(1)	0.033(1)	0.028(1)	0.003(1)	0.013(1)	-0.003(1)
C(4')	0.023(1)	0.038(1)	0.021(1)	0.003(1)	0.010(1)	0.001(1)
C(5')	0.021(1)	0.029(1)	0.020(1)	0.000(1)	0.009(1)	0.003(1)
C(6')	0.018(1)	0.025(1)	0.027(1)	-0.003(1)	0.011(1)	0.004(1)
C(7')	0.026(1)	0.040(1)	0.028(1)	-0.003(1)	0.010(1)	0.002(1)
C(8')	0.023(1)	0.050(2)	0.032(1)	0.011(1)	0.003(1)	0.004(1)
C(9')	0.020(1)	0.041(1)	0.051(2)	0.013(1)	0.010(1)	-0.003(1)
C(10')	0.024(1)	0.031(1)	0.050(2)	-0.004(1)	0.020(1)	0.000(1)
C(11')	0.021(1)	0.028(1)	0.033(1)	-0.003(1)	0.012(1)	0.004(1)
O(2)	0.050(1)	0.040(1)	0.040(1)	0.002(1)	0.033(1)	0.002(1)
O(3)	0.033(1)	0.028(1)	0.044(1)	-0.003(1)	0.028(1)	0.000(1)
O(4)	0.035(1)	0.026(1)	0.038(1)	-0.002(1)	0.018(1)	-0.001(1)
O(5)	0.034(1)	0.027(1)	0.053(1)	-0.010(1)	0.030(1)	-0.005(1)
C(12)	0.017(1)	0.028(1)	0.023(1)	-0.002(1)	0.007(1)	0.000(1)
C(13)	0.019(1)	0.030(1)	0.023(1)	-0.001(1)	0.010(1)	-0.001(1)
C(14)	0.020(1)	0.032(1)	0.022(1)	-0.002(1)	0.009(1)	-0.002(1)
C(15)	0.018(1)	0.029(1)	0.021(1)	-0.001(1)	0.006(1)	0.000(1)

Table 10. Hydrogen coordinates and isotropic displacement parameters ( $\text{\AA}^2$ ) for **51**.

Atom	x	y	z	$U_{eq}$
H(1)	0.0570(18)	0.1873(20)	0.1492(14)	0.027
H(2)	0.1971(19)	0.1723(20)	0.2849(14)	0.030
H(4)	0.0021(19)	-0.0882(21)	0.3503(15)	0.037
H(5A)	0.0545(21)	-0.1655(23)	0.2234(15)	0.043
H(5B)	-0.0878(21)	-0.1340(21)	0.1846(15)	0.043
H(6A)	-0.0471(21)	0.0157(20)	0.0833(16)	0.036
H(6B)	0.0827(21)	-0.0170(20)	0.1215(15)	0.036
H(7A)	-0.1319(20)	0.1692(20)	0.1475(15)	0.035
H(7B)	-0.0516(19)	0.2557(21)	0.2351(15)	0.035
H(8A)	-0.0767(21)	0.1207(21)	0.3442(16)	0.041
H(8B)	-0.1609(21)	0.0360(22)	0.2568(15)	0.041
H(3')	0.1474(20)	-0.1152(20)	0.5100(14)	0.033
H(4')	0.3286(19)	-0.0643(19)	0.6504(15)	0.032
H(7')	0.5113(20)	0.0452(21)	0.7298(16)	0.037
H(8')	0.6879(21)	0.1425(21)	0.8007(17)	0.044
H(9')	0.7696(22)	0.2666(21)	0.7055(16)	0.045
H(10')	0.6566(20)	0.2877(21)	0.5323(16)	0.040
H(11')	0.4840(19)	0.1880(19)	0.4710(15)	0.032
H(5O)	0.7961(21)	-0.2214(23)	-0.0262(16)	0.041
H(13)	0.6933(18)	0.0441(19)	0.0282(15)	0.028
H(14)	0.5983(19)	-0.1386(18)	0.1107(14)	0.029

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**$^1\text{H}$  NMR spectral data for compounds 3, 11, 23-24, 26-30, 32-34, 37, 39-41, 45, 47-53, 55-56, 58, 60-64, 67, 69, 73.**

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**3·0.5 fumarate** (270 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  7.16 (d,  $J = 3.6$  Hz, 1 H), 6.80-6.74 (m, 2 H), 6.69 (s, 1 H), 3.54-3.40 (m, 3 H), 3.12-2.96 (m, 2 H), 2.47 (d,  $J = 1.0$  Hz, 3 H), 2.14-1.99 (m, 2 H), 1.85-1.69 (m, 2 H).

**11** (270 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (d,  $J = 1$  Hz, 1 H), 7.60-7.44 (m, 3 H), 7.39-7.30 (m, 2 H), 7.19-7.11 (m, 1 H), 6.66 (d,  $J = 1$  Hz, 1 H).

**23·oxalate** (270 MHz,  $\text{D}_2\text{O}$ )  $\delta$  6.40 (d,  $J = 3.3$  Hz, 1 H), 6.32 (d,  $J = 3.3$  Hz, 1 H), 3.69 (d,  $J = 14.5$  Hz, 1 H), 3.35-2.99 (m, 5 H), 2.50-2.38 (m, 1 H), 2.25-2.17 (m, 1 H), 1.89-1.73 (m, 2 H), 1.65-1.50 (m, 1 H)

**24·0.5 oxalate** (270 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  7.41 (d,  $J = 1.8$  Hz, 1 H), 6.46 (d,  $J = 1.8$  Hz, 1 H), 4.09-3.82 (m, 5 H), 3.42-3.18<sup>a</sup> (m, 5 H), 2.60-2.34 (m, 2 H), 2.00-1.58<sup>a</sup> (m, 3 H), 1.70 (s, 3 H)

**26·fumarate** (270 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  6.64 (s, 1 H), 6.36 (d,  $J = 3.4$  Hz, 1 H), 6.04-6.0 (m, 1 H), 3.77 (dd,  $J = 1.7$  and 13.7 Hz, 1 H) 3.40-3.07<sup>a</sup> (m, 5 H), 2.70-2.58 (m, 2 H), 2.49-2.34 (m, 2 H), 1.95-1.58 (m, 3 H), 1.23 (t,  $J = 7.6$  Hz,  $\text{CH}_3$ )

**27** (free base, 270 MHz,  $\text{CDCl}_3$ )  $\delta$  6.13 (d,  $J = 3.2$  Hz, 1 H), 5.91 (app d,  $J = 3.2$  Hz, 1 H), 3.32 (dd,  $J = 2.0$  and 14.4 Hz, 1 H), 3.20-2.55 (m, 8 H), 2.22-2.07 (m, 2 H), 1.68-1.24 (m, 7 H), 0.92 (t,  $J = 7.4$  Hz, 3 H) .

**28** (free base, 270 MHz,  $\text{CD}_3\text{OD}$ )  $\delta$  7.62 (d,  $J = 2.0$  Hz, 1 H), 6.74 (d,  $J = 2.0$  Hz, 1 H), 3.63 (dd,  $J = 1.9$  and 14.4 Hz, 2-CH), 3.02-2.74 (m, 5 H), 2.36-2.13 (m, 2 H), 1.74-1.37 (m, 3 H)

**29** (free base, 270 MHz,  $\text{CDCl}_3$ )  $\delta$  7.08 (d,  $J = 3.6$  Hz, 1 H), 6.42 (d,  $J = 3.6$  Hz, 1 H), 4.63 (br s, 1 H, OH), 3.31 (dd,  $J = 1.9$  and 14.4 Hz, 1 H), 2.99-2.58 (m, 5 H), 2.22-2.06 (m, 2 H), 1.64-1.22 (m, 3 H)

**30** (free base, 270 MHz, CDCl<sub>3</sub>)  $\delta$  7.69-7.61 (m, 2 H), 7.42-7.34 (m, 2 H), 7.30-7.22<sup>a</sup> (m, 1 H), 6.60 (d,  $J$  = 3.3 Hz, 1 H), 6.37 (d,  $J$  = 3.3 Hz, 1 H), 3.47 (dd,  $J$  = 2.0 and 14.4 Hz, 1 H), 3.10-2.68 (m, 5 H), 2.50-2.12 (m, 3 H), 1.60-1.35 (m, 3 H)

**32.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.74 (s, 1 H), 7.02<sup>a</sup> (s, 1 H), 6.99<sup>a</sup> (s, 1 H), 3.78-3.40 (m, 3 H), 3.35-3.05<sup>a</sup> (m, 2 H), 2.25-2.00 (m, 2 H), 1.90-1.65 (m, 2 H)

**33.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  6.97-6.94 (m, 1 H), 6.88 (m, 1 H), 6.56 (d,  $J$  = 3.5 Hz, 1 H), 3.72-3.62 (m, 2 H), 3.48-3.40 (m, 1 H), 3.27-3.12 (m, 2 H), 2.22-2.07 (m, 2 H), 1.91-1.74 (m, 2 H).

**34.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.89 (app d, 1 H), 7.72 (d,  $J$  = 2.0 Hz, 1 H), 7.06 (d,  $J$  = 2.0 Hz, 1 H), 3.82-3.58 (m, 3 H), 3.34-3.10<sup>a</sup> (m, 2 H), 2.49 (s, 3 H), 2.24-2.06 (m, 2 H), 1.96-1.78 (m, 2 H)

**37.HCl** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.73 (d,  $J$  = 2.0 Hz, 1 H), 7.69-7.61 (m, 2 H), 7.53-7.49 (m, 1 H), 7.40-7.30 (m, 2 H), 7.20-7.11 (m, 2 H), 7.05 (d,  $J$  = 2.0 Hz, 1 H), 3.80-3.60 (m, 3 H), 3.29-3.13 (m, 2 H), 2.21-2.06 (m, 2 H), 1.99-1.82 (m, 2 H)

**39.oxalate** (270 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  10.22 (s, 1 H), 7.76-7.68 (m, 2 H), 7.42-7.29 (m, 4 H), 7.17-7.08 (m, 2 H), 3.57-3.40 (m, 3 H), 3.07-2.90 (m, 2 H), 2.08-1.91 (m, 2 H), 1.76-1.58 (m, 2 H)

**40.oxalate** (270 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.90 (d,  $J$  = 2.0 Hz, 1 H), 7.53 (app d, 1 H), 6.41 (d,  $J$  = 2.0 Hz, 1 H), 3.80 (s, 3 H), 3.61-3.38 (m, 3 H), 3.02-2.87 (m, 2 H), 2.04-1.86 (m, 2 H), 1.77-1.60 (m, 2 H)

**41.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  8.25 (s, 1 H), 7.19 (s, 1 H), 7.03 (br s, 1 H), 3.85 (s, 3 H), 3.74-3.45 (m, 3 H), 3.34-3.10<sup>a</sup> (m, 2 H), 2.23-2.06 (m, 2 H), 1.91-1.73 (m, 2 H)

**45.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.42 (d,  $J$  = 3.9 Hz, 1 H), 7.21 (app d, 1 H), 7.07 (d,  $J$  = 3.9 Hz, 1 H), 3.76-3.62 (m, 2 H), 3.59-3.52 (m, 1 H), 3.29-3.14<sup>a</sup> (m, 2 H), 2.25-2.09 (m, 2 H), 1.92-1.76 (m, 2 H)

**47.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.37 (m, 1 H), 6.89 (m, 1 H), 6.73 (s, 1 H), 3.72-3.56 (m, 2 H), 3.48-3.38 (m, 1 H), 3.25-3.08 (m, 2 H), 2.21-2.06<sup>a</sup> (m, 2 H), 2.05 (d,  $\underline{J}$  = 0.9 Hz, 3 H), 1.88-1.71 (m, 2 H)

**48.fumarate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  6.80 (br s, 1 H), 6.69 (s, 1H), 6.65 (d,  $\underline{J}$  = 3.3 Hz, 1 H), 6.14-6.11 (m, 1 H), 3.58-3.43 (m, 2 H), 3.37-3.28<sup>a</sup> (m, 1 H), 3.13-2.98 (m, 2 H), 2.31 (s, 3 H), 2.13-1.99 (m, 2 H), 1.82-1.76 (m, 2 H)

**49.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.65 (d,  $\underline{J}$  = 1.8 Hz, 1 H), 7.50-7.35 (m, 5 H), 6.88 (app d, 1 H), 6.61 (d,  $\underline{J}$  = 1.8 Hz, 1 H), 3.66-3.52 (m, 2 H), 3.24-3.08 (m, 3 H), 2.24-1.70 (m, 4 H)

**50.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  8.00 (s, 1 H), 7.62-7.55 (m, 2 H), 7.44-7.22 (m, 4 H), 6.99 (s, 1 H), 3.75-3.53 (m, 3 H), 3.38-3.12<sup>a</sup> (m, 2 H), 2.26-2.08 (m, 2 H), 1.95-1.76 (m, 2 H)

**51.fumarate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.80-7.70 (m, 2 H), 7.45-7.26 (m, 3 H), 7.01 (br s, 1 H), 6.90<sup>a</sup> (d,  $\underline{J}$  = 3.7 Hz, 1 H), 6.89<sup>a</sup> (d,  $\underline{J}$  = 3.7 Hz, 1 H), 6.71 (s, 2 H), 3.68-3.42 (m, 3 H), 3.36-3.06<sup>a</sup> (m, 2 H), 2.22-2.06 (m, 2 H), 1.92-1.86 (m, 2 H)

**52.fumarate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  6.82 (app d, 1 H), 6.73 (d,  $\underline{J}$  = 3.4 Hz, 1 H), 6.70 (s, 2 H), 6.16 (dt,  $\underline{J}$  = 3.4 and 1 Hz, 1 H), 3.67-3.53 (m, 2H, 2 H), 3.44-3.38 (m, 1 H), 3.22-3.08 (m, 2 H), 2.68 (m, 2 H), 2.19-2.05 (m, 2 H), 1.87-1.72 (m, 2 H), 1.24 (t,  $\underline{J}$  = 7.5 Hz, 3 H)

**53.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  6.84 (br s, 1 H), 6.74 (d,  $\underline{J}$  = 3.4 Hz, 1 H), 6.17 (dt,  $\underline{J}$  = 0.8 Hz and 3.4 Hz, 1 H), 3.72-3.57 (m, 2 H), 3.46-3.38 (m, 1 H), 3.26-3.10 (m, 2 H), 2.66 (m, 2 H), 2.21-2.06 (m, 2 H), 1.88-1.72 (m, 2 H), 1.70-1.57 (m, 2 H), 1.46-1.29 (m, 2 H), 0.94 (tr,  $\underline{J}$  = 7.3 Hz, 3 H)

**55.HCl** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.49-7.31 (m, 5 H), 6.80 (app d, 1 H), 6.23 (m, 1 H), 3.66-3.5 (m, 2 H), 3.24-3.06 (m, 3 H), 2.35 (d,  $\underline{J}$  = 0.7 Hz, 3 H), 2.01-1.68 (m, 4 H)

**56.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.76-6.74 (m, 4 H), 7.70 (d,  $J$  = 1.9 Hz, 1 H), 6.93 (app d, 1 H), 6.69 (d,  $J$  = 1.9 Hz, 1 H), 3.70-3.54 (m, 2 H), 3.26-3.04 (m, 3 H), 2.07-1.91 (m, 2 H), 1.88-1.71 (m, 2 H)

**58.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.63 (d,  $J$  = 1.9 Hz, 1 H), 7.45-7.20 (m, 1 H), 7.10-6.80 (m, 4 H), 6.59 (d,  $J$  = 1.9 Hz, 1 H), 3.99 (t,  $J$  = 6.3 Hz, 2 H), 3.75-3.45 (m, 2 H), 3.40-3.0<sup>a</sup> (m, 3 H), 2.10-1.40 (m, 8 H), 0.98 (t,  $J$  = 7.3 Hz, 3 H)

**60.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.64 (d,  $J$  = 2.0 Hz, 1 H), 7.42-7.15 (m, 4 H), 6.89(s, 1 H), 6.60 (d,  $J$  = 2.0 Hz, 1 H), 3.70-3.50 (m, 2 H), 3.25-3.05 (m, 2 H), 2.67 (q,  $J$  = 7.6 Hz, 2 H), 2.04-1.68 (m, 4 H), 1.25 (t,  $J$  = 7.6 Hz, 3 H)

**61.sesquioxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.63 (d,  $J$  = 1.8 Hz, 1 H), 7.37-7.24 (m, 4 H), 6.86 (app d, 1 H), 6.59 (d,  $J$  = 1.8 Hz, 1 H), 3.70-3.50 (m, 2 H), 3.25-3.07(m, 3 H), 2.69 (q,  $J$  = 7.6 Hz, 2 H), 2.05-1.89 (m, 2 H), 1.87-1.70 (m, 2 H), 1.26 (t,  $J$  = 7.6 Hz, 3 H)

**62.2HCl** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.95-7.52 (m, 5 H), 6.86 (app d, 1 H), 6.71 (d,  $J$  = 2.0 Hz, 1 H), 4.20-4.08 (m, 4 H), 3.77-3.53 (m, 6 H), 3.34-3.17<sup>a</sup> (m, 3 H), 2.12-1.76 (m, 4 H)

**63.2HCl** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.77-7.57 (m, 5 H), 6.86 (app d, 1 H), 6.66 (d,  $J$  = 2.0 Hz, 1 H), 4.14-4.05 (m, 4 H), 3.72-3.54 (m, 6 H), 3.31-3.12<sup>a</sup> (m, 3 H), 2.09-1.73 (m, 4 H)

**64.oxalate** (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.85-7.75 (m, 5 H), 6.89 (s, 1 H), 6.78 (d,  $J$  = 2.0 Hz, 1 H), 3.75-3.50 (m, 2 H), 3.35-3.05<sup>a</sup>(m, 3 H), 2.15-1.70 (m, 4 H)

**67.oxalate** (400 MHz, CD<sub>3</sub>OD)  $\delta$  7.66 (d,  $J$  = 2.0 Hz, 1 H), 7.50-7.40 (m, 2 H), 7.25-7.15 (m, 2 H), 6.86 (s, 1 H), 6.63 (d,  $J$  = 2.0 Hz, 1 H), 3.70-3.50 (m, 2 H), 3.30-3.05<sup>a</sup> (m, 3 H, 1 H), 2.30 (s, 3 H), 2.07-1.70 (m, 4 H)



**69**·sesquioxalate (270 MHz, CD<sub>3</sub>OD)  $\delta$  7.60 (d,  $J$  = 1.7 Hz, 1 H), 7.30-7.16 (m, 2 H), 6.93-6.77 (m, 3 H), 6.55 (d,  $J$  = 1.7 Hz, 1 H), 3.70-3.46 (m, 2 H), 3.40-3.10<sup>a</sup> (m, 3 H), 2.10-1.64 (m, 4 H).

**73**·0.5 fumarate (270 MHz, CD<sub>3</sub>OD)  $\delta$  6.92 (d,  $J$  = 3.6 Hz, 1 H), 6.67-6.30 (m, 2 H), 3.81 (dd,  $J$  = 1.9 and 13.8 Hz, 1 H), 3.40-3.10 (m, partly obscured, 5 H), 2.52-2.37 (m, 4 H), 2.33-2.24 (m, 1 H), 1.93-1.68 (m, 3 H).

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<sup>a</sup> partly obscured.

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**<sup>13</sup>C NMR spectral data for compounds 3, 11, 23, 24, 26-30, 32-34, 37, 39-41, 45, 47-53, 55, 56, 58, 60-64, 67, 69, 73.**

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**3**·0.5 fumarate (22.5 MHz, D<sub>2</sub>O)  $\delta$  175.91, 144.75, 142.95, 136.78, 134.59, 128.50, 127.88, 120.72, 52.34 (2C), 30.29, 24.15 (2C), 15.99.

**11** (67.9 MHz, CDCl<sub>3</sub>)  $\delta$  159.46, 146.07, 137.25, 129.16 (2C), 125.42, 124.92, 124.33, 120.41 (2C), 110.01.

**23**·Oxalate (67.9 MHz, D<sub>2</sub>O)  $\delta$  174.80, 157.62, 123.84, 113.8, 111.61, 69.79, 58.52, 47.77, 47.06, 31.11, 20.84, 18.93

**24**·0.5 oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  172.43, 152.34, 141.63, 126.56, 112.97, 108.01, 71.10, 65.88, 65.68, 59.80, 47.37, 46.67, 33.66, 27.82, 21.04, 19.69

**26**·fumarate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  174.44, 159.45, 155.25, 137.08, 108.60, 105.92, 69.59, 59.60, 47.56, 46.73, 32.19, 22.33, 21.59, 19.65, 12.70.

**27** (free base, 67.9 MHz, CDCl<sub>3</sub>)  $\delta$  156.46, 156.42, 106.34, 105.19, 70.15, 70.38, 47.13, 46.29, 32.18, 30.28, 27.94, 23.55, 23.78, 21.02, 13.99.

**28** (free base, 67.9 MHz, CD<sub>3</sub>OD)  $\delta$  169.45, 144.77, 139.60, 115.84, 114.69, 95.43, 72.77, 61.72, 48.32, 47.63, 33.89, 24.34, 22.31.

**29** (free base, 67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.88, 127.20, 125.13, 113.29, 109.91, 71.62, 61.74, 48.33, 47.58, 33.54, 24.49, 22.19.

**30** (free base, 67.9 MHz, CDCl<sub>3</sub>)  $\delta$  158.54, 153.81, 131.12, 129.10 (2C), 127.83, 124.09 (2C), 108.24, 105.91, 70.49, 60.32, 47.33, 46.55, 32.63, 23.98, 21.27.

**32.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.61, 149.77, 144.26, 137.79, 123.41, 114.73, 102.64, 51.84 (2C), 28.48, 24.28 (2C).

**33.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.52, 150.65, 137.55, 126.04, 122.21, 115.06, 114.54, 51.93 (2C), 28.25, 24.26 (2C).

**34.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  195.76, 166.59, 150.20, 144.85, 138.31, 129.94, 126.38, 114.66, 51.28 (2C), 29.72, 28.75, 24.28 (2C).

**37.HCl** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  163.70, 149.25, 144.90, 139.50, 138.67, 129.90 (2C), 127.83, 125.87, 123.04, 122.21 (2C), 113.08, 51.68 (2C), 28.89, 24.24 (2C).

**39.oxalate** (67.9 MHz, DMSO-*d*<sub>6</sub>, **ref 39.5**)  $\delta$  163.93, 155.72, 149.72, 147.58, 138.12, 136.00, 128.68 (2C), 127.40, 124.09, 120.77 (2C), 116.32, 111.51, 49.54 (2C), 26.42, 23.95 (2C).

**40.1.5 oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  165.11, 164.73, 151.52, 144.89, 138.17, 129.95, 118.54, 114.44, 52.56, 51.37 (2C), 28.82, 24.23 (2C).

**41.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.77, 164.35, 150.67, 150.15, 137.97, 123.66, 122.37, 111.10, 52.38, 51.93 (2C), 28.59, 24.29 (2C).

**45.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  164.22, 153.13, 137.30, 128.07, 126.22, 125.17, 112.74, 111.98, 51.77 (2C), 28.52 (C4), 24.22 (2C).

**47.oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.65, 148.62, 142.75, 138.67, 123.70, 121.27, 114.63, 52.02 (2C), 28.59, 24.31 (2C), 9.56.

**48.Fumarate** (22.5 MHz, CD<sub>3</sub>OD)  $\delta$  174.12, 155.84, 147.47, 138.61, 136.94, 121.65, 112.63, 109.02, 51.51 (2C), 28.51, 24.86 (2C), 13.53.

**49**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.66, 144.87, 143.23, 139.31, 134.55, 130.03 (2C), 129.92 (2C), 129.40, 129.20, 123.77, 115.83, 51.79 (2C), 28.07, 24.20 (2C).

**50**·oxalate (67.9 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  164.53, 148.64, 140.55, 136.17, 131.09, 128.80 (2C), 127.55, 127.26, 125.37 (2C), 123.81, 108.61, 49.47 (2C), 26.67, 23.67 (2C).

**51**·fumarate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  172.14, 156.96, 148.19, 138.52, 136.42, 131.27, 129.99 (2C), 129.43, 125.14 (2C), 122.30, 114.05, 108.30, 51.82 (2C), 28.54, 24.56 (2C).

**52**·Fumarate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  171.54, 161.82, 147.08, 138.76, 136.26, 120.38, 113.17, 107.73, 51.99 (2C), 28.52, 24.48 (2C), 22.38, 12.57.

**53**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.88, 160.59, 146.99, 138.60, 120.18, 113.26, 108.55, 52.15 (2C), 31.28, 28.68, 28.50, 24.35 (2C), 23.23, 14.11.

**55**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  165.01, 154.98, 141.51, 139.33, 134.89, 130.51, 129.94 (2C), 129.84 (2C), 129.27, 122.33, 112.22, 51.91 (2C), 27.94, 24.19 (2C), 13.41.

**56**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.54, 145.26, 143.86, 138.85, 135.69, 133.80, 132.19 (q,  $\underline{J}_{C,F}$  = 33 Hz), 130.96, 127.38, 126.62 (q,  $\underline{J}_{C,F}$  = 3.7 Hz), 126.01 (q,  $\underline{J}_{C,F}$  = 3.7 Hz), 125.48 (q,  $\underline{J}_{C,F}$  = 271 Hz, CF<sub>3</sub>), 124.78, 115.54, 51.64 (2C), 28.34, 24.20 (2C).

**58**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.54, 160.88, 144.74, 143.25, 139.23, 135.78, 130.94, 129.07, 123.86, 122.19, 116.23, 115.78, 115.22, 68.86, 51.73 (2C), 32.51, 28.05, 24.24 (2C), 20.32, 14.21.

**60**·oxalate (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  166.47, 147.04, 145.54, 143.89, 140.06, 135.27, 130.69, 130.23, 130.20, 129.70, 128.10, 124.38, 116.60, 52.56 (2C), 30.54, 28.74, 25.00 (2C), 17.04.

**61·sesquioxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  165.14, 145.87, 144.78, 143.03, 139.30, 131.75, 129.97 (2C), 129.36 (2C), 129.19, 123.57, 115.87, 51.77 (2C), 29.60, 27.98, 24.20 (2C), 16.08

**62·2HCl** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  145.45, 144.03, 143.69, 138.84, 136.97, 132.41, 131.62, 127.00, 124.00, 122.81, 121.79, 115.75, 65.37 (2C), 56.34 (2C), 51.84 (2C), 28.31, 24.14 (2C).

**63·2HCl** (100.5 MHz, CD<sub>3</sub>OD)  $\delta$  145.40, 143.62, 143.51, 139.05, 135.95, 127.28, 127.27, 124.06, 122.62, 115.63, 65.59 (2C), 56.02 (2C), 51.88 (2C), 28.25, 24.15 (2C).

**64·oxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  164.90, 145.37, 143.97, 138.81, 136.08, 134.68, 133.44, 132.99, 131.23, 126.77, 124.80, 119.28, 115.52, 114.19, 51.73 (2C), 28.41, 24.20 (2C).

**67·oxalate** (100.5 MHz, CD<sub>3</sub>OD)  $\delta$  171.14, 163.85, 152.32, 144.97, 143.41, 139.25, 132.15, 131.11 (2C), 128.25, 124.07, 123.37 (2C), 115.86, 51.79 (2C), 28.13, 24.27 (2C), 20.94

**69·sesquioxalate** (67.9 MHz, CD<sub>3</sub>OD)  $\delta$  165.16, 159.01, 144.68, 142.77, 139.56, 131.21 (2C), 129.48, 125.23, 122.94, 116.65 (2C), 115.99, 51.89 (2C), 27.83, 24.17 (2C).

**73·0.5 fumarate** (22.5 MHz, D<sub>2</sub>O)  $\delta$  175.94, 146.54, 142.77, 136.78, 126.37, 126.25, 71.77, 60.53, 47.71, 47.09, 34.28, 20.90, 19.42, 15.81.

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