Electronic Supporting Information

Novel Foldamer Structural Architecture from Cofacial Aromatic Building Blocks

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General Methods

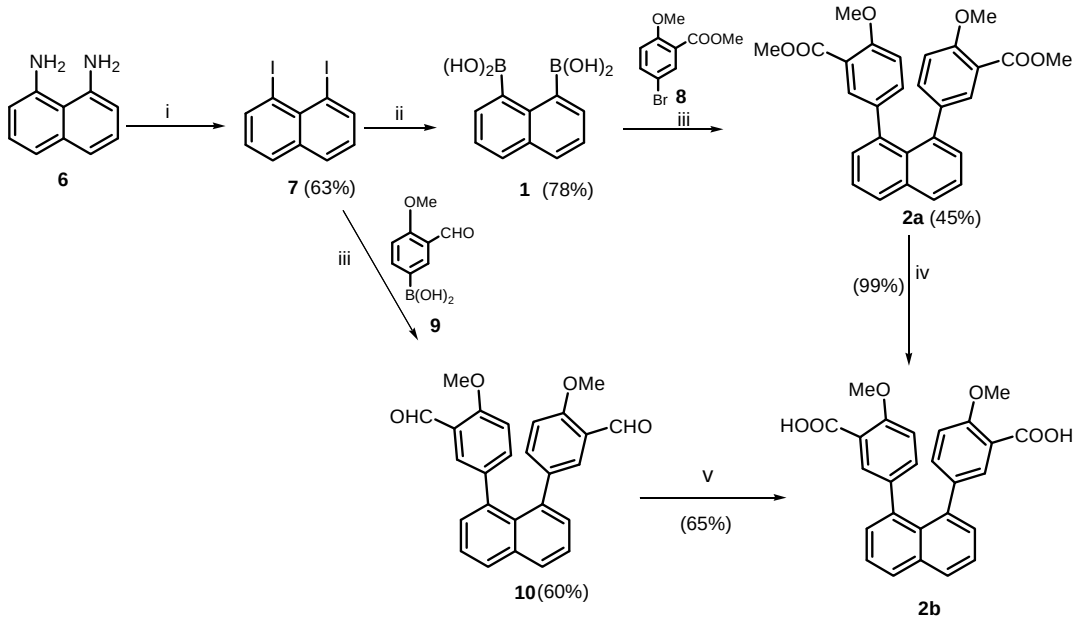
Unless otherwise stated, all the chemicals and reagents were obtained commercially. Dichloromethane was dried by distilling over P_2O_5 and keeping over 4 Å mol sieves. Analytical Thin Layer Chromatography was done on precoated silica gel plates (Kieselgel $60F_{254}$, Merck). Column chromatographic purifications were done with 100-200 Mesh Silica gel. NMR spectra were recorded in $CDCl_3$ on AV 200 MHz or AV 400 MHz or AV 500 MHz Bruker NMR spectrometers. All chemical shifts are reported in δ ppm downfield to TMS and peak multiplicities as singlet (s), doublet (d), quartet (q), broad (b), broad singlet (bs), and multiplet (m). Elemental analyses were performed on an Elmentar-Vario (Heraeus Company Ltd., Germany). IR spectra were recorded in nujol or $CHCl_3$ using Shimadzu FTIR-8400 spectrophotometer. Melting points were determined on a Buchi Melting Point B 540. MALDI-TOF spectrometric measurements were done with Voyager-DE STR Biospectrometer workstation using α-cyano-4-hydroxycinnamic acid (CHCA) as the matrix. Single crystal X-ray data were collected on a Bruker SMART APEX CCD Area diffractometer with graphite monochromatized (Mo Kα = 0.71073Å) radiation at room temperature. Since the quality of the crystals of **3** was poor and the diffraction at high angles was not observed, off limit is changed in the refinement. In the asymmetric unit, there is mainly one molecule along with 0.5CHCl2 and 0.25 water molecules. There are voids in the structure when the solvent molecules are not there. Merohedral twinning was checked in RLATT and the crystals are not twinned but the quality of crystals was poor and the high angle diffraction was not good which resulted in high R. All the data were corrected for Lorentzian, polarization, and

absorption effects using Bruker's SAINT and SADABS programs. SHELX-97[1] was used for structure solution and full matrix least squares refinement on F2. Hydrogen atoms were included in the refinement as per the riding model.

Experimental Methods

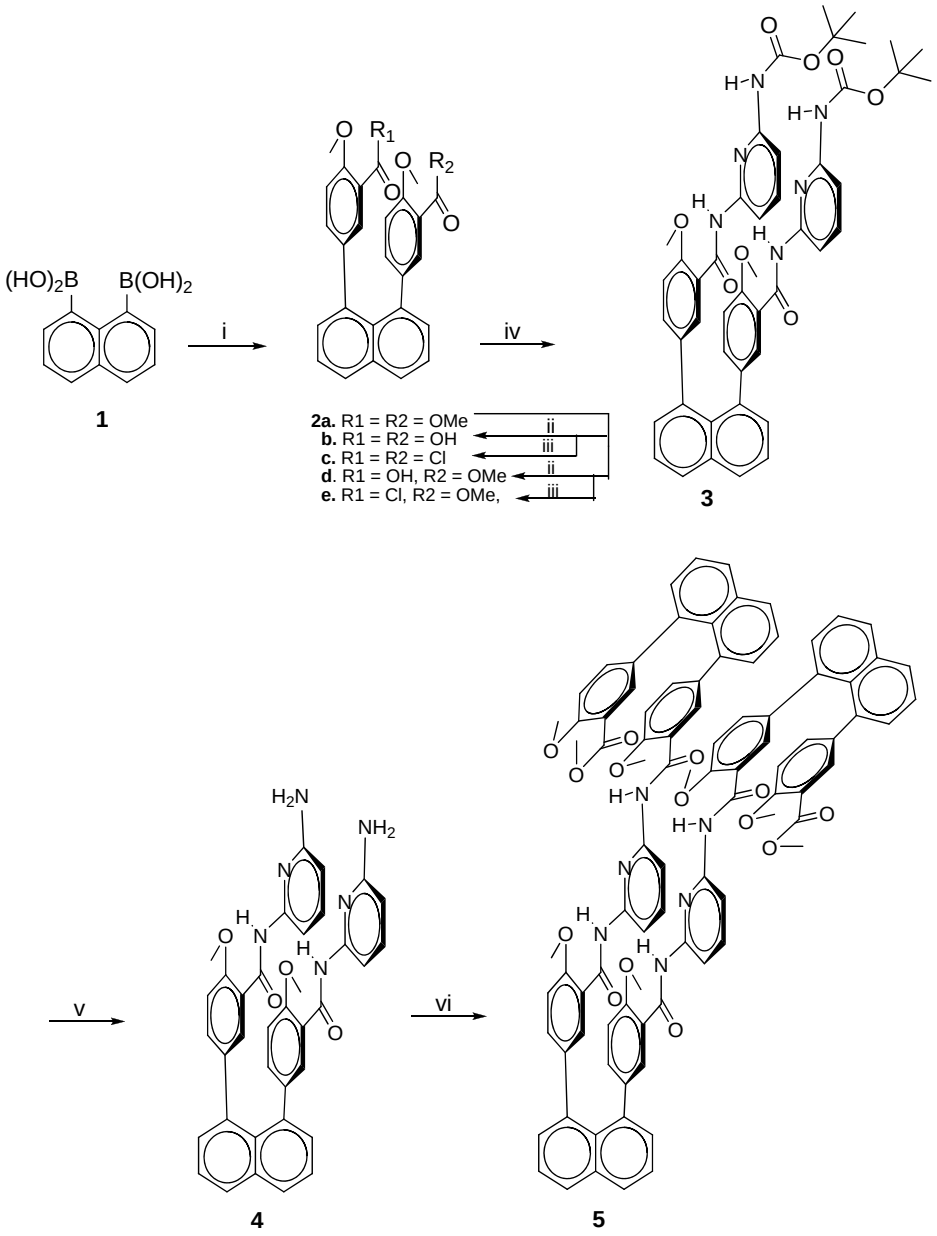
1,8-diaminonapthalene **6** and 3-formyl-4-methoxyphenyl boronic acid **9** were obtained from Aldrich. 1,8-diiodonapthalene **7**[2] and the naphthalene diboronic acid **1**[3] were prepared according to the literature procedures. Suzuki coupling of **1** with **8**, yielding **2a**, followed a recent procedure.[4] Alternatively, the acid **2b** could also be obtained from the reported bis-formyl compound[5] **10** (obtained by the Suzuki coupling of **7** with **9**) by Jones oxidation.

Scheme 1: Synthesis of the diacid **2b**[a]



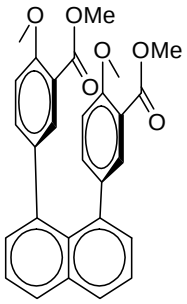
[a]**Reagents and conditions:** (i) (a) $NaNO_2$, H_2SO_4, H_2O,-15 to -20 °C; (b) KI in H_2O; (ii) BuLi, Trimethyl borate, -78 °C; (iii) $Pd(OAc)_2$ (12 mol%), K_2CO_3 (8 equiv.), PEG-400, DABCO (24 mol%), TBAB (0.1 equiv.), 110 °C, 15 h.; (iv) LiOH (2N), Dioxane/ H_2O; (v) CrO_3, H_2SO_4, acetone, rt, 3 h (Jones oxidation).

Scheme 2: Syntheses of **3** and **5**[b]



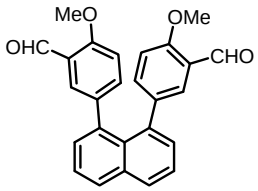
[b]**Reagents and conditions**: i) methyl-5-bromo-2-methoxy benzoic acid methyl ester, DABCO, Pd $(OAC)_2$, K_2CO_3, TBAB, PEG-400, 110 ^oC 15 h; ii) LiOH, dioxane, H_2O; iii) $(COCl)_2$, DMF (cat.), DCM, rt, 3h; iv) mono-boc-2,6-diamino pyridine, Et_3N, rt, 12 h; v) TFA, DCM, rt, 30 min; vi) **2e**, Et_3N, DCM, rt, 12 h.

1,8-Bis-(4-methoxy-3-methylcarboxyphenyl)-naphthalene 2a:



The Suzuki coupling of **1** with **8** yielding **2a** followed a recently reported procedure[4] as follows: A reaction mixture in PEG-400 (6 mL) containing naphthalene diboronic acid **1** (0.2 g, 0.9 mmol, 1 equiv.), methyl-5-bromo-2-methoxy-benzoic methyl ester **8** (0.68 g, 2.7 mmol, 3 equiv.), $Pd(OAc)_2$ (12 mol%), DABCO (24 mol%), TBAB (0.1 equiv.), and K_2CO_3 (8 equiv.) was sealed and heated at 110 °C for 15 h. After cooling to room temperature, the product was extracted into DCM (100 mL), and the crude compound obtained was purified by column chromatography (eluent: AcOEt / pet.ether: 25/75; R_f: 0.3) to yield **2a** (0.19 g, 45%). mp: 158-160 °C; Found: C, 73.82; H, 5.42. Calc. for $C_{28}H_{24}O_6$: C, 73.67; H, 5.30%; ν_{max} ($CHCl_3$) / (cm^{-1}): 3020, 2951, 2841, 1724, 1717, 1611, 1501, 1437, 1308, 1277, 1238, 1217, 1182, 1086, 1026; ^1H NMR (200 MHz, $CDCl_3$) δ: 7.98-7.93 (dd, *J* = 1.37 Hz, 2H), 7.59-7.51 (m, 2H), 7.46-7.39 (m, 4H), 7.08-7.03 (dd, *J* = 2.28 Hz, 1H), 6.98-6.93 (dd, *J* = 2.43 Hz, 1H), 3.85-3.81 (m, 12 H); ^{13}C NMR (50 MHz, $CDCl_3$) δ: 166.5, 166.0, 157.6, 157.4, 138.7, 135.4, 135.2, 135.1, 134.9, 134.4, 133.6, 132.6, 131.0, 130.7, 128.9, 125.2, 118.6, 111.4, 111.3, 56.3, 56.1, 51.9, 51.8; ESI-MS: 457.35 $(M+H)^+$, 479.28 $(M+Na)^+$, 496.26 $(M+K)^+$.

1,8-Bis-(3-formyl-4-methoxy-phenyl)-naphthalene 10[5]



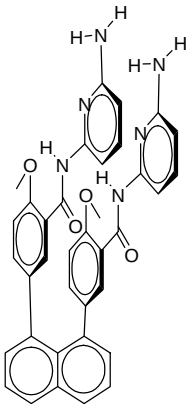
Following the same procedure for the preparation of **2a**, the Suzuki coupling of **7** (0.4 g, 1.5 mmol, 1 equiv.) with **9** (0.57 g, 3.1 mmol, 3 equiv.) yielded **10** (60%). ^{13}C (50 MHz,

$CDCl_3$) δ: 189.3, 159.7, 138.1, 137.3, 135.5, 135.2, 130.6, 129.4, 128.9, 125.1, 123.2, 110.7, 55.7; ESI-MS: 397.31 $(M+H)^+$, 419.30 $(M+Na)^+$, 435.28 $(M+K)^+$;

Synthesis of the short oligomer 3: To a stirred solution of the diacid **2b** (1g, 2.3 mmol, 1 equiv.) in dry DCM (15 ml), 2 drops of DMF were added followed by the drop-wise addition of oxalyl choride (1.2 ml, 9.2, 4 equiv.). After 3 h at room temperature, solvent and excess oxalyl chloride were removed from the reaction mixture under reduced pressure to get the crude acid chloride **2c** which was directly reacted with a reaction mixture containing mono-Boc-2,6-diaminopyridine[6] (9.2 mmol, 4 equiv.) and TEA (9.2 mmol, 4 equiv.) in DCM (10 ml). The reaction mixture was stirred overnight at rt. Work-up followed by column chromatographic purification afforded **3** (eluent: 80% dichlorometahane / pet.ether, R_f: 0.4) as a white solid (1.41 g, 75%), which could be crystallized from a solution of dichloromethane and MeOH. mp: 172 °C (decom.); Found: C, 68.26; H, 5.84; N, 10. 44. Calc. for $C_{46}H_{46}N_6O_8$: C, 68.13; H, 5.72; N, 10.36%; ν ($CHCl_3$)/ (cm^{-1}): 3421, 3356, 3018, 1730, 1587, 1506, 1497, 1456, 1369, 1305, 1217, 1153, 1053, 1028; ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 10.12, (s, 2H), 8.48 (bs, 2H), 8.08-8.06 (m, 2H), 7.98-7.96, *J* = 8.28 Hz, 2H), 7.77-7.73 (m, 6H), 7.58-7.54 (t, *J* = 7.54 Hz, 2H), 7.40-7.38 (d, *J* = 7.04 Hz, 2H), 7.18-7.16 (dd, *J* = 2.26 Hz, *J* = 6.29 Hz, 2H), 6.69-6.67 (d, *J* = 8.80 Hz, 2H), 3.73 (s, 6H), 1.38 (s, 18H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 163.1, 155.4, 152.5, 150.8, 150.1, 140.9, 138.7, 136.7, 135.6, 135.3, 133.2, 130.6, 130.0,

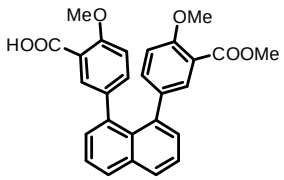
128.8, 125.2, 119.4, 110.6, 108.9, 107.7, 81.1, 56.1, 28.1; ESI MS: 810.96 $(M+H)^+$, 832.94 $(M+Na)^+$; 848.95 $(M+K)^+$.

Synthesis of bis-amine 4:



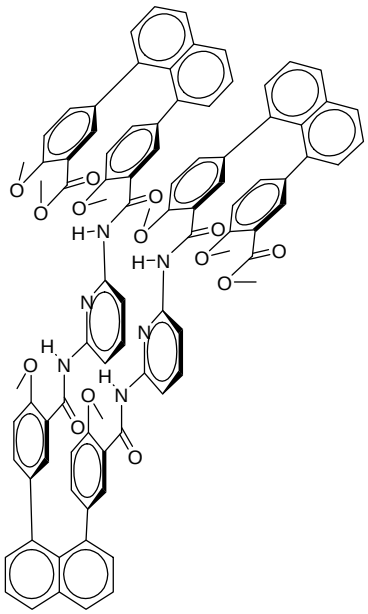
The compound **3** (0.5 g, 0.6 mmol) was subjected to the Boc-deprotection using TFA/DCM. After complete consumption of **3**, the solvent was stripped off from the reaction mixture. The residue was neutralized with sat. sodium bicarbonate solution and the white precipitate obtained was filtered, washed with water, and the residue was dried in KOH desiccator and taken for the further reaction without any purification.

Synthesis of monoacid 2d:

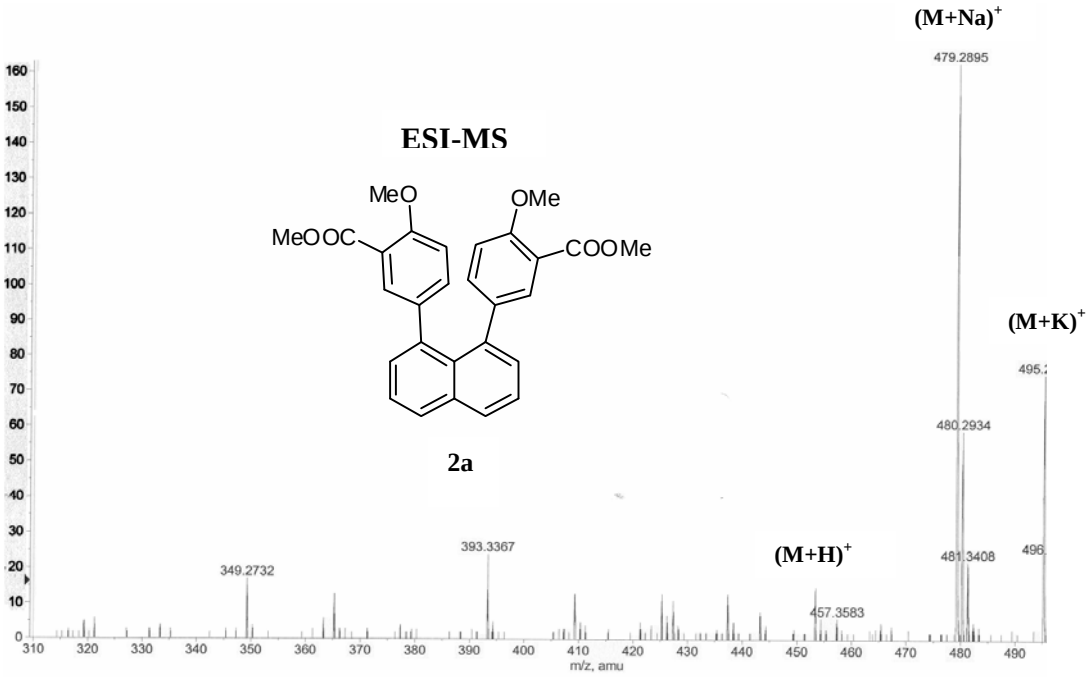


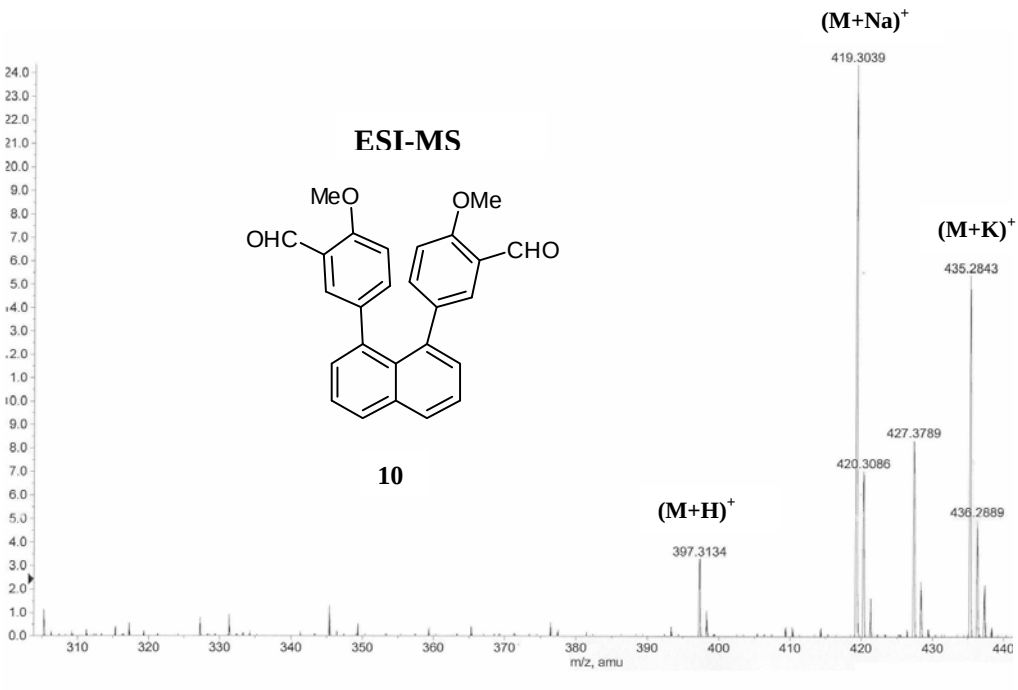
The bis-ester **2a** (0.6 g, 1.3 mmol, 1 equiv.) was subjected to careful saponification using $LiOH{\cdot}H_2O$ (56 mg, 1.3 mmol, 1 equiv.) dissolved in $MeOH/H_2O$ (9:1 mL). After stirring for 6 h, the reaction mixture was stripped off the solvent under reduced pressure. The residue was suspended in water and washed with DCM to remove any unreacted bis-ester **6**. The aqueous layer was neutralized with dil. HCl to get an off-white precipitate, which was taken in DCM and filtered to remove the undissolved material, which is presumably the bis-acid **2b**. The filtrate was evaporated to get the crude acid which was used for the next reaction without further purification.

Synthesis of 5: The monoacid **2d** (0.36 g, 0.8 mmol, 3 equiv.) was converted to the corresponding acid chloride **2e** using oxalyl chloride (4 equiv.) and cat. amount of



DMF in dihloromethane (15 mL) as the solvent. After stirring the reaction mixture for 3h at room temperature, the solvent and excess oxalyl chloride were removed under reduced pressure to get the crude acid chloride **2e** which was taken in a solution containing the bis-amine **4** (0.166 g, 0.27 mmol, 1 equiv.) and TEA (4 equiv.). The reaction mixture was allowed to stir for 12 h at rt. The insoluble product was filtered off and washed with DCM to get an off-white residue (62%) which could not be further purified owing to its inadequate solubility in various organic solvents. mp: > 295 °C, Found: 1459.89 $(M+H)^+$; 1481.84 $(M+Na)^+$; 1497.75 $(M+K)^+$. MALDI-TOF calc. for $C_{90}H_{70}N_6O_{14}$, 1459.50 $(M+H)^+$; ν (nujol) / (cm^{-1}): 3321, 3159, 2954, 2922, 2852, 2725, 1716, 1703, 1670, 1458, 1377, 1305, 1242, 1169, 1153, 1078, 1016.


ESI-MS
MeO
OMe
MeOOC
COOMe
2a
(M+Na)+
479.2895
(M+K)+
480.2934
(M+H)+
393.3367
349.2732
457.3583
481.3408
m/z, amu


ESI-MS
MeO
OMe
OHC
CHO
10
(M+Na)+
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(M+K)+
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427.3789
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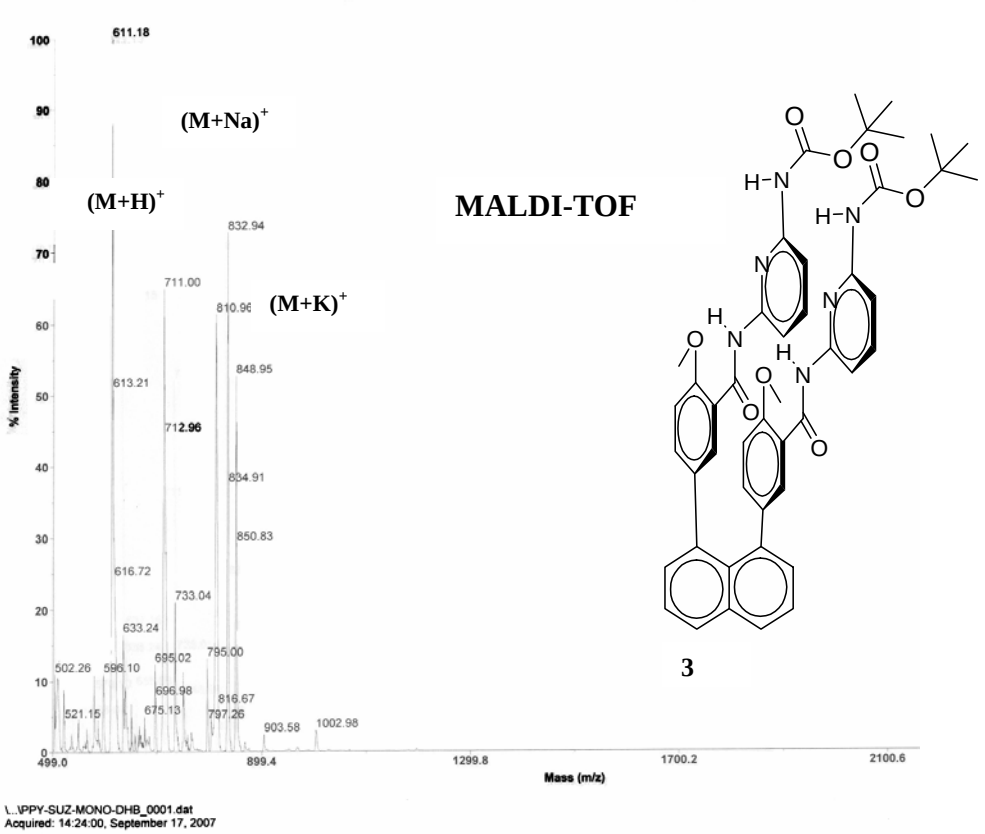
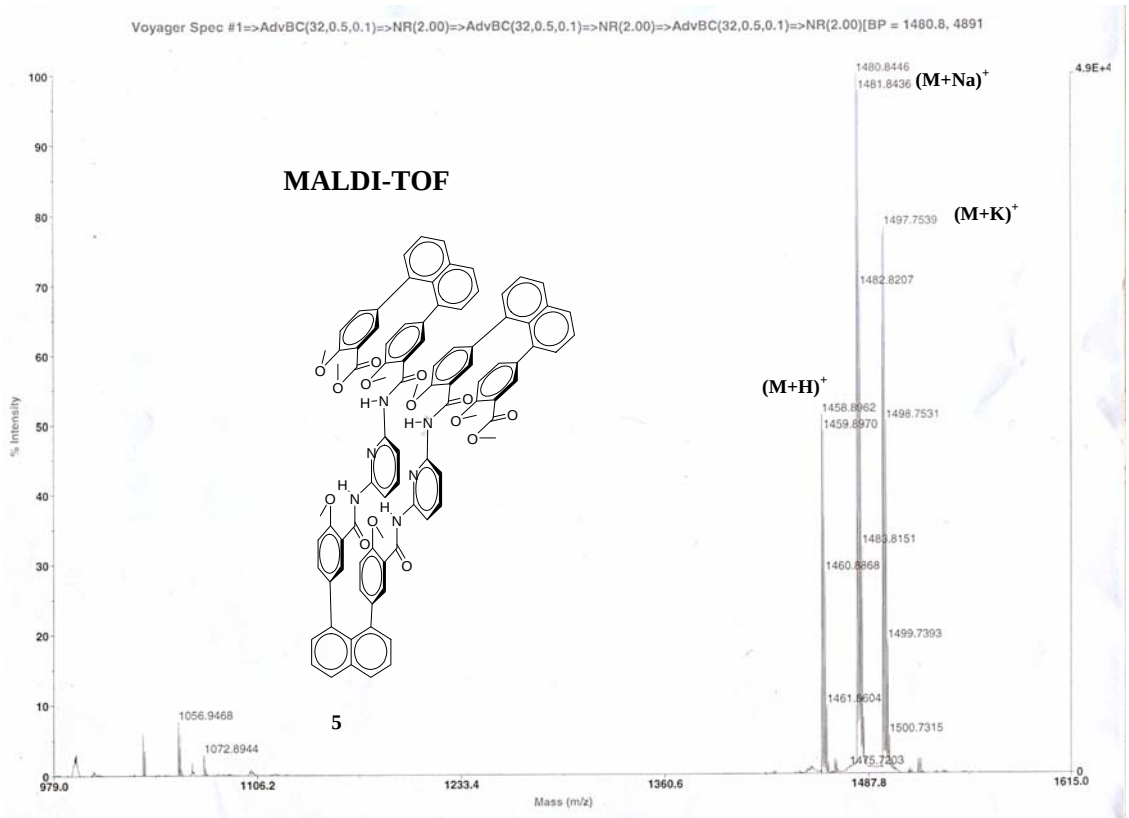
(M+H)+
397.3134
436.2889
m/z, amu


611.18
(M+Na)+
(M+H)+
832.94
711.00
(M+K)+
810.96
848.95
613.21
712.96
834.91
850.83
616.72
733.04
633.24
695.02
795.00
502.26
596.10
696.98
816.67
521.15
675.13
797.26
903.58
1002.98
% Intensity
499.0
899.4
1299.8
1700.2
2100.6
Mass (m/z)
MALDI-TOF
3
\...\PPY-SUZ-MONO-DHB_0001.dat
Acquired: 14:24:00, September 17, 2007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1480.8446
1481.8436
(M+Na)+
4.9E+4
MALDI-TOF
1497.7539
(M+K)+
1482.8207
(M+H)+
1458.8662
1459.8970
1498.7531
1483.8151
1460.8868
1499.7393
1461.8604
1056.9468
1072.8944
1500.7315
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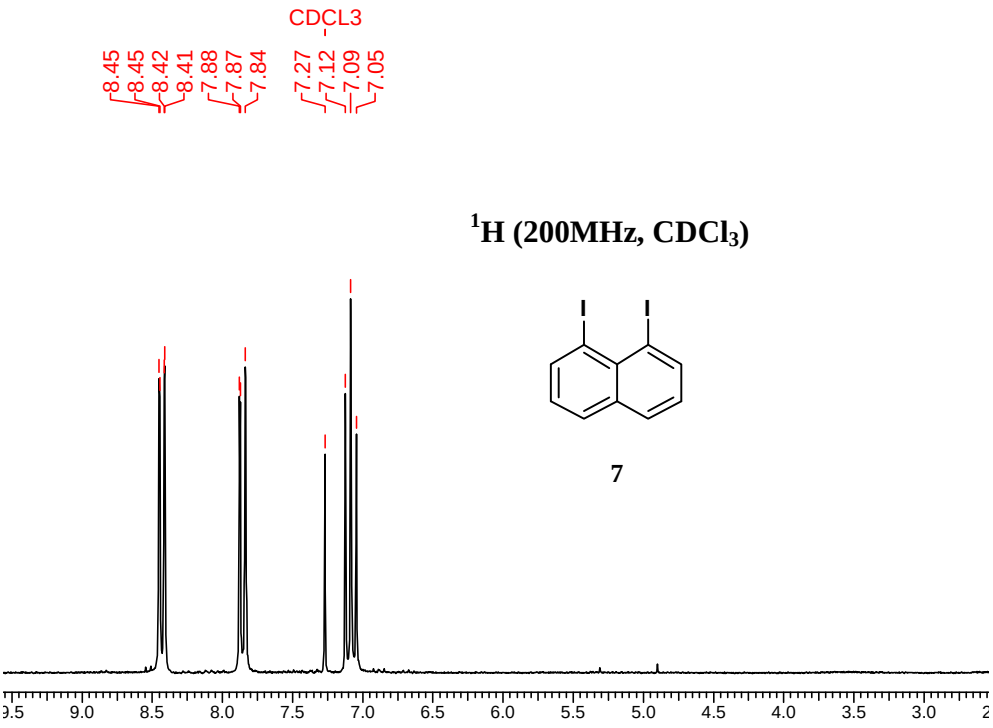
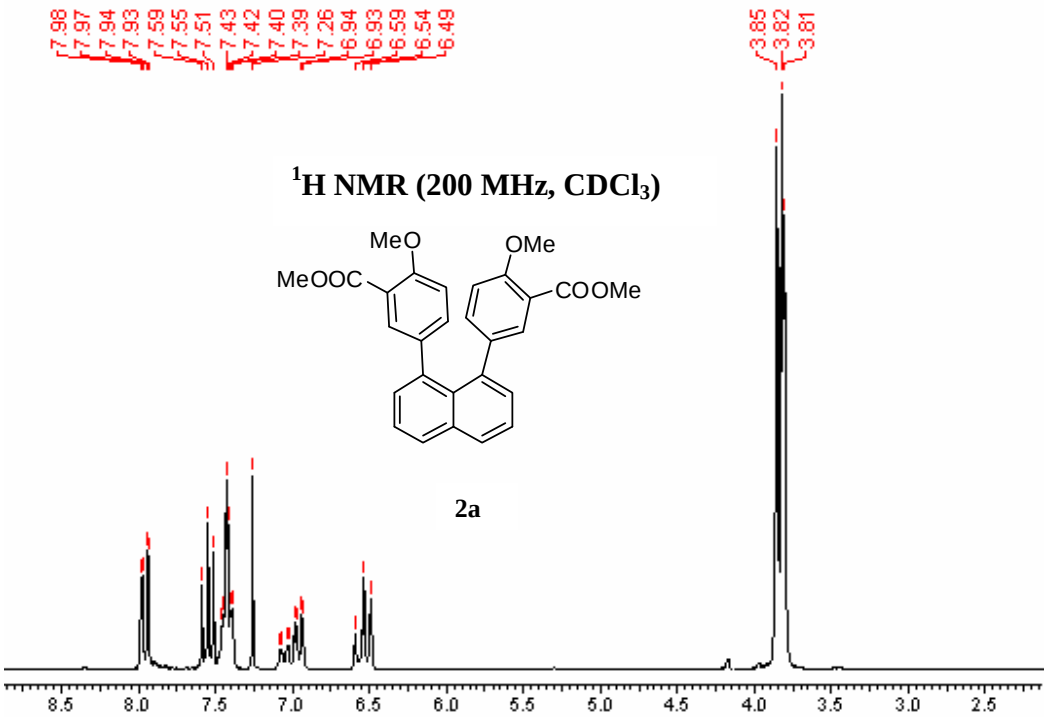
5
% Intensity
979.0
1106.2
1233.4
1360.6
1487.8
1615.0
Mass (m/z)



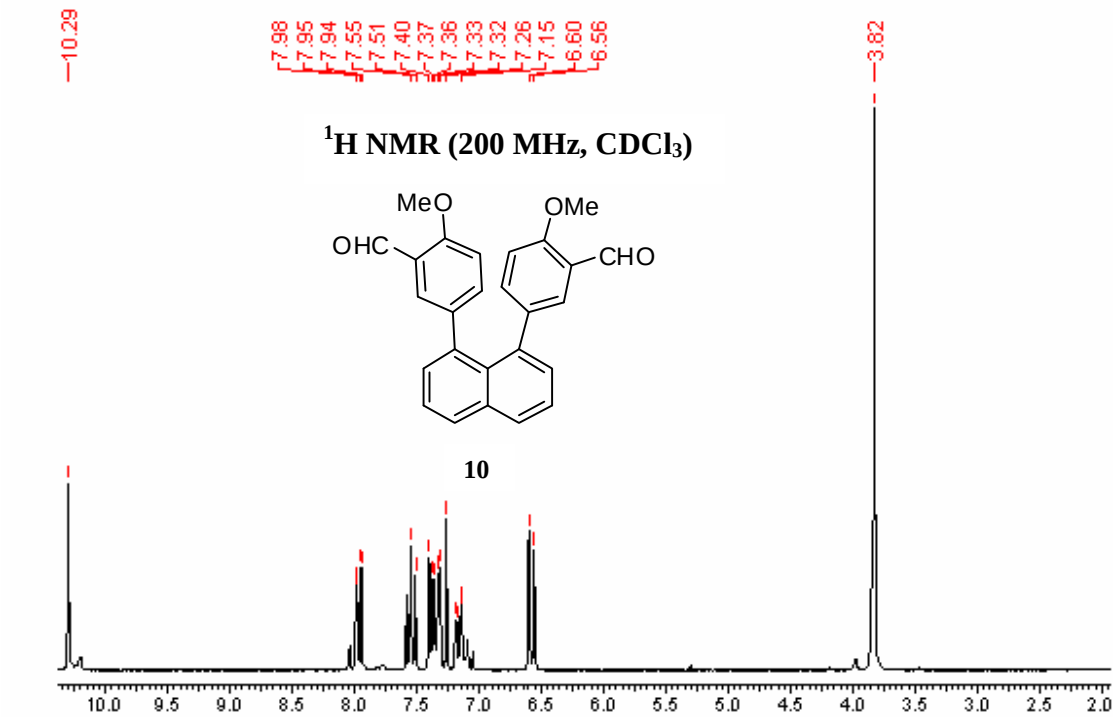
^{1}H (200MHz, $CDCl_3$)

7



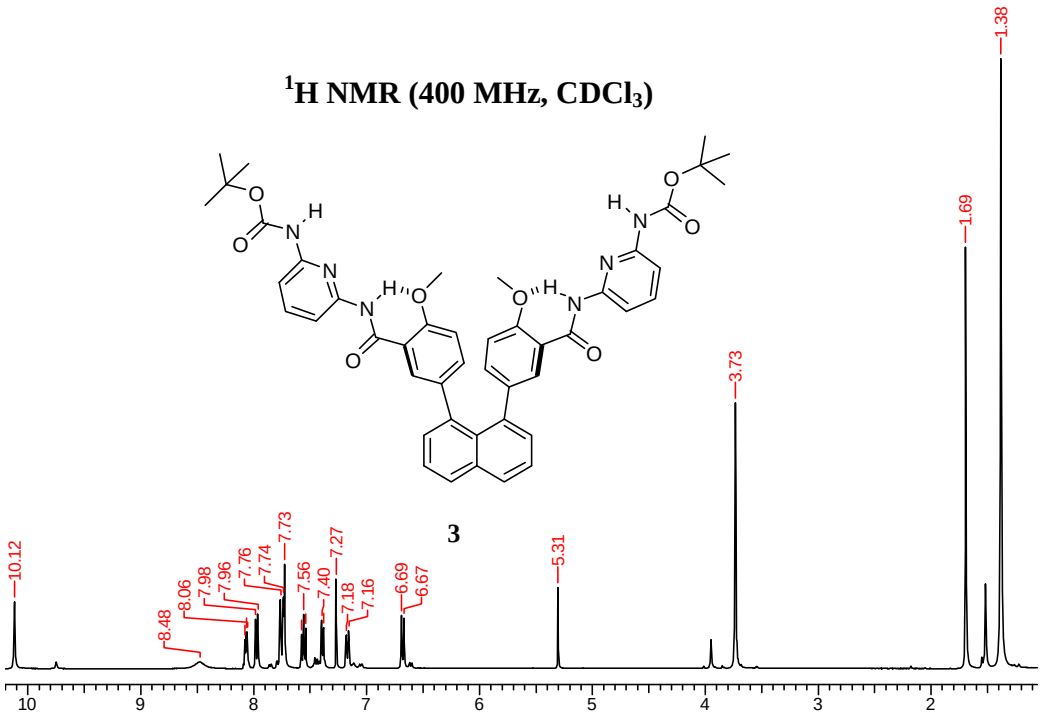
^{1}H NMR (200 MHz, $CDCl_3$)

2a



^{1}H NMR (200 MHz, $CDCl_3$)

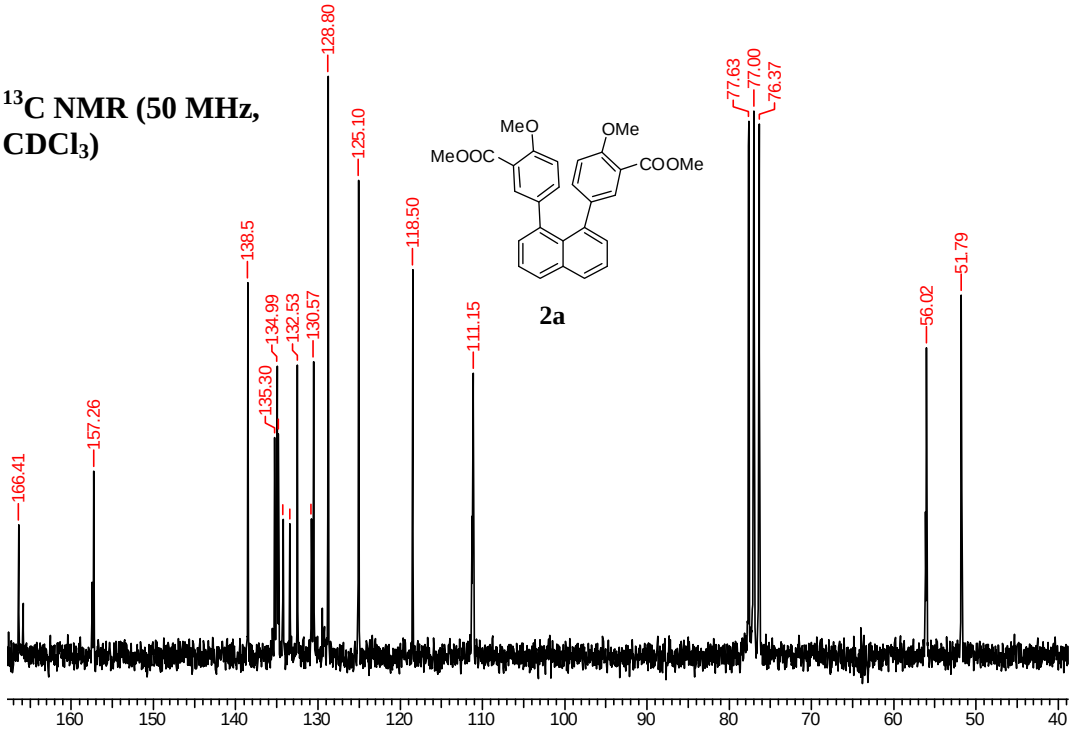
10



^{1}H NMR (400 MHz, $CDCl_3$)

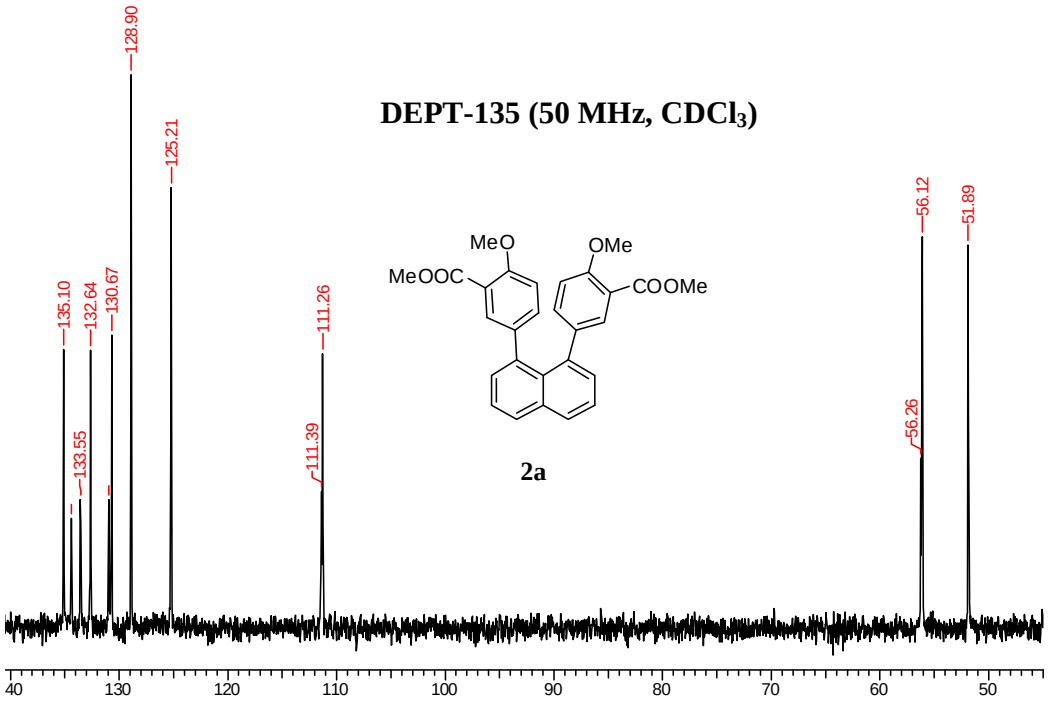
3

^{13}C NMR (50 MHz, $CDCl_3$)

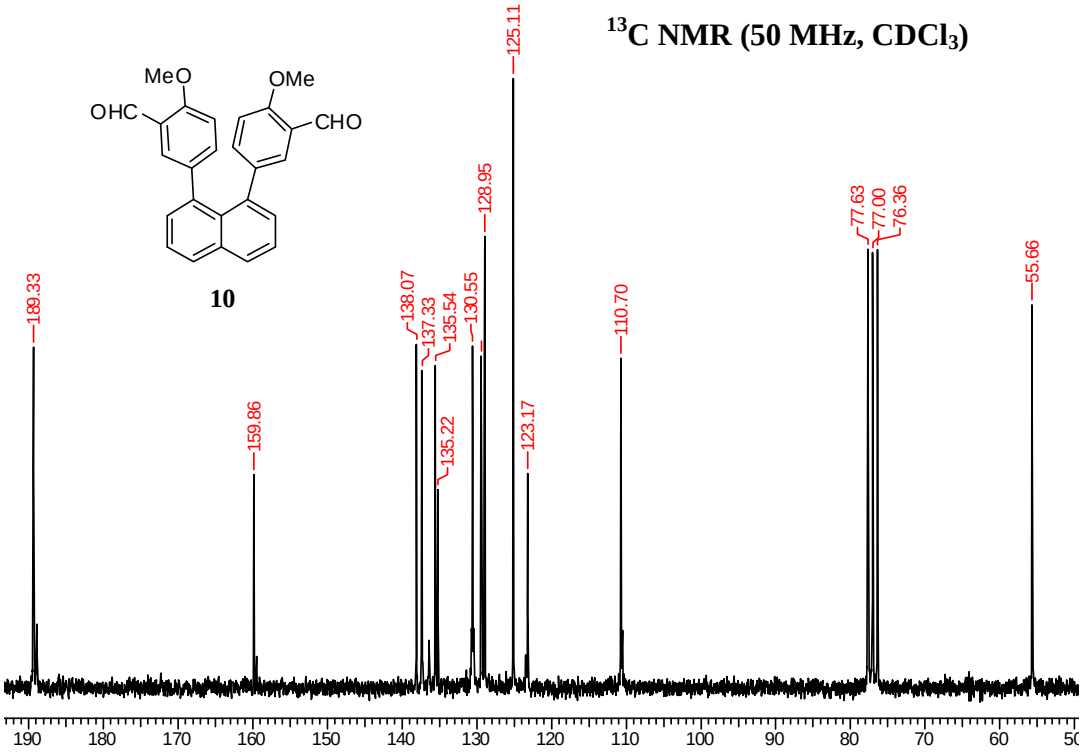


2a

DEPT-135 (50 MHz, $CDCl_3$)



2a


^{13}C NMR (50 MHz, CDCl$_3$)
MeO
OMe
OHC
CHO
10
189.33
159.86
138.07
137.33
135.54
135.22
130.55
128.95
125.11
123.17
110.70
77.63
77.00
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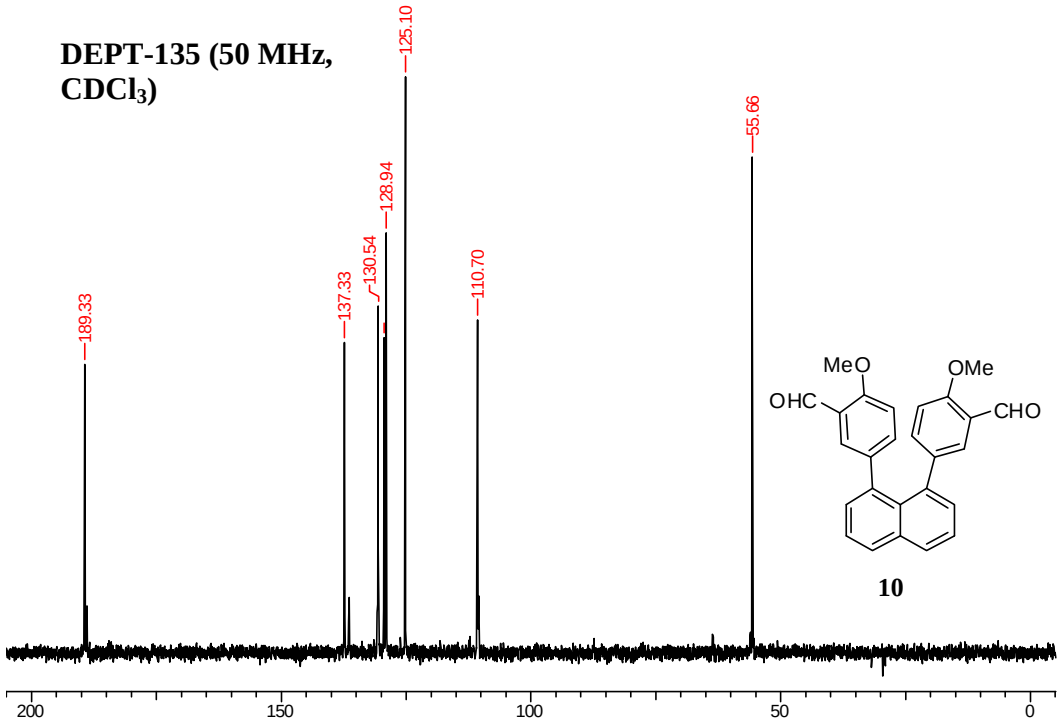
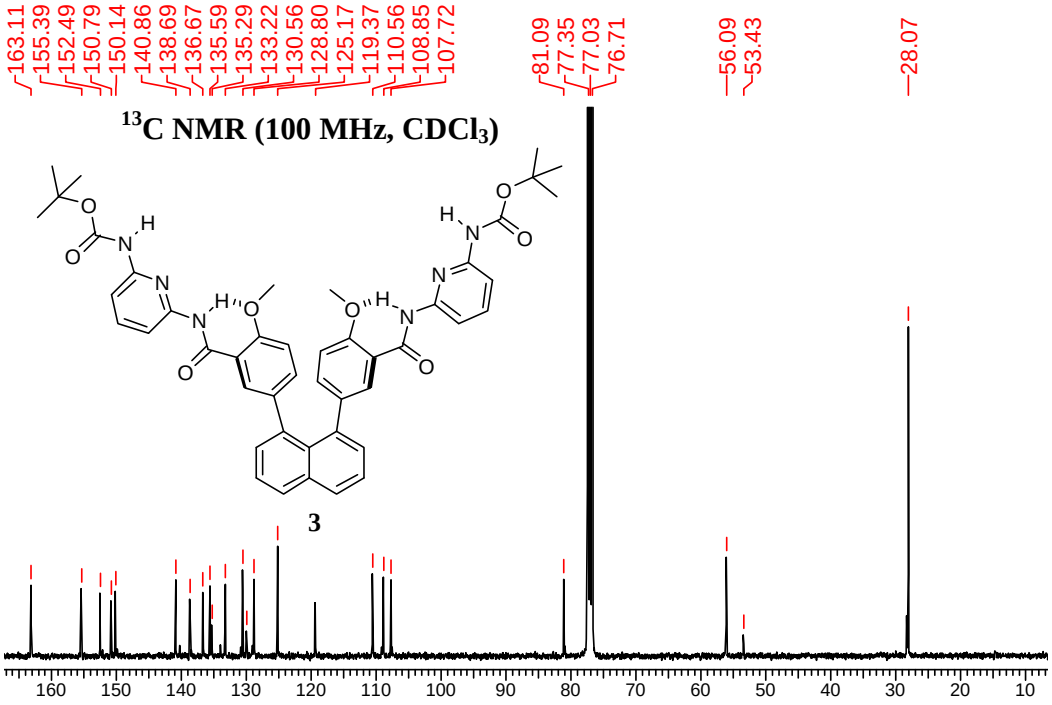
140
130
120
110
100
90
80
70
60
50


DEPT-135 (50 MHz, CDCl$_3$)
189.33
137.33
130.54
128.94
125.10
110.70
55.66
MeO
OMe
OHC
CHO
10
200
150
100
50
0



the peak at 53.43 ppm corresponds to DCM in the crystal lattice

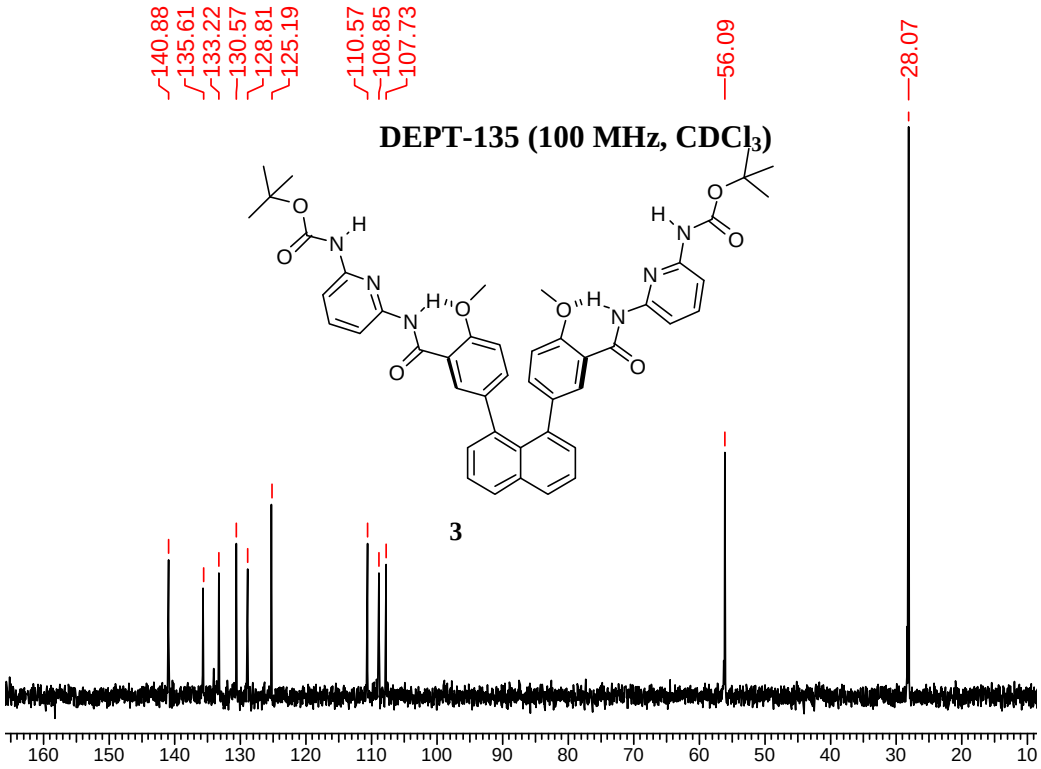
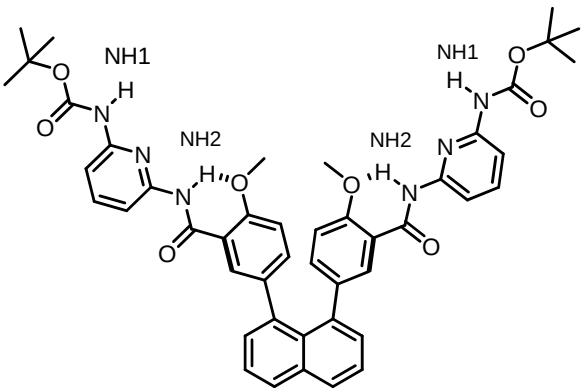
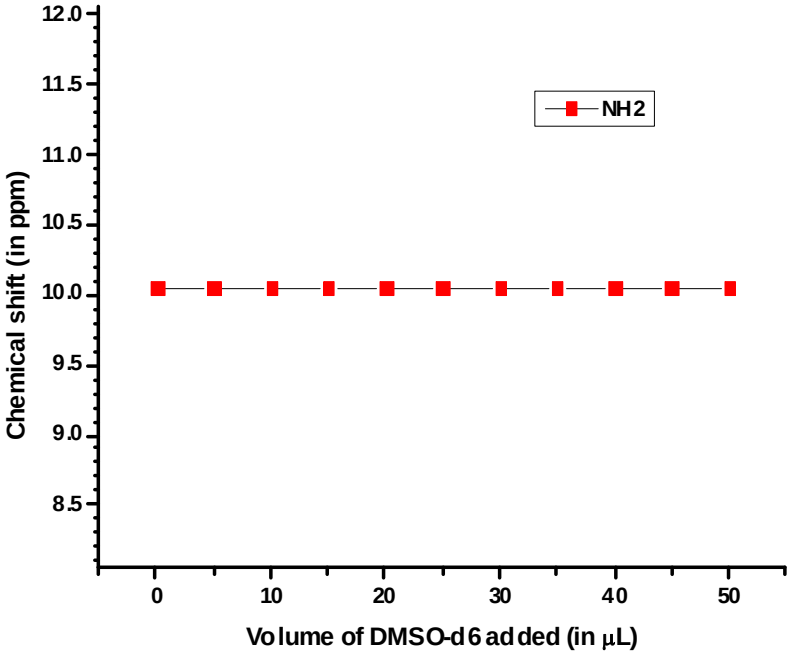


Table 1: Titration study of **3** in $CDCl_3$ ($V_{DMSO\text{-}d6}$ added at each step = 5 μl)

No	$V_{DMSO\text{-}d6}$ (in μl)	δ_{NH2}
1	0	10.05
2	5	10.05
3	10	10.05
4	15	10.05
5	20	10.05
6	25	10.05
7	30	10.05
8	35	10.05
9	40	10.05
10	45	10.05
11	50	10.05





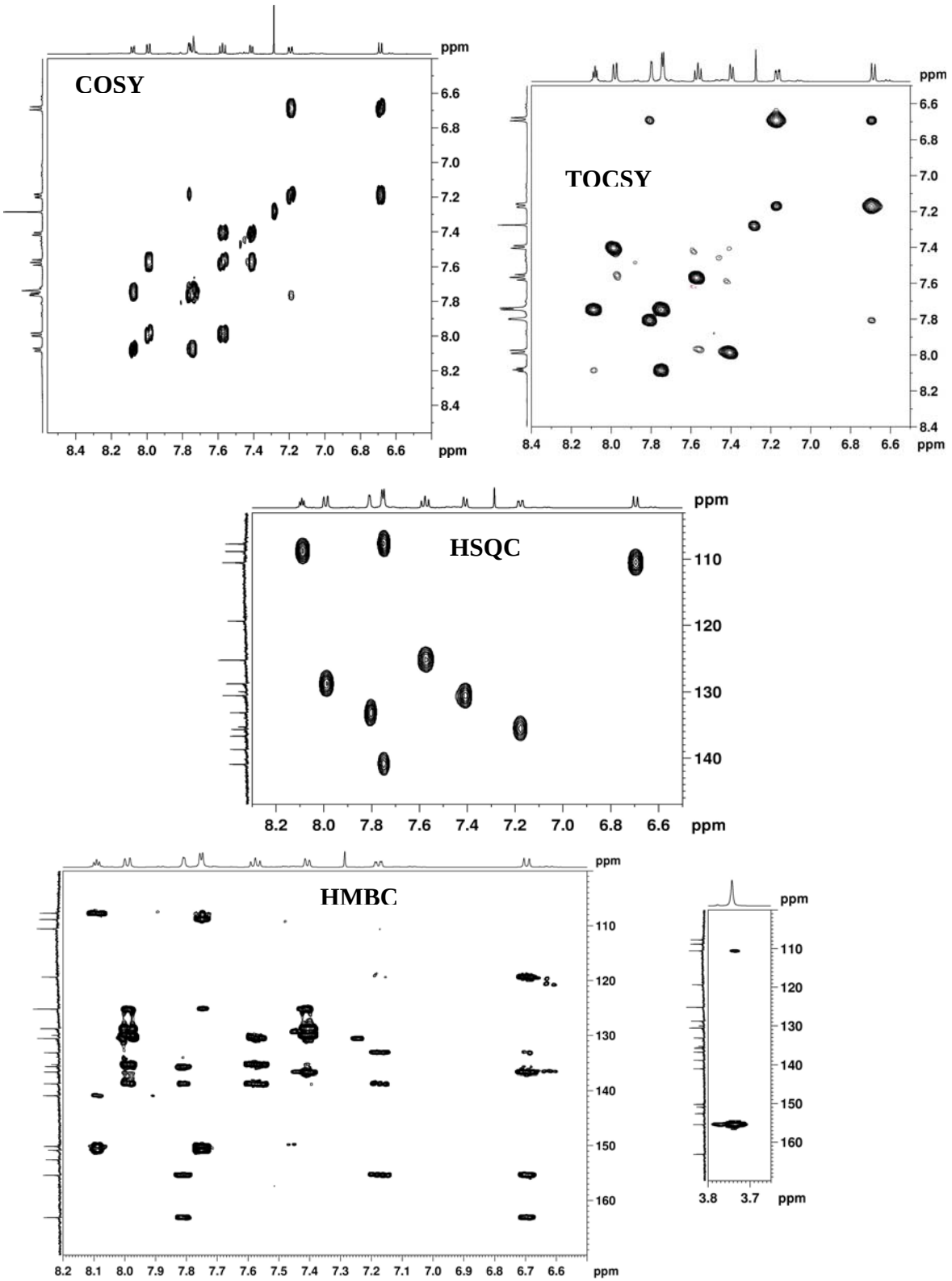


Figure S1. Partial COSY, TOCSY, HSQC, and HMBC spectra of **3**

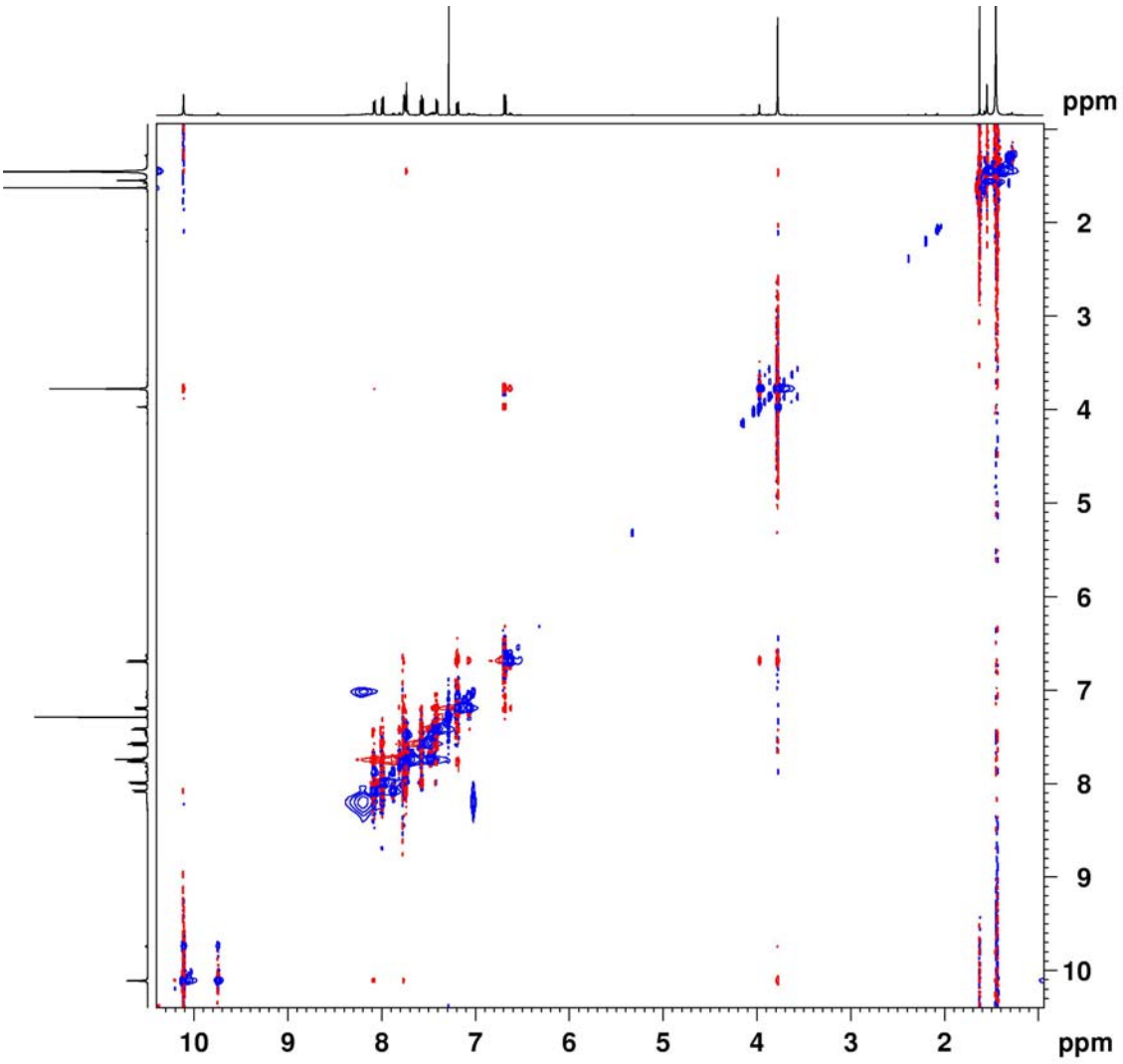


Figure S3. NOESY spectrum of 3 (500 MHz, $CDCl_3$)

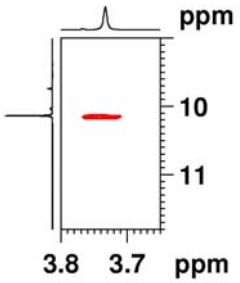


Figure S4. 2D NOESY extract of **3** showing nOe between OMe and NH (500 MHz, $CDCl_3$)

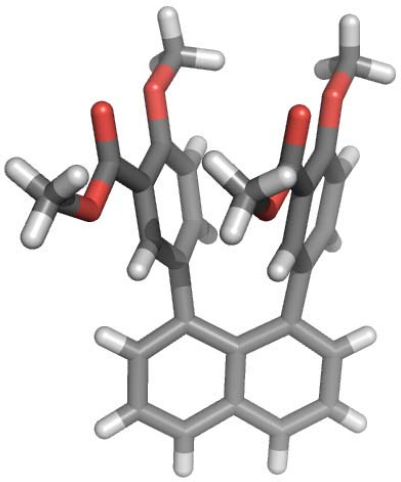


Figure S5. Crystal structure of **2a** with cofacial aryl rings containing the ester groups in *syn* orientation.

Details of the *ab initio* calculations

At first, a systematic conformational analysis for compound **3** was performed at the HF/6-31G* level of *ab initio* MO theory to test the reliability of the quantum chemical methods. Several conformational alternatives were considered as starting conformations of geometry optimization resulting from different torsion angles of the single bonds in the molecule. According to this analysis the anti-conformer with the side chains on the phenyl rings in the 1,8-positions pointing into opposite directions referred to the naphthalene ring is slightly favored over the syn-conformer, which corresponds to the X-ray structure having these groups in parallel orientation (ΔE = 10.0 kJ/mol in favour to anti). Considering correlation energy at the MP2//HF/6-31G* level, the stability order is reversed. The experimentally found syn-structure is clearly favoured by 9.0 kJ/mol over the anti-form now. This can be expected because of the influence of dispersion interactions between the parallel aromatic side chains in the syn-form, which is not considered at the Hartree-Fock level. Therefore, this structure was taken as the basis for the optimization of the much larger oligomer **5**. The geometry of compounds **3** (syn and anti) and **5** is given as pdb-files. All calculations were performed employing the Gaussian03 software package.

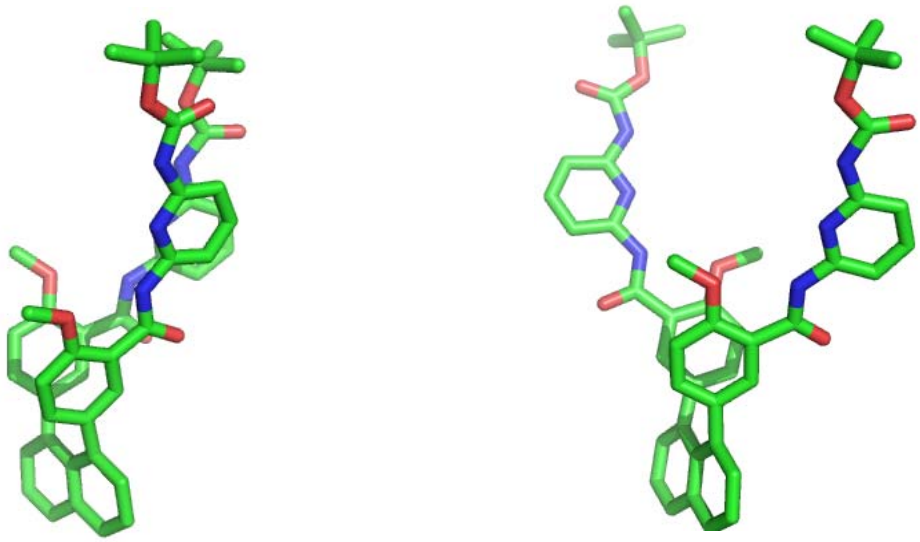


Figure S6. Possible isomers (*ab initio* models) of compound **3**: *Syn* (left) and *Anti* (right). *Note: The overlap of side arms (Pyridyl rings) is noticeable in the Syn isomer.*

Pdb-files for the most stable conformers of 3 and 5

Compound 3 *Syn* (E_T(HF/6-31G*) = -2694.483943 a.u.;
E_T(MP2//HF/6-31G*) = -2702.710143 a.u.)

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Compound 3 (*Anti*) (E_T(HF/6-31G*) = -2694.487753 a.u.;

E_T(MP2//6-31G*) = -2702.706700 a.u.)

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CONECT   22   42   53
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CONECT 77 35

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Compound 5 (E_T(HF/6-31G*) = -4823.810231 a.u.)

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HETATM    2  N   UNK  0001      0.709   2.895  -0.660
HETATM    3  N   UNK  0001      4.056  -1.990  -0.906
HETATM    4  N   UNK  0001      1.808  -2.031  -0.754
HETATM    5  N   UNK  0001     -0.382  -2.255  -0.269
HETATM    6  N   UNK  0001      2.944   2.653  -0.457
HETATM    7  C   UNK  0001     12.434  -0.698  -0.148
HETATM    8  C   UNK  0001     11.069  -0.758   0.232
HETATM    9  C   UNK  0001     12.873  -1.306  -1.353
HETATM   10  C   UNK  0001     13.380  -0.027   0.671
HETATM   11  C   UNK  0001     10.199  -1.593  -0.560
HETATM   12  C   UNK  0001     10.666   0.023   1.376
HETATM   13  C   UNK  0001      9.243   0.350   1.714
HETATM   14  C   UNK  0001      8.838  -2.050  -0.127
HETATM   15  C   UNK  0001     10.670  -2.142  -1.719
HETATM   16  C   UNK  0001     11.620   0.639   2.135
HETATM   17  C   UNK  0001     12.005  -1.976  -2.145
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HETATM	18	C	UNK	0001	12.991	0.593	1.809
HETATM	19	C	UNK	0001	7.704	-1.776	-0.870
HETATM	20	C	UNK	0001	6.450	-2.286	-0.532
HETATM	21	C	UNK	0001	8.710	-2.880	0.983
HETATM	22	C	UNK	0001	6.358	-3.126	0.577
HETATM	23	C	UNK	0001	5.307	-1.833	-1.411
HETATM	24	C	UNK	0001	7.486	-3.414	1.328
HETATM	25	C	UNK	0001	8.466	1.063	0.816
HETATM	26	C	UNK	0001	7.171	1.475	1.113
HETATM	27	C	UNK	0001	8.703	0.065	2.962
HETATM	28	C	UNK	0001	6.656	1.175	2.373
HETATM	29	C	UNK	0001	6.454	2.200	-0.002
HETATM	30	C	UNK	0001	7.424	0.474	3.288
HETATM	31	C	UNK	0001	-2.785	-3.669	-3.852
HETATM	32	C	UNK	0001	4.194	2.726	-0.877
HETATM	33	C	UNK	0001	4.544	3.219	-2.128
HETATM	34	C	UNK	0001	-0.942	-5.622	0.182
HETATM	35	C	UNK	0001	1.963	3.038	-1.254
HETATM	36	C	UNK	0001	2.184	3.540	-2.531
HETATM	37	C	UNK	0001	-2.954	8.152	2.570
HETATM	38	C	UNK	0001	3.502	3.622	-2.941
HETATM	39	C	UNK	0001	-0.517	3.065	-1.221
HETATM	40	C	UNK	0001	-1.708	2.770	-0.347
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HETATM	45	C	UNK	0001	-7.681	1.963	-1.719
HETATM	46	C	UNK	0001	-6.776	3.901	-0.538
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HETATM	48	C	UNK	0001	-4.060	2.223	1.038
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HETATM	51	C	UNK	0001	-8.037	4.431	-0.525
HETATM	52	C	UNK	0001	-7.543	0.717	-2.384
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HETATM	61	C	UNK	0001	-3.750	6.200	-0.396
HETATM	62	C	UNK	0001	-4.076	-8.257	-1.866
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HETATM	64	C	UNK	0001	2.696	-0.786	-2.579
HETATM	65	C	UNK	0001	-0.463	6.996	-1.832
HETATM	66	C	UNK	0001	0.582	-1.696	-1.113
HETATM	67	C	UNK	0001	0.310	-0.889	-2.209
HETATM	68	C	UNK	0001	-0.455	4.375	2.199
HETATM	69	C	UNK	0001	1.404	-0.445	-2.932
HETATM	70	C	UNK	0001	-1.729	-2.114	-0.298
HETATM	71	C	UNK	0001	-2.500	-2.834	0.779
HETATM	72	C	UNK	0001	-3.735	-2.285	1.119

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HETATM   76  C   UNK  0001      -8.231  -2.034   2.933
HETATM   77  C   UNK  0001      -7.507  -3.907   1.541
HETATM   78  C   UNK  0001      -6.569  -4.679   0.662
HETATM   79  C   UNK  0001      -4.118  -4.013   2.712
HETATM   80  C   UNK  0001      -2.092  -3.997   1.426
HETATM   81  C   UNK  0001      -5.674  -1.009   3.156
HETATM   82  C   UNK  0001      -8.801  -4.351   1.540
HETATM   83  C   UNK  0001      -8.000  -0.818   3.627
HETATM   84  C   UNK  0001      -9.556  -2.539   2.887
HETATM   85  C   UNK  0001      -2.900  -4.575   2.393
HETATM   86  C   UNK  0001      -6.754  -0.300   3.719
HETATM   87  C   UNK  0001      -9.836  -3.686   2.227
HETATM   88  C   UNK  0001      -6.325  -6.023   0.888
HETATM   89  C   UNK  0001      -6.015  -4.115  -0.481
HETATM   90  C   UNK  0001      -5.545  -6.780   0.026
HETATM   91  C   UNK  0001      -4.970  -6.195  -1.092
HETATM   92  C   UNK  0001      -5.204  -4.835  -1.340
HETATM   93  C   UNK  0001       5.278   2.737   3.468
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HETATM  127  H   UNK  0001      11.309   1.233   2.976
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HETATM  148  H   UNK  0001      -0.428   6.277  -2.635
HETATM  149  H   UNK  0001       0.508   4.444   2.681
HETATM  150  H   UNK  0001      -1.235   4.629   2.908
HETATM  151  H   UNK  0001      -0.500   5.058   1.361
HETATM  152  H   UNK  0001       4.227   2.875   3.672
HETATM  153  H   UNK  0001       5.651   3.578   2.895
HETATM  154  H   UNK  0001       5.824   2.666   4.401
HETATM  155  H   UNK  0001       3.958  -5.271   0.922
HETATM  156  H   UNK  0001       5.681  -5.667   0.907
HETATM  157  H   UNK  0001       4.905  -5.040  -0.553
HETATM  158  H   UNK  0001      -5.396  -7.820   0.238
HETATM  159  H   UNK  0001      -6.209  -3.085  -0.716
HETATM  160  H   UNK  0001      -6.749  -6.500   1.754
HETATM  161  H   UNK  0001     -10.837  -4.076   2.191
HETATM  162  H   UNK  0001      -6.574   0.623   4.240
HETATM  163  H   UNK  0001      -2.554  -5.462   2.891
HETATM  164  H   UNK  0001     -10.332  -1.989   3.389
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HETATM  179  H   UNK  0001      -2.874   2.479   2.803
HETATM  180  H   UNK  0001      -9.786   2.052  -2.144
CONECT    1   29   32  131
CONECT    2   35   39  132
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